



Full wwPDB EM Validation Report ⓘ

Nov 20, 2025 – 04:55 PM JST

PDB ID : 9L5V / pdb_00009l5v
EMDB ID : EMD-62846
Title : cryo-EM structure of PSII-ACPII from Rhodomonas sp. NIES-2332
Authors : Yonehara, N.; Akita, F.; Shen, J.R.
Deposited on : 2024-12-23
Resolution : 2.17 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

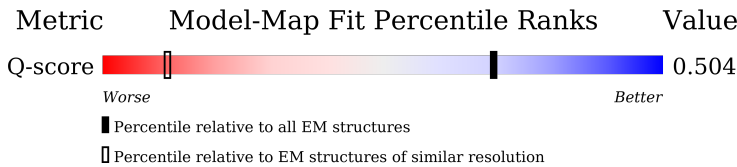
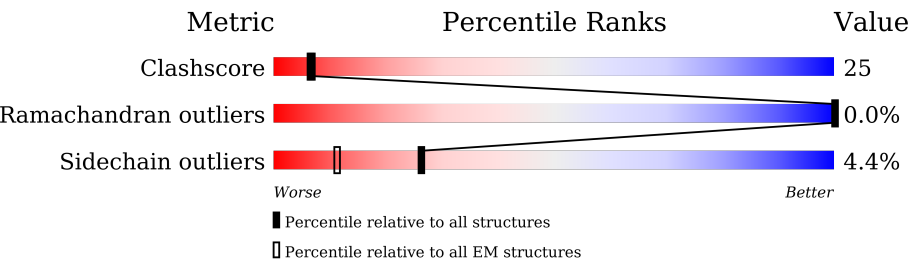
EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.17 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





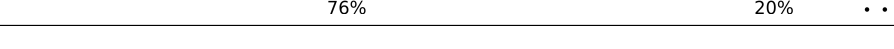
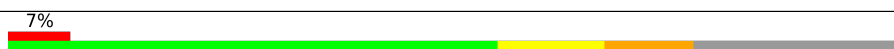

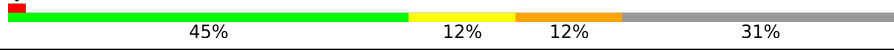

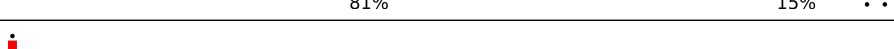



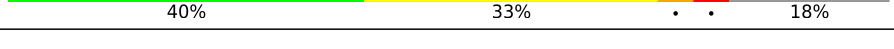




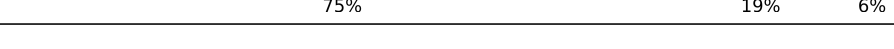







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	2651 (1.67 - 2.67)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	374	<div><div>60%</div><div>20%</div><div>19%</div></div>
1	a	374	<div><div>63%</div><div>18%</div><div>17%</div></div>
2	B	508	<div><div>65%</div><div>26%</div><div>5%</div></div>
2	b	508	<div><div>70%</div><div>22%</div><div>5%</div></div>

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Mol	Chain	Length	Quality of chain
3	C	486	
3	c	486	
4	D	351	
4	d	351	
5	E	84	
5	e	84	
6	F	42	
6	f	42	
7	H	67	
7	h	67	
8	I	38	
8	i	38	
9	K	45	
9	k	45	
10	L	38	
10	l	38	
11	M	118	
11	m	118	
12	T	32	
12	t	32	
13	W	121	
13	w	121	
14	X	39	
14	x	39	
15	Y	34	

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Mol	Chain	Length	Quality of chain
15	y	34	
16	Z	62	
16	z	62	
17	1	234	
17	N	234	
18	2	215	
18	O	215	
19	3	182	
19	P	182	
20	4	200	
20	Q	200	
21	5	228	
21	R	228	
22	6	174	
22	S	174	
23	G	292	
24	g	292	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	1	601	X	-	-	-
26	CLA	1	602	X	-	-	-
26	CLA	1	603	X	-	-	-
26	CLA	1	604	X	-	-	-
26	CLA	1	606	X	-	X	-
26	CLA	1	607	X	-	-	-
26	CLA	1	608	X	-	-	-
26	CLA	1	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	1	613	X	-	-	-
26	CLA	2	301	X	-	X	-
26	CLA	2	302	X	-	-	-
26	CLA	2	303	X	-	-	-
26	CLA	2	304	X	-	-	-
26	CLA	2	306	X	-	-	-
26	CLA	2	307	X	-	-	-
26	CLA	2	308	X	-	-	-
26	CLA	2	309	X	-	-	-
26	CLA	2	311	X	-	X	-
26	CLA	2	312	X	-	-	-
26	CLA	2	319	X	-	X	-
26	CLA	3	301	X	-	-	-
26	CLA	3	302	X	-	-	-
26	CLA	3	305	X	-	-	-
26	CLA	3	306	X	-	-	-
26	CLA	3	307	X	-	X	-
26	CLA	3	309	X	-	-	-
26	CLA	4	301	X	-	X	-
26	CLA	4	302	X	-	-	-
26	CLA	4	303	X	-	X	-
26	CLA	4	304	X	-	-	-
26	CLA	4	306	X	-	X	-
26	CLA	4	307	X	-	-	-
26	CLA	4	308	X	-	-	-
26	CLA	4	309	X	-	-	-
26	CLA	4	312	X	-	-	-
26	CLA	4	313	X	-	-	-
26	CLA	5	601	X	-	-	-
26	CLA	5	602	X	-	-	-
26	CLA	5	603	X	-	-	-
26	CLA	5	604	X	-	-	-
26	CLA	5	605	X	-	X	-
26	CLA	5	606	X	-	-	-
26	CLA	5	607	X	-	-	-
26	CLA	5	608	X	-	-	-
26	CLA	5	609	X	-	-	-
26	CLA	5	611	X	-	X	-
26	CLA	5	612	X	-	-	-
26	CLA	6	601	X	-	-	-
26	CLA	6	602	X	-	-	-
26	CLA	6	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	6	604	X	-	-	-
26	CLA	6	605	X	-	-	-
26	CLA	6	606	X	-	-	-
26	CLA	6	607	X	-	-	-
26	CLA	6	609	X	-	X	-
26	CLA	6	610	X	-	-	-
26	CLA	A	402	X	-	-	-
26	CLA	A	403	X	-	-	-
26	CLA	A	405	X	-	-	-
26	CLA	B	601	X	-	-	-
26	CLA	B	603	X	-	-	-
26	CLA	B	604	X	-	-	-
26	CLA	B	605	X	-	-	-
26	CLA	B	606	X	-	-	-
26	CLA	B	607	X	-	-	-
26	CLA	B	608	X	-	-	-
26	CLA	B	609	X	-	-	-
26	CLA	B	610	X	-	-	-
26	CLA	B	611	X	-	-	-
26	CLA	B	612	X	-	-	-
26	CLA	B	613	X	-	-	-
26	CLA	B	614	X	-	-	-
26	CLA	B	615	X	-	-	-
26	CLA	B	616	X	-	-	-
26	CLA	C	502	X	-	-	-
26	CLA	C	503	X	-	-	-
26	CLA	C	504	X	-	-	-
26	CLA	C	505	X	-	-	-
26	CLA	C	506	X	-	-	-
26	CLA	C	507	X	-	-	-
26	CLA	C	508	X	-	-	-
26	CLA	C	509	X	-	-	-
26	CLA	C	510	X	-	-	-
26	CLA	C	511	X	-	-	-
26	CLA	C	512	X	-	-	-
26	CLA	C	513	X	-	-	-
26	CLA	C	514	X	-	-	-
26	CLA	D	404	X	-	-	-
26	CLA	D	407	X	-	-	-
26	CLA	D	408	X	-	-	-
26	CLA	G	401	X	-	-	-
26	CLA	G	402	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	N	601	X	-	X	-
26	CLA	N	602	X	-	-	-
26	CLA	N	603	X	-	-	-
26	CLA	N	604	X	-	-	-
26	CLA	N	606	X	-	X	-
26	CLA	N	607	X	-	-	-
26	CLA	N	608	X	-	-	-
26	CLA	N	609	X	-	-	-
26	CLA	N	613	X	-	-	-
26	CLA	N	614	X	-	X	-
26	CLA	O	601	X	-	X	-
26	CLA	O	602	X	-	-	-
26	CLA	O	603	X	-	-	-
26	CLA	O	604	X	-	-	-
26	CLA	O	605	X	-	-	-
26	CLA	O	606	X	-	-	-
26	CLA	O	607	X	-	-	-
26	CLA	O	608	X	-	-	-
26	CLA	O	609	X	-	-	-
26	CLA	O	611	X	-	-	-
26	CLA	O	612	X	-	-	-
26	CLA	P	601	X	-	-	-
26	CLA	P	602	X	-	-	-
26	CLA	P	603	X	-	-	-
26	CLA	P	606	X	-	-	-
26	CLA	P	607	X	-	-	-
26	CLA	P	608	X	-	-	-
26	CLA	P	609	X	-	-	-
26	CLA	P	610	X	-	-	-
26	CLA	P	611	X	-	-	-
26	CLA	Q	301	X	-	-	-
26	CLA	Q	302	X	-	-	-
26	CLA	Q	303	X	-	-	-
26	CLA	Q	305	X	-	-	-
26	CLA	Q	306	X	-	-	-
26	CLA	Q	307	X	-	-	-
26	CLA	Q	308	X	-	-	-
26	CLA	Q	311	X	-	-	-
26	CLA	Q	312	X	-	-	-
26	CLA	R	302	X	-	-	-
26	CLA	R	303	X	-	-	-
26	CLA	R	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	R	305	X	-	-	-
26	CLA	R	306	X	-	X	-
26	CLA	R	307	X	-	-	-
26	CLA	R	308	X	-	-	-
26	CLA	R	309	X	-	-	-
26	CLA	R	310	X	-	-	-
26	CLA	R	312	X	-	-	-
26	CLA	R	313	X	-	-	-
26	CLA	S	601	X	-	-	-
26	CLA	S	602	X	-	-	-
26	CLA	S	603	X	-	-	-
26	CLA	S	604	X	-	-	-
26	CLA	S	605	X	-	-	-
26	CLA	S	606	X	-	-	-
26	CLA	S	607	X	-	-	-
26	CLA	S	609	X	-	-	-
26	CLA	S	610	X	-	-	-
26	CLA	a	402	X	-	-	-
26	CLA	a	403	X	-	-	-
26	CLA	a	405	X	-	-	-
26	CLA	b	601	X	-	-	-
26	CLA	b	603	X	-	-	-
26	CLA	b	604	X	-	-	-
26	CLA	b	605	X	-	-	-
26	CLA	b	606	X	-	-	-
26	CLA	b	607	X	-	-	-
26	CLA	b	608	X	-	-	-
26	CLA	b	609	X	-	-	-
26	CLA	b	610	X	-	-	-
26	CLA	b	611	X	-	-	-
26	CLA	b	612	X	-	-	-
26	CLA	b	613	X	-	-	-
26	CLA	b	614	X	-	-	-
26	CLA	b	615	X	-	-	-
26	CLA	b	616	X	-	-	-
26	CLA	c	503	X	-	-	-
26	CLA	c	504	X	-	-	-
26	CLA	c	505	X	-	-	-
26	CLA	c	506	X	-	-	-
26	CLA	c	507	X	-	-	-
26	CLA	c	508	X	-	-	-
26	CLA	c	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	c	510	X	-	-	-
26	CLA	c	511	X	-	-	-
26	CLA	c	512	X	-	-	-
26	CLA	c	513	X	-	-	-
26	CLA	c	514	X	-	-	-
26	CLA	c	515	X	-	-	-
26	CLA	d	402	X	-	-	-
26	CLA	d	405	X	-	-	-
26	CLA	d	406	X	-	-	-
26	CLA	g	401	X	-	-	-
26	CLA	g	402	X	-	-	-
28	WVN	3	313	-	-	X	-
28	WVN	C	516	-	X	-	-
34	LHG	1	620	-	-	X	-
34	LHG	2	321	-	-	X	-
34	LHG	N	621	-	-	X	-
38	KC2	N	612	-	-	X	-
38	KC2	Q	310	-	-	X	-
39	II0	3	310	-	-	X	-
39	II0	3	311	-	-	X	-
39	II0	4	320	-	-	X	-
40	IHT	1	619	-	X	-	-
40	IHT	2	317	-	-	X	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 69223 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	303	Total	C	N	O	S	1	0
			2377	1562	393	410	12		
1	a	311	Total	C	N	O	S	0	0
			2438	1603	401	422	12		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	482	Total	C	N	O	S	1	0
			3797	2479	650	656	12		
2	b	481	Total	C	N	O	S	0	0
			3782	2471	645	654	12		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	424	Total	C	N	O	S	1	0
			3331	2188	559	573	11		
3	c	421	Total	C	N	O	S	0	0
			3299	2164	555	569	11		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	1	0
			2713	1792	445	464	12		
4	d	341	Total	C	N	O	S	0	0
			2705	1788	443	462	12		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	64	Total	C	N	O	0	0
			525	345	85	95		
5	e	64	Total	C	N	O	0	0
			525	345	85	95		

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	29	Total	C	N	O	S	0	0
			235	159	40	35	1		
6	f	30	Total	C	N	O	S	0	0
			246	168	41	36	1		

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	65	Total	C	N	O	S	0	0
			508	337	81	88	2		
7	h	65	Total	C	N	O	S	0	0
			508	337	81	88	2		

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	35	Total	C	N	O	S	0	0
			284	188	46	49	1		
8	i	35	Total	C	N	O	S	0	0
			284	188	46	49	1		

- Molecule 9 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	K	37	Total	C	N	O	0	0
			296	209	44	43		
9	k	37	Total	C	N	O	0	0
			296	209	44	43		

- Molecule 10 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	37	Total	C	N	O	0	0
			301	204	47	50		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	l	37	Total	C	N	O	0	0
			301	204	47	50		

- Molecule 11 is a protein called Photosystem II protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	M	36	Total	C	N	O	0	0
			271	181	42	48		
11	m	36	Total	C	N	O	0	0
			271	181	42	48		

- Molecule 12 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	30	Total	C	N	O	S	0	0
			244	169	36	38	1		
12	t	30	Total	C	N	O	S	0	0
			244	169	36	38	1		

- Molecule 13 is a protein called Photosystem II protein W.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	W	45	Total	C	N	O	0	0
			361	233	58	70		
13	w	45	Total	C	N	O	0	0
			361	233	58	70		

- Molecule 14 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	X	34	Total	C	N	O	S	0	0
			249	167	36	45	1		
14	x	34	Total	C	N	O	S	0	0
			249	167	36	45	1		

- Molecule 15 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	Y	28	Total	C	N	O	0	0
			209	140	36	33		
15	y	28	Total	C	N	O	0	0
			209	140	36	33		

- Molecule 16 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Z	61	Total	C	N	O	S	0	0
			451	305	67	76	3		
16	z	61	Total	C	N	O	S	0	0
			460	314	67	76	3		

- Molecule 17 is a protein called ACPII-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1	192	Total	C	N	O	S	0	0
			1477	944	262	263	8		
17	N	192	Total	C	N	O	S	0	0
			1477	944	262	263	8		

- Molecule 18 is a protein called ACPII-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	2	172	Total	C	N	O	S	0	0
			1377	910	225	239	3		
18	O	172	Total	C	N	O	S	0	0
			1377	910	225	239	3		

- Molecule 19 is a protein called ACPII-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3	180	Total	C	N	O	S	0	0
			1388	898	232	249	9		
19	P	180	Total	C	N	O	S	0	0
			1388	898	232	249	9		

- Molecule 20 is a protein called ACPII-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	4	160	Total	C	N	O	S	0	0
			1226	787	210	219	10		
20	Q	160	Total	C	N	O	S	0	0
			1226	787	210	219	10		

- Molecule 21 is a protein called ACPII-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	5	189	Total	C	N	O	S	0	0
			1481	972	242	264	3		
21	R	189	Total	C	N	O	S	0	0
			1481	972	242	264	3		

- Molecule 22 is a protein called ACPII-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	6	173	Total	C	N	O	S	0	0
			1327	856	227	236	8		
22	S	173	Total	C	N	O	S	0	0
			1327	856	227	236	8		

- Molecule 23 is a protein called Psb-gama_linker.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	G	96	Total	C	N	O	0	0
			755	503	120	132		

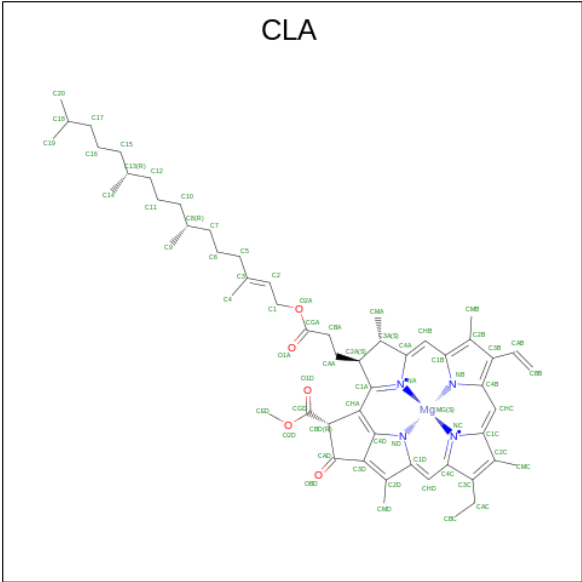
- Molecule 24 is a protein called Psb-gama_linker.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	g	95	Total	C	N	O	S	0	0
			747	499	118	129	1		

- Molecule 25 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
25	A	1	Total	Fe	0
			1	1	
25	a	1	Total	Fe	0
			1	1	

- Molecule 26 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
26	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	D	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 59	C 49	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 53	C 43	Mg 1	N 4	O 5	0
26	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	d	1	Total 61	C 51	Mg 1	N 4	O 5	0
26	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	1	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	1	1	Total 59	C 49	Mg 1	N 4	O 5	0
26	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	1	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	1	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
26	N	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	3	1	Total 62	C 52	Mg 1	N 4	O 5	0
26	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	3	1	Total 63	C 53	Mg 1	N 4	O 5	0
26	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	3	1	Total 53	C 43	Mg 1	N 4	O 5	0
26	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	4	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	4	1	Total 61	C 51	Mg 1	N 4	O 5	0
26	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	4	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	4	1	Total 56	C 46	Mg 1	N 4	O 5	0
26	4	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	4	1	Total 43	C 35	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
26	4	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	5	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	5	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	5	1	Total 59	C 49	Mg 1	N 4	O 5	0
26	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
26	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	6	1	Total 57	C 47	Mg 1	N 4	O 5	0
26	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	6	1	Total 53	C 43	Mg 1	N 4	O 5	0
26	6	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	O	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	O	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	O	1	Total 48	C 38	Mg 1	N 4	O 5	0
26	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	P	1	Total 62	C 52	Mg 1	N 4	O 5	0
26	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	P	1	Total 63	C 53	Mg 1	N 4	O 5	0
26	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	P	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	P	1	Total 53	C 43	Mg 1	N 4	O 5	0

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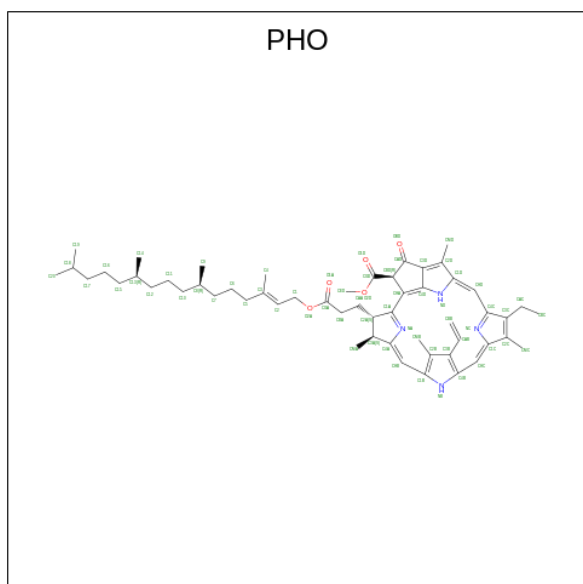
Mol	Chain	Residues	Atoms					AltConf
26	P	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Q	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
26	Q	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	Q	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
26	Q	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	Q	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
26	Q	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
26	Q	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
26	R	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
26	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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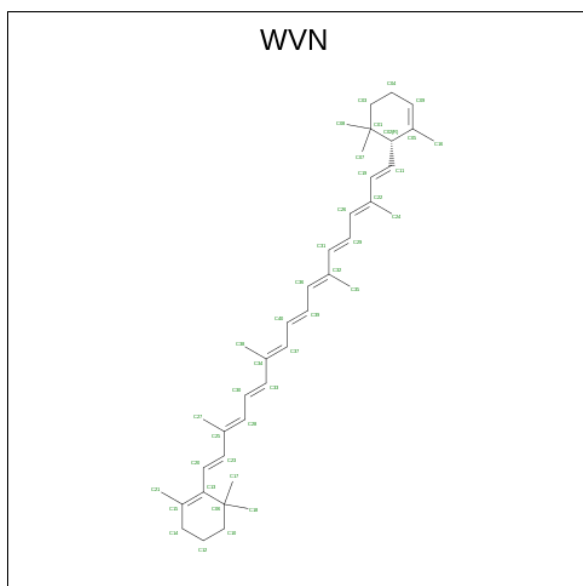
Mol	Chain	Residues	Atoms					AltConf
26	R	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 27 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	N	O	0
			64	55	4	5	
27	D	1	Total	C	N	O	0
			64	55	4	5	
27	a	1	Total	C	N	O	0
			64	55	4	5	
27	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 28 is 1,3,3-trimethyl-2-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-3,7,12,16-tetramethyl-18-[(1R)-2,6,6-trimethylcyclohex-2-en-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohexene (CCD ID: WVN) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



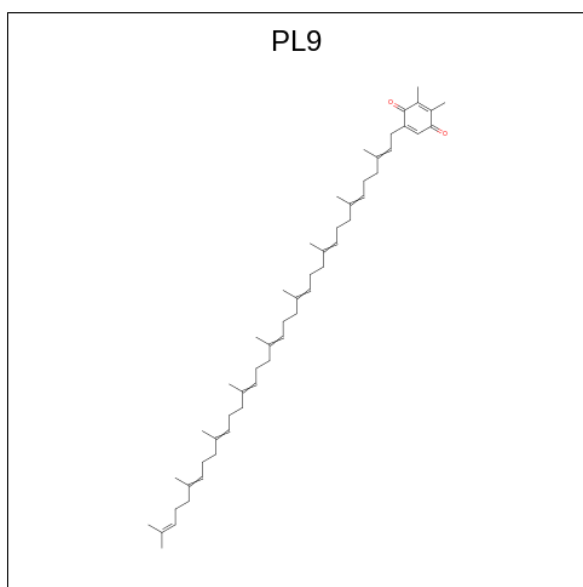
Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total	C	0
			40	40	
28	B	1	Total	C	0
			40	40	
28	B	1	Total	C	0
			40	40	
28	B	1	Total	C	0
			40	40	
28	C	1	Total	C	0
			40	40	
28	C	1	Total	C	0
			40	40	
28	D	1	Total	C	0
			40	40	

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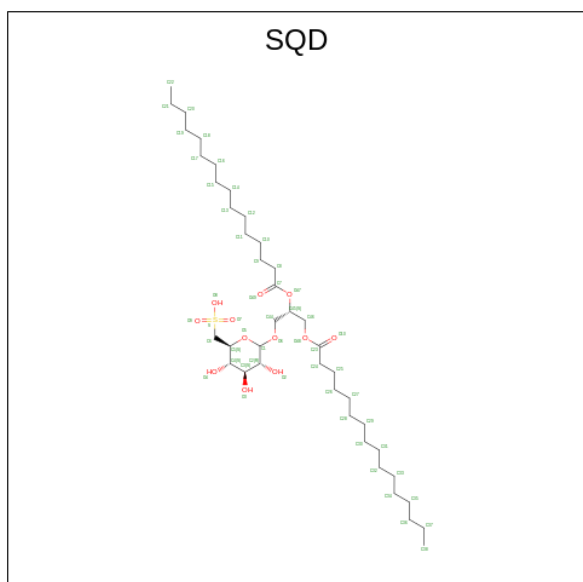
Mol	Chain	Residues	Atoms	AltConf
28	H	1	Total C 40 40	0
28	Y	1	Total C 40 40	0
28	Z	1	Total C 40 40	0
28	a	1	Total C 40 40	0
28	b	1	Total C 40 40	0
28	b	1	Total C 40 40	0
28	b	1	Total C 40 40	0
28	c	1	Total C 40 40	0
28	c	1	Total C 40 40	0
28	c	1	Total C 40 40	0
28	d	1	Total C 40 40	0
28	k	1	Total C 40 40	0
28	x	1	Total C 40 40	0
28	3	1	Total C 40 40	0
28	5	1	Total C 40 40	0
28	P	1	Total C 40 40	0
28	S	1	Total C 40 40	0

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			33	31	2	
29	D	1	Total	C	O	0
			55	53	2	
29	a	1	Total	C	O	0
			33	31	2	
29	d	1	Total	C	O	0
			55	53	2	

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	S	0
			40	27	12	1	
30	D	1	Total	C	O	S	0
			54	41	12	1	
30	a	1	Total	C	O	S	0
			40	27	12	1	
30	c	1	Total	C	O	S	0
			45	32	12	1	

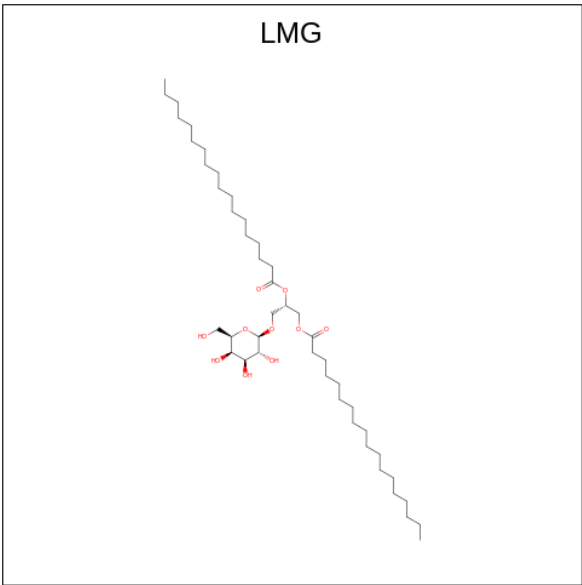
- Molecule 31 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
31	A	1	Total	Cl	0
			1	1	
31	a	1	Total	Cl	0
			1	1	
31	c	1	Total	Cl	0
			1	1	

- Molecule 32 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
32	A	2	Total	Mn	0
			2	2	
32	a	2	Total	Mn	0
			2	2	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



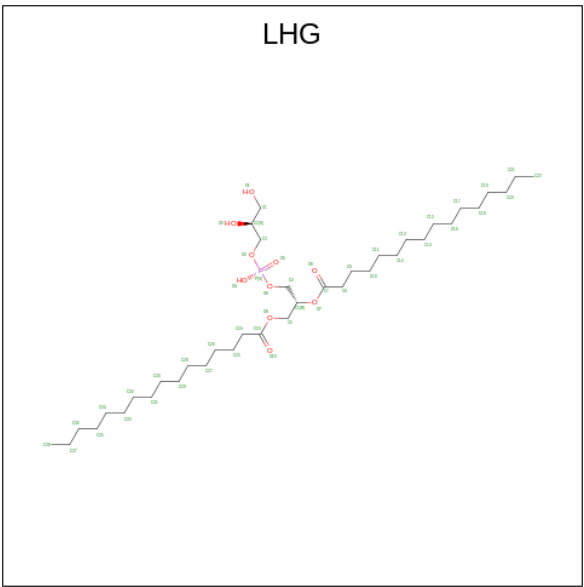
Mol	Chain	Residues	Atoms			AltConf
33	A	1	Total	C	O	0
			48	38	10	
33	B	1	Total	C	O	0
			51	41	10	
33	C	1	Total	C	O	0
			47	37	10	
33	C	1	Total	C	O	0
			31	21	10	
33	D	1	Total	C	O	0
			40	30	10	
33	D	1	Total	C	O	0
			37	27	10	
33	D	1	Total	C	O	0
			46	36	10	
33	M	1	Total	C	O	0
			40	30	10	
33	a	1	Total	C	O	0
			48	38	10	
33	b	1	Total	C	O	0
			51	41	10	
33	c	1	Total	C	O	0
			51	41	10	
33	c	1	Total	C	O	0
			31	21	10	
33	d	1	Total	C	O	0
			40	30	10	
33	d	1	Total	C	O	0
			37	27	10	

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Mol	Chain	Residues	Atoms			AltConf
33	d	1	Total	C	O	0
			46	36	10	
33	m	1	Total	C	O	0
			40	30	10	
33	2	1	Total	C	O	0
			40	30	10	
33	4	1	Total	C	O	0
			43	33	10	
33	5	1	Total	C	O	0
			40	30	10	
33	O	1	Total	C	O	0
			40	30	10	
33	Q	1	Total	C	O	0
			43	33	10	
33	R	1	Total	C	O	0
			40	30	10	

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



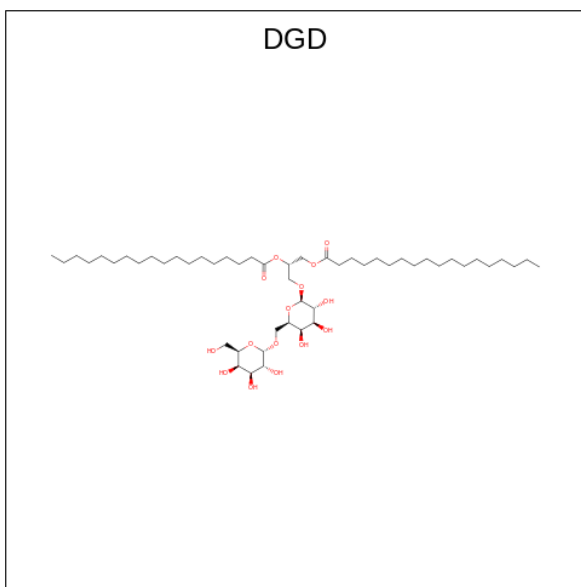
Mol	Chain	Residues	Atoms				AltConf
34	C	1	Total	C	O	P	0
			42	31	10	1	
34	C	1	Total	C	O	P	0
			40	29	10	1	
34	D	1	Total	C	O	P	0
			43	32	10	1	

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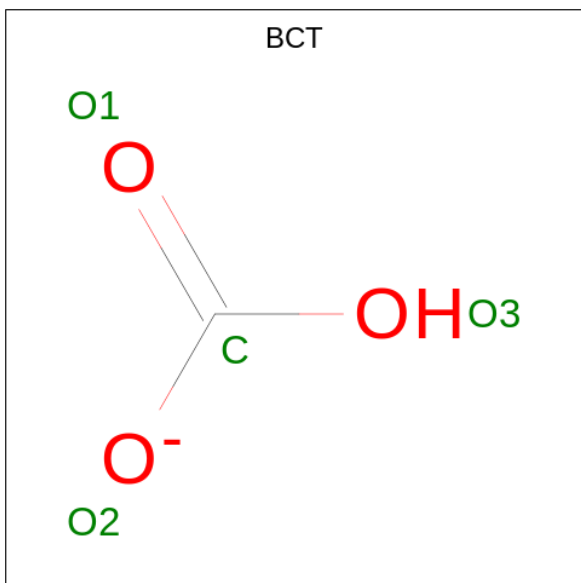
Mol	Chain	Residues	Atoms				AltConf
34	D	1	Total	C	O	P	0
			49	38	10	1	
34	L	1	Total	C	O	P	0
			49	38	10	1	
34	Z	1	Total	C	O	P	0
			25	14	10	1	
34	a	1	Total	C	O	P	0
			42	31	10	1	
34	b	1	Total	C	O	P	0
			43	32	10	1	
34	c	1	Total	C	O	P	0
			40	29	10	1	
34	d	1	Total	C	O	P	0
			49	38	10	1	
34	l	1	Total	C	O	P	0
			49	38	10	1	
34	z	1	Total	C	O	P	0
			25	14	10	1	
34	1	1	Total	C	O	P	0
			46	35	10	1	
34	N	1	Total	C	O	P	0
			46	35	10	1	
34	2	1	Total	C	O	P	0
			49	38	10	1	
34	5	1	Total	C	O	P	0
			40	29	10	1	
34	G	1	Total	C	O	P	0
			49	38	10	1	
34	R	1	Total	C	O	P	0
			40	29	10	1	

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



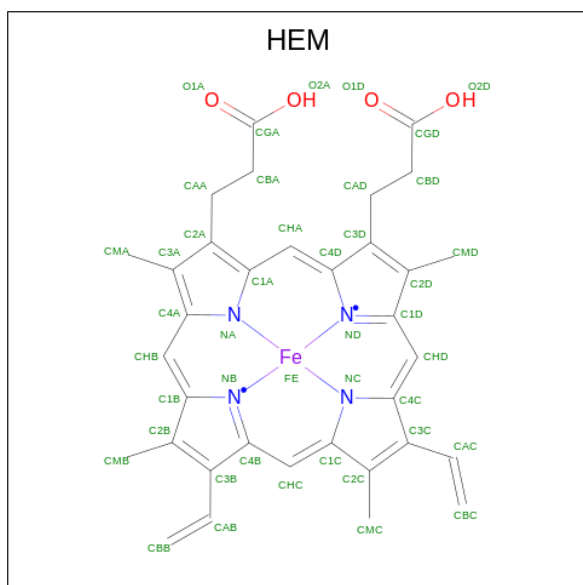
Mol	Chain	Residues	Atoms			AltConf
35	C	1	Total	C	O	0
			54	39	15	
35	H	1	Total	C	O	0
			62	47	15	
35	c	1	Total	C	O	0
			54	39	15	
35	h	1	Total	C	O	0
			62	47	15	

- Molecule 36 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



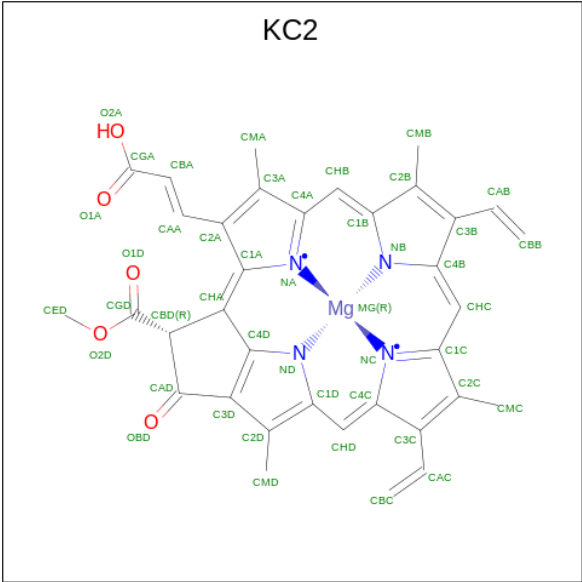
Mol	Chain	Residues	Atoms			AltConf
36	D	1	Total 4	C 1	O 3	0
36	d	1	Total 4	C 1	O 3	0

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
37	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
37	f	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 38 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



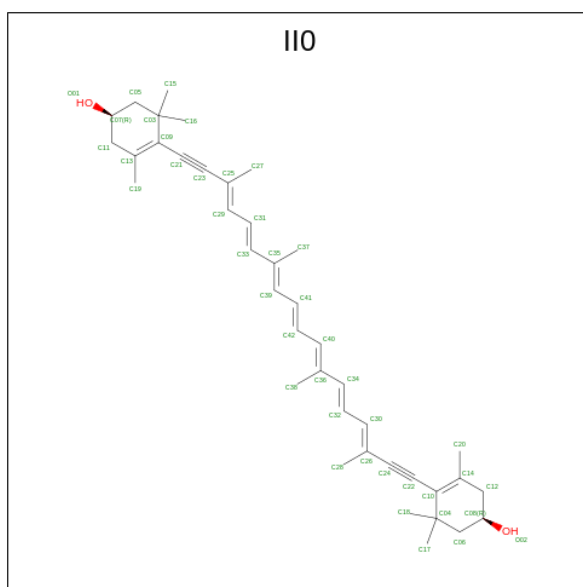
Mol	Chain	Residues	Atoms					AltConf
38	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
38	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 39 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (CCD ID: II0) (formula: C₄₀H₅₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
39	1	1	Total	C	O	0
			42	40	2	
39	1	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
39	1	1	Total	C	O	0
			42	40	2	
39	1	1	Total	C	O	0
			42	40	2	
39	N	1	Total	C	O	0
			42	40	2	
39	N	1	Total	C	O	0
			42	40	2	
39	N	1	Total	C	O	0
			42	40	2	
39	N	1	Total	C	O	0
			42	40	2	
39	N	1	Total	C	O	0
			42	40	2	
39	2	1	Total	C	O	0
			42	40	2	
39	2	1	Total	C	O	0
			42	40	2	
39	2	1	Total	C	O	0
			42	40	2	
39	2	1	Total	C	O	0
			42	40	2	
39	2	1	Total	C	O	0
			42	40	2	
39	2	1	Total	C	O	0
			42	40	2	
39	3	1	Total	C	O	0
			42	40	2	
39	3	1	Total	C	O	0
			42	40	2	
39	3	1	Total	C	O	0
			42	40	2	
39	4	1	Total	C	O	0
			42	40	2	
39	4	1	Total	C	O	0
			42	40	2	
39	4	1	Total	C	O	0
			42	40	2	
39	4	1	Total	C	O	0
			42	40	2	
39	4	1	Total	C	O	0
			42	40	2	
39	5	1	Total	C	O	0
			42	40	2	

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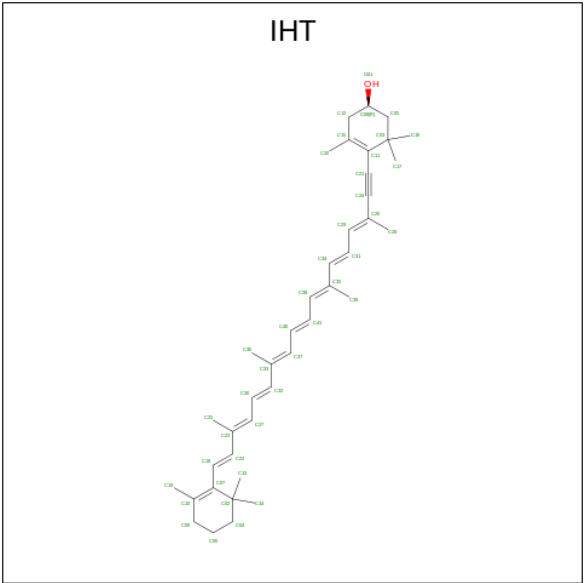
Mol	Chain	Residues	Atoms			AltConf
39	5	1	Total 42	C 40	O 2	0
39	5	1	Total 42	C 40	O 2	0
39	6	1	Total 42	C 40	O 2	0
39	6	1	Total 42	C 40	O 2	0
39	6	1	Total 42	C 40	O 2	0
39	O	1	Total 42	C 40	O 2	0
39	O	1	Total 42	C 40	O 2	0
39	O	1	Total 42	C 40	O 2	0
39	O	1	Total 42	C 40	O 2	0
39	P	1	Total 42	C 40	O 2	0
39	P	1	Total 42	C 40	O 2	0
39	P	1	Total 42	C 40	O 2	0
39	Q	1	Total 42	C 40	O 2	0
39	Q	1	Total 42	C 40	O 2	0
39	Q	1	Total 42	C 40	O 2	0
39	Q	1	Total 42	C 40	O 2	0
39	Q	1	Total 42	C 40	O 2	0
39	R	1	Total 42	C 40	O 2	0
39	R	1	Total 42	C 40	O 2	0
39	R	1	Total 42	C 40	O 2	0
39	R	1	Total 42	C 40	O 2	0

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Mol	Chain	Residues	Atoms			AltConf
39	S	1	Total	C	O	0
			42	40	2	
39	S	1	Total	C	O	0
			42	40	2	

- Molecule 40 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: IHT) (formula: C₄₀H₅₄O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
40	1	1	Total	C	O	0
			41	40	1	
40	N	1	Total	C	O	0
			41	40	1	
40	2	1	Total	C	O	0
			41	40	1	
40	4	1	Total	C	O	0
			41	40	1	
40	5	1	Total	C	O	0
			41	40	1	
40	O	1	Total	C	O	0
			41	40	1	
40	Q	1	Total	C	O	0
			41	40	1	
40	R	1	Total	C	O	0
			41	40	1	

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		AltConf
41	A	52	Total 52	O 52	0
41	B	117	Total 117	O 117	0
41	C	52	Total 52	O 52	0
41	D	70	Total 70	O 70	0
41	E	8	Total 8	O 8	0
41	F	2	Total 2	O 2	0
41	H	14	Total 14	O 14	0
41	I	1	Total 1	O 1	0
41	K	4	Total 4	O 4	0
41	L	7	Total 7	O 7	0
41	M	1	Total 1	O 1	0
41	T	4	Total 4	O 4	0
41	W	2	Total 2	O 2	0
41	X	3	Total 3	O 3	0
41	a	48	Total 48	O 48	0
41	b	125	Total 125	O 125	0
41	c	52	Total 52	O 52	0
41	d	71	Total 71	O 71	0
41	e	9	Total 9	O 9	0
41	h	14	Total 14	O 14	0
41	i	1	Total 1	O 1	0

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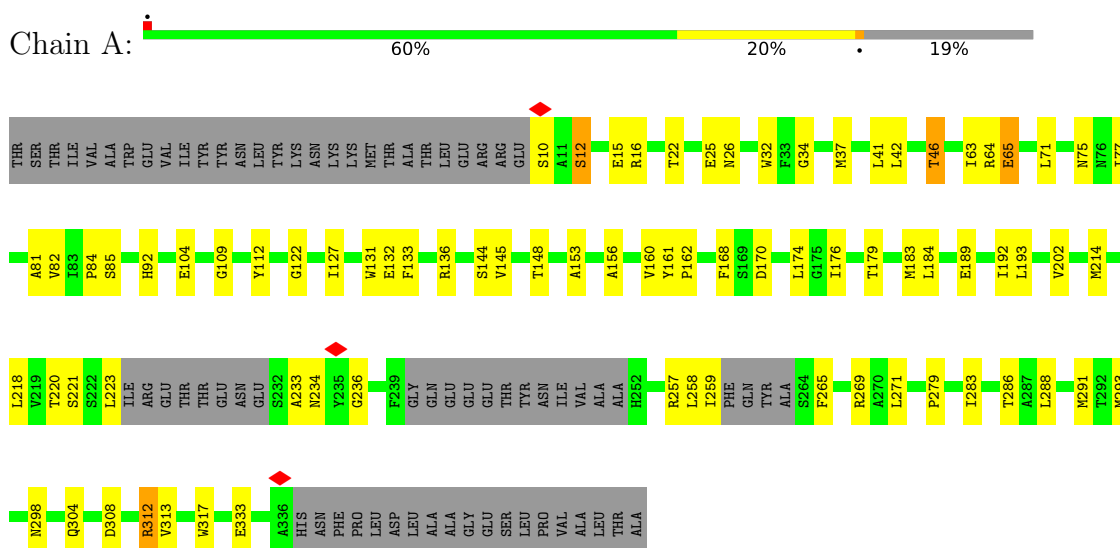
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Mol	Chain	Residues	Atoms		AltConf
41	k	3	Total 3	O 3	0
41	l	5	Total 5	O 5	0
41	m	4	Total 4	O 4	0
41	t	5	Total 5	O 5	0
41	w	1	Total 1	O 1	0
41	x	1	Total 1	O 1	0

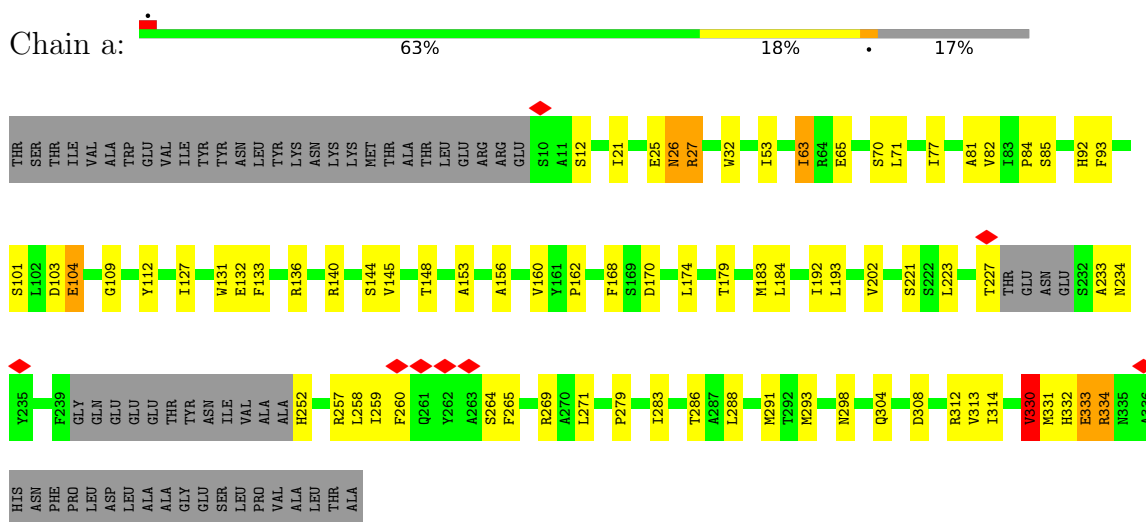
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Photosystem II protein D1



- Molecule 1: Photosystem II protein D1



- Molecule 2: Photosystem II CP47 reaction center protein

Response	Percentage
Yes	65%
No	26%
Don't know	5%



Frequency	Percentage
Daily	70%
Weekly	22%
Monthly	5%

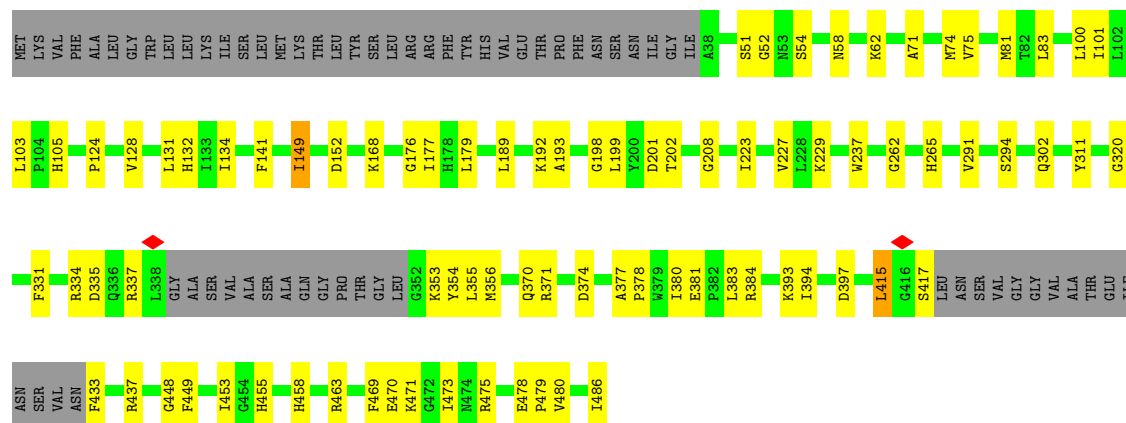


Frequency	Percentage
Daily	69%
Weekly	16%
Monthly	13%
Other	2%



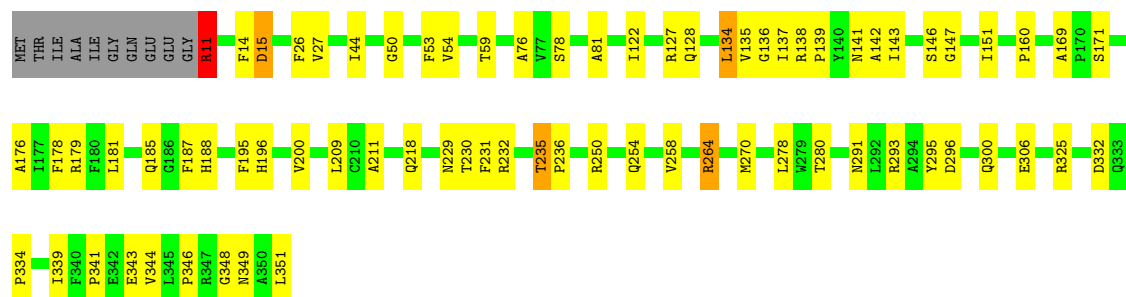
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 69% 17% 13%



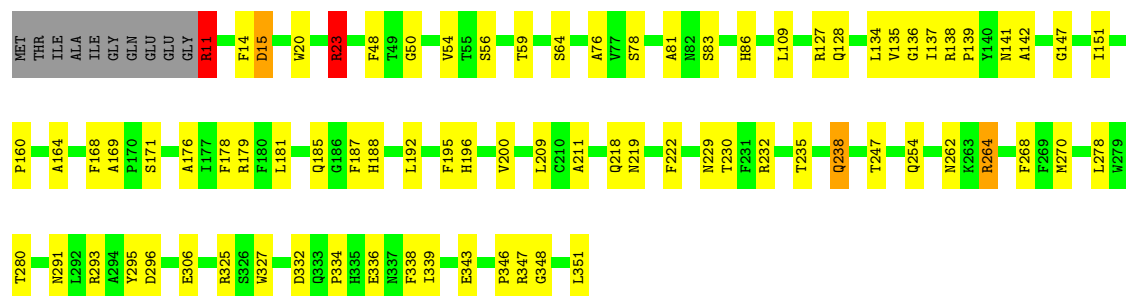
- Molecule 4: Photosystem II D2 protein

Chain D: 76% 20% . .

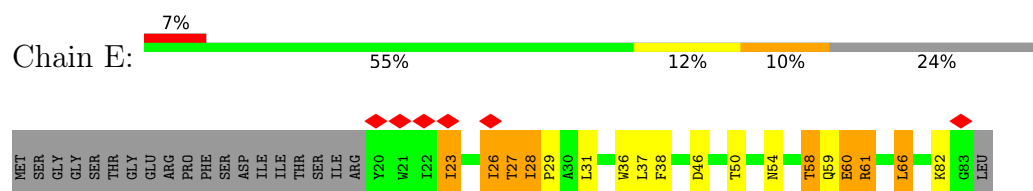


- Molecule 4: Photosystem II D2 protein

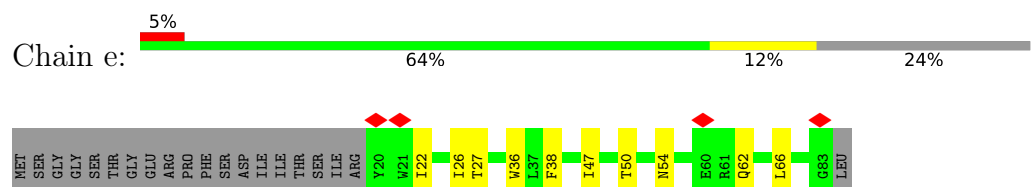
Chain d: 74% 21% ...



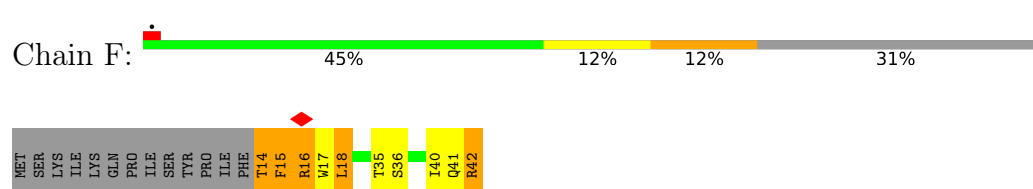
- Molecule 5: Cytochrome b559 subunit alpha



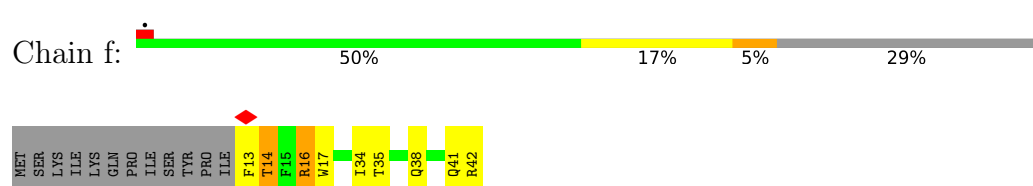
- Molecule 5: Cytochrome b559 subunit alpha



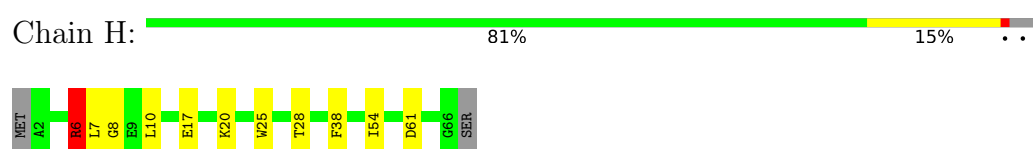
- Molecule 6: Cytochrome b559 subunit beta



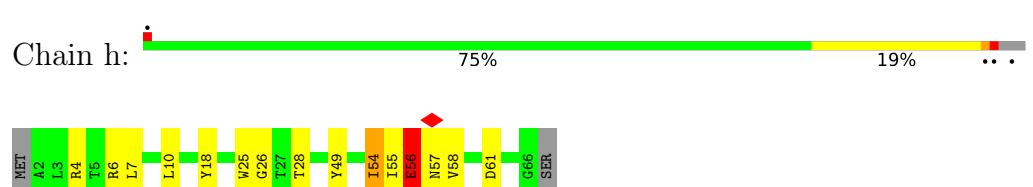
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I





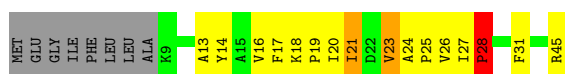
- Molecule 8: Photosystem II reaction center protein I

Chain i: 76% 13% 8%



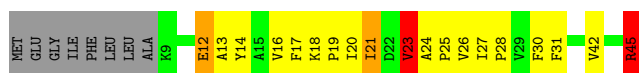
- Molecule 9: Photosystem II reaction center protein K

Chain K: 47% 29% 18%



- Molecule 9: Photosystem II reaction center protein K

Chain k: 40% 33% 18%



- Molecule 10: Photosystem II reaction center protein L

Chain L: 71% 24% 5%



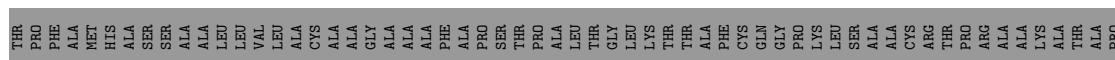
- Molecule 10: Photosystem II reaction center protein L

Chain l: 61% 32% 5%



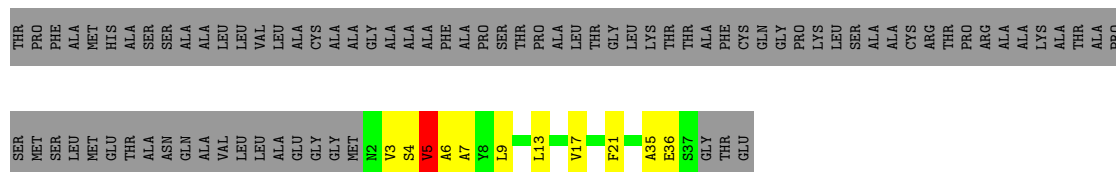
- Molecule 11: Photosystem II protein M

Chain M: 20% 10% 69%




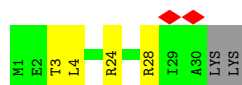
- Molecule 11: Photosystem II protein M

Chain m:  21% 8% 69%




• Molecule 12: Photosystem II reaction center protein T

Chain T:  6% 81% 12% 6%



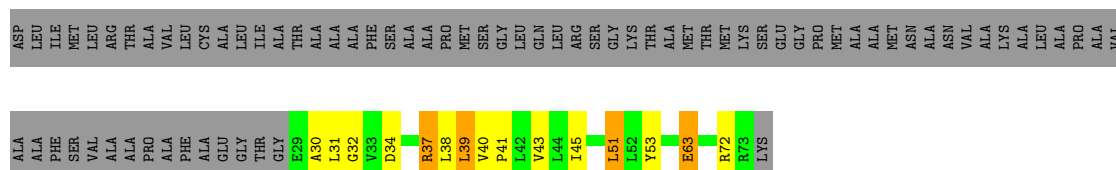
• Molecule 12: Photosystem II reaction center protein T

Chain t:  6% 75% 19% 6%



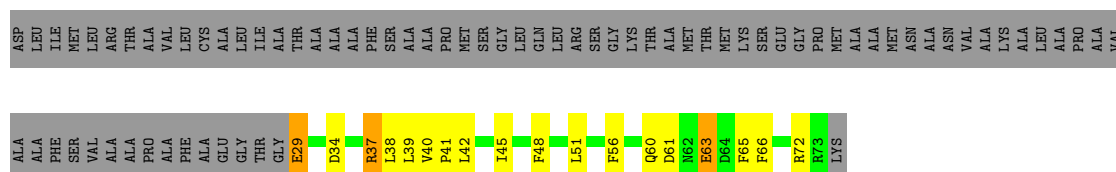
• Molecule 13: Photosystem II protein W

Chain W:  25% 9% 63%



• Molecule 13: Photosystem II protein W

Chain w:  22% 12% 63%



• Molecule 14: Photosystem II reaction center X protein

Chain X:  69% 10% 8% 13%



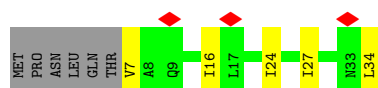
• Molecule 14: Photosystem II reaction center X protein

Chain x:  64% 15% 8% 13%



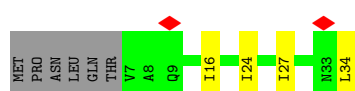
- Molecule 15: Photosystem II reaction center protein Psb30

Chain Y:  9% 68% 15% 18%



- Molecule 15: Photosystem II reaction center protein Psb30

Chain y:  6% 71% 12% 18%




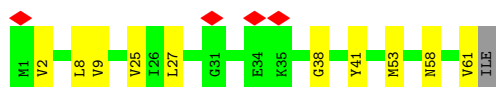
- Molecule 16: Photosystem II reaction center protein Z

Chain Z:  56% 31% 11% .




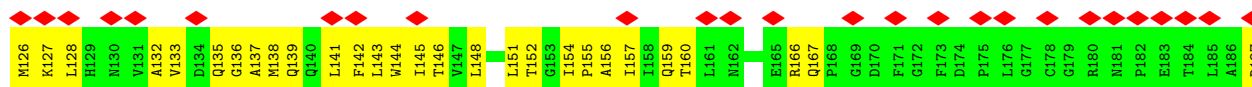
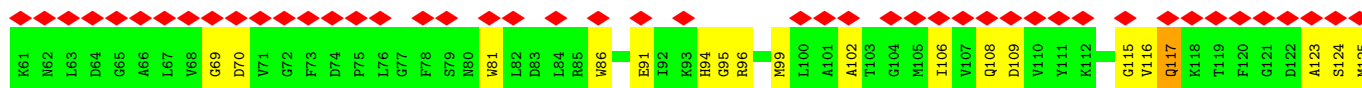
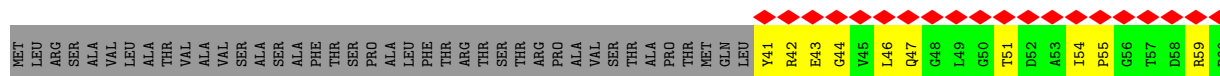
- Molecule 16: Photosystem II reaction center protein Z

Chain z:  6% 82% 16% .



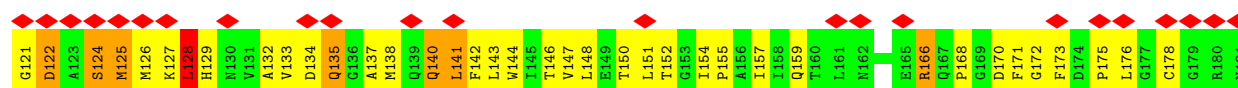
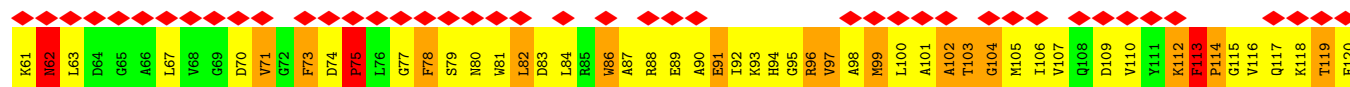
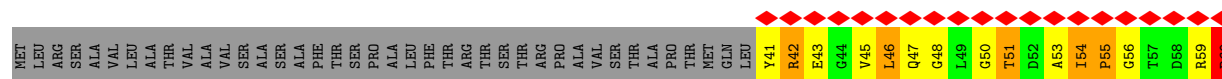
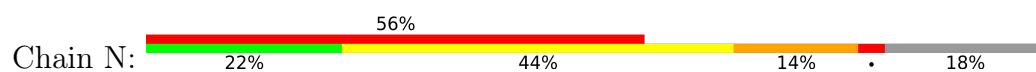
- Molecule 17: ACPH-1

Chain 1:  55% 45% 37% 18%

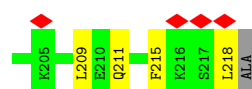
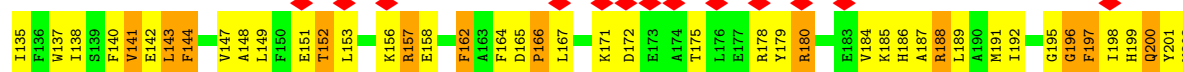
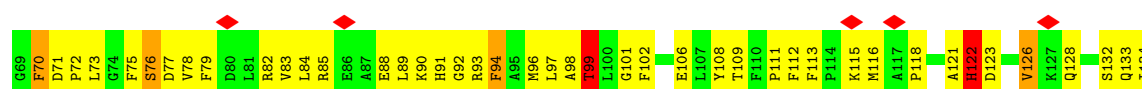
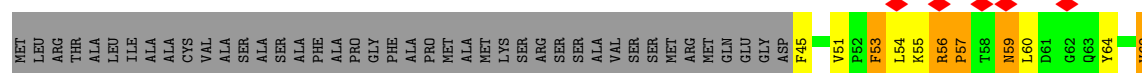




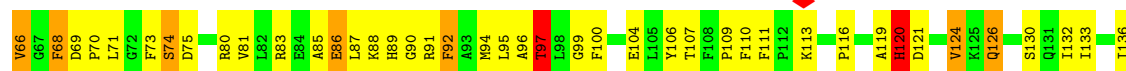
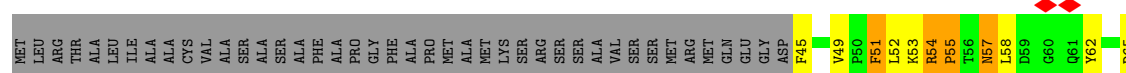
• Molecule 17: ACPII-1

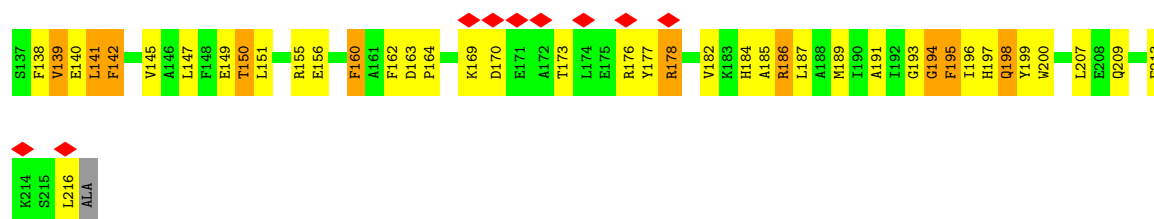


• Molecule 18: ACPII-2

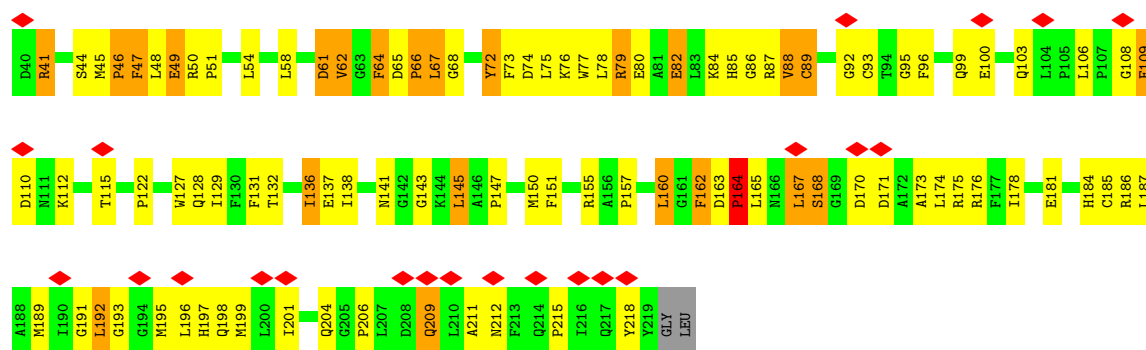
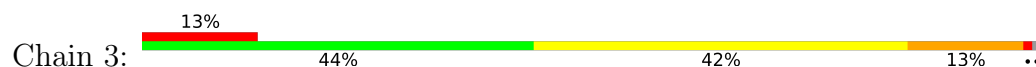


• Molecule 18: ACPII-2





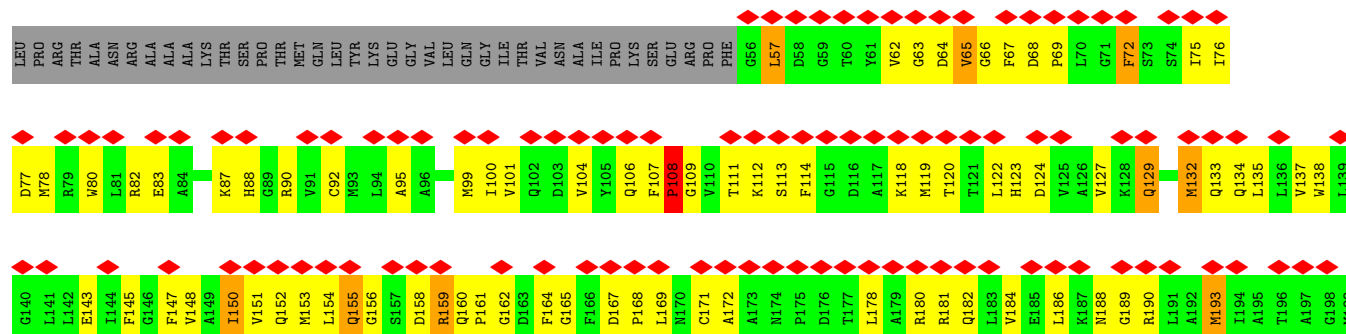
• Molecule 19: ACPH-3

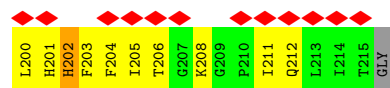


• Molecule 19: ACPH-3

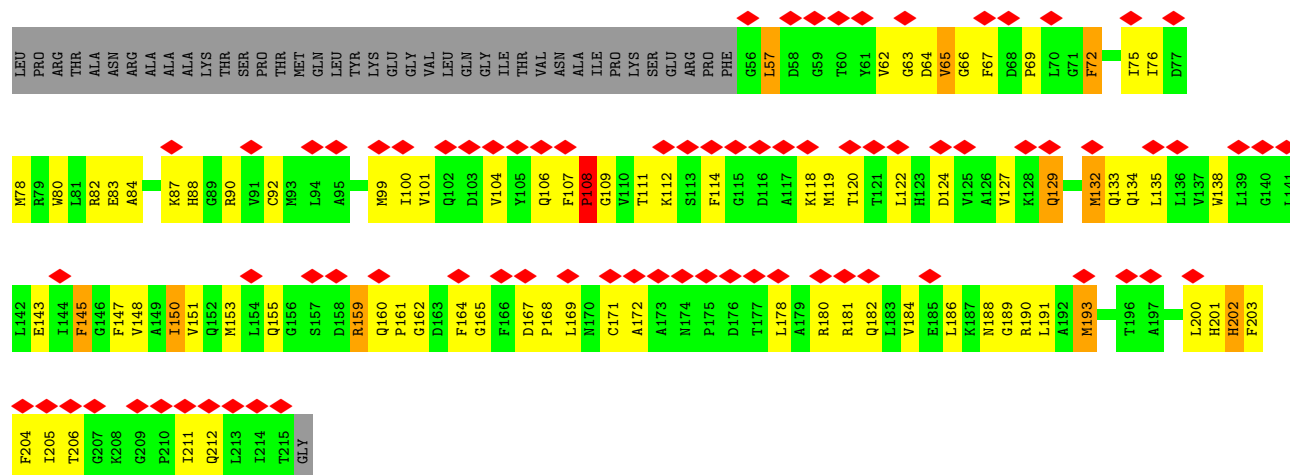
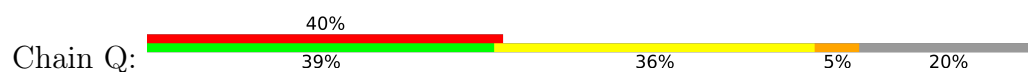


• Molecule 20: ACPH-4

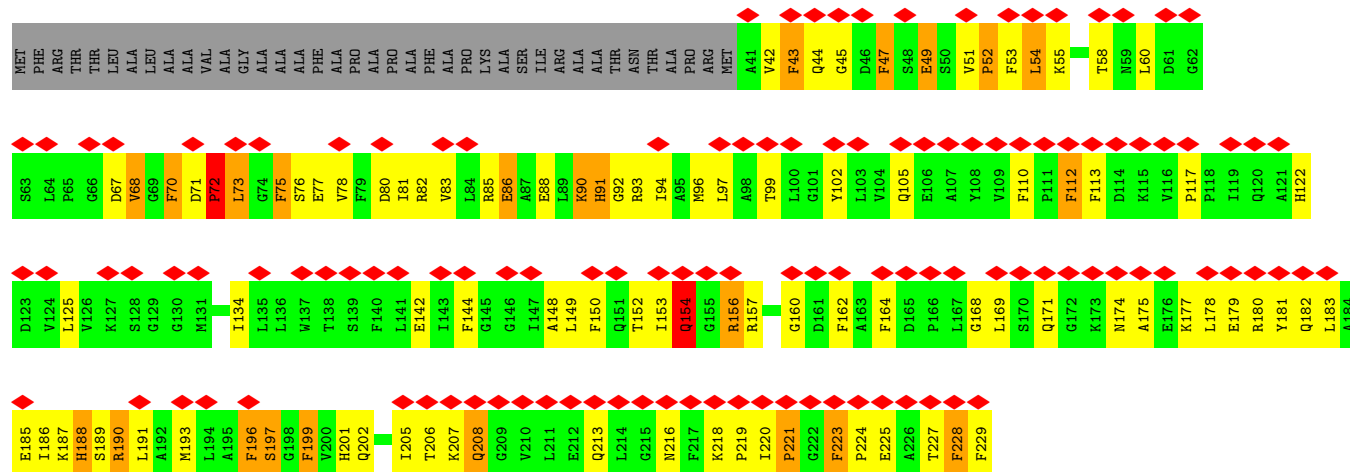




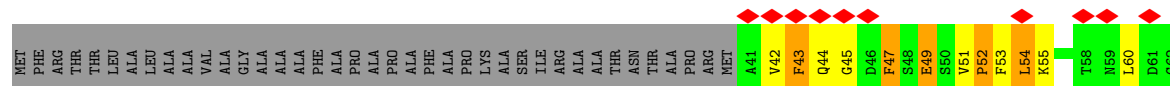
• Molecule 20: ACPII-4

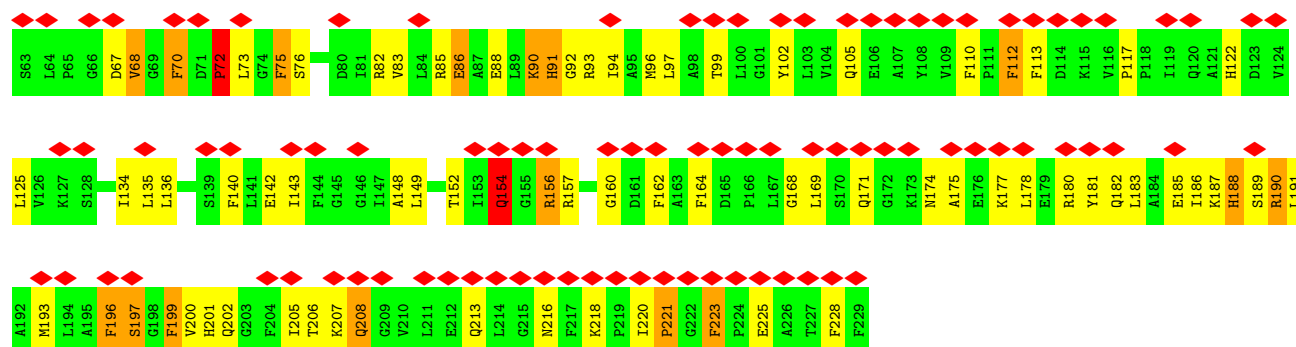


• Molecule 21: ACPII-5

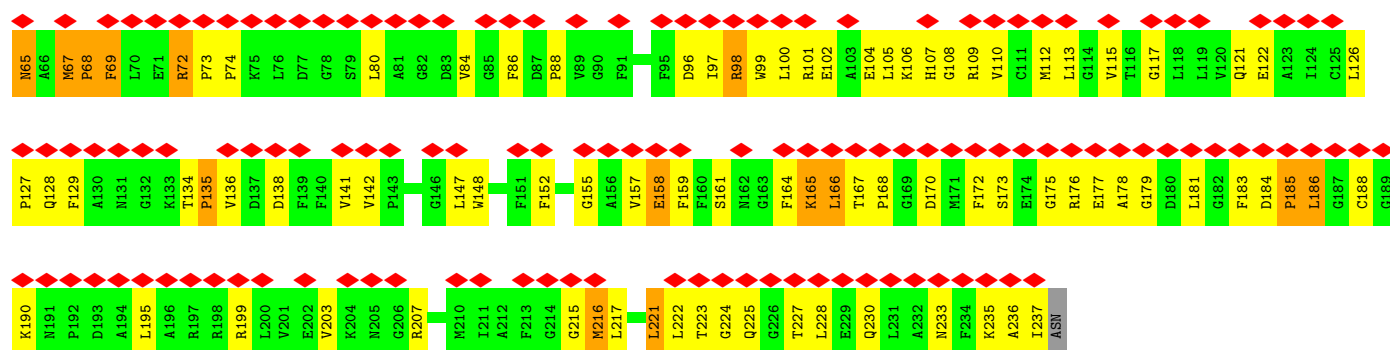
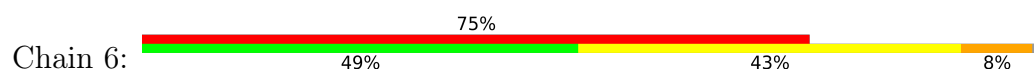


• Molecule 21: ACPII-5

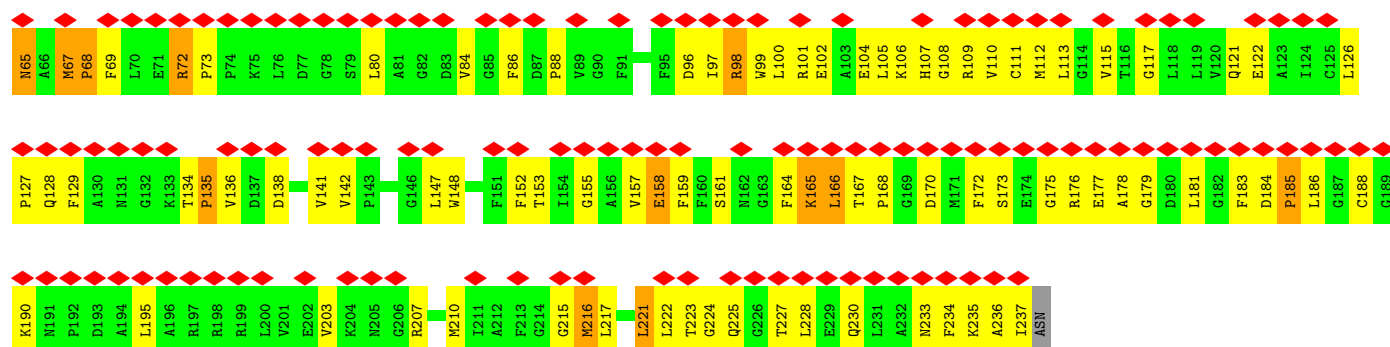




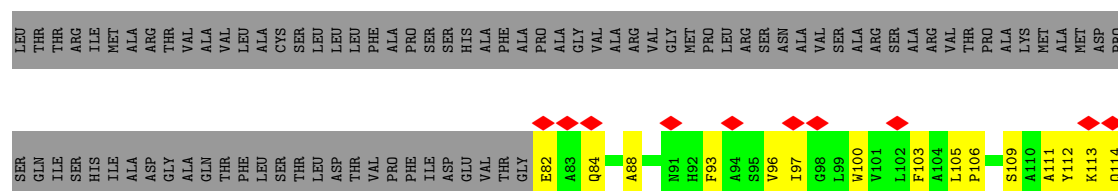
• Molecule 22: ACPH-6



• Molecule 22: ACPH-6



• Molecule 23: Psb-gama_linker



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28657	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.303	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	436.2, 436.2, 436.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MN, CLA, HEM, LMG, FE2, DGD, CL, BCT, WVN, LHG, PL9, IHT, SQD, KC2, PHO, IIO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	1/2452 (0.0%)	0.54	0/3339
1	a	0.37	0/2516	0.57	3/3428 (0.1%)
2	B	0.62	0/3927	0.94	11/5349 (0.2%)
2	b	0.44	0/3912	0.64	3/5330 (0.1%)
3	C	0.39	0/3442	0.54	1/4692 (0.0%)
3	c	0.29	0/3409	0.51	2/4647 (0.0%)
4	D	0.32	0/2806	0.48	0/3823
4	d	0.35	0/2798	0.53	0/3812
5	E	0.74	0/541	0.92	1/738 (0.1%)
5	e	0.35	0/541	0.49	0/738
6	F	0.75	0/242	1.04	0/328
6	f	0.65	0/254	0.87	0/344
7	H	0.38	0/519	0.61	0/707
7	h	0.48	0/519	0.73	1/707 (0.1%)
8	I	0.25	0/290	0.46	0/392
8	i	0.28	0/290	0.47	0/392
9	K	0.63	0/307	0.98	1/421 (0.2%)
9	k	0.75	0/307	1.07	1/421 (0.2%)
10	L	0.37	0/311	0.60	0/424
10	l	0.58	0/311	0.96	2/424 (0.5%)
11	M	0.65	0/275	0.93	0/375
11	m	0.55	0/275	0.93	2/375 (0.5%)
12	T	0.41	0/251	0.54	0/341
12	t	0.21	0/251	0.43	0/341
13	W	0.71	0/368	1.22	1/501 (0.2%)
13	w	0.77	0/368	1.33	2/501 (0.4%)
14	X	0.72	0/253	1.05	0/345
14	x	0.85	0/253	1.32	2/345 (0.6%)
15	Y	0.32	0/210	0.54	0/285
15	y	0.10	0/210	0.25	0/285
16	Z	0.77	0/460	1.12	2/628 (0.3%)
16	z	0.19	0/470	0.33	0/641

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	1	0.26	0/1510	0.57	0/2046
17	N	1.11	3/1510 (0.2%)	2.08	65/2046 (3.2%)
18	2	1.10	2/1416 (0.1%)	1.89	40/1915 (2.1%)
18	O	1.11	2/1416 (0.1%)	1.89	40/1915 (2.1%)
19	3	1.15	2/1424 (0.1%)	1.91	42/1925 (2.2%)
19	P	1.15	2/1424 (0.1%)	1.91	42/1925 (2.2%)
20	4	0.99	0/1251	1.95	30/1690 (1.8%)
20	Q	0.99	0/1251	1.95	29/1690 (1.7%)
21	5	1.08	1/1522 (0.1%)	1.99	54/2059 (2.6%)
21	R	1.08	1/1522 (0.1%)	1.99	53/2059 (2.6%)
22	6	0.90	0/1359	1.68	25/1836 (1.4%)
22	S	0.90	0/1359	1.68	25/1836 (1.4%)
23	G	0.92	0/784	1.14	1/1072 (0.1%)
24	g	0.31	0/777	0.52	2/1064 (0.2%)
All	All	0.70	14/51863 (0.0%)	1.19	483/70497 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	a	0	3
2	B	0	8
2	b	0	6
3	C	0	2
4	D	0	3
4	d	0	3
5	E	0	1
6	F	0	2
7	H	0	1
9	k	0	1
12	T	0	1
13	W	0	1
13	w	0	1
17	N	0	4
18	2	0	2
18	O	0	2
20	4	0	2
20	Q	0	2
23	G	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
24	g	0	1
All	All	0	50

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	P	44	SER	CA-CB	-6.26	1.43	1.53
19	3	44	SER	CA-CB	-6.26	1.43	1.53
1	A	10	SER	C-N	6.08	1.41	1.33
19	3	168	SER	CA-CB	-5.75	1.45	1.53
19	P	168	SER	CA-CB	-5.74	1.45	1.53
18	O	74	SER	CA-CB	-5.56	1.44	1.53
18	2	76	SER	CA-CB	-5.55	1.44	1.53
17	N	114	PRO	CA-C	-5.36	1.46	1.52
18	2	132	SER	CA-CB	-5.22	1.45	1.53
18	O	130	SER	CA-CB	-5.13	1.45	1.53
21	5	76	SER	CA-CB	-5.11	1.45	1.53
21	R	76	SER	CA-CB	-5.11	1.45	1.53
17	N	124	SER	CA-CB	-5.05	1.45	1.53
17	N	86	TRP	CA-C	-5.01	1.45	1.52

All (483) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	89	CYS	CB-CA-C	16.52	137.68	110.09
19	P	89	CYS	CB-CA-C	16.50	137.65	110.09
17	N	42	ARG	N-CA-C	-13.48	96.58	111.14
17	N	55	PRO	N-CA-C	-12.72	90.53	111.26
17	N	226	ASN	N-CA-C	-11.86	100.40	112.97
17	N	113	PHE	N-CA-CB	-11.81	95.30	109.59
21	R	75	PHE	N-CA-C	-11.66	99.58	114.04
21	5	75	PHE	N-CA-C	-11.65	99.59	114.04
17	N	91	GLU	CB-CA-C	-10.05	93.76	110.85
17	N	122	ASP	CB-CA-C	9.81	125.43	110.62
20	Q	159	ARG	N-CA-CB	-9.48	95.51	109.83
20	4	159	ARG	N-CA-CB	-9.46	95.54	109.83
21	R	49	GLU	CB-CA-C	-9.44	96.06	110.88
21	5	49	GLU	CB-CA-C	-9.42	96.10	110.88
17	N	86	TRP	CA-C-N	-9.41	106.93	120.29
17	N	86	TRP	C-N-CA	-9.41	106.93	120.29
17	N	103	THR	N-CA-C	-9.21	101.11	111.71
21	R	221	PRO	N-CA-CB	-9.06	95.11	103.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	221	PRO	N-CA-CB	-9.05	95.13	103.27
19	3	47	PHE	CA-CB-CG	9.03	122.83	113.80
19	P	47	PHE	CA-CB-CG	9.01	122.81	113.80
17	N	93	LYS	N-CA-CB	8.85	123.26	110.16
17	N	42	ARG	N-CA-CB	8.84	122.89	110.07
2	B	384	ARG	CB-CA-C	-8.75	96.72	109.84
7	h	56	GLU	CB-CG-CD	8.64	127.30	112.60
19	3	64	PHE	CB-CA-C	-8.49	98.78	112.03
19	P	64	PHE	CB-CA-C	-8.48	98.80	112.03
21	5	53	PHE	CA-CB-CG	8.34	122.14	113.80
21	R	53	PHE	CA-CB-CG	8.32	122.12	113.80
22	6	127	PRO	N-CA-C	-8.18	102.17	113.53
22	S	127	PRO	N-CA-C	-8.16	102.19	113.53
24	g	170	TRP	O-C-N	-8.13	112.54	122.71
18	2	152	THR	CA-CB-OG1	-8.13	97.41	109.60
22	6	128	GLN	N-CA-CB	-8.11	98.19	110.12
18	O	150	THR	CA-CB-OG1	-8.11	97.44	109.60
22	S	128	GLN	N-CA-CB	-8.11	98.20	110.12
17	N	86	TRP	N-CA-C	-8.06	103.23	113.23
17	N	142	PHE	N-CA-C	-8.03	104.01	113.88
2	B	135	LEU	O-C-N	8.02	126.72	120.38
11	m	5	VAL	N-CA-CB	-8.01	105.07	111.64
17	N	178	CYS	N-CA-C	-8.01	102.55	111.28
16	Z	34	GLU	N-CA-C	-7.93	104.21	114.04
20	4	155	GLN	N-CA-C	-7.89	100.11	110.53
19	P	164	PRO	N-CA-CB	-7.87	94.81	103.23
19	3	164	PRO	N-CA-CB	-7.86	94.82	103.23
22	6	98	ARG	N-CA-CB	-7.85	98.58	110.12
22	S	98	ARG	N-CA-CB	-7.85	98.58	110.12
20	Q	155	GLN	N-CA-C	-7.84	100.19	110.53
17	N	141	LEU	N-CA-C	-7.81	101.55	113.89
18	2	108	TYR	CB-CA-C	-7.80	94.23	109.68
18	O	106	TYR	CB-CA-C	-7.79	94.25	109.68
19	P	51	PRO	N-CA-C	-7.79	101.20	110.70
20	4	108	PRO	N-CA-CB	-7.79	94.77	103.33
18	O	120	HIS	N-CA-C	-7.78	102.77	111.71
20	4	65	VAL	N-CA-C	-7.77	105.14	112.83
20	Q	108	PRO	N-CA-CB	-7.77	94.78	103.33
20	Q	65	VAL	N-CA-C	-7.77	105.14	112.83
19	3	51	PRO	N-CA-C	-7.77	101.22	110.70
19	P	49	GLU	CB-CA-C	-7.75	96.26	109.51
18	2	122	HIS	N-CA-C	-7.74	102.81	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	60	PRO	N-CA-C	-7.74	98.65	111.26
19	3	49	GLU	CB-CA-C	-7.73	96.30	109.51
13	W	32	GLY	N-CA-C	-7.69	104.58	115.43
21	5	122	HIS	CA-CB-CG	7.68	121.48	113.80
21	R	122	HIS	CA-CB-CG	7.68	121.48	113.80
18	O	54	ARG	CA-CB-CG	7.65	129.40	114.10
18	2	56	ARG	CA-CB-CG	7.62	129.35	114.10
18	O	97	THR	CA-CB-OG1	-7.55	98.27	109.60
18	2	99	THR	CA-CB-OG1	-7.51	98.33	109.60
2	b	479	PHE	CA-CB-CG	-7.51	106.29	113.80
20	Q	72	PHE	CB-CA-C	7.49	123.22	110.79
20	4	72	PHE	CB-CA-C	7.48	123.21	110.79
21	5	207	LYS	N-CA-C	-7.46	103.75	112.86
18	2	57	PRO	N-CA-C	-7.43	99.57	111.38
21	R	207	LYS	N-CA-C	-7.43	103.80	112.86
18	O	55	PRO	N-CA-C	-7.42	99.59	111.38
19	P	206	PRO	N-CA-CB	-7.42	95.30	103.23
19	3	206	PRO	N-CA-CB	-7.40	95.31	103.23
19	3	89	CYS	N-CA-CB	-7.33	99.64	110.49
19	P	89	CYS	N-CA-CB	-7.33	99.64	110.49
20	4	202	HIS	N-CA-C	-7.30	103.26	111.07
17	N	75	PRO	CA-C-N	-7.25	111.28	122.60
17	N	75	PRO	C-N-CA	-7.25	111.28	122.60
20	Q	202	HIS	N-CA-C	-7.25	103.31	111.07
17	N	94	HIS	CA-CB-CG	7.23	121.03	113.80
19	P	157	PRO	N-CA-CB	-7.22	96.69	103.19
17	N	90	ALA	O-C-N	-7.21	114.47	122.12
19	3	157	PRO	N-CA-CB	-7.21	96.70	103.19
18	O	186	ARG	N-CA-CB	-7.18	99.59	110.01
19	P	62	VAL	N-CA-C	-7.17	105.36	112.17
18	2	188	ARG	N-CA-CB	-7.16	99.62	110.01
21	R	228	PHE	CB-CA-C	7.14	122.65	110.79
19	3	62	VAL	N-CA-C	-7.14	105.39	112.17
22	S	69	PHE	CA-CB-CG	7.14	120.94	113.80
1	a	330	VAL	CA-C-N	-7.12	111.21	123.25
1	a	330	VAL	C-N-CA	-7.12	111.21	123.25
22	6	69	PHE	CA-CB-CG	7.11	120.91	113.80
21	5	223	PHE	CA-CB-CG	-7.06	106.74	113.80
21	R	223	PHE	CA-CB-CG	-7.04	106.76	113.80
2	B	89	GLY	CA-C-O	-7.03	117.65	122.22
21	R	70	PHE	CA-CB-CG	6.97	120.77	113.80
19	3	88	VAL	CA-C-N	-6.97	111.04	122.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	88	VAL	C-N-CA	-6.97	111.04	122.54
19	P	88	VAL	CA-C-N	-6.97	111.04	122.54
19	P	88	VAL	C-N-CA	-6.97	111.04	122.54
21	5	228	PHE	CB-CA-C	6.97	122.69	110.85
21	5	70	PHE	CA-CB-CG	6.95	120.75	113.80
18	O	51	PHE	CB-CA-C	6.95	121.66	110.96
18	2	53	PHE	CB-CA-C	6.93	121.63	110.96
18	2	68	VAL	N-CA-C	-6.91	106.07	112.43
18	O	66	VAL	N-CA-C	-6.90	106.08	112.43
17	N	140	GLN	N-CA-CB	6.88	121.78	110.91
19	P	64	PHE	CA-CB-CG	6.86	120.66	113.80
19	3	64	PHE	CA-CB-CG	6.84	120.64	113.80
22	6	84	VAL	N-CA-C	-6.83	105.87	112.29
22	S	84	VAL	N-CA-C	-6.82	105.88	112.29
17	N	141	LEU	N-CA-CB	6.76	120.68	110.95
21	R	225	GLU	N-CA-CB	-6.72	100.22	110.16
21	5	225	GLU	N-CA-CB	-6.69	100.26	110.16
18	2	171	LYS	N-CA-CB	-6.63	100.35	110.16
3	c	479	PRO	N-CA-CB	-6.62	96.05	103.33
18	O	169	LYS	N-CA-CB	-6.60	100.39	110.16
21	5	208	GLN	N-CA-CB	-6.59	99.61	110.68
18	2	164	PHE	CA-CB-CG	6.58	120.38	113.80
21	R	208	GLN	N-CA-CB	-6.58	99.62	110.68
18	O	68	PHE	CA-CB-CG	6.54	120.34	113.80
18	2	70	PHE	CA-CB-CG	6.53	120.33	113.80
17	N	122	ASP	N-CA-C	-6.50	96.44	108.02
18	O	162	PHE	CA-CB-CG	6.50	120.30	113.80
20	4	108	PRO	N-CA-C	6.50	122.56	113.53
21	R	68	VAL	N-CA-C	-6.49	105.33	112.80
17	N	54	ILE	N-CA-C	-6.47	94.89	108.88
17	N	78	PHE	CA-CB-CG	6.47	120.28	113.80
22	S	68	PRO	N-CA-CB	-6.47	96.21	103.33
21	5	68	VAL	N-CA-C	-6.46	105.37	112.80
5	E	27	THR	CA-CB-OG1	-6.46	99.91	109.60
20	Q	108	PRO	N-CA-C	6.45	122.50	113.53
18	2	143	LEU	N-CA-CB	6.45	119.36	110.01
22	6	68	PRO	N-CA-CB	-6.44	96.25	103.33
21	R	90	LYS	N-CA-CB	6.43	119.58	110.12
18	O	141	LEU	N-CA-CB	6.43	119.33	110.01
21	5	90	LYS	N-CA-CB	6.43	119.57	110.12
17	N	135	GLN	N-CA-C	-6.36	104.62	112.38
17	N	100	LEU	N-CA-CB	6.36	119.57	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	71	VAL	N-CA-C	-6.35	106.55	112.83
3	C	469	PHE	CA-CB-CG	6.34	120.14	113.80
21	R	180	ARG	CB-CA-C	-6.33	100.28	110.79
21	5	180	ARG	CB-CA-C	-6.33	100.28	110.79
22	6	165	LYS	N-CA-CB	-6.33	102.48	110.45
18	O	155	ARG	CG-CD-NE	-6.32	98.09	112.00
19	P	209	GLN	CB-CA-C	-6.31	100.31	110.79
17	N	209	HIS	CB-CA-C	-6.31	100.97	110.88
18	2	157	ARG	CG-CD-NE	-6.30	98.13	112.00
22	S	96	ASP	CB-CA-C	-6.30	99.25	109.72
3	c	469	PHE	CA-CB-CG	6.30	120.10	113.80
22	S	165	LYS	N-CA-CB	-6.30	102.51	110.45
17	N	62	ASN	N-CA-C	-6.30	104.42	111.28
22	6	96	ASP	CB-CA-C	-6.30	99.27	109.72
17	N	215	ARG	N-CA-CB	-6.29	100.89	110.77
19	3	209	GLN	CB-CA-C	-6.29	100.35	110.79
21	R	73	LEU	N-CA-C	-6.29	98.48	108.73
18	2	59	ASN	CB-CA-C	6.28	120.58	110.09
18	O	57	ASN	CB-CA-C	6.28	120.58	110.09
18	O	142	PHE	CB-CA-C	6.26	122.22	110.63
19	P	46	PRO	N-CA-CB	-6.26	96.63	103.39
19	3	46	PRO	N-CA-CB	-6.25	96.64	103.39
18	2	144	PHE	CB-CA-C	6.25	122.20	110.63
21	5	73	LEU	N-CA-C	-6.25	98.54	108.73
21	R	72	PRO	N-CA-CB	-6.23	96.48	103.33
18	O	198	GLN	N-CA-C	-6.23	104.49	111.28
21	5	72	PRO	N-CA-CB	-6.20	96.51	103.33
21	R	54	LEU	N-CA-CB	-6.20	100.31	110.41
20	4	57	LEU	CB-CG-CD1	-6.18	92.16	110.70
21	5	54	LEU	N-CA-CB	-6.17	100.35	110.41
18	2	200	GLN	N-CA-C	-6.17	104.55	111.28
20	Q	57	LEU	CB-CG-CD1	-6.17	92.18	110.70
17	N	227	PHE	CA-CB-CG	6.16	119.96	113.80
2	B	219	VAL	N-CA-C	6.16	117.16	108.36
21	5	197	SER	N-CA-C	-6.16	103.72	111.11
21	R	197	SER	N-CA-C	-6.14	103.75	111.11
18	O	126	GLN	N-CA-C	-6.13	104.60	111.28
21	5	43	PHE	N-CA-CB	6.12	118.96	109.97
18	2	128	GLN	N-CA-C	-6.10	104.63	111.28
20	Q	83	GLU	N-CA-C	-6.10	104.63	111.28
20	4	83	GLU	N-CA-C	-6.09	104.65	111.28
21	R	43	PHE	N-CA-CB	6.08	118.91	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	481	GLY	CA-C-O	-6.07	118.27	122.22
17	N	171	PHE	N-CA-C	-6.07	105.05	112.88
23	G	120	PRO	N-CA-C	-6.07	105.46	113.65
17	N	42	ARG	CA-CB-CG	-6.06	101.98	114.10
22	S	158	GLU	CB-CA-C	-6.05	100.74	110.79
18	2	88	GLU	N-CA-C	-6.05	104.38	110.97
22	6	98	ARG	CA-CB-CG	6.04	126.18	114.10
18	O	124	VAL	N-CA-CB	6.04	120.98	110.65
22	6	158	GLU	CB-CA-C	-6.04	100.77	110.79
21	R	52	PRO	N-CA-CB	-6.03	96.69	103.33
22	S	98	ARG	CA-CB-CG	6.03	126.16	114.10
21	5	52	PRO	N-CA-CB	-6.03	96.70	103.33
18	2	126	VAL	N-CA-CB	6.03	120.96	110.65
18	O	155	ARG	CD-NE-CZ	-6.03	115.96	124.40
21	R	228	PHE	CA-CB-CG	-6.03	107.78	113.80
17	N	225	PRO	N-CA-C	6.02	119.94	111.33
18	O	86	GLU	N-CA-C	-6.01	104.42	110.97
18	2	112	PHE	CA-CB-CG	6.00	119.80	113.80
18	O	110	PHE	CA-CB-CG	5.99	119.79	113.80
21	R	225	GLU	CB-CG-CD	5.98	122.77	112.60
18	2	157	ARG	CD-NE-CZ	-5.98	116.03	124.40
21	5	228	PHE	CA-CB-CG	-5.98	107.82	113.80
21	R	122	HIS	N-CA-C	-5.97	104.78	111.28
21	5	122	HIS	N-CA-C	-5.96	104.78	111.28
21	5	225	GLU	CB-CG-CD	5.96	122.74	112.60
22	S	157	VAL	N-CA-C	-5.93	104.57	110.62
17	N	231	LEU	N-CA-CB	-5.93	101.45	110.11
22	6	157	VAL	N-CA-C	-5.92	104.58	110.62
21	5	154	GLN	CB-CA-C	-5.92	103.24	112.12
17	N	51	THR	CA-CB-OG1	-5.91	100.73	109.60
19	3	160	LEU	N-CA-C	-5.91	105.93	113.02
21	R	112	PHE	CA-CB-CG	5.91	119.71	113.80
9	K	28	PRO	N-CA-CB	-5.90	97.05	103.25
2	B	383	PHE	N-CA-C	-5.90	102.32	110.35
10	I	10	PRO	N-CA-CB	-5.90	97.84	103.33
19	P	87	ARG	N-CA-C	-5.90	104.85	111.28
19	P	160	LEU	N-CA-C	-5.90	105.94	113.02
21	5	117	PRO	N-CA-C	-5.90	103.51	110.70
21	R	154	GLN	CB-CA-C	-5.89	103.28	112.12
19	3	87	ARG	N-CA-C	-5.88	104.87	111.28
18	2	162	PHE	N-CA-C	-5.87	105.31	112.88
21	R	117	PRO	N-CA-C	-5.87	103.54	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	112	PHE	CA-CB-CG	5.87	119.67	113.80
22	6	67	MET	CB-CA-C	-5.86	103.66	110.17
22	S	67	MET	CB-CA-C	-5.86	103.67	110.17
18	O	160	PHE	N-CA-C	-5.84	105.35	112.88
20	Q	162	GLY	CA-C-N	-5.83	115.01	122.77
20	Q	162	GLY	C-N-CA	-5.83	115.01	122.77
17	N	128	LEU	N-CA-C	-5.83	104.93	111.28
17	N	99	MET	N-CA-C	-5.83	104.93	111.28
20	4	162	GLY	CA-C-N	-5.83	115.02	122.77
20	4	162	GLY	C-N-CA	-5.83	115.02	122.77
21	R	190	ARG	CB-CA-C	5.82	120.01	110.88
19	3	206	PRO	N-CD-CG	-5.80	94.49	103.20
19	P	109	PHE	N-CA-C	-5.80	106.43	112.93
19	P	206	PRO	N-CD-CG	-5.80	94.49	103.20
20	Q	63	GLY	CA-C-N	-5.79	114.72	122.42
20	Q	63	GLY	C-N-CA	-5.79	114.72	122.42
21	5	190	ARG	CB-CA-C	5.78	119.95	110.88
18	2	144	PHE	N-CA-C	-5.77	105.07	111.71
20	4	63	GLY	CA-C-N	-5.77	114.75	122.42
20	4	63	GLY	C-N-CA	-5.77	114.75	122.42
18	O	170	ASP	CB-CA-C	-5.77	97.97	109.79
21	R	122	HIS	CB-CA-C	-5.76	101.22	110.79
21	5	86	GLU	N-CA-C	-5.76	105.00	111.28
21	5	122	HIS	CB-CA-C	-5.76	101.23	110.79
21	5	202	GLN	N-CA-C	-5.76	105.00	111.28
17	N	114	PRO	N-CA-C	-5.76	101.88	111.26
18	O	142	PHE	N-CA-C	-5.76	105.09	111.71
21	R	86	GLU	N-CA-C	-5.76	105.01	111.28
18	2	172	ASP	CB-CA-C	-5.75	97.99	109.79
17	N	215	ARG	CD-NE-CZ	5.75	132.44	124.40
17	N	60	PRO	N-CA-CB	-5.74	98.02	103.19
19	P	82	GLU	CB-CG-CD	-5.74	102.84	112.60
17	N	102	ALA	CA-C-N	-5.74	112.02	120.28
17	N	102	ALA	C-N-CA	-5.74	112.02	120.28
19	3	109	PHE	N-CA-C	-5.73	106.51	112.93
18	2	158	GLU	CB-CA-C	-5.72	100.43	109.42
18	O	156	GLU	CB-CA-C	-5.72	100.44	109.42
21	R	202	GLN	N-CA-C	-5.72	105.05	111.28
17	N	97	VAL	N-CA-C	-5.71	104.94	110.42
19	3	82	GLU	CB-CG-CD	-5.69	102.93	112.60
13	w	66	PHE	N-CA-CB	5.68	120.63	111.65
21	5	102	TYR	N-CA-C	-5.68	105.09	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	R	102	TYR	N-CA-C	-5.68	105.09	111.28
18	2	197	PHE	CA-CB-CG	5.67	119.47	113.80
20	4	159	ARG	CA-CB-CG	5.67	125.44	114.10
22	6	165	LYS	CB-CA-C	5.67	119.87	111.88
20	Q	159	ARG	CA-CB-CG	5.66	125.43	114.10
17	N	104	GLY	N-CA-C	5.66	119.34	112.49
19	P	72	TYR	N-CA-CB	-5.66	101.87	110.92
14	x	13	LEU	CB-CG-CD1	-5.65	93.74	110.70
22	6	84	VAL	N-CA-CB	-5.65	103.85	112.15
22	S	165	LYS	CB-CA-C	5.65	119.84	111.88
24	g	171	LYS	N-CA-CB	5.65	118.60	109.90
19	3	72	TYR	N-CA-CB	-5.64	101.89	110.92
19	3	206	PRO	CA-N-CD	5.64	119.90	112.00
22	S	84	VAL	N-CA-CB	-5.64	103.86	112.15
19	P	206	PRO	CA-N-CD	5.64	119.89	112.00
13	w	65	PHE	CA-CB-CG	5.63	119.43	113.80
18	O	195	PHE	CA-CB-CG	5.62	119.42	113.80
22	6	216	MET	CB-CA-C	-5.62	102.06	110.88
22	6	88	PRO	N-CA-CB	-5.62	97.15	103.33
18	O	110	PHE	N-CA-CB	-5.62	101.57	110.22
18	O	110	PHE	CB-CA-C	5.61	121.01	110.63
18	2	112	PHE	CB-CA-C	5.61	121.01	110.63
18	2	112	PHE	N-CA-CB	-5.61	101.59	110.22
22	S	216	MET	CB-CA-C	-5.60	102.08	110.88
2	b	70	GLY	N-CA-C	5.59	121.41	114.37
19	P	67	LEU	N-CA-C	-5.59	106.44	113.20
19	3	41	ARG	CG-CD-NE	5.59	124.29	112.00
21	R	93	ARG	N-CA-C	-5.59	105.19	111.28
22	S	88	PRO	N-CA-CB	-5.58	97.19	103.33
21	5	93	ARG	N-CA-C	-5.58	105.20	111.28
21	R	93	ARG	CB-CA-C	5.58	120.05	110.79
19	P	41	ARG	CG-CD-NE	5.57	124.26	112.00
21	5	93	ARG	CB-CA-C	5.57	120.04	110.79
19	3	100	GLU	N-CA-CB	-5.57	101.94	110.01
2	B	405	LYS	CB-CA-C	-5.56	101.56	110.79
19	3	67	LEU	N-CA-C	-5.56	106.47	113.20
19	P	162	PHE	CA-CB-CG	5.56	119.36	113.80
19	P	100	GLU	N-CA-CB	-5.55	101.96	110.01
19	3	167	LEU	N-CA-C	-5.54	106.35	114.39
19	3	162	PHE	CA-CB-CG	5.54	119.34	113.80
19	3	215	PRO	N-CA-CB	-5.54	98.19	103.39
18	2	180	ARG	CA-CB-CG	5.52	125.14	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	P	167	LEU	N-CA-C	-5.52	106.39	114.39
18	O	178	ARG	CA-CB-CG	5.51	125.12	114.10
2	B	383	PHE	N-CA-CB	5.50	118.13	110.04
18	O	51	PHE	N-CA-CB	-5.50	101.88	109.91
18	2	53	PHE	N-CA-CB	-5.50	101.88	109.91
21	R	156	ARG	CB-CA-C	-5.50	109.75	117.23
21	5	156	ARG	CB-CA-C	-5.49	109.76	117.23
22	S	185	PRO	N-CA-C	-5.49	105.62	113.47
22	6	185	PRO	N-CA-C	-5.49	105.62	113.47
19	P	215	PRO	N-CA-CB	-5.49	98.23	103.39
2	B	70	GLY	N-CA-C	5.48	121.27	114.37
18	O	164	PRO	N-CA-CB	-5.48	97.37	103.23
21	R	162	PHE	N-CA-C	-5.47	106.19	112.92
19	3	61	ASP	CA-CB-CG	5.47	118.07	112.60
17	N	125	MET	CB-CA-C	-5.47	101.55	110.85
18	2	166	PRO	N-CA-CB	-5.46	97.39	103.23
20	4	145	PHE	CB-CA-C	5.46	119.86	110.79
22	6	135	PRO	N-CA-C	-5.45	105.95	113.53
20	Q	145	PHE	CB-CA-C	5.45	119.83	110.79
21	5	162	PHE	N-CA-C	-5.44	106.23	112.92
22	S	135	PRO	N-CA-C	-5.44	105.97	113.53
19	P	61	ASP	CA-CB-CG	5.43	118.03	112.60
17	N	78	PHE	N-CA-CB	-5.43	101.85	110.22
22	6	186	LEU	N-CA-C	-5.41	101.15	109.76
1	a	332	HIS	N-CA-C	-5.41	106.62	113.43
17	N	112	LYS	CB-CA-C	5.41	120.06	109.35
22	S	186	LEU	N-CA-C	-5.41	101.16	109.76
9	k	23	VAL	N-CA-CB	-5.40	104.83	112.12
17	N	46	LEU	N-CA-CB	5.40	118.25	110.20
22	6	221	LEU	N-CA-C	-5.40	105.39	111.28
17	N	92	ILE	CA-C-O	-5.39	115.14	120.85
20	4	155	GLN	CA-C-N	-5.38	110.86	121.41
20	4	155	GLN	C-N-CA	-5.38	110.86	121.41
20	Q	155	GLN	CA-C-N	-5.38	110.86	121.41
20	Q	155	GLN	C-N-CA	-5.38	110.86	121.41
22	S	221	LEU	N-CA-C	-5.38	105.42	111.28
21	5	105	GLN	CA-C-N	-5.37	113.33	120.63
21	5	105	GLN	C-N-CA	-5.37	113.33	120.63
20	Q	161	PRO	N-CA-CB	-5.37	98.53	103.31
20	Q	112	LYS	CB-CA-C	-5.35	102.48	110.88
22	6	100	LEU	N-CA-C	-5.34	105.38	111.14
17	N	78	PHE	CA-C-O	5.34	126.13	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	82	LEU	O-C-N	5.34	128.92	122.94
20	4	112	LYS	CB-CA-C	-5.34	102.50	110.88
18	O	139	VAL	N-CA-C	-5.33	104.38	111.05
21	R	105	GLN	CA-C-N	-5.33	113.39	120.63
21	R	105	GLN	C-N-CA	-5.33	113.39	120.63
19	3	157	PRO	N-CD-CG	-5.33	95.21	103.20
2	B	403	GLY	CA-C-O	-5.32	117.98	122.29
19	P	157	PRO	N-CD-CG	-5.32	95.22	103.20
20	4	161	PRO	N-CA-CB	-5.31	98.58	103.31
18	O	193	GLY	N-CA-C	-5.31	106.36	112.73
18	2	141	VAL	N-CA-C	-5.31	104.42	111.05
21	5	160	GLY	CA-C-N	-5.30	115.94	122.84
21	5	160	GLY	C-N-CA	-5.30	115.94	122.84
20	Q	88	HIS	CA-CB-CG	5.30	119.11	113.80
20	4	205	ILE	N-CA-C	5.30	115.51	110.42
22	S	100	LEU	N-CA-C	-5.29	105.42	111.14
21	R	160	GLY	CA-C-N	-5.29	115.96	122.84
21	R	160	GLY	C-N-CA	-5.29	115.96	122.84
17	N	50	GLY	N-CA-C	-5.29	108.42	115.40
18	2	118	PRO	N-CA-CB	-5.29	97.52	103.33
18	2	195	GLY	N-CA-C	-5.29	106.39	112.73
18	2	143	LEU	N-CA-C	-5.27	105.43	111.07
19	P	186	ARG	N-CA-CB	-5.27	102.38	110.12
19	P	218	TYR	N-CA-CB	-5.27	102.38	110.12
18	O	141	LEU	N-CA-C	-5.27	105.44	111.07
20	4	88	HIS	CA-CB-CG	5.26	119.06	113.80
21	R	199	PHE	CA-C-N	-5.26	113.82	120.56
21	R	199	PHE	C-N-CA	-5.26	113.82	120.56
22	6	68	PRO	N-CD-CG	-5.25	95.32	103.20
22	S	68	PRO	N-CD-CG	-5.25	95.32	103.20
21	5	199	PHE	CA-C-N	-5.25	113.84	120.56
21	5	199	PHE	C-N-CA	-5.25	113.84	120.56
21	R	88	GLU	CB-CG-CD	-5.25	103.67	112.60
21	5	88	GLU	CB-CG-CD	-5.25	103.67	112.60
21	5	47	PHE	N-CA-C	5.24	116.26	108.60
14	x	29	ILE	CB-CA-C	-5.24	105.26	111.97
19	3	218	TYR	N-CA-CB	-5.24	102.42	110.12
20	Q	205	ILE	N-CA-C	5.24	115.45	110.42
17	N	104	GLY	CA-C-N	-5.24	113.26	120.28
17	N	104	GLY	C-N-CA	-5.24	113.26	120.28
18	O	116	PRO	N-CA-CB	-5.24	97.57	103.33
17	N	222	LYS	CA-C-N	-5.23	116.04	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	222	LYS	C-N-CA	-5.23	116.04	122.84
19	3	186	ARG	N-CA-CB	-5.23	102.44	110.12
20	Q	129	GLN	N-CA-C	-5.23	105.58	111.28
16	Z	2	VAL	N-CA-C	-5.22	105.30	110.62
10	l	11	VAL	O-C-N	5.21	128.45	122.93
17	N	73	PHE	CB-CA-C	-5.20	102.94	111.68
19	3	85	HIS	CA-CB-CG	5.20	119.00	113.80
19	P	79	ARG	CG-CD-NE	5.20	123.44	112.00
19	3	79	ARG	CG-CD-NE	5.19	123.42	112.00
21	R	91	HIS	N-CA-C	-5.19	105.62	111.28
19	3	122	PRO	N-CA-CB	-5.19	98.69	103.31
21	R	47	PHE	N-CA-C	5.19	116.17	108.60
21	5	75	PHE	CA-CB-CG	5.19	118.99	113.80
20	4	129	GLN	N-CA-C	-5.18	105.63	111.28
21	R	75	PHE	CA-CB-CG	5.18	118.98	113.80
19	P	122	PRO	N-CA-CB	-5.17	98.70	103.31
2	b	89	GLY	CA-C-O	-5.16	117.85	121.88
19	P	85	HIS	CA-CB-CG	5.16	118.96	113.80
20	4	122	LEU	N-CA-C	-5.16	105.66	111.28
20	Q	122	LEU	N-CA-C	-5.16	105.66	111.28
17	N	142	PHE	CA-CB-CG	5.15	118.95	113.80
17	N	225	PRO	O-C-N	-5.15	116.53	122.71
11	m	6	ALA	N-CA-C	-5.15	106.10	112.38
17	N	140	GLN	CB-CA-C	-5.14	103.09	111.06
21	5	90	LYS	CB-CA-C	-5.14	102.26	110.79
21	5	91	HIS	N-CA-C	-5.14	105.68	111.28
22	S	173	SER	N-CA-C	-5.13	105.68	111.28
21	5	188	HIS	N-CA-C	-5.13	105.69	111.28
19	P	171	ASP	N-CA-C	-5.13	105.14	111.40
21	5	196	PHE	N-CA-C	-5.13	105.69	111.28
17	N	215	ARG	CG-CD-NE	5.13	123.28	112.00
21	R	196	PHE	N-CA-C	-5.12	105.70	111.28
20	4	165	GLY	CA-C-N	-5.12	115.74	122.85
20	4	165	GLY	C-N-CA	-5.12	115.74	122.85
21	R	188	HIS	N-CA-C	-5.12	105.70	111.28
20	Q	72	PHE	CA-CB-CG	-5.11	108.69	113.80
21	R	90	LYS	CB-CA-C	-5.11	102.30	110.79
18	2	94	PHE	N-CA-CB	5.11	117.63	110.12
22	6	173	SER	N-CA-C	-5.11	105.71	111.28
21	R	190	ARG	N-CA-C	-5.10	105.61	111.07
20	4	72	PHE	CA-CB-CG	-5.10	108.70	113.80
17	N	166	ARG	CB-CA-C	-5.09	101.95	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	R	185	GLU	CA-C-N	-5.09	113.48	120.46
21	R	185	GLU	C-N-CA	-5.09	113.48	120.46
18	O	68	PHE	CA-C-N	-5.09	116.99	123.15
18	O	68	PHE	C-N-CA	-5.09	116.99	123.15
18	O	92	PHE	N-CA-CB	5.09	117.61	110.12
19	3	171	ASP	N-CA-C	-5.09	105.19	111.40
17	N	103	THR	CA-CB-OG1	-5.09	101.97	109.60
20	4	167	ASP	CA-CB-CG	5.08	117.69	112.60
21	5	185	GLU	CA-C-N	-5.08	113.50	120.46
21	5	185	GLU	C-N-CA	-5.08	113.50	120.46
21	5	190	ARG	N-CA-C	-5.08	105.63	111.07
20	Q	165	GLY	CA-C-N	-5.08	115.79	122.85
20	Q	165	GLY	C-N-CA	-5.08	115.79	122.85
18	2	70	PHE	CA-C-N	-5.08	117.01	123.15
18	2	70	PHE	C-N-CA	-5.08	117.01	123.15
21	5	164	PHE	CA-C-N	-5.07	117.02	123.15
21	5	164	PHE	C-N-CA	-5.07	117.02	123.15
19	3	136	ILE	N-CA-C	-5.06	105.45	110.62
19	P	66	PRO	N-CA-CB	-5.06	97.76	103.33
19	P	145	LEU	N-CA-CB	-5.06	102.82	110.92
20	Q	190	ARG	N-CA-C	-5.06	105.76	111.28
20	Q	167	ASP	CA-CB-CG	5.06	117.66	112.60
19	3	66	PRO	N-CA-CB	-5.05	97.77	103.33
20	4	193	MET	N-CA-C	-5.05	105.77	111.28
20	Q	193	MET	N-CA-C	-5.05	105.77	111.28
19	3	181	GLU	N-CA-C	-5.05	105.67	111.07
19	3	145	LEU	N-CA-CB	-5.05	102.85	110.92
19	P	181	GLU	N-CA-C	-5.05	105.67	111.07
21	R	164	PHE	CA-C-N	-5.05	117.04	123.15
21	R	164	PHE	C-N-CA	-5.05	117.04	123.15
2	B	367	PRO	N-CA-CB	-5.04	98.82	103.31
18	O	109	PRO	N-CA-CB	-5.04	97.79	103.33
22	S	166	LEU	N-CA-CB	-5.04	102.70	110.16
19	3	186	ARG	CB-CA-C	5.04	119.15	110.79
18	2	111	PRO	N-CA-CB	-5.03	97.79	103.33
22	6	166	LEU	N-CA-CB	-5.03	102.71	110.16
19	P	136	ILE	N-CA-C	-5.03	105.49	110.62
22	6	216	MET	N-CA-C	-5.03	105.69	111.07
19	3	50	ARG	CB-CA-C	-5.03	101.73	109.62
20	4	123	HIS	CA-CB-CG	5.02	118.82	113.80
19	P	186	ARG	CB-CA-C	5.02	119.13	110.79
21	5	71	ASP	N-CA-C	-5.02	100.22	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	P	50	ARG	CB-CA-C	-5.01	101.75	109.62
22	S	216	MET	N-CA-C	-5.01	105.71	111.07
20	4	190	ARG	N-CA-C	-5.00	105.83	111.28

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	2	122	HIS	Mainchain
18	2	196	GLY	Mainchain
20	4	159	ARG	Sidechain
20	4	82	ARG	Sidechain
1	A	16	ARG	Sidechain
1	A	312[B]	ARG	Mainchain
1	A	64	ARG	Sidechain
2	B	151	PHE	Mainchain
2	B	227	ARG	Sidechain
2	B	230	ARG	Sidechain
2	B	304	ARG	Sidechain
2	B	357[A]	ARG	Sidechain
2	B	358	ARG	Sidechain
2	B	385	ARG	Sidechain
2	B	476	ARG	Sidechain
3	C	40	ARG	Sidechain
3	C	484	ARG	Sidechain
4	D	11	ARG	Sidechain
4	D	138	ARG	Sidechain
4	D	264	ARG	Sidechain
5	E	61	ARG	Sidechain
6	F	16	ARG	Sidechain
6	F	42	ARG	Sidechain
23	G	173	ARG	Sidechain
7	H	6	ARG	Sidechain
17	N	119	THR	Mainchain
17	N	225	PRO	Mainchain
17	N	75	PRO	Mainchain
17	N	96	ARG	Sidechain
18	O	120	HIS	Mainchain
18	O	194	GLY	Mainchain
20	Q	159	ARG	Sidechain
20	Q	82	ARG	Sidechain
12	T	28	ARG	Sidechain

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Mol	Chain	Res	Type	Group
13	W	37	ARG	Sidechain
1	a	27	ARG	Sidechain
1	a	330	VAL	Mainchain
1	a	334	ARG	Sidechain
2	b	230	ARG	Sidechain
2	b	304	ARG	Sidechain
2	b	378	ARG	Sidechain
2	b	384	ARG	Sidechain
2	b	385	ARG	Sidechain
2	b	476	ARG	Sidechain
4	d	11	ARG	Sidechain
4	d	138	ARG	Sidechain
4	d	23	ARG	Sidechain
24	g	173	ARG	Sidechain
9	k	45	ARG	Sidechain
13	w	37	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2377	0	2304	78	0
1	a	2438	0	2361	73	0
2	B	3797	0	3683	136	0
2	b	3782	0	3668	115	0
3	C	3331	0	3256	89	0
3	c	3299	0	3224	81	0
4	D	2713	0	2607	83	0
4	d	2705	0	2602	98	0
5	E	525	0	510	16	0
5	e	525	0	510	7	0
6	F	235	0	241	17	0
6	f	246	0	250	5	0
7	H	508	0	529	15	0
7	h	508	0	529	23	0
8	I	284	0	295	8	0
8	i	284	0	295	6	0
9	K	296	0	312	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	k	296	0	312	12	0
10	L	301	0	301	9	0
10	l	301	0	301	10	0
11	M	271	0	287	12	0
11	m	271	0	287	7	0
12	T	244	0	256	3	0
12	t	244	0	256	5	0
13	W	361	0	346	20	0
13	w	361	0	346	11	0
14	X	249	0	269	16	0
14	x	249	0	269	13	0
15	Y	209	0	243	4	0
15	y	209	0	243	3	0
16	Z	451	0	483	15	0
16	z	460	0	499	10	0
17	1	1477	0	1487	145	0
17	N	1477	0	1489	305	0
18	2	1377	0	1365	230	0
18	O	1377	0	1365	121	0
19	3	1388	0	1370	156	0
19	P	1388	0	1370	89	0
20	4	1226	0	1234	225	0
20	Q	1226	0	1234	116	0
21	5	1481	0	1466	136	0
21	R	1481	0	1466	83	0
22	6	1327	0	1311	70	0
22	S	1327	0	1311	80	0
23	G	755	0	724	43	0
24	g	747	0	720	157	0
25	A	1	0	0	0	0
25	a	1	0	0	0	0
26	1	510	0	428	66	0
26	2	678	0	647	174	0
26	3	473	0	471	91	0
26	4	534	0	488	147	0
26	5	620	0	589	101	0
26	6	525	0	510	52	0
26	A	174	0	170	13	0
26	B	1014	0	1092	50	0
26	C	827	0	894	32	0
26	D	190	0	203	11	0
26	G	110	0	105	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	N	509	0	426	135	0
26	O	633	0	614	105	0
26	P	570	0	547	56	0
26	Q	482	0	445	61	0
26	R	620	0	589	69	0
26	S	525	0	510	36	0
26	a	174	0	170	17	0
26	b	1014	0	1092	54	0
26	c	828	0	896	29	0
26	d	191	0	205	13	0
26	g	110	0	104	25	0
27	A	64	0	74	2	0
27	D	64	0	74	5	0
27	a	64	0	74	2	0
27	d	64	0	74	5	0
28	3	40	0	0	21	0
28	5	40	0	0	0	0
28	A	40	0	0	0	0
28	B	120	0	0	6	0
28	C	80	0	0	2	0
28	D	40	0	0	0	0
28	H	40	0	0	1	0
28	P	40	0	0	3	0
28	S	40	0	0	0	0
28	Y	40	0	0	0	0
28	Z	40	0	0	0	0
28	a	40	0	0	0	0
28	b	120	0	0	1	0
28	c	120	0	0	0	0
28	d	40	0	0	0	0
28	k	40	0	0	0	0
28	x	40	0	0	0	0
29	A	33	0	42	6	0
29	D	55	0	80	3	0
29	a	33	0	42	0	0
29	d	55	0	80	3	0
30	A	40	0	44	1	0
30	D	54	0	78	2	0
30	a	40	0	44	0	0
30	c	45	0	57	1	0
31	A	1	0	0	0	0
31	a	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	c	1	0	0	0	0
32	A	2	0	0	0	0
32	a	2	0	0	0	0
33	2	40	0	50	5	0
33	4	43	0	56	5	0
33	5	40	0	50	20	0
33	A	48	0	66	1	0
33	B	51	0	72	2	0
33	C	78	0	96	3	0
33	D	123	0	156	5	0
33	M	40	0	50	1	0
33	O	40	0	50	5	0
33	Q	43	0	56	2	0
33	R	40	0	50	9	0
33	a	48	0	66	3	0
33	b	51	0	72	1	0
33	c	82	0	104	8	0
33	d	123	0	156	6	0
33	m	40	0	50	2	0
34	1	46	0	65	48	0
34	2	49	0	74	23	0
34	5	40	0	53	8	0
34	C	82	0	107	3	0
34	D	92	0	133	12	0
34	G	49	0	74	11	0
34	L	49	0	74	7	0
34	N	46	0	65	26	0
34	R	40	0	53	12	0
34	Z	25	0	20	0	0
34	a	42	0	57	0	0
34	b	43	0	59	2	0
34	c	40	0	50	1	0
34	d	49	0	74	5	0
34	l	49	0	74	5	0
34	z	25	0	20	0	0
35	C	54	0	66	1	0
35	H	62	0	82	4	0
35	c	54	0	66	2	0
35	h	62	0	82	6	0
36	D	4	0	0	0	0
36	d	4	0	0	0	0
37	F	43	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	f	43	0	30	1	0
38	1	180	0	0	5	0
38	2	45	0	0	7	0
38	3	45	0	0	1	0
38	4	135	0	0	27	0
38	5	45	0	0	3	0
38	6	45	0	0	0	0
38	N	180	0	0	39	0
38	O	45	0	0	7	0
38	P	45	0	0	1	0
38	Q	135	0	0	28	0
38	R	45	0	0	3	0
38	S	45	0	0	0	0
39	1	168	0	0	1	0
39	2	210	0	0	33	0
39	3	126	0	0	60	0
39	4	210	0	0	48	0
39	5	126	0	0	7	0
39	6	126	0	0	1	0
39	N	210	0	0	39	0
39	O	168	0	0	28	0
39	P	126	0	0	13	0
39	Q	210	0	0	26	0
39	R	168	0	0	7	0
39	S	84	0	0	11	0
40	1	41	0	0	1	0
40	2	41	0	0	21	0
40	4	41	0	0	5	0
40	5	41	0	0	1	0
40	N	41	0	0	16	0
40	O	41	0	0	9	0
40	Q	41	0	0	4	0
40	R	41	0	0	4	0
41	A	52	0	0	6	0
41	B	117	0	0	20	0
41	C	52	0	0	8	0
41	D	70	0	0	12	0
41	E	8	0	0	2	0
41	F	2	0	0	6	0
41	H	14	0	0	1	0
41	I	1	0	0	0	0
41	K	4	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	L	7	0	0	4	0
41	M	1	0	0	0	0
41	T	4	0	0	2	0
41	W	2	0	0	0	0
41	X	3	0	0	1	0
41	a	48	0	0	8	0
41	b	125	0	0	36	0
41	c	52	0	0	8	0
41	d	71	0	0	16	0
41	e	9	0	0	5	0
41	h	14	0	0	4	0
41	i	1	0	0	0	0
41	k	3	0	0	1	0
41	l	5	0	0	2	0
41	m	4	0	0	0	0
41	t	5	0	0	1	0
41	w	1	0	0	1	0
41	x	1	0	0	1	0
All	All	69223	0	64352	3265	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (3265) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:196:LEU:HD11	28:3:313:WVN:C16	1.12	1.58
26:N:606:CLA:CBB	34:N:621:LHG:H172	1.37	1.54
26:5:605:CLA:HBB1	26:6:609:CLA:C6	1.41	1.49
1:a:331:MET:HE3	4:d:347:ARG:C	1.36	1.46
17:1:145:ILE:CD1	34:1:620:LHG:H221	1.49	1.42
19:3:196:LEU:CD1	28:3:313:WVN:C16	1.96	1.42
26:N:606:CLA:HBB1	34:N:621:LHG:C17	1.46	1.41
24:g:168:ILE:CG2	26:g:402:CLA:O2A	1.66	1.41
22:S:185:PRO:CD	39:S:611:II0:O02	1.71	1.37
26:O:601:CLA:HAC1	40:O:616:IHT:C04	1.56	1.33
1:a:331:MET:CE	4:d:347:ARG:O	1.75	1.32
17:N:73:PHE:CE1	26:N:601:CLA:HAC1	1.64	1.32
26:6:610:CLA:CMB	26:g:401:CLA:O1A	1.79	1.30
20:4:77:ASP:N	24:g:127:GLN:O	1.65	1.29
1:a:331:MET:CE	4:d:347:ARG:C	2.06	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:294:GLU:OE2	2:b:296:LEU:CD2	1.81	1.28
17:N:152:THR:OG1	18:O:51:PHE:CE1	1.79	1.27
6:F:16:ARG:CD	41:F:201:HOH:O	1.81	1.26
17:N:209:HIS:NE2	38:N:612:KC2:NC	1.81	1.26
17:N:86:TRP:CD1	26:N:603:CLA:O1A	1.88	1.26
18:2:137:TRP:CZ3	34:2:321:LHG:H372	1.70	1.26
17:1:145:ILE:HD13	34:1:620:LHG:C22	1.65	1.25
19:3:196:LEU:CD2	28:3:313:WVN:C26	2.14	1.24
17:1:145:ILE:CD1	34:1:620:LHG:C22	2.16	1.24
17:1:159:GLN:NE2	18:2:55:LYS:H	1.34	1.24
22:S:185:PRO:HD2	39:S:611:II0:O02	1.11	1.23
17:1:155:PRO:HB2	18:2:54:LEU:CD2	1.67	1.23
17:1:152:THR:CG2	34:1:620:LHG:C35	2.16	1.22
19:3:196:LEU:HD22	28:3:313:WVN:C26	1.69	1.22
17:N:212:LEU:HD21	26:N:614:CLA:O1D	1.34	1.21
26:4:301:CLA:CBA	26:4:303:CLA:H43	1.71	1.21
19:3:189:MET:HB3	39:3:311:II0:C36	1.72	1.19
18:2:144:PHE:CD1	26:2:319:CLA:HAC1	1.78	1.19
3:C:335:ASP:CG	3:C:354:TYR:HE2	1.52	1.18
26:4:306:CLA:CMB	26:5:611:CLA:HBA2	1.71	1.18
2:b:127:ARG:NH2	7:h:18:TYR:O	1.75	1.17
17:1:159:GLN:NE2	18:2:55:LYS:HD3	1.59	1.17
34:1:620:LHG:H241	26:2:301:CLA:C1D	1.73	1.17
34:N:621:LHG:H241	26:O:601:CLA:C1D	1.73	1.16
26:4:306:CLA:HMB1	26:5:611:CLA:HBA2	1.19	1.16
3:C:351:LEU:HD11	3:C:363:ILE:HD13	1.20	1.16
17:N:159:GLN:NE2	18:O:53:LYS:CD	2.09	1.16
26:N:606:CLA:CBB	34:N:621:LHG:C17	2.14	1.16
17:1:159:GLN:HE22	18:2:55:LYS:N	1.44	1.15
20:4:76:ILE:HG23	24:g:127:GLN:HG2	1.29	1.15
26:2:308:CLA:H41	38:2:310:KC2:CMA	1.76	1.15
17:N:159:GLN:NE2	18:O:53:LYS:HD3	1.58	1.15
26:1:606:CLA:HMA2	26:2:311:CLA:CAD	1.75	1.14
17:1:148:LEU:HD11	34:1:620:LHG:H341	1.14	1.14
17:1:152:THR:HG21	34:1:620:LHG:C35	1.77	1.14
17:N:208:HIS:HE1	40:N:619:IHT:C38	1.61	1.14
20:4:75:ILE:HD12	26:4:301:CLA:H3A	1.28	1.13
10:L:38:ASN:O	41:L:201:HOH:O	1.66	1.13
26:5:605:CLA:HBB1	26:6:609:CLA:C7	1.78	1.12
26:O:608:CLA:H41	38:O:610:KC2:CMA	1.76	1.12
24:g:168:ILE:HG23	26:g:402:CLA:O2A	1.24	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:45:ARG:NH2	41:K:101:HOH:O	1.81	1.12
26:1:606:CLA:C1C	26:2:311:CLA:H42	1.76	1.12
19:3:165:LEU:HD11	33:5:619:LMG:H382	1.25	1.12
21:5:55:LYS:HE2	24:g:121:ASP:HB3	1.24	1.12
7:h:6:ARG:NH2	24:g:155:GLU:OE2	1.81	1.11
26:N:606:CLA:H12	18:O:213:PHE:CZ	1.86	1.11
17:1:152:THR:HG23	34:1:620:LHG:C35	1.80	1.11
18:2:83:VAL:HG12	24:g:170:TRP:CH2	1.86	1.10
26:5:605:CLA:H161	26:6:609:CLA:H71	1.14	1.10
26:6:610:CLA:HMB3	26:g:401:CLA:O1A	1.48	1.10
17:N:73:PHE:HB2	26:N:601:CLA:HMD2	1.17	1.10
34:N:621:LHG:H261	26:O:601:CLA:NC	1.65	1.10
3:C:37:ILE:HG21	9:K:45:ARG:CZ	1.80	1.10
17:N:212:LEU:CG	26:N:614:CLA:HED3	1.82	1.10
17:1:144:TRP:CZ3	34:1:620:LHG:H172	1.87	1.09
20:4:129:GLN:HA	21:5:228:PHE:CZ	1.87	1.09
14:X:32:GLN:HB2	17:N:81:TRP:HB2	1.22	1.09
20:4:133:GLN:OE1	39:4:320:II0:C13	1.99	1.09
1:a:26:ASN:ND2	41:a:503:HOH:O	1.86	1.09
34:1:620:LHG:H261	26:2:301:CLA:NC	1.65	1.09
2:b:294:GLU:OE2	2:b:296:LEU:HD22	0.92	1.08
4:d:293:ARG:NH2	41:d:501:HOH:O	1.86	1.08
20:4:158:ASP:HB2	21:5:47:PHE:CZ	1.87	1.08
26:1:606:CLA:NC	26:2:311:CLA:H42	1.69	1.08
24:g:167:LEU:N	26:g:402:CLA:O1D	1.87	1.08
17:1:145:ILE:HD13	34:1:620:LHG:H221	1.19	1.07
17:1:159:GLN:NE2	18:2:55:LYS:CD	2.15	1.07
18:2:83:VAL:HG12	24:g:170:TRP:CZ2	1.89	1.07
22:S:183:PHE:CE2	39:S:611:II0:C08	2.38	1.07
26:4:301:CLA:HBA1	26:4:303:CLA:C4	1.84	1.06
26:1:606:CLA:CHB	26:2:311:CLA:HBA2	1.85	1.06
26:5:605:CLA:CBB	26:6:609:CLA:H61	1.85	1.06
26:4:301:CLA:H12	26:4:303:CLA:C2	1.85	1.06
1:a:331:MET:HE3	4:d:347:ARG:CA	1.84	1.05
17:N:213:VAL:CG2	38:N:612:KC2:CED	2.34	1.05
10:l:38:ASN:O	41:l:201:HOH:O	1.71	1.05
18:2:84:LEU:HD23	24:g:170:TRP:CZ3	1.91	1.05
20:4:154:LEU:CB	24:g:125:VAL:HB	1.87	1.05
20:4:134:GLN:HG2	39:4:320:II0:C19	1.87	1.04
26:3:302:CLA:H61	24:g:154:LEU:HD22	1.37	1.04
26:5:605:CLA:C1B	26:6:609:CLA:H11	1.87	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:611:CLA:HED3	41:B:751:HOH:O	1.57	1.04
26:b:611:CLA:HED3	41:b:755:HOH:O	1.56	1.03
24:g:168:ILE:HG22	26:g:402:CLA:O2A	1.59	1.03
14:x:21:ILE:HG23	26:1:603:CLA:C7	1.89	1.03
20:4:164:PHE:O	26:5:601:CLA:HBB2	1.58	1.03
26:4:301:CLA:H12	26:4:303:CLA:C1	1.88	1.03
1:A:218:LEU:HD23	29:A:407:PL9:C5	1.87	1.02
17:N:73:PHE:HE1	26:N:601:CLA:HAC1	0.87	1.02
17:N:208:HIS:CE1	40:N:619:IHT:C38	2.41	1.02
26:O:601:CLA:CAC	40:O:616:IHT:C04	2.36	1.02
3:C:335:ASP:OD2	3:C:354:TYR:CE2	2.13	1.02
17:N:212:LEU:HG	26:N:614:CLA:HED3	1.38	1.02
26:4:301:CLA:HBA1	26:4:303:CLA:H43	1.04	1.02
20:4:80:TRP:CB	24:g:127:GLN:HB2	1.90	1.02
26:4:306:CLA:HMA1	26:5:611:CLA:CAD	1.89	1.01
26:5:605:CLA:CBB	26:6:609:CLA:C6	2.38	1.01
2:B:472:ARG:HA	2:B:479:PHE:HE2	1.23	1.01
17:N:73:PHE:CD1	26:N:601:CLA:HHD	1.95	1.01
20:Q:135:LEU:HB2	26:Q:306:CLA:HBC1	1.41	1.01
14:X:32:GLN:CB	17:N:81:TRP:HB2	1.89	1.01
2:b:353:GLU:OE1	41:b:701:HOH:O	1.75	1.01
17:N:213:VAL:HG23	38:N:612:KC2:CED	1.90	1.01
2:b:294:GLU:CD	2:b:296:LEU:HD22	1.85	1.01
18:2:83:VAL:HG22	24:g:169:ALA:HB1	1.41	1.00
14:X:1:MET:HE1	26:N:607:CLA:CED	1.91	1.00
3:C:335:ASP:CG	3:C:354:TYR:CE2	2.38	1.00
26:6:610:CLA:HMB1	26:g:401:CLA:O1A	1.62	0.99
2:b:353:GLU:CD	41:b:701:HOH:O	2.01	0.99
18:2:137:TRP:CZ3	34:2:321:LHG:C37	2.44	0.99
17:N:86:TRP:HD1	26:N:603:CLA:O1A	1.34	0.99
18:2:84:LEU:CD2	24:g:170:TRP:HZ3	1.74	0.99
17:N:84:LEU:HA	17:N:87:ALA:HB3	1.41	0.99
41:a:526:HOH:O	4:d:141:ASN:HB2	1.61	0.99
18:2:84:LEU:CD2	24:g:170:TRP:CZ3	2.45	0.99
26:5:605:CLA:HBB1	26:6:609:CLA:H61	1.01	0.99
18:2:141:VAL:HG22	34:2:321:LHG:H321	1.44	0.99
20:4:135:LEU:HB2	26:4:307:CLA:HBC1	1.40	0.99
18:2:153:LEU:CD2	24:g:169:ALA:HA	1.92	0.99
3:C:37:ILE:CG2	9:K:45:ARG:CZ	2.41	0.98
20:4:80:TRP:HB2	24:g:127:GLN:HB2	1.45	0.98
26:3:307:CLA:CMD	26:4:303:CLA:H91	1.93	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:303:CLA:HBC1	40:R:317:IHT:C14	1.94	0.98
26:4:306:CLA:HED1	21:5:223:PHE:CD2	1.99	0.98
17:N:220:PHE:HE1	38:N:612:KC2:C4A	1.77	0.97
21:5:55:LYS:HE2	24:g:121:ASP:CB	1.92	0.97
17:1:155:PRO:HB2	18:2:54:LEU:HD21	1.43	0.97
9:k:45:ARG:C	41:k:202:HOH:O	2.06	0.97
3:c:331:PHE:HB3	3:c:354:TYR:CE1	1.99	0.97
17:N:128:LEU:HD21	26:N:604:CLA:HED2	1.43	0.97
17:N:212:LEU:HG	26:N:614:CLA:CED	1.93	0.97
34:1:620:LHG:H241	26:2:301:CLA:ND	1.81	0.96
38:N:605:KC2:NA	39:N:618:II0:C16	2.28	0.96
20:4:129:GLN:HA	21:5:228:PHE:CE1	1.99	0.96
6:F:16:ARG:HG2	41:F:201:HOH:O	1.65	0.96
26:N:606:CLA:H12	18:O:213:PHE:CE1	1.98	0.96
26:5:605:CLA:H172	34:5:618:LHG:H261	1.45	0.96
20:4:133:GLN:OE1	39:4:320:II0:C09	2.13	0.96
18:2:83:VAL:HG21	24:g:169:ALA:O	1.65	0.96
17:1:145:ILE:HD11	34:1:620:LHG:H221	1.46	0.95
21:5:80:ASP:H	24:g:111:ALA:HB1	1.29	0.95
2:b:410:VAL:O	41:b:702:HOH:O	1.83	0.95
1:a:331:MET:HE3	4:d:347:ARG:O	1.43	0.95
20:4:154:LEU:HB3	24:g:125:VAL:HB	1.45	0.95
18:2:83:VAL:HG11	24:g:170:TRP:CD2	2.01	0.95
26:4:306:CLA:HMB1	26:5:611:CLA:C1A	1.96	0.95
2:B:382:PRO:O	41:B:701:HOH:O	1.84	0.95
9:K:45:ARG:NH1	41:K:101:HOH:O	1.98	0.95
19:3:196:LEU:HD21	28:3:313:WVN:C16	1.97	0.95
18:2:83:VAL:CG1	24:g:170:TRP:CE2	2.50	0.95
26:3:306:CLA:H101	39:3:310:II0:C32	1.97	0.95
34:N:621:LHG:H241	26:O:601:CLA:ND	1.80	0.94
26:3:307:CLA:H52	20:4:80:TRP:HH2	1.29	0.94
22:S:183:PHE:CE2	39:S:611:II0:C06	2.51	0.94
26:A:402:CLA:HAB	26:A:403:CLA:HMD2	1.49	0.94
9:K:45:ARG:CZ	41:K:101:HOH:O	2.12	0.94
2:b:241:SER:O	2:b:245:VAL:HG23	1.66	0.94
26:5:605:CLA:CBB	26:6:609:CLA:H72	1.98	0.94
26:a:402:CLA:HAB	26:a:403:CLA:HMD2	1.49	0.93
17:N:155:PRO:HB2	18:O:52:LEU:HD22	1.47	0.93
26:4:301:CLA:H12	26:4:303:CLA:H12	1.48	0.93
20:Q:135:LEU:CB	26:Q:306:CLA:HBC1	1.99	0.93
38:Q:309:KC2:CHD	38:Q:310:KC2:CBC	2.47	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:306:GLU:HG2	41:D:563:HOH:O	1.68	0.93
4:d:229:ASN:HB3	41:d:521:HOH:O	1.66	0.93
26:N:614:CLA:CAC	40:N:619:IHT:C29	2.46	0.93
18:2:151:GLU:HG3	19:3:48:LEU:HD23	1.50	0.93
26:1:606:CLA:CMA	26:2:311:CLA:CAD	2.45	0.93
4:d:343:GLU:HG2	41:d:504:HOH:O	1.68	0.93
17:N:73:PHE:HD1	26:N:601:CLA:HHD	1.32	0.93
20:4:155:GLN:HE22	33:5:619:LMG:HC71	1.33	0.93
26:5:605:CLA:H161	26:6:609:CLA:C7	1.99	0.93
4:d:306:GLU:HG2	41:d:550:HOH:O	1.68	0.92
2:B:476:ARG:NH1	41:B:705:HOH:O	2.00	0.92
3:C:351:LEU:CD1	3:C:363:ILE:HD13	1.99	0.92
17:1:155:PRO:HB2	18:2:54:LEU:HD22	1.50	0.92
38:4:310:KC2:CHD	38:4:311:KC2:CBC	2.47	0.92
26:5:605:CLA:CBB	26:6:609:CLA:C7	2.48	0.92
20:4:135:LEU:CB	26:4:307:CLA:HBC1	1.99	0.92
26:O:603:CLA:H141	33:O:617:LMG:H382	1.52	0.92
19:3:192:LEU:HD11	39:3:311:II0:C29	1.99	0.92
2:b:218:ALA:HB1	24:g:172:PRO:HG3	1.51	0.91
18:2:83:VAL:CG2	24:g:169:ALA:HB1	2.00	0.91
17:N:73:PHE:HE1	26:N:601:CLA:CAC	1.81	0.91
2:B:472:ARG:HA	2:B:479:PHE:CE2	2.04	0.91
26:2:303:CLA:H141	33:2:318:LMG:H382	1.52	0.91
17:N:220:PHE:HZ	38:N:612:KC2:C1A	1.83	0.91
21:5:58:THR:HG21	24:g:119:THR:HG23	1.50	0.91
26:2:311:CLA:HBC2	39:2:315:II0:C31	2.01	0.91
18:2:144:PHE:CE1	26:2:319:CLA:CAC	2.53	0.91
7:h:6:ARG:HH22	24:g:155:GLU:CD	1.80	0.90
17:N:78:PHE:HA	17:N:81:TRP:HZ3	1.35	0.90
17:N:152:THR:OG1	18:O:51:PHE:HE1	1.51	0.90
17:1:148:LEU:HD11	34:1:620:LHG:H311	1.51	0.90
17:1:148:LEU:CD1	34:1:620:LHG:H341	1.99	0.90
17:N:212:LEU:CD2	26:N:614:CLA:O1D	2.20	0.90
18:2:83:VAL:HG21	24:g:169:ALA:C	1.96	0.90
23:G:141:ALA:HB3	19:P:58:LEU:HD23	1.51	0.90
17:N:78:PHE:HA	17:N:81:TRP:CZ3	2.07	0.90
17:N:155:PRO:HB2	18:O:52:LEU:CD2	2.03	0.89
19:3:193:GLY:HA3	28:3:313:WVN:C39	2.03	0.89
17:N:231:LEU:HD12	17:N:232:PRO:HD2	1.54	0.89
18:2:144:PHE:CG	26:2:319:CLA:HAC1	2.07	0.89
17:N:73:PHE:HB2	26:N:601:CLA:CMD	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:4:312:CLA:HBB1	39:4:314:II0:C20	2.02	0.89
17:N:209:HIS:NE2	38:N:612:KC2:C4C	2.35	0.89
18:2:144:PHE:CE1	26:2:319:CLA:HAC1	2.07	0.89
19:3:163:ASP:OD1	39:3:310:II0:O02	1.91	0.89
20:4:75:ILE:HD12	26:4:301:CLA:C3A	2.02	0.89
20:4:113:SER:O	21:5:227:THR:OG1	1.90	0.89
18:2:144:PHE:CZ	26:2:319:CLA:HBC1	2.08	0.88
20:Q:120:THR:HG23	40:Q:317:IHT:C20	2.03	0.88
2:B:15:ASP:OD1	41:B:702:HOH:O	1.91	0.88
14:X:1:MET:HE1	26:N:607:CLA:HED1	1.56	0.88
26:5:605:CLA:C16	26:6:609:CLA:H71	2.00	0.88
20:4:120:THR:HG23	40:4:318:IHT:C20	2.03	0.88
26:Q:311:CLA:HBB1	39:Q:313:II0:C20	2.02	0.88
22:S:185:PRO:HD3	39:S:611:II0:O02	1.74	0.88
3:C:331:PHE:HB3	3:C:354:TYR:CE1	2.09	0.88
17:N:220:PHE:CE1	38:N:612:KC2:C4A	2.57	0.88
20:4:156:GLY:H	24:g:123:PHE:HZ	1.22	0.88
21:5:55:LYS:NZ	33:5:619:LMG:HC62	1.89	0.87
18:O:81:VAL:HG13	26:O:607:CLA:HED1	1.56	0.87
17:1:144:TRP:HB3	34:1:620:LHG:H211	1.56	0.87
21:5:82:ARG:NH2	24:g:114:GLN:OE1	2.06	0.87
6:F:16:ARG:CG	41:F:201:HOH:O	2.07	0.87
18:2:151:GLU:HG3	19:3:48:LEU:CD2	2.03	0.87
20:4:154:LEU:HB2	24:g:125:VAL:CB	2.04	0.87
2:B:476:ARG:CZ	41:B:708:HOH:O	2.23	0.87
26:4:301:CLA:H52	26:4:303:CLA:H101	1.56	0.87
3:c:149:ILE:HD12	16:z:27:LEU:HB3	1.57	0.87
17:1:159:GLN:HE21	18:2:55:LYS:HD3	1.35	0.87
18:2:137:TRP:CE3	34:2:321:LHG:H372	2.09	0.87
19:3:196:LEU:CD2	28:3:313:WVN:C16	2.53	0.87
26:2:312:CLA:HHD	40:2:317:IHT:C20	2.05	0.87
20:4:133:GLN:OE1	39:4:320:II0:C21	2.23	0.87
9:K:45:ARG:C	41:K:103:HOH:O	2.18	0.86
26:R:306:CLA:H172	34:R:319:LHG:H261	1.55	0.86
22:S:183:PHE:CD2	39:S:611:II0:C06	2.58	0.86
1:a:331:MET:HE1	4:d:347:ARG:O	1.75	0.86
18:2:84:LEU:HD23	24:g:170:TRP:CH2	2.09	0.86
21:R:208:GLN:HE21	21:R:213:GLN:HA	1.39	0.86
17:1:148:LEU:CD1	34:1:620:LHG:H311	2.04	0.86
2:b:127:ARG:HH22	7:h:18:TYR:C	1.82	0.86
17:N:159:GLN:HE22	18:O:53:LYS:HD3	1.38	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:606:CLA:HBA1	18:2:218:LEU:HD13	1.57	0.85
26:N:614:CLA:HAC1	40:N:619:IHT:C29	2.04	0.85
26:2:311:CLA:CBC	39:2:315:II0:C31	2.54	0.85
18:2:70:PHE:CE1	40:2:317:IHT:C13	2.58	0.85
1:a:331:MET:HE3	4:d:347:ARG:N	1.92	0.85
20:4:154:LEU:HB2	24:g:125:VAL:HB	1.57	0.85
3:c:331:PHE:HB3	3:c:354:TYR:CZ	2.10	0.85
17:N:140:GLN:HE22	39:N:620:II0:C29	1.89	0.85
20:4:134:GLN:NE2	39:4:320:II0:C23	2.40	0.85
1:A:218:LEU:CD2	29:A:407:PL9:C5	2.55	0.85
4:D:293:ARG:NH2	41:D:503:HOH:O	2.08	0.85
21:5:208:GLN:HE21	21:5:213:GLN:HA	1.38	0.85
18:2:83:VAL:HG13	26:2:307:CLA:HED1	1.56	0.85
2:B:218:ALA:HB1	23:G:172:PRO:HG3	1.59	0.84
26:1:606:CLA:HHB	26:2:311:CLA:HBA2	1.56	0.84
18:2:153:LEU:HD21	24:g:169:ALA:HA	1.58	0.84
1:a:223:LEU:HD13	4:d:264:ARG:HD2	1.57	0.84
17:N:112:LYS:HE2	26:N:604:CLA:HED1	1.57	0.84
4:D:339:ILE:HA	41:D:509:HOH:O	1.74	0.84
26:4:306:CLA:CMA	26:5:611:CLA:OBD	2.25	0.84
2:B:162:TRP:CD1	41:B:769:HOH:O	2.30	0.84
14:X:1:MET:CE	26:N:607:CLA:CED	2.55	0.84
20:Q:134:GLN:HE22	39:Q:319:II0:C25	1.90	0.84
2:B:27:THR:HG22	2:B:107:LEU:HD13	1.60	0.84
39:1:618:II0:C40	26:2:311:CLA:C15	2.56	0.84
5:E:54:ASN:ND2	41:E:101:HOH:O	1.73	0.84
26:4:306:CLA:NC	26:5:611:CLA:C4	2.40	0.84
17:N:148:LEU:HD11	34:N:621:LHG:H341	1.60	0.84
19:3:67:LEU:HB3	24:g:160:PHE:CE2	2.13	0.84
2:B:476:ARG:NH1	41:B:708:HOH:O	2.11	0.83
22:S:185:PRO:HD2	39:S:611:II0:C08	2.08	0.83
18:2:109:THR:HG23	26:2:304:CLA:OBD	1.78	0.83
18:2:153:LEU:HD11	24:g:169:ALA:HB2	1.59	0.83
19:3:196:LEU:CG	28:3:313:WVN:C16	2.55	0.83
3:c:356:MET:SD	3:c:370:GLN:HG3	2.18	0.83
17:N:81:TRP:CE2	17:N:82:LEU:HB2	2.13	0.83
18:2:144:PHE:CE2	26:2:319:CLA:HBC1	2.14	0.83
17:N:81:TRP:CZ2	17:N:82:LEU:HD22	2.14	0.83
26:5:605:CLA:H203	34:5:618:LHG:C25	2.09	0.83
17:N:101:ALA:HA	26:N:604:CLA:CBB	2.09	0.83
26:3:306:CLA:O1A	39:3:310:II0:C12	2.27	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4:76:ILE:CG2	24:g:127:GLN:HG2	2.09	0.83
3:C:82:THR:O	3:C:86:VAL:HG13	1.79	0.83
26:2:308:CLA:H71	39:2:313:II0:C30	2.08	0.83
26:4:301:CLA:C1	26:4:303:CLA:H12	2.09	0.83
3:c:335:ASP:OD2	3:c:354:TYR:HE2	1.59	0.83
19:3:196:LEU:HD23	28:3:313:WVN:C26	2.07	0.83
26:5:605:CLA:CHB	26:6:609:CLA:H11	2.09	0.83
3:c:353:LYS:HD2	3:c:354:TYR:CD2	2.14	0.82
39:2:320:II0:C38	26:3:308:CLA:HAB	2.09	0.82
24:g:163:LYS:HG2	26:g:402:CLA:HMA3	1.60	0.82
1:A:223:LEU:HD13	4:D:264:ARG:HD2	1.61	0.82
17:1:155:PRO:CB	18:2:54:LEU:CD2	2.55	0.82
17:1:216:GLY:O	17:1:220:PHE:HB2	1.78	0.82
14:X:1:MET:CE	26:N:607:CLA:HED1	2.09	0.82
18:2:83:VAL:CG1	24:g:170:TRP:CD2	2.62	0.82
38:Q:309:KC2:CHA	38:Q:310:KC2:CMD	2.57	0.82
24:g:168:ILE:HG23	26:g:402:CLA:CGA	2.08	0.82
38:4:310:KC2:CHA	38:4:311:KC2:CMD	2.57	0.82
38:Q:309:KC2:C4D	38:Q:310:KC2:CMD	2.58	0.82
17:1:144:TRP:CE3	34:1:620:LHG:H172	2.15	0.82
17:N:151:LEU:HD23	18:O:71:LEU:HD11	1.61	0.82
18:2:83:VAL:HG12	24:g:170:TRP:CZ3	2.15	0.82
26:3:302:CLA:H61	24:g:154:LEU:CD2	2.07	0.82
20:4:164:PHE:O	26:5:601:CLA:CBB	2.28	0.82
3:C:335:ASP:OD2	3:C:354:TYR:HE2	1.52	0.82
26:2:301:CLA:HMD2	40:2:317:IHT:C14	2.09	0.82
17:1:159:GLN:NE2	18:2:55:LYS:HD2	1.93	0.81
6:F:16:ARG:HD2	41:F:201:HOH:O	1.52	0.81
2:b:227:ARG:HD2	41:b:795:HOH:O	1.80	0.81
17:N:73:PHE:CE1	26:N:601:CLA:CAC	2.57	0.81
17:N:159:GLN:NE2	18:O:53:LYS:HD2	1.92	0.81
17:N:212:LEU:CD1	26:N:614:CLA:HED3	2.09	0.81
18:2:144:PHE:CD1	26:2:319:CLA:CAC	2.62	0.81
26:3:307:CLA:CMD	26:4:303:CLA:C9	2.59	0.81
26:G:401:CLA:HBA2	26:S:610:CLA:H92	1.62	0.81
18:O:107:THR:HG23	26:O:604:CLA:OBD	1.78	0.81
1:A:220:THR:HG23	4:D:264:ARG:HH22	1.45	0.81
26:2:301:CLA:CMD	40:2:317:IHT:C14	2.58	0.81
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.14	0.81
17:1:145:ILE:HD13	34:1:620:LHG:H223	1.61	0.81
17:1:148:LEU:HD11	34:1:620:LHG:C34	2.06	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:4:310:KC2:C4D	38:4:311:KC2:CMD	2.58	0.81
18:2:83:VAL:HG12	24:g:170:TRP:CE2	2.14	0.81
3:c:335:ASP:OD2	3:c:354:TYR:CE2	2.33	0.81
18:2:153:LEU:HD21	24:g:169:ALA:CB	2.10	0.81
2:b:408:GLY:CA	41:b:754:HOH:O	2.28	0.81
26:5:605:CLA:C4B	26:6:609:CLA:H2	2.10	0.81
26:1:606:CLA:C4C	26:2:311:CLA:H42	2.11	0.80
18:2:138:ILE:HD12	26:2:307:CLA:HBC2	1.63	0.80
6:F:15:PHE:CE2	41:F:201:HOH:O	2.34	0.80
2:b:353:GLU:OE2	41:b:701:HOH:O	1.98	0.80
1:A:42:LEU:O	1:A:46:THR:CG2	2.30	0.80
38:Q:309:KC2:CAD	38:Q:310:KC2:C2D	2.60	0.80
3:c:331:PHE:CB	3:c:354:TYR:CE1	2.64	0.80
20:4:76:ILE:HA	24:g:128:VAL:HA	1.62	0.80
18:2:141:VAL:HG22	34:2:321:LHG:C32	2.10	0.80
22:6:122:GLU:HB3	22:6:135:PRO:HG3	1.64	0.80
19:3:189:MET:HB3	39:3:311:II0:C38	2.11	0.80
26:5:605:CLA:H203	34:5:618:LHG:H252	1.64	0.80
1:A:218:LEU:HD23	29:A:407:PL9:C4	2.11	0.80
18:2:153:LEU:HD21	24:g:169:ALA:CA	2.12	0.80
38:4:310:KC2:CAD	38:4:311:KC2:C2D	2.60	0.80
22:S:177:GLU:HG2	22:S:178:ALA:H	1.47	0.80
19:3:189:MET:CB	39:3:311:II0:C36	2.59	0.79
20:4:76:ILE:HD11	26:4:301:CLA:CBA	2.12	0.79
20:4:155:GLN:HA	24:g:123:PHE:CE2	2.16	0.79
17:N:54:ILE:O	17:N:55:PRO:C	2.23	0.79
17:N:144:TRP:HH2	39:N:620:II0:C41	1.95	0.79
24:g:163:LYS:CG	26:g:402:CLA:HMA3	2.11	0.79
2:b:179:GLN:OE1	41:b:703:HOH:O	2.00	0.79
6:f:41:GLN:O	6:f:42:ARG:C	2.25	0.79
18:2:148:ALA:HB2	19:3:47:PHE:CE2	2.17	0.79
26:O:605:CLA:CHC	26:P:610:CLA:H43	2.13	0.79
1:A:220:THR:HG23	4:D:264:ARG:NH2	1.98	0.79
19:3:67:LEU:HB3	24:g:160:PHE:CZ	2.17	0.79
2:b:390:TYR:CD2	4:d:343:GLU:OE2	2.36	0.79
17:1:159:GLN:HE21	18:2:55:LYS:CD	1.90	0.79
19:3:192:LEU:HD22	28:3:313:WVN:C35	2.13	0.79
17:1:144:TRP:HZ3	34:1:620:LHG:H172	1.47	0.79
17:1:155:PRO:CB	18:2:54:LEU:HD22	2.13	0.79
19:3:92:GLY:HA2	39:3:311:II0:C19	2.13	0.79
26:5:605:CLA:C3B	26:6:609:CLA:H2	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:h:56:GLU:HB2	41:h:207:HOH:O	1.82	0.79
17:N:159:GLN:CD	18:O:53:LYS:HD2	2.08	0.79
17:1:145:ILE:CD1	34:1:620:LHG:H223	2.10	0.79
26:4:304:CLA:H43	39:4:317:II0:C39	2.13	0.79
26:1:606:CLA:HMA2	26:2:311:CLA:OBD	1.81	0.78
26:1:606:CLA:CHB	26:2:311:CLA:CBA	2.60	0.78
19:3:164:PRO:HD2	39:3:310:II0:C06	2.14	0.78
19:P:96:PHE:CE2	19:P:192:LEU:HG	2.18	0.78
18:2:83:VAL:CG1	24:g:170:TRP:CZ2	2.64	0.78
26:4:306:CLA:NC	26:5:611:CLA:H42	1.98	0.78
2:b:412:THR:O	41:b:704:HOH:O	2.00	0.78
1:A:42:LEU:O	1:A:46:THR:HG23	1.84	0.78
7:h:10:LEU:HD11	24:g:162:TRP:CH2	2.18	0.78
17:N:73:PHE:CB	26:N:601:CLA:HMD2	2.08	0.78
2:B:27:THR:HG22	2:B:107:LEU:CD1	2.14	0.78
14:x:10:ASN:HA	14:x:13:LEU:HD12	1.65	0.78
17:N:135:GLN:NE2	26:N:606:CLA:OBD	2.17	0.78
20:4:154:LEU:HB2	24:g:125:VAL:CG2	2.13	0.78
2:b:49:ASP:OD2	41:b:705:HOH:O	2.00	0.78
18:2:153:LEU:HD22	24:g:169:ALA:HA	1.66	0.78
26:4:306:CLA:HMA1	26:5:611:CLA:OBD	1.83	0.78
22:S:122:GLU:HB3	22:S:135:PRO:HG3	1.64	0.78
20:4:138:TRP:CZ2	39:4:320:II0:C39	2.67	0.78
26:4:306:CLA:HED1	21:5:223:PHE:CE2	2.18	0.78
22:6:177:GLU:HG2	22:6:178:ALA:H	1.47	0.78
10:l:9:GLN:OE1	41:l:202:HOH:O	2.02	0.77
14:x:29:ILE:HG23	17:1:81:TRP:CD1	2.19	0.77
26:1:606:CLA:H12	18:2:215:PHE:HZ	1.48	0.77
19:3:106:LEU:CD1	39:3:312:II0:C23	2.62	0.77
17:1:132:ALA:HB1	17:1:137:ALA:HB3	1.65	0.77
20:4:155:GLN:N	24:g:125:VAL:HG11	1.99	0.77
26:4:306:CLA:HMB1	26:5:611:CLA:CHA	2.14	0.77
17:N:220:PHE:CZ	38:N:612:KC2:C1A	2.67	0.77
19:3:96:PHE:CE2	19:3:192:LEU:HG	2.18	0.77
18:O:136:ILE:HD12	26:O:607:CLA:HBC2	1.63	0.77
21:5:144:PHE:CE1	26:6:601:CLA:HAC1	2.19	0.77
17:N:129:HIS:HE1	26:N:607:CLA:NA	1.63	0.77
20:4:180:ARG:NH1	38:4:311:KC2:CBA	2.48	0.77
26:4:306:CLA:CED	21:5:223:PHE:CE2	2.68	0.77
20:Q:134:GLN:NE2	39:Q:319:II0:C23	2.48	0.77
2:b:46:ASP:O	41:b:706:HOH:O	2.03	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:433:PHE:HB3	41:c:632:HOH:O	1.83	0.77
17:N:140:GLN:NE2	39:N:620:II0:C29	2.46	0.77
26:Q:303:CLA:H43	39:Q:316:II0:C39	2.13	0.77
26:4:301:CLA:H52	26:4:303:CLA:C10	2.14	0.77
26:4:306:CLA:C2B	26:5:611:CLA:HBA2	2.14	0.77
4:d:229:ASN:CB	41:d:521:HOH:O	2.26	0.77
17:1:210:TYR:HE1	17:1:215:ARG:HA	1.48	0.77
26:N:606:CLA:H12	18:O:213:PHE:HZ	1.50	0.77
26:Q:305:CLA:HMB2	26:R:312:CLA:HBA2	1.64	0.77
2:B:80:ILE:HD13	2:B:93:PHE:HZ	1.51	0.76
3:C:37:ILE:HG21	9:K:45:ARG:NE	2.00	0.76
26:2:308:CLA:C9	38:2:310:KC2:CMB	2.63	0.76
20:Q:180:ARG:NH1	38:Q:310:KC2:CBA	2.48	0.76
2:b:408:GLY:C	41:b:754:HOH:O	2.28	0.76
17:1:135:GLN:OE1	17:1:137:ALA:N	2.19	0.76
14:x:21:ILE:CG2	26:1:603:CLA:C7	2.64	0.76
20:4:99:MET:HE3	20:4:119:MET:HE1	1.68	0.76
20:4:151:VAL:CG1	33:5:619:LMG:HC91	2.16	0.76
34:N:621:LHG:H261	26:O:601:CLA:C1C	2.16	0.76
18:O:141:LEU:HD11	33:O:617:LMG:C18	2.16	0.76
26:O:601:CLA:HHD	40:O:616:IHT:C04	2.16	0.76
26:O:608:CLA:C9	38:O:610:KC2:CMB	2.63	0.76
17:1:94:HIS:HB3	17:1:200:MET:HE1	1.67	0.76
2:B:399:THR:HG22	2:B:417:VAL:HG22	1.68	0.76
2:B:399:THR:HG23	2:B:411:PHE:HB2	1.67	0.76
26:4:306:CLA:CMA	26:5:611:CLA:CAD	2.63	0.76
17:N:86:TRP:NE1	26:N:603:CLA:O1A	2.19	0.76
3:C:37:ILE:CG2	9:K:45:ARG:NH1	2.48	0.76
19:3:184:HIS:HD2	39:3:310:II0:C37	1.99	0.76
26:3:302:CLA:H43	24:g:157:VAL:HG21	1.68	0.76
2:B:51:VAL:O	41:B:706:HOH:O	2.04	0.75
34:1:620:LHG:H261	26:2:301:CLA:C1C	2.16	0.75
19:3:165:LEU:HD11	33:5:619:LMG:C38	2.13	0.75
26:O:605:CLA:HAC1	39:O:615:II0:C41	2.16	0.75
20:4:151:VAL:HG11	33:5:619:LMG:HC91	1.66	0.75
18:2:143:LEU:HD11	33:2:318:LMG:C18	2.16	0.75
26:O:605:CLA:H3A	26:P:610:CLA:HBD	1.68	0.75
3:c:374:ASP:HB2	41:c:607:HOH:O	1.86	0.75
20:Q:99:MET:HE3	20:Q:119:MET:HE1	1.68	0.75
1:a:132:GLU:OE1	41:a:504:HOH:O	2.04	0.75
17:1:145:ILE:HD12	34:1:620:LHG:C22	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:189:MET:HB3	39:3:311:II0:C42	2.17	0.75
20:4:134:GLN:HE21	39:4:320:II0:C19	2.00	0.75
39:Q:316:II0:C27	26:R:312:CLA:H43	2.17	0.75
26:R:306:CLA:H203	34:R:319:LHG:C25	2.17	0.75
4:D:232:ARG:HD3	30:D:401:SQD:H62	1.69	0.75
26:2:308:CLA:H93	38:2:310:KC2:CMB	2.17	0.75
26:R:306:CLA:H2	26:S:609:CLA:O1A	1.86	0.75
18:2:162:PHE:O	26:2:319:CLA:HAB	1.86	0.74
26:3:307:CLA:H52	20:4:80:TRP:CH2	2.19	0.74
26:O:608:CLA:H93	38:O:610:KC2:CMB	2.17	0.74
26:1:606:CLA:C4C	26:2:311:CLA:C4	2.65	0.74
26:5:605:CLA:H141	26:6:609:CLA:C3	2.18	0.74
7:h:56:GLU:O	41:h:201:HOH:O	2.04	0.74
7:h:58:VAL:O	41:h:202:HOH:O	2.05	0.74
26:1:606:CLA:CBA	18:2:218:LEU:HD13	2.18	0.74
17:N:114:PRO:HB2	38:N:605:KC2:C1D	2.17	0.74
20:4:133:GLN:OE1	39:4:320:II0:C19	2.34	0.74
17:N:101:ALA:CA	26:N:604:CLA:CBB	2.65	0.74
26:2:305:CLA:HAC1	39:2:316:II0:C41	2.16	0.74
26:4:306:CLA:CHB	26:5:611:CLA:CGA	2.65	0.74
26:1:606:CLA:H11	18:2:215:PHE:CE1	2.22	0.74
3:C:196:LEU:HD12	26:C:503:CLA:H201	1.70	0.74
3:C:374:ASP:HB2	41:C:607:HOH:O	1.86	0.74
2:B:159:THR:O	2:B:180:PRO:HB3	1.87	0.74
18:2:151:GLU:CG	19:3:48:LEU:CD2	2.65	0.74
5:E:50:THR:O	41:E:102:HOH:O	2.06	0.74
2:b:405:LYS:O	41:b:707:HOH:O	2.05	0.74
17:N:207:VAL:HG11	40:N:619:IHT:C29	2.17	0.74
26:R:306:CLA:H12	26:S:609:CLA:HAA1	1.70	0.74
19:3:193:GLY:HA2	28:3:313:WVN:C32	2.18	0.74
1:a:331:MET:HE2	4:d:347:ARG:C	2.08	0.73
2:B:162:TRP:HD1	41:B:769:HOH:O	1.66	0.73
1:a:259:ILE:O	41:a:505:HOH:O	2.05	0.73
2:b:472:ARG:HD3	26:b:611:CLA:HED1	1.70	0.73
26:3:301:CLA:HMC1	39:3:311:II0:C34	2.18	0.73
3:C:351:LEU:N	3:C:351:LEU:HD23	2.02	0.73
26:2:319:CLA:HBA2	34:2:321:LHG:H242	1.70	0.73
3:C:353:LYS:HE2	3:C:354:TYR:H	1.53	0.73
18:2:92:GLY:HA3	18:2:187:ALA:HB1	1.71	0.73
17:N:152:THR:HG21	34:N:621:LHG:C35	2.19	0.73
20:4:129:GLN:HG2	21:5:228:PHE:CE2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4:155:GLN:NE2	33:5:619:LMG:HC71	2.03	0.73
17:N:132:ALA:HB1	17:N:138:MET:HG2	1.70	0.73
26:1:606:CLA:H3A	26:2:311:CLA:HBD	1.70	0.73
26:3:307:CLA:CED	26:4:303:CLA:CED	2.67	0.73
1:a:252:HIS:CD2	1:a:264:SER:OG	2.41	0.73
26:2:303:CLA:HAB	40:2:317:IHT:C39	2.19	0.73
18:O:90:GLY:HA3	18:O:185:ALA:HB1	1.71	0.72
2:B:241:SER:O	2:B:245:VAL:HG13	1.90	0.72
26:N:606:CLA:CBB	34:N:621:LHG:H171	2.17	0.72
20:4:152:GLN:CD	21:5:54:LEU:HD22	2.14	0.72
33:4:319:LMG:HC62	39:4:320:II0:C07	2.19	0.72
7:h:6:ARG:NH2	24:g:155:GLU:CD	2.45	0.72
17:1:155:PRO:HB2	18:2:54:LEU:CD1	2.19	0.72
1:a:314:ILE:O	41:a:506:HOH:O	2.06	0.72
17:N:159:GLN:HE21	18:O:53:LYS:NZ	1.87	0.72
26:1:606:CLA:H12	18:2:215:PHE:CZ	2.24	0.72
24:g:168:ILE:CG2	26:g:402:CLA:CGA	2.65	0.72
2:B:137:LYS:NZ	7:H:17:GLU:CD	2.48	0.72
17:1:59:ARG:NH2	17:1:70:ASP:OD2	2.23	0.72
17:N:89:GLU:HG2	17:N:157:ILE:HD13	1.72	0.72
26:2:303:CLA:H151	33:2:318:LMG:H372	1.71	0.72
1:a:257:ARG:O	41:a:505:HOH:O	2.08	0.72
26:N:604:CLA:C2B	39:N:616:II0:C19	2.67	0.72
18:2:140:PHE:HD2	34:2:321:LHG:H322	1.52	0.72
33:4:319:LMG:C6	39:4:320:II0:C07	2.66	0.72
26:5:605:CLA:C1B	26:6:609:CLA:C1	2.65	0.72
22:6:136:VAL:HG11	22:6:221:LEU:CD2	2.20	0.72
1:A:32:TRP:NE1	41:A:504:HOH:O	2.15	0.72
20:4:138:TRP:HZ2	39:4:320:II0:C39	2.02	0.72
22:6:172:PHE:HA	22:6:176:ARG:HG2	1.71	0.72
1:A:223:LEU:HD11	4:D:264:ARG:HG3	1.72	0.72
26:4:306:CLA:H3A	26:5:611:CLA:HBD	1.72	0.72
34:G:403:LHG:H242	26:P:601:CLA:HBA2	1.70	0.72
2:B:75:TRP:CD1	2:B:92:SER:HG	2.08	0.71
30:c:501:SQD:H62	4:d:232:ARG:HD3	1.70	0.71
20:Q:72:PHE:CD2	26:Q:301:CLA:H42	2.25	0.71
17:1:41:TYR:N	17:1:47:GLN:OE1	2.24	0.71
17:N:126:MET:CE	17:N:207:VAL:HG13	2.20	0.71
19:3:106:LEU:HD11	39:3:312:II0:C23	2.20	0.71
21:5:58:THR:CG2	24:g:119:THR:HG23	2.20	0.71
17:N:209:HIS:CD2	38:N:612:KC2:ND	2.59	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:55:PRO:HB2	18:O:58:LEU:HD13	1.72	0.71
19:P:197:HIS:HB3	26:P:611:CLA:HED1	1.73	0.71
13:W:43:VAL:HB	19:3:127:TRP:CZ3	2.26	0.71
18:2:45:PHE:N	18:2:55:LYS:HA	2.06	0.71
26:4:306:CLA:C4C	26:5:611:CLA:H41	2.20	0.71
20:Q:172:ALA:HB2	26:Q:308:CLA:HAA2	1.72	0.71
26:3:301:CLA:HMC1	39:3:311:II0:C30	2.20	0.71
20:4:172:ALA:HB2	26:4:309:CLA:HAA2	1.72	0.71
26:O:603:CLA:H151	33:O:617:LMG:H372	1.71	0.71
20:4:72:PHE:CD2	26:4:302:CLA:H42	2.25	0.71
26:4:306:CLA:C1B	26:5:611:CLA:CGA	2.68	0.71
17:1:54:ILE:HD12	17:1:55:PRO:HD2	1.73	0.71
1:A:236:GLY:O	41:A:501:HOH:O	2.09	0.71
3:C:37:ILE:HG22	9:K:45:ARG:NH1	2.06	0.71
17:N:99:MET:HB3	39:N:615:II0:C42	2.21	0.71
22:S:113:LEU:HD23	26:S:604:CLA:H8	1.73	0.71
17:1:159:GLN:HE22	18:2:55:LYS:H	0.73	0.70
26:O:603:CLA:HMD1	26:O:607:CLA:CHD	2.21	0.70
20:Q:120:THR:HG21	40:Q:317:IHT:C17	2.21	0.70
24:g:167:LEU:HB2	26:g:402:CLA:HBD	1.73	0.70
26:3:306:CLA:H72	39:3:310:II0:C30	2.20	0.70
22:S:136:VAL:HG11	22:S:221:LEU:CD2	2.20	0.70
23:G:167:LEU:HD21	26:O:607:CLA:H2	1.74	0.70
18:O:45:PHE:N	18:O:53:LYS:HA	2.06	0.70
17:1:155:PRO:C	18:2:54:LEU:CD2	2.65	0.70
18:2:134:ILE:HG13	26:2:305:CLA:HMD3	1.72	0.70
19:3:106:LEU:HD13	39:3:312:II0:C19	2.22	0.70
19:3:174:LEU:HD21	24:g:140:LYS:HE3	1.74	0.70
2:B:307:ASP:N	41:B:712:HOH:O	2.25	0.70
3:c:353:LYS:O	3:c:354:TYR:HB2	1.91	0.70
18:2:57:PRO:HB2	18:2:60:LEU:HD13	1.72	0.70
19:3:197:HIS:HB3	26:3:309:CLA:HED1	1.73	0.70
2:B:49:ASP:OD2	41:B:707:HOH:O	2.08	0.70
18:2:141:VAL:CG2	34:2:321:LHG:H332	2.21	0.70
26:2:303:CLA:HMD1	26:2:307:CLA:CHD	2.21	0.70
19:P:189:MET:HE3	26:P:602:CLA:HMC2	1.74	0.70
22:S:172:PHE:HA	22:S:176:ARG:HG2	1.71	0.70
14:x:29:ILE:HG23	17:1:81:TRP:NE1	2.06	0.70
19:3:189:MET:HE3	26:3:301:CLA:HMC2	1.74	0.70
20:4:120:THR:HG21	40:4:318:IHT:C17	2.21	0.70
1:A:257:ARG:O	41:A:502:HOH:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:59:ARG:NH2	17:N:70:ASP:O	2.25	0.70
21:5:72:PRO:O	33:5:619:LMG:O3	2.06	0.70
21:R:142:GLU:HG2	26:R:308:CLA:C4B	2.21	0.70
17:1:148:LEU:HB2	34:1:620:LHG:H202	1.73	0.70
26:2:319:CLA:ND	34:2:321:LHG:H251	2.07	0.70
17:N:71:VAL:HG11	26:N:601:CLA:CGD	2.22	0.70
20:4:80:TRP:CE3	24:g:127:GLN:HB3	2.26	0.70
1:a:234:ASN:HA	4:d:264:ARG:HD3	1.72	0.69
1:a:269:ARG:O	4:d:218:GLN:NE2	2.25	0.69
18:2:140:PHE:CD2	34:2:321:LHG:H322	2.27	0.69
18:2:144:PHE:CE1	26:2:319:CLA:HAC2	2.25	0.69
26:C:514:CLA:HBC1	33:C:520:LMG:H131	1.72	0.69
18:2:141:VAL:CG2	34:2:321:LHG:H321	2.20	0.69
26:O:603:CLA:HMD1	26:O:607:CLA:C1D	2.23	0.69
20:Q:76:ILE:CD1	26:Q:302:CLA:H11	2.22	0.69
20:Q:181:ARG:HB3	26:Q:308:CLA:HHB	1.75	0.69
17:N:213:VAL:HG21	38:N:612:KC2:CED	2.22	0.69
20:4:69:PRO:HD2	39:4:315:II0:C08	2.22	0.69
3:c:433:PHE:CB	41:c:632:HOH:O	2.40	0.69
17:N:212:LEU:HD11	26:N:614:CLA:HED3	1.74	0.69
26:3:307:CLA:HMB3	39:3:310:II0:C36	2.22	0.69
20:4:154:LEU:HB2	24:g:125:VAL:HG21	1.72	0.69
21:5:142:GLU:HG2	26:5:607:CLA:C4B	2.21	0.69
17:1:159:GLN:NE2	18:2:55:LYS:N	2.18	0.69
17:N:144:TRP:CH2	39:N:620:II0:C41	2.75	0.69
26:4:301:CLA:C7	26:4:303:CLA:H171	2.22	0.69
26:R:303:CLA:CBC	40:R:317:IHT:C14	2.69	0.69
17:N:81:TRP:CZ2	17:N:82:LEU:HD13	2.28	0.69
26:N:604:CLA:O1A	38:N:605:KC2:CBB	2.41	0.69
22:6:113:LEU:HD23	26:6:604:CLA:H8	1.73	0.69
1:A:189:GLU:OE1	41:A:503:HOH:O	2.09	0.69
1:A:269:ARG:O	4:D:218:GLN:NE2	2.25	0.69
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.74	0.69
1:a:331:MET:HE1	4:d:351:LEU:HG	1.75	0.69
17:N:211:LEU:HD13	26:N:614:CLA:HMD1	1.74	0.69
26:2:303:CLA:HMD1	26:2:307:CLA:C1D	2.23	0.69
38:Q:309:KC2:CAD	38:Q:310:KC2:C3D	2.71	0.69
14:x:3:PRO:O	41:x:201:HOH:O	2.10	0.69
18:2:70:PHE:CZ	40:2:317:IHT:C13	2.75	0.69
26:2:319:CLA:C3D	34:2:321:LHG:O10	2.41	0.69
20:Q:134:GLN:HE22	39:Q:319:II0:C29	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:303:CLA:HBB2	40:2:317:IHT:C38	2.23	0.69
19:3:89:CYS:SG	39:3:311:II0:C39	2.81	0.69
19:3:96:PHE:HD2	19:3:195:MET:HE3	1.58	0.69
34:G:403:LHG:H251	26:P:601:CLA:ND	2.07	0.69
7:h:10:LEU:HD11	24:g:162:TRP:HH2	1.57	0.68
20:4:76:ILE:CD1	26:4:303:CLA:H11	2.22	0.68
26:O:611:CLA:CBB	39:O:613:II0:C19	2.72	0.68
26:3:307:CLA:H41	20:4:150:ILE:CD1	2.23	0.68
34:G:403:LHG:O10	26:P:601:CLA:C3D	2.41	0.68
17:N:81:TRP:CZ2	17:N:82:LEU:HB2	2.28	0.68
19:P:96:PHE:HD2	19:P:195:MET:HE3	1.58	0.68
20:Q:145:PHE:HE1	21:R:72:PRO:HG2	1.59	0.68
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.75	0.68
3:c:353:LYS:HD3	3:c:354:TYR:N	2.09	0.68
17:1:144:TRP:CE3	34:1:620:LHG:H191	2.28	0.68
1:A:218:LEU:HD23	29:A:407:PL9:C52	2.22	0.68
9:K:17:PHE:O	9:K:18:LYS:C	2.36	0.68
2:b:476:ARG:HG2	41:b:737:HOH:O	1.93	0.68
1:A:77:ILE:HD13	10:L:30:VAL:HG13	1.74	0.68
14:X:1:MET:CE	26:N:607:CLA:HED2	2.22	0.68
17:1:159:GLN:CD	18:2:55:LYS:H	1.99	0.68
20:4:76:ILE:HD13	26:4:301:CLA:O1A	1.94	0.68
20:4:80:TRP:CG	24:g:127:GLN:HB2	2.29	0.68
23:G:84:GLN:HA	23:G:88:ALA:HB2	1.74	0.68
17:N:208:HIS:O	26:N:614:CLA:HED1	1.94	0.68
20:4:76:ILE:CD1	26:4:301:CLA:O1A	2.42	0.68
2:b:296:LEU:O	41:b:709:HOH:O	2.12	0.68
26:N:614:CLA:C3C	40:N:619:IHT:C29	2.72	0.68
38:4:310:KC2:CAD	38:4:311:KC2:C3D	2.71	0.68
2:B:118:TRP:O	41:B:702:HOH:O	2.12	0.68
17:1:133:VAL:O	17:1:139:GLN:NE2	2.27	0.68
17:N:209:HIS:NE2	38:N:612:KC2:C1C	2.56	0.68
18:2:198:ILE:HD13	40:2:317:IHT:C16	2.24	0.68
26:3:307:CLA:HAB	39:3:310:II0:C39	2.24	0.68
26:B:612:CLA:HBA1	41:B:754:HOH:O	1.94	0.68
6:F:16:ARG:NE	41:F:201:HOH:O	2.14	0.68
20:4:154:LEU:HD12	24:g:125:VAL:HG23	1.76	0.68
22:S:136:VAL:HG11	22:S:221:LEU:HD23	1.75	0.68
3:c:353:LYS:HD2	3:c:354:TYR:CE2	2.29	0.67
17:1:188:ARG:HH21	26:1:609:CLA:HBA1	1.59	0.67
26:1:606:CLA:C4A	26:2:311:CLA:O1A	2.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:N:606:CLA:HBA2	18:O:216:LEU:HD13	1.75	0.67
18:O:142:PHE:HE1	19:P:66:PRO:HG3	1.57	0.67
18:2:133:GLN:HG3	26:2:305:CLA:C4D	2.25	0.67
26:3:307:CLA:HED1	26:4:303:CLA:HED2	1.76	0.67
20:4:137:VAL:HG11	39:4:320:II0:C27	2.23	0.67
18:O:163:ASP:OD1	39:O:613:II0:O02	2.13	0.67
20:4:76:ILE:HD11	26:4:301:CLA:CGA	2.24	0.67
23:G:96:VAL:HG21	21:R:135:LEU:HD11	1.76	0.67
26:4:306:CLA:C2C	26:5:611:CLA:H61	2.24	0.67
18:2:218:LEU:HD12	26:2:311:CLA:HED1	1.76	0.67
26:3:307:CLA:HED1	26:4:303:CLA:CED	2.24	0.67
20:4:181:ARG:HB3	26:4:309:CLA:HHB	1.75	0.67
1:A:234:ASN:HA	4:D:264:ARG:HD3	1.76	0.67
2:b:409:GLN:NE2	41:b:716:HOH:O	2.26	0.67
26:1:606:CLA:CHB	26:2:311:CLA:CGA	2.73	0.67
17:N:225:PRO:HB2	17:N:227:PHE:HD2	1.60	0.67
2:b:51:VAL:O	41:b:708:HOH:O	2.11	0.67
2:b:170:ASP:OD2	41:b:710:HOH:O	2.13	0.67
18:2:60:LEU:HD11	18:2:76:SER:HB3	1.77	0.67
26:3:307:CLA:CAB	39:3:310:II0:C42	2.72	0.67
20:4:138:TRP:HH2	39:4:320:II0:C41	2.08	0.67
20:4:206:THR:HG23	26:4:312:CLA:HED1	1.76	0.67
1:A:220:THR:CG2	4:D:264:ARG:HH22	2.07	0.67
2:B:158:VAL:HG12	2:B:181:VAL:HG22	1.77	0.67
1:a:312:ARG:CD	41:e:102:HOH:O	2.42	0.67
26:1:606:CLA:C1	18:2:215:PHE:CZ	2.78	0.67
18:2:84:LEU:CG	24:g:170:TRP:HZ3	2.08	0.67
18:2:134:ILE:HB	26:2:306:CLA:HBC1	1.77	0.67
20:Q:75:ILE:HG13	20:Q:76:ILE:HG13	1.76	0.67
1:a:136:ARG:NH2	8:i:27:ASP:OD1	2.28	0.66
18:2:151:GLU:CG	19:3:48:LEU:HD22	2.24	0.66
38:4:310:KC2:C2D	38:4:311:KC2:CHD	2.73	0.66
26:6:610:CLA:C2B	26:g:401:CLA:O1A	2.43	0.66
20:Q:206:THR:HG23	26:Q:311:CLA:HED1	1.76	0.66
2:b:187:PRO:HB2	7:h:55:ILE:HG21	1.77	0.66
17:N:74:ASP:OD2	17:N:77:GLY:HA2	1.94	0.66
20:4:75:ILE:HG13	20:4:76:ILE:HG13	1.76	0.66
21:5:80:ASP:N	24:g:111:ALA:HB1	2.05	0.66
2:B:296:LEU:HD22	2:B:304:ARG:HD2	1.75	0.66
2:B:411:PHE:HB3	2:B:416:THR:CG2	2.26	0.66
14:X:1:MET:HE1	26:N:607:CLA:HED2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:408:GLY:HA2	41:b:754:HOH:O	1.93	0.66
21:5:78:VAL:O	24:g:112:TYR:CD1	2.49	0.66
20:4:184:VAL:HB	26:4:309:CLA:HMB2	1.77	0.66
21:5:68:VAL:HG22	26:5:602:CLA:HMD1	1.77	0.66
21:5:112:PHE:HB2	39:5:615:II0:C11	2.26	0.66
22:6:136:VAL:HG11	22:6:221:LEU:HD23	1.75	0.66
22:S:183:PHE:HE2	39:S:611:II0:C08	2.08	0.66
17:1:156:ALA:N	18:2:54:LEU:HD21	2.11	0.66
17:N:128:LEU:CD2	26:N:604:CLA:HED2	2.22	0.66
18:2:162:PHE:HB3	26:2:319:CLA:HBB2	1.76	0.66
20:4:138:TRP:CH2	39:4:320:II0:C41	2.78	0.66
38:Q:309:KC2:C2D	38:Q:310:KC2:CHD	2.73	0.66
20:4:160:GLN:HB2	21:5:43:PHE:CE2	2.30	0.66
21:R:68:VAL:HG22	26:R:303:CLA:HMD1	1.77	0.66
39:N:620:II0:C20	26:O:601:CLA:HMD2	2.24	0.66
19:3:75:LEU:HD23	19:3:78:LEU:HD12	1.78	0.66
20:Q:184:VAL:HB	26:Q:308:CLA:HMB2	1.77	0.66
22:S:159:PHE:CE1	22:S:166:LEU:HD11	2.31	0.66
3:c:334:ARG:HG2	3:c:337:ARG:HH12	1.61	0.66
27:d:403:PHO:H51	26:d:405:CLA:H13	1.78	0.66
26:4:306:CLA:O1A	21:5:220:ILE:HG13	1.96	0.66
17:1:69:GLY:HA3	17:1:193:LEU:HD23	1.77	0.65
22:6:159:PHE:CE1	22:6:166:LEU:HD11	2.31	0.65
18:O:216:LEU:HD12	26:O:611:CLA:HED1	1.76	0.65
20:Q:134:GLN:NE2	39:Q:319:II0:C25	2.57	0.65
26:Q:305:CLA:O1A	21:R:220:ILE:HG13	1.96	0.65
22:S:216:MET:SD	22:S:227:THR:HG21	2.36	0.65
9:K:27:ILE:HD11	15:Y:16:ILE:HD13	1.78	0.65
26:b:612:CLA:HBA1	41:b:793:HOH:O	1.97	0.65
18:2:53:PHE:HZ	26:2:301:CLA:HMC3	1.62	0.65
18:O:132:ILE:HB	26:O:606:CLA:HBC1	1.77	0.65
3:C:81:MET:HE2	41:C:635:HOH:O	1.97	0.65
26:N:606:CLA:H3A	26:O:611:CLA:HBD	1.78	0.65
18:2:137:TRP:CH2	26:2:305:CLA:HBB1	2.31	0.65
26:2:301:CLA:HMD3	40:2:317:IHT:C14	2.25	0.65
18:O:58:LEU:HD11	18:O:74:SER:HB3	1.77	0.65
24:g:166:ILE:HB	26:g:402:CLA:OBD	1.97	0.65
1:a:312:ARG:HD2	41:e:102:HOH:O	1.95	0.65
17:N:209:HIS:HD2	38:N:612:KC2:C1D	2.09	0.65
20:4:134:GLN:HE22	39:4:320:II0:C25	2.10	0.65
20:4:69:PRO:HG2	39:4:315:II0:C12	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:51:PHE:HZ	26:O:601:CLA:HMC3	1.62	0.65
26:R:306:CLA:H203	34:R:319:LHG:H251	1.78	0.65
26:R:306:CLA:HBB1	26:S:609:CLA:H61	1.78	0.65
13:W:40:VAL:HA	19:3:127:TRP:HH2	1.62	0.65
17:N:212:LEU:HD21	26:N:614:CLA:CGD	2.24	0.65
19:3:62:VAL:HG22	26:3:301:CLA:HMD1	1.79	0.65
21:5:55:LYS:HZ1	33:5:619:LMG:HC62	1.62	0.65
10:L:3:GLY:O	41:L:202:HOH:O	2.15	0.65
17:N:128:LEU:HD21	26:N:604:CLA:CED	2.24	0.65
22:6:216:MET:SD	22:6:227:THR:HG21	2.36	0.65
19:P:165:LEU:HD11	33:R:301:LMG:H382	1.77	0.65
26:Q:305:CLA:H3A	26:R:312:CLA:HBD	1.79	0.65
3:C:334:ARG:HG2	3:C:337:ARG:HH12	1.61	0.65
27:D:405:PHO:H51	26:D:407:CLA:H13	1.78	0.65
19:3:106:LEU:HD13	39:3:312:II0:C13	2.25	0.65
19:3:192:LEU:CD1	39:3:311:II0:C29	2.74	0.65
20:4:65:VAL:N	26:4:302:CLA:OBD	2.30	0.65
26:4:306:CLA:C1	21:5:219:PRO:HA	2.26	0.65
26:4:306:CLA:HHB	26:5:611:CLA:HBD	1.76	0.65
21:5:78:VAL:HG22	24:g:117:CYS:SG	2.37	0.65
19:P:62:VAL:HG22	26:P:602:CLA:HMD1	1.79	0.65
3:C:52:GLY:HA3	26:C:512:CLA:HMD2	1.77	0.65
2:b:475:PHE:CD2	4:d:139:PRO:HD3	2.32	0.65
17:N:227:PHE:CE1	17:N:228:LYS:HG3	2.32	0.65
20:Q:188:ASN:ND2	38:Q:310:KC2:NB	2.45	0.65
21:R:142:GLU:HG2	26:R:308:CLA:NB	2.12	0.65
4:d:178:PHE:HA	4:d:181:LEU:HD12	1.77	0.65
26:1:606:CLA:HMA2	26:2:311:CLA:CBD	2.26	0.65
19:3:193:GLY:CA	28:3:313:WVN:C32	2.74	0.65
26:3:307:CLA:H72	26:4:308:CLA:HBA2	1.78	0.65
20:4:184:VAL:HG22	38:4:310:KC2:CED	2.27	0.65
20:Q:184:VAL:HG22	38:Q:309:KC2:CED	2.27	0.65
22:S:222:LEU:HD21	22:S:237:ILE:HD11	1.79	0.65
11:M:9:LEU:HD23	11:m:9:LEU:HD23	1.79	0.64
3:c:52:GLY:HA3	26:c:513:CLA:HMD2	1.78	0.64
19:P:75:LEU:HD23	19:P:78:LEU:HD12	1.78	0.64
20:Q:65:VAL:N	26:Q:301:CLA:OBD	2.30	0.64
17:N:226:ASN:HB3	26:N:613:CLA:CED	2.27	0.64
20:4:134:GLN:HE21	39:4:320:II0:C21	2.11	0.64
26:4:306:CLA:CMB	26:5:611:CLA:C1A	2.74	0.64
21:R:112:PHE:HB2	39:R:316:II0:C11	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:LEU:HD21	2:B:93:PHE:HB2	1.79	0.64
2:b:425:GLN:NE2	41:b:717:HOH:O	2.28	0.64
3:c:128:VAL:HG22	33:c:521:LMG:H162	1.79	0.64
17:N:129:HIS:CE1	26:N:607:CLA:C4A	2.69	0.64
38:4:310:KC2:C3D	38:4:311:KC2:C2D	2.76	0.64
2:B:137:LYS:HZ2	7:H:17:GLU:CD	2.05	0.64
22:S:161:SER:HB3	22:S:181:LEU:HD22	1.80	0.64
2:B:27:THR:CG2	2:B:107:LEU:HD13	2.27	0.64
4:D:178:PHE:HA	4:D:181:LEU:HD12	1.77	0.64
4:D:230:THR:OG1	41:D:501:HOH:O	1.83	0.64
26:b:602:CLA:HBA2	41:b:743:HOH:O	1.98	0.64
26:N:614:CLA:C2C	40:N:619:IHT:C34	2.76	0.64
18:2:144:PHE:CE2	26:2:319:CLA:CBC	2.81	0.64
18:2:147:VAL:CG1	19:3:48:LEU:HD11	2.27	0.64
26:4:306:CLA:NC	26:5:611:CLA:H41	2.13	0.64
21:R:154:GLN:O	21:R:156:ARG:HD3	1.97	0.64
22:S:159:PHE:HE1	22:S:166:LEU:HD11	1.60	0.64
3:c:193:ALA:O	3:c:198:GLY:HA2	1.98	0.64
26:c:515:CLA:HBC1	33:c:522:LMG:H131	1.79	0.64
17:N:102:ALA:O	17:N:103:THR:C	2.32	0.64
26:3:307:CLA:HMD3	26:4:303:CLA:H91	1.78	0.64
20:4:78:MET:HE1	26:4:302:CLA:HMA2	1.79	0.64
20:4:133:GLN:HE22	39:4:320:II0:C23	2.11	0.64
20:4:134:GLN:HE22	39:4:320:II0:C23	2.08	0.64
22:6:222:LEU:HD21	22:6:237:ILE:HD11	1.79	0.64
20:Q:180:ARG:HH12	38:Q:310:KC2:CB D	2.10	0.64
17:1:156:ALA:N	18:2:54:LEU:CD2	2.61	0.64
26:1:606:CLA:C2C	26:2:311:CLA:H42	2.27	0.64
17:N:84:LEU:O	17:N:88:ARG:N	2.23	0.64
17:1:96:ARG:HA	17:1:99:MET:HE3	1.78	0.64
26:2:302:CLA:H141	40:2:317:IHT:C33	2.28	0.64
20:4:188:ASN:ND2	38:4:311:KC2:NB	2.45	0.64
17:1:144:TRP:HE3	34:1:620:LHG:H191	1.61	0.64
18:2:144:PHE:CZ	26:2:319:CLA:CBC	2.79	0.64
23:G:166:ILE:HG23	26:O:607:CLA:H3A	1.78	0.64
3:c:81:MET:HE2	41:c:633:HOH:O	1.98	0.63
17:N:119:THR:O	17:N:121:GLY:N	2.31	0.63
17:N:141:LEU:HB2	26:N:607:CLA:HBC1	1.80	0.63
19:3:66:PRO:HD2	39:3:311:II0:O02	1.97	0.63
20:4:100:ILE:HG23	20:4:211:ILE:HD11	1.80	0.63
21:5:154:GLN:O	21:5:156:ARG:HD3	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:189:MET:HB3	39:P:613:II0:C36	2.28	0.63
20:Q:100:ILE:HG23	20:Q:211:ILE:HD11	1.80	0.63
19:3:189:MET:HB3	39:3:311:II0:C40	2.28	0.63
20:4:76:ILE:HD11	26:4:301:CLA:HBA1	1.79	0.63
21:5:142:GLU:HG2	26:5:607:CLA:NB	2.12	0.63
26:5:605:CLA:H141	26:6:609:CLA:C5	2.28	0.63
22:6:159:PHE:HE1	22:6:166:LEU:HD11	1.60	0.63
38:Q:309:KC2:C3D	38:Q:310:KC2:C2D	2.76	0.63
13:w:29:GLU:O	41:w:101:HOH:O	2.15	0.63
17:N:196:GLY:O	17:N:200:MET:HG3	1.98	0.63
18:2:147:VAL:CG1	19:3:48:LEU:CD1	2.76	0.63
18:2:153:LEU:HD21	24:g:169:ALA:HB1	1.80	0.63
26:2:302:CLA:H142	26:2:312:CLA:HBB2	1.80	0.63
26:3:307:CLA:HBC1	26:4:303:CLA:H121	1.79	0.63
3:C:37:ILE:HG21	9:K:45:ARG:NH1	2.10	0.63
3:C:193:ALA:O	3:C:198:GLY:HA2	1.97	0.63
18:2:83:VAL:HG11	24:g:170:TRP:CE2	2.24	0.63
26:4:306:CLA:C1C	26:5:611:CLA:C4	2.76	0.63
2:B:71:VAL:HG21	2:B:96:VAL:HG21	1.80	0.63
2:B:91:TRP:CD1	26:B:606:CLA:HBD	2.33	0.63
17:N:126:MET:SD	17:N:211:LEU:HD21	2.38	0.63
26:3:307:CLA:HMD1	26:4:303:CLA:H91	1.75	0.63
20:4:92:CYS:SG	39:4:315:II0:C35	2.87	0.63
20:4:134:GLN:HE22	39:4:320:II0:C29	2.10	0.63
20:Q:150:ILE:HD12	20:Q:151:VAL:N	2.14	0.63
20:4:184:VAL:HG12	26:4:309:CLA:HBB1	1.81	0.63
26:4:306:CLA:HMA2	26:5:611:CLA:OBD	1.99	0.63
19:P:187:LEU:HG	39:P:612:II0:C27	2.28	0.63
21:R:136:LEU:HG	26:S:602:CLA:H201	1.81	0.63
26:R:309:CLA:H51	38:R:311:KC2:CMA	2.28	0.63
24:g:165:PRO:HA	26:g:402:CLA:CED	2.29	0.63
17:N:116:VAL:HG11	26:N:604:CLA:OBD	1.98	0.63
26:5:608:CLA:H51	38:5:610:KC2:CMA	2.28	0.63
22:6:161:SER:HB3	22:6:181:LEU:HD22	1.80	0.63
2:B:326:ARG:NH2	4:D:296:ASP:OD2	2.28	0.63
3:C:58:ASN:HB2	41:C:614:HOH:O	1.98	0.63
26:C:504:CLA:H172	26:C:511:CLA:HBB2	1.80	0.63
20:4:180:ARG:HH12	38:4:311:KC2:CBD	2.10	0.63
20:4:150:ILE:HD12	20:4:151:VAL:N	2.14	0.63
26:4:306:CLA:CED	21:5:223:PHE:CD2	2.77	0.63
18:O:68:PHE:CE1	40:O:616:IHT:C13	2.82	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Q:184:VAL:HG12	26:Q:308:CLA:HBB1	1.80	0.63
4:d:127:ARG:HG3	41:d:518:HOH:O	1.99	0.62
17:N:132:ALA:CB	17:N:138:MET:HG2	2.28	0.62
18:2:144:PHE:CZ	26:2:319:CLA:CAC	2.82	0.62
26:3:307:CLA:H41	20:4:150:ILE:HD13	1.79	0.62
22:S:183:PHE:HE2	39:S:611:II0:C06	2.06	0.62
17:N:140:GLN:NE2	39:N:620:II0:C25	2.62	0.62
39:O:615:II0:C37	26:P:610:CLA:H51	2.29	0.62
2:b:434:ARG:HA	41:b:742:HOH:O	1.98	0.62
5:e:27:THR:HB	37:f:101:HEM:HAB	1.81	0.62
18:2:141:VAL:HG22	34:2:321:LHG:C33	2.28	0.62
26:4:301:CLA:CGA	26:4:303:CLA:H43	2.30	0.62
20:Q:172:ALA:HB1	20:Q:178:LEU:HD13	1.81	0.62
4:D:127:ARG:HG3	41:D:519:HOH:O	1.99	0.62
2:b:382:PRO:HG3	2:b:388:SER:HB3	1.82	0.62
26:4:306:CLA:C1C	26:5:611:CLA:H42	2.29	0.62
4:D:135:VAL:HG12	4:D:137:ILE:HG23	1.81	0.62
4:d:343:GLU:OE2	41:d:504:HOH:O	2.16	0.62
17:N:81:TRP:C	17:N:81:TRP:CD1	2.71	0.62
26:N:606:CLA:CBA	18:O:216:LEU:HD13	2.29	0.62
20:4:152:GLN:HG2	33:5:619:LMG:O4	2.00	0.62
19:P:174:LEU:O	19:P:178:ILE:HG13	2.00	0.62
1:a:331:MET:HE2	4:d:347:ARG:O	1.92	0.62
3:c:480:VAL:HG21	4:d:247:THR:HA	1.81	0.62
18:O:66:VAL:HG22	26:O:602:CLA:HMD3	1.82	0.62
26:N:606:CLA:C1	18:O:213:PHE:CE1	2.81	0.62
20:4:137:VAL:HG21	39:4:320:II0:C27	2.30	0.62
26:4:301:CLA:H43	26:4:303:CLA:O1D	2.00	0.62
21:5:149:LEU:HD23	26:5:607:CLA:HMA2	1.81	0.62
4:d:135:VAL:HG12	4:d:137:ILE:HG23	1.82	0.62
17:N:59:ARG:O	17:N:60:PRO:C	2.41	0.62
17:N:78:PHE:HE2	39:N:616:II0:C18	2.12	0.62
19:3:106:LEU:HD13	39:3:312:II0:C23	2.28	0.62
19:3:115:THR:HG23	19:3:199:MET:HE3	1.82	0.62
21:R:149:LEU:HD23	26:R:308:CLA:HMA2	1.81	0.62
1:A:92:HIS:NE2	3:C:374:ASP:OD2	2.33	0.62
10:L:14:ASN:ND2	10:L:17:SER:H	1.98	0.62
17:1:187:ARG:O	17:1:191:VAL:HG23	2.00	0.62
19:3:73:PHE:CZ	26:3:302:CLA:H12	2.35	0.62
19:3:174:LEU:O	19:3:178:ILE:HG13	2.00	0.62
20:4:134:GLN:CG	39:4:320:II0:C19	2.73	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:O:603:CLA:CMD	26:O:607:CLA:C1D	2.78	0.62
26:P:608:CLA:H12	26:Q:302:CLA:H12	1.82	0.62
10:L:14:ASN:HD22	10:L:17:SER:H	1.46	0.62
20:4:80:TRP:CG	24:g:127:GLN:CB	2.83	0.62
17:1:47:GLN:HE21	17:1:190:LEU:HD13	1.65	0.61
17:N:151:LEU:HD22	39:O:614:II0:C17	2.30	0.61
19:P:73:PHE:CZ	26:P:603:CLA:H12	2.35	0.61
20:Q:78:MET:HE1	26:Q:301:CLA:HMA2	1.80	0.61
3:c:149:ILE:HD11	16:z:27:LEU:HD13	1.83	0.61
17:1:142:PHE:O	17:1:146:THR:OG1	2.17	0.61
17:N:209:HIS:CD2	38:N:612:KC2:C4C	2.84	0.61
17:N:215:ARG:O	17:N:219:GLU:HB2	2.00	0.61
19:3:92:GLY:CA	39:3:311:II0:C19	2.79	0.61
20:4:206:THR:CG2	26:4:312:CLA:HED1	2.30	0.61
26:O:605:CLA:HBA2	26:P:610:CLA:HBD	1.82	0.61
19:P:106:LEU:HD13	39:P:614:II0:C13	2.30	0.61
2:b:326:ARG:NH2	4:d:296:ASP:OD2	2.30	0.61
17:N:81:TRP:CH2	17:N:82:LEU:HD22	2.34	0.61
17:N:86:TRP:HE1	26:N:603:CLA:CGA	2.14	0.61
20:4:172:ALA:HB1	20:4:178:LEU:HD13	1.81	0.61
21:5:77:GLU:OE1	24:g:122:TRP:CE3	2.53	0.61
19:P:115:THR:HG23	19:P:199:MET:HE3	1.82	0.61
26:B:602:CLA:HBA2	41:B:756:HOH:O	2.00	0.61
2:b:183:PRO:O	41:b:712:HOH:O	2.16	0.61
20:Q:132:MET:HE2	20:Q:132:MET:HA	1.82	0.61
3:c:320:GLY:HA3	3:c:415:LEU:HD12	1.82	0.61
26:c:505:CLA:H172	26:c:512:CLA:HBB2	1.81	0.61
18:2:83:VAL:CG1	24:g:170:TRP:CE3	2.84	0.61
26:2:303:CLA:CMD	26:2:307:CLA:C1D	2.78	0.61
26:2:319:CLA:C4D	34:2:321:LHG:O10	2.49	0.61
19:3:67:LEU:O	24:g:160:PHE:HZ	1.84	0.61
26:4:309:CLA:HED1	21:5:42:VAL:HB	1.82	0.61
26:O:602:CLA:H142	26:O:612:CLA:HBB2	1.80	0.61
20:4:132:MET:HA	20:4:132:MET:HE2	1.82	0.61
17:1:123:ALA:HB1	17:1:127:LYS:HB3	1.83	0.61
22:S:105:LEU:HD21	22:S:203:VAL:HG12	1.82	0.61
2:B:411:PHE:HB3	2:B:416:THR:HG21	1.82	0.61
26:4:306:CLA:HBB	26:5:611:CLA:CBD	2.30	0.61
18:O:141:LEU:H	18:O:141:LEU:HD12	1.66	0.61
20:Q:133:GLN:O	20:Q:134:GLN:C	2.43	0.61
3:c:58:ASN:HB2	41:c:614:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:189:LEU:HD21	39:2:313:II0:C27	2.31	0.61
20:4:152:GLN:OE1	21:5:54:LEU:HA	2.01	0.61
20:4:155:GLN:HG3	24:g:125:VAL:CG1	2.31	0.61
34:G:403:LHG:O10	26:P:601:CLA:C4D	2.49	0.61
19:P:96:PHE:HE2	19:P:192:LEU:HG	1.66	0.61
21:R:191:LEU:HD21	39:R:314:II0:C27	2.31	0.61
2:B:345:ILE:HG23	2:B:353:GLU:OE2	2.01	0.61
4:D:171:SER:HB2	4:D:176:ALA:HB1	1.83	0.61
3:c:229:LYS:HB3	3:c:237:TRP:HA	1.83	0.61
17:N:141:LEU:CB	26:N:607:CLA:HBC1	2.30	0.61
26:2:305:CLA:H3A	26:3:308:CLA:HAA1	1.82	0.61
4:d:171:SER:HB2	4:d:176:ALA:HB1	1.83	0.60
17:1:151:LEU:HB3	26:2:301:CLA:CBC	2.30	0.60
17:N:129:HIS:HE1	26:N:607:CLA:C4A	2.11	0.60
26:N:603:CLA:HED3	26:N:603:CLA:H2	1.83	0.60
26:2:311:CLA:HBC3	39:2:315:II0:C35	2.31	0.60
26:4:306:CLA:C2B	26:5:611:CLA:CBA	2.79	0.60
18:O:62:TYR:OH	18:O:80:ARG:HG2	2.01	0.60
20:Q:206:THR:CG2	26:Q:311:CLA:HED1	2.30	0.60
26:R:306:CLA:H11	22:S:234:PHE:CE2	2.36	0.60
17:N:109:ASP:OD2	17:N:216:GLY:HA3	2.01	0.60
17:N:115:GLY:O	17:N:117:GLN:N	2.28	0.60
17:N:225:PRO:HB2	17:N:227:PHE:CD2	2.35	0.60
26:2:311:CLA:HBC3	39:2:315:II0:C31	2.31	0.60
19:3:58:LEU:HD23	24:g:141:ALA:HB3	1.84	0.60
2:b:307:ASP:N	41:b:715:HOH:O	2.23	0.60
34:1:620:LHG:H142	40:2:317:IHT:C09	2.32	0.60
17:N:99:MET:HE3	26:N:609:CLA:HMC3	1.82	0.60
9:K:13:ALA:HB2	16:Z:61:VAL:HG11	1.83	0.60
2:b:362:PHE:CD1	4:d:187:PHE:CD2	2.89	0.60
17:1:125:MET:HE2	17:1:125:MET:N	2.16	0.60
17:1:202:ALA:O	17:1:206:MET:HG2	2.02	0.60
5:E:27:THR:OG1	37:F:101:HEM:HAB	2.01	0.60
17:1:143:LEU:HD21	26:2:302:CLA:H201	1.83	0.60
22:6:105:LEU:HD21	22:6:203:VAL:HG12	1.82	0.60
7:H:38:PHE:HB2	28:H:101:WVN:C26	2.31	0.60
3:c:149:ILE:CD1	16:z:27:LEU:HD13	2.32	0.60
13:w:40:VAL:HB	13:w:41:PRO:HD3	1.83	0.60
17:1:215:ARG:O	17:1:219:GLU:HB3	2.01	0.60
17:N:152:THR:CB	18:O:51:PHE:CE1	2.83	0.60
17:N:159:GLN:HE21	18:O:53:LYS:HZ3	1.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:307:CLA:HAB	39:3:310:II0:C42	2.32	0.60
22:S:115:VAL:HG13	22:S:216:MET:HE3	1.84	0.60
24:g:168:ILE:N	26:g:402:CLA:O1A	2.35	0.60
2:b:399:THR:HG22	2:b:417:VAL:HG22	1.84	0.60
20:4:129:GLN:CA	21:5:228:PHE:CE1	2.78	0.60
21:5:181:TYR:HB3	26:5:608:CLA:HBB	1.84	0.60
26:B:614:CLA:OBD	10:L:11:VAL:HG21	2.02	0.60
18:2:143:LEU:H	18:2:143:LEU:HD12	1.66	0.60
26:5:603:CLA:HBC1	26:5:607:CLA:HAC1	1.84	0.60
23:G:160:PHE:HZ	19:P:67:LEU:O	1.84	0.60
3:C:335:ASP:CB	3:C:354:TYR:HE2	2.14	0.60
9:K:24:ALA:N	9:K:25:PRO:HD2	2.17	0.60
18:2:133:GLN:HB3	26:2:305:CLA:C1D	2.32	0.60
26:2:303:CLA:HBB2	40:2:317:IHT:C35	2.32	0.60
20:4:158:ASP:CB	21:5:47:PHE:CZ	2.74	0.60
26:R:306:CLA:H172	34:R:319:LHG:H282	1.84	0.60
22:S:97:ILE:HD12	22:S:98:ARG:N	2.17	0.60
1:A:131:TRP:CH2	26:C:506:CLA:HAA2	2.37	0.59
17:N:67:LEU:HD12	26:N:602:CLA:HED1	1.83	0.59
17:N:225:PRO:HB2	17:N:227:PHE:H	1.67	0.59
19:3:96:PHE:HE2	19:3:192:LEU:HG	1.66	0.59
20:4:155:GLN:NE2	24:g:123:PHE:O	2.35	0.59
21:5:77:GLU:OE1	24:g:122:TRP:HE3	1.85	0.59
21:5:186:ILE:HD12	21:5:187:LYS:N	2.17	0.59
1:a:92:HIS:NE2	3:c:374:ASP:OD2	2.34	0.59
20:4:76:ILE:HD12	26:4:303:CLA:H11	1.83	0.59
18:O:194:GLY:O	18:O:195:PHE:C	2.44	0.59
21:R:186:ILE:HD12	21:R:187:LYS:N	2.17	0.59
11:M:35:ALA:HB1	11:m:36:GLU:HG3	1.84	0.59
2:b:157:HIS:HA	2:b:163:GLY:HA3	1.83	0.59
18:2:64:TYR:OH	18:2:82:ARG:HG2	2.01	0.59
18:2:94:PHE:CE1	26:2:307:CLA:HBC3	2.37	0.59
26:5:605:CLA:C17	34:5:618:LHG:H261	2.27	0.59
22:6:115:VAL:HG13	22:6:216:MET:HE3	1.84	0.59
18:O:92:PHE:CE1	26:O:607:CLA:HBC3	2.37	0.59
26:P:610:CLA:HBC1	26:P:611:CLA:HMA1	1.85	0.59
34:N:621:LHG:C26	26:O:601:CLA:NC	2.55	0.59
18:2:137:TRP:CZ2	26:2:305:CLA:HBB1	2.38	0.59
20:4:134:GLN:HE21	39:4:320:II0:C23	2.15	0.59
26:4:306:CLA:CMB	26:5:611:CLA:CBA	2.64	0.59
26:4:312:CLA:CBB	39:4:314:II0:C20	2.79	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:G:154:LEU:HD22	26:P:603:CLA:H61	1.83	0.59
17:N:105:MET:HB3	17:N:125:MET:SD	2.43	0.59
20:4:133:GLN:O	20:4:134:GLN:C	2.43	0.59
21:5:191:LEU:HD21	39:5:613:II0:C27	2.31	0.59
26:5:605:CLA:HBB2	26:6:609:CLA:H72	1.79	0.59
19:P:86:GLY:HA3	19:P:185:CYS:HB3	1.84	0.59
20:Q:171:CYS:HB3	20:Q:181:ARG:NH1	2.17	0.59
21:R:181:TYR:HB3	26:R:309:CLA:HBB	1.84	0.59
26:R:304:CLA:HBC1	26:R:308:CLA:HAC1	1.84	0.59
19:3:198:GLN:OE1	26:3:308:CLA:MG	1.45	0.59
26:3:301:CLA:CMC	39:3:311:II0:C26	2.81	0.59
26:C:514:CLA:H61	22:6:166:LEU:HD12	1.85	0.59
17:N:53:ALA:HB3	26:N:601:CLA:O1D	2.03	0.59
20:4:80:TRP:CD2	24:g:127:GLN:HB3	2.38	0.59
21:5:58:THR:CB	24:g:119:THR:CG2	2.80	0.59
26:P:610:CLA:CBC	26:P:611:CLA:HMA1	2.32	0.59
20:Q:134:GLN:HE21	39:Q:319:II0:C23	2.15	0.59
24:g:105:LEU:O	24:g:109:SER:CB	2.51	0.59
3:c:179:LEU:HD21	26:c:508:CLA:HAB	1.85	0.59
20:4:75:ILE:HB	26:4:301:CLA:HMA2	1.85	0.59
22:6:97:ILE:HD12	22:6:98:ARG:N	2.17	0.59
41:L:207:HOH:O	11:M:3:VAL:HG21	2.01	0.59
33:M:101:LMG:H141	11:m:21:PHE:HD1	1.68	0.59
17:N:226:ASN:CA	38:N:612:KC2:O2A	2.50	0.59
38:N:610:KC2:CHD	39:N:617:II0:C18	2.80	0.59
19:3:86:GLY:HA3	19:3:185:CYS:HB3	1.84	0.59
26:P:601:CLA:HBC2	28:P:615:WVN:C12	2.33	0.59
2:B:330:MET:HG3	41:B:766:HOH:O	2.02	0.58
38:N:605:KC2:C4A	39:N:618:II0:C16	2.81	0.58
20:4:171:CYS:HB3	20:4:181:ARG:NH1	2.17	0.58
20:Q:201:HIS:HE1	40:Q:317:IHT:C38	2.16	0.58
2:B:27:THR:HG23	26:B:605:CLA:HAC1	1.86	0.58
2:B:28:ALA:HB2	2:B:107:LEU:HB2	1.85	0.58
3:C:332:LEU:HA	3:C:354:TYR:CD2	2.38	0.58
14:X:25:THR:OG1	26:N:603:CLA:H52	2.03	0.58
1:a:131:TRP:CH2	26:c:507:CLA:HAA2	2.38	0.58
1:a:145:VAL:O	1:a:148:THR:OG1	2.21	0.58
19:3:66:PRO:HD2	39:3:311:II0:C06	2.33	0.58
21:5:144:PHE:CZ	26:6:601:CLA:HAC1	2.39	0.58
21:5:178:LEU:HD12	26:5:608:CLA:HMA2	1.84	0.58
1:A:42:LEU:O	1:A:46:THR:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:40:ARG:HB3	9:K:45:ARG:HH12	1.68	0.58
9:k:24:ALA:N	9:k:25:PRO:HD2	2.18	0.58
18:2:96:MET:HE3	26:2:308:CLA:HMC3	1.86	0.58
2:B:30:VAL:HG12	26:B:605:CLA:HHD	1.86	0.58
2:B:153:PHE:HB2	26:B:606:CLA:HBB1	1.84	0.58
2:B:320:ALA:HB1	4:D:291:ASN:HD22	1.69	0.58
1:a:233:ALA:HB3	4:d:264:ARG:HH11	1.67	0.58
17:1:152:THR:CG2	26:2:301:CLA:CMC	2.80	0.58
26:1:606:CLA:CMA	26:2:311:CLA:CBD	2.81	0.58
21:5:58:THR:HB	24:g:119:THR:HG21	1.86	0.58
23:G:111:ALA:HA	23:G:114:GLN:HE21	1.68	0.58
18:O:68:PHE:CZ	40:O:616:IHT:C13	2.86	0.58
26:O:608:CLA:O1A	39:O:613:II0:C20	2.51	0.58
21:R:178:LEU:HD12	26:R:309:CLA:HMA2	1.84	0.58
2:b:70:GLY:HA2	2:b:178:VAL:HG11	1.86	0.58
2:b:478:VAL:HG21	4:d:136:GLY:O	2.04	0.58
17:N:151:LEU:HD23	18:O:71:LEU:CD1	2.30	0.58
17:N:213:VAL:HB	38:N:612:KC2:CED	2.32	0.58
20:4:57:LEU:HD21	26:4:302:CLA:HBD	1.86	0.58
13:W:43:VAL:CB	19:3:127:TRP:CZ3	2.86	0.58
26:b:605:CLA:HBC3	26:b:612:CLA:H42	1.86	0.58
3:c:311:TYR:O	3:c:437:ARG:NH2	2.36	0.58
8:i:6:ILE:HD12	13:w:38:LEU:HD23	1.84	0.58
17:N:225:PRO:CB	17:N:227:PHE:HB3	2.34	0.58
18:2:167:LEU:N	39:2:313:II0:O02	2.36	0.58
21:5:134:ILE:HA	26:5:605:CLA:HBC3	1.86	0.58
4:d:339:ILE:HA	41:d:530:HOH:O	2.04	0.58
23:G:100:TRP:HH2	26:R:308:CLA:H172	1.68	0.58
20:Q:76:ILE:HD12	26:Q:302:CLA:H11	1.84	0.58
3:C:475:ARG:HG2	41:C:649:HOH:O	2.03	0.58
41:L:207:HOH:O	11:M:3:VAL:CG2	2.52	0.58
33:d:404:LMG:H132	33:d:409:LMG:H312	1.86	0.58
29:d:407:PL9:H111	34:d:408:LHG:H102	1.86	0.58
17:1:155:PRO:HB2	18:2:54:LEU:CG	2.30	0.58
17:1:155:PRO:CB	18:2:54:LEU:HD21	2.26	0.58
18:2:196:GLY:O	18:2:197:PHE:C	2.45	0.58
21:5:55:LYS:HZ2	33:5:619:LMG:HC62	1.68	0.58
19:P:141:ASN:HB2	19:P:145:LEU:HD23	1.85	0.58
20:4:77:ASP:CB	24:g:127:GLN:O	2.51	0.58
26:4:306:CLA:CHB	26:5:611:CLA:O1A	2.52	0.58
21:5:75:PHE:CE1	33:5:619:LMG:H172	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:g:105:LEU:O	24:g:109:SER:HB2	2.03	0.58
1:A:81:ALA:HB2	41:A:522:HOH:O	2.03	0.58
1:A:145:VAL:O	1:A:148:THR:OG1	2.22	0.58
7:H:25:TRP:HB3	7:H:28:THR:OG1	2.04	0.58
1:a:81:ALA:HB2	41:a:527:HOH:O	2.03	0.58
1:a:227:THR:HG21	1:a:233:ALA:HA	1.86	0.58
17:N:126:MET:SD	40:N:619:IHT:C17	2.92	0.58
19:3:96:PHE:HE1	39:3:311:II0:C09	2.17	0.58
26:3:307:CLA:C3B	39:3:310:II0:C42	2.82	0.58
21:R:206:THR:HB	21:R:208:GLN:HB3	1.86	0.58
29:D:409:PL9:H111	34:D:410:LHG:H102	1.86	0.57
17:N:188:ARG:HB3	26:N:609:CLA:HNB	1.86	0.57
20:4:201:HIS:HE1	40:4:318:IHT:C38	2.16	0.57
26:O:608:CLA:H62	38:O:610:KC2:CMA	2.34	0.57
20:Q:67:PHE:CD2	39:Q:314:II0:C18	2.87	0.57
3:C:148:LEU:HD11	26:C:512:CLA:H92	1.85	0.57
34:1:620:LHG:C24	26:2:301:CLA:C1D	2.67	0.57
17:N:105:MET:HG2	17:N:125:MET:SD	2.44	0.57
19:3:196:LEU:HD22	28:3:313:WVN:C22	2.34	0.57
20:4:180:ARG:HH12	38:4:311:KC2:CBA	2.16	0.57
20:Q:145:PHE:CE1	21:R:72:PRO:HG2	2.39	0.57
22:S:183:PHE:CD2	39:S:611:II0:C08	2.88	0.57
3:C:179:LEU:HD21	26:C:507:CLA:HAB	1.85	0.57
3:C:229:LYS:HB3	3:C:237:TRP:HA	1.86	0.57
33:D:406:LMG:H132	33:D:411:LMG:H312	1.85	0.57
2:b:155:ALA:O	2:b:159:THR:OG1	2.21	0.57
17:N:78:PHE:CE2	26:N:602:CLA:H61	2.39	0.57
17:N:212:LEU:CD2	26:N:614:CLA:HED3	2.33	0.57
20:Q:57:LEU:HD21	26:Q:301:CLA:HBD	1.86	0.57
17:1:159:GLN:CD	18:2:55:LYS:HD2	2.28	0.57
26:1:606:CLA:NB	26:2:311:CLA:H11	2.19	0.57
17:N:110:VAL:HG23	17:N:218:ILE:HG13	1.86	0.57
18:2:153:LEU:HD11	24:g:169:ALA:CB	2.32	0.57
18:2:185:LYS:HG2	39:2:315:II0:C06	2.34	0.57
19:3:165:LEU:O	39:3:310:II0:O02	2.22	0.57
23:G:166:ILE:CG2	26:O:607:CLA:HBA1	2.34	0.57
18:O:94:MET:HE3	26:O:608:CLA:HMC3	1.86	0.57
17:N:73:PHE:CE1	26:N:601:CLA:HHD	2.40	0.57
38:4:310:KC2:C3D	38:4:311:KC2:C1D	2.83	0.57
38:Q:309:KC2:C3D	38:Q:310:KC2:C1D	2.83	0.57
26:Q:311:CLA:CBB	39:Q:313:II0:C20	2.79	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:262:ASN:OD1	4:d:264:ARG:HB2	2.04	0.57
14:x:25:THR:O	14:x:29:ILE:HG12	2.03	0.57
17:N:115:GLY:C	17:N:117:GLN:H	2.12	0.57
21:5:206:THR:HB	21:5:208:GLN:HB3	1.86	0.57
26:5:605:CLA:HBA2	26:6:609:CLA:O1A	2.04	0.57
22:S:138:ASP:O	22:S:142:VAL:HG23	2.04	0.57
7:h:56:GLU:CB	41:h:207:HOH:O	2.47	0.57
34:1:620:LHG:HC62	26:2:301:CLA:CAD	2.35	0.57
17:N:81:TRP:CE2	17:N:82:LEU:HD13	2.39	0.57
17:N:175:PRO:HD2	39:N:615:II0:C12	2.35	0.57
17:N:204:GLY:HA2	40:N:619:IHT:C39	2.35	0.57
17:N:220:PHE:HE1	38:N:612:KC2:CHB	2.15	0.57
18:2:83:VAL:CG2	24:g:169:ALA:O	2.49	0.57
26:2:308:CLA:H62	38:2:310:KC2:CMA	2.34	0.57
20:4:151:VAL:HA	24:g:125:VAL:HG21	1.87	0.57
22:6:106:LYS:O	22:6:110:VAL:HG23	2.05	0.57
24:g:167:LEU:C	26:g:402:CLA:O1A	2.48	0.57
21:R:134:ILE:HA	26:R:306:CLA:HBC3	1.86	0.57
26:B:605:CLA:HBC3	26:B:612:CLA:H42	1.86	0.57
3:C:291:VAL:HB	3:C:455:HIS:CG	2.39	0.57
2:b:330:MET:HG3	41:b:770:HOH:O	2.04	0.57
26:b:614:CLA:H2	28:b:617:WVN:C23	2.35	0.57
18:2:147:VAL:HG11	19:3:48:LEU:CD1	2.34	0.57
19:3:141:ASN:HB2	19:3:145:LEU:HD23	1.85	0.57
22:6:138:ASP:O	22:6:142:VAL:HG23	2.04	0.57
3:c:291:VAL:HB	3:c:455:HIS:CG	2.40	0.57
8:i:10:THR:HG23	13:w:45:ILE:HD11	1.85	0.57
17:1:152:THR:HG21	26:2:301:CLA:HMC3	1.86	0.57
17:N:78:PHE:CA	17:N:81:TRP:CZ3	2.85	0.57
21:5:67:ASP:HA	26:5:602:CLA:O1D	2.05	0.57
22:S:106:LYS:O	22:S:110:VAL:HG23	2.05	0.57
26:C:507:CLA:HBB2	26:C:508:CLA:H52	1.87	0.56
17:N:51:THR:HG22	26:N:601:CLA:HED2	1.86	0.56
19:P:41:ARG:NH2	19:P:49:GLU:OE1	2.38	0.56
2:B:80:ILE:HD13	2:B:93:PHE:CZ	2.35	0.56
2:B:478:VAL:HG22	2:B:482:ILE:HG22	1.87	0.56
1:a:223:LEU:CD1	4:d:264:ARG:HD2	2.30	0.56
17:N:81:TRP:CE2	17:N:82:LEU:CB	2.88	0.56
19:3:128:GLN:NE2	38:3:304:KC2:O1D	2.39	0.56
21:5:58:THR:CB	24:g:119:THR:HG23	2.35	0.56
26:a:402:CLA:HMC3	26:d:405:CLA:HBC3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:30:VAL:HG12	26:b:605:CLA:HHD	1.86	0.56
26:c:508:CLA:HBB2	26:c:509:CLA:H52	1.87	0.56
17:1:191:VAL:HG11	38:1:611:KC2:CHA	2.35	0.56
34:1:620:LHG:C26	26:2:301:CLA:NC	2.55	0.56
17:N:209:HIS:HD2	38:N:612:KC2:ND	2.01	0.56
26:2:311:CLA:CBC	39:2:315:II0:C33	2.82	0.56
26:3:307:CLA:H72	26:4:308:CLA:CBA	2.35	0.56
19:P:155:ARG:HH12	19:P:160:LEU:HD23	1.69	0.56
26:Q:305:CLA:CMB	26:R:312:CLA:HBA2	2.35	0.56
26:Q:308:CLA:O2D	21:R:42:VAL:HB	2.05	0.56
4:D:188:HIS:HA	4:D:293:ARG:HD2	1.88	0.56
17:N:70:ASP:HA	26:N:602:CLA:O1D	2.06	0.56
17:N:129:HIS:O	17:N:129:HIS:CG	2.58	0.56
19:3:155:ARG:HH12	19:3:160:LEU:HD23	1.69	0.56
18:O:133:ILE:HD13	18:O:136:ILE:HD11	1.88	0.56
11:M:35:ALA:HB3	11:m:35:ALA:HB3	1.86	0.56
17:N:86:TRP:NE1	26:N:603:CLA:CGA	2.68	0.56
26:N:603:CLA:HAB	39:N:616:II0:C42	2.35	0.56
18:2:83:VAL:CG1	26:2:307:CLA:HED1	2.32	0.56
22:6:190:LYS:HE2	22:6:190:LYS:HA	1.87	0.56
26:P:608:CLA:HBA1	26:Q:302:CLA:H43	1.87	0.56
21:R:67:ASP:HA	26:R:303:CLA:O1D	2.05	0.56
2:B:414:ALA:N	2:B:415:PRO:HD2	2.20	0.56
3:C:355:LEU:HD22	3:C:363:ILE:HD11	1.88	0.56
17:N:53:ALA:HB1	26:N:601:CLA:HMA2	1.87	0.56
18:2:147:VAL:HG12	19:3:48:LEU:CD1	2.36	0.56
26:Q:306:CLA:HMD3	33:Q:318:LMG:HC8	1.87	0.56
21:R:92:GLY:HA3	21:R:189:SER:HB3	1.87	0.56
2:B:311:PHE:O	2:B:317:ASN:ND2	2.38	0.56
4:D:229[B]:ASN:OD1	4:D:231:PHE:HD2	1.89	0.56
1:a:279:PRO:HG2	4:d:211:ALA:HB2	1.88	0.56
17:N:71:VAL:HG11	26:N:601:CLA:CAD	2.35	0.56
17:N:159:GLN:HE21	18:O:53:LYS:CD	2.13	0.56
34:N:621:LHG:HC62	26:O:601:CLA:CAD	2.35	0.56
26:2:303:CLA:H151	33:2:318:LMG:C37	2.36	0.56
39:P:613:II0:C15	28:P:615:WVN:C07	2.83	0.56
1:A:170:ASP:OD2	3:C:371:ARG:NH1	2.35	0.56
17:1:196:GLY:O	17:1:200:MET:HG2	2.06	0.56
17:N:42:ARG:NH2	38:N:610:KC2:O1A	2.39	0.56
17:N:63:LEU:HD11	17:N:74:ASP:HB2	1.88	0.56
17:N:138:MET:HE3	26:N:607:CLA:C4C	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:225:PRO:C	38:N:612:KC2:O2A	2.48	0.56
18:2:188:ARG:HB2	39:2:315:II0:C17	2.36	0.56
19:3:41:ARG:NH2	19:3:49:GLU:OE1	2.38	0.56
22:6:101:ARG:HH21	22:6:203:VAL:HG11	1.71	0.56
19:P:128:GLN:NE2	38:P:605:KC2:O1D	2.38	0.56
20:Q:180:ARG:HH12	38:Q:310:KC2:CBA	2.16	0.56
22:S:138:ASP:HA	22:S:141:VAL:HG22	1.88	0.56
1:a:170:ASP:OD2	3:c:371:ARG:NH1	2.35	0.56
26:2:308:CLA:C4	38:2:310:KC2:CMA	2.70	0.56
26:O:601:CLA:CHD	40:O:616:IHT:C04	2.83	0.56
22:S:101:ARG:NH2	22:S:203:VAL:HG11	2.21	0.56
3:c:168:LYS:NZ	41:c:605:HOH:O	2.30	0.56
20:4:75:ILE:O	24:g:128:VAL:CG1	2.54	0.56
26:4:301:CLA:C1	26:4:303:CLA:C1	2.71	0.56
23:G:142:ALA:HB1	19:P:76:LYS:HD3	1.87	0.56
26:R:306:CLA:H192	34:R:319:LHG:H261	1.87	0.56
2:B:135:LEU:HB2	2:B:136:PRO:HD3	1.88	0.55
5:e:50:THR:O	41:e:103:HOH:O	2.18	0.55
22:S:101:ARG:HH21	22:S:203:VAL:HG11	1.71	0.55
17:1:42:ARG:HD2	17:1:43:GLU:HG3	1.87	0.55
26:N:603:CLA:HMB2	39:N:616:II0:C34	2.37	0.55
34:N:621:LHG:H331	26:O:601:CLA:HBB2	1.89	0.55
21:5:92:GLY:HA3	21:5:189:SER:HB3	1.87	0.55
19:P:199:MET:HG2	19:P:204:GLN:O	2.07	0.55
20:Q:138:TRP:HZ2	39:Q:319:II0:C39	2.19	0.55
22:S:190:LYS:HE2	22:S:190:LYS:HA	1.87	0.55
4:D:334:PRO:HB2	5:E:66:LEU:HD21	1.89	0.55
17:N:113:PHE:CD2	38:N:605:KC2:CMC	2.89	0.55
17:N:202:ALA:HB1	39:N:615:II0:C23	2.36	0.55
17:N:223:ASN:O	17:N:223:ASN:ND2	2.37	0.55
19:3:64:PHE:CZ	39:3:311:II0:C17	2.90	0.55
20:4:135:LEU:HB3	26:4:307:CLA:HBC1	1.86	0.55
17:N:213:VAL:CB	38:N:612:KC2:CED	2.83	0.55
20:4:138:TRP:CZ2	39:4:320:II0:C35	2.89	0.55
34:5:618:LHG:H121	26:6:601:CLA:C1C	2.36	0.55
22:6:138:ASP:HA	22:6:141:VAL:HG22	1.88	0.55
20:Q:203:PHE:O	20:Q:204:PHE:C	2.49	0.55
17:1:44:GLY:O	17:1:51:THR:OG1	2.18	0.55
17:N:129:HIS:HE1	26:N:607:CLA:C1A	2.20	0.55
26:2:304:CLA:H192	39:2:316:II0:C17	2.37	0.55
26:4:307:CLA:HMD3	33:4:319:LMG:HC8	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Q:80:TRP:CD2	26:Q:307:CLA:HED1	2.42	0.55
28:B:617:WVN:C23	28:B:617:WVN:C17	2.85	0.55
1:a:140:ARG:HB2	4:d:219:ASN:HA	1.89	0.55
2:b:458:PHE:HB3	26:b:604:CLA:HBC2	1.89	0.55
17:1:108:GLN:OE1	26:1:604:CLA:NA	2.39	0.55
17:N:225:PRO:HB2	17:N:227:PHE:HB3	1.88	0.55
18:2:60:LEU:HD21	18:2:71:ASP:HB2	1.89	0.55
18:2:135:ILE:HD13	18:2:138:ILE:HD11	1.88	0.55
26:2:312:CLA:HAC2	40:2:317:IHT:C20	2.36	0.55
22:6:101:ARG:NH2	22:6:203:VAL:HG11	2.21	0.55
23:G:167:LEU:HD21	26:O:607:CLA:C2	2.35	0.55
26:G:401:CLA:HBC3	26:G:401:CLA:H71	1.89	0.55
26:O:603:CLA:H151	33:O:617:LMG:C37	2.36	0.55
1:a:257:ARG:C	41:a:505:HOH:O	2.48	0.55
4:d:188:HIS:HA	4:d:293:ARG:HD2	1.87	0.55
17:1:115:GLY:O	17:1:117:GLN:N	2.34	0.55
17:1:210:TYR:CE1	17:1:215:ARG:HA	2.37	0.55
26:1:606:CLA:C1B	26:2:311:CLA:HBA2	2.34	0.55
19:3:199:MET:HG2	19:3:204:GLN:O	2.07	0.55
1:A:279:PRO:HG2	4:D:211:ALA:HB2	1.89	0.55
2:B:256:MET:HA	2:B:263:THR:HG21	1.89	0.55
5:E:36:TRP:HA	6:F:36:SER:HB2	1.88	0.55
2:b:128:THR:OG1	2:b:130:ASN:ND2	2.40	0.55
17:1:155:PRO:C	18:2:54:LEU:HD22	2.32	0.55
17:N:190:LEU:HD11	17:N:194:LYS:HE3	1.88	0.55
26:N:604:CLA:CMB	39:N:616:II0:C19	2.85	0.55
21:5:171:GLN:O	21:5:175:ALA:N	2.39	0.55
18:O:141:LEU:HD12	18:O:141:LEU:N	2.21	0.55
19:P:77:TRP:CE3	19:P:147:PRO:HA	2.42	0.55
20:Q:69:PRO:HD2	39:Q:314:II0:C08	2.37	0.55
21:R:171:GLN:O	21:R:175:ALA:N	2.39	0.55
26:R:306:CLA:C17	34:R:319:LHG:H261	2.34	0.55
34:R:319:LHG:H121	26:S:601:CLA:C1C	2.36	0.55
3:C:311:TYR:O	3:C:437:ARG:NH2	2.36	0.55
4:D:27:VAL:HB	6:F:15:PHE:HZ	1.71	0.55
5:E:23:ILE:H	5:E:23:ILE:HD12	1.72	0.55
17:N:132:ALA:O	17:N:134:ASP:N	2.40	0.55
17:N:141:LEU:HD23	26:N:606:CLA:HBC3	1.87	0.55
17:N:152:THR:CG2	34:N:621:LHG:C35	2.85	0.55
17:N:226:ASN:HA	38:N:612:KC2:O2A	2.05	0.55
20:4:67:PHE:CD2	39:4:315:II0:C18	2.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4:80:TRP:CD2	26:4:308:CLA:HED1	2.42	0.55
21:5:75:PHE:CD1	33:5:619:LMG:H172	2.42	0.55
39:P:613:II0:C19	39:P:613:II0:C23	2.85	0.55
2:B:74:SER:HA	2:B:92:SER:HB2	1.89	0.55
17:N:73:PHE:CD1	26:N:601:CLA:HMD1	2.42	0.55
26:2:306:CLA:H71	26:2:312:CLA:HBC1	1.89	0.55
19:3:77:TRP:CE3	19:3:147:PRO:HA	2.41	0.55
26:3:307:CLA:HMD2	26:4:303:CLA:C9	2.34	0.55
21:5:196:PHE:O	21:5:197:SER:C	2.48	0.55
22:6:177:GLU:HG2	22:6:178:ALA:N	2.21	0.55
26:G:401:CLA:H91	21:R:143:ILE:HD11	1.88	0.55
2:b:42:LEU:HD13	2:b:94:GLU:HG3	1.89	0.54
2:b:330:MET:HA	2:b:444:ARG:HB2	1.88	0.54
17:1:151:LEU:HD13	26:2:301:CLA:HBC1	1.89	0.54
17:1:187:ARG:NH2	38:1:611:KC2:OBD	2.41	0.54
34:1:620:LHG:H331	26:2:301:CLA:HBB2	1.89	0.54
18:2:79:PHE:HB3	24:g:170:TRP:HE3	1.72	0.54
20:4:77:ASP:CA	24:g:127:GLN:O	2.54	0.54
23:G:122:TRP:NE1	19:P:166:ASN:O	2.40	0.54
1:A:136:ARG:O	8:I:32:PRO:HD3	2.07	0.54
14:X:4:SER:HB2	41:X:101:HOH:O	2.07	0.54
2:b:256:MET:HA	2:b:263:THR:HG21	1.89	0.54
2:b:390:TYR:HD2	4:d:343:GLU:OE2	1.89	0.54
5:e:62:GLN:NE2	41:e:102:HOH:O	1.98	0.54
18:2:60:LEU:HD11	18:2:76:SER:CB	2.37	0.54
20:4:155:GLN:HE22	33:5:619:LMG:C7	2.14	0.54
20:Q:180:ARG:HH11	38:Q:310:KC2:CBA	2.20	0.54
2:B:103:LEU:HD21	26:B:605:CLA:HMC2	1.90	0.54
2:B:330:MET:HA	2:B:444:ARG:HB2	1.88	0.54
6:F:14:THR:HG23	6:F:17:TRP:H	1.71	0.54
34:1:620:LHG:H261	26:2:301:CLA:C4C	2.35	0.54
40:2:317:IHT:C16	40:2:317:IHT:C24	2.85	0.54
19:3:45:MET:SD	19:3:66:PRO:HB3	2.47	0.54
19:3:162:PHE:HE2	39:3:310:II0:C22	2.21	0.54
19:3:189:MET:CB	39:3:311:II0:C42	2.85	0.54
20:4:114:PHE:O	21:5:229:PHE:O	2.24	0.54
2:B:458:PHE:HB3	26:B:604:CLA:HBC2	1.89	0.54
3:C:168:LYS:NZ	41:C:605:HOH:O	2.30	0.54
26:a:402:CLA:H151	26:d:402:CLA:H151	1.90	0.54
33:a:413:LMG:H362	35:c:519:DGD:C8A	2.37	0.54
34:d:408:LHG:O1	34:l:101:LHG:O4	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:137:GLU:HG3	26:3:305:CLA:NB	2.22	0.54
26:O:605:CLA:CBA	26:P:610:CLA:HBD	2.38	0.54
19:P:137:GLU:HG3	26:P:606:CLA:NB	2.23	0.54
28:B:617:WVN:C08	28:B:617:WVN:C09	2.85	0.54
3:c:51:SER:OG	26:c:510:CLA:O1D	2.25	0.54
26:1:606:CLA:C3C	26:2:311:CLA:C4	2.86	0.54
26:N:614:CLA:HAC2	40:N:619:IHT:C24	2.37	0.54
34:N:621:LHG:H241	26:O:601:CLA:CHD	2.35	0.54
18:2:141:VAL:HG22	34:2:321:LHG:H332	1.87	0.54
26:4:306:CLA:CMB	26:5:611:CLA:NA	2.71	0.54
22:6:136:VAL:HG11	22:6:221:LEU:HD21	1.89	0.54
18:O:58:LEU:HD21	18:O:69:ASP:HB2	1.89	0.54
3:C:59:VAL:CG2	3:C:62:LYS:HB2	2.37	0.54
7:h:25:TRP:HB3	7:h:28:THR:OG1	2.08	0.54
17:N:116:VAL:HG13	17:N:120:PHE:HD2	1.72	0.54
34:N:621:LHG:H261	26:O:601:CLA:C4C	2.35	0.54
18:2:192:ILE:HD13	39:2:315:II0:C34	2.38	0.54
39:3:311:II0:C19	39:3:311:II0:C23	2.85	0.54
26:4:306:CLA:C4A	26:5:611:CLA:O1A	2.56	0.54
26:R:309:CLA:H71	38:R:311:KC2:CMA	2.38	0.54
2:B:446:SER:CB	41:B:709:HOH:O	2.52	0.54
2:B:461:LEU:HD13	26:B:613:CLA:H111	1.90	0.54
28:B:618:WVN:C08	28:B:618:WVN:C09	2.86	0.54
34:D:410:LHG:O1	34:L:101:LHG:O4	2.23	0.54
17:N:220:PHE:CE1	38:N:612:KC2:NA	2.75	0.54
39:3:312:II0:C23	39:3:312:II0:C16	2.85	0.54
20:4:80:TRP:CD2	24:g:127:GLN:CB	2.91	0.54
22:6:108:GLY:O	22:6:112:MET:HG3	2.08	0.54
20:Q:182:GLN:N	26:Q:308:CLA:HMA1	2.23	0.54
26:R:306:CLA:HBB2	34:R:319:LHG:C29	2.37	0.54
3:C:470:GLU:OE2	3:C:471:LYS:NZ	2.35	0.54
26:N:614:CLA:HAC2	40:N:619:IHT:C29	2.37	0.54
18:2:143:LEU:HD12	18:2:143:LEU:N	2.21	0.54
18:2:166:PRO:HD2	39:2:313:II0:C12	2.37	0.54
22:6:225:GLN:OE1	22:6:230:GLN:HA	2.08	0.54
20:Q:109:GLY:HA3	38:Q:304:KC2:NA	2.23	0.54
20:Q:151:VAL:HG11	33:R:301:LMG:HC91	1.90	0.54
26:R:306:CLA:H203	34:R:319:LHG:H252	1.90	0.54
26:R:306:CLA:H143	26:S:609:CLA:H71	1.89	0.54
22:S:136:VAL:HG11	22:S:221:LEU:HD21	1.89	0.54
34:1:620:LHG:C14	40:2:317:IHT:C09	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:43:GLU:HB3	17:N:45:VAL:HG12	1.90	0.54
18:2:84:LEU:HD21	24:g:170:TRP:CZ3	2.38	0.54
19:3:89:CYS:SG	19:3:189:MET:HA	2.48	0.54
26:3:307:CLA:CED	26:4:303:CLA:HED2	2.34	0.54
39:3:310:II0:C19	39:3:310:II0:C23	2.85	0.54
18:O:58:LEU:HD11	18:O:74:SER:CB	2.37	0.54
18:O:81:VAL:CG1	26:O:607:CLA:HED1	2.32	0.54
2:B:369:ILE:HD11	4:D:344:VAL:HG11	1.90	0.54
17:1:102:ALA:O	17:1:106:ILE:HG23	2.08	0.54
17:1:148:LEU:HD13	34:1:620:LHG:H311	1.89	0.54
20:4:180:ARG:NH1	38:4:311:KC2:CBD	2.71	0.54
20:4:203:PHE:O	20:4:204:PHE:C	2.49	0.54
26:O:606:CLA:H71	26:O:612:CLA:HBC1	1.89	0.54
19:P:45:MET:SD	19:P:66:PRO:HB3	2.47	0.54
20:Q:135:LEU:HB3	26:Q:306:CLA:HBC1	1.86	0.54
20:Q:178:LEU:HD12	26:Q:308:CLA:HMA2	1.90	0.54
26:1:606:CLA:C1C	26:2:311:CLA:C4	2.69	0.53
17:N:53:ALA:HB3	26:N:601:CLA:H2A	1.89	0.53
17:N:138:MET:HE3	26:N:607:CLA:C3C	2.38	0.53
26:2:311:CLA:HBC3	39:2:315:II0:C33	2.38	0.53
20:4:155:GLN:N	24:g:125:VAL:CG1	2.71	0.53
26:4:306:CLA:H3A	26:5:611:CLA:CBD	2.38	0.53
21:5:58:THR:HB	24:g:119:THR:CG2	2.38	0.53
19:P:89:CYS:SG	19:P:189:MET:HA	2.49	0.53
26:R:306:CLA:HBB1	26:S:609:CLA:C6	2.38	0.53
22:S:225:GLN:OE1	22:S:230:GLN:HA	2.08	0.53
1:A:136:ARG:HH22	8:I:27:ASP:CG	2.14	0.53
18:2:147:VAL:HG11	19:3:48:LEU:HD11	1.90	0.53
23:G:105:LEU:HB2	23:G:106:PRO:HD3	1.90	0.53
21:R:140:PHE:CE2	26:S:601:CLA:HBC1	2.42	0.53
4:D:179:ARG:NE	4:D:332:ASP:OD1	2.41	0.53
13:W:40:VAL:HA	19:3:127:TRP:CH2	2.44	0.53
2:b:475:PHE:CE2	4:d:139:PRO:HB3	2.44	0.53
3:c:201:ASP:O	3:c:208:GLY:HA2	2.08	0.53
33:c:521:LMG:H142	33:c:521:LMG:H321	1.90	0.53
34:1:620:LHG:C33	26:2:301:CLA:HBB2	2.38	0.53
17:N:113:PHE:O	17:N:114:PRO:C	2.48	0.53
34:N:621:LHG:C33	26:O:601:CLA:HBB2	2.38	0.53
19:3:211:ALA:O	19:3:212:ASN:C	2.51	0.53
20:4:182:GLN:N	26:4:309:CLA:HMA1	2.23	0.53
1:A:223:LEU:CD1	4:D:264:ARG:HD2	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:VAL:HG23	26:B:606:CLA:HMA2	1.90	0.53
2:B:356:VAL:HG22	2:B:370:LEU:HG	1.89	0.53
2:b:153:PHE:HB2	26:b:606:CLA:HBB1	1.90	0.53
2:b:223:GLN:NE2	2:b:227:ARG:NH2	2.56	0.53
18:2:97:LEU:HD12	39:2:316:II0:C28	2.39	0.53
18:2:137:TRP:HZ3	34:2:321:LHG:H372	1.56	0.53
20:Q:180:ARG:NH1	38:Q:310:KC2:CBD	2.71	0.53
3:C:351:LEU:HD12	3:C:355:LEU:HD13	1.89	0.53
3:c:374:ASP:CB	41:c:607:HOH:O	2.50	0.53
17:N:67:LEU:HB2	26:N:602:CLA:HED2	1.90	0.53
19:3:162:PHE:CZ	26:3:303:CLA:H141	2.44	0.53
19:P:162:PHE:CZ	26:P:604:CLA:H141	2.44	0.53
24:g:163:LYS:CG	26:g:402:CLA:CMA	2.84	0.53
3:C:374:ASP:CB	41:C:607:HOH:O	2.50	0.53
4:D:348:GLY:HA2	4:D:351:LEU:HD12	1.89	0.53
7:H:10:LEU:HD11	23:G:162:TRP:HH2	1.73	0.53
13:W:63:GLU:O	13:W:72:ARG:NH2	2.34	0.53
1:a:133:PHE:CE2	4:d:254:GLN:HB2	2.44	0.53
2:b:320:ALA:HB1	4:d:291:ASN:HD22	1.73	0.53
26:2:308:CLA:H91	38:2:310:KC2:CMB	2.38	0.53
20:4:75:ILE:O	24:g:128:VAL:HG13	2.09	0.53
20:4:80:TRP:HB2	24:g:127:GLN:CB	2.31	0.53
20:4:129:GLN:CG	21:5:228:PHE:CE2	2.92	0.53
20:4:155:GLN:HA	24:g:123:PHE:CZ	2.43	0.53
20:4:169:LEU:HD23	39:4:314:II0:C05	2.39	0.53
17:1:152:THR:CG2	26:2:301:CLA:HMC3	2.39	0.53
26:3:307:CLA:CMC	39:3:310:II0:C31	2.87	0.53
26:4:306:CLA:O1A	21:5:220:ILE:N	2.34	0.53
22:6:217:LEU:C	22:6:217:LEU:HD23	2.34	0.53
2:B:391:SER:HB3	2:B:394:GLN:HG3	1.91	0.53
4:D:264:ARG:NH2	34:D:403:LHG:O2	2.42	0.53
1:a:53:ILE:O	1:a:70:SER:OG	2.27	0.53
2:b:368:VAL:HG21	2:b:422:ARG:HG2	1.91	0.53
20:4:109:GLY:HA3	38:4:305:KC2:NA	2.23	0.53
20:4:178:LEU:HD12	26:4:309:CLA:HMA2	1.90	0.53
26:5:608:CLA:H71	38:5:610:KC2:CMA	2.38	0.53
20:Q:180:ARG:NH1	38:Q:310:KC2:CGA	2.72	0.53
1:A:25:GLU:HA	3:C:484:ARG:HH22	1.74	0.53
2:B:135:LEU:N	2:B:136:PRO:CD	2.72	0.53
17:1:144:TRP:CH2	34:1:620:LHG:H151	2.44	0.53
18:2:70:PHE:HE1	40:2:317:IHT:C13	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Q:72:PHE:CG	26:Q:301:CLA:H42	2.44	0.53
28:B:618:WVN:C14	28:B:618:WVN:C18	2.85	0.53
5:E:23:ILE:HD12	5:E:23:ILE:N	2.22	0.53
17:N:211:LEU:CD1	26:N:614:CLA:CMD	2.87	0.53
19:3:176:ARG:HD3	24:g:130:GLU:HA	1.90	0.53
26:3:307:CLA:HBC1	26:4:303:CLA:C12	2.39	0.53
21:5:78:VAL:O	24:g:112:TYR:HD1	1.91	0.53
26:5:605:CLA:H203	34:5:618:LHG:H261	1.90	0.53
18:O:66:VAL:CG2	26:O:602:CLA:HMD3	2.39	0.53
20:Q:169:LEU:HD23	39:Q:313:II0:C05	2.39	0.53
21:R:196:PHE:O	21:R:197:SER:C	2.48	0.53
13:W:51:LEU:CD2	26:3:305:CLA:HBA1	2.39	0.52
14:X:32:GLN:HB3	17:N:81:TRP:HB2	1.87	0.52
1:a:131:TRP:HZ2	3:c:463:ARG:HG3	1.74	0.52
7:h:54:ILE:HD12	7:h:54:ILE:N	2.25	0.52
9:k:18:LYS:N	9:k:19:PRO:HD2	2.24	0.52
17:N:74:ASP:OD2	17:N:77:GLY:CA	2.57	0.52
17:N:101:ALA:HB2	26:N:604:CLA:CBB	2.39	0.52
17:N:226:ASN:HB3	26:N:613:CLA:HED3	1.90	0.52
18:2:78:VAL:O	24:g:172:PRO:HA	2.08	0.52
26:3:307:CLA:HMC1	39:3:310:II0:C31	2.39	0.52
20:4:64:ASP:HA	26:4:302:CLA:O1D	2.09	0.52
20:4:75:ILE:CD1	26:4:301:CLA:HBB	2.38	0.52
20:Q:168:PRO:HG2	20:Q:169:LEU:HD22	1.92	0.52
22:S:217:LEU:HD23	22:S:217:LEU:C	2.34	0.52
2:B:142:HIS:HE1	26:B:610:CLA:H202	1.74	0.52
3:C:177:ILE:HD13	26:C:513:CLA:HAB	1.92	0.52
3:c:177:ILE:HD13	26:c:514:CLA:HAB	1.91	0.52
4:d:235:THR:OG1	4:d:238:GLN:HG3	2.09	0.52
17:N:53:ALA:HB1	26:N:601:CLA:CMA	2.39	0.52
17:N:226:ASN:HB3	26:N:613:CLA:HED2	1.91	0.52
18:2:149:LEU:O	18:2:152:THR:N	2.43	0.52
20:4:180:ARG:NH1	38:4:311:KC2:CGA	2.72	0.52
21:5:80:ASP:H	24:g:111:ALA:CB	2.12	0.52
18:O:147:LEU:O	18:O:150:THR:N	2.43	0.52
26:O:602:CLA:HBB2	26:O:603:CLA:C1B	2.39	0.52
21:R:99:THR:HG23	21:R:199:PHE:CE2	2.43	0.52
26:R:306:CLA:HBA2	26:S:609:CLA:O1A	2.09	0.52
1:A:131:TRP:HZ2	3:C:463:ARG:HG3	1.74	0.52
2:B:154:GLY:O	2:B:159:THR:HG23	2.09	0.52
4:d:338:PHE:N	41:d:508:HOH:O	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1:124:SER:O	17:1:128:LEU:HG	2.09	0.52
17:N:91:GLU:OE1	17:N:193:LEU:HD11	2.10	0.52
21:5:99:THR:HG23	21:5:199:PHE:CE2	2.43	0.52
2:B:150:CYS:HB2	26:B:603:CLA:CMC	2.40	0.52
2:b:471:SER:HB2	4:d:139:PRO:HG2	1.92	0.52
13:w:56:PHE:O	13:w:60:GLN:HG2	2.10	0.52
17:N:74:ASP:OD1	39:N:616:II0:O02	2.28	0.52
18:2:156:LYS:HB3	19:3:49:GLU:OE1	2.09	0.52
20:Q:64:ASP:HA	26:Q:301:CLA:O1D	2.09	0.52
26:A:402:CLA:H151	26:D:404:CLA:H151	1.91	0.52
17:1:47:GLN:NE2	17:1:69:GLY:H	2.08	0.52
17:N:152:THR:OG1	18:O:51:PHE:CZ	2.33	0.52
17:N:208:HIS:CD2	26:N:614:CLA:NA	2.78	0.52
18:2:83:VAL:HG21	24:g:169:ALA:HB1	1.89	0.52
20:4:72:PHE:CG	26:4:302:CLA:H42	2.44	0.52
26:6:603:CLA:HBB1	26:6:610:CLA:H122	1.92	0.52
21:R:201:HIS:HE1	40:R:317:IHT:C38	2.22	0.52
22:S:104:GLU:OE2	22:S:207:ARG:NE	2.35	0.52
22:S:108:GLY:O	22:S:112:MET:HG3	2.08	0.52
1:A:133:PHE:CE2	4:D:254:GLN:HB2	2.45	0.52
1:a:293:MET:HG2	1:a:298:ASN:HA	1.92	0.52
26:1:606:CLA:NC	26:2:311:CLA:C4	2.57	0.52
17:N:54:ILE:HG22	17:N:55:PRO:HD2	1.92	0.52
17:N:54:ILE:CD1	17:N:73:PHE:HA	2.40	0.52
17:N:125:MET:SD	17:N:217:PRO:HD3	2.50	0.52
20:4:80:TRP:CH2	26:4:308:CLA:HAA2	2.45	0.52
26:5:605:CLA:H203	34:5:618:LHG:C26	2.38	0.52
2:b:57:ARG:NH2	2:b:334:ASP:OD1	2.39	0.52
2:b:311:PHE:O	2:b:317:ASN:ND2	2.43	0.52
26:1:606:CLA:CMA	26:2:311:CLA:HBD	2.39	0.52
26:1:606:CLA:C2C	26:2:311:CLA:C4	2.88	0.52
19:3:129:ILE:HD11	26:3:303:CLA:HBA1	1.92	0.52
22:6:186:LEU:O	39:6:611:II0:O02	2.28	0.52
26:O:608:CLA:H91	38:O:610:KC2:CMB	2.38	0.52
26:A:402:CLA:HMC3	26:D:407:CLA:HBC3	1.91	0.52
3:C:51:SER:OG	26:C:509:CLA:O1D	2.25	0.52
33:D:406:LMG:HC3	33:D:411:LMG:HC3	1.92	0.52
7:H:61:ASP:OD1	35:H:102:DGD:O4E	2.27	0.52
1:a:82:VAL:HB	1:a:174:LEU:HB2	1.91	0.52
17:1:144:TRP:CZ3	34:1:620:LHG:C17	2.79	0.52
26:1:606:CLA:H11	18:2:215:PHE:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:116:VAL:O	17:N:119:THR:O	2.28	0.52
18:2:83:VAL:HG12	24:g:170:TRP:CE3	2.43	0.52
23:G:167:LEU:HD23	26:O:607:CLA:O1A	2.10	0.52
19:P:211:ALA:O	19:P:212:ASN:C	2.51	0.52
26:S:603:CLA:HBB1	26:S:610:CLA:H122	1.92	0.52
3:C:201:ASP:O	3:C:208:GLY:HA2	2.08	0.52
3:C:475:ARG:CG	41:C:649:HOH:O	2.57	0.52
1:a:21:ILE:HG21	1:a:32:TRP:CE3	2.45	0.52
6:f:14:THR:H	6:f:17:TRP:HB3	1.74	0.52
17:N:54:ILE:HG12	26:N:601:CLA:C1D	2.40	0.52
17:N:84:LEU:HA	17:N:87:ALA:CB	2.26	0.52
17:N:126:MET:HE1	17:N:207:VAL:HG13	1.90	0.52
26:N:604:CLA:C3B	39:N:616:II0:C19	2.88	0.52
18:2:68:VAL:HG22	26:2:302:CLA:HMD1	1.92	0.52
26:2:303:CLA:CBC	26:2:307:CLA:HAC1	2.39	0.52
23:G:143:PRO:HG2	19:P:75:LEU:HB2	1.92	0.52
4:D:258:VAL:HG21	34:D:410:LHG:H291	1.91	0.52
9:k:27:ILE:HD11	15:y:16:ILE:HD13	1.91	0.52
17:1:155:PRO:CB	18:2:54:LEU:CD1	2.88	0.52
17:N:215:ARG:NH2	17:N:215:ARG:HB2	2.25	0.52
26:2:302:CLA:HBB2	26:2:303:CLA:C1B	2.39	0.52
19:3:138:ILE:HA	19:3:145:LEU:HD21	1.91	0.52
21:5:189:SER:O	21:5:190:ARG:C	2.52	0.52
2:B:222:PRO:HB3	7:H:25:TRP:C	2.35	0.51
3:C:141:PHE:CG	33:C:520:LMG:H292	2.45	0.51
20:4:119:MET:CE	20:4:200:LEU:HD23	2.40	0.51
20:4:148:VAL:HG22	21:5:73:LEU:HD23	1.91	0.51
26:O:603:CLA:CBC	26:O:607:CLA:HAC1	2.39	0.51
19:P:129:ILE:HD11	26:P:604:CLA:HBA1	1.92	0.51
21:R:55:LYS:NZ	33:R:301:LMG:HC62	2.25	0.51
2:B:425:GLN:NE2	41:B:725:HOH:O	2.43	0.51
3:C:193:ALA:HA	3:C:199:LEU:HG	1.92	0.51
2:b:241:SER:O	2:b:245:VAL:CG2	2.51	0.51
2:b:434:ARG:NH2	41:b:713:HOH:O	2.17	0.51
3:c:331:PHE:HB2	3:c:354:TYR:CE1	2.43	0.51
4:d:343:GLU:CG	41:d:504:HOH:O	2.38	0.51
19:P:84:LYS:HD2	26:P:606:CLA:C3D	2.40	0.51
20:Q:119:MET:HE1	20:Q:200:LEU:HD23	1.92	0.51
26:Q:305:CLA:HMA1	26:R:312:CLA:CAD	2.40	0.51
21:R:75:PHE:CE1	33:R:301:LMG:H172	2.45	0.51
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:470:GLU:OE2	3:c:471:LYS:NZ	2.36	0.51
17:N:195:ASN:HD22	17:N:195:ASN:H	1.57	0.51
19:P:64:PHE:CD1	19:P:66:PRO:HD3	2.45	0.51
3:C:228:LEU:HB3	13:W:30:ALA:O	2.09	0.51
9:k:26:VAL:HG13	9:k:30:PHE:CE2	2.46	0.51
10:l:19:PHE:CE2	12:t:20:ALA:HA	2.45	0.51
19:P:138:ILE:HA	19:P:145:LEU:HD21	1.91	0.51
20:Q:119:MET:CE	20:Q:200:LEU:HD23	2.40	0.51
22:S:175:GLY:O	22:S:176:ARG:HG2	2.11	0.51
26:B:614:CLA:H11	33:m:101:LMG:O10	2.11	0.51
26:C:507:CLA:HMC2	26:C:508:CLA:H101	1.93	0.51
11:M:3:VAL:HG12	11:M:4:SER:N	2.25	0.51
4:d:128:GLN:HB2	4:d:142:ALA:HB2	1.91	0.51
17:N:101:ALA:HA	26:N:604:CLA:CAB	2.40	0.51
26:N:606:CLA:HBB2	34:N:621:LHG:H141	1.93	0.51
39:2:314:II0:C42	40:2:317:IHT:C39	2.88	0.51
19:3:99:GLN:NE2	26:3:303:CLA:NA	2.58	0.51
26:5:605:CLA:H141	26:6:609:CLA:H52	1.91	0.51
23:G:158:PHE:CD2	23:G:162:TRP:NE1	2.78	0.51
18:O:142:PHE:CE1	19:P:66:PRO:HG3	2.42	0.51
19:P:106:LEU:HD13	39:P:614:II0:C19	2.40	0.51
21:R:49:GLU:HB3	26:R:302:CLA:HED1	1.92	0.51
1:A:233:ALA:HB3	4:D:264:ARG:HH11	1.75	0.51
2:B:369:ILE:HD11	4:D:344:VAL:HG21	1.93	0.51
5:E:28:ILE:HB	5:E:29:PRO:HD3	1.92	0.51
13:W:43:VAL:HB	19:3:127:TRP:HZ3	1.76	0.51
4:d:334:PRO:HB2	5:e:66:LEU:HD11	1.91	0.51
17:1:46:LEU:HD11	38:1:610:KC2:CBA	2.40	0.51
17:N:140:GLN:HE21	39:N:620:II0:C25	2.23	0.51
18:2:144:PHE:HB3	26:2:319:CLA:HMC2	1.92	0.51
26:3:307:CLA:HAB	39:3:310:II0:C41	2.40	0.51
20:4:133:GLN:NE2	39:4:320:II0:C23	2.72	0.51
18:O:92:PHE:CZ	26:O:607:CLA:HBC3	2.46	0.51
19:P:77:TRP:CD1	26:P:603:CLA:HBA1	2.46	0.51
26:Q:308:CLA:HED2	21:R:43:PHE:CE2	2.45	0.51
22:S:126:LEU:HG	26:S:604:CLA:OBD	2.10	0.51
4:D:128:GLN:HB2	4:D:142:ALA:HB2	1.91	0.51
17:N:54:ILE:HD11	17:N:73:PHE:HA	1.93	0.51
19:3:54:LEU:HB3	19:3:61:ASP:OD2	2.11	0.51
20:4:68:ASP:OD1	39:4:315:II0:O02	2.29	0.51
20:4:134:GLN:NE2	39:4:320:II0:C21	2.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4:168:PRO:HG2	20:4:169:LEU:HD22	1.91	0.51
17:1:152:THR:HB	26:2:301:CLA:CMC	2.40	0.51
26:1:606:CLA:C1	18:2:215:PHE:CE1	2.93	0.51
34:1:620:LHG:H241	26:2:301:CLA:CHD	2.34	0.51
17:N:41:TYR:N	17:N:47:GLN:NE2	2.59	0.51
17:N:54:ILE:O	17:N:56:GLY:N	2.44	0.51
40:2:317:IHT:C06	40:2:317:IHT:C18	2.88	0.51
19:3:64:PHE:CD1	19:3:66:PRO:HD3	2.45	0.51
21:5:58:THR:CB	24:g:119:THR:HG21	2.40	0.51
22:6:126:LEU:HG	26:6:604:CLA:OBD	2.10	0.51
18:O:95:LEU:HD12	39:O:615:II0:C28	2.41	0.51
2:B:369:ILE:HG23	2:B:377:ILE:HG23	1.92	0.51
26:C:511:CLA:HED2	26:C:511:CLA:H52	1.92	0.51
9:K:45:ARG:NH2	15:Y:34:LEU:O	2.44	0.51
2:b:27:THR:CG2	41:b:793:HOH:O	2.59	0.51
2:b:221:PRO:HA	26:b:609:CLA:HED2	1.93	0.51
2:b:253:THR:HG23	2:b:452:THR:HG23	1.93	0.51
19:3:170:ASP:HB3	19:3:173:ALA:HB3	1.93	0.51
38:4:305:KC2:CMA	21:5:224:PRO:HA	2.40	0.51
26:5:605:CLA:C14	26:6:609:CLA:H52	2.40	0.51
19:P:99:GLN:NE2	26:P:604:CLA:NA	2.59	0.51
20:Q:80:TRP:CH2	26:Q:307:CLA:HAA2	2.45	0.51
33:A:412:LMG:H372	26:C:507:CLA:H203	1.93	0.51
2:B:72:THR:HG22	2:B:80:ILE:HD11	1.93	0.51
2:B:75:TRP:HA	2:B:88:PRO:HG3	1.92	0.51
2:B:253:THR:HG23	2:B:452:THR:HG23	1.92	0.51
11:M:3:VAL:HG12	11:M:4:SER:H	1.76	0.51
3:c:331:PHE:HB3	3:c:354:TYR:OH	2.09	0.51
34:N:621:LHG:C33	26:O:601:CLA:CBB	2.89	0.51
18:O:73:PHE:CZ	26:O:602:CLA:H92	2.45	0.51
20:Q:134:GLN:HG2	39:Q:319:II0:C19	2.40	0.51
22:S:183:PHE:HD2	39:S:611:II0:C06	2.21	0.51
2:B:216:HIS:HE1	26:B:609:CLA:NC	2.09	0.50
2:b:216:HIS:HE1	26:b:609:CLA:NC	2.10	0.50
17:1:160:THR:OG1	17:1:166:ARG:NH1	2.44	0.50
17:N:209:HIS:CD2	38:N:612:KC2:C1D	2.91	0.50
18:2:75:PHE:CZ	26:2:302:CLA:H92	2.45	0.50
20:4:119:MET:HE1	20:4:200:LEU:HD23	1.92	0.50
21:5:150:PHE:CZ	24:g:103:PHE:CE2	2.99	0.50
21:5:181:TYR:HE1	38:5:610:KC2:O1A	1.94	0.50
22:6:117:GLY:O	22:6:121:GLN:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:ARG:O	2:B:10:THR:OG1	2.18	0.50
3:C:227:VAL:O	3:C:237:TRP:NE1	2.36	0.50
17:1:42:ARG:CZ	17:1:187:ARG:HD2	2.41	0.50
17:1:225:PRO:HB2	17:1:227:PHE:HD1	1.76	0.50
34:1:620:LHG:C33	26:2:301:CLA:CBB	2.89	0.50
17:N:119:THR:C	17:N:121:GLY:N	2.68	0.50
18:2:106:GLU:OE2	18:2:209:LEU:HB2	2.10	0.50
26:4:306:CLA:C1C	26:5:611:CLA:H41	2.41	0.50
19:P:170:ASP:HB3	19:P:173:ALA:HB3	1.93	0.50
21:R:181:TYR:HE1	38:R:311:KC2:O1A	1.94	0.50
1:A:233:ALA:HB3	4:D:264:ARG:NE	2.26	0.50
1:A:317:TRP:CZ3	4:D:179:ARG:HD2	2.47	0.50
2:b:413:ASP:HB3	2:b:416:THR:HG22	1.92	0.50
9:k:13:ALA:HB2	16:z:61:VAL:HG11	1.93	0.50
11:m:4:SER:HB2	11:m:7:ALA:HB2	1.93	0.50
26:N:606:CLA:HMB1	26:O:611:CLA:NA	2.27	0.50
19:3:72:TYR:HB3	24:g:153:GLY:HA2	1.93	0.50
19:3:84:LYS:HD2	26:3:305:CLA:C3D	2.40	0.50
20:4:180:ARG:HH11	38:4:311:KC2:CBA	2.20	0.50
22:6:122:GLU:OE2	22:6:228:LEU:HD13	2.12	0.50
23:G:100:TRP:HE1	26:R:308:CLA:C4B	2.25	0.50
20:Q:106:GLN:OE1	20:Q:111:THR:HG22	2.11	0.50
20:Q:132:MET:HE2	26:Q:306:CLA:HBC3	1.93	0.50
26:b:614:CLA:OBD	10:l:11:VAL:HG21	2.11	0.50
33:d:404:LMG:HC3	33:d:409:LMG:HC3	1.93	0.50
17:1:154:ILE:HG23	17:1:155:PRO:HD3	1.93	0.50
17:N:120:PHE:O	17:N:121:GLY:C	2.53	0.50
17:N:132:ALA:O	17:N:133:VAL:C	2.52	0.50
19:3:78:LEU:HD13	26:3:301:CLA:O1A	2.12	0.50
19:3:96:PHE:CD2	19:3:195:MET:HE3	2.44	0.50
20:4:75:ILE:CD1	26:4:301:CLA:H3A	2.20	0.50
20:4:156:GLY:N	24:g:123:PHE:HZ	2.00	0.50
23:G:165:PRO:O	23:G:168:ILE:HG12	2.12	0.50
18:O:104:GLU:OE2	18:O:207:LEU:HB2	2.10	0.50
18:O:182:VAL:HG12	18:O:186:ARG:NE	2.27	0.50
24:g:163:LYS:HG3	26:g:402:CLA:CMA	2.42	0.50
17:N:42:ARG:NH2	17:N:43:GLU:OE2	2.34	0.50
17:N:210:TYR:HD1	17:N:216:GLY:H	1.58	0.50
17:N:210:TYR:CD1	17:N:215:ARG:HA	2.46	0.50
26:N:604:CLA:HBB1	39:N:616:II0:C19	2.40	0.50
19:3:77:TRP:CD1	26:3:302:CLA:HBA1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:192:LEU:HD21	28:3:313:WVN:C24	2.41	0.50
20:4:155:GLN:HG2	24:g:123:PHE:O	2.11	0.50
21:5:49:GLU:HB3	26:5:601:CLA:HED1	1.92	0.50
23:G:100:TRP:CH2	26:R:308:CLA:H172	2.45	0.50
19:P:54:LEU:HB3	19:P:61:ASP:OD2	2.11	0.50
2:B:272:ARG:NH1	41:B:719:HOH:O	2.36	0.50
3:C:83:LEU:HB3	9:K:21:ILE:HD13	1.93	0.50
3:C:109:LEU:HD12	3:C:199:LEU:HD22	1.94	0.50
10:L:24:LEU:HD13	34:L:101:LHG:H151	1.93	0.50
3:c:354:TYR:O	3:c:355:LEU:HD23	2.11	0.50
17:N:59:ARG:HH21	17:N:70:ASP:CG	2.19	0.50
18:2:162:PHE:O	26:2:319:CLA:CAB	2.58	0.50
26:2:302:CLA:H172	40:2:317:IHT:C25	2.41	0.50
40:2:317:IHT:C14	40:2:317:IHT:C19	2.90	0.50
26:3:307:CLA:HED3	26:4:303:CLA:CED	2.40	0.50
19:P:78:LEU:HD13	26:P:602:CLA:O1A	2.12	0.50
20:Q:206:THR:CG2	26:Q:311:CLA:CED	2.90	0.50
2:B:137:LYS:NZ	7:H:17:GLU:OE2	2.39	0.50
26:B:613:CLA:H52	34:D:403:LHG:H352	1.94	0.50
4:D:250:ARG:NE	4:D:254:GLN:OE1	2.35	0.50
26:c:508:CLA:HMC2	26:c:509:CLA:H101	1.93	0.50
26:c:512:CLA:H52	26:c:512:CLA:HED2	1.92	0.50
34:l:101:LHG:H342	11:m:17:VAL:HG12	1.93	0.50
12:t:1:MET:N	41:t:101:HOH:O	1.78	0.50
17:N:106:ILE:HG23	17:N:218:ILE:HD11	1.94	0.50
26:N:606:CLA:H3A	26:O:611:CLA:CBD	2.42	0.50
19:3:175:ARG:NE	24:g:136:GLY:O	2.42	0.50
18:O:199:TYR:O	18:O:200:TRP:C	2.52	0.50
2:B:135:LEU:N	2:B:136:PRO:HD2	2.27	0.50
18:2:94:PHE:CZ	26:2:307:CLA:HBC3	2.46	0.50
18:2:121:ALA:O	18:2:122:HIS:C	2.54	0.50
18:2:184:VAL:HG12	18:2:188:ARG:NE	2.27	0.50
19:3:58:LEU:HB2	26:3:301:CLA:HED2	1.94	0.50
19:3:176:ARG:NH1	24:g:128:VAL:O	2.45	0.50
26:3:301:CLA:H41	26:3:302:CLA:HMA3	1.92	0.50
26:3:307:CLA:HMD3	26:4:303:CLA:C9	2.38	0.50
20:4:181:ARG:HD3	26:4:309:CLA:H11	1.94	0.50
22:6:175:GLY:O	22:6:176:ARG:HG2	2.11	0.50
21:R:205:ILE:HG12	21:R:220:ILE:HD13	1.94	0.50
24:g:83:PRO:HB2	24:g:88:SER:HA	1.93	0.50
3:C:331:PHE:HB3	3:C:354:TYR:CZ	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:235:THR:HG22	4:D:236:PRO:HD2	1.92	0.50
3:c:331:PHE:CB	3:c:354:TYR:HE1	2.24	0.50
17:1:124:SER:HB2	17:1:210:TYR:OH	2.11	0.50
17:N:209:HIS:CD2	38:N:612:KC2:CHD	2.95	0.50
18:2:102:PHE:CE2	18:2:198:ILE:HG12	2.47	0.50
19:3:65:ASP:HB2	26:3:301:CLA:HBA2	1.93	0.50
20:4:106:GLN:OE1	20:4:111:THR:HG22	2.11	0.50
20:4:206:THR:CG2	26:4:312:CLA:CED	2.90	0.50
21:5:205:ILE:HG12	21:5:220:ILE:HD13	1.94	0.50
19:P:58:LEU:HB2	26:P:602:CLA:HED2	1.94	0.50
4:D:14:PHE:CE2	33:D:406:LMG:HC72	2.47	0.49
4:D:143:ILE:O	4:D:146:SER:OG	2.26	0.49
15:Y:27:ILE:HD11	16:Z:25:VAL:HA	1.93	0.49
16:Z:26:ILE:HD13	16:Z:40:VAL:HG23	1.93	0.49
2:b:103:LEU:HD22	26:b:606:CLA:H51	1.94	0.49
26:b:612:CLA:H13	26:b:613:CLA:HBB2	1.94	0.49
4:d:200:VAL:HG22	26:d:405:CLA:C1B	2.42	0.49
26:1:603:CLA:HBB2	26:1:614:CLA:HAB	1.94	0.49
38:N:610:KC2:C4C	39:N:617:II0:C18	2.90	0.49
21:5:72:PRO:HD2	39:5:614:II0:C17	2.42	0.49
22:S:117:GLY:O	22:S:121:GLN:HG3	2.11	0.49
9:K:14:TYR:OH	16:Z:58:ASN:HB2	2.11	0.49
3:c:193:ALA:HA	3:c:199:LEU:HG	1.94	0.49
17:N:225:PRO:C	17:N:227:PHE:H	2.20	0.49
18:2:122:HIS:O	18:2:126:VAL:HG13	2.12	0.49
26:2:306:CLA:HMB2	40:2:317:IHT:C11	2.41	0.49
20:4:80:TRP:CD1	24:g:127:GLN:HG3	2.46	0.49
20:4:132:MET:HE2	26:4:307:CLA:HBC3	1.93	0.49
26:4:306:CLA:CMC	26:5:611:CLA:H61	2.42	0.49
18:O:119:ALA:O	18:O:120:HIS:C	2.54	0.49
19:P:65:ASP:HB2	26:P:602:CLA:HBA2	1.93	0.49
20:Q:72:PHE:CB	26:Q:301:CLA:H42	2.42	0.49
13:W:39:LEU:O	19:3:127:TRP:CH2	2.65	0.49
26:a:405:CLA:H3A	33:a:413:LMG:C13	2.42	0.49
26:1:606:CLA:C1B	26:2:311:CLA:CGA	2.89	0.49
20:4:75:ILE:O	24:g:129:ALA:N	2.37	0.49
20:4:129:GLN:CA	21:5:228:PHE:CZ	2.78	0.49
23:G:168:ILE:HG23	26:G:402:CLA:O1D	2.12	0.49
23:G:170:TRP:CZ3	18:O:81:VAL:HG12	2.47	0.49
20:Q:108:PRO:HD2	38:Q:304:KC2:C4C	2.43	0.49
1:A:85:SER:HA	1:A:109:GLY:HA3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:HIS:CE1	2:B:164:PRO:HG2	2.47	0.49
2:B:158:VAL:HG13	2:B:166:ILE:HD13	1.95	0.49
2:B:388:SER:HB2	4:D:343:GLU:OE1	2.11	0.49
2:B:471:SER:HB2	4:D:139:PRO:HG2	1.94	0.49
26:B:612:CLA:H13	26:B:613:CLA:HBB2	1.94	0.49
4:d:14:PHE:CE2	33:d:404:LMG:HC72	2.47	0.49
18:2:83:VAL:CG1	24:g:170:TRP:CZ3	2.92	0.49
19:3:65:ASP:HA	39:3:311:II0:O02	2.12	0.49
20:Q:87:LYS:HD2	26:Q:307:CLA:C4D	2.43	0.49
1:A:63:ILE:HG13	1:A:65:GLU:HB2	1.94	0.49
26:a:405:CLA:HBA1	33:a:413:LMG:H132	1.93	0.49
2:b:472:ARG:HA	2:b:479:PHE:CE1	2.48	0.49
17:N:102:ALA:C	17:N:104:GLY:N	2.65	0.49
22:6:86:PHE:CZ	26:6:601:CLA:HAC2	2.47	0.49
4:D:141:ASN:HB2	41:D:561:HOH:O	2.10	0.49
6:F:41:GLN:O	6:F:42:ARG:C	2.56	0.49
3:c:105:HIS:NE2	26:c:504:CLA:O1D	2.46	0.49
17:N:211:LEU:CD1	26:N:614:CLA:HMD1	2.42	0.49
18:2:102:PHE:HE2	18:2:198:ILE:HG12	1.78	0.49
18:2:175:THR:HG23	18:2:178:ARG:HH21	1.77	0.49
21:5:168:GLY:HA2	21:5:171:GLN:HE21	1.77	0.49
18:O:138:PHE:O	18:O:139:VAL:C	2.56	0.49
26:R:306:CLA:H172	34:R:319:LHG:C26	2.36	0.49
1:A:286:THR:OG1	26:A:402:CLA:O1D	2.27	0.49
4:d:11:ARG:HH21	4:d:15:ASP:HB3	1.78	0.49
17:1:148:LEU:HD11	34:1:620:LHG:C31	2.35	0.49
17:1:151:LEU:HB3	26:2:301:CLA:HBC2	1.93	0.49
19:3:165:LEU:O	19:3:167:LEU:HG	2.13	0.49
21:5:154:GLN:HE21	21:5:154:GLN:N	2.11	0.49
22:6:99:TRP:CZ3	22:6:168:PRO:HA	2.47	0.49
22:6:104:GLU:OE2	22:6:207:ARG:NE	2.35	0.49
20:Q:120:THR:HG23	40:Q:317:IHT:C15	2.43	0.49
21:R:75:PHE:CD1	33:R:301:LMG:H172	2.48	0.49
22:S:86:PHE:CZ	26:S:601:CLA:HAC2	2.47	0.49
1:A:179:THR:O	1:A:183:MET:HG3	2.13	0.49
4:D:200:VAL:HG22	26:D:407:CLA:C1B	2.42	0.49
1:a:162:PRO:HB3	1:a:168:PHE:HA	1.94	0.49
16:z:38:GLY:HA2	16:z:41:TYR:HD2	1.78	0.49
17:N:198:LEU:HB2	39:N:617:II0:C17	2.42	0.49
26:3:307:CLA:HMD2	26:4:303:CLA:H93	1.94	0.49
26:4:306:CLA:H12	21:5:219:PRO:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:94:MET:HE3	26:O:608:CLA:CMC	2.43	0.49
18:O:120:HIS:O	18:O:124:VAL:HG13	2.12	0.49
20:Q:181:ARG:HD3	26:Q:308:CLA:H11	1.94	0.49
2:B:142:HIS:CE1	26:B:610:CLA:H202	2.47	0.49
2:B:162:TRP:HA	2:B:162:TRP:CE3	2.48	0.49
2:b:7:ARG:O	2:b:10:THR:OG1	2.18	0.49
17:N:115:GLY:C	17:N:117:GLN:N	2.65	0.49
18:2:134:ILE:CG1	26:2:305:CLA:HMD3	2.40	0.49
20:4:134:GLN:NE2	39:4:320:II0:C19	2.73	0.49
21:R:168:GLY:HA2	21:R:171:GLN:HE21	1.78	0.49
22:S:122:GLU:OE2	22:S:228:LEU:HD13	2.12	0.49
5:E:26:ILE:C	5:E:26:ILE:HD12	2.38	0.49
3:c:62:LYS:NZ	3:c:152:ASP:OD1	2.46	0.49
17:1:144:TRP:CZ3	34:1:620:LHG:H151	2.48	0.49
18:2:144:PHE:CD2	26:2:319:CLA:HAC1	2.48	0.49
20:4:75:ILE:HB	26:4:301:CLA:CMA	2.42	0.49
19:P:65:ASP:OD2	19:P:68:GLY:HA2	2.13	0.49
20:Q:92:CYS:SG	39:Q:314:II0:C35	3.01	0.49
22:S:177:GLU:HG2	22:S:178:ALA:N	2.21	0.49
8:I:10:THR:HG23	13:W:45:ILE:HD11	1.95	0.48
1:a:85:SER:HA	1:a:109:GLY:HA3	1.93	0.48
17:N:223:ASN:HB2	17:N:227:PHE:HE2	1.78	0.48
39:N:620:II0:O02	18:O:186:ARG:NH1	2.35	0.48
18:2:140:PHE:HD2	34:2:321:LHG:C32	2.24	0.48
18:2:140:PHE:O	18:2:141:VAL:C	2.56	0.48
20:4:62:VAL:HG23	20:4:186:LEU:HD11	1.95	0.48
34:G:403:LHG:O3	34:G:403:LHG:O1	2.26	0.48
18:O:100:PHE:HE2	18:O:196:ILE:HG12	1.78	0.48
2:b:377:ILE:HD11	4:d:339:ILE:CG2	2.42	0.48
3:c:335:ASP:CG	3:c:354:TYR:CE2	2.91	0.48
17:1:94:HIS:HE1	26:1:603:CLA:C4D	2.26	0.48
17:N:63:LEU:HD22	26:N:602:CLA:O2D	2.13	0.48
18:2:96:MET:HE3	26:2:308:CLA:CMC	2.43	0.48
20:4:154:LEU:HD12	24:g:125:VAL:CG2	2.43	0.48
20:4:158:ASP:HB2	21:5:47:PHE:CE1	2.45	0.48
38:4:310:KC2:CMD	38:4:311:KC2:CHD	2.91	0.48
2:B:158:VAL:HA	2:B:166:ILE:HG23	1.96	0.48
3:C:105:HIS:NE2	26:C:503:CLA:O1D	2.46	0.48
3:C:380:ILE:HG23	3:C:384:ARG:HH12	1.78	0.48
17:1:126:MET:HA	17:1:126:MET:HE3	1.95	0.48
19:3:184:HIS:CD2	39:3:310:II0:C37	2.88	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4:72:PHE:CB	26:4:302:CLA:H42	2.42	0.48
21:5:110:PHE:HE2	26:5:604:CLA:H11	1.79	0.48
26:R:306:CLA:H11	22:S:234:PHE:HE2	1.75	0.48
22:S:105:LEU:CD2	22:S:203:VAL:HG12	2.43	0.48
1:A:84:PRO:HA	1:A:112:TYR:CG	2.49	0.48
28:C:516:WVN:C21	28:C:516:WVN:C23	2.91	0.48
11:M:21:PHE:HD1	33:m:101:LMG:H141	1.76	0.48
1:a:127:ILE:HG23	1:a:144:SER:HB2	1.94	0.48
2:b:127:ARG:NH2	7:h:18:TYR:HB3	2.28	0.48
7:h:61:ASP:OD1	35:h:101:DGD:O4E	2.27	0.48
34:1:620:LHG:C26	26:2:301:CLA:C4C	2.92	0.48
26:3:305:CLA:H92	26:3:305:CLA:H61	1.75	0.48
26:G:401:CLA:H121	21:R:143:ILE:HG13	1.96	0.48
18:O:173:THR:HG23	18:O:176:ARG:HH21	1.77	0.48
26:O:608:CLA:C4	38:O:610:KC2:CMA	2.70	0.48
21:R:189:SER:O	21:R:190:ARG:C	2.52	0.48
22:S:99:TRP:CZ3	22:S:168:PRO:HA	2.48	0.48
4:D:11:ARG:HH21	4:D:15:ASP:HB3	1.79	0.48
4:d:76:ALA:HB2	41:d:562:HOH:O	2.13	0.48
7:h:56:GLU:OE1	7:h:57:ASN:N	2.46	0.48
17:N:82:LEU:HD12	17:N:83:ASP:H	1.77	0.48
18:2:147:VAL:CG1	19:3:48:LEU:HD13	2.43	0.48
18:2:201:TYR:O	18:2:202:TRP:C	2.52	0.48
20:4:108:PRO:HD2	38:4:305:KC2:C4C	2.43	0.48
18:O:100:PHE:CE2	18:O:196:ILE:HG12	2.47	0.48
21:R:72:PRO:HD2	39:R:315:II0:C17	2.43	0.48
24:g:168:ILE:HG22	26:g:402:CLA:CGA	2.40	0.48
1:A:127:ILE:HG23	1:A:144:SER:HB2	1.95	0.48
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.94	0.48
2:B:369:ILE:CD1	4:D:344:VAL:HG11	2.42	0.48
1:a:179:THR:O	1:a:183:MET:HG3	2.13	0.48
26:a:402:CLA:NB	26:d:405:CLA:HBB1	2.29	0.48
2:b:373:LYS:HE3	2:b:373:LYS:HB2	1.52	0.48
3:c:475:ARG:HG2	4:d:222:PHE:CD1	2.48	0.48
14:x:1:MET:HE3	14:x:1:MET:HB3	1.73	0.48
17:N:46:LEU:C	17:N:51:THR:HG21	2.39	0.48
17:N:81:TRP:NE1	17:N:82:LEU:HD13	2.29	0.48
17:N:132:ALA:C	17:N:134:ASP:N	2.68	0.48
21:5:75:PHE:CD2	26:5:602:CLA:H2	2.48	0.48
22:6:105:LEU:CD2	22:6:203:VAL:HG12	2.43	0.48
22:6:183:PHE:HB3	26:6:606:CLA:HMD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:O:605:CLA:CAC	39:O:615:II0:C37	2.91	0.48
20:Q:62:VAL:HG23	20:Q:186:LEU:HD11	1.95	0.48
21:R:110:PHE:HE2	26:R:305:CLA:H11	1.79	0.48
26:b:615:CLA:CBB	26:g:402:CLA:HBB1	2.44	0.48
17:N:146:THR:HG23	26:N:608:CLA:HAB	1.96	0.48
34:N:621:LHG:C26	26:O:601:CLA:C4C	2.92	0.48
26:O:603:CLA:HMD3	26:O:607:CLA:ND	2.29	0.48
26:O:605:CLA:HMB3	26:P:610:CLA:ND	2.29	0.48
20:Q:57:LEU:HA	20:Q:57:LEU:HD12	1.43	0.48
2:b:384:ARG:HB3	2:b:385:ARG:H	1.52	0.48
10:l:21:GLY:HA2	34:l:101:LHG:H262	1.96	0.48
18:2:79:PHE:HD1	24:g:170:TRP:HB3	1.79	0.48
20:4:87:LYS:HD2	26:4:308:CLA:C4D	2.43	0.48
23:G:170:TRP:CH2	18:O:81:VAL:HG12	2.49	0.48
39:O:618:II0:C33	26:P:610:CLA:HBC3	2.42	0.48
2:B:162:TRP:HA	2:B:162:TRP:HE3	1.79	0.48
3:C:62:LYS:NZ	3:C:152:ASP:OD1	2.46	0.48
1:a:84:PRO:HA	1:a:112:TYR:CG	2.48	0.48
17:1:86:TRP:HZ3	17:1:157:ILE:HG12	1.79	0.48
17:N:46:LEU:HD11	38:N:610:KC2:CBA	2.44	0.48
17:N:81:TRP:CG	17:N:82:LEU:N	2.75	0.48
26:N:607:CLA:HBB2	39:N:616:II0:C25	2.43	0.48
18:2:186:HIS:ND1	26:2:309:CLA:HMD1	2.28	0.48
22:6:167:THR:HB	22:6:168:PRO:HD2	1.96	0.48
22:6:188:CYS:HB2	26:6:606:CLA:O1A	2.14	0.48
38:Q:309:KC2:CMD	38:Q:310:KC2:CHD	2.91	0.48
21:R:154:GLN:N	21:R:154:GLN:HE21	2.11	0.48
22:S:183:PHE:HB3	26:S:606:CLA:HMD3	1.96	0.48
22:S:188:CYS:HB2	26:S:606:CLA:O1A	2.14	0.48
1:A:12:SER:HB3	1:A:15:GLU:HB3	1.96	0.48
3:C:59:VAL:HG23	3:C:152:ASP:O	2.14	0.48
4:d:187:PHE:O	4:d:293:ARG:NH1	2.47	0.48
29:d:407:PL9:H221	34:l:101:LHG:H192	1.95	0.48
18:2:199:HIS:CD2	26:2:312:CLA:NA	2.82	0.48
19:3:155:ARG:HH11	19:3:155:ARG:HG2	1.79	0.48
23:G:82:GLU:OE1	23:G:82:GLU:N	2.46	0.48
23:G:103:PHE:C	23:G:106:PRO:HD2	2.39	0.48
18:O:121:ASP:O	18:O:124:VAL:HG22	2.14	0.48
26:O:608:CLA:O1A	39:O:613:II0:C12	2.62	0.48
19:P:66:PRO:HD2	39:P:613:II0:C06	2.43	0.48
20:Q:67:PHE:CD1	20:Q:69:PRO:HD3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:VAL:HG12	2:B:181:VAL:CG2	2.42	0.47
26:B:607:CLA:HBA2	33:B:620:LMG:H121	1.96	0.47
9:K:28:PRO:O	9:K:31:PHE:HB2	2.14	0.47
3:c:141:PHE:CG	33:c:522:LMG:H292	2.49	0.47
9:k:23:VAL:O	9:k:26:VAL:HG12	2.14	0.47
17:N:97:VAL:HG11	39:N:616:II0:C27	2.43	0.47
26:3:307:CLA:CBC	26:4:303:CLA:C12	2.92	0.47
20:4:67:PHE:CD1	20:4:69:PRO:HD3	2.49	0.47
20:4:155:GLN:CG	24:g:125:VAL:CG1	2.92	0.47
26:4:306:CLA:CHB	26:5:611:CLA:HBD	2.42	0.47
19:P:165:LEU:O	19:P:167:LEU:HG	2.13	0.47
1:A:32:TRP:O	8:I:19:PHE:HD1	1.97	0.47
4:D:27:VAL:HB	6:F:15:PHE:CZ	2.49	0.47
33:D:406:LMG:H111	7:H:25:TRP:HZ3	1.80	0.47
26:1:606:CLA:HMA1	26:2:311:CLA:CAD	2.38	0.47
17:N:150:THR:O	17:N:154:ILE:HG22	2.13	0.47
18:2:123:ASP:O	18:2:126:VAL:HG22	2.14	0.47
20:4:120:THR:HG23	40:4:318:IHT:C15	2.43	0.47
20:4:129:GLN:HG2	21:5:228:PHE:CZ	2.48	0.47
18:O:57:ASN:OD1	18:O:57:ASN:N	2.43	0.47
18:O:184:HIS:ND1	26:O:609:CLA:HMD1	2.28	0.47
20:Q:78:MET:HB3	20:Q:78:MET:HE3	1.60	0.47
26:R:306:CLA:H161	26:S:609:CLA:H71	1.96	0.47
2:b:287:ARG:HD3	41:b:718:HOH:O	2.13	0.47
13:w:48:PHE:O	13:w:51:LEU:HB2	2.15	0.47
17:1:216:GLY:O	17:1:220:PHE:CB	2.56	0.47
17:N:98:ALA:O	17:N:99:MET:C	2.56	0.47
17:N:101:ALA:CB	26:N:604:CLA:CBB	2.92	0.47
17:N:151:LEU:O	18:O:70:PRO:HB3	2.15	0.47
17:N:185:LEU:HD23	17:N:189:GLN:HG3	1.96	0.47
18:2:79:PHE:CD1	24:g:170:TRP:HB3	2.49	0.47
26:2:319:CLA:HMD2	28:3:313:WVN:C12	2.45	0.47
1:A:161:TYR:OH	41:A:503:HOH:O	2.20	0.47
4:D:209:LEU:HB3	4:D:270:MET:HG2	1.96	0.47
11:M:17:VAL:HB	11:M:18:PRO:HD3	1.96	0.47
2:b:446:SER:CB	41:b:723:HOH:O	2.61	0.47
26:b:613:CLA:H142	26:b:613:CLA:H111	1.76	0.47
17:N:104:GLY:O	17:N:105:MET:C	2.56	0.47
17:N:209:HIS:CE1	39:N:615:II0:C11	2.97	0.47
26:N:606:CLA:CHB	26:O:611:CLA:HBA2	2.45	0.47
18:2:156:LYS:NZ	19:3:49:GLU:HG3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:65:ASP:OD2	19:3:68:GLY:HA2	2.13	0.47
26:3:302:CLA:C4	24:g:157:VAL:HG21	2.41	0.47
21:5:86:GLU:HG2	21:5:149:LEU:HD13	1.97	0.47
26:O:608:CLA:HBA2	26:O:608:CLA:H3A	1.53	0.47
19:P:96:PHE:CZ	19:P:192:LEU:HG	2.50	0.47
20:Q:160:GLN:N	20:Q:160:GLN:OE1	2.48	0.47
2:B:137:LYS:HZ3	7:H:17:GLU:HG2	1.80	0.47
2:B:221:PRO:HA	26:B:609:CLA:HED2	1.96	0.47
3:C:228:LEU:O	13:W:30:ALA:O	2.32	0.47
1:a:71:LEU:HB3	12:t:3:THR:HG23	1.94	0.47
2:b:359:MET:CE	41:b:777:HOH:O	2.62	0.47
9:k:12:GLU:H	9:k:12:GLU:HG2	1.40	0.47
9:k:17:PHE:CZ	16:z:9:VAL:HG13	2.49	0.47
26:1:606:CLA:HMA1	26:2:311:CLA:C3D	2.44	0.47
17:N:220:PHE:CZ	38:N:612:KC2:NA	2.83	0.47
18:O:111:PHE:HE1	39:O:615:II0:C15	2.28	0.47
19:P:155:ARG:HG2	19:P:155:ARG:HH11	1.79	0.47
21:R:75:PHE:CD2	26:R:303:CLA:H2	2.49	0.47
21:R:169:LEU:HD13	26:R:309:CLA:H42	1.97	0.47
17:N:144:TRP:HH2	39:N:620:II0:C42	2.27	0.47
26:2:303:CLA:HMD3	26:2:307:CLA:ND	2.29	0.47
19:3:79:ARG:O	19:3:80:GLU:C	2.57	0.47
20:4:133:GLN:CD	39:4:320:II0:C21	2.87	0.47
20:4:158:ASP:HB2	21:5:47:PHE:HZ	1.66	0.47
26:O:603:CLA:OBD	26:O:607:CLA:HBA2	2.15	0.47
19:P:74:ASP:OD2	19:P:76:LYS:HB2	2.15	0.47
26:Q:306:CLA:C4D	33:Q:318:LMG:H291	2.45	0.47
22:S:165:LYS:HA	22:S:170:ASP:OD2	2.14	0.47
22:S:167:THR:HB	22:S:168:PRO:HD2	1.96	0.47
1:A:308:ASP:OD1	1:A:312[B]:ARG:N	2.48	0.47
3:C:302:GLN:HG3	35:C:517:DGD:HB42	1.96	0.47
9:K:18:LYS:N	9:K:19:PRO:HD2	2.29	0.47
15:Y:24:ILE:HG23	15:Y:34:LEU:HD11	1.97	0.47
3:c:75:VAL:HG13	3:c:132:HIS:CD2	2.49	0.47
5:e:54:ASN:ND2	41:e:101:HOH:O	1.62	0.47
15:y:24:ILE:HG23	15:y:34:LEU:HD11	1.96	0.47
17:N:71:VAL:HG21	26:N:601:CLA:OBD	2.14	0.47
17:N:107:VAL:O	17:N:107:VAL:HG12	2.15	0.47
17:N:112:LYS:HD2	17:N:117:GLN:OE1	2.15	0.47
17:N:119:THR:C	17:N:121:GLY:H	2.21	0.47
17:N:152:THR:CB	18:O:51:PHE:HE1	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:211:LEU:HD13	26:N:614:CLA:CMD	2.43	0.47
17:N:213:VAL:HG21	17:N:226:ASN:OD1	2.15	0.47
26:N:603:CLA:CAB	39:N:616:II0:C36	2.92	0.47
26:2:303:CLA:OBD	26:2:307:CLA:HBA2	2.15	0.47
39:2:320:II0:C32	28:3:313:WVN:C17	2.93	0.47
26:3:307:CLA:C4	20:4:80:TRP:HZ3	2.27	0.47
20:4:76:ILE:HD11	26:4:301:CLA:CAA	2.45	0.47
26:4:306:CLA:C4C	26:5:611:CLA:C4	2.86	0.47
26:4:306:CLA:C3A	26:5:611:CLA:HBD	2.43	0.47
26:4:307:CLA:C4D	33:4:319:LMG:H291	2.45	0.47
21:5:99:THR:HG23	21:5:199:PHE:HE2	1.79	0.47
21:5:169:LEU:HD13	26:5:608:CLA:H42	1.97	0.47
23:G:157:VAL:HG21	26:P:603:CLA:H43	1.95	0.47
26:P:608:CLA:H43	26:Q:302:CLA:HED3	1.97	0.47
21:R:99:THR:HG23	21:R:199:PHE:HE2	1.79	0.47
2:B:75:TRP:CG	2:B:92:SER:HG	2.33	0.47
2:b:331:ASN:HB3	2:b:336:ILE:HG12	1.97	0.47
3:c:302:GLN:HG3	35:c:519:DGD:HB42	1.96	0.47
17:N:78:PHE:O	17:N:81:TRP:CE3	2.68	0.47
17:N:210:TYR:HD1	17:N:215:ARG:HA	1.80	0.47
26:N:603:CLA:C3B	39:N:616:II0:C40	2.92	0.47
18:2:133:GLN:CB	26:2:305:CLA:C1D	2.92	0.47
19:3:92:GLY:O	39:3:311:II0:C19	2.63	0.47
26:3:307:CLA:H41	20:4:150:ILE:HD11	1.95	0.47
20:4:160:GLN:OE1	20:4:160:GLN:N	2.48	0.47
21:5:55:LYS:NZ	33:5:619:LMG:C6	2.72	0.47
21:5:70:PHE:HE1	26:5:601:CLA:HAC2	1.80	0.47
26:Q:302:CLA:H92	26:Q:302:CLA:H62	1.78	0.47
1:a:283:ILE:HA	1:a:286:THR:HG22	1.96	0.47
2:b:383:PHE:CD1	4:d:346:PRO:HA	2.50	0.47
4:d:127:ARG:CG	41:d:518:HOH:O	2.62	0.47
26:1:606:CLA:C3A	26:2:311:CLA:HBD	2.42	0.47
17:N:129:HIS:O	17:N:129:HIS:ND1	2.48	0.47
18:2:137:TRP:CE2	26:2:305:CLA:CHC	2.98	0.47
26:3:307:CLA:H43	20:4:80:TRP:CZ3	2.50	0.47
23:G:135:ILE:HD13	19:P:176:ARG:HG2	1.97	0.47
19:P:106:LEU:HD22	39:P:614:II0:C11	2.45	0.47
24:g:157:VAL:O	24:g:160:PHE:HB2	2.15	0.47
1:A:156:ALA:HA	1:A:160:VAL:HB	1.97	0.47
1:A:218:LEU:CD2	29:A:407:PL9:C6	2.93	0.47
1:A:265:PHE:HB3	1:A:271:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:GLU:O	2:B:98:LEU:HG	2.15	0.47
26:b:605:CLA:H92	26:b:605:CLA:H61	1.76	0.47
4:d:48:PHE:HZ	33:d:411:LMG:H341	1.80	0.47
4:d:209:LEU:HB3	4:d:270:MET:HG2	1.96	0.47
4:d:343:GLU:CD	41:d:504:HOH:O	2.55	0.47
17:1:159:GLN:HE22	18:2:55:LYS:HD3	1.65	0.47
17:N:96:ARG:HA	17:N:99:MET:HE2	1.97	0.47
17:N:124:SER:HB3	17:N:210:TYR:CE1	2.51	0.47
17:N:215:ARG:HB2	17:N:215:ARG:HH21	1.79	0.47
18:2:133:GLN:HE21	39:2:320:II0:C19	2.28	0.47
26:2:311:CLA:HBC2	39:2:315:II0:C29	2.44	0.47
21:5:78:VAL:HG13	24:g:112:TYR:HE1	1.80	0.47
22:6:225:GLN:NE2	22:6:235:LYS:HD2	2.30	0.47
19:P:96:PHE:CD2	19:P:195:MET:HE3	2.44	0.47
20:Q:67:PHE:CE2	39:Q:314:II0:C18	2.97	0.47
2:B:137:LYS:NZ	7:H:17:GLU:CG	2.77	0.46
4:D:147:GLY:O	4:D:151:ILE:HG12	2.15	0.46
4:D:325:ARG:NH1	41:D:516:HOH:O	2.46	0.46
26:b:615:CLA:H162	7:h:7:LEU:HD21	1.96	0.46
26:d:405:CLA:H3A	26:d:405:CLA:HBA1	1.62	0.46
17:N:61:LYS:HG3	17:N:62:ASN:N	2.30	0.46
17:N:166:ARG:NE	17:N:170:ASP:O	2.48	0.46
26:N:603:CLA:OBD	26:N:608:CLA:HAA1	2.15	0.46
34:N:621:LHG:C24	26:O:601:CLA:C1D	2.67	0.46
26:3:306:CLA:H3A	26:3:306:CLA:HBA2	1.44	0.46
22:6:165:LYS:HA	22:6:170:ASP:OD2	2.14	0.46
23:G:157:VAL:O	23:G:160:PHE:HB2	2.15	0.46
18:O:197:HIS:CD2	26:O:612:CLA:NA	2.82	0.46
2:B:331:ASN:HB3	2:B:336:ILE:HG12	1.97	0.46
4:D:187:PHE:O	4:D:293:ARG:NH1	2.48	0.46
1:a:234:ASN:OD1	4:d:264:ARG:NE	2.48	0.46
2:b:127:ARG:HE	2:b:127:ARG:HB3	1.41	0.46
26:c:514:CLA:HBA2	26:c:514:CLA:H3A	1.66	0.46
17:1:209:HIS:NE2	38:1:612:KC2:NC	2.63	0.46
17:N:220:PHE:CZ	38:N:612:KC2:C2A	2.98	0.46
26:N:608:CLA:H3A	26:N:608:CLA:HBA2	1.41	0.46
19:3:74:ASP:OD2	19:3:76:LYS:HB2	2.15	0.46
26:3:307:CLA:CBC	26:4:303:CLA:H121	2.44	0.46
20:4:80:TRP:CZ2	26:4:308:CLA:HAA2	2.50	0.46
20:4:109:GLY:HA3	38:4:305:KC2:C4A	2.45	0.46
21:5:55:LYS:CE	24:g:121:ASP:CB	2.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:O:601:CLA:CAC	40:O:616:IHT:C06	2.92	0.46
21:R:86:GLU:HG2	21:R:149:LEU:HD13	1.97	0.46
1:A:223:LEU:CD1	4:D:264:ARG:CD	2.93	0.46
10:L:21:GLY:HA2	34:L:101:LHG:H262	1.96	0.46
2:b:121:GLU:HG3	7:h:4:ARG:HG2	1.96	0.46
2:b:201:HIS:HE2	26:b:603:CLA:C2B	2.28	0.46
3:c:265:HIS:HE1	26:c:508:CLA:NA	2.13	0.46
4:d:147:GLY:O	4:d:151:ILE:HG12	2.15	0.46
4:d:187:PHE:HA	4:d:325:ARG:HD3	1.97	0.46
17:1:109:ASP:OD1	17:1:217:PRO:HD2	2.16	0.46
17:1:115:GLY:C	17:1:117:GLN:H	2.22	0.46
26:1:606:CLA:C1B	26:2:311:CLA:CBA	2.93	0.46
18:2:137:TRP:CZ2	26:2:305:CLA:CHC	2.98	0.46
26:3:303:CLA:H62	39:3:312:II0:C36	2.46	0.46
20:4:114:PHE:C	21:5:229:PHE:O	2.57	0.46
20:Q:148:VAL:HG12	21:R:54:LEU:HD22	1.97	0.46
21:R:208:GLN:NE2	21:R:213:GLN:HA	2.19	0.46
26:C:511:CLA:HBA1	26:C:511:CLA:H11	1.70	0.46
4:D:264:ARG:NE	34:D:403:LHG:O2	2.48	0.46
6:F:18:LEU:HD22	6:F:18:LEU:HA	1.78	0.46
2:b:71:VAL:HG21	2:b:96:VAL:HG21	1.98	0.46
17:1:152:THR:HG21	26:2:301:CLA:CMC	2.44	0.46
17:N:42:ARG:NH1	17:N:43:GLU:HG3	2.31	0.46
17:N:67:LEU:HD12	17:N:84:LEU:HD13	1.97	0.46
21:5:55:LYS:CE	33:5:619:LMG:HC62	2.45	0.46
21:5:80:ASP:OD2	24:g:114:GLN:CD	2.58	0.46
26:Q:308:CLA:CED	21:R:42:VAL:HB	2.44	0.46
21:R:193:MET:HE3	26:R:303:CLA:HMC2	1.97	0.46
22:S:225:GLN:NE2	22:S:235:LYS:HD2	2.30	0.46
24:g:165:PRO:CA	26:g:402:CLA:CED	2.94	0.46
26:C:511:CLA:H41	26:C:511:CLA:H61	1.76	0.46
2:b:27:THR:HG22	41:b:793:HOH:O	2.14	0.46
2:b:362:PHE:CE1	4:d:187:PHE:CB	2.98	0.46
26:b:604:CLA:C1C	26:b:613:CLA:HBB1	2.45	0.46
26:c:505:CLA:H41	26:c:505:CLA:H62	1.70	0.46
9:k:14:TYR:HE2	16:z:58:ASN:ND2	2.14	0.46
18:2:133:GLN:HG3	26:2:305:CLA:CHA	2.45	0.46
26:O:605:CLA:HAC1	39:O:615:II0:C37	2.45	0.46
26:O:608:CLA:HHC	39:O:613:II0:C34	2.46	0.46
20:Q:133:GLN:OE1	39:Q:319:II0:C21	2.63	0.46
2:B:413:ASP:O	2:B:417:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:17:TRP:HA	37:F:101:HEM:O1D	2.16	0.46
2:b:272:ARG:NH1	41:b:720:HOH:O	2.38	0.46
3:c:124:PRO:HB3	33:c:521:LMG:HC71	1.97	0.46
3:c:380:ILE:HG23	3:c:384:ARG:HH12	1.80	0.46
4:d:20:TRP:CD1	4:d:23:ARG:HH22	2.34	0.46
4:d:179:ARG:HD3	4:d:332:ASP:OD1	2.16	0.46
26:1:604:CLA:H93	26:1:604:CLA:H111	1.70	0.46
17:N:132:ALA:C	17:N:134:ASP:H	2.24	0.46
26:N:606:CLA:HBB2	34:N:621:LHG:C17	2.34	0.46
19:3:66:PRO:HD2	39:3:311:II0:C08	2.46	0.46
26:3:307:CLA:C3B	39:3:310:II0:C41	2.93	0.46
20:4:138:TRP:CH2	39:4:320:II0:C39	2.99	0.46
18:O:99:GLY:O	18:O:100:PHE:C	2.56	0.46
18:O:160:PHE:O	26:P:601:CLA:HAB	2.15	0.46
20:Q:80:TRP:CZ2	26:Q:307:CLA:HAA2	2.50	0.46
2:B:201:HIS:HE2	26:B:603:CLA:C2B	2.28	0.46
26:B:607:CLA:H162	26:B:607:CLA:H141	1.72	0.46
26:a:403:CLA:HBA2	26:a:403:CLA:H3A	1.71	0.46
26:b:613:CLA:H62	26:b:613:CLA:H2	1.60	0.46
17:N:202:ALA:O	17:N:206:MET:HG3	2.15	0.46
18:2:157:ARG:HH11	18:2:157:ARG:HD3	1.56	0.46
20:4:80:TRP:CG	24:g:127:GLN:HG3	2.50	0.46
20:4:155:GLN:HG3	24:g:125:VAL:HG11	1.96	0.46
21:5:45:GLY:HA3	21:5:47:PHE:CE2	2.51	0.46
21:5:148:ALA:HB1	21:5:157:ARG:HD3	1.98	0.46
22:6:172:PHE:HE1	22:6:178:ALA:HA	1.80	0.46
22:6:236:ALA:O	22:6:237:ILE:C	2.59	0.46
20:Q:109:GLY:HA3	38:Q:304:KC2:C4A	2.45	0.46
1:A:160:VAL:HG11	1:A:291:MET:HG2	1.98	0.46
26:B:615:CLA:H162	7:H:7:LEU:HD21	1.97	0.46
3:C:351:LEU:N	3:C:351:LEU:CD2	2.73	0.46
2:b:124:ARG:HA	2:b:131:PRO:HA	1.98	0.46
3:c:75:VAL:HG13	3:c:132:HIS:HD2	1.81	0.46
17:1:146:THR:HG23	26:1:608:CLA:CAB	2.46	0.46
17:N:208:HIS:CE1	26:N:614:CLA:NB	2.72	0.46
18:2:83:VAL:CG2	24:g:169:ALA:CB	2.86	0.46
22:6:99:TRP:CE3	22:6:168:PRO:HA	2.51	0.46
18:O:187:LEU:HD21	39:O:613:II0:C27	2.46	0.46
19:P:103:GLN:HB3	19:P:109:PHE:O	2.16	0.46
20:Q:168:PRO:HD2	39:Q:313:II0:C05	2.46	0.46
1:A:283:ILE:HA	1:A:286:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:225:PRO:CB	17:N:227:PHE:H	2.28	0.46
17:N:227:PHE:CG	17:N:228:LYS:N	2.84	0.46
18:2:148:ALA:HB2	19:3:47:PHE:HE2	1.76	0.46
33:5:619:LMG:H121	33:5:619:LMG:H361	1.98	0.46
22:6:98:ARG:HG2	22:6:172:PHE:CE1	2.51	0.46
1:A:304:GLN:HG2	1:A:313:VAL:HG11	1.98	0.46
2:B:159:THR:HA	2:B:181:VAL:O	2.16	0.46
3:C:75:VAL:HG13	3:C:132:HIS:CD2	2.50	0.46
4:D:50:GLY:HA2	4:D:54:VAL:HB	1.98	0.46
4:D:264:ARG:CZ	34:D:403:LHG:O2	2.63	0.46
7:H:6:ARG:HB3	7:H:6:ARG:CZ	2.45	0.46
2:b:476:ARG:HD2	2:b:476:ARG:HA	1.55	0.46
34:N:621:LHG:H161	26:O:611:CLA:HMB2	1.98	0.46
18:2:137:TRP:HE3	34:2:321:LHG:H342	1.81	0.46
26:2:303:CLA:H3A	26:2:303:CLA:HBA1	1.68	0.46
21:5:201:HIS:HE1	40:5:616:IHT:C38	2.29	0.46
23:G:140:LYS:HE3	19:P:174:LEU:HD21	1.98	0.46
20:Q:135:LEU:HB2	26:Q:306:CLA:CBC	2.29	0.46
20:Q:160:GLN:HB2	21:R:43:PHE:CE2	2.51	0.46
21:R:148:ALA:HB1	21:R:157:ARG:HD3	1.98	0.46
26:R:305:CLA:H12	39:R:316:II0:C39	2.46	0.46
1:a:160:VAL:HG11	1:a:291:MET:HG2	1.98	0.45
3:c:71:ALA:O	3:c:75:VAL:HG23	2.16	0.45
3:c:353:LYS:O	3:c:354:TYR:CB	2.61	0.45
10:l:5:ASN:HA	10:l:6:PRO:HD3	1.81	0.45
10:l:24:LEU:HD13	34:l:101:LHG:H151	1.98	0.45
26:1:603:CLA:OBD	26:1:608:CLA:HAA1	2.16	0.45
20:4:118:LYS:HE3	20:4:212:GLN:NE2	2.30	0.45
20:4:119:MET:HB3	20:4:119:MET:HE3	1.72	0.45
21:5:113:PHE:HE1	39:5:615:II0:C15	2.29	0.45
26:5:605:CLA:NB	26:6:609:CLA:H11	2.27	0.45
23:G:93:PHE:O	23:G:97:ILE:HG12	2.15	0.45
21:R:70:PHE:HE1	26:R:302:CLA:HAC2	1.80	0.45
22:S:98:ARG:HG2	22:S:172:PHE:CE1	2.51	0.45
26:A:402:CLA:NB	26:D:407:CLA:HBB1	2.31	0.45
2:B:35:GLY:HA3	2:B:101:ILE:HG13	1.99	0.45
1:a:156:ALA:HA	1:a:160:VAL:HB	1.97	0.45
26:a:402:CLA:H142	26:a:402:CLA:H112	1.83	0.45
17:1:188:ARG:HE	26:1:609:CLA:CGA	2.29	0.45
17:1:188:ARG:HG2	26:1:609:CLA:H3A	1.98	0.45
17:1:208:HIS:HD2	26:1:614:CLA:HED2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:609:CLA:H62	26:1:609:CLA:H41	1.77	0.45
26:2:311:CLA:HBC2	39:2:315:II0:C33	2.44	0.45
19:3:103:GLN:HB3	19:3:109:PHE:O	2.16	0.45
19:3:145:LEU:HD22	26:3:305:CLA:HMA1	1.99	0.45
19:3:150:MET:O	19:3:155:ARG:HD3	2.17	0.45
26:3:307:CLA:H43	20:4:80:TRP:HZ3	1.81	0.45
20:4:168:PRO:HD2	39:4:314:II0:C05	2.46	0.45
20:4:180:ARG:O	20:4:184:VAL:HG23	2.17	0.45
26:4:301:CLA:H2	26:4:303:CLA:H71	1.97	0.45
38:4:310:KC2:OBD	38:4:311:KC2:C4D	2.64	0.45
26:O:605:CLA:H3A	26:P:610:CLA:CBD	2.41	0.45
19:P:145:LEU:HD22	26:P:606:CLA:HMA1	1.99	0.45
20:Q:118:LYS:HE3	20:Q:212:GLN:NE2	2.30	0.45
20:Q:202:HIS:HE1	26:Q:311:CLA:C1B	2.29	0.45
22:S:172:PHE:HE1	22:S:178:ALA:HA	1.80	0.45
2:B:242:ILE:HA	2:B:245:VAL:HG22	1.97	0.45
34:C:518:LHG:HC11	19:3:143:GLY:HA3	1.99	0.45
14:X:1:MET:HE2	26:N:607:CLA:HED2	1.93	0.45
1:a:184:LEU:HD21	4:d:185:GLN:HG2	1.97	0.45
3:c:192:LYS:HD3	26:c:504:CLA:H192	1.99	0.45
26:1:603:CLA:H62	26:1:603:CLA:H2	1.62	0.45
18:2:147:VAL:HG12	19:3:48:LEU:CD2	2.47	0.45
26:2:308:CLA:H161	26:2:308:CLA:H141	1.71	0.45
19:3:141:ASN:HB2	19:3:145:LEU:CD2	2.47	0.45
20:4:180:ARG:HH12	38:4:311:KC2:CGD	2.30	0.45
21:5:193:MET:HE3	26:5:602:CLA:HMC2	1.97	0.45
20:Q:201:HIS:HA	20:Q:204:PHE:CD2	2.51	0.45
26:Q:307:CLA:H3A	26:Q:307:CLA:HBA2	1.40	0.45
26:S:604:CLA:H151	26:S:606:CLA:HBC1	1.98	0.45
26:S:607:CLA:H3A	26:S:607:CLA:HBA2	1.65	0.45
16:Z:8:LEU:HD21	16:Z:53:MET:HB3	1.98	0.45
3:c:294:SER:OG	3:c:448:GLY:O	2.33	0.45
34:c:520:LHG:H262	34:c:520:LHG:H291	1.72	0.45
4:d:56:SER:OG	4:d:64:SER:OG	2.27	0.45
17:1:108:GLN:OE1	26:1:604:CLA:ND	2.50	0.45
34:1:620:LHG:C24	26:2:301:CLA:ND	2.67	0.45
17:N:226:ASN:N	38:N:612:KC2:O2A	2.49	0.45
18:2:165:ASP:HA	39:2:313:II0:C12	2.47	0.45
19:3:95:GLY:O	19:3:99:GLN:HG3	2.17	0.45
19:3:103:GLN:N	19:3:103:GLN:OE1	2.50	0.45
20:4:75:ILE:HD12	26:4:301:CLA:HHB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4:143:GLU:HG3	26:4:308:CLA:CHC	2.47	0.45
20:4:202:HIS:HE1	26:4:312:CLA:C1B	2.29	0.45
22:6:159:PHE:HE1	22:6:166:LEU:CD1	2.29	0.45
26:P:607:CLA:H3A	26:P:607:CLA:HBA2	1.44	0.45
1:A:32:TRP:CE3	8:I:22:GLY:HA3	2.51	0.45
2:B:42:LEU:HD11	2:B:93:PHE:C	2.41	0.45
2:B:94:GLU:OE1	2:B:94:GLU:N	2.40	0.45
4:D:325:ARG:NH2	41:D:502:HOH:O	2.49	0.45
9:K:17:PHE:CZ	16:Z:9:VAL:HG13	2.51	0.45
2:b:222:PRO:HG3	7:h:26:GLY:HA3	1.97	0.45
3:c:83:LEU:HB3	9:k:21:ILE:HD13	1.99	0.45
4:d:20:TRP:HA	4:d:23:ARG:NH1	2.30	0.45
4:d:264:ARG:HH21	4:d:268:PHE:HB2	1.81	0.45
8:i:6:ILE:HD11	13:w:41:PRO:HG2	1.98	0.45
9:k:28:PRO:O	9:k:31:PHE:HB2	2.16	0.45
20:4:201:HIS:HA	20:4:204:PHE:CD2	2.52	0.45
22:6:107:HIS:CD2	26:6:602:CLA:HBB2	2.52	0.45
18:O:87:LEU:HD21	18:O:182:VAL:HG22	1.99	0.45
19:P:89:CYS:SG	19:P:189:MET:HG2	2.57	0.45
33:R:301:LMG:H361	33:R:301:LMG:H121	1.98	0.45
22:S:107:HIS:CD2	26:S:602:CLA:HBB2	2.52	0.45
26:B:604:CLA:C1C	26:B:613:CLA:HBB1	2.46	0.45
3:C:71:ALA:O	3:C:75:VAL:HG23	2.16	0.45
14:x:10:ASN:HA	14:x:13:LEU:CD1	2.41	0.45
17:1:187:ARG:NH1	38:1:611:KC2:O1A	2.50	0.45
17:1:213:VAL:HG11	17:1:226:ASN:OD1	2.16	0.45
17:N:118:LYS:NZ	38:N:605:KC2:O2A	2.30	0.45
21:5:208:GLN:NE2	21:5:213:GLN:HA	2.19	0.45
23:G:100:TRP:HE1	26:R:308:CLA:CHC	2.30	0.45
34:G:403:LHG:H382	28:P:615:WVN:C17	2.47	0.45
19:P:79:ARG:O	19:P:80:GLU:C	2.57	0.45
19:P:103:GLN:OE1	19:P:103:GLN:N	2.50	0.45
20:Q:57:LEU:HD11	26:Q:301:CLA:O2D	2.16	0.45
22:S:236:ALA:O	22:S:237:ILE:C	2.59	0.45
2:B:383:PHE:CD2	4:D:346:PRO:HA	2.51	0.45
34:C:518:LHG:H262	34:C:518:LHG:H291	1.74	0.45
26:b:603:CLA:H41	26:b:603:CLA:H61	1.72	0.45
26:b:607:CLA:HBA2	33:b:620:LMG:H121	1.99	0.45
26:b:610:CLA:H193	26:b:612:CLA:HMD2	1.99	0.45
17:1:208:HIS:HA	26:1:614:CLA:HED3	1.98	0.45
26:1:606:CLA:HMA2	26:2:311:CLA:HBD	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:147:VAL:HG22	26:O:602:CLA:H18	1.98	0.45
39:2:320:II0:C16	19:3:201:ILE:HD11	2.47	0.45
20:4:57:LEU:HD12	20:4:57:LEU:HA	1.43	0.45
20:4:76:ILE:CG2	24:g:127:GLN:CG	2.88	0.45
18:O:191:ALA:HA	39:O:613:II0:C19	2.47	0.45
19:P:141:ASN:HB2	19:P:145:LEU:CD2	2.47	0.45
21:R:45:GLY:HA3	21:R:47:PHE:CE2	2.51	0.45
21:R:75:PHE:CG	26:R:303:CLA:H2	2.52	0.45
26:S:605:CLA:H2	26:S:605:CLA:H61	1.68	0.45
1:A:223:LEU:CD1	4:D:264:ARG:HG3	2.44	0.45
1:A:233:ALA:CB	4:D:264:ARG:HH11	2.30	0.45
2:B:296:LEU:HD23	2:B:300:GLU:HB3	1.99	0.45
4:D:341:PRO:HD2	4:D:344:VAL:HG21	1.99	0.45
1:a:265:PHE:HB3	1:a:271:LEU:HB2	1.99	0.45
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.98	0.45
3:c:54:SER:OG	26:c:510:CLA:H2A	2.17	0.45
13:w:40:VAL:HA	19:P:127:TRP:HH2	1.81	0.45
17:1:152:THR:HB	26:2:301:CLA:HMC1	1.98	0.45
17:1:155:PRO:C	18:2:54:LEU:HD21	2.38	0.45
17:N:172:GLY:N	26:N:609:CLA:OBD	2.49	0.45
17:N:191:VAL:O	17:N:195:ASN:ND2	2.44	0.45
17:N:227:PHE:CD1	17:N:228:LYS:HG3	2.51	0.45
38:N:612:KC2:CBC	39:N:617:II0:C42	2.95	0.45
20:4:69:PRO:HD2	39:4:315:II0:C18	2.47	0.45
20:4:76:ILE:HD11	26:4:301:CLA:HAA2	1.99	0.45
18:O:182:VAL:HG12	18:O:186:ARG:CZ	2.47	0.45
26:O:611:CLA:HBB1	39:O:613:II0:C19	2.45	0.45
2:B:341:LEU:HD23	2:B:405:LYS:HG3	1.99	0.45
2:B:372:ASP:OD2	2:B:376:ILE:HB	2.16	0.45
26:a:403:CLA:HMD3	4:d:181:LEU:HD11	1.97	0.45
26:b:613:CLA:HBA1	26:b:613:CLA:H3A	1.74	0.45
13:w:38:LEU:O	13:w:41:PRO:HD2	2.17	0.45
14:x:32:GLN:HB2	17:1:81:TRP:HB2	1.99	0.45
26:1:606:CLA:C3C	26:2:311:CLA:H42	2.45	0.45
17:N:81:TRP:CD2	17:N:82:LEU:HB2	2.50	0.45
17:N:116:VAL:O	17:N:117:GLN:C	2.59	0.45
18:2:89:LEU:HD21	18:2:184:VAL:HG22	1.99	0.45
26:2:311:CLA:HBC3	39:2:315:II0:C37	2.47	0.45
19:3:58:LEU:HB2	26:3:301:CLA:CED	2.47	0.45
21:5:82:ARG:NH1	21:5:152:THR:O	2.50	0.45
21:5:96:MET:HE3	26:5:608:CLA:HMC3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:95:GLY:O	19:P:99:GLN:HG3	2.17	0.45
21:R:72:PRO:O	33:R:301:LMG:O3	2.26	0.45
21:R:83:VAL:CG1	26:R:308:CLA:HED1	2.47	0.45
21:R:205:ILE:HG12	21:R:220:ILE:CD1	2.47	0.45
1:A:22:THR:HB	1:A:136:ARG:HE	1.82	0.45
26:C:513:CLA:HBA2	26:C:513:CLA:H3A	1.66	0.45
4:D:295:TYR:OH	41:D:502:HOH:O	2.07	0.45
1:a:223:LEU:HD13	4:d:264:ARG:CD	2.37	0.45
16:z:8:LEU:HD21	16:z:53:MET:HB3	1.99	0.45
17:N:42:ARG:CZ	38:N:610:KC2:O1A	2.65	0.45
17:N:144:TRP:CZ2	39:N:620:II0:C35	3.00	0.45
18:2:167:LEU:HB2	39:2:313:II0:C06	2.47	0.45
18:2:184:VAL:HG12	18:2:188:ARG:CZ	2.47	0.45
20:4:57:LEU:HD11	26:4:302:CLA:O2D	2.17	0.45
20:4:66:GLY:N	26:4:302:CLA:OBD	2.50	0.45
20:4:155:GLN:O	20:4:156:GLY:C	2.55	0.45
21:5:181:TYR:CB	26:5:608:CLA:HMA1	2.47	0.45
26:5:605:CLA:C4A	26:6:609:CLA:H11	2.46	0.45
39:O:618:II0:C31	26:P:610:CLA:HBC3	2.47	0.45
20:Q:135:LEU:HD23	20:Q:135:LEU:HA	1.82	0.45
26:S:603:CLA:HMD2	26:S:605:CLA:H8	1.99	0.45
24:g:171:LYS:HG2	24:g:172:PRO:HD2	1.98	0.45
3:C:192:LYS:HD3	26:C:503:CLA:H192	1.99	0.44
4:D:78:SER:HA	4:D:171:SER:HB3	2.00	0.44
16:Z:16:SER:OG	16:Z:47:TRP:NE1	2.47	0.44
3:c:202:THR:HB	3:c:378:PRO:HG2	1.99	0.44
4:d:192:LEU:HD13	41:d:545:HOH:O	2.17	0.44
17:N:61:LYS:HG3	17:N:62:ASN:ND2	2.31	0.44
33:2:318:LMG:H161	33:2:318:LMG:H131	1.86	0.44
19:3:88:VAL:HG12	39:3:311:II0:C31	2.47	0.44
19:3:89:CYS:SG	19:3:189:MET:HG2	2.57	0.44
26:3:302:CLA:H41	24:g:157:VAL:HG11	1.99	0.44
21:5:75:PHE:CG	26:5:602:CLA:H2	2.52	0.44
21:5:205:ILE:HG12	21:5:220:ILE:CD1	2.47	0.44
26:O:603:CLA:H3A	26:O:603:CLA:HBA1	1.68	0.44
26:P:606:CLA:H92	26:P:606:CLA:H61	1.75	0.44
21:R:181:TYR:CB	26:R:309:CLA:HMA1	2.47	0.44
22:S:99:TRP:CE3	22:S:168:PRO:HA	2.51	0.44
1:A:221:SER:HB3	4:D:137:ILE:HD12	1.99	0.44
2:b:357:ARG:NH2	4:d:336:GLU:O	2.29	0.44
26:c:515:CLA:H62	22:S:166:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:606:CLA:C3C	26:2:311:CLA:H41	2.47	0.44
18:2:153:LEU:HD11	24:g:169:ALA:CA	2.48	0.44
19:3:96:PHE:CZ	19:3:192:LEU:HG	2.50	0.44
19:P:58:LEU:HB2	26:P:602:CLA:CED	2.47	0.44
19:P:150:MET:O	19:P:155:ARG:HD3	2.17	0.44
20:Q:164:PHE:O	26:R:302:CLA:HBB2	2.17	0.44
20:Q:180:ARG:HH12	38:Q:310:KC2:CGD	2.30	0.44
38:Q:309:KC2:OBD	38:Q:310:KC2:C4D	2.65	0.44
21:R:113:PHE:HE1	39:R:316:II0:C15	2.29	0.44
26:S:605:CLA:H3A	26:S:605:CLA:HBA2	1.43	0.44
26:g:401:CLA:H141	26:g:401:CLA:H162	1.75	0.44
3:C:202:THR:HB	3:C:378:PRO:HG2	1.99	0.44
26:C:504:CLA:H62	26:C:504:CLA:H41	1.70	0.44
4:D:76:ALA:HB2	41:D:562:HOH:O	2.16	0.44
16:Z:22:SER:O	16:Z:23:VAL:C	2.60	0.44
1:a:63:ILE:HG13	1:a:65:GLU:HG2	1.98	0.44
1:a:304:GLN:HG2	1:a:313:VAL:HG11	1.98	0.44
26:b:615:CLA:H92	26:b:615:CLA:H61	1.87	0.44
5:e:38:PHE:HE1	5:e:47:ILE:HD12	1.83	0.44
17:1:136:GLY:HA2	17:1:139:GLN:NE2	2.32	0.44
26:5:604:CLA:H12	39:5:615:II0:C39	2.46	0.44
26:6:604:CLA:H112	26:6:604:CLA:H152	1.69	0.44
20:Q:143:GLU:HG3	26:Q:307:CLA:CHC	2.47	0.44
20:Q:180:ARG:O	20:Q:184:VAL:HG23	2.17	0.44
21:R:96:MET:HE3	26:R:309:CLA:HMC3	1.98	0.44
1:A:71:LEU:HB3	12:T:3:THR:HG23	1.98	0.44
1:A:308:ASP:OD1	1:A:312[A]:ARG:N	2.51	0.44
3:C:374:ASP:CG	41:C:607:HOH:O	2.61	0.44
1:a:223:LEU:CD1	4:d:264:ARG:CD	2.96	0.44
26:b:606:CLA:H122	26:b:606:CLA:H162	1.85	0.44
26:c:512:CLA:HBA1	26:c:512:CLA:H11	1.71	0.44
26:d:402:CLA:H141	26:d:402:CLA:H161	1.82	0.44
14:x:1:MET:SD	26:1:607:CLA:HED1	2.57	0.44
17:1:145:ILE:HD12	34:1:620:LHG:H223	1.89	0.44
17:N:88:ARG:HG3	17:N:168:PRO:HB2	1.98	0.44
17:N:225:PRO:HB2	17:N:227:PHE:CB	2.47	0.44
18:2:84:LEU:HA	24:g:170:TRP:HH2	1.82	0.44
18:2:137:TRP:NE1	26:2:305:CLA:C1C	2.81	0.44
20:4:90:ARG:CB	39:4:317:II0:C20	2.96	0.44
20:4:152:GLN:OE1	21:5:54:LEU:CA	2.65	0.44
26:4:308:CLA:HBA2	26:4:308:CLA:H3A	1.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:6:603:CLA:HMD2	26:6:605:CLA:H8	1.98	0.44
26:O:606:CLA:H61	26:O:606:CLA:H2	1.78	0.44
26:O:611:CLA:CAB	39:O:613:II0:C19	2.95	0.44
20:Q:114:PHE:CE2	38:Q:304:KC2:CBB	3.01	0.44
20:Q:129:GLN:NE2	39:Q:316:II0:C15	2.81	0.44
21:R:168:GLY:O	21:R:171:GLN:HB2	2.18	0.44
26:A:403:CLA:HMD3	4:D:181:LEU:HD11	1.99	0.44
3:C:54:SER:OG	26:C:509:CLA:H2A	2.17	0.44
26:C:506:CLA:H101	26:C:506:CLA:H13	1.74	0.44
8:I:6:ILE:HD12	13:W:38:LEU:HD23	1.99	0.44
1:a:221:SER:HB3	4:d:137:ILE:HD12	1.99	0.44
13:w:63:GLU:O	13:w:72:ARG:NH2	2.38	0.44
19:3:191:GLY:HA2	39:3:310:II0:C19	2.47	0.44
26:3:303:CLA:H92	39:3:312:II0:C34	2.48	0.44
22:6:105:LEU:O	22:6:109:ARG:HG3	2.18	0.44
20:Q:66:GLY:N	26:Q:301:CLA:OBD	2.50	0.44
20:Q:90:ARG:CB	39:Q:316:II0:C20	2.96	0.44
2:B:42:LEU:HD21	2:B:93:PHE:CB	2.45	0.44
2:B:134:ASP:O	2:B:138:ILE:HG13	2.18	0.44
6:F:40:ILE:HG22	6:F:42:ARG:H	1.83	0.44
3:c:227:VAL:O	3:c:237:TRP:NE1	2.38	0.44
4:d:50:GLY:HA2	4:d:54:VAL:HB	1.98	0.44
17:N:83:ASP:O	17:N:87:ALA:N	2.46	0.44
17:N:137:ALA:O	17:N:138:MET:C	2.56	0.44
18:2:59:ASN:OD1	18:2:59:ASN:N	2.43	0.44
26:2:319:CLA:ND	34:2:321:LHG:C25	2.80	0.44
19:3:168:SER:HB3	26:3:306:CLA:HBA1	1.99	0.44
26:5:605:CLA:C4B	26:6:609:CLA:C2	2.91	0.44
26:6:604:CLA:H151	26:6:606:CLA:HBC1	1.98	0.44
23:G:158:PHE:CD2	23:G:162:TRP:CD1	3.05	0.44
19:P:82:GLU:HB2	26:P:602:CLA:C1B	2.48	0.44
19:P:89:CYS:HB2	19:P:192:LEU:HD13	2.00	0.44
1:A:184:LEU:HD21	4:D:185:GLN:HG2	2.00	0.44
26:C:512:CLA:HBA1	28:C:516:WVN:C09	2.48	0.44
13:W:39:LEU:HB3	19:3:127:TRP:CZ2	2.52	0.44
1:a:77:ILE:HD11	12:t:6:TYR:HB3	1.99	0.44
2:b:69:ILE:HD11	26:b:605:CLA:HBA1	2.00	0.44
26:b:616:CLA:H143	26:b:616:CLA:H161	1.74	0.44
18:2:53:PHE:CD1	18:2:54:LEU:HG	2.53	0.44
20:4:72:PHE:HD1	20:4:72:PHE:HA	1.69	0.44
20:4:76:ILE:CD1	26:4:301:CLA:CGA	2.92	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:5:85:ARG:NH1	21:5:186:ILE:HG21	2.33	0.44
21:5:168:GLY:O	21:5:171:GLN:HB2	2.18	0.44
21:5:216:ASN:ND2	21:5:218:LYS:HE3	2.33	0.44
22:6:67:MET:HE1	26:6:601:CLA:HMC2	2.00	0.44
26:G:401:CLA:H141	26:G:401:CLA:H162	1.69	0.44
26:O:603:CLA:HBC2	26:O:607:CLA:HAC1	2.00	0.44
19:P:189:MET:HB3	39:P:613:II0:C38	2.48	0.44
20:Q:119:MET:HE3	20:Q:119:MET:HB3	1.72	0.44
38:Q:309:KC2:C3D	38:Q:310:KC2:CMD	2.95	0.44
21:R:51:VAL:HG22	26:R:302:CLA:C4C	2.48	0.44
1:A:293:MET:HG2	1:A:298:ASN:HA	2.00	0.44
26:B:616:CLA:H143	26:B:616:CLA:H161	1.73	0.44
16:Z:37:LYS:HB3	16:Z:37:LYS:HE3	1.63	0.44
4:d:78:SER:HA	4:d:171:SER:HB3	2.00	0.44
26:1:603:CLA:HBA1	26:1:603:CLA:H11	1.74	0.44
26:2:303:CLA:HBC2	26:2:307:CLA:HAC1	2.00	0.44
21:5:113:PHE:CE1	39:5:615:II0:C15	3.01	0.44
21:5:153:ILE:HG21	24:g:110:ALA:HB1	1.98	0.44
22:6:98:ARG:HG3	22:6:178:ALA:HB2	2.00	0.44
26:6:605:CLA:H3A	26:6:605:CLA:HBA2	1.43	0.44
18:O:96:ALA:O	18:O:97:THR:C	2.60	0.44
18:O:213:PHE:CE1	26:O:611:CLA:HED3	2.53	0.44
2:B:80:ILE:CD1	2:B:93:PHE:HZ	2.28	0.44
2:B:434:ARG:HB3	2:B:439:SER:HB2	2.00	0.44
2:B:437:LEU:HD23	2:B:437:LEU:HA	1.78	0.44
26:B:606:CLA:H122	26:B:606:CLA:H162	1.84	0.44
9:K:17:PHE:C	9:K:19:PRO:HD2	2.43	0.44
13:W:51:LEU:HD22	26:3:305:CLA:HBA1	1.99	0.44
16:Z:20:VAL:O	16:Z:24:PRO:HG3	2.18	0.44
2:b:69:ILE:HG21	26:b:603:CLA:OBD	2.18	0.44
26:b:610:CLA:H11	26:b:612:CLA:H191	2.00	0.44
17:1:167:GLN:OE1	17:1:167:GLN:HA	2.18	0.44
19:3:89:CYS:HB2	19:3:192:LEU:HD13	2.00	0.44
19:3:138:ILE:HG12	19:3:145:LEU:HD11	2.00	0.44
19:3:193:GLY:CA	28:3:313:WVN:C39	2.87	0.44
20:4:78:MET:HB3	20:4:78:MET:HE3	1.60	0.44
20:4:80:TRP:HB3	24:g:127:GLN:HB2	1.92	0.44
20:4:114:PHE:CE2	38:4:305:KC2:CBB	3.01	0.44
26:4:306:CLA:HHB	26:5:611:CLA:CHA	2.48	0.44
23:G:167:LEU:CD2	26:O:607:CLA:H2	2.46	0.44
18:O:187:LEU:HD11	39:O:613:II0:C27	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:168:SER:HB3	26:P:607:CLA:HBA1	1.99	0.44
26:Q:311:CLA:HMB1	39:Q:313:II0:C20	2.48	0.44
22:S:99:TRP:CZ2	26:S:605:CLA:HED3	2.53	0.44
22:S:105:LEU:O	22:S:109:ARG:HG3	2.18	0.44
2:B:74:SER:O	2:B:88:PRO:HB3	2.18	0.43
2:B:103:LEU:O	2:B:107:LEU:HG	2.18	0.43
2:b:6:TYR:HB2	34:b:621:LHG:H382	2.00	0.43
17:1:148:LEU:HD13	34:1:620:LHG:H291	2.00	0.43
17:1:204:GLY:HA3	40:1:619:IHT:C40	2.48	0.43
26:3:307:CLA:C4	20:4:80:TRP:CZ3	3.01	0.43
20:4:78:MET:CE	26:4:302:CLA:HMA2	2.48	0.43
20:4:129:GLN:NE2	39:4:317:II0:C15	2.81	0.43
21:5:83:VAL:CG1	26:5:607:CLA:HED1	2.47	0.43
22:6:99:TRP:CZ2	26:6:605:CLA:HED3	2.53	0.43
23:G:143:PRO:HD2	19:P:76:LYS:HG3	2.00	0.43
21:R:113:PHE:CE1	39:R:316:II0:C15	3.01	0.43
26:g:401:CLA:H112	26:g:401:CLA:H142	1.76	0.43
3:C:393:LYS:HG3	3:C:397:ASP:HB2	2.01	0.43
4:D:195:PHE:HB3	4:D:280:THR:O	2.19	0.43
3:c:374:ASP:CG	41:c:607:HOH:O	2.60	0.43
3:c:393:LYS:HG3	3:c:397:ASP:HB2	2.00	0.43
26:c:504:CLA:H12	26:c:504:CLA:H51	1.84	0.43
4:d:264:ARG:NH2	4:d:268:PHE:HB2	2.33	0.43
8:i:6:ILE:CD1	13:w:38:LEU:HA	2.48	0.43
8:i:35:LYS:HA	8:i:35:LYS:HD2	1.81	0.43
17:N:75:PRO:HG2	39:N:616:II0:C06	2.48	0.43
17:N:151:LEU:CD2	39:O:614:II0:C17	2.96	0.43
26:N:607:CLA:HHC	26:N:607:CLA:HBB1	2.00	0.43
18:2:101:GLY:O	18:2:102:PHE:C	2.56	0.43
18:2:109:THR:CG2	26:2:304:CLA:OBD	2.60	0.43
19:3:82:GLU:HB2	26:3:301:CLA:C1B	2.48	0.43
21:5:51:VAL:HG22	26:5:601:CLA:C4C	2.48	0.43
21:5:97:LEU:HD13	26:5:604:CLA:H91	2.00	0.43
18:O:189:MET:HB3	39:O:614:II0:C42	2.48	0.43
19:P:138:ILE:HG12	19:P:145:LEU:HD11	2.00	0.43
34:R:319:LHG:H142	26:S:601:CLA:CHC	2.48	0.43
3:C:145:TYR:CE1	33:C:520:LMG:HC61	2.53	0.43
17:1:155:PRO:HB2	18:2:54:LEU:HD11	2.00	0.43
18:2:191:MET:HB3	39:2:314:II0:C42	2.48	0.43
21:5:55:LYS:CE	33:5:619:LMG:C6	2.95	0.43
21:5:188:HIS:HD2	26:5:608:CLA:CBB	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:70:PRO:HB2	18:O:71:LEU:HD12	2.00	0.43
18:O:177:TYR:CE1	38:O:610:KC2:CGA	3.01	0.43
19:P:62:VAL:N	26:P:602:CLA:OBD	2.51	0.43
20:Q:138:TRP:CZ2	39:Q:319:II0:C39	3.00	0.43
26:Q:305:CLA:CMA	26:R:312:CLA:CAD	2.96	0.43
21:R:97:LEU:HD13	26:R:305:CLA:H91	2.00	0.43
22:S:67:MET:HE3	22:S:67:MET:HB3	1.76	0.43
26:b:615:CLA:H11	26:b:616:CLA:HBB2	2.00	0.43
3:c:179:LEU:HG	26:c:509:CLA:HED1	2.00	0.43
26:c:512:CLA:H61	26:c:512:CLA:H41	1.77	0.43
27:d:403:PHO:H3A	26:d:405:CLA:H142	2.00	0.43
17:1:145:ILE:HA	34:1:620:LHG:H223	2.00	0.43
17:N:73:PHE:CB	26:N:601:CLA:CMD	2.81	0.43
17:N:78:PHE:O	17:N:81:TRP:CZ3	2.71	0.43
17:N:135:GLN:OE1	17:N:137:ALA:HB2	2.18	0.43
17:N:215:ARG:HB3	17:N:219:GLU:OE1	2.18	0.43
34:N:621:LHG:H241	26:O:601:CLA:C4D	2.46	0.43
18:2:144:PHE:HE1	19:3:64:PHE:CZ	2.36	0.43
26:3:307:CLA:H52	26:4:308:CLA:HBA1	2.00	0.43
20:4:180:ARG:HH11	38:4:311:KC2:CGA	2.31	0.43
38:4:310:KC2:C3D	38:4:311:KC2:CMD	2.95	0.43
21:5:94:ILE:HD13	26:5:607:CLA:HBC3	2.01	0.43
21:5:148:ALA:HB2	22:6:69:PHE:CD2	2.54	0.43
21:5:205:ILE:HG13	21:5:220:ILE:HG23	2.00	0.43
26:G:401:CLA:CBA	26:S:610:CLA:H92	2.41	0.43
18:O:51:PHE:CD1	18:O:52:LEU:HG	2.53	0.43
19:P:58:LEU:HD12	19:P:75:LEU:HD13	2.00	0.43
26:P:608:CLA:H62	26:P:608:CLA:H41	1.55	0.43
21:R:216:ASN:ND2	21:R:218:LYS:HE3	2.33	0.43
26:R:303:CLA:H41	26:R:303:CLA:H62	1.58	0.43
22:S:68:PRO:HG2	26:S:601:CLA:HMB3	2.01	0.43
26:S:607:CLA:H41	26:S:607:CLA:H61	1.55	0.43
4:D:53:PHE:O	5:E:50:THR:OG1	2.35	0.43
3:c:100:LEU:HD13	3:c:103:LEU:HD22	2.01	0.43
3:c:101:ILE:O	3:c:105:HIS:ND1	2.43	0.43
3:c:132:HIS:CE1	33:c:521:LMG:H191	2.53	0.43
5:e:36:TRP:HZ3	6:f:35:THR:HG22	1.83	0.43
17:N:204:GLY:CA	40:N:619:IHT:C39	2.97	0.43
18:2:57:PRO:HG2	18:2:71:ASP:HB3	2.01	0.43
26:2:306:CLA:H61	26:2:306:CLA:H2	1.77	0.43
19:3:132:THR:O	19:3:136:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:209:GLN:HE22	26:3:308:CLA:CGD	2.32	0.43
20:4:90:ARG:HB3	39:4:317:II0:C20	2.48	0.43
19:P:106:LEU:HD13	39:P:614:II0:C21	2.49	0.43
19:P:163:ASP:OD1	39:P:612:II0:O02	2.36	0.43
19:P:187:LEU:CG	39:P:612:II0:C27	2.97	0.43
21:R:188:HIS:HD2	26:R:309:CLA:CBB	2.32	0.43
22:S:98:ARG:HG3	22:S:178:ALA:HB2	2.00	0.43
26:S:604:CLA:H152	26:S:604:CLA:H112	1.69	0.43
26:S:604:CLA:H2	26:S:604:CLA:H62	1.67	0.43
26:B:609:CLA:H141	26:B:609:CLA:H161	1.79	0.43
12:T:24:ARG:HD2	41:T:101:HOH:O	2.18	0.43
1:a:308:ASP:OD1	1:a:312:ARG:N	2.51	0.43
2:b:71:VAL:HG23	26:b:606:CLA:HMA2	2.00	0.43
14:x:1:MET:CE	26:1:607:CLA:HED1	2.48	0.43
20:4:147:PHE:HA	26:4:308:CLA:HMA2	2.01	0.43
26:4:312:CLA:HMB1	39:4:314:II0:C20	2.48	0.43
26:6:610:CLA:H101	26:6:610:CLA:H13	1.83	0.43
21:R:60:LEU:HA	21:R:60:LEU:HD12	1.80	0.43
21:R:90:LYS:O	21:R:91:HIS:C	2.61	0.43
1:A:131:TRP:CZ3	26:C:506:CLA:HAA2	2.54	0.43
34:D:403:LHG:O3	34:D:403:LHG:O1	2.25	0.43
12:T:24:ARG:CD	41:T:101:HOH:O	2.66	0.43
13:W:43:VAL:HG21	19:3:127:TRP:CE3	2.54	0.43
3:c:458:HIS:HE1	26:c:510:CLA:NA	2.12	0.43
15:y:27:ILE:HD11	16:z:25:VAL:HA	2.00	0.43
18:2:84:LEU:HG	24:g:170:TRP:HZ3	1.80	0.43
19:3:96:PHE:CE1	39:3:311:II0:C09	2.99	0.43
20:4:67:PHE:CE2	39:4:315:II0:C18	3.01	0.43
20:4:107:PHE:HB3	20:4:108:PRO:CD	2.49	0.43
26:6:604:CLA:H2	26:6:604:CLA:H62	1.67	0.43
19:P:132:THR:O	19:P:136:ILE:HG13	2.19	0.43
21:R:85:ARG:NH1	21:R:186:ILE:HG21	2.33	0.43
26:S:609:CLA:H61	26:S:609:CLA:H2	1.70	0.43
5:E:23:ILE:H	5:E:23:ILE:CD1	2.30	0.43
11:M:5:VAL:HG21	11:m:5:VAL:O	2.19	0.43
1:a:331:MET:HG2	4:d:347:ARG:HA	2.01	0.43
3:c:353:LYS:CD	3:c:354:TYR:CD2	2.96	0.43
27:d:403:PHO:H51	26:d:405:CLA:H111	2.01	0.43
26:N:604:CLA:HMB1	39:N:616:II0:C19	2.49	0.43
26:N:614:CLA:CMC	40:N:619:IHT:C34	2.97	0.43
26:2:319:CLA:C4D	34:2:321:LHG:H251	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:301:CLA:HMC1	39:3:311:II0:C32	2.47	0.43
20:4:135:LEU:HB2	26:4:307:CLA:CB2	2.29	0.43
26:6:605:CLA:H2	26:6:605:CLA:H61	1.68	0.43
22:S:166:LEU:HD22	26:S:605:CLA:HMA1	2.01	0.43
1:A:26:ASN:O	4:D:254:GLN:NE2	2.52	0.43
1:A:176:ILE:HG12	26:D:404:CLA:HED1	2.00	0.43
2:B:223:GLN:HG2	2:B:227:ARG:HE	1.84	0.43
2:B:347:GLN:HE21	2:B:347:GLN:HB3	1.63	0.43
26:B:605:CLA:H101	26:B:605:CLA:H13	1.90	0.43
26:C:503:CLA:H62	26:C:503:CLA:H41	1.73	0.43
7:H:54:ILE:O	14:X:2:THR:HG21	2.18	0.43
13:W:51:LEU:HD21	26:3:305:CLA:HBA1	2.00	0.43
2:b:192:PRO:HG3	7:h:49:TYR:CZ	2.54	0.43
2:b:374:ASP:OD1	2:b:374:ASP:N	2.51	0.43
17:N:105:MET:C	17:N:217:PRO:HG3	2.44	0.43
18:2:179:TYR:CE1	38:2:310:KC2:CGA	3.01	0.43
22:6:67:MET:HB3	22:6:67:MET:HE3	1.76	0.43
18:O:119:ALA:C	18:O:121:ASP:N	2.72	0.43
21:R:83:VAL:HG13	26:R:308:CLA:HED1	2.01	0.43
21:R:223:PHE:HD1	21:R:223:PHE:HA	1.67	0.43
26:R:306:CLA:H192	34:R:319:LHG:C26	2.49	0.43
26:A:402:CLA:H142	26:A:402:CLA:H112	1.83	0.43
2:B:65:PHE:HE2	26:B:604:CLA:HED2	1.83	0.43
2:B:91:TRP:HA	2:B:91:TRP:CE3	2.53	0.43
2:B:411:PHE:HB3	2:B:416:THR:HG23	2.01	0.43
26:B:610:CLA:H193	26:B:612:CLA:HMD2	2.00	0.43
26:B:610:CLA:H43	26:B:612:CLA:H51	2.00	0.43
3:C:355:LEU:HB3	3:C:363:ILE:CD1	2.49	0.43
3:C:449:PHE:CZ	3:C:453:ILE:HD11	2.53	0.43
3:C:480:VAL:HG12	3:C:480:VAL:O	2.19	0.43
4:D:196:HIS:HD2	41:D:533:HOH:O	2.01	0.43
14:X:13:LEU:HD12	14:X:13:LEU:HA	1.88	0.43
16:Z:33:TRP:O	16:Z:33:TRP:CG	2.71	0.43
1:a:132:GLU:O	1:a:136:ARG:HG2	2.19	0.43
2:b:362:PHE:CE1	4:d:187:PHE:HB3	2.53	0.43
2:b:476:ARG:NH1	41:b:737:HOH:O	2.51	0.43
17:N:71:VAL:CG1	26:N:601:CLA:CGD	2.96	0.43
18:2:72:PRO:HB2	18:2:73:LEU:HD12	2.00	0.43
18:2:121:ALA:C	18:2:123:ASP:N	2.72	0.43
20:4:189:GLY:O	20:4:193:MET:HG3	2.19	0.43
26:4:301:CLA:H62	26:4:301:CLA:H41	1.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:4:303:CLA:H92	26:4:303:CLA:H62	1.78	0.43
34:G:403:LHG:H251	26:P:601:CLA:C4D	2.49	0.43
26:P:608:CLA:H12	26:Q:302:CLA:C1	2.46	0.43
20:Q:189:GLY:O	20:Q:193:MET:HG3	2.19	0.43
21:R:183:LEU:HD23	26:R:310:CLA:HED2	2.01	0.43
21:R:205:ILE:HG13	21:R:220:ILE:HG23	2.01	0.43
26:B:609:CLA:H43	26:B:610:CLA:HBB2	2.01	0.42
3:C:75:VAL:HG13	3:C:132:HIS:HD2	1.84	0.42
26:C:504:CLA:H151	26:C:511:CLA:HBB2	2.00	0.42
4:D:341:PRO:HD2	4:D:344:VAL:CG2	2.49	0.42
1:a:193:LEU:HD11	26:a:402:CLA:HMC2	2.01	0.42
2:b:201:HIS:HB2	26:b:602:CLA:CHB	2.49	0.42
26:b:611:CLA:H72	26:b:611:CLA:H112	1.78	0.42
4:d:196:HIS:HD2	41:d:532:HOH:O	2.02	0.42
17:N:231:LEU:CD1	17:N:232:PRO:HD2	2.36	0.42
18:2:215:PHE:CE1	26:2:311:CLA:HED3	2.53	0.42
34:5:618:LHG:H142	26:6:601:CLA:CHC	2.48	0.42
23:G:109:SER:O	23:G:113:LYS:HG3	2.19	0.42
18:O:57:ASN:HD21	18:O:75:ASP:HA	1.84	0.42
26:O:608:CLA:H202	26:O:608:CLA:H162	1.84	0.42
20:Q:147:PHE:HA	26:Q:307:CLA:HMA2	2.01	0.42
21:R:174:ASN:HB3	21:R:177:LYS:CE	2.49	0.42
21:R:182:GLN:N	26:R:309:CLA:HMA1	2.34	0.42
1:A:75:ASN:HA	4:D:300:GLN:HE22	1.84	0.42
1:A:193:LEU:HD11	26:A:402:CLA:HMC2	2.01	0.42
3:C:477:ASN:OD1	3:C:477:ASN:N	2.53	0.42
13:W:40:VAL:HB	13:W:41:PRO:HD3	2.01	0.42
1:a:131:TRP:CZ2	3:c:463:ARG:HG3	2.55	0.42
1:a:288:LEU:HD21	3:c:449:PHE:HD2	1.84	0.42
26:a:402:CLA:HBD	26:d:402:CLA:HAC2	2.01	0.42
2:b:187:PRO:CB	7:h:55:ILE:HG21	2.48	0.42
41:b:719:HOH:O	4:d:325:ARG:NH1	2.51	0.42
3:c:383:LEU:HD22	3:c:394:ILE:HA	2.00	0.42
3:c:449:PHE:CZ	3:c:453:ILE:HD11	2.53	0.42
33:d:411:LMG:H191	33:d:411:LMG:H161	1.76	0.42
6:f:34:ILE:O	6:f:38:GLN:HG2	2.19	0.42
17:N:77:GLY:O	17:N:78:PHE:C	2.59	0.42
17:N:128:LEU:HD12	17:N:128:LEU:HA	1.71	0.42
18:2:71:ASP:HA	39:2:314:II0:C12	2.49	0.42
34:2:321:LHG:H223	26:3:308:CLA:HBA1	2.00	0.42
19:3:192:LEU:C	19:3:192:LEU:HD23	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:4:307:CLA:HHC	26:4:307:CLA:HBB1	2.01	0.42
22:6:80:LEU:HD11	22:6:97:ILE:HD13	2.01	0.42
22:6:155:GLY:O	22:6:158:GLU:HB2	2.19	0.42
23:G:136:GLY:HA2	19:P:56:GLY:O	2.20	0.42
19:P:86:GLY:O	19:P:90:MET:N	2.51	0.42
20:Q:101:VAL:O	20:Q:104:VAL:HG22	2.20	0.42
21:R:200:VAL:HG21	40:R:317:IHT:C31	2.49	0.42
22:S:80:LEU:HD11	22:S:97:ILE:HD13	2.01	0.42
1:A:132:GLU:O	1:A:136:ARG:HG2	2.19	0.42
1:A:153:ALA:HB1	26:A:402:CLA:HED1	2.00	0.42
2:B:135:LEU:O	2:B:139:PHE:N	2.37	0.42
26:B:603:CLA:H61	26:B:603:CLA:H41	1.72	0.42
14:X:1:MET:HE2	26:N:607:CLA:CED	2.42	0.42
26:b:610:CLA:H43	26:b:612:CLA:H51	2.01	0.42
3:c:189:LEU:HD22	26:c:503:CLA:C1D	2.49	0.42
17:1:154:ILE:CG2	17:1:155:PRO:HD3	2.49	0.42
26:1:606:CLA:C4A	26:2:311:CLA:CGA	2.96	0.42
17:N:67:LEU:HB2	26:N:602:CLA:CED	2.50	0.42
17:N:141:LEU:HB3	26:N:607:CLA:HBC1	1.99	0.42
17:N:173:PHE:H	26:N:609:CLA:CAD	2.28	0.42
17:N:220:PHE:CE1	38:N:612:KC2:C3A	3.02	0.42
18:2:199:HIS:O	18:2:200:GLN:C	2.62	0.42
26:2:308:CLA:HBA2	26:2:308:CLA:H3A	1.53	0.42
19:3:58:LEU:HD12	19:3:75:LEU:HD13	2.00	0.42
19:3:187:LEU:HG	39:3:310:II0:C27	2.50	0.42
21:5:174:ASN:HB3	21:5:177:LYS:CE	2.49	0.42
18:O:91:ARG:HA	18:O:94:MET:HE2	2.01	0.42
19:P:192:LEU:HD23	19:P:192:LEU:C	2.44	0.42
19:P:216:ILE:N	26:P:610:CLA:HED1	2.34	0.42
20:Q:153:MET:HB3	20:Q:153:MET:HE2	1.74	0.42
26:Q:306:CLA:HHC	26:Q:306:CLA:HBB1	2.01	0.42
21:R:94:ILE:HD13	26:R:308:CLA:HBC3	2.01	0.42
26:R:306:CLA:C1	26:S:609:CLA:HAA1	2.46	0.42
22:S:155:GLY:O	22:S:158:GLU:HB2	2.19	0.42
26:B:605:CLA:H92	26:B:605:CLA:H61	1.77	0.42
3:C:189:LEU:HD22	26:C:502:CLA:C1D	2.49	0.42
34:D:403:LHG:HC91	34:L:101:LHG:HC81	2.00	0.42
27:D:405:PHO:H3A	26:D:407:CLA:H142	2.00	0.42
34:D:410:LHG:H251	34:D:410:LHG:H281	1.87	0.42
35:H:102:DGD:O5D	35:H:102:DGD:O4D	2.37	0.42
16:Z:35:LYS:H	16:Z:35:LYS:HG2	1.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:330:VAL:HG21	4:d:327:TRP:CE2	2.53	0.42
4:d:86:HIS:HB2	35:h:101:DGD:HG11	2.02	0.42
4:d:195:PHE:HB3	4:d:280:THR:O	2.19	0.42
33:d:404:LMG:H171	33:d:404:LMG:H142	1.94	0.42
17:N:73:PHE:CD1	26:N:601:CLA:HAC1	2.38	0.42
18:2:93:ARG:HA	18:2:96:MET:HE2	2.01	0.42
18:2:115:LYS:HE2	18:2:115:LYS:HB3	1.70	0.42
20:4:132:MET:HE2	20:4:135:LEU:HD12	2.00	0.42
20:4:155:GLN:HG3	24:g:125:VAL:HG13	2.00	0.42
26:O:603:CLA:HAB	39:O:614:II0:C42	2.50	0.42
20:Q:107:PHE:HB3	20:Q:108:PRO:CD	2.49	0.42
21:R:169:LEU:HD12	39:R:314:II0:C06	2.50	0.42
26:R:309:CLA:H142	26:R:309:CLA:H111	1.86	0.42
22:S:72:ARG:HA	22:S:73:PRO:HD3	1.91	0.42
26:g:401:CLA:H2	26:g:401:CLA:H62	1.75	0.42
26:B:611:CLA:H61	26:B:611:CLA:H2	1.83	0.42
3:C:179:LEU:HG	26:C:508:CLA:HED1	2.01	0.42
34:L:101:LHG:H342	11:M:17:VAL:HG12	2.01	0.42
26:a:402:CLA:H72	26:a:402:CLA:H111	1.80	0.42
27:a:404:PHO:H92	27:a:404:PHO:H62	1.75	0.42
26:b:607:CLA:H162	26:b:607:CLA:H141	1.74	0.42
26:b:611:CLA:H202	26:b:611:CLA:H161	1.88	0.42
17:1:205:GLY:O	17:1:209:HIS:CG	2.73	0.42
17:N:78:PHE:HD1	17:N:81:TRP:HZ3	1.66	0.42
18:2:90:LYS:HG2	18:2:94:PHE:HE2	1.85	0.42
18:2:113:PHE:HE1	39:2:316:II0:C15	2.33	0.42
20:4:135:LEU:HD23	20:4:135:LEU:HA	1.82	0.42
21:5:182:GLN:N	26:5:608:CLA:HMA1	2.34	0.42
22:6:166:LEU:HD22	26:6:605:CLA:HMA1	2.01	0.42
18:O:69:ASP:HA	39:O:614:II0:C12	2.49	0.42
2:B:70:GLY:HA2	2:B:178:VAL:HG11	2.01	0.42
26:B:610:CLA:H11	26:B:612:CLA:H191	2.01	0.42
5:E:58:THR:O	5:E:59:GLN:C	2.62	0.42
1:a:153:ALA:HB1	26:a:402:CLA:HED1	2.01	0.42
1:a:259:ILE:HG22	1:a:260:PHE:H	1.84	0.42
2:b:253:THR:HG22	35:h:101:DGD:HBH1	2.02	0.42
2:b:377:ILE:HD11	4:d:339:ILE:HB	2.01	0.42
26:b:615:CLA:H112	26:b:615:CLA:H152	1.77	0.42
26:c:505:CLA:H151	26:c:512:CLA:HBB2	2.01	0.42
26:d:402:CLA:H3A	26:d:402:CLA:HBA2	1.78	0.42
26:d:406:CLA:H2	14:x:11:SER:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:t:7:THR:O	12:t:11:ILE:HG12	2.19	0.42
17:N:81:TRP:CZ2	17:N:82:LEU:CD2	2.96	0.42
18:2:153:LEU:CD1	24:g:169:ALA:CA	2.98	0.42
22:6:65:ASN:OD1	22:6:72:ARG:HB2	2.20	0.42
22:6:68:PRO:HG2	26:6:601:CLA:HMB3	2.00	0.42
18:O:68:PHE:HE1	40:O:616:IHT:C13	2.30	0.42
18:O:209:GLN:NE2	26:O:611:CLA:O1D	2.53	0.42
26:P:610:CLA:H62	26:P:610:CLA:H41	1.83	0.42
20:Q:90:ARG:HB3	39:Q:316:II0:C20	2.48	0.42
21:R:82:ARG:NH1	21:R:152:THR:O	2.50	0.42
22:S:68:PRO:HG2	26:S:601:CLA:CMB	2.50	0.42
1:A:258:LEU:C	1:A:259:ILE:HD13	2.44	0.42
2:B:366:PHE:O	41:B:711:HOH:O	2.22	0.42
3:C:294:SER:OG	3:C:448:GLY:O	2.33	0.42
34:D:403:LHG:HC81	34:D:403:LHG:H362	2.02	0.42
27:D:405:PHO:H51	26:D:407:CLA:H111	2.00	0.42
9:K:23:VAL:O	9:K:26:VAL:HG22	2.19	0.42
1:a:131:TRP:CZ3	26:c:507:CLA:HAA2	2.54	0.42
26:b:612:CLA:H91	26:b:613:CLA:HAB	2.02	0.42
26:b:613:CLA:H61	26:b:613:CLA:H102	1.64	0.42
4:d:230:THR:OG1	41:d:502:HOH:O	2.05	0.42
18:2:188:ARG:NH1	39:2:315:II0:O02	2.43	0.42
26:2:302:CLA:H142	26:2:312:CLA:CBB	2.49	0.42
26:2:319:CLA:HHD	28:3:313:WVN:C14	2.49	0.42
19:3:64:PHE:CE2	39:3:311:II0:C17	3.03	0.42
20:4:152:GLN:NE2	33:5:619:LMG:O3	2.43	0.42
21:5:125:LEU:HG	26:5:604:CLA:HAA2	2.02	0.42
21:5:169:LEU:HD12	39:5:613:II0:C06	2.50	0.42
20:Q:180:ARG:HH11	38:Q:310:KC2:CGA	2.31	0.42
26:Q:301:CLA:H161	26:Q:301:CLA:H141	1.87	0.42
21:R:125:LEU:HG	26:R:305:CLA:HAA2	2.02	0.42
22:S:106:LYS:NZ	22:S:158:GLU:OE1	2.52	0.42
2:B:151:PHE:O	2:B:151:PHE:CG	2.72	0.42
3:C:383:LEU:HD22	3:C:394:ILE:HA	2.00	0.42
4:D:122:ILE:HD11	35:H:102:DGD:HAH2	2.02	0.42
26:D:407:CLA:HBA1	26:D:407:CLA:H3A	1.62	0.42
26:b:615:CLA:H202	26:b:615:CLA:H161	1.81	0.42
16:z:2:VAL:HG22	16:z:61:VAL:HG13	2.02	0.42
17:1:155:PRO:HG2	18:2:54:LEU:HD11	2.02	0.42
17:N:184:THR:HB	17:N:188:ARG:HH12	1.84	0.42
19:3:108:GLY:C	19:3:110:ASP:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:4:306:CLA:HED1	21:5:223:PHE:HD2	1.71	0.42
26:4:306:CLA:HED2	21:5:223:PHE:CE2	2.50	0.42
23:G:138:LEU:HD12	23:G:138:LEU:O	2.19	0.42
18:O:55:PRO:HG2	18:O:69:ASP:HB3	2.01	0.42
19:P:73:PHE:CE2	26:P:603:CLA:H12	2.55	0.42
21:R:52:PRO:HG2	26:R:302:CLA:C2B	2.50	0.42
22:S:65:ASN:OD1	22:S:72:ARG:HB2	2.20	0.42
22:S:102:GLU:OE1	22:S:179:GLY:HA2	2.20	0.42
3:C:100:LEU:HD13	3:C:103:LEU:HD22	2.01	0.42
29:D:409:PL9:H122	29:D:409:PL9:H101	1.89	0.42
13:W:43:VAL:HG21	19:3:127:TRP:CZ3	2.54	0.42
16:Z:7:LEU:O	16:Z:11:MET:HG3	2.20	0.42
17:1:189:GLN:HG3	26:1:609:CLA:HMA2	2.01	0.42
17:N:95:GLY:O	17:N:99:MET:HG3	2.20	0.42
26:3:307:CLA:HMC3	39:3:310:II0:C31	2.50	0.42
26:3:309:CLA:H3A	26:3:309:CLA:HBA2	1.72	0.42
20:4:114:PHE:HE2	38:4:305:KC2:CBB	2.33	0.42
20:4:154:LEU:CB	24:g:125:VAL:CB	2.65	0.42
22:S:215:GLY:O	22:S:216:MET:C	2.62	0.42
1:A:202:VAL:HG22	26:A:402:CLA:C1B	2.50	0.42
26:A:402:CLA:H122	27:A:404:PHO:H3A	2.01	0.42
2:B:366:PHE:HA	2:B:367:PRO:HD3	1.92	0.42
26:B:605:CLA:H142	26:B:610:CLA:H2	2.02	0.42
26:B:613:CLA:H62	26:B:613:CLA:H2	1.69	0.42
3:C:74:MET:HE3	26:C:511:CLA:HAB	2.02	0.42
3:C:458:HIS:HE1	26:C:509:CLA:NA	2.13	0.42
4:D:59:THR:HG22	4:D:81:ALA:HB2	2.02	0.42
26:D:408:CLA:H2	14:X:11:SER:O	2.19	0.42
3:c:473:ILE:HG21	3:c:478:GLU:HG3	2.01	0.42
17:N:71:VAL:O	17:N:71:VAL:HG12	2.19	0.42
18:2:83:VAL:HG12	24:g:170:TRP:CD2	2.42	0.42
18:2:142:GLU:O	18:2:143:LEU:C	2.63	0.42
21:5:81:ILE:HD12	21:5:81:ILE:HA	1.95	0.42
21:5:150:PHE:HZ	24:g:103:PHE:CE2	2.38	0.42
34:G:403:LHG:C6	26:P:601:CLA:HBD	2.50	0.42
18:O:126:GLN:O	26:O:605:CLA:HED2	2.20	0.42
20:Q:99:MET:HE3	20:Q:119:MET:CE	2.45	0.42
20:Q:124:ASP:O	20:Q:127:VAL:HG22	2.20	0.42
20:Q:132:MET:HE2	20:Q:135:LEU:HD12	2.00	0.42
21:R:68:VAL:CG2	26:R:303:CLA:HMD1	2.49	0.42
26:A:405:CLA:H42	13:W:31:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:ALA:HB1	23:G:172:PRO:CG	2.40	0.41
4:D:134:LEU:HA	4:D:134:LEU:HD22	1.77	0.41
5:E:37:LEU:O	5:E:38:PHE:C	2.62	0.41
4:d:192:LEU:O	10:l:35:TYR:OH	2.25	0.41
10:l:8:LYS:HB3	10:l:8:LYS:HE2	1.64	0.41
17:1:151:LEU:HD13	26:2:301:CLA:CAC	2.50	0.41
17:1:154:ILE:HB	26:1:608:CLA:HMA1	2.02	0.41
17:1:223:ASN:HD22	17:1:228:LYS:HE3	1.85	0.41
17:N:77:GLY:O	17:N:80:ASN:N	2.38	0.41
17:N:126:MET:O	17:N:127:LYS:C	2.63	0.41
17:N:159:GLN:CD	18:O:53:LYS:CD	2.74	0.41
17:N:191:VAL:O	17:N:192:GLU:C	2.63	0.41
26:N:602:CLA:H142	26:N:602:CLA:H112	1.86	0.41
26:N:603:CLA:CAB	39:N:616:II0:C40	2.98	0.41
39:N:620:II0:C20	26:O:601:CLA:CMD	2.95	0.41
18:2:59:ASN:HD21	18:2:77:ASP:HA	1.83	0.41
18:2:211:GLN:NE2	26:2:311:CLA:O1D	2.53	0.41
26:2:319:CLA:HBD	34:2:321:LHG:C6	2.50	0.41
26:3:307:CLA:CMD	26:4:303:CLA:H93	2.44	0.41
26:3:307:CLA:CMB	39:3:310:II0:C36	2.95	0.41
20:4:120:THR:CG2	40:4:318:IHT:C17	2.97	0.41
26:5:602:CLA:H41	26:5:602:CLA:H62	1.58	0.41
22:6:73:PRO:HA	22:6:74:PRO:HD3	1.84	0.41
22:6:101:ARG:HD2	22:6:101:ARG:HA	1.89	0.41
26:O:608:CLA:H71	39:O:613:II0:C30	2.50	0.41
33:R:301:LMG:H121	33:R:301:LMG:H331	2.02	0.41
2:B:201:HIS:HB2	26:B:602:CLA:CHB	2.50	0.41
2:B:369:ILE:CG2	2:B:377:ILE:HD12	2.50	0.41
2:B:371:VAL:HG12	2:B:377:ILE:HD12	2.01	0.41
34:C:518:LHG:C23	13:W:53:TYR:HE1	2.33	0.41
2:b:201:HIS:HB2	26:b:602:CLA:C1B	2.50	0.41
17:1:144:TRP:HB3	34:1:620:LHG:C21	2.38	0.41
17:N:199:ALA:HB2	39:N:615:II0:C35	2.50	0.41
26:2:303:CLA:HAB	39:2:314:II0:C42	2.50	0.41
19:3:80:GLU:HB2	19:3:151:PHE:HZ	1.86	0.41
28:3:313:WVN:C08	28:3:313:WVN:C09	2.98	0.41
20:4:124:ASP:O	20:4:127:VAL:HG22	2.20	0.41
20:4:155:GLN:H	24:g:125:VAL:HG11	1.79	0.41
22:6:148:TRP:O	22:6:152:PHE:HD2	2.03	0.41
18:O:83:ARG:HH11	18:O:83:ARG:HD2	1.68	0.41
18:O:88:LYS:HG2	18:O:92:PHE:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:89:HIS:O	18:O:90:GLY:C	2.62	0.41
26:P:607:CLA:H91	26:P:607:CLA:H112	1.78	0.41
22:S:184:ASP:N	22:S:185:PRO:HD3	2.35	0.41
1:A:34:GLY:HA2	1:A:37:MET:HB3	2.02	0.41
29:A:407:PL9:HC8	29:A:407:PL9:HC2	1.92	0.41
26:B:615:CLA:H112	26:B:615:CLA:H152	1.77	0.41
4:D:127:ARG:CG	41:D:519:HOH:O	2.62	0.41
16:Z:25:VAL:O	16:Z:29:SER:HB3	2.21	0.41
26:a:402:CLA:H122	27:a:404:PHO:H3A	2.01	0.41
4:d:348:GLY:HA2	4:d:351:LEU:HD12	2.03	0.41
17:1:86:TRP:HH2	26:1:608:CLA:HAA2	1.84	0.41
17:1:151:LEU:HB3	26:2:301:CLA:HBC1	2.00	0.41
18:2:70:PHE:CE2	39:2:314:II0:C14	3.03	0.41
18:2:85:ARG:HH11	18:2:85:ARG:HD2	1.67	0.41
18:2:147:VAL:O	18:2:151:GLU:HG2	2.20	0.41
26:2:302:CLA:CBB	26:2:303:CLA:CHB	2.98	0.41
20:4:202:HIS:HE1	26:4:312:CLA:NB	2.16	0.41
21:5:183:LEU:HD23	26:5:609:CLA:HED2	2.00	0.41
33:5:619:LMG:H121	33:5:619:LMG:H331	2.02	0.41
18:O:68:PHE:CE2	39:O:614:II0:C14	3.03	0.41
19:P:108:GLY:C	19:P:110:ASP:H	2.28	0.41
2:B:201:HIS:HB2	26:B:602:CLA:C1B	2.51	0.41
2:B:478:VAL:HG21	4:D:136:GLY:O	2.20	0.41
3:C:149:ILE:HD13	16:Z:27:LEU:HD22	2.03	0.41
26:C:506:CLA:H162	26:C:506:CLA:H122	1.87	0.41
4:D:128:GLN:NE2	27:D:405:PHO:OBD	2.53	0.41
1:a:202:VAL:HG22	26:a:402:CLA:C1B	2.50	0.41
2:b:22:VAL:HG11	26:b:614:CLA:HMA1	2.03	0.41
2:b:341:LEU:HD12	2:b:429:VAL:HG12	2.02	0.41
2:b:341:LEU:HD22	2:b:406:LEU:HD13	2.01	0.41
26:b:608:CLA:H152	26:b:609:CLA:H172	2.02	0.41
26:b:609:CLA:H43	26:b:610:CLA:HBB2	2.01	0.41
17:N:75:PRO:HD2	39:N:616:II0:C08	2.51	0.41
17:N:95:GLY:N	17:N:200:MET:HE2	2.35	0.41
18:2:144:PHE:HE1	19:3:64:PHE:CE1	2.38	0.41
19:3:73:PHE:CE2	26:3:302:CLA:H12	2.55	0.41
26:4:301:CLA:C5	26:4:303:CLA:H101	2.38	0.41
26:4:308:CLA:H92	26:4:308:CLA:H62	1.84	0.41
21:5:174:ASN:HB3	21:5:177:LYS:HE2	2.03	0.41
34:G:403:LHG:H321	18:O:139:VAL:HG22	2.02	0.41
18:O:95:LEU:CD1	39:O:615:II0:C28	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:145:VAL:O	18:O:149:GLU:HG2	2.20	0.41
26:O:605:CLA:HBA2	26:P:610:CLA:HAA1	2.02	0.41
22:S:80:LEU:HB3	22:S:101:ARG:NH1	2.35	0.41
22:S:134:THR:HG22	22:S:224:GLY:O	2.20	0.41
22:S:195:LEU:HD12	26:S:606:CLA:HMA2	2.02	0.41
4:D:293:ARG:HG3	4:D:295:TYR:HB2	2.02	0.41
5:E:36:TRP:HZ3	6:F:35:THR:HG22	1.85	0.41
34:L:101:LHG:H341	34:L:101:LHG:H371	1.83	0.41
1:a:101:SER:H	1:a:104:GLU:HG2	1.85	0.41
3:c:74:MET:HE3	26:c:512:CLA:HAB	2.03	0.41
17:N:46:LEU:HD23	17:N:46:LEU:HA	1.89	0.41
17:N:48:GLY:O	17:N:51:THR:HB	2.20	0.41
17:N:155:PRO:HB2	18:O:52:LEU:HD21	1.95	0.41
17:N:212:LEU:HD21	26:N:614:CLA:HED3	2.03	0.41
17:N:212:LEU:HD11	39:N:617:II0:C15	2.51	0.41
26:N:614:CLA:HAC1	40:N:619:IHT:C26	2.46	0.41
26:2:302:CLA:H192	26:2:302:CLA:H162	1.92	0.41
26:3:306:CLA:H121	39:3:310:II0:C28	2.50	0.41
20:4:95:ALA:HA	39:4:315:II0:C19	2.50	0.41
20:4:119:MET:HG3	20:4:203:PHE:CD1	2.56	0.41
33:4:319:LMG:HC61	39:4:320:II0:C11	2.50	0.41
22:6:184:ASP:N	22:6:185:PRO:HD3	2.35	0.41
18:O:85:ALA:O	18:O:86:GLU:C	2.63	0.41
26:O:602:CLA:CBB	26:O:603:CLA:CHB	2.98	0.41
19:P:103:GLN:NE2	19:P:112:LYS:HD3	2.35	0.41
33:R:301:LMG:H161	33:R:301:LMG:H132	1.85	0.41
26:B:615:CLA:H92	26:B:615:CLA:H61	1.85	0.41
3:C:109:LEU:HD12	3:C:109:LEU:HA	1.82	0.41
4:D:26:PHE:HB3	6:F:16:ARG:HD2	2.02	0.41
11:M:3:VAL:CG1	11:M:4:SER:H	2.34	0.41
17:N:119:THR:HG22	17:N:120:PHE:N	2.36	0.41
17:N:143:LEU:HD11	26:O:602:CLA:H201	2.01	0.41
26:N:606:CLA:C1	18:O:213:PHE:HE1	2.32	0.41
18:2:153:LEU:CD1	24:g:169:ALA:HB2	2.42	0.41
19:3:196:LEU:HD22	28:3:313:WVN:C19	2.51	0.41
21:5:83:VAL:HG13	26:5:607:CLA:HED1	2.01	0.41
21:5:171:GLN:O	21:5:174:ASN:N	2.54	0.41
22:6:134:THR:HG22	22:6:224:GLY:O	2.20	0.41
18:O:88:LYS:HE3	18:O:88:LYS:HB2	1.83	0.41
19:P:80:GLU:HB2	19:P:151:PHE:HZ	1.86	0.41
20:Q:78:MET:CE	26:Q:301:CLA:HMA2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Q:138:TRP:CH2	39:Q:319:II0:C41	3.04	0.41
20:Q:164:PHE:O	26:R:302:CLA:CBB	2.68	0.41
20:Q:180:ARG:HH22	38:Q:310:KC2:CGD	2.33	0.41
22:S:165:LYS:HA	22:S:170:ASP:CG	2.46	0.41
1:A:41:LEU:CD2	1:A:122:GLY:HA3	2.51	0.41
2:B:71:VAL:HG11	2:B:96:VAL:HG21	2.03	0.41
2:B:296:LEU:CD2	2:B:304:ARG:HD2	2.49	0.41
2:B:325:PHE:CG	10:L:35:TYR:HB3	2.56	0.41
2:B:341:LEU:HD12	2:B:429:VAL:HG12	2.02	0.41
2:B:469:HIS:HE1	26:B:611:CLA:NA	2.19	0.41
5:E:60:GLU:CD	5:E:60:GLU:H	2.29	0.41
1:a:93:PHE:HZ	26:a:405:CLA:HAA2	1.85	0.41
2:b:266:GLU:HB2	41:b:741:HOH:O	2.19	0.41
2:b:377:ILE:CD1	4:d:339:ILE:CG2	2.97	0.41
4:d:128:GLN:NE2	27:d:403:PHO:OBD	2.54	0.41
4:d:164:ALA:HB3	4:d:168:PHE:HE2	1.86	0.41
17:1:102:ALA:HB2	17:1:203:VAL:HG23	2.03	0.41
17:N:159:GLN:NE2	18:O:53:LYS:H	2.19	0.41
17:N:207:VAL:HG21	40:N:619:IHT:C28	2.51	0.41
26:N:614:CLA:HMC1	40:N:619:IHT:C31	2.51	0.41
18:2:83:VAL:CG2	18:2:153:LEU:HD21	2.50	0.41
18:2:98:ALA:O	18:2:99:THR:C	2.60	0.41
20:4:69:PRO:CD	39:4:315:II0:C08	2.97	0.41
20:4:153:MET:HB3	20:4:153:MET:HE2	1.74	0.41
21:5:153:ILE:HG21	24:g:110:ALA:CB	2.51	0.41
26:5:609:CLA:H141	26:5:609:CLA:H203	2.03	0.41
22:6:165:LYS:HA	22:6:170:ASP:CG	2.46	0.41
22:6:215:GLY:O	22:6:216:MET:C	2.62	0.41
22:6:223:THR:OG1	22:6:224:GLY:N	2.53	0.41
22:S:223:THR:OG1	22:S:224:GLY:N	2.53	0.41
24:g:117:CYS:HB3	24:g:122:TRP:CD1	2.56	0.41
26:A:405:CLA:HBC1	30:A:408:SQD:H312	2.02	0.41
3:C:353:LYS:HD2	3:C:353:LYS:HA	1.24	0.41
7:H:8:GLY:HA3	41:H:210:HOH:O	2.21	0.41
26:a:403:CLA:CHC	26:d:405:CLA:H2	2.51	0.41
2:b:343:HIS:HA	2:b:344:PRO:HD3	1.96	0.41
26:b:611:CLA:H92	26:b:611:CLA:H62	1.94	0.41
4:d:59:THR:HG22	4:d:81:ALA:HB2	2.02	0.41
6:f:14:THR:HG21	6:f:16:ARG:NH1	2.35	0.41
17:1:201:ILE:H	17:1:201:ILE:HG13	1.71	0.41
26:1:606:CLA:NA	26:2:311:CLA:O1A	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:159:GLN:HE22	18:O:53:LYS:H	1.68	0.41
18:2:116:MET:HE3	18:2:116:MET:HB2	1.81	0.41
18:2:179:TYR:O	18:2:180:ARG:C	2.63	0.41
19:3:89:CYS:HB2	19:3:192:LEU:CD1	2.51	0.41
21:5:60:LEU:HG	21:5:67:ASP:OD2	2.21	0.41
22:6:68:PRO:HG2	26:6:601:CLA:CMB	2.50	0.41
22:6:80:LEU:HB3	22:6:101:ARG:NH1	2.35	0.41
26:B:608:CLA:H152	26:B:609:CLA:H172	2.03	0.41
26:B:611:CLA:H92	26:B:611:CLA:H62	1.94	0.41
3:C:201:ASP:O	3:C:208:GLY:CA	2.69	0.41
30:D:401:SQD:H142	30:D:401:SQD:H171	1.93	0.41
26:D:404:CLA:H161	26:D:404:CLA:H141	1.82	0.41
34:D:410:LHG:H352	34:D:410:LHG:H322	1.89	0.41
2:b:65:PHE:HE2	26:b:604:CLA:HED2	1.85	0.41
2:b:192:PRO:HG3	7:h:49:TYR:CE2	2.56	0.41
26:b:601:CLA:H2	26:b:601:CLA:H3A	2.03	0.41
26:b:605:CLA:H142	26:b:610:CLA:H2	2.02	0.41
34:d:408:LHG:HC62	10:l:16:THR:HG23	2.03	0.41
35:h:101:DGD:O5D	35:h:101:DGD:O4D	2.37	0.41
17:1:99:MET:HE2	17:1:196:GLY:CA	2.51	0.41
26:1:603:CLA:HBC1	26:1:608:CLA:HBC2	2.03	0.41
17:N:54:ILE:HG23	26:N:601:CLA:C4C	2.51	0.41
26:2:303:CLA:H41	26:2:303:CLA:H61	1.90	0.41
19:3:103:GLN:NE2	19:3:112:LYS:HD3	2.35	0.41
19:3:155:ARG:NH1	19:3:160:LEU:HD23	2.34	0.41
26:3:307:CLA:CAB	39:3:310:II0:C41	2.98	0.41
26:3:307:CLA:CBC	26:4:303:CLA:H122	2.51	0.41
26:3:308:CLA:HED2	26:3:308:CLA:HBD	1.67	0.41
20:4:101:VAL:O	20:4:104:VAL:HG22	2.20	0.41
26:4:312:CLA:C2B	39:4:314:II0:C20	2.99	0.41
21:5:52:PRO:HG2	26:5:601:CLA:C2B	2.50	0.41
21:5:152:THR:OG1	21:5:157:ARG:HG3	2.21	0.41
23:G:138:LEU:HD12	23:G:141:ALA:HB2	2.02	0.41
34:G:403:LHG:C25	26:P:601:CLA:ND	2.80	0.41
18:O:197:HIS:O	18:O:198:GLN:C	2.62	0.41
26:O:603:CLA:HBC1	26:O:607:CLA:HAC1	2.02	0.41
26:O:605:CLA:HMA1	26:P:610:CLA:C3D	2.50	0.41
19:P:80:GLU:HB3	26:P:606:CLA:HED2	2.03	0.41
19:P:89:CYS:HB2	19:P:192:LEU:CD1	2.51	0.41
20:Q:202:HIS:HE1	26:Q:311:CLA:NB	2.16	0.41
22:S:148:TRP:O	22:S:152:PHE:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:g:105:LEU:O	24:g:109:SER:HB3	2.21	0.41
27:A:404:PHO:H62	27:A:404:PHO:H92	1.75	0.41
2:B:69:ILE:HD11	26:B:605:CLA:HBA1	2.03	0.41
28:B:617:WVN:C21	33:B:620:LMG:H111	2.51	0.41
34:L:101:LHG:H162	34:L:101:LHG:H131	1.92	0.41
26:b:612:CLA:HBA1	26:b:612:CLA:H3A	1.98	0.41
3:c:201:ASP:O	3:c:208:GLY:CA	2.69	0.41
33:c:521:LMG:H201	33:c:521:LMG:H382	2.03	0.41
17:1:159:GLN:CD	18:2:55:LYS:N	2.72	0.41
17:1:211:LEU:HB2	26:1:614:CLA:HED1	2.02	0.41
26:1:606:CLA:HMB2	26:2:311:CLA:NA	2.36	0.41
17:N:59:ARG:NH2	17:N:70:ASP:OD2	2.47	0.41
17:N:79:SER:HA	17:N:84:LEU:HD21	2.03	0.41
17:N:118:LYS:HE2	17:N:118:LYS:HB3	1.83	0.41
18:2:70:PHE:C	18:2:72:PRO:HD3	2.46	0.41
18:2:134:ILE:HD11	26:2:304:CLA:CBA	2.51	0.41
21:5:60:LEU:HA	21:5:60:LEU:HD12	1.80	0.41
26:O:605:CLA:C3C	39:O:615:II0:C37	2.99	0.41
19:P:96:PHE:CE1	39:P:613:II0:C19	3.04	0.41
26:P:609:CLA:H41	20:Q:150:ILE:CD1	2.51	0.41
26:Q:311:CLA:C2B	39:Q:313:II0:C20	2.99	0.41
22:S:111:CYS:SG	22:S:210:MET:HG2	2.61	0.41
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.90	0.40
3:C:59:VAL:HG22	3:C:62:LYS:HB2	2.03	0.40
26:C:504:CLA:H193	26:C:504:CLA:H161	1.77	0.40
5:E:82:LYS:HE3	5:E:82:LYS:HB2	1.86	0.40
1:a:333:GLU:H	1:a:333:GLU:HG3	1.66	0.40
2:b:373:LYS:H	2:b:373:LYS:HG3	1.55	0.40
4:d:109:LEU:HD12	4:d:109:LEU:HA	1.94	0.40
4:d:160:PRO:HB3	4:d:169:ALA:HB2	2.03	0.40
4:d:293:ARG:HG3	4:d:295:TYR:HB2	2.03	0.40
17:1:91:GLU:CD	17:1:197:ARG:HH21	2.29	0.40
18:2:51:VAL:HG23	18:2:54:LEU:HB2	2.03	0.40
18:2:83:VAL:HG21	24:g:169:ALA:CB	2.48	0.40
18:2:147:VAL:HG11	19:3:48:LEU:HD13	2.01	0.40
18:2:151:GLU:HG2	19:3:48:LEU:CD2	2.46	0.40
26:2:308:CLA:H162	26:2:308:CLA:H202	1.84	0.40
19:3:45:MET:HE2	19:3:45:MET:HB3	1.92	0.40
23:G:140:LYS:HB3	19:P:156:ALA:CB	2.51	0.40
18:O:132:ILE:HD11	26:O:604:CLA:CBA	2.51	0.40
18:O:133:ILE:HG12	26:O:606:CLA:HAC1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:178:ARG:HH11	18:O:178:ARG:HD3	1.76	0.40
18:O:198:GLN:NE2	39:O:613:II0:O01	2.49	0.40
33:O:617:LMG:H131	33:O:617:LMG:H161	1.86	0.40
20:Q:84:ALA:HA	26:Q:307:CLA:OBD	2.21	0.40
20:Q:114:PHE:HE2	38:Q:304:KC2:CBB	2.33	0.40
21:R:171:GLN:O	21:R:174:ASN:N	2.53	0.40
1:A:32:TRP:CD2	8:I:22:GLY:HA3	2.56	0.40
1:A:288:LEU:HD21	3:C:449:PHE:HD2	1.86	0.40
2:B:120:LEU:HD12	2:B:123:PHE:CE2	2.56	0.40
3:C:351:LEU:HD12	3:C:355:LEU:CD1	2.50	0.40
4:D:160:PRO:HB3	4:D:169:ALA:HB2	2.03	0.40
33:D:413:LMG:H231	33:D:413:LMG:H202	1.87	0.40
2:b:464:LEU:HD21	34:b:621:LHG:H261	2.02	0.40
26:c:504:CLA:H2	26:c:505:CLA:H193	2.04	0.40
29:d:407:PL9:H401	34:d:408:LHG:H202	2.03	0.40
34:d:408:LHG:H352	34:d:408:LHG:H322	1.90	0.40
17:l:95:GLY:HA2	17:l:200:MET:SD	2.60	0.40
34:N:621:LHG:H192	34:N:621:LHG:H162	1.60	0.40
18:2:91:HIS:O	18:2:92:GLY:C	2.62	0.40
18:2:137:TRP:CE3	34:2:321:LHG:H342	2.57	0.40
26:4:312:CLA:HBA1	26:4:312:CLA:H3A	1.86	0.40
21:5:90:LYS:O	21:5:91:HIS:C	2.61	0.40
21:5:178:LEU:O	21:5:179:GLU:C	2.64	0.40
18:O:58:LEU:HD12	18:O:58:LEU:N	2.37	0.40
18:O:58:LEU:HB3	18:O:65:ASP:OD1	2.21	0.40
18:O:68:PHE:C	18:O:70:PRO:HD3	2.46	0.40
18:O:81:VAL:CG2	18:O:151:LEU:HD21	2.50	0.40
18:O:140:GLU:O	18:O:141:LEU:C	2.63	0.40
26:O:608:CLA:H91	26:O:608:CLA:H112	1.85	0.40
20:Q:119:MET:HG3	20:Q:203:PHE:CD1	2.56	0.40
2:B:254:GLY:HA3	35:H:102:DGD:HB52	2.02	0.40
2:B:324:LEU:HD21	4:D:195:PHE:HE2	1.86	0.40
26:B:601:CLA:H2	26:B:601:CLA:H3A	2.02	0.40
4:D:278:LEU:HD12	27:D:405:PHO:HBC3	2.02	0.40
2:b:461:LEU:HD13	26:b:613:CLA:H111	2.03	0.40
26:b:605:CLA:H101	26:b:605:CLA:H13	1.89	0.40
26:b:605:CLA:HMA1	26:b:606:CLA:H3A	2.04	0.40
3:c:131:LEU:HD13	33:c:521:LMG:H372	2.03	0.40
3:c:176:GLY:HA2	3:c:262:GLY:HA2	2.02	0.40
3:c:291:VAL:HB	3:c:455:HIS:CD2	2.56	0.40
26:c:503:CLA:H93	26:c:503:CLA:HBB1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:504:CLA:H62	26:c:504:CLA:H41	1.73	0.40
17:1:138:MET:HA	17:1:138:MET:HE3	2.03	0.40
18:2:144:PHE:CZ	26:2:319:CLA:HAC1	2.51	0.40
26:2:305:CLA:HAC1	39:2:316:II0:C37	2.50	0.40
26:3:307:CLA:CBB	26:4:308:CLA:H101	2.51	0.40
20:4:206:THR:O	20:4:208:LYS:HG2	2.22	0.40
26:4:302:CLA:H142	26:4:302:CLA:H111	1.85	0.40
22:6:102:GLU:OE1	22:6:179:GLY:HA2	2.20	0.40
22:6:195:LEU:O	22:6:199:ARG:HG3	2.21	0.40
26:G:401:CLA:CMA	26:S:610:CLA:H43	2.52	0.40
18:O:113:LYS:HB3	18:O:113:LYS:HE2	1.71	0.40
20:Q:108:PRO:HD2	38:Q:304:KC2:CHD	2.52	0.40
20:Q:191:LEU:HD21	39:Q:313:II0:C28	2.52	0.40
26:Q:307:CLA:H92	26:Q:307:CLA:H62	1.84	0.40
26:R:310:CLA:H203	26:R:310:CLA:H141	2.03	0.40
1:A:176:ILE:HD11	29:D:409:PL9:H452	2.03	0.40
2:B:80:ILE:H	2:B:80:ILE:HG12	1.66	0.40
2:B:173:GLY:HA3	2:B:265:ILE:HD11	2.03	0.40
26:B:612:CLA:H91	26:B:613:CLA:HAB	2.03	0.40
3:C:37:ILE:HG22	9:K:45:ARG:CZ	2.33	0.40
3:C:291:VAL:HB	3:C:455:HIS:CD2	2.56	0.40
4:D:11:ARG:HB2	4:D:15:ASP:HB2	2.04	0.40
2:b:87:ASN:HA	2:b:88:PRO:HD2	1.91	0.40
17:N:152:THR:HB	26:O:601:CLA:HMC1	2.04	0.40
18:2:51:VAL:HG12	26:2:301:CLA:C1C	2.52	0.40
26:2:303:CLA:HBC1	26:2:307:CLA:HAC1	2.02	0.40
19:3:115:THR:HA	28:3:313:WVN:C04	2.51	0.40
22:6:195:LEU:HD12	26:6:606:CLA:HMA2	2.03	0.40
23:G:112:TYR:O	23:G:116:GLY:N	2.45	0.40
2:B:33:TRP:HB2	28:B:618:WVN:C34	2.51	0.40
2:B:408:GLY:CA	41:B:745:HOH:O	2.68	0.40
6:F:14:THR:OG1	6:F:15:PHE:N	2.53	0.40
1:a:258:LEU:C	1:a:259:ILE:HD13	2.47	0.40
2:b:63:MET:HA	2:b:66:MET:HE3	2.04	0.40
2:b:254:GLY:HA3	35:h:101:DGD:HB52	2.02	0.40
3:c:377:ALA:O	3:c:381:GLU:HG2	2.22	0.40
4:d:278:LEU:HD12	27:d:403:PHO:HBC3	2.02	0.40
35:h:101:DGD:HBN1	35:h:101:DGD:HBW2	1.93	0.40
17:1:137:ALA:O	17:1:141:LEU:HD12	2.21	0.40
17:1:152:THR:HB	26:2:301:CLA:HMC3	2.03	0.40
17:N:112:LYS:NZ	17:N:122:ASP:HA	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:N:606:CLA:HBB1	34:N:621:LHG:H172	0.52	0.40
26:N:606:CLA:HMA1	26:O:611:CLA:C3D	2.52	0.40
26:3:308:CLA:HBA1	26:3:308:CLA:H3A	1.90	0.40
26:3:308:CLA:HBB1	39:3:310:II0:C13	2.51	0.40
20:4:152:GLN:HE22	21:5:54:LEU:HB3	1.87	0.40
26:5:608:CLA:H142	26:5:608:CLA:H111	1.86	0.40
34:G:403:LHG:C3	26:P:601:CLA:HED1	2.52	0.40
18:O:49:VAL:HG12	26:O:601:CLA:C1C	2.51	0.40
26:O:601:CLA:C3C	40:O:616:IHT:C04	2.98	0.40
21:R:60:LEU:HG	21:R:67:ASP:OD2	2.21	0.40
22:S:152:PHE:O	22:S:153:THR:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	296/374 (79%)	291 (98%)	5 (2%)	0	100	100
1	a	305/374 (82%)	299 (98%)	6 (2%)	0	100	100
2	B	481/508 (95%)	472 (98%)	9 (2%)	0	100	100
2	b	479/508 (94%)	472 (98%)	7 (2%)	0	100	100
3	C	419/486 (86%)	415 (99%)	4 (1%)	0	100	100
3	c	415/486 (85%)	406 (98%)	9 (2%)	0	100	100
4	D	340/351 (97%)	332 (98%)	8 (2%)	0	100	100
4	d	339/351 (97%)	331 (98%)	8 (2%)	0	100	100
5	E	62/84 (74%)	57 (92%)	5 (8%)	0	100	100
5	e	62/84 (74%)	62 (100%)	0	0	100	100
6	F	27/42 (64%)	26 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	f	28/42 (67%)	28 (100%)	0	0	100	100
7	H	63/67 (94%)	58 (92%)	5 (8%)	0	100	100
7	h	63/67 (94%)	60 (95%)	3 (5%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
9	K	35/45 (78%)	34 (97%)	1 (3%)	0	100	100
9	k	35/45 (78%)	35 (100%)	0	0	100	100
10	L	35/38 (92%)	35 (100%)	0	0	100	100
10	l	35/38 (92%)	35 (100%)	0	0	100	100
11	M	34/118 (29%)	33 (97%)	1 (3%)	0	100	100
11	m	34/118 (29%)	32 (94%)	2 (6%)	0	100	100
12	T	28/32 (88%)	28 (100%)	0	0	100	100
12	t	28/32 (88%)	28 (100%)	0	0	100	100
13	W	43/121 (36%)	43 (100%)	0	0	100	100
13	w	43/121 (36%)	43 (100%)	0	0	100	100
14	X	32/39 (82%)	32 (100%)	0	0	100	100
14	x	32/39 (82%)	32 (100%)	0	0	100	100
15	Y	26/34 (76%)	25 (96%)	1 (4%)	0	100	100
15	y	26/34 (76%)	26 (100%)	0	0	100	100
16	Z	59/62 (95%)	56 (95%)	2 (3%)	1 (2%)	7	4
16	z	59/62 (95%)	59 (100%)	0	0	100	100
17	1	190/234 (81%)	181 (95%)	8 (4%)	1 (0%)	25	26
17	N	190/234 (81%)	182 (96%)	8 (4%)	0	100	100
18	2	170/215 (79%)	168 (99%)	2 (1%)	0	100	100
18	O	170/215 (79%)	168 (99%)	2 (1%)	0	100	100
19	3	178/182 (98%)	176 (99%)	2 (1%)	0	100	100
19	P	178/182 (98%)	176 (99%)	2 (1%)	0	100	100
20	4	158/200 (79%)	157 (99%)	1 (1%)	0	100	100
20	Q	158/200 (79%)	157 (99%)	1 (1%)	0	100	100
21	5	187/228 (82%)	185 (99%)	2 (1%)	0	100	100
21	R	187/228 (82%)	185 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	6	171/174 (98%)	166 (97%)	5 (3%)	0	100	100
22	S	171/174 (98%)	166 (97%)	5 (3%)	0	100	100
23	G	92/292 (32%)	88 (96%)	4 (4%)	0	100	100
24	g	91/292 (31%)	87 (96%)	4 (4%)	0	100	100
All	All	6320/7928 (80%)	6191 (98%)	127 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Z	33	TRP
17	1	116	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	246/305 (81%)	240 (98%)	6 (2%)	44	54
1	a	252/305 (83%)	243 (96%)	9 (4%)	30	37
2	B	384/403 (95%)	356 (93%)	28 (7%)	11	11
2	b	383/403 (95%)	362 (94%)	21 (6%)	18	20
3	C	337/387 (87%)	319 (95%)	18 (5%)	19	21
3	c	334/387 (86%)	328 (98%)	6 (2%)	54	66
4	D	274/280 (98%)	268 (98%)	6 (2%)	47	58
4	d	273/280 (98%)	266 (97%)	7 (3%)	41	51
5	E	56/73 (77%)	47 (84%)	9 (16%)	2	1
5	e	56/73 (77%)	54 (96%)	2 (4%)	30	37
6	F	24/37 (65%)	21 (88%)	3 (12%)	3	2
6	f	25/37 (68%)	22 (88%)	3 (12%)	4	3
7	H	55/57 (96%)	53 (96%)	2 (4%)	30	37
7	h	55/57 (96%)	53 (96%)	2 (4%)	30	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	33/36 (92%)	31 (94%)	2 (6%)	15	16
8	i	33/36 (92%)	30 (91%)	3 (9%)	7	7
9	K	30/36 (83%)	25 (83%)	5 (17%)	2	1
9	k	30/36 (83%)	23 (77%)	7 (23%)	0	0
10	L	34/35 (97%)	32 (94%)	2 (6%)	16	17
10	l	34/35 (97%)	31 (91%)	3 (9%)	8	7
11	M	29/83 (35%)	25 (86%)	4 (14%)	3	2
11	m	29/83 (35%)	26 (90%)	3 (10%)	6	5
12	T	26/28 (93%)	25 (96%)	1 (4%)	28	34
12	t	26/28 (93%)	26 (100%)	0	100	100
13	W	39/88 (44%)	34 (87%)	5 (13%)	3	2
13	w	39/88 (44%)	32 (82%)	7 (18%)	1	1
14	X	29/34 (85%)	26 (90%)	3 (10%)	6	5
14	x	29/34 (85%)	28 (97%)	1 (3%)	32	39
15	Y	23/29 (79%)	22 (96%)	1 (4%)	25	29
15	y	23/29 (79%)	23 (100%)	0	100	100
16	Z	49/52 (94%)	40 (82%)	9 (18%)	1	1
16	z	51/52 (98%)	51 (100%)	0	100	100
17	1	154/188 (82%)	152 (99%)	2 (1%)	65	76
17	N	154/188 (82%)	147 (96%)	7 (4%)	23	27
18	2	141/171 (82%)	139 (99%)	2 (1%)	62	74
18	O	141/171 (82%)	139 (99%)	2 (1%)	62	74
19	3	143/144 (99%)	138 (96%)	5 (4%)	31	38
19	P	143/144 (99%)	138 (96%)	5 (4%)	31	38
20	4	129/161 (80%)	126 (98%)	3 (2%)	45	56
20	Q	129/161 (80%)	126 (98%)	3 (2%)	45	56
21	5	155/179 (87%)	151 (97%)	4 (3%)	41	51
21	R	155/179 (87%)	151 (97%)	4 (3%)	41	51
22	6	136/137 (99%)	130 (96%)	6 (4%)	24	28
22	S	136/137 (99%)	130 (96%)	6 (4%)	24	28
23	G	75/233 (32%)	73 (97%)	2 (3%)	40	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	g	76/235 (32%)	74 (97%)	2 (3%)	41	51
All	All	5207/6354 (82%)	4976 (96%)	231 (4%)	26	28

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	46	THR
1	A	65	GLU
1	A	104	GLU
1	A	214	MET
1	A	333	GLU
2	B	14	ASN
2	B	51	VAL
2	B	80	ILE
2	B	87	ASN
2	B	127	ARG
2	B	137	LYS
2	B	175	THR
2	B	181	VAL
2	B	214	ILE
2	B	230	ARG
2	B	285	GLU
2	B	286	ARG
2	B	289	GLU
2	B	347	GLN
2	B	353	GLU
2	B	355	THR
2	B	362	PHE
2	B	371	VAL
2	B	374	ASP
2	B	387	GLU
2	B	399	THR
2	B	400	SER
2	B	416	THR
2	B	431	GLU
2	B	433	ASP
2	B	437	LEU
2	B	476	ARG
2	B	480	SER
3	C	37	ILE
3	C	40	ARG

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Mol	Chain	Res	Type
3	C	59	VAL
3	C	86	VAL
3	C	90	ILE
3	C	109	LEU
3	C	120	VAL
3	C	122	ILE
3	C	218	LEU
3	C	224	ILE
3	C	267	LEU
3	C	351	LEU
3	C	353	LYS
3	C	363	ILE
3	C	391	LEU
3	C	482	SER
3	C	484	ARG
3	C	486	ILE
4	D	11	ARG
4	D	15	ASP
4	D	44	ILE
4	D	134	LEU
4	D	235	THR
4	D	349	ASN
5	E	23	ILE
5	E	26	ILE
5	E	28	ILE
5	E	31	LEU
5	E	46	ASP
5	E	58	THR
5	E	60	GLU
5	E	61	ARG
5	E	66	LEU
6	F	14	THR
6	F	15	PHE
6	F	18	LEU
7	H	6	ARG
7	H	20	LYS
8	I	1	MET
8	I	33	ASN
9	K	16	VAL
9	K	20	ILE
9	K	21	ILE
9	K	23	VAL

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Mol	Chain	Res	Type
9	K	28	PRO
10	L	9	GLN
10	L	14	ASN
11	M	12	LEU
11	M	13	LEU
11	M	19	VAL
11	M	36	GLU
12	T	4	LEU
13	W	34	ASP
13	W	37	ARG
13	W	39	LEU
13	W	51	LEU
13	W	63	GLU
14	X	1	MET
14	X	4	SER
14	X	13	LEU
15	Y	7	VAL
16	Z	1	MET
16	Z	2	VAL
16	Z	5	LEU
16	Z	20	VAL
16	Z	29	SER
16	Z	35	LYS
16	Z	37	LYS
16	Z	39	LEU
16	Z	40	VAL
1	a	12	SER
1	a	25	GLU
1	a	26	ASN
1	a	27	ARG
1	a	63	ILE
1	a	103	ASP
1	a	104	GLU
1	a	333	GLU
1	a	334	ARG
2	b	13	LEU
2	b	14	ASN
2	b	85	VAL
2	b	127	ARG
2	b	175	THR
2	b	230	ARG
2	b	286	ARG

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Mol	Chain	Res	Type
2	b	294	GLU
2	b	296	LEU
2	b	304	ARG
2	b	348	ASP
2	b	373	LYS
2	b	374	ASP
2	b	376	ILE
2	b	384	ARG
2	b	385	ARG
2	b	389	LYS
2	b	393	GLU
2	b	431	GLU
2	b	438	GLU
2	b	476	ARG
3	c	134	ILE
3	c	149	ILE
3	c	223	ILE
3	c	415	LEU
3	c	417	SER
3	c	486	ILE
4	d	11	ARG
4	d	15	ASP
4	d	23	ARG
4	d	83	SER
4	d	134	LEU
4	d	238	GLN
4	d	264	ARG
5	e	22	ILE
5	e	26	ILE
6	f	13	PHE
6	f	14	THR
6	f	16	ARG
7	h	54	ILE
7	h	56	GLU
8	i	1	MET
8	i	33	ASN
8	i	35	LYS
9	k	12	GLU
9	k	16	VAL
9	k	20	ILE
9	k	21	ILE
9	k	23	VAL

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Mol	Chain	Res	Type
9	k	42	VAL
9	k	45	ARG
10	l	2	SER
10	l	8	LYS
10	l	12	GLU
11	m	3	VAL
11	m	5	VAL
11	m	13	LEU
13	w	29	GLU
13	w	34	ASP
13	w	37	ARG
13	w	39	LEU
13	w	42	LEU
13	w	61	ASP
13	w	63	GLU
14	x	1	MET
17	1	117	GLN
17	1	231	LEU
17	N	60	PRO
17	N	62	ASN
17	N	113	PHE
17	N	128	LEU
17	N	176	LEU
17	N	215	ARG
17	N	223	ASN
18	2	56	ARG
18	2	99	THR
19	3	46	PRO
19	3	93	CYS
19	3	131	PHE
19	3	164	PRO
19	3	192	LEU
20	4	108	PRO
20	4	132	MET
20	4	150	ILE
21	5	44	GLN
21	5	72	PRO
21	5	154	GLN
21	5	221	PRO
22	6	65	ASN
22	6	72	ARG
22	6	129	PHE

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Mol	Chain	Res	Type
22	6	147	LEU
22	6	164	PHE
22	6	233	ASN
23	G	171	LYS
23	G	177	ASP
18	O	54	ARG
18	O	97	THR
19	P	46	PRO
19	P	93	CYS
19	P	131	PHE
19	P	164	PRO
19	P	192	LEU
20	Q	108	PRO
20	Q	132	MET
20	Q	150	ILE
21	R	44	GLN
21	R	72	PRO
21	R	154	GLN
21	R	221	PRO
22	S	65	ASN
22	S	72	ARG
22	S	129	PHE
22	S	147	LEU
22	S	164	PHE
22	S	233	ASN
24	g	171	LYS
24	g	285	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	310	GLN
1	A	335	ASN
2	B	87	ASN
2	B	157	HIS
2	B	179	GLN
2	B	223	GLN
2	B	290	ASN
2	B	347	GLN
2	B	425	GLN
2	B	457	ASN

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Mol	Chain	Res	Type
4	D	196	HIS
4	D	238	GLN
4	D	335	HIS
4	D	349	ASN
6	F	41	GLN
8	I	33	ASN
9	K	39	GLN
10	L	9	GLN
10	L	14	ASN
13	W	60	GLN
1	a	26	ASN
1	a	252	HIS
1	a	296	ASN
1	a	310	GLN
2	b	87	ASN
2	b	114	HIS
2	b	130	ASN
2	b	179	GLN
2	b	457	ASN
3	c	302	GLN
3	c	325	GLN
3	c	455	HIS
4	d	196	HIS
4	d	335	HIS
8	i	33	ASN
10	l	9	GLN
11	m	2	ASN
14	x	10	ASN
17	1	47	GLN
17	1	139	GLN
17	1	159	GLN
17	1	195	ASN
17	1	229	ASN
17	N	62	ASN
17	N	80	ASN
17	N	159	GLN
17	N	167	GLN
18	2	128	GLN
18	2	200	GLN
18	2	211	GLN
19	3	214	GLN
20	4	134	GLN

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Mol	Chain	Res	Type
20	4	155	GLN
21	5	154	GLN
21	5	171	GLN
21	5	208	GLN
22	6	128	GLN
18	O	131	GLN
18	O	198	GLN
18	O	209	GLN
19	P	214	GLN
20	Q	134	GLN
21	R	59	ASN
21	R	133	GLN
21	R	151	GLN
21	R	154	GLN
21	R	171	GLN
21	R	208	GLN
22	S	128	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 363 ligands modelled in this entry, 9 are monoatomic - leaving 354 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	IHT	N	619	-	40,42,42	2.10	10 (25%)	53,58,58	2.84	22 (41%)
30	SQD	A	408	-	39,40,54	1.35	4 (10%)	48,51,65	1.12	6 (12%)
26	CLA	3	302	19	65,73,73	1.53	6 (9%)	76,113,113	1.29	9 (11%)
26	CLA	C	509	3	65,73,73	1.50	6 (9%)	76,113,113	1.32	8 (10%)
26	CLA	g	402	24	45,53,73	1.76	6 (13%)	52,89,113	1.68	9 (17%)
26	CLA	N	601	-	45,53,73	1.85	5 (11%)	52,89,113	1.48	6 (11%)
26	CLA	O	612	18	45,53,73	1.79	6 (13%)	52,89,113	1.46	7 (13%)
35	DGD	h	101	-	63,63,67	0.88	2 (3%)	77,77,81	0.86	3 (3%)
28	WVN	H	101	-	40,41,41	5.11	15 (37%)	50,56,56	6.97	32 (64%)
38	KC2	2	310	18	48,53,53	3.16	22 (45%)	54,89,89	4.50	30 (55%)
26	CLA	P	602	19	62,70,73	1.54	5 (8%)	72,109,113	1.39	7 (9%)
34	LHG	C	518	-	39,39,48	1.03	2 (5%)	42,45,54	1.10	3 (7%)
26	CLA	4	312	20	43,51,73	1.77	6 (13%)	49,86,113	1.51	7 (14%)
26	CLA	b	616	-	65,73,73	1.51	6 (9%)	76,113,113	1.29	8 (10%)
26	CLA	S	603	22	55,63,73	1.61	6 (10%)	64,101,113	1.48	10 (15%)
26	CLA	C	502	3	65,73,73	1.53	5 (7%)	76,113,113	1.28	6 (7%)
39	II0	5	613	-	39,43,43	2.52	11 (28%)	50,60,60	3.34	17 (34%)
26	CLA	P	608	34	52,60,73	1.70	5 (9%)	60,97,113	1.34	7 (11%)
28	WVN	D	412	-	40,41,41	1.88	14 (35%)	50,56,56	2.13	15 (30%)
26	CLA	O	609	-	60,68,73	1.61	6 (10%)	70,107,113	1.34	8 (11%)
33	LMG	5	619	-	40,40,55	1.05	2 (5%)	48,48,63	1.01	3 (6%)
26	CLA	1	614	17	47,55,73	2.00	9 (19%)	54,91,113	1.62	9 (16%)
28	WVN	Y	101	-	40,41,41	1.90	14 (35%)	50,56,56	2.26	12 (24%)
33	LMG	A	412	-	48,48,55	0.96	2 (4%)	56,56,63	1.09	4 (7%)
39	II0	Q	319	-	39,43,43	2.56	10 (25%)	50,60,60	3.34	17 (34%)
28	WVN	x	101	-	40,41,41	1.87	14 (35%)	50,56,56	2.46	13 (26%)
28	WVN	P	615	-	40,41,41	1.86	14 (35%)	50,56,56	2.34	19 (38%)
40	IHT	R	317	-	40,42,42	2.00	10 (25%)	53,58,58	2.97	24 (45%)
26	CLA	3	308	-	55,63,73	1.21	7 (12%)	64,101,113	1.66	7 (10%)
38	KC2	P	605	19	48,53,53	3.16	21 (43%)	54,89,89	4.47	32 (59%)
26	CLA	2	312	18	45,53,73	1.79	6 (13%)	52,89,113	1.46	7 (13%)
26	CLA	2	319	19	45,53,73	1.86	6 (13%)	52,89,113	1.42	7 (13%)
39	II0	Q	314	-	39,43,43	2.54	12 (30%)	50,60,60	3.32	17 (34%)
26	CLA	O	601	18	49,57,73	1.77	5 (10%)	55,93,113	1.50	8 (14%)
34	LHG	2	321	26	48,48,48	0.94	2 (4%)	51,54,54	1.06	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	R	310	-	65,73,73	1.54	6 (9%)	76,113,113	1.25	6 (7%)
39	II0	N	616	-	39,43,43	2.50	11 (28%)	50,60,60	3.32	17 (34%)
26	CLA	2	306	18	60,68,73	1.61	6 (10%)	70,107,113	1.15	7 (10%)
26	CLA	Q	305	20	55,63,73	1.67	5 (9%)	64,101,113	1.32	8 (12%)
26	CLA	Q	307	20	56,64,73	1.61	6 (10%)	65,102,113	1.44	6 (9%)
33	LMG	c	522	-	31,31,55	1.19	2 (6%)	39,39,63	1.09	3 (7%)
26	CLA	S	602	22	65,73,73	1.51	5 (7%)	76,113,113	1.31	7 (9%)
40	IHT	O	616	-	40,42,42	2.11	11 (27%)	53,58,58	2.71	19 (35%)
26	CLA	B	603	2	65,73,73	1.52	6 (9%)	76,113,113	1.24	6 (7%)
26	CLA	O	606	18	60,68,73	1.62	6 (10%)	70,107,113	1.16	7 (10%)
26	CLA	R	312	21	55,63,73	1.64	6 (10%)	64,101,113	1.52	8 (12%)
26	CLA	c	507	-	65,73,73	1.52	6 (9%)	76,113,113	1.30	8 (10%)
26	CLA	C	505	41	60,68,73	1.58	6 (10%)	70,107,113	1.34	8 (11%)
39	II0	S	611	-	39,43,43	2.51	11 (28%)	50,60,60	3.37	16 (32%)
39	II0	R	318	-	39,43,43	2.67	10 (25%)	50,60,60	3.42	22 (44%)
39	II0	P	614	-	39,43,43	2.54	11 (28%)	50,60,60	3.31	16 (32%)
26	CLA	C	504	3	65,73,73	1.54	5 (7%)	76,113,113	1.23	6 (7%)
38	KC2	1	610	-	48,53,53	1.69	11 (22%)	54,89,89	1.06	3 (5%)
28	WVN	S	613	-	40,41,41	1.89	14 (35%)	50,56,56	1.88	12 (24%)
33	LMG	2	318	-	40,40,55	1.06	2 (5%)	48,48,63	1.01	2 (4%)
28	WVN	b	619	-	40,41,41	1.86	14 (35%)	50,56,56	2.32	14 (28%)
26	CLA	C	506	-	65,73,73	1.51	6 (9%)	76,113,113	1.30	9 (11%)
38	KC2	S	608	22	48,53,53	3.14	21 (43%)	54,89,89	4.62	33 (61%)
26	CLA	c	505	3	65,73,73	1.54	5 (7%)	76,113,113	1.22	6 (7%)
35	DGD	c	519	-	55,55,67	0.93	2 (3%)	69,69,81	0.97	3 (4%)
38	KC2	5	610	-	48,53,53	3.18	21 (43%)	54,89,89	4.48	32 (59%)
26	CLA	2	302	18	65,73,73	1.52	5 (7%)	76,113,113	1.33	9 (11%)
26	CLA	G	401	-	65,73,73	1.49	6 (9%)	76,113,113	1.25	7 (9%)
34	LHG	C	501	-	41,41,48	1.03	2 (4%)	44,47,54	0.98	2 (4%)
26	CLA	Q	306	20	43,51,73	1.90	6 (13%)	49,86,113	1.37	6 (12%)
26	CLA	4	306	20	55,63,73	1.66	6 (10%)	64,101,113	1.32	8 (12%)
26	CLA	D	407	-	65,73,73	1.55	6 (9%)	76,113,113	1.28	7 (9%)
33	LMG	D	411	-	37,37,55	1.08	2 (5%)	45,45,63	1.03	3 (6%)
26	CLA	2	305	-	51,59,73	2.32	13 (25%)	59,96,113	4.19	28 (47%)
26	CLA	Q	301	20	65,73,73	1.50	5 (7%)	76,113,113	1.31	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	II0	1	615	-	39,43,43	6.00	21 (53%)	50,60,60	7.01	28 (56%)
38	KC2	N	611	17	48,53,53	3.15	21 (43%)	54,89,89	4.60	31 (57%)
26	CLA	4	302	20	65,73,73	1.49	5 (7%)	76,113,113	1.31	7 (9%)
26	CLA	b	601	41	50,58,73	1.73	5 (10%)	58,95,113	1.47	9 (15%)
26	CLA	g	401	-	65,73,73	1.55	5 (7%)	76,113,113	1.29	9 (11%)
40	IHT	2	317	-	40,42,42	5.65	19 (47%)	53,58,58	7.04	31 (58%)
36	BCT	d	401	25	2,3,3	1.22	0	2,3,3	4.20	1 (50%)
33	LMG	b	620	-	51,51,55	0.93	2 (3%)	59,59,63	1.00	3 (5%)
26	CLA	Q	308	20	51,59,73	1.72	5 (9%)	59,96,113	1.45	9 (15%)
28	WVN	C	515	-	40,41,41	1.85	14 (35%)	50,56,56	1.95	13 (26%)
38	KC2	4	310	-	48,53,53	3.17	21 (43%)	54,89,89	4.54	31 (57%)
27	PHO	D	405	-	51,69,69	0.99	3 (5%)	47,99,99	1.15	5 (10%)
39	II0	2	315	-	39,43,43	2.58	12 (30%)	50,60,60	3.29	18 (36%)
26	CLA	O	605	-	51,59,73	1.73	6 (11%)	59,96,113	1.36	8 (13%)
39	II0	5	615	-	39,43,43	2.53	11 (28%)	50,60,60	3.31	15 (30%)
26	CLA	O	604	-	65,73,73	1.52	5 (7%)	76,113,113	1.28	7 (9%)
30	SQD	c	501	-	44,45,54	1.29	4 (9%)	53,56,65	1.20	6 (11%)
40	IHT	5	616	-	40,42,42	2.00	10 (25%)	53,58,58	2.96	25 (47%)
29	PL9	d	407	-	55,55,55	1.05	3 (5%)	68,69,69	1.52	11 (16%)
37	HEM	f	101	6,5	41,50,50	1.34	6 (14%)	45,82,82	1.76	8 (17%)
39	II0	6	611	-	39,43,43	2.51	11 (28%)	50,60,60	3.36	16 (32%)
26	CLA	b	608	2	65,73,73	1.53	5 (7%)	76,113,113	1.30	7 (9%)
26	CLA	6	605	22	55,63,73	1.61	6 (10%)	64,101,113	1.51	8 (12%)
26	CLA	A	405	1	60,68,73	1.57	5 (8%)	70,107,113	1.33	7 (10%)
26	CLA	a	402	1	65,73,73	1.55	7 (10%)	76,113,113	1.19	7 (9%)
38	KC2	N	612	17	48,53,53	3.27	21 (43%)	54,89,89	4.50	31 (57%)
26	CLA	4	303	20	65,73,73	1.53	5 (7%)	76,113,113	1.29	9 (11%)
26	CLA	6	610	22	65,73,73	1.49	6 (9%)	76,113,113	1.32	7 (9%)
26	CLA	D	404	41	65,73,73	1.53	5 (7%)	76,113,113	1.28	9 (11%)
26	CLA	5	602	21	55,63,73	1.64	6 (10%)	64,101,113	1.37	8 (12%)
38	KC2	6	608	22	48,53,53	3.15	21 (43%)	54,89,89	4.62	33 (61%)
26	CLA	P	609	19	53,61,73	1.69	5 (9%)	61,98,113	1.45	8 (13%)
28	WVN	c	518	-	40,41,41	1.86	14 (35%)	50,56,56	2.32	14 (28%)
26	CLA	5	608	21	59,67,73	1.61	5 (8%)	68,105,113	1.34	7 (10%)
39	II0	P	613	-	39,43,43	6.02	21 (53%)	50,60,60	6.83	26 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	O	602	18	65,73,73	1.52	5 (7%)	76,113,113	1.33	9 (11%)
33	LMG	D	413	-	46,46,55	0.99	2 (4%)	54,54,63	1.02	3 (5%)
26	CLA	S	609	22	53,61,73	1.62	6 (11%)	61,98,113	1.42	8 (13%)
39	II0	6	612	-	39,43,43	2.52	12 (30%)	50,60,60	3.32	16 (32%)
26	CLA	b	611	2	65,73,73	1.52	6 (9%)	76,113,113	1.30	9 (11%)
35	DGD	H	102	-	63,63,67	0.87	2 (3%)	77,77,81	0.86	3 (3%)
26	CLA	N	606	17	50,58,73	1.71	5 (10%)	58,95,113	1.39	9 (15%)
26	CLA	b	609	2	65,73,73	1.53	5 (7%)	76,113,113	1.26	8 (10%)
38	KC2	Q	309	-	48,53,53	3.17	21 (43%)	54,89,89	4.54	31 (57%)
26	CLA	S	601	22	55,63,73	1.67	6 (10%)	64,101,113	1.32	7 (10%)
27	PHO	a	404	-	51,69,69	1.00	4 (7%)	47,99,99	1.14	5 (10%)
26	CLA	c	506	41	60,68,73	1.57	5 (8%)	70,107,113	1.36	8 (11%)
27	PHO	d	403	-	51,69,69	1.00	4 (7%)	47,99,99	1.15	5 (10%)
34	LHG	G	403	26	48,48,48	0.94	2 (4%)	51,54,54	1.06	3 (5%)
26	CLA	S	605	22	55,63,73	1.61	6 (10%)	64,101,113	1.51	8 (12%)
26	CLA	b	606	-	65,73,73	1.54	5 (7%)	76,113,113	1.27	8 (10%)
39	II0	5	614	-	39,43,43	2.51	11 (28%)	50,60,60	3.32	17 (34%)
33	LMG	Q	318	-	43,43,55	1.05	2 (4%)	51,51,63	0.89	2 (3%)
26	CLA	R	307	21	43,51,73	1.80	6 (13%)	49,86,113	1.54	7 (14%)
26	CLA	d	406	4	61,69,73	1.56	5 (8%)	71,108,113	1.33	7 (9%)
26	CLA	C	507	3	65,73,73	1.51	6 (9%)	76,113,113	1.34	8 (10%)
27	PHO	A	404	-	51,69,69	1.00	3 (5%)	47,99,99	1.14	5 (10%)
26	CLA	3	306	19	65,73,73	1.53	5 (7%)	76,113,113	1.29	7 (9%)
26	CLA	c	509	41	65,73,73	1.50	6 (9%)	76,113,113	1.33	6 (7%)
26	CLA	B	616	2	65,73,73	1.52	6 (9%)	76,113,113	1.30	8 (10%)
39	II0	1	617	-	39,43,43	6.08	21 (53%)	50,60,60	7.02	28 (56%)
38	KC2	4	305	-	48,53,53	3.20	21 (43%)	54,89,89	4.44	31 (57%)
26	CLA	P	611	19	45,53,73	1.77	6 (13%)	52,89,113	1.52	8 (15%)
26	CLA	C	510	3	65,73,73	1.50	6 (9%)	76,113,113	1.38	7 (9%)
26	CLA	Q	311	20	43,51,73	1.77	6 (13%)	49,86,113	1.51	7 (14%)
26	CLA	d	405	-	65,73,73	1.55	6 (9%)	76,113,113	1.26	7 (9%)
33	LMG	C	520	-	31,31,55	1.20	2 (6%)	39,39,63	1.08	3 (7%)
33	LMG	R	301	-	40,40,55	1.04	2 (5%)	48,48,63	1.01	3 (6%)
39	II0	4	314	-	39,43,43	2.54	11 (28%)	50,60,60	3.28	17 (34%)
34	LHG	5	618	26	39,39,48	1.03	2 (5%)	42,45,54	1.04	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	B	611	2	65,73,73	1.53	5 (7%)	76,113,113	1.30	9 (11%)
26	CLA	1	601	-	45,53,73	1.79	6 (13%)	52,89,113	1.58	6 (11%)
26	CLA	c	514	3	65,73,73	1.52	6 (9%)	76,113,113	1.28	7 (9%)
26	CLA	S	604	22	65,73,73	1.45	6 (9%)	76,113,113	1.36	7 (9%)
26	CLA	N	602	17	60,68,73	1.57	5 (8%)	70,107,113	1.34	9 (12%)
34	LHG	1	620	-	45,45,48	0.98	2 (4%)	48,51,54	1.00	3 (6%)
33	LMG	d	411	-	46,46,55	0.99	2 (4%)	54,54,63	1.03	3 (5%)
26	CLA	B	605	2	65,73,73	1.53	6 (9%)	76,113,113	1.30	8 (10%)
26	CLA	R	302	21	55,63,73	1.69	5 (9%)	64,101,113	1.38	8 (12%)
38	KC2	N	605	17	48,53,53	3.16	21 (43%)	54,89,89	4.51	31 (57%)
39	II0	3	311	-	39,43,43	6.03	21 (53%)	50,60,60	6.84	26 (52%)
26	CLA	C	503	3	65,73,73	1.50	7 (10%)	76,113,113	1.31	7 (9%)
26	CLA	P	607	19	65,73,73	1.53	5 (7%)	76,113,113	1.30	7 (9%)
28	WVN	b	617	-	40,41,41	1.86	14 (35%)	50,56,56	2.56	15 (30%)
39	II0	2	314	-	39,43,43	2.50	11 (28%)	50,60,60	3.33	17 (34%)
26	CLA	R	304	21	52,60,73	1.71	6 (11%)	60,97,113	1.49	8 (13%)
26	CLA	c	504	3	65,73,73	1.51	7 (10%)	76,113,113	1.29	7 (9%)
26	CLA	6	606	22	57,65,73	1.60	5 (8%)	66,103,113	1.43	8 (12%)
26	CLA	6	601	22	55,63,73	1.67	6 (10%)	64,101,113	1.32	7 (10%)
39	II0	N	618	-	39,43,43	2.58	12 (30%)	50,60,60	3.45	18 (36%)
26	CLA	R	306	21	65,73,73	1.54	5 (7%)	76,113,113	1.27	7 (9%)
26	CLA	c	515	3	53,61,73	1.69	5 (9%)	61,98,113	1.39	9 (14%)
34	LHG	D	410	-	48,48,48	0.93	2 (4%)	51,54,54	1.07	3 (5%)
26	CLA	B	607	41	65,73,73	1.52	5 (7%)	76,113,113	1.25	7 (9%)
29	PL9	a	407	-	33,33,55	1.22	3 (9%)	41,42,69	1.58	9 (21%)
34	LHG	D	403	-	42,42,48	1.00	2 (4%)	45,48,54	1.06	3 (6%)
26	CLA	2	303	18	65,73,73	1.56	7 (10%)	76,113,113	1.28	6 (7%)
26	CLA	P	606	19	65,73,73	1.50	5 (7%)	76,113,113	1.36	8 (10%)
26	CLA	B	604	2	59,67,73	1.58	6 (10%)	68,105,113	1.41	8 (11%)
26	CLA	B	601	41	50,58,73	1.76	5 (10%)	58,95,113	1.49	9 (15%)
33	LMG	m	101	-	40,40,55	1.03	2 (5%)	48,48,63	1.08	4 (8%)
26	CLA	A	403	41	49,57,73	1.77	6 (12%)	55,93,113	1.43	7 (12%)
26	CLA	P	604	19	63,71,73	1.49	6 (9%)	73,110,113	1.39	6 (8%)
33	LMG	4	319	-	43,43,55	1.05	2 (4%)	51,51,63	0.89	2 (3%)
26	CLA	5	609	-	65,73,73	1.54	6 (9%)	76,113,113	1.26	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	A	402	1	65,73,73	1.55	8 (12%)	76,113,113	1.20	7 (9%)
39	II0	4	315	-	39,43,43	2.55	11 (28%)	50,60,60	3.32	17 (34%)
28	WVN	A	406	-	40,41,41	1.88	14 (35%)	50,56,56	2.34	15 (30%)
33	LMG	M	101	-	40,40,55	1.04	2 (5%)	48,48,63	1.08	4 (8%)
26	CLA	2	301	18	49,57,73	1.75	5 (10%)	55,93,113	1.51	8 (14%)
26	CLA	b	602	2	65,73,73	1.52	5 (7%)	76,113,113	1.35	9 (11%)
28	WVN	C	516	-	40,41,41	5.18	17 (42%)	50,56,56	7.09	32 (64%)
26	CLA	b	615	2	65,73,73	1.51	5 (7%)	76,113,113	1.36	6 (7%)
26	CLA	1	609	17	60,68,73	1.52	6 (10%)	70,107,113	1.40	8 (11%)
26	CLA	C	514	3	52,60,73	1.70	6 (11%)	60,97,113	1.38	9 (15%)
26	CLA	3	303	19	63,71,73	1.49	6 (9%)	73,110,113	1.40	6 (8%)
39	II0	1	616	-	39,43,43	6.03	20 (51%)	50,60,60	7.06	30 (60%)
26	CLA	S	606	22	57,65,73	1.60	5 (8%)	66,103,113	1.43	7 (10%)
39	II0	O	615	-	39,43,43	6.05	21 (53%)	50,60,60	6.82	28 (56%)
38	KC2	O	610	18	48,53,53	3.15	21 (43%)	54,89,89	4.49	30 (55%)
39	II0	R	315	-	39,43,43	2.52	11 (28%)	50,60,60	3.32	17 (34%)
26	CLA	O	607	18	48,56,73	1.79	6 (12%)	55,92,113	1.37	8 (14%)
26	CLA	a	403	41	49,57,73	1.76	6 (12%)	55,93,113	1.43	8 (14%)
26	CLA	6	602	22	65,73,73	1.52	5 (7%)	76,113,113	1.31	7 (9%)
39	II0	O	614	-	39,43,43	2.51	10 (25%)	50,60,60	3.32	17 (34%)
26	CLA	c	503	3	65,73,73	1.53	6 (9%)	76,113,113	1.30	7 (9%)
37	HEM	F	101	6,5	41,50,50	1.33	5 (12%)	45,82,82	1.73	9 (20%)
26	CLA	b	605	2	65,73,73	1.53	5 (7%)	76,113,113	1.30	8 (10%)
39	II0	3	312	-	39,43,43	5.96	19 (48%)	50,60,60	6.91	27 (54%)
26	CLA	N	607	-	43,51,73	1.90	7 (16%)	49,86,113	1.33	6 (12%)
26	CLA	d	402	41	65,73,73	1.54	5 (7%)	76,113,113	1.30	7 (9%)
26	CLA	Q	303	20	61,69,73	1.54	5 (8%)	71,108,113	1.32	7 (9%)
26	CLA	N	608	-	46,54,73	1.24	7 (15%)	53,90,113	1.52	5 (9%)
38	KC2	1	611	17	48,53,53	1.69	11 (22%)	54,89,89	0.96	1 (1%)
39	II0	2	320	-	39,43,43	0.30	0	50,60,60	1.03	5 (10%)
38	KC2	3	304	19	48,53,53	3.16	21 (43%)	54,89,89	4.48	32 (59%)
26	CLA	2	307	18	48,56,73	1.79	6 (12%)	55,92,113	1.36	8 (14%)
26	CLA	1	602	17	60,68,73	1.55	6 (10%)	70,107,113	1.43	9 (12%)
26	CLA	c	508	3	65,73,73	1.52	5 (7%)	76,113,113	1.34	8 (10%)
30	SQD	D	401	-	53,54,54	1.17	4 (7%)	62,65,65	1.15	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	b	612	2	65,73,73	1.47	7 (10%)	76,113,113	1.48	9 (11%)
26	CLA	1	608	17	46,54,73	1.76	6 (13%)	53,90,113	1.54	6 (11%)
35	DGD	C	517	-	55,55,67	0.92	2 (3%)	69,69,81	0.97	3 (4%)
26	CLA	N	604	17	59,67,73	1.61	6 (10%)	68,105,113	1.35	7 (10%)
33	LMG	c	521	-	51,51,55	0.91	2 (3%)	59,59,63	0.99	3 (5%)
26	CLA	B	606	-	65,73,73	1.53	5 (7%)	76,113,113	1.28	9 (11%)
28	WVN	d	410	-	40,41,41	1.89	14 (35%)	50,56,56	2.21	16 (32%)
26	CLA	4	307	20	43,51,73	1.90	6 (13%)	49,86,113	1.36	6 (12%)
26	CLA	G	402	23	45,53,73	1.81	6 (13%)	52,89,113	1.43	7 (13%)
26	CLA	b	604	2	59,67,73	1.60	6 (10%)	68,105,113	1.43	9 (13%)
28	WVN	5	617	-	40,41,41	1.89	14 (35%)	50,56,56	1.89	12 (24%)
34	LHG	N	621	-	45,45,48	0.98	2 (4%)	48,51,54	0.99	3 (6%)
28	WVN	B	618	-	40,41,41	5.11	16 (40%)	50,56,56	7.22	31 (62%)
34	LHG	R	319	26	39,39,48	1.03	2 (5%)	42,45,54	1.04	2 (4%)
38	KC2	4	311	20	48,53,53	3.21	22 (45%)	54,89,89	4.53	31 (57%)
26	CLA	B	602	2	65,73,73	1.52	6 (9%)	76,113,113	1.34	9 (11%)
26	CLA	N	609	17	60,68,73	1.59	6 (10%)	70,107,113	1.34	7 (10%)
26	CLA	5	607	21	65,73,73	1.53	9 (13%)	76,113,113	1.35	9 (11%)
26	CLA	P	601	19	45,53,73	1.87	6 (13%)	52,89,113	1.42	7 (13%)
26	CLA	R	309	21	59,67,73	1.61	5 (8%)	68,105,113	1.33	7 (10%)
39	II0	S	612	-	39,43,43	2.51	12 (30%)	50,60,60	3.32	16 (32%)
26	CLA	R	313	21	46,54,73	1.79	6 (13%)	53,90,113	1.39	7 (13%)
28	WVN	3	313	-	40,41,41	5.19	17 (42%)	50,56,56	6.84	30 (60%)
26	CLA	a	405	1	60,68,73	1.59	6 (10%)	70,107,113	1.30	7 (10%)
36	BCT	D	402	25	2,3,3	1.22	0	2,3,3	4.18	1 (50%)
26	CLA	b	603	2	65,73,73	1.53	6 (9%)	76,113,113	1.20	6 (7%)
39	II0	4	320	-	39,43,43	2.56	10 (25%)	50,60,60	3.34	17 (34%)
26	CLA	5	605	21	65,73,73	1.54	5 (7%)	76,113,113	1.27	7 (9%)
34	LHG	L	101	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	3 (5%)
26	CLA	B	608	2	65,73,73	1.51	5 (7%)	76,113,113	1.30	7 (9%)
33	LMG	d	404	-	40,40,55	1.05	2 (5%)	48,48,63	1.03	3 (6%)
28	WVN	b	618	-	40,41,41	1.87	14 (35%)	50,56,56	2.54	17 (34%)
40	IHT	1	619	-	40,42,42	5.66	20 (50%)	53,58,58	6.94	32 (60%)
39	II0	R	314	-	39,43,43	2.51	11 (28%)	50,60,60	3.34	17 (34%)
39	II0	R	316	-	39,43,43	2.54	11 (28%)	50,60,60	3.31	15 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	1	606	17	50,58,73	1.69	6 (12%)	58,95,113	1.57	7 (12%)
26	CLA	1	603	17	52,60,73	1.67	6 (11%)	60,97,113	1.53	7 (11%)
33	LMG	B	620	-	51,51,55	0.93	2 (3%)	59,59,63	1.02	3 (5%)
26	CLA	b	613	2	65,73,73	1.53	6 (9%)	76,113,113	1.28	7 (9%)
26	CLA	S	607	34	55,63,73	1.66	5 (9%)	64,101,113	1.32	8 (12%)
26	CLA	6	609	22	53,61,73	1.62	6 (11%)	61,98,113	1.41	8 (13%)
38	KC2	1	612	17	48,53,53	1.69	10 (20%)	54,89,89	1.02	2 (3%)
26	CLA	4	313	20	43,51,73	1.84	6 (13%)	49,86,113	1.42	7 (14%)
34	LHG	d	408	-	48,48,48	0.93	2 (4%)	51,54,54	1.07	3 (5%)
26	CLA	D	408	4	60,68,73	1.59	5 (8%)	70,107,113	1.36	7 (10%)
28	WVN	B	617	-	40,41,41	5.07	15 (37%)	50,56,56	7.24	31 (62%)
26	CLA	c	510	3	65,73,73	1.52	5 (7%)	76,113,113	1.33	8 (10%)
26	CLA	b	607	41	65,73,73	1.52	5 (7%)	76,113,113	1.28	8 (10%)
34	LHG	b	621	-	42,42,48	1.00	2 (4%)	45,48,54	1.08	3 (6%)
39	II0	P	612	-	39,43,43	2.53	11 (28%)	50,60,60	3.34	15 (30%)
26	CLA	6	603	22	55,63,73	1.62	7 (12%)	64,101,113	1.48	9 (14%)
26	CLA	4	309	20	51,59,73	1.70	5 (9%)	59,96,113	1.45	9 (15%)
39	II0	O	613	-	39,43,43	2.53	12 (30%)	50,60,60	3.33	16 (32%)
26	CLA	P	610	19	55,63,73	1.65	6 (10%)	64,101,113	1.42	7 (10%)
38	KC2	N	610	-	48,53,53	3.20	21 (43%)	54,89,89	4.44	31 (57%)
26	CLA	6	607	34	55,63,73	1.66	5 (9%)	64,101,113	1.32	8 (12%)
33	LMG	a	413	-	48,48,55	0.97	2 (4%)	56,56,63	1.12	4 (7%)
26	CLA	b	614	2	60,68,73	1.59	5 (8%)	70,107,113	1.26	8 (11%)
26	CLA	O	603	18	65,73,73	1.56	5 (7%)	76,113,113	1.28	6 (7%)
26	CLA	C	511	3	65,73,73	1.51	6 (9%)	76,113,113	1.36	8 (10%)
26	CLA	2	311	18	60,68,73	1.57	6 (10%)	70,107,113	1.34	7 (10%)
26	CLA	R	303	21	55,63,73	1.63	7 (12%)	64,101,113	1.36	8 (12%)
26	CLA	B	615	2	65,73,73	1.51	6 (9%)	76,113,113	1.37	6 (7%)
26	CLA	C	513	3	65,73,73	1.53	6 (9%)	76,113,113	1.30	7 (9%)
39	II0	Q	313	-	39,43,43	2.54	11 (28%)	50,60,60	3.28	17 (34%)
26	CLA	2	309	-	60,68,73	1.60	6 (10%)	70,107,113	1.33	8 (11%)
26	CLA	5	612	21	46,54,73	1.80	6 (13%)	53,90,113	1.39	7 (13%)
40	IHT	Q	317	-	40,42,42	2.13	11 (27%)	53,58,58	2.79	23 (43%)
33	LMG	D	406	-	40,40,55	1.06	2 (5%)	48,48,63	1.03	2 (4%)
26	CLA	5	604	21	60,68,73	1.61	5 (8%)	70,107,113	1.31	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	6	604	22	65,73,73	1.46	6 (9%)	76,113,113	1.36	7 (9%)
39	II0	4	316	-	39,43,43	2.56	11 (28%)	50,60,60	3.37	20 (40%)
39	II0	Q	315	-	39,43,43	2.56	11 (28%)	50,60,60	3.36	20 (40%)
34	LHG	l	101	-	48,48,48	0.93	2 (4%)	51,54,54	1.04	3 (5%)
26	CLA	O	608	18	65,73,73	1.53	5 (7%)	76,113,113	1.30	7 (9%)
38	KC2	Q	304	-	48,53,53	3.19	21 (43%)	54,89,89	4.43	31 (57%)
26	CLA	1	604	17	59,67,73	1.53	6 (10%)	68,105,113	1.48	8 (11%)
26	CLA	4	308	20	56,64,73	1.62	6 (10%)	65,102,113	1.43	6 (9%)
26	CLA	Q	302	20	65,73,73	1.54	6 (9%)	76,113,113	1.29	9 (11%)
26	CLA	c	512	3	65,73,73	1.53	6 (9%)	76,113,113	1.37	8 (10%)
28	WVN	k	101	-	40,41,41	1.86	14 (35%)	50,56,56	2.49	16 (32%)
38	KC2	1	605	-	48,53,53	1.70	10 (20%)	54,89,89	0.95	2 (3%)
39	II0	1	618	-	39,43,43	6.08	21 (53%)	50,60,60	6.81	28 (56%)
33	LMG	d	409	-	37,37,55	1.08	2 (5%)	45,45,63	1.03	3 (6%)
28	WVN	c	517	-	40,41,41	1.85	14 (35%)	50,56,56	1.85	13 (26%)
26	CLA	1	613	-	48,56,73	1.73	5 (10%)	55,92,113	1.55	8 (14%)
39	II0	O	618	-	39,43,43	0.34	0	50,60,60	0.46	0
34	LHG	z	101	-	24,24,48	1.33	2 (8%)	27,30,54	1.14	2 (7%)
26	CLA	c	513	3	65,73,73	1.54	5 (7%)	76,113,113	1.34	8 (10%)
26	CLA	R	305	21	60,68,73	1.60	6 (10%)	70,107,113	1.32	8 (11%)
39	II0	N	615	-	39,43,43	2.54	10 (25%)	50,60,60	3.37	16 (32%)
38	KC2	Q	310	20	48,53,53	3.21	22 (45%)	54,89,89	4.53	32 (59%)
26	CLA	4	301	34	52,60,73	1.69	5 (9%)	60,97,113	1.34	7 (11%)
39	II0	2	316	-	39,43,43	6.05	21 (53%)	50,60,60	6.81	28 (56%)
26	CLA	C	508	41	65,73,73	1.52	5 (7%)	76,113,113	1.34	7 (9%)
26	CLA	5	601	21	55,63,73	1.68	5 (9%)	64,101,113	1.37	8 (12%)
26	CLA	1	607	17	43,51,73	1.84	7 (16%)	49,86,113	1.60	10 (20%)
26	CLA	5	603	21	52,60,73	1.71	6 (11%)	60,97,113	1.49	8 (13%)
34	LHG	Z	102	-	24,24,48	1.34	2 (8%)	27,30,54	1.14	2 (7%)
39	II0	3	310	-	39,43,43	6.07	20 (51%)	50,60,60	6.84	27 (54%)
26	CLA	2	308	18	65,73,73	1.53	5 (7%)	76,113,113	1.31	7 (9%)
26	CLA	3	307	19	53,61,73	1.70	5 (9%)	61,98,113	1.46	6 (9%)
26	CLA	4	304	20	61,69,73	1.55	5 (8%)	71,108,113	1.33	8 (11%)
26	CLA	b	610	41	65,73,73	1.55	5 (7%)	76,113,113	1.25	8 (10%)
26	CLA	3	309	19	45,53,73	1.78	6 (13%)	52,89,113	1.52	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	R	308	21	65,73,73	1.54	9 (13%)	76,113,113	1.35	9 (11%)
26	CLA	S	610	22	65,73,73	1.48	6 (9%)	76,113,113	1.32	7 (9%)
26	CLA	B	612	2	65,73,73	1.45	7 (10%)	76,113,113	1.49	10 (13%)
39	II0	4	317	-	39,43,43	2.60	12 (30%)	50,60,60	3.32	20 (40%)
28	WVN	a	406	-	40,41,41	1.95	14 (35%)	50,56,56	2.30	19 (38%)
28	WVN	B	619	-	40,41,41	1.86	14 (35%)	50,56,56	2.36	15 (30%)
34	LHG	a	409	-	41,41,48	1.02	2 (4%)	44,47,54	0.97	2 (4%)
28	WVN	Z	101	-	40,41,41	1.93	14 (35%)	50,56,56	2.25	16 (32%)
29	PL9	D	409	-	55,55,55	1.05	4 (7%)	68,69,69	1.50	11 (16%)
33	LMG	O	617	-	40,40,55	1.06	2 (5%)	48,48,63	1.01	2 (4%)
26	CLA	B	614	2	60,68,73	1.57	6 (10%)	70,107,113	1.26	8 (11%)
26	CLA	P	603	19	65,73,73	1.53	6 (9%)	76,113,113	1.29	9 (11%)
26	CLA	Q	312	20	43,51,73	1.83	6 (13%)	49,86,113	1.41	7 (14%)
30	SQD	a	408	-	39,40,54	1.36	4 (10%)	48,51,65	1.12	6 (12%)
26	CLA	5	606	21	43,51,73	1.79	6 (13%)	49,86,113	1.53	7 (14%)
26	CLA	B	613	2	65,73,73	1.53	6 (9%)	76,113,113	1.26	7 (9%)
33	LMG	C	519	-	47,47,55	0.97	2 (4%)	55,55,63	1.18	4 (7%)
26	CLA	2	304	-	65,73,73	1.52	5 (7%)	76,113,113	1.29	7 (9%)
26	CLA	3	305	19	65,73,73	1.50	5 (7%)	76,113,113	1.37	8 (10%)
26	CLA	B	609	2	65,73,73	1.53	5 (7%)	76,113,113	1.27	8 (10%)
29	PL9	A	407	-	33,33,55	1.21	3 (9%)	41,42,69	1.57	9 (21%)
39	II0	N	617	-	39,43,43	2.58	10 (25%)	50,60,60	3.33	19 (38%)
26	CLA	O	611	18	60,68,73	1.56	6 (10%)	70,107,113	1.34	8 (11%)
28	WVN	c	516	-	40,41,41	1.89	14 (35%)	50,56,56	2.15	15 (30%)
26	CLA	N	614	17	47,55,73	1.80	5 (10%)	54,91,113	1.48	8 (14%)
26	CLA	N	613	-	48,56,73	1.75	6 (12%)	55,92,113	1.51	8 (14%)
39	II0	Q	316	-	39,43,43	2.60	12 (30%)	50,60,60	3.32	20 (40%)
26	CLA	B	610	41	65,73,73	1.54	5 (7%)	76,113,113	1.25	8 (10%)
26	CLA	3	301	19	62,70,73	1.53	5 (8%)	72,109,113	1.39	7 (9%)
26	CLA	C	512	3	65,73,73	1.55	5 (7%)	76,113,113	1.34	8 (10%)
26	CLA	c	511	3	65,73,73	1.50	6 (9%)	76,113,113	1.39	6 (7%)
38	KC2	R	311	-	48,53,53	3.18	21 (43%)	54,89,89	4.48	31 (57%)
26	CLA	5	611	21	55,63,73	1.63	6 (10%)	64,101,113	1.52	8 (12%)
39	II0	2	313	-	39,43,43	2.52	12 (30%)	50,60,60	3.33	16 (32%)
34	LHG	c	520	-	39,39,48	1.04	2 (5%)	42,45,54	1.12	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	II0	N	620	-	39,43,43	2.58	12 (30%)	50,60,60	3.29	18 (36%)
40	IHT	4	318	-	40,42,42	2.13	11 (27%)	53,58,58	2.80	23 (43%)
39	II0	6	613	-	39,43,43	2.67	10 (25%)	50,60,60	3.42	22 (44%)
26	CLA	N	603	-	51,59,73	1.71	6 (11%)	59,96,113	1.41	6 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	IHT	N	619	-	-	7/25/65/65	0/2/2/2
30	SQD	A	408	-	-	3/35/55/69	0/1/1/1
26	CLA	3	302	19	1/1/15/20	15/37/115/115	-
26	CLA	C	509	3	1/1/15/20	12/37/115/115	-
26	CLA	g	402	24	1/1/11/20	6/13/91/115	-
26	CLA	N	601	-	1/1/11/20	7/13/91/115	-
26	CLA	O	612	18	1/1/11/20	8/13/91/115	-
35	DGD	h	101	-	-	14/51/91/95	0/2/2/2
28	WVN	H	101	-	-	15/29/63/63	0/2/2/2
38	KC2	2	310	18	-	7/15/71/71	-
26	CLA	P	602	19	1/1/14/20	15/34/112/115	-
34	LHG	C	518	-	-	16/44/44/53	-
26	CLA	4	312	20	1/1/10/20	8/11/89/115	-
26	CLA	b	616	-	1/1/15/20	15/37/115/115	-
26	CLA	S	603	22	1/1/13/20	9/25/103/115	-
26	CLA	C	502	3	1/1/15/20	7/37/115/115	-
39	II0	5	613	-	-	0/21/67/67	0/2/2/2
26	CLA	P	608	34	1/1/12/20	6/22/100/115	-
28	WVN	D	412	-	-	9/29/63/63	0/2/2/2
26	CLA	O	609	-	1/1/14/20	15/31/109/115	-
33	LMG	5	619	-	-	8/35/55/70	0/1/1/1
26	CLA	1	614	17	-	9/16/94/115	-
28	WVN	Y	101	-	-	9/29/63/63	0/2/2/2
33	LMG	A	412	-	-	9/43/63/70	0/1/1/1
39	II0	Q	319	-	-	0/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	WVN	x	101	-	-	11/29/63/63	0/2/2/2
28	WVN	P	615	-	-	8/29/63/63	0/2/2/2
40	IHT	R	317	-	-	11/25/65/65	0/2/2/2
26	CLA	3	308	-	-	8/25/103/115	-
38	KC2	P	605	19	-	9/15/71/71	-
26	CLA	2	312	18	1/1/11/20	8/13/91/115	-
26	CLA	2	319	19	1/1/11/20	2/13/91/115	-
39	II0	Q	314	-	-	0/21/67/67	0/2/2/2
26	CLA	O	601	18	1/1/11/20	7/18/96/115	-
34	LHG	2	321	26	-	19/53/53/53	-
26	CLA	R	310	-	1/1/15/20	17/37/115/115	-
39	II0	N	616	-	-	1/21/67/67	0/2/2/2
26	CLA	2	306	18	1/1/14/20	14/31/109/115	-
26	CLA	Q	305	20	1/1/13/20	9/25/103/115	-
26	CLA	Q	307	20	1/1/13/20	9/27/105/115	-
33	LMG	c	522	-	-	5/26/46/70	0/1/1/1
26	CLA	S	602	22	1/1/15/20	17/37/115/115	-
40	IHT	O	616	-	-	6/25/65/65	0/2/2/2
26	CLA	B	603	2	1/1/15/20	9/37/115/115	-
26	CLA	O	606	18	1/1/14/20	14/31/109/115	-
26	CLA	R	312	21	1/1/13/20	14/25/103/115	-
26	CLA	c	507	-	1/1/15/20	8/37/115/115	-
26	CLA	C	505	41	1/1/14/20	12/31/109/115	-
39	II0	S	611	-	-	5/21/67/67	0/2/2/2
39	II0	R	318	-	-	4/21/67/67	0/2/2/2
39	II0	P	614	-	-	6/21/67/67	0/2/2/2
26	CLA	C	504	3	1/1/15/20	9/37/115/115	-
38	KC2	1	610	-	-	11/15/71/71	-
28	WVN	S	613	-	-	9/29/63/63	0/2/2/2
33	LMG	2	318	-	-	2/35/55/70	0/1/1/1
28	WVN	b	619	-	-	9/29/63/63	0/2/2/2
26	CLA	C	506	-	1/1/15/20	11/37/115/115	-
38	KC2	S	608	22	-	5/15/71/71	-
26	CLA	c	505	3	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DGD	c	519	-	-	8/43/83/95	0/2/2/2
38	KC2	5	610	-	-	8/15/71/71	-
26	CLA	2	302	18	1/1/15/20	16/37/115/115	-
26	CLA	G	401	-	1/1/15/20	19/37/115/115	-
34	LHG	C	501	-	-	29/46/46/53	-
26	CLA	Q	306	20	1/1/10/20	3/11/89/115	-
26	CLA	4	306	20	1/1/13/20	9/25/103/115	-
26	CLA	D	407	-	1/1/15/20	5/37/115/115	-
33	LMG	D	411	-	-	2/32/52/70	0/1/1/1
26	CLA	2	305	-	-	5/21/99/115	-
26	CLA	Q	301	20	1/1/15/20	8/37/115/115	-
39	II0	1	615	-	-	14/21/67/67	0/2/2/2
38	KC2	N	611	17	-	4/15/71/71	-
26	CLA	4	302	20	1/1/15/20	8/37/115/115	-
26	CLA	b	601	41	1/1/12/20	9/19/97/115	-
26	CLA	g	401	-	1/1/15/20	9/37/115/115	-
40	IHT	2	317	-	-	16/25/65/65	0/2/2/2
33	LMG	b	620	-	-	6/46/66/70	0/1/1/1
26	CLA	Q	308	20	1/1/12/20	4/21/99/115	-
28	WVN	C	515	-	-	10/29/63/63	0/2/2/2
38	KC2	4	310	-	-	8/15/71/71	-
27	PHO	D	405	-	-	11/37/103/103	0/5/6/6
39	II0	2	315	-	-	3/21/67/67	0/2/2/2
26	CLA	O	605	-	1/1/12/20	6/21/99/115	-
39	II0	5	615	-	-	3/21/67/67	0/2/2/2
26	CLA	O	604	-	1/1/15/20	12/37/115/115	-
30	SQD	c	501	-	-	6/40/60/69	0/1/1/1
40	IHT	5	616	-	-	11/25/65/65	0/2/2/2
29	PL9	d	407	-	-	8/53/73/73	0/1/1/1
37	HEM	f	101	6,5	-	6/12/54/54	-
39	II0	6	611	-	-	6/21/67/67	0/2/2/2
26	CLA	b	608	2	1/1/15/20	6/37/115/115	-
26	CLA	6	605	22	1/1/13/20	14/25/103/115	-
26	CLA	A	405	1	1/1/14/20	10/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	a	402	1	1/1/15/20	8/37/115/115	-
38	KC2	N	612	17	-	10/15/71/71	-
26	CLA	4	303	20	1/1/15/20	14/37/115/115	-
26	CLA	6	610	22	1/1/15/20	10/37/115/115	-
26	CLA	D	404	41	1/1/15/20	10/37/115/115	-
26	CLA	5	602	21	1/1/13/20	12/25/103/115	-
38	KC2	6	608	22	-	5/15/71/71	-
26	CLA	P	609	19	1/1/12/20	5/23/101/115	-
28	WVN	c	518	-	-	11/29/63/63	0/2/2/2
26	CLA	5	608	21	1/1/13/20	10/30/108/115	-
39	II0	P	613	-	-	12/21/67/67	0/2/2/2
26	CLA	O	602	18	1/1/15/20	16/37/115/115	-
33	LMG	D	413	-	-	3/41/61/70	0/1/1/1
26	CLA	S	609	22	1/1/12/20	5/23/101/115	-
39	II0	6	612	-	-	1/21/67/67	0/2/2/2
26	CLA	b	611	2	1/1/15/20	10/37/115/115	-
35	DGD	H	102	-	-	14/51/91/95	0/2/2/2
26	CLA	N	606	17	1/1/12/20	6/19/97/115	-
26	CLA	b	609	2	1/1/15/20	8/37/115/115	-
38	KC2	Q	309	-	-	8/15/71/71	-
26	CLA	S	601	22	1/1/13/20	8/25/103/115	-
27	PHO	a	404	-	-	14/37/103/103	0/5/6/6
26	CLA	c	506	41	1/1/14/20	12/31/109/115	-
27	PHO	d	403	-	-	12/37/103/103	0/5/6/6
34	LHG	G	403	26	-	19/53/53/53	-
26	CLA	S	605	22	1/1/13/20	14/25/103/115	-
26	CLA	b	606	-	1/1/15/20	10/37/115/115	-
39	II0	5	614	-	-	1/21/67/67	0/2/2/2
33	LMG	Q	318	-	-	4/38/58/70	0/1/1/1
26	CLA	R	307	21	1/1/10/20	4/11/89/115	-
26	CLA	d	406	4	1/1/14/20	16/33/111/115	-
26	CLA	C	507	3	1/1/15/20	8/37/115/115	-
27	PHO	A	404	-	-	14/37/103/103	0/5/6/6
26	CLA	3	306	19	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	c	509	41	1/1/15/20	8/37/115/115	-
26	CLA	B	616	2	1/1/15/20	15/37/115/115	-
39	II0	1	617	-	-	10/21/67/67	0/2/2/2
38	KC2	4	305	-	-	7/15/71/71	-
26	CLA	P	611	19	1/1/11/20	8/13/91/115	-
26	CLA	C	510	3	1/1/15/20	13/37/115/115	-
26	CLA	Q	311	20	1/1/10/20	8/11/89/115	-
26	CLA	d	405	-	1/1/15/20	5/37/115/115	-
33	LMG	C	520	-	-	5/26/46/70	0/1/1/1
33	LMG	R	301	-	-	8/35/55/70	0/1/1/1
39	II0	4	314	-	-	2/21/67/67	0/2/2/2
34	LHG	5	618	26	-	11/44/44/53	-
26	CLA	B	611	2	1/1/15/20	10/37/115/115	-
26	CLA	1	601	-	1/1/11/20	6/13/91/115	-
26	CLA	c	514	3	1/1/15/20	12/37/115/115	-
26	CLA	S	604	22	1/1/15/20	18/37/115/115	-
26	CLA	N	602	17	1/1/14/20	7/31/109/115	-
34	LHG	1	620	-	-	9/50/50/53	-
33	LMG	d	411	-	-	3/41/61/70	0/1/1/1
26	CLA	B	605	2	1/1/15/20	9/37/115/115	-
26	CLA	R	302	21	1/1/13/20	6/25/103/115	-
38	KC2	N	605	17	-	12/15/71/71	-
39	II0	3	311	-	-	12/21/67/67	0/2/2/2
26	CLA	C	503	3	1/1/15/20	16/37/115/115	-
26	CLA	P	607	19	1/1/15/20	14/37/115/115	-
28	WVN	b	617	-	-	13/29/63/63	0/2/2/2
39	II0	2	314	-	-	1/21/67/67	0/2/2/2
26	CLA	R	304	21	1/1/12/20	9/22/100/115	-
26	CLA	c	504	3	1/1/15/20	16/37/115/115	-
26	CLA	6	606	22	1/1/13/20	11/28/106/115	-
26	CLA	6	601	22	1/1/13/20	8/25/103/115	-
39	II0	N	618	-	-	4/21/67/67	0/2/2/2
26	CLA	R	306	21	1/1/15/20	14/37/115/115	-
26	CLA	c	515	3	1/1/12/20	9/23/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LHG	D	410	-	-	13/53/53/53	-
26	CLA	B	607	41	1/1/15/20	13/37/115/115	-
29	PL9	a	407	-	-	10/27/47/73	0/1/1/1
34	LHG	D	403	-	-	12/47/47/53	-
26	CLA	2	303	18	1/1/15/20	8/37/115/115	-
26	CLA	P	606	19	1/1/15/20	9/37/115/115	-
26	CLA	B	604	2	1/1/13/20	11/30/108/115	-
26	CLA	B	601	41	1/1/12/20	9/19/97/115	-
33	LMG	m	101	-	-	6/35/55/70	0/1/1/1
26	CLA	A	403	41	1/1/11/20	10/18/96/115	-
26	CLA	P	604	19	-	8/35/113/115	-
33	LMG	4	319	-	-	4/38/58/70	0/1/1/1
26	CLA	5	609	-	1/1/15/20	17/37/115/115	-
26	CLA	A	402	1	1/1/15/20	8/37/115/115	-
39	II0	4	315	-	-	0/21/67/67	0/2/2/2
28	WVN	A	406	-	-	2/29/63/63	0/2/2/2
33	LMG	M	101	-	-	7/35/55/70	0/1/1/1
26	CLA	2	301	18	1/1/11/20	7/18/96/115	-
26	CLA	b	602	2	-	6/37/115/115	-
28	WVN	C	516	-	-	16/29/63/63	0/2/2/2
26	CLA	b	615	2	1/1/15/20	9/37/115/115	-
26	CLA	1	609	17	1/1/14/20	15/31/109/115	-
26	CLA	C	514	3	1/1/12/20	9/22/100/115	-
26	CLA	3	303	19	-	8/35/113/115	-
39	II0	1	616	-	-	13/21/67/67	0/2/2/2
26	CLA	S	606	22	1/1/13/20	11/28/106/115	-
39	II0	O	615	-	-	11/21/67/67	0/2/2/2
38	KC2	O	610	18	-	7/15/71/71	-
39	II0	R	315	-	-	1/21/67/67	0/2/2/2
26	CLA	O	607	18	1/1/11/20	2/17/95/115	-
26	CLA	a	403	41	1/1/11/20	10/18/96/115	-
26	CLA	6	602	22	1/1/15/20	17/37/115/115	-
39	II0	O	614	-	-	1/21/67/67	0/2/2/2
26	CLA	c	503	3	1/1/15/20	8/37/115/115	-
37	HEM	F	101	6,5	-	6/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	b	605	2	1/1/15/20	9/37/115/115	-
39	II0	3	312	-	-	10/21/67/67	0/2/2/2
26	CLA	N	607	-	1/1/10/20	5/11/89/115	-
26	CLA	d	402	41	1/1/15/20	10/37/115/115	-
26	CLA	Q	303	20	1/1/14/20	16/33/111/115	-
26	CLA	N	608	-	1/1/11/20	5/15/93/115	-
38	KC2	1	611	17	-	8/15/71/71	-
39	II0	2	320	-	-	3/21/67/67	0/2/2/2
38	KC2	3	304	19	-	9/15/71/71	-
26	CLA	2	307	18	1/1/11/20	2/17/95/115	-
26	CLA	1	602	17	1/1/14/20	6/31/109/115	-
26	CLA	c	508	3	1/1/15/20	7/37/115/115	-
30	SQD	D	401	-	-	7/49/69/69	0/1/1/1
26	CLA	b	612	2	1/1/15/20	12/37/115/115	-
26	CLA	1	608	17	1/1/11/20	7/15/93/115	-
35	DGD	C	517	-	-	8/43/83/95	0/2/2/2
26	CLA	N	604	17	1/1/13/20	8/30/108/115	-
33	LMG	c	521	-	-	19/46/66/70	0/1/1/1
26	CLA	B	606	-	1/1/15/20	12/37/115/115	-
28	WVN	d	410	-	-	12/29/63/63	0/2/2/2
26	CLA	4	307	20	1/1/10/20	3/11/89/115	-
26	CLA	G	402	23	1/1/11/20	4/13/91/115	-
26	CLA	b	604	2	1/1/13/20	12/30/108/115	-
28	WVN	5	617	-	-	9/29/63/63	0/2/2/2
34	LHG	N	621	-	-	12/50/50/53	-
28	WVN	B	618	-	-	17/29/63/63	0/2/2/2
34	LHG	R	319	26	-	12/44/44/53	-
38	KC2	4	311	20	-	3/15/71/71	-
26	CLA	B	602	2	-	6/37/115/115	-
26	CLA	N	609	17	1/1/14/20	7/31/109/115	-
26	CLA	5	607	21	1/1/15/20	10/37/115/115	-
26	CLA	P	601	19	1/1/11/20	2/13/91/115	-
26	CLA	R	309	21	1/1/13/20	10/30/108/115	-
39	II0	S	612	-	-	1/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	R	313	21	1/1/11/20	5/15/93/115	-
28	WVN	3	313	-	-	16/29/63/63	0/2/2/2
26	CLA	a	405	1	1/1/14/20	11/31/109/115	-
26	CLA	b	603	2	1/1/15/20	9/37/115/115	-
39	II0	4	320	-	-	0/21/67/67	0/2/2/2
26	CLA	5	605	21	1/1/15/20	14/37/115/115	-
34	LHG	L	101	-	-	7/53/53/53	-
26	CLA	B	608	2	1/1/15/20	4/37/115/115	-
33	LMG	d	404	-	-	9/35/55/70	0/1/1/1
28	WVN	b	618	-	-	10/29/63/63	0/2/2/2
40	IHT	1	619	-	-	15/25/65/65	0/2/2/2
39	II0	R	314	-	-	0/21/67/67	0/2/2/2
39	II0	R	316	-	-	3/21/67/67	0/2/2/2
26	CLA	1	606	17	1/1/12/20	8/19/97/115	-
26	CLA	1	603	17	1/1/12/20	7/22/100/115	-
33	LMG	B	620	-	-	7/46/66/70	0/1/1/1
26	CLA	b	613	2	1/1/15/20	16/37/115/115	-
26	CLA	S	607	34	1/1/13/20	11/25/103/115	-
26	CLA	6	609	22	1/1/12/20	5/23/101/115	-
38	KC2	1	612	17	-	9/15/71/71	-
26	CLA	4	313	20	1/1/10/20	2/11/89/115	-
34	LHG	d	408	-	-	13/53/53/53	-
26	CLA	D	408	4	1/1/14/20	13/31/109/115	-
28	WVN	B	617	-	-	15/29/63/63	0/2/2/2
26	CLA	c	510	3	1/1/15/20	12/37/115/115	-
26	CLA	b	607	41	1/1/15/20	12/37/115/115	-
34	LHG	b	621	-	-	20/47/47/53	-
39	II0	P	612	-	-	2/21/67/67	0/2/2/2
26	CLA	6	603	22	1/1/13/20	9/25/103/115	-
26	CLA	4	309	20	1/1/12/20	4/21/99/115	-
39	II0	O	613	-	-	2/21/67/67	0/2/2/2
26	CLA	P	610	19	1/1/13/20	11/25/103/115	-
38	KC2	N	610	-	-	4/15/71/71	-
26	CLA	6	607	34	1/1/13/20	11/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	a	413	-	-	8/43/63/70	0/1/1/1
26	CLA	b	614	2	1/1/14/20	12/31/109/115	-
26	CLA	O	603	18	1/1/15/20	8/37/115/115	-
26	CLA	C	511	3	1/1/15/20	11/37/115/115	-
26	CLA	2	311	18	1/1/14/20	10/31/109/115	-
26	CLA	R	303	21	1/1/13/20	12/25/103/115	-
26	CLA	B	615	2	1/1/15/20	10/37/115/115	-
26	CLA	C	513	3	1/1/15/20	11/37/115/115	-
39	II0	Q	313	-	-	2/21/67/67	0/2/2/2
26	CLA	2	309	-	1/1/14/20	15/31/109/115	-
26	CLA	5	612	21	1/1/11/20	5/15/93/115	-
40	IHT	Q	317	-	-	10/25/65/65	0/2/2/2
33	LMG	D	406	-	-	9/35/55/70	0/1/1/1
26	CLA	5	604	21	1/1/14/20	11/31/109/115	-
26	CLA	6	604	22	1/1/15/20	18/37/115/115	-
39	II0	4	316	-	-	2/21/67/67	0/2/2/2
39	II0	Q	315	-	-	1/21/67/67	0/2/2/2
34	LHG	l	101	-	-	6/53/53/53	-
26	CLA	O	608	18	1/1/15/20	10/37/115/115	-
38	KC2	Q	304	-	-	7/15/71/71	-
26	CLA	1	604	17	1/1/13/20	15/30/108/115	-
26	CLA	4	308	20	1/1/13/20	9/27/105/115	-
26	CLA	Q	302	20	1/1/15/20	14/37/115/115	-
26	CLA	c	512	3	1/1/15/20	11/37/115/115	-
28	WVN	k	101	-	-	8/29/63/63	0/2/2/2
38	KC2	1	605	-	-	12/15/71/71	-
39	II0	1	618	-	-	14/21/67/67	0/2/2/2
33	LMG	d	409	-	-	2/32/52/70	0/1/1/1
28	WVN	c	517	-	-	10/29/63/63	0/2/2/2
26	CLA	1	613	-	1/1/11/20	8/17/95/115	-
39	II0	O	618	-	-	1/21/67/67	0/2/2/2
34	LHG	z	101	-	-	8/29/29/53	-
26	CLA	c	513	3	1/1/15/20	11/37/115/115	-
26	CLA	R	305	21	1/1/14/20	11/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	II0	N	615	-	-	4/21/67/67	0/2/2/2
38	KC2	Q	310	20	-	3/15/71/71	-
26	CLA	4	301	34	1/1/12/20	6/22/100/115	-
39	II0	2	316	-	-	11/21/67/67	0/2/2/2
26	CLA	C	508	41	1/1/15/20	8/37/115/115	-
26	CLA	5	601	21	1/1/13/20	6/25/103/115	-
26	CLA	1	607	17	1/1/10/20	5/11/89/115	-
26	CLA	5	603	21	1/1/12/20	9/22/100/115	-
34	LHG	Z	102	-	-	8/29/29/53	-
39	II0	3	310	-	-	10/21/67/67	0/2/2/2
26	CLA	2	308	18	1/1/15/20	10/37/115/115	-
26	CLA	3	307	19	1/1/12/20	5/23/101/115	-
26	CLA	4	304	20	1/1/14/20	17/33/111/115	-
26	CLA	b	610	41	1/1/15/20	9/37/115/115	-
26	CLA	3	309	19	1/1/11/20	8/13/91/115	-
26	CLA	R	308	21	1/1/15/20	10/37/115/115	-
26	CLA	S	610	22	1/1/15/20	10/37/115/115	-
26	CLA	B	612	2	1/1/15/20	12/37/115/115	-
39	II0	4	317	-	-	5/21/67/67	0/2/2/2
28	WVN	a	406	-	-	9/29/63/63	0/2/2/2
28	WVN	B	619	-	-	10/29/63/63	0/2/2/2
34	LHG	a	409	-	-	28/46/46/53	-
28	WVN	Z	101	-	-	10/29/63/63	0/2/2/2
29	PL9	D	409	-	-	7/53/73/73	0/1/1/1
33	LMG	O	617	-	-	2/35/55/70	0/1/1/1
26	CLA	B	614	2	1/1/14/20	11/31/109/115	-
26	CLA	P	603	19	1/1/15/20	15/37/115/115	-
26	CLA	Q	312	20	1/1/10/20	2/11/89/115	-
30	SQD	a	408	-	-	4/35/55/69	0/1/1/1
26	CLA	5	606	21	1/1/10/20	4/11/89/115	-
26	CLA	B	613	2	1/1/15/20	15/37/115/115	-
33	LMG	C	519	-	-	20/42/62/70	0/1/1/1
26	CLA	2	304	-	1/1/15/20	12/37/115/115	-
26	CLA	3	305	19	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	B	609	2	1/1/15/20	9/37/115/115	-
29	PL9	A	407	-	-	10/27/47/73	0/1/1/1
39	II0	N	617	-	-	3/21/67/67	0/2/2/2
26	CLA	O	611	18	1/1/14/20	10/31/109/115	-
28	WVN	c	516	-	-	10/29/63/63	0/2/2/2
26	CLA	N	614	17	1/1/11/20	10/16/94/115	-
26	CLA	N	613	-	1/1/11/20	6/17/95/115	-
39	II0	Q	316	-	-	5/21/67/67	0/2/2/2
26	CLA	B	610	41	1/1/15/20	9/37/115/115	-
26	CLA	3	301	19	1/1/14/20	15/34/112/115	-
26	CLA	C	512	3	1/1/15/20	13/37/115/115	-
26	CLA	c	511	3	1/1/15/20	13/37/115/115	-
38	KC2	R	311	-	-	8/15/71/71	-
26	CLA	5	611	21	1/1/13/20	14/25/103/115	-
39	II0	2	313	-	-	1/21/67/67	0/2/2/2
34	LHG	c	520	-	-	13/44/44/53	-
39	II0	N	620	-	-	3/21/67/67	0/2/2/2
40	IHT	4	318	-	-	10/25/65/65	0/2/2/2
39	II0	6	613	-	-	4/21/67/67	0/2/2/2
26	CLA	N	603	-	1/1/12/20	7/21/99/115	-

All (2712) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	1	616	II0	C14-C10	18.08	1.55	1.34
39	2	316	II0	C14-C10	17.59	1.54	1.34
39	O	615	II0	C14-C10	17.57	1.54	1.34
40	1	619	IHT	C15-C11	17.56	1.54	1.34
39	1	618	II0	C14-C10	17.39	1.54	1.34
40	2	317	IHT	C15-C11	17.36	1.54	1.34
39	1	617	II0	C13-C09	17.27	1.54	1.34
39	3	311	II0	C13-C09	17.22	1.54	1.34
39	P	613	II0	C13-C09	17.22	1.54	1.34
39	1	617	II0	C14-C10	17.20	1.54	1.34
39	3	311	II0	C14-C10	17.16	1.54	1.34
39	P	613	II0	C14-C10	17.16	1.54	1.34
39	3	310	II0	C13-C09	17.15	1.54	1.34
39	1	615	II0	C14-C10	17.14	1.54	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	1	618	II0	C13-C09	16.97	1.53	1.34
39	3	312	II0	C14-C10	16.90	1.53	1.34
39	3	310	II0	C14-C10	16.90	1.53	1.34
39	O	615	II0	C13-C09	16.84	1.53	1.34
39	2	316	II0	C13-C09	16.84	1.53	1.34
39	1	615	II0	C13-C09	16.82	1.53	1.34
39	1	616	II0	C13-C09	16.81	1.53	1.34
39	3	312	II0	C13-C09	16.14	1.52	1.34
28	B	618	WVN	C26-C22	14.29	1.54	1.35
28	3	313	WVN	C26-C22	14.13	1.54	1.35
28	C	516	WVN	C26-C22	13.94	1.54	1.35
28	H	101	WVN	C26-C22	13.91	1.54	1.35
39	1	618	II0	C39-C35	13.88	1.54	1.35
39	1	617	II0	C39-C35	13.81	1.54	1.35
39	1	615	II0	C39-C35	13.80	1.54	1.35
28	C	516	WVN	C28-C25	13.75	1.54	1.35
28	B	617	WVN	C26-C22	13.68	1.53	1.35
39	1	618	II0	C40-C36	13.61	1.53	1.35
40	1	619	IHT	C27-C23	13.59	1.53	1.35
40	1	619	IHT	C38-C35	13.58	1.53	1.35
40	2	317	IHT	C38-C35	13.51	1.53	1.35
39	1	617	II0	C40-C36	13.49	1.53	1.35
39	1	616	II0	C39-C35	13.45	1.53	1.35
40	2	317	IHT	C37-C33	13.41	1.53	1.35
28	B	618	WVN	C28-C25	13.37	1.53	1.35
39	1	615	II0	C40-C36	13.36	1.53	1.35
28	H	101	WVN	C28-C25	13.35	1.53	1.35
40	2	317	IHT	C27-C23	13.34	1.53	1.35
39	3	310	II0	C39-C35	13.34	1.53	1.35
28	B	617	WVN	C28-C25	13.29	1.53	1.35
28	3	313	WVN	C28-C25	13.28	1.53	1.35
39	3	312	II0	C39-C35	13.28	1.53	1.35
39	3	310	II0	C40-C36	13.27	1.53	1.35
39	1	616	II0	C40-C36	13.27	1.53	1.35
28	3	313	WVN	C37-C34	13.22	1.53	1.35
40	1	619	IHT	C37-C33	13.16	1.53	1.35
39	3	311	II0	C39-C35	13.14	1.53	1.35
39	P	613	II0	C39-C35	13.14	1.53	1.35
39	2	316	II0	C40-C36	13.13	1.53	1.35
39	O	615	II0	C40-C36	13.13	1.53	1.35
28	C	516	WVN	C37-C34	13.11	1.53	1.35
39	3	311	II0	C40-C36	13.07	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	3	312	II0	C40-C36	13.03	1.53	1.35
39	P	613	II0	C40-C36	13.02	1.53	1.35
39	2	316	II0	C39-C35	13.01	1.53	1.35
39	O	615	II0	C39-C35	12.95	1.53	1.35
28	H	101	WVN	C37-C34	12.82	1.52	1.35
28	B	617	WVN	C37-C34	12.65	1.52	1.35
28	B	618	WVN	C37-C34	12.57	1.52	1.35
28	3	313	WVN	C36-C32	12.54	1.52	1.35
28	B	618	WVN	C36-C32	12.21	1.52	1.35
28	H	101	WVN	C36-C32	12.20	1.52	1.35
28	B	617	WVN	C36-C32	12.07	1.51	1.35
28	C	516	WVN	C36-C32	12.06	1.51	1.35
28	C	516	WVN	C15-C13	11.18	1.53	1.34
40	2	317	IHT	C10-C07	11.13	1.53	1.34
28	3	313	WVN	C15-C13	11.03	1.53	1.34
28	B	617	WVN	C15-C13	11.03	1.53	1.34
28	H	101	WVN	C15-C13	11.02	1.53	1.34
39	6	613	II0	C13-C09	-10.90	1.22	1.34
39	R	318	II0	C13-C09	-10.88	1.22	1.34
40	1	619	IHT	C10-C07	10.88	1.53	1.34
28	B	618	WVN	C15-C13	10.84	1.53	1.34
26	2	305	CLA	C1D-ND	10.64	1.50	1.37
28	B	617	WVN	C09-C05	10.34	1.53	1.32
28	3	313	WVN	C09-C05	10.26	1.52	1.32
28	C	516	WVN	C09-C05	10.25	1.52	1.32
28	H	101	WVN	C09-C05	10.19	1.52	1.32
39	Q	319	II0	C13-C09	-10.14	1.23	1.34
39	4	320	II0	C13-C09	-10.14	1.23	1.34
39	N	617	II0	C13-C09	-10.12	1.23	1.34
28	B	618	WVN	C09-C05	10.10	1.52	1.32
39	4	317	II0	C13-C09	-10.00	1.23	1.34
39	2	315	II0	C13-C09	-9.99	1.23	1.34
39	Q	315	II0	C13-C09	-9.98	1.23	1.34
39	Q	316	II0	C13-C09	-9.98	1.23	1.34
39	N	620	II0	C13-C09	-9.95	1.23	1.34
39	N	618	II0	C13-C09	-9.95	1.23	1.34
39	4	316	II0	C13-C09	-9.92	1.23	1.34
39	4	315	II0	C13-C09	-9.91	1.23	1.34
39	Q	314	II0	C13-C09	-9.90	1.23	1.34
39	R	315	II0	C13-C09	-9.86	1.23	1.34
39	P	612	II0	C13-C09	-9.85	1.23	1.34
39	P	614	II0	C13-C09	-9.85	1.24	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	N	615	II0	C13-C09	-9.83	1.24	1.34
39	4	314	II0	C13-C09	-9.80	1.24	1.34
39	5	614	II0	C13-C09	-9.79	1.24	1.34
39	Q	313	II0	C13-C09	-9.79	1.24	1.34
39	R	316	II0	C13-C09	-9.75	1.24	1.34
39	5	615	II0	C13-C09	-9.72	1.24	1.34
39	O	614	II0	C13-C09	-9.72	1.24	1.34
39	O	613	II0	C13-C09	-9.68	1.24	1.34
39	2	313	II0	C13-C09	-9.65	1.24	1.34
39	2	314	II0	C13-C09	-9.65	1.24	1.34
39	6	612	II0	C13-C09	-9.64	1.24	1.34
39	S	612	II0	C13-C09	-9.61	1.24	1.34
39	5	613	II0	C13-C09	-9.60	1.24	1.34
39	N	616	II0	C13-C09	-9.59	1.24	1.34
39	R	314	II0	C13-C09	-9.57	1.24	1.34
39	6	611	II0	C13-C09	-9.42	1.24	1.34
39	S	611	II0	C13-C09	-9.39	1.24	1.34
26	1	614	CLA	C4B-NB	9.15	1.43	1.35
39	3	310	II0	C29-C25	9.07	1.56	1.37
39	P	613	II0	C29-C25	8.56	1.55	1.37
39	3	311	II0	C29-C25	8.55	1.55	1.37
39	O	615	II0	C29-C25	8.54	1.54	1.37
39	2	316	II0	C29-C25	8.54	1.54	1.37
39	3	312	II0	C29-C25	8.54	1.54	1.37
38	4	311	KC2	C4D-ND	8.53	1.42	1.35
38	Q	310	KC2	C4D-ND	8.52	1.42	1.35
39	1	615	II0	C30-C26	8.29	1.54	1.37
39	1	617	II0	C30-C26	8.29	1.54	1.37
39	1	618	II0	C30-C26	8.24	1.54	1.37
38	N	612	KC2	C4D-ND	8.21	1.42	1.35
40	2	317	IHT	C29-C26	8.21	1.54	1.37
26	N	607	CLA	C4B-NB	8.20	1.42	1.35
39	1	616	II0	C30-C26	8.19	1.54	1.37
38	N	612	KC2	C4C-NC	8.19	1.50	1.37
26	D	407	CLA	C4B-NB	8.16	1.42	1.35
26	P	601	CLA	C4B-NB	8.15	1.42	1.35
38	N	610	KC2	C4D-ND	8.11	1.42	1.35
26	5	604	CLA	C4B-NB	8.10	1.42	1.35
26	2	319	CLA	C4B-NB	8.09	1.42	1.35
26	4	307	CLA	C4B-NB	8.07	1.42	1.35
38	O	610	KC2	C4D-ND	8.07	1.42	1.35
26	C	512	CLA	C4B-NB	8.07	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	2	310	KC2	C4D-ND	8.05	1.42	1.35
26	d	405	CLA	C4B-NB	8.05	1.42	1.35
40	1	619	IHT	C29-C26	8.04	1.53	1.37
39	1	617	II0	C29-C25	8.01	1.53	1.37
38	4	305	KC2	C4D-ND	8.01	1.42	1.35
38	N	611	KC2	C4D-ND	8.01	1.42	1.35
26	R	305	CLA	C4B-NB	8.00	1.42	1.35
26	B	601	CLA	C4B-NB	8.00	1.42	1.35
38	R	311	KC2	C4D-ND	8.00	1.42	1.35
39	3	312	II0	C30-C26	8.00	1.53	1.37
39	O	615	II0	C30-C26	8.00	1.53	1.37
26	g	401	CLA	C4B-NB	7.99	1.42	1.35
26	R	302	CLA	C4B-NB	7.99	1.42	1.35
38	5	610	KC2	C4D-ND	7.99	1.42	1.35
26	Q	306	CLA	C4B-NB	7.99	1.42	1.35
39	2	316	II0	C30-C26	7.99	1.53	1.37
26	O	603	CLA	C4B-NB	7.99	1.42	1.35
38	Q	304	KC2	C4D-ND	7.98	1.42	1.35
26	B	610	CLA	C4B-NB	7.98	1.42	1.35
26	b	608	CLA	C4B-NB	7.98	1.42	1.35
26	2	303	CLA	C4B-NB	7.97	1.42	1.35
26	c	503	CLA	C4B-NB	7.97	1.42	1.35
26	A	403	CLA	C4B-NB	7.97	1.42	1.35
26	N	604	CLA	C4B-NB	7.97	1.42	1.35
26	B	611	CLA	C4B-NB	7.96	1.42	1.35
26	b	610	CLA	C4B-NB	7.96	1.42	1.35
26	a	405	CLA	C4B-NB	7.96	1.42	1.35
26	5	609	CLA	C4B-NB	7.95	1.42	1.35
26	c	505	CLA	C4B-NB	7.95	1.42	1.35
26	5	601	CLA	C4B-NB	7.94	1.42	1.35
38	4	305	KC2	C4C-NC	7.94	1.49	1.37
39	1	618	II0	C29-C25	7.94	1.53	1.37
26	R	310	CLA	C4B-NB	7.94	1.42	1.35
26	b	613	CLA	C4B-NB	7.94	1.42	1.35
26	2	302	CLA	C4B-NB	7.94	1.42	1.35
26	O	601	CLA	C4B-NB	7.93	1.42	1.35
26	O	606	CLA	C4B-NB	7.93	1.42	1.35
39	3	310	II0	C30-C26	7.92	1.53	1.37
38	5	610	KC2	C4C-NC	7.92	1.49	1.37
38	Q	304	KC2	C4C-NC	7.92	1.49	1.37
26	P	610	CLA	C4B-NB	7.91	1.42	1.35
38	6	608	KC2	C4D-ND	7.91	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	S	608	KC2	C4D-ND	7.91	1.42	1.35
26	R	309	CLA	C4B-NB	7.91	1.42	1.35
38	4	311	KC2	C4C-NC	7.91	1.49	1.37
26	D	404	CLA	C4B-NB	7.91	1.42	1.35
26	d	402	CLA	C4B-NB	7.91	1.42	1.35
26	O	602	CLA	C4B-NB	7.91	1.42	1.35
26	C	513	CLA	C4B-NB	7.90	1.42	1.35
39	1	616	II0	C29-C25	7.90	1.53	1.37
26	O	609	CLA	C4B-NB	7.90	1.42	1.35
38	2	310	KC2	C4C-NC	7.90	1.49	1.37
26	5	608	CLA	C4B-NB	7.89	1.42	1.35
26	P	607	CLA	C4B-NB	7.89	1.42	1.35
26	b	606	CLA	C4B-NB	7.89	1.42	1.35
38	N	610	KC2	C4C-NC	7.89	1.49	1.37
26	R	306	CLA	C4B-NB	7.89	1.42	1.35
26	6	607	CLA	C4B-NB	7.88	1.42	1.35
26	N	614	CLA	C4B-NB	7.88	1.42	1.35
26	3	307	CLA	C4B-NB	7.88	1.42	1.35
26	b	607	CLA	C4B-NB	7.87	1.42	1.35
26	C	504	CLA	C4B-NB	7.87	1.42	1.35
38	R	311	KC2	C4C-NC	7.87	1.49	1.37
26	b	611	CLA	C4B-NB	7.87	1.42	1.35
26	2	307	CLA	C4B-NB	7.87	1.42	1.35
26	a	403	CLA	C4B-NB	7.86	1.42	1.35
26	O	607	CLA	C4B-NB	7.86	1.42	1.35
26	3	306	CLA	C4B-NB	7.86	1.42	1.35
26	B	609	CLA	C4B-NB	7.86	1.42	1.35
38	Q	310	KC2	C4C-NC	7.85	1.49	1.37
26	2	309	CLA	C4B-NB	7.85	1.42	1.35
26	c	512	CLA	C4B-NB	7.85	1.42	1.35
26	D	408	CLA	C4B-NB	7.84	1.42	1.35
26	c	513	CLA	C4B-NB	7.83	1.42	1.35
26	S	607	CLA	C4B-NB	7.83	1.42	1.35
38	O	610	KC2	C4C-NC	7.83	1.49	1.37
26	B	607	CLA	C4B-NB	7.83	1.42	1.35
39	1	615	II0	C29-C25	7.83	1.53	1.37
26	B	613	CLA	C4B-NB	7.83	1.42	1.35
26	C	514	CLA	C4B-NB	7.83	1.42	1.35
26	6	601	CLA	C4B-NB	7.83	1.42	1.35
38	N	605	KC2	C4C-NC	7.82	1.49	1.37
26	b	605	CLA	C4B-NB	7.82	1.42	1.35
26	S	601	CLA	C4B-NB	7.82	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	603	CLA	C4B-NB	7.82	1.42	1.35
26	4	313	CLA	C4B-NB	7.82	1.42	1.35
26	2	306	CLA	C4B-NB	7.82	1.42	1.35
38	3	304	KC2	C4C-NC	7.81	1.49	1.37
38	P	605	KC2	C4D-ND	7.80	1.42	1.35
26	d	406	CLA	C4B-NB	7.80	1.42	1.35
26	P	609	CLA	C4B-NB	7.80	1.42	1.35
26	C	502	CLA	C4B-NB	7.80	1.42	1.35
26	N	601	CLA	C4B-NB	7.80	1.42	1.35
26	P	603	CLA	C4B-NB	7.79	1.42	1.35
26	2	301	CLA	C4B-NB	7.79	1.42	1.35
26	b	614	CLA	C4B-NB	7.79	1.42	1.35
26	c	515	CLA	C4B-NB	7.79	1.42	1.35
38	P	605	KC2	C4C-NC	7.79	1.49	1.37
26	R	312	CLA	C4B-NB	7.79	1.42	1.35
26	R	308	CLA	C4B-NB	7.79	1.42	1.35
38	4	310	KC2	C4C-NC	7.79	1.49	1.37
38	N	605	KC2	C4D-ND	7.78	1.42	1.35
26	B	615	CLA	C4B-NB	7.78	1.42	1.35
26	B	605	CLA	C4B-NB	7.78	1.42	1.35
26	3	302	CLA	C4B-NB	7.78	1.42	1.35
26	B	608	CLA	C4B-NB	7.77	1.42	1.35
26	B	606	CLA	C4B-NB	7.77	1.42	1.35
26	c	508	CLA	C4B-NB	7.77	1.42	1.35
26	Q	308	CLA	C4B-NB	7.77	1.42	1.35
26	5	605	CLA	C4B-NB	7.77	1.42	1.35
26	B	603	CLA	C4B-NB	7.76	1.42	1.35
26	b	609	CLA	C4B-NB	7.76	1.42	1.35
26	O	604	CLA	C4B-NB	7.76	1.42	1.35
38	Q	309	KC2	C4C-NC	7.76	1.49	1.37
38	Q	309	KC2	C4D-ND	7.75	1.42	1.35
26	c	507	CLA	C4B-NB	7.74	1.42	1.35
26	N	609	CLA	C4B-NB	7.74	1.42	1.35
26	5	611	CLA	C4B-NB	7.74	1.42	1.35
26	c	514	CLA	C4B-NB	7.74	1.42	1.35
26	5	607	CLA	C4B-NB	7.74	1.42	1.35
26	a	402	CLA	C4B-NB	7.73	1.42	1.35
26	C	511	CLA	C4B-NB	7.73	1.42	1.35
26	A	402	CLA	C4B-NB	7.73	1.42	1.35
26	O	608	CLA	C4B-NB	7.73	1.42	1.35
26	P	608	CLA	C4B-NB	7.73	1.42	1.35
26	Q	312	CLA	C4B-NB	7.73	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	506	CLA	C4B-NB	7.72	1.42	1.35
26	C	505	CLA	C4B-NB	7.72	1.42	1.35
26	b	604	CLA	C4B-NB	7.72	1.42	1.35
26	b	616	CLA	C4B-NB	7.72	1.42	1.35
26	2	311	CLA	C4B-NB	7.72	1.42	1.35
26	N	613	CLA	C4B-NB	7.71	1.42	1.35
26	6	602	CLA	C4B-NB	7.71	1.42	1.35
26	b	601	CLA	C4B-NB	7.71	1.42	1.35
26	b	615	CLA	C4B-NB	7.71	1.42	1.35
26	B	616	CLA	C4B-NB	7.70	1.42	1.35
26	c	510	CLA	C4B-NB	7.70	1.42	1.35
26	P	602	CLA	C4B-NB	7.70	1.42	1.35
26	2	304	CLA	C4B-NB	7.70	1.42	1.35
26	C	508	CLA	C4B-NB	7.69	1.42	1.35
39	3	311	II0	C21-C09	7.69	1.58	1.42
26	O	611	CLA	C4B-NB	7.69	1.42	1.35
26	R	304	CLA	C4B-NB	7.69	1.42	1.35
26	Q	305	CLA	C4B-NB	7.68	1.42	1.35
26	S	602	CLA	C4B-NB	7.68	1.42	1.35
26	S	606	CLA	C4B-NB	7.68	1.42	1.35
38	3	304	KC2	C4D-ND	7.68	1.42	1.35
26	B	602	CLA	C4B-NB	7.67	1.42	1.35
26	6	606	CLA	C4B-NB	7.67	1.42	1.35
26	C	510	CLA	C4B-NB	7.67	1.42	1.35
26	c	504	CLA	C4B-NB	7.67	1.42	1.35
26	O	605	CLA	C4B-NB	7.67	1.42	1.35
26	b	602	CLA	C4B-NB	7.66	1.42	1.35
38	4	310	KC2	C4D-ND	7.66	1.42	1.35
26	C	506	CLA	C4B-NB	7.66	1.42	1.35
26	2	308	CLA	C4B-NB	7.66	1.42	1.35
38	6	608	KC2	C4C-NC	7.65	1.49	1.37
26	4	309	CLA	C4B-NB	7.65	1.42	1.35
39	P	613	II0	C21-C09	7.65	1.58	1.42
26	5	603	CLA	C4B-NB	7.64	1.42	1.35
26	4	301	CLA	C4B-NB	7.64	1.42	1.35
26	A	405	CLA	C4B-NB	7.63	1.42	1.35
26	4	304	CLA	C4B-NB	7.63	1.42	1.35
39	3	311	II0	C30-C26	7.62	1.53	1.37
39	P	613	II0	C30-C26	7.62	1.53	1.37
26	R	313	CLA	C4B-NB	7.62	1.42	1.35
38	S	608	KC2	C4C-NC	7.61	1.49	1.37
26	C	509	CLA	C4B-NB	7.61	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	612	CLA	C4B-NB	7.61	1.42	1.35
26	C	507	CLA	C4B-NB	7.61	1.42	1.35
26	G	402	CLA	C4B-NB	7.60	1.42	1.35
26	N	603	CLA	C4B-NB	7.59	1.42	1.35
26	3	301	CLA	C4B-NB	7.58	1.42	1.35
26	P	606	CLA	C4B-NB	7.58	1.42	1.35
26	N	606	CLA	C4B-NB	7.58	1.42	1.35
26	R	303	CLA	C4B-NB	7.58	1.42	1.35
26	N	602	CLA	C4B-NB	7.57	1.42	1.35
26	1	603	CLA	C4B-NB	7.56	1.42	1.35
26	Q	303	CLA	C4B-NB	7.56	1.42	1.35
26	B	614	CLA	C4B-NB	7.56	1.42	1.35
26	4	306	CLA	C4B-NB	7.55	1.41	1.35
38	N	611	KC2	C4C-NC	7.55	1.49	1.37
39	3	310	II0	C21-C09	7.55	1.58	1.42
26	C	503	CLA	C4B-NB	7.55	1.41	1.35
26	3	305	CLA	C4B-NB	7.54	1.41	1.35
26	5	602	CLA	C4B-NB	7.54	1.41	1.35
26	B	604	CLA	C4B-NB	7.54	1.41	1.35
26	G	401	CLA	C4B-NB	7.52	1.41	1.35
26	4	308	CLA	C4B-NB	7.51	1.41	1.35
26	2	312	CLA	C4B-NB	7.50	1.41	1.35
26	1	607	CLA	C4B-NB	7.50	1.41	1.35
26	O	612	CLA	C4B-NB	7.50	1.41	1.35
26	3	309	CLA	C4B-NB	7.49	1.41	1.35
26	Q	301	CLA	C4B-NB	7.49	1.41	1.35
26	Q	302	CLA	C4B-NB	7.49	1.41	1.35
39	3	312	II0	C21-C09	7.48	1.58	1.42
26	c	511	CLA	C4B-NB	7.47	1.41	1.35
26	1	606	CLA	C4B-NB	7.47	1.41	1.35
26	1	601	CLA	C4B-NB	7.46	1.41	1.35
39	3	311	II0	C23-C25	7.46	1.56	1.42
26	P	611	CLA	C4B-NB	7.45	1.41	1.35
26	c	509	CLA	C4B-NB	7.45	1.41	1.35
26	4	302	CLA	C4B-NB	7.45	1.41	1.35
26	1	613	CLA	C4B-NB	7.44	1.41	1.35
26	4	303	CLA	C4B-NB	7.44	1.41	1.35
26	Q	307	CLA	C4B-NB	7.44	1.41	1.35
39	P	613	II0	C23-C25	7.42	1.56	1.42
26	6	610	CLA	C4B-NB	7.42	1.41	1.35
26	S	605	CLA	C4B-NB	7.42	1.41	1.35
26	1	608	CLA	C4B-NB	7.40	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	3	303	CLA	C4B-NB	7.39	1.41	1.35
26	6	605	CLA	C4B-NB	7.39	1.41	1.35
40	Q	317	IHT	C38-C35	7.38	1.45	1.35
40	4	318	IHT	C38-C35	7.38	1.45	1.35
26	6	603	CLA	C4B-NB	7.37	1.41	1.35
26	S	610	CLA	C4B-NB	7.37	1.41	1.35
40	O	616	IHT	C38-C35	7.37	1.45	1.35
26	b	612	CLA	C4B-NB	7.35	1.41	1.35
39	O	615	II0	C23-C25	7.35	1.56	1.42
26	S	603	CLA	C4B-NB	7.34	1.41	1.35
26	P	604	CLA	C4B-NB	7.34	1.41	1.35
39	2	316	II0	C23-C25	7.33	1.56	1.42
26	1	602	CLA	C4B-NB	7.33	1.41	1.35
26	R	307	CLA	C4B-NB	7.32	1.41	1.35
39	3	312	II0	C23-C25	7.31	1.56	1.42
26	6	604	CLA	C4B-NB	7.30	1.41	1.35
26	5	606	CLA	C4B-NB	7.27	1.41	1.35
26	S	609	CLA	C4B-NB	7.25	1.41	1.35
40	N	619	IHT	C38-C35	7.23	1.45	1.35
39	O	615	II0	C21-C09	7.23	1.57	1.42
40	R	317	IHT	C38-C35	7.22	1.45	1.35
26	1	604	CLA	C4B-NB	7.22	1.41	1.35
26	6	609	CLA	C4B-NB	7.22	1.41	1.35
39	2	316	II0	C21-C09	7.21	1.57	1.42
40	5	616	IHT	C38-C35	7.21	1.45	1.35
26	g	402	CLA	C4B-NB	7.21	1.41	1.35
26	S	604	CLA	C4B-NB	7.19	1.41	1.35
39	3	310	II0	C23-C25	7.15	1.56	1.42
26	Q	311	CLA	C4B-NB	7.13	1.41	1.35
26	1	609	CLA	C4B-NB	7.08	1.41	1.35
26	B	612	CLA	C4B-NB	7.06	1.41	1.35
26	4	312	CLA	C4B-NB	7.04	1.41	1.35
39	1	618	II0	C23-C25	6.77	1.55	1.42
39	1	617	II0	C23-C25	6.71	1.55	1.42
39	1	616	II0	C23-C25	6.63	1.55	1.42
40	2	317	IHT	C21-C11	6.61	1.56	1.42
39	1	615	II0	C23-C25	6.58	1.55	1.42
39	1	618	II0	C21-C09	6.52	1.56	1.42
40	2	317	IHT	C24-C26	6.45	1.54	1.42
39	1	617	II0	C21-C09	6.44	1.56	1.42
39	1	618	II0	C22-C10	6.42	1.55	1.42
39	1	616	II0	C21-C09	6.41	1.55	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	1	615	II0	C21-C09	6.37	1.55	1.42
40	1	619	IHT	C21-C11	6.23	1.55	1.42
39	1	617	II0	C22-C10	6.22	1.55	1.42
39	1	616	II0	C22-C10	6.18	1.55	1.42
38	4	305	KC2	C2A-C3A	6.07	1.49	1.37
39	1	617	II0	C24-C26	6.06	1.54	1.42
38	Q	304	KC2	C2A-C3A	6.03	1.49	1.37
39	P	613	II0	C23-C21	5.99	1.37	1.20
40	1	619	IHT	C24-C26	5.98	1.54	1.42
39	3	311	II0	C23-C21	5.96	1.37	1.20
39	1	615	II0	C22-C10	5.96	1.55	1.42
39	3	312	II0	C23-C21	5.94	1.37	1.20
39	1	618	II0	C24-C26	5.93	1.54	1.42
39	3	310	II0	C23-C21	5.92	1.37	1.20
39	1	615	II0	C24-C26	5.92	1.53	1.42
39	2	316	II0	C23-C21	5.91	1.37	1.20
39	O	615	II0	C23-C21	5.91	1.37	1.20
38	4	310	KC2	C2A-C3A	5.82	1.49	1.37
38	Q	309	KC2	C2A-C3A	5.81	1.49	1.37
38	N	610	KC2	C2A-C3A	5.80	1.49	1.37
38	N	612	KC2	OBD-CAD	5.78	1.30	1.22
38	N	605	KC2	C2A-C3A	5.75	1.48	1.37
39	3	312	II0	C22-C10	5.73	1.54	1.42
39	O	615	II0	C22-C10	5.73	1.54	1.42
39	3	310	II0	C24-C26	5.72	1.53	1.42
39	2	316	II0	C24-C26	5.71	1.53	1.42
38	3	304	KC2	C2A-C3A	5.71	1.48	1.37
39	O	615	II0	C24-C26	5.71	1.53	1.42
39	1	616	II0	C24-C26	5.70	1.53	1.42
38	N	612	KC2	C2A-C3A	5.70	1.48	1.37
39	3	310	II0	C22-C10	5.67	1.54	1.42
39	2	316	II0	C22-C10	5.66	1.54	1.42
38	N	605	KC2	CHD-C4C	5.65	1.49	1.35
38	P	605	KC2	C2A-C3A	5.65	1.48	1.37
38	N	612	KC2	CHD-C4C	5.63	1.49	1.35
38	P	605	KC2	CHD-C4C	5.63	1.49	1.35
38	3	304	KC2	CHD-C4C	5.61	1.49	1.35
38	S	608	KC2	C2A-C3A	5.60	1.48	1.37
38	R	311	KC2	C2A-C3A	5.60	1.48	1.37
38	4	310	KC2	CHD-C4C	5.60	1.49	1.35
38	6	608	KC2	C2A-C3A	5.59	1.48	1.37
38	Q	309	KC2	CHD-C4C	5.58	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	5	610	KC2	C2A-C3A	5.57	1.48	1.37
40	N	619	IHT	C24-C26	5.56	1.53	1.42
38	O	610	KC2	CHD-C4C	5.54	1.49	1.35
38	N	610	KC2	CHD-C4C	5.54	1.49	1.35
38	Q	310	KC2	C2A-C3A	5.54	1.48	1.37
38	4	305	KC2	CHD-C4C	5.53	1.49	1.35
38	2	310	KC2	CHD-C4C	5.53	1.49	1.35
38	Q	304	KC2	CHD-C4C	5.53	1.49	1.35
38	4	311	KC2	C1A-NA	5.52	1.48	1.38
38	Q	310	KC2	CHD-C4C	5.51	1.49	1.35
38	4	311	KC2	CHD-C4C	5.51	1.49	1.35
38	4	311	KC2	C2A-C3A	5.50	1.48	1.37
39	3	312	II0	C24-C26	5.49	1.53	1.42
38	R	311	KC2	CHD-C4C	5.49	1.49	1.35
38	Q	310	KC2	C1A-NA	5.49	1.48	1.38
38	N	611	KC2	C2A-C3A	5.49	1.48	1.37
39	3	311	II0	C24-C26	5.48	1.53	1.42
38	6	608	KC2	OBD-CAD	5.48	1.30	1.22
39	1	617	II0	C23-C21	5.48	1.36	1.20
38	N	611	KC2	CHD-C4C	5.48	1.49	1.35
38	5	610	KC2	CHD-C4C	5.48	1.49	1.35
38	N	605	KC2	OBD-CAD	5.47	1.30	1.22
39	1	615	II0	C23-C21	5.46	1.36	1.20
39	P	613	II0	C24-C26	5.44	1.53	1.42
39	1	618	II0	C23-C21	5.43	1.36	1.20
38	S	608	KC2	OBD-CAD	5.42	1.29	1.22
38	S	608	KC2	CHD-C4C	5.41	1.48	1.35
39	1	616	II0	C23-C21	5.40	1.36	1.20
38	6	608	KC2	CHD-C4C	5.39	1.48	1.35
39	3	311	II0	C22-C10	5.37	1.53	1.42
39	P	613	II0	C22-C10	5.37	1.53	1.42
38	N	611	KC2	OBD-CAD	5.36	1.29	1.22
38	N	610	KC2	OBD-CAD	5.35	1.29	1.22
38	P	605	KC2	OBD-CAD	5.35	1.29	1.22
38	Q	309	KC2	OBD-CAD	5.35	1.29	1.22
38	3	304	KC2	OBD-CAD	5.34	1.29	1.22
38	O	610	KC2	C2A-C3A	5.33	1.48	1.37
38	N	612	KC2	C3D-C2D	5.33	1.49	1.39
38	4	305	KC2	OBD-CAD	5.32	1.29	1.22
38	2	310	KC2	C2A-C3A	5.31	1.48	1.37
38	N	611	KC2	C1A-NA	5.31	1.48	1.38
38	4	310	KC2	OBD-CAD	5.31	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	Q	304	KC2	OBD-CAD	5.30	1.29	1.22
38	S	608	KC2	C1A-NA	5.29	1.48	1.38
39	1	617	II0	C24-C22	5.28	1.35	1.20
38	O	610	KC2	OBD-CAD	5.28	1.29	1.22
38	2	310	KC2	OBD-CAD	5.28	1.29	1.22
39	N	618	II0	C24-C26	5.27	1.52	1.42
39	4	316	II0	C24-C26	5.26	1.52	1.42
39	1	618	II0	C24-C22	5.26	1.35	1.20
39	Q	315	II0	C24-C26	5.24	1.52	1.42
38	6	608	KC2	C1A-NA	5.24	1.48	1.38
39	R	316	II0	C24-C26	5.23	1.52	1.42
38	R	311	KC2	OBD-CAD	5.23	1.29	1.22
38	4	310	KC2	C1A-NA	5.23	1.48	1.38
38	N	605	KC2	C1A-NA	5.23	1.48	1.38
39	5	615	II0	C24-C26	5.23	1.52	1.42
38	2	310	KC2	C1A-NA	5.22	1.48	1.38
38	5	610	KC2	C1A-NA	5.21	1.48	1.38
38	N	610	KC2	C1A-NA	5.21	1.48	1.38
38	Q	309	KC2	C1A-NA	5.20	1.48	1.38
38	5	610	KC2	OBD-CAD	5.20	1.29	1.22
38	N	612	KC2	C3C-C2C	5.20	1.47	1.37
38	R	311	KC2	C1A-NA	5.19	1.48	1.38
39	N	620	II0	C24-C26	5.19	1.52	1.42
38	O	610	KC2	C1A-NA	5.19	1.48	1.38
39	6	611	II0	C24-C26	5.19	1.52	1.42
39	S	611	II0	C24-C26	5.19	1.52	1.42
39	4	317	II0	C24-C26	5.19	1.52	1.42
39	Q	316	II0	C24-C26	5.18	1.52	1.42
39	6	613	II0	C24-C26	5.18	1.52	1.42
38	Q	310	KC2	OBD-CAD	5.18	1.29	1.22
39	R	318	II0	C24-C26	5.17	1.52	1.42
38	4	311	KC2	OBD-CAD	5.17	1.29	1.22
38	2	310	KC2	C3C-C2C	5.17	1.47	1.37
39	2	313	II0	C24-C26	5.16	1.52	1.42
39	4	315	II0	C24-C26	5.16	1.52	1.42
39	2	315	II0	C24-C26	5.16	1.52	1.42
39	R	314	II0	C24-C26	5.16	1.52	1.42
39	Q	313	II0	C24-C26	5.16	1.52	1.42
39	5	613	II0	C24-C26	5.15	1.52	1.42
39	N	617	II0	C24-C26	5.15	1.52	1.42
38	N	610	KC2	C3C-C2C	5.15	1.47	1.37
38	N	611	KC2	C3C-C2C	5.14	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Q	314	II0	C24-C26	5.14	1.52	1.42
38	P	605	KC2	C1A-NA	5.14	1.48	1.38
39	P	612	II0	C24-C26	5.14	1.52	1.42
40	1	619	IHT	C24-C21	5.14	1.35	1.20
38	3	304	KC2	C1A-NA	5.13	1.48	1.38
39	4	314	II0	C24-C26	5.13	1.52	1.42
38	6	608	KC2	C3C-C2C	5.13	1.47	1.37
38	5	610	KC2	C3C-C2C	5.12	1.47	1.37
39	O	613	II0	C24-C26	5.12	1.52	1.42
39	4	320	II0	C24-C26	5.12	1.52	1.42
39	6	612	II0	C24-C26	5.12	1.52	1.42
38	O	610	KC2	C3C-C2C	5.11	1.47	1.37
39	Q	319	II0	C24-C26	5.11	1.52	1.42
38	Q	309	KC2	C3C-C2C	5.11	1.47	1.37
38	4	311	KC2	C3C-C2C	5.10	1.47	1.37
39	N	615	II0	C24-C26	5.10	1.52	1.42
39	2	314	II0	C24-C26	5.10	1.52	1.42
38	R	311	KC2	C3C-C2C	5.10	1.47	1.37
39	N	616	II0	C24-C26	5.10	1.52	1.42
38	S	608	KC2	C3C-C2C	5.10	1.47	1.37
39	S	612	II0	C24-C26	5.09	1.52	1.42
39	1	615	II0	C24-C22	5.09	1.35	1.20
38	3	304	KC2	C3C-C2C	5.09	1.47	1.37
39	1	616	II0	C24-C22	5.09	1.35	1.20
38	P	605	KC2	C3C-C2C	5.09	1.47	1.37
38	4	310	KC2	C3C-C2C	5.08	1.47	1.37
39	P	614	II0	C24-C26	5.07	1.52	1.42
38	Q	310	KC2	C3C-C2C	5.07	1.47	1.37
38	Q	304	KC2	C1A-NA	5.07	1.47	1.38
40	4	318	IHT	C21-C11	5.07	1.53	1.42
38	R	311	KC2	C3B-C2B	5.06	1.47	1.37
38	N	611	KC2	C3B-C2B	5.06	1.47	1.37
38	4	305	KC2	C3B-C2B	5.05	1.47	1.37
38	N	612	KC2	C3B-C2B	5.05	1.47	1.37
38	Q	304	KC2	C3D-C2D	5.05	1.48	1.39
39	N	618	II0	C21-C09	5.04	1.53	1.42
39	R	315	II0	C24-C26	5.04	1.52	1.42
38	5	610	KC2	C3B-C2B	5.04	1.47	1.37
39	5	614	II0	C24-C26	5.04	1.52	1.42
40	Q	317	IHT	C24-C26	5.04	1.52	1.42
38	2	310	KC2	C3B-C2B	5.03	1.47	1.37
40	Q	317	IHT	C21-C11	5.03	1.53	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	O	614	II0	C24-C26	5.03	1.52	1.42
38	Q	304	KC2	C3C-C2C	5.03	1.47	1.37
38	4	305	KC2	C1A-NA	5.03	1.47	1.38
39	O	614	II0	C21-C09	5.02	1.53	1.42
39	2	314	II0	C21-C09	5.02	1.53	1.42
38	P	605	KC2	C3D-C2D	5.02	1.48	1.39
40	4	318	IHT	C24-C26	5.02	1.52	1.42
38	Q	304	KC2	C3B-C2B	5.02	1.47	1.37
40	N	619	IHT	C21-C11	5.01	1.53	1.42
38	3	304	KC2	C3D-C2D	5.01	1.48	1.39
39	2	315	II0	C21-C09	5.00	1.52	1.42
38	4	305	KC2	C3C-C2C	5.00	1.47	1.37
38	O	610	KC2	C3B-C2B	5.00	1.47	1.37
38	4	310	KC2	C3D-C2D	4.99	1.48	1.39
39	N	620	II0	C21-C09	4.99	1.52	1.42
39	6	611	II0	C21-C09	4.99	1.52	1.42
40	O	616	IHT	C24-C26	4.99	1.52	1.42
38	N	610	KC2	C3D-C2D	4.99	1.48	1.39
38	N	605	KC2	C3C-C2C	4.98	1.47	1.37
38	N	605	KC2	C3D-C2D	4.98	1.48	1.39
38	4	305	KC2	C3D-C2D	4.97	1.48	1.39
39	4	317	II0	C21-C09	4.97	1.52	1.42
38	Q	309	KC2	C3D-C2D	4.96	1.48	1.39
40	2	317	IHT	C24-C21	4.95	1.34	1.20
39	S	611	II0	C21-C09	4.95	1.52	1.42
39	P	614	II0	C21-C09	4.94	1.52	1.42
39	N	617	II0	C21-C09	4.94	1.52	1.42
39	N	615	II0	C21-C09	4.94	1.52	1.42
39	4	320	II0	C21-C09	4.94	1.52	1.42
39	Q	316	II0	C21-C09	4.93	1.52	1.42
38	S	608	KC2	C3B-C2B	4.92	1.47	1.37
39	6	613	II0	C21-C09	4.92	1.52	1.42
38	6	608	KC2	C3B-C2B	4.91	1.47	1.37
39	R	318	II0	C21-C09	4.91	1.52	1.42
38	Q	310	KC2	C3D-C2D	4.91	1.48	1.39
39	Q	319	II0	C21-C09	4.90	1.52	1.42
39	O	613	II0	C21-C09	4.90	1.52	1.42
38	5	610	KC2	C3D-C2D	4.89	1.48	1.39
39	5	613	II0	C21-C09	4.89	1.52	1.42
38	N	612	KC2	C1A-NA	4.89	1.47	1.38
39	2	313	II0	C21-C09	4.88	1.52	1.42
38	4	311	KC2	C3D-C2D	4.88	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	R	311	KC2	C3D-C2D	4.88	1.48	1.39
39	4	316	II0	C21-C09	4.88	1.52	1.42
39	R	316	II0	C21-C09	4.88	1.52	1.42
39	R	314	II0	C21-C09	4.87	1.52	1.42
39	5	615	II0	C21-C09	4.86	1.52	1.42
39	Q	313	II0	C21-C09	4.84	1.52	1.42
40	O	616	IHT	C21-C11	4.83	1.52	1.42
38	4	310	KC2	C3B-C2B	4.83	1.47	1.37
39	N	616	II0	C21-C09	4.83	1.52	1.42
38	Q	309	KC2	C3B-C2B	4.83	1.47	1.37
38	N	612	KC2	O2D-CGD	4.82	1.45	1.33
39	4	317	II0	C20-C14	-4.82	1.43	1.50
39	4	314	II0	C21-C09	4.82	1.52	1.42
39	5	614	II0	C21-C09	4.81	1.52	1.42
39	Q	315	II0	C21-C09	4.81	1.52	1.42
38	4	311	KC2	C3B-C2B	4.80	1.47	1.37
39	6	612	II0	C21-C09	4.80	1.52	1.42
39	R	315	II0	C21-C09	4.80	1.52	1.42
39	Q	316	II0	C20-C14	-4.80	1.43	1.50
39	P	612	II0	C21-C09	4.79	1.52	1.42
38	N	605	KC2	O2D-CGD	4.79	1.44	1.33
39	S	612	II0	C21-C09	4.79	1.52	1.42
38	6	608	KC2	C3D-C2D	4.78	1.48	1.39
38	Q	310	KC2	C3B-C2B	4.78	1.47	1.37
39	3	310	II0	C24-C22	4.78	1.34	1.20
39	R	316	II0	C20-C14	-4.77	1.43	1.50
40	R	317	IHT	C24-C26	4.77	1.51	1.42
38	N	610	KC2	C3B-C2B	4.77	1.46	1.37
38	S	608	KC2	C3D-C2D	4.76	1.48	1.39
26	2	305	CLA	C3D-C4D	-4.76	1.33	1.44
39	Q	314	II0	C21-C09	4.76	1.52	1.42
40	5	616	IHT	C24-C26	4.75	1.51	1.42
38	O	610	KC2	C3D-C2D	4.75	1.47	1.39
38	4	310	KC2	O2D-CGD	4.74	1.44	1.33
38	P	605	KC2	C3B-C2B	4.73	1.46	1.37
39	3	312	II0	C24-C22	4.73	1.34	1.20
39	4	315	II0	C21-C09	4.73	1.52	1.42
39	S	611	II0	C20-C14	-4.73	1.43	1.50
38	2	310	KC2	C3D-C2D	4.73	1.47	1.39
38	5	610	KC2	O2D-CGD	4.72	1.44	1.33
38	N	605	KC2	C3B-C2B	4.72	1.46	1.37
39	5	615	II0	C20-C14	-4.72	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	R	311	KC2	O2D-CGD	4.71	1.44	1.33
39	2	316	II0	C24-C22	4.70	1.34	1.20
38	Q	309	KC2	O2D-CGD	4.70	1.44	1.33
39	Q	314	II0	C20-C14	-4.69	1.43	1.50
39	O	615	II0	C24-C22	4.69	1.34	1.20
39	Q	313	II0	C20-C14	-4.69	1.43	1.50
38	4	305	KC2	O2D-CGD	4.68	1.44	1.33
38	Q	304	KC2	O2D-CGD	4.68	1.44	1.33
38	3	304	KC2	C3B-C2B	4.68	1.46	1.37
39	N	618	II0	C20-C14	-4.68	1.43	1.50
39	6	611	II0	C20-C14	-4.67	1.43	1.50
38	N	610	KC2	O2D-CGD	4.67	1.44	1.33
39	N	616	II0	C20-C14	-4.67	1.43	1.50
38	6	608	KC2	O2D-CGD	4.67	1.44	1.33
39	4	315	II0	C20-C14	-4.67	1.43	1.50
38	1	611	KC2	C4D-ND	-4.66	1.31	1.35
30	c	501	SQD	O8-S	4.66	1.64	1.47
38	N	611	KC2	C3D-C2D	4.66	1.47	1.39
39	O	613	II0	C20-C14	-4.65	1.43	1.50
39	Q	315	II0	C20-C14	-4.65	1.43	1.50
39	2	314	II0	C20-C14	-4.65	1.43	1.50
39	P	612	II0	C20-C14	-4.65	1.43	1.50
39	4	316	II0	C20-C14	-4.65	1.43	1.50
38	N	611	KC2	O2D-CGD	4.65	1.44	1.33
38	S	608	KC2	O2D-CGD	4.64	1.44	1.33
38	N	612	KC2	CHB-C1B	4.64	1.47	1.38
38	Q	310	KC2	O2D-CGD	4.64	1.44	1.33
39	O	614	II0	C20-C14	-4.64	1.43	1.50
39	N	620	II0	C20-C14	-4.62	1.43	1.50
39	4	314	II0	C20-C14	-4.62	1.43	1.50
38	4	311	KC2	O2D-CGD	4.62	1.44	1.33
30	a	408	SQD	O8-S	4.62	1.63	1.47
40	R	317	IHT	C21-C11	4.62	1.52	1.42
30	D	401	SQD	O8-S	4.62	1.63	1.47
39	P	614	II0	C20-C14	-4.61	1.43	1.50
40	5	616	IHT	C21-C11	4.61	1.52	1.42
38	P	605	KC2	O2D-CGD	4.61	1.44	1.33
26	2	305	CLA	O2D-CGD	4.59	1.44	1.33
38	3	304	KC2	O2D-CGD	4.59	1.44	1.33
39	2	313	II0	C20-C14	-4.59	1.43	1.50
39	2	315	II0	C20-C14	-4.59	1.43	1.50
38	2	310	KC2	O2D-CGD	4.58	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	O	610	KC2	O2D-CGD	4.57	1.44	1.33
30	A	408	SQD	O8-S	4.57	1.63	1.47
39	N	617	II0	C20-C14	-4.57	1.43	1.50
39	R	318	II0	C20-C14	-4.56	1.43	1.50
39	3	311	II0	C24-C22	4.56	1.33	1.20
39	P	613	II0	C24-C22	4.56	1.33	1.20
26	3	308	CLA	C4D-ND	-4.55	1.31	1.37
39	N	615	II0	C20-C14	-4.55	1.43	1.50
39	5	613	II0	C20-C14	-4.55	1.43	1.50
39	Q	319	II0	C20-C14	-4.55	1.43	1.50
39	6	613	II0	C20-C14	-4.55	1.43	1.50
39	R	314	II0	C20-C14	-4.55	1.43	1.50
39	4	320	II0	C20-C14	-4.53	1.43	1.50
39	6	612	II0	C20-C14	-4.52	1.43	1.50
39	S	612	II0	C20-C14	-4.51	1.43	1.50
33	Q	318	LMG	O7-C10	4.48	1.46	1.34
26	N	608	CLA	C4D-ND	-4.48	1.31	1.37
33	4	319	LMG	O7-C10	4.47	1.46	1.34
39	R	315	II0	C20-C14	-4.44	1.43	1.50
39	3	310	II0	C42-C40	4.42	1.57	1.43
38	1	605	KC2	C4D-ND	-4.42	1.31	1.35
39	5	614	II0	C20-C14	-4.42	1.43	1.50
39	3	310	II0	C31-C29	4.42	1.57	1.43
38	4	305	KC2	CHB-C1B	4.41	1.47	1.38
34	Z	102	LHG	O7-C7	4.41	1.46	1.34
38	1	612	KC2	C4D-ND	-4.37	1.31	1.35
39	3	310	II0	C41-C39	4.37	1.57	1.43
34	z	101	LHG	O7-C7	4.37	1.46	1.34
39	3	311	II0	C41-C39	4.37	1.57	1.43
26	1	614	CLA	C1D-ND	4.37	1.43	1.37
38	Q	304	KC2	CHB-C1B	4.37	1.46	1.38
39	P	613	II0	C41-C39	4.35	1.56	1.43
39	3	312	II0	C41-C39	4.34	1.56	1.43
33	2	318	LMG	O8-C28	4.34	1.46	1.33
33	D	406	LMG	O8-C28	4.33	1.46	1.33
33	O	617	LMG	O8-C28	4.33	1.46	1.33
39	O	615	II0	C41-C39	4.32	1.56	1.43
38	1	605	KC2	C1D-ND	4.32	1.39	1.35
39	3	312	II0	C31-C29	4.32	1.56	1.43
38	1	610	KC2	C4D-ND	-4.32	1.31	1.35
38	R	311	KC2	CHB-C1B	4.32	1.46	1.38
39	2	316	II0	C41-C39	4.32	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	3	312	II0	C42-C40	4.32	1.56	1.43
33	C	520	LMG	O8-C28	4.31	1.45	1.33
34	G	403	LHG	O8-C23	4.30	1.45	1.33
33	D	413	LMG	O8-C28	4.30	1.45	1.33
38	5	610	KC2	CHB-C1B	4.30	1.46	1.38
33	d	411	LMG	O8-C28	4.29	1.45	1.33
33	b	620	LMG	O8-C28	4.29	1.45	1.33
38	N	605	KC2	CHB-C1B	4.29	1.46	1.38
34	2	321	LHG	O8-C23	4.29	1.45	1.33
39	3	311	II0	C31-C29	4.29	1.56	1.43
39	P	613	II0	C31-C29	4.29	1.56	1.43
39	O	615	II0	C42-C40	4.29	1.56	1.43
33	4	319	LMG	O8-C28	4.28	1.45	1.33
34	1	620	LHG	O8-C23	4.27	1.45	1.33
33	c	522	LMG	O8-C28	4.27	1.45	1.33
38	1	612	KC2	C1D-ND	4.27	1.39	1.35
34	C	501	LHG	O8-C23	4.27	1.45	1.33
38	N	610	KC2	CHB-C1B	4.26	1.46	1.38
33	Q	318	LMG	O8-C28	4.26	1.45	1.33
33	d	404	LMG	O8-C28	4.26	1.45	1.33
40	2	317	IHT	C31-C29	4.26	1.56	1.43
34	N	621	LHG	O8-C23	4.26	1.45	1.33
33	5	619	LMG	O8-C28	4.25	1.45	1.33
34	c	520	LHG	O8-C23	4.25	1.45	1.33
39	2	316	II0	C42-C40	4.25	1.56	1.43
33	B	620	LMG	O8-C28	4.25	1.45	1.33
33	D	411	LMG	O8-C28	4.25	1.45	1.33
39	3	310	II0	C33-C35	4.24	1.55	1.45
34	D	403	LHG	O8-C23	4.24	1.45	1.33
33	d	409	LMG	O8-C28	4.24	1.45	1.33
35	H	102	DGD	O1G-C1A	4.24	1.45	1.33
34	l	101	LHG	O8-C23	4.23	1.45	1.33
39	2	316	II0	C31-C29	4.23	1.56	1.43
33	M	101	LMG	O8-C28	4.23	1.45	1.33
34	d	408	LHG	O8-C23	4.23	1.45	1.33
30	A	408	SQD	O48-C23	4.23	1.45	1.33
34	b	621	LHG	O7-C7	4.23	1.46	1.34
35	c	519	DGD	O1G-C1A	4.23	1.45	1.33
33	R	301	LMG	O8-C28	4.22	1.45	1.33
34	R	319	LHG	O8-C23	4.22	1.45	1.33
34	a	409	LHG	O8-C23	4.22	1.45	1.33
38	4	311	KC2	CHC-C4B	4.22	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Q	306	CLA	C1D-ND	4.21	1.43	1.37
33	C	519	LMG	O8-C28	4.21	1.45	1.33
39	3	311	II0	C42-C40	4.21	1.56	1.43
39	P	613	II0	C42-C40	4.21	1.56	1.43
33	m	101	LMG	O8-C28	4.21	1.45	1.33
30	c	501	SQD	O48-C23	4.20	1.45	1.33
34	5	618	LHG	O8-C23	4.20	1.45	1.33
34	L	101	LHG	O8-C23	4.20	1.45	1.33
38	Q	310	KC2	CHC-C4B	4.20	1.46	1.38
35	h	101	DGD	O1G-C1A	4.20	1.45	1.33
33	A	412	LMG	O8-C28	4.20	1.45	1.33
34	D	410	LHG	O8-C23	4.20	1.45	1.33
39	O	615	II0	C31-C29	4.20	1.56	1.43
26	4	307	CLA	C1D-ND	4.19	1.42	1.37
26	N	601	CLA	C1D-ND	4.19	1.42	1.37
35	C	517	DGD	O1G-C1A	4.19	1.45	1.33
30	a	408	SQD	O48-C23	4.19	1.45	1.33
34	Z	102	LHG	O8-C23	4.19	1.45	1.33
30	D	401	SQD	O48-C23	4.19	1.45	1.33
38	5	610	KC2	CBC-CAC	4.18	1.51	1.30
34	z	101	LHG	O8-C23	4.18	1.45	1.33
33	d	404	LMG	O7-C10	4.18	1.46	1.34
38	R	311	KC2	CBC-CAC	4.18	1.51	1.30
33	2	318	LMG	O7-C10	4.17	1.46	1.34
33	D	413	LMG	O7-C10	4.17	1.46	1.34
35	c	519	DGD	O2G-C1B	4.17	1.46	1.34
26	4	303	CLA	C1D-ND	4.17	1.42	1.37
34	a	409	LHG	O7-C7	4.17	1.46	1.34
38	N	610	KC2	CBC-CAC	4.16	1.50	1.30
34	N	621	LHG	O7-C7	4.16	1.46	1.34
33	a	413	LMG	O8-C28	4.16	1.45	1.33
34	1	620	LHG	O7-C7	4.16	1.46	1.34
33	c	522	LMG	O7-C10	4.16	1.46	1.34
33	O	617	LMG	O7-C10	4.16	1.46	1.34
34	C	501	LHG	O7-C7	4.16	1.46	1.34
38	P	605	KC2	CHB-C1B	4.16	1.46	1.38
38	Q	304	KC2	CBC-CAC	4.15	1.50	1.30
38	3	304	KC2	CBC-CAC	4.15	1.50	1.30
38	N	605	KC2	CBC-CAC	4.15	1.50	1.30
38	4	310	KC2	CBC-CAC	4.15	1.50	1.30
38	4	310	KC2	CHB-C1B	4.15	1.46	1.38
38	Q	309	KC2	CBC-CAC	4.15	1.50	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	520	LMG	O7-C10	4.15	1.46	1.34
38	4	305	KC2	CBC-CAC	4.15	1.50	1.30
38	S	608	KC2	CHB-C1B	4.15	1.46	1.38
38	P	605	KC2	CBC-CAC	4.15	1.50	1.30
26	4	312	CLA	C1D-ND	4.14	1.42	1.37
38	N	605	KC2	CHC-C4B	4.14	1.46	1.38
38	6	608	KC2	CHB-C1B	4.14	1.46	1.38
34	c	520	LHG	O7-C7	4.14	1.46	1.34
38	Q	309	KC2	CHC-C4B	4.14	1.46	1.38
26	Q	302	CLA	C1D-ND	4.14	1.42	1.37
38	Q	309	KC2	CHB-C1B	4.13	1.46	1.38
26	R	302	CLA	C1D-ND	4.13	1.42	1.37
38	N	611	KC2	CBC-CAC	4.13	1.50	1.30
34	L	101	LHG	O7-C7	4.13	1.45	1.34
33	a	413	LMG	O7-C10	4.13	1.45	1.34
26	2	303	CLA	C1D-ND	4.13	1.42	1.37
38	3	304	KC2	CHB-C1B	4.13	1.46	1.38
33	D	406	LMG	O7-C10	4.12	1.45	1.34
38	S	608	KC2	CBC-CAC	4.12	1.50	1.30
38	4	310	KC2	CHC-C4B	4.12	1.46	1.38
38	N	612	KC2	CBC-CAC	4.12	1.50	1.30
33	d	411	LMG	O7-C10	4.12	1.45	1.34
26	b	610	CLA	C1D-ND	4.12	1.42	1.37
34	C	518	LHG	O8-C23	4.12	1.45	1.33
40	1	619	IHT	C22-C23	4.12	1.54	1.45
34	R	319	LHG	O7-C7	4.11	1.45	1.34
38	4	311	KC2	CBC-CAC	4.11	1.50	1.30
38	2	310	KC2	CHB-C1B	4.11	1.46	1.38
34	5	618	LHG	O7-C7	4.11	1.45	1.34
38	O	610	KC2	CHB-C1B	4.11	1.46	1.38
33	c	521	LMG	O8-C28	4.11	1.45	1.33
38	Q	310	KC2	CBC-CAC	4.11	1.50	1.30
34	C	518	LHG	O7-C7	4.11	1.45	1.34
26	2	308	CLA	C1D-ND	4.11	1.42	1.37
26	Q	311	CLA	C1D-ND	4.11	1.42	1.37
38	6	608	KC2	CBC-CAC	4.11	1.50	1.30
29	a	407	PL9	C7-C3	-4.11	1.47	1.51
34	D	403	LHG	O7-C7	4.11	1.45	1.34
38	P	605	KC2	CHC-C4B	4.11	1.46	1.38
38	O	610	KC2	CBC-CAC	4.11	1.50	1.30
38	2	310	KC2	CBC-CAC	4.11	1.50	1.30
38	O	610	KC2	CHC-C4B	4.10	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A	412	LMG	O7-C10	4.10	1.45	1.34
35	h	101	DGD	O2G-C1B	4.10	1.45	1.34
26	2	305	CLA	O2A-CGA	4.10	1.45	1.33
34	D	410	LHG	O7-C7	4.09	1.45	1.34
33	B	620	LMG	O7-C10	4.09	1.45	1.34
26	5	605	CLA	C1D-ND	4.09	1.42	1.37
33	b	620	LMG	O7-C10	4.09	1.45	1.34
26	3	302	CLA	C1D-ND	4.09	1.42	1.37
30	a	408	SQD	O47-C7	4.08	1.45	1.34
38	3	304	KC2	CHC-C4B	4.08	1.46	1.38
33	D	411	LMG	O7-C10	4.08	1.45	1.34
39	1	617	II0	C31-C29	4.08	1.56	1.43
26	O	609	CLA	C1D-ND	4.08	1.42	1.37
26	O	603	CLA	C1D-ND	4.08	1.42	1.37
33	C	519	LMG	O7-C10	4.08	1.45	1.34
26	c	513	CLA	C1D-ND	4.07	1.42	1.37
33	d	409	LMG	O7-C10	4.07	1.45	1.34
26	b	615	CLA	C1D-ND	4.07	1.42	1.37
33	c	521	LMG	O7-C10	4.07	1.45	1.34
38	R	311	KC2	CHC-C4B	4.07	1.46	1.38
35	H	102	DGD	O2G-C1B	4.07	1.45	1.34
33	M	101	LMG	O7-C10	4.07	1.45	1.34
38	2	310	KC2	CHC-C4B	4.07	1.46	1.38
26	2	301	CLA	C1D-ND	4.07	1.42	1.37
26	O	608	CLA	C1D-ND	4.07	1.42	1.37
30	c	501	SQD	O47-C7	4.06	1.45	1.34
26	A	403	CLA	C1D-ND	4.06	1.42	1.37
26	R	306	CLA	C1D-ND	4.06	1.42	1.37
35	C	517	DGD	O2G-C1B	4.06	1.45	1.34
30	D	401	SQD	O47-C7	4.06	1.45	1.34
34	l	101	LHG	O7-C7	4.05	1.45	1.34
26	O	601	CLA	C1D-ND	4.05	1.42	1.37
26	5	601	CLA	C1D-ND	4.05	1.42	1.37
38	N	611	KC2	CHB-C1B	4.05	1.46	1.38
38	6	608	KC2	CHC-C4B	4.05	1.46	1.38
33	5	619	LMG	O7-C10	4.05	1.45	1.34
26	b	602	CLA	C1D-ND	4.05	1.42	1.37
38	5	610	KC2	CHC-C4B	4.05	1.46	1.38
34	b	621	LHG	O8-C23	4.05	1.45	1.33
26	g	401	CLA	C1D-ND	4.04	1.42	1.37
26	C	512	CLA	C1D-ND	4.04	1.42	1.37
26	Q	305	CLA	C1D-ND	4.04	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	505	CLA	C1D-ND	4.04	1.42	1.37
26	2	309	CLA	C1D-ND	4.04	1.42	1.37
39	1	615	II0	C32-C30	4.04	1.56	1.43
39	3	311	II0	C33-C35	4.04	1.54	1.45
26	B	601	CLA	C1D-ND	4.04	1.42	1.37
33	R	301	LMG	O7-C10	4.04	1.45	1.34
26	N	614	CLA	C1D-ND	4.04	1.42	1.37
34	G	403	LHG	O7-C7	4.04	1.45	1.34
39	1	618	II0	C31-C29	4.04	1.56	1.43
26	d	402	CLA	C1D-ND	4.04	1.42	1.37
26	3	305	CLA	C1D-ND	4.04	1.42	1.37
26	P	603	CLA	C1D-ND	4.04	1.42	1.37
26	a	403	CLA	C1D-ND	4.03	1.42	1.37
26	b	606	CLA	C1D-ND	4.03	1.42	1.37
29	A	407	PL9	C7-C3	-4.03	1.47	1.51
26	c	512	CLA	C1D-ND	4.03	1.42	1.37
26	P	606	CLA	C1D-ND	4.03	1.42	1.37
34	d	408	LHG	O7-C7	4.03	1.45	1.34
38	1	611	KC2	C1D-ND	4.03	1.38	1.35
39	1	618	II0	C32-C30	4.03	1.55	1.43
30	A	408	SQD	O47-C7	4.02	1.45	1.34
26	O	604	CLA	C1D-ND	4.02	1.42	1.37
26	D	408	CLA	C1D-ND	4.02	1.42	1.37
26	5	612	CLA	C1D-ND	4.02	1.42	1.37
26	5	603	CLA	C1D-ND	4.02	1.42	1.37
39	1	616	II0	C31-C29	4.02	1.55	1.43
26	B	604	CLA	C1D-ND	4.01	1.42	1.37
26	2	304	CLA	C1D-ND	4.01	1.42	1.37
39	P	613	II0	C33-C35	4.01	1.54	1.45
38	1	605	KC2	C3B-C4B	-4.01	1.38	1.46
26	c	503	CLA	C1D-ND	4.01	1.42	1.37
33	m	101	LMG	O7-C10	4.01	1.45	1.34
34	2	321	LHG	O7-C7	4.01	1.45	1.34
38	S	608	KC2	CHC-C4B	4.01	1.46	1.38
26	4	306	CLA	C1D-ND	4.01	1.42	1.37
26	B	606	CLA	C1D-ND	4.01	1.42	1.37
26	B	614	CLA	C1D-ND	4.01	1.42	1.37
26	2	307	CLA	C1D-ND	4.00	1.42	1.37
40	1	619	IHT	C30-C27	4.00	1.55	1.43
26	N	602	CLA	C1D-ND	4.00	1.42	1.37
26	B	610	CLA	C1D-ND	3.99	1.42	1.37
26	C	508	CLA	C1D-ND	3.99	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	605	CLA	C1D-ND	3.99	1.42	1.37
26	N	609	CLA	C1D-ND	3.99	1.42	1.37
38	4	311	KC2	CHB-C1B	3.98	1.46	1.38
26	D	404	CLA	C1D-ND	3.98	1.42	1.37
38	N	612	KC2	CHC-C4B	3.98	1.46	1.38
39	1	617	II0	C32-C30	3.98	1.55	1.43
26	B	616	CLA	C1D-ND	3.98	1.42	1.37
38	N	611	KC2	CHC-C4B	3.98	1.46	1.38
26	C	502	CLA	C1D-ND	3.98	1.42	1.37
26	N	613	CLA	C1D-ND	3.98	1.42	1.37
26	c	514	CLA	C1D-ND	3.97	1.42	1.37
39	1	615	II0	C31-C29	3.97	1.55	1.43
26	3	309	CLA	C1D-ND	3.97	1.42	1.37
38	N	610	KC2	CHC-C4B	3.97	1.46	1.38
26	b	604	CLA	C1D-ND	3.97	1.42	1.37
38	Q	310	KC2	CHB-C1B	3.97	1.46	1.38
26	N	604	CLA	C1D-ND	3.96	1.42	1.37
26	3	306	CLA	C1D-ND	3.96	1.42	1.37
26	c	509	CLA	C1D-ND	3.96	1.42	1.37
26	R	305	CLA	C1D-ND	3.95	1.42	1.37
26	C	507	CLA	C1D-ND	3.95	1.42	1.37
26	B	608	CLA	C1D-ND	3.95	1.42	1.37
28	H	101	WVN	C23-C25	3.95	1.54	1.45
26	5	609	CLA	C1D-ND	3.95	1.42	1.37
39	R	318	II0	C06-C08	-3.95	1.46	1.52
26	O	607	CLA	C1D-ND	3.94	1.42	1.37
26	R	304	CLA	C1D-ND	3.94	1.42	1.37
26	b	608	CLA	C1D-ND	3.94	1.42	1.37
39	6	613	II0	C06-C08	-3.94	1.46	1.52
26	B	615	CLA	C1D-ND	3.94	1.42	1.37
26	4	301	CLA	C1D-ND	3.94	1.42	1.37
26	B	602	CLA	C1D-ND	3.94	1.42	1.37
26	C	504	CLA	C1D-ND	3.94	1.42	1.37
26	c	515	CLA	C1D-ND	3.94	1.42	1.37
26	C	505	CLA	C1D-ND	3.93	1.42	1.37
26	C	511	CLA	C1D-ND	3.93	1.42	1.37
26	O	606	CLA	C1D-ND	3.93	1.42	1.37
26	Q	308	CLA	C1D-ND	3.93	1.42	1.37
26	2	306	CLA	C1D-ND	3.93	1.42	1.37
38	1	610	KC2	C3B-C4B	-3.93	1.39	1.46
26	b	611	CLA	C1D-ND	3.93	1.42	1.37
26	5	604	CLA	C1D-ND	3.93	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	3	312	II0	C33-C35	3.93	1.54	1.45
26	b	614	CLA	C1D-ND	3.93	1.42	1.37
26	c	506	CLA	C1D-ND	3.92	1.42	1.37
26	P	608	CLA	C1D-ND	3.92	1.42	1.37
26	B	607	CLA	C1D-ND	3.92	1.42	1.37
26	C	510	CLA	C1D-ND	3.92	1.42	1.37
26	P	601	CLA	C1D-ND	3.92	1.42	1.37
26	6	605	CLA	C1D-ND	3.92	1.42	1.37
26	S	607	CLA	C1D-ND	3.92	1.42	1.37
39	O	615	II0	C33-C35	3.92	1.54	1.45
26	c	508	CLA	C1D-ND	3.92	1.42	1.37
26	1	601	CLA	C1D-ND	3.92	1.42	1.37
26	R	313	CLA	C1D-ND	3.92	1.42	1.37
40	1	619	IHT	C41-C38	3.92	1.55	1.43
28	B	618	WVN	C29-C26	3.92	1.55	1.43
26	C	509	CLA	C1D-ND	3.91	1.42	1.37
26	c	510	CLA	C1D-ND	3.91	1.42	1.37
26	P	607	CLA	C1D-ND	3.91	1.42	1.37
26	6	607	CLA	C1D-ND	3.91	1.42	1.37
26	1	613	CLA	C1D-ND	3.91	1.42	1.37
26	P	611	CLA	C1D-ND	3.91	1.42	1.37
26	2	319	CLA	C1D-ND	3.91	1.42	1.37
26	b	601	CLA	C1D-ND	3.90	1.42	1.37
26	R	310	CLA	C1D-ND	3.90	1.42	1.37
39	N	618	II0	C06-C08	-3.90	1.46	1.52
26	R	307	CLA	C1D-ND	3.90	1.42	1.37
26	B	613	CLA	C1D-ND	3.90	1.42	1.37
26	b	613	CLA	C1D-ND	3.90	1.42	1.37
26	c	511	CLA	C1D-ND	3.90	1.42	1.37
26	B	605	CLA	C1D-ND	3.90	1.42	1.37
26	O	605	CLA	C1D-ND	3.90	1.42	1.37
28	a	406	WVN	C02-C11	3.89	1.56	1.50
26	a	402	CLA	C1D-ND	3.89	1.42	1.37
26	d	406	CLA	C1D-ND	3.89	1.42	1.37
39	1	616	II0	C32-C30	3.89	1.55	1.43
26	C	503	CLA	C1D-ND	3.88	1.42	1.37
28	C	516	WVN	C23-C25	3.88	1.54	1.45
26	B	609	CLA	C1D-ND	3.88	1.42	1.37
26	R	309	CLA	C1D-ND	3.88	1.42	1.37
26	3	301	CLA	C1D-ND	3.88	1.42	1.37
26	4	313	CLA	C1D-ND	3.88	1.42	1.37
38	1	611	KC2	C3B-C4B	-3.87	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	606	CLA	C1D-ND	3.87	1.42	1.37
40	2	317	IHT	C34-C35	3.87	1.54	1.45
26	B	611	CLA	C1D-ND	3.87	1.42	1.37
26	P	602	CLA	C1D-ND	3.87	1.42	1.37
26	5	602	CLA	C1D-ND	3.87	1.42	1.37
26	b	609	CLA	C1D-ND	3.87	1.42	1.37
26	Q	303	CLA	C1D-ND	3.87	1.42	1.37
26	4	304	CLA	C1D-ND	3.87	1.42	1.37
26	1	607	CLA	C1D-ND	3.87	1.42	1.37
26	N	603	CLA	C1D-ND	3.87	1.42	1.37
26	4	309	CLA	C1D-ND	3.87	1.42	1.37
26	C	514	CLA	C1D-ND	3.86	1.42	1.37
26	b	603	CLA	C1D-ND	3.86	1.42	1.37
26	Q	312	CLA	C1D-ND	3.86	1.42	1.37
26	P	609	CLA	C1D-ND	3.86	1.42	1.37
26	6	609	CLA	C1D-ND	3.86	1.42	1.37
26	S	605	CLA	C1D-ND	3.86	1.42	1.37
26	A	405	CLA	C1D-ND	3.86	1.42	1.37
38	1	610	KC2	C1D-ND	3.86	1.38	1.35
26	3	307	CLA	C1D-ND	3.86	1.42	1.37
29	D	409	PL9	C7-C3	-3.85	1.47	1.51
39	2	316	II0	C33-C35	3.85	1.54	1.45
28	3	313	WVN	C29-C26	3.85	1.55	1.43
38	1	612	KC2	C3B-C4B	-3.85	1.39	1.46
26	A	402	CLA	C1D-ND	3.85	1.42	1.37
26	2	302	CLA	C1D-ND	3.85	1.42	1.37
26	R	308	CLA	C1D-ND	3.85	1.42	1.37
26	C	513	CLA	C1D-ND	3.85	1.42	1.37
26	b	616	CLA	C1D-ND	3.85	1.42	1.37
40	1	619	IHT	C32-C33	3.84	1.54	1.45
26	6	602	CLA	C1D-ND	3.84	1.42	1.37
26	S	601	CLA	C1D-ND	3.84	1.42	1.37
38	Q	304	KC2	CHC-C4B	3.84	1.45	1.38
39	1	618	II0	C42-C40	3.84	1.55	1.43
26	O	602	CLA	C1D-ND	3.84	1.42	1.37
26	6	601	CLA	C1D-ND	3.83	1.42	1.37
26	5	611	CLA	C1D-ND	3.83	1.42	1.37
26	S	609	CLA	C1D-ND	3.83	1.42	1.37
26	R	312	CLA	C1D-ND	3.83	1.42	1.37
38	4	305	KC2	CHC-C4B	3.83	1.45	1.38
39	N	620	II0	C06-C08	-3.83	1.46	1.52
40	1	619	IHT	C31-C29	3.83	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S	602	CLA	C1D-ND	3.82	1.42	1.37
26	1	608	CLA	C1D-ND	3.82	1.42	1.37
26	b	607	CLA	C1D-ND	3.82	1.42	1.37
26	6	606	CLA	C1D-ND	3.82	1.42	1.37
28	C	516	WVN	C31-C32	3.81	1.54	1.45
39	3	312	II0	C32-C30	3.81	1.55	1.43
26	5	607	CLA	C1D-ND	3.81	1.42	1.37
26	N	606	CLA	C1D-ND	3.81	1.42	1.37
26	N	607	CLA	C1D-ND	3.81	1.42	1.37
39	P	614	II0	C06-C08	-3.81	1.46	1.52
26	Q	301	CLA	C1D-ND	3.80	1.42	1.37
26	c	504	CLA	C1D-ND	3.80	1.42	1.37
39	1	617	II0	C42-C40	3.80	1.55	1.43
26	S	606	CLA	C1D-ND	3.79	1.42	1.37
26	5	608	CLA	C1D-ND	3.79	1.42	1.37
39	1	615	II0	C42-C40	3.79	1.55	1.43
28	3	313	WVN	C23-C25	3.79	1.54	1.45
26	B	603	CLA	C1D-ND	3.79	1.42	1.37
39	Q	315	II0	C06-C08	-3.79	1.46	1.52
39	1	618	II0	C33-C35	3.78	1.54	1.45
26	a	405	CLA	C1D-ND	3.78	1.42	1.37
26	3	303	CLA	C1D-ND	3.78	1.42	1.37
26	R	303	CLA	C1D-ND	3.78	1.42	1.37
26	4	302	CLA	C1D-ND	3.77	1.42	1.37
39	4	315	II0	C06-C08	-3.77	1.46	1.52
39	N	617	II0	C06-C08	-3.77	1.46	1.52
39	Q	314	II0	C06-C08	-3.77	1.46	1.52
28	C	516	WVN	C40-C37	3.76	1.55	1.43
26	P	604	CLA	C1D-ND	3.76	1.42	1.37
26	6	604	CLA	C1D-ND	3.76	1.42	1.37
40	1	619	IHT	C40-C37	3.76	1.55	1.43
28	3	313	WVN	C39-C36	3.76	1.55	1.43
26	S	604	CLA	C1D-ND	3.76	1.42	1.37
26	1	602	CLA	C1D-ND	3.75	1.42	1.37
39	1	616	II0	C42-C40	3.75	1.55	1.43
40	2	317	IHT	C30-C27	3.75	1.55	1.43
39	2	315	II0	C06-C08	-3.74	1.46	1.52
39	4	316	II0	C06-C08	-3.74	1.46	1.52
38	1	611	KC2	C1B-C2B	-3.73	1.38	1.45
39	1	618	II0	C41-C39	3.73	1.55	1.43
26	G	402	CLA	C1D-ND	3.73	1.42	1.37
39	4	314	II0	C06-C08	-3.73	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	2	316	II0	C32-C30	3.73	1.55	1.43
39	1	617	II0	C34-C36	3.73	1.53	1.45
39	1	617	II0	C33-C35	3.73	1.53	1.45
39	N	616	II0	C06-C08	-3.72	1.47	1.52
26	B	612	CLA	C1D-ND	3.72	1.42	1.37
26	C	506	CLA	C1D-ND	3.72	1.42	1.37
39	1	617	II0	C41-C39	3.72	1.55	1.43
38	1	605	KC2	C1B-C2B	-3.71	1.38	1.45
26	2	312	CLA	C1D-ND	3.71	1.42	1.37
26	4	308	CLA	C1D-ND	3.71	1.42	1.37
26	O	611	CLA	C1D-ND	3.71	1.42	1.37
39	1	615	II0	C41-C39	3.71	1.54	1.43
26	Q	307	CLA	C1D-ND	3.71	1.42	1.37
39	6	612	II0	C06-C08	-3.71	1.47	1.52
28	B	618	WVN	C31-C32	3.71	1.53	1.45
39	Q	313	II0	C06-C08	-3.71	1.47	1.52
39	O	615	II0	C32-C30	3.71	1.54	1.43
26	1	603	CLA	C1D-ND	3.70	1.42	1.37
28	Z	101	WVN	C02-C11	3.70	1.55	1.50
39	4	320	II0	C06-C08	-3.70	1.47	1.52
26	O	612	CLA	C1D-ND	3.70	1.42	1.37
26	d	405	CLA	C1D-ND	3.70	1.42	1.37
28	3	313	WVN	C31-C32	3.69	1.53	1.45
39	5	613	II0	C06-C08	-3.69	1.47	1.52
39	1	616	II0	C33-C35	3.69	1.53	1.45
26	S	603	CLA	C1D-ND	3.69	1.42	1.37
29	d	407	PL9	C7-C3	-3.68	1.47	1.51
28	H	101	WVN	C29-C26	3.68	1.54	1.43
28	3	313	WVN	C40-C37	3.68	1.54	1.43
26	1	609	CLA	C1D-ND	3.68	1.42	1.37
40	2	317	IHT	C41-C38	3.67	1.54	1.43
38	1	611	KC2	C4A-C3A	-3.67	1.37	1.44
40	2	317	IHT	C40-C37	3.67	1.54	1.43
28	C	516	WVN	C29-C26	3.67	1.54	1.43
39	1	618	II0	C34-C36	3.67	1.53	1.45
39	1	616	II0	C41-C39	3.67	1.54	1.43
26	6	603	CLA	C1D-ND	3.67	1.42	1.37
39	3	310	II0	C32-C30	3.66	1.54	1.43
39	Q	319	II0	C06-C08	-3.66	1.47	1.52
26	2	311	CLA	C1D-ND	3.66	1.42	1.37
39	S	612	II0	C06-C08	-3.66	1.47	1.52
26	6	610	CLA	C1D-ND	3.65	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H	101	WVN	C31-C32	3.65	1.53	1.45
26	1	604	CLA	C1D-ND	3.64	1.42	1.37
26	S	610	CLA	C1D-ND	3.64	1.42	1.37
26	N	608	CLA	C1C-NC	3.64	1.43	1.37
39	R	314	II0	C06-C08	-3.63	1.47	1.52
39	S	611	II0	C06-C08	-3.63	1.47	1.52
28	B	617	WVN	C40-C37	3.63	1.54	1.43
26	b	612	CLA	C1D-ND	3.63	1.42	1.37
26	D	407	CLA	C1D-ND	3.62	1.42	1.37
38	1	605	KC2	C4A-C3A	-3.62	1.37	1.44
28	C	516	WVN	C39-C36	3.62	1.54	1.43
28	B	617	WVN	C29-C26	3.62	1.54	1.43
39	2	313	II0	C06-C08	-3.61	1.47	1.52
39	Q	315	II0	C22-C10	3.61	1.50	1.42
39	1	615	II0	C33-C35	3.61	1.53	1.45
26	c	507	CLA	C1D-ND	3.60	1.42	1.37
26	G	401	CLA	C1D-ND	3.60	1.42	1.37
39	N	615	II0	C06-C08	-3.60	1.47	1.52
26	P	610	CLA	C1D-ND	3.60	1.42	1.37
39	6	611	II0	C22-C10	3.60	1.50	1.42
38	1	610	KC2	C4A-C3A	-3.60	1.37	1.44
38	1	605	KC2	C1C-C2C	-3.60	1.37	1.44
37	f	101	HEM	C1B-NB	-3.59	1.34	1.40
39	4	317	II0	C22-C10	3.59	1.50	1.42
39	S	611	II0	C22-C10	3.59	1.50	1.42
39	4	316	II0	C22-C10	3.59	1.50	1.42
39	Q	316	II0	C22-C10	3.59	1.50	1.42
28	H	101	WVN	C39-C36	3.59	1.54	1.43
28	B	617	WVN	C23-C25	3.58	1.53	1.45
39	R	318	II0	C22-C10	3.58	1.50	1.42
26	1	606	CLA	C1D-ND	3.58	1.42	1.37
28	B	617	WVN	C39-C36	3.57	1.54	1.43
39	R	315	II0	C06-C08	-3.57	1.47	1.52
39	P	612	II0	C06-C08	-3.56	1.47	1.52
39	6	611	II0	C06-C08	-3.56	1.47	1.52
39	1	615	II0	C34-C36	3.56	1.53	1.45
38	1	612	KC2	C1B-C2B	-3.56	1.38	1.45
28	B	618	WVN	C39-C36	3.55	1.54	1.43
39	O	613	II0	C06-C08	-3.55	1.47	1.52
38	1	610	KC2	C1B-C2B	-3.55	1.38	1.45
40	1	619	IHT	C34-C35	3.55	1.53	1.45
39	R	316	II0	C06-C08	-3.54	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	2	317	IHT	C32-C33	3.54	1.53	1.45
28	H	101	WVN	C40-C37	3.54	1.54	1.43
40	5	616	IHT	C37-C33	-3.54	1.31	1.35
39	5	613	II0	C22-C10	3.54	1.49	1.42
39	N	618	II0	C22-C10	3.54	1.49	1.42
39	6	613	II0	C22-C10	3.54	1.49	1.42
39	R	314	II0	C22-C10	3.54	1.49	1.42
28	B	618	WVN	C40-C37	3.53	1.54	1.43
39	Q	316	II0	C06-C08	-3.52	1.47	1.52
39	4	317	II0	C06-C08	-3.52	1.47	1.52
39	5	615	II0	C06-C08	-3.52	1.47	1.52
26	g	402	CLA	C1D-ND	3.52	1.42	1.37
39	N	617	II0	C22-C10	3.52	1.49	1.42
28	b	617	WVN	C28-C25	-3.51	1.31	1.35
40	R	317	IHT	C37-C33	-3.51	1.31	1.35
39	6	612	II0	C22-C10	3.51	1.49	1.42
39	O	613	II0	C22-C10	3.51	1.49	1.42
28	3	313	WVN	C19-C22	3.51	1.53	1.45
39	R	315	II0	C22-C10	3.50	1.49	1.42
39	2	316	II0	C34-C36	3.50	1.53	1.45
39	P	613	II0	C32-C30	3.50	1.54	1.43
39	4	315	II0	C22-C10	3.50	1.49	1.42
39	2	313	II0	C22-C10	3.50	1.49	1.42
37	F	101	HEM	C4D-ND	-3.50	1.34	1.40
39	3	311	II0	C32-C30	3.50	1.54	1.43
26	3	308	CLA	MG-NA	3.50	2.14	2.06
39	2	315	II0	C22-C10	3.49	1.49	1.42
39	S	612	II0	C22-C10	3.49	1.49	1.42
39	3	312	II0	C34-C36	3.49	1.53	1.45
39	5	614	II0	C06-C08	-3.48	1.47	1.52
39	N	620	II0	C22-C10	3.48	1.49	1.42
40	Q	317	IHT	C37-C33	-3.47	1.31	1.35
28	B	618	WVN	C23-C25	3.47	1.53	1.45
39	4	320	II0	C22-C10	3.47	1.49	1.42
39	O	615	II0	C34-C36	3.46	1.53	1.45
39	5	614	II0	C22-C10	3.46	1.49	1.42
39	N	615	II0	C22-C10	3.46	1.49	1.42
39	Q	314	II0	C22-C10	3.46	1.49	1.42
39	Q	319	II0	C22-C10	3.46	1.49	1.42
38	1	612	KC2	C4A-C3A	-3.45	1.37	1.44
28	B	617	WVN	C31-C32	3.45	1.53	1.45
39	P	614	II0	C22-C10	3.45	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	O	614	II0	C06-C08	-3.44	1.47	1.52
39	R	316	II0	C22-C10	3.44	1.49	1.42
28	D	412	WVN	C33-C34	3.44	1.53	1.45
37	f	101	HEM	C4D-ND	-3.44	1.34	1.40
38	N	610	KC2	C4D-CHA	3.44	1.49	1.45
38	1	612	KC2	C1C-C2C	-3.42	1.37	1.44
39	5	615	II0	C22-C10	3.42	1.49	1.42
39	4	314	II0	C22-C10	3.42	1.49	1.42
39	1	616	II0	C34-C36	3.42	1.53	1.45
40	2	317	IHT	C22-C23	3.42	1.53	1.45
38	N	612	KC2	C4D-CHA	3.42	1.49	1.45
37	F	101	HEM	C1B-NB	-3.41	1.34	1.40
39	Q	313	II0	C22-C10	3.41	1.49	1.42
38	N	605	KC2	CHB-C4A	3.41	1.47	1.39
28	B	619	WVN	C26-C22	-3.40	1.31	1.35
39	2	314	II0	C22-C10	3.40	1.49	1.42
40	4	318	IHT	C37-C33	-3.40	1.31	1.35
38	3	304	KC2	CHB-C4A	3.39	1.47	1.39
39	O	614	II0	C22-C10	3.39	1.49	1.42
39	P	612	II0	C22-C10	3.38	1.49	1.42
38	Q	310	KC2	CHC-C1C	3.37	1.46	1.39
28	C	516	WVN	C33-C34	3.37	1.53	1.45
38	N	611	KC2	CHB-C4A	3.37	1.46	1.39
28	5	617	WVN	C31-C32	3.37	1.53	1.45
28	a	406	WVN	C33-C34	3.37	1.53	1.45
28	A	406	WVN	C36-C32	-3.37	1.31	1.35
38	1	611	KC2	C1C-C2C	-3.37	1.38	1.44
39	3	310	II0	C34-C36	3.37	1.53	1.45
39	2	314	II0	C06-C08	-3.36	1.47	1.52
38	5	610	KC2	CHB-C4A	3.36	1.46	1.39
28	Y	101	WVN	C19-C22	3.36	1.53	1.45
38	Q	304	KC2	CHB-C4A	3.35	1.46	1.39
38	N	610	KC2	CHB-C4A	3.35	1.46	1.39
38	4	311	KC2	CHC-C1C	3.35	1.46	1.39
40	O	616	IHT	C32-C33	3.35	1.53	1.45
38	P	605	KC2	CHB-C4A	3.34	1.46	1.39
28	S	613	WVN	C31-C32	3.34	1.53	1.45
28	C	516	WVN	C19-C22	3.34	1.53	1.45
39	N	616	II0	C22-C10	3.34	1.49	1.42
38	N	612	KC2	CHB-C4A	3.34	1.46	1.39
38	4	305	KC2	CHB-C4A	3.34	1.46	1.39
38	R	311	KC2	CHB-C4A	3.34	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	2	305	CLA	CHC-C1C	3.33	1.43	1.35
38	3	304	KC2	CHC-C1C	3.33	1.46	1.39
38	1	610	KC2	C1C-C2C	-3.33	1.38	1.44
28	d	410	WVN	C33-C34	3.32	1.53	1.45
38	4	310	KC2	CHB-C4A	3.32	1.46	1.39
38	Q	310	KC2	C4D-CHA	3.31	1.49	1.45
28	A	406	WVN	C37-C34	-3.31	1.31	1.35
28	c	517	WVN	C26-C22	-3.31	1.31	1.35
26	2	305	CLA	C3C-C2C	3.31	1.43	1.36
28	5	617	WVN	C29-C26	3.31	1.53	1.43
38	O	610	KC2	CHB-C4A	3.30	1.46	1.39
28	Y	101	WVN	C23-C25	3.30	1.53	1.45
38	2	310	KC2	CHB-C4A	3.30	1.46	1.39
28	b	619	WVN	C33-C34	3.30	1.53	1.45
38	6	608	KC2	CHB-C4A	3.30	1.46	1.39
38	S	608	KC2	CHB-C4A	3.30	1.46	1.39
28	H	101	WVN	C19-C22	3.30	1.53	1.45
28	P	615	WVN	C28-C25	-3.29	1.31	1.35
38	2	310	KC2	CHC-C1C	3.29	1.46	1.39
38	O	610	KC2	CHC-C1C	3.29	1.46	1.39
38	4	305	KC2	C4D-CHA	3.29	1.49	1.45
28	3	313	WVN	C33-C34	3.28	1.53	1.45
38	Q	304	KC2	C4D-CHA	3.28	1.49	1.45
28	S	613	WVN	C29-C26	3.28	1.53	1.43
38	N	605	KC2	CHC-C1C	3.28	1.46	1.39
28	B	618	WVN	C19-C22	3.28	1.53	1.45
38	Q	309	KC2	CHB-C4A	3.28	1.46	1.39
28	S	613	WVN	C23-C25	3.28	1.53	1.45
26	3	308	CLA	MG-NC	3.27	2.14	2.06
28	B	617	WVN	C33-C34	3.27	1.53	1.45
28	D	412	WVN	C23-C25	3.27	1.53	1.45
28	5	617	WVN	C23-C25	3.27	1.53	1.45
38	P	605	KC2	CHC-C1C	3.26	1.46	1.39
28	C	516	WVN	C30-C28	3.26	1.53	1.43
39	3	311	II0	C34-C36	3.26	1.52	1.45
28	a	406	WVN	C31-C32	3.26	1.52	1.45
38	4	311	KC2	CHB-C4A	3.25	1.46	1.39
38	R	311	KC2	CHC-C1C	3.25	1.46	1.39
28	B	618	WVN	C33-C34	3.25	1.52	1.45
28	b	617	WVN	C37-C34	-3.25	1.31	1.35
26	2	305	CLA	CHD-C1D	3.24	1.44	1.38
38	5	610	KC2	CHC-C1C	3.24	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	4	311	KC2	C4D-CHA	3.23	1.49	1.45
38	Q	310	KC2	CHB-C4A	3.23	1.46	1.39
26	2	305	CLA	OBD-CAD	3.23	1.28	1.22
28	Z	101	WVN	C31-C32	3.23	1.52	1.45
39	P	613	II0	C34-C36	3.23	1.52	1.45
38	4	310	KC2	CHC-C1C	3.23	1.46	1.39
28	A	406	WVN	C28-C25	-3.22	1.31	1.35
38	Q	309	KC2	CHC-C1C	3.22	1.46	1.39
28	c	516	WVN	C31-C32	3.22	1.52	1.45
28	P	615	WVN	C26-C22	-3.22	1.31	1.35
26	1	614	CLA	C1B-NB	3.22	1.38	1.35
28	a	406	WVN	C30-C28	3.21	1.53	1.43
38	6	608	KC2	CHC-C1C	3.21	1.46	1.39
28	b	618	WVN	C33-C34	3.21	1.52	1.45
38	S	608	KC2	CHC-C1C	3.20	1.46	1.39
38	Q	304	KC2	CHC-C1C	3.20	1.46	1.39
26	1	609	CLA	C4D-ND	-3.20	1.33	1.37
28	b	619	WVN	C30-C28	3.19	1.53	1.43
28	d	410	WVN	C30-C28	3.19	1.53	1.43
28	C	515	WVN	C28-C25	-3.19	1.31	1.35
28	d	410	WVN	C23-C25	3.19	1.52	1.45
28	Y	101	WVN	C30-C28	3.19	1.53	1.43
38	4	305	KC2	CHC-C1C	3.19	1.46	1.39
28	Y	101	WVN	C33-C34	3.18	1.52	1.45
28	b	617	WVN	C19-C22	3.18	1.52	1.45
28	P	615	WVN	C37-C34	-3.18	1.31	1.35
28	k	101	WVN	C19-C22	3.18	1.52	1.45
28	5	617	WVN	C39-C36	3.17	1.53	1.43
28	c	517	WVN	C33-C34	3.17	1.52	1.45
38	N	610	KC2	CHC-C1C	3.17	1.46	1.39
26	G	402	CLA	C4D-ND	-3.17	1.33	1.37
28	x	101	WVN	C30-C28	3.16	1.53	1.43
26	5	602	CLA	CHC-C1C	3.16	1.43	1.35
28	C	515	WVN	C26-C22	-3.16	1.31	1.35
26	1	613	CLA	CHC-C1C	3.16	1.43	1.35
38	N	611	KC2	CHC-C1C	3.16	1.46	1.39
28	D	412	WVN	C30-C28	3.16	1.53	1.43
28	Z	101	WVN	C29-C26	3.16	1.53	1.43
38	3	304	KC2	C4D-CHA	3.16	1.49	1.45
28	S	613	WVN	C39-C36	3.15	1.53	1.43
28	c	516	WVN	C33-C34	3.15	1.52	1.45
26	P	606	CLA	CHC-C1C	3.15	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	516	WVN	C23-C25	3.15	1.52	1.45
28	d	410	WVN	C31-C32	3.15	1.52	1.45
28	b	619	WVN	C23-C25	3.15	1.52	1.45
26	2	308	CLA	CHC-C1C	3.15	1.43	1.35
28	x	101	WVN	C23-C25	3.15	1.52	1.45
28	x	101	WVN	C33-C34	3.15	1.52	1.45
26	R	303	CLA	CHC-C1C	3.15	1.43	1.35
40	N	619	IHT	C32-C33	3.15	1.52	1.45
28	c	518	WVN	C19-C22	3.14	1.52	1.45
28	S	613	WVN	C30-C28	3.14	1.53	1.43
28	A	406	WVN	C26-C22	-3.14	1.31	1.35
40	1	619	IHT	C18-C07	3.14	1.56	1.45
28	5	617	WVN	C33-C34	3.14	1.52	1.45
28	Y	101	WVN	C29-C26	3.13	1.53	1.43
28	c	516	WVN	C39-C36	3.13	1.53	1.43
38	N	612	KC2	CHC-C1C	3.13	1.46	1.39
26	1	602	CLA	CHC-C1C	3.13	1.43	1.35
28	5	617	WVN	C30-C28	3.13	1.53	1.43
26	1	602	CLA	C4D-ND	-3.13	1.33	1.37
40	O	616	IHT	C37-C33	-3.13	1.31	1.35
28	x	101	WVN	C31-C32	3.13	1.52	1.45
28	H	101	WVN	C30-C28	3.13	1.53	1.43
38	P	605	KC2	C4D-CHA	3.12	1.48	1.45
28	d	410	WVN	C19-C22	3.12	1.52	1.45
28	Z	101	WVN	C33-C34	3.12	1.52	1.45
28	a	406	WVN	C36-C32	-3.12	1.31	1.35
28	a	406	WVN	C23-C25	3.12	1.52	1.45
28	b	618	WVN	C23-C25	3.12	1.52	1.45
26	3	305	CLA	CHC-C1C	3.12	1.43	1.35
26	O	605	CLA	CHC-C1C	3.12	1.43	1.35
28	D	412	WVN	C19-C22	3.11	1.52	1.45
28	S	613	WVN	C33-C34	3.11	1.52	1.45
26	1	601	CLA	CHC-C1C	3.11	1.42	1.35
28	A	406	WVN	C31-C32	3.11	1.52	1.45
38	O	610	KC2	C4D-CHA	3.11	1.48	1.45
26	6	604	CLA	CHC-C1C	3.11	1.42	1.35
26	O	608	CLA	CHC-C1C	3.11	1.42	1.35
26	Q	305	CLA	CHC-C1C	3.11	1.42	1.35
28	5	617	WVN	C40-C37	3.11	1.53	1.43
28	b	619	WVN	C31-C32	3.11	1.52	1.45
26	B	614	CLA	CHC-C1C	3.11	1.42	1.35
26	S	606	CLA	CHC-C1C	3.10	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	x	101	WVN	C39-C36	3.10	1.53	1.43
38	4	310	KC2	C4D-CHA	3.10	1.48	1.45
26	R	306	CLA	CHC-C1C	3.10	1.42	1.35
28	c	518	WVN	C31-C32	3.10	1.52	1.45
28	Z	101	WVN	C19-C22	3.10	1.52	1.45
26	O	602	CLA	CHC-C1C	3.10	1.42	1.35
40	N	619	IHT	C37-C33	-3.10	1.31	1.35
38	Q	309	KC2	C4D-CHA	3.10	1.48	1.45
26	d	405	CLA	CHC-C1C	3.10	1.42	1.35
26	N	614	CLA	CHC-C1C	3.10	1.42	1.35
26	2	302	CLA	CHC-C1C	3.10	1.42	1.35
28	x	101	WVN	C29-C26	3.09	1.53	1.43
28	b	619	WVN	C26-C22	-3.09	1.31	1.35
26	4	306	CLA	CHC-C1C	3.09	1.42	1.35
28	b	617	WVN	C29-C26	3.09	1.53	1.43
26	B	607	CLA	CHC-C1C	3.09	1.42	1.35
26	Q	302	CLA	CHC-C1C	3.09	1.42	1.35
28	c	516	WVN	C40-C37	3.09	1.53	1.43
28	S	613	WVN	C40-C37	3.09	1.53	1.43
26	c	507	CLA	CHC-C1C	3.09	1.42	1.35
26	S	604	CLA	CHC-C1C	3.09	1.42	1.35
26	5	605	CLA	CHC-C1C	3.09	1.42	1.35
26	4	303	CLA	CHC-C1C	3.08	1.42	1.35
26	b	601	CLA	CHC-C1C	3.08	1.42	1.35
26	6	606	CLA	CHC-C1C	3.08	1.42	1.35
26	b	613	CLA	CHC-C1C	3.08	1.42	1.35
28	c	516	WVN	C29-C26	3.08	1.53	1.43
39	N	618	II0	C41-C39	3.08	1.53	1.43
26	2	307	CLA	CHC-C1C	3.08	1.42	1.35
28	B	619	WVN	C33-C34	3.08	1.52	1.45
26	C	506	CLA	CHC-C1C	3.08	1.42	1.35
28	x	101	WVN	C26-C22	-3.08	1.31	1.35
28	D	412	WVN	C31-C32	3.08	1.52	1.45
28	S	613	WVN	C19-C22	3.08	1.52	1.45
26	5	608	CLA	CHC-C1C	3.07	1.42	1.35
28	d	410	WVN	C37-C34	-3.07	1.31	1.35
26	c	512	CLA	CHC-C1C	3.07	1.42	1.35
26	C	509	CLA	CHC-C1C	3.07	1.42	1.35
26	R	309	CLA	CHC-C1C	3.07	1.42	1.35
38	2	310	KC2	C4D-CHA	3.07	1.48	1.45
28	Z	101	WVN	C39-C36	3.07	1.53	1.43
39	4	317	II0	C42-C40	3.07	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	518	WVN	C37-C34	-3.07	1.31	1.35
28	b	618	WVN	C39-C36	3.07	1.52	1.43
39	Q	316	II0	C42-C40	3.07	1.52	1.43
28	k	101	WVN	C33-C34	3.06	1.52	1.45
28	B	619	WVN	C19-C22	3.06	1.52	1.45
26	4	304	CLA	CHC-C1C	3.06	1.42	1.35
26	B	606	CLA	CHC-C1C	3.06	1.42	1.35
40	Q	317	IHT	C32-C33	3.06	1.52	1.45
26	3	302	CLA	CHC-C1C	3.06	1.42	1.35
26	1	609	CLA	CHC-C1C	3.06	1.42	1.35
28	c	518	WVN	C33-C34	3.06	1.52	1.45
26	c	510	CLA	CHC-C1C	3.06	1.42	1.35
26	P	604	CLA	CHC-C1C	3.06	1.42	1.35
26	1	604	CLA	CHC-C1C	3.06	1.42	1.35
39	4	316	II0	C42-C40	3.05	1.52	1.43
26	O	607	CLA	CHC-C1C	3.05	1.42	1.35
26	S	601	CLA	CHC-C1C	3.05	1.42	1.35
39	P	614	II0	C42-C40	3.05	1.52	1.43
28	k	101	WVN	C29-C26	3.05	1.52	1.43
39	S	611	II0	C42-C40	3.05	1.52	1.43
26	1	608	CLA	CHC-C1C	3.05	1.42	1.35
39	Q	315	II0	C42-C40	3.05	1.52	1.43
38	1	610	KC2	MG-NA	3.05	2.13	2.06
26	3	308	CLA	C1D-C2D	-3.05	1.39	1.45
26	b	614	CLA	CHC-C1C	3.05	1.42	1.35
26	S	610	CLA	CHC-C1C	3.05	1.42	1.35
28	Z	101	WVN	C28-C25	-3.05	1.31	1.35
28	c	516	WVN	C30-C28	3.05	1.52	1.43
39	6	611	II0	C42-C40	3.05	1.52	1.43
28	b	619	WVN	C19-C22	3.05	1.52	1.45
26	b	611	CLA	C4D-ND	-3.05	1.33	1.37
26	6	602	CLA	C4D-ND	-3.05	1.33	1.37
28	c	516	WVN	C19-C22	3.05	1.52	1.45
26	b	611	CLA	CHC-C1C	3.05	1.42	1.35
26	Q	303	CLA	CHC-C1C	3.05	1.42	1.35
28	k	101	WVN	C37-C34	-3.05	1.31	1.35
26	2	311	CLA	CHC-C1C	3.05	1.42	1.35
40	5	616	IHT	C32-C33	3.05	1.52	1.45
28	B	619	WVN	C36-C32	-3.05	1.31	1.35
28	Z	101	WVN	C40-C37	3.04	1.52	1.43
26	6	601	CLA	CHC-C1C	3.04	1.42	1.35
26	N	602	CLA	CHC-C1C	3.04	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	604	CLA	CHC-C1C	3.04	1.42	1.35
26	P	607	CLA	CHC-C1C	3.04	1.42	1.35
26	Q	308	CLA	CHC-C1C	3.04	1.42	1.35
26	5	603	CLA	CHC-C1C	3.04	1.42	1.35
26	R	304	CLA	CHC-C1C	3.04	1.42	1.35
26	B	611	CLA	C4D-ND	-3.04	1.33	1.37
28	Z	101	WVN	C23-C25	3.04	1.52	1.45
28	c	517	WVN	C19-C22	3.04	1.52	1.45
28	5	617	WVN	C19-C22	3.04	1.52	1.45
26	3	307	CLA	CHC-C1C	3.04	1.42	1.35
26	5	609	CLA	CHC-C1C	3.04	1.42	1.35
26	6	610	CLA	CHC-C1C	3.04	1.42	1.35
26	B	601	CLA	CHC-C1C	3.04	1.42	1.35
28	b	618	WVN	C40-C37	3.04	1.52	1.43
26	C	511	CLA	CHC-C1C	3.04	1.42	1.35
26	d	406	CLA	CHC-C1C	3.04	1.42	1.35
26	3	306	CLA	CHC-C1C	3.04	1.42	1.35
26	4	309	CLA	CHC-C1C	3.04	1.42	1.35
26	R	305	CLA	CHC-C1C	3.04	1.42	1.35
39	4	314	II0	C42-C40	3.04	1.52	1.43
26	B	602	CLA	CHC-C1C	3.04	1.42	1.35
28	k	101	WVN	C36-C32	-3.04	1.31	1.35
28	S	613	WVN	C28-C25	-3.04	1.31	1.35
26	b	606	CLA	CHC-C1C	3.04	1.42	1.35
26	P	610	CLA	CHC-C1C	3.04	1.42	1.35
28	D	412	WVN	C39-C36	3.04	1.52	1.43
28	b	618	WVN	C30-C28	3.04	1.52	1.43
28	c	517	WVN	C30-C28	3.04	1.52	1.43
28	b	617	WVN	C31-C32	3.04	1.52	1.45
26	b	616	CLA	CHC-C1C	3.03	1.42	1.35
26	c	510	CLA	C4D-ND	-3.03	1.33	1.37
26	B	605	CLA	CHC-C1C	3.03	1.42	1.35
28	C	515	WVN	C33-C34	3.03	1.52	1.45
28	S	613	WVN	C02-C11	3.03	1.54	1.50
26	2	319	CLA	C4D-ND	-3.03	1.33	1.37
26	S	602	CLA	C4D-ND	-3.03	1.33	1.37
26	C	507	CLA	CHC-C1C	3.03	1.42	1.35
26	P	603	CLA	CHC-C1C	3.03	1.42	1.35
39	Q	313	II0	C42-C40	3.03	1.52	1.43
39	N	618	II0	C42-C40	3.03	1.52	1.43
26	1	608	CLA	C4D-ND	-3.03	1.33	1.37
26	g	401	CLA	CHC-C1C	3.03	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	4	318	IHT	C32-C33	3.03	1.52	1.45
26	N	606	CLA	CHC-C1C	3.03	1.42	1.35
28	b	618	WVN	C31-C32	3.03	1.52	1.45
28	5	617	WVN	C02-C11	3.03	1.54	1.50
26	O	612	CLA	CHC-C1C	3.03	1.42	1.35
26	c	503	CLA	CHC-C1C	3.03	1.42	1.35
26	c	508	CLA	CHC-C1C	3.03	1.42	1.35
28	H	101	WVN	C33-C34	3.02	1.52	1.45
26	R	310	CLA	CHC-C1C	3.02	1.42	1.35
26	C	502	CLA	C4D-ND	-3.02	1.33	1.37
26	P	609	CLA	CHC-C1C	3.02	1.42	1.35
26	3	303	CLA	CHC-C1C	3.02	1.42	1.35
26	Q	307	CLA	CHC-C1C	3.02	1.42	1.35
28	b	618	WVN	C29-C26	3.02	1.52	1.43
26	B	616	CLA	CHC-C1C	3.02	1.42	1.35
26	C	505	CLA	CHC-C1C	3.02	1.42	1.35
26	2	309	CLA	CHC-C1C	3.02	1.42	1.35
26	P	602	CLA	CHC-C1C	3.02	1.42	1.35
28	B	617	WVN	C30-C28	3.02	1.52	1.43
26	3	309	CLA	CHC-C1C	3.02	1.42	1.35
26	O	611	CLA	CHC-C1C	3.02	1.42	1.35
26	1	613	CLA	C4D-ND	-3.02	1.33	1.37
28	Y	101	WVN	C39-C36	3.02	1.52	1.43
39	4	316	II0	C41-C39	3.02	1.52	1.43
28	C	516	WVN	C20-C13	3.02	1.55	1.45
26	C	502	CLA	CHC-C1C	3.02	1.42	1.35
39	5	615	II0	C42-C40	3.02	1.52	1.43
26	b	608	CLA	CHC-C1C	3.02	1.42	1.35
26	4	308	CLA	CHC-C1C	3.02	1.42	1.35
28	C	515	WVN	C31-C32	3.02	1.52	1.45
26	b	605	CLA	CHC-C1C	3.02	1.42	1.35
26	O	609	CLA	CHC-C1C	3.02	1.42	1.35
28	5	617	WVN	C28-C25	-3.02	1.31	1.35
28	D	412	WVN	C29-C26	3.02	1.52	1.43
28	c	518	WVN	C39-C36	3.02	1.52	1.43
26	O	603	CLA	C4D-ND	-3.02	1.33	1.37
38	R	311	KC2	C4D-CHA	3.02	1.48	1.45
26	4	302	CLA	CHC-C1C	3.02	1.42	1.35
28	b	617	WVN	C36-C32	-3.01	1.31	1.35
39	N	615	II0	C42-C40	3.01	1.52	1.43
26	1	606	CLA	CHC-C1C	3.01	1.42	1.35
26	S	602	CLA	CHC-C1C	3.01	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	619	WVN	C40-C37	3.01	1.52	1.43
39	2	315	II0	C42-C40	3.01	1.52	1.43
28	c	518	WVN	C36-C32	-3.01	1.31	1.35
26	b	603	CLA	CHC-C1C	3.01	1.42	1.35
26	2	312	CLA	CHC-C1C	3.01	1.42	1.35
26	c	508	CLA	C4D-ND	-3.01	1.33	1.37
26	6	602	CLA	CHC-C1C	3.01	1.42	1.35
28	c	516	WVN	C28-C25	-3.01	1.31	1.35
28	d	410	WVN	C26-C22	-3.01	1.31	1.35
26	B	613	CLA	CHC-C1C	3.01	1.42	1.35
26	1	603	CLA	CHC-C1C	3.01	1.42	1.35
28	3	313	WVN	C30-C28	3.01	1.52	1.43
39	R	316	II0	C42-C40	3.01	1.52	1.43
28	b	618	WVN	C19-C22	3.01	1.52	1.45
26	C	513	CLA	CHC-C1C	3.01	1.42	1.35
39	R	318	II0	C42-C40	3.01	1.52	1.43
26	B	611	CLA	CHC-C1C	3.01	1.42	1.35
26	N	604	CLA	CHC-C1C	3.01	1.42	1.35
28	B	619	WVN	C30-C28	3.01	1.52	1.43
28	d	410	WVN	C29-C26	3.00	1.52	1.43
26	C	512	CLA	CHC-C1C	3.00	1.42	1.35
26	S	607	CLA	CHC-C1C	3.00	1.42	1.35
40	R	317	IHT	C32-C33	3.00	1.52	1.45
39	6	613	II0	C42-C40	3.00	1.52	1.43
28	d	410	WVN	C39-C36	3.00	1.52	1.43
26	C	504	CLA	CHC-C1C	3.00	1.42	1.35
28	b	619	WVN	C39-C36	3.00	1.52	1.43
39	5	613	II0	C42-C40	3.00	1.52	1.43
26	A	403	CLA	CHC-C1C	3.00	1.42	1.35
28	B	618	WVN	C30-C28	3.00	1.52	1.43
26	N	609	CLA	CHC-C1C	3.00	1.42	1.35
26	3	301	CLA	CHC-C1C	3.00	1.42	1.35
28	b	618	WVN	C37-C34	-3.00	1.31	1.35
26	G	401	CLA	C4D-ND	-3.00	1.33	1.37
26	C	503	CLA	C4D-ND	-3.00	1.33	1.37
39	N	617	II0	C42-C40	3.00	1.52	1.43
39	P	614	II0	C41-C39	3.00	1.52	1.43
26	C	514	CLA	CHC-C1C	3.00	1.42	1.35
26	a	403	CLA	CHC-C1C	3.00	1.42	1.35
26	Q	312	CLA	CHC-C1C	3.00	1.42	1.35
28	x	101	WVN	C40-C37	3.00	1.52	1.43
39	4	315	II0	C42-C40	3.00	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	510	CLA	CHC-C1C	3.00	1.42	1.35
26	b	610	CLA	CHC-C1C	3.00	1.42	1.35
39	Q	316	II0	C41-C39	3.00	1.52	1.43
28	c	518	WVN	C26-C22	-3.00	1.31	1.35
26	a	405	CLA	CHC-C1C	2.99	1.42	1.35
26	6	607	CLA	CHC-C1C	2.99	1.42	1.35
26	O	604	CLA	CHC-C1C	2.99	1.42	1.35
28	a	406	WVN	C29-C26	2.99	1.52	1.43
26	b	607	CLA	CHC-C1C	2.99	1.42	1.35
39	N	620	II0	C42-C40	2.99	1.52	1.43
26	C	505	CLA	C4D-ND	-2.99	1.33	1.37
26	c	511	CLA	CHC-C1C	2.99	1.42	1.35
28	k	101	WVN	C23-C25	2.99	1.52	1.45
39	O	613	II0	C42-C40	2.99	1.52	1.43
26	b	612	CLA	CHC-C1C	2.99	1.42	1.35
26	b	602	CLA	CHC-C1C	2.99	1.42	1.35
26	2	304	CLA	CHC-C1C	2.99	1.42	1.35
40	O	616	IHT	C34-C35	2.99	1.52	1.45
26	B	608	CLA	CHC-C1C	2.99	1.42	1.35
26	1	607	CLA	C4D-ND	-2.99	1.33	1.37
28	P	615	WVN	C36-C32	-2.99	1.31	1.35
26	5	602	CLA	C4D-ND	-2.99	1.33	1.37
26	R	305	CLA	C4D-ND	-2.99	1.33	1.37
26	Q	301	CLA	CHC-C1C	2.99	1.42	1.35
28	D	412	WVN	C40-C37	2.99	1.52	1.43
39	4	317	II0	C41-C39	2.99	1.52	1.43
28	x	101	WVN	C36-C32	-2.99	1.31	1.35
26	B	609	CLA	CHC-C1C	2.99	1.42	1.35
26	c	513	CLA	CHC-C1C	2.99	1.42	1.35
26	2	303	CLA	CHC-C1C	2.99	1.42	1.35
28	B	617	WVN	C20-C13	2.99	1.55	1.45
28	c	517	WVN	C40-C37	2.98	1.52	1.43
26	5	608	CLA	C4D-ND	-2.98	1.33	1.37
28	c	517	WVN	C37-C34	-2.98	1.31	1.35
39	6	612	II0	C42-C40	2.98	1.52	1.43
26	D	407	CLA	CHC-C1C	2.98	1.42	1.35
26	P	611	CLA	CHC-C1C	2.98	1.42	1.35
28	P	615	WVN	C40-C37	2.98	1.52	1.43
39	Q	315	II0	C41-C39	2.98	1.52	1.43
38	N	611	KC2	C4D-CHA	2.98	1.48	1.45
38	5	610	KC2	C4D-CHA	2.98	1.48	1.45
28	a	406	WVN	C39-C36	2.98	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Q	319	II0	C42-C40	2.98	1.52	1.43
26	C	509	CLA	C4D-ND	-2.98	1.33	1.37
28	k	101	WVN	C39-C36	2.98	1.52	1.43
39	Q	314	II0	C42-C40	2.98	1.52	1.43
28	B	619	WVN	C40-C37	2.98	1.52	1.43
26	O	603	CLA	CHC-C1C	2.98	1.42	1.35
28	P	615	WVN	C19-C22	2.98	1.52	1.45
28	D	412	WVN	C37-C34	-2.98	1.31	1.35
26	2	303	CLA	C4D-ND	-2.98	1.33	1.37
28	d	410	WVN	C40-C37	2.98	1.52	1.43
39	N	620	II0	C41-C39	2.98	1.52	1.43
28	P	615	WVN	C31-C32	2.98	1.52	1.45
26	B	610	CLA	CHC-C1C	2.98	1.42	1.35
28	C	515	WVN	C36-C32	-2.98	1.31	1.35
26	D	408	CLA	CHC-C1C	2.98	1.42	1.35
26	4	313	CLA	CHC-C1C	2.98	1.42	1.35
39	R	315	II0	C42-C40	2.98	1.52	1.43
26	c	507	CLA	C4D-ND	-2.97	1.33	1.37
26	C	508	CLA	CHC-C1C	2.97	1.42	1.35
26	1	607	CLA	CHC-C1C	2.97	1.42	1.35
26	N	603	CLA	CHC-C1C	2.97	1.42	1.35
26	B	603	CLA	CHC-C1C	2.97	1.42	1.35
26	5	612	CLA	CHC-C1C	2.97	1.42	1.35
28	c	518	WVN	C29-C26	2.97	1.52	1.43
26	5	606	CLA	CHC-C1C	2.97	1.42	1.35
26	5	604	CLA	C4D-ND	-2.97	1.33	1.37
39	Q	313	II0	C41-C39	2.97	1.52	1.43
28	Z	101	WVN	C30-C28	2.97	1.52	1.43
39	R	314	II0	C42-C40	2.97	1.52	1.43
28	d	410	WVN	C36-C32	-2.97	1.31	1.35
28	c	517	WVN	C31-C32	2.97	1.52	1.45
26	B	602	CLA	C4D-ND	-2.97	1.33	1.37
26	a	402	CLA	CHC-C1C	2.97	1.42	1.35
26	6	605	CLA	CHC-C1C	2.97	1.42	1.35
26	b	615	CLA	CHC-C1C	2.97	1.42	1.35
28	k	101	WVN	C26-C22	-2.97	1.31	1.35
26	A	402	CLA	CHC-C1C	2.97	1.42	1.35
28	B	619	WVN	C39-C36	2.97	1.52	1.43
26	c	504	CLA	C4D-ND	-2.97	1.33	1.37
28	B	619	WVN	C37-C34	-2.97	1.31	1.35
28	c	517	WVN	C29-C26	2.97	1.52	1.43
38	S	608	KC2	C4D-CHA	2.96	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	4	314	II0	C41-C39	2.96	1.52	1.43
28	k	101	WVN	C30-C28	2.96	1.52	1.43
28	k	101	WVN	C31-C32	2.96	1.52	1.45
28	c	518	WVN	C40-C37	2.96	1.52	1.43
26	S	605	CLA	CHC-C1C	2.96	1.42	1.35
39	S	612	II0	C42-C40	2.96	1.52	1.43
26	c	505	CLA	CHC-C1C	2.96	1.42	1.35
26	B	612	CLA	CHC-C1C	2.96	1.42	1.35
26	a	402	CLA	C4D-ND	-2.96	1.33	1.37
28	A	406	WVN	C33-C34	2.96	1.52	1.45
28	C	515	WVN	C19-C22	2.96	1.52	1.45
26	b	609	CLA	CHC-C1C	2.96	1.42	1.35
39	2	313	II0	C42-C40	2.96	1.52	1.43
28	C	515	WVN	C37-C34	-2.96	1.31	1.35
26	2	305	CLA	C3B-C2B	2.96	1.44	1.40
26	B	615	CLA	CHC-C1C	2.96	1.42	1.35
26	c	514	CLA	CHC-C1C	2.96	1.42	1.35
26	c	515	CLA	CHC-C1C	2.96	1.42	1.35
28	c	518	WVN	C30-C28	2.96	1.52	1.43
26	c	509	CLA	C4D-ND	-2.96	1.33	1.37
39	2	315	II0	C41-C39	2.96	1.52	1.43
26	R	313	CLA	CHC-C1C	2.96	1.42	1.35
28	a	406	WVN	C19-C22	2.96	1.52	1.45
28	P	615	WVN	C39-C36	2.96	1.52	1.43
40	4	318	IHT	C34-C35	2.95	1.52	1.45
26	R	307	CLA	CHC-C1C	2.95	1.42	1.35
28	H	101	WVN	C20-C13	2.95	1.55	1.45
28	a	406	WVN	C37-C34	-2.95	1.31	1.35
39	4	320	II0	C42-C40	2.95	1.52	1.43
39	5	614	II0	C42-C40	2.95	1.52	1.43
26	N	613	CLA	CHC-C1C	2.95	1.42	1.35
28	C	515	WVN	C40-C37	2.95	1.52	1.43
26	P	602	CLA	C4D-ND	-2.95	1.33	1.37
28	B	619	WVN	C29-C26	2.95	1.52	1.43
26	A	405	CLA	CHC-C1C	2.95	1.42	1.35
28	x	101	WVN	C37-C34	-2.95	1.31	1.35
26	R	309	CLA	C4D-ND	-2.95	1.33	1.37
26	R	308	CLA	CHC-C1C	2.95	1.42	1.35
26	d	402	CLA	C4D-ND	-2.95	1.33	1.37
28	A	406	WVN	C29-C26	2.95	1.52	1.43
26	N	604	CLA	C4D-ND	-2.95	1.33	1.37
26	b	605	CLA	C4D-ND	-2.95	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	2	314	II0	C42-C40	2.95	1.52	1.43
26	P	608	CLA	CHC-C1C	2.95	1.42	1.35
26	P	601	CLA	C4D-ND	-2.95	1.33	1.37
28	C	515	WVN	C29-C26	2.94	1.52	1.43
26	B	610	CLA	C4D-ND	-2.94	1.33	1.37
26	R	303	CLA	C4D-ND	-2.94	1.33	1.37
39	O	614	II0	C42-C40	2.94	1.52	1.43
26	c	506	CLA	CHC-C1C	2.94	1.42	1.35
39	N	616	II0	C42-C40	2.94	1.52	1.43
26	B	609	CLA	C4D-ND	-2.94	1.33	1.37
26	b	609	CLA	C4D-ND	-2.94	1.33	1.37
26	1	604	CLA	C4D-ND	-2.94	1.33	1.37
30	c	501	SQD	C6-S	-2.94	1.66	1.77
26	C	506	CLA	C4D-ND	-2.94	1.33	1.37
30	D	401	SQD	C6-S	-2.94	1.66	1.77
28	a	406	WVN	C40-C37	2.94	1.52	1.43
26	4	312	CLA	CHC-C1C	2.94	1.42	1.35
39	O	614	II0	C41-C39	2.94	1.52	1.43
26	3	301	CLA	C4D-ND	-2.94	1.33	1.37
26	Q	303	CLA	C4D-ND	-2.94	1.33	1.37
39	N	617	II0	C41-C39	2.94	1.52	1.43
29	d	407	PL9	C3-C4	-2.94	1.44	1.49
26	4	301	CLA	CHC-C1C	2.94	1.42	1.35
28	Y	101	WVN	C31-C32	2.93	1.52	1.45
38	1	611	KC2	C3C-C4C	-2.93	1.39	1.44
40	Q	317	IHT	C34-C35	2.93	1.52	1.45
26	D	404	CLA	C4D-ND	-2.93	1.33	1.37
26	5	607	CLA	C4D-ND	-2.93	1.33	1.37
26	N	601	CLA	CHC-C1C	2.93	1.42	1.35
28	b	619	WVN	C29-C26	2.93	1.52	1.43
38	6	608	KC2	C4D-CHA	2.93	1.48	1.45
39	6	611	II0	C41-C39	2.93	1.52	1.43
39	P	612	II0	C42-C40	2.93	1.52	1.43
26	5	607	CLA	CHC-C1C	2.93	1.42	1.35
28	Y	101	WVN	C40-C37	2.93	1.52	1.43
26	2	312	CLA	C4D-ND	-2.93	1.33	1.37
26	O	612	CLA	C4D-ND	-2.93	1.33	1.37
26	2	306	CLA	CHC-C1C	2.93	1.42	1.35
28	C	515	WVN	C30-C28	2.92	1.52	1.43
26	A	405	CLA	C4D-ND	-2.92	1.33	1.37
26	5	609	CLA	C4D-ND	-2.92	1.33	1.37
39	2	314	II0	C41-C39	2.92	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	R	314	II0	C41-C39	2.92	1.52	1.43
26	4	307	CLA	C4D-ND	-2.92	1.33	1.37
26	P	607	CLA	C4D-ND	-2.92	1.33	1.37
39	5	613	II0	C41-C39	2.92	1.52	1.43
39	R	318	II0	C41-C39	2.92	1.52	1.43
26	R	308	CLA	C4D-ND	-2.92	1.33	1.37
26	R	302	CLA	C4D-ND	-2.92	1.33	1.37
26	P	601	CLA	CHC-C1C	2.92	1.42	1.35
38	1	605	KC2	C3C-C4C	-2.92	1.39	1.44
28	P	615	WVN	C33-C34	2.92	1.52	1.45
28	b	617	WVN	C26-C22	-2.92	1.31	1.35
38	1	610	KC2	C3C-C4C	-2.92	1.39	1.44
26	5	601	CLA	C4D-ND	-2.92	1.33	1.37
28	B	617	WVN	C19-C22	2.92	1.52	1.45
39	P	612	II0	C41-C39	2.91	1.52	1.43
28	3	313	WVN	C20-C13	2.91	1.55	1.45
28	Y	101	WVN	C36-C32	-2.91	1.31	1.35
26	R	307	CLA	C4D-ND	-2.91	1.33	1.37
39	S	611	II0	C41-C39	2.91	1.52	1.43
26	C	504	CLA	C4D-ND	-2.91	1.33	1.37
26	O	608	CLA	C4D-ND	-2.91	1.33	1.37
26	G	402	CLA	CHC-C1C	2.91	1.42	1.35
39	6	613	II0	C41-C39	2.91	1.52	1.43
37	F	101	HEM	FE-NB	2.91	2.11	1.96
28	k	101	WVN	C40-C37	2.91	1.52	1.43
26	2	308	CLA	C4D-ND	-2.91	1.33	1.37
39	R	316	II0	C41-C39	2.91	1.52	1.43
26	O	601	CLA	CHC-C1C	2.91	1.42	1.35
28	Y	101	WVN	C37-C34	-2.91	1.31	1.35
39	Q	319	II0	C41-C39	2.91	1.52	1.43
28	A	406	WVN	C19-C22	2.91	1.52	1.45
26	D	404	CLA	CHC-C1C	2.91	1.42	1.35
26	2	306	CLA	C4D-ND	-2.91	1.33	1.37
26	d	402	CLA	CHC-C1C	2.91	1.42	1.35
26	B	603	CLA	C4D-ND	-2.91	1.33	1.37
28	Y	101	WVN	C28-C25	-2.91	1.31	1.35
28	c	518	WVN	C28-C25	-2.91	1.31	1.35
26	O	606	CLA	CHC-C1C	2.90	1.42	1.35
26	B	616	CLA	C4D-ND	-2.90	1.33	1.37
26	N	601	CLA	C4D-ND	-2.90	1.33	1.37
26	Q	306	CLA	C4D-ND	-2.90	1.33	1.37
28	A	406	WVN	C39-C36	2.90	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	2	301	CLA	CHC-C1C	2.90	1.42	1.35
26	2	319	CLA	CHC-C1C	2.90	1.42	1.35
26	6	609	CLA	CHC-C1C	2.90	1.42	1.35
26	S	609	CLA	CHC-C1C	2.90	1.42	1.35
26	b	616	CLA	C4D-ND	-2.90	1.33	1.37
26	P	608	CLA	C4D-ND	-2.90	1.33	1.37
28	k	101	WVN	C28-C25	-2.90	1.31	1.35
28	c	517	WVN	C39-C36	2.90	1.52	1.43
28	C	515	WVN	C39-C36	2.90	1.52	1.43
28	b	617	WVN	C39-C36	2.90	1.52	1.43
28	P	615	WVN	C29-C26	2.90	1.52	1.43
26	C	511	CLA	C4D-ND	-2.90	1.33	1.37
26	g	402	CLA	CHC-C1C	2.90	1.42	1.35
26	Q	311	CLA	CHC-C1C	2.89	1.42	1.35
28	k	101	WVN	C02-C11	2.89	1.54	1.50
26	4	301	CLA	C4D-ND	-2.89	1.33	1.37
39	O	613	II0	C41-C39	2.89	1.52	1.43
30	A	408	SQD	C6-S	-2.89	1.66	1.77
26	c	509	CLA	CHC-C1C	2.89	1.42	1.35
26	A	402	CLA	C4D-ND	-2.89	1.33	1.37
26	d	405	CLA	C4D-ND	-2.89	1.33	1.37
26	P	610	CLA	C4D-ND	-2.89	1.33	1.37
26	Q	308	CLA	C4D-ND	-2.89	1.33	1.37
26	S	603	CLA	CHC-C1C	2.89	1.42	1.35
26	4	304	CLA	C4D-ND	-2.89	1.33	1.37
39	4	320	II0	C41-C39	2.89	1.52	1.43
26	O	604	CLA	C4D-ND	-2.89	1.33	1.37
28	B	619	WVN	C28-C25	-2.89	1.32	1.35
26	C	503	CLA	CHC-C1C	2.89	1.42	1.35
26	Q	301	CLA	C4D-ND	-2.89	1.33	1.37
28	Z	101	WVN	C26-C22	-2.88	1.32	1.35
38	1	612	KC2	C3C-C4C	-2.88	1.39	1.44
28	B	619	WVN	C31-C32	2.88	1.52	1.45
26	b	610	CLA	C4D-ND	-2.88	1.33	1.37
28	b	619	WVN	C37-C34	-2.88	1.32	1.35
39	5	615	II0	C41-C39	2.88	1.52	1.43
26	B	605	CLA	C4D-ND	-2.88	1.33	1.37
26	S	605	CLA	C4D-ND	-2.88	1.33	1.37
28	b	618	WVN	C28-C25	-2.88	1.32	1.35
28	b	618	WVN	C26-C22	-2.88	1.32	1.35
26	b	602	CLA	C4D-ND	-2.88	1.33	1.37
28	Z	101	WVN	C36-C32	-2.88	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	506	CLA	C4D-ND	-2.88	1.33	1.37
26	S	603	CLA	C4D-ND	-2.88	1.33	1.37
28	B	618	WVN	C20-C13	2.88	1.55	1.45
26	6	603	CLA	CHC-C1C	2.88	1.42	1.35
26	N	602	CLA	C4D-ND	-2.88	1.33	1.37
26	6	603	CLA	C4D-ND	-2.87	1.33	1.37
39	N	615	II0	C41-C39	2.87	1.52	1.43
37	f	101	HEM	FE-NB	2.87	2.11	1.96
28	x	101	WVN	C28-C25	-2.87	1.32	1.35
39	R	315	II0	C41-C39	2.87	1.52	1.43
26	C	512	CLA	C4D-ND	-2.87	1.33	1.37
39	4	315	II0	C41-C39	2.87	1.52	1.43
30	a	408	SQD	C6-S	-2.87	1.66	1.77
28	B	619	WVN	C23-C25	2.87	1.52	1.45
39	N	616	II0	C41-C39	2.87	1.52	1.43
38	N	605	KC2	C4A-C3A	2.87	1.50	1.44
26	c	504	CLA	CHC-C1C	2.87	1.42	1.35
26	g	401	CLA	C4D-ND	-2.87	1.33	1.37
26	N	609	CLA	C4D-ND	-2.87	1.33	1.37
26	b	603	CLA	C4D-ND	-2.86	1.33	1.37
26	C	507	CLA	C4D-ND	-2.86	1.33	1.37
26	O	606	CLA	C4D-ND	-2.86	1.33	1.37
28	c	517	WVN	C23-C25	2.86	1.52	1.45
26	R	310	CLA	C4D-ND	-2.86	1.33	1.37
26	1	614	CLA	CHC-C1C	2.86	1.42	1.35
26	6	605	CLA	C4D-ND	-2.86	1.33	1.37
26	1	603	CLA	C4D-ND	-2.86	1.33	1.37
26	N	607	CLA	CHC-C1C	2.86	1.42	1.35
26	C	514	CLA	C4D-ND	-2.86	1.33	1.37
26	3	306	CLA	C4D-ND	-2.86	1.33	1.37
26	S	606	CLA	C4D-ND	-2.86	1.33	1.37
26	a	403	CLA	C4D-ND	-2.86	1.33	1.37
26	2	304	CLA	C4D-ND	-2.86	1.33	1.37
38	N	611	KC2	C1B-NB	-2.86	1.34	1.37
38	6	608	KC2	C1B-NB	-2.86	1.34	1.37
26	6	606	CLA	C4D-ND	-2.85	1.33	1.37
26	N	607	CLA	C4D-ND	-2.85	1.33	1.37
26	5	606	CLA	C4D-ND	-2.85	1.33	1.37
26	b	607	CLA	C4D-ND	-2.85	1.33	1.37
26	d	406	CLA	C4D-ND	-2.85	1.33	1.37
39	5	614	II0	C41-C39	2.85	1.52	1.43
26	R	312	CLA	CHC-C1C	2.85	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	607	CLA	C4D-ND	-2.85	1.33	1.37
39	2	313	II0	C41-C39	2.85	1.52	1.43
26	1	601	CLA	C4D-ND	-2.85	1.33	1.37
26	a	405	CLA	C4D-ND	-2.85	1.33	1.37
28	P	615	WVN	C23-C25	2.85	1.52	1.45
38	N	605	KC2	C4D-CHA	2.84	1.48	1.45
26	c	505	CLA	C4D-ND	-2.84	1.33	1.37
26	b	608	CLA	C4D-ND	-2.84	1.33	1.37
26	Q	311	CLA	C4D-ND	-2.84	1.33	1.37
39	Q	314	II0	C41-C39	2.84	1.52	1.43
26	g	402	CLA	C4D-ND	-2.84	1.33	1.37
26	C	513	CLA	C4D-ND	-2.83	1.33	1.37
26	c	511	CLA	C4D-ND	-2.83	1.33	1.37
38	S	608	KC2	C1B-NB	-2.83	1.34	1.37
26	B	614	CLA	C4D-ND	-2.83	1.33	1.37
26	4	306	CLA	C4D-ND	-2.83	1.33	1.37
26	B	613	CLA	C4D-ND	-2.83	1.33	1.37
26	4	309	CLA	C4D-ND	-2.83	1.33	1.37
26	Q	302	CLA	C4D-ND	-2.83	1.33	1.37
26	O	607	CLA	C4D-ND	-2.83	1.33	1.37
26	Q	312	CLA	C4D-ND	-2.83	1.33	1.37
26	G	401	CLA	CHC-C1C	2.83	1.42	1.35
29	D	409	PL9	C3-C4	-2.83	1.44	1.49
39	N	620	II0	C40-C36	-2.82	1.32	1.35
26	6	609	CLA	C4D-ND	-2.82	1.33	1.37
26	S	607	CLA	C4D-ND	-2.82	1.33	1.37
26	c	513	CLA	C4D-ND	-2.82	1.33	1.37
26	Q	305	CLA	C4D-ND	-2.82	1.33	1.37
26	C	508	CLA	C4D-ND	-2.81	1.33	1.37
28	b	618	WVN	C36-C32	-2.81	1.32	1.35
26	2	309	CLA	C4D-ND	-2.81	1.33	1.37
26	6	610	CLA	C4D-ND	-2.81	1.33	1.37
28	c	517	WVN	C28-C25	-2.81	1.32	1.35
26	Q	306	CLA	CHC-C1C	2.81	1.42	1.35
26	R	306	CLA	C4D-ND	-2.81	1.33	1.37
26	6	607	CLA	C4D-ND	-2.81	1.33	1.37
26	c	512	CLA	C4D-ND	-2.81	1.33	1.37
26	N	613	CLA	C4D-ND	-2.81	1.33	1.37
28	C	515	WVN	C23-C25	2.81	1.52	1.45
26	B	608	CLA	C4D-ND	-2.81	1.33	1.37
26	D	408	CLA	C4D-ND	-2.81	1.33	1.37
26	3	307	CLA	C4D-ND	-2.81	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	O	605	CLA	C4D-ND	-2.81	1.33	1.37
26	b	604	CLA	C4D-ND	-2.81	1.33	1.37
26	b	614	CLA	C4D-ND	-2.81	1.33	1.37
26	O	611	CLA	C4D-ND	-2.81	1.33	1.37
28	c	516	WVN	C26-C22	-2.81	1.32	1.35
26	B	604	CLA	CHC-C1C	2.81	1.42	1.35
26	B	601	CLA	C4D-ND	-2.81	1.33	1.37
28	b	617	WVN	C33-C34	2.81	1.52	1.45
26	5	611	CLA	CHC-C1C	2.80	1.42	1.35
28	D	412	WVN	C26-C22	-2.80	1.32	1.35
26	D	407	CLA	C4D-ND	-2.80	1.33	1.37
26	S	601	CLA	C4D-ND	-2.80	1.33	1.37
38	3	304	KC2	C1D-CHD	2.80	1.48	1.41
38	P	605	KC2	C1D-CHD	2.80	1.48	1.41
28	P	615	WVN	C30-C28	2.80	1.52	1.43
39	6	612	II0	C41-C39	2.80	1.52	1.43
26	O	602	CLA	C4D-ND	-2.80	1.33	1.37
26	4	312	CLA	C4D-ND	-2.80	1.33	1.37
38	5	610	KC2	C1B-NB	-2.79	1.34	1.37
28	b	617	WVN	C40-C37	2.79	1.52	1.43
26	P	609	CLA	C4D-ND	-2.79	1.33	1.37
26	2	311	CLA	C4D-ND	-2.79	1.33	1.37
26	6	601	CLA	C4D-ND	-2.79	1.33	1.37
26	c	514	CLA	C4D-ND	-2.79	1.33	1.37
26	S	609	CLA	C4D-ND	-2.79	1.33	1.37
39	2	315	II0	C40-C36	-2.79	1.32	1.35
26	N	606	CLA	C4D-ND	-2.79	1.33	1.37
26	5	605	CLA	C4D-ND	-2.79	1.33	1.37
26	4	302	CLA	C4D-ND	-2.79	1.33	1.37
28	x	101	WVN	C19-C22	2.79	1.51	1.45
39	S	612	II0	C41-C39	2.79	1.52	1.43
26	O	601	CLA	C4D-ND	-2.78	1.33	1.37
28	c	517	WVN	C36-C32	-2.78	1.32	1.35
26	1	606	CLA	C4D-ND	-2.78	1.33	1.37
26	O	609	CLA	C4D-ND	-2.78	1.33	1.37
26	2	307	CLA	C4D-ND	-2.78	1.33	1.37
28	c	518	WVN	C23-C25	2.78	1.51	1.45
26	c	515	CLA	C4D-ND	-2.78	1.33	1.37
26	b	604	CLA	CHC-C1C	2.78	1.42	1.35
26	4	307	CLA	CHC-C1C	2.78	1.42	1.35
26	c	503	CLA	C4D-ND	-2.78	1.33	1.37
28	Y	101	WVN	C26-C22	-2.78	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	516	WVN	C37-C34	-2.78	1.32	1.35
26	4	313	CLA	C4D-ND	-2.78	1.33	1.37
39	Q	313	II0	C40-C36	-2.77	1.32	1.35
29	a	407	PL9	C3-C4	-2.77	1.45	1.49
26	4	303	CLA	C4D-ND	-2.77	1.33	1.37
26	R	304	CLA	C4D-ND	-2.77	1.33	1.37
38	N	612	KC2	C4A-C3A	2.77	1.49	1.44
26	2	302	CLA	C4D-ND	-2.76	1.33	1.37
26	2	301	CLA	C4D-ND	-2.76	1.33	1.37
26	B	612	CLA	C4D-ND	-2.76	1.33	1.37
26	5	612	CLA	C4D-ND	-2.76	1.33	1.37
28	A	406	WVN	C23-C25	2.76	1.51	1.45
28	a	406	WVN	C28-C25	-2.76	1.32	1.35
26	S	610	CLA	C4D-ND	-2.75	1.33	1.37
28	D	412	WVN	C02-C11	2.75	1.54	1.50
28	D	412	WVN	C36-C32	-2.75	1.32	1.35
26	N	603	CLA	C4D-ND	-2.75	1.33	1.37
26	N	614	CLA	C4D-ND	-2.75	1.33	1.37
26	5	611	CLA	C4D-ND	-2.75	1.33	1.37
38	Q	304	KC2	C4A-C3A	2.75	1.49	1.44
26	b	612	CLA	C4D-ND	-2.75	1.33	1.37
26	P	603	CLA	C4D-ND	-2.75	1.33	1.37
26	5	601	CLA	CHC-C1C	2.75	1.42	1.35
26	P	606	CLA	C4D-ND	-2.75	1.33	1.37
38	4	305	KC2	C4A-C3A	2.75	1.49	1.44
38	N	612	KC2	C3C-C4C	2.75	1.50	1.44
28	A	406	WVN	C30-C28	2.75	1.52	1.43
28	c	516	WVN	C36-C32	-2.74	1.32	1.35
26	R	302	CLA	CHC-C1C	2.74	1.42	1.35
28	A	406	WVN	C40-C37	2.74	1.51	1.43
26	b	615	CLA	C4D-ND	-2.74	1.33	1.37
26	R	312	CLA	C4D-ND	-2.74	1.33	1.37
39	6	612	II0	C40-C36	-2.74	1.32	1.35
39	4	314	II0	C40-C36	-2.74	1.32	1.35
39	O	614	II0	C40-C36	-2.73	1.32	1.35
26	3	309	CLA	C4D-ND	-2.73	1.33	1.37
28	b	619	WVN	C36-C32	-2.73	1.32	1.35
26	Q	307	CLA	C4D-ND	-2.73	1.33	1.37
26	b	601	CLA	C4D-ND	-2.73	1.33	1.37
38	P	605	KC2	C4A-C3A	2.72	1.49	1.44
28	b	617	WVN	C30-C28	2.72	1.51	1.43
38	R	311	KC2	C4A-C3A	2.72	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	R	315	II0	C40-C36	-2.72	1.32	1.35
38	R	311	KC2	C1B-NB	-2.72	1.34	1.37
38	N	612	KC2	C1D-CHD	2.72	1.48	1.41
39	2	314	II0	C40-C36	-2.72	1.32	1.35
26	R	313	CLA	C4D-ND	-2.72	1.34	1.37
26	B	604	CLA	C4D-ND	-2.71	1.34	1.37
39	5	613	II0	C40-C36	-2.71	1.32	1.35
28	a	406	WVN	C26-C22	-2.71	1.32	1.35
26	b	606	CLA	C4D-ND	-2.71	1.34	1.37
29	A	407	PL9	C3-C4	-2.71	1.45	1.49
26	5	603	CLA	C4D-ND	-2.71	1.34	1.37
38	5	610	KC2	C4A-C3A	2.71	1.49	1.44
28	b	619	WVN	C28-C25	-2.70	1.32	1.35
26	P	611	CLA	C4D-ND	-2.70	1.34	1.37
39	S	612	II0	C40-C36	-2.70	1.32	1.35
26	3	302	CLA	C4D-ND	-2.70	1.34	1.37
26	b	613	CLA	C4D-ND	-2.70	1.34	1.37
39	5	614	II0	C40-C36	-2.70	1.32	1.35
26	C	510	CLA	C4D-ND	-2.69	1.34	1.37
38	Q	310	KC2	C1D-CHD	2.69	1.48	1.41
26	B	615	CLA	C4D-ND	-2.69	1.34	1.37
38	N	610	KC2	C1B-NB	-2.69	1.34	1.37
26	4	308	CLA	C4D-ND	-2.68	1.34	1.37
26	3	305	CLA	C4D-ND	-2.68	1.34	1.37
39	R	314	II0	C40-C36	-2.68	1.32	1.35
38	3	304	KC2	C4A-C3A	2.68	1.49	1.44
38	2	310	KC2	C1B-NB	-2.68	1.34	1.37
38	4	310	KC2	C4A-C3A	2.67	1.49	1.44
39	4	315	II0	C40-C36	-2.67	1.32	1.35
39	N	617	II0	C40-C36	-2.67	1.32	1.35
28	Y	101	WVN	C02-C11	2.67	1.54	1.50
40	O	616	IHT	C22-C23	2.67	1.51	1.45
38	Q	309	KC2	C1D-CHD	2.67	1.48	1.41
26	B	606	CLA	C4D-ND	-2.67	1.34	1.37
39	N	615	II0	C40-C36	-2.67	1.32	1.35
38	4	311	KC2	C1D-CHD	2.67	1.48	1.41
38	4	310	KC2	C1B-NB	-2.66	1.34	1.37
38	Q	309	KC2	C1B-NB	-2.66	1.34	1.37
26	A	403	CLA	C4D-ND	-2.66	1.34	1.37
38	Q	309	KC2	C4A-C3A	2.66	1.49	1.44
28	5	617	WVN	C36-C32	-2.66	1.32	1.35
38	4	310	KC2	C1D-CHD	2.66	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	2	317	IHT	C18-C07	2.65	1.54	1.45
39	Q	319	II0	C40-C36	-2.65	1.32	1.35
26	6	604	CLA	C4D-ND	-2.65	1.34	1.37
28	S	613	WVN	C36-C32	-2.64	1.32	1.35
38	N	612	KC2	C1A-CHA	2.64	1.47	1.40
38	S	608	KC2	C4A-C3A	2.64	1.49	1.44
26	1	614	CLA	C4D-ND	-2.64	1.34	1.37
39	5	615	II0	C40-C36	-2.64	1.32	1.35
39	S	611	II0	C40-C36	-2.64	1.32	1.35
39	Q	314	II0	C40-C36	-2.64	1.32	1.35
38	N	605	KC2	C1D-CHD	2.63	1.48	1.41
39	6	613	II0	C40-C36	-2.63	1.32	1.35
38	5	610	KC2	C1D-CHD	2.63	1.48	1.41
38	R	311	KC2	C1D-CHD	2.63	1.48	1.41
39	R	318	II0	C40-C36	-2.62	1.32	1.35
26	S	604	CLA	C4D-ND	-2.62	1.34	1.37
38	Q	310	KC2	C3C-C4C	2.62	1.50	1.44
28	Z	101	WVN	C37-C34	-2.62	1.32	1.35
38	N	610	KC2	C1D-CHD	2.62	1.48	1.41
28	c	516	WVN	C02-C11	2.62	1.54	1.50
38	4	305	KC2	C1D-CHD	2.61	1.48	1.41
38	Q	304	KC2	C1D-CHD	2.61	1.48	1.41
39	4	316	II0	C40-C36	-2.61	1.32	1.35
38	N	605	KC2	C1B-NB	-2.61	1.34	1.37
39	6	611	II0	C40-C36	-2.60	1.32	1.35
27	A	404	PHO	CAC-C3C	-2.60	1.47	1.52
38	6	608	KC2	C1D-CHD	2.60	1.48	1.41
26	2	306	CLA	CMB-C2B	-2.60	1.46	1.51
39	P	614	II0	C40-C36	-2.60	1.32	1.35
39	R	316	II0	C40-C36	-2.60	1.32	1.35
38	6	608	KC2	C4A-C3A	2.60	1.49	1.44
39	Q	315	II0	C40-C36	-2.60	1.32	1.35
26	S	603	CLA	CMB-C2B	-2.60	1.46	1.51
38	P	605	KC2	C1B-NB	-2.60	1.34	1.37
38	N	610	KC2	C4A-C3A	2.59	1.49	1.44
28	d	410	WVN	C02-C11	2.59	1.54	1.50
39	4	320	II0	C40-C36	-2.59	1.32	1.35
38	S	608	KC2	C1D-CHD	2.58	1.48	1.41
26	6	603	CLA	CMB-C2B	-2.58	1.46	1.51
38	4	305	KC2	C1B-NB	-2.58	1.34	1.37
39	P	612	II0	C40-C36	-2.58	1.32	1.35
28	5	617	WVN	C26-C22	-2.57	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	611	CLA	CMB-C2B	-2.57	1.46	1.51
26	2	304	CLA	CMB-C2B	-2.57	1.46	1.51
26	O	606	CLA	CMB-C2B	-2.57	1.46	1.51
40	1	619	IHT	C19-C10	2.57	1.55	1.50
28	b	619	WVN	C20-C13	2.57	1.54	1.45
28	S	613	WVN	C26-C22	-2.57	1.32	1.35
38	4	311	KC2	C3C-C4C	2.56	1.50	1.44
38	O	610	KC2	C1B-NB	-2.56	1.34	1.37
26	b	604	CLA	CMB-C2B	-2.56	1.46	1.51
27	a	404	PHO	CAC-C3C	-2.55	1.47	1.52
38	3	304	KC2	C1B-NB	-2.55	1.34	1.37
26	1	603	CLA	CMB-C2B	-2.55	1.46	1.51
38	Q	304	KC2	C1B-NB	-2.55	1.34	1.37
38	N	611	KC2	C4A-C3A	2.54	1.49	1.44
26	c	508	CLA	CMB-C2B	-2.54	1.46	1.51
38	N	611	KC2	C1D-CHD	2.54	1.48	1.41
38	3	304	KC2	C3C-C4C	2.54	1.49	1.44
40	Q	317	IHT	C22-C23	2.54	1.51	1.45
26	P	604	CLA	C4D-ND	-2.54	1.34	1.37
28	c	518	WVN	C02-C11	2.53	1.54	1.50
40	4	318	IHT	C22-C23	2.53	1.51	1.45
38	O	610	KC2	C1D-CHD	2.53	1.48	1.41
40	N	619	IHT	C34-C35	2.53	1.51	1.45
38	6	608	KC2	C3C-C4C	2.53	1.49	1.44
27	D	405	PHO	CAC-C3C	-2.53	1.47	1.52
26	N	607	CLA	CMB-C2B	-2.53	1.46	1.51
26	O	604	CLA	CMB-C2B	-2.53	1.46	1.51
26	4	308	CLA	CMB-C2B	-2.53	1.46	1.51
40	N	619	IHT	C22-C23	2.52	1.51	1.45
38	Q	310	KC2	C1B-NB	-2.52	1.34	1.37
38	4	311	KC2	C1B-NB	-2.52	1.34	1.37
26	R	312	CLA	CMB-C2B	-2.52	1.46	1.51
26	R	308	CLA	CMB-C2B	-2.52	1.46	1.51
39	2	313	II0	C40-C36	-2.52	1.32	1.35
26	5	601	CLA	CMB-C2B	-2.51	1.46	1.51
27	d	403	PHO	CAC-C3C	-2.51	1.47	1.52
26	B	604	CLA	CMB-C2B	-2.51	1.46	1.51
26	5	607	CLA	CMB-C2B	-2.51	1.46	1.51
26	R	304	CLA	CMB-C2B	-2.51	1.46	1.51
38	P	605	KC2	C3C-C4C	2.51	1.49	1.44
38	4	311	KC2	C4A-C3A	2.51	1.49	1.44
38	N	611	KC2	C3C-C4C	2.50	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	503	CLA	CMB-C2B	-2.50	1.46	1.51
28	d	410	WVN	C28-C25	-2.50	1.32	1.35
28	5	617	WVN	C37-C34	-2.50	1.32	1.35
28	c	516	WVN	C20-C13	2.50	1.54	1.45
38	2	310	KC2	C1D-CHD	2.50	1.47	1.41
38	1	612	KC2	CHD-C4C	2.50	1.41	1.35
28	S	613	WVN	C37-C34	-2.50	1.32	1.35
28	d	410	WVN	C20-C13	2.50	1.54	1.45
26	1	604	CLA	CMB-C2B	-2.50	1.46	1.51
38	S	608	KC2	C3C-C4C	2.50	1.49	1.44
28	Z	101	WVN	C20-C13	2.50	1.54	1.45
26	5	603	CLA	CMB-C2B	-2.50	1.46	1.51
28	c	517	WVN	C02-C11	2.49	1.54	1.50
26	c	504	CLA	CMB-C2B	-2.49	1.46	1.51
26	Q	306	CLA	CMB-C2B	-2.49	1.46	1.51
28	D	412	WVN	C28-C25	-2.49	1.32	1.35
38	N	610	KC2	C3C-C4C	2.49	1.49	1.44
39	O	613	II0	C40-C36	-2.49	1.32	1.35
38	O	610	KC2	C4A-C3A	2.48	1.49	1.44
26	1	609	CLA	CMB-C2B	-2.48	1.46	1.51
28	b	617	WVN	C23-C25	2.48	1.51	1.45
26	P	609	CLA	CMB-C2B	-2.48	1.46	1.51
38	1	610	KC2	CHD-C4C	2.48	1.41	1.35
26	Q	307	CLA	CMB-C2B	-2.48	1.46	1.51
28	D	412	WVN	C20-C13	2.47	1.53	1.45
39	N	618	II0	C40-C36	-2.47	1.32	1.35
26	3	303	CLA	C4D-ND	-2.47	1.34	1.37
28	x	101	WVN	C02-C11	2.47	1.53	1.50
26	4	307	CLA	CMB-C2B	-2.47	1.46	1.51
38	2	310	KC2	C4A-C3A	2.47	1.49	1.44
26	R	302	CLA	CMB-C2B	-2.47	1.46	1.51
28	x	101	WVN	C20-C13	2.47	1.53	1.45
38	Q	309	KC2	C3C-C4C	2.47	1.49	1.44
38	4	310	KC2	C3C-C4C	2.46	1.49	1.44
39	N	616	II0	C40-C36	-2.46	1.32	1.35
26	G	401	CLA	CMB-C2B	-2.46	1.46	1.51
26	Q	308	CLA	CMB-C2B	-2.46	1.46	1.51
26	A	402	CLA	CMB-C2B	-2.46	1.46	1.51
40	R	317	IHT	C34-C35	2.46	1.51	1.45
26	C	507	CLA	CMB-C2B	-2.46	1.46	1.51
26	B	608	CLA	CMB-C2B	-2.46	1.46	1.51
28	B	619	WVN	C20-C13	2.46	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	601	CLA	CMB-C2B	-2.46	1.46	1.51
40	N	619	IHT	C22-C18	2.46	1.40	1.33
38	Q	310	KC2	C4A-C3A	2.45	1.49	1.44
26	C	509	CLA	CMB-C2B	-2.45	1.46	1.51
26	b	608	CLA	CMB-C2B	-2.45	1.46	1.51
26	2	301	CLA	CMB-C2B	-2.45	1.46	1.51
26	N	601	CLA	CMB-C2B	-2.45	1.46	1.51
26	Q	302	CLA	CMB-C2B	-2.45	1.46	1.51
26	B	606	CLA	CMB-C2B	-2.45	1.46	1.51
26	B	609	CLA	CMB-C2B	-2.45	1.46	1.51
28	Y	101	WVN	C20-C13	2.45	1.53	1.45
26	Q	305	CLA	CMB-C2B	-2.45	1.46	1.51
26	O	607	CLA	CMB-C2B	-2.45	1.46	1.51
26	B	613	CLA	CMB-C2B	-2.45	1.46	1.51
26	S	601	CLA	CMB-C2B	-2.45	1.46	1.51
38	5	610	KC2	C3C-C4C	2.44	1.49	1.44
38	R	311	KC2	C3C-C4C	2.44	1.49	1.44
26	1	607	CLA	CMB-C2B	-2.44	1.46	1.51
26	N	603	CLA	CMB-C2B	-2.44	1.46	1.51
38	O	610	KC2	C3C-C4C	2.44	1.49	1.44
28	a	406	WVN	C20-C13	2.44	1.53	1.45
26	B	603	CLA	CMB-C2B	-2.44	1.46	1.51
38	1	605	KC2	CHD-C4C	2.44	1.41	1.35
26	b	607	CLA	CMB-C2B	-2.44	1.46	1.51
28	k	101	WVN	C20-C13	2.44	1.53	1.45
26	B	602	CLA	CMB-C2B	-2.44	1.46	1.51
26	4	303	CLA	CMB-C2B	-2.44	1.46	1.51
26	G	402	CLA	CMB-C2B	-2.44	1.46	1.51
26	g	402	CLA	CMB-C2B	-2.44	1.46	1.51
26	3	307	CLA	CMB-C2B	-2.44	1.46	1.51
39	Q	316	II0	C40-C36	-2.43	1.32	1.35
26	C	513	CLA	CMB-C2B	-2.43	1.46	1.51
40	1	619	IHT	C20-C15	2.43	1.54	1.50
26	g	401	CLA	CMB-C2B	-2.43	1.46	1.51
26	5	612	CLA	CMB-C2B	-2.43	1.46	1.51
26	b	610	CLA	CMB-C2B	-2.43	1.46	1.51
26	O	601	CLA	CMB-C2B	-2.43	1.46	1.51
26	d	402	CLA	CMB-C2B	-2.43	1.46	1.51
39	4	317	II0	C40-C36	-2.43	1.32	1.35
26	4	309	CLA	CMB-C2B	-2.43	1.46	1.51
26	P	603	CLA	CMB-C2B	-2.43	1.46	1.51
26	c	510	CLA	CMB-C2B	-2.43	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	517	WVN	C20-C13	2.43	1.53	1.45
26	N	609	CLA	CMB-C2B	-2.43	1.46	1.51
26	4	306	CLA	CMB-C2B	-2.43	1.46	1.51
26	a	402	CLA	CMB-C2B	-2.43	1.46	1.51
26	R	305	CLA	CMB-C2B	-2.43	1.46	1.51
26	2	305	CLA	C1D-C2D	2.42	1.50	1.45
26	5	604	CLA	CMB-C2B	-2.42	1.46	1.51
28	C	515	WVN	C20-C13	2.42	1.53	1.45
26	R	313	CLA	CMB-C2B	-2.42	1.46	1.51
26	b	609	CLA	CMB-C2B	-2.42	1.46	1.51
39	1	616	II0	C20-C14	2.42	1.54	1.50
26	b	601	CLA	CMB-C2B	-2.42	1.46	1.51
40	4	318	IHT	C22-C18	2.42	1.40	1.33
26	3	302	CLA	CMB-C2B	-2.42	1.46	1.51
38	1	611	KC2	CHD-C4C	2.42	1.41	1.35
26	Q	301	CLA	CMB-C2B	-2.41	1.46	1.51
26	c	513	CLA	CMB-C2B	-2.41	1.46	1.51
26	2	303	CLA	CMB-C2B	-2.41	1.46	1.51
28	5	617	WVN	C20-C13	2.41	1.53	1.45
38	2	310	KC2	C3C-C4C	2.41	1.49	1.44
26	2	307	CLA	CMB-C2B	-2.41	1.46	1.51
28	S	613	WVN	C20-C13	2.41	1.53	1.45
39	1	617	II0	C19-C13	2.41	1.54	1.50
26	C	506	CLA	CMB-C2B	-2.41	1.46	1.51
26	b	606	CLA	CMB-C2B	-2.40	1.46	1.51
40	R	317	IHT	C22-C18	2.40	1.40	1.33
40	5	616	IHT	C34-C35	2.40	1.51	1.45
26	2	319	CLA	CMB-C2B	-2.40	1.46	1.51
38	N	605	KC2	C3C-C4C	2.40	1.49	1.44
26	B	601	CLA	CMB-C2B	-2.40	1.46	1.51
26	5	609	CLA	CMB-C2B	-2.40	1.46	1.51
26	O	603	CLA	CMB-C2B	-2.40	1.46	1.51
26	C	512	CLA	CMB-C2B	-2.40	1.46	1.51
40	5	616	IHT	C22-C18	2.39	1.40	1.33
26	b	613	CLA	CMB-C2B	-2.39	1.46	1.51
40	Q	317	IHT	C22-C18	2.39	1.40	1.33
26	c	507	CLA	CMB-C2B	-2.39	1.46	1.51
26	b	612	CLA	CMB-C2B	-2.39	1.46	1.51
26	S	607	CLA	CMB-C2B	-2.39	1.46	1.51
26	A	405	CLA	CMB-C2B	-2.39	1.46	1.51
26	c	514	CLA	CMB-C2B	-2.39	1.46	1.51
26	R	310	CLA	CMB-C2B	-2.39	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S	602	CLA	CMB-C2B	-2.39	1.46	1.51
26	D	407	CLA	CMB-C2B	-2.39	1.46	1.51
26	1	601	CLA	CMB-C2B	-2.39	1.46	1.51
26	d	405	CLA	CMD-C2D	-2.39	1.45	1.50
26	b	603	CLA	CMB-C2B	-2.39	1.46	1.51
28	B	619	WVN	C02-C11	2.38	1.53	1.50
26	c	515	CLA	CMB-C2B	-2.38	1.46	1.51
26	a	405	CLA	CMB-C2B	-2.38	1.46	1.51
26	1	602	CLA	CMB-C2B	-2.38	1.46	1.51
26	2	302	CLA	CMB-C2B	-2.38	1.46	1.51
26	1	608	CLA	CMB-C2B	-2.38	1.46	1.51
26	C	502	CLA	CMB-C2B	-2.38	1.46	1.51
26	N	606	CLA	CMB-C2B	-2.38	1.46	1.51
26	6	602	CLA	CMB-C2B	-2.38	1.46	1.51
38	Q	309	KC2	C1A-CHA	2.37	1.46	1.40
26	O	605	CLA	CMB-C2B	-2.37	1.46	1.51
26	B	611	CLA	CMB-C2B	-2.37	1.46	1.51
26	b	615	CLA	CMB-C2B	-2.37	1.46	1.51
28	b	618	WVN	C20-C13	2.37	1.53	1.45
38	N	610	KC2	C1A-CHA	2.37	1.46	1.40
38	4	305	KC2	C3C-C4C	2.37	1.49	1.44
26	6	607	CLA	CMB-C2B	-2.37	1.46	1.51
38	3	304	KC2	C1A-CHA	2.37	1.46	1.40
26	b	602	CLA	CMB-C2B	-2.37	1.46	1.51
26	5	605	CLA	CMB-C2B	-2.37	1.46	1.51
26	c	506	CLA	CMB-C2B	-2.37	1.46	1.51
38	1	612	KC2	MG-NA	2.36	2.11	2.06
26	c	505	CLA	CMB-C2B	-2.36	1.46	1.51
38	Q	304	KC2	C3C-C4C	2.36	1.49	1.44
26	B	610	CLA	CMB-C2B	-2.36	1.46	1.51
26	1	613	CLA	CMB-C2B	-2.36	1.46	1.51
26	2	305	CLA	CHD-C4C	2.36	1.44	1.39
26	A	403	CLA	CMB-C2B	-2.36	1.46	1.51
38	4	310	KC2	C1A-CHA	2.36	1.46	1.40
26	c	509	CLA	CMB-C2B	-2.36	1.46	1.51
26	P	608	CLA	CMB-C2B	-2.36	1.46	1.51
40	O	616	IHT	C22-C18	2.36	1.40	1.33
26	4	301	CLA	CMB-C2B	-2.36	1.46	1.51
26	P	601	CLA	CMB-C2B	-2.36	1.46	1.51
26	R	306	CLA	CMB-C2B	-2.36	1.46	1.51
39	6	612	II0	C39-C35	-2.36	1.32	1.35
26	C	504	CLA	CMB-C2B	-2.36	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S	606	CLA	CMB-C2B	-2.35	1.46	1.51
38	N	612	KC2	C1B-NB	-2.35	1.34	1.37
28	A	406	WVN	C20-C13	2.35	1.53	1.45
26	B	605	CLA	CMB-C2B	-2.35	1.46	1.51
26	N	613	CLA	CMB-C2B	-2.35	1.46	1.51
26	4	302	CLA	CMB-C2B	-2.35	1.46	1.51
26	O	609	CLA	CMB-C2B	-2.35	1.46	1.51
26	c	512	CLA	CMB-C2B	-2.35	1.46	1.51
26	d	405	CLA	CMB-C2B	-2.35	1.46	1.51
26	P	610	CLA	CMB-C2B	-2.34	1.46	1.51
26	R	307	CLA	CMB-C2B	-2.34	1.46	1.51
39	3	310	II0	C20-C14	2.34	1.54	1.50
26	6	606	CLA	CMB-C2B	-2.34	1.46	1.51
26	b	605	CLA	CMB-C2B	-2.34	1.46	1.51
26	2	306	CLA	C3B-C2B	-2.34	1.37	1.40
39	1	615	II0	C19-C13	2.34	1.54	1.50
26	4	313	CLA	CMB-C2B	-2.34	1.46	1.51
26	N	602	CLA	CMB-C2B	-2.34	1.46	1.51
40	R	317	IHT	C22-C23	2.34	1.51	1.45
26	D	404	CLA	CMB-C2B	-2.34	1.46	1.51
26	1	614	CLA	C3B-C2B	-2.34	1.37	1.40
26	O	602	CLA	CMB-C2B	-2.33	1.46	1.51
26	N	614	CLA	CMB-C2B	-2.33	1.46	1.51
38	4	305	KC2	C1A-CHA	2.33	1.46	1.40
26	5	608	CLA	CMB-C2B	-2.33	1.46	1.51
39	O	615	II0	C20-C14	2.33	1.54	1.50
26	3	301	CLA	CMB-C2B	-2.33	1.46	1.51
26	5	606	CLA	CMB-C2B	-2.33	1.46	1.51
26	B	616	CLA	CMB-C2B	-2.33	1.46	1.51
26	1	606	CLA	CMB-C2B	-2.33	1.46	1.51
26	c	503	CLA	CMB-C2B	-2.33	1.46	1.51
26	c	511	CLA	CMB-C2B	-2.33	1.46	1.51
38	P	605	KC2	C1A-CHA	2.33	1.46	1.40
26	B	614	CLA	CMB-C2B	-2.33	1.46	1.51
26	Q	312	CLA	CMB-C2B	-2.33	1.46	1.51
26	B	615	CLA	CMB-C2B	-2.32	1.46	1.51
26	b	614	CLA	CMB-C2B	-2.32	1.46	1.51
26	4	304	CLA	CMB-C2B	-2.32	1.46	1.51
38	Q	304	KC2	C1A-CHA	2.32	1.46	1.40
26	O	606	CLA	C3B-C2B	-2.32	1.37	1.40
39	3	312	II0	C20-C14	2.32	1.54	1.50
26	S	605	CLA	CMB-C2B	-2.32	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	N	604	CLA	CMB-C2B	-2.32	1.46	1.51
39	S	612	II0	C39-C35	-2.32	1.32	1.35
39	N	615	II0	C39-C35	-2.32	1.32	1.35
28	c	518	WVN	C20-C13	2.32	1.53	1.45
26	d	406	CLA	CMB-C2B	-2.32	1.46	1.51
28	b	618	WVN	C02-C11	2.32	1.53	1.50
38	R	311	KC2	C1A-CHA	2.31	1.46	1.40
26	b	611	CLA	CMB-C2B	-2.31	1.46	1.51
40	5	616	IHT	C22-C23	2.31	1.50	1.45
26	Q	303	CLA	CMB-C2B	-2.31	1.46	1.51
38	5	610	KC2	C1A-CHA	2.31	1.46	1.40
26	4	307	CLA	C3B-C2B	-2.31	1.37	1.40
26	Q	306	CLA	C3B-C2B	-2.31	1.37	1.40
26	C	505	CLA	CMB-C2B	-2.31	1.46	1.51
26	R	309	CLA	CMB-C2B	-2.31	1.46	1.51
26	D	407	CLA	CMD-C2D	-2.31	1.45	1.50
39	2	316	II0	C11-C13	2.31	1.54	1.51
40	2	317	IHT	C20-C15	2.31	1.54	1.50
39	6	613	II0	C39-C35	-2.30	1.32	1.35
26	6	605	CLA	CMB-C2B	-2.30	1.46	1.51
40	2	317	IHT	C19-C10	2.30	1.54	1.50
26	O	608	CLA	CMB-C2B	-2.30	1.46	1.51
26	C	510	CLA	CMB-C2B	-2.30	1.46	1.51
39	6	611	II0	C39-C35	-2.30	1.32	1.35
26	a	403	CLA	CMB-C2B	-2.30	1.46	1.51
26	O	612	CLA	CMB-C2B	-2.30	1.46	1.51
39	1	618	II0	C19-C13	2.30	1.54	1.50
26	B	607	CLA	CMB-C2B	-2.30	1.46	1.51
26	5	607	CLA	C3B-C2B	-2.30	1.37	1.40
26	2	305	CLA	C3D-C2D	2.30	1.45	1.39
39	2	314	II0	C39-C35	-2.30	1.32	1.35
26	b	616	CLA	CMB-C2B	-2.29	1.46	1.51
26	1	614	CLA	CMB-C2B	-2.29	1.46	1.51
26	C	508	CLA	CMB-C2B	-2.29	1.46	1.51
39	1	616	II0	C19-C13	2.29	1.54	1.50
39	O	614	II0	C39-C35	-2.29	1.32	1.35
26	C	514	CLA	CMB-C2B	-2.29	1.46	1.51
26	D	408	CLA	CMB-C2B	-2.29	1.46	1.51
26	P	602	CLA	CMB-C2B	-2.29	1.46	1.51
26	B	612	CLA	CMB-C2B	-2.28	1.46	1.51
26	S	610	CLA	CMD-C2D	-2.28	1.46	1.50
26	N	607	CLA	C3B-C2B	-2.28	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	2	316	II0	C20-C14	2.28	1.54	1.50
26	O	611	CLA	CMB-C2B	-2.28	1.46	1.51
39	O	613	II0	C39-C35	-2.28	1.32	1.35
26	P	607	CLA	CMB-C2B	-2.28	1.46	1.51
26	C	511	CLA	CMB-C2B	-2.28	1.46	1.51
28	P	615	WVN	C20-C13	2.28	1.53	1.45
39	R	318	II0	C39-C35	-2.28	1.32	1.35
26	2	308	CLA	CMB-C2B	-2.28	1.46	1.51
26	2	312	CLA	CMB-C2B	-2.27	1.46	1.51
28	3	313	WVN	C02-C11	2.27	1.53	1.50
26	2	311	CLA	CMB-C2B	-2.27	1.46	1.51
26	a	403	CLA	CMD-C2D	-2.27	1.46	1.50
26	3	306	CLA	CMB-C2B	-2.27	1.46	1.51
28	b	619	WVN	C02-C11	2.27	1.53	1.50
26	6	610	CLA	CMD-C2D	-2.27	1.46	1.50
39	O	615	II0	C11-C13	2.27	1.54	1.51
26	6	610	CLA	CMB-C2B	-2.26	1.46	1.51
39	Q	316	II0	C29-C25	-2.26	1.32	1.37
26	N	608	CLA	C1D-C2D	-2.26	1.40	1.45
26	2	309	CLA	CMB-C2B	-2.26	1.46	1.51
26	R	303	CLA	CMB-C2B	-2.26	1.46	1.51
26	P	606	CLA	CMB-C2B	-2.26	1.46	1.51
26	N	608	CLA	MG-NA	2.25	2.11	2.06
40	5	616	IHT	C05-C08	2.25	1.55	1.52
26	S	609	CLA	CMB-C2B	-2.25	1.47	1.51
39	4	317	II0	C29-C25	-2.25	1.32	1.37
39	S	611	II0	C39-C35	-2.25	1.32	1.35
39	2	313	II0	C39-C35	-2.24	1.32	1.35
39	P	612	II0	C39-C35	-2.24	1.32	1.35
38	Q	310	KC2	C1A-CHA	2.24	1.46	1.40
26	4	312	CLA	CMB-C2B	-2.24	1.47	1.51
39	Q	316	II0	C30-C26	2.24	1.41	1.37
38	4	311	KC2	C1A-CHA	2.24	1.46	1.40
39	1	615	II0	C20-C14	2.24	1.54	1.50
26	S	610	CLA	CMB-C2B	-2.24	1.47	1.51
26	3	308	CLA	C1C-NC	2.23	1.41	1.37
26	Q	311	CLA	CMB-C2B	-2.23	1.47	1.51
26	6	609	CLA	CMB-C2B	-2.23	1.47	1.51
39	1	617	II0	C20-C14	2.23	1.54	1.50
26	5	602	CLA	CMB-C2B	-2.23	1.47	1.51
26	1	607	CLA	CMD-C2D	-2.23	1.46	1.50
38	O	610	KC2	C1A-CHA	2.23	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	3	305	CLA	CMB-C2B	-2.22	1.47	1.51
38	6	608	KC2	C1A-CHA	2.22	1.46	1.40
26	R	308	CLA	C3B-C2B	-2.22	1.37	1.40
28	b	617	WVN	C02-C11	2.22	1.53	1.50
26	c	507	CLA	CMD-C2D	-2.22	1.46	1.50
39	R	315	II0	C39-C35	-2.22	1.32	1.35
26	P	604	CLA	CMB-C2B	-2.22	1.47	1.51
26	N	608	CLA	C1D-ND	-2.21	1.35	1.37
38	2	310	KC2	C1A-CHA	2.21	1.46	1.40
28	A	406	WVN	C02-C11	2.21	1.53	1.50
40	Q	317	IHT	C05-C08	2.21	1.55	1.52
39	R	316	II0	C39-C35	-2.21	1.32	1.35
39	4	315	II0	C39-C35	-2.21	1.32	1.35
38	1	610	KC2	C1B-NB	-2.21	1.35	1.37
39	Q	319	II0	C39-C35	-2.21	1.32	1.35
40	R	317	IHT	C05-C08	2.20	1.55	1.52
39	N	620	II0	C39-C35	-2.20	1.32	1.35
39	2	315	II0	C39-C35	-2.20	1.32	1.35
38	S	608	KC2	C1A-CHA	2.20	1.46	1.40
26	2	311	CLA	CMD-C2D	-2.20	1.46	1.50
37	f	101	HEM	C1D-ND	-2.20	1.34	1.38
26	N	608	CLA	C4B-NB	2.20	1.37	1.35
26	3	303	CLA	CMB-C2B	-2.19	1.47	1.51
40	N	619	IHT	C36-C33	2.19	1.55	1.50
26	C	506	CLA	CMD-C2D	-2.19	1.46	1.50
29	A	407	PL9	C53-C6	-2.19	1.46	1.50
39	1	618	II0	C20-C14	2.19	1.54	1.50
26	O	611	CLA	CMD-C2D	-2.19	1.46	1.50
39	Q	316	II0	C14-C10	-2.19	1.32	1.34
26	A	403	CLA	CMD-C2D	-2.19	1.46	1.50
39	4	317	II0	C30-C26	2.19	1.41	1.37
39	4	316	II0	C39-C35	-2.19	1.32	1.35
40	4	318	IHT	C05-C08	2.18	1.55	1.52
26	a	402	CLA	C3B-C2B	-2.18	1.37	1.40
39	5	613	II0	C39-C35	-2.18	1.32	1.35
39	5	615	II0	C39-C35	-2.18	1.32	1.35
26	P	611	CLA	CMB-C2B	-2.18	1.47	1.51
26	N	607	CLA	CMD-C2D	-2.18	1.46	1.50
27	d	403	PHO	CMC-C2C	-2.17	1.46	1.51
26	b	604	CLA	CMD-C2D	-2.17	1.46	1.50
39	5	614	II0	C39-C35	-2.17	1.32	1.35
26	B	612	CLA	CMD-C2D	-2.17	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C	515	WVN	C02-C11	2.17	1.53	1.50
26	a	402	CLA	CMD-C2D	-2.17	1.46	1.50
39	R	314	II0	C39-C35	-2.16	1.32	1.35
39	4	316	II0	C30-C26	2.16	1.41	1.37
39	N	616	II0	C39-C35	-2.16	1.32	1.35
39	Q	315	II0	C30-C26	2.16	1.41	1.37
38	N	611	KC2	C1A-CHA	2.16	1.46	1.40
26	S	604	CLA	CMB-C2B	-2.15	1.47	1.51
26	1	606	CLA	CMD-C2D	-2.15	1.46	1.50
26	3	308	CLA	C4B-NB	2.15	1.37	1.35
27	D	405	PHO	CMD-C2D	-2.15	1.46	1.51
39	4	317	II0	C14-C10	-2.15	1.32	1.34
39	4	320	II0	C39-C35	-2.15	1.32	1.35
39	P	613	II0	C20-C14	2.15	1.54	1.50
26	3	309	CLA	CMD-C2D	-2.15	1.46	1.50
28	P	615	WVN	C02-C11	2.15	1.53	1.50
26	6	604	CLA	CMB-C2B	-2.15	1.47	1.51
39	R	316	II0	C30-C26	2.15	1.41	1.37
39	P	614	II0	C30-C26	2.15	1.41	1.37
40	O	616	IHT	C36-C33	2.14	1.55	1.50
39	Q	313	II0	C39-C35	-2.14	1.32	1.35
26	1	614	CLA	CMD-C2D	-2.14	1.46	1.50
39	4	314	II0	C39-C35	-2.14	1.32	1.35
26	R	313	CLA	CMD-C2D	-2.14	1.46	1.50
28	b	617	WVN	C20-C13	2.14	1.52	1.45
26	3	309	CLA	CMB-C2B	-2.14	1.47	1.51
40	O	616	IHT	C30-C27	2.14	1.50	1.43
26	1	607	CLA	C3C-C2C	2.14	1.41	1.36
29	d	407	PL9	C6-C1	-2.14	1.44	1.48
39	2	313	II0	C30-C26	2.13	1.41	1.37
38	N	605	KC2	C1A-CHA	2.13	1.46	1.40
29	a	407	PL9	C53-C6	-2.13	1.46	1.50
26	5	612	CLA	CMD-C2D	-2.13	1.46	1.50
26	B	616	CLA	CMC-C2C	-2.13	1.46	1.50
28	B	618	WVN	C21-C15	2.13	1.54	1.50
39	P	614	II0	C39-C35	-2.13	1.33	1.35
39	3	311	II0	C20-C14	2.13	1.54	1.50
39	Q	314	II0	C39-C35	-2.13	1.33	1.35
26	A	402	CLA	C3B-C2B	-2.13	1.37	1.40
27	a	404	PHO	CMC-C2C	-2.12	1.46	1.51
26	c	511	CLA	CMD-C2D	-2.12	1.46	1.50
26	4	308	CLA	CMD-C2D	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	603	CLA	CMD-C2D	-2.12	1.46	1.50
27	d	403	PHO	CMD-C2D	-2.12	1.46	1.51
39	Q	315	II0	C39-C35	-2.12	1.33	1.35
39	1	617	II0	C11-C13	2.12	1.54	1.51
26	b	612	CLA	CMD-C2D	-2.12	1.46	1.50
39	N	620	II0	C30-C26	2.12	1.41	1.37
29	D	409	PL9	C6-C1	-2.11	1.44	1.48
39	5	615	II0	C30-C26	2.11	1.41	1.37
26	P	611	CLA	CMD-C2D	-2.11	1.46	1.50
39	N	618	II0	C30-C26	2.11	1.41	1.37
39	3	310	II0	C19-C13	2.11	1.54	1.50
39	5	613	II0	C30-C26	2.11	1.41	1.37
26	Q	307	CLA	CMD-C2D	-2.11	1.46	1.50
26	b	603	CLA	CMD-C2D	-2.11	1.46	1.50
38	1	611	KC2	MG-NA	2.11	2.11	2.06
40	Q	317	IHT	C36-C33	2.11	1.55	1.50
39	O	613	II0	C30-C26	2.10	1.41	1.37
26	P	601	CLA	CMD-C2D	-2.10	1.46	1.50
26	2	305	CLA	C4D-ND	2.10	1.40	1.37
39	S	611	II0	C30-C26	2.10	1.41	1.37
26	R	304	CLA	CMD-C2D	-2.10	1.46	1.50
39	N	617	II0	C30-C26	2.10	1.41	1.37
39	1	618	II0	C12-C14	2.10	1.54	1.51
26	c	504	CLA	CMD-C2D	-2.10	1.46	1.50
26	b	616	CLA	CMC-C2C	-2.09	1.46	1.50
38	1	611	KC2	C1B-NB	-2.09	1.35	1.37
39	2	315	II0	C30-C26	2.09	1.41	1.37
26	3	308	CLA	C1D-ND	-2.09	1.35	1.37
39	R	314	II0	C30-C26	2.09	1.41	1.37
38	1	612	KC2	C1A-CHA	2.09	1.46	1.40
26	C	503	CLA	CMD-C2D	-2.09	1.46	1.50
39	1	615	II0	C12-C14	2.09	1.54	1.51
39	6	611	II0	C30-C26	2.09	1.41	1.37
26	5	603	CLA	CMD-C2D	-2.09	1.46	1.50
39	S	612	II0	C30-C26	2.09	1.41	1.37
39	N	616	II0	C30-C26	2.09	1.41	1.37
40	4	318	IHT	C36-C33	2.09	1.55	1.50
26	2	319	CLA	CMD-C2D	-2.09	1.46	1.50
39	6	612	II0	C30-C26	2.08	1.41	1.37
26	G	401	CLA	CMD-C2D	-2.08	1.46	1.50
26	P	610	CLA	CMD-C2D	-2.08	1.46	1.50
26	N	608	CLA	MG-NC	2.08	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	N	620	II0	C29-C25	-2.08	1.32	1.37
26	5	606	CLA	CMD-C2D	-2.08	1.46	1.50
26	c	504	CLA	CMC-C2C	-2.08	1.46	1.50
39	3	311	II0	C19-C13	2.07	1.54	1.50
26	c	512	CLA	CMD-C2D	-2.07	1.46	1.50
26	2	309	CLA	CMC-C2C	-2.07	1.46	1.50
26	A	402	CLA	CMD-C2D	-2.07	1.46	1.50
26	B	604	CLA	CMD-C2D	-2.07	1.46	1.50
39	Q	313	II0	C30-C26	2.07	1.41	1.37
27	a	404	PHO	CMB-C2B	-2.07	1.46	1.51
26	O	612	CLA	CMD-C2D	-2.07	1.46	1.50
37	F	101	HEM	C1D-ND	-2.07	1.34	1.38
28	3	313	WVN	C16-C05	2.07	1.54	1.50
26	B	613	CLA	C3B-C2B	-2.07	1.37	1.40
38	1	605	KC2	C1A-CHA	2.07	1.46	1.40
38	1	605	KC2	MG-NA	2.06	2.11	2.06
39	4	314	II0	C30-C26	2.06	1.41	1.37
26	5	607	CLA	CMC-C2C	-2.06	1.46	1.50
26	S	605	CLA	CMD-C2D	-2.06	1.46	1.50
26	C	511	CLA	CMD-C2D	-2.06	1.46	1.50
26	Q	312	CLA	CMD-C2D	-2.06	1.46	1.50
37	f	101	HEM	CHB-C1B	2.06	1.40	1.35
38	Q	310	KC2	C1D-ND	2.06	1.37	1.35
26	N	613	CLA	C3D-C4D	2.06	1.48	1.44
37	F	101	HEM	C4B-NB	-2.06	1.34	1.38
26	P	604	CLA	CMD-C2D	-2.06	1.46	1.50
39	O	615	II0	C19-C13	2.05	1.54	1.50
26	R	303	CLA	CMC-C2C	-2.05	1.46	1.50
26	4	312	CLA	CMD-C2D	-2.05	1.46	1.50
40	N	619	IHT	C30-C27	2.05	1.49	1.43
27	D	405	PHO	CMC-C2C	-2.05	1.46	1.51
26	c	503	CLA	CMD-C2D	-2.05	1.46	1.50
39	S	612	II0	C29-C25	-2.05	1.32	1.37
26	S	604	CLA	CMD-C2D	-2.05	1.46	1.50
26	R	308	CLA	CMD-C2D	-2.05	1.46	1.50
38	1	611	KC2	C1A-CHA	2.05	1.46	1.40
26	1	602	CLA	CMD-C2D	-2.05	1.46	1.50
39	6	612	II0	C29-C25	-2.05	1.32	1.37
38	4	311	KC2	C1D-ND	2.04	1.37	1.35
26	6	605	CLA	CMD-C2D	-2.04	1.46	1.50
26	6	604	CLA	CMD-C2D	-2.04	1.46	1.50
39	N	618	II0	C29-C25	-2.04	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	3	302	CLA	CMD-C2D	-2.04	1.46	1.50
26	A	402	CLA	C3B-CAB	-2.04	1.43	1.47
26	P	603	CLA	CMD-C2D	-2.04	1.46	1.50
39	O	613	II0	C29-C25	-2.04	1.32	1.37
26	5	607	CLA	CMD-C2D	-2.04	1.46	1.50
26	R	307	CLA	CMD-C2D	-2.04	1.46	1.50
39	3	311	II0	C11-C13	2.04	1.54	1.51
39	P	613	II0	C11-C13	2.04	1.54	1.51
26	C	514	CLA	CMD-C2D	-2.04	1.46	1.50
26	1	608	CLA	CMD-C2D	-2.04	1.46	1.50
39	2	316	II0	C19-C13	2.04	1.54	1.50
39	P	613	II0	C19-C13	2.04	1.54	1.50
26	a	405	CLA	CMD-C2D	-2.04	1.46	1.50
26	2	303	CLA	CMD-C2D	-2.04	1.46	1.50
26	5	602	CLA	CMC-C2C	-2.04	1.46	1.50
27	A	404	PHO	CMD-C2D	-2.04	1.46	1.51
26	B	612	CLA	C3D-C4D	2.04	1.48	1.44
28	C	516	WVN	C16-C05	2.04	1.54	1.50
26	R	308	CLA	CMC-C2C	-2.04	1.46	1.50
26	c	509	CLA	CMD-C2D	-2.04	1.46	1.50
26	g	402	CLA	CMD-C2D	-2.04	1.46	1.50
26	S	609	CLA	CMD-C2D	-2.03	1.46	1.50
39	R	315	II0	C30-C26	2.03	1.41	1.37
26	C	513	CLA	CMD-C2D	-2.03	1.46	1.50
26	3	303	CLA	CMD-C2D	-2.03	1.46	1.50
38	1	610	KC2	C1A-CHA	2.03	1.46	1.40
26	2	303	CLA	CMC-C2C	-2.03	1.46	1.50
26	4	313	CLA	CMD-C2D	-2.03	1.46	1.50
26	R	308	CLA	C3B-CAB	-2.03	1.43	1.47
26	6	603	CLA	CMD-C2D	-2.03	1.46	1.50
26	2	312	CLA	CMD-C2D	-2.03	1.46	1.50
26	C	503	CLA	CMC-C2C	-2.03	1.46	1.50
26	b	611	CLA	CMD-C2D	-2.03	1.46	1.50
39	Q	314	II0	C29-C25	-2.03	1.32	1.37
39	4	315	II0	C30-C26	2.03	1.41	1.37
28	C	516	WVN	C21-C15	2.03	1.54	1.50
40	1	619	IHT	C12-C15	2.03	1.54	1.51
26	5	607	CLA	C3B-CAB	-2.03	1.43	1.47
26	Q	311	CLA	CMD-C2D	-2.02	1.46	1.50
26	B	615	CLA	CMD-C2D	-2.02	1.46	1.50
39	2	313	II0	C29-C25	-2.02	1.32	1.37
40	Q	317	IHT	C30-C27	2.02	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	614	CLA	CMD-C2D	-2.02	1.46	1.50
39	Q	314	II0	C30-C26	2.02	1.41	1.37
26	S	603	CLA	CMD-C2D	-2.02	1.46	1.50
37	f	101	HEM	C4B-NB	-2.02	1.34	1.38
26	O	609	CLA	CMC-C2C	-2.02	1.46	1.50
26	R	303	CLA	CMD-C2D	-2.02	1.46	1.50
26	6	609	CLA	CMD-C2D	-2.02	1.46	1.50
26	G	402	CLA	CMD-C2D	-2.02	1.46	1.50
40	R	317	IHT	C36-C33	2.02	1.55	1.50
38	2	310	KC2	C1D-ND	2.02	1.37	1.35
26	5	611	CLA	CMD-C2D	-2.02	1.46	1.50
29	D	409	PL9	C53-C6	-2.01	1.46	1.50
26	b	612	CLA	C3D-C4D	2.01	1.48	1.44
26	B	605	CLA	CMD-C2D	-2.01	1.46	1.50
39	N	618	II0	C39-C35	-2.01	1.33	1.35
26	B	602	CLA	CMD-C2D	-2.01	1.46	1.50
26	1	604	CLA	CMD-C2D	-2.01	1.46	1.50
26	6	601	CLA	C3B-C2B	-2.01	1.37	1.40
26	S	601	CLA	C3B-C2B	-2.01	1.37	1.40
27	a	404	PHO	CMD-C2D	-2.01	1.46	1.51
26	N	603	CLA	CMD-C2D	-2.01	1.46	1.50
26	N	609	CLA	CMC-C2C	-2.01	1.46	1.50
26	6	603	CLA	CMC-C2C	-2.01	1.46	1.50
39	P	612	II0	C30-C26	2.01	1.41	1.37
26	1	609	CLA	CMD-C2D	-2.01	1.46	1.50
26	R	305	CLA	CMD-C2D	-2.01	1.46	1.50
26	N	604	CLA	CMD-C2D	-2.01	1.46	1.50
26	R	310	CLA	CMD-C2D	-2.01	1.46	1.50
26	Q	302	CLA	C3D-C4D	2.01	1.48	1.44
39	5	614	II0	C30-C26	2.01	1.41	1.37
26	c	514	CLA	CMD-C2D	-2.01	1.46	1.50
26	C	510	CLA	CMD-C2D	-2.01	1.46	1.50
39	2	315	II0	C29-C25	-2.01	1.32	1.37
26	R	312	CLA	CMD-C2D	-2.01	1.46	1.50
26	C	507	CLA	CMD-C2D	-2.01	1.46	1.50
26	1	614	CLA	CMC-C2C	-2.01	1.46	1.50
26	O	605	CLA	CMD-C2D	-2.01	1.46	1.50
40	4	318	IHT	C30-C27	2.01	1.49	1.43
39	2	314	II0	C14-C10	-2.01	1.32	1.34
26	b	613	CLA	C3B-C2B	-2.01	1.37	1.40
26	2	307	CLA	C3B-C2B	-2.00	1.37	1.40
40	5	616	IHT	C36-C33	2.00	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	505	CLA	CMD-C2D	-2.00	1.46	1.50
27	d	403	PHO	CMB-C2B	-2.00	1.46	1.51
26	1	601	CLA	CMD-C2D	-2.00	1.46	1.50
26	1	603	CLA	CMD-C2D	-2.00	1.46	1.50
26	O	607	CLA	C3B-C2B	-2.00	1.37	1.40
26	5	609	CLA	CMD-C2D	-2.00	1.46	1.50
40	O	616	IHT	C05-C08	2.00	1.55	1.52
26	4	306	CLA	CMD-C2D	-2.00	1.46	1.50
27	A	404	PHO	CMC-C2C	-2.00	1.46	1.51
26	C	509	CLA	CMD-C2D	-2.00	1.46	1.50

All (3792) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	617	WVN	C20-C23-C25	-27.60	84.52	126.23
28	B	618	WVN	C20-C23-C25	-26.81	85.73	126.23
28	C	516	WVN	C20-C23-C25	-26.79	85.76	126.23
39	3	312	II0	C24-C22-C10	-25.49	110.88	175.43
39	3	310	II0	C23-C21-C09	-25.28	111.43	175.43
39	1	616	II0	C24-C22-C10	-25.05	112.01	175.43
39	1	617	II0	C23-C21-C09	-24.93	112.31	175.43
39	1	615	II0	C23-C21-C09	-24.91	112.36	175.43
39	1	618	II0	C23-C21-C09	-24.89	112.40	175.43
39	1	616	II0	C23-C21-C09	-24.87	112.46	175.43
28	H	101	WVN	C20-C23-C25	-24.69	88.93	126.23
40	2	317	IHT	C24-C21-C11	-24.41	113.61	175.43
39	1	617	II0	C24-C22-C10	-24.40	113.64	175.43
40	1	619	IHT	C24-C21-C11	-24.39	113.66	175.43
39	3	311	II0	C24-C22-C10	-24.33	113.83	175.43
39	P	613	II0	C24-C22-C10	-24.33	113.83	175.43
39	O	615	II0	C23-C21-C09	-24.31	113.89	175.43
39	2	316	II0	C23-C21-C09	-24.29	113.92	175.43
39	3	312	II0	C23-C21-C09	-24.23	114.07	175.43
39	1	615	II0	C24-C22-C10	-24.09	114.44	175.43
39	3	310	II0	C24-C22-C10	-23.92	114.87	175.43
28	3	313	WVN	C20-C23-C25	-23.82	90.24	126.23
39	3	311	II0	C23-C21-C09	-23.72	115.38	175.43
39	P	613	II0	C23-C21-C09	-23.71	115.39	175.43
39	O	615	II0	C24-C22-C10	-23.51	115.90	175.43
39	2	316	II0	C24-C22-C10	-23.48	115.99	175.43
39	1	618	II0	C24-C22-C10	-22.46	118.55	175.43
40	1	619	IHT	C18-C22-C23	17.46	152.61	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	2	317	IHT	C18-C22-C23	16.72	151.50	126.23
26	2	305	CLA	C1D-ND-C4D	-14.94	95.72	106.33
28	B	617	WVN	C21-C15-C13	-14.77	107.94	124.53
28	B	618	WVN	C21-C15-C13	-14.66	108.07	124.53
28	C	516	WVN	C21-C15-C13	-14.13	108.66	124.53
28	3	313	WVN	C04-C09-C05	-14.07	111.36	124.85
28	B	618	WVN	C04-C09-C05	-14.06	111.37	124.85
40	2	317	IHT	C19-C10-C07	-13.93	108.89	124.53
40	2	317	IHT	C31-C34-C35	-13.91	87.33	126.42
28	B	617	WVN	C04-C09-C05	-13.81	111.61	124.85
40	1	619	IHT	C19-C10-C07	-13.51	109.35	124.53
28	H	101	WVN	C21-C15-C13	-13.41	109.47	124.53
28	C	516	WVN	C04-C09-C05	-13.12	112.27	124.85
28	H	101	WVN	C04-C09-C05	-13.07	112.32	124.85
28	B	617	WVN	C29-C26-C22	-13.06	108.67	127.31
38	6	608	KC2	C1A-NA-C4A	-12.57	101.06	106.71
28	3	313	WVN	C21-C15-C13	-12.56	110.42	124.53
38	S	608	KC2	C1A-NA-C4A	-12.56	101.06	106.71
39	3	310	II0	C20-C14-C10	-12.52	107.34	124.35
38	2	310	KC2	C1A-NA-C4A	-12.46	101.10	106.71
38	N	611	KC2	C1A-NA-C4A	-12.43	101.12	106.71
38	4	311	KC2	C1A-NA-C4A	-12.42	101.12	106.71
38	Q	310	KC2	C1A-NA-C4A	-12.38	101.14	106.71
38	O	610	KC2	C1A-NA-C4A	-12.38	101.14	106.71
38	N	605	KC2	C1A-NA-C4A	-12.20	101.22	106.71
28	C	516	WVN	C40-C37-C34	-12.17	109.94	127.31
39	1	616	II0	C42-C40-C36	-12.09	110.06	127.31
39	P	613	II0	C20-C14-C10	-12.04	107.98	124.35
39	3	311	II0	C20-C14-C10	-12.03	108.00	124.35
28	B	618	WVN	C39-C36-C32	-11.94	110.27	127.31
39	3	311	II0	C42-C40-C36	-11.92	110.30	127.31
39	P	613	II0	C42-C40-C36	-11.89	110.35	127.31
39	1	617	II0	C20-C14-C10	-11.88	108.20	124.35
38	4	310	KC2	C1A-NA-C4A	-11.85	101.38	106.71
39	1	618	II0	C20-C14-C10	-11.82	108.29	124.35
38	Q	309	KC2	C1A-NA-C4A	-11.80	101.40	106.71
39	1	615	II0	C20-C14-C10	-11.75	108.39	124.35
28	H	101	WVN	C40-C37-C34	-11.71	110.60	127.31
28	C	516	WVN	C30-C28-C25	-11.66	110.67	127.31
28	B	618	WVN	C40-C37-C34	-11.66	110.67	127.31
39	O	615	II0	C19-C13-C09	-11.63	108.54	124.35
39	2	316	II0	C19-C13-C09	-11.63	108.54	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	3	312	II0	C19-C13-C09	-11.63	108.55	124.35
28	B	618	WVN	C29-C26-C22	-11.56	110.82	127.31
39	2	314	II0	C06-C08-C12	11.44	125.97	110.30
39	O	614	II0	C06-C08-C12	11.43	125.96	110.30
39	4	316	II0	C06-C08-C12	11.40	125.91	110.30
39	Q	315	II0	C06-C08-C12	11.40	125.91	110.30
39	3	310	II0	C41-C39-C35	-11.38	111.06	127.31
28	H	101	WVN	C30-C28-C25	-11.35	111.12	127.31
28	B	617	WVN	C40-C37-C34	-11.34	111.13	127.31
39	1	615	II0	C42-C40-C36	-11.33	111.13	127.31
38	5	610	KC2	C1A-NA-C4A	-11.32	101.62	106.71
39	1	616	II0	C19-C13-C09	-11.31	108.97	124.35
39	N	617	II0	C06-C08-C12	11.29	125.75	110.30
28	B	617	WVN	C30-C28-C25	-11.28	111.21	127.31
28	C	516	WVN	C29-C26-C22	-11.27	111.22	127.31
39	3	311	II0	C19-C13-C09	-11.24	109.07	124.35
39	N	615	II0	C06-C08-C12	11.23	125.67	110.30
39	1	617	II0	C42-C40-C36	-11.22	111.29	127.31
39	P	613	II0	C19-C13-C09	-11.22	109.10	124.35
38	R	311	KC2	C1A-NA-C4A	-11.21	101.67	106.71
39	R	315	II0	C06-C08-C12	11.18	125.61	110.30
28	B	618	WVN	C30-C28-C25	-11.17	111.37	127.31
38	3	304	KC2	C1A-NA-C4A	-11.17	101.69	106.71
39	5	614	II0	C06-C08-C12	11.15	125.57	110.30
39	1	618	II0	C19-C13-C09	-11.15	109.20	124.35
38	P	605	KC2	C1A-NA-C4A	-11.14	101.70	106.71
39	R	314	II0	C06-C08-C12	11.12	125.53	110.30
39	1	615	II0	C19-C13-C09	-11.12	109.24	124.35
39	5	613	II0	C06-C08-C12	11.10	125.50	110.30
28	3	313	WVN	C40-C37-C34	-11.10	111.47	127.31
39	N	616	II0	C06-C08-C12	11.10	125.50	110.30
39	1	617	II0	C19-C13-C09	-11.09	109.27	124.35
39	4	317	II0	C06-C08-C12	11.05	125.44	110.30
39	Q	319	II0	C06-C08-C12	11.05	125.43	110.30
39	Q	316	II0	C06-C08-C12	11.05	125.42	110.30
39	4	320	II0	C06-C08-C12	11.04	125.42	110.30
39	3	310	II0	C42-C40-C36	-11.03	111.57	127.31
39	6	611	II0	C06-C08-C12	11.02	125.39	110.30
39	S	611	II0	C06-C08-C12	11.02	125.39	110.30
39	R	316	II0	C06-C08-C12	10.99	125.35	110.30
39	5	615	II0	C06-C08-C12	10.98	125.34	110.30
39	Q	313	II0	C06-C08-C12	10.97	125.32	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	4	314	II0	C06-C08-C12	10.96	125.31	110.30
39	2	313	II0	C06-C08-C12	10.95	125.29	110.30
28	H	101	WVN	C39-C36-C32	-10.95	111.69	127.31
39	O	613	II0	C06-C08-C12	10.94	125.28	110.30
39	3	311	II0	C41-C39-C35	-10.94	111.70	127.31
39	P	613	II0	C41-C39-C35	-10.94	111.70	127.31
39	N	620	II0	C06-C08-C12	10.92	125.25	110.30
39	Q	314	II0	C06-C08-C12	10.87	125.19	110.30
39	2	315	II0	C06-C08-C12	10.85	125.15	110.30
39	4	315	II0	C06-C08-C12	10.84	125.14	110.30
39	P	614	II0	C06-C08-C12	10.80	125.09	110.30
40	1	619	IHT	C41-C38-C35	-10.76	111.95	127.31
26	2	305	CLA	C2C-C1C-NC	10.75	120.05	109.97
39	O	615	II0	C41-C39-C35	-10.75	111.97	127.31
39	2	316	II0	C41-C39-C35	-10.74	111.98	127.31
39	6	612	II0	C06-C08-C12	10.73	124.99	110.30
39	N	618	II0	C06-C08-C12	10.72	124.98	110.30
39	P	612	II0	C06-C08-C12	10.71	124.96	110.30
39	S	612	II0	C06-C08-C12	10.71	124.96	110.30
39	6	613	II0	C06-C08-C12	10.68	124.92	110.30
39	R	318	II0	C06-C08-C12	10.66	124.89	110.30
40	1	619	IHT	C30-C27-C23	-10.52	112.29	127.31
28	C	516	WVN	C39-C36-C32	-10.47	112.36	127.31
40	2	317	IHT	C30-C27-C23	-10.47	112.37	127.31
40	2	317	IHT	C20-C15-C11	-10.43	110.17	124.35
38	N	610	KC2	C1A-NA-C4A	-10.43	102.02	106.71
28	3	313	WVN	C39-C36-C32	-10.43	112.42	127.31
39	Q	313	II0	C41-C39-C35	-10.43	112.43	127.31
40	2	317	IHT	C40-C37-C33	-10.42	112.44	127.31
39	N	618	II0	C41-C39-C35	-10.41	112.45	127.31
39	4	314	II0	C41-C39-C35	-10.40	112.47	127.31
28	B	617	WVN	C39-C36-C32	-10.38	112.50	127.31
28	H	101	WVN	C27-C25-C28	-10.36	108.41	122.92
39	1	616	II0	C20-C14-C10	-10.30	110.36	124.35
39	O	615	II0	C42-C40-C36	-10.29	112.62	127.31
38	Q	309	KC2	CHC-C4B-NB	10.28	133.90	124.45
39	2	316	II0	C42-C40-C36	-10.27	112.65	127.31
38	3	304	KC2	CHC-C4B-NB	10.27	133.89	124.45
38	6	608	KC2	CHC-C4B-NB	10.26	133.89	124.45
40	1	619	IHT	C39-C35-C38	-10.26	108.55	122.92
39	O	615	II0	C20-C14-C10	-10.25	110.42	124.35
40	1	619	IHT	C40-C37-C33	-10.24	112.69	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	2	316	II0	C20-C14-C10	-10.24	110.43	124.35
38	S	608	KC2	CHC-C4B-NB	10.24	133.87	124.45
38	P	605	KC2	CHC-C4B-NB	10.23	133.86	124.45
38	5	610	KC2	CHC-C4B-NB	10.23	133.85	124.45
38	N	612	KC2	CHC-C4B-NB	10.23	133.85	124.45
40	1	619	IHT	C36-C33-C37	-10.22	108.61	122.92
38	4	310	KC2	CHC-C4B-NB	10.20	133.83	124.45
39	1	617	II0	C41-C39-C35	-10.17	112.80	127.31
39	S	611	II0	C42-C40-C36	-10.16	112.81	127.31
38	R	311	KC2	CHC-C4B-NB	10.16	133.79	124.45
38	N	611	KC2	CHC-C4B-NB	10.15	133.78	124.45
39	6	611	II0	C42-C40-C36	-10.15	112.82	127.31
28	B	617	WVN	C02-C05-C09	-10.14	108.99	121.47
39	N	617	II0	C41-C39-C35	-10.13	112.86	127.31
38	Q	304	KC2	C1A-NA-C4A	-10.11	102.16	106.71
38	N	612	KC2	C1A-NA-C4A	-10.11	102.16	106.71
39	3	312	II0	C20-C14-C10	-10.10	110.62	124.35
28	3	313	WVN	C29-C26-C22	-10.09	112.91	127.31
39	1	616	II0	C38-C36-C40	-10.09	108.79	122.92
39	1	615	II0	C41-C39-C35	-10.05	112.97	127.31
38	4	305	KC2	C1A-NA-C4A	-10.02	102.20	106.71
39	5	613	II0	C41-C39-C35	-10.02	113.01	127.31
39	R	314	II0	C41-C39-C35	-10.02	113.01	127.31
38	Q	304	KC2	CHC-C4B-NB	10.02	133.66	124.45
38	N	610	KC2	CHC-C4B-NB	10.00	133.65	124.45
38	4	305	KC2	CHC-C4B-NB	9.99	133.64	124.45
40	2	317	IHT	C39-C35-C38	-9.99	108.92	122.92
39	N	615	II0	C42-C40-C36	-9.98	113.06	127.31
38	N	605	KC2	CHC-C4B-NB	9.93	133.58	124.45
39	1	616	II0	C37-C35-C39	-9.90	109.05	122.92
38	2	310	KC2	CHC-C4B-NB	9.90	133.55	124.45
39	4	320	II0	C41-C39-C35	-9.90	113.18	127.31
39	4	316	II0	C41-C39-C35	-9.89	113.19	127.31
39	Q	319	II0	C41-C39-C35	-9.89	113.20	127.31
39	P	612	II0	C41-C39-C35	-9.85	113.25	127.31
28	H	101	WVN	C29-C26-C22	-9.85	113.25	127.31
39	Q	315	II0	C41-C39-C35	-9.84	113.26	127.31
39	1	615	II0	C32-C34-C36	9.84	154.06	126.42
39	R	318	II0	C42-C40-C36	-9.84	113.27	127.31
28	3	313	WVN	C29-C31-C32	9.83	154.04	126.42
39	R	318	II0	C41-C39-C35	-9.83	113.28	127.31
39	6	613	II0	C42-C40-C36	-9.83	113.29	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	2	317	IHT	C41-C38-C35	-9.82	113.29	127.31
28	H	101	WVN	C29-C31-C32	9.82	154.00	126.42
39	6	613	II0	C41-C39-C35	-9.81	113.31	127.31
39	4	316	II0	C42-C40-C36	-9.80	113.32	127.31
40	2	317	IHT	C25-C23-C27	-9.80	109.20	122.92
38	O	610	KC2	CHC-C4B-NB	9.79	133.45	124.45
39	Q	315	II0	C42-C40-C36	-9.78	113.36	127.31
39	Q	316	II0	C41-C39-C35	-9.77	113.36	127.31
38	4	311	KC2	CHC-C4B-NB	9.77	133.43	124.45
39	4	315	II0	C42-C40-C36	-9.76	113.38	127.31
38	Q	310	KC2	CHC-C4B-NB	9.76	133.42	124.45
39	4	317	II0	C41-C39-C35	-9.76	113.38	127.31
39	1	615	II0	C38-C36-C40	-9.76	109.25	122.92
39	1	618	II0	C41-C39-C35	-9.76	113.39	127.31
39	1	616	II0	C41-C39-C35	-9.74	113.40	127.31
39	4	315	II0	C41-C39-C35	-9.73	113.42	127.31
39	O	613	II0	C42-C40-C36	-9.73	113.42	127.31
39	3	310	II0	C37-C35-C39	-9.73	109.29	122.92
39	Q	314	II0	C41-C39-C35	-9.72	113.44	127.31
39	Q	314	II0	C42-C40-C36	-9.71	113.45	127.31
39	2	313	II0	C42-C40-C36	-9.71	113.46	127.31
38	N	612	KC2	OBD-CAD-CBD	9.70	139.75	125.89
39	1	617	II0	C38-C36-C40	-9.69	109.35	122.92
26	3	308	CLA	C4A-NA-C1A	9.67	111.06	106.71
39	O	615	II0	C32-C34-C36	9.66	153.55	126.42
39	2	316	II0	C32-C34-C36	9.65	153.53	126.42
28	C	516	WVN	C27-C25-C28	-9.64	109.42	122.92
39	1	617	II0	C37-C35-C39	-9.64	109.42	122.92
39	S	611	II0	C41-C39-C35	-9.63	113.57	127.31
28	3	313	WVN	C24-C22-C26	-9.62	109.45	122.92
40	1	619	IHT	C20-C15-C11	-9.61	111.29	124.35
39	6	611	II0	C41-C39-C35	-9.61	113.59	127.31
39	1	618	II0	C42-C40-C36	-9.61	113.59	127.31
40	2	317	IHT	C36-C33-C37	-9.60	109.47	122.92
39	5	614	II0	C41-C39-C35	-9.60	113.61	127.31
39	R	315	II0	C41-C39-C35	-9.58	113.63	127.31
39	N	618	II0	C42-C40-C36	-9.58	113.64	127.31
39	3	312	II0	C41-C39-C35	-9.56	113.66	127.31
39	N	620	II0	C41-C39-C35	-9.54	113.69	127.31
39	2	315	II0	C41-C39-C35	-9.54	113.69	127.31
39	6	612	II0	C42-C40-C36	-9.53	113.71	127.31
39	S	612	II0	C42-C40-C36	-9.53	113.72	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	R	315	II0	C42-C40-C36	-9.52	113.72	127.31
39	2	314	II0	C42-C40-C36	-9.51	113.73	127.31
39	1	618	II0	C37-C35-C39	-9.49	109.63	122.92
39	5	614	II0	C42-C40-C36	-9.49	113.77	127.31
28	B	618	WVN	C29-C31-C32	9.47	153.03	126.42
39	O	614	II0	C42-C40-C36	-9.47	113.79	127.31
39	O	613	II0	C41-C39-C35	-9.42	113.86	127.31
39	1	616	II0	C32-C34-C36	9.42	152.87	126.42
39	3	310	II0	C19-C13-C09	-9.41	111.57	124.35
38	N	611	KC2	OBD-CAD-CBD	9.40	139.33	125.89
39	2	313	II0	C41-C39-C35	-9.40	113.89	127.31
38	4	310	KC2	OBD-CAD-CBD	9.39	139.31	125.89
39	1	615	II0	C31-C33-C35	9.38	152.78	126.42
39	3	312	II0	C42-C40-C36	-9.38	113.92	127.31
40	1	619	IHT	C25-C23-C27	-9.38	109.79	122.92
39	O	614	II0	C41-C39-C35	-9.35	113.96	127.31
28	3	313	WVN	C30-C28-C25	-9.35	113.97	127.31
38	Q	309	KC2	OBD-CAD-CBD	9.34	139.24	125.89
39	2	314	II0	C41-C39-C35	-9.33	113.99	127.31
39	N	616	II0	C42-C40-C36	-9.32	114.01	127.31
39	Q	319	II0	C42-C40-C36	-9.31	114.02	127.31
39	2	316	II0	C37-C35-C39	-9.31	109.89	122.92
39	P	613	II0	C38-C36-C40	-9.31	109.89	122.92
39	1	617	II0	C31-C33-C35	9.30	152.54	126.42
39	1	618	II0	C32-C34-C36	9.28	152.50	126.42
39	O	615	II0	C37-C35-C39	-9.28	109.92	122.92
38	N	610	KC2	OBD-CAD-CBD	9.28	139.15	125.89
28	B	618	WVN	C24-C22-C26	-9.27	109.93	122.92
39	3	311	II0	C38-C36-C40	-9.27	109.93	122.92
39	5	615	II0	C42-C40-C36	-9.27	114.08	127.31
39	1	617	II0	C32-C34-C36	9.26	152.43	126.42
39	S	612	II0	C41-C39-C35	-9.26	114.10	127.31
39	4	320	II0	C42-C40-C36	-9.25	114.11	127.31
39	3	312	II0	C38-C36-C40	-9.25	109.97	122.92
28	C	516	WVN	C38-C34-C37	-9.25	109.97	122.92
39	R	316	II0	C42-C40-C36	-9.23	114.14	127.31
39	6	612	II0	C41-C39-C35	-9.22	114.15	127.31
39	3	312	II0	C32-C34-C36	9.22	152.31	126.42
39	N	615	II0	C41-C39-C35	-9.21	114.17	127.31
39	1	618	II0	C31-C33-C35	9.20	152.26	126.42
39	R	314	II0	C42-C40-C36	-9.20	114.18	127.31
39	P	614	II0	C41-C39-C35	-9.19	114.19	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	2	317	IHT	C30-C32-C33	9.19	152.23	126.42
39	5	613	II0	C42-C40-C36	-9.19	114.20	127.31
40	1	619	IHT	C30-C32-C33	9.18	152.21	126.42
38	N	605	KC2	OBD-CAD-CBD	9.17	139.00	125.89
28	B	618	WVN	C35-C32-C36	-9.16	110.10	122.92
38	R	311	KC2	OBD-CAD-CBD	9.15	138.96	125.89
39	P	613	II0	C31-C33-C35	9.14	152.09	126.42
38	5	610	KC2	OBD-CAD-CBD	9.14	138.95	125.89
40	1	619	IHT	C31-C34-C35	9.14	152.08	126.42
39	3	311	II0	C31-C33-C35	9.14	152.08	126.42
38	4	311	KC2	OBD-CAD-CBD	9.13	138.95	125.89
39	P	612	II0	C42-C40-C36	-9.13	114.28	127.31
38	Q	310	KC2	OBD-CAD-CBD	9.13	138.93	125.89
39	1	616	II0	C31-C33-C35	9.08	151.93	126.42
28	B	618	WVN	C38-C34-C37	-9.06	110.23	122.92
39	1	618	II0	C38-C36-C40	-9.05	110.25	122.92
28	C	516	WVN	C35-C32-C36	-9.05	110.25	122.92
39	1	615	II0	C37-C35-C39	-9.04	110.26	122.92
38	Q	304	KC2	CHD-C4C-NC	9.04	137.91	124.20
38	N	612	KC2	CHD-C4C-NC	9.02	137.89	124.20
38	4	305	KC2	CHD-C4C-NC	9.02	137.89	124.20
38	O	610	KC2	CHD-C4C-NC	9.00	137.85	124.20
40	1	619	IHT	C03-C11-C15	-8.99	109.93	122.63
28	b	618	WVN	C04-C09-C05	-8.99	116.23	124.85
39	3	312	II0	C31-C33-C35	8.99	151.67	126.42
38	2	310	KC2	CHD-C4C-NC	8.99	137.84	124.20
28	3	313	WVN	C38-C34-C37	-8.96	110.36	122.92
28	3	313	WVN	C27-C25-C28	-8.95	110.38	122.92
39	3	311	II0	C32-C34-C36	8.95	151.56	126.42
39	P	613	II0	C32-C34-C36	8.94	151.53	126.42
39	N	616	II0	C41-C39-C35	-8.94	114.55	127.31
26	2	305	CLA	CMD-C2D-C1D	8.94	140.47	124.71
38	4	305	KC2	OBD-CAD-CBD	8.93	138.66	125.89
38	3	304	KC2	OBD-CAD-CBD	8.93	138.65	125.89
38	3	304	KC2	CHD-C4C-NC	8.93	137.75	124.20
39	N	620	II0	C42-C40-C36	-8.93	114.57	127.31
39	2	315	II0	C42-C40-C36	-8.92	114.58	127.31
38	R	311	KC2	CHD-C4C-NC	8.92	137.74	124.20
38	P	605	KC2	CHD-C4C-NC	8.91	137.72	124.20
38	5	610	KC2	CHD-C4C-NC	8.91	137.72	124.20
38	Q	304	KC2	OBD-CAD-CBD	8.91	138.63	125.89
38	P	605	KC2	OBD-CAD-CBD	8.90	138.61	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	2	310	KC2	OBD-CAD-CBD	8.90	138.61	125.89
39	R	316	II0	C41-C39-C35	-8.90	114.61	127.31
38	S	608	KC2	OBD-CAD-CBD	8.90	138.60	125.89
28	H	101	WVN	C24-C22-C26	-8.89	110.47	122.92
39	5	615	II0	C41-C39-C35	-8.89	114.63	127.31
38	6	608	KC2	CHD-C4C-NC	8.86	137.65	124.20
38	6	608	KC2	OBD-CAD-CBD	8.86	138.55	125.89
39	P	613	II0	C37-C35-C39	-8.86	110.51	122.92
38	S	608	KC2	CHD-C4C-NC	8.86	137.64	124.20
39	3	311	II0	C37-C35-C39	-8.84	110.53	122.92
38	O	610	KC2	OBD-CAD-CBD	8.83	138.51	125.89
38	4	310	KC2	CHD-C4C-NC	8.81	137.57	124.20
38	Q	309	KC2	CHD-C4C-NC	8.80	137.55	124.20
39	N	617	II0	C42-C40-C36	-8.78	114.79	127.31
38	N	605	KC2	CHD-C4C-NC	8.76	137.50	124.20
38	N	610	KC2	CHD-C4C-NC	8.73	137.45	124.20
38	N	611	KC2	CHD-C4C-NC	8.73	137.45	124.20
38	N	612	KC2	CHB-C1B-NB	8.73	132.47	124.45
39	3	310	II0	C31-C33-C35	8.72	150.90	126.42
28	C	516	WVN	C24-C22-C26	-8.70	110.74	122.92
28	B	617	WVN	C24-C22-C26	-8.67	110.78	122.92
39	Q	316	II0	C42-C40-C36	-8.67	114.94	127.31
39	4	317	II0	C42-C40-C36	-8.66	114.95	127.31
40	2	317	IHT	C09-C10-C07	-8.62	110.21	122.73
28	C	516	WVN	C29-C31-C32	8.61	150.61	126.42
39	Q	313	II0	C42-C40-C36	-8.58	115.07	127.31
39	2	316	II0	C04-C10-C14	-8.56	110.54	122.63
38	3	304	KC2	CHB-C1B-NB	8.56	132.32	124.45
39	4	314	II0	C42-C40-C36	-8.55	115.10	127.31
39	O	615	II0	C38-C36-C40	-8.55	110.95	122.92
39	O	615	II0	C04-C10-C14	-8.55	110.56	122.63
28	A	406	WVN	C04-C09-C05	-8.54	116.66	124.85
38	N	605	KC2	CHB-C1B-NB	8.53	132.30	124.45
39	2	316	II0	C38-C36-C40	-8.53	110.98	122.92
38	P	605	KC2	CHB-C1B-NB	8.52	132.28	124.45
38	Q	304	KC2	CHB-C1B-NB	8.50	132.27	124.45
38	4	305	KC2	CHB-C1B-NB	8.50	132.26	124.45
39	P	614	II0	C42-C40-C36	-8.49	115.20	127.31
38	N	610	KC2	CHB-C1B-NB	8.48	132.25	124.45
39	3	310	II0	C38-C36-C40	-8.45	111.09	122.92
28	3	313	WVN	C23-C25-C28	-8.45	105.98	118.94
28	3	313	WVN	C30-C33-C34	8.45	150.14	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	Q	310	KC2	CHD-C4C-NC	8.44	137.01	124.20
28	H	101	WVN	C30-C33-C34	8.42	150.08	126.42
28	B	617	WVN	C35-C32-C36	-8.42	111.14	122.92
38	4	311	KC2	CHD-C4C-NC	8.41	136.96	124.20
28	B	617	WVN	C27-C25-C28	-8.38	111.19	122.92
28	B	617	WVN	C38-C34-C37	-8.37	111.20	122.92
39	O	615	II0	C31-C33-C35	8.34	149.84	126.42
39	3	312	II0	C37-C35-C39	-8.34	111.25	122.92
39	2	316	II0	C31-C33-C35	8.33	149.82	126.42
28	3	313	WVN	C35-C32-C36	-8.33	111.25	122.92
38	N	611	KC2	CHB-C1B-NB	8.22	132.01	124.45
38	4	310	KC2	CHB-C1B-NB	8.20	131.99	124.45
38	Q	309	KC2	CHB-C1B-NB	8.20	131.99	124.45
38	5	610	KC2	CHB-C1B-NB	8.19	131.98	124.45
38	N	605	KC2	OBD-CAD-C3D	-8.18	114.39	127.98
38	R	311	KC2	CHB-C1B-NB	8.18	131.97	124.45
39	3	312	II0	C03-C09-C13	-8.11	111.18	122.63
38	4	305	KC2	OBD-CAD-C3D	-8.11	114.52	127.98
38	Q	304	KC2	OBD-CAD-C3D	-8.07	114.58	127.98
38	2	310	KC2	CHB-C1B-NB	8.06	131.86	124.45
28	H	101	WVN	C14-C15-C13	-8.06	111.03	122.73
38	6	608	KC2	CHB-C1B-NB	8.06	131.86	124.45
38	3	304	KC2	OBD-CAD-C3D	-8.06	114.60	127.98
38	O	610	KC2	CHB-C1B-NB	8.06	131.86	124.45
28	B	618	WVN	C27-C25-C28	-8.05	111.64	122.92
38	S	608	KC2	CHB-C1B-NB	8.05	131.85	124.45
28	B	617	WVN	C30-C33-C34	8.04	148.99	126.42
38	P	605	KC2	OBD-CAD-C3D	-8.03	114.65	127.98
28	B	617	WVN	C29-C31-C32	8.02	148.94	126.42
38	N	612	KC2	CMD-C2D-C1D	-8.01	116.16	128.46
40	1	619	IHT	C09-C10-C07	-7.97	111.16	122.73
40	R	317	IHT	C05-C03-C11	7.96	125.76	109.62
40	5	616	IHT	C05-C03-C11	7.94	125.72	109.62
26	2	305	CLA	C3C-C4C-NC	7.93	119.46	110.57
38	S	608	KC2	OBD-CAD-C3D	-7.92	114.83	127.98
38	6	608	KC2	OBD-CAD-C3D	-7.90	114.87	127.98
28	H	101	WVN	C35-C32-C36	-7.90	111.86	122.92
39	3	310	II0	C32-C34-C36	7.86	148.50	126.42
28	k	101	WVN	C04-C09-C05	-7.84	117.33	124.85
28	C	516	WVN	C30-C33-C34	7.78	148.28	126.42
28	B	618	WVN	C14-C15-C13	-7.76	111.47	122.73
38	4	311	KC2	CHB-C1B-NB	7.74	131.57	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	Q	310	KC2	CHB-C1B-NB	7.73	131.56	124.45
28	B	618	WVN	C30-C33-C34	7.73	148.12	126.42
39	1	615	II0	C03-C09-C13	-7.73	111.72	122.63
38	N	612	KC2	OBD-CAD-C3D	-7.72	115.17	127.98
28	b	617	WVN	C04-C09-C05	-7.69	117.47	124.85
28	B	619	WVN	C04-C09-C05	-7.68	117.48	124.85
38	N	610	KC2	OBD-CAD-C3D	-7.68	115.23	127.98
39	1	617	II0	C03-C09-C13	-7.66	111.81	122.63
28	B	618	WVN	C02-C05-C09	-7.63	112.08	121.47
40	2	317	IHT	C02-C07-C10	-7.63	111.87	122.61
28	H	101	WVN	C38-C34-C37	-7.62	112.25	122.92
38	4	310	KC2	OBD-CAD-C3D	-7.60	115.36	127.98
38	5	610	KC2	OBD-CAD-C3D	-7.59	115.39	127.98
38	R	311	KC2	OBD-CAD-C3D	-7.58	115.39	127.98
38	Q	309	KC2	OBD-CAD-C3D	-7.58	115.39	127.98
28	3	313	WVN	C14-C15-C13	-7.57	111.73	122.73
38	4	311	KC2	OBD-CAD-C3D	-7.57	115.42	127.98
38	Q	310	KC2	OBD-CAD-C3D	-7.57	115.42	127.98
40	N	619	IHT	C09-C10-C07	-7.56	111.76	122.73
39	1	616	II0	C03-C09-C13	-7.55	111.97	122.63
28	x	101	WVN	C04-C09-C05	-7.52	117.64	124.85
28	b	619	WVN	C30-C28-C25	-7.51	116.60	127.31
38	N	611	KC2	OBD-CAD-C3D	-7.49	115.54	127.98
28	P	615	WVN	C04-C09-C05	-7.49	117.67	124.85
40	1	619	IHT	C02-C07-C10	-7.48	112.08	122.61
38	2	310	KC2	OBD-CAD-C3D	-7.48	115.57	127.98
39	3	312	II0	C04-C10-C14	-7.47	112.09	122.63
38	O	610	KC2	OBD-CAD-C3D	-7.43	115.65	127.98
28	3	313	WVN	C02-C05-C09	-7.38	112.39	121.47
28	H	101	WVN	C19-C22-C26	-7.37	107.62	118.94
39	1	618	II0	C03-C09-C13	-7.36	112.25	122.63
38	N	610	KC2	C2C-C1C-NC	7.32	118.57	110.57
38	N	612	KC2	C2C-C1C-NC	7.32	118.57	110.57
40	5	616	IHT	C09-C10-C07	-7.27	112.17	122.73
40	R	317	IHT	C09-C10-C07	-7.26	112.19	122.73
28	H	101	WVN	C23-C25-C28	-7.23	107.84	118.94
38	Q	310	KC2	C4C-C3C-C2C	-7.23	101.38	107.11
38	4	311	KC2	C4C-C3C-C2C	-7.22	101.38	107.11
38	N	611	KC2	C2C-C1C-NC	7.22	118.45	110.57
38	6	608	KC2	C2C-C1C-NC	7.20	118.44	110.57
38	S	608	KC2	C2C-C1C-NC	7.19	118.42	110.57
28	Z	101	WVN	C02-C05-C09	-7.14	112.69	121.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	305	KC2	C2C-C1C-NC	7.09	118.31	110.57
38	Q	310	KC2	C2C-C1C-NC	7.09	118.31	110.57
38	Q	304	KC2	C2C-C1C-NC	7.07	118.29	110.57
38	3	304	KC2	C2C-C1C-NC	7.06	118.28	110.57
38	4	311	KC2	C2C-C1C-NC	7.06	118.28	110.57
38	5	610	KC2	C2C-C1C-NC	7.06	118.28	110.57
38	4	310	KC2	C2C-C1C-NC	7.04	118.25	110.57
38	R	311	KC2	C2C-C1C-NC	7.03	118.25	110.57
38	Q	309	KC2	C2C-C1C-NC	7.02	118.23	110.57
38	4	305	KC2	C1A-C2A-C3A	-7.01	101.55	107.11
38	Q	309	KC2	C1A-C2A-C3A	-7.01	101.55	107.11
38	Q	304	KC2	C1A-C2A-C3A	-7.01	101.55	107.11
38	P	605	KC2	C2C-C1C-NC	7.00	118.22	110.57
38	S	608	KC2	CMD-C2D-C1D	-6.96	117.76	128.46
38	4	310	KC2	C1A-C2A-C3A	-6.96	101.59	107.11
28	Y	101	WVN	C21-C15-C13	-6.96	116.72	124.53
39	N	618	II0	C28-C26-C24	-6.96	103.06	116.84
39	3	310	II0	C03-C09-C13	-6.95	112.81	122.63
38	6	608	KC2	CMD-C2D-C1D	-6.95	117.78	128.46
38	N	612	KC2	C4C-C3C-C2C	-6.94	101.61	107.11
38	N	612	KC2	CMD-C2D-C3D	6.91	137.61	124.68
38	2	310	KC2	C2C-C1C-NC	6.91	118.11	110.57
38	N	611	KC2	CHC-C4B-C3B	-6.88	113.48	125.26
38	O	610	KC2	C2C-C1C-NC	6.88	118.08	110.57
38	N	611	KC2	CMD-C2D-C1D	-6.87	117.90	128.46
26	1	606	CLA	C4A-NA-C1A	6.86	109.79	106.71
38	6	608	KC2	CHC-C4B-C3B	-6.86	113.53	125.26
38	6	608	KC2	C4C-C3C-C2C	-6.83	101.69	107.11
38	S	608	KC2	CHC-C4B-C3B	-6.83	113.57	125.26
39	4	316	II0	C28-C26-C24	-6.82	103.33	116.84
39	N	618	II0	C17-C04-C10	6.82	121.31	110.47
40	O	616	IHT	C05-C03-C11	6.82	123.44	109.62
38	S	608	KC2	C4C-C3C-C2C	-6.81	101.71	107.11
39	P	614	II0	C28-C26-C24	-6.81	103.35	116.84
38	6	608	KC2	C1A-C2A-C3A	-6.81	101.71	107.11
26	1	604	CLA	C4A-NA-C1A	6.81	109.77	106.71
39	Q	315	II0	C28-C26-C24	-6.80	103.36	116.84
38	Q	309	KC2	CHC-C4B-C3B	-6.80	113.63	125.26
38	N	610	KC2	CMD-C2D-C1D	-6.80	118.01	128.46
38	4	305	KC2	CMD-C2D-C1D	-6.80	118.02	128.46
39	Q	319	II0	C17-C04-C10	6.79	121.26	110.47
38	5	610	KC2	CHC-C4B-C3B	-6.79	113.65	125.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	N	605	KC2	C1A-C2A-C3A	-6.78	101.73	107.11
38	N	610	KC2	C1A-C2A-C3A	-6.78	101.73	107.11
28	H	101	WVN	C06-C13-C15	-6.78	113.06	122.61
38	Q	310	KC2	CHB-C4A-C3A	-6.78	114.38	124.98
38	R	311	KC2	CHC-C4B-C3B	-6.78	113.66	125.26
38	N	612	KC2	CHC-C4B-C3B	-6.78	113.66	125.26
39	5	615	II0	C28-C26-C24	-6.78	103.42	116.84
38	4	310	KC2	CHC-C4B-C3B	-6.77	113.67	125.26
38	Q	309	KC2	CMD-C2D-C1D	-6.77	118.05	128.46
38	4	310	KC2	CMD-C2D-C1D	-6.77	118.06	128.46
39	R	316	II0	C28-C26-C24	-6.77	103.44	116.84
39	4	320	II0	C17-C04-C10	6.77	121.22	110.47
39	5	615	II0	C17-C04-C10	6.76	121.21	110.47
39	P	612	II0	C17-C04-C10	6.76	121.21	110.47
38	S	608	KC2	C1A-C2A-C3A	-6.76	101.75	107.11
38	4	311	KC2	CHB-C4A-C3A	-6.76	114.42	124.98
39	2	313	II0	C28-C26-C24	-6.76	103.45	116.84
38	Q	304	KC2	CMD-C2D-C1D	-6.76	118.08	128.46
28	3	313	WVN	C23-C20-C13	-6.76	108.23	127.20
39	O	615	II0	C03-C09-C13	-6.75	113.10	122.63
39	O	613	II0	C28-C26-C24	-6.75	103.47	116.84
40	2	317	IHT	C22-C23-C27	-6.75	108.58	118.94
39	R	316	II0	C17-C04-C10	6.74	121.18	110.47
38	Q	310	KC2	C1A-C2A-C3A	-6.74	101.76	107.11
38	N	611	KC2	C1A-C2A-C3A	-6.74	101.77	107.11
39	2	316	II0	C03-C09-C13	-6.74	113.12	122.63
39	1	617	II0	C04-C10-C14	-6.73	113.13	122.63
39	4	317	II0	C28-C26-C24	-6.73	103.51	116.84
39	P	612	II0	C28-C26-C24	-6.73	103.51	116.84
39	S	611	II0	C28-C26-C24	-6.72	103.52	116.84
39	Q	316	II0	C28-C26-C24	-6.72	103.53	116.84
39	6	611	II0	C28-C26-C24	-6.72	103.54	116.84
38	R	311	KC2	CMD-C2D-C1D	-6.71	118.15	128.46
38	O	610	KC2	CHB-C4A-C3A	-6.71	114.50	124.98
38	5	610	KC2	CMD-C2D-C1D	-6.70	118.16	128.46
38	2	310	KC2	CHB-C4A-C3A	-6.69	114.52	124.98
38	4	311	KC2	C1A-C2A-C3A	-6.69	101.80	107.11
28	B	618	WVN	C06-C13-C15	-6.69	113.19	122.61
38	N	611	KC2	C4C-C3C-C2C	-6.69	101.80	107.11
39	S	612	II0	C17-C04-C10	6.68	121.09	110.47
38	3	304	KC2	CMD-C2D-C1D	-6.68	118.19	128.46
39	N	617	II0	C28-C26-C24	-6.68	103.61	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	P	605	KC2	CMD-C2D-C1D	-6.68	118.20	128.46
39	6	612	II0	C17-C04-C10	6.68	121.08	110.47
39	5	613	II0	C28-C26-C24	-6.67	103.63	116.84
40	N	619	IHT	C05-C03-C11	6.67	123.14	109.62
38	3	304	KC2	CHC-C4B-C3B	-6.67	113.85	125.26
38	P	605	KC2	CHC-C4B-C3B	-6.67	113.86	125.26
38	O	610	KC2	C1A-C2A-C3A	-6.66	101.83	107.11
39	N	615	II0	C28-C26-C24	-6.66	103.65	116.84
38	2	310	KC2	CHC-C4B-C3B	-6.66	113.87	125.26
39	R	314	II0	C28-C26-C24	-6.66	103.66	116.84
40	Q	317	IHT	C05-C03-C11	6.66	123.11	109.62
39	Q	314	II0	C28-C26-C24	-6.65	103.66	116.84
38	O	610	KC2	CHC-C4B-C3B	-6.65	113.89	125.26
39	N	616	II0	C28-C26-C24	-6.64	103.68	116.84
38	N	605	KC2	C2C-C1C-NC	6.64	117.82	110.57
28	H	101	WVN	C02-C05-C09	-6.64	113.30	121.47
38	N	605	KC2	CMD-C2D-C1D	-6.64	118.27	128.46
38	R	311	KC2	C1A-C2A-C3A	-6.63	101.85	107.11
39	4	315	II0	C28-C26-C24	-6.63	103.71	116.84
38	N	610	KC2	CHC-C4B-C3B	-6.63	113.92	125.26
40	2	317	IHT	C25-C23-C22	-6.63	107.64	118.08
40	4	318	IHT	C05-C03-C11	6.63	123.05	109.62
39	4	314	II0	C28-C26-C24	-6.62	103.72	116.84
39	Q	313	II0	C28-C26-C24	-6.62	103.73	116.84
26	2	305	CLA	CHD-C4C-C3C	-6.61	115.13	124.84
39	O	613	II0	C17-C04-C10	6.60	120.96	110.47
38	2	310	KC2	C1A-C2A-C3A	-6.60	101.87	107.11
38	3	304	KC2	C1A-C2A-C3A	-6.60	101.88	107.11
28	B	617	WVN	C14-C15-C13	-6.60	113.16	122.73
38	P	605	KC2	C1A-C2A-C3A	-6.59	101.88	107.11
38	5	610	KC2	C1A-C2A-C3A	-6.59	101.88	107.11
38	Q	304	KC2	CHC-C4B-C3B	-6.59	113.99	125.26
39	2	313	II0	C17-C04-C10	6.59	120.93	110.47
38	4	305	KC2	CHC-C4B-C3B	-6.58	114.00	125.26
38	N	611	KC2	CHB-C4A-C3A	-6.58	114.70	124.98
38	4	311	KC2	CHC-C4B-C3B	-6.58	114.00	125.26
39	O	615	II0	C37-C35-C33	-6.58	107.72	118.08
38	4	305	KC2	C4C-C3C-C2C	-6.57	101.89	107.11
39	P	614	II0	C42-C41-C39	-6.57	110.01	123.47
39	5	614	II0	C17-C04-C10	6.56	120.90	110.47
39	S	611	II0	C17-C04-C10	6.56	120.90	110.47
26	1	613	CLA	C4A-NA-C1A	6.56	109.66	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	2	316	II0	C37-C35-C33	-6.56	107.73	118.08
39	R	318	II0	C28-C26-C24	-6.56	103.84	116.84
28	C	515	WVN	C04-C09-C05	-6.56	118.56	124.85
38	Q	310	KC2	CHC-C4B-C3B	-6.55	114.05	125.26
38	Q	304	KC2	C4C-C3C-C2C	-6.55	101.91	107.11
26	Q	307	CLA	C4A-NA-C1A	6.55	109.65	106.71
39	6	613	II0	C28-C26-C24	-6.55	103.86	116.84
28	B	617	WVN	C35-C32-C31	-6.55	107.75	118.08
26	4	308	CLA	C4A-NA-C1A	6.55	109.65	106.71
39	6	611	II0	C17-C04-C10	6.55	120.87	110.47
39	R	315	II0	C17-C04-C10	6.55	120.87	110.47
39	5	614	II0	C28-C26-C24	-6.54	103.89	116.84
39	R	315	II0	C28-C26-C24	-6.52	103.92	116.84
38	R	311	KC2	C4C-C3C-C2C	-6.52	101.94	107.11
28	B	618	WVN	C23-C25-C28	-6.52	108.94	118.94
26	1	601	CLA	C4A-NA-C1A	6.51	109.64	106.71
39	N	620	II0	C28-C26-C24	-6.51	103.95	116.84
39	2	315	II0	C28-C26-C24	-6.51	103.95	116.84
39	N	615	II0	C42-C41-C39	-6.50	110.16	123.47
26	1	609	CLA	C4A-NA-C1A	6.50	109.63	106.71
38	N	610	KC2	C4C-C3C-C2C	-6.50	101.95	107.11
38	5	610	KC2	C4C-C3C-C2C	-6.50	101.95	107.11
39	R	314	II0	C17-C04-C10	6.50	120.80	110.47
40	N	619	IHT	C16-C03-C11	-6.50	100.14	110.47
39	5	613	II0	C17-C04-C10	6.48	120.77	110.47
38	4	310	KC2	C4C-C3C-C2C	-6.46	101.98	107.11
38	4	310	KC2	CHB-C4A-C3A	-6.46	114.89	124.98
38	S	608	KC2	CHB-C4A-C3A	-6.46	114.89	124.98
38	Q	309	KC2	CHB-C4A-C3A	-6.45	114.91	124.98
38	Q	309	KC2	C4C-C3C-C2C	-6.44	102.00	107.11
39	2	315	II0	C17-C04-C10	6.44	120.70	110.47
38	2	310	KC2	CMD-C2D-C1D	-6.44	118.57	128.46
39	S	612	II0	C42-C41-C39	-6.44	110.29	123.47
38	O	610	KC2	CMD-C2D-C1D	-6.43	118.58	128.46
39	6	612	II0	C42-C41-C39	-6.43	110.30	123.47
39	N	620	II0	C17-C04-C10	6.43	120.69	110.47
38	N	612	KC2	C1A-C2A-C3A	-6.43	102.01	107.11
39	1	615	II0	C04-C10-C14	-6.42	113.56	122.63
38	6	608	KC2	CHB-C4A-C3A	-6.42	114.95	124.98
39	2	314	II0	C28-C26-C24	-6.41	104.14	116.84
38	6	608	KC2	CMD-C2D-C3D	6.41	136.67	124.68
39	6	611	II0	C42-C41-C39	-6.41	110.34	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	S	608	KC2	CMD-C2D-C3D	6.41	136.66	124.68
39	S	611	II0	C42-C41-C39	-6.40	110.36	123.47
39	O	614	II0	C28-C26-C24	-6.39	104.18	116.84
38	4	311	KC2	CMD-C2D-C1D	-6.38	118.65	128.46
38	Q	310	KC2	CMD-C2D-C1D	-6.37	118.67	128.46
28	c	518	WVN	C04-C09-C05	-6.37	118.75	124.85
39	Q	316	II0	C17-C04-C10	6.36	120.57	110.47
40	4	318	IHT	C16-C03-C11	-6.36	100.36	110.47
40	Q	317	IHT	C16-C03-C11	-6.36	100.36	110.47
28	C	516	WVN	C02-C05-C09	-6.36	113.65	121.47
39	4	317	II0	C17-C04-C10	6.34	120.55	110.47
39	1	616	II0	C33-C35-C39	-6.34	109.21	118.94
38	N	611	KC2	CMD-C2D-C3D	6.33	136.53	124.68
26	1	608	CLA	C4A-NA-C1A	6.33	109.55	106.71
39	S	612	II0	C28-C26-C24	-6.32	104.32	116.84
39	1	615	II0	C33-C35-C39	-6.32	109.25	118.94
26	1	602	CLA	C4A-NA-C1A	6.31	109.54	106.71
39	6	612	II0	C28-C26-C24	-6.31	104.34	116.84
26	2	305	CLA	O2D-CGD-CBD	6.31	122.48	111.27
39	N	615	II0	C17-C04-C10	6.30	120.48	110.47
28	c	516	WVN	C04-C09-C05	-6.30	118.81	124.85
28	C	516	WVN	C06-C13-C15	-6.29	113.75	122.61
26	S	603	CLA	C4A-NA-C1A	6.29	109.53	106.71
38	O	610	KC2	CMD-C2D-C3D	6.29	136.44	124.68
39	3	311	II0	C04-C10-C14	-6.28	113.76	122.63
39	P	613	II0	C04-C10-C14	-6.28	113.76	122.63
40	2	317	IHT	C03-C11-C15	-6.28	113.77	122.63
38	2	310	KC2	CMD-C2D-C3D	6.27	136.41	124.68
26	6	603	CLA	C4A-NA-C1A	6.27	109.53	106.71
28	P	615	WVN	C39-C36-C32	-6.27	118.36	127.31
26	N	608	CLA	C4A-NA-C1A	6.25	109.52	106.71
40	1	619	IHT	C22-C23-C27	-6.25	109.34	118.94
39	2	314	II0	C42-C41-C39	-6.25	110.67	123.47
39	O	614	II0	C42-C41-C39	-6.25	110.67	123.47
38	N	605	KC2	CHC-C4B-C3B	-6.25	114.57	125.26
38	N	605	KC2	CMD-C2D-C3D	6.22	136.31	124.68
38	Q	309	KC2	CMD-C2D-C3D	6.22	136.31	124.68
40	2	317	IHT	C34-C35-C38	-6.22	109.40	118.94
38	R	311	KC2	CMD-C2D-C3D	6.21	136.30	124.68
39	O	613	II0	C42-C41-C39	-6.21	110.75	123.47
38	N	610	KC2	CMD-C2D-C3D	6.21	136.30	124.68
38	N	610	KC2	CHB-C4A-C3A	-6.21	115.28	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	Y	101	WVN	C04-C09-C05	-6.21	118.90	124.85
38	3	304	KC2	C4C-C3C-C2C	-6.20	102.19	107.11
38	4	310	KC2	CMD-C2D-C3D	6.20	136.27	124.68
38	R	311	KC2	CHB-C4A-C3A	-6.20	115.30	124.98
39	R	316	II0	C42-C41-C39	-6.19	110.78	123.47
39	2	313	II0	C42-C41-C39	-6.19	110.79	123.47
38	5	610	KC2	CHB-C4A-C3A	-6.19	115.31	124.98
38	P	605	KC2	C4C-C3C-C2C	-6.19	102.20	107.11
26	2	305	CLA	CHD-C1D-ND	-6.19	118.77	124.45
38	5	610	KC2	CMD-C2D-C3D	6.19	136.25	124.68
39	N	616	II0	C42-C41-C39	-6.18	110.81	123.47
38	Q	304	KC2	CMD-C2D-C3D	6.17	136.22	124.68
28	B	617	WVN	C24-C22-C19	-6.16	108.36	118.08
28	Y	101	WVN	C20-C23-C25	-6.16	116.92	126.23
39	5	615	II0	C42-C41-C39	-6.16	110.85	123.47
26	1	603	CLA	C4A-NA-C1A	6.16	109.48	106.71
38	4	305	KC2	CMD-C2D-C3D	6.16	136.20	124.68
38	N	605	KC2	C4C-C3C-C2C	-6.15	102.23	107.11
38	3	304	KC2	CHB-C4A-C3A	-6.15	115.38	124.98
39	1	618	II0	C04-C10-C14	-6.13	113.97	122.63
26	5	611	CLA	C4A-NA-C1A	6.13	109.46	106.71
38	P	605	KC2	CHB-C4A-C3A	-6.13	115.41	124.98
40	1	619	IHT	C32-C33-C37	-6.12	109.55	118.94
39	R	318	II0	C42-C41-C39	-6.12	110.93	123.47
40	1	619	IHT	C39-C35-C34	-6.12	108.44	118.08
39	6	613	II0	C42-C41-C39	-6.10	110.99	123.47
39	N	616	II0	C17-C04-C10	6.09	120.15	110.47
39	4	320	II0	C28-C26-C24	-6.08	104.79	116.84
28	C	516	WVN	C14-C15-C13	-6.08	113.91	122.73
28	a	406	WVN	C29-C26-C22	-6.08	118.64	127.31
39	N	617	II0	C17-C04-C10	6.08	120.12	110.47
39	Q	319	II0	C28-C26-C24	-6.08	104.81	116.84
39	P	612	II0	C42-C41-C39	-6.06	111.05	123.47
28	B	617	WVN	C20-C13-C15	-6.06	106.78	121.46
39	5	614	II0	C42-C41-C39	-6.05	111.08	123.47
39	R	315	II0	C42-C41-C39	-6.05	111.09	123.47
38	3	304	KC2	CMD-C2D-C3D	6.03	135.95	124.68
26	R	312	CLA	C4A-NA-C1A	6.02	109.41	106.71
39	3	310	II0	C38-C36-C34	-6.02	108.59	118.08
38	P	605	KC2	CMD-C2D-C3D	6.02	135.94	124.68
39	Q	315	II0	C17-C04-C10	6.02	120.03	110.47
28	H	101	WVN	C23-C20-C13	-6.01	110.32	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	1	616	II0	C38-C36-C34	-6.01	108.61	118.08
28	b	619	WVN	C21-C15-C13	-6.00	117.79	124.53
39	4	316	II0	C42-C41-C39	-6.00	111.19	123.47
39	4	316	II0	C17-C04-C10	5.99	119.99	110.47
38	2	310	KC2	C4C-C3C-C2C	-5.99	102.36	107.11
40	2	317	IHT	C39-C35-C34	-5.98	108.65	118.08
39	Q	315	II0	C42-C41-C39	-5.98	111.22	123.47
38	O	610	KC2	C4C-C3C-C2C	-5.97	102.38	107.11
26	S	605	CLA	C4A-NA-C1A	5.96	109.39	106.71
38	N	605	KC2	CHB-C4A-C3A	-5.95	115.68	124.98
39	4	315	II0	C42-C41-C39	-5.95	111.29	123.47
39	O	614	II0	C17-C04-C10	5.95	119.92	110.47
39	2	314	II0	C17-C04-C10	5.94	119.91	110.47
39	Q	314	II0	C42-C41-C39	-5.92	111.34	123.47
26	2	305	CLA	C3B-C4B-NB	5.92	116.87	109.21
39	P	614	II0	C17-C04-C10	5.92	119.87	110.47
26	6	605	CLA	C4A-NA-C1A	5.92	109.37	106.71
40	R	317	IHT	C17-C03-C11	-5.91	101.07	110.47
39	R	314	II0	C42-C41-C39	-5.91	111.36	123.47
28	B	618	WVN	C38-C34-C33	-5.91	108.77	118.08
38	4	311	KC2	CMD-C2D-C3D	5.91	135.73	124.68
39	5	613	II0	C42-C41-C39	-5.90	111.39	123.47
38	Q	310	KC2	CMD-C2D-C3D	5.89	135.71	124.68
39	1	618	II0	C33-C35-C39	-5.89	109.90	118.94
39	O	615	II0	C38-C36-C34	-5.89	108.80	118.08
39	2	316	II0	C38-C36-C34	-5.88	108.81	118.08
40	5	616	IHT	C17-C03-C11	-5.86	101.15	110.47
38	4	305	KC2	CHB-C4A-C3A	-5.86	115.82	124.98
40	1	619	IHT	C36-C33-C32	-5.86	108.84	118.08
26	N	613	CLA	C4A-NA-C1A	5.86	109.34	106.71
38	Q	304	KC2	CHB-C4A-C3A	-5.86	115.83	124.98
28	B	617	WVN	C23-C25-C28	-5.86	109.95	118.94
40	O	616	IHT	C09-C10-C07	-5.86	114.22	122.73
39	1	617	II0	C33-C35-C39	-5.83	109.99	118.94
28	B	619	WVN	C30-C28-C25	-5.83	118.99	127.31
26	g	402	CLA	C4A-NA-C1A	5.83	109.33	106.71
40	O	616	IHT	C41-C38-C35	-5.81	119.02	127.31
40	O	616	IHT	C16-C03-C11	-5.80	101.25	110.47
39	Q	319	II0	C42-C41-C39	-5.80	111.60	123.47
39	4	320	II0	C42-C41-C39	-5.80	111.60	123.47
26	3	303	CLA	C4A-NA-C1A	5.79	109.31	106.71
28	3	313	WVN	C38-C34-C33	-5.79	108.96	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	3	305	CLA	C4A-NA-C1A	5.78	109.31	106.71
28	a	406	WVN	C06-C13-C15	-5.78	114.47	122.61
40	2	317	IHT	C36-C33-C32	-5.78	108.97	118.08
26	2	301	CLA	C4A-NA-C1A	5.77	109.30	106.71
26	2	305	CLA	C1D-CHD-C4C	-5.77	113.61	126.06
26	P	606	CLA	C4A-NA-C1A	5.75	109.29	106.71
26	c	511	CLA	C4A-NA-C1A	5.75	109.29	106.71
39	4	315	II0	C17-C04-C10	5.74	119.58	110.47
40	4	318	IHT	C25-C23-C27	-5.73	114.90	122.92
39	Q	314	II0	C17-C04-C10	5.73	119.57	110.47
39	1	618	II0	C38-C36-C34	-5.72	109.06	118.08
26	1	607	CLA	C4A-NA-C1A	5.72	109.28	106.71
28	H	101	WVN	C35-C32-C31	-5.71	109.08	118.08
26	2	305	CLA	C3D-C4D-ND	5.71	119.47	110.24
39	1	617	II0	C38-C36-C34	-5.70	109.09	118.08
39	3	311	II0	C37-C35-C33	-5.70	109.09	118.08
39	3	312	II0	C37-C35-C33	-5.70	109.10	118.08
40	Q	317	IHT	C25-C23-C27	-5.70	114.94	122.92
39	P	613	II0	C37-C35-C33	-5.69	109.11	118.08
28	c	516	WVN	C29-C26-C22	-5.69	119.19	127.31
26	O	601	CLA	C4A-NA-C1A	5.69	109.26	106.71
26	P	604	CLA	C4A-NA-C1A	5.69	109.26	106.71
39	1	618	II0	C37-C35-C33	-5.69	109.12	118.08
26	2	305	CLA	C4D-CHA-C1A	-5.69	114.33	121.25
28	c	517	WVN	C04-C09-C05	-5.68	119.40	124.85
26	2	305	CLA	C1B-CHB-C4A	-5.67	118.90	130.12
28	C	516	WVN	C24-C22-C19	-5.66	109.15	118.08
39	1	615	II0	C38-C36-C34	-5.65	109.17	118.08
26	b	601	CLA	C4A-NA-C1A	5.65	109.25	106.71
26	b	604	CLA	C4A-NA-C1A	5.64	109.24	106.71
40	O	616	IHT	C25-C23-C27	-5.63	115.04	122.92
40	R	317	IHT	C16-C03-C11	-5.63	101.53	110.47
39	3	310	II0	C04-C10-C14	-5.62	114.70	122.63
28	x	101	WVN	C20-C23-C25	-5.62	117.75	126.23
39	2	315	II0	C42-C41-C39	-5.62	111.97	123.47
40	5	616	IHT	C16-C03-C11	-5.61	101.55	110.47
36	d	401	BCT	O2-C-O1	5.61	134.11	119.55
40	N	619	IHT	C25-C23-C27	-5.61	115.06	122.92
36	D	402	BCT	O2-C-O1	5.61	134.10	119.55
39	R	318	II0	C17-C04-C10	5.61	119.38	110.47
39	N	618	II0	C42-C41-C39	-5.61	111.99	123.47
39	6	613	II0	C17-C04-C10	5.61	119.38	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	x	101	WVN	C20-C13-C15	-5.60	107.89	121.46
28	H	101	WVN	C38-C34-C33	-5.59	109.26	118.08
39	3	311	II0	C38-C36-C34	-5.59	109.27	118.08
26	B	612	CLA	CMB-C2B-C1B	-5.59	119.87	128.46
39	N	620	II0	C42-C41-C39	-5.59	112.02	123.47
40	1	619	IHT	C31-C29-C26	-5.59	110.35	126.58
38	N	612	KC2	CHB-C4A-C3A	-5.58	116.25	124.98
39	1	617	II0	C37-C35-C33	-5.58	109.29	118.08
26	c	509	CLA	C4A-NA-C1A	5.57	109.21	106.71
40	2	317	IHT	C18-C07-C10	-5.57	107.97	121.46
39	P	613	II0	C38-C36-C34	-5.56	109.31	118.08
40	4	318	IHT	C09-C10-C07	-5.56	114.66	122.73
40	2	317	IHT	C32-C33-C37	-5.55	110.42	118.94
28	c	518	WVN	C30-C28-C25	-5.54	119.40	127.31
40	2	317	IHT	C22-C18-C07	-5.54	111.66	127.20
28	C	516	WVN	C38-C34-C33	-5.54	109.36	118.08
26	C	510	CLA	C4A-NA-C1A	5.53	109.19	106.71
40	Q	317	IHT	C09-C10-C07	-5.53	114.71	122.73
39	3	310	II0	C32-C30-C26	-5.52	110.55	126.58
28	B	618	WVN	C24-C22-C19	-5.52	109.39	118.08
28	3	313	WVN	C19-C22-C26	-5.52	110.48	118.94
40	1	619	IHT	C25-C23-C22	-5.51	109.39	118.08
28	d	410	WVN	C20-C13-C15	-5.51	108.11	121.46
40	5	616	IHT	C25-C23-C27	-5.51	115.21	122.92
39	4	317	II0	C42-C41-C39	-5.50	112.22	123.47
39	Q	316	II0	C42-C41-C39	-5.49	112.22	123.47
28	B	618	WVN	C23-C20-C13	-5.49	111.78	127.20
40	R	317	IHT	C25-C23-C27	-5.49	115.24	122.92
26	b	612	CLA	CMB-C2B-C1B	-5.49	120.03	128.46
28	b	618	WVN	C39-C36-C32	-5.48	119.48	127.31
39	4	314	II0	C17-C04-C10	5.48	119.17	110.47
39	Q	313	II0	C17-C04-C10	5.47	119.17	110.47
28	k	101	WVN	C40-C37-C34	-5.47	119.50	127.31
39	1	615	II0	C37-C35-C33	-5.47	109.45	118.08
39	3	312	II0	C33-C35-C39	-5.47	110.55	118.94
26	c	512	CLA	C4A-NA-C1A	5.47	109.16	106.71
28	C	516	WVN	C23-C25-C28	-5.45	110.58	118.94
28	c	516	WVN	C39-C36-C32	-5.45	119.53	127.31
26	B	601	CLA	C4A-NA-C1A	5.44	109.15	106.71
26	O	609	CLA	C4A-NA-C1A	5.44	109.15	106.71
26	C	503	CLA	C4A-NA-C1A	5.44	109.15	106.71
28	B	617	WVN	C06-C13-C15	-5.44	114.96	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	1	616	II0	C37-C35-C33	-5.43	109.52	118.08
26	C	508	CLA	C4A-NA-C1A	5.42	109.14	106.71
28	b	618	WVN	C40-C37-C34	-5.42	119.57	127.31
39	1	618	II0	C34-C36-C40	-5.40	110.65	118.94
39	3	312	II0	C34-C36-C40	-5.40	110.66	118.94
40	4	318	IHT	C40-C37-C33	-5.39	119.61	127.31
26	2	305	CLA	C2D-C1D-ND	5.39	114.08	110.10
40	Q	317	IHT	C40-C37-C33	-5.38	119.63	127.31
28	B	619	WVN	C21-C15-C13	-5.37	118.49	124.53
28	k	101	WVN	C20-C13-C15	-5.36	108.47	121.46
26	b	613	CLA	C4A-NA-C1A	5.36	109.12	106.71
26	S	610	CLA	C4A-NA-C1A	5.36	109.11	106.71
40	4	318	IHT	C17-C03-C11	-5.36	101.96	110.47
40	Q	317	IHT	C17-C03-C11	-5.35	101.96	110.47
39	3	312	II0	C38-C36-C34	-5.35	109.64	118.08
26	2	308	CLA	C4A-NA-C1A	5.34	109.11	106.71
28	C	516	WVN	C35-C32-C31	-5.34	109.67	118.08
26	5	605	CLA	C4A-NA-C1A	5.33	109.10	106.71
26	6	610	CLA	C4A-NA-C1A	5.32	109.10	106.71
28	b	617	WVN	C20-C13-C15	-5.32	108.58	121.46
26	B	604	CLA	C4A-NA-C1A	5.32	109.10	106.71
26	2	309	CLA	C4A-NA-C1A	5.32	109.10	106.71
39	N	617	II0	C42-C41-C39	-5.32	112.58	123.47
26	R	306	CLA	C4A-NA-C1A	5.30	109.09	106.71
26	S	604	CLA	C4A-NA-C1A	5.30	109.09	106.71
26	3	301	CLA	C4A-NA-C1A	5.30	109.09	106.71
28	B	618	WVN	C35-C32-C31	-5.29	109.74	118.08
26	D	407	CLA	C4A-NA-C1A	5.28	109.08	106.71
26	6	604	CLA	C4A-NA-C1A	5.28	109.08	106.71
26	B	616	CLA	C4A-NA-C1A	5.27	109.08	106.71
26	C	511	CLA	C4A-NA-C1A	5.27	109.08	106.71
26	b	615	CLA	C4A-NA-C1A	5.27	109.08	106.71
39	2	316	II0	C31-C29-C25	-5.25	111.32	126.58
39	1	618	II0	C32-C30-C26	-5.25	111.33	126.58
39	O	615	II0	C31-C29-C25	-5.25	111.33	126.58
26	c	507	CLA	C4A-NA-C1A	5.25	109.07	106.71
38	N	611	KC2	C3A-C4A-NA	5.25	116.30	110.57
40	N	619	IHT	C17-C03-C11	-5.24	102.14	110.47
26	c	504	CLA	C4A-NA-C1A	5.24	109.06	106.71
26	P	602	CLA	C4A-NA-C1A	5.24	109.06	106.71
40	1	619	IHT	C18-C07-C10	-5.23	108.78	121.46
38	S	608	KC2	C3A-C4A-NA	5.23	116.28	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	5	603	CLA	C4A-NA-C1A	5.23	109.06	106.71
29	d	407	PL9	C7-C3-C4	5.23	121.13	116.88
26	b	612	CLA	C4A-NA-C1A	5.22	109.05	106.71
26	O	608	CLA	C4A-NA-C1A	5.22	109.05	106.71
39	3	312	II0	C32-C30-C26	-5.22	111.42	126.58
26	4	302	CLA	C4A-NA-C1A	5.22	109.05	106.71
39	3	310	II0	C37-C35-C33	-5.21	109.86	118.08
38	6	608	KC2	C3A-C4A-NA	5.21	116.26	110.57
26	3	307	CLA	C4A-NA-C1A	5.20	109.05	106.71
39	1	616	II0	C32-C30-C26	-5.20	111.49	126.58
28	d	410	WVN	C21-C15-C13	-5.19	118.69	124.53
26	N	608	CLA	C1D-ND-C4D	-5.19	102.64	106.33
29	A	407	PL9	C7-C3-C4	5.19	121.10	116.88
26	N	614	CLA	C4A-NA-C1A	5.18	109.04	106.71
26	Q	301	CLA	C4A-NA-C1A	5.17	109.03	106.71
28	a	406	WVN	C08-C01-C02	5.17	117.38	109.55
26	P	607	CLA	C4A-NA-C1A	5.17	109.03	106.71
29	a	407	PL9	C7-C3-C4	5.17	121.08	116.88
38	Q	310	KC2	C3A-C4A-NA	5.17	116.21	110.57
26	R	304	CLA	C4A-NA-C1A	5.16	109.03	106.71
40	1	619	IHT	C22-C18-C07	-5.16	112.70	127.20
28	Z	101	WVN	C04-C09-C05	-5.16	119.90	124.85
26	B	612	CLA	C4A-NA-C1A	5.16	109.03	106.71
28	B	617	WVN	C38-C34-C33	-5.16	109.94	118.08
39	1	617	II0	C34-C36-C40	-5.16	111.02	118.94
28	P	615	WVN	C14-C15-C13	-5.16	115.24	122.73
26	S	606	CLA	C4A-NA-C1A	5.15	109.02	106.71
28	D	412	WVN	C20-C13-C15	-5.15	108.98	121.46
28	B	617	WVN	C31-C32-C36	-5.15	111.04	118.94
28	C	516	WVN	C27-C25-C23	-5.15	109.97	118.08
38	4	311	KC2	C3A-C4A-NA	5.15	116.19	110.57
26	C	513	CLA	C4A-NA-C1A	5.14	109.02	106.71
39	1	615	II0	C34-C36-C40	-5.14	111.05	118.94
26	O	611	CLA	C4A-NA-C1A	5.14	109.02	106.71
28	b	617	WVN	C29-C26-C22	-5.14	119.97	127.31
28	B	618	WVN	C27-C25-C23	-5.14	109.98	118.08
28	Z	101	WVN	C40-C37-C34	-5.14	119.98	127.31
26	N	601	CLA	C4A-NA-C1A	5.13	109.01	106.71
28	3	313	WVN	C35-C32-C31	-5.13	109.99	118.08
38	2	310	KC2	C3A-C4A-NA	5.12	116.16	110.57
26	2	302	CLA	C4A-NA-C1A	5.12	109.01	106.71
26	O	602	CLA	C4A-NA-C1A	5.11	109.00	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	310	KC2	C3A-C4A-NA	5.11	116.15	110.57
26	b	602	CLA	C4A-NA-C1A	5.11	109.00	106.71
26	P	610	CLA	C4A-NA-C1A	5.10	109.00	106.71
28	D	412	WVN	C21-C15-C13	-5.10	118.80	124.53
26	3	306	CLA	C4A-NA-C1A	5.10	109.00	106.71
26	S	602	CLA	C4A-NA-C1A	5.10	109.00	106.71
26	6	602	CLA	C4A-NA-C1A	5.10	109.00	106.71
38	O	610	KC2	C3A-C4A-NA	5.09	116.13	110.57
38	Q	309	KC2	C3A-C4A-NA	5.09	116.13	110.57
28	k	101	WVN	C20-C23-C25	-5.08	118.55	126.23
38	S	608	KC2	CHC-C1C-NC	-5.08	116.20	124.20
38	Q	310	KC2	CHC-C1C-NC	-5.08	116.21	124.20
26	6	606	CLA	C4A-NA-C1A	5.08	108.99	106.71
38	4	311	KC2	CHC-C1C-NC	-5.07	116.22	124.20
28	b	619	WVN	C04-C09-C05	-5.07	119.99	124.85
26	N	602	CLA	C4A-NA-C1A	5.07	108.99	106.71
26	2	304	CLA	C4A-NA-C1A	5.07	108.99	106.71
26	2	311	CLA	C4A-NA-C1A	5.07	108.98	106.71
26	5	607	CLA	C4A-NA-C1A	5.07	108.98	106.71
39	3	312	II0	C31-C29-C25	-5.07	111.86	126.58
26	B	615	CLA	C4A-NA-C1A	5.07	108.98	106.71
38	6	608	KC2	CHC-C1C-NC	-5.06	116.23	124.20
39	3	311	II0	C03-C09-C13	-5.06	115.49	122.63
39	P	613	II0	C03-C09-C13	-5.06	115.49	122.63
38	5	610	KC2	CHC-C1C-NC	-5.06	116.24	124.20
37	f	101	HEM	CHC-C4B-NB	5.05	129.92	124.43
28	3	313	WVN	C31-C32-C36	-5.05	111.19	118.94
38	R	311	KC2	CHC-C1C-NC	-5.05	116.25	124.20
26	b	616	CLA	C4A-NA-C1A	5.04	108.97	106.71
26	2	305	CLA	C4A-NA-C1A	-5.04	104.44	106.71
28	b	617	WVN	C40-C37-C34	-5.03	120.13	127.31
40	R	317	IHT	C41-C38-C35	-5.03	120.13	127.31
26	N	604	CLA	C4A-NA-C1A	5.02	108.97	106.71
26	P	609	CLA	C4A-NA-C1A	5.02	108.97	106.71
38	N	611	KC2	CHC-C1C-NC	-5.02	116.30	124.20
26	R	308	CLA	C4A-NA-C1A	5.02	108.96	106.71
39	3	311	II0	C32-C30-C26	-5.01	112.02	126.58
39	6	612	II0	C19-C13-C09	-5.01	117.54	124.35
26	B	602	CLA	C4A-NA-C1A	5.01	108.96	106.71
26	O	604	CLA	C4A-NA-C1A	5.01	108.96	106.71
38	N	605	KC2	CHC-C1C-NC	-5.00	116.32	124.20
39	S	612	II0	C19-C13-C09	-5.00	117.55	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	506	CLA	C4A-NA-C1A	5.00	108.95	106.71
26	c	514	CLA	C4A-NA-C1A	5.00	108.95	106.71
38	Q	304	KC2	CHD-C4C-C3C	-5.00	107.99	126.11
39	P	613	II0	C32-C30-C26	-5.00	112.07	126.58
26	d	405	CLA	C4A-NA-C1A	5.00	108.95	106.71
26	g	401	CLA	C4A-NA-C1A	5.00	108.95	106.71
38	4	305	KC2	CHD-C4C-C3C	-5.00	108.00	126.11
38	N	605	KC2	C3A-C4A-NA	4.99	116.03	110.57
26	C	506	CLA	C4A-NA-C1A	4.99	108.95	106.71
26	B	610	CLA	C4A-NA-C1A	4.99	108.95	106.71
28	x	101	WVN	C39-C36-C32	-4.99	120.19	127.31
40	5	616	IHT	C41-C38-C35	-4.98	120.20	127.31
29	D	409	PL9	C7-C3-C4	4.98	120.92	116.88
40	O	616	IHT	C17-C03-C11	-4.98	102.56	110.47
28	D	412	WVN	C39-C36-C32	-4.97	120.21	127.31
38	N	612	KC2	CHD-C4C-C3C	-4.97	108.09	126.11
40	N	619	IHT	C40-C37-C33	-4.97	120.22	127.31
38	6	608	KC2	CHD-C4C-C3C	-4.96	108.13	126.11
38	S	608	KC2	CHD-C4C-C3C	-4.96	108.13	126.11
38	4	310	KC2	CHC-C1C-NC	-4.96	116.40	124.20
38	Q	309	KC2	CHC-C1C-NC	-4.94	116.42	124.20
28	b	617	WVN	C21-C15-C13	-4.94	118.98	124.53
28	3	313	WVN	C24-C22-C19	-4.94	110.29	118.08
39	1	616	II0	C31-C29-C25	-4.93	112.25	126.58
26	B	613	CLA	C4A-NA-C1A	4.93	108.92	106.71
40	1	619	IHT	C34-C35-C38	-4.93	111.38	118.94
28	x	101	WVN	C29-C26-C22	-4.92	120.28	127.31
38	2	310	KC2	CHC-C1C-NC	-4.92	116.45	124.20
28	k	101	WVN	C21-C15-C13	-4.92	119.01	124.53
28	c	518	WVN	C40-C37-C34	-4.91	120.30	127.31
39	1	618	II0	C31-C29-C25	-4.91	112.32	126.58
28	C	516	WVN	C23-C20-C13	-4.90	113.43	127.20
26	B	608	CLA	CMB-C2B-C1B	-4.89	120.95	128.46
38	N	612	KC2	C4B-CHC-C1C	-4.89	115.52	126.06
38	3	304	KC2	CHC-C1C-NC	-4.88	116.51	124.20
37	F	101	HEM	CHC-C4B-NB	4.88	129.73	124.43
26	b	608	CLA	CMB-C2B-C1B	-4.88	120.96	128.46
26	C	512	CLA	C4A-NA-C1A	4.88	108.90	106.71
38	P	605	KC2	CHC-C1C-NC	-4.88	116.52	124.20
38	O	610	KC2	C4B-CHC-C1C	-4.88	115.54	126.06
38	O	610	KC2	CHC-C1C-NC	-4.88	116.52	124.20
28	b	619	WVN	C40-C37-C34	-4.88	120.35	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	N	611	KC2	CHD-C4C-C3C	-4.87	108.45	126.11
38	2	310	KC2	C4B-CHC-C1C	-4.87	115.55	126.06
39	3	310	II0	C31-C29-C25	-4.87	112.44	126.58
39	1	615	II0	C31-C29-C25	-4.87	112.45	126.58
38	R	311	KC2	CHD-C4C-C3C	-4.86	108.48	126.11
26	A	405	CLA	C4A-NA-C1A	4.86	108.89	106.71
38	5	610	KC2	CHD-C4C-C3C	-4.86	108.49	126.11
39	1	617	II0	C32-C30-C26	-4.86	112.47	126.58
28	C	516	WVN	C20-C13-C15	-4.86	109.69	121.46
39	4	314	II0	C42-C41-C39	-4.85	113.53	123.47
28	x	101	WVN	C30-C28-C25	-4.85	120.39	127.31
38	Q	310	KC2	CHD-C4C-C3C	-4.84	108.56	126.11
38	N	610	KC2	CHD-C4C-C3C	-4.84	108.56	126.11
39	Q	313	II0	C42-C41-C39	-4.84	113.56	123.47
28	S	613	WVN	C04-C09-C05	-4.84	120.21	124.85
38	4	311	KC2	CHD-C4C-C3C	-4.84	108.58	126.11
26	O	605	CLA	C4A-NA-C1A	4.84	108.88	106.71
26	b	610	CLA	C4A-NA-C1A	4.83	108.88	106.71
28	5	617	WVN	C04-C09-C05	-4.83	120.22	124.85
26	D	408	CLA	C4A-NA-C1A	4.83	108.88	106.71
26	Q	308	CLA	C4A-NA-C1A	4.83	108.88	106.71
38	3	304	KC2	C3A-C4A-NA	4.83	115.84	110.57
39	1	615	II0	C32-C30-C26	-4.83	112.57	126.58
28	B	619	WVN	C40-C37-C34	-4.82	120.43	127.31
40	Q	317	IHT	C03-C11-C15	-4.82	115.83	122.63
38	N	610	KC2	C4B-CHC-C1C	-4.81	115.68	126.06
38	N	610	KC2	C3A-C4A-NA	4.80	115.81	110.57
39	2	314	II0	C19-C13-C09	-4.80	117.82	124.35
28	H	101	WVN	C24-C22-C19	-4.80	110.51	118.08
26	N	609	CLA	C4A-NA-C1A	4.80	108.86	106.71
28	b	617	WVN	C39-C36-C32	-4.79	120.47	127.31
39	O	614	II0	C19-C13-C09	-4.79	117.84	124.35
26	c	508	CLA	CMB-C2B-C1B	-4.79	121.10	128.46
26	c	510	CLA	CMB-C2B-C1B	-4.79	121.10	128.46
38	Q	309	KC2	CHD-C4C-C3C	-4.79	108.75	126.11
38	4	310	KC2	CHD-C4C-C3C	-4.79	108.76	126.11
38	Q	304	KC2	C4B-CHC-C1C	-4.79	115.73	126.06
38	6	608	KC2	C4B-CHC-C1C	-4.78	115.74	126.06
38	4	305	KC2	CHC-C1C-NC	-4.78	116.67	124.20
26	b	605	CLA	C4A-NA-C1A	4.78	108.86	106.71
39	O	615	II0	C33-C35-C39	-4.77	111.61	118.94
38	P	605	KC2	C3A-C4A-NA	4.77	115.78	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	305	KC2	C4B-CHC-C1C	-4.77	115.76	126.06
26	C	507	CLA	CMB-C2B-C1B	-4.77	121.13	128.46
39	P	613	II0	C19-C13-C11	-4.77	105.52	114.36
28	3	313	WVN	C06-C13-C15	-4.77	115.90	122.61
28	b	618	WVN	C30-C28-C25	-4.77	120.51	127.31
39	3	311	II0	C19-C13-C11	-4.76	105.53	114.36
38	S	608	KC2	C4B-CHC-C1C	-4.76	115.78	126.06
38	N	611	KC2	C4B-CHC-C1C	-4.76	115.79	126.06
26	c	513	CLA	C4A-NA-C1A	4.76	108.85	106.71
38	3	304	KC2	CHD-C4C-C3C	-4.76	108.87	126.11
38	Q	304	KC2	CHC-C1C-NC	-4.76	116.71	124.20
38	P	605	KC2	CHD-C4C-C3C	-4.76	108.87	126.11
26	C	509	CLA	CMB-C2B-C1B	-4.75	121.16	128.46
40	4	318	IHT	C03-C11-C15	-4.75	115.93	122.63
26	2	305	CLA	C1C-C2C-C3C	-4.75	101.97	106.96
38	O	610	KC2	CHD-C4C-C3C	-4.75	108.91	126.11
26	a	405	CLA	C4A-NA-C1A	4.74	108.84	106.71
39	3	312	II0	C12-C14-C10	-4.74	109.81	120.57
26	B	612	CLA	CMB-C2B-C3B	4.74	133.54	124.68
38	2	310	KC2	CHD-C4C-C3C	-4.74	108.94	126.11
40	O	616	IHT	C03-C11-C15	-4.74	115.94	122.63
38	5	610	KC2	C3A-C4A-NA	4.74	115.74	110.57
39	2	316	II0	C33-C35-C39	-4.74	111.67	118.94
26	P	601	CLA	C4A-NA-C1A	4.73	108.83	106.71
38	N	610	KC2	CHC-C1C-NC	-4.73	116.75	124.20
26	5	609	CLA	C4A-NA-C1A	4.73	108.83	106.71
38	5	610	KC2	C4B-CHC-C1C	-4.73	115.86	126.06
26	R	303	CLA	C4A-NA-C1A	4.72	108.83	106.71
26	C	505	CLA	C4A-NA-C1A	4.72	108.83	106.71
38	R	311	KC2	C4B-CHC-C1C	-4.72	115.88	126.06
26	3	309	CLA	C4A-NA-C1A	4.71	108.82	106.71
26	5	608	CLA	C4A-NA-C1A	4.71	108.82	106.71
38	N	605	KC2	CHD-C4C-C3C	-4.70	109.07	126.11
28	A	406	WVN	C30-C28-C25	-4.70	120.60	127.31
26	d	402	CLA	C4A-NA-C1A	4.70	108.82	106.71
26	R	310	CLA	C4A-NA-C1A	4.70	108.82	106.71
39	O	615	II0	C32-C30-C26	-4.70	112.95	126.58
39	2	316	II0	C32-C30-C26	-4.69	112.95	126.58
38	R	311	KC2	C3A-C4A-NA	4.69	115.70	110.57
26	B	605	CLA	C4A-NA-C1A	4.69	108.82	106.71
26	5	602	CLA	C4A-NA-C1A	4.69	108.81	106.71
26	N	606	CLA	C4A-NA-C1A	4.68	108.81	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	3	311	II0	C31-C29-C25	-4.68	112.98	126.58
26	G	402	CLA	C4A-NA-C1A	4.68	108.81	106.71
39	P	613	II0	C31-C29-C25	-4.67	113.02	126.58
28	Y	101	WVN	C39-C36-C32	-4.67	120.64	127.31
38	3	304	KC2	C4B-CHC-C1C	-4.66	116.00	126.06
39	1	617	II0	C31-C29-C25	-4.66	113.06	126.58
40	N	619	IHT	C08-C12-C15	4.65	121.12	111.85
26	4	309	CLA	C4A-NA-C1A	4.65	108.80	106.71
38	4	311	KC2	C1B-CHB-C4A	-4.64	116.04	126.06
38	P	605	KC2	C4B-CHC-C1C	-4.64	116.05	126.06
26	b	612	CLA	CMB-C2B-C3B	4.64	133.36	124.68
38	Q	309	KC2	C4B-CHC-C1C	-4.64	116.05	126.06
38	Q	310	KC2	C1B-CHB-C4A	-4.64	116.06	126.06
38	4	311	KC2	CHB-C1B-C2B	-4.64	115.75	125.48
40	O	616	IHT	C08-C12-C15	4.63	121.08	111.85
26	b	609	CLA	C4A-NA-C1A	4.63	108.79	106.71
26	d	406	CLA	C4A-NA-C1A	4.63	108.79	106.71
26	P	611	CLA	C4A-NA-C1A	4.63	108.79	106.71
39	N	616	II0	C19-C13-C09	-4.63	118.06	124.35
38	Q	304	KC2	C3A-C4A-NA	4.62	115.62	110.57
38	4	310	KC2	C4B-CHC-C1C	-4.62	116.08	126.06
26	B	609	CLA	C4A-NA-C1A	4.62	108.78	106.71
26	2	319	CLA	C4A-NA-C1A	4.62	108.78	106.71
38	N	612	KC2	C3A-C4A-NA	4.62	115.62	110.57
39	2	316	II0	C34-C36-C40	-4.62	111.85	118.94
40	N	619	IHT	C30-C27-C23	-4.62	120.72	127.31
38	4	305	KC2	C3A-C4A-NA	4.62	115.61	110.57
38	N	612	KC2	CHC-C1C-NC	-4.62	116.93	124.20
39	O	615	II0	C34-C36-C40	-4.62	111.86	118.94
26	1	614	CLA	C4A-NA-C1A	4.62	108.78	106.71
38	Q	310	KC2	CHB-C1B-C2B	-4.62	115.80	125.48
26	G	401	CLA	C4A-NA-C1A	4.61	108.78	106.71
26	c	515	CLA	C4A-NA-C1A	4.61	108.78	106.71
26	R	309	CLA	C4A-NA-C1A	4.60	108.78	106.71
38	N	610	KC2	CHB-C1B-C2B	-4.60	115.82	125.48
38	4	311	KC2	C4B-CHC-C1C	-4.60	116.13	126.06
38	4	305	KC2	CHB-C1B-C2B	-4.60	115.84	125.48
38	Q	310	KC2	C4B-CHC-C1C	-4.60	116.14	126.06
39	P	614	II0	C19-C13-C09	-4.59	118.11	124.35
38	N	605	KC2	C1B-CHB-C4A	-4.59	116.16	126.06
38	S	608	KC2	C1B-CHB-C4A	-4.58	116.18	126.06
38	P	605	KC2	CHB-C1B-C2B	-4.57	115.89	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	N	611	KC2	CHB-C1B-C2B	-4.57	115.89	125.48
38	Q	304	KC2	CHB-C1B-C2B	-4.57	115.90	125.48
38	6	608	KC2	C1B-CHB-C4A	-4.57	116.21	126.06
38	3	304	KC2	CHB-C1B-C2B	-4.56	115.92	125.48
28	H	101	WVN	C31-C32-C36	-4.56	111.95	118.94
26	O	607	CLA	C4A-NA-C1A	4.55	108.75	106.71
26	R	302	CLA	C4A-NA-C1A	4.55	108.75	106.71
26	S	601	CLA	C4A-NA-C1A	4.55	108.75	106.71
26	2	305	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
28	b	617	WVN	C30-C28-C25	-4.55	120.82	127.31
28	c	516	WVN	C20-C13-C15	-4.55	110.45	121.46
26	4	306	CLA	C4A-NA-C1A	4.54	108.75	106.71
26	b	611	CLA	CMB-C2B-C1B	-4.54	121.49	128.46
38	N	611	KC2	C1B-CHB-C4A	-4.54	116.27	126.06
26	R	305	CLA	C4A-NA-C1A	4.53	108.74	106.71
28	5	617	WVN	C39-C36-C32	-4.53	120.85	127.31
38	S	608	KC2	CHB-C1B-C2B	-4.53	115.98	125.48
33	a	413	LMG	O7-C10-C11	4.53	121.26	111.50
26	c	508	CLA	C4A-NA-C1A	4.53	108.74	106.71
26	3	305	CLA	CMB-C2B-C1B	-4.53	121.51	128.46
28	C	516	WVN	C19-C22-C26	-4.52	112.00	118.94
40	4	318	IHT	C41-C38-C35	-4.52	120.86	127.31
28	d	410	WVN	C39-C36-C32	-4.52	120.86	127.31
38	6	608	KC2	CHB-C1B-C2B	-4.51	116.01	125.48
28	S	613	WVN	C39-C36-C32	-4.51	120.87	127.31
26	6	601	CLA	C4A-NA-C1A	4.51	108.73	106.71
38	N	612	KC2	C4B-C3B-C2B	-4.51	103.05	106.75
40	Q	317	IHT	C41-C38-C35	-4.50	120.89	127.31
26	4	304	CLA	C4A-NA-C1A	4.50	108.73	106.71
28	A	406	WVN	C20-C13-C15	-4.49	110.58	121.46
38	N	605	KC2	CHB-C1B-C2B	-4.49	116.07	125.48
39	6	613	II0	C06-C04-C10	4.48	118.71	109.62
26	5	601	CLA	C4A-NA-C1A	4.48	108.72	106.71
28	c	518	WVN	C14-C15-C13	-4.48	116.23	122.73
40	R	317	IHT	C41-C40-C37	-4.48	114.30	123.47
38	O	610	KC2	C4B-C3B-C2B	-4.48	103.08	106.75
38	5	610	KC2	CHB-C1B-C2B	-4.48	116.09	125.48
39	R	318	II0	C06-C04-C10	4.48	118.69	109.62
38	4	310	KC2	CHB-C1B-C2B	-4.47	116.10	125.48
28	b	618	WVN	C29-C26-C22	-4.47	120.92	127.31
28	C	516	WVN	C31-C32-C36	-4.47	112.08	118.94
26	1	614	CLA	C1B-CHB-C4A	-4.47	121.26	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Q	305	CLA	C4A-NA-C1A	4.47	108.72	106.71
28	B	619	WVN	C39-C40-C37	-4.47	114.31	123.47
40	5	616	IHT	C41-C40-C37	-4.47	114.31	123.47
26	6	607	CLA	C4A-NA-C1A	4.47	108.72	106.71
38	2	310	KC2	C4B-C3B-C2B	-4.47	103.08	106.75
38	R	311	KC2	CHB-C1B-C2B	-4.47	116.11	125.48
26	P	606	CLA	CMB-C2B-C1B	-4.47	121.60	128.46
39	3	312	II0	C11-C13-C09	-4.47	110.43	120.57
28	B	618	WVN	C20-C13-C15	-4.46	110.65	121.46
26	5	606	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
26	2	307	CLA	C4A-NA-C1A	4.46	108.71	106.71
26	5	604	CLA	C4A-NA-C1A	4.46	108.71	106.71
26	B	611	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
26	C	507	CLA	C4A-NA-C1A	4.46	108.71	106.71
39	R	314	II0	C19-C13-C09	-4.45	118.30	124.35
28	B	619	WVN	C20-C13-C15	-4.45	110.69	121.46
26	R	307	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
38	Q	309	KC2	CHB-C1B-C2B	-4.44	116.17	125.48
28	B	617	WVN	C27-C25-C23	-4.44	111.08	118.08
26	P	608	CLA	C4A-NA-C1A	4.43	108.70	106.71
26	S	606	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
39	P	612	II0	C19-C13-C09	-4.43	118.33	124.35
39	5	613	II0	C19-C13-C09	-4.43	118.33	124.35
26	b	607	CLA	C4A-NA-C1A	4.42	108.69	106.71
38	N	605	KC2	C4B-CHC-C1C	-4.42	116.52	126.06
26	4	301	CLA	C4A-NA-C1A	4.42	108.69	106.71
38	4	310	KC2	C1B-CHB-C4A	-4.42	116.53	126.06
28	S	613	WVN	C20-C13-C15	-4.42	110.76	121.46
26	Q	303	CLA	C4A-NA-C1A	4.41	108.69	106.71
26	S	609	CLA	C4A-NA-C1A	4.41	108.69	106.71
26	6	606	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
28	5	617	WVN	C20-C13-C15	-4.41	110.78	121.46
39	Q	316	II0	C19-C13-C09	-4.40	118.36	124.35
38	Q	309	KC2	C1B-CHB-C4A	-4.40	116.57	126.06
39	4	317	II0	C19-C13-C09	-4.39	118.38	124.35
40	R	317	IHT	C03-C11-C15	-4.39	116.44	122.63
26	S	607	CLA	C4A-NA-C1A	4.38	108.68	106.71
26	6	609	CLA	C4A-NA-C1A	4.38	108.67	106.71
39	1	616	II0	C06-C04-C10	4.37	118.49	109.62
28	c	518	WVN	C20-C23-C25	-4.37	119.63	126.23
40	5	616	IHT	C03-C11-C15	-4.37	116.46	122.63
39	1	616	II0	C34-C36-C40	-4.37	112.24	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	3	301	CLA	CMB-C2B-C1B	-4.36	121.76	128.46
26	P	602	CLA	CMB-C2B-C1B	-4.36	121.76	128.46
26	D	404	CLA	C4A-NA-C1A	4.36	108.67	106.71
26	c	503	CLA	C4A-NA-C1A	4.36	108.67	106.71
39	N	618	II0	C19-C13-C09	-4.35	118.43	124.35
26	c	506	CLA	CMB-C2B-C1B	-4.34	121.79	128.46
26	A	403	CLA	C4A-NA-C1A	4.34	108.66	106.71
26	S	604	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
28	b	617	WVN	C40-C39-C36	-4.34	114.59	123.47
26	6	604	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
39	1	615	II0	C28-C26-C24	-4.33	108.27	116.84
26	Q	311	CLA	C4A-NA-C1A	4.32	108.65	106.71
28	B	617	WVN	C33-C34-C37	-4.31	112.32	118.94
28	B	618	WVN	C31-C32-C36	-4.31	112.33	118.94
38	N	611	KC2	C4B-C3B-C2B	-4.31	103.22	106.75
26	O	603	CLA	CMB-C2B-C1B	-4.30	121.85	128.46
33	A	412	LMG	O7-C10-C11	4.30	120.77	111.50
38	N	612	KC2	CHB-C1B-C2B	-4.30	116.47	125.48
26	C	510	CLA	CMB-C2B-C1B	-4.29	121.87	128.46
26	B	611	CLA	C4A-NA-C1A	4.29	108.64	106.71
26	C	505	CLA	CMB-C2B-C1B	-4.29	121.87	128.46
26	R	313	CLA	C4A-NA-C1A	4.29	108.63	106.71
26	B	606	CLA	C4A-NA-C1A	4.28	108.63	106.71
40	N	619	IHT	C03-C11-C15	-4.28	116.59	122.63
38	5	610	KC2	C4B-C3B-C2B	-4.28	103.24	106.75
26	B	607	CLA	C4A-NA-C1A	4.27	108.63	106.71
28	k	101	WVN	C39-C36-C32	-4.27	121.22	127.31
38	O	610	KC2	C1B-CHB-C4A	-4.27	116.86	126.06
26	2	303	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
35	c	519	DGD	O2G-C1B-C2B	4.26	120.67	111.50
39	O	613	II0	C19-C13-C09	-4.26	118.57	124.35
39	2	313	II0	C19-C13-C09	-4.25	118.57	124.35
38	2	310	KC2	C1B-CHB-C4A	-4.25	116.89	126.06
26	b	606	CLA	C4A-NA-C1A	4.25	108.62	106.71
26	B	603	CLA	C4A-NA-C1A	4.25	108.61	106.71
26	5	612	CLA	C4A-NA-C1A	4.25	108.61	106.71
34	l	101	LHG	O7-C7-C8	4.25	120.65	111.50
37	f	101	HEM	C1B-NB-C4B	4.24	109.46	105.07
38	R	311	KC2	C4B-C3B-C2B	-4.24	103.27	106.75
38	5	610	KC2	C1B-CHB-C4A	-4.23	116.92	126.06
38	R	311	KC2	C1B-CHB-C4A	-4.23	116.92	126.06
26	3	303	CLA	CMB-C2B-C1B	-4.23	121.96	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P	604	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
26	3	307	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
26	c	511	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
26	P	610	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
28	c	517	WVN	C20-C13-C15	-4.23	111.22	121.46
38	P	605	KC2	C1B-CHB-C4A	-4.23	116.94	126.06
34	L	101	LHG	O7-C7-C8	4.22	120.60	111.50
40	Q	317	IHT	C30-C27-C23	-4.22	121.28	127.31
38	3	304	KC2	C1B-CHB-C4A	-4.22	116.95	126.06
26	C	514	CLA	C4A-NA-C1A	4.22	108.60	106.71
26	4	312	CLA	C4A-NA-C1A	4.22	108.60	106.71
26	Q	311	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
26	O	612	CLA	C4A-NA-C1A	4.21	108.60	106.71
26	P	609	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
39	Q	314	II0	C19-C13-C09	-4.21	118.63	124.35
28	3	313	WVN	C27-C25-C23	-4.20	111.45	118.08
28	3	313	WVN	C33-C34-C37	-4.20	112.49	118.94
26	a	403	CLA	C4A-NA-C1A	4.20	108.59	106.71
40	4	318	IHT	C30-C27-C23	-4.20	121.32	127.31
26	4	312	CLA	CMB-C2B-C1B	-4.20	122.02	128.46
26	6	605	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
35	C	517	DGD	O2G-C1B-C2B	4.19	120.53	111.50
26	S	605	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
38	6	608	KC2	C4B-C3B-C2B	-4.18	103.32	106.75
26	C	502	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
26	2	305	CLA	C2A-C1A-CHA	-4.18	116.55	123.86
38	2	310	KC2	CHB-C1B-C2B	-4.17	116.72	125.48
39	4	315	II0	C19-C13-C09	-4.17	118.68	124.35
38	O	610	KC2	CHB-C1B-C2B	-4.17	116.73	125.48
26	B	607	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
26	D	408	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
26	c	503	CLA	CMB-C2B-C1B	-4.16	122.06	128.46
28	Z	101	WVN	C29-C26-C22	-4.16	121.37	127.31
26	2	312	CLA	C4A-NA-C1A	4.15	108.57	106.71
28	3	313	WVN	C20-C13-C15	-4.15	111.41	121.46
39	S	611	II0	C19-C13-C09	-4.15	118.71	124.35
26	4	309	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
40	R	317	IHT	C19-C10-C07	-4.14	119.88	124.53
33	C	519	LMG	O7-C10-C11	4.14	120.42	111.50
26	S	609	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
39	P	613	II0	C33-C35-C39	-4.13	112.60	118.94
38	N	610	KC2	C1B-CHB-C4A	-4.13	117.15	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	S	608	KC2	C4B-C3B-C2B	-4.13	103.36	106.75
39	6	611	II0	C19-C13-C09	-4.12	118.75	124.35
26	Q	308	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
28	a	406	WVN	C20-C23-C25	-4.12	120.01	126.23
26	6	609	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
28	B	618	WVN	C19-C22-C26	-4.12	112.62	118.94
37	f	101	HEM	CHD-C1D-ND	4.11	128.90	124.43
39	3	311	II0	C33-C35-C39	-4.11	112.63	118.94
33	D	413	LMG	O7-C10-C11	4.11	120.37	111.50
33	B	620	LMG	O7-C10-C11	4.11	120.36	111.50
26	C	502	CLA	C4A-NA-C1A	4.11	108.55	106.71
33	d	411	LMG	O7-C10-C11	4.11	120.36	111.50
26	Q	312	CLA	C4A-NA-C1A	4.10	108.55	106.71
26	C	511	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
34	c	520	LHG	O7-C7-C8	4.09	120.32	111.50
39	N	616	II0	C06-C04-C10	4.09	117.91	109.62
30	D	401	SQD	O47-C7-C8	4.09	120.32	111.50
26	b	611	CLA	C4A-NA-C1A	4.09	108.54	106.71
39	3	311	II0	C34-C36-C40	-4.09	112.67	118.94
26	b	607	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
26	d	406	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
28	A	406	WVN	C02-C05-C09	-4.09	116.44	121.47
39	P	613	II0	C34-C36-C40	-4.09	112.67	118.94
28	Y	101	WVN	C40-C37-C34	-4.08	121.49	127.31
26	2	305	CLA	CHC-C1C-C2C	-4.08	115.44	126.72
26	1	603	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
37	F	101	HEM	CHD-C1D-ND	4.07	128.86	124.43
34	b	621	LHG	O7-C7-C8	4.07	120.28	111.50
28	c	518	WVN	C39-C36-C32	-4.07	121.50	127.31
34	d	408	LHG	O7-C7-C8	4.07	120.27	111.50
26	4	313	CLA	C4A-NA-C1A	4.07	108.53	106.71
26	6	604	CLA	CMB-C2B-C3B	4.07	132.29	124.68
39	P	614	II0	C06-C04-C10	4.07	117.86	109.62
40	5	616	IHT	C19-C10-C07	-4.06	119.97	124.53
30	c	501	SQD	O47-C7-C8	4.06	120.25	111.50
33	c	522	LMG	O7-C10-C11	4.06	120.24	111.50
26	4	304	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
26	S	604	CLA	CMB-C2B-C3B	4.06	132.27	124.68
26	3	302	CLA	C4A-NA-C1A	4.05	108.53	106.71
34	D	410	LHG	O7-C7-C8	4.05	120.22	111.50
28	b	617	WVN	C23-C20-C13	-4.05	115.84	127.20
38	4	305	KC2	C1B-CHB-C4A	-4.04	117.34	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	305	KC2	C4B-C3B-C2B	-4.04	103.43	106.75
39	R	315	II0	C19-C13-C09	-4.04	118.86	124.35
38	Q	304	KC2	C1B-CHB-C4A	-4.04	117.35	126.06
28	x	101	WVN	C40-C37-C34	-4.04	121.55	127.31
26	c	512	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
28	3	313	WVN	C16-C05-C09	-4.02	108.02	122.33
26	N	603	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
39	2	316	II0	C11-C13-C09	-4.02	111.44	120.57
38	Q	304	KC2	C4B-C3B-C2B	-4.02	103.45	106.75
33	C	520	LMG	O7-C10-C11	4.02	120.16	111.50
39	2	313	II0	C20-C14-C10	-4.02	118.89	124.35
33	D	406	LMG	O7-C10-C11	4.02	120.16	111.50
33	b	620	LMG	O7-C10-C11	4.02	120.16	111.50
39	1	618	II0	C20-C14-C12	-4.01	106.92	114.36
26	Q	303	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
39	5	614	II0	C19-C13-C09	-4.01	118.90	124.35
26	2	312	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
26	B	608	CLA	CMB-C2B-C3B	4.01	132.18	124.68
26	R	305	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
39	O	615	II0	C11-C13-C09	-4.00	111.49	120.57
33	d	404	LMG	O7-C10-C11	4.00	120.12	111.50
28	Y	101	WVN	C29-C26-C22	-4.00	121.60	127.31
26	c	510	CLA	CMB-C2B-C3B	3.99	132.15	124.68
39	Q	313	II0	C19-C13-C09	-3.99	118.93	124.35
39	1	617	II0	C27-C25-C23	-3.99	108.94	116.84
26	5	604	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
26	B	614	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
26	b	608	CLA	CMB-C2B-C3B	3.99	132.14	124.68
39	P	612	II0	C20-C14-C10	-3.98	118.94	124.35
26	3	302	CLA	CMB-C2B-C1B	-3.98	122.34	128.46
26	C	509	CLA	CMB-C2B-C3B	3.98	132.12	124.68
26	O	612	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
26	P	603	CLA	C4A-NA-C1A	3.98	108.49	106.71
26	2	311	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
39	O	613	II0	C20-C14-C10	-3.97	118.95	124.35
38	Q	309	KC2	C4B-C3B-C2B	-3.97	103.49	106.75
26	P	603	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
33	c	521	LMG	O7-C10-C11	3.97	120.05	111.50
26	N	609	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
26	b	615	CLA	CMB-C2B-C1B	-3.96	122.37	128.46
26	O	611	CLA	CMB-C2B-C1B	-3.96	122.37	128.46
39	4	314	II0	C19-C13-C09	-3.96	118.97	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	614	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
28	d	410	WVN	C30-C28-C25	-3.95	121.68	127.31
38	4	310	KC2	C4B-C3B-C2B	-3.95	103.51	106.75
39	N	615	II0	C19-C13-C09	-3.95	118.99	124.35
26	c	508	CLA	CMB-C2B-C3B	3.94	132.06	124.68
39	3	310	II0	C27-C25-C23	-3.94	109.03	116.84
26	2	305	CLA	CAC-C3C-C4C	3.94	129.92	124.81
38	N	612	KC2	C1B-CHB-C4A	-3.94	117.56	126.06
33	M	101	LMG	O7-C10-C11	3.94	119.98	111.50
38	N	610	KC2	C4B-C3B-C2B	-3.93	103.53	106.75
28	a	406	WVN	C04-C09-C05	-3.93	121.08	124.85
26	C	507	CLA	CMB-C2B-C3B	3.93	132.02	124.68
26	B	615	CLA	CMB-C2B-C1B	-3.92	122.43	128.46
26	3	305	CLA	CMB-C2B-C3B	3.92	132.02	124.68
26	c	510	CLA	C4A-NA-C1A	3.92	108.47	106.71
40	2	317	IHT	C29-C31-C34	-3.92	110.98	123.22
26	5	606	CLA	CMB-C2B-C3B	3.92	132.01	124.68
26	P	611	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
39	N	618	II0	C20-C14-C10	-3.92	119.03	124.35
28	Z	101	WVN	C14-C15-C13	-3.92	117.04	122.73
40	N	619	IHT	C41-C38-C35	-3.92	121.72	127.31
26	R	310	CLA	CMB-C2B-C1B	-3.92	122.45	128.46
26	3	303	CLA	CMB-C2B-C3B	3.92	132.00	124.68
26	A	402	CLA	C4A-NA-C1A	3.91	108.47	106.71
26	P	604	CLA	CMB-C2B-C3B	3.91	132.00	124.68
38	N	605	KC2	O2D-CGD-CBD	3.91	118.21	111.27
28	H	101	WVN	C26-C29-C31	-3.91	111.02	123.22
26	R	307	CLA	CMB-C2B-C3B	3.91	131.99	124.68
38	S	608	KC2	O2D-CGD-CBD	3.91	118.21	111.27
39	4	315	II0	C20-C14-C10	-3.90	119.04	124.35
26	3	309	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
26	N	603	CLA	C4A-NA-C1A	3.90	108.46	106.71
40	2	317	IHT	C12-C15-C11	-3.90	111.72	120.57
28	d	410	WVN	C20-C23-C25	-3.90	120.34	126.23
39	Q	314	II0	C20-C14-C10	-3.90	119.05	124.35
28	d	410	WVN	C40-C37-C34	-3.90	121.75	127.31
39	3	310	II0	C19-C13-C11	-3.90	107.14	114.36
26	N	604	CLA	CMB-C2B-C1B	-3.90	122.48	128.46
26	P	606	CLA	CMB-C2B-C3B	3.89	131.97	124.68
26	5	609	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
26	1	602	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
39	1	618	II0	C27-C25-C23	-3.89	109.13	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	605	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
38	6	608	KC2	O2D-CGD-CBD	3.88	118.17	111.27
28	H	101	WVN	C20-C13-C15	-3.88	112.06	121.46
28	C	516	WVN	C16-C05-C09	-3.88	108.53	122.33
26	b	611	CLA	CMB-C2B-C3B	3.88	131.93	124.68
39	S	612	II0	C20-C14-C10	-3.88	119.08	124.35
26	B	616	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
33	5	619	LMG	O7-C10-C11	3.87	119.85	111.50
39	6	612	II0	C20-C14-C10	-3.87	119.10	124.35
33	d	409	LMG	O7-C10-C11	3.86	119.83	111.50
33	O	617	LMG	O7-C10-C11	3.86	119.82	111.50
28	A	406	WVN	C39-C36-C32	-3.86	121.80	127.31
26	a	403	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
38	P	605	KC2	C4B-C3B-C2B	-3.86	103.58	106.75
28	C	515	WVN	C23-C20-C13	-3.86	116.37	127.20
35	H	102	DGD	O2G-C1B-C2B	3.86	119.81	111.50
33	2	318	LMG	O7-C10-C11	3.85	119.81	111.50
26	B	602	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
33	R	301	LMG	O7-C10-C11	3.85	119.81	111.50
40	O	616	IHT	C19-C10-C07	-3.85	120.20	124.53
39	4	314	II0	C20-C14-C10	-3.85	119.12	124.35
39	1	616	II0	C27-C25-C23	-3.85	109.22	116.84
39	Q	319	II0	C03-C09-C13	-3.84	117.20	122.63
33	D	411	LMG	O7-C10-C11	3.84	119.78	111.50
26	b	616	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
39	4	314	II0	C41-C42-C40	-3.84	115.61	123.47
26	O	604	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
39	4	320	II0	C03-C09-C13	-3.84	117.22	122.63
26	4	303	CLA	CMB-C2B-C1B	-3.84	122.57	128.46
39	Q	313	II0	C41-C42-C40	-3.83	115.62	123.47
33	m	101	LMG	O7-C10-C11	3.83	119.76	111.50
26	Q	302	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
34	C	518	LHG	O7-C7-C8	3.83	119.76	111.50
34	2	321	LHG	O7-C7-C8	3.83	119.76	111.50
38	3	304	KC2	C4B-C3B-C2B	-3.83	103.61	106.75
39	3	310	II0	C28-C26-C24	-3.83	109.25	116.84
26	b	605	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
26	S	606	CLA	CMB-C2B-C3B	3.82	131.83	124.68
26	b	602	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
39	4	315	II0	C06-C04-C10	3.82	117.36	109.62
39	Q	314	II0	C06-C04-C10	3.82	117.36	109.62
28	A	406	WVN	C14-C15-C13	-3.82	117.19	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	618	WVN	C21-C15-C13	-3.82	120.24	124.53
26	O	608	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
26	2	304	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
39	4	317	II0	C20-C14-C10	-3.81	119.17	124.35
39	Q	313	II0	C20-C14-C10	-3.80	119.18	124.35
26	2	308	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
39	Q	316	II0	C20-C14-C10	-3.80	119.18	124.35
35	h	101	DGD	O2G-C1B-C2B	3.80	119.69	111.50
28	B	617	WVN	C23-C20-C13	-3.80	116.53	127.20
26	B	611	CLA	CMB-C2B-C3B	3.80	131.78	124.68
34	D	403	LHG	O7-C7-C8	3.80	119.68	111.50
34	G	403	LHG	O7-C7-C8	3.80	119.68	111.50
26	O	602	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
26	A	403	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
26	C	504	CLA	C4A-NA-C1A	3.79	108.41	106.71
39	5	615	II0	C20-C14-C10	-3.79	119.20	124.35
34	N	621	LHG	O7-C7-C8	3.79	119.66	111.50
26	N	613	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
39	1	615	II0	C11-C13-C09	-3.79	111.97	120.57
26	6	606	CLA	CMB-C2B-C3B	3.79	131.76	124.68
26	3	306	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
26	C	509	CLA	C4A-NA-C1A	3.78	108.41	106.71
26	a	402	CLA	C4A-NA-C1A	3.78	108.41	106.71
26	P	607	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
26	B	603	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
39	1	616	II0	C04-C10-C14	-3.77	117.31	122.63
26	c	506	CLA	CMB-C2B-C3B	3.77	131.73	124.68
34	1	620	LHG	O7-C7-C8	3.77	119.63	111.50
39	N	620	II0	C19-C13-C09	-3.77	119.23	124.35
39	1	617	II0	C28-C26-C24	-3.77	109.38	116.84
37	F	101	HEM	C1B-NB-C4B	3.77	108.96	105.07
38	N	605	KC2	C2A-C1A-NA	3.76	115.44	109.40
26	S	609	CLA	CMB-C2B-C3B	3.76	131.72	124.68
26	2	302	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
26	C	503	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
26	R	313	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
39	N	617	II0	C06-C04-C10	3.76	117.24	109.62
39	5	613	II0	C20-C14-C10	-3.76	119.24	124.35
26	3	301	CLA	CMB-C2B-C3B	3.76	131.71	124.68
28	D	412	WVN	C30-C28-C25	-3.76	121.95	127.31
26	6	609	CLA	CMB-C2B-C3B	3.76	131.71	124.68
39	5	615	II0	C19-C13-C09	-3.76	119.25	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	402	CLA	CMB-C2B-C1B	-3.75	122.69	128.46
26	2	303	CLA	C4A-NA-C1A	3.75	108.39	106.71
39	1	616	II0	C20-C14-C12	-3.75	107.40	114.36
26	Q	311	CLA	CMB-C2B-C3B	3.75	131.70	124.68
28	3	313	WVN	C26-C29-C31	-3.75	111.51	123.22
34	5	618	LHG	O7-C7-C8	3.75	119.59	111.50
28	H	101	WVN	C33-C34-C37	-3.75	113.19	118.94
26	4	312	CLA	CMB-C2B-C3B	3.75	131.69	124.68
26	P	602	CLA	CMB-C2B-C3B	3.75	131.69	124.68
39	1	615	II0	C27-C25-C23	-3.75	109.42	116.84
26	S	610	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
39	R	314	II0	C20-C14-C10	-3.74	119.26	124.35
39	5	614	II0	C20-C14-C10	-3.74	119.27	124.35
26	c	505	CLA	C4A-NA-C1A	3.74	108.39	106.71
40	2	317	IHT	C20-C15-C12	-3.74	107.42	114.36
26	c	504	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
26	1	604	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
26	6	610	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
39	1	618	II0	C28-C26-C24	-3.74	109.44	116.84
34	R	319	LHG	O7-C7-C8	3.74	119.55	111.50
26	D	404	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
26	C	510	CLA	CMB-C2B-C3B	3.73	131.66	124.68
28	c	516	WVN	C40-C37-C34	-3.73	121.99	127.31
39	R	315	II0	C20-C14-C10	-3.73	119.28	124.35
26	1	613	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
26	b	614	CLA	C4A-NA-C1A	3.73	108.38	106.71
28	C	515	WVN	C14-C15-C13	-3.73	117.32	122.73
39	N	616	II0	C20-C14-C10	-3.73	119.28	124.35
39	P	614	II0	C20-C14-C10	-3.73	119.29	124.35
26	C	508	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
39	2	315	II0	C19-C13-C09	-3.72	119.29	124.35
40	4	318	IHT	C08-C12-C15	3.72	119.27	111.85
39	R	316	II0	C20-C14-C10	-3.72	119.29	124.35
26	B	614	CLA	C4A-NA-C1A	3.72	108.38	106.71
26	c	511	CLA	CMB-C2B-C3B	3.72	131.64	124.68
39	R	316	II0	C19-C13-C09	-3.72	119.29	124.35
40	1	619	IHT	C12-C15-C11	-3.72	112.13	120.57
26	5	612	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
38	4	311	KC2	C4B-C3B-C2B	-3.72	103.70	106.75
26	b	603	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
38	Q	310	KC2	C4B-C3B-C2B	-3.71	103.70	106.75
39	1	618	II0	C11-C13-C09	-3.71	112.14	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	R	317	IHT	C02-C07-C10	-3.71	117.38	122.61
26	C	512	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
40	Q	317	IHT	C08-C12-C15	3.71	119.24	111.85
39	1	616	II0	C11-C13-C09	-3.71	112.16	120.57
26	6	603	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
40	5	616	IHT	C02-C07-C10	-3.70	117.40	122.61
26	O	603	CLA	C4A-NA-C1A	3.70	108.37	106.71
39	1	617	II0	C20-C14-C12	-3.70	107.50	114.36
29	A	407	PL9	C7-C3-C2	-3.70	118.44	123.30
26	A	405	CLA	CMB-C2B-C1B	-3.69	122.78	128.46
26	2	305	CLA	O2D-CGD-O1D	-3.69	116.62	123.84
39	1	616	II0	C28-C26-C24	-3.69	109.53	116.84
26	C	505	CLA	CMB-C2B-C3B	3.69	131.58	124.68
26	a	405	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
38	6	608	KC2	C2A-C1A-NA	3.68	115.30	109.40
26	b	604	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
26	P	611	CLA	CMB-C2B-C3B	3.68	131.56	124.68
39	3	312	II0	C28-C26-C24	-3.68	109.56	116.84
26	S	603	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
26	4	302	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
28	a	406	WVN	C39-C36-C32	-3.67	122.08	127.31
26	3	309	CLA	CMB-C2B-C3B	3.66	131.53	124.68
39	1	616	II0	C30-C32-C34	-3.66	111.78	123.22
38	S	608	KC2	C2A-C1A-NA	3.66	115.28	109.40
26	Q	301	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
39	1	617	II0	C11-C13-C09	-3.66	112.26	120.57
28	c	518	WVN	C01-C02-C11	-3.66	108.08	112.70
26	c	513	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
26	6	602	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
26	C	506	CLA	CMB-C2B-C1B	-3.66	122.85	128.46
26	B	604	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
40	N	619	IHT	C04-C06-C09	3.65	119.54	111.38
26	P	610	CLA	CMB-C2B-C3B	3.65	131.51	124.68
26	1	608	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
26	C	513	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
28	b	618	WVN	C21-C15-C14	3.65	120.62	113.62
38	N	605	KC2	C4B-C3B-C2B	-3.65	103.76	106.75
38	N	605	KC2	CBC-CAC-C3C	-3.64	109.49	127.62
38	3	304	KC2	CBC-CAC-C3C	-3.64	109.49	127.62
29	a	407	PL9	C7-C3-C2	-3.64	118.51	123.30
39	N	615	II0	C20-C14-C10	-3.64	119.40	124.35
40	1	619	IHT	C28-C26-C24	-3.64	109.62	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	P	605	KC2	CBC-CAC-C3C	-3.64	109.51	127.62
39	4	316	II0	C03-C09-C13	-3.64	117.50	122.63
26	S	602	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
38	N	611	KC2	O2D-CGD-CBD	3.64	117.73	111.27
26	b	609	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
26	R	312	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
26	c	512	CLA	CMB-C2B-C3B	3.63	131.46	124.68
26	c	507	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
39	2	316	II0	C30-C32-C34	-3.63	111.90	123.22
39	1	615	II0	C30-C32-C34	-3.62	111.91	123.22
26	Q	302	CLA	C4A-NA-C1A	3.62	108.33	106.71
26	b	608	CLA	C4A-NA-C1A	3.62	108.33	106.71
26	C	511	CLA	CMB-C2B-C3B	3.62	131.45	124.68
39	3	310	II0	C11-C13-C09	-3.62	112.35	120.57
38	4	310	KC2	C2A-C1A-NA	3.62	115.20	109.40
39	O	615	II0	C30-C32-C34	-3.62	111.93	123.22
38	Q	309	KC2	C2A-C1A-NA	3.61	115.20	109.40
26	g	402	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
26	5	611	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
26	R	303	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
38	Q	304	KC2	O2D-CGD-CBD	3.61	117.68	111.27
26	N	602	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
39	Q	315	II0	C03-C09-C13	-3.60	117.55	122.63
28	P	615	WVN	C23-C20-C13	-3.60	117.08	127.20
26	C	502	CLA	CMB-C2B-C3B	3.60	131.42	124.68
26	b	603	CLA	C4A-NA-C1A	3.60	108.33	106.71
26	c	503	CLA	CMB-C2B-C3B	3.60	131.41	124.68
26	5	608	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
26	5	611	CLA	O2D-CGD-O1D	-3.60	116.81	123.84
26	B	606	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
28	Z	101	WVN	C08-C01-C02	3.60	114.99	109.55
34	C	501	LHG	O7-C7-C8	3.59	119.25	111.50
26	S	605	CLA	O2D-CGD-O1D	-3.59	116.82	123.84
26	5	602	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
38	4	305	KC2	O2D-CGD-CBD	3.59	117.65	111.27
26	R	312	CLA	O2D-CGD-O1D	-3.59	116.82	123.84
26	c	513	CLA	O2D-CGD-O1D	-3.59	116.82	123.84
26	c	514	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
26	4	303	CLA	C4A-NA-C1A	3.59	108.32	106.71
26	R	309	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
26	6	605	CLA	O2D-CGD-O1D	-3.59	116.83	123.84
26	4	304	CLA	CMB-C2B-C3B	3.59	131.39	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	618	WVN	C06-C13-C15	-3.58	117.57	122.61
26	C	514	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
40	Q	317	IHT	C28-C26-C24	3.57	123.92	116.84
26	C	512	CLA	O2D-CGD-O1D	-3.57	116.85	123.84
39	6	613	II0	C20-C14-C10	-3.57	119.50	124.35
26	b	606	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
26	O	603	CLA	CMB-C2B-C3B	3.57	131.35	124.68
30	a	408	SQD	O47-C7-C8	3.57	119.19	111.50
26	S	605	CLA	CMB-C2B-C3B	3.57	131.35	124.68
38	O	610	KC2	C2A-C1A-NA	3.57	115.12	109.40
26	2	312	CLA	CMB-C2B-C3B	3.56	131.34	124.68
29	d	407	PL9	C7-C3-C2	-3.56	118.62	123.30
26	6	605	CLA	CMB-C2B-C3B	3.56	131.34	124.68
28	k	101	WVN	C26-C29-C31	-3.56	112.11	123.22
26	B	609	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
26	c	505	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
38	2	310	KC2	C2A-C1A-NA	3.55	115.10	109.40
26	2	303	CLA	CMB-C2B-C3B	3.55	131.33	124.68
26	3	307	CLA	CMB-C2B-C3B	3.55	131.32	124.68
39	N	618	II0	C18-C04-C10	-3.55	104.83	110.47
39	4	316	II0	C20-C14-C10	-3.54	119.53	124.35
26	Q	303	CLA	CMB-C2B-C3B	3.54	131.31	124.68
40	4	318	IHT	C28-C26-C24	3.54	123.86	116.84
38	N	611	KC2	C2A-C1A-NA	3.54	115.08	109.40
39	1	615	II0	C29-C31-C33	-3.54	112.16	123.22
38	2	310	KC2	O2D-CGD-CBD	3.54	117.56	111.27
26	R	307	CLA	C4A-NA-C1A	3.54	108.30	106.71
26	O	612	CLA	CMB-C2B-C3B	3.54	131.30	124.68
26	P	609	CLA	CMB-C2B-C3B	3.54	131.30	124.68
39	Q	315	II0	C20-C14-C10	-3.54	119.54	124.35
39	R	318	II0	C20-C14-C10	-3.54	119.54	124.35
37	f	101	HEM	CHA-C4D-ND	3.53	128.75	124.38
26	B	608	CLA	C4A-NA-C1A	3.53	108.30	106.71
30	A	408	SQD	O47-C7-C8	3.53	119.12	111.50
39	S	611	II0	C20-C14-C10	-3.53	119.55	124.35
26	g	401	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
26	D	408	CLA	CMB-C2B-C3B	3.53	131.28	124.68
26	4	313	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
28	c	518	WVN	C26-C29-C31	-3.53	112.21	123.22
26	c	515	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
26	R	304	CLA	CAA-C2A-C3A	-3.52	103.14	112.78
38	4	311	KC2	C3B-C2B-C1B	-3.52	103.72	107.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	518	WVN	C02-C05-C09	-3.52	117.14	121.47
39	6	611	II0	C20-C14-C10	-3.52	119.57	124.35
28	5	617	WVN	C29-C26-C22	-3.52	122.29	127.31
26	5	603	CLA	CAA-C2A-C3A	-3.52	103.15	112.78
26	Q	312	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
38	4	311	KC2	C2A-C1A-NA	3.51	115.03	109.40
38	Q	310	KC2	C2A-C1A-NA	3.51	115.03	109.40
26	1	614	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
38	O	610	KC2	O2D-CGD-CBD	3.50	117.50	111.27
28	S	613	WVN	C29-C26-C22	-3.50	122.31	127.31
38	4	311	KC2	C2B-C1B-NB	3.49	112.68	110.10
34	a	409	LHG	O7-C7-C8	3.49	119.03	111.50
38	4	310	KC2	CBC-CAC-C3C	-3.49	110.25	127.62
26	G	401	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
26	d	406	CLA	CMB-C2B-C3B	3.49	131.21	124.68
39	Q	315	II0	C19-C13-C09	-3.49	119.61	124.35
39	4	316	II0	C19-C13-C09	-3.49	119.61	124.35
40	1	619	IHT	C27-C30-C32	-3.49	112.33	123.22
26	c	509	CLA	CMB-C2B-C1B	-3.49	123.11	128.46
39	3	311	II0	C28-C26-C24	-3.48	109.94	116.84
39	P	613	II0	C28-C26-C24	-3.48	109.94	116.84
26	B	607	CLA	CMB-C2B-C3B	3.48	131.20	124.68
28	b	617	WVN	C12-C14-C15	-3.48	107.86	114.08
26	b	607	CLA	CMB-C2B-C3B	3.48	131.19	124.68
38	R	311	KC2	CBC-CAC-C3C	-3.48	110.30	127.62
38	Q	309	KC2	CBC-CAC-C3C	-3.48	110.30	127.62
39	1	618	II0	C12-C14-C10	-3.48	112.67	120.57
26	2	305	CLA	C4C-C3C-C2C	-3.48	101.83	106.90
38	5	610	KC2	CBC-CAC-C3C	-3.48	110.32	127.62
38	3	304	KC2	C2A-C1A-NA	3.47	114.97	109.40
26	C	504	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
38	N	611	KC2	CBC-CAC-C3C	-3.47	110.35	127.62
39	N	618	II0	C03-C09-C13	-3.47	117.73	122.63
37	F	101	HEM	CHA-C4D-ND	3.47	128.67	124.38
38	2	310	KC2	CBC-CAC-C3C	-3.47	110.36	127.62
26	Q	306	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
38	O	610	KC2	CBC-CAC-C3C	-3.47	110.37	127.62
38	P	605	KC2	C2A-C1A-NA	3.47	114.96	109.40
38	Q	310	KC2	C3B-C2B-C1B	-3.46	103.77	107.08
28	b	619	WVN	C20-C13-C15	-3.46	113.07	121.46
38	Q	304	KC2	CBC-CAC-C3C	-3.46	110.39	127.62
26	3	308	CLA	C1D-CHD-C4C	-3.46	118.59	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	305	KC2	CBC-CAC-C3C	-3.46	110.39	127.62
26	R	305	CLA	CMB-C2B-C3B	3.46	131.15	124.68
26	5	604	CLA	CMB-C2B-C3B	3.46	131.14	124.68
26	4	307	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
26	C	514	CLA	O2D-CGD-O1D	-3.45	117.08	123.84
39	3	310	II0	C20-C14-C12	-3.45	107.96	114.36
38	R	311	KC2	C2A-C1A-NA	3.45	114.94	109.40
28	d	410	WVN	C29-C26-C22	-3.45	122.38	127.31
26	b	615	CLA	CMB-C2B-C3B	3.45	131.13	124.68
38	5	610	KC2	C2A-C1A-NA	3.45	114.93	109.40
28	D	412	WVN	C29-C26-C22	-3.45	122.39	127.31
38	Q	310	KC2	C2B-C1B-NB	3.45	112.64	110.10
40	R	317	IHT	C18-C22-C23	-3.45	121.03	126.23
38	Q	310	KC2	O2D-CGD-CBD	3.44	117.39	111.27
26	5	606	CLA	C4A-NA-C1A	3.44	108.25	106.71
40	R	317	IHT	C04-C06-C09	3.44	119.07	111.38
34	z	101	LHG	O7-C7-C8	3.44	118.92	111.50
40	5	616	IHT	C04-C06-C09	3.44	119.06	111.38
37	F	101	HEM	CHB-C1B-NB	3.43	128.62	124.38
34	Z	102	LHG	O7-C7-C8	3.43	118.89	111.50
28	k	101	WVN	C30-C28-C25	-3.43	122.42	127.31
40	5	616	IHT	C31-C34-C35	-3.43	116.79	126.42
28	c	518	WVN	C39-C40-C37	-3.43	116.45	123.47
26	S	601	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
26	B	614	CLA	CMB-C2B-C3B	3.42	131.09	124.68
26	6	601	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
26	c	515	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
28	x	101	WVN	C02-C05-C09	-3.42	117.26	121.47
26	5	605	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
38	4	311	KC2	O2D-CGD-CBD	3.42	117.34	111.27
26	B	601	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
26	2	309	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
26	Q	305	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
26	N	604	CLA	CMB-C2B-C3B	3.41	131.07	124.68
40	R	317	IHT	C31-C34-C35	-3.41	116.83	126.42
26	B	615	CLA	CMB-C2B-C3B	3.41	131.06	124.68
26	R	306	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
39	3	311	II0	C30-C32-C34	-3.41	112.57	123.22
28	c	518	WVN	C20-C13-C15	-3.41	113.20	121.46
39	P	613	II0	C30-C32-C34	-3.41	112.57	123.22
26	1	609	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
40	5	616	IHT	C18-C22-C23	-3.41	121.08	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	R	318	II0	C18-C04-C10	-3.41	105.05	110.47
38	Q	310	KC2	CBC-CAC-C3C	-3.41	110.67	127.62
28	k	101	WVN	C03-C04-C09	-3.41	106.34	112.00
38	4	311	KC2	CBC-CAC-C3C	-3.41	110.67	127.62
26	O	609	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
40	4	318	IHT	C18-C22-C23	-3.40	121.09	126.23
38	4	305	KC2	C2A-C1A-NA	3.40	114.86	109.40
38	Q	304	KC2	C2A-C1A-NA	3.40	114.86	109.40
38	P	605	KC2	O2D-CGD-CBD	3.40	117.31	111.27
26	S	610	CLA	CMB-C2B-C3B	3.40	131.04	124.68
26	4	306	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
26	6	610	CLA	CMB-C2B-C3B	3.39	131.03	124.68
26	6	607	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
39	1	616	II0	C12-C14-C10	-3.39	112.87	120.57
26	1	601	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
39	6	613	II0	C18-C04-C10	-3.39	105.08	110.47
38	3	304	KC2	O2D-CGD-CBD	3.39	117.29	111.27
28	P	615	WVN	C20-C13-C15	-3.39	113.26	121.46
26	G	402	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
26	4	309	CLA	CMB-C2B-C3B	3.38	131.01	124.68
26	N	603	CLA	CMB-C2B-C3B	3.38	131.01	124.68
26	3	302	CLA	CMB-C2B-C3B	3.38	131.01	124.68
26	1	614	CLA	CMB-C2B-C3B	3.38	131.01	124.68
26	b	610	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
40	Q	317	IHT	C18-C22-C23	-3.38	121.13	126.23
26	P	603	CLA	CMB-C2B-C3B	3.38	131.00	124.68
26	Q	308	CLA	CMB-C2B-C3B	3.38	131.00	124.68
28	D	412	WVN	C20-C23-C25	-3.38	121.13	126.23
28	H	101	WVN	C27-C25-C23	-3.38	112.76	118.08
29	D	409	PL9	C7-C3-C2	-3.37	118.87	123.30
26	b	614	CLA	CMB-C2B-C3B	3.37	130.98	124.68
26	N	601	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
26	a	403	CLA	CMB-C2B-C3B	3.37	130.98	124.68
26	B	610	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
26	N	607	CLA	C4A-NA-C1A	3.36	108.22	106.71
39	N	616	II0	C18-C04-C10	-3.36	105.13	110.47
26	S	607	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
26	1	606	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
40	O	616	IHT	C40-C37-C33	-3.36	122.52	127.31
39	Q	319	II0	C18-C04-C10	-3.36	105.14	110.47
26	N	606	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
26	P	601	CLA	CMB-C2B-C1B	-3.35	123.31	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	601	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
26	2	305	CLA	CMD-C2D-C3D	-3.35	119.91	127.61
26	B	616	CLA	CMB-C2B-C3B	3.35	130.94	124.68
40	2	317	IHT	C27-C30-C32	-3.35	112.77	123.22
39	4	320	II0	C18-C04-C10	-3.34	105.15	110.47
28	d	410	WVN	C29-C31-C32	-3.34	117.03	126.42
26	4	301	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
28	H	101	WVN	C28-C30-C33	-3.34	112.79	123.22
39	1	617	II0	C30-C32-C34	-3.34	112.79	123.22
26	5	609	CLA	CMB-C2B-C3B	3.34	130.93	124.68
26	R	310	CLA	CMB-C2B-C3B	3.34	130.93	124.68
26	2	319	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
28	D	412	WVN	C39-C40-C37	-3.34	116.64	123.47
40	O	616	IHT	C30-C27-C23	-3.34	122.55	127.31
26	P	608	CLA	CMB-C2B-C1B	-3.34	123.34	128.46
39	4	320	II0	C20-C14-C10	-3.34	119.82	124.35
28	a	406	WVN	C40-C37-C34	-3.33	122.55	127.31
28	5	617	WVN	C20-C23-C25	-3.33	121.20	126.23
26	2	301	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
39	1	616	II0	C19-C13-C11	-3.33	108.18	114.36
39	Q	319	II0	C20-C14-C10	-3.33	119.82	124.35
28	S	613	WVN	C20-C23-C25	-3.33	121.20	126.23
26	N	607	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
39	N	620	II0	C20-C14-C10	-3.33	119.83	124.35
40	4	318	IHT	C04-C06-C09	3.33	118.81	111.38
39	N	617	II0	C20-C14-C10	-3.33	119.83	124.35
26	R	312	CLA	O2D-CGD-CBD	3.33	117.18	111.27
26	A	403	CLA	CMB-C2B-C3B	3.33	130.90	124.68
28	B	617	WVN	C16-C05-C09	-3.32	110.50	122.33
39	3	311	II0	C29-C31-C33	-3.32	112.84	123.22
26	N	614	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
26	B	605	CLA	CMB-C2B-C3B	3.32	130.90	124.68
26	N	609	CLA	CMB-C2B-C3B	3.32	130.90	124.68
28	c	517	WVN	C23-C20-C13	-3.32	117.87	127.20
26	d	405	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
28	A	406	WVN	C23-C20-C13	-3.32	117.87	127.20
26	b	616	CLA	CMB-C2B-C3B	3.32	130.89	124.68
26	b	605	CLA	CMB-C2B-C3B	3.32	130.89	124.68
39	5	615	II0	C03-C09-C13	-3.32	117.95	122.63
39	N	620	II0	C03-C09-C13	-3.32	117.95	122.63
26	6	610	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
28	b	619	WVN	C29-C26-C22	-3.31	122.58	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	P	613	II0	C29-C31-C33	-3.31	112.88	123.22
40	Q	317	IHT	C04-C06-C09	3.31	118.78	111.38
38	S	608	KC2	CBC-CAC-C3C	-3.31	111.15	127.62
26	D	407	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
38	6	608	KC2	CBC-CAC-C3C	-3.31	111.17	127.62
26	1	614	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
40	Q	317	IHT	C30-C32-C33	-3.30	117.14	126.42
28	P	615	WVN	C30-C33-C34	-3.30	117.14	126.42
26	Q	301	CLA	CMB-C2B-C3B	3.30	130.85	124.68
28	H	101	WVN	C16-C05-C09	-3.30	110.59	122.33
38	Q	310	KC2	CHB-C4A-NA	3.30	129.40	124.20
28	P	615	WVN	C30-C28-C25	-3.30	122.60	127.31
40	4	318	IHT	C30-C32-C33	-3.30	117.15	126.42
26	O	601	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
28	B	617	WVN	C19-C22-C26	-3.30	113.88	118.94
26	1	607	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
39	1	615	II0	C20-C14-C12	-3.30	108.25	114.36
28	b	618	WVN	C12-C14-C15	-3.29	108.19	114.08
26	R	302	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
26	S	610	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
28	C	515	WVN	C39-C36-C32	-3.29	122.61	127.31
39	R	316	II0	C03-C09-C13	-3.29	117.98	122.63
38	4	311	KC2	CHB-C4A-NA	3.29	129.39	124.20
26	5	611	CLA	O2D-CGD-CBD	3.29	117.11	111.27
39	3	312	II0	C29-C31-C33	-3.29	112.96	123.22
39	1	617	II0	C29-C31-C33	-3.29	112.96	123.22
40	R	317	IHT	C30-C27-C23	-3.28	122.62	127.31
26	4	312	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
26	1	603	CLA	CMB-C2B-C3B	3.28	130.82	124.68
39	2	315	II0	C20-C14-C10	-3.28	119.89	124.35
28	a	406	WVN	C21-C15-C14	3.28	119.92	113.62
38	N	612	KC2	C2A-C1A-NA	3.28	114.66	109.40
40	5	616	IHT	C30-C27-C23	-3.28	122.63	127.31
39	O	614	II0	C20-C14-C10	-3.28	119.90	124.35
26	4	302	CLA	CMB-C2B-C3B	3.28	130.81	124.68
26	P	607	CLA	CMB-C2B-C3B	3.27	130.80	124.68
26	O	606	CLA	CMB-C2B-C1B	-3.27	123.43	128.46
38	O	610	KC2	CHB-C4A-NA	3.27	129.36	124.20
39	2	315	II0	C03-C09-C13	-3.27	118.01	122.63
26	2	306	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
39	P	612	II0	O02-C08-C12	3.27	116.69	109.68
26	3	306	CLA	CMB-C2B-C3B	3.27	130.80	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	4	303	CLA	CMB-C2B-C3B	3.27	130.80	124.68
39	R	318	II0	C19-C13-C09	-3.27	119.91	124.35
39	N	617	II0	C19-C13-C09	-3.27	119.91	124.35
38	N	610	KC2	O2D-CGD-CBD	3.27	117.07	111.27
26	O	611	CLA	CMB-C2B-C3B	3.26	130.79	124.68
26	2	311	CLA	CMB-C2B-C3B	3.26	130.78	124.68
26	Q	302	CLA	CMB-C2B-C3B	3.26	130.78	124.68
26	5	606	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
28	P	615	WVN	C12-C14-C15	-3.26	108.25	114.08
37	f	101	HEM	CHB-C1B-NB	3.26	128.41	124.38
26	Q	311	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
26	R	307	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
28	Z	101	WVN	C39-C36-C32	-3.26	122.66	127.31
39	N	620	II0	C06-C04-C10	3.26	116.22	109.62
39	2	315	II0	C06-C04-C10	3.26	116.22	109.62
26	O	608	CLA	CMB-C2B-C3B	3.25	130.76	124.68
39	1	618	II0	C19-C13-C11	-3.25	108.33	114.36
39	1	618	II0	C30-C32-C34	-3.25	113.07	123.22
39	3	310	II0	C33-C35-C39	-3.25	113.95	118.94
40	N	619	IHT	C28-C26-C24	3.25	123.28	116.84
39	4	316	II0	C06-C04-C10	3.25	116.20	109.62
26	P	604	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
39	2	314	II0	C20-C14-C10	-3.24	119.94	124.35
39	6	613	II0	C19-C13-C09	-3.24	119.94	124.35
38	2	310	KC2	CHB-C4A-NA	3.24	129.31	124.20
28	D	412	WVN	C40-C37-C34	-3.24	122.68	127.31
33	Q	318	LMG	O7-C10-C11	3.24	118.49	111.50
38	N	610	KC2	CBC-CAC-C3C	-3.24	111.50	127.62
27	d	403	PHO	CMB-C2B-C3B	3.24	130.74	124.68
28	P	615	WVN	C39-C40-C37	-3.24	116.84	123.47
28	a	406	WVN	C30-C28-C25	-3.24	122.69	127.31
26	D	408	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
26	d	402	CLA	CMB-C2B-C3B	3.24	130.73	124.68
26	5	607	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
26	5	601	CLA	CMB-C2B-C1B	-3.23	123.49	128.46
38	N	610	KC2	C2A-C1A-NA	3.23	114.59	109.40
26	N	606	CLA	C1B-CHB-C4A	-3.23	123.71	130.12
26	A	405	CLA	CMB-C2B-C3B	3.23	130.72	124.68
39	N	617	II0	C18-C04-C10	-3.23	105.33	110.47
26	C	508	CLA	CMB-C2B-C3B	3.23	130.72	124.68
26	1	602	CLA	CMB-C2B-C3B	3.23	130.72	124.68
33	4	319	LMG	O7-C10-C11	3.23	118.46	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	618	WVN	C33-C34-C37	-3.23	113.99	118.94
26	B	602	CLA	CMB-C2B-C3B	3.23	130.72	124.68
39	O	613	II0	O02-C08-C12	3.23	116.59	109.68
26	D	404	CLA	CMB-C2B-C3B	3.23	130.71	124.68
26	Q	306	CLA	O2D-CGD-O1D	-3.22	117.53	123.84
28	b	619	WVN	C30-C33-C34	-3.22	117.36	126.42
26	b	602	CLA	CMB-C2B-C3B	3.22	130.71	124.68
39	2	313	II0	O02-C08-C12	3.22	116.58	109.68
28	Z	101	WVN	C20-C13-C15	-3.22	113.66	121.46
28	d	410	WVN	C12-C14-C15	-3.22	108.32	114.08
26	d	406	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
26	R	308	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
26	4	308	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
26	4	306	CLA	C1B-CHB-C4A	-3.22	123.75	130.12
26	3	303	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
39	Q	315	II0	C06-C04-C10	3.21	116.14	109.62
26	Q	302	CLA	C1B-CHB-C4A	-3.21	123.75	130.12
28	P	615	WVN	C40-C37-C34	-3.21	122.72	127.31
26	N	613	CLA	CMB-C2B-C3B	3.21	130.69	124.68
26	2	308	CLA	CMB-C2B-C3B	3.21	130.69	124.68
26	Q	307	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
28	B	618	WVN	C26-C29-C31	-3.21	113.19	123.22
26	S	604	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
28	b	619	WVN	C23-C25-C28	3.21	123.87	118.94
26	6	604	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
26	6	602	CLA	CMB-C2B-C3B	3.21	130.68	124.68
26	4	307	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
26	2	302	CLA	CMB-C2B-C3B	3.20	130.67	124.68
26	g	402	CLA	CMB-C2B-C3B	3.20	130.67	124.68
28	b	618	WVN	C02-C05-C09	-3.20	117.53	121.47
26	G	401	CLA	C1B-CHB-C4A	-3.20	123.78	130.12
40	O	616	IHT	C28-C26-C24	3.20	123.18	116.84
26	B	606	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
39	P	612	II0	C18-C04-C10	-3.20	105.39	110.47
26	O	605	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
27	D	405	PHO	CMB-C2B-C3B	3.19	130.65	124.68
26	O	602	CLA	CMB-C2B-C3B	3.19	130.65	124.68
26	4	303	CLA	C1B-CHB-C4A	-3.19	123.81	130.12
28	C	516	WVN	C06-C13-C20	-3.19	106.76	115.78
26	b	606	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
26	Q	305	CLA	C1B-CHB-C4A	-3.18	123.82	130.12
26	S	602	CLA	CMB-C2B-C3B	3.18	130.63	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	O	616	IHT	C25-C23-C22	3.18	123.09	118.08
26	2	305	CLA	C4-C3-C5	3.18	119.62	115.98
40	5	616	IHT	C08-C12-C15	3.18	118.19	111.85
39	3	310	II0	C34-C36-C40	-3.18	114.06	118.94
26	O	606	CLA	C1B-CHB-C4A	-3.18	123.82	130.12
28	5	617	WVN	C08-C01-C02	3.18	114.36	109.55
26	a	405	CLA	CMB-C2B-C3B	3.18	130.62	124.68
26	1	608	CLA	CMB-C2B-C3B	3.18	130.62	124.68
26	1	614	CLA	C1D-ND-C4D	-3.17	104.08	106.33
26	B	614	CLA	C1B-CHB-C4A	-3.17	123.83	130.12
28	S	613	WVN	C08-C01-C02	3.17	114.35	109.55
39	1	617	II0	C12-C14-C10	-3.17	113.37	120.57
28	C	515	WVN	C20-C13-C15	-3.17	113.79	121.46
40	R	317	IHT	C08-C12-C15	3.17	118.17	111.85
26	g	402	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
26	b	602	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
28	A	406	WVN	C29-C26-C22	-3.17	122.79	127.31
28	x	101	WVN	C21-C15-C13	-3.16	120.97	124.53
38	Q	309	KC2	O2D-CGD-CBD	3.16	116.89	111.27
26	O	607	CLA	CMB-C2B-C1B	-3.16	123.60	128.46
26	B	602	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
26	C	512	CLA	CMB-C2B-C3B	3.16	130.59	124.68
39	N	618	II0	C32-C30-C26	-3.16	117.41	126.58
26	2	305	CLA	CMC-C2C-C1C	3.16	129.85	125.04
26	2	307	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
39	1	616	II0	C29-C31-C33	-3.16	113.37	123.22
40	1	619	IHT	C20-C15-C12	-3.15	108.51	114.36
26	b	607	CLA	C1B-CHB-C4A	-3.15	123.87	130.12
28	c	518	WVN	C28-C30-C33	-3.15	113.38	123.22
26	A	402	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
39	4	314	II0	C06-C04-C10	3.15	116.01	109.62
26	5	603	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
38	4	310	KC2	O2D-CGD-CBD	3.15	116.86	111.27
39	Q	314	II0	O02-C08-C12	3.15	116.42	109.68
39	2	320	II0	C06-C08-C12	3.15	114.61	110.30
39	Q	313	II0	C06-C04-C10	3.14	115.99	109.62
26	2	306	CLA	C1B-CHB-C4A	-3.14	123.90	130.12
28	Y	101	WVN	C20-C13-C15	-3.14	113.86	121.46
26	C	513	CLA	CMB-C2B-C3B	3.14	130.55	124.68
28	d	410	WVN	C04-C09-C05	-3.14	121.84	124.85
39	4	315	II0	O02-C08-C12	3.14	116.40	109.68
26	R	304	CLA	CMB-C2B-C1B	-3.13	123.65	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	R	303	CLA	CMB-C2B-C3B	3.13	130.54	124.68
39	1	617	II0	C19-C13-C11	-3.13	108.56	114.36
26	a	402	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
26	c	513	CLA	CMB-C2B-C3B	3.13	130.53	124.68
28	b	617	WVN	C14-C15-C13	-3.13	118.19	122.73
39	R	318	II0	O02-C08-C12	3.13	116.38	109.68
34	G	403	LHG	C5-O7-C7	-3.12	110.10	117.79
26	1	604	CLA	CMB-C2B-C3B	3.12	130.52	124.68
39	N	617	II0	C03-C09-C13	-3.12	118.23	122.63
39	1	618	II0	C29-C31-C33	-3.12	113.48	123.22
26	5	602	CLA	CMB-C2B-C3B	3.12	130.52	124.68
39	6	613	II0	O02-C08-C12	3.12	116.36	109.68
26	b	614	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
28	c	516	WVN	C02-C05-C09	-3.12	117.63	121.47
26	N	614	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
26	4	313	CLA	CMB-C2B-C3B	3.11	130.50	124.68
26	R	308	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
26	d	402	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
39	N	615	II0	C06-C04-C10	3.11	115.92	109.62
26	b	613	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
26	5	607	CLA	C1B-CHB-C4A	-3.11	123.97	130.12
26	C	506	CLA	CMB-C2B-C3B	3.10	130.49	124.68
26	N	602	CLA	CMB-C2B-C3B	3.10	130.48	124.68
26	c	507	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
26	6	603	CLA	CMB-C2B-C3B	3.10	130.48	124.68
28	S	613	WVN	C14-C15-C13	-3.10	118.23	122.73
34	2	321	LHG	C5-O7-C7	-3.10	110.16	117.79
26	B	607	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
26	D	404	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
26	c	505	CLA	CMB-C2B-C3B	3.10	130.48	124.68
26	S	609	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
26	2	304	CLA	CMB-C2B-C3B	3.10	130.47	124.68
26	b	608	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
26	P	608	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
39	P	614	II0	C18-C04-C10	-3.10	105.55	110.47
26	A	405	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
39	Q	319	II0	C19-C13-C09	-3.10	120.14	124.35
26	B	603	CLA	CMB-C2B-C3B	3.09	130.47	124.68
26	c	509	CLA	CMB-C2B-C3B	3.09	130.47	124.68
26	Q	312	CLA	CMB-C2B-C3B	3.09	130.47	124.68
26	B	613	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
39	2	316	II0	C29-C31-C33	-3.09	113.57	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	4	320	II0	C19-C13-C09	-3.09	120.15	124.35
26	B	608	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
26	1	613	CLA	CMB-C2B-C3B	3.09	130.45	124.68
26	O	604	CLA	CMB-C2B-C3B	3.09	130.45	124.68
26	S	603	CLA	CMB-C2B-C3B	3.09	130.45	124.68
39	R	318	II0	C03-C09-C13	-3.09	118.28	122.63
28	5	617	WVN	C14-C15-C13	-3.08	118.25	122.73
39	O	615	II0	C28-C26-C24	-3.08	110.73	116.84
28	3	313	WVN	C28-C30-C33	-3.08	113.60	123.22
39	O	615	II0	C29-C31-C33	-3.08	113.60	123.22
26	5	608	CLA	CMB-C2B-C3B	3.08	130.44	124.68
26	a	402	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
26	C	509	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
26	d	402	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
26	5	602	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
39	2	316	II0	C28-C26-C24	-3.08	110.75	116.84
26	Q	303	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
38	N	605	KC2	C3D-CAD-CBD	-3.07	103.56	107.61
26	R	303	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
26	C	504	CLA	CMB-C2B-C3B	3.07	130.43	124.68
26	A	405	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
26	N	614	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
26	A	402	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
26	C	509	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
26	5	604	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
26	6	609	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
26	5	602	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
26	2	312	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
33	C	519	LMG	C8-O7-C10	-3.07	110.24	117.79
26	B	603	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
26	c	510	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
28	D	412	WVN	C04-C09-C05	-3.07	121.91	124.85
26	Q	306	CLA	C1B-CHB-C4A	-3.07	124.05	130.12
26	R	305	CLA	C1B-CHB-C4A	-3.07	124.05	130.12
39	R	316	II0	C18-C04-C10	-3.07	105.60	110.47
28	b	619	WVN	C39-C36-C32	-3.06	122.94	127.31
26	B	609	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
26	D	404	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
26	b	604	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
39	5	615	II0	C18-C04-C10	-3.06	105.60	110.47
26	G	401	CLA	CMB-C2B-C3B	3.06	130.40	124.68
26	R	313	CLA	CMB-C2B-C3B	3.06	130.40	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	404	PHO	CMB-C2B-C3B	3.06	130.40	124.68
38	N	612	KC2	O2D-CGD-O1D	-3.06	117.86	123.84
38	N	611	KC2	C3B-C2B-C1B	-3.06	104.15	107.08
26	4	301	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
26	5	611	CLA	CMB-C2B-C3B	3.06	130.40	124.68
39	S	612	II0	O02-C08-C12	3.06	116.23	109.68
28	P	615	WVN	C21-C15-C14	3.06	119.49	113.62
38	S	608	KC2	C3B-C2B-C1B	-3.06	104.16	107.08
39	2	316	II0	C19-C13-C11	-3.06	108.69	114.36
26	N	607	CLA	C1B-CHB-C4A	-3.06	124.07	130.12
39	P	614	II0	O02-C08-C12	3.06	116.22	109.68
39	O	615	II0	C19-C13-C11	-3.06	108.69	114.36
28	B	617	WVN	C28-C30-C33	-3.05	113.69	123.22
39	4	317	II0	O02-C08-C12	3.05	116.22	109.68
39	Q	316	II0	O02-C08-C12	3.05	116.22	109.68
26	b	603	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
26	O	607	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
28	C	515	WVN	C40-C37-C34	-3.05	122.96	127.31
26	O	605	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
26	2	305	CLA	O2A-CGA-CBA	3.05	121.47	111.91
28	c	517	WVN	C39-C36-C32	-3.05	122.96	127.31
39	6	613	II0	C03-C09-C13	-3.05	118.33	122.63
38	R	311	KC2	CHB-C4A-NA	3.05	129.00	124.20
26	O	612	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
38	N	611	KC2	CHB-C4A-NA	3.05	129.00	124.20
26	a	405	CLA	C1B-CHB-C4A	-3.05	124.09	130.12
26	C	514	CLA	CMB-C2B-C3B	3.04	130.38	124.68
26	b	602	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
39	3	311	II0	C27-C25-C23	-3.04	110.81	116.84
26	c	507	CLA	CMB-C2B-C3B	3.04	130.37	124.68
27	A	404	PHO	CMB-C2B-C3B	3.04	130.37	124.68
26	C	503	CLA	CMB-C2B-C3B	3.04	130.37	124.68
26	c	504	CLA	CMB-C2B-C3B	3.04	130.37	124.68
26	S	601	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
39	N	618	II0	O02-C08-C12	3.04	116.19	109.68
26	4	307	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
26	R	309	CLA	CMB-C2B-C3B	3.04	130.37	124.68
26	2	307	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
40	5	616	IHT	C28-C26-C24	3.04	122.86	116.84
26	R	312	CLA	CMB-C2B-C3B	3.04	130.36	124.68
26	N	607	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
39	P	613	II0	C27-C25-C23	-3.04	110.83	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P	606	CLA	C1B-CHB-C4A	-3.04	124.11	130.12
26	R	303	CLA	C1B-CHB-C4A	-3.04	124.11	130.12
26	5	612	CLA	CMB-C2B-C3B	3.04	130.36	124.68
26	4	304	CLA	C1B-CHB-C4A	-3.04	124.11	130.12
40	1	619	IHT	C29-C31-C34	-3.03	113.75	123.22
39	N	616	II0	O02-C08-C12	3.03	116.18	109.68
39	2	315	II0	O02-C08-C12	3.03	116.18	109.68
39	6	612	II0	O02-C08-C12	3.03	116.18	109.68
26	C	508	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
39	N	620	II0	C18-C04-C10	-3.03	105.65	110.47
26	6	601	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
26	2	301	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
26	c	510	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
26	g	401	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
26	c	509	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
26	b	603	CLA	CMB-C2B-C3B	3.03	130.34	124.68
26	2	319	CLA	C1B-CHB-C4A	-3.03	124.12	130.12
26	c	514	CLA	CMB-C2B-C3B	3.03	130.34	124.68
26	a	405	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
39	Q	319	II0	C30-C32-C34	-3.03	113.78	123.22
38	4	310	KC2	C3B-C2B-C1B	-3.02	104.19	107.08
28	C	516	WVN	C21-C15-C14	-3.02	107.81	113.62
26	P	611	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
39	4	320	II0	C30-C32-C34	-3.02	113.79	123.22
39	6	613	II0	C03-C05-C07	3.02	120.47	113.64
39	N	620	II0	O02-C08-C12	3.02	116.15	109.68
38	4	310	KC2	CHB-C4A-NA	3.02	128.96	124.20
28	B	618	WVN	C16-C05-C09	-3.02	111.60	122.33
26	g	402	CLA	O2D-CGD-CBD	3.02	116.63	111.27
26	P	602	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
38	Q	309	KC2	CHB-C4A-NA	3.02	128.96	124.20
26	C	507	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
28	A	406	WVN	C40-C37-C34	-3.02	123.01	127.31
26	b	609	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
39	R	318	II0	C03-C05-C07	3.01	120.45	113.64
28	B	619	WVN	C39-C36-C32	-3.01	123.01	127.31
26	b	611	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
40	R	317	IHT	C25-C23-C22	3.01	122.83	118.08
39	2	315	II0	C18-C04-C10	-3.01	105.68	110.47
38	5	610	KC2	CHB-C4A-NA	3.01	128.95	124.20
26	c	515	CLA	CMB-C2B-C3B	3.01	130.31	124.68
26	O	601	CLA	O2D-CGD-O1D	-3.01	117.95	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	5	616	IHT	C25-C23-C22	3.01	122.82	118.08
26	3	305	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
26	G	402	CLA	CMB-C2B-C3B	3.01	130.31	124.68
26	3	309	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
26	B	611	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
26	B	602	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
39	3	311	II0	C11-C13-C09	-3.01	113.75	120.57
39	P	613	II0	C11-C13-C09	-3.01	113.75	120.57
38	6	608	KC2	C3B-C2B-C1B	-3.01	104.21	107.08
40	2	317	IHT	C31-C29-C26	-3.00	117.86	126.58
28	c	517	WVN	C14-C15-C13	-3.00	118.37	122.73
26	B	604	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
38	N	610	KC2	C3B-C2B-C1B	-3.00	104.21	107.08
26	4	307	CLA	C4A-NA-C1A	3.00	108.05	106.71
38	R	311	KC2	O2D-CGD-CBD	3.00	116.60	111.27
26	C	514	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
26	C	506	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
39	5	614	II0	O02-C08-C12	2.99	116.09	109.68
26	Q	306	CLA	C4A-NA-C1A	2.99	108.05	106.71
28	b	617	WVN	C01-C02-C11	-2.99	108.92	112.70
26	P	601	CLA	C1B-CHB-C4A	-2.99	124.19	130.12
38	Q	309	KC2	C3B-C2B-C1B	-2.99	104.22	107.08
40	N	619	IHT	C06-C09-C10	-2.99	108.74	114.08
26	N	614	CLA	CMB-C2B-C3B	2.99	130.27	124.68
26	G	402	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
38	N	610	KC2	CHB-C4A-NA	2.99	128.91	124.20
39	2	314	II0	O02-C08-C12	2.99	116.08	109.68
26	B	606	CLA	CMB-C2B-C3B	2.98	130.26	124.68
26	3	301	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
39	R	314	II0	O02-C08-C12	2.98	116.07	109.68
26	b	604	CLA	CMB-C2B-C3B	2.98	130.26	124.68
39	5	613	II0	O02-C08-C12	2.98	116.06	109.68
26	c	508	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
26	5	607	CLA	CHB-C4A-NA	2.98	128.63	124.51
26	6	607	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
26	S	607	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
39	6	611	II0	O02-C08-C12	2.98	116.06	109.68
28	c	517	WVN	C39-C40-C37	-2.98	117.37	123.47
40	R	317	IHT	C28-C26-C24	2.98	122.74	116.84
26	B	601	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
39	R	315	II0	O02-C08-C12	2.98	116.06	109.68
26	C	504	CLA	C1B-CHB-C4A	-2.98	124.22	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	609	CLA	CMB-C2B-C3B	2.97	130.24	124.68
33	a	413	LMG	C8-O7-C10	-2.97	110.47	117.79
26	b	614	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
26	b	611	CLA	C1B-CHB-C4A	-2.97	124.23	130.12
40	N	619	IHT	C18-C22-C23	-2.97	121.75	126.23
26	S	607	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
26	B	601	CLA	CMB-C2B-C3B	2.97	130.23	124.68
39	R	316	II0	O02-C08-C12	2.97	116.04	109.68
26	c	505	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
39	N	615	II0	C18-C04-C10	-2.97	105.75	110.47
39	N	615	II0	O02-C08-C12	2.97	116.03	109.68
26	G	402	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
38	5	610	KC2	O2D-CGD-CBD	2.97	116.54	111.27
26	N	609	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
26	6	602	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
26	B	605	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
26	S	602	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
39	5	615	II0	O02-C08-C12	2.96	116.03	109.68
39	N	617	II0	C41-C42-C40	-2.96	117.41	123.47
39	O	614	II0	O02-C08-C12	2.96	116.02	109.68
28	a	406	WVN	C14-C15-C13	-2.96	118.43	122.73
26	6	607	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
39	3	312	II0	C30-C32-C34	-2.96	113.98	123.22
39	1	615	II0	C19-C13-C11	-2.96	108.87	114.36
26	B	611	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
39	S	611	II0	O02-C08-C12	2.96	116.02	109.68
34	D	410	LHG	C5-O7-C7	-2.96	110.51	117.79
26	2	302	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
26	2	301	CLA	CMB-C2B-C3B	2.96	130.21	124.68
26	R	308	CLA	CHB-C4A-NA	2.95	128.60	124.51
26	B	606	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
26	N	604	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
39	2	316	II0	C12-C14-C10	-2.95	113.87	120.57
26	Q	305	CLA	CMB-C2B-C3B	2.95	130.20	124.68
26	B	604	CLA	CMB-C2B-C3B	2.95	130.20	124.68
26	g	401	CLA	CMB-C2B-C3B	2.95	130.20	124.68
26	b	601	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
38	4	305	KC2	C3B-C2B-C1B	-2.95	104.26	107.08
40	O	616	IHT	C41-C40-C37	-2.95	117.44	123.47
26	4	306	CLA	CMB-C2B-C3B	2.95	130.19	124.68
26	5	605	CLA	CMB-C2B-C3B	2.95	130.19	124.68
26	R	306	CLA	CMB-C2B-C3B	2.95	130.19	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	614	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
26	5	601	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
39	O	615	II0	C12-C14-C10	-2.94	113.89	120.57
26	O	602	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
26	O	604	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
26	b	605	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
33	A	412	LMG	C8-O7-C10	-2.94	110.55	117.79
29	D	409	PL9	C40-C39-C41	2.94	120.22	115.27
33	m	101	LMG	O8-C28-C29	2.94	121.14	111.91
26	5	612	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
26	c	515	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
39	Q	313	II0	O02-C08-C12	2.94	115.98	109.68
26	b	606	CLA	CMB-C2B-C3B	2.94	130.18	124.68
26	b	606	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
26	R	313	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
26	4	313	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
28	b	618	WVN	C30-C33-C34	-2.94	118.17	126.42
40	2	317	IHT	C02-C07-C18	-2.93	107.47	115.78
38	S	608	KC2	CHB-C4A-NA	2.93	128.82	124.20
27	a	404	PHO	O1D-CGD-CBD	2.93	129.62	124.74
26	O	601	CLA	CMB-C2B-C3B	2.93	130.16	124.68
33	M	101	LMG	O8-C28-C29	2.93	121.10	111.91
29	d	407	PL9	C40-C39-C41	2.93	120.20	115.27
26	d	406	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
26	g	402	CLA	CHB-C4A-NA	2.93	128.56	124.51
26	5	608	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
26	2	304	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
26	c	507	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
40	5	616	IHT	C20-C15-C11	-2.93	120.37	124.35
26	R	302	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
40	R	317	IHT	C20-C15-C11	-2.92	120.38	124.35
26	2	309	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
38	P	605	KC2	CHB-C4A-NA	2.92	128.81	124.20
26	B	609	CLA	CMB-C2B-C3B	2.92	130.14	124.68
26	A	403	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
26	O	602	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
26	P	602	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
26	a	403	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
26	2	302	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
26	C	506	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
26	4	301	CLA	CMB-C2B-C3B	2.92	130.13	124.68
26	b	609	CLA	CMB-C2B-C3B	2.91	130.13	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	Q	316	II0	C32-C30-C26	-2.91	118.12	126.58
38	6	608	KC2	CHB-C4A-NA	2.91	128.79	124.20
26	2	304	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
26	O	609	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
26	5	603	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
26	b	601	CLA	CMB-C2B-C3B	2.91	130.13	124.68
26	3	301	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
26	6	607	CLA	CMB-C2B-C3B	2.91	130.12	124.68
26	O	604	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
26	O	606	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
26	S	607	CLA	CMB-C2B-C3B	2.91	130.12	124.68
26	6	602	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
28	c	516	WVN	C21-C15-C13	-2.91	121.26	124.53
26	C	507	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
40	Q	317	IHT	C25-C23-C22	2.91	122.66	118.08
26	Q	312	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
26	2	306	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
26	Q	301	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
26	b	610	CLA	CMB-C2B-C3B	2.91	130.12	124.68
26	S	602	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
26	O	606	CLA	C4A-NA-C1A	2.90	108.01	106.71
38	3	304	KC2	CHB-C4A-NA	2.90	128.78	124.20
38	Q	304	KC2	C3B-C2B-C1B	-2.90	104.30	107.08
34	d	408	LHG	C5-O7-C7	-2.90	110.64	117.79
26	R	309	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
26	P	608	CLA	CMB-C2B-C3B	2.90	130.11	124.68
26	4	302	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
39	4	314	II0	O02-C08-C12	2.90	115.89	109.68
26	N	606	CLA	CMB-C2B-C3B	2.90	130.10	124.68
26	R	304	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
26	c	506	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
26	C	502	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
40	4	318	IHT	C25-C23-C22	2.90	122.64	118.08
39	Q	319	II0	O02-C08-C12	2.90	115.88	109.68
38	P	605	KC2	C3B-C2B-C1B	-2.90	104.31	107.08
27	A	404	PHO	O1D-CGD-CBD	2.89	129.56	124.74
26	a	403	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
39	4	317	II0	C32-C30-C26	-2.89	118.18	126.58
26	D	408	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
26	6	609	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
38	R	311	KC2	C3B-C2B-C1B	-2.89	104.31	107.08
26	O	609	CLA	CMB-C2B-C3B	2.89	130.09	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	503	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
39	P	614	II0	C30-C32-C34	-2.89	114.20	123.22
26	c	508	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
26	P	610	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
26	B	610	CLA	CMB-C2B-C3B	2.89	130.08	124.68
26	S	609	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
26	5	604	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
26	5	609	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
26	b	610	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
26	N	602	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
26	6	606	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
26	4	309	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
26	R	305	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
26	R	310	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
26	2	309	CLA	CMB-C2B-C3B	2.88	130.07	124.68
39	4	320	II0	O02-C08-C12	2.88	115.85	109.68
26	6	601	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
26	g	401	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
28	d	410	WVN	C39-C40-C37	-2.88	117.58	123.47
26	B	610	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
26	S	606	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
26	6	601	CLA	CMB-C2B-C3B	2.87	130.06	124.68
26	4	309	CLA	C1B-CHB-C4A	-2.87	124.42	130.12
26	Q	301	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
26	5	607	CLA	CMB-C2B-C3B	2.87	130.05	124.68
26	5	609	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
33	a	413	LMG	O8-C28-C29	2.87	120.92	111.91
26	6	606	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
26	N	601	CLA	CMB-C2B-C3B	2.87	130.05	124.68
26	5	608	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
26	N	602	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
26	C	505	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
26	A	403	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
26	1	603	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
26	O	611	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
26	S	606	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
26	4	302	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
26	O	612	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
26	R	309	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
26	S	601	CLA	CMB-C2B-C3B	2.87	130.04	124.68
38	N	612	KC2	CBC-CAC-C3C	-2.86	113.38	127.62
26	N	603	CLA	C1B-CHB-C4A	-2.86	124.45	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	407	CLA	CMB-C2B-C3B	2.86	130.03	124.68
26	Q	307	CLA	CHB-C4A-NA	2.86	128.47	124.51
28	x	101	WVN	C01-C02-C11	-2.86	109.08	112.70
26	S	601	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
26	2	311	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
39	O	615	II0	C20-C14-C12	-2.86	109.06	114.36
39	2	316	II0	C20-C14-C12	-2.86	109.06	114.36
39	N	615	II0	C32-C30-C26	-2.86	118.28	126.58
28	b	619	WVN	C40-C39-C36	-2.85	117.63	123.47
26	b	603	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
39	N	617	II0	O02-C08-C12	2.85	115.79	109.68
26	c	504	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
26	P	608	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
26	2	312	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
26	Q	308	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
26	R	310	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
26	C	503	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
39	1	618	II0	C18-C04-C10	-2.85	105.94	110.47
38	3	304	KC2	C3B-C2B-C1B	-2.85	104.35	107.08
26	b	607	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
26	4	308	CLA	CHB-C4A-NA	2.85	128.45	124.51
26	B	615	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
26	c	512	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
26	3	309	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
26	4	301	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
26	b	608	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
26	2	319	CLA	CMB-C2B-C3B	2.85	130.00	124.68
26	b	613	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
38	5	610	KC2	C3B-C2B-C1B	-2.84	104.36	107.08
26	O	608	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
28	C	516	WVN	C26-C29-C31	-2.84	114.35	123.22
26	2	303	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
26	1	609	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
39	4	316	II0	O02-C08-C12	2.84	115.76	109.68
26	d	405	CLA	CMB-C2B-C3B	2.84	129.99	124.68
26	B	603	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
26	C	510	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
26	O	603	CLA	C1B-CHB-C4A	-2.83	124.50	130.12
26	1	601	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
26	R	308	CLA	CMB-C2B-C3B	2.83	129.98	124.68
28	D	412	WVN	C29-C31-C32	-2.83	118.46	126.42
26	1	606	CLA	O2D-CGD-O1D	-2.83	118.30	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Q	308	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
26	P	610	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
26	b	613	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
26	c	509	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
26	P	611	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
39	3	311	II0	C12-C14-C10	-2.83	114.15	120.57
26	c	511	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
26	1	601	CLA	CMB-C2B-C3B	2.83	129.96	124.68
26	c	511	CLA	O2D-CGD-O1D	-2.82	118.31	123.84
39	N	615	II0	C03-C09-C13	-2.82	118.65	122.63
39	Q	315	II0	O02-C08-C12	2.82	115.73	109.68
26	2	308	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
26	B	608	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
26	B	615	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
26	c	503	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
26	P	601	CLA	CMB-C2B-C3B	2.82	129.95	124.68
39	P	613	II0	C12-C14-C10	-2.82	114.17	120.57
26	B	613	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
26	B	613	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
26	Q	305	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
26	b	615	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
26	B	616	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
26	5	607	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
26	P	607	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
29	a	407	PL9	C7-C8-C9	-2.81	122.11	126.79
26	D	407	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
26	c	506	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
26	R	308	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
28	B	617	WVN	C01-C02-C11	2.81	116.25	112.70
26	2	307	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
28	H	101	WVN	C21-C15-C14	-2.81	108.22	113.62
26	O	607	CLA	CMB-C2B-C3B	2.81	129.93	124.68
26	b	609	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
26	C	513	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
26	b	616	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
26	5	603	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
29	A	407	PL9	C7-C8-C9	-2.81	122.12	126.79
39	O	614	II0	C30-C32-C34	-2.81	114.46	123.22
39	6	613	II0	C32-C30-C26	-2.80	118.44	126.58
38	1	610	KC2	CHB-C1B-NB	-2.80	121.88	124.45
26	O	607	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
39	N	620	II0	C30-C32-C34	-2.80	114.48	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	3	306	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
39	N	617	II0	C32-C30-C26	-2.80	118.45	126.58
26	C	502	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
26	R	306	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
39	R	318	II0	C32-C30-C26	-2.80	118.46	126.58
28	b	618	WVN	C20-C23-C25	-2.80	122.01	126.23
26	1	604	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
26	B	615	CLA	CHB-C4A-NA	2.80	128.38	124.51
26	A	402	CLA	CMB-C2B-C3B	2.80	129.91	124.68
26	C	510	CLA	C1B-CHB-C4A	-2.79	124.58	130.12
26	1	602	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
38	S	608	KC2	C2B-C1B-NB	2.79	112.16	110.10
38	N	611	KC2	C3D-CAD-CBD	-2.79	103.93	107.61
26	b	610	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
39	4	317	II0	C18-C04-C10	-2.79	106.03	110.47
39	2	315	II0	C41-C42-C40	-2.79	117.75	123.47
39	2	314	II0	C30-C32-C34	-2.79	114.50	123.22
26	c	504	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
26	P	601	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
26	a	402	CLA	CMB-C2B-C3B	2.79	129.90	124.68
39	2	315	II0	C30-C32-C34	-2.79	114.51	123.22
26	C	511	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
26	4	308	CLA	CMB-C2B-C3B	2.79	129.90	124.68
26	N	601	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
33	O	617	LMG	O8-C28-C29	2.79	120.66	111.91
26	B	607	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
27	d	403	PHO	O2D-CGD-O1D	-2.79	118.39	123.84
26	N	609	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
26	b	615	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
26	2	319	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
26	R	306	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
28	A	406	WVN	C39-C40-C37	-2.78	117.78	123.47
26	C	503	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
26	4	306	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
26	C	504	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
26	1	607	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
33	2	318	LMG	O8-C28-C29	2.78	120.64	111.91
28	C	516	WVN	C33-C34-C37	-2.78	114.67	118.94
39	N	620	II0	C41-C42-C40	-2.78	117.78	123.47
39	3	312	II0	C27-C25-C23	-2.78	111.33	116.84
26	2	307	CLA	CMB-C2B-C3B	2.78	129.88	124.68
39	Q	316	II0	C18-C04-C10	-2.78	106.05	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	509	CLA	CHB-C4A-NA	2.78	128.35	124.51
39	N	618	II0	C31-C33-C35	-2.78	118.61	126.42
26	R	304	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
26	b	615	CLA	CHB-C4A-NA	2.78	128.35	124.51
26	c	511	CLA	CHB-C4A-NA	2.78	128.35	124.51
26	d	405	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
26	1	613	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
28	D	412	WVN	C12-C14-C15	-2.77	109.12	114.08
26	R	312	CLA	CHB-C4A-NA	2.77	128.35	124.51
26	O	603	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
27	D	405	PHO	O2D-CGD-O1D	-2.77	118.42	123.84
26	2	303	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
26	O	605	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
26	5	605	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
38	4	305	KC2	CHB-C4A-NA	2.77	128.57	124.20
26	B	609	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
38	N	605	KC2	C3B-C2B-C1B	-2.77	104.43	107.08
26	C	511	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
28	Z	101	WVN	C28-C30-C33	-2.76	114.59	123.22
26	R	307	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
39	P	612	II0	C06-C04-C10	2.76	115.22	109.62
26	5	611	CLA	CHB-C4A-NA	2.76	128.33	124.51
26	C	508	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
26	Q	307	CLA	CMB-C2B-C3B	2.76	129.84	124.68
26	O	608	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
38	Q	304	KC2	CHB-C4A-NA	2.76	128.55	124.20
28	5	617	WVN	C39-C40-C37	-2.76	117.82	123.47
26	5	611	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
26	C	505	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
26	b	616	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
26	P	603	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
26	G	401	CLA	CHB-C4A-NA	2.76	128.32	124.51
26	N	601	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
26	R	312	CLA	C1B-CHB-C4A	-2.75	124.66	130.12
26	O	609	CLA	C1B-CHB-C4A	-2.75	124.66	130.12
26	N	603	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
39	P	614	II0	C31-C33-C35	-2.75	118.68	126.42
39	N	618	II0	C41-C42-C40	-2.75	117.84	123.47
26	2	308	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
28	P	615	WVN	C20-C23-C25	-2.75	122.08	126.23
39	5	613	II0	C41-C42-C40	-2.75	117.84	123.47
26	N	604	CLA	O2D-CGD-O1D	-2.75	118.46	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	512	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
26	5	612	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
39	R	314	II0	C41-C42-C40	-2.75	117.84	123.47
26	O	605	CLA	CMB-C2B-C3B	2.75	129.82	124.68
28	S	613	WVN	C39-C40-C37	-2.75	117.84	123.47
39	P	614	II0	C05-C03-C09	2.75	115.19	109.62
26	1	606	CLA	CMB-C2B-C3B	2.75	129.82	124.68
33	C	519	LMG	O8-C28-C29	2.75	120.53	111.91
26	c	514	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
26	5	605	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
26	5	606	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
39	2	316	II0	C27-C25-C23	-2.75	111.40	116.84
26	R	313	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
26	2	306	CLA	C4A-NA-C1A	2.74	107.94	106.71
38	6	608	KC2	C2B-C1B-NB	2.74	112.13	110.10
39	N	617	II0	C30-C32-C34	-2.74	114.66	123.22
27	d	403	PHO	O1D-CGD-CBD	2.74	129.31	124.74
28	C	515	WVN	C39-C40-C37	-2.74	117.86	123.47
26	R	302	CLA	CMB-C2B-C3B	2.74	129.81	124.68
26	S	605	CLA	CHB-C4A-NA	2.74	128.30	124.51
26	b	612	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
26	5	604	CLA	CHD-C1D-ND	-2.73	121.94	124.45
26	2	309	CLA	C1B-CHB-C4A	-2.73	124.70	130.12
26	6	605	CLA	CHB-C4A-NA	2.73	128.29	124.51
40	5	616	IHT	C40-C37-C33	-2.73	123.41	127.31
26	1	607	CLA	CMB-C2B-C3B	2.73	129.79	124.68
26	B	616	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
28	B	618	WVN	C28-C30-C33	-2.73	114.70	123.22
26	O	611	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
39	O	615	II0	C27-C25-C23	-2.73	111.43	116.84
26	2	311	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
34	G	403	LHG	O8-C23-C24	2.73	120.47	111.91
39	R	318	II0	C05-C07-C11	2.73	114.04	110.30
26	3	302	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
26	5	603	CLA	CMB-C2B-C3B	2.73	129.78	124.68
26	c	513	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
27	D	405	PHO	O1D-CGD-CBD	2.73	129.28	124.74
26	R	305	CLA	CHD-C1D-ND	-2.73	121.95	124.45
39	Q	316	II0	C06-C04-C10	2.72	115.14	109.62
35	c	519	DGD	C2G-O2G-C1B	-2.72	111.09	117.79
26	C	510	CLA	CHB-C4A-NA	2.72	128.28	124.51
39	6	613	II0	C05-C07-C11	2.72	114.03	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	D	406	LMG	O8-C28-C29	2.72	120.45	111.91
39	4	317	II0	C06-C04-C10	2.72	115.14	109.62
26	A	402	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
26	2	301	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
26	Q	312	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
39	6	612	II0	C29-C31-C33	-2.72	114.73	123.22
34	c	520	LHG	O8-C23-C24	2.72	120.44	111.91
39	O	613	II0	C06-C04-C10	2.72	115.13	109.62
26	1	608	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
26	S	610	CLA	C1B-CHB-C4A	-2.72	124.74	130.12
39	S	612	II0	C29-C31-C33	-2.72	114.74	123.22
39	R	316	II0	C32-C30-C26	-2.72	118.70	126.58
26	4	313	CLA	C1B-CHB-C4A	-2.71	124.74	130.12
28	c	518	WVN	C29-C26-C22	-2.71	123.44	127.31
39	Q	316	II0	C30-C32-C34	-2.71	114.75	123.22
34	2	321	LHG	O8-C23-C24	2.71	120.42	111.91
40	R	317	IHT	C40-C37-C33	-2.71	123.44	127.31
39	2	313	II0	C06-C04-C10	2.71	115.12	109.62
26	O	601	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
39	R	314	II0	C06-C04-C10	2.71	115.12	109.62
26	C	511	CLA	C1-C2-C3	-2.71	121.35	126.04
26	Q	307	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
26	R	304	CLA	CMB-C2B-C3B	2.71	129.75	124.68
26	B	610	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
26	C	508	CLA	CHB-C4A-NA	2.71	128.26	124.51
26	c	505	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
26	c	512	CLA	C1-C2-C3	-2.71	121.36	126.04
26	C	512	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
39	N	618	II0	C06-C04-C10	2.71	115.11	109.62
39	4	314	II0	C03-C09-C13	-2.71	118.81	122.63
39	6	612	II0	C30-C32-C34	-2.71	114.77	123.22
38	N	611	KC2	C2B-C1B-NB	2.71	112.10	110.10
39	Q	319	II0	C41-C42-C40	-2.70	117.94	123.47
26	1	607	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
33	d	404	LMG	O8-C28-C29	2.70	120.39	111.91
26	3	307	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
39	5	615	II0	C32-C30-C26	-2.70	118.73	126.58
26	4	304	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
39	Q	316	II0	C31-C33-C35	-2.70	118.82	126.42
26	g	402	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
28	a	406	WVN	C20-C13-C15	-2.70	114.92	121.46
26	5	601	CLA	CMB-C2B-C3B	2.70	129.73	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	R	317	IHT	C02-C07-C18	2.70	123.42	115.78
39	4	317	II0	C31-C33-C35	-2.70	118.83	126.42
39	S	611	II0	C32-C30-C26	-2.70	118.74	126.58
39	6	611	II0	C32-C30-C26	-2.70	118.74	126.58
39	Q	313	II0	C03-C09-C13	-2.70	118.82	122.63
40	5	616	IHT	C02-C07-C18	2.70	123.41	115.78
26	Q	307	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
39	5	613	II0	C06-C04-C10	2.70	115.09	109.62
35	C	517	DGD	C2G-O2G-C1B	-2.70	111.15	117.79
39	S	612	II0	C30-C32-C34	-2.70	114.80	123.22
26	P	609	CLA	C1B-CHB-C4A	-2.70	124.78	130.12
29	d	407	PL9	C7-C8-C9	-2.70	122.31	126.79
26	4	308	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
33	A	412	LMG	O8-C28-C29	2.69	120.36	111.91
26	5	601	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
26	Q	311	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
40	N	619	IHT	C25-C23-C22	2.69	122.32	118.08
26	4	312	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
39	4	317	II0	C30-C32-C34	-2.69	114.81	123.22
26	6	610	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
26	B	601	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
26	C	513	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
26	b	601	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
28	k	101	WVN	C12-C14-C15	-2.69	109.28	114.08
26	3	306	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
26	a	402	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
26	Q	303	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
38	Q	309	KC2	O2D-CGD-O1D	-2.68	118.59	123.84
26	b	612	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
39	4	317	II0	C20-C14-C12	2.68	119.32	114.36
26	P	607	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
26	R	302	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
26	S	604	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
40	Q	317	IHT	C03-C05-C08	-2.68	107.59	113.64
26	N	613	CLA	CHB-C4A-NA	2.68	128.21	124.51
26	b	613	CLA	CMB-C2B-C3B	2.68	129.69	124.68
26	B	605	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
40	O	616	IHT	C03-C05-C08	-2.67	107.61	113.64
39	4	320	II0	C41-C42-C40	-2.67	118.00	123.47
28	b	619	WVN	C23-C20-C13	-2.67	119.70	127.20
39	1	615	II0	C12-C14-C10	-2.67	114.51	120.57
38	4	310	KC2	O2D-CGD-O1D	-2.67	118.62	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	3	307	CLA	CHB-C4A-NA	2.67	128.20	124.51
34	D	403	LHG	O8-C23-C24	2.67	120.27	111.91
26	1	608	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
39	O	614	II0	C18-C04-C10	-2.66	106.23	110.47
39	Q	316	II0	C20-C14-C12	2.66	119.29	114.36
26	6	604	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
39	2	314	II0	C18-C04-C10	-2.66	106.24	110.47
26	3	307	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
26	S	603	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
29	D	409	PL9	C7-C8-C9	-2.66	122.36	126.79
40	4	318	IHT	C03-C05-C08	-2.66	107.64	113.64
26	4	308	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
26	P	604	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
26	O	602	CLA	CHD-C1D-ND	-2.66	122.01	124.45
26	b	604	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
26	S	604	CLA	CHB-C4A-NA	2.65	128.18	124.51
26	b	605	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
26	c	514	CLA	C1B-CHB-C4A	-2.65	124.88	130.12
26	3	308	CLA	C3D-C4D-ND	-2.65	105.96	110.24
26	B	613	CLA	CMB-C2B-C3B	2.65	129.63	124.68
26	5	603	CLA	CHB-C4A-NA	2.64	128.17	124.51
26	6	605	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
26	B	612	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
34	D	403	LHG	C5-O7-C7	-2.64	111.29	117.79
26	P	609	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
26	6	603	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
26	S	605	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
28	B	619	WVN	C23-C20-C13	-2.64	119.78	127.20
26	3	303	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
26	B	604	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
26	B	612	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
39	2	313	II0	C32-C30-C26	-2.64	118.92	126.58
29	D	409	PL9	C22-C23-C24	-2.64	121.31	127.66
30	D	401	SQD	O48-C23-C24	2.64	120.18	111.91
28	Z	101	WVN	C23-C20-C13	-2.63	119.80	127.20
39	O	613	II0	C32-C30-C26	-2.63	118.93	126.58
26	Q	303	CLA	CHB-C4A-NA	2.63	128.15	124.51
28	a	406	WVN	C21-C15-C13	-2.63	121.57	124.53
28	x	101	WVN	C39-C40-C37	-2.63	118.08	123.47
26	c	515	CLA	O2D-CGD-CBD	2.63	115.94	111.27
39	R	315	II0	C41-C42-C40	-2.63	118.09	123.47
38	N	605	KC2	CMB-C2B-C1B	2.63	129.35	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	O	609	CLA	CHB-C4A-NA	2.63	128.15	124.51
26	6	603	CLA	CHB-C4A-NA	2.63	128.15	124.51
26	2	302	CLA	CHD-C1D-ND	-2.63	122.04	124.45
26	4	304	CLA	CHD-C1D-ND	-2.63	122.04	124.45
39	3	312	II0	C20-C14-C12	-2.63	109.49	114.36
40	4	318	IHT	C36-C33-C37	-2.63	119.24	122.92
39	4	320	II0	C06-C04-C10	2.62	114.94	109.62
26	P	609	CLA	CHB-C4A-NA	2.62	128.14	124.51
34	R	319	LHG	O8-C23-C24	2.62	120.14	111.91
29	d	407	PL9	C22-C23-C24	-2.62	121.34	127.66
39	P	612	II0	C41-C42-C40	-2.62	118.10	123.47
26	S	603	CLA	CHB-C4A-NA	2.62	128.14	124.51
28	d	410	WVN	C01-C02-C11	-2.62	109.39	112.70
28	d	410	WVN	C14-C15-C13	-2.62	118.92	122.73
28	c	517	WVN	C40-C37-C34	-2.62	123.57	127.31
34	5	618	LHG	O8-C23-C24	2.62	120.13	111.91
26	N	613	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
26	4	304	CLA	CHB-C4A-NA	2.62	128.13	124.51
39	Q	314	II0	C18-C04-C10	-2.62	106.31	110.47
39	3	312	II0	C19-C13-C11	-2.62	109.51	114.36
39	R	316	II0	C06-C04-C10	2.62	114.92	109.62
39	Q	319	II0	C06-C04-C10	2.62	114.92	109.62
26	C	513	CLA	CHB-C4A-NA	2.62	128.13	124.51
26	6	604	CLA	CHB-C4A-NA	2.61	128.13	124.51
38	N	611	KC2	CAB-C3B-C2B	2.61	137.22	128.60
26	6	609	CLA	CHB-C4A-NA	2.61	128.13	124.51
38	4	305	KC2	CBD-CHA-C1A	2.61	133.75	128.88
39	4	315	II0	C18-C04-C10	-2.61	106.32	110.47
39	5	614	II0	C41-C42-C40	-2.61	118.13	123.47
30	c	501	SQD	O48-C23-C24	2.61	120.10	111.91
39	4	315	II0	C32-C30-C26	-2.61	119.00	126.58
26	1	603	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
26	d	405	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
40	Q	317	IHT	C36-C33-C37	-2.61	119.27	122.92
28	Z	101	WVN	C01-C02-C11	-2.61	109.41	112.70
33	d	411	LMG	O8-C28-C29	2.61	120.08	111.91
38	R	311	KC2	O2D-CGD-O1D	-2.61	118.74	123.84
28	c	518	WVN	C23-C20-C13	-2.60	119.89	127.20
26	4	307	CLA	CMB-C2B-C3B	2.60	129.55	124.68
26	S	609	CLA	CHB-C4A-NA	2.60	128.11	124.51
26	R	304	CLA	CHB-C4A-NA	2.60	128.11	124.51
28	D	412	WVN	C07-C01-C02	2.60	113.49	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Q	303	CLA	CHD-C1D-ND	-2.60	122.06	124.45
34	C	501	LHG	O8-C23-C24	2.60	120.06	111.91
34	a	409	LHG	O8-C23-C24	2.60	120.06	111.91
40	N	619	IHT	C41-C40-C37	-2.60	118.15	123.47
39	2	314	II0	C06-C04-C10	2.60	114.89	109.62
38	N	605	KC2	CHB-C4A-NA	2.60	128.30	124.20
26	Q	306	CLA	CMB-C2B-C3B	2.59	129.53	124.68
26	2	309	CLA	CHB-C4A-NA	2.59	128.10	124.51
39	5	614	II0	C06-C04-C10	2.59	114.87	109.62
39	Q	313	II0	C30-C32-C34	-2.59	115.13	123.22
26	C	514	CLA	O2D-CGD-CBD	2.59	115.87	111.27
28	k	101	WVN	C24-C22-C19	2.59	122.16	118.08
39	5	615	II0	C06-C04-C10	2.59	114.87	109.62
28	5	617	WVN	C40-C37-C34	-2.59	123.61	127.31
28	C	515	WVN	C02-C05-C09	-2.59	118.28	121.47
39	P	613	II0	C20-C14-C12	-2.59	109.56	114.36
39	Q	314	II0	C32-C30-C26	-2.59	119.07	126.58
26	R	308	CLA	C1-C2-C3	-2.59	121.57	126.04
29	a	407	PL9	C22-C23-C24	-2.59	121.43	127.66
26	D	407	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
39	O	614	II0	C06-C04-C10	2.58	114.86	109.62
27	A	404	PHO	O2D-CGD-O1D	-2.58	118.79	123.84
33	m	101	LMG	C8-O7-C10	-2.58	111.43	117.79
39	4	314	II0	C30-C32-C34	-2.58	115.16	123.22
28	b	618	WVN	C23-C20-C13	-2.58	119.96	127.20
38	Q	304	KC2	CBD-CHA-C1A	2.58	133.69	128.88
39	R	318	II0	C41-C42-C40	-2.58	118.19	123.47
38	5	610	KC2	O2D-CGD-O1D	-2.58	118.80	123.84
39	3	310	II0	C29-C31-C33	-2.58	115.17	123.22
28	S	613	WVN	C40-C37-C34	-2.58	123.64	127.31
33	D	413	LMG	O8-C28-C29	2.57	119.98	111.91
40	2	317	IHT	C28-C26-C24	-2.57	111.75	116.84
26	O	607	CLA	CHB-C4A-NA	2.57	128.07	124.51
26	6	606	CLA	CHB-C4A-NA	2.57	128.07	124.51
40	1	619	IHT	C19-C10-C09	-2.57	108.68	113.62
26	3	303	CLA	CHB-C4A-NA	2.57	128.06	124.51
39	3	311	II0	C20-C14-C12	-2.57	109.60	114.36
26	S	606	CLA	CHB-C4A-NA	2.57	128.06	124.51
26	4	306	CLA	CHB-C4A-NA	2.57	128.06	124.51
26	S	603	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
26	N	606	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
39	4	315	II0	C41-C42-C40	-2.57	118.22	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	3	309	CLA	CHB-C4A-NA	2.56	128.06	124.51
26	1	606	CLA	CHB-C4A-NA	2.56	128.06	124.51
26	1	604	CLA	CHB-C4A-NA	2.56	128.06	124.51
26	Q	302	CLA	CHB-C4A-NA	2.56	128.06	124.51
26	5	607	CLA	C1-C2-C3	-2.56	121.61	126.04
39	R	315	II0	C06-C04-C10	2.56	114.81	109.62
26	P	603	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
26	6	603	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
33	D	413	LMG	C8-O7-C10	-2.56	111.49	117.79
26	b	601	CLA	CHB-C4A-NA	2.56	128.05	124.51
34	C	518	LHG	O8-C23-C24	2.56	119.93	111.91
39	4	316	II0	C32-C30-C26	-2.56	119.16	126.58
26	3	302	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
26	N	608	CLA	C1D-CHD-C4C	-2.55	120.55	126.06
39	6	613	II0	C41-C42-C40	-2.55	118.24	123.47
37	F	101	HEM	CHD-C1D-C2D	-2.55	120.99	124.98
28	k	101	WVN	C40-C39-C36	-2.55	118.25	123.47
26	6	606	CLA	CHD-C1D-ND	-2.55	122.11	124.45
28	k	101	WVN	C19-C22-C26	-2.55	115.03	118.94
26	S	606	CLA	CHD-C1D-ND	-2.55	122.11	124.45
26	A	405	CLA	CHB-C4A-NA	2.55	128.04	124.51
39	P	614	II0	C32-C30-C26	-2.55	119.18	126.58
26	P	604	CLA	CHB-C4A-NA	2.55	128.04	124.51
26	1	603	CLA	O2A-CGA-O1A	-2.55	117.16	123.59
33	d	411	LMG	C8-O7-C10	-2.55	111.52	117.79
28	B	617	WVN	C26-C29-C31	-2.55	115.27	123.22
33	d	409	LMG	O8-C28-C29	2.55	119.90	111.91
35	H	102	DGD	O1G-C1A-C2A	2.55	119.90	111.91
34	l	101	LHG	O8-C23-C24	2.55	119.90	111.91
35	h	101	DGD	O1G-C1A-C2A	2.55	119.89	111.91
29	A	407	PL9	C22-C23-C24	-2.54	121.53	127.66
39	4	314	II0	C31-C33-C35	-2.54	119.27	126.42
39	Q	313	II0	C31-C33-C35	-2.54	119.27	126.42
29	a	407	PL9	C20-C19-C21	2.54	119.55	115.27
26	Q	311	CLA	CHB-C4A-NA	2.54	128.03	124.51
39	N	616	II0	C32-C30-C26	-2.54	119.20	126.58
26	3	305	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
39	Q	314	II0	C41-C42-C40	-2.54	118.27	123.47
39	P	612	II0	C03-C09-C13	-2.54	119.05	122.63
38	4	311	KC2	C3D-CAD-CBD	-2.54	104.26	107.61
26	Q	302	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
33	D	411	LMG	O8-C28-C29	2.54	119.87	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	3	304	KC2	O2D-CGD-O1D	-2.53	118.88	123.84
39	O	613	II0	C18-C04-C10	-2.53	106.44	110.47
39	Q	315	II0	C32-C30-C26	-2.53	119.22	126.58
34	L	101	LHG	O8-C23-C24	2.53	119.86	111.91
38	P	605	KC2	O2D-CGD-O1D	-2.53	118.89	123.84
26	Q	305	CLA	CHB-C4A-NA	2.53	128.01	124.51
26	P	606	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
28	b	619	WVN	C08-C01-C02	2.53	113.38	109.55
38	Q	310	KC2	C3D-CAD-CBD	-2.53	104.27	107.61
40	O	616	IHT	C22-C18-C07	-2.53	120.10	127.20
33	B	620	LMG	C8-O7-C10	-2.53	111.56	117.79
26	N	604	CLA	CHB-C4A-NA	2.53	128.01	124.51
26	4	303	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
39	2	313	II0	C18-C04-C10	-2.53	106.45	110.47
39	R	318	II0	C19-C13-C11	2.53	119.04	114.36
39	2	320	II0	C41-C42-C40	2.53	128.65	123.47
26	4	312	CLA	CHB-C4A-NA	2.53	128.00	124.51
39	6	612	II0	C41-C42-C40	-2.53	118.30	123.47
33	M	101	LMG	C8-O7-C10	-2.53	111.57	117.79
28	A	406	WVN	C20-C23-C25	-2.53	122.42	126.23
33	C	519	LMG	C7-O1-C1	-2.52	108.81	113.74
26	1	601	CLA	CHB-C4A-NA	2.52	128.00	124.51
27	a	404	PHO	O2D-CGD-O1D	-2.52	118.90	123.84
26	c	514	CLA	CHB-C4A-NA	2.52	128.00	124.51
26	4	303	CLA	CHB-C4A-NA	2.52	128.00	124.51
26	P	611	CLA	CHB-C4A-NA	2.52	128.00	124.51
39	6	613	II0	C19-C13-C11	2.52	119.03	114.36
39	S	612	II0	C41-C42-C40	-2.52	118.31	123.47
39	3	310	II0	C30-C32-C34	-2.52	115.35	123.22
28	P	615	WVN	C07-C01-C02	2.52	113.36	109.55
39	R	315	II0	C30-C32-C34	-2.52	115.36	123.22
28	D	412	WVN	C23-C20-C13	-2.52	120.13	127.20
34	b	621	LHG	C5-O7-C7	-2.52	111.59	117.79
26	c	515	CLA	CHB-C4A-NA	2.52	127.99	124.51
26	N	609	CLA	CHB-C4A-NA	2.51	127.99	124.51
39	5	614	II0	C30-C32-C34	-2.51	115.37	123.22
26	N	601	CLA	CHB-C4A-NA	2.51	127.98	124.51
37	f	101	HEM	CHD-C1D-C2D	-2.51	121.06	124.98
39	6	613	II0	C30-C32-C34	-2.51	115.38	123.22
28	B	619	WVN	C26-C29-C31	-2.51	115.39	123.22
26	R	303	CLA	CHD-C1D-ND	-2.51	122.15	124.45
28	Y	101	WVN	C28-C30-C33	-2.51	115.39	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	613	CLA	CHB-C4A-NA	2.51	127.98	124.51
26	P	603	CLA	CHB-C4A-NA	2.51	127.98	124.51
26	2	307	CLA	CHB-C4A-NA	2.51	127.98	124.51
26	6	607	CLA	CHB-C4A-NA	2.51	127.98	124.51
26	1	613	CLA	CHB-C4A-NA	2.51	127.98	124.51
26	2	301	CLA	CHB-C4A-NA	2.51	127.98	124.51
34	d	408	LHG	O8-C23-C24	2.51	119.77	111.91
33	5	619	LMG	O8-C28-C29	2.50	119.77	111.91
38	6	608	KC2	CAA-CBA-CGA	-2.50	114.39	127.26
26	N	609	CLA	CHD-C1D-ND	-2.50	122.15	124.45
28	C	516	WVN	C28-C30-C33	-2.50	115.41	123.22
38	S	608	KC2	CAA-CBA-CGA	-2.50	114.40	127.26
39	R	318	II0	C30-C32-C34	-2.50	115.41	123.22
26	g	402	CLA	C3A-C2A-C1A	2.50	105.08	101.34
39	2	320	II0	C03-C05-C07	2.50	119.29	113.64
39	N	615	II0	C31-C33-C35	-2.50	119.40	126.42
39	P	612	II0	C30-C32-C34	-2.50	115.42	123.22
26	6	602	CLA	CHB-C4A-NA	2.50	127.97	124.51
26	b	612	CLA	CHD-C1D-ND	-2.49	122.16	124.45
34	D	410	LHG	O8-C23-C24	2.49	119.73	111.91
38	O	610	KC2	CAB-C3B-C2B	2.49	136.81	128.60
33	R	301	LMG	O8-C28-C29	2.49	119.73	111.91
26	5	602	CLA	CHD-C1D-ND	-2.49	122.16	124.45
28	b	618	WVN	C14-C15-C13	-2.49	119.11	122.73
28	5	617	WVN	C23-C20-C13	-2.49	120.21	127.20
38	2	310	KC2	CAB-C3B-C2B	2.49	136.81	128.60
26	G	401	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
26	C	512	CLA	O2D-CGD-CBD	2.49	115.69	111.27
28	a	406	WVN	C16-C05-C09	-2.49	113.48	122.33
38	1	605	KC2	C3C-C2C-C1C	2.49	108.33	106.49
40	R	317	IHT	C12-C15-C11	-2.49	114.92	120.57
26	B	612	CLA	CHD-C1D-ND	-2.49	122.17	124.45
38	N	612	KC2	CHB-C4A-NA	2.49	128.12	124.20
28	B	617	WVN	C21-C15-C14	-2.49	108.84	113.62
26	B	601	CLA	CHB-C4A-NA	2.48	127.95	124.51
40	1	619	IHT	C02-C07-C18	-2.48	108.75	115.78
38	N	610	KC2	O2D-CGD-O1D	-2.48	118.98	123.84
40	2	317	IHT	C19-C10-C09	-2.48	108.85	113.62
26	O	601	CLA	CHB-C4A-NA	2.48	127.94	124.51
30	a	408	SQD	O9-S-C6	2.48	109.89	106.94
38	6	608	KC2	C3D-CAD-CBD	-2.48	104.34	107.61
26	c	513	CLA	O2D-CGD-CBD	2.48	115.67	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	3	308	CLA	CHA-C1A-NA	-2.48	120.72	126.40
38	N	610	KC2	C2B-C1B-NB	2.48	111.93	110.10
28	b	617	WVN	C02-C05-C09	-2.48	118.42	121.47
38	S	608	KC2	C3D-CAD-CBD	-2.48	104.34	107.61
33	C	520	LMG	O8-C28-C29	2.48	119.68	111.91
28	S	613	WVN	C23-C20-C13	-2.48	120.25	127.20
34	L	101	LHG	C5-O7-C7	-2.48	111.69	117.79
26	4	302	CLA	CHB-C4A-NA	2.48	127.94	124.51
26	Q	301	CLA	CHB-C4A-NA	2.48	127.94	124.51
26	3	302	CLA	CHB-C4A-NA	2.48	127.94	124.51
26	S	602	CLA	CHB-C4A-NA	2.48	127.94	124.51
26	S	607	CLA	CHB-C4A-NA	2.47	127.93	124.51
38	5	610	KC2	C2B-C1B-NB	2.47	111.93	110.10
28	C	516	WVN	C10-C06-C13	2.47	114.29	110.48
28	b	617	WVN	C28-C30-C33	-2.47	115.50	123.22
26	D	408	CLA	CHB-C4A-NA	2.47	127.93	124.51
26	P	607	CLA	CHB-C4A-NA	2.47	127.93	124.51
33	b	620	LMG	C8-O7-C10	-2.47	111.71	117.79
26	N	603	CLA	CHB-C4A-NA	2.47	127.93	124.51
39	N	620	II0	C31-C33-C35	-2.47	119.48	126.42
39	P	612	II0	C32-C30-C26	-2.47	119.41	126.58
39	2	314	II0	C41-C42-C40	-2.47	118.42	123.47
26	C	514	CLA	CHB-C4A-NA	2.47	127.93	124.51
33	c	521	LMG	O8-C28-C29	2.47	119.66	111.91
28	c	516	WVN	C14-C15-C13	-2.47	119.15	122.73
40	1	619	IHT	C04-C02-C07	2.47	114.28	110.48
26	b	607	CLA	CHB-C4A-NA	2.47	127.93	124.51
26	a	405	CLA	CHB-C4A-NA	2.47	127.92	124.51
26	b	602	CLA	CHB-C4A-NA	2.47	127.92	124.51
26	N	606	CLA	CHB-C4A-NA	2.47	127.92	124.51
39	O	614	II0	C41-C42-C40	-2.47	118.42	123.47
39	6	612	II0	C06-C04-C10	2.47	114.62	109.62
26	B	613	CLA	CHB-C4A-NA	2.47	127.92	124.51
38	N	610	KC2	CMB-C2B-C1B	2.47	129.06	124.71
40	4	318	IHT	C22-C18-C07	-2.47	120.28	127.20
39	S	612	II0	C06-C04-C10	2.47	114.62	109.62
38	R	311	KC2	C2B-C1B-NB	2.47	111.92	110.10
28	H	101	WVN	C06-C13-C20	-2.47	108.80	115.78
39	2	315	II0	C31-C33-C35	-2.46	119.49	126.42
26	N	613	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
26	5	608	CLA	CHB-C4A-NA	2.46	127.92	124.51
39	R	315	II0	C03-C09-C13	-2.46	119.16	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	522	LMG	O8-C28-C29	2.46	119.64	111.91
38	5	610	KC2	CAB-C3B-C2B	2.46	136.72	128.60
26	B	612	CLA	CHB-C4A-NA	2.46	127.92	124.51
39	4	314	II0	C17-C04-C06	-2.46	98.00	109.05
40	5	616	IHT	C12-C15-C11	-2.46	114.99	120.57
39	Q	313	II0	C17-C04-C06	-2.46	98.00	109.05
38	N	605	KC2	O2D-CGD-O1D	-2.46	119.03	123.84
39	5	614	II0	C03-C09-C13	-2.46	119.16	122.63
38	N	612	KC2	O2D-CGD-CBD	2.46	115.64	111.27
38	N	612	KC2	CAB-C3B-C2B	2.46	136.71	128.60
38	2	310	KC2	C3B-C2B-C1B	-2.46	104.73	107.08
40	Q	317	IHT	C22-C18-C07	-2.46	120.30	127.20
26	b	605	CLA	CHD-C1D-ND	-2.46	122.20	124.45
34	l	101	LHG	C5-O7-C7	-2.46	111.74	117.79
38	P	605	KC2	CMB-C2B-C1B	2.46	129.04	124.71
26	1	604	CLA	C1-C2-C3	-2.46	121.80	126.04
26	2	304	CLA	CHD-C1D-ND	-2.46	122.20	124.45
28	C	515	WVN	C23-C25-C28	-2.45	115.17	118.94
38	4	310	KC2	C2B-C1B-NB	2.45	111.91	110.10
26	N	604	CLA	CHD-C1D-ND	-2.45	122.20	124.45
26	2	304	CLA	CHB-C4A-NA	2.45	127.90	124.51
26	P	608	CLA	CHB-C4A-NA	2.45	127.90	124.51
26	d	406	CLA	CHB-C4A-NA	2.45	127.90	124.51
26	C	512	CLA	CHB-C4A-NA	2.45	127.90	124.51
29	A	407	PL9	C20-C19-C21	2.45	119.39	115.27
37	f	101	HEM	C4D-ND-C1D	2.45	107.60	105.07
28	x	101	WVN	C12-C14-C15	-2.45	109.71	114.08
26	P	602	CLA	CHB-C4A-NA	2.45	127.90	124.51
38	R	311	KC2	CAB-C3B-C2B	2.45	136.66	128.60
26	3	306	CLA	CHB-C4A-NA	2.45	127.89	124.51
39	4	320	II0	C31-C33-C35	-2.45	119.55	126.42
26	3	301	CLA	CHB-C4A-NA	2.44	127.89	124.51
34	b	621	LHG	O8-C23-C24	2.44	119.58	111.91
28	Y	101	WVN	C30-C28-C25	-2.44	123.82	127.31
28	b	619	WVN	C27-C25-C28	-2.44	119.50	122.92
39	1	615	II0	C06-C04-C10	2.44	114.57	109.62
38	Q	309	KC2	CBD-CHA-C1A	2.44	133.43	128.88
39	Q	316	II0	C41-C42-C40	-2.44	118.47	123.47
26	3	308	CLA	C1D-ND-C4D	-2.44	104.60	106.33
39	Q	319	II0	C19-C13-C11	2.44	118.87	114.36
26	b	612	CLA	CHB-C4A-NA	2.44	127.88	124.51
26	5	602	CLA	CHB-C4A-NA	2.44	127.88	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	406	WVN	C40-C39-C36	-2.44	118.48	123.47
38	N	611	KC2	O2D-CGD-O1D	-2.44	119.07	123.84
26	B	602	CLA	CHB-C4A-NA	2.44	127.88	124.51
26	C	503	CLA	CHB-C4A-NA	2.44	127.88	124.51
26	N	602	CLA	CHB-C4A-NA	2.44	127.88	124.51
26	O	602	CLA	CHB-C4A-NA	2.44	127.88	124.51
38	6	608	KC2	CAB-C3B-C2B	2.44	136.63	128.60
30	A	408	SQD	O9-S-C6	2.44	109.83	106.94
38	3	304	KC2	CMB-C2B-C1B	2.44	129.01	124.71
26	S	605	CLA	O1D-CGD-CBD	2.44	129.47	124.48
39	N	616	II0	C41-C42-C40	-2.43	118.49	123.47
26	1	609	CLA	CHB-C4A-NA	2.43	127.88	124.51
38	4	305	KC2	C2B-C1B-NB	2.43	111.90	110.10
39	4	320	II0	C19-C13-C11	2.43	118.86	114.36
38	O	610	KC2	C3B-C2B-C1B	-2.43	104.76	107.08
38	R	311	KC2	CAA-CBA-CGA	-2.43	114.78	127.26
38	5	610	KC2	CAA-CBA-CGA	-2.43	114.78	127.26
38	4	310	KC2	CBD-CHA-C1A	2.43	133.41	128.88
39	4	317	II0	C41-C42-C40	-2.43	118.50	123.47
26	1	602	CLA	CHB-C4A-NA	2.42	127.86	124.51
38	S	608	KC2	CAB-C3B-C2B	2.42	136.59	128.60
26	6	605	CLA	O1D-CGD-CBD	2.42	129.44	124.48
26	2	302	CLA	CHB-C4A-NA	2.42	127.86	124.51
26	1	602	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
39	Q	319	II0	C31-C33-C35	-2.42	119.61	126.42
26	R	309	CLA	CHB-C4A-NA	2.42	127.86	124.51
28	B	619	WVN	C24-C22-C19	2.42	121.89	118.08
29	D	409	PL9	C27-C28-C29	-2.42	121.83	127.66
33	d	409	LMG	C8-O7-C10	-2.42	111.83	117.79
26	4	301	CLA	CHB-C4A-NA	2.42	127.86	124.51
26	R	303	CLA	CHB-C4A-NA	2.42	127.85	124.51
33	D	411	LMG	C8-O7-C10	-2.42	111.84	117.79
39	5	614	II0	C32-C30-C26	-2.42	119.57	126.58
26	3	302	CLA	C1-C2-C3	-2.41	121.87	126.04
39	S	611	II0	C06-C04-C10	2.41	114.51	109.62
28	Z	101	WVN	C12-C14-C15	-2.41	109.77	114.08
26	b	604	CLA	CHB-C4A-NA	2.41	127.85	124.51
26	b	606	CLA	CHB-C4A-NA	2.41	127.85	124.51
26	O	604	CLA	CHB-C4A-NA	2.41	127.85	124.51
39	3	312	II0	C05-C07-C11	2.41	113.60	110.30
38	S	608	KC2	O2D-CGD-O1D	-2.41	119.13	123.84
33	4	319	LMG	O8-C28-C29	2.41	119.46	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	6	608	KC2	O2D-CGD-O1D	-2.40	119.14	123.84
30	A	408	SQD	O48-C23-C24	2.40	119.45	111.91
26	5	609	CLA	CHB-C4A-NA	2.40	127.84	124.51
26	C	507	CLA	CHD-C1D-ND	-2.40	122.25	124.45
26	1	607	CLA	CBC-CAC-C3C	2.40	119.06	112.43
26	4	313	CLA	CHB-C4A-NA	2.40	127.83	124.51
26	B	614	CLA	CHB-C4A-NA	2.40	127.83	124.51
39	6	611	II0	C06-C04-C10	2.40	114.49	109.62
26	C	504	CLA	CHB-C4A-NA	2.40	127.83	124.51
33	Q	318	LMG	O8-C28-C29	2.40	119.44	111.91
26	c	506	CLA	CHB-C4A-NA	2.40	127.83	124.51
26	c	507	CLA	CHB-C4A-NA	2.40	127.83	124.51
39	5	613	II0	C30-C32-C34	-2.40	115.73	123.22
26	N	608	CLA	C3D-C4D-ND	-2.40	106.36	110.24
26	2	306	CLA	CMB-C2B-C3B	2.40	129.17	124.68
39	R	315	II0	C32-C30-C26	-2.40	119.62	126.58
40	N	619	IHT	C22-C23-C27	2.40	122.62	118.94
26	4	302	CLA	CHD-C1D-ND	-2.40	122.25	124.45
26	D	407	CLA	CHB-C4A-NA	2.39	127.82	124.51
39	R	314	II0	C30-C32-C34	-2.39	115.75	123.22
38	2	310	KC2	C3D-CAD-CBD	-2.39	104.45	107.61
28	B	619	WVN	C02-C05-C09	-2.39	118.52	121.47
26	A	403	CLA	CHB-C4A-NA	2.39	127.82	124.51
26	B	605	CLA	CHD-C1D-ND	-2.39	122.26	124.45
26	O	606	CLA	CMB-C2B-C3B	2.39	129.15	124.68
26	c	505	CLA	CHB-C4A-NA	2.39	127.81	124.51
38	4	305	KC2	O2D-CGD-O1D	-2.39	119.17	123.84
26	P	603	CLA	C1-C2-C3	-2.39	121.91	126.04
28	c	516	WVN	C28-C30-C33	-2.39	115.77	123.22
40	N	619	IHT	C03-C05-C08	-2.39	108.25	113.64
38	Q	304	KC2	O2D-CGD-O1D	-2.39	119.17	123.84
26	c	513	CLA	CHB-C4A-NA	2.39	127.81	124.51
39	3	310	II0	C12-C14-C10	-2.39	115.16	120.57
39	R	314	II0	C18-C04-C10	-2.39	106.68	110.47
26	Q	312	CLA	CHB-C4A-NA	2.38	127.81	124.51
26	b	605	CLA	CHB-C4A-NA	2.38	127.81	124.51
26	R	306	CLA	CHB-C4A-NA	2.38	127.81	124.51
38	O	610	KC2	C3D-CAD-CBD	-2.38	104.47	107.61
38	N	612	KC2	C3D-CAD-CBD	-2.38	104.47	107.61
26	B	606	CLA	CHB-C4A-NA	2.38	127.81	124.51
28	Y	101	WVN	C39-C40-C37	-2.38	118.60	123.47
40	4	318	IHT	C41-C40-C37	-2.38	118.60	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	407	PL9	C27-C28-C29	-2.38	121.93	127.66
39	R	314	II0	C32-C30-C26	-2.38	119.67	126.58
26	O	604	CLA	CHD-C1D-ND	-2.38	122.27	124.45
26	2	308	CLA	CHB-C4A-NA	2.38	127.80	124.51
26	P	602	CLA	CHD-C1D-ND	-2.38	122.27	124.45
40	Q	317	IHT	C41-C40-C37	-2.38	118.61	123.47
26	d	405	CLA	CHB-C4A-NA	2.37	127.80	124.51
26	O	608	CLA	CHB-C4A-NA	2.37	127.80	124.51
26	P	610	CLA	CHB-C4A-NA	2.37	127.80	124.51
39	S	611	II0	C03-C09-C13	-2.37	119.28	122.63
35	c	519	DGD	O1G-C1A-C2A	2.37	119.36	111.91
26	R	302	CLA	CHD-C1D-ND	-2.37	122.27	124.45
26	b	607	CLA	CHD-C1D-ND	-2.37	122.27	124.45
39	5	613	II0	C32-C30-C26	-2.37	119.69	126.58
26	B	607	CLA	CHB-C4A-NA	2.37	127.79	124.51
39	5	613	II0	C18-C04-C10	-2.37	106.70	110.47
26	C	506	CLA	CHB-C4A-NA	2.37	127.79	124.51
39	Q	314	II0	C03-C09-C13	-2.37	119.29	122.63
28	D	412	WVN	C01-C02-C11	-2.37	109.70	112.70
26	3	301	CLA	CHD-C1D-ND	-2.37	122.28	124.45
26	P	601	CLA	CHB-C4A-NA	2.37	127.79	124.51
26	c	512	CLA	CHB-C4A-NA	2.37	127.79	124.51
30	a	408	SQD	O48-C23-C24	2.37	119.34	111.91
26	R	310	CLA	CHB-C4A-NA	2.37	127.79	124.51
39	N	617	II0	C31-C33-C35	-2.37	119.77	126.42
33	c	521	LMG	C8-O7-C10	-2.37	111.96	117.79
26	2	319	CLA	CHB-C4A-NA	2.37	127.78	124.51
26	S	610	CLA	CHB-C4A-NA	2.37	127.78	124.51
26	O	605	CLA	CHB-C4A-NA	2.36	127.78	124.51
26	R	302	CLA	CHB-C4A-NA	2.36	127.78	124.51
28	B	619	WVN	C28-C30-C33	-2.36	115.84	123.22
38	Q	309	KC2	C2B-C1B-NB	2.36	111.84	110.10
26	O	608	CLA	CHD-C1D-ND	-2.36	122.28	124.45
28	Z	101	WVN	C27-C25-C23	2.36	121.80	118.08
26	1	601	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
26	B	605	CLA	CHB-C4A-NA	2.36	127.78	124.51
26	6	602	CLA	CHD-C1D-ND	-2.36	122.28	124.45
26	G	402	CLA	O2D-CGD-CBD	2.36	115.46	111.27
38	4	310	KC2	CMB-C2B-C1B	2.36	128.87	124.71
26	1	604	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
26	2	303	CLA	CHB-C4A-NA	2.36	127.77	124.51
26	N	607	CLA	CMB-C2B-C3B	2.36	129.09	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	4	315	II0	C03-C09-C13	-2.36	119.31	122.63
26	1	606	CLA	C1-C2-C3	-2.36	122.94	126.75
26	d	402	CLA	CHB-C4A-NA	2.36	127.77	124.51
29	D	409	PL9	C20-C19-C21	2.36	119.23	115.27
40	5	616	IHT	C06-C09-C10	-2.36	109.87	114.08
26	O	603	CLA	CHB-C4A-NA	2.36	127.77	124.51
38	4	311	KC2	CMB-C2B-C1B	2.36	128.86	124.71
26	2	308	CLA	CHD-C1D-ND	-2.35	122.29	124.45
26	B	604	CLA	CHB-C4A-NA	2.35	127.77	124.51
28	d	410	WVN	C07-C01-C02	2.35	113.11	109.55
39	2	313	II0	C03-C09-C13	-2.35	119.31	122.63
40	R	317	IHT	C06-C09-C10	-2.35	109.88	114.08
26	P	607	CLA	CHD-C1D-ND	-2.35	122.29	124.45
26	5	601	CLA	CHB-C4A-NA	2.35	127.76	124.51
38	Q	309	KC2	CMB-C2B-C1B	2.35	128.86	124.71
39	R	316	II0	C41-C42-C40	-2.35	118.66	123.47
26	Q	301	CLA	CHD-C1D-ND	-2.35	122.29	124.45
26	b	616	CLA	CHB-C4A-NA	2.35	127.76	124.51
28	S	613	WVN	C28-C30-C33	-2.35	115.88	123.22
39	Q	314	II0	C17-C04-C06	-2.35	98.50	109.05
35	C	517	DGD	O1G-C1A-C2A	2.35	119.28	111.91
39	O	613	II0	C03-C09-C13	-2.35	119.32	122.63
26	2	305	CLA	C1-C2-C3	-2.35	121.98	126.04
26	O	611	CLA	CHB-C4A-NA	2.35	127.76	124.51
28	A	406	WVN	C30-C33-C34	-2.35	119.82	126.42
39	4	315	II0	C17-C04-C06	-2.35	98.51	109.05
26	3	308	CLA	C1-C2-C3	-2.35	121.98	126.04
39	6	611	II0	C03-C09-C13	-2.35	119.32	122.63
40	O	616	IHT	C31-C34-C35	-2.35	119.83	126.42
28	c	517	WVN	C26-C29-C31	-2.35	115.90	123.22
26	5	605	CLA	CHB-C4A-NA	2.35	127.75	124.51
26	4	309	CLA	CHD-C1D-ND	-2.34	122.30	124.45
39	4	316	II0	C41-C42-C40	-2.34	118.67	123.47
28	5	617	WVN	C28-C30-C33	-2.34	115.90	123.22
39	R	316	II0	C30-C32-C34	-2.34	115.90	123.22
38	P	605	KC2	CBD-CHA-C1A	2.34	133.25	128.88
26	g	401	CLA	CHB-C4A-NA	2.34	127.75	124.51
38	P	605	KC2	C2B-C1B-NB	2.34	111.83	110.10
38	Q	304	KC2	C2B-C1B-NB	2.34	111.83	110.10
26	B	604	CLA	O2D-CGD-CBD	2.34	115.43	111.27
38	N	610	KC2	CBD-CHA-C1A	2.34	133.24	128.88
26	1	614	CLA	O1D-CGD-CBD	2.34	129.27	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	Q	310	KC2	CMB-C2B-C1B	2.34	128.83	124.71
26	C	507	CLA	CHB-C4A-NA	2.34	127.74	124.51
26	2	311	CLA	CHB-C4A-NA	2.34	127.74	124.51
26	3	306	CLA	CHD-C1D-ND	-2.34	122.31	124.45
26	6	610	CLA	CHB-C4A-NA	2.33	127.74	124.51
26	1	603	CLA	CHB-C4A-NA	2.33	127.74	124.51
28	C	515	WVN	C28-C30-C33	-2.33	115.94	123.22
38	3	304	KC2	CBD-CHA-C1A	2.33	133.23	128.88
39	Q	315	II0	C41-C42-C40	-2.33	118.70	123.47
28	Z	101	WVN	C16-C05-C09	-2.33	114.04	122.33
28	P	615	WVN	C29-C31-C32	-2.33	119.87	126.42
40	O	616	IHT	C30-C32-C33	-2.33	119.87	126.42
40	R	317	IHT	C14-C02-C07	-2.33	106.52	110.30
26	R	305	CLA	CHB-C4A-NA	2.33	127.73	124.51
26	S	602	CLA	CHD-C1D-ND	-2.33	122.31	124.45
28	d	410	WVN	C23-C20-C13	-2.33	120.67	127.20
39	5	615	II0	C41-C42-C40	-2.33	118.71	123.47
26	S	601	CLA	CHB-C4A-NA	2.32	127.73	124.51
28	c	517	WVN	C02-C05-C09	-2.32	118.61	121.47
39	1	617	II0	C06-C08-C12	2.32	113.49	110.30
26	G	402	CLA	CHB-C4A-NA	2.32	127.73	124.51
39	N	616	II0	C30-C32-C34	-2.32	115.97	123.22
26	g	401	CLA	CHD-C1D-ND	-2.32	122.32	124.45
26	C	505	CLA	CHB-C4A-NA	2.32	127.72	124.51
26	4	309	CLA	C1-C2-C3	-2.32	122.03	126.04
39	5	615	II0	C30-C32-C34	-2.32	115.98	123.22
26	a	403	CLA	CHB-C4A-NA	2.32	127.72	124.51
26	P	606	CLA	CHB-C4A-NA	2.32	127.72	124.51
40	N	619	IHT	C39-C35-C34	2.32	121.73	118.08
26	6	601	CLA	CHB-C4A-NA	2.32	127.71	124.51
39	N	617	II0	C17-C04-C06	-2.32	98.65	109.05
39	5	614	II0	C18-C04-C10	-2.31	106.79	110.47
26	b	614	CLA	CHB-C4A-NA	2.31	127.71	124.51
26	5	604	CLA	CHB-C4A-NA	2.31	127.71	124.51
26	A	405	CLA	CHD-C1D-ND	-2.31	122.33	124.45
26	Q	308	CLA	CHB-C4A-NA	2.31	127.71	124.51
26	d	402	CLA	O2D-CGD-CBD	2.31	115.38	111.27
28	b	617	WVN	C18-C06-C13	-2.31	106.55	110.30
40	4	318	IHT	C17-C03-C05	2.31	119.42	109.05
26	3	305	CLA	CHB-C4A-NA	2.31	127.70	124.51
30	A	408	SQD	O8-S-C6	2.31	109.42	105.74
26	b	604	CLA	O2D-CGD-CBD	2.31	115.37	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	407	PL9	C20-C19-C21	2.31	119.15	115.27
26	c	508	CLA	CHD-C1D-ND	-2.31	122.33	124.45
26	4	301	CLA	CHD-C1D-ND	-2.31	122.33	124.45
26	c	510	CLA	CHB-C4A-NA	2.31	127.70	124.51
28	B	619	WVN	C18-C06-C13	2.31	114.04	110.30
39	N	618	II0	C31-C29-C25	-2.30	119.89	126.58
28	b	618	WVN	C29-C31-C32	-2.30	119.94	126.42
28	C	515	WVN	C27-C25-C23	2.30	121.71	118.08
40	5	616	IHT	C14-C02-C07	-2.30	106.56	110.30
40	Q	317	IHT	C17-C03-C05	2.30	119.39	109.05
26	R	308	CLA	CHD-C1D-ND	-2.30	122.34	124.45
26	3	308	CLA	C2C-C1C-NC	-2.30	107.82	109.97
26	A	402	CLA	CHD-C1D-ND	-2.30	122.34	124.45
26	R	309	CLA	CHD-C1D-ND	-2.30	122.34	124.45
26	Q	308	CLA	C1-C2-C3	-2.30	122.07	126.04
39	Q	315	II0	C17-C04-C06	-2.30	98.73	109.05
26	4	306	CLA	CHD-C1D-ND	-2.30	122.34	124.45
26	c	508	CLA	CHB-C4A-NA	2.30	127.69	124.51
38	N	612	KC2	CBD-CHA-C1A	2.30	133.16	128.88
26	B	610	CLA	CHB-C4A-NA	2.30	127.69	124.51
26	b	606	CLA	CHD-C1D-ND	-2.30	122.34	124.45
26	b	610	CLA	CHD-C1D-ND	-2.30	122.34	124.45
39	4	316	II0	C17-C04-C06	-2.30	98.74	109.05
26	5	601	CLA	CHD-C1D-ND	-2.29	122.35	124.45
40	4	318	IHT	C22-C23-C27	2.29	122.46	118.94
26	O	612	CLA	CHB-C4A-NA	2.29	127.68	124.51
26	c	504	CLA	CHB-C4A-NA	2.29	127.68	124.51
26	Q	305	CLA	CHD-C1D-ND	-2.29	122.35	124.45
39	P	614	II0	C17-C04-C06	-2.29	98.77	109.05
26	B	603	CLA	CHB-C4A-NA	2.29	127.68	124.51
26	1	609	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
30	c	501	SQD	O7-S-C6	2.29	109.66	106.94
26	D	404	CLA	CHB-C4A-NA	2.29	127.67	124.51
39	R	315	II0	C18-C04-C10	-2.28	106.84	110.47
37	F	101	HEM	CHA-C4D-C3D	-2.28	121.04	125.33
26	N	614	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
39	1	615	II0	C05-C07-C11	2.28	113.42	110.30
26	D	408	CLA	CHD-C1D-ND	-2.28	122.36	124.45
28	c	516	WVN	C12-C14-C15	-2.28	110.01	114.08
26	P	608	CLA	CHD-C1D-ND	-2.28	122.36	124.45
39	6	613	II0	C17-C04-C06	-2.28	98.82	109.05
26	6	603	CLA	C1-C2-C3	-2.28	122.11	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	Q	310	KC2	CAA-CBA-CGA	-2.28	115.56	127.26
39	O	614	II0	C20-C14-C12	2.28	118.57	114.36
26	B	606	CLA	CHD-C1D-ND	-2.28	122.36	124.45
26	2	312	CLA	CHB-C4A-NA	2.27	127.66	124.51
26	N	602	CLA	CHD-C1D-ND	-2.27	122.36	124.45
39	R	318	II0	C17-C04-C06	-2.27	98.85	109.05
26	4	309	CLA	CHB-C4A-NA	2.27	127.65	124.51
38	4	311	KC2	CAA-CBA-CGA	-2.27	115.59	127.26
33	R	301	LMG	C8-O7-C10	-2.27	112.20	117.79
26	Q	308	CLA	CHD-C1D-ND	-2.27	122.37	124.45
34	C	518	LHG	C6-C5-C4	-2.27	106.42	111.79
26	b	602	CLA	CHD-C1D-ND	-2.27	122.37	124.45
26	5	608	CLA	CHD-C1D-ND	-2.27	122.37	124.45
26	S	603	CLA	C1-C2-C3	-2.27	122.12	126.04
26	C	511	CLA	CHB-C4A-NA	2.27	127.65	124.51
39	N	617	II0	C19-C13-C11	2.27	118.55	114.36
26	B	616	CLA	CHB-C4A-NA	2.27	127.64	124.51
34	Z	102	LHG	O8-C23-C24	2.27	119.02	111.91
38	4	305	KC2	CAB-C3B-C2B	2.26	136.06	128.60
26	R	313	CLA	CHB-C4A-NA	2.26	127.64	124.51
39	1	616	II0	C05-C07-C11	2.26	113.40	110.30
28	A	406	WVN	C40-C39-C36	-2.26	118.84	123.47
26	b	610	CLA	CHB-C4A-NA	2.26	127.64	124.51
38	Q	304	KC2	CAB-C3B-C2B	2.26	136.05	128.60
28	k	101	WVN	C30-C33-C34	-2.26	120.07	126.42
38	2	310	KC2	CAA-CBA-CGA	-2.26	115.66	127.26
39	2	314	II0	C20-C14-C12	2.26	118.54	114.36
38	O	610	KC2	CAA-CBA-CGA	-2.26	115.66	127.26
26	1	608	CLA	CHB-C4A-NA	2.26	127.63	124.51
30	D	401	SQD	O7-S-C6	2.26	109.62	106.94
26	5	612	CLA	CHB-C4A-NA	2.26	127.63	124.51
26	N	606	CLA	CHD-C1D-ND	-2.25	122.38	124.45
26	5	607	CLA	CHD-C1D-ND	-2.25	122.38	124.45
34	1	620	LHG	C5-O7-C7	-2.25	112.24	117.79
39	6	612	II0	C27-C25-C23	2.25	121.30	116.84
28	D	412	WVN	C14-C15-C13	-2.25	119.46	122.73
38	3	304	KC2	C2B-C1B-NB	2.25	111.76	110.10
40	O	616	IHT	C18-C22-C23	-2.25	122.84	126.23
26	5	612	CLA	CHD-C1D-ND	-2.25	122.39	124.45
26	B	608	CLA	CHB-C4A-NA	2.25	127.62	124.51
34	N	621	LHG	O8-C23-C24	2.25	118.96	111.91
40	Q	317	IHT	C22-C23-C27	2.25	122.39	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	404	CLA	O2D-CGD-CBD	2.25	115.26	111.27
39	S	612	II0	C27-C25-C23	2.25	121.29	116.84
38	1	605	KC2	OBD-CAD-CBD	-2.25	122.69	125.89
39	R	318	II0	C31-C33-C35	-2.25	120.11	126.42
26	A	402	CLA	CHB-C4A-NA	2.24	127.62	124.51
28	A	406	WVN	C26-C29-C31	-2.24	116.21	123.22
26	C	509	CLA	CHB-C4A-NA	2.24	127.61	124.51
34	z	101	LHG	O8-C23-C24	2.24	118.95	111.91
34	1	620	LHG	O8-C23-C24	2.24	118.95	111.91
38	4	305	KC2	CMB-C2B-C1B	2.24	128.66	124.71
33	a	413	LMG	O8-C28-O10	-2.24	117.93	123.59
33	c	522	LMG	C8-O7-C10	-2.24	112.27	117.79
26	B	609	CLA	CHD-C1D-ND	-2.24	122.40	124.45
38	3	304	KC2	CAA-CBA-CGA	-2.24	115.75	127.26
26	g	401	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
26	a	402	CLA	CHD-C1D-ND	-2.24	122.40	124.45
26	b	608	CLA	CHB-C4A-NA	2.24	127.61	124.51
29	a	407	PL9	O2-C1-C6	2.24	124.47	120.59
34	N	621	LHG	C5-O7-C7	-2.24	112.29	117.79
26	R	313	CLA	CHD-C1D-ND	-2.24	122.40	124.45
26	O	602	CLA	C1-C2-C3	-2.23	122.18	126.04
26	1	613	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
33	B	620	LMG	O8-C28-C29	2.23	118.92	111.91
26	c	503	CLA	CHB-C4A-NA	2.23	127.60	124.51
26	C	505	CLA	CHD-C1D-ND	-2.23	122.40	124.45
39	O	614	II0	C03-C09-C13	-2.23	119.48	122.63
30	D	401	SQD	O8-S-C6	2.23	109.30	105.74
26	2	312	CLA	CHD-C1D-ND	-2.23	122.40	124.45
40	N	619	IHT	C22-C18-C07	-2.23	120.94	127.20
39	6	613	II0	C31-C33-C35	-2.23	120.15	126.42
26	b	602	CLA	O2D-CGD-CBD	2.23	115.23	111.27
26	1	604	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
39	N	617	II0	C20-C14-C12	2.23	118.48	114.36
30	a	408	SQD	O8-S-C6	2.23	109.29	105.74
39	5	613	II0	C31-C33-C35	-2.22	120.17	126.42
38	P	605	KC2	CAA-CBA-CGA	-2.22	115.83	127.26
38	Q	310	KC2	CAB-C3B-C2B	2.22	135.93	128.60
39	2	314	II0	C03-C09-C13	-2.22	119.49	122.63
39	O	614	II0	C27-C25-C23	2.22	121.24	116.84
26	R	306	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
39	O	613	II0	C41-C42-C40	-2.22	118.92	123.47
26	5	605	CLA	O2A-CGA-O1A	-2.22	117.98	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	4	315	II0	C30-C32-C34	-2.22	116.28	123.22
33	b	620	LMG	O8-C28-C29	2.22	118.87	111.91
28	c	517	WVN	C30-C28-C25	-2.22	124.14	127.31
28	5	617	WVN	C21-C15-C14	2.22	117.88	113.62
37	f	101	HEM	CHA-C4D-C3D	-2.22	121.17	125.33
38	N	605	KC2	CBD-CHA-C1A	2.22	133.01	128.88
26	2	302	CLA	C1-C2-C3	-2.21	122.22	126.04
39	N	616	II0	C17-C04-C06	-2.21	99.11	109.05
33	5	619	LMG	C8-O7-C10	-2.21	112.34	117.79
29	d	407	PL9	O1-C4-C3	-2.21	118.28	120.72
26	B	602	CLA	CHD-C1D-ND	-2.21	122.42	124.45
26	a	402	CLA	CHB-C4A-NA	2.21	127.57	124.51
28	a	406	WVN	C38-C34-C33	2.21	121.56	118.08
26	b	614	CLA	CHD-C1D-ND	-2.21	122.42	124.45
26	3	309	CLA	CHD-C1D-ND	-2.21	122.42	124.45
28	c	516	WVN	C23-C20-C13	-2.21	121.00	127.20
26	a	405	CLA	CHD-C1D-ND	-2.21	122.42	124.45
26	c	506	CLA	CHD-C1D-ND	-2.21	122.42	124.45
38	Q	304	KC2	CMB-C2B-C1B	2.21	128.60	124.71
26	a	403	CLA	C2D-C1D-ND	-2.21	108.48	110.10
38	4	310	KC2	CAA-CBA-CGA	-2.21	115.92	127.26
38	1	611	KC2	OBD-CAD-CBD	-2.21	122.74	125.89
28	S	613	WVN	C21-C15-C14	2.21	117.85	113.62
28	Y	101	WVN	C14-C15-C13	-2.21	119.53	122.73
38	N	611	KC2	CAB-C3B-C4B	-2.21	119.57	124.90
39	4	314	II0	C38-C36-C34	2.20	121.55	118.08
38	4	311	KC2	CAB-C3B-C2B	2.20	135.87	128.60
26	b	613	CLA	CHD-C1D-ND	-2.20	122.43	124.45
38	Q	309	KC2	CAA-CBA-CGA	-2.20	115.94	127.26
39	2	313	II0	C41-C42-C40	-2.20	118.96	123.47
39	2	314	II0	C27-C25-C23	2.20	121.20	116.84
28	A	406	WVN	C35-C32-C31	2.20	121.55	118.08
26	b	612	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
26	1	602	CLA	CHD-C1D-ND	-2.20	122.43	124.45
39	R	314	II0	C31-C33-C35	-2.20	120.24	126.42
26	C	502	CLA	CHB-C4A-NA	2.20	127.55	124.51
39	Q	315	II0	C18-C04-C10	-2.20	106.97	110.47
28	Z	101	WVN	C40-C39-C36	-2.20	118.97	123.47
26	6	601	CLA	CHD-C1D-ND	-2.20	122.44	124.45
26	B	602	CLA	O2D-CGD-CBD	2.20	115.17	111.27
30	c	501	SQD	O8-S-C6	2.20	109.24	105.74
26	g	402	CLA	CAA-C2A-C3A	-2.20	106.76	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	N	608	CLA	C2C-C1C-NC	-2.20	107.92	109.97
39	Q	314	II0	C30-C32-C34	-2.19	116.37	123.22
28	k	101	WVN	C14-C15-C13	-2.19	119.55	122.73
26	1	614	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
26	S	607	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
26	b	609	CLA	CHD-C1D-ND	-2.19	122.44	124.45
26	B	611	CLA	CHB-C4A-NA	2.19	127.54	124.51
39	3	310	II0	C18-C04-C10	-2.19	106.99	110.47
39	O	613	II0	C30-C32-C34	-2.19	116.39	123.22
26	B	613	CLA	CHD-C1D-ND	-2.19	122.44	124.45
26	1	607	CLA	C2D-C1D-ND	-2.19	108.49	110.10
39	Q	313	II0	C38-C36-C34	2.19	121.52	118.08
38	Q	309	KC2	CAB-C3B-C2B	2.19	135.81	128.60
27	d	403	PHO	CMC-C2C-C3C	2.19	129.06	124.94
26	R	303	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
26	6	607	CLA	O2A-CGA-O1A	-2.19	118.08	123.59
30	D	401	SQD	O9-S-C6	2.19	109.54	106.94
39	S	611	II0	C18-C04-C10	-2.18	107.00	110.47
26	G	401	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
38	4	310	KC2	CAB-C3B-C2B	2.18	135.80	128.60
26	N	614	CLA	CHB-C4A-NA	2.18	127.53	124.51
26	B	609	CLA	CHB-C4A-NA	2.18	127.53	124.51
39	4	316	II0	C18-C04-C10	-2.18	107.00	110.47
26	O	601	CLA	O2D-CGD-CBD	2.18	115.14	111.27
26	c	512	CLA	CHD-C1D-ND	-2.18	122.45	124.45
26	O	612	CLA	CHD-C1D-ND	-2.18	122.45	124.45
26	B	612	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
26	P	611	CLA	CHD-C1D-ND	-2.18	122.45	124.45
26	S	601	CLA	CHD-C1D-ND	-2.18	122.45	124.45
28	P	615	WVN	C29-C26-C22	-2.18	124.20	127.31
26	B	607	CLA	CHD-C1D-ND	-2.18	122.45	124.45
30	A	408	SQD	C45-O47-C7	-2.18	112.43	117.79
26	2	301	CLA	O2D-CGD-CBD	2.18	115.14	111.27
38	1	612	KC2	OBD-CAD-CBD	-2.18	122.79	125.89
33	C	520	LMG	C8-O7-C10	-2.18	112.44	117.79
26	B	605	CLA	C1-C2-C3	-2.17	122.29	126.04
26	5	602	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
26	b	609	CLA	CHB-C4A-NA	2.17	127.52	124.51
26	N	606	CLA	C1-C2-C3	-2.17	123.24	126.75
39	2	313	II0	C30-C32-C34	-2.17	116.44	123.22
39	N	618	II0	C30-C32-C34	-2.17	116.44	123.22
40	N	619	IHT	C17-C03-C05	2.17	118.79	109.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	516	WVN	C20-C23-C25	-2.17	122.96	126.23
26	N	607	CLA	CHB-C4A-NA	2.17	127.51	124.51
39	1	616	II0	C42-C41-C39	-2.17	119.03	123.47
40	Q	317	IHT	C31-C34-C35	-2.17	120.32	126.42
40	4	318	IHT	C31-C34-C35	-2.17	120.33	126.42
30	a	408	SQD	C45-O47-C7	-2.17	112.45	117.79
38	S	608	KC2	CMB-C2B-C1B	2.17	128.53	124.71
26	P	603	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
38	N	611	KC2	CAA-CBA-CGA	-2.17	116.12	127.26
38	N	612	KC2	C3B-C2B-C1B	-2.17	105.01	107.08
29	A	407	PL9	O2-C1-C6	2.17	124.34	120.59
28	b	618	WVN	C38-C34-C37	-2.17	119.89	122.92
26	3	302	CLA	O2A-CGA-O1A	-2.17	118.13	123.59
28	a	406	WVN	C30-C33-C34	-2.17	120.33	126.42
26	c	503	CLA	CHD-C1D-ND	-2.16	122.47	124.45
26	b	609	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
26	4	303	CLA	CAC-C3C-C4C	2.16	127.62	124.81
28	d	410	WVN	C10-C06-C13	2.16	113.81	110.48
26	b	616	CLA	CHD-C1D-ND	-2.16	122.47	124.45
38	1	612	KC2	CHC-C4B-NB	-2.16	122.47	124.45
39	4	316	II0	C31-C33-C35	-2.16	120.34	126.42
26	B	601	CLA	CHD-C1D-ND	-2.16	122.47	124.45
39	Q	315	II0	C31-C33-C35	-2.16	120.35	126.42
38	6	608	KC2	CMB-C2B-C1B	2.16	128.52	124.71
39	N	620	II0	C32-C30-C26	-2.16	120.31	126.58
26	Q	302	CLA	CAC-C3C-C4C	2.16	127.61	124.81
26	b	611	CLA	CHB-C4A-NA	2.16	127.50	124.51
27	D	405	PHO	O2A-CGA-O1A	-2.16	118.15	123.59
38	2	310	KC2	O2D-CGD-O1D	-2.16	119.62	123.84
28	C	515	WVN	C12-C14-C15	-2.16	110.23	114.08
26	B	609	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
40	N	619	IHT	C20-C15-C11	-2.16	121.42	124.35
26	1	606	CLA	C1B-CHB-C4A	-2.16	125.85	130.12
38	N	605	KC2	CAA-CBA-CGA	-2.16	116.19	127.26
38	N	612	KC2	CAA-CBA-CGA	-2.15	116.19	127.26
26	b	611	CLA	C1-C2-C3	-2.15	122.32	126.04
28	c	516	WVN	C29-C31-C32	-2.15	120.38	126.42
26	B	610	CLA	CHD-C1D-ND	-2.15	122.48	124.45
26	b	603	CLA	CHB-C4A-NA	2.15	127.48	124.51
26	Q	302	CLA	C1-C2-C3	-2.15	122.33	126.04
26	N	606	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
39	N	616	II0	C05-C07-C11	-2.15	107.36	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	514	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
30	c	501	SQD	C45-O47-C7	-2.15	112.51	117.79
39	6	611	II0	C18-C04-C10	-2.15	107.06	110.47
38	O	610	KC2	O2D-CGD-O1D	-2.14	119.65	123.84
27	a	404	PHO	CMC-C2C-C3C	2.14	128.98	124.94
39	1	617	II0	C06-C04-C10	2.14	113.96	109.62
39	2	315	II0	C32-C30-C26	-2.14	120.36	126.58
26	N	614	CLA	CHD-C1D-ND	-2.14	122.49	124.45
30	D	401	SQD	C45-O47-C7	-2.14	112.52	117.79
27	D	405	PHO	CMC-C2C-C3C	2.14	128.98	124.94
26	c	507	CLA	O2D-CGD-CBD	2.14	115.07	111.27
28	b	618	WVN	C39-C40-C37	-2.14	119.09	123.47
39	2	314	II0	C32-C30-C26	-2.14	120.38	126.58
26	b	605	CLA	C1-C2-C3	-2.14	122.35	126.04
26	C	506	CLA	O2D-CGD-CBD	2.13	115.06	111.27
29	D	409	PL9	O1-C4-C3	-2.13	118.37	120.72
26	A	403	CLA	C2D-C1D-ND	-2.13	108.53	110.10
30	c	501	SQD	O9-S-C6	2.13	109.47	106.94
26	B	616	CLA	CHD-C1D-ND	-2.13	122.50	124.45
26	b	611	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
26	C	512	CLA	CHD-C1D-ND	-2.13	122.50	124.45
30	A	408	SQD	O7-S-C6	2.13	109.47	106.94
28	P	615	WVN	C24-C22-C19	2.13	121.43	118.08
39	O	614	II0	C32-C30-C26	-2.13	120.41	126.58
30	a	408	SQD	O7-S-C6	2.13	109.47	106.94
26	1	602	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
26	4	303	CLA	C1-C2-C3	-2.12	122.37	126.04
26	C	506	CLA	CHD-C1D-ND	-2.12	122.50	124.45
26	d	406	CLA	CHD-C1D-ND	-2.12	122.50	124.45
26	b	616	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
28	H	101	WVN	C01-C02-C11	-2.12	110.02	112.70
26	b	611	CLA	CHD-C1D-ND	-2.12	122.50	124.45
38	N	610	KC2	CAA-CBA-CGA	-2.12	116.36	127.26
38	2	310	KC2	CMB-C2B-C1B	2.12	128.45	124.71
39	4	316	II0	C30-C32-C34	-2.12	116.61	123.22
40	R	317	IHT	C27-C30-C32	-2.12	116.61	123.22
26	6	610	CLA	CHD-C1D-ND	-2.12	122.51	124.45
26	R	307	CLA	CHB-C4A-NA	2.12	127.44	124.51
38	5	610	KC2	CBD-CHA-C1A	2.12	132.83	128.88
37	F	101	HEM	C4D-ND-C1D	2.12	107.26	105.07
33	A	412	LMG	O8-C28-O10	-2.12	118.25	123.59
28	B	619	WVN	C21-C15-C14	2.12	117.68	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	514	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
26	2	306	CLA	CHD-C1D-ND	-2.11	122.51	124.45
26	R	307	CLA	CHD-C1D-ND	-2.11	122.51	124.45
38	1	610	KC2	OBD-CAD-CBD	-2.11	122.88	125.89
26	C	509	CLA	CHD-C1D-ND	-2.11	122.51	124.45
26	1	609	CLA	CHD-C1D-ND	-2.11	122.51	124.45
39	2	316	II0	C17-C04-C10	-2.11	107.12	110.47
28	a	406	WVN	C12-C14-C15	-2.11	110.31	114.08
29	D	409	PL9	O2-C1-C6	2.11	124.24	120.59
28	c	517	WVN	C12-C14-C15	-2.11	110.31	114.08
26	B	614	CLA	CHD-C1D-ND	-2.11	122.52	124.45
26	5	603	CLA	CAA-C2A-C1A	-2.11	105.07	111.97
39	R	314	II0	C03-C09-C13	-2.11	119.66	122.63
28	x	101	WVN	C19-C22-C26	2.10	122.17	118.94
26	c	513	CLA	CHD-C1D-ND	-2.10	122.52	124.45
26	B	611	CLA	C1-C2-C3	-2.10	122.41	126.04
38	R	311	KC2	CBD-CHA-C1A	2.10	132.80	128.88
26	O	605	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
26	B	611	CLA	CHD-C1D-ND	-2.10	122.52	124.45
26	B	604	CLA	CAA-CBA-CGA	-2.10	107.11	113.25
26	6	603	CLA	C3A-C2A-C1A	2.10	104.48	101.34
26	O	606	CLA	CHD-C1D-ND	-2.10	122.52	124.45
26	O	606	CLA	CHB-C4A-NA	2.10	127.42	124.51
26	g	401	CLA	C1-C2-C3	-2.10	122.41	126.04
26	2	305	CLA	CMB-C2B-C1B	2.10	131.69	128.46
28	P	615	WVN	C03-C04-C09	-2.10	108.51	112.00
28	c	517	WVN	C28-C30-C33	-2.10	116.67	123.22
40	5	616	IHT	C27-C30-C32	-2.10	116.67	123.22
26	1	607	CLA	CMC-C2C-C1C	-2.10	121.84	125.04
26	B	601	CLA	C1-C2-C3	-2.10	123.36	126.75
26	C	513	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
26	S	609	CLA	O1D-CGD-CBD	2.10	128.77	124.48
26	6	609	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
26	R	304	CLA	CAA-C2A-C1A	-2.10	105.11	111.97
39	5	613	II0	C03-C09-C13	-2.10	119.67	122.63
38	N	612	KC2	CMB-C2B-C1B	2.10	128.41	124.71
39	Q	315	II0	C20-C14-C12	2.09	118.24	114.36
39	O	615	II0	C06-C04-C10	2.09	113.86	109.62
26	S	610	CLA	CHD-C1D-ND	-2.09	122.53	124.45
39	O	615	II0	C17-C04-C10	-2.09	107.14	110.47
26	C	506	CLA	C1-C2-C3	-2.09	122.42	126.04
39	2	320	II0	C03-C09-C13	-2.09	119.68	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	407	PL9	O2-C1-C2	-2.09	116.99	121.78
26	R	312	CLA	CAA-CBA-CGA	-2.09	107.14	113.25
26	S	609	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
27	d	403	PHO	O2A-CGA-O1A	-2.09	118.31	123.59
26	6	609	CLA	O1D-CGD-CBD	2.09	128.76	124.48
39	R	315	II0	C29-C31-C33	-2.09	116.69	123.22
26	C	514	CLA	CHD-C1D-ND	-2.09	122.53	124.45
29	A	407	PL9	O2-C1-C2	-2.09	116.99	121.78
28	C	515	WVN	C26-C29-C31	-2.09	116.69	123.22
35	h	101	DGD	C2G-O2G-C1B	-2.09	112.65	117.79
38	O	610	KC2	CMB-C2B-C1B	2.09	128.40	124.71
26	B	616	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
35	H	102	DGD	C2G-O2G-C1B	-2.09	112.65	117.79
33	M	101	LMG	O8-C28-O10	-2.09	118.32	123.59
39	4	316	II0	C20-C14-C12	2.09	118.22	114.36
26	S	603	CLA	C3A-C2A-C1A	2.09	104.47	101.34
26	5	606	CLA	CHB-C4A-NA	2.09	127.40	124.51
29	d	407	PL9	O2-C1-C6	2.09	124.20	120.59
28	a	406	WVN	C06-C13-C20	2.09	121.68	115.78
26	5	611	CLA	CAA-CBA-CGA	-2.09	107.16	113.25
26	b	602	CLA	C1-C2-C3	-2.09	122.43	126.04
26	B	606	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
39	2	316	II0	C06-C04-C10	2.09	113.85	109.62
26	6	604	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
39	1	618	II0	C05-C07-C11	2.09	113.16	110.30
27	A	404	PHO	CMC-C2C-C3C	2.09	128.87	124.94
39	2	320	II0	C05-C07-C11	2.08	113.16	110.30
39	Q	315	II0	C30-C32-C34	-2.08	116.72	123.22
26	d	405	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
26	B	611	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
26	b	601	CLA	C1-C2-C3	-2.08	123.39	126.75
39	5	614	II0	C29-C31-C33	-2.08	116.73	123.22
26	C	509	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
26	P	610	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
26	4	313	CLA	CHD-C1D-ND	-2.08	122.54	124.45
39	4	315	II0	C27-C25-C23	2.08	120.95	116.84
27	a	404	PHO	O2A-CGA-O1A	-2.08	118.35	123.59
26	R	305	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
26	6	605	CLA	CHD-C1D-ND	-2.08	122.55	124.45
26	c	515	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
26	C	507	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
38	N	605	KC2	C2B-C1B-NB	2.07	111.63	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	N	613	CLA	CHD-C1D-ND	-2.07	122.55	124.45
26	6	607	CLA	CHD-C1D-ND	-2.07	122.55	124.45
39	N	615	II0	C17-C04-C06	-2.07	99.75	109.05
39	N	620	II0	C19-C13-C11	2.07	118.19	114.36
39	6	611	II0	C17-C04-C06	-2.07	99.75	109.05
26	D	407	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
26	B	606	CLA	C1-C2-C3	-2.07	122.46	126.04
38	1	610	KC2	C3C-C2C-C1C	2.07	108.02	106.49
39	Q	316	II0	C19-C13-C11	2.07	118.19	114.36
26	c	507	CLA	CHD-C1D-ND	-2.07	122.55	124.45
33	d	404	LMG	C8-O7-C10	-2.07	112.70	117.79
26	S	604	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
26	R	308	CLA	O1D-CGD-CBD	2.07	128.72	124.48
28	Y	101	WVN	C40-C39-C36	-2.07	119.24	123.47
39	Q	316	II0	C31-C29-C25	-2.07	120.58	126.58
26	1	607	CLA	CMC-C2C-C3C	2.07	131.72	126.12
26	S	607	CLA	CHD-C1D-ND	-2.07	122.56	124.45
28	P	615	WVN	C27-C25-C23	2.07	121.33	118.08
39	Q	316	II0	C17-C04-C06	-2.06	99.78	109.05
38	4	305	KC2	CAA-CBA-CGA	-2.06	116.65	127.26
26	2	319	CLA	CHD-C1D-ND	-2.06	122.56	124.45
26	5	604	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
39	N	615	II0	C30-C32-C34	-2.06	116.78	123.22
38	Q	304	KC2	CAA-CBA-CGA	-2.06	116.66	127.26
29	A	407	PL9	O1-C4-C3	-2.06	118.45	120.72
26	b	601	CLA	CHD-C1D-ND	-2.06	122.56	124.45
39	4	317	II0	C31-C29-C25	-2.06	120.59	126.58
39	2	315	II0	C19-C13-C11	2.06	118.17	114.36
39	R	318	II0	C31-C29-C25	-2.06	120.60	126.58
26	5	607	CLA	O1D-CGD-CBD	2.06	128.70	124.48
26	C	503	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
26	5	606	CLA	CHD-C1D-ND	-2.06	122.56	124.45
26	O	609	CLA	CHD-C1D-ND	-2.06	122.56	124.45
26	2	311	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
26	P	601	CLA	CHD-C1D-ND	-2.06	122.56	124.45
26	b	604	CLA	CAA-CBA-CGA	-2.06	107.24	113.25
28	B	618	WVN	C06-C13-C20	-2.06	109.96	115.78
39	N	618	II0	C04-C06-C08	-2.06	109.00	113.64
39	6	612	II0	C17-C04-C06	-2.06	99.81	109.05
39	S	611	II0	C17-C04-C06	-2.06	99.81	109.05
39	4	317	II0	C17-C04-C06	-2.06	99.81	109.05
39	6	612	II0	C32-C30-C26	-2.06	120.61	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	P	615	WVN	C26-C29-C31	-2.06	116.80	123.22
26	B	601	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
26	P	606	CLA	CHD-C1D-ND	-2.06	122.56	124.45
26	B	602	CLA	C1-C2-C3	-2.05	122.49	126.04
26	c	515	CLA	CHD-C1D-ND	-2.05	122.57	124.45
26	1	614	CLA	CHA-C1A-NA	-2.05	121.70	126.40
38	3	304	KC2	CAB-C3B-C2B	2.05	135.37	128.60
33	m	101	LMG	O8-C28-O10	-2.05	118.41	123.59
29	d	407	PL9	O2-C1-C2	-2.05	117.08	121.78
39	4	317	II0	C04-C10-C14	-2.05	119.74	122.63
39	S	612	II0	C17-C04-C06	-2.05	99.84	109.05
27	A	404	PHO	O2A-CGA-O1A	-2.05	118.41	123.59
39	Q	316	II0	C04-C10-C14	-2.05	119.74	122.63
39	S	612	II0	C32-C30-C26	-2.05	120.62	126.58
26	O	611	CLA	CHD-C1D-ND	-2.05	122.57	124.45
39	6	613	II0	C20-C14-C12	2.05	118.16	114.36
26	1	613	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
28	c	516	WVN	C39-C40-C37	-2.05	119.27	123.47
26	c	510	CLA	CHD-C1D-ND	-2.05	122.57	124.45
26	O	605	CLA	CHD-C1D-ND	-2.05	122.57	124.45
39	4	317	II0	C19-C13-C11	2.05	118.15	114.36
26	b	607	CLA	C1-C2-C3	-2.05	122.50	126.04
39	6	613	II0	C31-C29-C25	-2.05	120.63	126.58
26	Q	302	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
38	P	605	KC2	CAB-C3B-C2B	2.05	135.35	128.60
26	c	510	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
40	Q	317	IHT	C39-C35-C34	2.05	121.30	118.08
26	O	611	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
26	4	303	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
38	R	311	KC2	CMB-C2B-C1B	2.05	128.32	124.71
28	3	313	WVN	C01-C02-C11	-2.05	110.11	112.70
26	O	601	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
29	d	407	PL9	C36-C34-C33	-2.05	116.98	121.12
26	S	605	CLA	CHD-C1D-ND	-2.05	122.57	124.45
26	C	505	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
26	3	305	CLA	CHD-C1D-ND	-2.04	122.58	124.45
38	5	610	KC2	CMB-C2B-C1B	2.04	128.31	124.71
38	N	610	KC2	CAB-C3B-C2B	2.04	135.34	128.60
26	O	607	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
28	a	406	WVN	C29-C31-C32	-2.04	120.68	126.42
37	F	101	HEM	CHB-C1B-C2B	-2.04	121.08	126.72
26	4	312	CLA	O1D-CGD-CBD	2.04	128.66	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	508	CLA	CHD-C1D-ND	-2.04	122.58	124.45
29	D	409	PL9	O2-C1-C2	-2.04	117.11	121.78
26	2	302	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
26	1	609	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
40	4	318	IHT	C39-C35-C34	2.04	121.29	118.08
26	O	607	CLA	CHD-C1D-ND	-2.04	122.58	124.45
39	R	315	II0	C17-C04-C06	-2.04	99.90	109.05
26	B	610	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
26	2	307	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
26	B	612	CLA	C3A-C2A-C1A	2.04	104.39	101.34
39	R	318	II0	C20-C14-C12	2.04	118.13	114.36
29	D	409	PL9	C36-C34-C33	-2.04	117.00	121.12
39	5	614	II0	C17-C04-C06	-2.04	99.91	109.05
28	Z	101	WVN	C23-C25-C28	-2.03	115.82	118.94
26	Q	312	CLA	CHD-C1D-ND	-2.03	122.58	124.45
26	Q	306	CLA	CHB-C4A-NA	2.03	127.32	124.51
26	B	612	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
26	2	306	CLA	CHB-C4A-NA	2.03	127.32	124.51
39	4	316	II0	C31-C29-C25	-2.03	120.68	126.58
26	N	602	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
26	Q	311	CLA	O1D-CGD-CBD	2.03	128.64	124.48
26	D	404	CLA	CHD-C1D-ND	-2.03	122.59	124.45
26	3	305	CLA	O1D-CGD-CBD	2.03	128.64	124.48
38	S	608	KC2	CBD-CHA-C1A	2.03	132.67	128.88
26	c	506	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
26	Q	308	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
26	b	610	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
26	3	302	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
28	b	619	WVN	C06-C13-C20	-2.03	110.04	115.78
38	P	605	KC2	C3D-CAD-CBD	-2.03	104.94	107.61
26	b	601	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
26	4	309	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
26	b	612	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
38	6	608	KC2	CBD-CHA-C1A	2.03	132.66	128.88
39	4	314	II0	C34-C36-C40	-2.03	115.83	118.94
26	b	614	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
40	5	616	IHT	C39-C35-C34	2.03	121.27	118.08
26	C	510	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
26	N	613	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
26	P	603	CLA	CAA-C2A-C3A	-2.02	107.23	112.78
39	N	616	II0	C03-C09-C13	-2.02	119.78	122.63
26	S	603	CLA	CHD-C1D-ND	-2.02	122.59	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	Q	314	II0	C27-C25-C23	2.02	120.84	116.84
26	O	602	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
39	1	616	II0	C17-C04-C10	-2.02	107.25	110.47
29	A	407	PL9	C12-C13-C14	-2.02	122.79	127.66
26	c	508	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
26	B	608	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
38	Q	310	KC2	O2D-CGD-O1D	-2.02	119.89	123.84
39	Q	313	II0	C34-C36-C40	-2.02	115.84	118.94
28	c	516	WVN	C27-C25-C23	2.02	121.26	118.08
26	C	511	CLA	CHD-C1D-ND	-2.02	122.60	124.45
26	2	309	CLA	CHD-C1D-ND	-2.02	122.60	124.45
38	3	304	KC2	C3D-CAD-CBD	-2.02	104.95	107.61
26	b	606	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
39	S	611	II0	C30-C32-C34	-2.02	116.92	123.22
39	Q	315	II0	C31-C29-C25	-2.02	120.72	126.58
39	2	313	II0	C17-C04-C06	-2.02	99.99	109.05
39	4	320	II0	C04-C10-C14	-2.02	119.79	122.63
39	O	613	II0	C17-C04-C06	-2.02	99.99	109.05
26	a	403	CLA	O2D-CGD-CBD	2.02	114.85	111.27
26	P	609	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
26	2	301	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
26	2	309	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
29	a	407	PL9	C12-C13-C14	-2.01	122.81	127.66
39	Q	315	II0	C19-C13-C11	2.01	118.09	114.36
38	4	311	KC2	CAC-C3C-C4C	2.01	133.85	124.47
39	Q	319	II0	C04-C10-C14	-2.01	119.79	122.63
26	N	602	CLA	C1-C2-C3	-2.01	122.56	126.04
39	S	611	II0	C20-C14-C12	2.01	118.08	114.36
26	P	606	CLA	O1D-CGD-CBD	2.01	128.60	124.48
39	6	611	II0	C30-C32-C34	-2.01	116.94	123.22
28	B	618	WVN	C21-C15-C14	-2.01	109.75	113.62
26	1	607	CLA	CHB-C4A-NA	2.01	127.29	124.51
26	Q	305	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
39	R	314	II0	C17-C04-C06	-2.01	100.02	109.05
26	R	302	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
26	S	603	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
28	k	101	WVN	C23-C20-C13	-2.01	121.56	127.20
39	2	315	II0	C17-C04-C06	-2.01	100.03	109.05
38	5	610	KC2	CAB-C3B-C4B	-2.01	120.04	124.90
26	c	504	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
26	b	604	CLA	C1-C2-C3	-2.01	122.57	126.04
26	P	609	CLA	C1-C2-C3	-2.01	122.57	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	S	608	KC2	CAB-C3B-C4B	-2.01	120.04	124.90
26	1	613	CLA	CHD-C1D-ND	-2.01	122.61	124.45
26	2	307	CLA	CHD-C1D-ND	-2.01	122.61	124.45
29	a	407	PL9	O1-C4-C3	-2.01	118.51	120.72
26	b	608	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
39	6	611	II0	C20-C14-C12	2.01	118.08	114.36
26	3	309	CLA	O1A-CGA-CBA	2.01	129.53	123.08
26	6	603	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
28	B	619	WVN	C19-C22-C26	-2.01	115.86	118.94
26	2	305	CLA	CMB-C2B-C3B	2.01	128.43	124.68
26	4	307	CLA	CHB-C4A-NA	2.01	127.29	124.51
38	6	608	KC2	CAB-C3B-C4B	-2.01	120.05	124.90
26	D	404	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
26	P	611	CLA	O1A-CGA-CBA	2.01	129.52	123.08
26	6	606	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
38	Q	310	KC2	CAC-C3C-C4C	2.01	133.81	124.47
28	c	517	WVN	C03-C04-C09	-2.00	108.67	112.00
39	N	620	II0	C17-C04-C06	-2.00	100.05	109.05
26	1	602	CLA	C1-C2-C3	-2.00	122.58	126.04
39	5	613	II0	C17-C04-C06	-2.00	100.05	109.05
26	B	614	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
26	O	609	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
26	4	304	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
39	4	316	II0	C19-C13-C11	2.00	118.06	114.36
26	5	601	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
26	4	306	CLA	O2A-CGA-O1A	-2.00	118.54	123.59

All (187) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
26	A	402	CLA	ND
26	A	403	CLA	ND
26	A	405	CLA	ND
26	B	601	CLA	ND
26	B	603	CLA	ND
26	B	604	CLA	ND
26	B	605	CLA	ND
26	B	606	CLA	ND
26	B	607	CLA	ND
26	B	608	CLA	ND
26	B	609	CLA	ND
26	B	610	CLA	ND

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Mol	Chain	Res	Type	Atom
26	B	611	CLA	ND
26	B	612	CLA	ND
26	B	613	CLA	ND
26	B	614	CLA	ND
26	B	615	CLA	ND
26	B	616	CLA	ND
26	C	502	CLA	ND
26	C	503	CLA	ND
26	C	504	CLA	ND
26	C	505	CLA	ND
26	C	506	CLA	ND
26	C	507	CLA	ND
26	C	508	CLA	ND
26	C	509	CLA	ND
26	C	510	CLA	ND
26	C	511	CLA	ND
26	C	512	CLA	ND
26	C	513	CLA	ND
26	C	514	CLA	ND
26	D	404	CLA	ND
26	D	407	CLA	ND
26	D	408	CLA	ND
26	a	402	CLA	ND
26	a	403	CLA	ND
26	a	405	CLA	ND
26	b	601	CLA	ND
26	b	603	CLA	ND
26	b	604	CLA	ND
26	b	605	CLA	ND
26	b	606	CLA	ND
26	b	607	CLA	ND
26	b	608	CLA	ND
26	b	609	CLA	ND
26	b	610	CLA	ND
26	b	611	CLA	ND
26	b	612	CLA	ND
26	b	613	CLA	ND
26	b	614	CLA	ND
26	b	615	CLA	ND
26	b	616	CLA	ND
26	c	503	CLA	ND
26	c	504	CLA	ND

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Mol	Chain	Res	Type	Atom
26	c	505	CLA	ND
26	c	506	CLA	ND
26	c	507	CLA	ND
26	c	508	CLA	ND
26	c	509	CLA	ND
26	c	510	CLA	ND
26	c	511	CLA	ND
26	c	512	CLA	ND
26	c	513	CLA	ND
26	c	514	CLA	ND
26	c	515	CLA	ND
26	d	402	CLA	ND
26	d	405	CLA	ND
26	d	406	CLA	ND
26	1	601	CLA	ND
26	1	602	CLA	ND
26	1	603	CLA	ND
26	1	604	CLA	ND
26	1	606	CLA	ND
26	1	607	CLA	ND
26	1	608	CLA	ND
26	1	609	CLA	ND
26	1	613	CLA	ND
26	N	601	CLA	ND
26	N	602	CLA	ND
26	N	603	CLA	ND
26	N	604	CLA	ND
26	N	606	CLA	ND
26	N	607	CLA	ND
26	N	608	CLA	ND
26	N	609	CLA	ND
26	N	613	CLA	ND
26	N	614	CLA	ND
26	2	301	CLA	ND
26	2	302	CLA	ND
26	2	303	CLA	ND
26	2	304	CLA	ND
26	2	306	CLA	ND
26	2	307	CLA	ND
26	2	308	CLA	ND
26	2	309	CLA	ND
26	2	311	CLA	ND

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Mol	Chain	Res	Type	Atom
26	2	312	CLA	ND
26	2	319	CLA	ND
26	3	301	CLA	ND
26	3	302	CLA	ND
26	3	305	CLA	ND
26	3	306	CLA	ND
26	3	307	CLA	ND
26	3	309	CLA	ND
26	4	301	CLA	ND
26	4	302	CLA	ND
26	4	303	CLA	ND
26	4	304	CLA	ND
26	4	306	CLA	ND
26	4	307	CLA	ND
26	4	308	CLA	ND
26	4	309	CLA	ND
26	4	312	CLA	ND
26	4	313	CLA	ND
26	5	601	CLA	ND
26	5	602	CLA	ND
26	5	603	CLA	ND
26	5	604	CLA	ND
26	5	605	CLA	ND
26	5	606	CLA	ND
26	5	607	CLA	ND
26	5	608	CLA	ND
26	5	609	CLA	ND
26	5	611	CLA	ND
26	5	612	CLA	ND
26	6	601	CLA	ND
26	6	602	CLA	ND
26	6	603	CLA	ND
26	6	604	CLA	ND
26	6	605	CLA	ND
26	6	606	CLA	ND
26	6	607	CLA	ND
26	6	609	CLA	ND
26	6	610	CLA	ND
26	G	401	CLA	ND
26	G	402	CLA	ND
26	O	601	CLA	ND
26	O	602	CLA	ND

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Mol	Chain	Res	Type	Atom
26	O	603	CLA	ND
26	O	604	CLA	ND
26	O	605	CLA	ND
26	O	606	CLA	ND
26	O	607	CLA	ND
26	O	608	CLA	ND
26	O	609	CLA	ND
26	O	611	CLA	ND
26	O	612	CLA	ND
26	P	601	CLA	ND
26	P	602	CLA	ND
26	P	603	CLA	ND
26	P	606	CLA	ND
26	P	607	CLA	ND
26	P	608	CLA	ND
26	P	609	CLA	ND
26	P	610	CLA	ND
26	P	611	CLA	ND
26	Q	301	CLA	ND
26	Q	302	CLA	ND
26	Q	303	CLA	ND
26	Q	305	CLA	ND
26	Q	306	CLA	ND
26	Q	307	CLA	ND
26	Q	308	CLA	ND
26	Q	311	CLA	ND
26	Q	312	CLA	ND
26	R	302	CLA	ND
26	R	303	CLA	ND
26	R	304	CLA	ND
26	R	305	CLA	ND
26	R	306	CLA	ND
26	R	307	CLA	ND
26	R	308	CLA	ND
26	R	309	CLA	ND
26	R	310	CLA	ND
26	R	312	CLA	ND
26	R	313	CLA	ND
26	S	601	CLA	ND
26	S	602	CLA	ND
26	S	603	CLA	ND
26	S	604	CLA	ND

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Mol	Chain	Res	Type	Atom
26	S	605	CLA	ND
26	S	606	CLA	ND
26	S	607	CLA	ND
26	S	609	CLA	ND
26	S	610	CLA	ND
26	g	401	CLA	ND
26	g	402	CLA	ND

All (3158) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A	403	CLA	C1A-C2A-CAA-CBA
26	A	403	CLA	C3A-C2A-CAA-CBA
26	A	405	CLA	C1A-C2A-CAA-CBA
26	A	405	CLA	C3A-C2A-CAA-CBA
26	A	405	CLA	CBD-CGD-O2D-CED
26	B	601	CLA	CHA-CBD-CGD-O1D
26	B	601	CLA	CHA-CBD-CGD-O2D
26	B	601	CLA	CAD-CBD-CGD-O1D
26	B	602	CLA	CHA-CBD-CGD-O1D
26	B	602	CLA	CHA-CBD-CGD-O2D
26	B	606	CLA	CHA-CBD-CGD-O1D
26	B	606	CLA	CHA-CBD-CGD-O2D
26	B	606	CLA	CAD-CBD-CGD-O1D
26	B	606	CLA	CAD-CBD-CGD-O2D
26	B	609	CLA	C1A-C2A-CAA-CBA
26	B	609	CLA	C3A-C2A-CAA-CBA
26	B	611	CLA	CBD-CGD-O2D-CED
26	B	614	CLA	CHA-CBD-CGD-O1D
26	B	614	CLA	CHA-CBD-CGD-O2D
26	B	614	CLA	CAD-CBD-CGD-O1D
26	B	615	CLA	C1A-C2A-CAA-CBA
26	B	615	CLA	C3A-C2A-CAA-CBA
26	C	502	CLA	C1A-C2A-CAA-CBA
26	C	502	CLA	CBD-CGD-O2D-CED
26	C	503	CLA	CHA-CBD-CGD-O1D
26	C	503	CLA	CHA-CBD-CGD-O2D
26	C	503	CLA	CAD-CBD-CGD-O1D
26	C	503	CLA	CBD-CGD-O2D-CED
26	C	512	CLA	CHA-CBD-CGD-O1D
26	C	512	CLA	CAD-CBD-CGD-O1D
26	C	512	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
26	C	514	CLA	CHA-CBD-CGD-O1D
26	C	514	CLA	CHA-CBD-CGD-O2D
26	C	514	CLA	C3-C5-C6-C7
26	D	404	CLA	C1A-C2A-CAA-CBA
26	D	404	CLA	C3A-C2A-CAA-CBA
26	D	408	CLA	CHA-CBD-CGD-O1D
26	D	408	CLA	CAD-CBD-CGD-O1D
26	D	408	CLA	CAD-CBD-CGD-O2D
26	a	403	CLA	C1A-C2A-CAA-CBA
26	a	403	CLA	C3A-C2A-CAA-CBA
26	a	405	CLA	C1A-C2A-CAA-CBA
26	a	405	CLA	C3A-C2A-CAA-CBA
26	a	405	CLA	CBD-CGD-O2D-CED
26	b	601	CLA	CHA-CBD-CGD-O1D
26	b	601	CLA	CHA-CBD-CGD-O2D
26	b	601	CLA	CAD-CBD-CGD-O1D
26	b	602	CLA	CHA-CBD-CGD-O1D
26	b	602	CLA	CHA-CBD-CGD-O2D
26	b	606	CLA	CHA-CBD-CGD-O1D
26	b	606	CLA	CHA-CBD-CGD-O2D
26	b	606	CLA	CAD-CBD-CGD-O1D
26	b	606	CLA	CAD-CBD-CGD-O2D
26	b	609	CLA	C1A-C2A-CAA-CBA
26	b	609	CLA	C3A-C2A-CAA-CBA
26	b	611	CLA	CBD-CGD-O2D-CED
26	b	614	CLA	CHA-CBD-CGD-O1D
26	b	614	CLA	CHA-CBD-CGD-O2D
26	b	614	CLA	CAD-CBD-CGD-O1D
26	b	615	CLA	C1A-C2A-CAA-CBA
26	c	503	CLA	C1A-C2A-CAA-CBA
26	c	503	CLA	CBD-CGD-O2D-CED
26	c	504	CLA	CHA-CBD-CGD-O1D
26	c	504	CLA	CHA-CBD-CGD-O2D
26	c	504	CLA	CAD-CBD-CGD-O1D
26	c	504	CLA	CBD-CGD-O2D-CED
26	c	512	CLA	O1A-CGA-O2A-C1
26	c	513	CLA	CHA-CBD-CGD-O1D
26	c	513	CLA	CAD-CBD-CGD-O1D
26	c	513	CLA	CAD-CBD-CGD-O2D
26	c	515	CLA	CHA-CBD-CGD-O2D
26	d	402	CLA	C1A-C2A-CAA-CBA
26	d	402	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	d	406	CLA	CHA-CBD-CGD-O1D
26	d	406	CLA	CAD-CBD-CGD-O1D
26	d	406	CLA	CAD-CBD-CGD-O2D
26	1	603	CLA	O1A-CGA-O2A-C1
26	1	604	CLA	CHA-CBD-CGD-O1D
26	1	604	CLA	CHA-CBD-CGD-O2D
26	1	604	CLA	CAD-CBD-CGD-O1D
26	1	606	CLA	CHA-CBD-CGD-O1D
26	1	606	CLA	CHA-CBD-CGD-O2D
26	1	606	CLA	CBD-CGD-O2D-CED
26	1	607	CLA	CBD-CGD-O2D-CED
26	1	608	CLA	C1A-C2A-CAA-CBA
26	1	608	CLA	C3A-C2A-CAA-CBA
26	1	609	CLA	C1A-C2A-CAA-CBA
26	1	609	CLA	C2-C3-C5-C6
26	1	609	CLA	C4-C3-C5-C6
26	1	613	CLA	CBD-CGD-O2D-CED
26	1	614	CLA	C1A-C2A-CAA-CBA
26	N	602	CLA	CHA-CBD-CGD-O1D
26	N	602	CLA	CHA-CBD-CGD-O2D
26	N	603	CLA	C2-C3-C5-C6
26	N	604	CLA	CHA-CBD-CGD-O1D
26	N	604	CLA	CHA-CBD-CGD-O2D
26	N	604	CLA	CAD-CBD-CGD-O1D
26	N	607	CLA	CBD-CGD-O2D-CED
26	N	608	CLA	C1A-C2A-CAA-CBA
26	N	608	CLA	C3A-C2A-CAA-CBA
26	N	608	CLA	CHA-CBD-CGD-O1D
26	N	608	CLA	CHA-CBD-CGD-O2D
26	N	613	CLA	CBD-CGD-O2D-CED
26	N	614	CLA	C1A-C2A-CAA-CBA
26	N	614	CLA	CBD-CGD-O2D-CED
26	2	302	CLA	CHA-CBD-CGD-O1D
26	2	302	CLA	CHA-CBD-CGD-O2D
26	2	308	CLA	C1A-C2A-CAA-CBA
26	2	308	CLA	C3A-C2A-CAA-CBA
26	2	308	CLA	CHA-CBD-CGD-O1D
26	2	308	CLA	CHA-CBD-CGD-O2D
26	2	309	CLA	C1A-C2A-CAA-CBA
26	2	309	CLA	CBD-CGD-O2D-CED
26	2	312	CLA	C1A-C2A-CAA-CBA
26	3	306	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	3	308	CLA	CBD-CGD-O2D-CED
26	3	308	CLA	O1D-CGD-O2D-CED
26	3	309	CLA	C1A-C2A-CAA-CBA
26	3	309	CLA	C3A-C2A-CAA-CBA
26	4	301	CLA	C4-C3-C5-C6
26	4	306	CLA	CHA-CBD-CGD-O1D
26	4	306	CLA	CHA-CBD-CGD-O2D
26	4	308	CLA	C1A-C2A-CAA-CBA
26	4	308	CLA	C3A-C2A-CAA-CBA
26	4	312	CLA	C1A-C2A-CAA-CBA
26	4	312	CLA	C3A-C2A-CAA-CBA
26	4	312	CLA	CHA-CBD-CGD-O1D
26	4	312	CLA	CHA-CBD-CGD-O2D
26	4	312	CLA	CAD-CBD-CGD-O1D
26	4	312	CLA	CAD-CBD-CGD-O2D
26	4	313	CLA	CBD-CGD-O2D-CED
26	5	602	CLA	CHA-CBD-CGD-O1D
26	5	602	CLA	CHA-CBD-CGD-O2D
26	5	602	CLA	C2-C3-C5-C6
26	5	602	CLA	C4-C3-C5-C6
26	5	605	CLA	C1A-C2A-CAA-CBA
26	5	605	CLA	C3A-C2A-CAA-CBA
26	5	606	CLA	C1A-C2A-CAA-CBA
26	5	607	CLA	CHA-CBD-CGD-O1D
26	5	607	CLA	CHA-CBD-CGD-O2D
26	5	608	CLA	CHA-CBD-CGD-O1D
26	5	608	CLA	CBD-CGD-O2D-CED
26	5	611	CLA	C1A-C2A-CAA-CBA
26	5	611	CLA	CHA-CBD-CGD-O1D
26	5	611	CLA	CHA-CBD-CGD-O2D
26	5	611	CLA	CAD-CBD-CGD-O1D
26	6	602	CLA	CHA-CBD-CGD-O1D
26	6	602	CLA	CHA-CBD-CGD-O2D
26	6	603	CLA	C1A-C2A-CAA-CBA
26	6	604	CLA	CHA-CBD-CGD-O1D
26	6	604	CLA	CAD-CBD-CGD-O1D
26	6	604	CLA	CAD-CBD-CGD-O2D
26	6	605	CLA	C1A-C2A-CAA-CBA
26	6	605	CLA	C3A-C2A-CAA-CBA
26	6	605	CLA	C2A-CAA-CBA-CGA
26	6	606	CLA	CHA-CBD-CGD-O1D
26	6	606	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
26	6	607	CLA	C1A-C2A-CAA-CBA
26	6	607	CLA	C3A-C2A-CAA-CBA
26	6	607	CLA	CHA-CBD-CGD-O1D
26	6	607	CLA	CHA-CBD-CGD-O2D
26	6	607	CLA	C4-C3-C5-C6
26	6	609	CLA	CBD-CGD-O2D-CED
26	6	610	CLA	CBD-CGD-O2D-CED
26	O	602	CLA	CHA-CBD-CGD-O1D
26	O	602	CLA	CHA-CBD-CGD-O2D
26	O	605	CLA	C1A-C2A-CAA-CBA
26	O	605	CLA	C3A-C2A-CAA-CBA
26	O	608	CLA	C1A-C2A-CAA-CBA
26	O	608	CLA	C3A-C2A-CAA-CBA
26	O	608	CLA	CHA-CBD-CGD-O1D
26	O	608	CLA	CHA-CBD-CGD-O2D
26	O	609	CLA	C1A-C2A-CAA-CBA
26	O	609	CLA	CBD-CGD-O2D-CED
26	O	612	CLA	C1A-C2A-CAA-CBA
26	P	607	CLA	C3A-C2A-CAA-CBA
26	P	608	CLA	C4-C3-C5-C6
26	P	610	CLA	C1A-C2A-CAA-CBA
26	P	610	CLA	C2-C3-C5-C6
26	P	610	CLA	C4-C3-C5-C6
26	P	611	CLA	C1A-C2A-CAA-CBA
26	P	611	CLA	C3A-C2A-CAA-CBA
26	Q	305	CLA	CHA-CBD-CGD-O1D
26	Q	305	CLA	CHA-CBD-CGD-O2D
26	Q	307	CLA	C1A-C2A-CAA-CBA
26	Q	307	CLA	C3A-C2A-CAA-CBA
26	Q	311	CLA	C1A-C2A-CAA-CBA
26	Q	311	CLA	C3A-C2A-CAA-CBA
26	Q	311	CLA	CHA-CBD-CGD-O1D
26	Q	311	CLA	CHA-CBD-CGD-O2D
26	Q	311	CLA	CAD-CBD-CGD-O1D
26	Q	311	CLA	CAD-CBD-CGD-O2D
26	Q	312	CLA	CBD-CGD-O2D-CED
26	R	303	CLA	CHA-CBD-CGD-O1D
26	R	303	CLA	CHA-CBD-CGD-O2D
26	R	303	CLA	C2-C3-C5-C6
26	R	303	CLA	C4-C3-C5-C6
26	R	306	CLA	C1A-C2A-CAA-CBA
26	R	306	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	R	307	CLA	C1A-C2A-CAA-CBA
26	R	308	CLA	CHA-CBD-CGD-O1D
26	R	308	CLA	CHA-CBD-CGD-O2D
26	R	309	CLA	CHA-CBD-CGD-O1D
26	R	309	CLA	CBD-CGD-O2D-CED
26	R	312	CLA	C1A-C2A-CAA-CBA
26	R	312	CLA	CHA-CBD-CGD-O1D
26	R	312	CLA	CHA-CBD-CGD-O2D
26	R	312	CLA	CAD-CBD-CGD-O1D
26	S	602	CLA	CHA-CBD-CGD-O1D
26	S	602	CLA	CHA-CBD-CGD-O2D
26	S	603	CLA	C1A-C2A-CAA-CBA
26	S	604	CLA	CHA-CBD-CGD-O1D
26	S	604	CLA	CAD-CBD-CGD-O1D
26	S	604	CLA	CAD-CBD-CGD-O2D
26	S	605	CLA	C1A-C2A-CAA-CBA
26	S	605	CLA	C3A-C2A-CAA-CBA
26	S	605	CLA	C2A-CAA-CBA-CGA
26	S	606	CLA	CHA-CBD-CGD-O1D
26	S	606	CLA	CHA-CBD-CGD-O2D
26	S	607	CLA	C1A-C2A-CAA-CBA
26	S	607	CLA	C3A-C2A-CAA-CBA
26	S	607	CLA	CHA-CBD-CGD-O1D
26	S	607	CLA	CHA-CBD-CGD-O2D
26	S	607	CLA	C4-C3-C5-C6
26	S	609	CLA	CBD-CGD-O2D-CED
26	S	610	CLA	CBD-CGD-O2D-CED
27	D	405	PHO	C2-C1-O2A-CGA
27	d	403	PHO	C2-C1-O2A-CGA
28	A	406	WVN	C06-C13-C20-C23
28	A	406	WVN	C15-C13-C20-C23
28	B	617	WVN	C19-C22-C26-C29
28	B	617	WVN	C20-C23-C25-C27
28	B	617	WVN	C20-C23-C25-C28
28	B	617	WVN	C23-C25-C28-C30
28	B	617	WVN	C22-C26-C29-C31
28	B	617	WVN	C29-C31-C32-C36
28	B	617	WVN	C35-C32-C36-C39
28	B	617	WVN	C30-C33-C34-C38
28	B	617	WVN	C38-C34-C37-C40
28	B	618	WVN	C24-C22-C26-C29
28	B	618	WVN	C20-C23-C25-C27

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Mol	Chain	Res	Type	Atoms
28	B	618	WVN	C20-C23-C25-C28
28	B	618	WVN	C23-C25-C28-C30
28	B	618	WVN	C29-C31-C32-C35
28	B	618	WVN	C29-C31-C32-C36
28	B	618	WVN	C35-C32-C36-C39
28	B	618	WVN	C30-C33-C34-C37
28	B	618	WVN	C38-C34-C37-C40
28	B	619	WVN	C11-C19-C22-C24
28	B	619	WVN	C11-C19-C22-C26
28	C	515	WVN	C01-C02-C11-C19
28	C	515	WVN	C15-C13-C20-C23
28	C	515	WVN	C22-C26-C29-C31
28	C	515	WVN	C29-C31-C32-C35
28	C	515	WVN	C29-C31-C32-C36
28	C	515	WVN	C30-C33-C34-C37
28	C	515	WVN	C30-C33-C34-C38
28	C	516	WVN	C19-C22-C26-C29
28	C	516	WVN	C20-C23-C25-C27
28	C	516	WVN	C20-C23-C25-C28
28	C	516	WVN	C27-C25-C28-C30
28	C	516	WVN	C35-C32-C36-C39
28	C	516	WVN	C30-C33-C34-C38
28	C	516	WVN	C38-C34-C37-C40
28	D	412	WVN	C15-C13-C20-C23
28	D	412	WVN	C11-C19-C22-C26
28	D	412	WVN	C20-C23-C25-C27
28	D	412	WVN	C20-C23-C25-C28
28	D	412	WVN	C30-C33-C34-C37
28	D	412	WVN	C30-C33-C34-C38
28	H	101	WVN	C15-C13-C20-C23
28	H	101	WVN	C11-C19-C22-C24
28	H	101	WVN	C11-C19-C22-C26
28	H	101	WVN	C24-C22-C26-C29
28	H	101	WVN	C27-C25-C28-C30
28	H	101	WVN	C22-C26-C29-C31
28	H	101	WVN	C29-C31-C32-C35
28	H	101	WVN	C29-C31-C32-C36
28	H	101	WVN	C35-C32-C36-C39
28	H	101	WVN	C30-C33-C34-C37
28	H	101	WVN	C38-C34-C37-C40
28	Y	101	WVN	C01-C02-C11-C19
28	Y	101	WVN	C05-C02-C11-C19

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Mol	Chain	Res	Type	Atoms
28	Y	101	WVN	C20-C23-C25-C27
28	Y	101	WVN	C20-C23-C25-C28
28	Y	101	WVN	C29-C31-C32-C35
28	Y	101	WVN	C29-C31-C32-C36
28	Z	101	WVN	C15-C13-C20-C23
28	Z	101	WVN	C11-C19-C22-C24
28	Z	101	WVN	C11-C19-C22-C26
28	Z	101	WVN	C30-C33-C34-C38
28	Z	101	WVN	C34-C37-C40-C39
28	a	406	WVN	C11-C19-C22-C24
28	a	406	WVN	C11-C19-C22-C26
28	a	406	WVN	C30-C33-C34-C37
28	a	406	WVN	C30-C33-C34-C38
28	b	617	WVN	C11-C19-C22-C24
28	b	617	WVN	C11-C19-C22-C26
28	b	617	WVN	C20-C23-C25-C27
28	b	617	WVN	C20-C23-C25-C28
28	b	617	WVN	C22-C26-C29-C31
28	b	617	WVN	C29-C31-C32-C35
28	b	617	WVN	C29-C31-C32-C36
28	b	617	WVN	C30-C33-C34-C38
28	b	617	WVN	C32-C36-C39-C40
28	b	618	WVN	C06-C13-C20-C23
28	b	618	WVN	C11-C19-C22-C24
28	b	618	WVN	C11-C19-C22-C26
28	b	618	WVN	C22-C26-C29-C31
28	b	618	WVN	C29-C31-C32-C35
28	b	618	WVN	C29-C31-C32-C36
28	b	619	WVN	C15-C13-C20-C23
28	b	619	WVN	C29-C31-C32-C35
28	b	619	WVN	C30-C33-C34-C37
28	b	619	WVN	C30-C33-C34-C38
28	c	516	WVN	C15-C13-C20-C23
28	c	516	WVN	C29-C31-C32-C35
28	c	516	WVN	C29-C31-C32-C36
28	c	517	WVN	C01-C02-C11-C19
28	c	517	WVN	C15-C13-C20-C23
28	c	517	WVN	C22-C26-C29-C31
28	c	517	WVN	C29-C31-C32-C35
28	c	517	WVN	C29-C31-C32-C36
28	c	517	WVN	C30-C33-C34-C37
28	c	517	WVN	C30-C33-C34-C38

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Mol	Chain	Res	Type	Atoms
28	c	518	WVN	C15-C13-C20-C23
28	c	518	WVN	C11-C19-C22-C24
28	c	518	WVN	C11-C19-C22-C26
28	c	518	WVN	C22-C26-C29-C31
28	c	518	WVN	C30-C33-C34-C37
28	c	518	WVN	C30-C33-C34-C38
28	d	410	WVN	C15-C13-C20-C23
28	d	410	WVN	C20-C23-C25-C27
28	d	410	WVN	C20-C23-C25-C28
28	d	410	WVN	C29-C31-C32-C35
28	d	410	WVN	C29-C31-C32-C36
28	d	410	WVN	C30-C33-C34-C37
28	d	410	WVN	C30-C33-C34-C38
28	k	101	WVN	C15-C13-C20-C23
28	x	101	WVN	C15-C13-C20-C23
28	x	101	WVN	C29-C31-C32-C35
28	x	101	WVN	C29-C31-C32-C36
28	x	101	WVN	C30-C33-C34-C37
28	x	101	WVN	C30-C33-C34-C38
28	3	313	WVN	C05-C02-C11-C19
28	3	313	WVN	C24-C22-C26-C29
28	3	313	WVN	C27-C25-C28-C30
28	3	313	WVN	C29-C31-C32-C35
28	3	313	WVN	C35-C32-C36-C39
28	3	313	WVN	C38-C34-C37-C40
28	5	617	WVN	C15-C13-C20-C23
28	5	617	WVN	C29-C31-C32-C35
28	5	617	WVN	C29-C31-C32-C36
28	P	615	WVN	C30-C33-C34-C37
28	P	615	WVN	C30-C33-C34-C38
28	S	613	WVN	C15-C13-C20-C23
28	S	613	WVN	C29-C31-C32-C35
28	S	613	WVN	C29-C31-C32-C36
29	A	407	PL9	C7-C8-C9-C11
29	A	407	PL9	C19-C21-C22-C23
29	A	407	PL9	C22-C23-C24-C26
29	a	407	PL9	C7-C8-C9-C11
29	a	407	PL9	C19-C21-C22-C23
29	a	407	PL9	C22-C23-C24-C26
33	A	412	LMG	O6-C1-O1-C7
33	A	412	LMG	O7-C8-C9-O8
33	a	413	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
33	a	413	LMG	O7-C8-C9-O8
33	c	521	LMG	C2-C1-O1-C7
33	c	521	LMG	O6-C1-O1-C7
34	C	501	LHG	C3-O3-P-O4
34	C	501	LHG	C4-O6-P-O5
34	C	518	LHG	C4-O6-P-O3
34	C	518	LHG	C4-O6-P-O4
34	C	518	LHG	C4-O6-P-O5
34	Z	102	LHG	C4-O6-P-O5
34	a	409	LHG	C3-O3-P-O4
34	a	409	LHG	C4-O6-P-O5
34	b	621	LHG	C3-O3-P-O4
34	b	621	LHG	C3-O3-P-O5
34	b	621	LHG	C4-O6-P-O5
34	c	520	LHG	O1-C1-C2-C3
34	c	520	LHG	C3-O3-P-O5
34	z	101	LHG	C4-O6-P-O5
34	1	620	LHG	C3-O3-P-O5
34	N	621	LHG	C3-O3-P-O5
34	2	321	LHG	C3-O3-P-O5
34	G	403	LHG	C3-O3-P-O5
37	F	101	HEM	C2B-C3B-CAB-CBB
37	f	101	HEM	C2B-C3B-CAB-CBB
37	f	101	HEM	C4B-C3B-CAB-CBB
38	1	605	KC2	C1A-C2A-CAA-CBA
38	1	605	KC2	C3A-C2A-CAA-CBA
38	1	605	KC2	C2A-CAA-CBA-CGA
38	1	610	KC2	C2B-C3B-CAB-CBB
38	1	610	KC2	C4B-C3B-CAB-CBB
38	1	610	KC2	C2C-C3C-CAC-CBC
38	1	610	KC2	C4C-C3C-CAC-CBC
38	1	610	KC2	CBD-CGD-O2D-CED
38	1	611	KC2	C1A-C2A-CAA-CBA
38	1	611	KC2	C3A-C2A-CAA-CBA
38	1	611	KC2	C2C-C3C-CAC-CBC
38	1	611	KC2	C4C-C3C-CAC-CBC
38	1	612	KC2	C1A-C2A-CAA-CBA
38	1	612	KC2	C2C-C3C-CAC-CBC
38	1	612	KC2	CBD-CGD-O2D-CED
38	N	605	KC2	C2B-C3B-CAB-CBB
38	N	605	KC2	C4B-C3B-CAB-CBB
38	N	605	KC2	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
38	N	605	KC2	C4C-C3C-CAC-CBC
38	N	605	KC2	C2A-CAA-CBA-CGA
38	N	610	KC2	C2B-C3B-CAB-CBB
38	N	610	KC2	C4B-C3B-CAB-CBB
38	N	610	KC2	C2C-C3C-CAC-CBC
38	N	611	KC2	C2C-C3C-CAC-CBC
38	N	611	KC2	C4C-C3C-CAC-CBC
38	N	612	KC2	C2B-C3B-CAB-CBB
38	N	612	KC2	C4B-C3B-CAB-CBB
38	N	612	KC2	CBD-CGD-O2D-CED
38	2	310	KC2	C1A-C2A-CAA-CBA
38	2	310	KC2	C3A-C2A-CAA-CBA
38	2	310	KC2	C2C-C3C-CAC-CBC
38	2	310	KC2	C4C-C3C-CAC-CBC
38	2	310	KC2	C2A-CAA-CBA-CGA
38	3	304	KC2	C1A-C2A-CAA-CBA
38	3	304	KC2	C2B-C3B-CAB-CBB
38	3	304	KC2	C4B-C3B-CAB-CBB
38	3	304	KC2	C2C-C3C-CAC-CBC
38	3	304	KC2	C4C-C3C-CAC-CBC
38	3	304	KC2	C2A-CAA-CBA-CGA
38	4	305	KC2	C2C-C3C-CAC-CBC
38	4	305	KC2	C4C-C3C-CAC-CBC
38	4	305	KC2	C2A-CAA-CBA-CGA
38	4	310	KC2	C2C-C3C-CAC-CBC
38	4	310	KC2	C4C-C3C-CAC-CBC
38	4	310	KC2	CBD-CGD-O2D-CED
38	4	310	KC2	O1D-CGD-O2D-CED
38	4	311	KC2	C2C-C3C-CAC-CBC
38	4	311	KC2	C4C-C3C-CAC-CBC
38	5	610	KC2	C1A-C2A-CAA-CBA
38	5	610	KC2	C2C-C3C-CAC-CBC
38	5	610	KC2	C4C-C3C-CAC-CBC
38	5	610	KC2	C2A-CAA-CBA-CGA
38	5	610	KC2	CAA-CBA-CGA-O2A
38	6	608	KC2	C2C-C3C-CAC-CBC
38	6	608	KC2	C4C-C3C-CAC-CBC
38	O	610	KC2	C1A-C2A-CAA-CBA
38	O	610	KC2	C3A-C2A-CAA-CBA
38	O	610	KC2	C2C-C3C-CAC-CBC
38	O	610	KC2	C4C-C3C-CAC-CBC
38	O	610	KC2	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
38	P	605	KC2	C1A-C2A-CAA-CBA
38	P	605	KC2	C2B-C3B-CAB-CBB
38	P	605	KC2	C4B-C3B-CAB-CBB
38	P	605	KC2	C2C-C3C-CAC-CBC
38	P	605	KC2	C4C-C3C-CAC-CBC
38	P	605	KC2	C2A-CAA-CBA-CGA
38	Q	304	KC2	C2C-C3C-CAC-CBC
38	Q	304	KC2	C4C-C3C-CAC-CBC
38	Q	304	KC2	C2A-CAA-CBA-CGA
38	Q	309	KC2	C2C-C3C-CAC-CBC
38	Q	309	KC2	C4C-C3C-CAC-CBC
38	Q	309	KC2	CBD-CGD-O2D-CED
38	Q	309	KC2	O1D-CGD-O2D-CED
38	Q	310	KC2	C2C-C3C-CAC-CBC
38	Q	310	KC2	C4C-C3C-CAC-CBC
38	R	311	KC2	C1A-C2A-CAA-CBA
38	R	311	KC2	C2C-C3C-CAC-CBC
38	R	311	KC2	C4C-C3C-CAC-CBC
38	R	311	KC2	C2A-CAA-CBA-CGA
38	R	311	KC2	CAA-CBA-CGA-O2A
38	S	608	KC2	C2C-C3C-CAC-CBC
38	S	608	KC2	C4C-C3C-CAC-CBC
39	1	615	II0	C23-C25-C29-C31
39	1	615	II0	C27-C25-C29-C31
39	1	615	II0	C24-C26-C30-C32
39	1	615	II0	C32-C34-C36-C38
39	1	615	II0	C38-C36-C40-C42
39	1	616	II0	C23-C25-C29-C31
39	1	616	II0	C27-C25-C29-C31
39	1	616	II0	C24-C26-C30-C32
39	1	616	II0	C26-C30-C32-C34
39	1	616	II0	C31-C33-C35-C39
39	1	616	II0	C32-C34-C36-C38
39	1	616	II0	C32-C34-C36-C40
39	1	616	II0	C37-C35-C39-C41
39	1	616	II0	C38-C36-C40-C42
39	1	616	II0	C36-C40-C42-C41
39	1	617	II0	C23-C25-C29-C31
39	1	617	II0	C28-C26-C30-C32
39	1	617	II0	C31-C33-C35-C37
39	1	617	II0	C31-C33-C35-C39
39	1	617	II0	C32-C34-C36-C40

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Mol	Chain	Res	Type	Atoms
39	1	617	II0	C37-C35-C39-C41
39	1	617	II0	C38-C36-C40-C42
39	1	618	II0	C23-C25-C29-C31
39	1	618	II0	C27-C25-C29-C31
39	1	618	II0	C28-C26-C30-C32
39	1	618	II0	C25-C29-C31-C33
39	1	618	II0	C31-C33-C35-C37
39	1	618	II0	C31-C33-C35-C39
39	1	618	II0	C32-C34-C36-C40
39	1	618	II0	C37-C35-C39-C41
39	1	618	II0	C34-C36-C40-C42
39	N	615	II0	C09-C21-C23-C25
39	N	617	II0	C10-C22-C24-C26
39	2	316	II0	C23-C25-C29-C31
39	2	316	II0	C24-C26-C30-C32
39	2	316	II0	C26-C30-C32-C34
39	2	316	II0	C32-C34-C36-C38
39	2	316	II0	C32-C34-C36-C40
39	2	316	II0	C37-C35-C39-C41
39	2	316	II0	C38-C36-C40-C42
39	2	320	II0	C32-C34-C36-C38
39	2	320	II0	C32-C34-C36-C40
39	3	310	II0	C23-C25-C29-C31
39	3	310	II0	C27-C25-C29-C31
39	3	310	II0	C24-C26-C30-C32
39	3	310	II0	C32-C34-C36-C38
39	3	310	II0	C32-C34-C36-C40
39	3	310	II0	C37-C35-C39-C41
39	3	310	II0	C38-C36-C40-C42
39	3	311	II0	C23-C25-C29-C31
39	3	311	II0	C24-C26-C30-C32
39	3	311	II0	C28-C26-C30-C32
39	3	311	II0	C32-C34-C36-C40
39	3	311	II0	C37-C35-C39-C41
39	3	311	II0	C38-C36-C40-C42
39	3	312	II0	C23-C25-C29-C31
39	3	312	II0	C24-C26-C30-C32
39	3	312	II0	C28-C26-C30-C32
39	3	312	II0	C37-C35-C39-C41
39	3	312	II0	C38-C36-C40-C42
39	4	314	II0	C32-C34-C36-C38
39	4	314	II0	C32-C34-C36-C40

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Mol	Chain	Res	Type	Atoms
39	4	317	II0	C09-C21-C23-C25
39	4	317	II0	C31-C33-C35-C37
39	4	317	II0	C31-C33-C35-C39
39	6	611	II0	C31-C33-C35-C37
39	6	611	II0	C31-C33-C35-C39
39	O	615	II0	C23-C25-C29-C31
39	O	615	II0	C24-C26-C30-C32
39	O	615	II0	C26-C30-C32-C34
39	O	615	II0	C32-C34-C36-C38
39	O	615	II0	C32-C34-C36-C40
39	O	615	II0	C37-C35-C39-C41
39	O	615	II0	C38-C36-C40-C42
39	P	613	II0	C23-C25-C29-C31
39	P	613	II0	C24-C26-C30-C32
39	P	613	II0	C28-C26-C30-C32
39	P	613	II0	C32-C34-C36-C40
39	P	613	II0	C37-C35-C39-C41
39	P	613	II0	C38-C36-C40-C42
39	P	614	II0	C09-C21-C23-C25
39	P	614	II0	C31-C33-C35-C37
39	P	614	II0	C31-C33-C35-C39
39	Q	313	II0	C32-C34-C36-C38
39	Q	313	II0	C32-C34-C36-C40
39	Q	316	II0	C31-C33-C35-C37
39	Q	316	II0	C31-C33-C35-C39
39	S	611	II0	C31-C33-C35-C37
39	S	611	II0	C31-C33-C35-C39
40	1	619	IHT	C10-C07-C18-C22
40	1	619	IHT	C25-C23-C27-C30
40	1	619	IHT	C28-C26-C29-C31
40	1	619	IHT	C30-C32-C33-C36
40	1	619	IHT	C30-C32-C33-C37
40	1	619	IHT	C36-C33-C37-C40
40	1	619	IHT	C31-C34-C35-C38
40	1	619	IHT	C31-C34-C35-C39
40	1	619	IHT	C39-C35-C38-C41
40	N	619	IHT	C18-C22-C23-C25
40	N	619	IHT	C18-C22-C23-C27
40	N	619	IHT	C30-C32-C33-C36
40	N	619	IHT	C30-C32-C33-C37
40	N	619	IHT	C35-C38-C41-C40
40	2	317	IHT	C18-C22-C23-C27

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Mol	Chain	Res	Type	Atoms
40	2	317	IHT	C25-C23-C27-C30
40	2	317	IHT	C28-C26-C29-C31
40	2	317	IHT	C30-C32-C33-C36
40	2	317	IHT	C30-C32-C33-C37
40	2	317	IHT	C36-C33-C37-C40
40	2	317	IHT	C31-C34-C35-C38
40	2	317	IHT	C34-C35-C38-C41
40	4	318	IHT	C30-C32-C33-C36
40	4	318	IHT	C30-C32-C33-C37
40	5	616	IHT	C30-C32-C33-C36
40	5	616	IHT	C30-C32-C33-C37
40	5	616	IHT	C31-C34-C35-C38
40	5	616	IHT	C31-C34-C35-C39
40	Q	317	IHT	C30-C32-C33-C36
40	Q	317	IHT	C30-C32-C33-C37
40	R	317	IHT	C30-C32-C33-C36
40	R	317	IHT	C30-C32-C33-C37
40	R	317	IHT	C31-C34-C35-C38
40	R	317	IHT	C31-C34-C35-C39
26	A	402	CLA	O1D-CGD-O2D-CED
26	B	609	CLA	O1D-CGD-O2D-CED
26	a	402	CLA	O1D-CGD-O2D-CED
26	b	609	CLA	O1D-CGD-O2D-CED
26	1	606	CLA	O1D-CGD-O2D-CED
26	1	614	CLA	O1D-CGD-O2D-CED
26	2	309	CLA	O1D-CGD-O2D-CED
26	5	605	CLA	O1D-CGD-O2D-CED
26	5	608	CLA	O1D-CGD-O2D-CED
26	O	609	CLA	O1D-CGD-O2D-CED
26	R	306	CLA	O1D-CGD-O2D-CED
26	R	309	CLA	O1D-CGD-O2D-CED
38	1	610	KC2	O1D-CGD-O2D-CED
26	1	607	CLA	C4C-C3C-CAC-CBC
26	B	605	CLA	O1D-CGD-O2D-CED
26	b	605	CLA	O1D-CGD-O2D-CED
26	c	515	CLA	O1D-CGD-O2D-CED
26	1	607	CLA	O1D-CGD-O2D-CED
26	N	607	CLA	O1D-CGD-O2D-CED
26	4	313	CLA	O1D-CGD-O2D-CED
26	Q	312	CLA	O1D-CGD-O2D-CED
26	A	402	CLA	CBD-CGD-O2D-CED
26	B	603	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	B	605	CLA	CBD-CGD-O2D-CED
26	B	607	CLA	CBD-CGD-O2D-CED
26	B	609	CLA	CBD-CGD-O2D-CED
26	B	613	CLA	CBD-CGD-O2D-CED
26	B	616	CLA	CBD-CGD-O2D-CED
26	C	507	CLA	CBD-CGD-O2D-CED
26	C	509	CLA	CBD-CGD-O2D-CED
26	C	514	CLA	CBD-CGD-O2D-CED
26	a	402	CLA	CBD-CGD-O2D-CED
26	b	605	CLA	CBD-CGD-O2D-CED
26	b	607	CLA	CBD-CGD-O2D-CED
26	b	609	CLA	CBD-CGD-O2D-CED
26	b	616	CLA	CBD-CGD-O2D-CED
26	c	508	CLA	CBD-CGD-O2D-CED
26	c	510	CLA	CBD-CGD-O2D-CED
26	c	515	CLA	CBD-CGD-O2D-CED
26	1	608	CLA	CBD-CGD-O2D-CED
26	1	614	CLA	CBD-CGD-O2D-CED
26	N	606	CLA	CBD-CGD-O2D-CED
26	2	304	CLA	CBD-CGD-O2D-CED
26	3	309	CLA	CBD-CGD-O2D-CED
26	4	303	CLA	CBD-CGD-O2D-CED
26	4	304	CLA	CBD-CGD-O2D-CED
26	4	312	CLA	CBD-CGD-O2D-CED
26	5	605	CLA	CBD-CGD-O2D-CED
26	5	607	CLA	CBD-CGD-O2D-CED
26	5	611	CLA	CBD-CGD-O2D-CED
26	6	604	CLA	CBD-CGD-O2D-CED
26	6	605	CLA	CBD-CGD-O2D-CED
26	O	604	CLA	CBD-CGD-O2D-CED
26	P	610	CLA	CBD-CGD-O2D-CED
26	P	611	CLA	CBD-CGD-O2D-CED
26	Q	302	CLA	CBD-CGD-O2D-CED
26	Q	303	CLA	CBD-CGD-O2D-CED
26	Q	311	CLA	CBD-CGD-O2D-CED
26	R	306	CLA	CBD-CGD-O2D-CED
26	R	308	CLA	CBD-CGD-O2D-CED
26	R	312	CLA	CBD-CGD-O2D-CED
26	S	604	CLA	CBD-CGD-O2D-CED
26	S	605	CLA	CBD-CGD-O2D-CED
38	N	605	KC2	CBD-CGD-O2D-CED
26	B	615	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	C	511	CLA	O1A-CGA-O2A-C1
26	b	615	CLA	O1A-CGA-O2A-C1
26	b	616	CLA	O1A-CGA-O2A-C1
26	2	306	CLA	O1A-CGA-O2A-C1
26	4	306	CLA	O1A-CGA-O2A-C1
26	O	606	CLA	O1A-CGA-O2A-C1
26	Q	305	CLA	O1A-CGA-O2A-C1
27	A	404	PHO	O1A-CGA-O2A-C1
27	a	404	PHO	O1A-CGA-O2A-C1
26	1	607	CLA	C2C-C3C-CAC-CBC
26	C	507	CLA	O1D-CGD-O2D-CED
26	C	514	CLA	O1D-CGD-O2D-CED
26	c	508	CLA	O1D-CGD-O2D-CED
26	4	303	CLA	O1D-CGD-O2D-CED
26	Q	302	CLA	O1D-CGD-O2D-CED
26	B	611	CLA	O1D-CGD-O2D-CED
26	C	502	CLA	O1D-CGD-O2D-CED
26	b	611	CLA	O1D-CGD-O2D-CED
26	c	503	CLA	O1D-CGD-O2D-CED
26	1	613	CLA	O1D-CGD-O2D-CED
26	3	309	CLA	O1D-CGD-O2D-CED
26	6	605	CLA	O1D-CGD-O2D-CED
26	6	609	CLA	O1D-CGD-O2D-CED
26	6	610	CLA	O1D-CGD-O2D-CED
26	P	611	CLA	O1D-CGD-O2D-CED
26	S	605	CLA	O1D-CGD-O2D-CED
26	S	609	CLA	O1D-CGD-O2D-CED
26	S	610	CLA	O1D-CGD-O2D-CED
26	B	616	CLA	CBA-CGA-O2A-C1
26	b	616	CLA	CBA-CGA-O2A-C1
26	4	306	CLA	CBA-CGA-O2A-C1
26	Q	305	CLA	CBA-CGA-O2A-C1
27	A	404	PHO	CBA-CGA-O2A-C1
27	a	404	PHO	CBA-CGA-O2A-C1
26	B	606	CLA	CBD-CGD-O2D-CED
26	B	614	CLA	CBD-CGD-O2D-CED
26	b	603	CLA	CBD-CGD-O2D-CED
26	b	606	CLA	CBD-CGD-O2D-CED
26	b	613	CLA	CBD-CGD-O2D-CED
26	b	614	CLA	CBD-CGD-O2D-CED
26	1	604	CLA	CBD-CGD-O2D-CED
26	2	302	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	2	311	CLA	CBD-CGD-O2D-CED
26	5	609	CLA	CBD-CGD-O2D-CED
26	G	401	CLA	CBD-CGD-O2D-CED
26	O	602	CLA	CBD-CGD-O2D-CED
26	O	611	CLA	CBD-CGD-O2D-CED
26	R	310	CLA	CBD-CGD-O2D-CED
27	D	405	PHO	CBD-CGD-O2D-CED
27	d	403	PHO	CBD-CGD-O2D-CED
38	1	605	KC2	CBD-CGD-O2D-CED
26	A	403	CLA	O1A-CGA-O2A-C1
26	A	405	CLA	O1A-CGA-O2A-C1
26	B	616	CLA	O1A-CGA-O2A-C1
26	C	505	CLA	O1A-CGA-O2A-C1
26	a	403	CLA	O1A-CGA-O2A-C1
26	a	405	CLA	O1A-CGA-O2A-C1
26	c	506	CLA	O1A-CGA-O2A-C1
26	1	613	CLA	O1A-CGA-O2A-C1
26	N	603	CLA	O1A-CGA-O2A-C1
26	N	613	CLA	O1A-CGA-O2A-C1
26	5	601	CLA	O1A-CGA-O2A-C1
26	5	605	CLA	O1A-CGA-O2A-C1
26	6	603	CLA	O1A-CGA-O2A-C1
26	6	607	CLA	O1A-CGA-O2A-C1
26	O	605	CLA	O1A-CGA-O2A-C1
26	R	302	CLA	O1A-CGA-O2A-C1
26	R	306	CLA	O1A-CGA-O2A-C1
26	S	603	CLA	O1A-CGA-O2A-C1
26	S	607	CLA	O1A-CGA-O2A-C1
26	g	401	CLA	O1A-CGA-O2A-C1
27	D	405	PHO	O1A-CGA-O2A-C1
27	d	403	PHO	O1A-CGA-O2A-C1
26	A	405	CLA	O1D-CGD-O2D-CED
26	a	405	CLA	O1D-CGD-O2D-CED
26	N	613	CLA	O1D-CGD-O2D-CED
26	N	614	CLA	O1D-CGD-O2D-CED
38	1	612	KC2	O1D-CGD-O2D-CED
26	C	503	CLA	O1D-CGD-O2D-CED
26	c	504	CLA	O1D-CGD-O2D-CED
26	Q	303	CLA	O1D-CGD-O2D-CED
26	4	304	CLA	O1D-CGD-O2D-CED
26	A	405	CLA	C3-C5-C6-C7
26	B	604	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
26	B	614	CLA	C3-C5-C6-C7
26	B	616	CLA	C3-C5-C6-C7
26	C	505	CLA	C3-C5-C6-C7
26	a	405	CLA	C3-C5-C6-C7
26	b	604	CLA	C3-C5-C6-C7
26	b	613	CLA	C3-C5-C6-C7
26	b	614	CLA	C3-C5-C6-C7
26	b	616	CLA	C3-C5-C6-C7
26	c	506	CLA	C3-C5-C6-C7
26	3	301	CLA	C3-C5-C6-C7
26	4	308	CLA	C3-C5-C6-C7
26	5	601	CLA	C3-C5-C6-C7
26	5	602	CLA	C3-C5-C6-C7
26	5	608	CLA	C3-C5-C6-C7
26	5	609	CLA	C3-C5-C6-C7
26	6	601	CLA	C3-C5-C6-C7
26	6	605	CLA	C3-C5-C6-C7
26	6	606	CLA	C3-C5-C6-C7
26	6	609	CLA	C3-C5-C6-C7
26	P	602	CLA	C3-C5-C6-C7
26	P	610	CLA	C3-C5-C6-C7
26	Q	307	CLA	C3-C5-C6-C7
26	R	302	CLA	C3-C5-C6-C7
26	R	303	CLA	C3-C5-C6-C7
26	R	309	CLA	C3-C5-C6-C7
26	R	310	CLA	C3-C5-C6-C7
26	S	601	CLA	C3-C5-C6-C7
26	S	605	CLA	C3-C5-C6-C7
26	S	606	CLA	C3-C5-C6-C7
26	S	609	CLA	C3-C5-C6-C7
27	D	405	PHO	C3-C5-C6-C7
27	d	403	PHO	C3-C5-C6-C7
26	A	402	CLA	CBA-CGA-O2A-C1
26	A	403	CLA	CBA-CGA-O2A-C1
26	B	615	CLA	CBA-CGA-O2A-C1
26	C	511	CLA	CBA-CGA-O2A-C1
26	a	402	CLA	CBA-CGA-O2A-C1
26	a	403	CLA	CBA-CGA-O2A-C1
26	b	615	CLA	CBA-CGA-O2A-C1
26	c	512	CLA	CBA-CGA-O2A-C1
26	1	603	CLA	CBA-CGA-O2A-C1
26	1	613	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	N	603	CLA	CBA-CGA-O2A-C1
26	N	613	CLA	CBA-CGA-O2A-C1
26	N	614	CLA	CBA-CGA-O2A-C1
26	2	306	CLA	CBA-CGA-O2A-C1
26	5	605	CLA	CBA-CGA-O2A-C1
26	6	603	CLA	CBA-CGA-O2A-C1
26	6	607	CLA	CBA-CGA-O2A-C1
26	O	605	CLA	CBA-CGA-O2A-C1
26	O	606	CLA	CBA-CGA-O2A-C1
26	R	306	CLA	CBA-CGA-O2A-C1
26	S	603	CLA	CBA-CGA-O2A-C1
26	S	607	CLA	CBA-CGA-O2A-C1
26	g	401	CLA	CBA-CGA-O2A-C1
26	1	608	CLA	O1D-CGD-O2D-CED
26	2	304	CLA	O1D-CGD-O2D-CED
26	5	607	CLA	O1D-CGD-O2D-CED
26	O	604	CLA	O1D-CGD-O2D-CED
26	R	308	CLA	O1D-CGD-O2D-CED
26	D	408	CLA	CBD-CGD-O2D-CED
26	d	406	CLA	CBD-CGD-O2D-CED
38	1	605	KC2	CAA-CBA-CGA-O1A
38	1	605	KC2	CAA-CBA-CGA-O2A
38	N	605	KC2	CAA-CBA-CGA-O1A
38	4	305	KC2	CAA-CBA-CGA-O2A
38	Q	304	KC2	CAA-CBA-CGA-O2A
26	1	603	CLA	C3-C5-C6-C7
26	4	301	CLA	C3-C5-C6-C7
26	P	608	CLA	C3-C5-C6-C7
26	C	504	CLA	C4-C3-C5-C6
26	c	505	CLA	C4-C3-C5-C6
26	4	301	CLA	C2-C3-C5-C6
26	6	607	CLA	C2-C3-C5-C6
26	P	608	CLA	C2-C3-C5-C6
26	S	607	CLA	C2-C3-C5-C6
26	S	603	CLA	CBD-CGD-O2D-CED
26	B	606	CLA	C2A-CAA-CBA-CGA
26	B	615	CLA	C2A-CAA-CBA-CGA
26	C	503	CLA	C2A-CAA-CBA-CGA
26	C	510	CLA	C2A-CAA-CBA-CGA
26	C	511	CLA	C2A-CAA-CBA-CGA
26	D	404	CLA	C2A-CAA-CBA-CGA
26	b	606	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
26	b	615	CLA	C2A-CAA-CBA-CGA
26	c	504	CLA	C2A-CAA-CBA-CGA
26	c	511	CLA	C2A-CAA-CBA-CGA
26	c	512	CLA	C2A-CAA-CBA-CGA
26	d	402	CLA	C2A-CAA-CBA-CGA
26	1	608	CLA	C2A-CAA-CBA-CGA
26	3	307	CLA	C2A-CAA-CBA-CGA
26	4	302	CLA	C2A-CAA-CBA-CGA
26	5	611	CLA	C2A-CAA-CBA-CGA
26	6	607	CLA	C2A-CAA-CBA-CGA
26	P	609	CLA	C2A-CAA-CBA-CGA
26	Q	301	CLA	C2A-CAA-CBA-CGA
26	R	312	CLA	C2A-CAA-CBA-CGA
26	S	607	CLA	C2A-CAA-CBA-CGA
26	g	401	CLA	C2A-CAA-CBA-CGA
26	C	508	CLA	C3-C5-C6-C7
26	c	509	CLA	C3-C5-C6-C7
26	A	405	CLA	CBA-CGA-O2A-C1
26	C	505	CLA	CBA-CGA-O2A-C1
26	a	405	CLA	CBA-CGA-O2A-C1
26	c	506	CLA	CBA-CGA-O2A-C1
26	3	306	CLA	CBA-CGA-O2A-C1
26	5	601	CLA	CBA-CGA-O2A-C1
26	5	603	CLA	CBA-CGA-O2A-C1
26	P	607	CLA	CBA-CGA-O2A-C1
26	R	302	CLA	CBA-CGA-O2A-C1
26	R	304	CLA	CBA-CGA-O2A-C1
27	D	405	PHO	CBA-CGA-O2A-C1
27	d	403	PHO	CBA-CGA-O2A-C1
29	A	407	PL9	C17-C18-C19-C20
29	a	407	PL9	C17-C18-C19-C20
26	6	603	CLA	CBD-CGD-O2D-CED
33	c	521	LMG	C13-C14-C15-C16
26	B	607	CLA	O1D-CGD-O2D-CED
26	b	607	CLA	O1D-CGD-O2D-CED
26	4	312	CLA	O1D-CGD-O2D-CED
26	5	611	CLA	O1D-CGD-O2D-CED
26	P	610	CLA	O1D-CGD-O2D-CED
26	Q	311	CLA	O1D-CGD-O2D-CED
26	R	312	CLA	O1D-CGD-O2D-CED
26	A	402	CLA	O1A-CGA-O2A-C1
26	a	402	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	1	614	CLA	O1A-CGA-O2A-C1
26	N	614	CLA	O1A-CGA-O2A-C1
26	2	307	CLA	O1A-CGA-O2A-C1
26	3	306	CLA	O1A-CGA-O2A-C1
26	4	302	CLA	O1A-CGA-O2A-C1
26	O	607	CLA	O1A-CGA-O2A-C1
26	P	607	CLA	O1A-CGA-O2A-C1
26	Q	301	CLA	O1A-CGA-O2A-C1
28	B	618	WVN	C32-C36-C39-C40
28	B	619	WVN	C25-C28-C30-C33
28	B	619	WVN	C34-C37-C40-C39
28	Z	101	WVN	C22-C26-C29-C31
28	a	406	WVN	C25-C28-C30-C33
28	b	617	WVN	C25-C28-C30-C33
28	c	516	WVN	C34-C37-C40-C39
28	c	518	WVN	C25-C28-C30-C33
39	1	617	II0	C26-C30-C32-C34
39	N	615	II0	C25-C29-C31-C33
39	2	320	II0	C26-C30-C32-C34
39	3	310	II0	C26-C30-C32-C34
39	3	312	II0	C26-C30-C32-C34
40	2	317	IHT	C23-C27-C30-C32
26	b	604	CLA	CBD-CGD-O2D-CED
26	1	602	CLA	CBD-CGD-O2D-CED
26	N	601	CLA	CBD-CGD-O2D-CED
26	5	603	CLA	CBD-CGD-O2D-CED
26	6	602	CLA	CBD-CGD-O2D-CED
26	R	304	CLA	CBD-CGD-O2D-CED
26	S	602	CLA	CBD-CGD-O2D-CED
38	5	610	KC2	CBD-CGD-O2D-CED
38	R	311	KC2	CBD-CGD-O2D-CED
26	B	616	CLA	O1D-CGD-O2D-CED
26	N	606	CLA	O1D-CGD-O2D-CED
34	C	501	LHG	O2-C2-C3-O3
34	a	409	LHG	O2-C2-C3-O3
26	B	613	CLA	C3-C5-C6-C7
26	N	604	CLA	C3-C5-C6-C7
26	2	311	CLA	C3-C5-C6-C7
26	6	603	CLA	C3-C5-C6-C7
26	6	604	CLA	C3-C5-C6-C7
26	O	611	CLA	C3-C5-C6-C7
26	S	603	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
26	S	604	CLA	C3-C5-C6-C7
26	B	612	CLA	CBA-CGA-O2A-C1
26	C	514	CLA	CBA-CGA-O2A-C1
26	b	612	CLA	CBA-CGA-O2A-C1
26	2	305	CLA	CBA-CGA-O2A-C1
34	C	518	LHG	C24-C23-O8-C6
26	C	509	CLA	O1D-CGD-O2D-CED
26	b	616	CLA	O1D-CGD-O2D-CED
26	6	604	CLA	O1D-CGD-O2D-CED
26	S	604	CLA	O1D-CGD-O2D-CED
26	c	510	CLA	O1D-CGD-O2D-CED
26	b	610	CLA	CBD-CGD-O2D-CED
26	1	601	CLA	CBD-CGD-O2D-CED
26	4	308	CLA	CBD-CGD-O2D-CED
26	Q	307	CLA	CBD-CGD-O2D-CED
26	C	514	CLA	O1A-CGA-O2A-C1
34	N	621	LHG	C16-C17-C18-C19
26	1	614	CLA	CBA-CGA-O2A-C1
26	2	307	CLA	CBA-CGA-O2A-C1
26	4	302	CLA	CBA-CGA-O2A-C1
26	O	607	CLA	CBA-CGA-O2A-C1
26	Q	301	CLA	CBA-CGA-O2A-C1
38	2	310	KC2	CAA-CBA-CGA-O1A
38	4	310	KC2	CAA-CBA-CGA-O2A
38	O	610	KC2	CAA-CBA-CGA-O1A
38	Q	309	KC2	CAA-CBA-CGA-O2A
26	B	612	CLA	O1A-CGA-O2A-C1
26	b	612	CLA	O1A-CGA-O2A-C1
26	5	603	CLA	O1A-CGA-O2A-C1
26	R	304	CLA	O1A-CGA-O2A-C1
26	B	604	CLA	CBD-CGD-O2D-CED
26	S	601	CLA	CBD-CGD-O2D-CED
26	B	610	CLA	C2A-CAA-CBA-CGA
26	b	610	CLA	C2A-CAA-CBA-CGA
26	1	603	CLA	C2A-CAA-CBA-CGA
26	B	613	CLA	O1D-CGD-O2D-CED
26	2	305	CLA	O1A-CGA-O2A-C1
26	B	610	CLA	CBD-CGD-O2D-CED
26	b	602	CLA	CBD-CGD-O2D-CED
26	6	601	CLA	CBD-CGD-O2D-CED
26	B	603	CLA	O1D-CGD-O2D-CED
26	b	613	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	B	614	CLA	O1D-CGD-O2D-CED
26	b	603	CLA	O1D-CGD-O2D-CED
26	5	609	CLA	O1D-CGD-O2D-CED
26	R	310	CLA	O1D-CGD-O2D-CED
38	N	605	KC2	CAA-CBA-CGA-O2A
34	C	501	LHG	C1-C2-C3-O3
34	C	518	LHG	C1-C2-C3-O3
34	a	409	LHG	C1-C2-C3-O3
29	A	407	PL9	C17-C18-C19-C21
29	a	407	PL9	C17-C18-C19-C21
26	6	602	CLA	C3-C5-C6-C7
26	S	602	CLA	C3-C5-C6-C7
26	2	311	CLA	O1D-CGD-O2D-CED
26	O	611	CLA	O1D-CGD-O2D-CED
38	1	605	KC2	O1D-CGD-O2D-CED
26	B	604	CLA	CBA-CGA-O2A-C1
26	B	614	CLA	CBA-CGA-O2A-C1
26	C	506	CLA	CBA-CGA-O2A-C1
26	C	510	CLA	CBA-CGA-O2A-C1
26	D	404	CLA	CBA-CGA-O2A-C1
26	D	407	CLA	CBA-CGA-O2A-C1
26	b	604	CLA	CBA-CGA-O2A-C1
26	b	614	CLA	CBA-CGA-O2A-C1
26	c	507	CLA	CBA-CGA-O2A-C1
26	c	511	CLA	CBA-CGA-O2A-C1
26	d	402	CLA	CBA-CGA-O2A-C1
26	d	405	CLA	CBA-CGA-O2A-C1
26	N	602	CLA	CBA-CGA-O2A-C1
26	2	301	CLA	CBA-CGA-O2A-C1
26	3	307	CLA	CBA-CGA-O2A-C1
26	5	602	CLA	CBA-CGA-O2A-C1
26	5	611	CLA	CBA-CGA-O2A-C1
26	O	601	CLA	CBA-CGA-O2A-C1
26	P	609	CLA	CBA-CGA-O2A-C1
26	R	303	CLA	CBA-CGA-O2A-C1
26	R	312	CLA	CBA-CGA-O2A-C1
34	b	621	LHG	C24-C23-O8-C6
26	B	602	CLA	CBD-CGD-O2D-CED
26	2	319	CLA	CBD-CGD-O2D-CED
26	3	301	CLA	CBD-CGD-O2D-CED
26	P	601	CLA	CBD-CGD-O2D-CED
26	P	602	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	B	619	WVN	C32-C36-C39-C40
28	x	101	WVN	C32-C36-C39-C40
39	1	616	II0	C25-C29-C31-C33
39	N	617	II0	C26-C30-C32-C34
39	3	311	II0	C26-C30-C32-C34
39	P	613	II0	C26-C30-C32-C34
40	4	318	IHT	C23-C27-C30-C32
40	Q	317	IHT	C23-C27-C30-C32
33	5	619	LMG	C28-C29-C30-C31
33	R	301	LMG	C28-C29-C30-C31
38	3	304	KC2	CAA-CBA-CGA-O2A
38	5	610	KC2	CAA-CBA-CGA-O1A
38	P	605	KC2	CAA-CBA-CGA-O2A
38	R	311	KC2	CAA-CBA-CGA-O1A
26	B	613	CLA	C10-C11-C12-C13
34	1	620	LHG	O2-C2-C3-O3
34	N	621	LHG	O2-C2-C3-O3
26	1	613	CLA	O2A-C1-C2-C3
26	6	606	CLA	CBA-CGA-O2A-C1
26	S	606	CLA	CBA-CGA-O2A-C1
26	B	614	CLA	O1A-CGA-O2A-C1
26	5	602	CLA	O1A-CGA-O2A-C1
26	R	303	CLA	O1A-CGA-O2A-C1
34	C	518	LHG	O10-C23-O8-C6
26	B	603	CLA	C4-C3-C5-C6
26	b	603	CLA	C4-C3-C5-C6
26	C	504	CLA	C2-C3-C5-C6
26	c	505	CLA	C2-C3-C5-C6
26	2	306	CLA	C6-C7-C8-C9
26	3	305	CLA	C6-C7-C8-C9
26	G	401	CLA	C14-C13-C15-C16
26	O	606	CLA	C6-C7-C8-C9
26	P	606	CLA	C6-C7-C8-C9
26	G	401	CLA	O1D-CGD-O2D-CED
38	N	605	KC2	O1D-CGD-O2D-CED
26	6	604	CLA	C5-C6-C7-C8
26	S	604	CLA	C5-C6-C7-C8
26	A	403	CLA	C2A-CAA-CBA-CGA
26	a	403	CLA	C2A-CAA-CBA-CGA
28	B	619	WVN	C20-C23-C25-C27
28	D	412	WVN	C11-C19-C22-C24
28	H	101	WVN	C20-C23-C25-C27

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Mol	Chain	Res	Type	Atoms
28	Y	101	WVN	C11-C19-C22-C24
28	c	516	WVN	C30-C33-C34-C38
28	c	518	WVN	C29-C31-C32-C35
28	d	410	WVN	C11-C19-C22-C24
28	k	101	WVN	C29-C31-C32-C35
28	3	313	WVN	C20-C23-C25-C27
28	5	617	WVN	C11-C19-C22-C24
28	P	615	WVN	C11-C19-C22-C24
28	S	613	WVN	C11-C19-C22-C24
39	1	615	II0	C31-C33-C35-C37
39	1	618	II0	C32-C34-C36-C38
39	N	618	II0	C31-C33-C35-C37
39	3	311	II0	C32-C34-C36-C38
39	3	312	II0	C31-C33-C35-C37
39	5	615	II0	C31-C33-C35-C37
39	6	613	II0	C31-C33-C35-C37
39	P	613	II0	C32-C34-C36-C38
39	R	316	II0	C31-C33-C35-C37
39	R	318	II0	C31-C33-C35-C37
40	2	317	IHT	C18-C22-C23-C25
40	2	317	IHT	C31-C34-C35-C39
40	4	318	IHT	C18-C22-C23-C25
40	5	616	IHT	C18-C22-C23-C25
40	O	616	IHT	C30-C32-C33-C36
40	Q	317	IHT	C18-C22-C23-C25
40	R	317	IHT	C18-C22-C23-C25
28	B	617	WVN	C11-C19-C22-C26
28	B	619	WVN	C20-C23-C25-C28
28	C	516	WVN	C11-C19-C22-C26
28	C	516	WVN	C29-C31-C32-C36
28	Y	101	WVN	C11-C19-C22-C26
28	Z	101	WVN	C30-C33-C34-C37
28	c	516	WVN	C30-C33-C34-C37
28	c	518	WVN	C29-C31-C32-C36
28	d	410	WVN	C11-C19-C22-C26
28	3	313	WVN	C30-C33-C34-C37
28	5	617	WVN	C11-C19-C22-C26
28	P	615	WVN	C11-C19-C22-C26
28	S	613	WVN	C11-C19-C22-C26
39	1	615	II0	C32-C34-C36-C40
39	N	615	II0	C31-C33-C35-C39
39	2	316	II0	C31-C33-C35-C39

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Mol	Chain	Res	Type	Atoms
39	3	310	II0	C31-C33-C35-C39
39	3	311	II0	C31-C33-C35-C39
39	3	312	II0	C32-C34-C36-C40
39	O	615	II0	C31-C33-C35-C39
39	P	613	II0	C31-C33-C35-C39
40	4	318	IHT	C18-C22-C23-C27
40	Q	317	IHT	C18-C22-C23-C27
34	b	621	LHG	C8-C7-O7-C5
26	B	604	CLA	O1A-CGA-O2A-C1
26	C	510	CLA	O1A-CGA-O2A-C1
26	b	604	CLA	O1A-CGA-O2A-C1
26	b	614	CLA	O1A-CGA-O2A-C1
26	c	511	CLA	O1A-CGA-O2A-C1
26	3	307	CLA	O1A-CGA-O2A-C1
26	O	601	CLA	O1A-CGA-O2A-C1
26	P	609	CLA	O1A-CGA-O2A-C1
26	b	614	CLA	O1D-CGD-O2D-CED
26	1	608	CLA	CBA-CGA-O2A-C1
38	1	611	KC2	CAA-CBA-CGA-O1A
38	1	611	KC2	CAA-CBA-CGA-O2A
38	2	310	KC2	CAA-CBA-CGA-O2A
38	O	610	KC2	CAA-CBA-CGA-O2A
26	3	305	CLA	CBA-CGA-O2A-C1
26	4	301	CLA	CBA-CGA-O2A-C1
26	6	605	CLA	CBA-CGA-O2A-C1
26	P	606	CLA	CBA-CGA-O2A-C1
26	P	608	CLA	CBA-CGA-O2A-C1
26	S	605	CLA	CBA-CGA-O2A-C1
26	B	613	CLA	C5-C6-C7-C8
26	N	604	CLA	C5-C6-C7-C8
26	6	602	CLA	C10-C11-C12-C13
26	O	606	CLA	C5-C6-C7-C8
26	S	601	CLA	C5-C6-C7-C8
26	S	602	CLA	C10-C11-C12-C13
33	M	101	LMG	C10-C11-C12-C13
34	a	409	LHG	C7-C8-C9-C10
26	2	301	CLA	O1A-CGA-O2A-C1
26	b	613	CLA	C5-C6-C7-C8
26	2	306	CLA	C5-C6-C7-C8
26	3	305	CLA	C5-C6-C7-C8
26	3	305	CLA	C13-C15-C16-C17
26	3	306	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	6	601	CLA	C5-C6-C7-C8
26	6	604	CLA	C13-C15-C16-C17
26	P	606	CLA	C5-C6-C7-C8
26	P	606	CLA	C13-C15-C16-C17
26	P	607	CLA	C10-C11-C12-C13
26	S	604	CLA	C13-C15-C16-C17
26	C	506	CLA	O1A-CGA-O2A-C1
33	m	101	LMG	C10-C11-C12-C13
34	C	501	LHG	C7-C8-C9-C10
34	b	621	LHG	C23-C24-C25-C26
35	H	102	DGD	C1A-C2A-C3A-C4A
35	h	101	DGD	C1A-C2A-C3A-C4A
26	5	602	CLA	CBD-CGD-O2D-CED
26	R	303	CLA	CBD-CGD-O2D-CED
26	b	606	CLA	O1D-CGD-O2D-CED
26	C	509	CLA	C13-C15-C16-C17
26	b	613	CLA	C13-C15-C16-C17
26	c	510	CLA	C13-C15-C16-C17
26	1	604	CLA	C8-C10-C11-C12
27	A	404	PHO	C3-C5-C6-C7
26	c	515	CLA	CBA-CGA-O2A-C1
26	1	604	CLA	O1D-CGD-O2D-CED
26	2	302	CLA	O1D-CGD-O2D-CED
26	O	602	CLA	O1D-CGD-O2D-CED
26	C	510	CLA	C2-C1-O2A-CGA
26	c	511	CLA	C2-C1-O2A-CGA
26	5	605	CLA	C2-C1-O2A-CGA
26	R	306	CLA	C2-C1-O2A-CGA
26	3	301	CLA	C13-C15-C16-C17
26	P	602	CLA	C13-C15-C16-C17
26	2	303	CLA	C10-C11-C12-C13
26	O	603	CLA	C10-C11-C12-C13
26	B	612	CLA	C6-C7-C8-C10
26	C	508	CLA	C12-C13-C15-C16
26	b	612	CLA	C6-C7-C8-C10
26	c	509	CLA	C12-C13-C15-C16
26	N	609	CLA	C11-C10-C8-C7
26	G	401	CLA	C11-C10-C8-C7
26	2	302	CLA	C3-C5-C6-C7
26	3	305	CLA	C3-C5-C6-C7
26	O	602	CLA	C3-C5-C6-C7
26	P	606	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
27	a	404	PHO	C3-C5-C6-C7
26	D	407	CLA	O1A-CGA-O2A-C1
26	c	507	CLA	O1A-CGA-O2A-C1
26	d	405	CLA	O1A-CGA-O2A-C1
26	5	611	CLA	O1A-CGA-O2A-C1
26	R	312	CLA	O1A-CGA-O2A-C1
28	B	617	WVN	C34-C37-C40-C39
28	x	101	WVN	C25-C28-C30-C33
39	1	615	II0	C25-C29-C31-C33
39	1	615	II0	C26-C30-C32-C34
39	1	617	II0	C25-C29-C31-C33
39	1	618	II0	C26-C30-C32-C34
40	1	619	IHT	C23-C27-C30-C32
40	1	619	IHT	C33-C37-C40-C41
40	N	619	IHT	C33-C37-C40-C41
40	2	317	IHT	C35-C38-C41-C40
40	5	616	IHT	C26-C29-C31-C34
40	O	616	IHT	C26-C29-C31-C34
40	R	317	IHT	C26-C29-C31-C34
26	1	614	CLA	C2A-CAA-CBA-CGA
26	B	606	CLA	O1D-CGD-O2D-CED
27	D	405	PHO	O1D-CGD-O2D-CED
27	d	403	PHO	O1D-CGD-O2D-CED
26	B	611	CLA	C15-C16-C17-C18
26	C	504	CLA	C15-C16-C17-C18
26	b	613	CLA	C10-C11-C12-C13
26	c	505	CLA	C15-C16-C17-C18
26	N	609	CLA	C5-C6-C7-C8
26	3	306	CLA	C13-C15-C16-C17
26	P	607	CLA	C13-C15-C16-C17
26	g	401	CLA	C10-C11-C12-C13
26	6	606	CLA	O1A-CGA-O2A-C1
34	b	621	LHG	O10-C23-O8-C6
26	2	308	CLA	CBD-CGD-O2D-CED
26	O	608	CLA	CBD-CGD-O2D-CED
26	b	611	CLA	C15-C16-C17-C18
33	D	406	LMG	C10-C11-C12-C13
33	d	404	LMG	C10-C11-C12-C13
38	N	612	KC2	O1D-CGD-O2D-CED
34	b	621	LHG	O9-C7-O7-C5
26	C	508	CLA	C15-C16-C17-C18
26	c	509	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
26	6	610	CLA	C13-C15-C16-C17
26	S	610	CLA	C13-C15-C16-C17
26	D	404	CLA	O1A-CGA-O2A-C1
26	d	402	CLA	O1A-CGA-O2A-C1
26	N	602	CLA	O1A-CGA-O2A-C1
26	4	301	CLA	O1A-CGA-O2A-C1
26	P	608	CLA	O1A-CGA-O2A-C1
26	S	606	CLA	O1A-CGA-O2A-C1
26	b	616	CLA	C15-C16-C17-C18
26	1	603	CLA	CBD-CGD-O2D-CED
26	c	515	CLA	O1A-CGA-O2A-C1
26	3	305	CLA	O1A-CGA-O2A-C1
30	A	408	SQD	C8-C7-O47-C45
30	a	408	SQD	C8-C7-O47-C45
33	C	519	LMG	C11-C10-O7-C8
26	B	615	CLA	C5-C6-C7-C8
26	3	301	CLA	C10-C11-C12-C13
26	5	604	CLA	C5-C6-C7-C8
26	5	604	CLA	C10-C11-C12-C13
26	5	609	CLA	C10-C11-C12-C13
26	P	602	CLA	C10-C11-C12-C13
26	R	305	CLA	C5-C6-C7-C8
26	R	305	CLA	C10-C11-C12-C13
26	R	310	CLA	C10-C11-C12-C13
26	g	401	CLA	C8-C10-C11-C12
34	C	501	LHG	C3-O3-P-O6
34	C	501	LHG	C4-O6-P-O3
34	D	403	LHG	C3-O3-P-O6
34	a	409	LHG	C3-O3-P-O6
34	a	409	LHG	C4-O6-P-O3
34	b	621	LHG	C3-O3-P-O6
26	B	613	CLA	CBA-CGA-O2A-C1
26	C	507	CLA	CBA-CGA-O2A-C1
26	b	613	CLA	CBA-CGA-O2A-C1
26	c	508	CLA	CBA-CGA-O2A-C1
26	P	606	CLA	O1A-CGA-O2A-C1
26	N	613	CLA	O2A-C1-C2-C3
33	c	521	LMG	C10-C11-C12-C13
26	D	408	CLA	O1D-CGD-O2D-CED
26	d	406	CLA	O1D-CGD-O2D-CED
26	6	603	CLA	O1D-CGD-O2D-CED
26	S	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	C	503	CLA	C5-C6-C7-C8
26	c	504	CLA	C5-C6-C7-C8
26	P	602	CLA	C8-C10-C11-C12
26	N	608	CLA	C2A-CAA-CBA-CGA
26	6	610	CLA	C2A-CAA-CBA-CGA
26	S	610	CLA	C2A-CAA-CBA-CGA
26	B	607	CLA	C16-C17-C18-C20
26	C	510	CLA	C16-C17-C18-C20
38	3	304	KC2	CAA-CBA-CGA-O1A
38	6	608	KC2	CAA-CBA-CGA-O2A
38	P	605	KC2	CAA-CBA-CGA-O1A
38	S	608	KC2	CAA-CBA-CGA-O2A
26	1	606	CLA	CBA-CGA-O2A-C1
26	4	309	CLA	CBA-CGA-O2A-C1
26	6	610	CLA	CBA-CGA-O2A-C1
26	Q	308	CLA	CBA-CGA-O2A-C1
26	S	610	CLA	CBA-CGA-O2A-C1
26	3	301	CLA	C8-C10-C11-C12
39	1	615	II0	C28-C26-C30-C32
39	1	616	II0	C28-C26-C30-C32
39	1	617	II0	C27-C25-C29-C31
39	2	316	II0	C28-C26-C30-C32
39	O	615	II0	C28-C26-C30-C32
28	C	516	WVN	C22-C26-C29-C31
28	D	412	WVN	C25-C28-C30-C33
28	d	410	WVN	C25-C28-C30-C33
28	3	313	WVN	C22-C26-C29-C31
28	3	313	WVN	C25-C28-C30-C33
39	1	615	II0	C36-C40-C42-C41
40	N	619	IHT	C23-C27-C30-C32
40	2	317	IHT	C26-C29-C31-C34
40	4	318	IHT	C35-C38-C41-C40
40	O	616	IHT	C23-C27-C30-C32
40	Q	317	IHT	C35-C38-C41-C40
35	C	517	DGD	C1B-C2B-C3B-C4B
33	C	520	LMG	C11-C10-O7-C8
33	c	522	LMG	C11-C10-O7-C8
34	C	501	LHG	C8-C7-O7-C5
34	a	409	LHG	C8-C7-O7-C5
28	B	617	WVN	C24-C22-C26-C29
28	C	516	WVN	C24-C22-C26-C29
39	1	615	II0	C37-C35-C39-C41

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Mol	Chain	Res	Type	Atoms
34	D	410	LHG	C31-C32-C33-C34
34	d	408	LHG	C31-C32-C33-C34
26	6	605	CLA	O1A-CGA-O2A-C1
26	S	605	CLA	O1A-CGA-O2A-C1
38	1	610	KC2	C2A-CAA-CBA-CGA
38	4	310	KC2	C2A-CAA-CBA-CGA
38	Q	309	KC2	C2A-CAA-CBA-CGA
26	b	607	CLA	C16-C17-C18-C20
34	N	621	LHG	C15-C16-C17-C18
30	A	408	SQD	O49-C7-O47-C45
30	a	408	SQD	O49-C7-O47-C45
33	C	519	LMG	O9-C10-O7-C8
33	C	520	LMG	O9-C10-O7-C8
33	c	522	LMG	O9-C10-O7-C8
34	C	501	LHG	O9-C7-O7-C5
34	a	409	LHG	O9-C7-O7-C5
34	D	410	LHG	C7-C8-C9-C10
35	c	519	DGD	C1B-C2B-C3B-C4B
26	N	602	CLA	CBD-CGD-O2D-CED
26	P	604	CLA	CBD-CGD-O2D-CED
34	C	518	LHG	O2-C2-C3-O3
26	1	604	CLA	C3-C5-C6-C7
26	3	303	CLA	CBD-CGD-O2D-CED
28	B	618	WVN	C19-C22-C26-C29
28	B	618	WVN	C33-C34-C37-C40
28	H	101	WVN	C19-C22-C26-C29
39	1	615	II0	C33-C35-C39-C41
39	1	618	II0	C33-C35-C39-C41
39	2	316	II0	C34-C36-C40-C42
39	3	312	II0	C33-C35-C39-C41
39	O	615	II0	C34-C36-C40-C42
40	1	619	IHT	C22-C23-C27-C30
40	2	317	IHT	C22-C23-C27-C30
33	C	519	LMG	O1-C7-C8-O7
26	5	609	CLA	CBA-CGA-O2A-C1
26	R	310	CLA	CBA-CGA-O2A-C1
34	b	621	LHG	C26-C27-C28-C29
35	H	102	DGD	C2B-C3B-C4B-C5B
26	1	606	CLA	O1A-CGA-O2A-C1
26	B	607	CLA	C16-C17-C18-C19
26	B	613	CLA	C16-C17-C18-C19
26	B	616	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
26	c	511	CLA	C16-C17-C18-C20
26	1	609	CLA	C11-C12-C13-C15
26	G	401	CLA	C16-C17-C18-C19
35	h	101	DGD	C2B-C3B-C4B-C5B
26	B	602	CLA	C6-C7-C8-C9
26	B	605	CLA	C11-C12-C13-C14
26	C	503	CLA	C11-C12-C13-C14
26	b	602	CLA	C6-C7-C8-C9
26	b	605	CLA	C11-C12-C13-C14
26	b	608	CLA	C14-C13-C15-C16
26	c	504	CLA	C11-C12-C13-C14
26	2	306	CLA	C11-C10-C8-C9
26	O	606	CLA	C11-C10-C8-C9
34	a	409	LHG	C32-C33-C34-C35
34	c	520	LHG	C24-C25-C26-C27
26	b	616	CLA	C13-C15-C16-C17
38	4	310	KC2	CAA-CBA-CGA-O1A
38	Q	309	KC2	CAA-CBA-CGA-O1A
26	6	603	CLA	C2A-CAA-CBA-CGA
26	S	603	CLA	C2A-CAA-CBA-CGA
26	C	507	CLA	O1A-CGA-O2A-C1
26	c	508	CLA	O1A-CGA-O2A-C1
28	B	619	WVN	C30-C33-C34-C38
39	N	615	II0	C31-C33-C35-C37
40	1	619	IHT	C18-C22-C23-C25
33	b	620	LMG	C17-C18-C19-C20
34	C	501	LHG	C32-C33-C34-C35
34	b	621	LHG	O1-C1-C2-C3
28	B	618	WVN	C11-C19-C22-C26
28	B	619	WVN	C30-C33-C34-C37
28	b	619	WVN	C29-C31-C32-C36
28	3	313	WVN	C11-C19-C22-C26
28	3	313	WVN	C29-C31-C32-C36
39	1	615	II0	C31-C33-C35-C39
40	1	619	IHT	C18-C22-C23-C27
40	O	616	IHT	C30-C32-C33-C37
26	4	303	CLA	C3-C5-C6-C7
26	Q	302	CLA	C3-C5-C6-C7
26	S	602	CLA	O1D-CGD-O2D-CED
29	D	409	PL9	C47-C48-C49-C51
29	d	407	PL9	C47-C48-C49-C51
33	D	406	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
33	d	404	LMG	C31-C32-C33-C34
35	H	102	DGD	C7B-C8B-C9B-CAB
35	h	101	DGD	C7B-C8B-C9B-CAB
26	b	607	CLA	C16-C17-C18-C19
26	5	609	CLA	C16-C17-C18-C20
26	6	604	CLA	C16-C17-C18-C20
26	R	310	CLA	C16-C17-C18-C20
26	S	604	CLA	C16-C17-C18-C20
26	B	616	CLA	C15-C16-C17-C18
26	G	401	CLA	C5-C6-C7-C8
26	6	602	CLA	O1D-CGD-O2D-CED
33	C	519	LMG	C33-C34-C35-C36
33	C	519	LMG	C34-C35-C36-C37
34	D	410	LHG	C26-C27-C28-C29
34	d	408	LHG	C26-C27-C28-C29
34	2	321	LHG	C31-C32-C33-C34
34	G	403	LHG	C31-C32-C33-C34
34	C	501	LHG	C24-C25-C26-C27
34	C	501	LHG	C28-C29-C30-C31
34	a	409	LHG	C24-C25-C26-C27
34	a	409	LHG	C28-C29-C30-C31
34	2	321	LHG	C27-C28-C29-C30
34	G	403	LHG	C27-C28-C29-C30
26	B	605	CLA	C5-C6-C7-C8
26	b	605	CLA	C5-C6-C7-C8
38	N	612	KC2	CAA-CBA-CGA-O1A
26	b	613	CLA	O1A-CGA-O2A-C1
26	N	607	CLA	C2C-C3C-CAC-CBC
26	C	502	CLA	C3A-C2A-CAA-CBA
26	C	510	CLA	C3A-C2A-CAA-CBA
26	b	615	CLA	C3A-C2A-CAA-CBA
26	c	503	CLA	C3A-C2A-CAA-CBA
26	c	511	CLA	C3A-C2A-CAA-CBA
26	1	601	CLA	C3A-C2A-CAA-CBA
26	N	601	CLA	C3A-C2A-CAA-CBA
26	N	614	CLA	C3A-C2A-CAA-CBA
26	2	312	CLA	C3A-C2A-CAA-CBA
26	3	302	CLA	C3A-C2A-CAA-CBA
26	4	306	CLA	C3A-C2A-CAA-CBA
26	4	307	CLA	C3A-C2A-CAA-CBA
26	5	603	CLA	C3A-C2A-CAA-CBA
26	5	606	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	6	603	CLA	C3A-C2A-CAA-CBA
26	O	612	CLA	C3A-C2A-CAA-CBA
26	P	603	CLA	C3A-C2A-CAA-CBA
26	P	610	CLA	C3A-C2A-CAA-CBA
26	Q	305	CLA	C3A-C2A-CAA-CBA
26	Q	306	CLA	C3A-C2A-CAA-CBA
26	R	304	CLA	C3A-C2A-CAA-CBA
26	R	307	CLA	C3A-C2A-CAA-CBA
26	S	603	CLA	C3A-C2A-CAA-CBA
33	c	521	LMG	O6-C5-C6-O5
26	1	602	CLA	O1D-CGD-O2D-CED
26	5	609	CLA	C16-C17-C18-C19
26	6	604	CLA	C16-C17-C18-C19
26	R	310	CLA	C16-C17-C18-C19
26	S	604	CLA	C16-C17-C18-C19
33	B	620	LMG	C17-C18-C19-C20
33	C	519	LMG	C16-C17-C18-C19
33	c	521	LMG	C30-C31-C32-C33
26	5	603	CLA	O1D-CGD-O2D-CED
26	R	304	CLA	O1D-CGD-O2D-CED
38	1	611	KC2	CBD-CGD-O2D-CED
26	A	402	CLA	O2A-C1-C2-C3
26	a	402	CLA	O2A-C1-C2-C3
26	2	306	CLA	C4-C3-C5-C6
26	6	605	CLA	C4-C3-C5-C6
26	O	606	CLA	C4-C3-C5-C6
26	S	605	CLA	C4-C3-C5-C6
26	2	306	CLA	C2-C3-C5-C6
26	6	605	CLA	C2-C3-C5-C6
26	O	606	CLA	C2-C3-C5-C6
26	S	605	CLA	C2-C3-C5-C6
29	a	407	PL9	C23-C24-C26-C27
26	N	601	CLA	O1D-CGD-O2D-CED
26	1	613	CLA	C2A-CAA-CBA-CGA
34	c	520	LHG	O1-C1-C2-O2
34	b	621	LHG	C29-C30-C31-C32
26	B	613	CLA	O1A-CGA-O2A-C1
26	4	309	CLA	O1A-CGA-O2A-C1
26	6	610	CLA	O1A-CGA-O2A-C1
26	Q	308	CLA	O1A-CGA-O2A-C1
26	S	610	CLA	O1A-CGA-O2A-C1
34	d	408	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
26	6	602	CLA	C8-C10-C11-C12
26	S	602	CLA	C8-C10-C11-C12
34	Z	102	LHG	O9-C7-O7-C5
34	z	101	LHG	O9-C7-O7-C5
26	A	403	CLA	C2-C1-O2A-CGA
26	a	403	CLA	C2-C1-O2A-CGA
26	5	609	CLA	C2-C1-O2A-CGA
26	R	310	CLA	C2-C1-O2A-CGA
33	c	521	LMG	C17-C18-C19-C20
33	5	619	LMG	C32-C33-C34-C35
33	R	301	LMG	C32-C33-C34-C35
34	D	410	LHG	C9-C10-C11-C12
26	C	504	CLA	C8-C10-C11-C12
26	c	505	CLA	C8-C10-C11-C12
26	5	609	CLA	O1A-CGA-O2A-C1
26	R	310	CLA	O1A-CGA-O2A-C1
28	B	618	WVN	C15-C13-C20-C23
28	C	516	WVN	C06-C13-C20-C23
28	a	406	WVN	C15-C13-C20-C23
28	b	617	WVN	C15-C13-C20-C23
28	3	313	WVN	C06-C13-C20-C23
28	3	313	WVN	C15-C13-C20-C23
28	P	615	WVN	C15-C13-C20-C23
40	5	616	IHT	C02-C07-C18-C22
40	5	616	IHT	C10-C07-C18-C22
40	R	317	IHT	C02-C07-C18-C22
40	R	317	IHT	C10-C07-C18-C22
34	b	621	LHG	C25-C26-C27-C28
26	B	616	CLA	C13-C15-C16-C17
26	C	505	CLA	C5-C6-C7-C8
26	c	506	CLA	C5-C6-C7-C8
26	3	302	CLA	C13-C15-C16-C17
26	4	303	CLA	C13-C15-C16-C17
26	G	401	CLA	C13-C15-C16-C17
26	Q	302	CLA	C13-C15-C16-C17
33	D	413	LMG	C15-C16-C17-C18
33	2	318	LMG	C12-C13-C14-C15
33	O	617	LMG	C12-C13-C14-C15
26	d	406	CLA	C14-C13-C15-C16
26	4	304	CLA	C14-C13-C15-C16
26	Q	303	CLA	C14-C13-C15-C16
26	P	603	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	b	604	CLA	O1D-CGD-O2D-CED
38	N	612	KC2	CAA-CBA-CGA-O2A
26	B	604	CLA	C4-C3-C5-C6
26	C	506	CLA	C4-C3-C5-C6
26	b	604	CLA	C4-C3-C5-C6
26	5	607	CLA	C4-C3-C5-C6
26	R	308	CLA	C4-C3-C5-C6
26	B	602	CLA	C6-C7-C8-C10
26	B	603	CLA	C6-C7-C8-C10
26	B	605	CLA	C11-C12-C13-C15
26	B	607	CLA	C11-C10-C8-C7
26	C	503	CLA	C11-C12-C13-C15
26	b	602	CLA	C6-C7-C8-C10
26	b	603	CLA	C6-C7-C8-C10
26	b	605	CLA	C11-C12-C13-C15
26	b	607	CLA	C11-C10-C8-C7
26	c	504	CLA	C11-C12-C13-C15
26	1	609	CLA	C11-C10-C8-C7
26	2	304	CLA	C11-C10-C8-C7
26	3	307	CLA	C2-C3-C5-C6
26	5	607	CLA	C11-C12-C13-C15
26	6	602	CLA	C6-C7-C8-C10
26	6	602	CLA	C11-C12-C13-C15
26	O	604	CLA	C11-C10-C8-C7
26	P	609	CLA	C2-C3-C5-C6
26	R	308	CLA	C11-C12-C13-C15
26	S	602	CLA	C6-C7-C8-C10
26	S	602	CLA	C11-C12-C13-C15
27	A	404	PHO	C11-C10-C8-C7
27	a	404	PHO	C11-C10-C8-C7
29	A	407	PL9	C23-C24-C26-C27
29	d	407	PL9	C43-C44-C46-C47
26	D	408	CLA	C3-C5-C6-C7
26	d	406	CLA	C3-C5-C6-C7
34	2	321	LHG	C9-C10-C11-C12
34	G	403	LHG	C9-C10-C11-C12
28	B	618	WVN	C22-C26-C29-C31
28	d	410	WVN	C22-C26-C29-C31
39	6	613	II0	C26-C30-C32-C34
39	R	318	II0	C26-C30-C32-C34
26	B	616	CLA	C16-C17-C18-C20
26	2	309	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	O	609	CLA	C11-C12-C13-C14
26	b	610	CLA	O1D-CGD-O2D-CED
26	4	308	CLA	O1D-CGD-O2D-CED
26	Q	307	CLA	O1D-CGD-O2D-CED
33	M	101	LMG	O9-C10-O7-C8
33	m	101	LMG	O9-C10-O7-C8
33	5	619	LMG	C10-C11-C12-C13
33	R	301	LMG	C10-C11-C12-C13
26	1	608	CLA	O1A-CGA-O2A-C1
26	B	607	CLA	CBA-CGA-O2A-C1
26	b	607	CLA	CBA-CGA-O2A-C1
26	C	505	CLA	C2A-CAA-CBA-CGA
26	C	506	CLA	C2A-CAA-CBA-CGA
26	c	506	CLA	C2A-CAA-CBA-CGA
26	c	507	CLA	C2A-CAA-CBA-CGA
26	N	602	CLA	C2A-CAA-CBA-CGA
26	3	309	CLA	C2A-CAA-CBA-CGA
26	P	611	CLA	C2A-CAA-CBA-CGA
34	L	101	LHG	C33-C34-C35-C36
34	l	101	LHG	C33-C34-C35-C36
33	d	411	LMG	C15-C16-C17-C18
34	d	408	LHG	C9-C10-C11-C12
27	A	404	PHO	C13-C15-C16-C17
27	a	404	PHO	C13-C15-C16-C17
38	1	605	KC2	C2B-C3B-CAB-CBB
26	1	601	CLA	O1D-CGD-O2D-CED
26	6	601	CLA	O1D-CGD-O2D-CED
34	a	409	LHG	C26-C27-C28-C29
27	A	404	PHO	CBD-CGD-O2D-CED
26	G	401	CLA	C16-C17-C18-C20
26	S	601	CLA	O1D-CGD-O2D-CED
34	C	501	LHG	C26-C27-C28-C29
34	a	409	LHG	C25-C26-C27-C28
33	M	101	LMG	C11-C10-O7-C8
33	m	101	LMG	C11-C10-O7-C8
34	Z	102	LHG	C8-C7-O7-C5
34	z	101	LHG	C8-C7-O7-C5
34	2	321	LHG	C8-C7-O7-C5
34	G	403	LHG	C8-C7-O7-C5
37	F	101	HEM	C4B-C3B-CAB-CBB
38	1	612	KC2	C4C-C3C-CAC-CBC
38	N	610	KC2	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
26	B	616	CLA	C5-C6-C7-C8
26	c	510	CLA	C15-C16-C17-C18
26	C	511	CLA	CBD-CGD-O2D-CED
27	a	404	PHO	CBD-CGD-O2D-CED
38	P	605	KC2	CBD-CGD-O2D-CED
34	C	501	LHG	C25-C26-C27-C28
34	2	321	LHG	O9-C7-O7-C5
34	G	403	LHG	O9-C7-O7-C5
33	m	101	LMG	C28-C29-C30-C31
35	c	519	DGD	C3A-C4A-C5A-C6A
33	C	520	LMG	O7-C8-C9-O8
33	c	522	LMG	O7-C8-C9-O8
26	c	511	CLA	C16-C17-C18-C19
34	L	101	LHG	C32-C33-C34-C35
35	h	101	DGD	O6E-C5E-C6E-O5E
26	C	509	CLA	C15-C16-C17-C18
26	b	616	CLA	C5-C6-C7-C8
26	3	307	CLA	C4-C3-C5-C6
26	P	609	CLA	C4-C3-C5-C6
26	g	401	CLA	C4-C3-C5-C6
29	A	407	PL9	C12-C11-C9-C10
29	a	407	PL9	C12-C11-C9-C10
26	B	603	CLA	C2-C3-C5-C6
26	b	603	CLA	C2-C3-C5-C6
26	5	607	CLA	C2-C3-C5-C6
26	R	308	CLA	C2-C3-C5-C6
29	D	409	PL9	C43-C44-C46-C47
29	D	409	PL9	C4-C3-C7-C8
29	d	407	PL9	C4-C3-C7-C8
39	4	317	II0	C10-C22-C24-C26
39	6	613	II0	C10-C22-C24-C26
39	O	613	II0	C09-C21-C23-C25
39	O	614	II0	C09-C21-C23-C25
39	P	614	II0	C10-C22-C24-C26
39	Q	316	II0	C09-C21-C23-C25
39	Q	316	II0	C10-C22-C24-C26
39	R	318	II0	C10-C22-C24-C26
40	4	318	IHT	C11-C21-C24-C26
40	Q	317	IHT	C11-C21-C24-C26
26	B	603	CLA	C6-C7-C8-C9
26	B	608	CLA	C14-C13-C15-C16
26	B	612	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
26	C	508	CLA	C14-C13-C15-C16
26	b	603	CLA	C6-C7-C8-C9
26	b	612	CLA	C6-C7-C8-C9
26	c	509	CLA	C14-C13-C15-C16
26	N	609	CLA	C11-C10-C8-C9
26	2	304	CLA	C11-C10-C8-C9
26	3	303	CLA	C11-C10-C8-C9
26	5	605	CLA	C11-C10-C8-C9
26	6	602	CLA	C6-C7-C8-C9
26	6	602	CLA	C11-C12-C13-C14
26	G	401	CLA	C11-C10-C8-C9
26	O	604	CLA	C11-C10-C8-C9
26	P	604	CLA	C11-C10-C8-C9
26	R	306	CLA	C11-C10-C8-C9
26	S	602	CLA	C6-C7-C8-C9
26	S	602	CLA	C11-C12-C13-C14
27	A	404	PHO	C11-C10-C8-C9
27	a	404	PHO	C11-C10-C8-C9
38	3	304	KC2	CBD-CGD-O2D-CED
33	a	413	LMG	O6-C5-C6-O5
35	H	102	DGD	O6E-C5E-C6E-O5E
26	B	610	CLA	O1D-CGD-O2D-CED
26	N	604	CLA	C2A-CAA-CBA-CGA
26	N	614	CLA	C2A-CAA-CBA-CGA
26	4	304	CLA	C2A-CAA-CBA-CGA
26	4	308	CLA	C2A-CAA-CBA-CGA
26	6	606	CLA	C2A-CAA-CBA-CGA
26	Q	303	CLA	C2A-CAA-CBA-CGA
26	Q	307	CLA	C2A-CAA-CBA-CGA
26	S	606	CLA	C2A-CAA-CBA-CGA
34	l	101	LHG	C32-C33-C34-C35
33	A	412	LMG	O6-C5-C6-O5
28	b	618	WVN	C20-C23-C25-C27
26	2	303	CLA	C8-C10-C11-C12
26	O	603	CLA	C8-C10-C11-C12
34	D	403	LHG	C25-C26-C27-C28
28	b	617	WVN	C30-C33-C34-C37
28	b	618	WVN	C20-C23-C25-C28
39	N	618	II0	C31-C33-C35-C39
26	B	601	CLA	C1A-C2A-CAA-CBA
26	B	607	CLA	C1A-C2A-CAA-CBA
26	C	504	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	C	510	CLA	C1A-C2A-CAA-CBA
26	C	512	CLA	C1A-C2A-CAA-CBA
26	b	601	CLA	C1A-C2A-CAA-CBA
26	b	607	CLA	C1A-C2A-CAA-CBA
26	c	505	CLA	C1A-C2A-CAA-CBA
26	c	511	CLA	C1A-C2A-CAA-CBA
26	c	513	CLA	C1A-C2A-CAA-CBA
26	1	601	CLA	C1A-C2A-CAA-CBA
26	N	601	CLA	C1A-C2A-CAA-CBA
26	3	302	CLA	C1A-C2A-CAA-CBA
26	3	306	CLA	C1A-C2A-CAA-CBA
26	4	306	CLA	C1A-C2A-CAA-CBA
26	4	307	CLA	C1A-C2A-CAA-CBA
26	5	603	CLA	C1A-C2A-CAA-CBA
26	5	612	CLA	C1A-C2A-CAA-CBA
26	P	603	CLA	C1A-C2A-CAA-CBA
26	P	607	CLA	C1A-C2A-CAA-CBA
26	Q	305	CLA	C1A-C2A-CAA-CBA
26	Q	306	CLA	C1A-C2A-CAA-CBA
26	R	304	CLA	C1A-C2A-CAA-CBA
26	R	313	CLA	C1A-C2A-CAA-CBA
26	1	609	CLA	C11-C12-C13-C14
26	3	308	CLA	C6-C7-C8-C9
34	5	618	LHG	C11-C10-C9-C8
34	R	319	LHG	C11-C10-C9-C8
28	B	618	WVN	C25-C28-C30-C33
28	b	617	WVN	C34-C37-C40-C39
26	2	306	CLA	C10-C11-C12-C13
26	2	308	CLA	C13-C15-C16-C17
26	O	606	CLA	C10-C11-C12-C13
26	O	608	CLA	C13-C15-C16-C17
34	b	621	LHG	C4-O6-P-O3
26	b	602	CLA	O1D-CGD-O2D-CED
33	c	521	LMG	C15-C16-C17-C18
26	C	508	CLA	C13-C15-C16-C17
26	c	509	CLA	C13-C15-C16-C17
26	R	312	CLA	C5-C6-C7-C8
34	b	621	LHG	O6-C4-C5-C6
34	5	618	LHG	O6-C4-C5-C6
34	R	319	LHG	O6-C4-C5-C6
26	2	319	CLA	O1D-CGD-O2D-CED
35	C	517	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
26	5	611	CLA	C5-C6-C7-C8
26	C	510	CLA	C16-C17-C18-C19
26	b	616	CLA	C16-C17-C18-C19
26	N	609	CLA	C11-C12-C13-C15
26	c	506	CLA	CBD-CGD-O2D-CED
26	c	512	CLA	CBD-CGD-O2D-CED
26	C	502	CLA	CBA-CGA-O2A-C1
26	c	503	CLA	CBA-CGA-O2A-C1
26	C	506	CLA	C2-C3-C5-C6
26	b	611	CLA	C13-C15-C16-C17
26	P	601	CLA	O1D-CGD-O2D-CED
26	b	607	CLA	O1A-CGA-O2A-C1
26	3	306	CLA	C2A-CAA-CBA-CGA
26	P	607	CLA	C2A-CAA-CBA-CGA
26	B	613	CLA	C16-C17-C18-C20
26	2	311	CLA	C11-C12-C13-C15
26	O	611	CLA	C11-C12-C13-C15
26	B	602	CLA	O1D-CGD-O2D-CED
33	A	412	LMG	C7-C8-C9-O8
33	C	519	LMG	O1-C7-C8-C9
33	a	413	LMG	C7-C8-C9-O8
33	4	319	LMG	C7-C8-C9-O8
33	Q	318	LMG	C7-C8-C9-O8
26	B	611	CLA	C13-C15-C16-C17
33	C	519	LMG	C32-C33-C34-C35
26	B	604	CLA	O1D-CGD-O2D-CED
33	C	519	LMG	C22-C23-C24-C25
35	H	102	DGD	O2G-C1B-C2B-C3B
35	h	101	DGD	O2G-C1B-C2B-C3B
26	C	513	CLA	C3-C5-C6-C7
26	c	514	CLA	C3-C5-C6-C7
26	B	607	CLA	O1A-CGA-O2A-C1
35	C	517	DGD	O6E-C5E-C6E-O5E
35	c	519	DGD	O6E-C5E-C6E-O5E
35	h	101	DGD	C4B-C5B-C6B-C7B
26	3	301	CLA	O1D-CGD-O2D-CED
26	3	302	CLA	C5-C6-C7-C8
26	P	603	CLA	C5-C6-C7-C8
33	d	411	LMG	O6-C5-C6-O5
39	1	618	II0	C38-C36-C40-C42
26	3	308	CLA	C4-C3-C5-C6
29	D	409	PL9	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
29	d	407	PL9	C15-C14-C16-C17
26	3	308	CLA	C2-C3-C5-C6
26	P	602	CLA	O1D-CGD-O2D-CED
26	2	309	CLA	C11-C12-C13-C15
26	O	609	CLA	C11-C12-C13-C15
26	4	303	CLA	CBA-CGA-O2A-C1
26	Q	302	CLA	CBA-CGA-O2A-C1
34	C	501	LHG	C35-C36-C37-C38
26	C	505	CLA	CBD-CGD-O2D-CED
26	b	615	CLA	C5-C6-C7-C8
34	Z	102	LHG	C4-C5-O7-C7
34	z	101	LHG	C4-C5-O7-C7
33	D	413	LMG	O6-C5-C6-O5
26	N	603	CLA	C2A-CAA-CBA-CGA
26	4	302	CLA	C13-C15-C16-C17
26	Q	301	CLA	C13-C15-C16-C17
35	H	102	DGD	C4B-C5B-C6B-C7B
26	5	602	CLA	O1D-CGD-O2D-CED
34	c	520	LHG	C14-C15-C16-C17
26	R	303	CLA	O1D-CGD-O2D-CED
34	a	409	LHG	C35-C36-C37-C38
34	a	409	LHG	C24-C23-O8-C6
26	b	616	CLA	C16-C17-C18-C20
26	1	609	CLA	CBD-CGD-O2D-CED
33	m	101	LMG	C29-C30-C31-C32
26	B	612	CLA	C15-C16-C17-C18
26	b	612	CLA	C15-C16-C17-C18
26	G	401	CLA	C10-C11-C12-C13
28	3	313	WVN	C31-C32-C36-C39
39	2	316	II0	C33-C35-C39-C41
39	O	615	II0	C33-C35-C39-C41
40	1	619	IHT	C34-C35-C38-C41
26	c	503	CLA	O1A-CGA-O2A-C1
26	C	509	CLA	C12-C13-C15-C16
26	C	510	CLA	C6-C7-C8-C10
26	c	510	CLA	C12-C13-C15-C16
26	c	511	CLA	C6-C7-C8-C10
26	2	302	CLA	C6-C7-C8-C10
26	2	306	CLA	C6-C7-C8-C10
26	3	301	CLA	C6-C7-C8-C10
26	3	303	CLA	C11-C10-C8-C7
26	5	605	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
26	5	608	CLA	C6-C7-C8-C10
26	6	602	CLA	C11-C10-C8-C7
26	O	602	CLA	C6-C7-C8-C10
26	O	606	CLA	C6-C7-C8-C10
26	P	602	CLA	C6-C7-C8-C10
26	P	604	CLA	C11-C10-C8-C7
26	R	306	CLA	C11-C10-C8-C7
26	R	309	CLA	C6-C7-C8-C10
26	S	602	CLA	C11-C10-C8-C7
26	g	401	CLA	C2-C3-C5-C6
29	A	407	PL9	C12-C11-C9-C8
29	a	407	PL9	C12-C11-C9-C8
26	C	502	CLA	O1A-CGA-O2A-C1
26	C	503	CLA	C6-C7-C8-C9
26	b	613	CLA	C11-C12-C13-C14
26	c	504	CLA	C6-C7-C8-C9
26	1	609	CLA	C11-C10-C8-C9
26	2	302	CLA	C6-C7-C8-C9
26	2	302	CLA	C11-C10-C8-C9
26	2	302	CLA	C11-C12-C13-C14
26	2	309	CLA	C6-C7-C8-C9
26	3	301	CLA	C6-C7-C8-C9
26	5	608	CLA	C6-C7-C8-C9
26	5	609	CLA	C6-C7-C8-C9
26	O	602	CLA	C6-C7-C8-C9
26	O	602	CLA	C11-C10-C8-C9
26	O	602	CLA	C11-C12-C13-C14
26	O	602	CLA	C14-C13-C15-C16
26	O	609	CLA	C6-C7-C8-C9
26	P	602	CLA	C6-C7-C8-C9
26	R	309	CLA	C6-C7-C8-C9
26	R	310	CLA	C6-C7-C8-C9
26	2	308	CLA	CBA-CGA-O2A-C1
26	O	608	CLA	CBA-CGA-O2A-C1
26	P	610	CLA	CBA-CGA-O2A-C1
34	C	501	LHG	C24-C23-O8-C6
28	k	101	WVN	C20-C23-C25-C27
28	x	101	WVN	C11-C19-C22-C24
26	N	609	CLA	C11-C12-C13-C14
26	2	311	CLA	C11-C12-C13-C14
26	O	611	CLA	C11-C12-C13-C14
34	C	518	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
26	2	308	CLA	O1D-CGD-O2D-CED
26	O	608	CLA	O1D-CGD-O2D-CED
28	k	101	WVN	C20-C23-C25-C28
34	C	518	LHG	C12-C13-C14-C15
34	N	621	LHG	C13-C14-C15-C16
26	1	603	CLA	O1D-CGD-O2D-CED
26	1	609	CLA	C10-C11-C12-C13
26	c	513	CLA	CBA-CGA-O2A-C1
26	1	609	CLA	CBA-CGA-O2A-C1
33	D	406	LMG	C29-C28-O8-C9
34	1	620	LHG	C7-C8-C9-C10
34	N	621	LHG	C7-C8-C9-C10
26	B	609	CLA	C15-C16-C17-C18
26	C	513	CLA	C5-C6-C7-C8
26	b	609	CLA	C15-C16-C17-C18
34	D	403	LHG	O6-C4-C5-C6
34	L	101	LHG	O6-C4-C5-C6
34	l	101	LHG	O6-C4-C5-C6
35	c	519	DGD	C6B-C7B-C8B-C9B
26	C	512	CLA	CBA-CGA-O2A-C1
33	d	404	LMG	C29-C28-O8-C9
26	c	514	CLA	C5-C6-C7-C8
26	4	304	CLA	C10-C11-C12-C13
26	Q	303	CLA	C10-C11-C12-C13
35	C	517	DGD	C6B-C7B-C8B-C9B
33	M	101	LMG	C29-C30-C31-C32
26	C	513	CLA	CBA-CGA-O2A-C1
26	c	514	CLA	CBA-CGA-O2A-C1
26	3	303	CLA	O1D-CGD-O2D-CED
26	P	604	CLA	O1D-CGD-O2D-CED
38	1	611	KC2	O1D-CGD-O2D-CED
26	B	612	CLA	C3A-C2A-CAA-CBA
26	C	513	CLA	C3A-C2A-CAA-CBA
26	b	612	CLA	C3A-C2A-CAA-CBA
26	c	514	CLA	C3A-C2A-CAA-CBA
26	2	303	CLA	C3A-C2A-CAA-CBA
26	2	309	CLA	C3A-C2A-CAA-CBA
26	3	308	CLA	C3A-C2A-CAA-CBA
26	O	603	CLA	C3A-C2A-CAA-CBA
26	O	609	CLA	C3A-C2A-CAA-CBA
26	B	611	CLA	C8-C10-C11-C12
28	B	618	WVN	C34-C37-C40-C39

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Mol	Chain	Res	Type	Atoms
28	c	516	WVN	C25-C28-C30-C33
28	c	517	WVN	C34-C37-C40-C39
28	k	101	WVN	C22-C26-C29-C31
28	P	615	WVN	C25-C28-C30-C33
40	4	318	IHT	C33-C37-C40-C41
40	5	616	IHT	C23-C27-C30-C32
40	Q	317	IHT	C33-C37-C40-C41
40	R	317	IHT	C23-C27-C30-C32
26	b	611	CLA	C8-C10-C11-C12
33	A	412	LMG	C29-C28-O8-C9
34	2	321	LHG	C13-C14-C15-C16
34	G	403	LHG	C13-C14-C15-C16
33	B	620	LMG	C7-C8-C9-O8
33	C	520	LMG	C7-C8-C9-O8
33	b	620	LMG	C7-C8-C9-O8
33	c	521	LMG	C7-C8-C9-O8
33	c	522	LMG	C7-C8-C9-O8
34	C	518	LHG	C4-C5-C6-O8
35	H	102	DGD	C6A-C7A-C8A-C9A
35	h	101	DGD	C6A-C7A-C8A-C9A
26	1	604	CLA	C5-C6-C7-C8
26	N	602	CLA	O1D-CGD-O2D-CED
33	R	301	LMG	C29-C30-C31-C32
26	Q	302	CLA	O1A-CGA-O2A-C1
26	2	311	CLA	C5-C6-C7-C8
26	O	611	CLA	C5-C6-C7-C8
26	C	503	CLA	C4-C3-C5-C6
26	C	514	CLA	C4-C3-C5-C6
35	h	101	DGD	C8A-C9A-CAA-CBA
26	4	303	CLA	O1A-CGA-O2A-C1
34	b	621	LHG	O1-C1-C2-O2
34	b	621	LHG	C28-C29-C30-C31
34	b	621	LHG	O6-C4-C5-O7
34	5	618	LHG	O6-C4-C5-O7
34	R	319	LHG	O6-C4-C5-O7
38	1	612	KC2	C3A-C2A-CAA-CBA
38	N	611	KC2	C3A-C2A-CAA-CBA
38	4	311	KC2	C3A-C2A-CAA-CBA
38	Q	310	KC2	C3A-C2A-CAA-CBA
26	3	308	CLA	C6-C7-C8-C10
26	b	606	CLA	C8-C10-C11-C12
34	a	409	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
33	5	619	LMG	C29-C30-C31-C32
30	D	401	SQD	O47-C45-C46-O48
30	c	501	SQD	O47-C45-C46-O48
33	B	620	LMG	O7-C8-C9-O8
33	D	406	LMG	O7-C8-C9-O8
33	b	620	LMG	O7-C8-C9-O8
33	d	404	LMG	O7-C8-C9-O8
35	H	102	DGD	C8A-C9A-CAA-CBA
26	C	513	CLA	C16-C17-C18-C20
26	c	514	CLA	C16-C17-C18-C20
29	D	409	PL9	C45-C44-C46-C47
26	3	302	CLA	C2-C1-O2A-CGA
26	P	603	CLA	C2-C1-O2A-CGA
26	P	610	CLA	O1A-CGA-O2A-C1
26	B	616	CLA	C11-C12-C13-C14
26	D	408	CLA	C11-C10-C8-C9
26	b	616	CLA	C11-C12-C13-C14
26	c	512	CLA	C6-C7-C8-C9
26	d	406	CLA	C11-C10-C8-C9
26	1	604	CLA	C11-C10-C8-C9
26	2	302	CLA	C14-C13-C15-C16
26	3	302	CLA	C6-C7-C8-C9
26	3	306	CLA	C6-C7-C8-C9
26	4	303	CLA	C11-C12-C13-C14
26	5	609	CLA	C14-C13-C15-C16
26	6	602	CLA	C11-C10-C8-C9
26	6	606	CLA	C6-C7-C8-C9
26	6	610	CLA	C11-C12-C13-C14
26	P	603	CLA	C6-C7-C8-C9
26	P	607	CLA	C6-C7-C8-C9
26	Q	302	CLA	C11-C12-C13-C14
26	R	310	CLA	C14-C13-C15-C16
26	S	602	CLA	C11-C10-C8-C9
26	S	606	CLA	C6-C7-C8-C9
26	S	610	CLA	C11-C12-C13-C14
27	D	405	PHO	C6-C7-C8-C9
27	d	403	PHO	C6-C7-C8-C9
33	a	413	LMG	C29-C28-O8-C9
34	C	518	LHG	C11-C10-C9-C8
26	2	304	CLA	C8-C10-C11-C12
26	O	604	CLA	C8-C10-C11-C12
38	1	610	KC2	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	3	303	CLA	C2A-CAA-CBA-CGA
26	6	604	CLA	C2A-CAA-CBA-CGA
26	P	604	CLA	C2A-CAA-CBA-CGA
26	S	604	CLA	C2A-CAA-CBA-CGA
28	B	617	WVN	C06-C13-C20-C23
28	c	517	WVN	C06-C13-C20-C23
40	2	317	IHT	C10-C07-C18-C22
30	c	501	SQD	C11-C10-C9-C8
27	A	404	PHO	O1D-CGD-O2D-CED
39	5	615	II0	C31-C33-C35-C39
39	6	613	II0	C31-C33-C35-C39
39	R	316	II0	C31-C33-C35-C39
39	R	318	II0	C31-C33-C35-C39
26	C	512	CLA	C8-C10-C11-C12
27	a	404	PHO	O1D-CGD-O2D-CED
30	D	401	SQD	C11-C10-C9-C8
34	C	501	LHG	O10-C23-O8-C6
34	C	501	LHG	C12-C13-C14-C15
26	C	511	CLA	O1D-CGD-O2D-CED
38	4	305	KC2	CAA-CBA-CGA-O1A
38	Q	304	KC2	CAA-CBA-CGA-O1A
26	c	504	CLA	C4-C3-C5-C6
29	d	407	PL9	C45-C44-C46-C47
26	g	402	CLA	C4C-C3C-CAC-CBC
26	B	606	CLA	C6-C7-C8-C10
26	B	607	CLA	C6-C7-C8-C10
26	C	503	CLA	C6-C7-C8-C10
26	C	505	CLA	C6-C7-C8-C10
26	D	404	CLA	C11-C10-C8-C7
26	D	408	CLA	C11-C10-C8-C7
26	b	607	CLA	C6-C7-C8-C10
26	c	504	CLA	C6-C7-C8-C10
26	c	506	CLA	C6-C7-C8-C10
26	d	402	CLA	C11-C10-C8-C7
26	d	406	CLA	C11-C10-C8-C7
26	2	302	CLA	C11-C10-C8-C7
26	2	302	CLA	C11-C12-C13-C15
26	2	302	CLA	C12-C13-C15-C16
26	3	302	CLA	C6-C7-C8-C10
26	3	305	CLA	C12-C13-C15-C16
26	3	306	CLA	C6-C7-C8-C10
26	4	303	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
26	4	303	CLA	C11-C12-C13-C15
26	5	604	CLA	C6-C7-C8-C10
26	5	609	CLA	C6-C7-C8-C10
26	5	609	CLA	C12-C13-C15-C16
26	6	604	CLA	C12-C13-C15-C16
26	O	602	CLA	C11-C10-C8-C7
26	O	602	CLA	C11-C12-C13-C15
26	O	602	CLA	C12-C13-C15-C16
26	P	603	CLA	C6-C7-C8-C10
26	P	606	CLA	C12-C13-C15-C16
26	P	607	CLA	C6-C7-C8-C10
26	Q	302	CLA	C11-C10-C8-C7
26	Q	302	CLA	C11-C12-C13-C15
26	R	305	CLA	C6-C7-C8-C10
26	R	310	CLA	C6-C7-C8-C10
26	R	310	CLA	C12-C13-C15-C16
26	S	604	CLA	C12-C13-C15-C16
27	D	405	PHO	C6-C7-C8-C10
27	d	403	PHO	C6-C7-C8-C10
26	2	308	CLA	O1A-CGA-O2A-C1
26	O	608	CLA	O1A-CGA-O2A-C1
28	C	515	WVN	C34-C37-C40-C39
28	b	619	WVN	C32-C36-C39-C40
28	k	101	WVN	C34-C37-C40-C39
28	x	101	WVN	C22-C26-C29-C31
39	5	615	II0	C26-C30-C32-C34
39	6	611	II0	C25-C29-C31-C33
39	R	316	II0	C26-C30-C32-C34
39	S	611	II0	C25-C29-C31-C33
26	5	611	CLA	C6-C7-C8-C9
26	R	312	CLA	C6-C7-C8-C9
34	G	403	LHG	C32-C33-C34-C35
33	2	318	LMG	C10-C11-C12-C13
33	O	617	LMG	C10-C11-C12-C13
26	c	512	CLA	O1D-CGD-O2D-CED
34	2	321	LHG	C32-C33-C34-C35
38	N	612	KC2	C2A-CAA-CBA-CGA
26	C	513	CLA	C16-C17-C18-C19
26	2	311	CLA	CBA-CGA-O2A-C1
26	G	401	CLA	CBA-CGA-O2A-C1
26	4	304	CLA	C12-C13-C15-C16
26	Q	303	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
26	O	603	CLA	C15-C16-C17-C18
33	5	619	LMG	C12-C13-C14-C15
26	B	608	CLA	CAD-CBD-CGD-O2D
26	C	503	CLA	CAD-CBD-CGD-O2D
26	b	608	CLA	CAD-CBD-CGD-O2D
26	c	504	CLA	CAD-CBD-CGD-O2D
26	c	505	CLA	CAD-CBD-CGD-O2D
26	N	601	CLA	CAD-CBD-CGD-O2D
26	N	613	CLA	CAD-CBD-CGD-O2D
26	3	306	CLA	CAD-CBD-CGD-O2D
26	5	601	CLA	CAD-CBD-CGD-O2D
26	P	607	CLA	CAD-CBD-CGD-O2D
26	R	302	CLA	CAD-CBD-CGD-O2D
38	1	605	KC2	C2C-C3C-CAC-CBC
38	1	605	KC2	CAD-CBD-CGD-O2D
38	1	610	KC2	CAD-CBD-CGD-O2D
38	N	612	KC2	C2C-C3C-CAC-CBC
38	N	612	KC2	CAD-CBD-CGD-O2D
38	4	305	KC2	CAD-CBD-CGD-O2D
38	Q	304	KC2	CAD-CBD-CGD-O2D
33	R	301	LMG	C12-C13-C14-C15
26	C	511	CLA	C8-C10-C11-C12
26	2	303	CLA	C15-C16-C17-C18
26	4	303	CLA	C5-C6-C7-C8
26	Q	302	CLA	C5-C6-C7-C8
33	c	521	LMG	C18-C19-C20-C21
26	O	611	CLA	CBA-CGA-O2A-C1
26	C	510	CLA	C4-C3-C5-C6
26	c	511	CLA	C4-C3-C5-C6
26	c	514	CLA	C16-C17-C18-C19
26	2	304	CLA	C15-C16-C17-C18
26	O	604	CLA	C15-C16-C17-C18
26	b	604	CLA	C2-C3-C5-C6
33	C	519	LMG	C7-C8-C9-O8
26	1	609	CLA	O1A-CGA-O2A-C1
26	c	507	CLA	C5-C6-C7-C8
38	1	605	KC2	C4B-C3B-CAB-CBB
38	1	612	KC2	C4B-C3B-CAB-CBB
26	4	304	CLA	CBA-CGA-O2A-C1
26	Q	303	CLA	CBA-CGA-O2A-C1
26	3	302	CLA	C16-C17-C18-C19
26	3	302	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
26	P	603	CLA	C16-C17-C18-C19
26	P	603	CLA	C16-C17-C18-C20
33	D	411	LMG	O9-C10-O7-C8
26	B	605	CLA	CHA-CBD-CGD-O1D
26	B	605	CLA	CHA-CBD-CGD-O2D
26	B	609	CLA	CHA-CBD-CGD-O1D
26	B	611	CLA	CHA-CBD-CGD-O1D
26	B	611	CLA	CHA-CBD-CGD-O2D
26	C	506	CLA	CHA-CBD-CGD-O1D
26	C	506	CLA	CHA-CBD-CGD-O2D
26	C	512	CLA	CHA-CBD-CGD-O2D
26	D	408	CLA	CHA-CBD-CGD-O2D
26	b	605	CLA	CHA-CBD-CGD-O1D
26	b	605	CLA	CHA-CBD-CGD-O2D
26	b	611	CLA	CHA-CBD-CGD-O1D
26	b	611	CLA	CHA-CBD-CGD-O2D
26	c	507	CLA	CHA-CBD-CGD-O1D
26	c	507	CLA	CHA-CBD-CGD-O2D
26	c	515	CLA	CHA-CBD-CGD-O1D
26	d	406	CLA	CHA-CBD-CGD-O2D
26	3	302	CLA	CHA-CBD-CGD-O1D
26	3	306	CLA	CHA-CBD-CGD-O1D
26	4	304	CLA	CHA-CBD-CGD-O1D
26	4	304	CLA	CHA-CBD-CGD-O2D
26	4	308	CLA	CHA-CBD-CGD-O1D
26	5	604	CLA	CHA-CBD-CGD-O1D
26	5	608	CLA	CHA-CBD-CGD-O2D
26	6	601	CLA	CHA-CBD-CGD-O1D
26	6	604	CLA	CHA-CBD-CGD-O2D
26	G	402	CLA	CHA-CBD-CGD-O1D
26	P	603	CLA	CHA-CBD-CGD-O1D
26	P	607	CLA	CHA-CBD-CGD-O1D
26	Q	303	CLA	CHA-CBD-CGD-O1D
26	Q	303	CLA	CHA-CBD-CGD-O2D
26	Q	307	CLA	CHA-CBD-CGD-O1D
26	R	305	CLA	CHA-CBD-CGD-O1D
26	R	309	CLA	CHA-CBD-CGD-O2D
26	S	601	CLA	CHA-CBD-CGD-O1D
26	S	604	CLA	CHA-CBD-CGD-O2D
26	g	402	CLA	CHA-CBD-CGD-O1D
26	g	402	CLA	CHA-CBD-CGD-O2D
38	N	605	KC2	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
38	N	605	KC2	CHA-CBD-CGD-O2D
26	c	513	CLA	O1A-CGA-O2A-C1
33	D	406	LMG	O10-C28-O8-C9
33	d	404	LMG	O10-C28-O8-C9
26	B	609	CLA	C13-C15-C16-C17
26	b	609	CLA	C13-C15-C16-C17
33	C	519	LMG	O7-C8-C9-O8
33	4	319	LMG	O7-C8-C9-O8
33	Q	318	LMG	O7-C8-C9-O8
34	C	518	LHG	O7-C5-C6-O8
26	c	512	CLA	C8-C10-C11-C12
26	C	512	CLA	O1A-CGA-O2A-C1
26	c	514	CLA	O1A-CGA-O2A-C1
33	A	412	LMG	O10-C28-O8-C9
26	c	506	CLA	O1D-CGD-O2D-CED
34	5	618	LHG	C15-C16-C17-C18
34	R	319	LHG	C15-C16-C17-C18
26	c	515	CLA	C3-C5-C6-C7
33	D	411	LMG	C11-C10-O7-C8
33	d	409	LMG	C11-C10-O7-C8
27	A	404	PHO	C4-C3-C5-C6
27	a	404	PHO	C4-C3-C5-C6
26	C	513	CLA	O1A-CGA-O2A-C1
26	B	604	CLA	C2-C3-C5-C6
39	N	618	II0	C09-C21-C23-C25
39	N	620	II0	C09-C21-C23-C25
39	N	620	II0	C10-C22-C24-C26
39	2	313	II0	C09-C21-C23-C25
39	2	314	II0	C09-C21-C23-C25
39	2	315	II0	C09-C21-C23-C25
39	2	315	II0	C10-C22-C24-C26
39	4	316	II0	C10-C22-C24-C26
39	5	614	II0	C10-C22-C24-C26
39	6	611	II0	C10-C22-C24-C26
39	6	612	II0	C09-C21-C23-C25
39	O	613	II0	C10-C22-C24-C26
39	O	618	II0	C10-C22-C24-C26
39	P	612	II0	C10-C22-C24-C26
39	Q	315	II0	C10-C22-C24-C26
39	R	315	II0	C10-C22-C24-C26
39	S	611	II0	C09-C21-C23-C25
39	S	612	II0	C09-C21-C23-C25

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Mol	Chain	Res	Type	Atoms
33	d	409	LMG	O9-C10-O7-C8
26	C	511	CLA	C6-C7-C8-C9
26	2	304	CLA	C11-C12-C13-C14
26	3	305	CLA	C14-C13-C15-C16
26	5	605	CLA	C14-C13-C15-C16
26	6	604	CLA	C14-C13-C15-C16
26	O	604	CLA	C11-C12-C13-C14
26	P	606	CLA	C14-C13-C15-C16
26	R	306	CLA	C14-C13-C15-C16
26	S	604	CLA	C14-C13-C15-C16
26	C	505	CLA	O1D-CGD-O2D-CED
33	C	519	LMG	C12-C13-C14-C15
33	c	521	LMG	C29-C30-C31-C32
34	5	618	LHG	C14-C15-C16-C17
34	R	319	LHG	C14-C15-C16-C17
26	A	402	CLA	C2A-CAA-CBA-CGA
28	B	617	WVN	C11-C19-C22-C24
28	b	618	WVN	C30-C33-C34-C38
28	b	619	WVN	C20-C23-C25-C27
28	c	516	WVN	C11-C19-C22-C24
34	C	501	LHG	C30-C31-C32-C33
28	B	617	WVN	C30-C33-C34-C37
28	b	618	WVN	C30-C33-C34-C37
28	b	619	WVN	C20-C23-C25-C28
28	c	516	WVN	C11-C19-C22-C26
28	x	101	WVN	C11-C19-C22-C26
40	5	616	IHT	C18-C22-C23-C27
40	R	317	IHT	C18-C22-C23-C27
26	B	611	CLA	C1A-C2A-CAA-CBA
26	B	612	CLA	C1A-C2A-CAA-CBA
26	C	513	CLA	C1A-C2A-CAA-CBA
26	b	611	CLA	C1A-C2A-CAA-CBA
26	c	514	CLA	C1A-C2A-CAA-CBA
26	1	602	CLA	C1A-C2A-CAA-CBA
26	2	302	CLA	C1A-C2A-CAA-CBA
26	3	301	CLA	C1A-C2A-CAA-CBA
26	6	609	CLA	C1A-C2A-CAA-CBA
26	O	602	CLA	C1A-C2A-CAA-CBA
26	P	602	CLA	C1A-C2A-CAA-CBA
26	S	609	CLA	C1A-C2A-CAA-CBA
26	2	303	CLA	C16-C17-C18-C19
26	O	603	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
26	P	610	CLA	C6-C7-C8-C10
28	c	518	WVN	C34-C37-C40-C39
34	c	520	LHG	C3-O3-P-O6
34	d	408	LHG	C4-O6-P-O3
34	5	618	LHG	C4-O6-P-O3
34	R	319	LHG	C4-O6-P-O3
34	a	409	LHG	C30-C31-C32-C33
26	2	309	CLA	C4-C3-C5-C6
26	O	609	CLA	C4-C3-C5-C6
34	C	501	LHG	C5-C4-O6-P
34	a	409	LHG	C5-C4-O6-P
34	a	409	LHG	C31-C32-C33-C34
26	2	311	CLA	O1A-CGA-O2A-C1
33	a	413	LMG	O10-C28-O8-C9
34	C	501	LHG	C4-O6-P-O4
34	D	403	LHG	C3-O3-P-O5
34	a	409	LHG	C4-O6-P-O4
34	c	520	LHG	C10-C11-C12-C13
26	A	403	CLA	O2A-C1-C2-C3
26	a	403	CLA	O2A-C1-C2-C3
26	6	604	CLA	CBA-CGA-O2A-C1
26	S	604	CLA	CBA-CGA-O2A-C1
26	O	611	CLA	O1A-CGA-O2A-C1
34	C	501	LHG	C31-C32-C33-C34
26	B	605	CLA	CAD-CBD-CGD-O1D
26	B	611	CLA	CAD-CBD-CGD-O1D
26	C	506	CLA	CAD-CBD-CGD-O1D
26	b	605	CLA	CAD-CBD-CGD-O1D
26	b	611	CLA	CAD-CBD-CGD-O1D
26	c	507	CLA	CAD-CBD-CGD-O1D
26	1	614	CLA	CAD-CBD-CGD-O1D
26	2	305	CLA	C2-C3-C5-C6
26	4	304	CLA	CAD-CBD-CGD-O1D
26	Q	303	CLA	CAD-CBD-CGD-O1D
38	N	605	KC2	CAD-CBD-CGD-O1D
33	M	101	LMG	C28-C29-C30-C31
26	4	303	CLA	C8-C10-C11-C12
26	Q	302	CLA	C8-C10-C11-C12
26	4	304	CLA	O1A-CGA-O2A-C1
26	Q	303	CLA	O1A-CGA-O2A-C1
26	1	609	CLA	O1D-CGD-O2D-CED
26	A	405	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
26	C	504	CLA	C11-C10-C8-C7
26	b	606	CLA	C6-C7-C8-C10
26	c	505	CLA	C11-C10-C8-C7
26	2	304	CLA	C11-C12-C13-C15
26	3	301	CLA	C11-C12-C13-C15
26	3	302	CLA	C11-C10-C8-C7
26	4	304	CLA	C11-C12-C13-C15
26	5	604	CLA	C11-C10-C8-C7
26	6	602	CLA	C12-C13-C15-C16
26	6	606	CLA	C6-C7-C8-C10
26	G	401	CLA	C12-C13-C15-C16
26	O	604	CLA	C11-C12-C13-C15
26	P	602	CLA	C11-C12-C13-C15
26	P	603	CLA	C11-C10-C8-C7
26	Q	303	CLA	C11-C12-C13-C15
26	R	305	CLA	C11-C10-C8-C7
26	S	602	CLA	C12-C13-C15-C16
26	S	606	CLA	C6-C7-C8-C10
28	C	515	WVN	C05-C02-C11-C19
28	C	516	WVN	C05-C02-C11-C19
28	c	517	WVN	C05-C02-C11-C19
28	5	617	WVN	C05-C02-C11-C19
28	S	613	WVN	C05-C02-C11-C19
34	D	410	LHG	O6-C4-C5-O7
34	L	101	LHG	O6-C4-C5-O7
34	l	101	LHG	O6-C4-C5-O7
39	3	311	II0	C36-C40-C42-C41
39	P	613	II0	C36-C40-C42-C41
33	C	519	LMG	C17-C18-C19-C20
26	B	606	CLA	C8-C10-C11-C12
34	2	321	LHG	C7-C8-C9-C10
26	g	402	CLA	C2C-C3C-CAC-CBC
33	d	404	LMG	C13-C14-C15-C16
26	a	402	CLA	C2A-CAA-CBA-CGA
26	2	301	CLA	C2A-CAA-CBA-CGA
26	O	601	CLA	C2A-CAA-CBA-CGA
33	B	620	LMG	C14-C15-C16-C17
34	G	403	LHG	C7-C8-C9-C10
26	C	508	CLA	C16-C17-C18-C20
34	C	501	LHG	C2-C3-O3-P
26	6	604	CLA	O1A-CGA-O2A-C1
33	D	406	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
33	c	521	LMG	C32-C33-C34-C35
27	A	404	PHO	C2-C3-C5-C6
27	a	404	PHO	C2-C3-C5-C6
26	5	608	CLA	C8-C10-C11-C12
26	R	309	CLA	C8-C10-C11-C12
26	B	606	CLA	C6-C7-C8-C9
26	B	614	CLA	C11-C10-C8-C9
26	C	505	CLA	C6-C7-C8-C9
26	D	404	CLA	C11-C10-C8-C9
26	b	610	CLA	C11-C12-C13-C14
26	b	614	CLA	C11-C10-C8-C9
26	c	506	CLA	C6-C7-C8-C9
26	d	402	CLA	C11-C10-C8-C9
26	4	303	CLA	C11-C10-C8-C9
26	Q	302	CLA	C11-C10-C8-C9
26	S	604	CLA	O1A-CGA-O2A-C1
26	5	612	CLA	CBA-CGA-O2A-C1
26	c	509	CLA	C16-C17-C18-C20
28	S	613	WVN	C22-C26-C29-C31
26	G	401	CLA	O1A-CGA-O2A-C1
28	k	101	WVN	C29-C31-C32-C36
26	C	506	CLA	C5-C6-C7-C8
26	R	313	CLA	CBA-CGA-O2A-C1
26	b	607	CLA	C8-C10-C11-C12
26	c	513	CLA	C8-C10-C11-C12
26	b	615	CLA	C15-C16-C17-C18
26	A	403	CLA	C1-C2-C3-C4
26	a	403	CLA	C1-C2-C3-C4
33	c	521	LMG	C12-C13-C14-C15
34	2	321	LHG	C35-C36-C37-C38
26	4	309	CLA	C2A-CAA-CBA-CGA
26	5	604	CLA	C2A-CAA-CBA-CGA
26	Q	308	CLA	C2A-CAA-CBA-CGA
26	R	305	CLA	C2A-CAA-CBA-CGA
26	B	610	CLA	O1A-CGA-O2A-C1
26	b	610	CLA	O1A-CGA-O2A-C1
26	B	610	CLA	CBA-CGA-O2A-C1
26	D	408	CLA	CBA-CGA-O2A-C1
26	6	603	CLA	C2-C1-O2A-CGA
26	S	603	CLA	C2-C1-O2A-CGA
34	a	409	LHG	C9-C10-C11-C12
34	G	403	LHG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
33	5	619	LMG	C4-C5-C6-O5
33	R	301	LMG	C4-C5-C6-O5
26	B	607	CLA	C8-C10-C11-C12
34	a	409	LHG	C2-C3-O3-P
34	a	409	LHG	C10-C11-C12-C13
26	b	610	CLA	CBA-CGA-O2A-C1
26	d	406	CLA	CBA-CGA-O2A-C1
28	5	617	WVN	C22-C26-C29-C31
26	D	408	CLA	O1A-CGA-O2A-C1
26	d	406	CLA	O1A-CGA-O2A-C1
34	D	403	LHG	O6-C4-C5-O7
26	B	615	CLA	C15-C16-C17-C18
26	5	609	CLA	C13-C15-C16-C17
26	R	310	CLA	C13-C15-C16-C17
28	B	619	WVN	C06-C13-C20-C23
28	d	410	WVN	C06-C13-C20-C23
28	x	101	WVN	C06-C13-C20-C23
26	c	511	CLA	C2-C3-C5-C6
33	5	619	LMG	C34-C35-C36-C37
33	R	301	LMG	C34-C35-C36-C37
33	d	404	LMG	C28-C29-C30-C31
26	N	607	CLA	C4C-C3C-CAC-CBC
26	6	605	CLA	C6-C7-C8-C9
26	S	605	CLA	C6-C7-C8-C9
26	1	609	CLA	C2A-CAA-CBA-CGA
33	5	619	LMG	O1-C7-C8-O7
34	D	403	LHG	C4-O6-P-O3
34	D	410	LHG	C3-O3-P-O6
34	D	410	LHG	C4-O6-P-O3
34	L	101	LHG	C3-O3-P-O6
34	Z	102	LHG	C3-O3-P-O6
34	Z	102	LHG	C4-O6-P-O3
34	d	408	LHG	C3-O3-P-O6
34	l	101	LHG	C3-O3-P-O6
34	z	101	LHG	C3-O3-P-O6
34	z	101	LHG	C4-O6-P-O3
34	1	620	LHG	C3-O3-P-O6
34	1	620	LHG	C4-O6-P-O3
34	N	621	LHG	C3-O3-P-O6
34	N	621	LHG	C4-O6-P-O3
34	2	321	LHG	C3-O3-P-O6
34	2	321	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
34	5	618	LHG	C3-O3-P-O6
34	G	403	LHG	C3-O3-P-O6
34	G	403	LHG	C4-O6-P-O3
34	R	319	LHG	C3-O3-P-O6
33	D	406	LMG	C28-C29-C30-C31
27	D	405	PHO	CHA-CBD-CGD-O2D
27	d	403	PHO	CHA-CBD-CGD-O2D
26	C	510	CLA	C2-C3-C5-C6
26	c	510	CLA	C11-C10-C8-C7
26	6	610	CLA	C11-C12-C13-C15
26	G	401	CLA	C6-C7-C8-C10
26	S	610	CLA	C11-C12-C13-C15
33	b	620	LMG	C14-C15-C16-C17
26	B	607	CLA	C11-C10-C8-C9
26	C	504	CLA	C11-C10-C8-C9
26	C	509	CLA	C14-C13-C15-C16
26	b	606	CLA	C6-C7-C8-C9
26	b	607	CLA	C11-C10-C8-C9
26	c	505	CLA	C11-C10-C8-C9
26	c	510	CLA	C14-C13-C15-C16
26	2	308	CLA	C14-C13-C15-C16
26	3	302	CLA	C11-C10-C8-C9
26	4	304	CLA	C11-C12-C13-C14
26	5	604	CLA	C11-C10-C8-C9
26	6	602	CLA	C14-C13-C15-C16
26	P	603	CLA	C11-C10-C8-C9
26	Q	303	CLA	C11-C12-C13-C14
26	R	305	CLA	C11-C10-C8-C9
26	S	602	CLA	C14-C13-C15-C16
28	H	101	WVN	C32-C36-C39-C40
28	P	615	WVN	C34-C37-C40-C39
39	1	618	II0	C36-C40-C42-C41
39	3	311	II0	C35-C39-C41-C42
39	P	613	II0	C35-C39-C41-C42
34	C	518	LHG	C26-C27-C28-C29
33	c	521	LMG	C31-C32-C33-C34
34	N	621	LHG	C11-C10-C9-C8
34	C	501	LHG	O1-C1-C2-C3
33	4	319	LMG	C33-C34-C35-C36
33	Q	318	LMG	C33-C34-C35-C36
26	d	406	CLA	C12-C13-C15-C16
34	1	620	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
34	N	621	LHG	C1-C2-C3-O3
26	C	510	CLA	C13-C15-C16-C17
29	D	409	PL9	C13-C14-C16-C17
29	d	407	PL9	C13-C14-C16-C17
26	a	405	CLA	C11-C12-C13-C15
26	P	610	CLA	C6-C7-C8-C9
26	C	509	CLA	CBA-CGA-O2A-C1
34	C	501	LHG	C9-C10-C11-C12
34	G	403	LHG	C11-C10-C9-C8
34	2	321	LHG	C11-C10-C9-C8
26	b	604	CLA	C11-C12-C13-C14
26	6	604	CLA	C15-C16-C17-C18
26	S	604	CLA	C15-C16-C17-C18
26	b	601	CLA	CBD-CGD-O2D-CED
26	6	601	CLA	CBA-CGA-O2A-C1
26	S	601	CLA	CBA-CGA-O2A-C1
26	c	510	CLA	C16-C17-C18-C20
28	C	516	WVN	C34-C37-C40-C39
28	a	406	WVN	C22-C26-C29-C31
28	b	619	WVN	C34-C37-C40-C39
28	P	615	WVN	C32-C36-C39-C40
39	4	317	II0	C26-C30-C32-C34
39	P	614	II0	C36-C40-C42-C41
39	Q	316	II0	C26-C30-C32-C34
26	C	509	CLA	O1A-CGA-O2A-C1
30	A	408	SQD	C11-C10-C9-C8
26	c	514	CLA	C15-C16-C17-C18
26	4	303	CLA	C15-C16-C17-C18
26	Q	302	CLA	C15-C16-C17-C18
37	F	101	HEM	CAD-CBD-CGD-O2D
34	d	408	LHG	O6-C4-C5-O7
26	C	513	CLA	C15-C16-C17-C18
30	a	408	SQD	C11-C10-C9-C8
26	N	606	CLA	CAA-CBA-CGA-O2A
38	N	612	KC2	C4C-C3C-CAC-CBC
26	O	603	CLA	CAA-CBA-CGA-O2A
26	D	408	CLA	C2-C1-O2A-CGA
26	d	406	CLA	C2-C1-O2A-CGA
26	3	306	CLA	C2-C1-O2A-CGA
26	6	606	CLA	C2-C1-O2A-CGA
26	P	607	CLA	C2-C1-O2A-CGA
26	S	606	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
26	C	508	CLA	C16-C17-C18-C19
26	C	509	CLA	C16-C17-C18-C20
26	6	610	CLA	C16-C17-C18-C20
26	S	610	CLA	C16-C17-C18-C20
26	B	603	CLA	C2A-CAA-CBA-CGA
26	B	616	CLA	C2A-CAA-CBA-CGA
26	b	603	CLA	C2A-CAA-CBA-CGA
26	1	602	CLA	C2A-CAA-CBA-CGA
26	1	604	CLA	C2A-CAA-CBA-CGA
26	N	609	CLA	C2A-CAA-CBA-CGA
26	2	304	CLA	C2A-CAA-CBA-CGA
26	5	602	CLA	C2A-CAA-CBA-CGA
26	O	604	CLA	C2A-CAA-CBA-CGA
26	R	303	CLA	C2A-CAA-CBA-CGA
26	B	604	CLA	C11-C12-C13-C14
26	c	511	CLA	C13-C15-C16-C17
34	C	501	LHG	C10-C11-C12-C13
35	H	102	DGD	O1B-C1B-C2B-C3B
26	D	407	CLA	C3A-C2A-CAA-CBA
26	d	405	CLA	C3A-C2A-CAA-CBA
26	1	614	CLA	C3A-C2A-CAA-CBA
26	5	611	CLA	C3A-C2A-CAA-CBA
26	R	312	CLA	C3A-C2A-CAA-CBA
26	c	509	CLA	C16-C17-C18-C19
26	2	304	CLA	C16-C17-C18-C19
26	O	604	CLA	C16-C17-C18-C19
33	C	519	LMG	C28-C29-C30-C31
34	1	620	LHG	C11-C10-C9-C8
35	H	102	DGD	C3B-C4B-C5B-C6B
35	h	101	DGD	O1B-C1B-C2B-C3B
28	Z	101	WVN	C32-C36-C39-C40
28	5	617	WVN	C25-C28-C30-C33
28	S	613	WVN	C25-C28-C30-C33
39	P	612	II0	C26-C30-C32-C34
40	5	616	IHT	C33-C37-C40-C41
40	R	317	IHT	C33-C37-C40-C41
30	D	401	SQD	C33-C34-C35-C36
37	f	101	HEM	CAA-CBA-CGA-O1A
35	h	101	DGD	CBB-CCB-CDB-CEB
29	A	407	PL9	C4-C3-C7-C8
29	a	407	PL9	C4-C3-C7-C8
39	4	316	II0	C09-C21-C23-C25

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Mol	Chain	Res	Type	Atoms
39	6	611	II0	C09-C21-C23-C25
40	O	616	IHT	C11-C21-C24-C26
33	c	521	LMG	C19-C20-C21-C22
26	2	303	CLA	CAA-CBA-CGA-O2A
26	B	603	CLA	C11-C12-C13-C14
26	B	610	CLA	C11-C12-C13-C14
26	B	616	CLA	C14-C13-C15-C16
26	b	603	CLA	C11-C12-C13-C14
26	2	309	CLA	C11-C10-C8-C9
26	G	401	CLA	C11-C12-C13-C14
26	O	608	CLA	C14-C13-C15-C16
26	O	609	CLA	C11-C10-C8-C9
27	a	404	PHO	C6-C7-C8-C9
26	A	405	CLA	C11-C12-C13-C14
33	m	101	LMG	C34-C35-C36-C37
28	3	313	WVN	C01-C02-C11-C19
26	B	612	CLA	C2A-CAA-CBA-CGA
33	A	412	LMG	C34-C35-C36-C37
38	1	612	KC2	C2A-CAA-CBA-CGA
35	H	102	DGD	CBB-CCB-CDB-CEB
26	6	605	CLA	C6-C7-C8-C10
26	S	605	CLA	C6-C7-C8-C10
26	5	603	CLA	O2A-C1-C2-C3
26	R	304	CLA	O2A-C1-C2-C3
26	G	402	CLA	CAA-CBA-CGA-O1A
37	f	101	HEM	CAD-CBD-CGD-O2D
33	M	101	LMG	C34-C35-C36-C37
34	1	620	LHG	C24-C25-C26-C27
34	N	621	LHG	C24-C25-C26-C27
26	B	604	CLA	C1A-C2A-CAA-CBA
26	C	507	CLA	C1A-C2A-CAA-CBA
26	D	407	CLA	C1A-C2A-CAA-CBA
26	b	604	CLA	C1A-C2A-CAA-CBA
26	b	612	CLA	C1A-C2A-CAA-CBA
26	b	614	CLA	C1A-C2A-CAA-CBA
26	c	508	CLA	C1A-C2A-CAA-CBA
26	d	405	CLA	C1A-C2A-CAA-CBA
26	N	607	CLA	C1A-C2A-CAA-CBA
26	2	303	CLA	C1A-C2A-CAA-CBA
26	3	308	CLA	C1A-C2A-CAA-CBA
26	4	302	CLA	C1A-C2A-CAA-CBA
26	4	309	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	6	602	CLA	C1A-C2A-CAA-CBA
26	O	603	CLA	C1A-C2A-CAA-CBA
26	Q	308	CLA	C1A-C2A-CAA-CBA
26	S	602	CLA	C1A-C2A-CAA-CBA
34	D	403	LHG	O9-C7-O7-C5
26	B	612	CLA	C11-C10-C8-C7
26	C	509	CLA	C11-C10-C8-C7
26	b	612	CLA	C11-C10-C8-C7
26	4	304	CLA	C6-C7-C8-C10
26	5	607	CLA	C12-C13-C15-C16
26	6	604	CLA	C11-C12-C13-C15
26	Q	303	CLA	C6-C7-C8-C10
26	R	308	CLA	C12-C13-C15-C16
26	S	604	CLA	C11-C12-C13-C15
26	2	309	CLA	C8-C10-C11-C12
26	O	609	CLA	C8-C10-C11-C12
26	6	601	CLA	O1A-CGA-O2A-C1
26	S	601	CLA	O1A-CGA-O2A-C1
26	G	402	CLA	CAA-CBA-CGA-O2A
37	f	101	HEM	CAA-CBA-CGA-O2A
28	H	101	WVN	C34-C37-C40-C39
35	h	101	DGD	C3B-C4B-C5B-C6B
29	d	407	PL9	C47-C48-C49-C50
26	5	611	CLA	C6-C7-C8-C10
26	R	312	CLA	C6-C7-C8-C10
26	b	612	CLA	C2A-CAA-CBA-CGA
26	3	301	CLA	C2A-CAA-CBA-CGA
26	4	306	CLA	C2A-CAA-CBA-CGA
26	P	602	CLA	C2A-CAA-CBA-CGA
26	Q	305	CLA	C2A-CAA-CBA-CGA
26	3	303	CLA	C10-C11-C12-C13
26	P	604	CLA	C10-C11-C12-C13
34	C	501	LHG	C23-C24-C25-C26
26	O	612	CLA	O1D-CGD-O2D-CED
34	2	321	LHG	O6-C4-C5-O7
34	G	403	LHG	O6-C4-C5-O7
26	b	601	CLA	O1D-CGD-O2D-CED
38	4	305	KC2	C3A-C2A-CAA-CBA
38	5	610	KC2	C3A-C2A-CAA-CBA
38	Q	304	KC2	C3A-C2A-CAA-CBA
38	R	311	KC2	C3A-C2A-CAA-CBA
26	C	507	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
26	b	605	CLA	C15-C16-C17-C18
26	2	312	CLA	O1D-CGD-O2D-CED
26	G	401	CLA	C4-C3-C5-C6
33	c	522	LMG	C10-C11-C12-C13
34	a	409	LHG	C23-C24-C25-C26
33	C	519	LMG	C29-C30-C31-C32
35	h	101	DGD	C5B-C6B-C7B-C8B
26	1	601	CLA	CAA-CBA-CGA-O1A
26	B	605	CLA	C15-C16-C17-C18
29	D	409	PL9	C47-C48-C49-C50
35	H	102	DGD	C5B-C6B-C7B-C8B
26	5	602	CLA	C6-C7-C8-C10
26	R	303	CLA	C6-C7-C8-C10
33	A	412	LMG	C11-C12-C13-C14
33	c	521	LMG	O7-C8-C9-O8
33	R	301	LMG	O1-C7-C8-O7
28	C	516	WVN	C25-C28-C30-C33
28	Y	101	WVN	C25-C28-C30-C33
28	a	406	WVN	C32-C36-C39-C40
39	N	617	II0	C36-C40-C42-C41
39	N	618	II0	C26-C30-C32-C34
39	3	312	II0	C25-C29-C31-C33
37	F	101	HEM	CAD-CBD-CGD-O1D
26	b	613	CLA	C16-C17-C18-C19
34	b	621	LHG	C27-C28-C29-C30
34	L	101	LHG	C1-C2-C3-O3
34	l	101	LHG	C1-C2-C3-O3
26	g	401	CLA	C3-C5-C6-C7
26	G	401	CLA	C2C-C3C-CAC-CBC
26	a	405	CLA	C2-C1-O2A-CGA
26	2	305	CLA	C2-C1-O2A-CGA
26	6	607	CLA	C2-C1-O2A-CGA
26	S	607	CLA	C2-C1-O2A-CGA
26	1	604	CLA	O1A-CGA-O2A-C1
26	4	302	CLA	C10-C11-C12-C13
26	Q	301	CLA	C10-C11-C12-C13
26	N	601	CLA	CAA-CBA-CGA-O2A
37	f	101	HEM	CAD-CBD-CGD-O1D
27	A	404	PHO	C6-C7-C8-C9
35	H	102	DGD	C5A-C6A-C7A-C8A
26	N	603	CLA	C4-C3-C5-C6
26	2	305	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	N	614	CLA	C2-C1-O2A-CGA
27	a	404	PHO	C10-C11-C12-C13
26	2	302	CLA	C2A-CAA-CBA-CGA
26	5	605	CLA	C2A-CAA-CBA-CGA
26	O	602	CLA	C2A-CAA-CBA-CGA
26	c	510	CLA	O1A-CGA-O2A-C1
28	C	515	WVN	C06-C13-C20-C23
28	c	516	WVN	C06-C13-C20-C23
28	k	101	WVN	C06-C13-C20-C23
40	2	317	IHT	C02-C07-C18-C22
40	4	318	IHT	C02-C07-C18-C22
40	Q	317	IHT	C02-C07-C18-C22
26	R	309	CLA	C10-C11-C12-C13
26	1	601	CLA	CAA-CBA-CGA-O2A
35	h	101	DGD	C5A-C6A-C7A-C8A
28	Z	101	WVN	C25-C28-C30-C33
39	3	311	II0	C25-C29-C31-C33
39	P	613	II0	C25-C29-C31-C33
39	P	614	II0	C26-C30-C32-C34
26	C	511	CLA	C4-C3-C5-C6
26	b	616	CLA	C10-C11-C12-C13
26	C	503	CLA	C2-C3-C5-C6
26	C	514	CLA	C2-C3-C5-C6
26	5	608	CLA	C10-C11-C12-C13
27	A	404	PHO	C10-C11-C12-C13
38	6	608	KC2	CAA-CBA-CGA-O1A
38	S	608	KC2	CAA-CBA-CGA-O1A
26	c	510	CLA	C16-C17-C18-C19
34	a	409	LHG	C12-C13-C14-C15
26	2	309	CLA	C2A-CAA-CBA-CGA
26	O	609	CLA	C2A-CAA-CBA-CGA
26	R	306	CLA	C2A-CAA-CBA-CGA
26	B	601	CLA	O1D-CGD-O2D-CED
26	c	513	CLA	CBD-CGD-O2D-CED
26	c	510	CLA	CBA-CGA-O2A-C1
34	5	618	LHG	O9-C7-O7-C5
38	1	610	KC2	CAA-CBA-CGA-O2A
26	2	304	CLA	C16-C17-C18-C20
26	B	601	CLA	CBD-CGD-O2D-CED
34	D	410	LHG	O6-C4-C5-C6
34	d	408	LHG	O6-C4-C5-C6
26	c	512	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	2	311	CLA	C4-C3-C5-C6
26	4	306	CLA	C4-C3-C5-C6
26	Q	305	CLA	C4-C3-C5-C6
26	B	603	CLA	C11-C12-C13-C15
26	B	616	CLA	C11-C10-C8-C7
26	C	506	CLA	C11-C10-C8-C7
26	b	603	CLA	C11-C12-C13-C15
26	c	504	CLA	C2-C3-C5-C6
26	c	507	CLA	C11-C10-C8-C7
26	3	301	CLA	C12-C13-C15-C16
26	P	602	CLA	C12-C13-C15-C16
26	C	512	CLA	CBD-CGD-O2D-CED
27	D	405	PHO	C8-C10-C11-C12
33	c	521	LMG	C39-C40-C41-C42
28	C	516	WVN	C32-C36-C39-C40
39	6	611	II0	C36-C40-C42-C41
26	O	604	CLA	C16-C17-C18-C20
26	1	614	CLA	C2-C1-O2A-CGA
34	D	403	LHG	O7-C5-C6-O8
34	R	319	LHG	O9-C7-O7-C5
26	3	302	CLA	CBA-CGA-O2A-C1
27	d	403	PHO	C8-C10-C11-C12
26	6	607	CLA	C3-C5-C6-C7
26	S	607	CLA	C3-C5-C6-C7
26	b	613	CLA	CAA-CBA-CGA-O2A
26	1	606	CLA	C2A-CAA-CBA-CGA
26	C	509	CLA	C16-C17-C18-C19
26	6	610	CLA	C16-C17-C18-C19
26	1	604	CLA	CBA-CGA-O2A-C1
26	P	603	CLA	CBA-CGA-O2A-C1
34	z	101	LHG	C24-C23-O8-C6
30	D	401	SQD	C7-C8-C9-C10
26	A	402	CLA	CAA-CBA-CGA-O2A
26	a	402	CLA	CAA-CBA-CGA-O2A
26	N	603	CLA	CAA-CBA-CGA-O2A
26	c	513	CLA	C4-C3-C5-C6
26	O	611	CLA	C4-C3-C5-C6
26	P	607	CLA	C4-C3-C5-C6
29	A	407	PL9	C15-C14-C16-C17
29	a	407	PL9	C15-C14-C16-C17
26	B	616	CLA	C10-C11-C12-C13
27	a	404	PHO	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	2	309	CLA	C2-C3-C5-C6
26	O	609	CLA	C2-C3-C5-C6
34	d	408	LHG	C11-C10-C9-C8
26	S	610	CLA	C16-C17-C18-C19
33	C	519	LMG	C19-C20-C21-C22
26	B	609	CLA	C6-C7-C8-C9
26	B	611	CLA	C11-C12-C13-C14
26	B	612	CLA	C11-C10-C8-C9
26	b	607	CLA	C6-C7-C8-C9
26	b	609	CLA	C6-C7-C8-C9
26	b	611	CLA	C11-C12-C13-C14
26	b	612	CLA	C11-C10-C8-C9
26	b	616	CLA	C14-C13-C15-C16
26	3	306	CLA	C11-C10-C8-C9
26	4	304	CLA	C6-C7-C8-C9
26	5	607	CLA	C11-C12-C13-C14
26	G	401	CLA	C6-C7-C8-C9
26	P	607	CLA	C11-C10-C8-C9
26	Q	303	CLA	C6-C7-C8-C9
26	R	308	CLA	C11-C12-C13-C14
38	1	610	KC2	CAA-CBA-CGA-O1A
30	c	501	SQD	C7-C8-C9-C10
26	2	301	CLA	C3A-C2A-CAA-CBA
26	O	601	CLA	C3A-C2A-CAA-CBA
26	O	609	CLA	O1A-CGA-O2A-C1
26	B	613	CLA	CAA-CBA-CGA-O2A
34	5	618	LHG	O7-C7-C8-C9
34	R	319	LHG	O7-C7-C8-C9
26	N	601	CLA	CAA-CBA-CGA-O1A
26	A	405	CLA	CAD-CBD-CGD-O2D
26	B	601	CLA	CAD-CBD-CGD-O2D
26	B	609	CLA	CAD-CBD-CGD-O2D
26	B	614	CLA	CAD-CBD-CGD-O2D
26	C	502	CLA	CAD-CBD-CGD-O2D
26	C	504	CLA	CAD-CBD-CGD-O2D
26	C	507	CLA	CAD-CBD-CGD-O2D
26	a	405	CLA	CAD-CBD-CGD-O2D
26	b	601	CLA	CAD-CBD-CGD-O2D
26	b	604	CLA	CAD-CBD-CGD-O2D
26	b	609	CLA	CAD-CBD-CGD-O2D
26	b	614	CLA	CAD-CBD-CGD-O2D
26	c	503	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
26	c	508	CLA	CAD-CBD-CGD-O2D
26	1	604	CLA	CAD-CBD-CGD-O2D
26	1	607	CLA	CAD-CBD-CGD-O2D
26	1	613	CLA	CAD-CBD-CGD-O2D
26	N	614	CLA	CAD-CBD-CGD-O2D
26	2	309	CLA	CAD-CBD-CGD-O2D
26	3	309	CLA	CAD-CBD-CGD-O2D
26	4	301	CLA	CAD-CBD-CGD-O2D
26	4	307	CLA	CAD-CBD-CGD-O2D
26	5	611	CLA	CAD-CBD-CGD-O2D
26	6	609	CLA	CAD-CBD-CGD-O2D
26	O	609	CLA	CAD-CBD-CGD-O2D
26	P	608	CLA	CAD-CBD-CGD-O2D
26	P	611	CLA	CAD-CBD-CGD-O2D
26	Q	306	CLA	CAD-CBD-CGD-O2D
26	R	312	CLA	CAD-CBD-CGD-O2D
26	S	609	CLA	CAD-CBD-CGD-O2D
27	A	404	PHO	CAD-CBD-CGD-O2D
27	a	404	PHO	CAD-CBD-CGD-O2D
38	4	310	KC2	CAD-CBD-CGD-O2D
38	6	608	KC2	CAD-CBD-CGD-O2D
38	Q	309	KC2	CAD-CBD-CGD-O2D
38	S	608	KC2	CAD-CBD-CGD-O2D
26	a	405	CLA	C11-C12-C13-C14
39	S	611	II0	C36-C40-C42-C41
26	2	309	CLA	O1A-CGA-O2A-C1
26	B	615	CLA	C2-C1-O2A-CGA
26	g	402	CLA	CAA-CBA-CGA-O2A
26	b	610	CLA	CAA-CBA-CGA-O2A
34	Z	102	LHG	C24-C23-O8-C6
33	B	620	LMG	C19-C20-C21-C22
34	b	621	LHG	C35-C36-C37-C38
26	C	512	CLA	C4-C3-C5-C6
26	3	306	CLA	C4-C3-C5-C6
33	A	412	LMG	C29-C30-C31-C32
26	G	401	CLA	C2-C3-C5-C6
26	B	610	CLA	CAA-CBA-CGA-O2A
26	c	506	CLA	CAA-CBA-CGA-O2A
34	c	520	LHG	O7-C7-C8-C9
30	D	401	SQD	C44-C45-C46-O48
30	c	501	SQD	C44-C45-C46-O48
33	D	406	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
33	d	404	LMG	C7-C8-C9-O8
26	O	612	CLA	CBD-CGD-O2D-CED
26	C	506	CLA	C10-C11-C12-C13
26	A	403	CLA	CAA-CBA-CGA-O2A
26	B	612	CLA	CAA-CBA-CGA-O2A
26	C	505	CLA	CAA-CBA-CGA-O2A
26	b	612	CLA	CAA-CBA-CGA-O2A
26	2	301	CLA	O2A-C1-C2-C3
26	2	312	CLA	CBD-CGD-O2D-CED
26	B	613	CLA	O2A-C1-C2-C3
26	D	404	CLA	O2A-C1-C2-C3
26	D	407	CLA	O2A-C1-C2-C3
26	b	613	CLA	O2A-C1-C2-C3
26	d	402	CLA	O2A-C1-C2-C3
26	d	405	CLA	O2A-C1-C2-C3
26	d	406	CLA	O2A-C1-C2-C3
26	5	609	CLA	O2A-C1-C2-C3
26	R	310	CLA	O2A-C1-C2-C3
27	d	403	PHO	O2A-C1-C2-C3
38	1	605	KC2	C4C-C3C-CAC-CBC
34	D	403	LHG	C24-C23-O8-C6
26	b	616	CLA	C2A-CAA-CBA-CGA
26	2	303	CLA	C2A-CAA-CBA-CGA
26	O	603	CLA	C2A-CAA-CBA-CGA
26	2	302	CLA	C13-C15-C16-C17
26	a	403	CLA	CAA-CBA-CGA-O2A
34	d	408	LHG	O8-C23-C24-C25
26	3	302	CLA	O1A-CGA-O2A-C1
37	F	101	HEM	CAA-CBA-CGA-O2A
26	C	507	CLA	C16-C17-C18-C19
26	b	613	CLA	C16-C17-C18-C20
26	b	615	CLA	C16-C17-C18-C20
34	c	520	LHG	C29-C30-C31-C32
26	5	612	CLA	O1A-CGA-O2A-C1
26	R	313	CLA	O1A-CGA-O2A-C1
34	c	520	LHG	C23-C24-C25-C26
26	B	604	CLA	CHA-CBD-CGD-O1D
26	C	511	CLA	CHA-CBD-CGD-O2D
26	b	604	CLA	CHA-CBD-CGD-O1D
26	c	512	CLA	CHA-CBD-CGD-O2D
26	c	513	CLA	CHA-CBD-CGD-O2D
26	1	602	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
26	1	602	CLA	CHA-CBD-CGD-O2D
26	N	606	CLA	CHA-CBD-CGD-O1D
26	N	606	CLA	CHA-CBD-CGD-O2D
26	2	301	CLA	CHA-CBD-CGD-O2D
26	2	306	CLA	CHA-CBD-CGD-O1D
26	2	312	CLA	CHA-CBD-CGD-O1D
26	2	312	CLA	CHA-CBD-CGD-O2D
26	3	301	CLA	CHA-CBD-CGD-O1D
26	3	301	CLA	CHA-CBD-CGD-O2D
26	3	302	CLA	CHA-CBD-CGD-O2D
26	3	303	CLA	CHA-CBD-CGD-O1D
26	4	302	CLA	CHA-CBD-CGD-O1D
26	4	302	CLA	CHA-CBD-CGD-O2D
26	4	308	CLA	CHA-CBD-CGD-O2D
26	5	604	CLA	CHA-CBD-CGD-O2D
26	5	605	CLA	CHA-CBD-CGD-O1D
26	5	605	CLA	CHA-CBD-CGD-O2D
26	5	606	CLA	CHA-CBD-CGD-O1D
26	6	601	CLA	CHA-CBD-CGD-O2D
26	G	402	CLA	CHA-CBD-CGD-O2D
26	O	601	CLA	CHA-CBD-CGD-O2D
26	O	606	CLA	CHA-CBD-CGD-O1D
26	O	612	CLA	CHA-CBD-CGD-O1D
26	O	612	CLA	CHA-CBD-CGD-O2D
26	P	602	CLA	CHA-CBD-CGD-O1D
26	P	602	CLA	CHA-CBD-CGD-O2D
26	P	603	CLA	CHA-CBD-CGD-O2D
26	P	604	CLA	CHA-CBD-CGD-O1D
26	Q	301	CLA	CHA-CBD-CGD-O1D
26	Q	301	CLA	CHA-CBD-CGD-O2D
26	Q	307	CLA	CHA-CBD-CGD-O2D
26	R	305	CLA	CHA-CBD-CGD-O2D
26	R	306	CLA	CHA-CBD-CGD-O1D
26	R	306	CLA	CHA-CBD-CGD-O2D
26	R	307	CLA	CHA-CBD-CGD-O1D
26	S	601	CLA	CHA-CBD-CGD-O2D
26	g	402	CLA	CAA-CBA-CGA-O1A
26	1	606	CLA	CAA-CBA-CGA-O2A
26	6	605	CLA	CAA-CBA-CGA-O2A
26	S	605	CLA	CAA-CBA-CGA-O2A
34	C	518	LHG	O8-C23-C24-C25
34	D	410	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
26	2	309	CLA	CBA-CGA-O2A-C1
26	O	609	CLA	CBA-CGA-O2A-C1
26	B	613	CLA	C2-C3-C5-C6
26	c	512	CLA	C3-C5-C6-C7
26	b	608	CLA	CBD-CGD-O2D-CED
34	2	321	LHG	O6-C4-C5-C6
34	G	403	LHG	O6-C4-C5-C6
26	O	602	CLA	C13-C15-C16-C17
26	5	603	CLA	CAA-CBA-CGA-O2A
26	5	612	CLA	CAA-CBA-CGA-O2A
26	R	304	CLA	CAA-CBA-CGA-O2A
33	C	519	LMG	O7-C10-C11-C12
34	2	321	LHG	O7-C5-C6-O8
34	G	403	LHG	O7-C5-C6-O8
26	P	603	CLA	O1A-CGA-O2A-C1
26	b	608	CLA	O1D-CGD-O2D-CED
26	c	508	CLA	C13-C15-C16-C17
26	5	609	CLA	C5-C6-C7-C8
26	5	604	CLA	C3-C5-C6-C7
26	R	305	CLA	C3-C5-C6-C7
37	F	101	HEM	CAA-CBA-CGA-O1A
26	R	310	CLA	C5-C6-C7-C8
27	A	404	PHO	C5-C6-C7-C8
26	R	313	CLA	CAA-CBA-CGA-O2A
35	C	517	DGD	O2G-C1B-C2B-C3B
26	b	613	CLA	C2A-CAA-CBA-CGA
27	D	405	PHO	CHA-CBD-CGD-O1D
27	d	403	PHO	CHA-CBD-CGD-O1D
26	D	408	CLA	C8-C10-C11-C12
34	c	520	LHG	C26-C27-C28-C29
26	R	307	CLA	O1D-CGD-O2D-CED
26	C	511	CLA	C3-C5-C6-C7
34	5	618	LHG	C8-C7-O7-C5
34	R	319	LHG	C8-C7-O7-C5
26	B	601	CLA	CAA-CBA-CGA-O2A
26	C	503	CLA	CAA-CBA-CGA-O2A
26	c	504	CLA	CAA-CBA-CGA-O2A
35	c	519	DGD	O2G-C1B-C2B-C3B
26	C	512	CLA	C2-C3-C5-C6
26	c	513	CLA	C2-C3-C5-C6
26	3	305	CLA	C6-C7-C8-C10
26	4	306	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	5	605	CLA	C12-C13-C15-C16
26	R	306	CLA	C12-C13-C15-C16
39	N	616	II0	C10-C22-C24-C26
33	c	521	LMG	C35-C36-C37-C38
26	b	601	CLA	CAA-CBA-CGA-O2A
26	R	310	CLA	CAA-CBA-CGA-O2A
26	B	607	CLA	C6-C7-C8-C9
26	B	610	CLA	C14-C13-C15-C16
26	C	509	CLA	C11-C10-C8-C9
26	C	513	CLA	C14-C13-C15-C16
26	b	610	CLA	C14-C13-C15-C16
26	c	510	CLA	C11-C10-C8-C9
26	c	514	CLA	C14-C13-C15-C16
26	N	604	CLA	C6-C7-C8-C9
26	3	301	CLA	C11-C12-C13-C14
26	5	607	CLA	C14-C13-C15-C16
26	P	602	CLA	C11-C12-C13-C14
26	d	406	CLA	C8-C10-C11-C12
26	O	601	CLA	O2A-C1-C2-C3
34	D	410	LHG	C11-C10-C9-C8
30	D	401	SQD	C5-C6-S-O8
30	c	501	SQD	C5-C6-S-O8
26	B	615	CLA	C16-C17-C18-C20
26	5	602	CLA	C6-C7-C8-C9
26	R	303	CLA	C6-C7-C8-C9
26	5	606	CLA	O1D-CGD-O2D-CED
34	D	403	LHG	C8-C7-O7-C5
26	O	612	CLA	CAA-CBA-CGA-O2A
26	B	608	CLA	C2A-CAA-CBA-CGA
34	5	618	LHG	O9-C7-C8-C9
33	M	101	LMG	C35-C36-C37-C38
26	2	306	CLA	CAA-CBA-CGA-O2A
26	5	609	CLA	CAA-CBA-CGA-O2A
26	O	606	CLA	CAA-CBA-CGA-O2A
39	3	310	II0	C28-C26-C30-C32
26	2	312	CLA	CAA-CBA-CGA-O2A
39	1	616	II0	C31-C33-C35-C37
26	A	402	CLA	CAA-CBA-CGA-O1A
26	b	612	CLA	CAA-CBA-CGA-O1A
34	R	319	LHG	O9-C7-C8-C9
26	Q	305	CLA	C2-C3-C5-C6
26	A	403	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
26	C	505	CLA	CAA-CBA-CGA-O1A
26	a	402	CLA	CAA-CBA-CGA-O1A
26	2	301	CLA	C1A-C2A-CAA-CBA
26	2	306	CLA	C1A-C2A-CAA-CBA
26	O	601	CLA	C1A-C2A-CAA-CBA
26	O	606	CLA	C1A-C2A-CAA-CBA
26	Q	301	CLA	C1A-C2A-CAA-CBA
33	a	413	LMG	C11-C12-C13-C14
26	B	612	CLA	CAA-CBA-CGA-O1A
26	c	506	CLA	CAA-CBA-CGA-O1A
26	N	603	CLA	CAA-CBA-CGA-O1A
34	d	408	LHG	O10-C23-C24-C25
26	N	604	CLA	C8-C10-C11-C12
34	C	518	LHG	C29-C30-C31-C32
35	C	517	DGD	C4A-C5A-C6A-C7A
35	H	102	DGD	CCA-CDA-CEA-CFA
26	a	403	CLA	CAA-CBA-CGA-O1A
26	b	610	CLA	CAA-CBA-CGA-O1A
33	c	521	LMG	C34-C35-C36-C37
35	h	101	DGD	CCA-CDA-CEA-CFA
26	6	606	CLA	CAA-CBA-CGA-O2A
26	S	606	CLA	CAA-CBA-CGA-O2A
33	B	620	LMG	O8-C28-C29-C30
26	B	613	CLA	C2A-CAA-CBA-CGA
26	b	608	CLA	C2A-CAA-CBA-CGA
26	6	602	CLA	C2A-CAA-CBA-CGA
26	S	602	CLA	C2A-CAA-CBA-CGA
26	2	306	CLA	C11-C12-C13-C15
26	O	606	CLA	C11-C12-C13-C15
26	b	613	CLA	CAA-CBA-CGA-O1A
26	D	404	CLA	C13-C15-C16-C17
26	d	402	CLA	C13-C15-C16-C17
30	a	408	SQD	C28-C29-C30-C31
26	B	613	CLA	CAA-CBA-CGA-O1A
26	2	306	CLA	CAA-CBA-CGA-O1A
33	C	519	LMG	C2-C1-O1-C7
33	a	413	LMG	C34-C35-C36-C37
34	D	403	LHG	C4-O6-P-O5
34	D	410	LHG	C3-O3-P-O5
34	L	101	LHG	C4-O6-P-O4
34	d	408	LHG	C3-O3-P-O5
34	1	620	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
34	N	621	LHG	C4-O6-P-O5
34	2	321	LHG	C4-O6-P-O5
34	G	403	LHG	C4-O6-P-O5
26	B	610	CLA	CAA-CBA-CGA-O1A
26	6	605	CLA	CAA-CBA-CGA-O1A
26	O	606	CLA	CAA-CBA-CGA-O1A
26	S	605	CLA	CAA-CBA-CGA-O1A
33	C	519	LMG	O9-C10-C11-C12
34	D	410	LHG	O10-C23-C24-C25
35	C	517	DGD	O6D-C5D-C6D-O5D
40	4	318	IHT	C10-C07-C18-C22
40	Q	317	IHT	C10-C07-C18-C22
26	C	513	CLA	C13-C15-C16-C17
26	c	514	CLA	C13-C15-C16-C17
26	5	612	CLA	CAA-CBA-CGA-O1A
26	R	313	CLA	CAA-CBA-CGA-O1A
34	z	101	LHG	O10-C23-O8-C6
26	P	611	CLA	CAA-CBA-CGA-O2A
33	C	520	LMG	C10-C11-C12-C13
26	c	509	CLA	C2A-CAA-CBA-CGA
26	3	309	CLA	CAA-CBA-CGA-O2A
26	1	603	CLA	CAA-CBA-CGA-O2A
33	C	519	LMG	O8-C28-C29-C30
26	C	512	CLA	O1D-CGD-O2D-CED
26	c	504	CLA	CAA-CBA-CGA-O1A
26	B	606	CLA	C4-C3-C5-C6
26	C	505	CLA	CAD-CBD-CGD-O1D
26	c	506	CLA	CAD-CBD-CGD-O1D
26	c	515	CLA	CAD-CBD-CGD-O1D
26	1	609	CLA	CAD-CBD-CGD-O1D
26	N	606	CLA	CAD-CBD-CGD-O1D
26	N	609	CLA	CAD-CBD-CGD-O1D
26	3	303	CLA	CAD-CBD-CGD-O1D
26	4	308	CLA	CAD-CBD-CGD-O1D
26	5	604	CLA	CAD-CBD-CGD-O1D
26	P	604	CLA	CAD-CBD-CGD-O1D
26	Q	307	CLA	CAD-CBD-CGD-O1D
26	R	305	CLA	CAD-CBD-CGD-O1D
30	D	401	SQD	C5-C6-S-O7
30	c	501	SQD	C5-C6-S-O7
33	4	319	LMG	C9-C8-O7-C10
33	Q	318	LMG	C9-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
38	N	611	KC2	CAD-CBD-CGD-O1D
34	D	403	LHG	O10-C23-O8-C6
34	Z	102	LHG	O10-C23-O8-C6
26	C	503	CLA	CAA-CBA-CGA-O1A
26	5	603	CLA	CAA-CBA-CGA-O1A
34	D	410	LHG	C32-C33-C34-C35
26	g	401	CLA	CAA-CBA-CGA-O2A
35	c	519	DGD	O6D-C5D-C6D-O5D
26	C	510	CLA	C6-C7-C8-C9
26	c	503	CLA	C11-C10-C8-C9
26	c	511	CLA	C6-C7-C8-C9
26	2	311	CLA	C6-C7-C8-C9
26	5	604	CLA	C6-C7-C8-C9
26	O	611	CLA	C6-C7-C8-C9
26	R	305	CLA	C6-C7-C8-C9
26	R	308	CLA	C14-C13-C15-C16
33	B	620	LMG	C31-C32-C33-C34
33	d	404	LMG	C34-C35-C36-C37
33	b	620	LMG	C31-C32-C33-C34
26	1	609	CLA	C5-C6-C7-C8
26	R	304	CLA	CAA-CBA-CGA-O1A
35	C	517	DGD	O1B-C1B-C2B-C3B
34	d	408	LHG	C32-C33-C34-C35
26	B	604	CLA	CAA-CBA-CGA-O2A
26	b	604	CLA	CAA-CBA-CGA-O2A
26	c	505	CLA	CAA-CBA-CGA-O2A
33	b	620	LMG	O8-C28-C29-C30
34	c	520	LHG	O8-C23-C24-C25
33	D	406	LMG	C34-C35-C36-C37
33	D	413	LMG	C13-C14-C15-C16
26	C	508	CLA	C2A-CAA-CBA-CGA
38	1	612	KC2	CAA-CBA-CGA-O1A
26	4	303	CLA	CAA-CBA-CGA-O2A
26	4	304	CLA	CAA-CBA-CGA-O2A
26	O	605	CLA	CAA-CBA-CGA-O2A
26	Q	302	CLA	CAA-CBA-CGA-O2A
34	a	409	LHG	O8-C23-C24-C25
26	B	606	CLA	C10-C11-C12-C13
26	B	607	CLA	C13-C15-C16-C17
26	B	615	CLA	C10-C11-C12-C13
35	c	519	DGD	O1B-C1B-C2B-C3B
26	B	613	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	d	407	PL9	C35-C34-C36-C37
33	d	411	LMG	C13-C14-C15-C16
26	B	608	CLA	C11-C10-C8-C7
26	B	614	CLA	C11-C10-C8-C7
26	C	511	CLA	C11-C10-C8-C7
26	C	512	CLA	C3A-C2A-CAA-CBA
26	b	608	CLA	C11-C10-C8-C7
26	b	613	CLA	C6-C7-C8-C10
26	b	614	CLA	C11-C10-C8-C7
26	b	616	CLA	C11-C10-C8-C7
26	c	512	CLA	C11-C10-C8-C7
26	c	514	CLA	C12-C13-C15-C16
26	1	604	CLA	C11-C10-C8-C7
26	P	606	CLA	C6-C7-C8-C10
28	Z	101	WVN	C05-C02-C11-C19
28	a	406	WVN	C05-C02-C11-C19
26	5	601	CLA	CAA-CBA-CGA-O1A
26	2	312	CLA	CAA-CBA-CGA-O1A
26	3	309	CLA	CAA-CBA-CGA-O1A
26	O	612	CLA	CAA-CBA-CGA-O1A
26	P	611	CLA	CAA-CBA-CGA-O1A
26	5	601	CLA	CAA-CBA-CGA-O2A
26	Q	303	CLA	CAA-CBA-CGA-O2A
26	R	302	CLA	CAA-CBA-CGA-O2A
34	C	501	LHG	O8-C23-C24-C25
34	2	321	LHG	O7-C7-C8-C9
34	G	403	LHG	O7-C7-C8-C9
28	5	617	WVN	C20-C23-C25-C28
28	S	613	WVN	C20-C23-C25-C28
26	b	601	CLA	CAA-CBA-CGA-O1A
26	R	302	CLA	CAA-CBA-CGA-O1A
34	a	409	LHG	O10-C23-C24-C25
34	2	321	LHG	O9-C7-C8-C9
34	G	403	LHG	O9-C7-C8-C9
28	D	412	WVN	C22-C26-C29-C31
28	c	518	WVN	C32-C36-C39-C40
39	N	620	II0	C26-C30-C32-C34
39	2	315	II0	C26-C30-C32-C34
40	O	616	IHT	C33-C37-C40-C41
26	N	614	CLA	CAA-CBA-CGA-O2A
35	c	519	DGD	C4A-C5A-C6A-C7A
26	B	601	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
26	O	605	CLA	CAA-CBA-CGA-O1A
34	C	518	LHG	O10-C23-C24-C25
34	c	520	LHG	O10-C23-C24-C25
26	C	504	CLA	CAA-CBA-CGA-O2A
26	d	402	CLA	CAA-CBA-CGA-O2A
26	1	604	CLA	CAA-CBA-CGA-O2A
26	2	304	CLA	CAA-CBA-CGA-O2A
26	O	604	CLA	CAA-CBA-CGA-O2A
26	b	615	CLA	C10-C11-C12-C13
26	6	606	CLA	CAA-CBA-CGA-O1A
26	S	606	CLA	CAA-CBA-CGA-O1A
34	C	501	LHG	O10-C23-C24-C25
26	c	515	CLA	C2A-CAA-CBA-CGA
26	5	608	CLA	C2A-CAA-CBA-CGA
26	R	309	CLA	C2A-CAA-CBA-CGA
34	R	319	LHG	C16-C17-C18-C19
26	4	304	CLA	CAA-CBA-CGA-O1A
26	D	404	CLA	CAA-CBA-CGA-O2A
26	1	613	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

301 monomers are involved in 1707 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	N	619	IHT	16	0
30	A	408	SQD	1	0
26	3	302	CLA	9	0
26	C	509	CLA	3	0
26	g	402	CLA	18	0
26	N	601	CLA	24	0
26	O	612	CLA	3	0
35	h	101	DGD	6	0
28	H	101	WVN	1	0
38	2	310	KC2	7	0
26	P	602	CLA	8	0
34	C	518	LHG	3	0
26	4	312	CLA	10	0
26	b	616	CLA	2	0
26	S	603	CLA	2	0
26	C	502	CLA	1	0
39	5	613	II0	2	0
26	P	608	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	O	609	CLA	1	0
33	5	619	LMG	20	0
26	1	614	CLA	4	0
33	A	412	LMG	1	0
39	Q	319	II0	10	0
28	P	615	WVN	3	0
40	R	317	IHT	4	0
26	3	308	CLA	8	0
38	P	605	KC2	1	0
26	2	312	CLA	6	0
26	2	319	CLA	26	0
39	Q	314	II0	4	0
26	O	601	CLA	25	0
34	2	321	LHG	23	0
26	R	310	CLA	2	0
39	N	616	II0	16	0
26	2	306	CLA	4	0
26	Q	305	CLA	6	0
26	Q	307	CLA	9	0
33	c	522	LMG	2	0
26	S	602	CLA	2	0
40	O	616	IHT	9	0
26	B	603	CLA	3	0
26	O	606	CLA	4	0
26	R	312	CLA	6	0
26	c	507	CLA	2	0
39	S	611	II0	11	0
39	P	614	II0	4	0
26	C	504	CLA	4	0
38	1	610	KC2	1	0
33	2	318	LMG	5	0
26	C	506	CLA	4	0
26	c	505	CLA	4	0
35	c	519	DGD	2	0
38	5	610	KC2	3	0
26	2	302	CLA	10	0
26	G	401	CLA	7	0
26	Q	306	CLA	8	0
26	4	306	CLA	45	0
26	D	407	CLA	7	0
33	D	411	LMG	2	0
26	2	305	CLA	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	Q	301	CLA	11	0
26	4	302	CLA	11	0
26	b	601	CLA	1	0
26	g	401	CLA	7	0
40	2	317	IHT	21	0
33	b	620	LMG	1	0
26	Q	308	CLA	10	0
38	4	310	KC2	12	0
27	D	405	PHO	5	0
39	2	315	II0	13	0
26	O	605	CLA	13	0
39	5	615	II0	4	0
26	O	604	CLA	2	0
30	c	501	SQD	1	0
40	5	616	IHT	1	0
29	d	407	PL9	3	0
37	f	101	HEM	1	0
39	6	611	II0	1	0
26	b	608	CLA	1	0
26	6	605	CLA	5	0
26	A	405	CLA	2	0
26	a	402	CLA	11	0
38	N	612	KC2	28	0
26	4	303	CLA	36	0
26	6	610	CLA	6	0
26	D	404	CLA	3	0
26	5	602	CLA	6	0
26	P	609	CLA	1	0
26	5	608	CLA	10	0
39	P	613	II0	6	0
26	O	602	CLA	8	0
33	D	413	LMG	1	0
26	S	609	CLA	9	0
26	b	611	CLA	5	0
35	H	102	DGD	4	0
26	N	606	CLA	21	0
26	b	609	CLA	4	0
38	Q	309	KC2	12	0
26	S	601	CLA	6	0
27	a	404	PHO	2	0
27	d	403	PHO	5	0
34	G	403	LHG	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	S	605	CLA	5	0
26	b	606	CLA	5	0
39	5	614	II0	1	0
33	Q	318	LMG	2	0
26	d	406	CLA	1	0
26	C	507	CLA	4	0
27	A	404	PHO	2	0
26	3	306	CLA	6	0
26	c	509	CLA	3	0
26	B	616	CLA	1	0
38	4	305	KC2	6	0
26	P	611	CLA	3	0
26	Q	311	CLA	9	0
26	d	405	CLA	8	0
33	C	520	LMG	3	0
33	R	301	LMG	9	0
39	4	314	II0	6	0
34	5	618	LHG	8	0
26	B	611	CLA	4	0
26	c	514	CLA	2	0
26	S	604	CLA	5	0
26	N	602	CLA	7	0
34	1	620	LHG	48	0
33	d	411	LMG	2	0
26	B	605	CLA	8	0
26	R	302	CLA	6	0
38	N	605	KC2	6	0
39	3	311	II0	26	0
26	C	503	CLA	4	0
26	P	607	CLA	3	0
28	b	617	WVN	1	0
39	2	314	II0	5	0
26	R	304	CLA	1	0
26	c	504	CLA	5	0
26	6	606	CLA	4	0
26	6	601	CLA	8	0
39	N	618	II0	2	0
26	R	306	CLA	21	0
26	c	515	CLA	2	0
34	D	410	LHG	5	0
26	B	607	CLA	2	0
34	D	403	LHG	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	2	303	CLA	19	0
26	P	606	CLA	5	0
26	B	604	CLA	3	0
26	B	601	CLA	1	0
33	m	101	LMG	2	0
26	A	403	CLA	2	0
26	P	604	CLA	3	0
33	4	319	LMG	5	0
26	5	609	CLA	2	0
26	A	402	CLA	10	0
39	4	315	II0	9	0
33	M	101	LMG	1	0
26	2	301	CLA	31	0
26	b	602	CLA	3	0
28	C	516	WVN	2	0
26	b	615	CLA	6	0
26	1	609	CLA	5	0
26	C	514	CLA	2	0
26	3	303	CLA	5	0
26	S	606	CLA	4	0
39	O	615	II0	8	0
38	O	610	KC2	7	0
39	R	315	II0	1	0
26	O	607	CLA	19	0
26	a	403	CLA	4	0
26	6	602	CLA	1	0
39	O	614	II0	6	0
26	c	503	CLA	2	0
37	F	101	HEM	2	0
26	b	605	CLA	7	0
39	3	312	II0	8	0
26	N	607	CLA	19	0
26	d	402	CLA	4	0
26	Q	303	CLA	1	0
26	N	608	CLA	3	0
38	1	611	KC2	3	0
39	2	320	II0	4	0
38	3	304	KC2	1	0
26	2	307	CLA	13	0
26	c	508	CLA	4	0
30	D	401	SQD	2	0
26	b	612	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	1	608	CLA	5	0
35	C	517	DGD	1	0
26	N	604	CLA	16	0
33	c	521	LMG	6	0
26	B	606	CLA	4	0
26	4	307	CLA	8	0
26	G	402	CLA	1	0
26	b	604	CLA	3	0
34	N	621	LHG	26	0
28	B	618	WVN	3	0
34	R	319	LHG	12	0
38	4	311	KC2	20	0
26	B	602	CLA	3	0
26	N	609	CLA	4	0
26	5	607	CLA	7	0
26	P	601	CLA	10	0
26	R	309	CLA	10	0
28	3	313	WVN	21	0
26	a	405	CLA	3	0
26	b	603	CLA	3	0
39	4	320	II0	29	0
26	5	605	CLA	31	0
34	L	101	LHG	7	0
26	B	608	CLA	1	0
33	d	404	LMG	4	0
40	1	619	IHT	1	0
39	R	314	II0	2	0
39	R	316	II0	4	0
26	1	606	CLA	42	0
26	1	603	CLA	8	0
33	B	620	LMG	2	0
26	b	613	CLA	8	0
26	S	607	CLA	2	0
26	6	609	CLA	24	0
38	1	612	KC2	1	0
34	d	408	LHG	5	0
26	D	408	CLA	1	0
28	B	617	WVN	3	0
26	c	510	CLA	3	0
26	b	607	CLA	2	0
34	b	621	LHG	2	0
39	P	612	II0	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	6	603	CLA	2	0
26	4	309	CLA	8	0
39	O	613	II0	12	0
26	P	610	CLA	15	0
38	N	610	KC2	5	0
33	a	413	LMG	3	0
26	b	614	CLA	3	0
26	O	603	CLA	15	0
26	C	511	CLA	6	0
26	2	311	CLA	47	0
26	R	303	CLA	9	0
26	B	615	CLA	3	0
26	C	513	CLA	2	0
39	Q	313	II0	7	0
26	2	309	CLA	1	0
40	Q	317	IHT	4	0
33	D	406	LMG	4	0
26	5	604	CLA	4	0
26	6	604	CLA	5	0
34	l	101	LHG	5	0
26	O	608	CLA	15	0
38	Q	304	KC2	6	0
26	1	604	CLA	3	0
26	4	308	CLA	12	0
26	Q	302	CLA	7	0
26	c	512	CLA	6	0
39	1	618	II0	1	0
33	d	409	LMG	2	0
39	O	618	II0	2	0
26	c	513	CLA	1	0
26	R	305	CLA	4	0
39	N	615	II0	5	0
38	Q	310	KC2	21	0
26	4	301	CLA	31	0
39	2	316	II0	5	0
26	C	508	CLA	3	0
26	5	601	CLA	6	0
26	1	607	CLA	2	0
26	5	603	CLA	1	0
39	3	310	II0	26	0
26	2	308	CLA	12	0
26	3	307	CLA	43	0

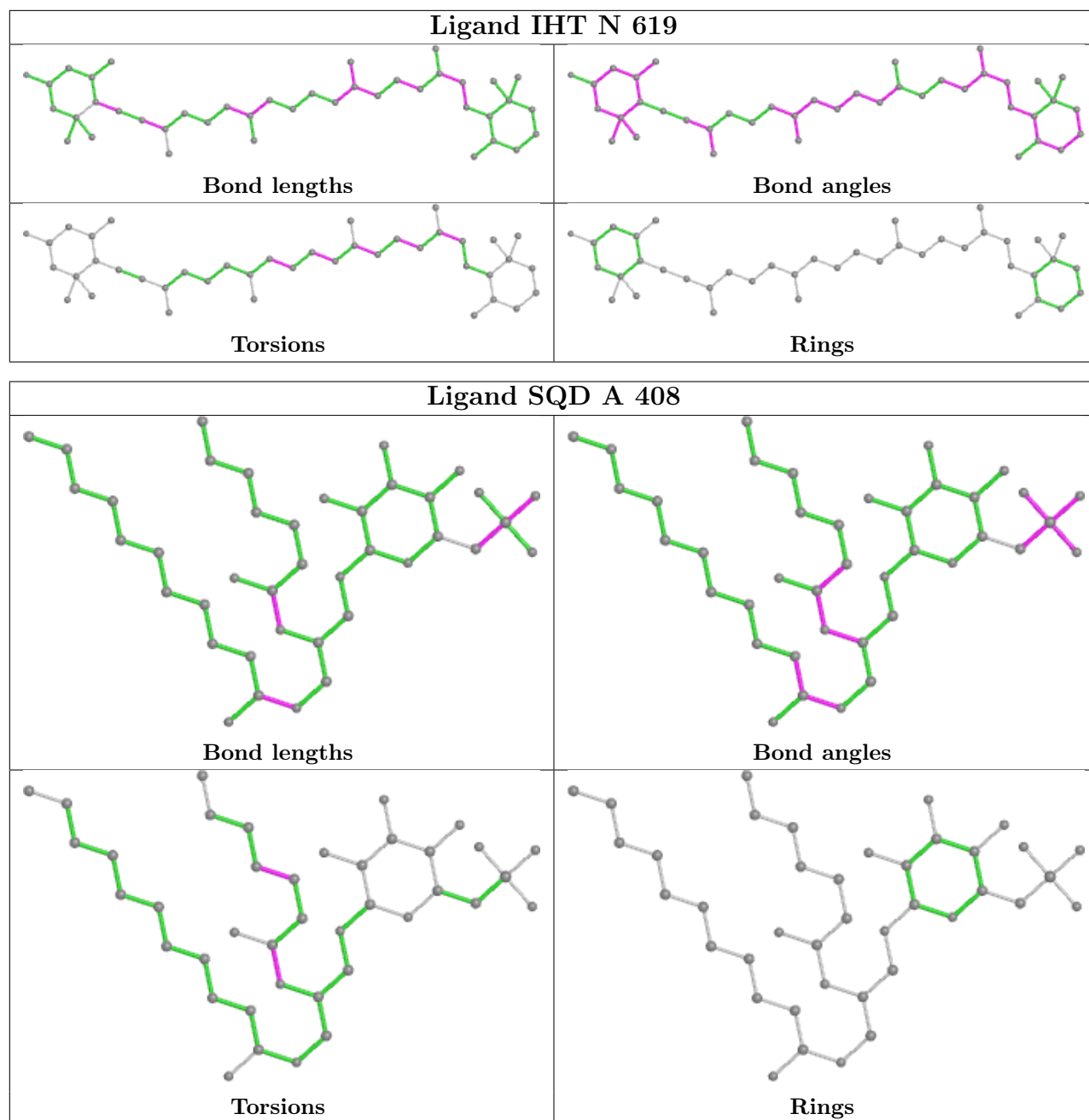
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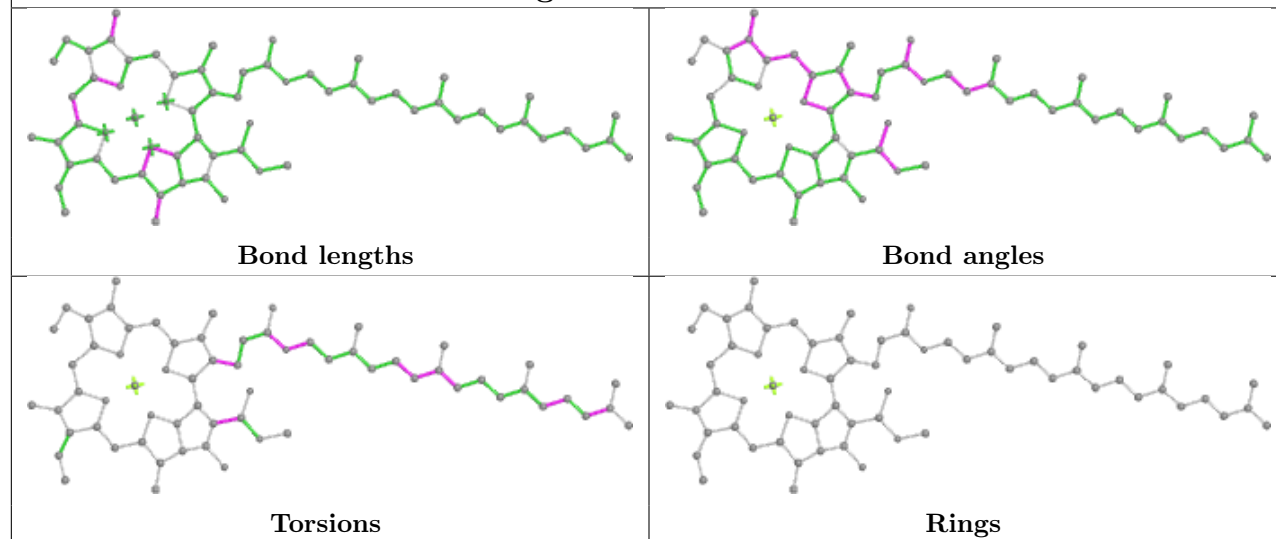
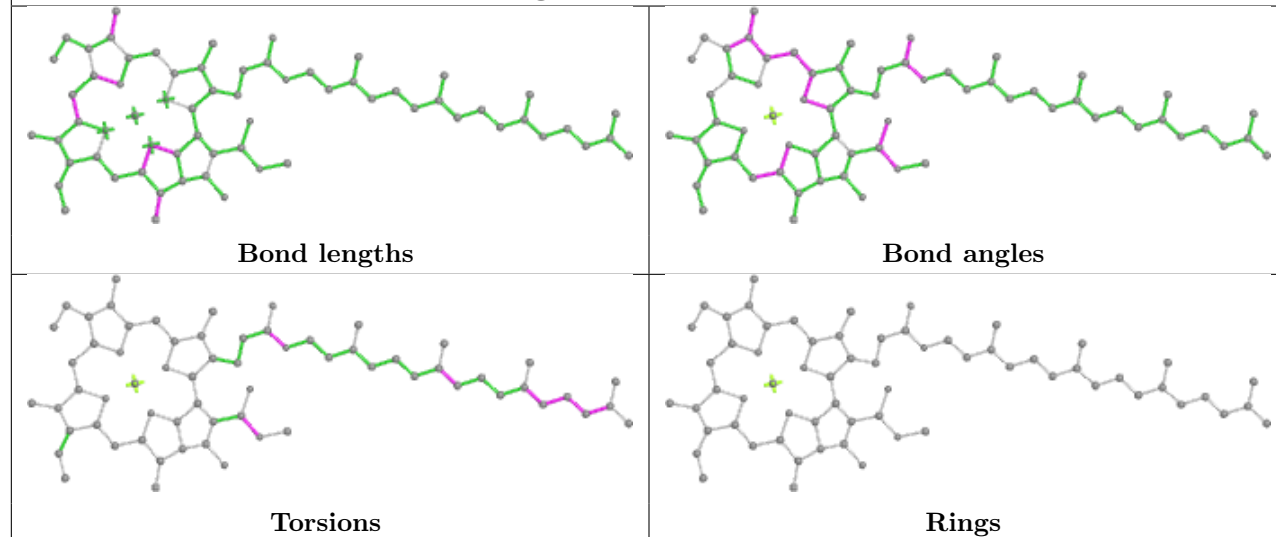
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	4	304	CLA	1	0
26	b	610	CLA	5	0
26	3	309	CLA	2	0
26	R	308	CLA	11	0
26	S	610	CLA	4	0
26	B	612	CLA	7	0
39	4	317	II0	4	0
29	D	409	PL9	3	0
33	O	617	LMG	5	0
26	B	614	CLA	2	0
26	P	603	CLA	5	0
26	B	613	CLA	6	0
26	2	304	CLA	4	0
26	3	305	CLA	7	0
26	B	609	CLA	5	0
29	A	407	PL9	6	0
39	N	617	II0	5	0
26	O	611	CLA	12	0
26	N	614	CLA	26	0
26	N	613	CLA	3	0
39	Q	316	II0	5	0
26	B	610	CLA	7	0
26	3	301	CLA	12	0
26	C	512	CLA	3	0
38	R	311	KC2	3	0
26	5	611	CLA	35	0
39	2	313	II0	6	0
34	c	520	LHG	1	0
39	N	620	II0	11	0
40	4	318	IHT	5	0
26	N	603	CLA	13	0

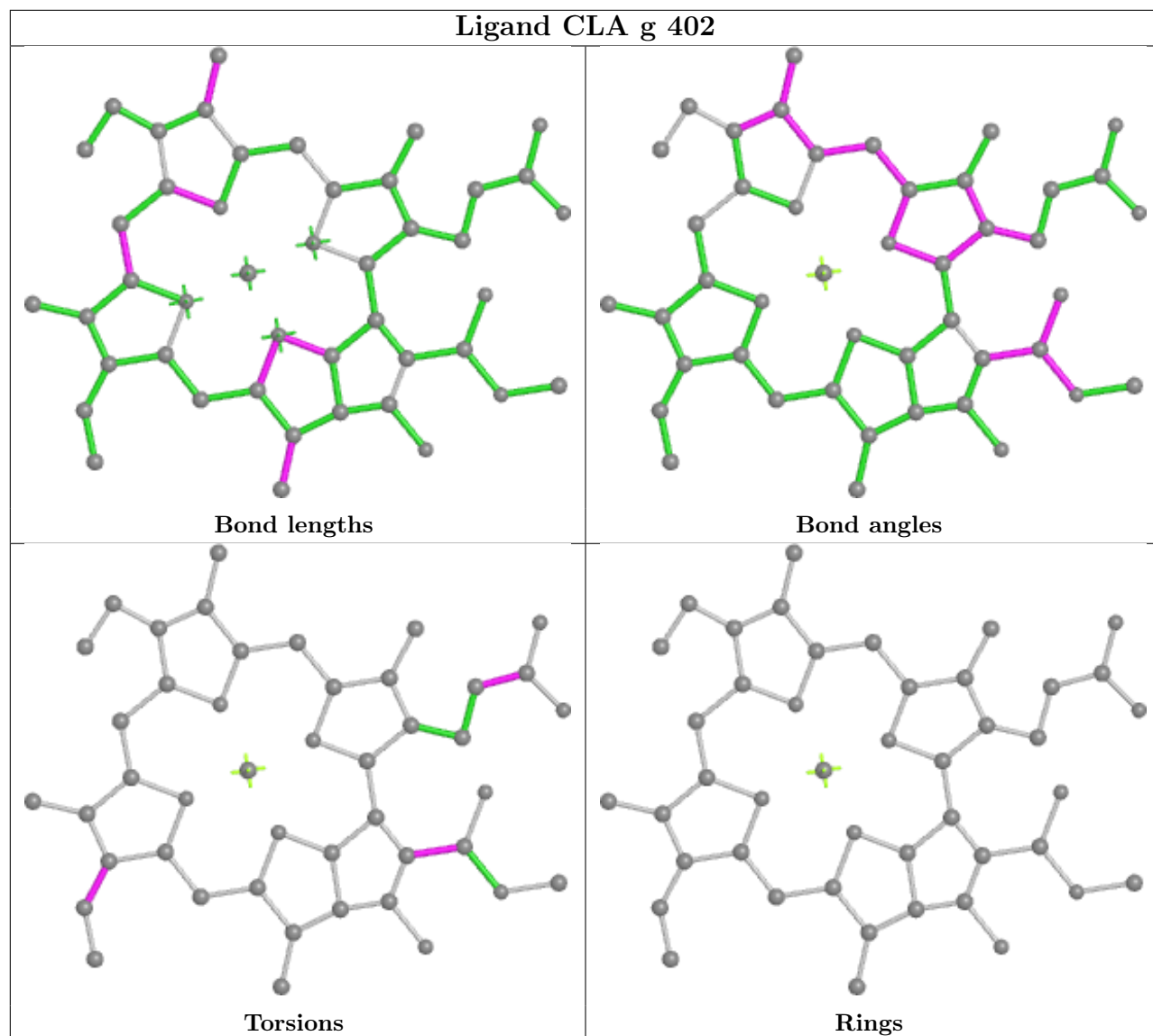
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

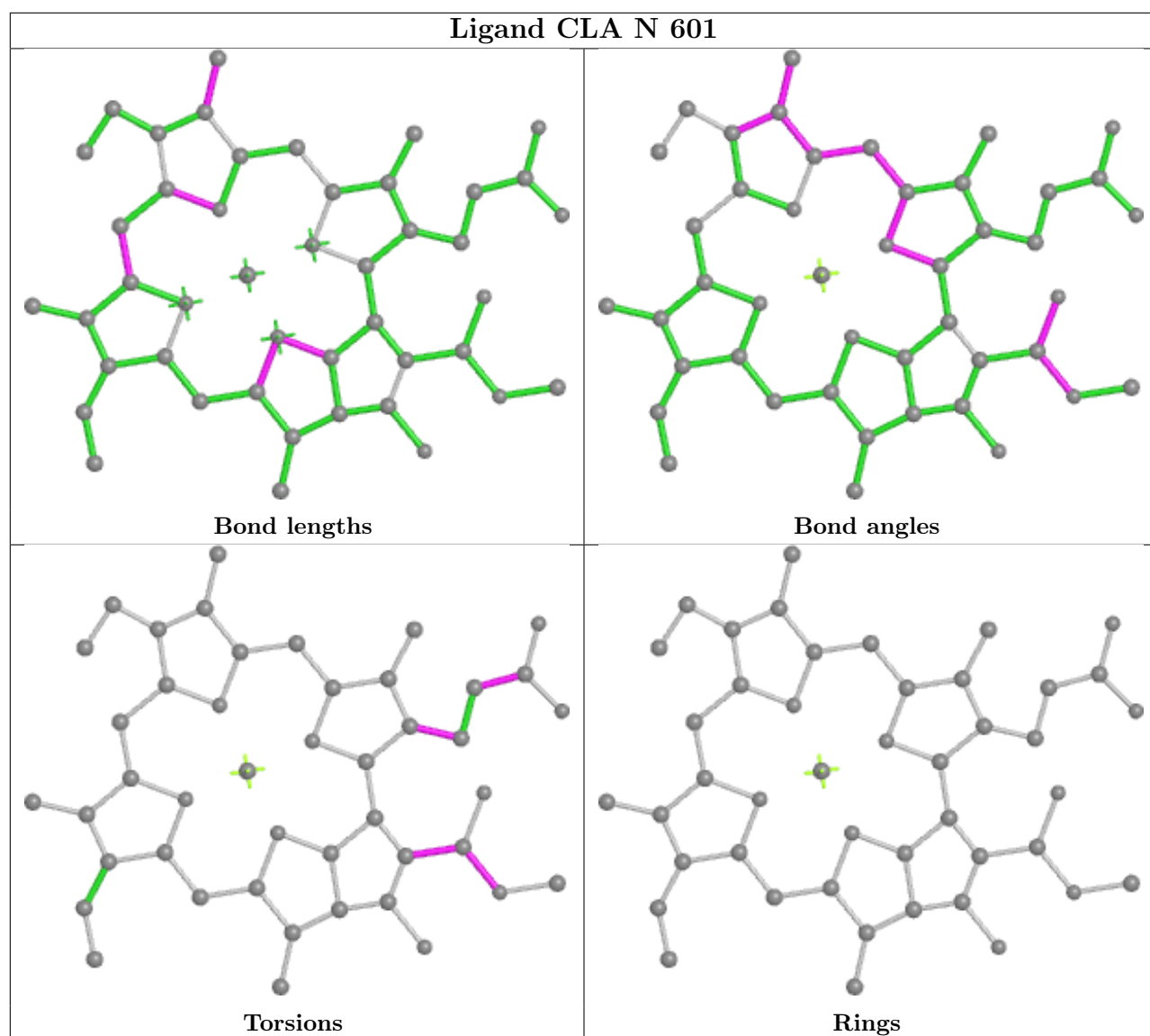
equivalents in the CSD to analyse the geometry.



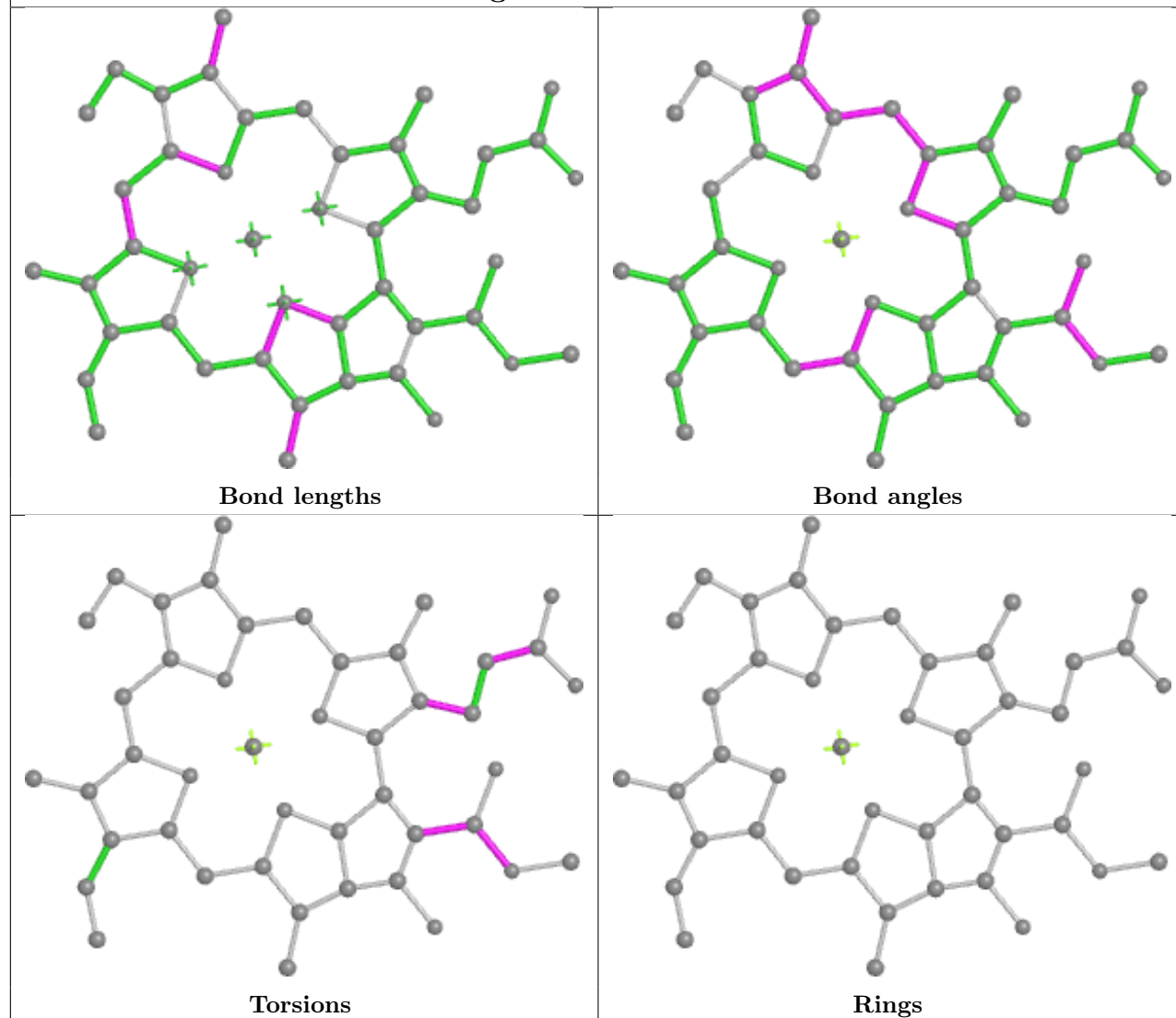
Ligand CLA 3 302**Ligand CLA C 509**

Ligand CLA g 402

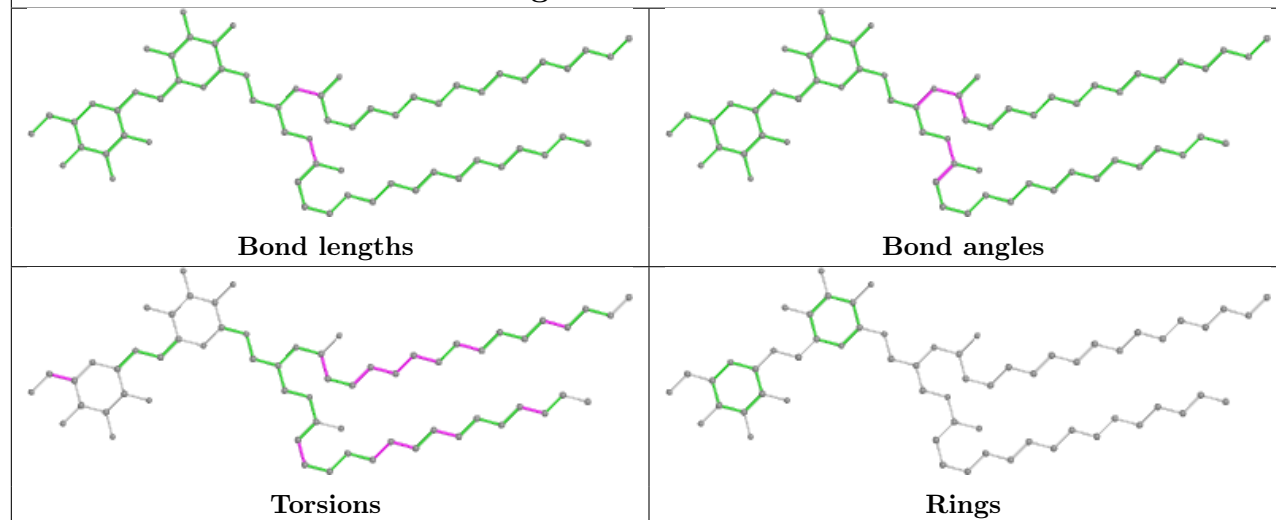


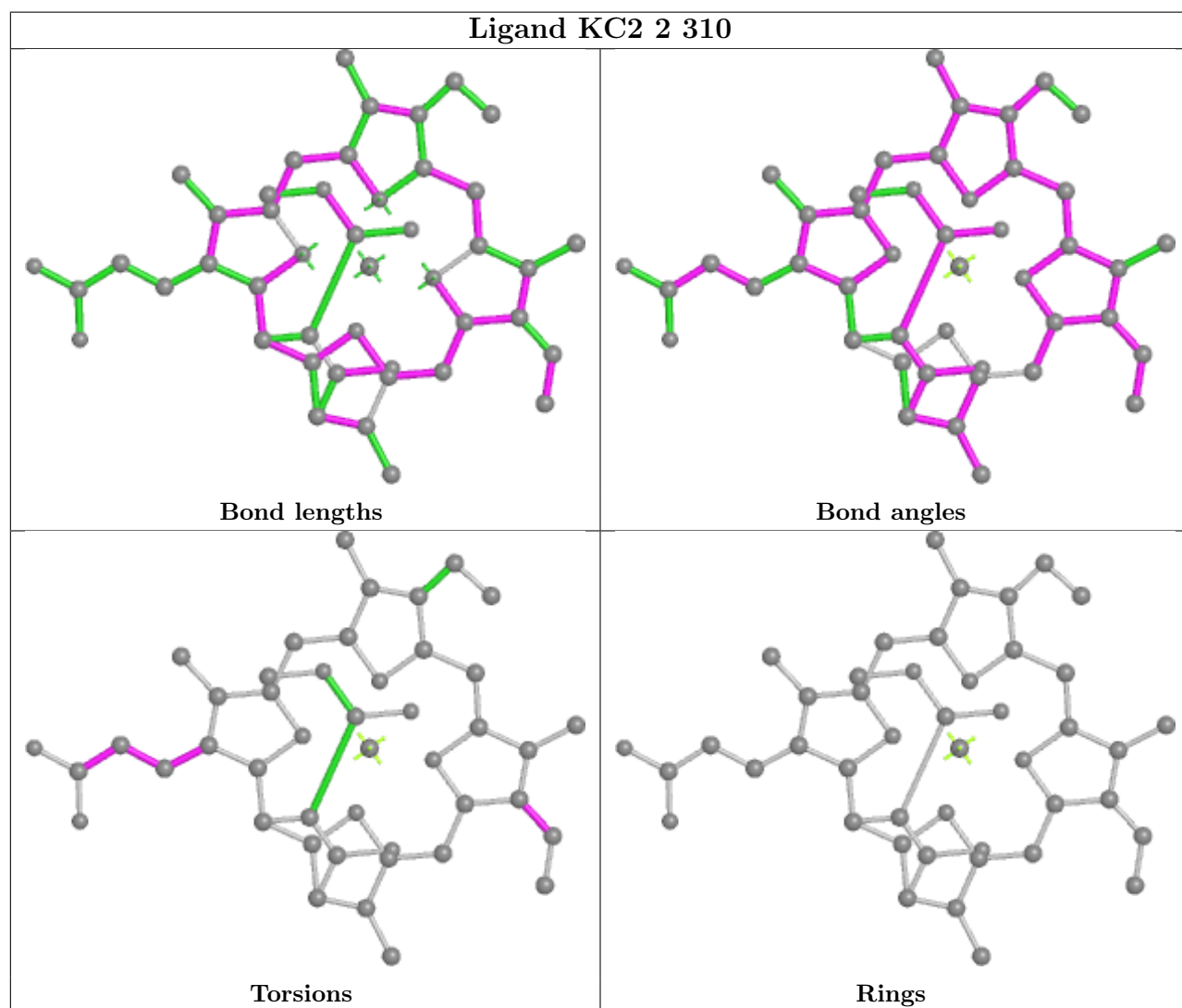
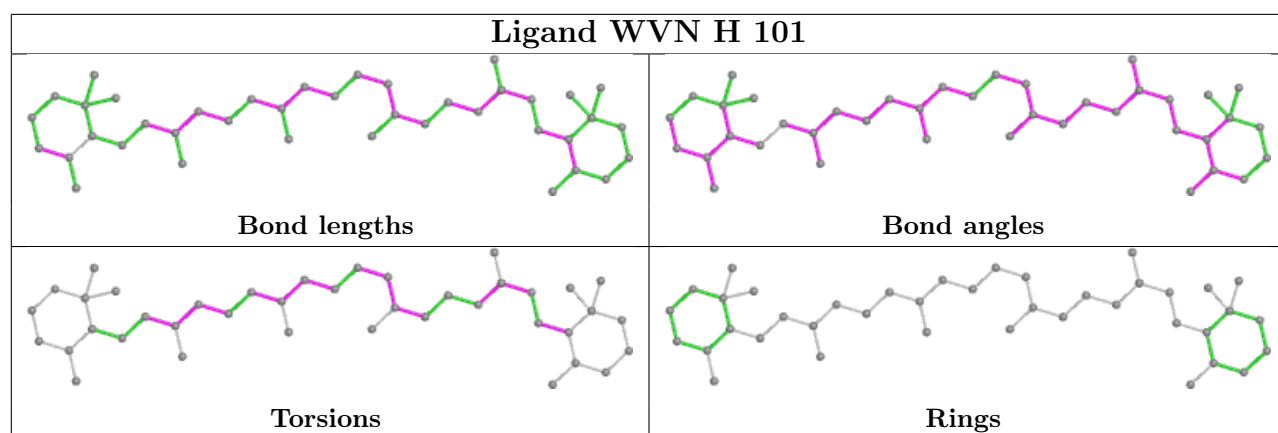


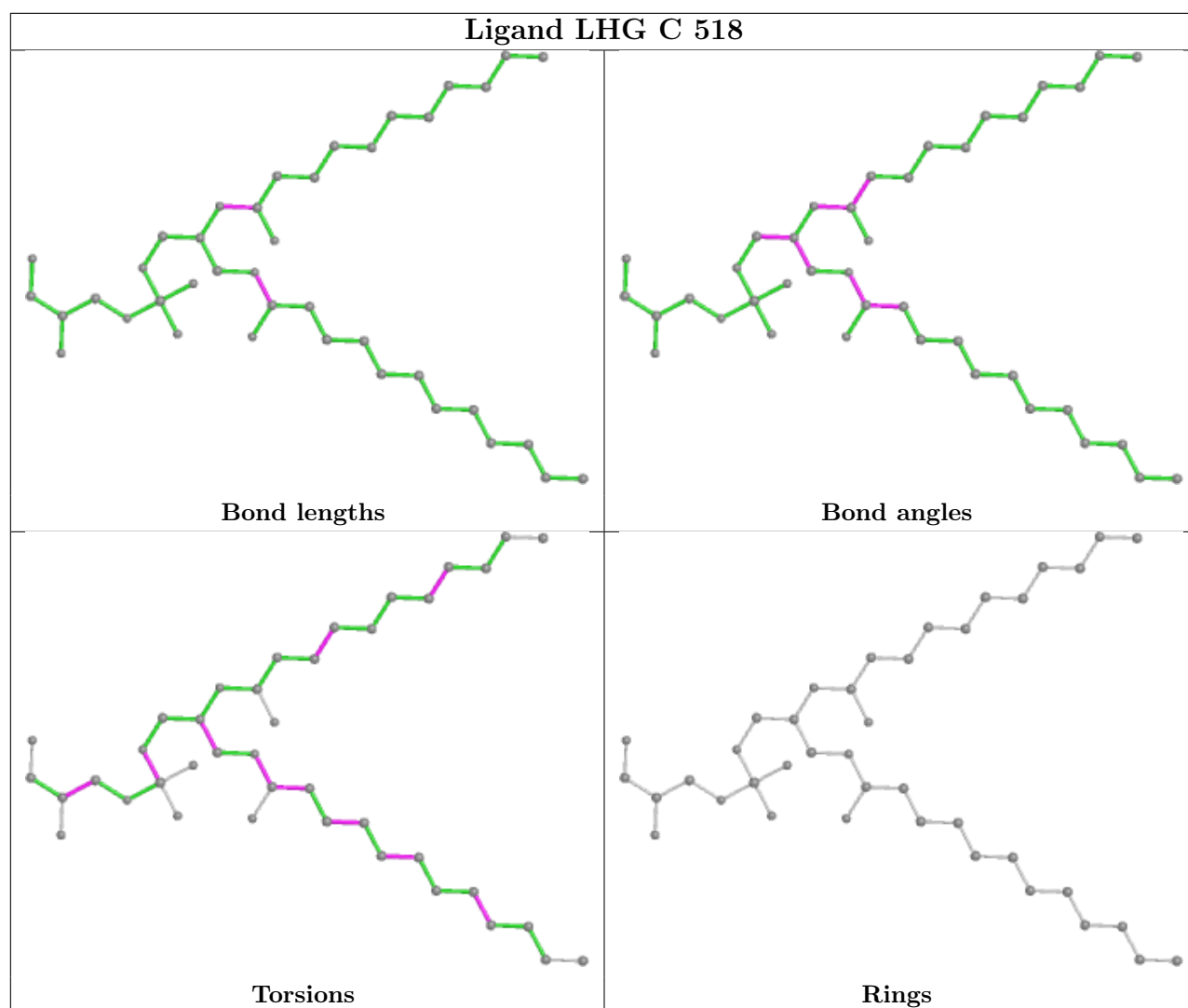
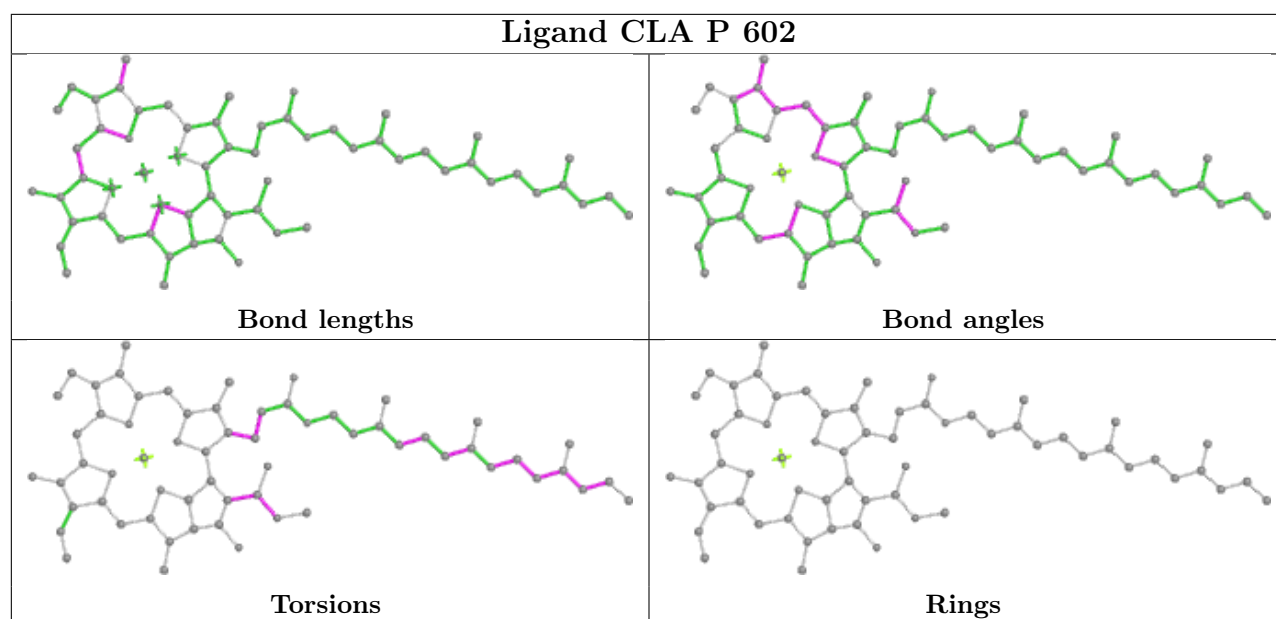
Ligand CLA O 612



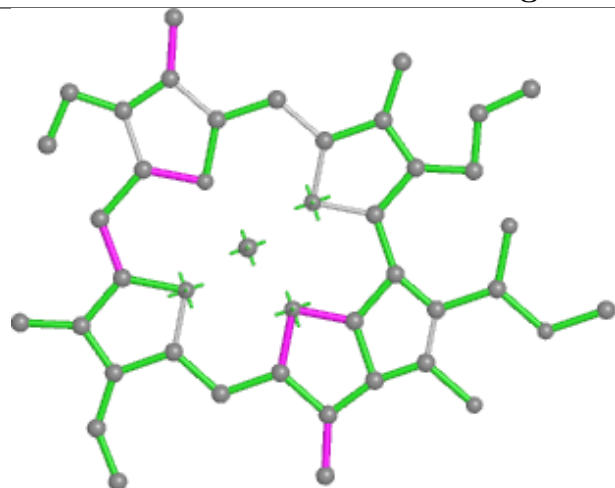
Ligand DGD h 101



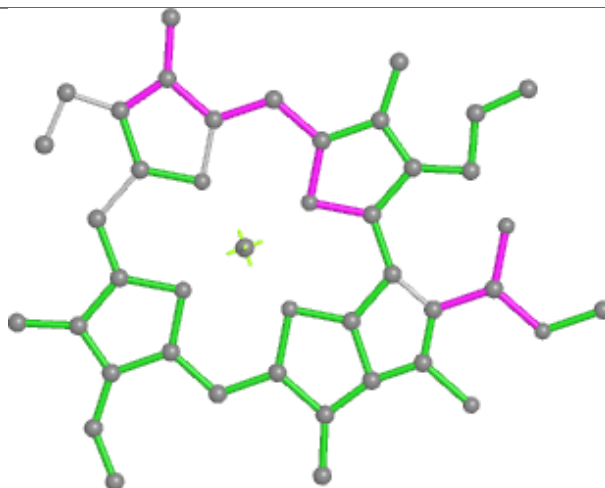




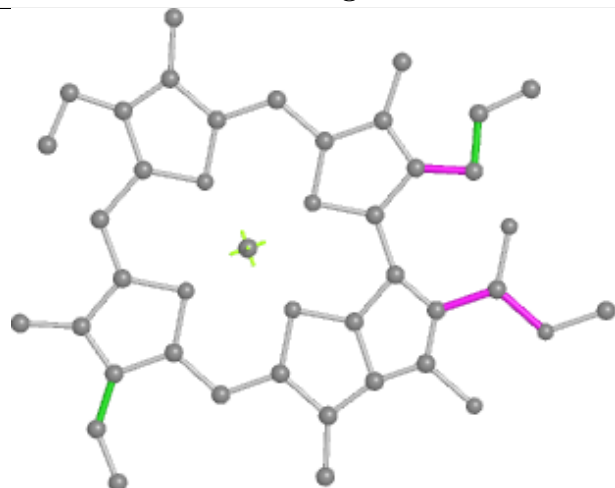
Ligand CLA 4 312



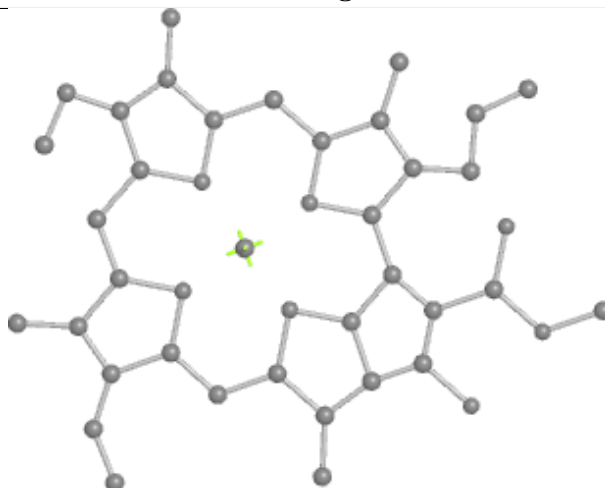
Bond lengths



Bond angles

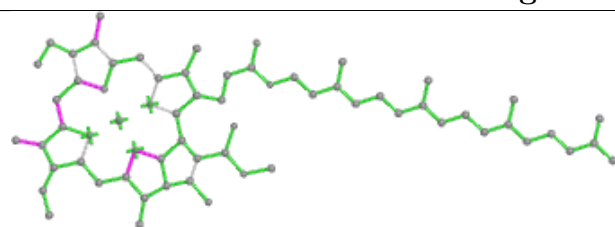


Torsions

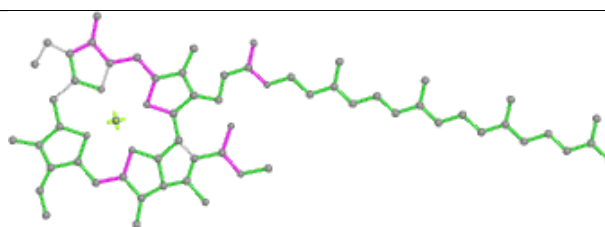


Rings

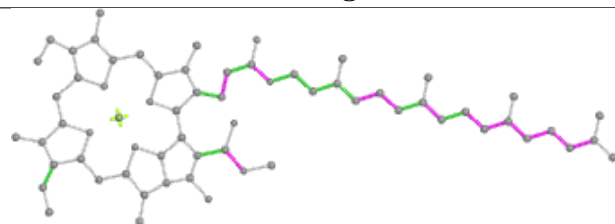
Ligand CLA b 616



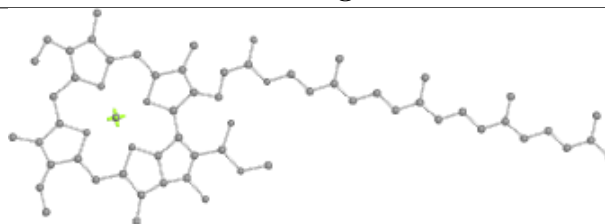
Bond lengths



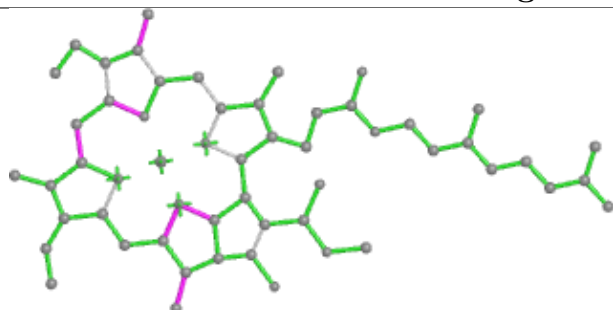
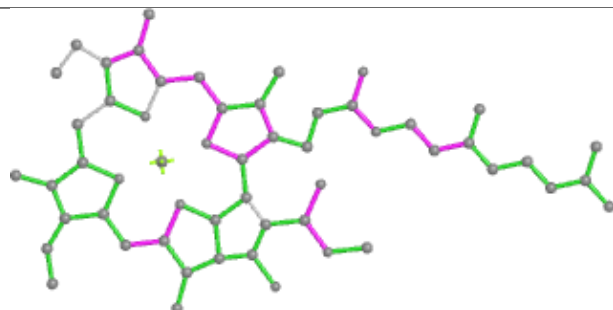
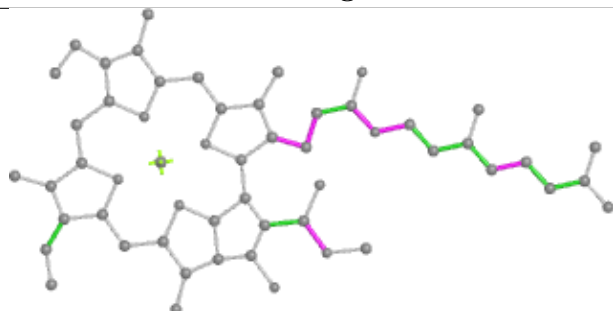
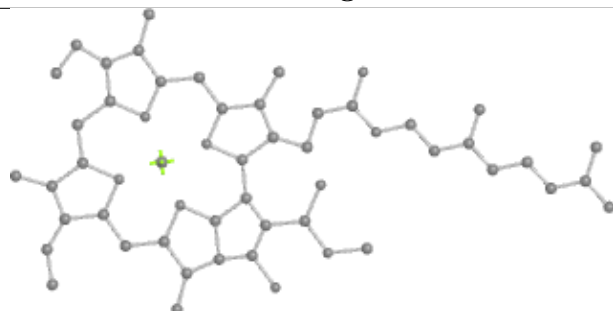
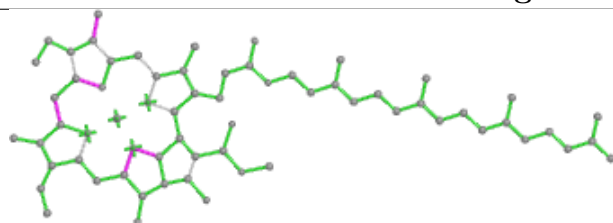
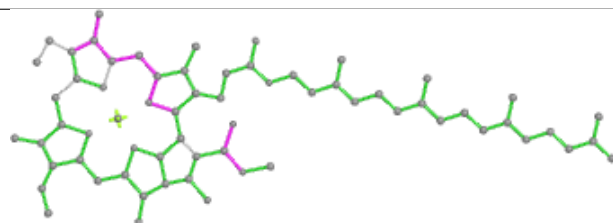
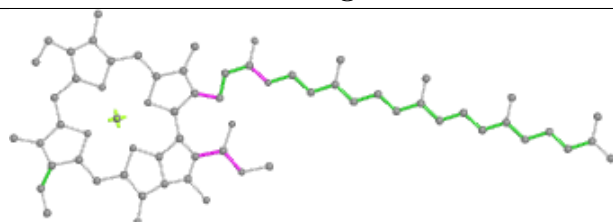
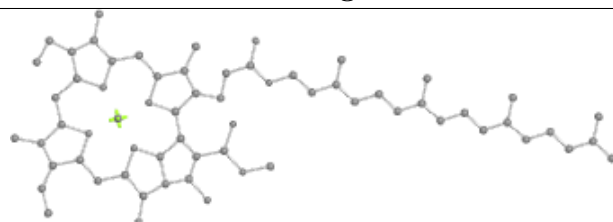
Bond angles



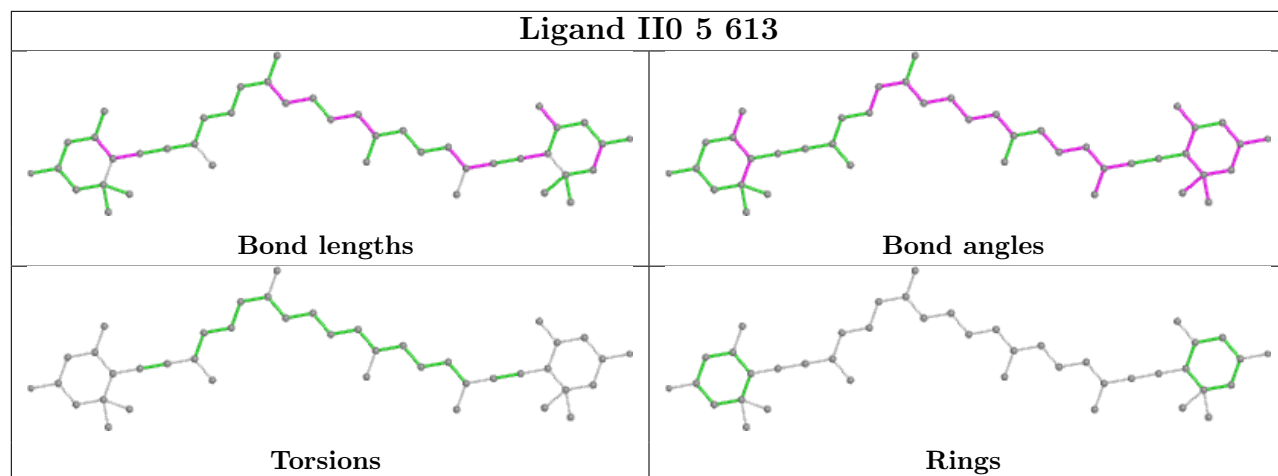
Torsions



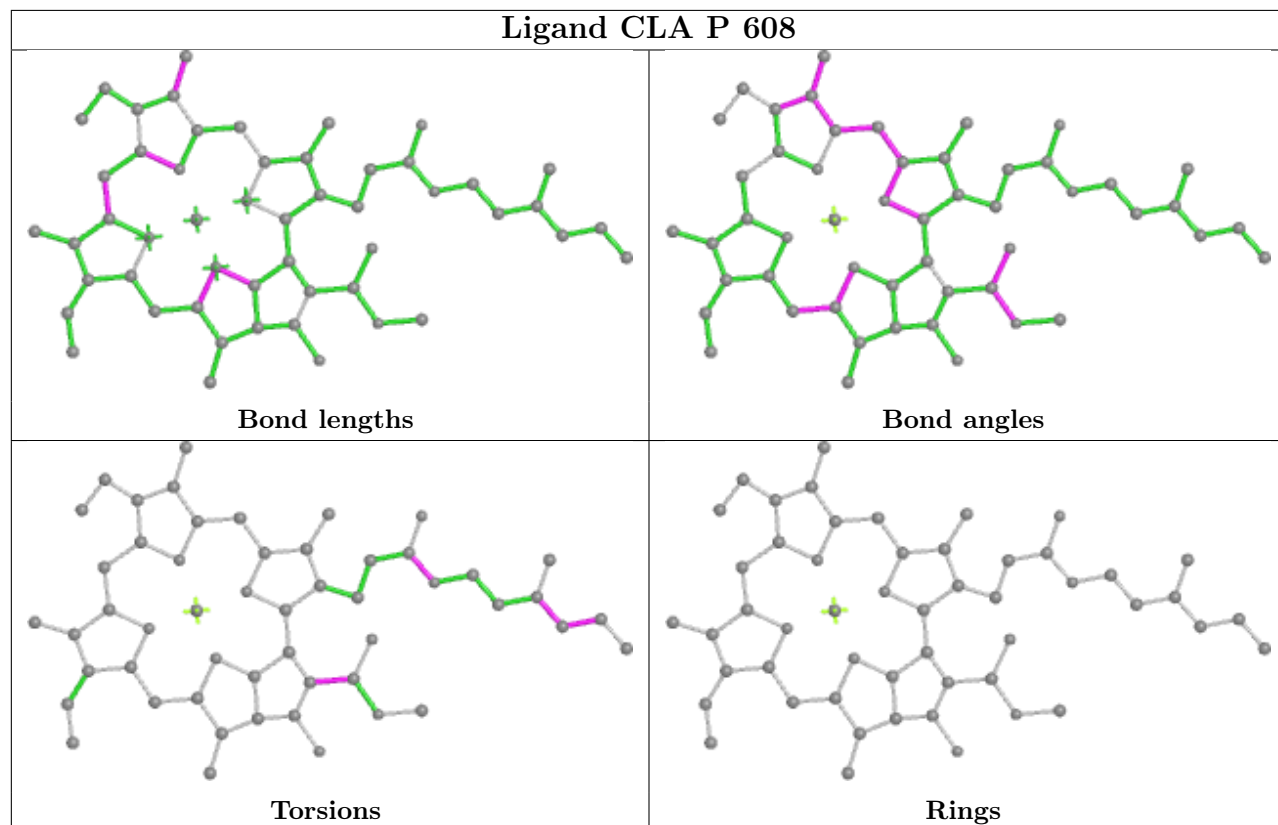
Rings

Ligand CLA S 603**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA C 502****Bond lengths****Bond angles****Torsions****Rings**

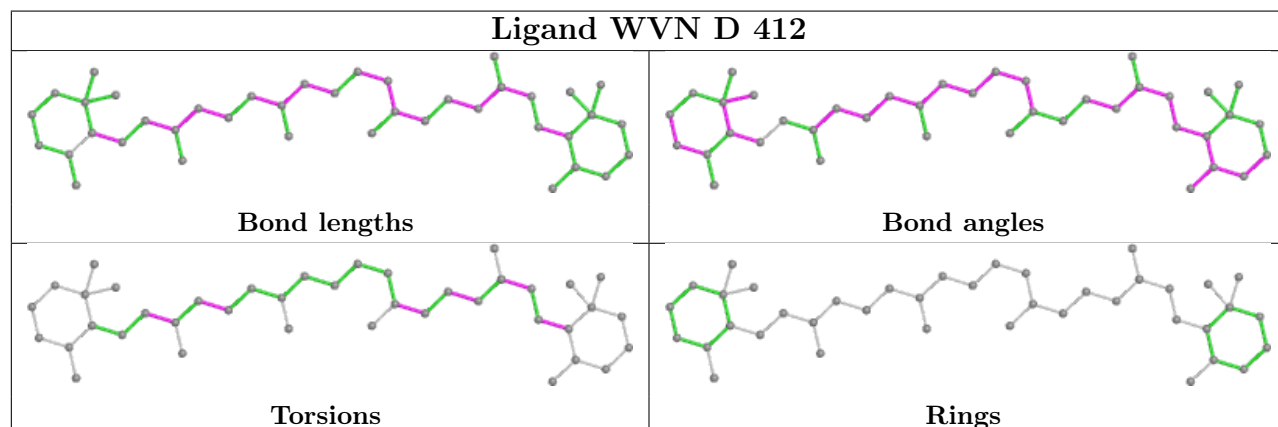
Ligand II0 5 613

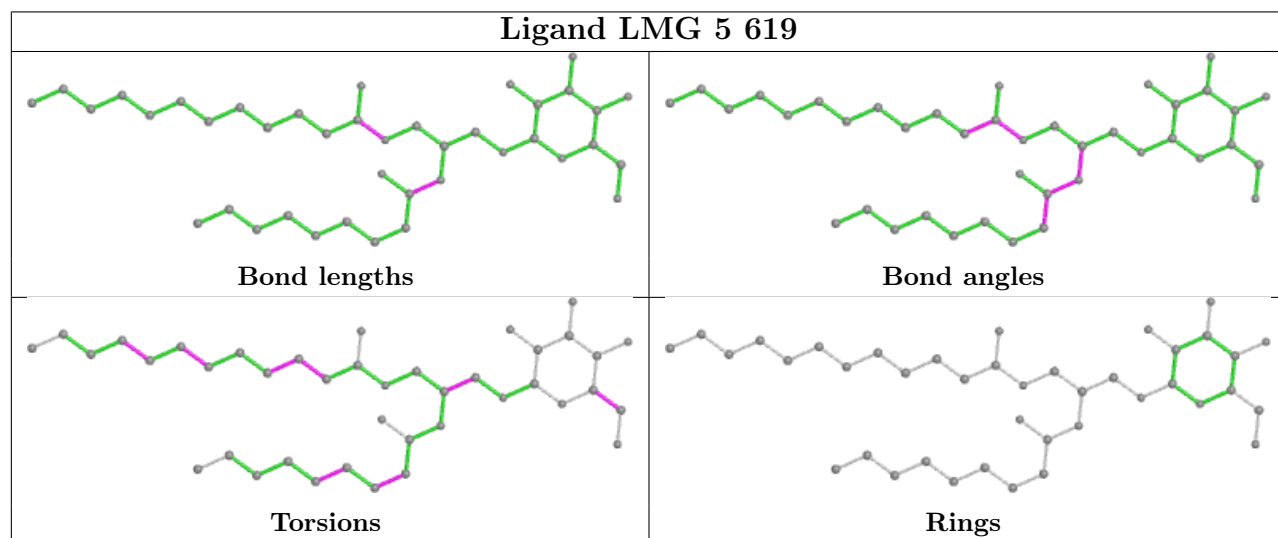
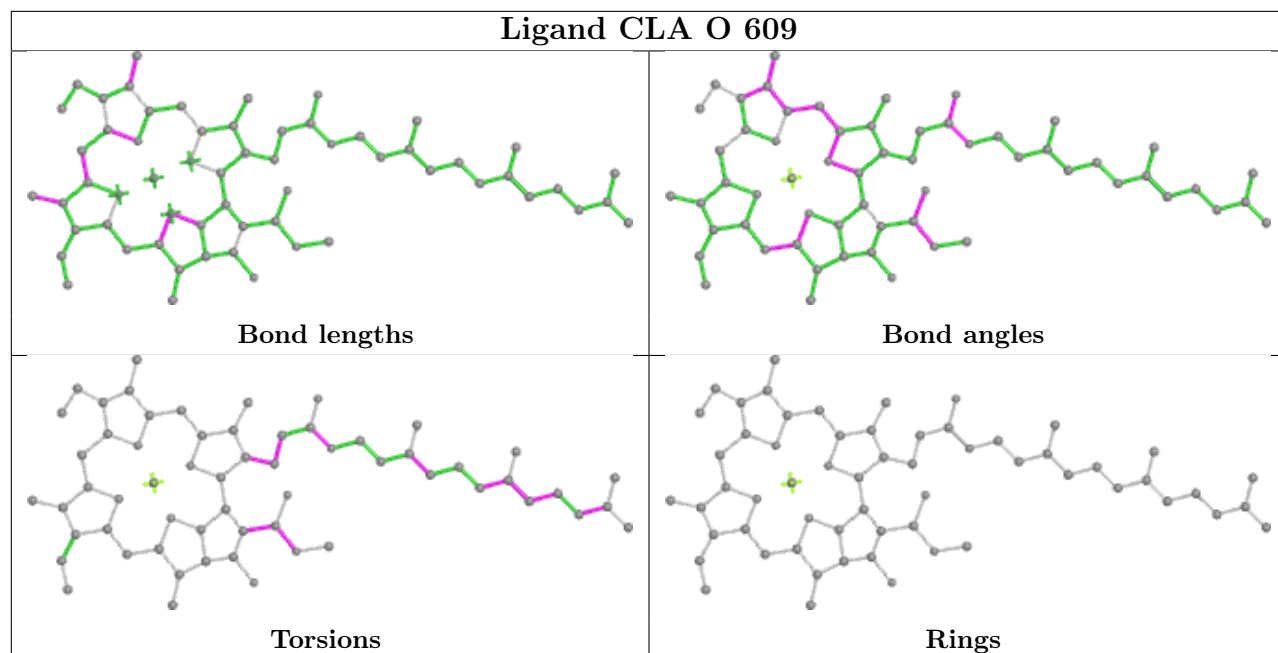


Ligand CLA P 608

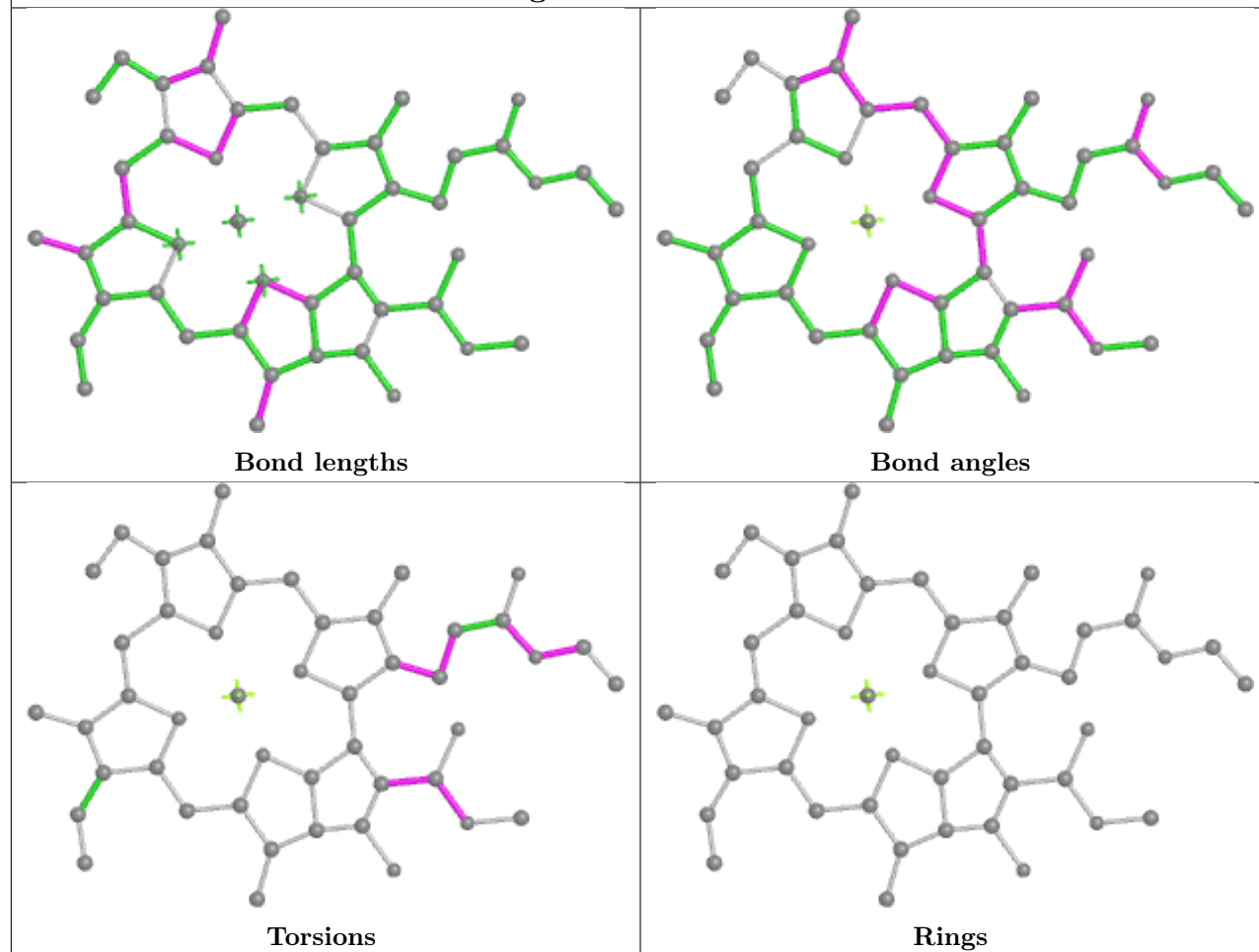


Ligand WVN D 412

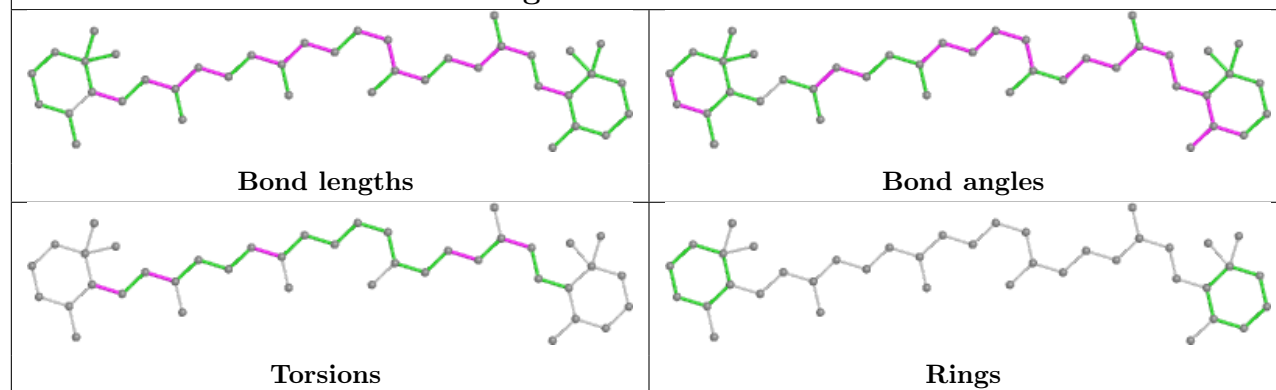


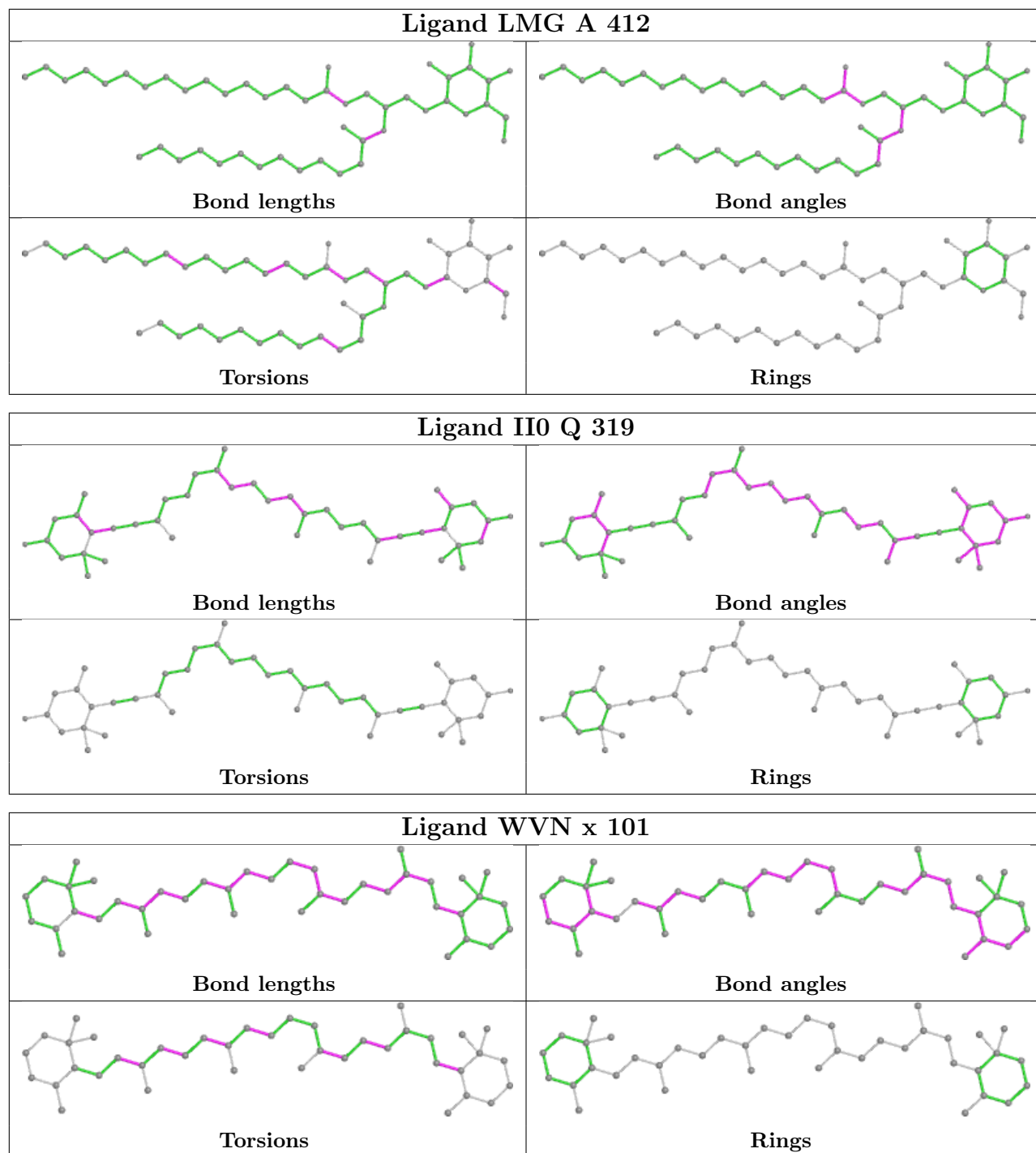


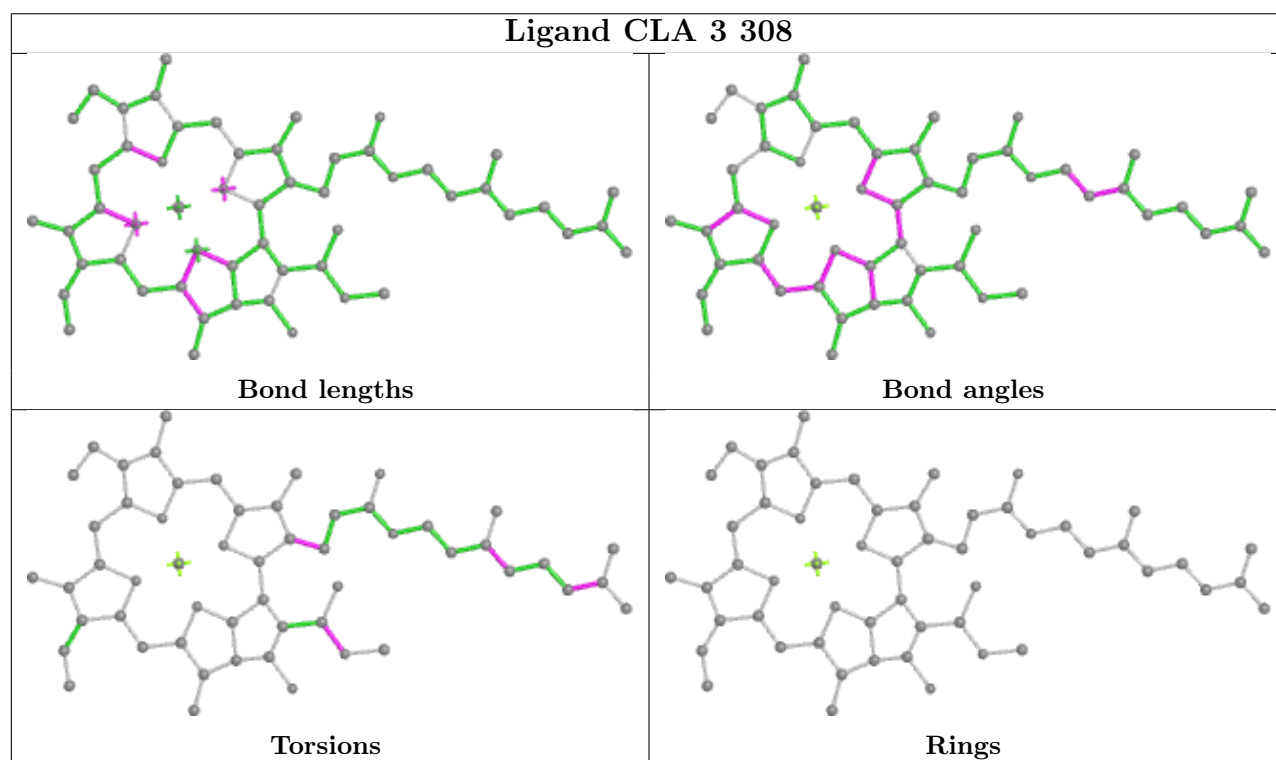
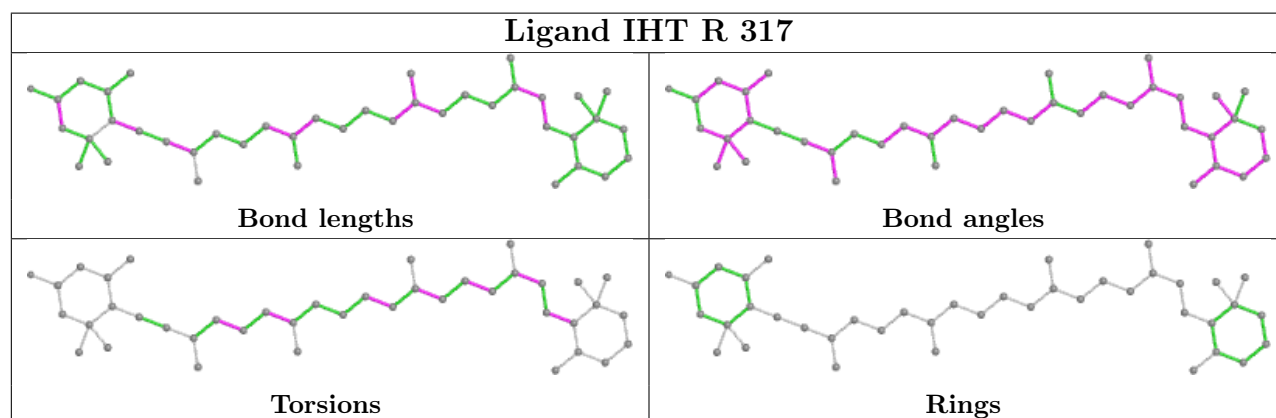
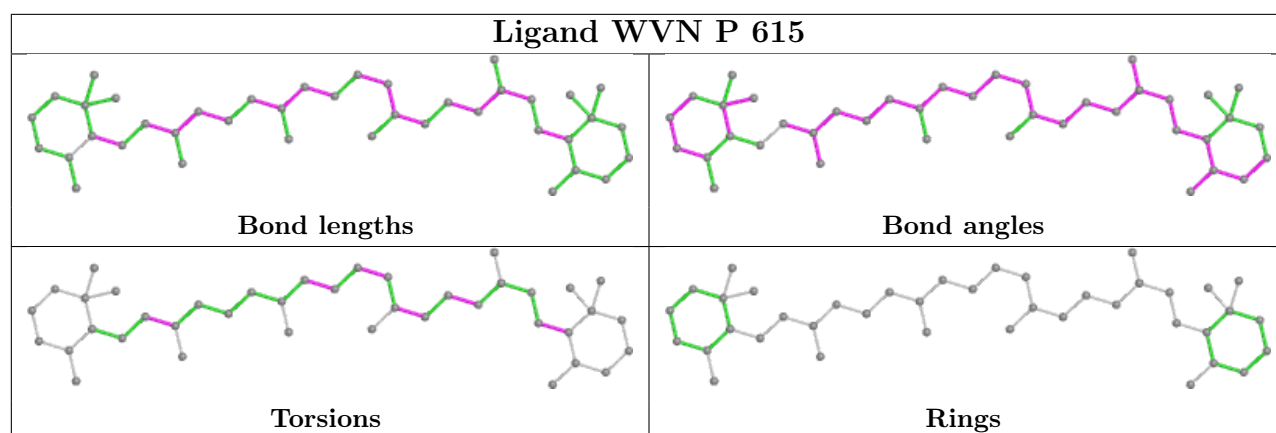
Ligand CLA 1 614



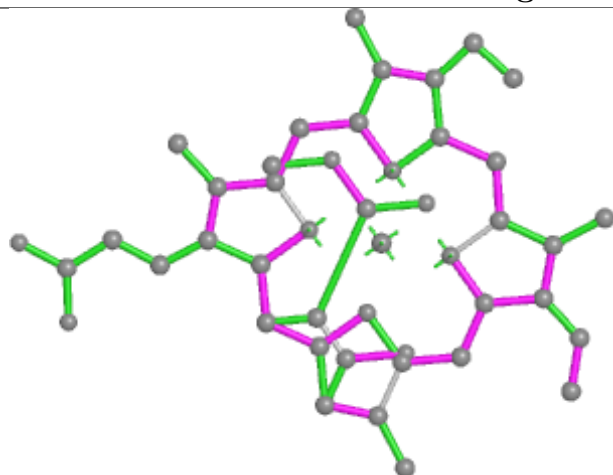
Ligand WVN Y 101



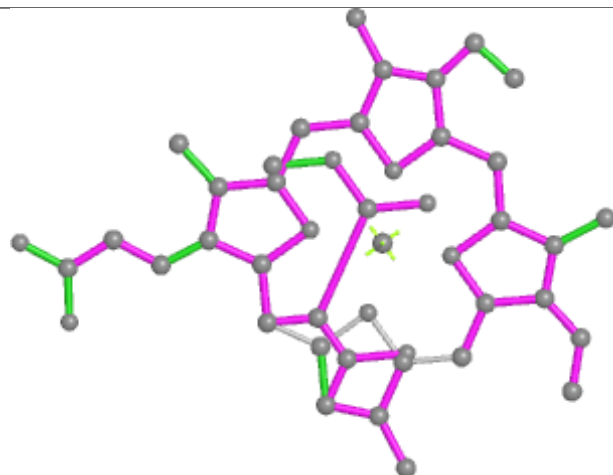




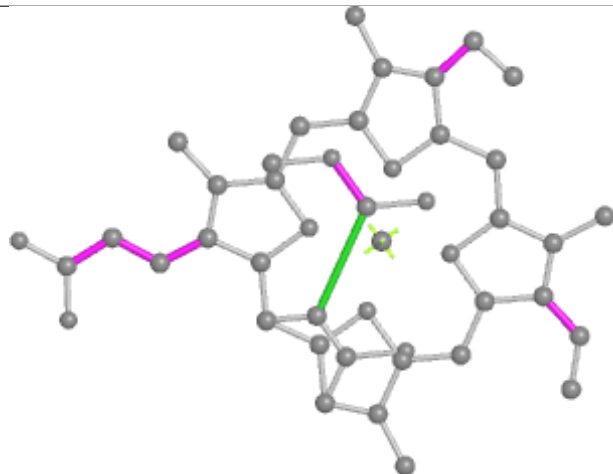
Ligand KC2 P 605



Bond lengths



Bond angles

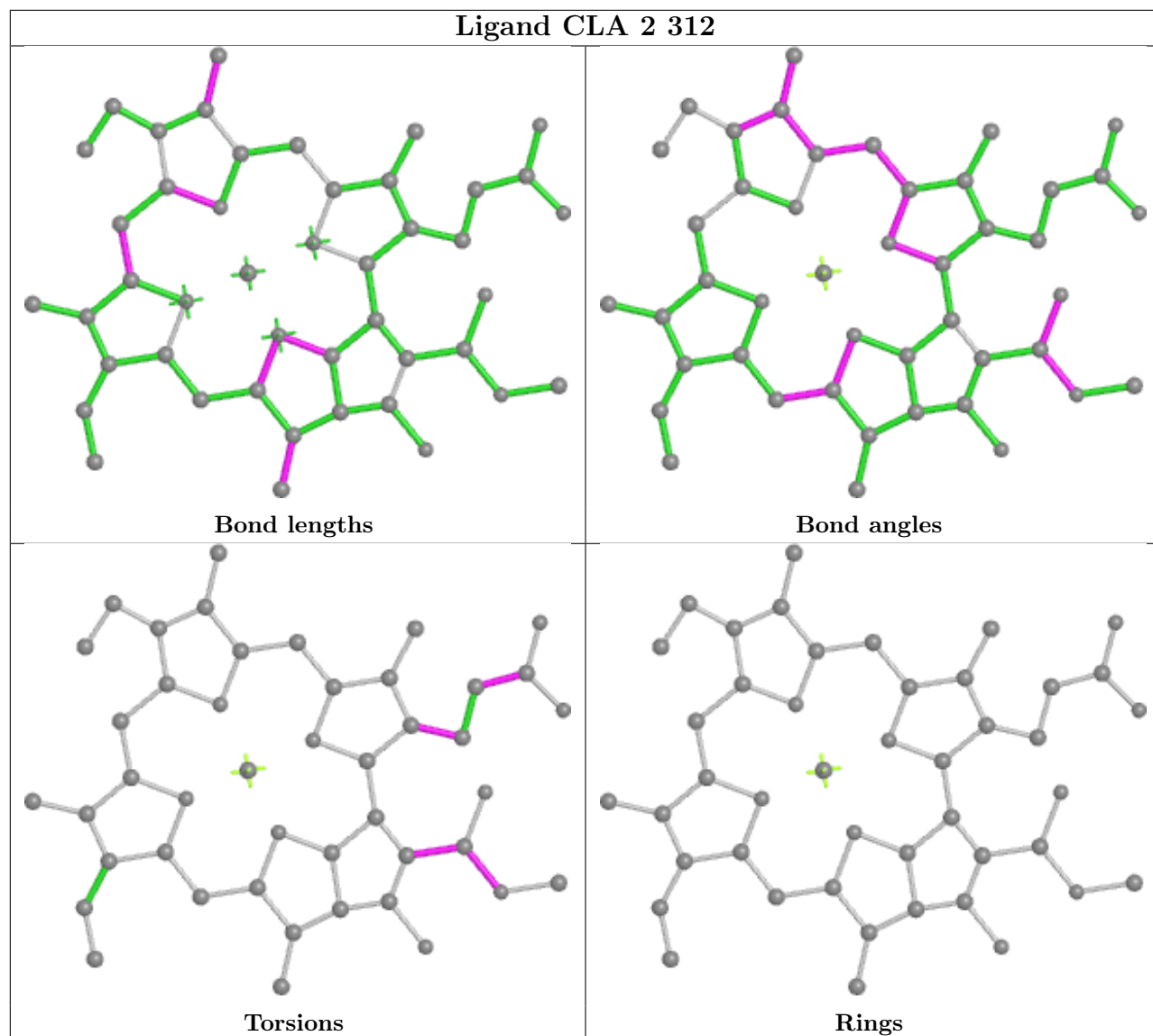


Torsions

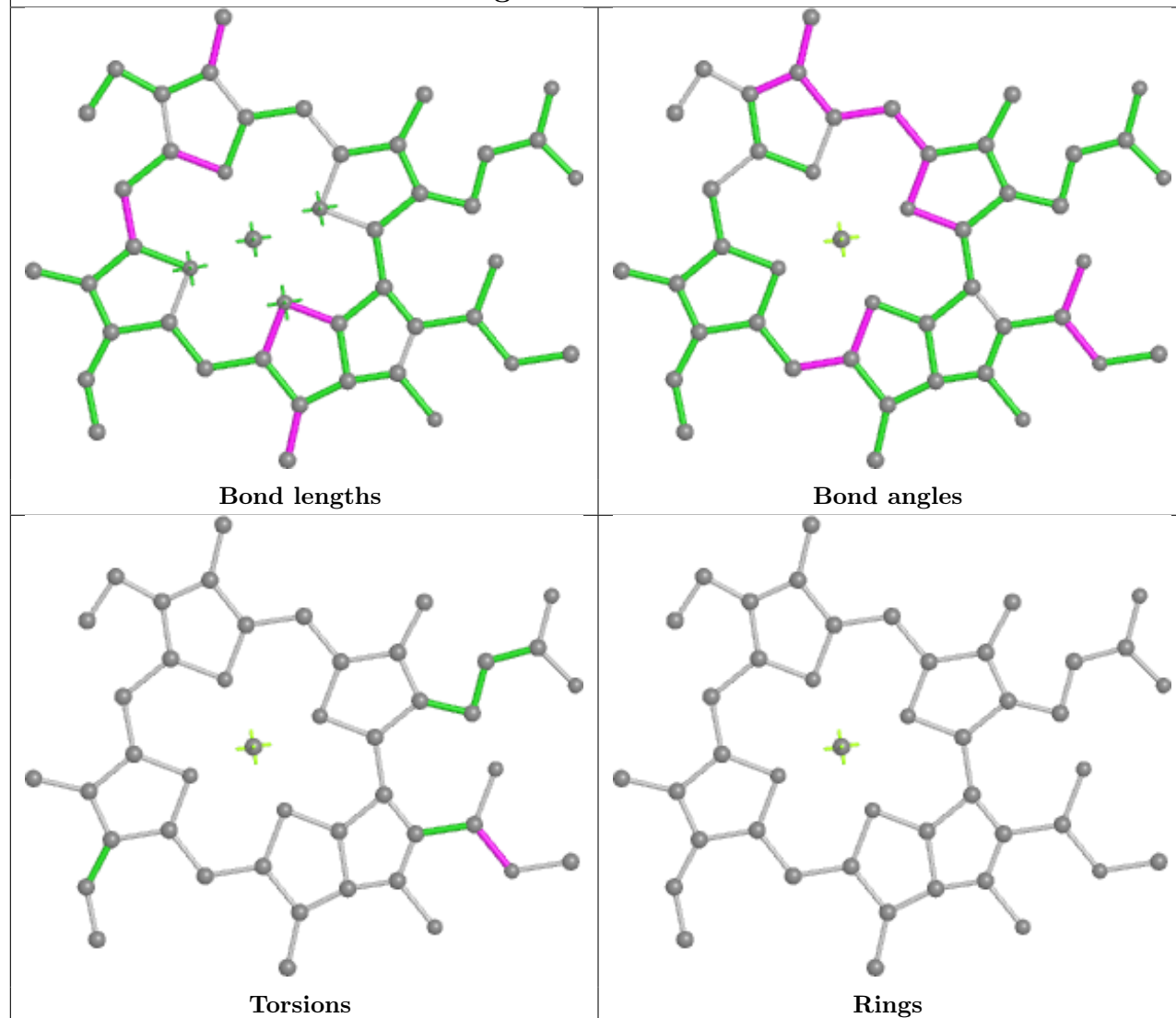


Rings

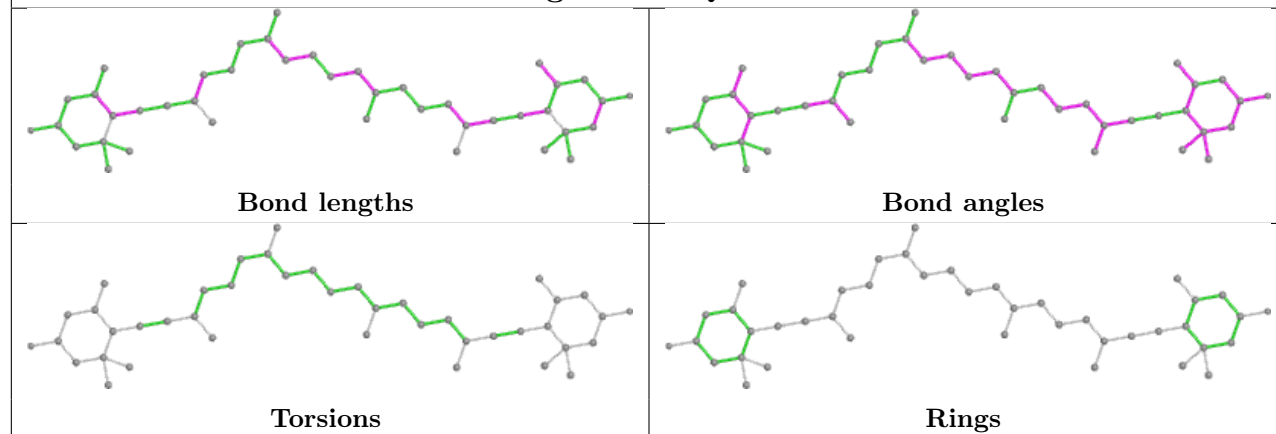
Ligand CLA 2 312

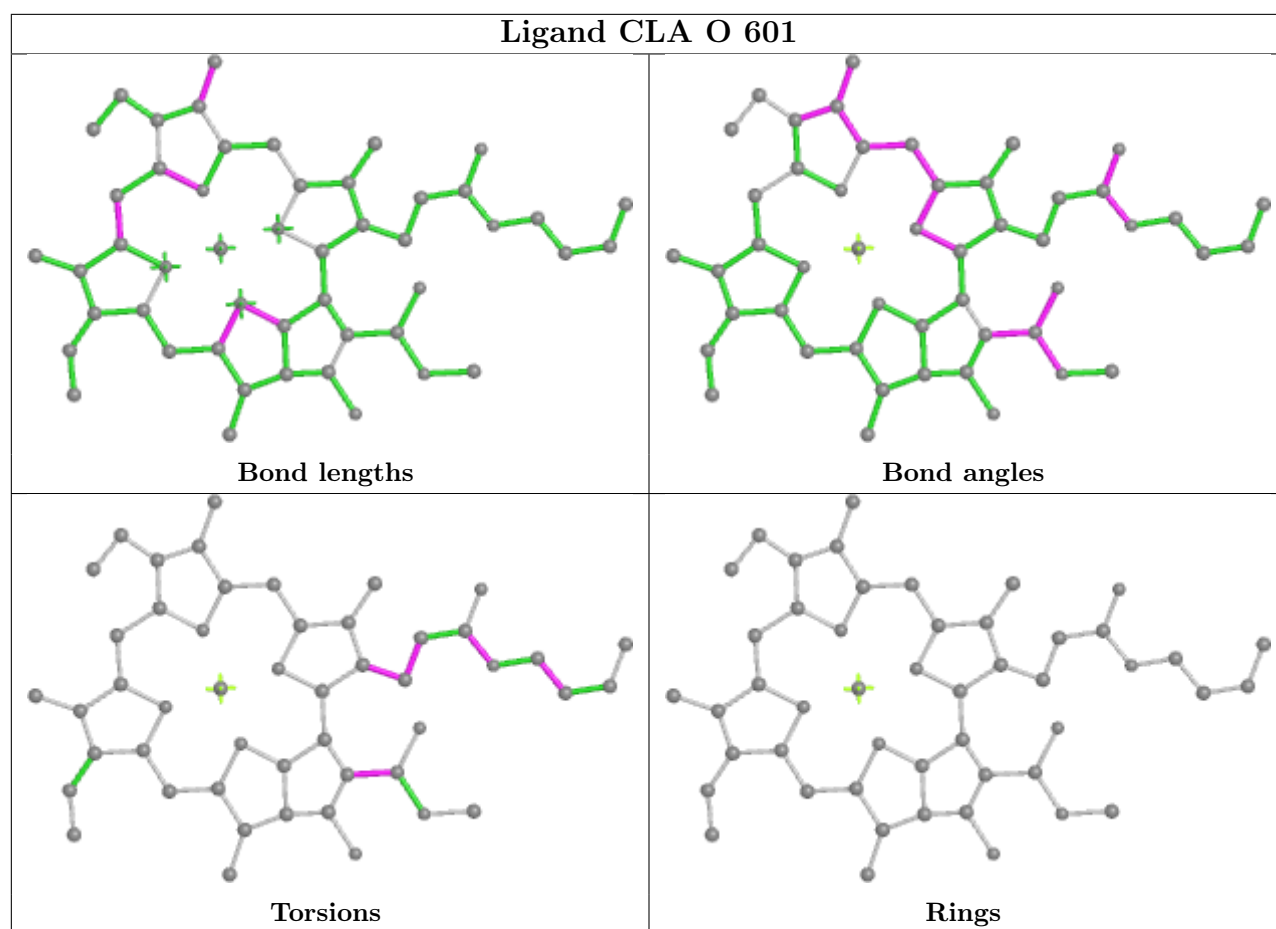


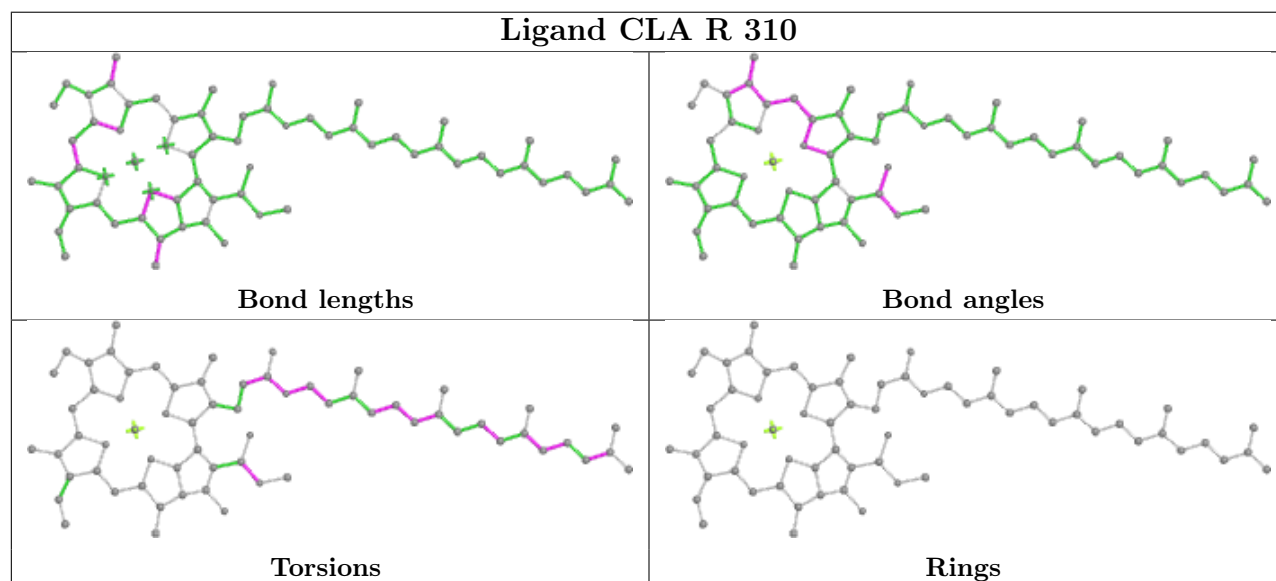
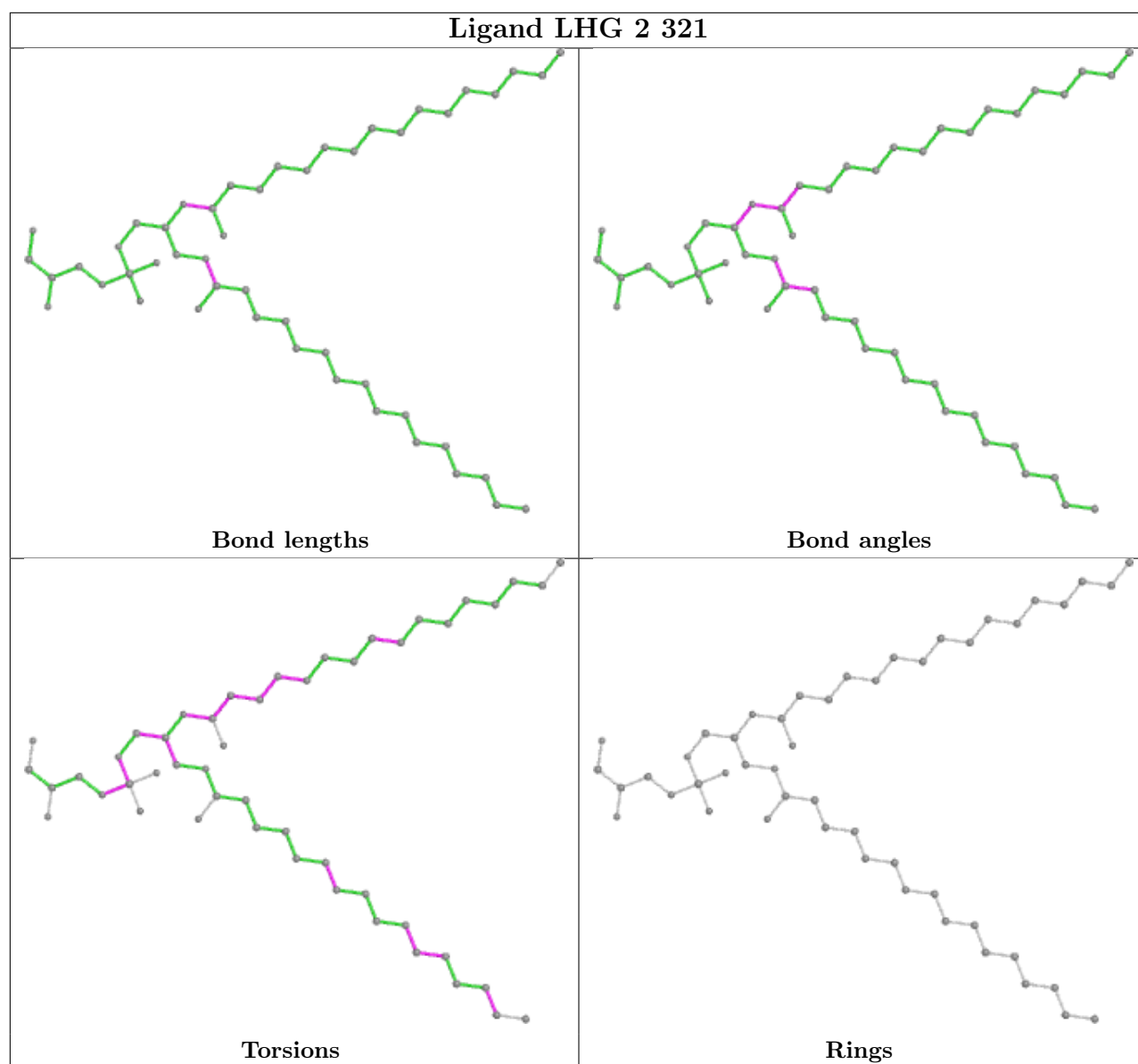
Ligand CLA 2 319

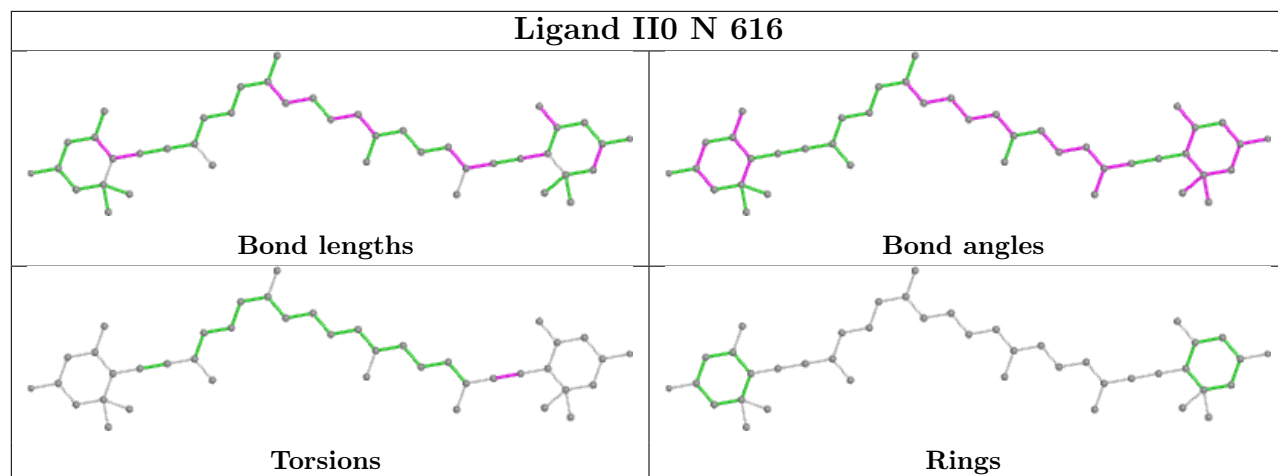
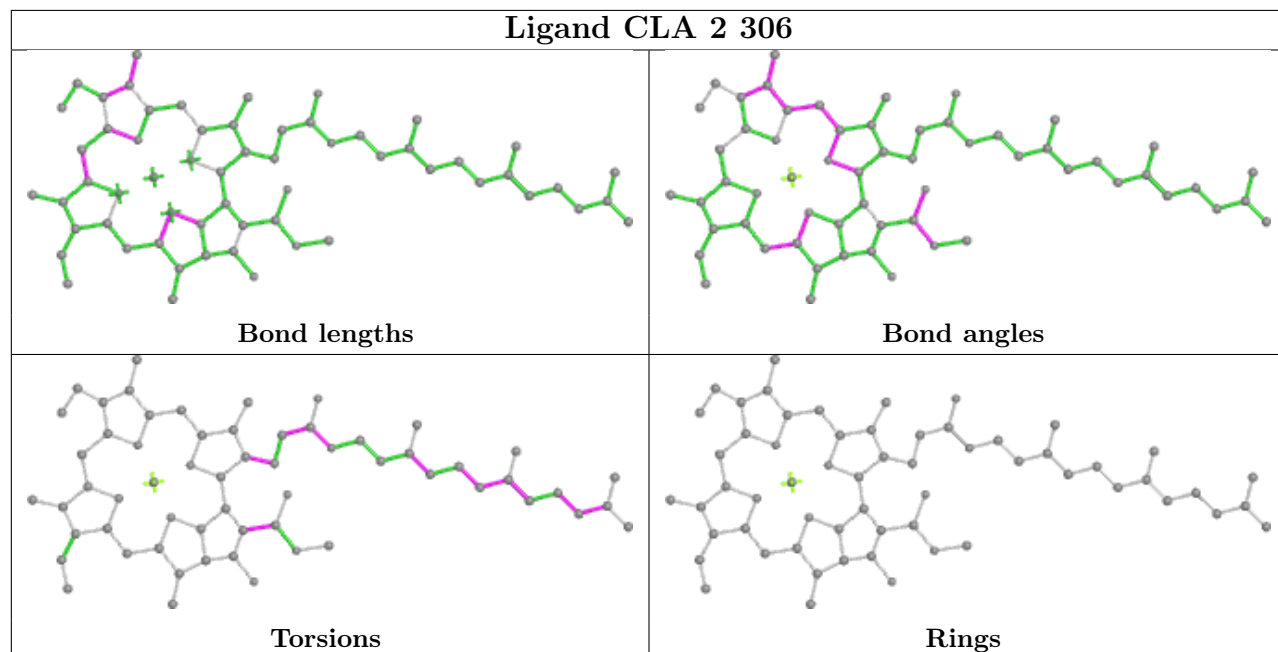


Ligand II0 Q 314

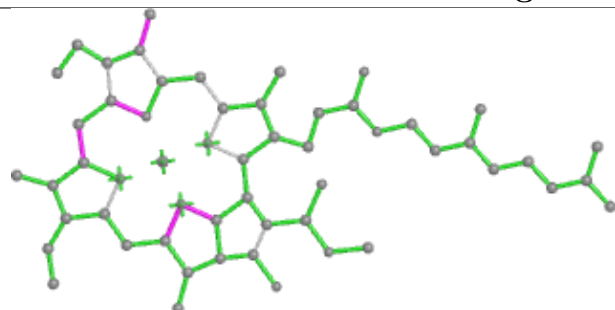




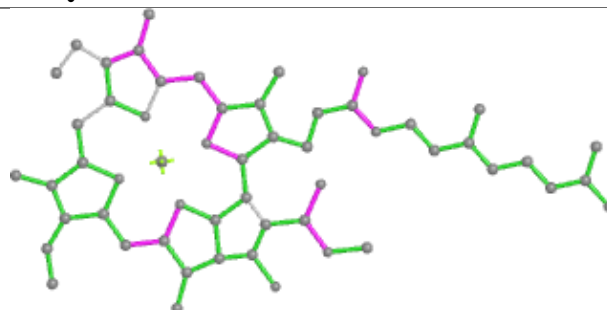


Ligand II0 N 616**Ligand CLA 2 306**

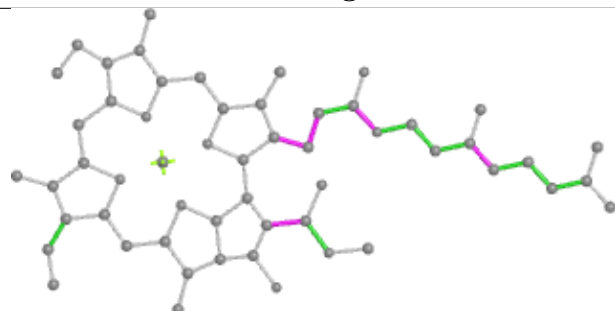
Ligand CLA Q 305



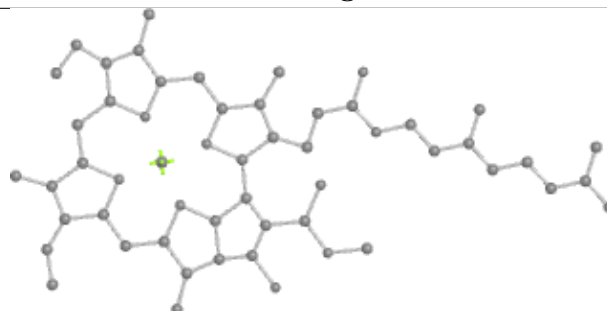
Bond lengths



Bond angles

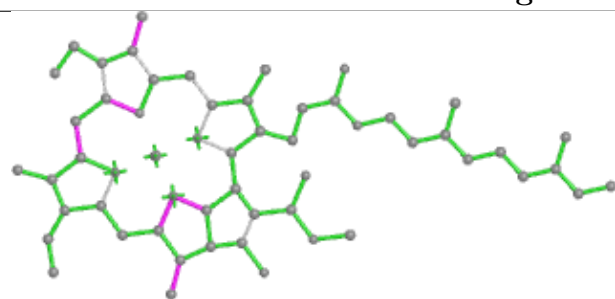


Torsions

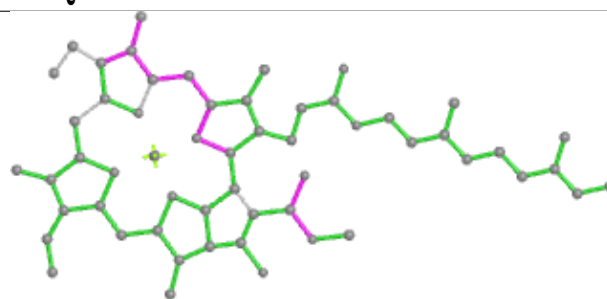


Rings

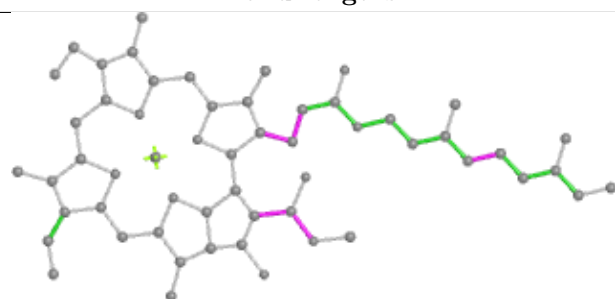
Ligand CLA Q 307



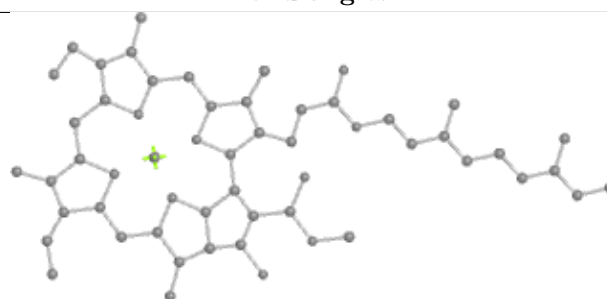
Bond lengths



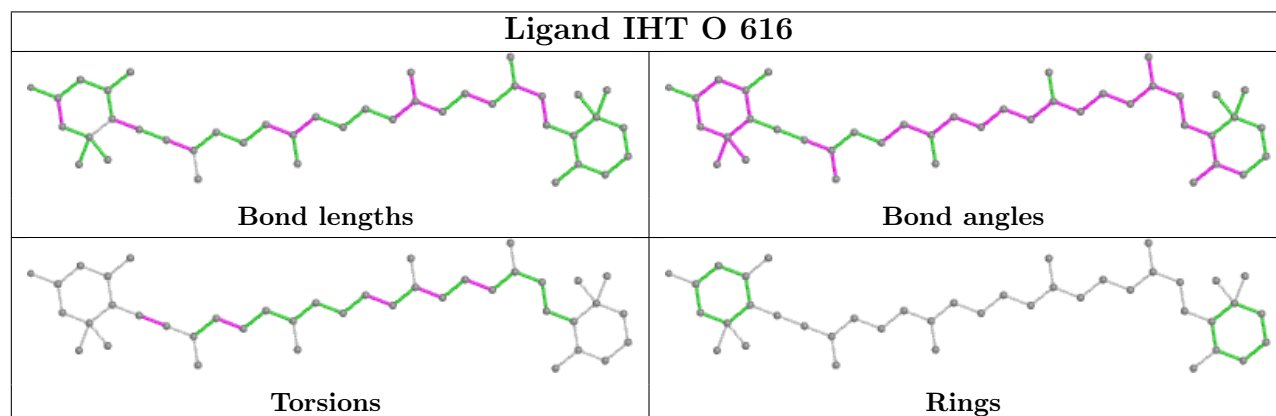
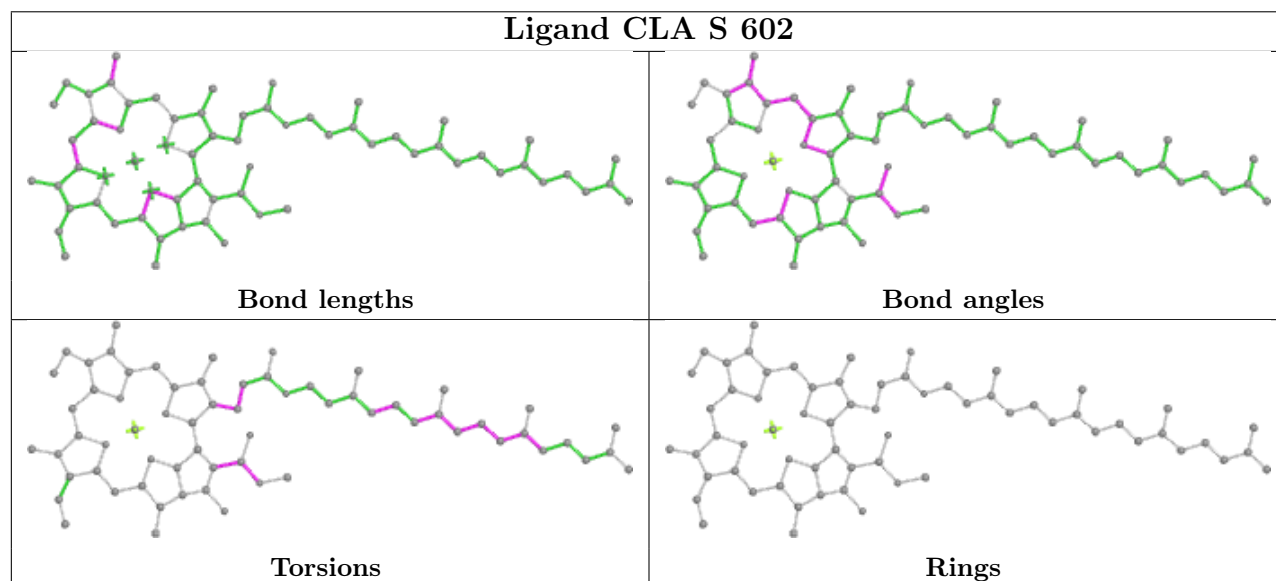
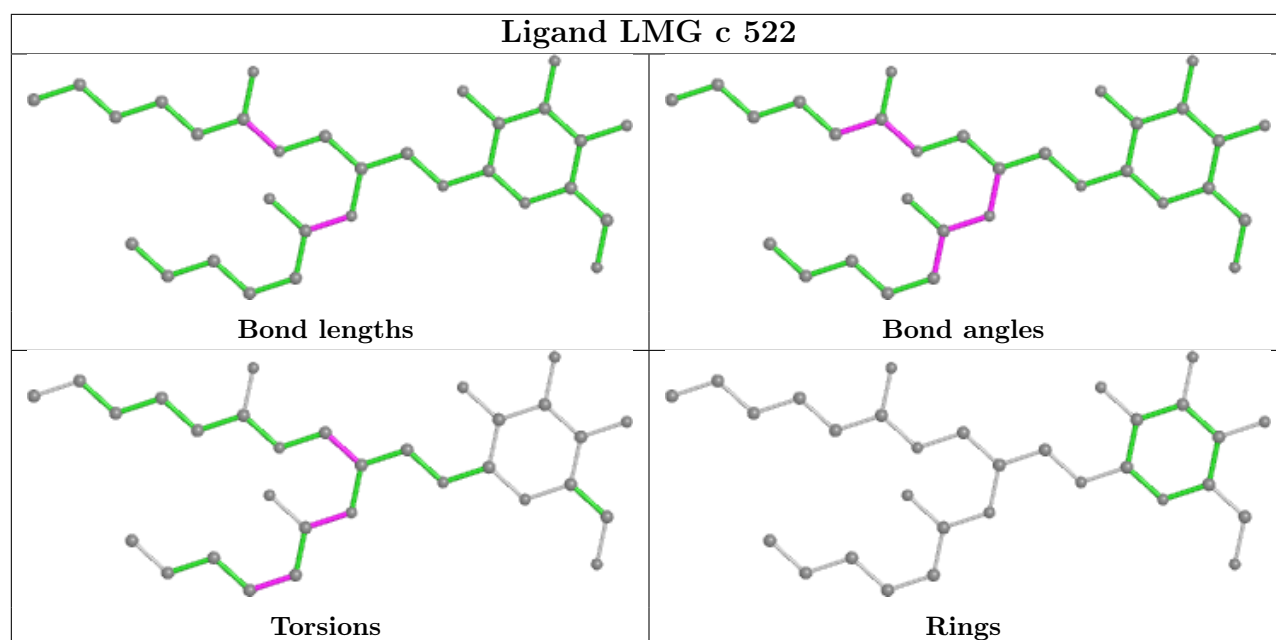
Bond angles

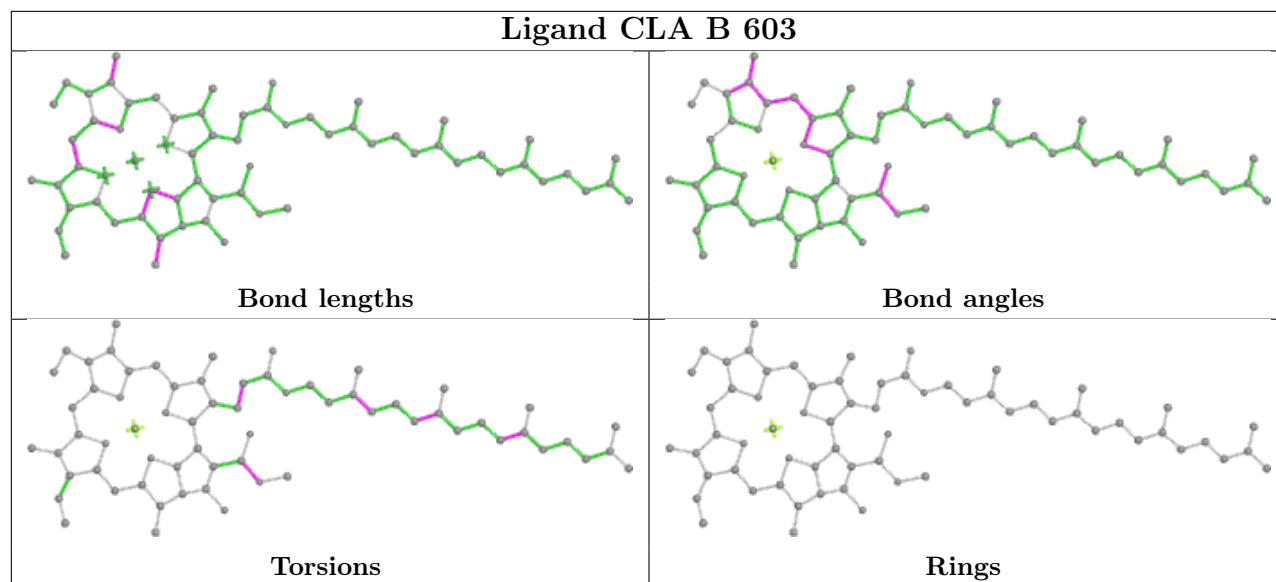
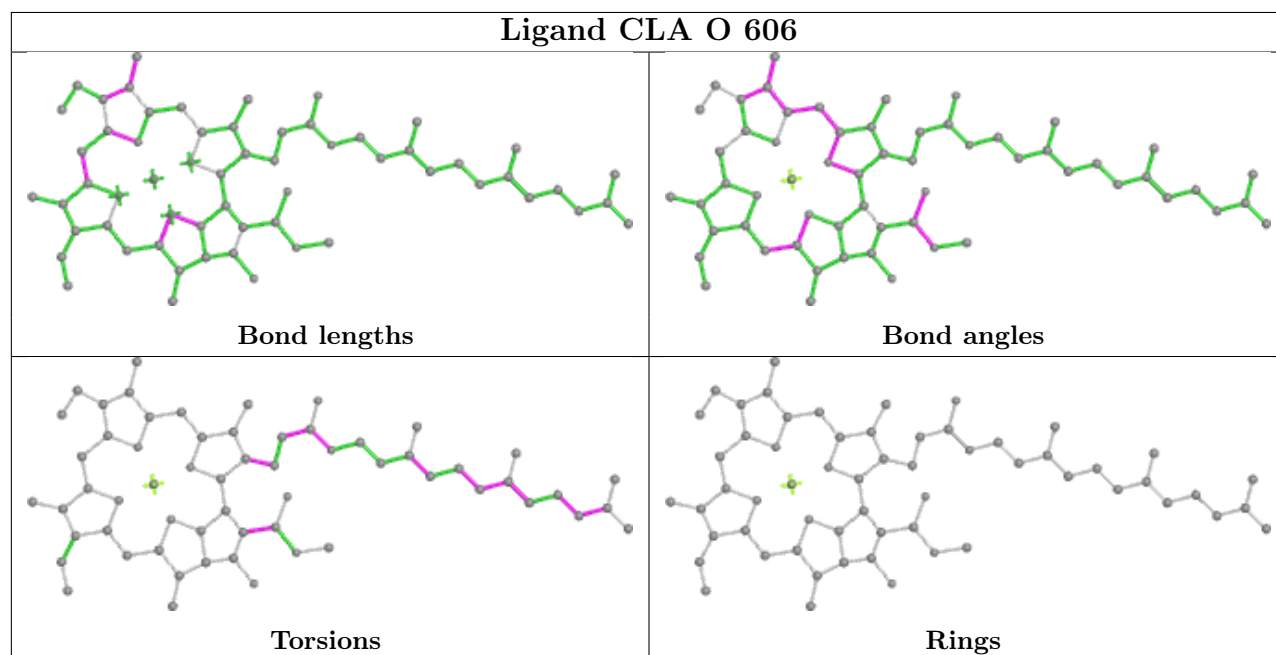


Torsions

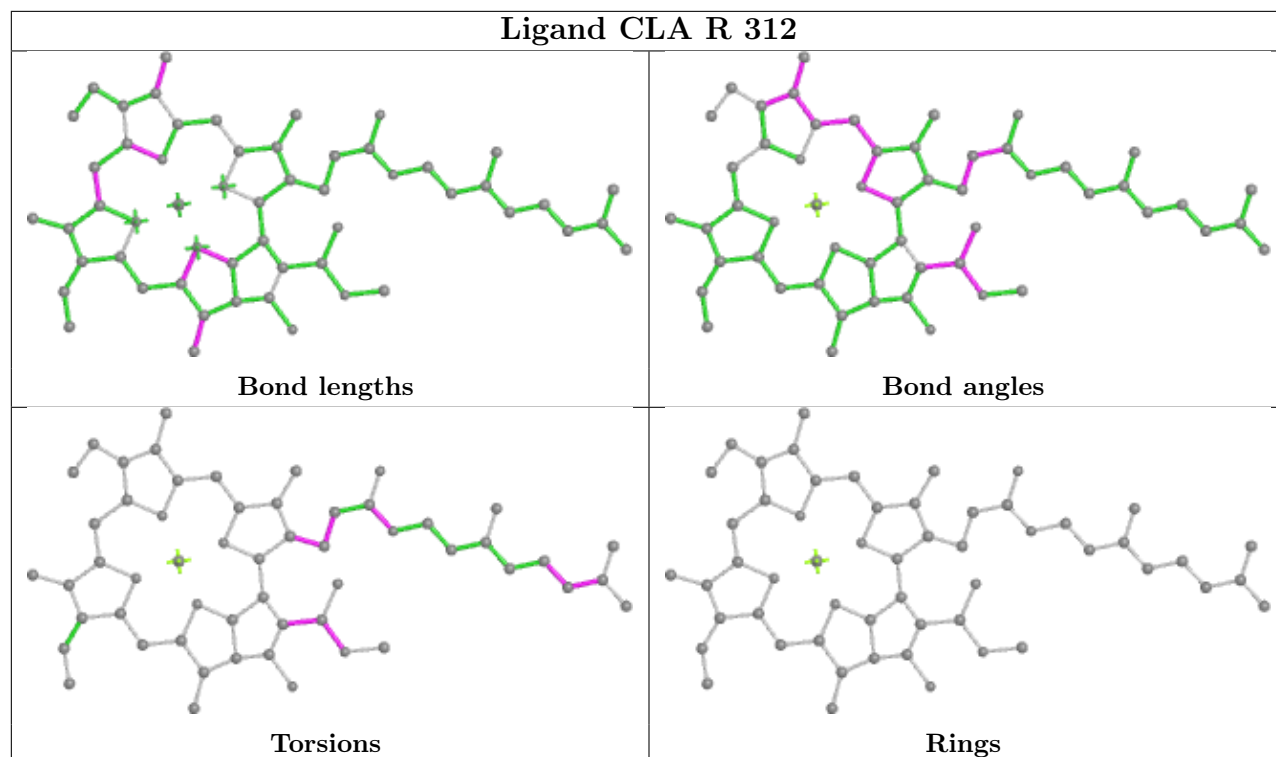


Rings

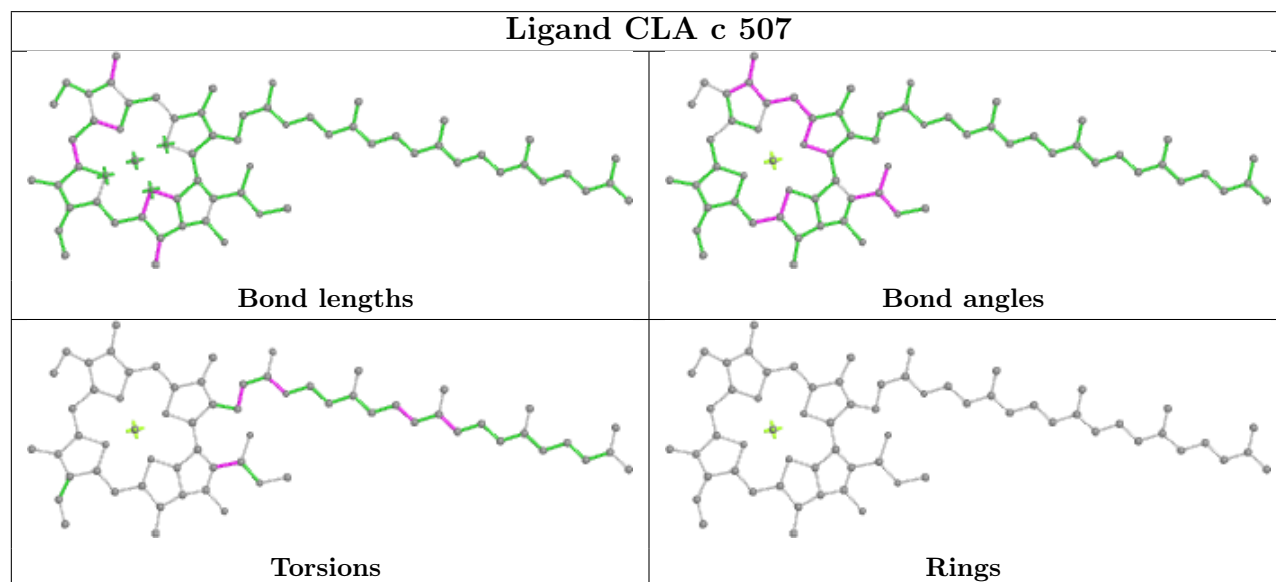


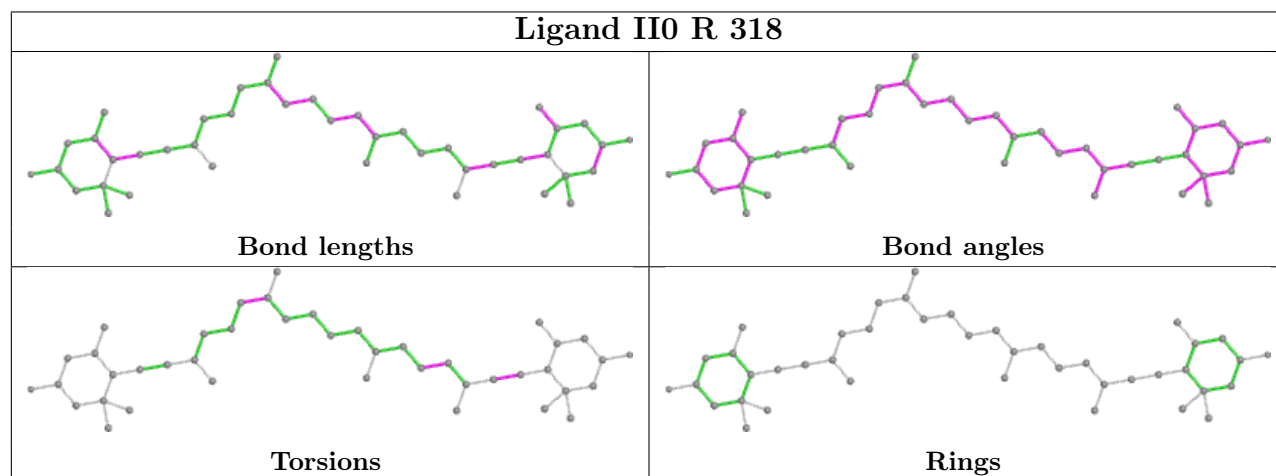
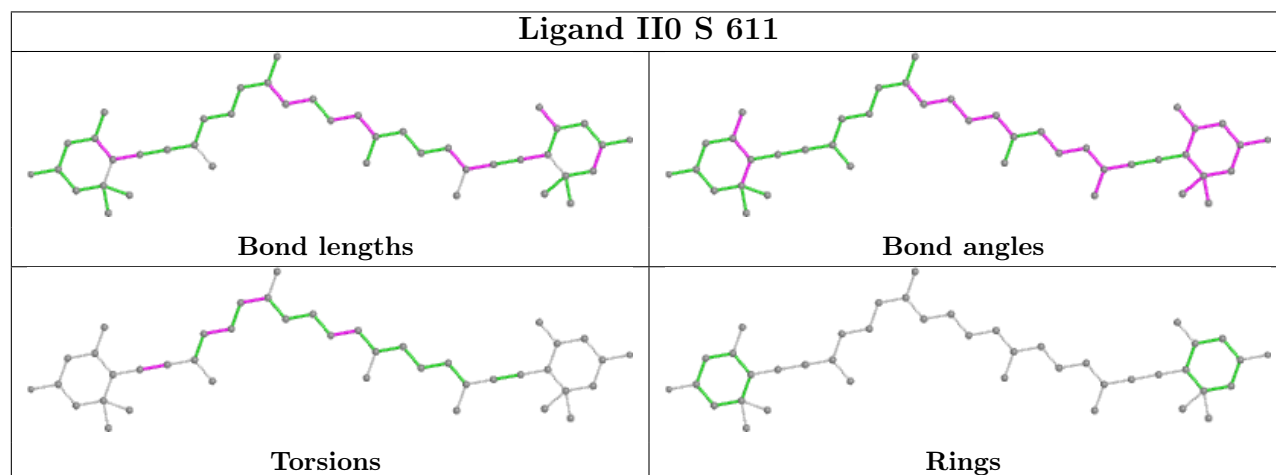
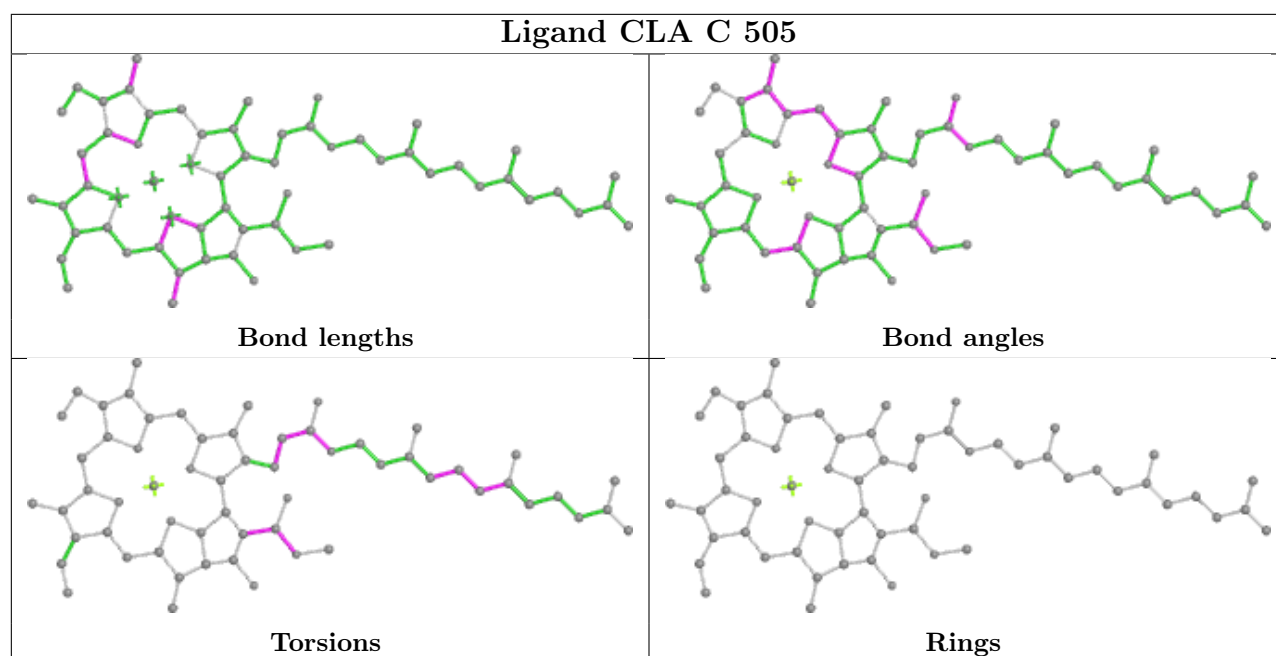
Ligand CLA B 603**Ligand CLA O 606**

Ligand CLA R 312

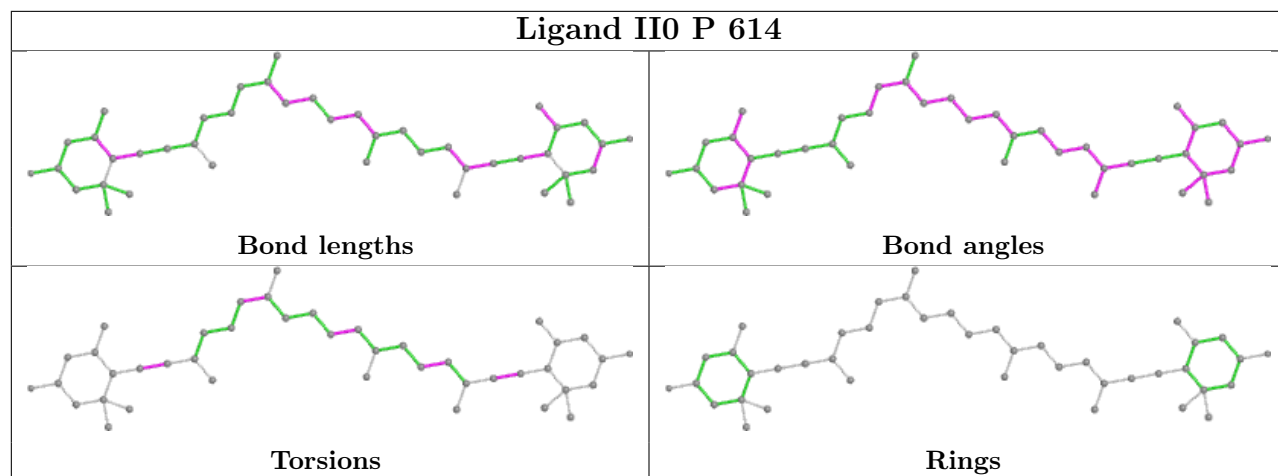


Ligand CLA c 507

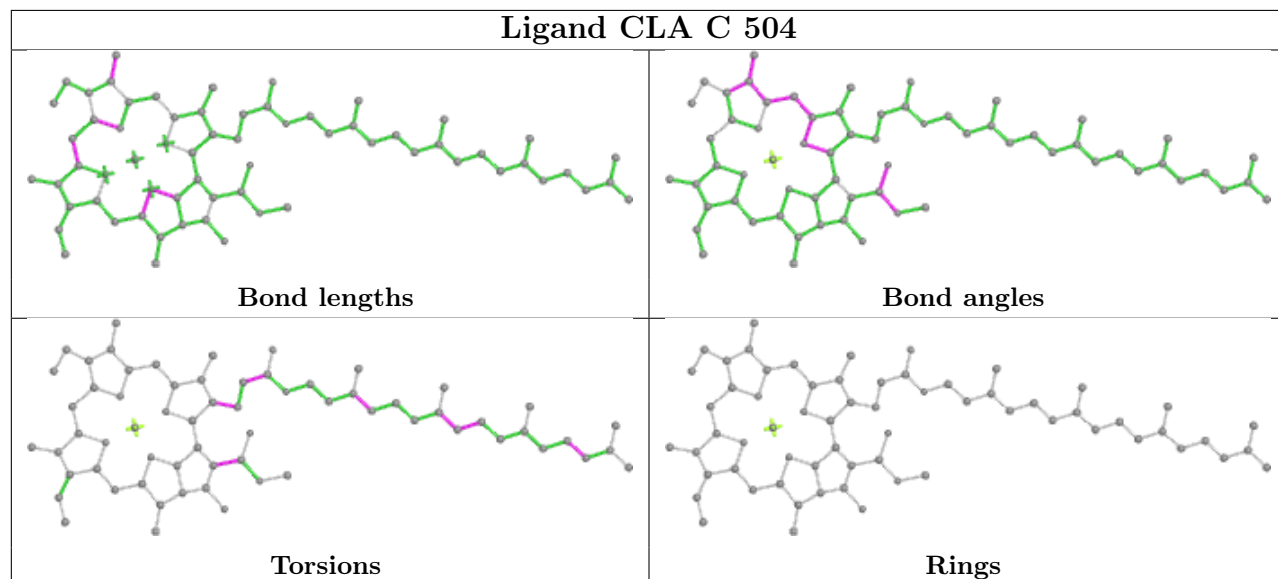




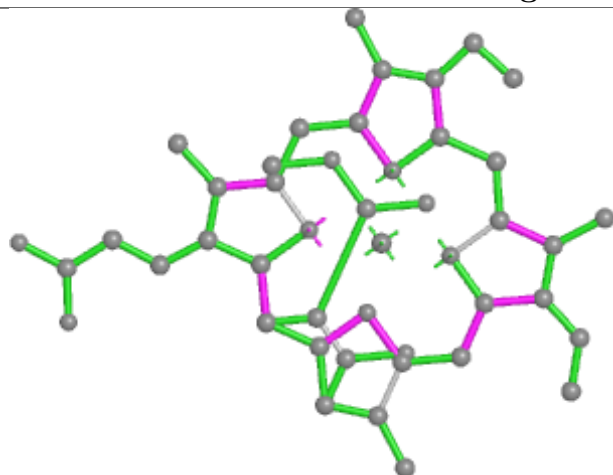
Ligand II0 P 614



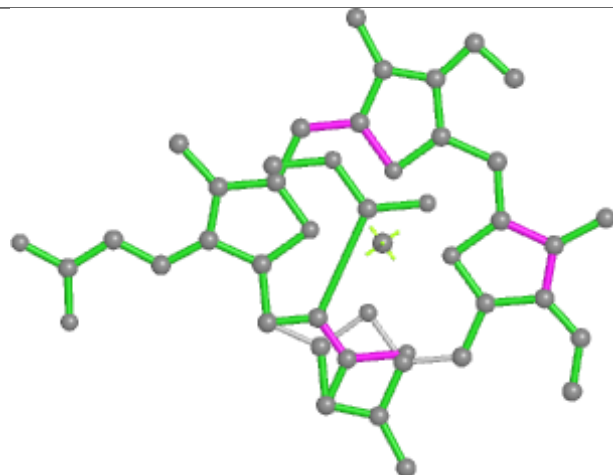
Ligand CLA C 504



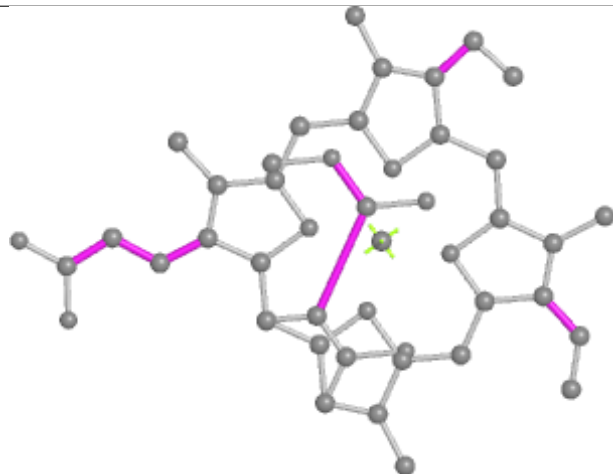
Ligand KC2 1 610



Bond lengths



Bond angles

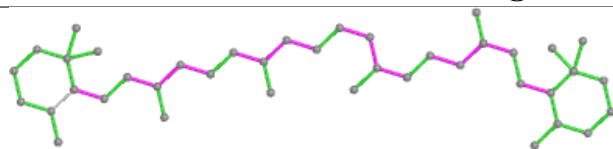


Torsions

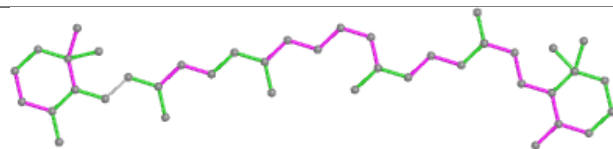


Rings

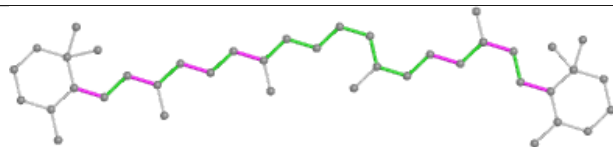
Ligand WVN S 613



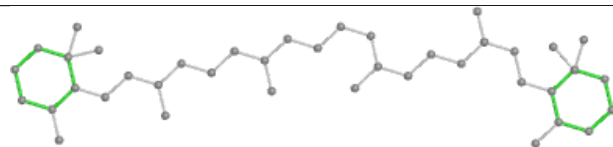
Bond lengths



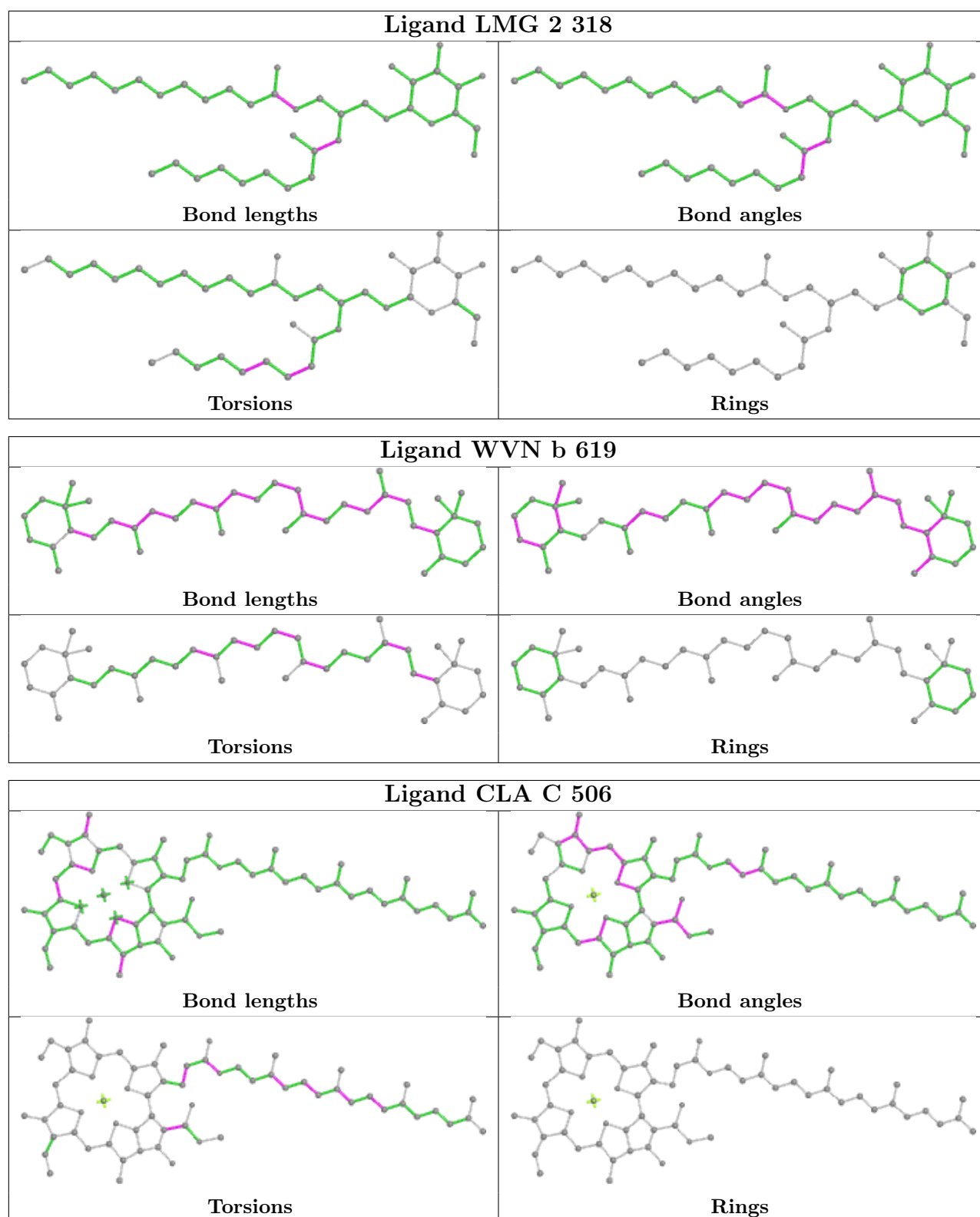
Bond angles



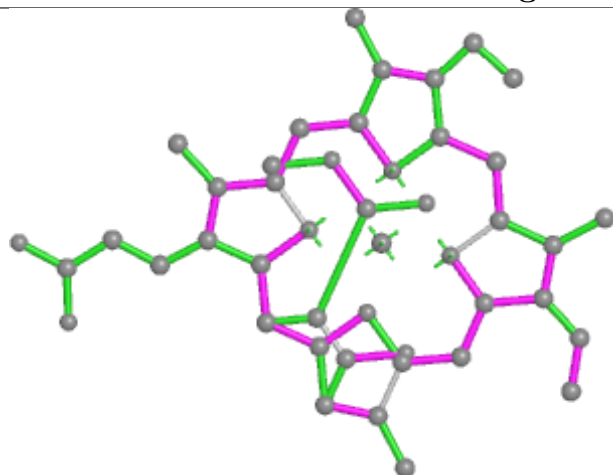
Torsions



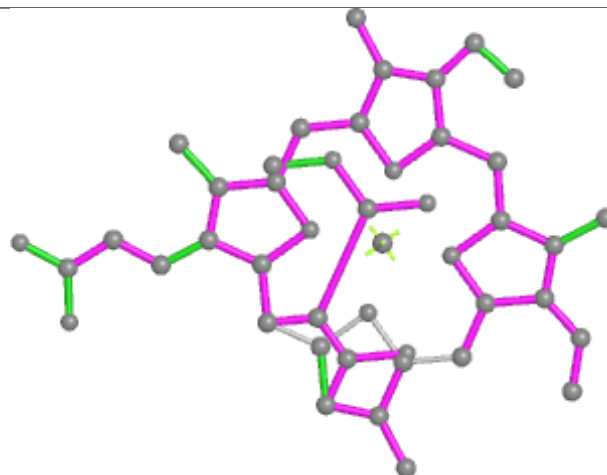
Rings



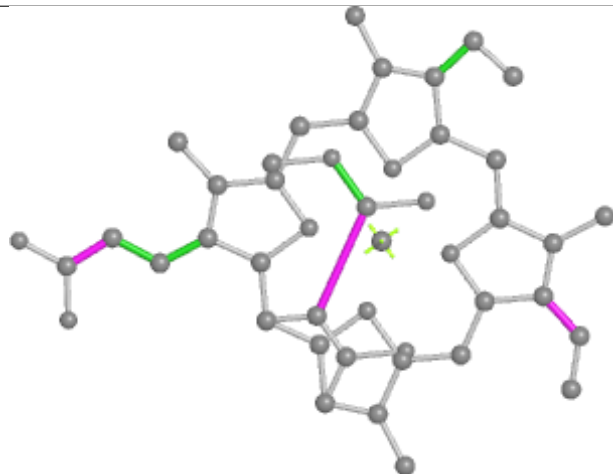
Ligand KC2 S 608



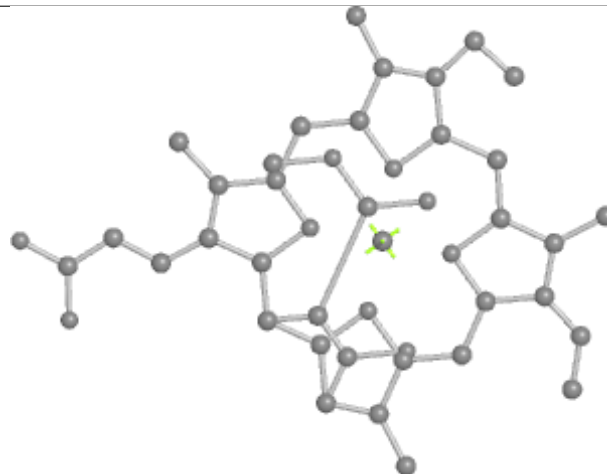
Bond lengths



Bond angles

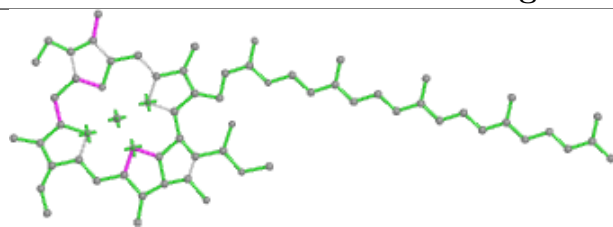


Torsions

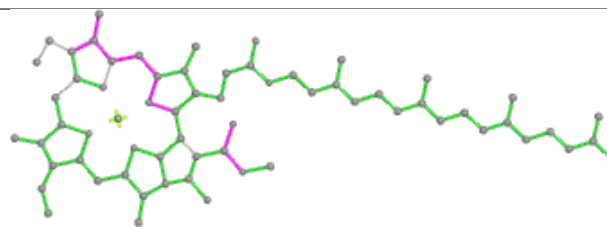


Rings

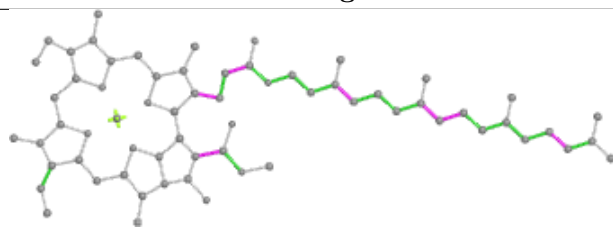
Ligand CLA c 505



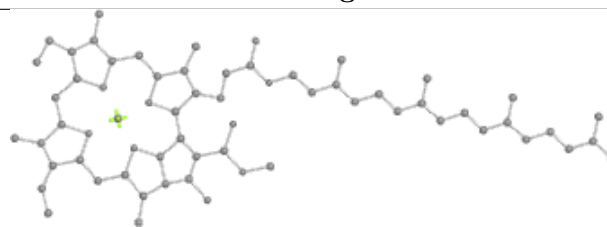
Bond lengths



Bond angles

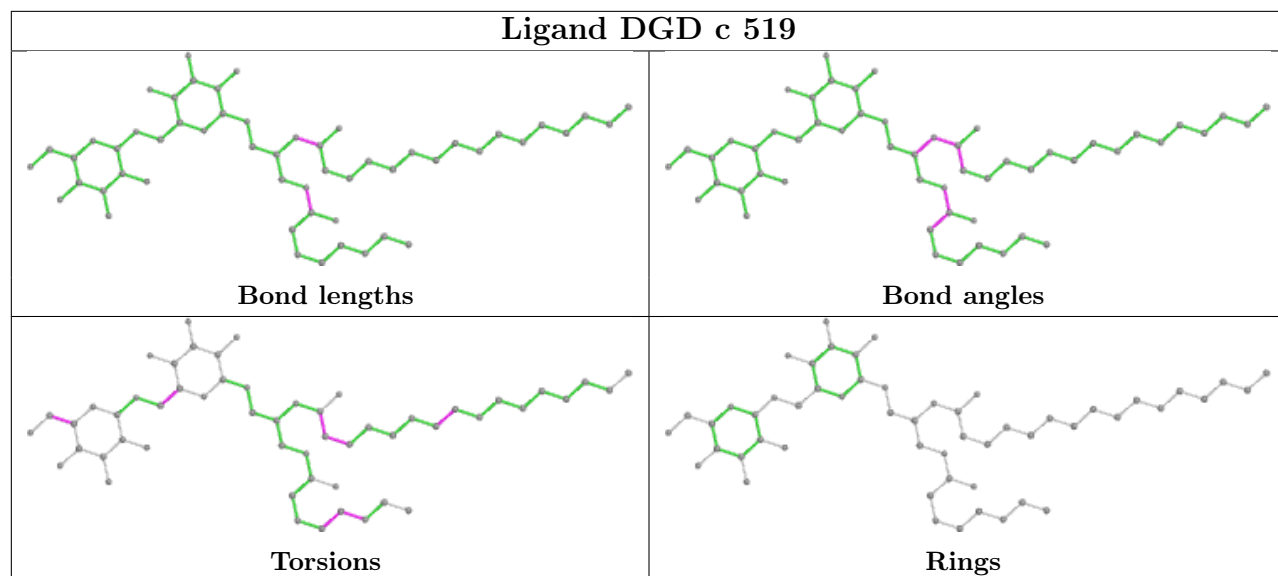


Torsions

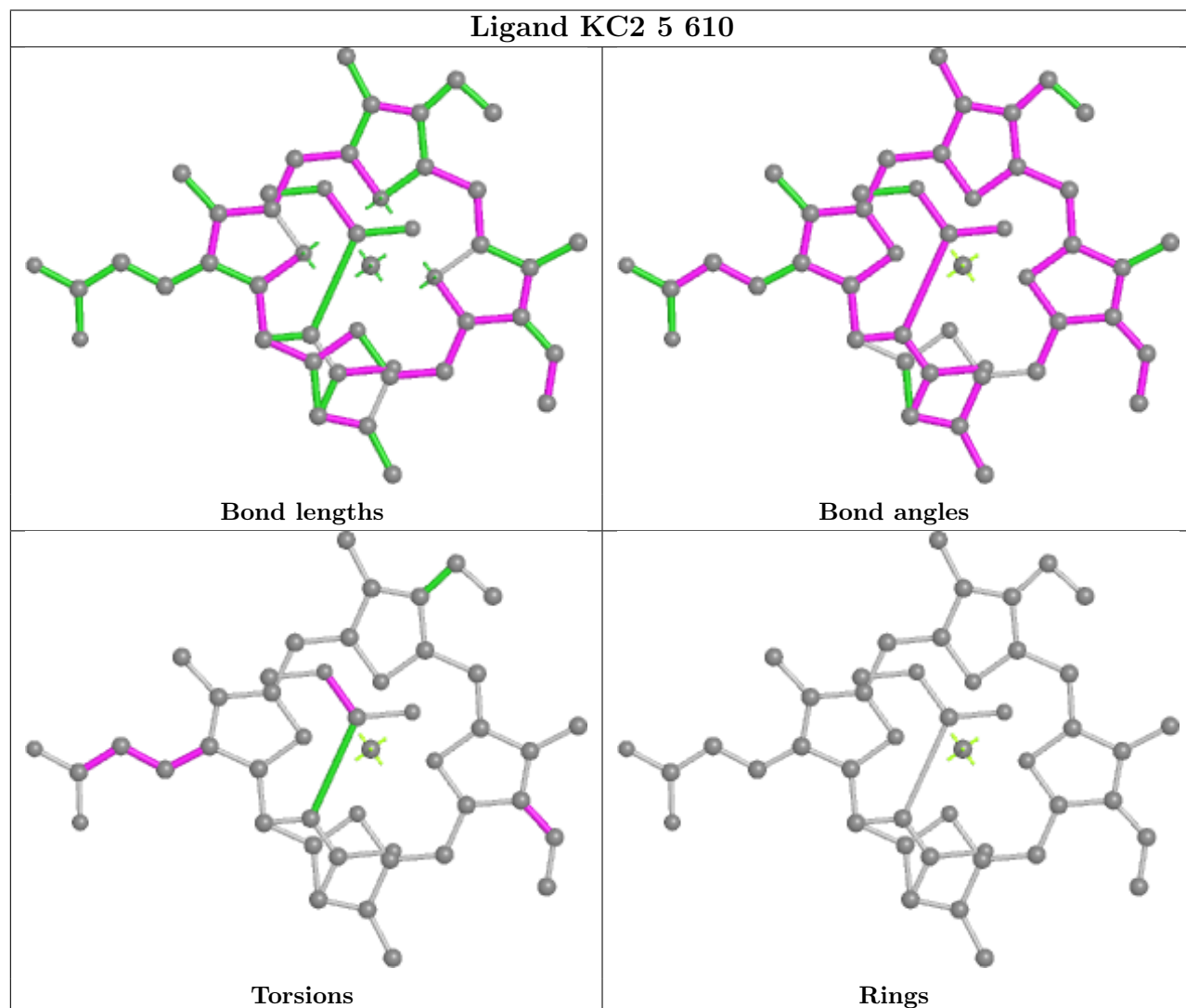


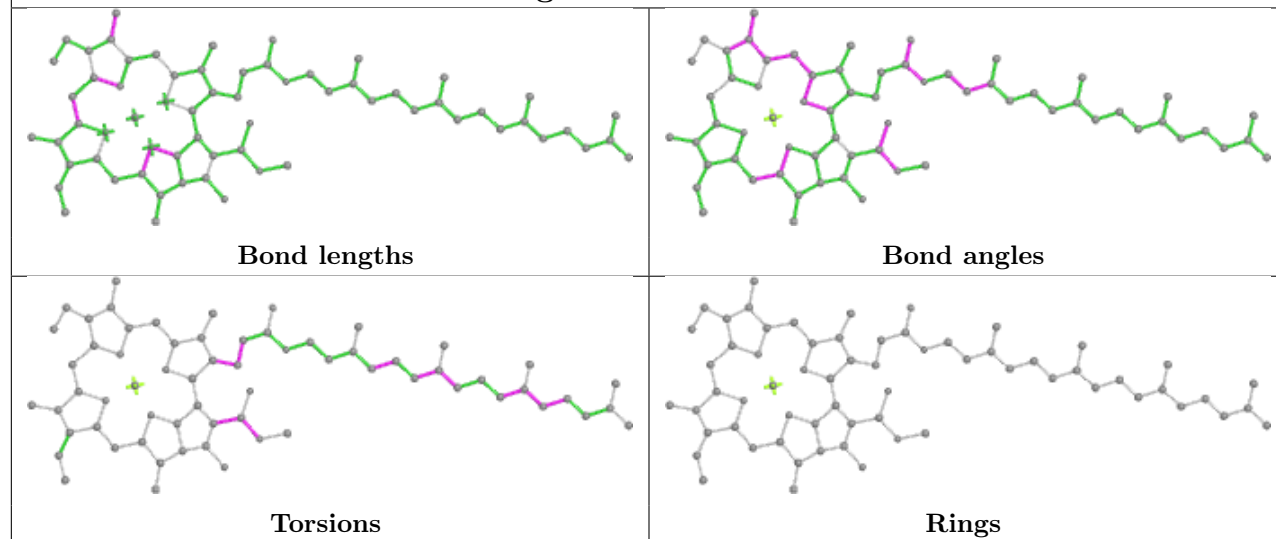
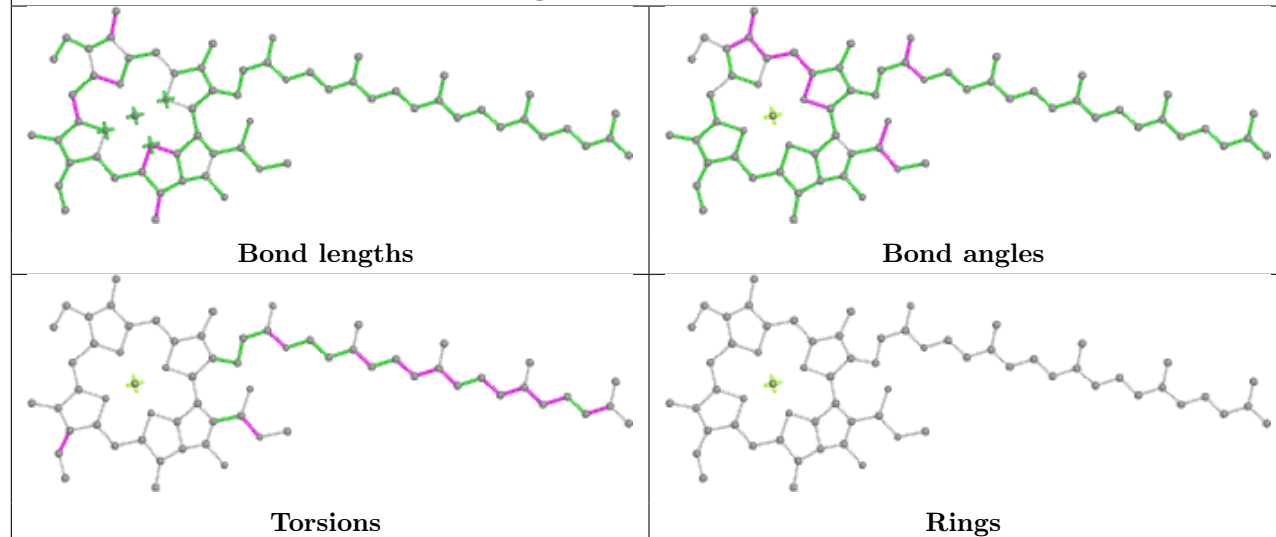
Rings

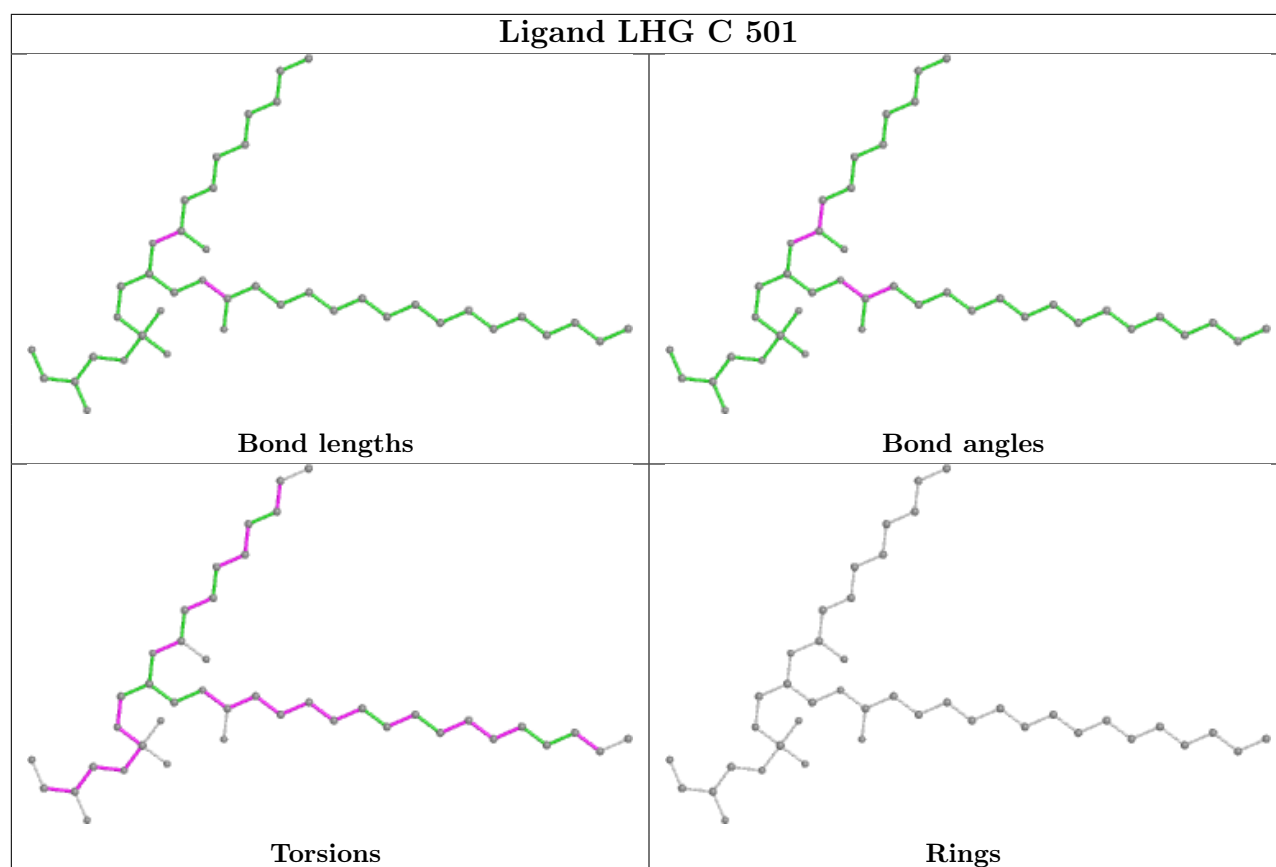
Ligand DGD c 519

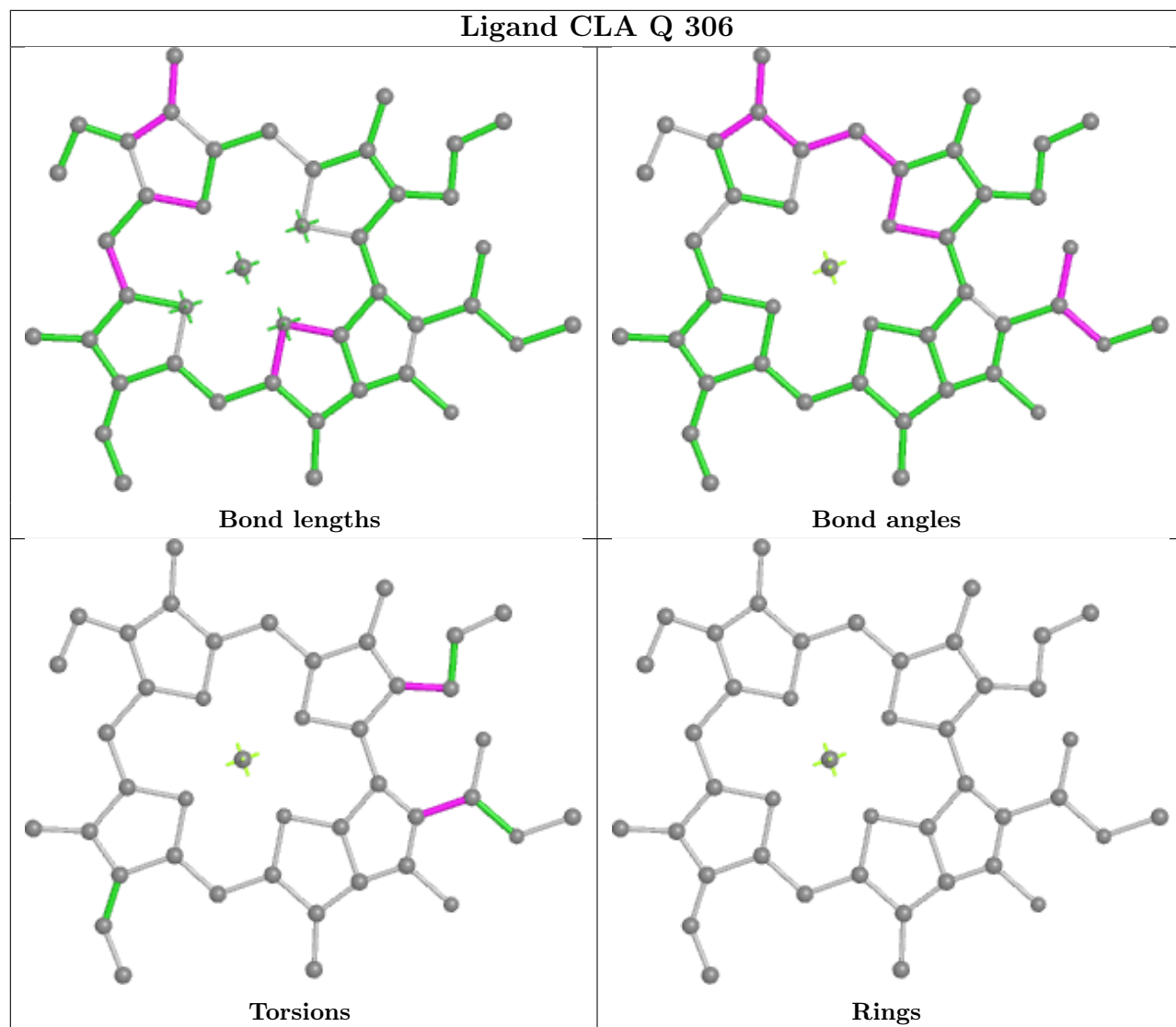


Ligand KC2 5 610

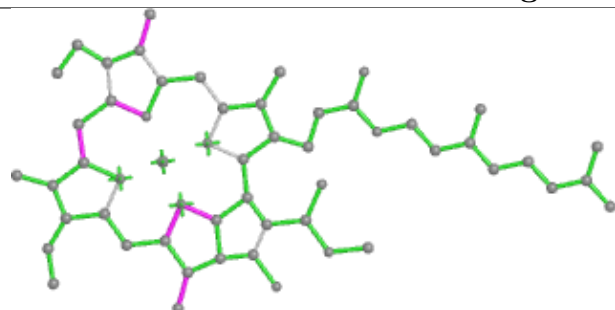


Ligand CLA 2 302**Ligand CLA G 401**

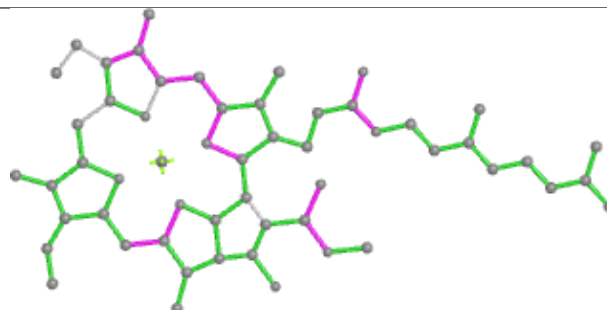




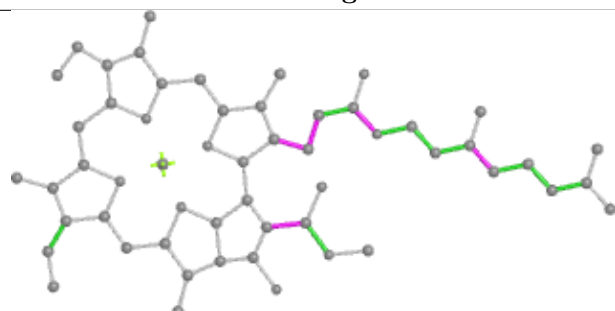
Ligand CLA 4 306



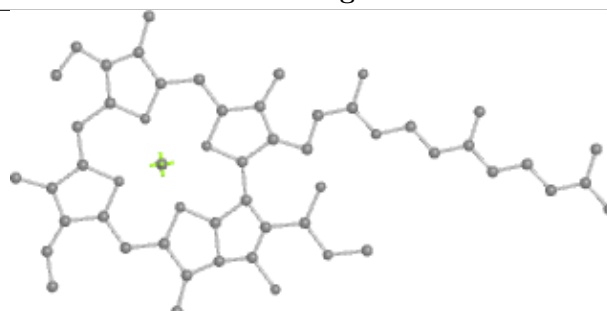
Bond lengths



Bond angles

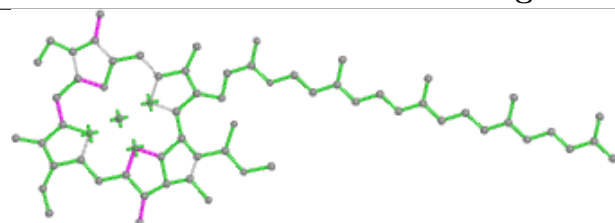


Torsions

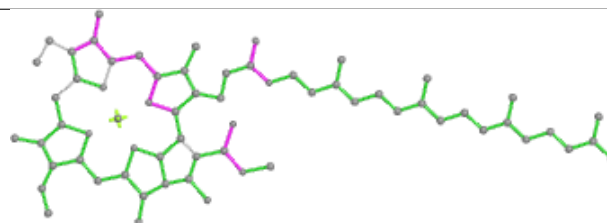


Rings

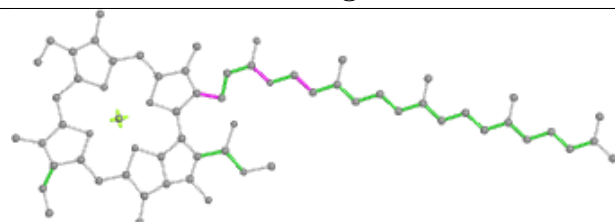
Ligand CLA D 407



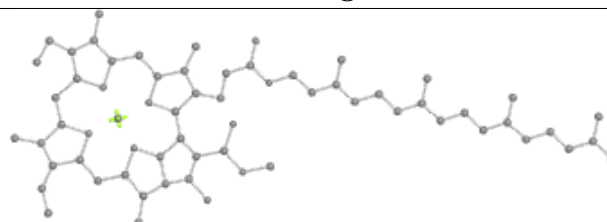
Bond lengths



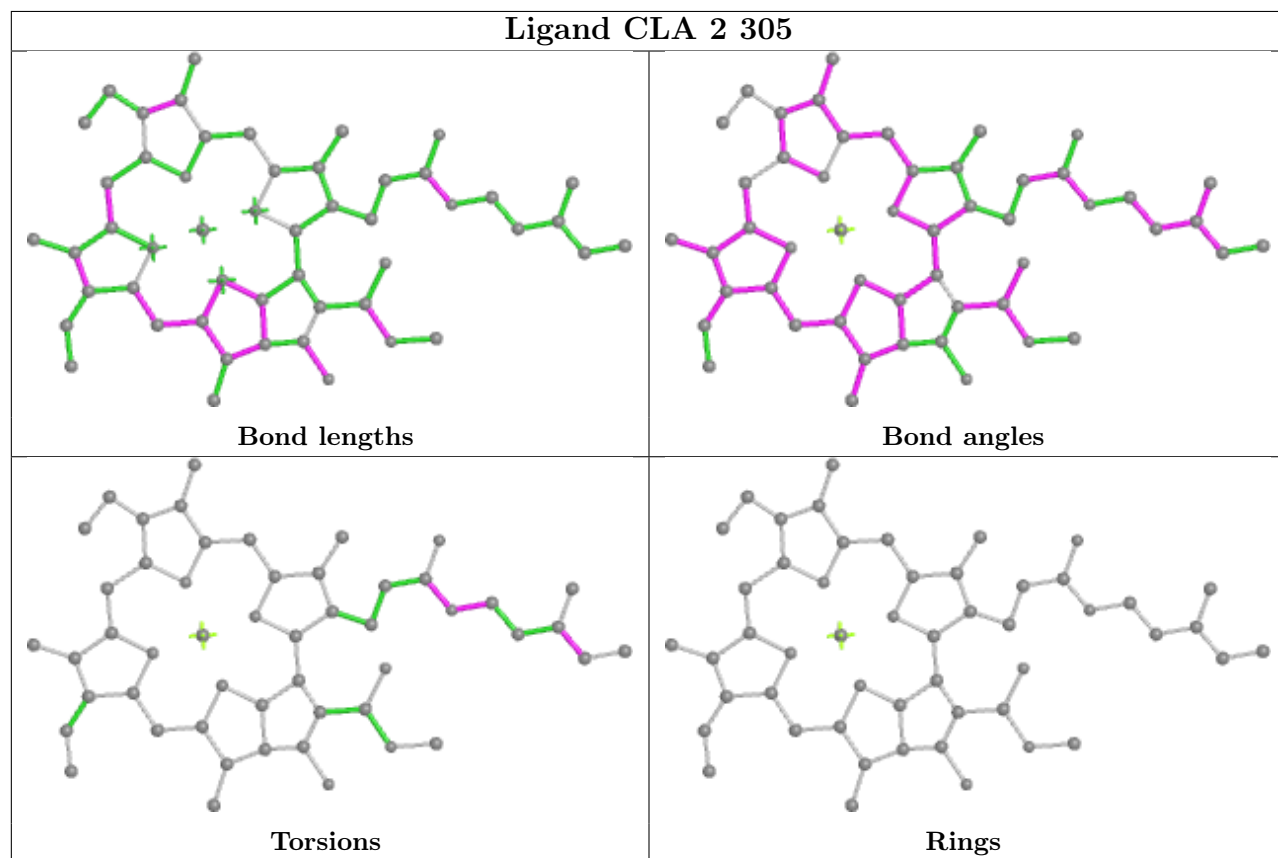
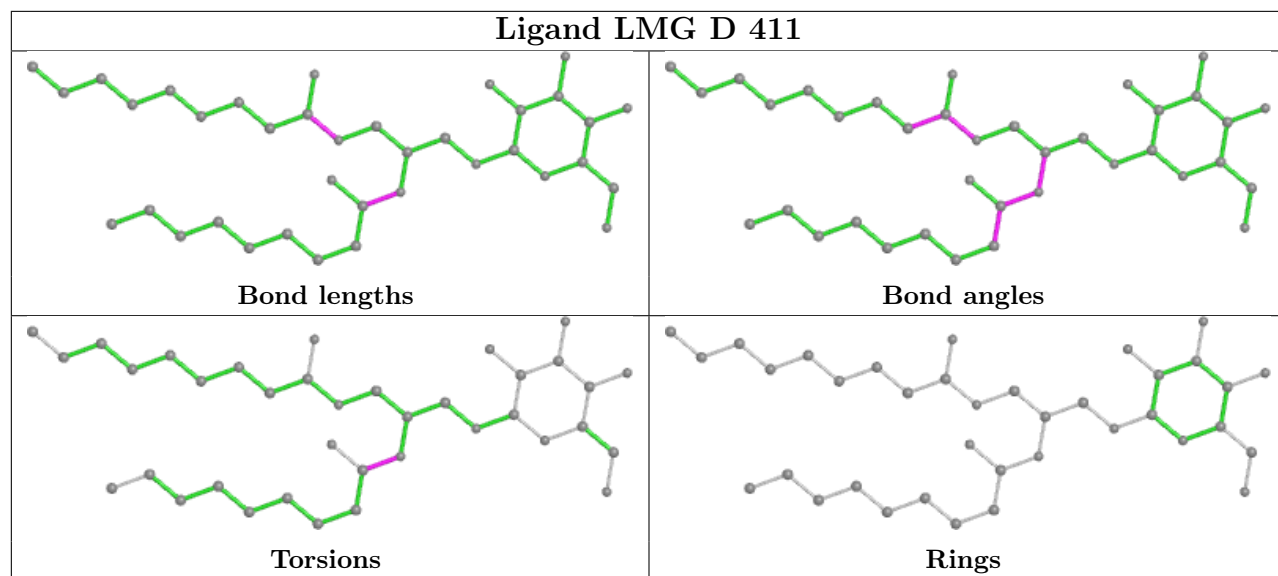
Bond angles

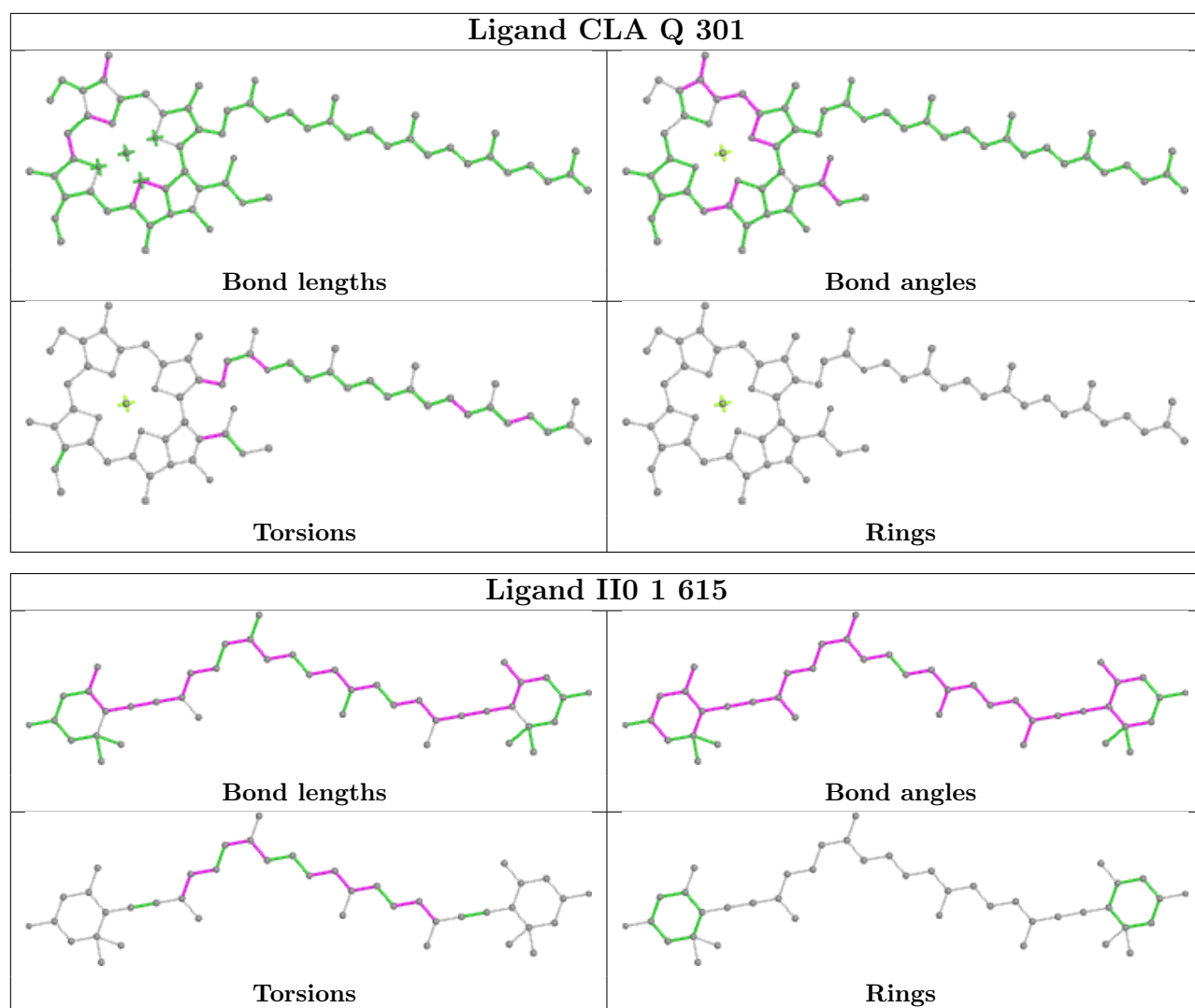


Torsions

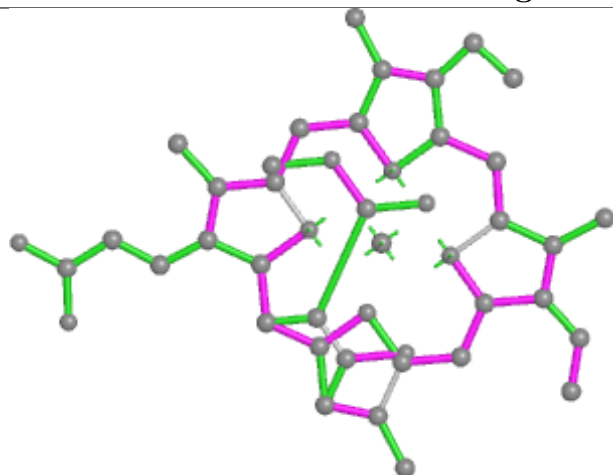


Rings

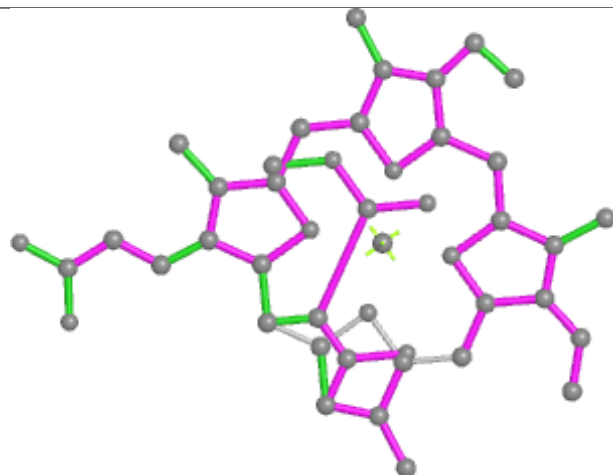




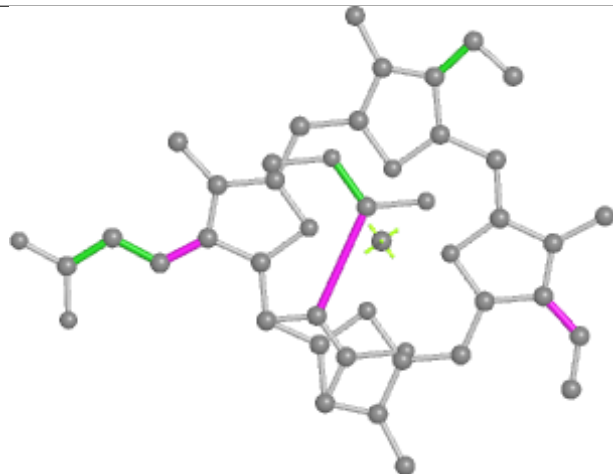
Ligand KC2 N 611



Bond lengths



Bond angles

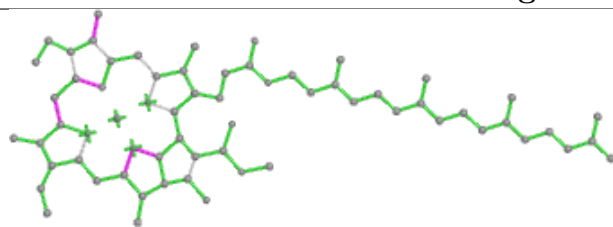


Torsions

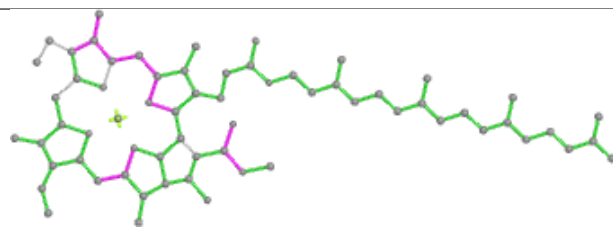


Rings

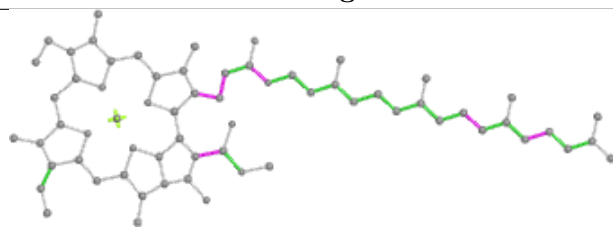
Ligand CLA 4 302



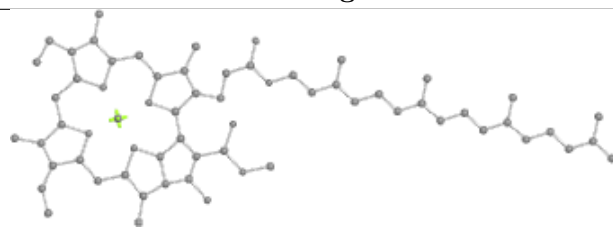
Bond lengths



Bond angles

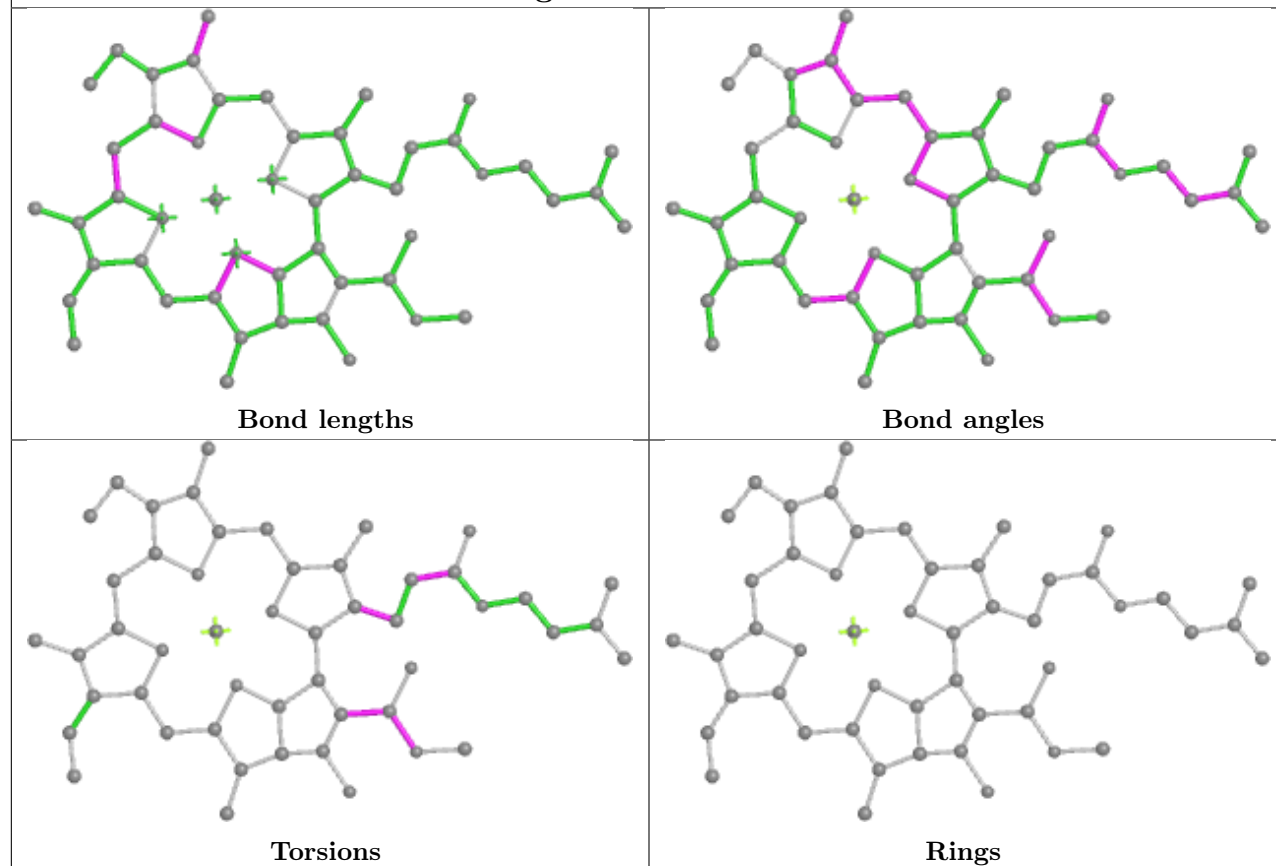


Torsions

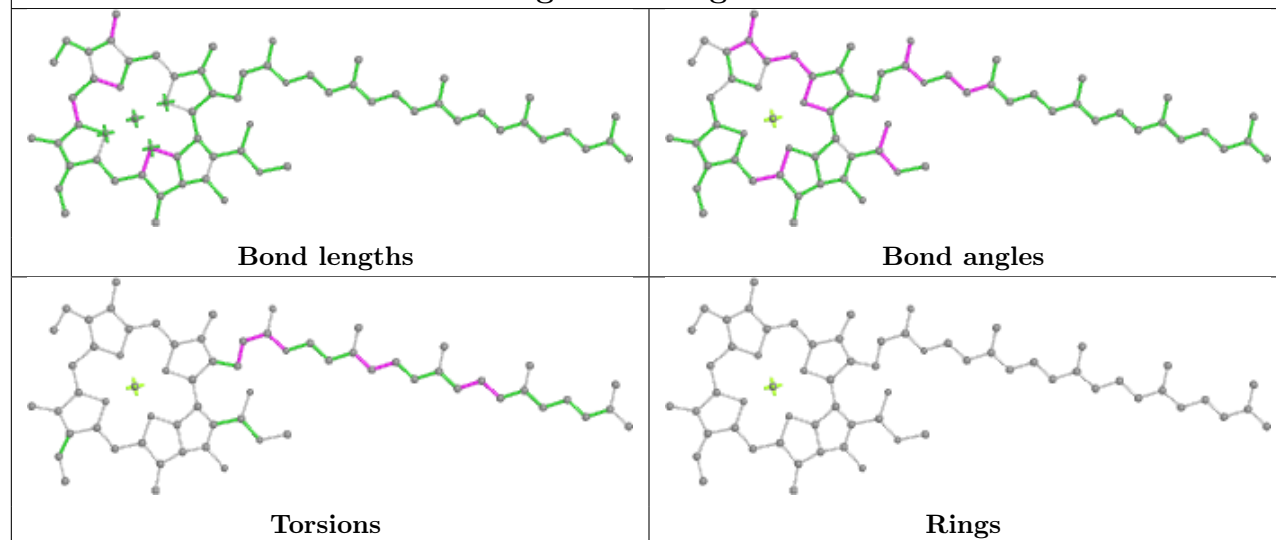


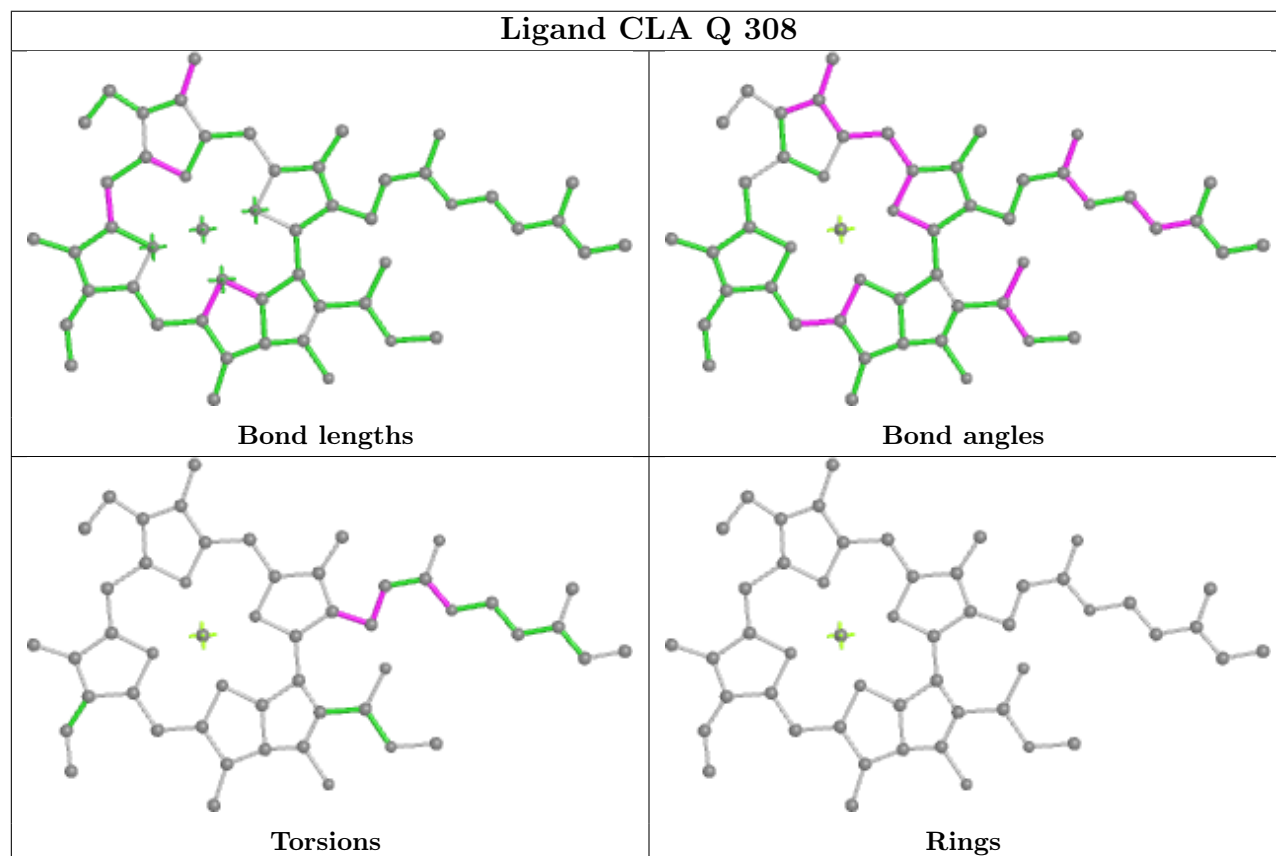
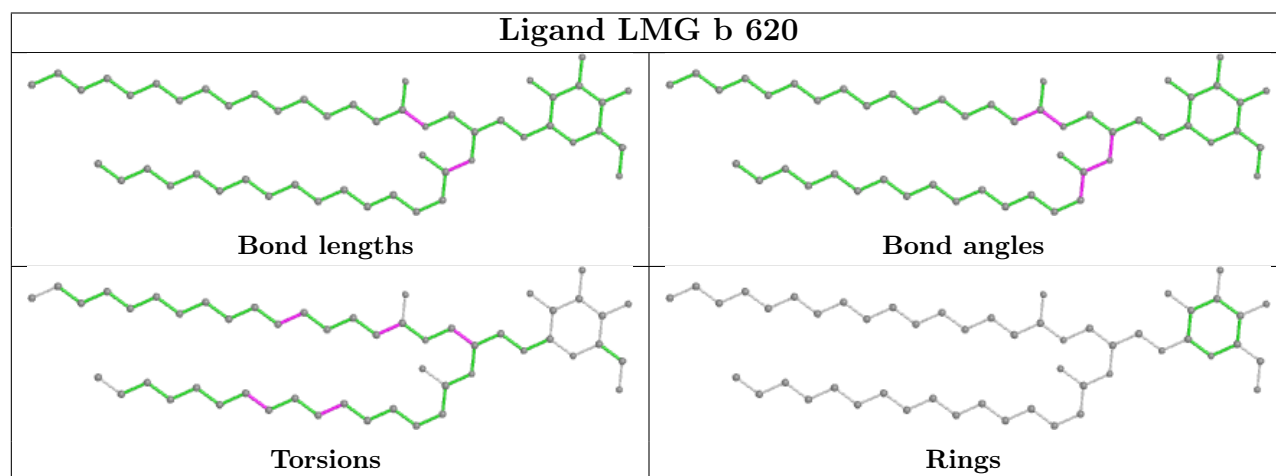
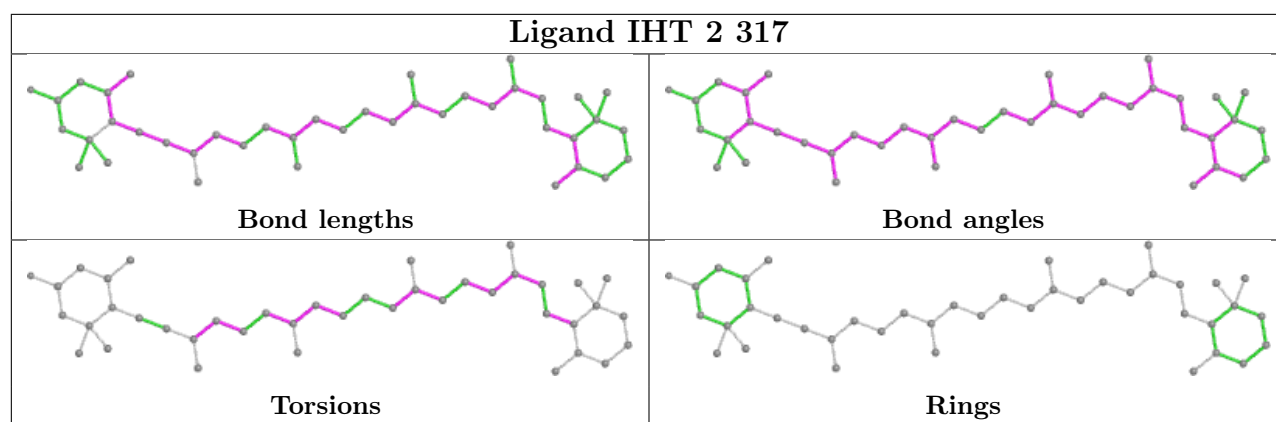
Rings

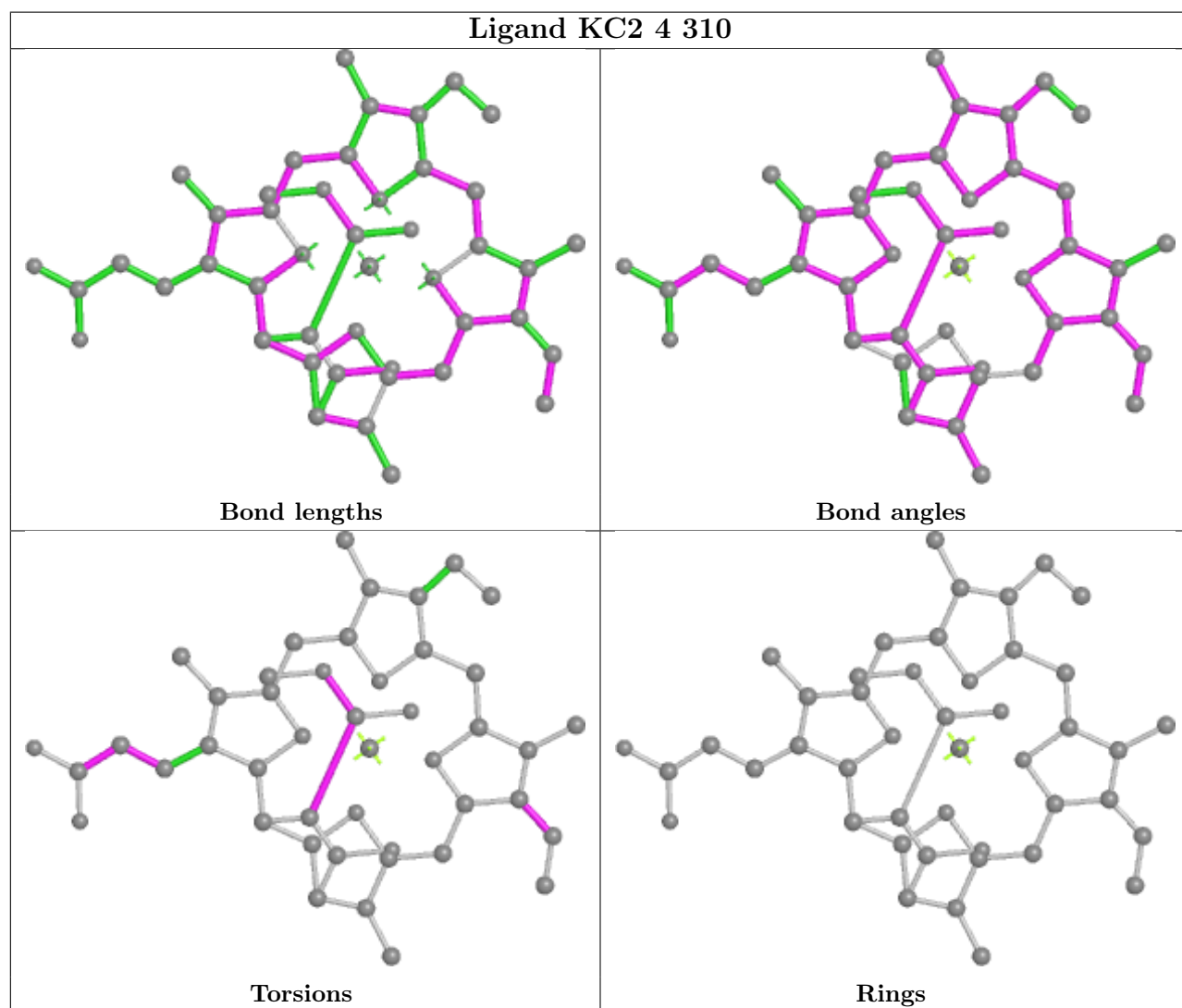
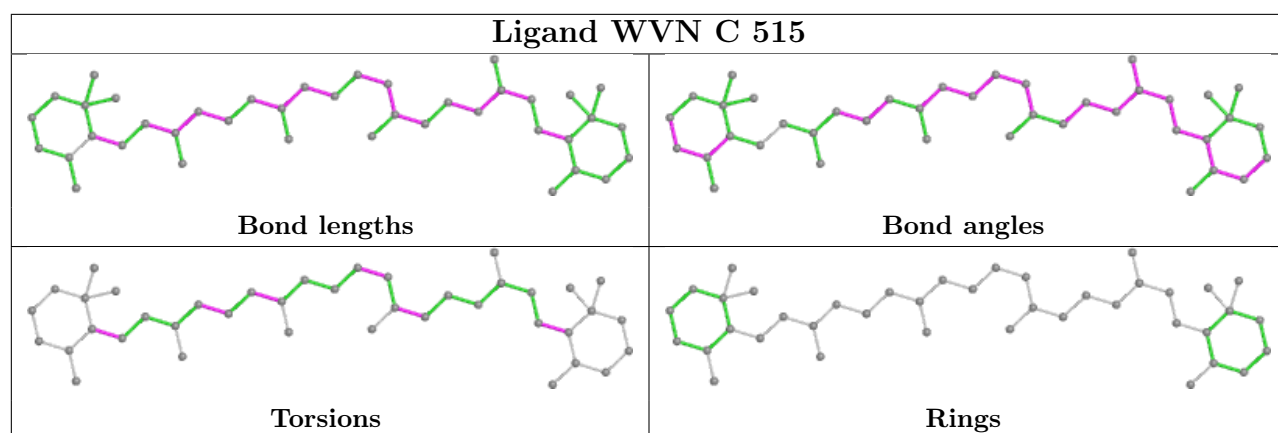
Ligand CLA b 601

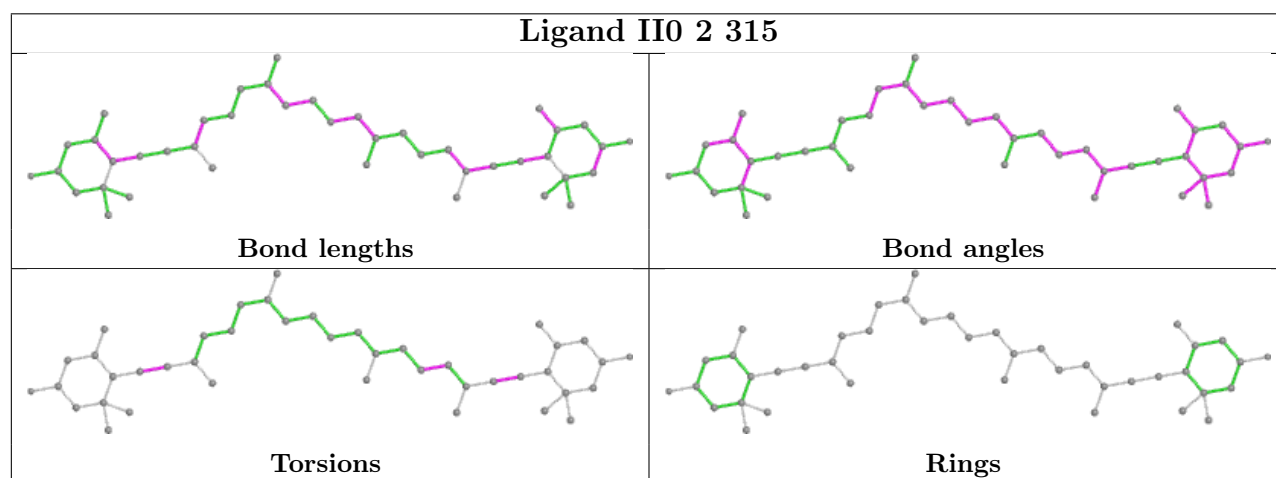
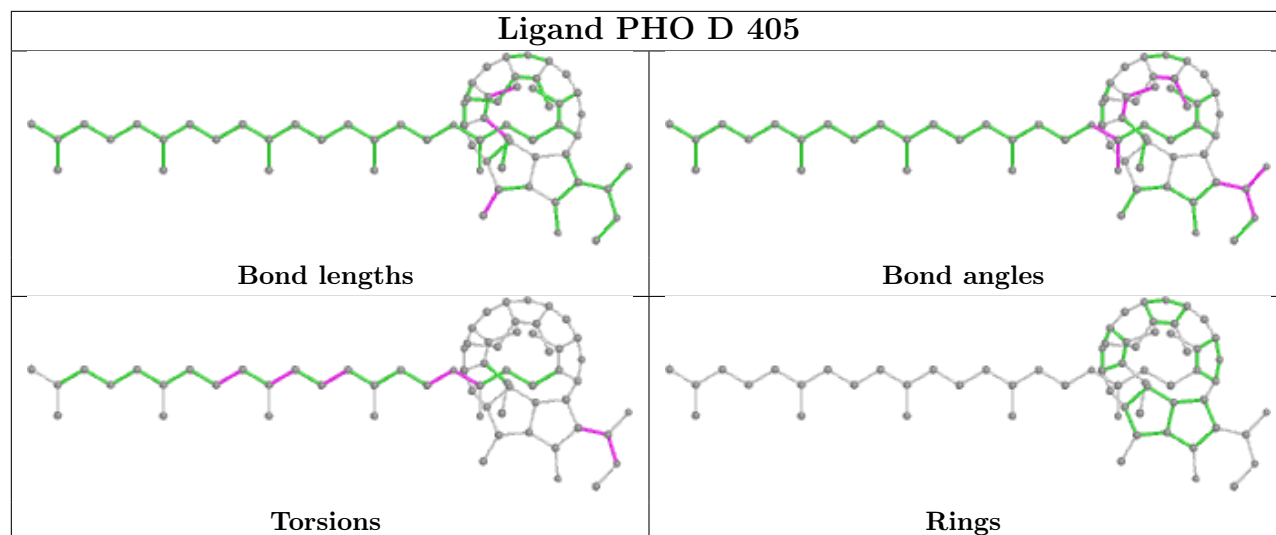


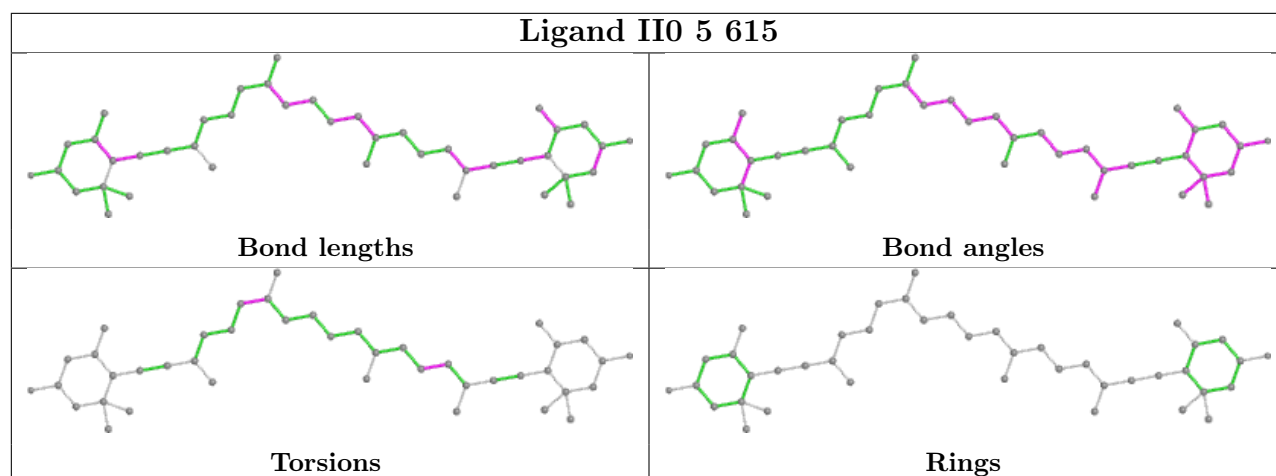
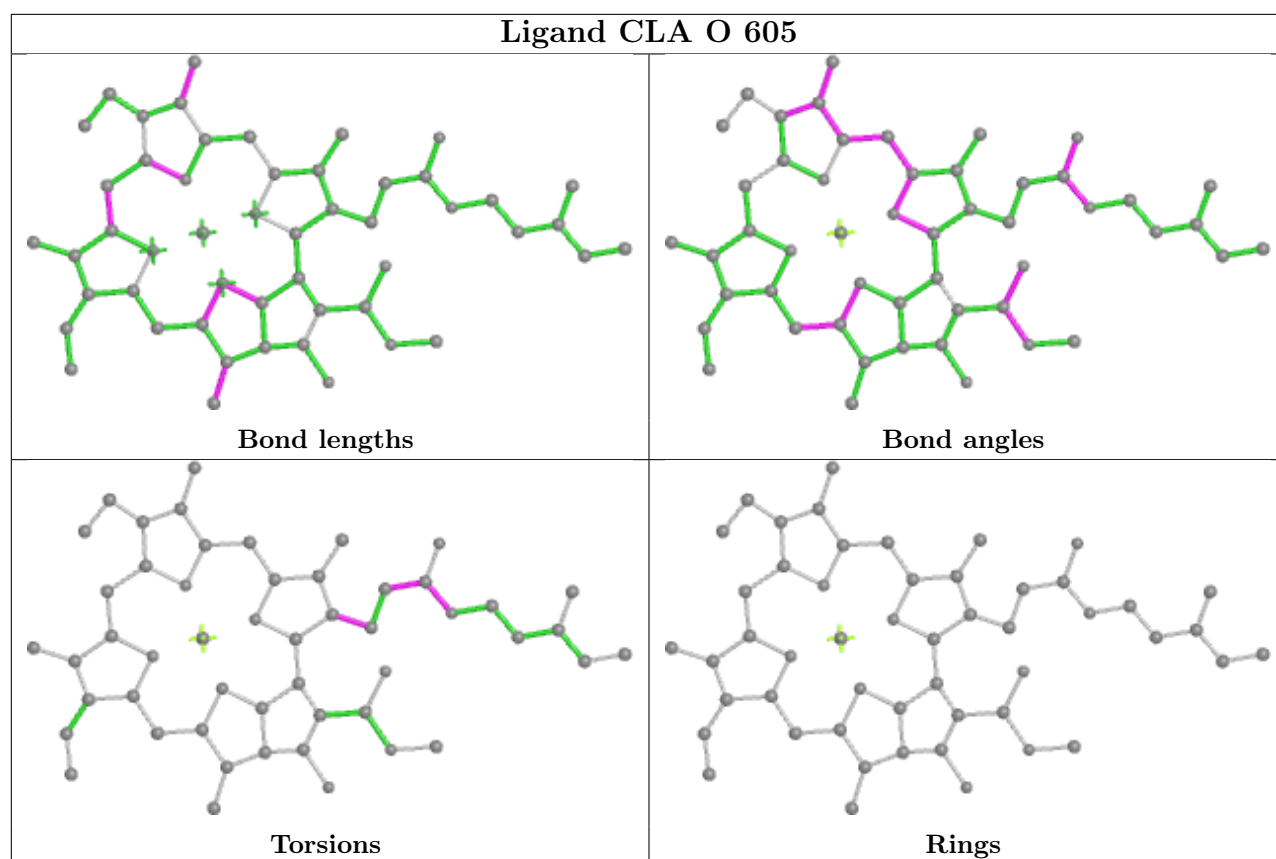
Ligand CLA g 401

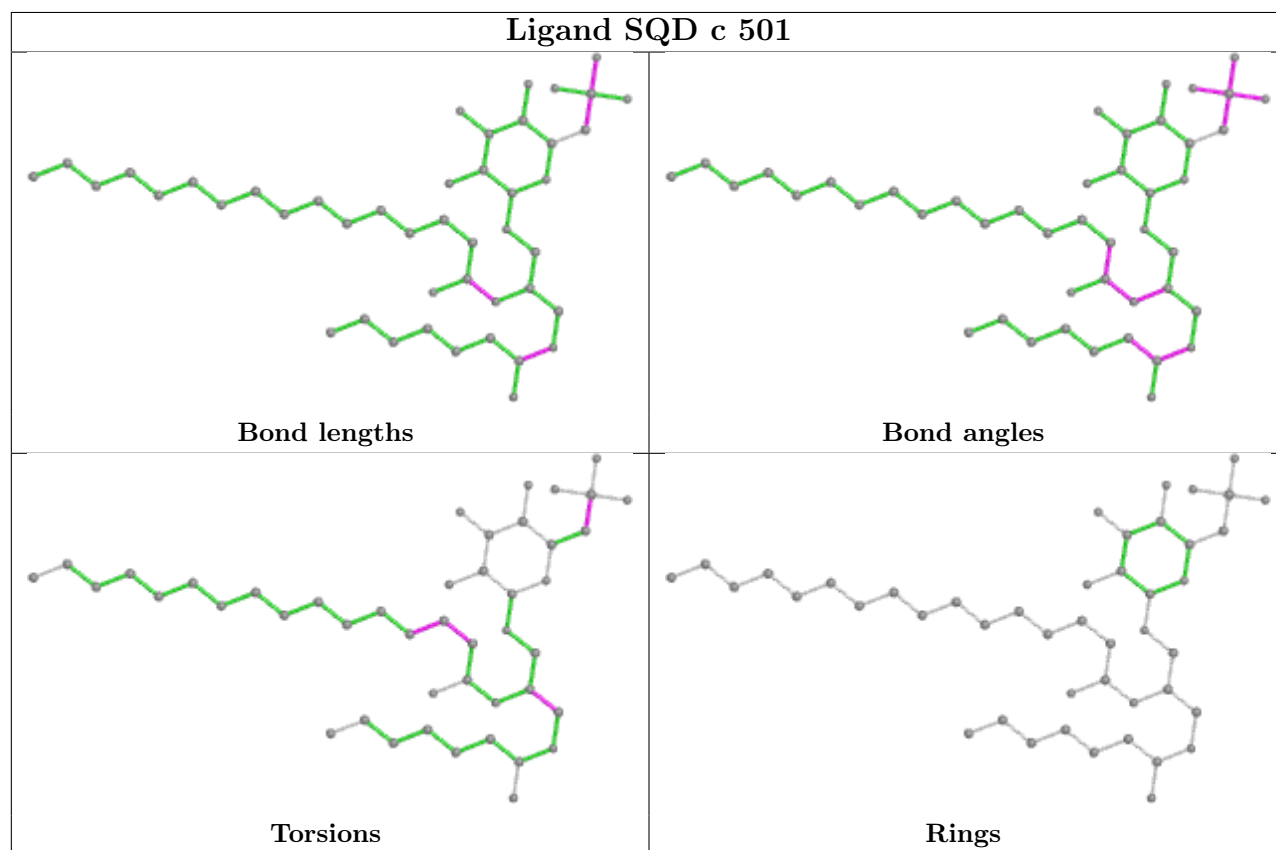
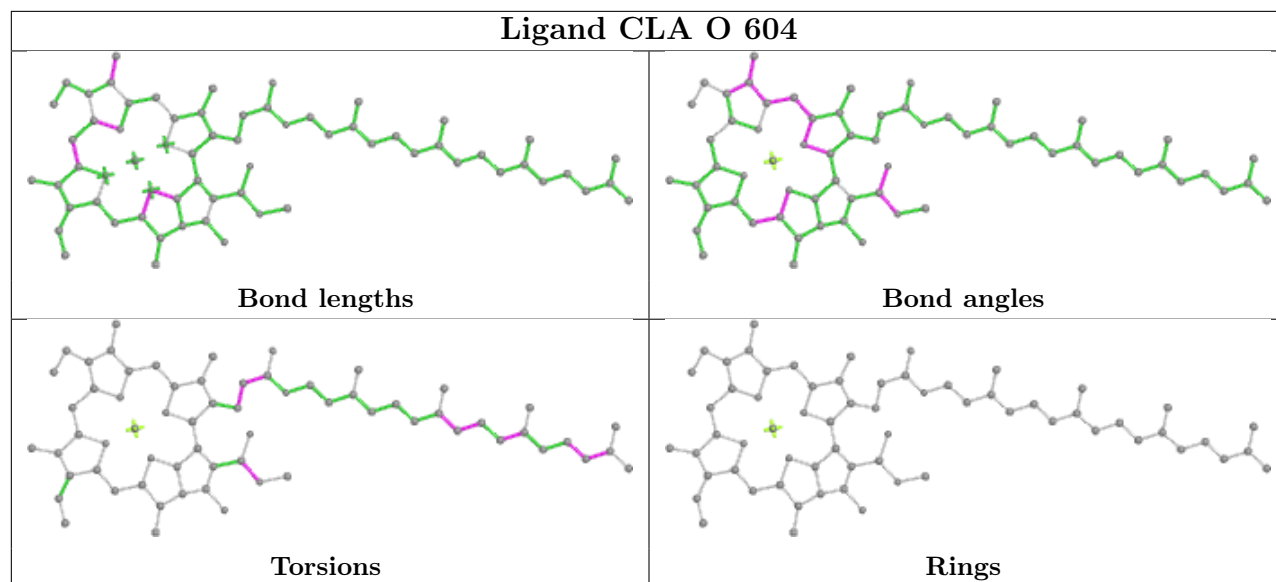


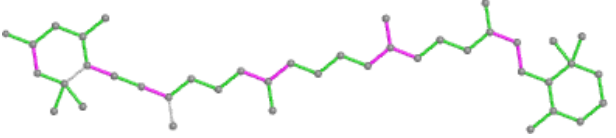
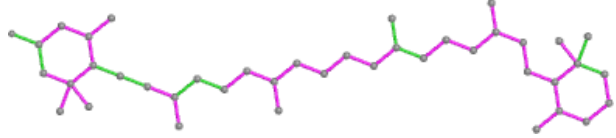
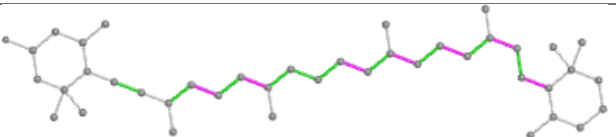
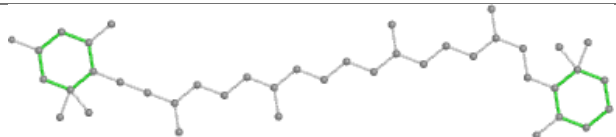
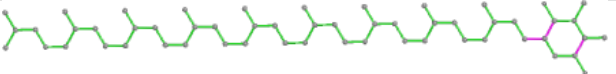
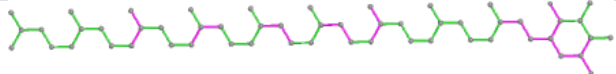
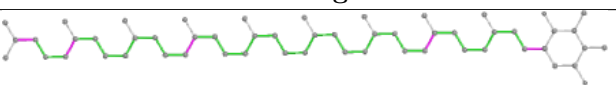
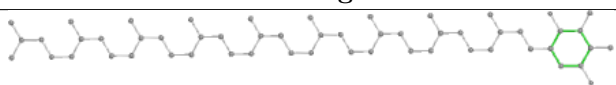




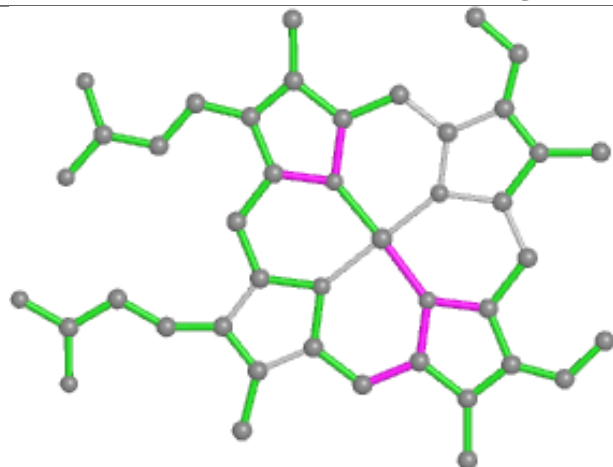




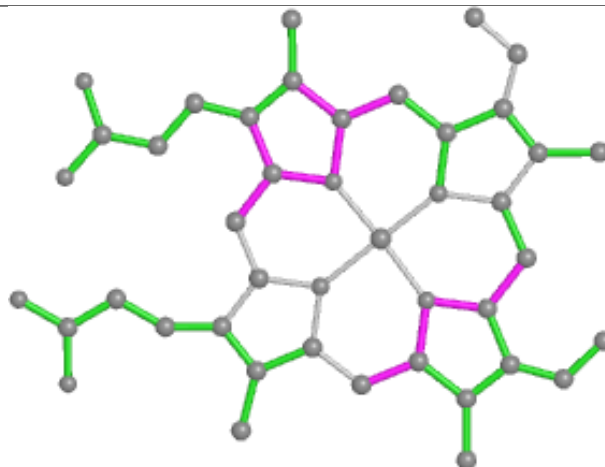


Ligand IHT 5 616	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PL9 d 407	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

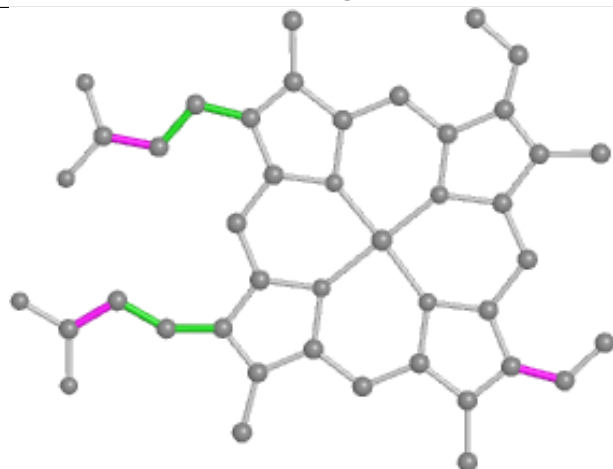
Ligand HEM f 101



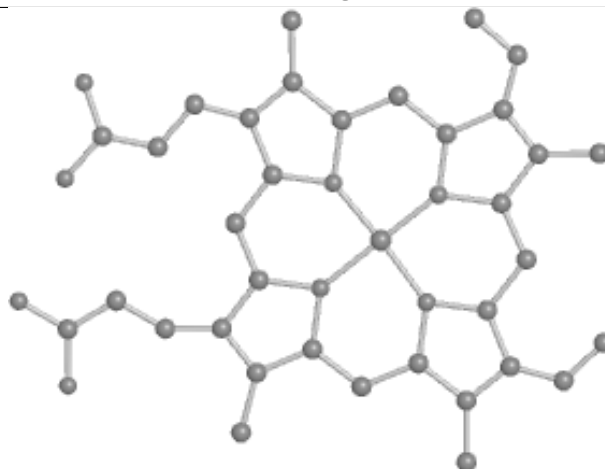
Bond lengths



Bond angles

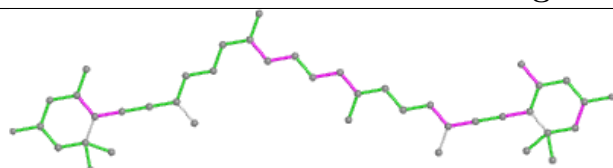


Torsions

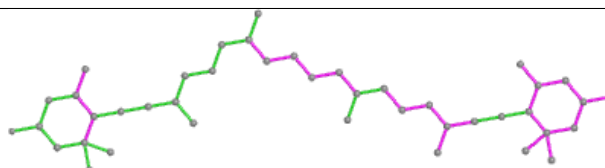


Rings

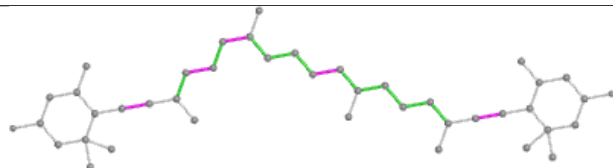
Ligand II0 6 611



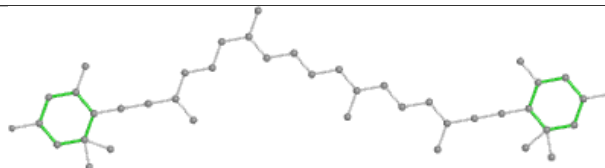
Bond lengths



Bond angles

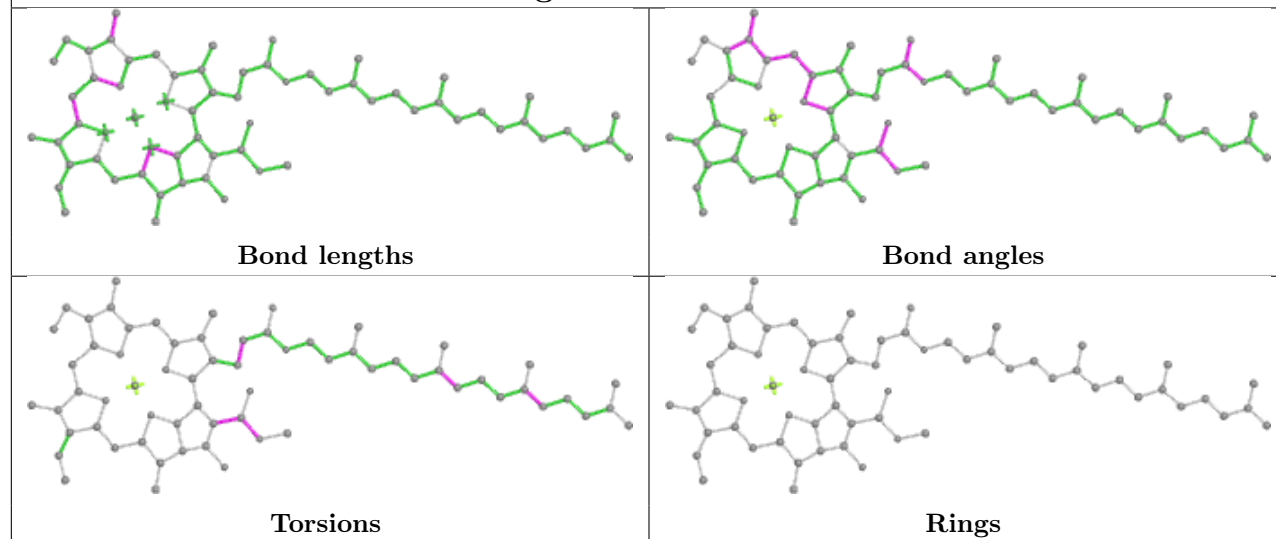


Torsions

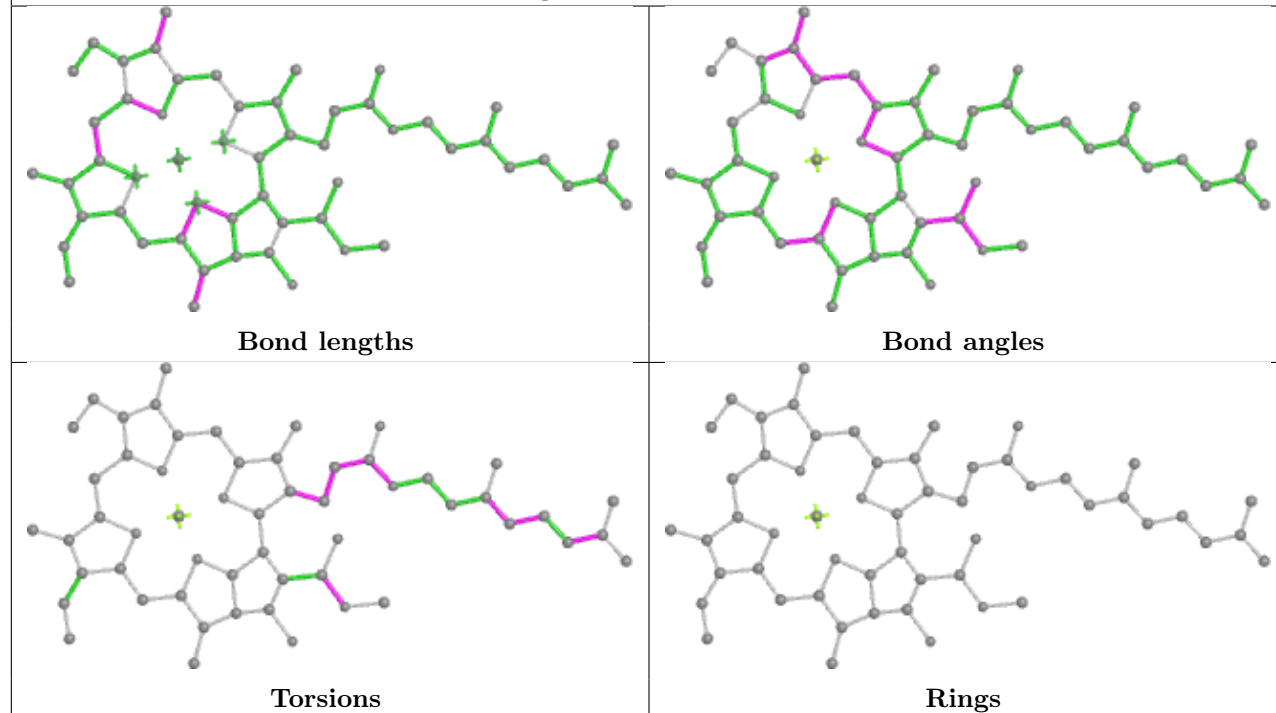


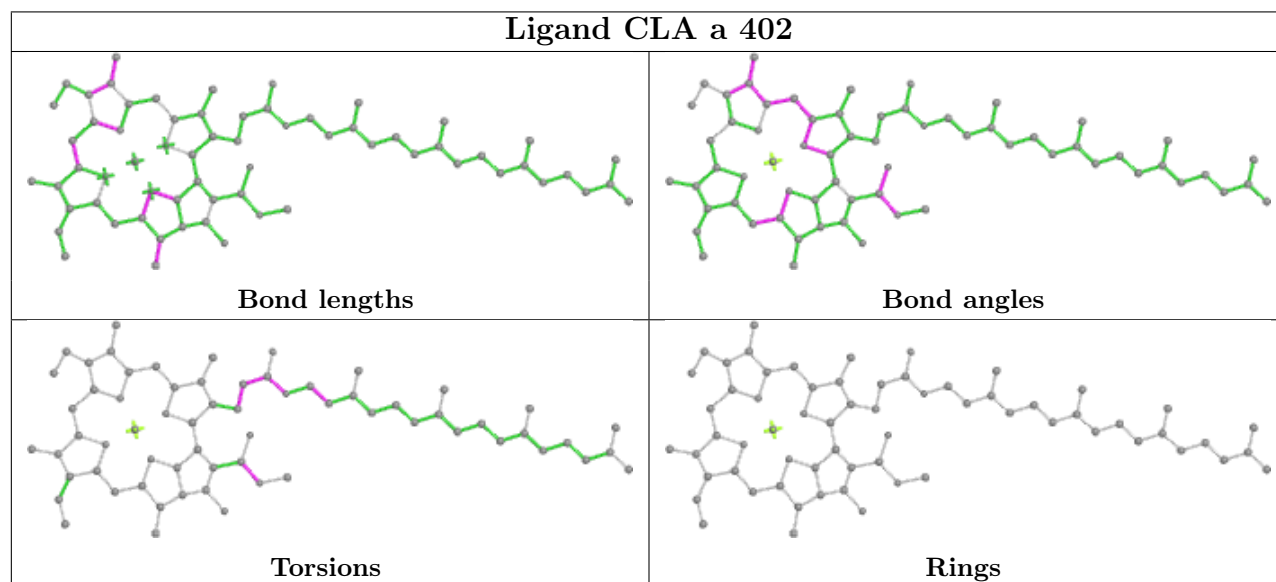
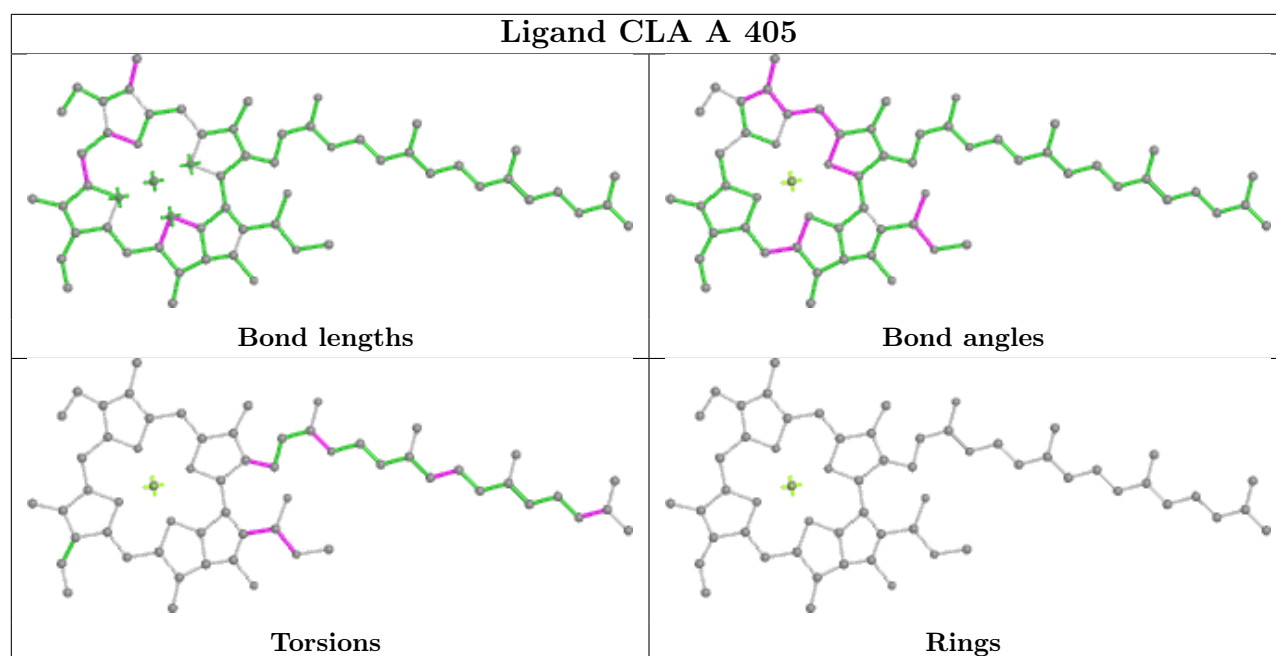
Rings

Ligand CLA b 608

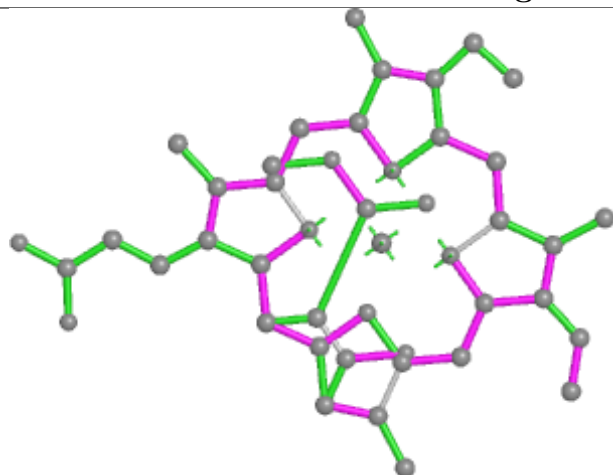


Ligand CLA 6 605

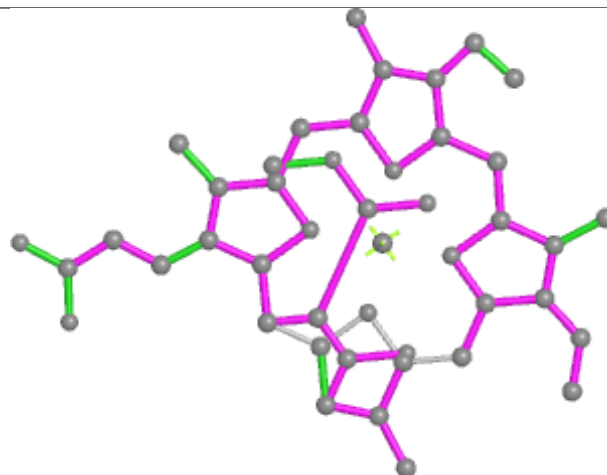




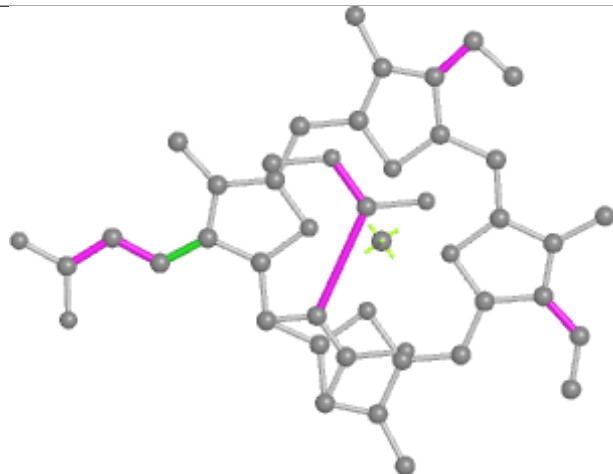
Ligand KC2 N 612



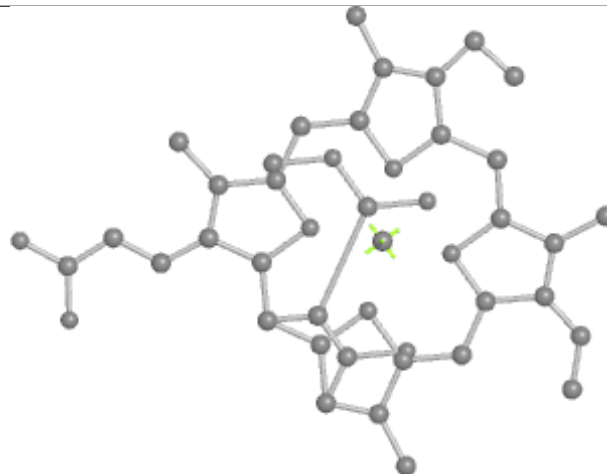
Bond lengths



Bond angles

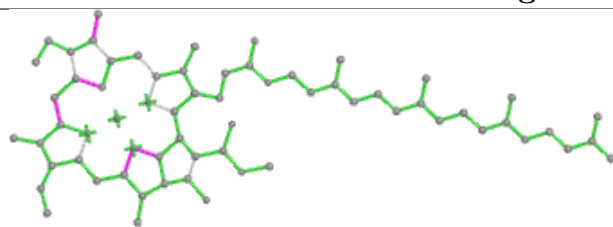


Torsions

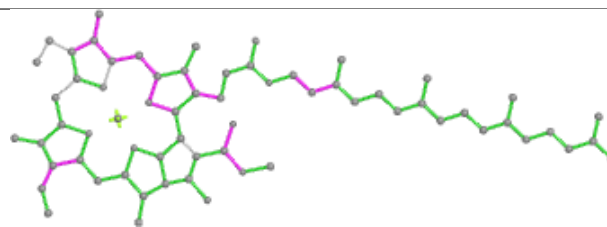


Rings

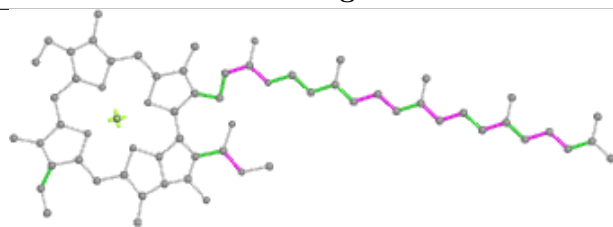
Ligand CLA 4 303



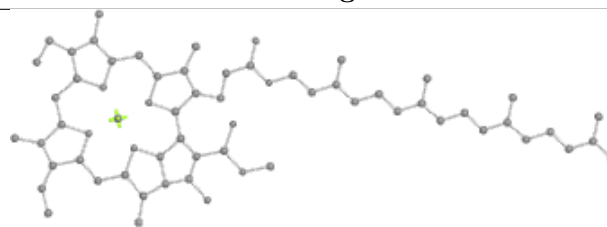
Bond lengths



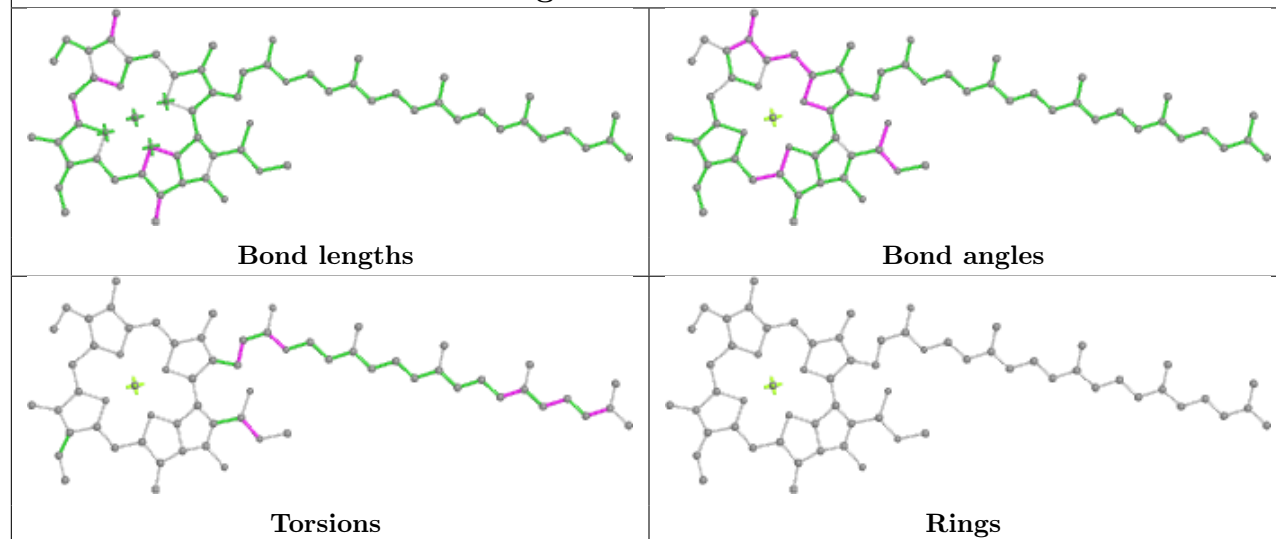
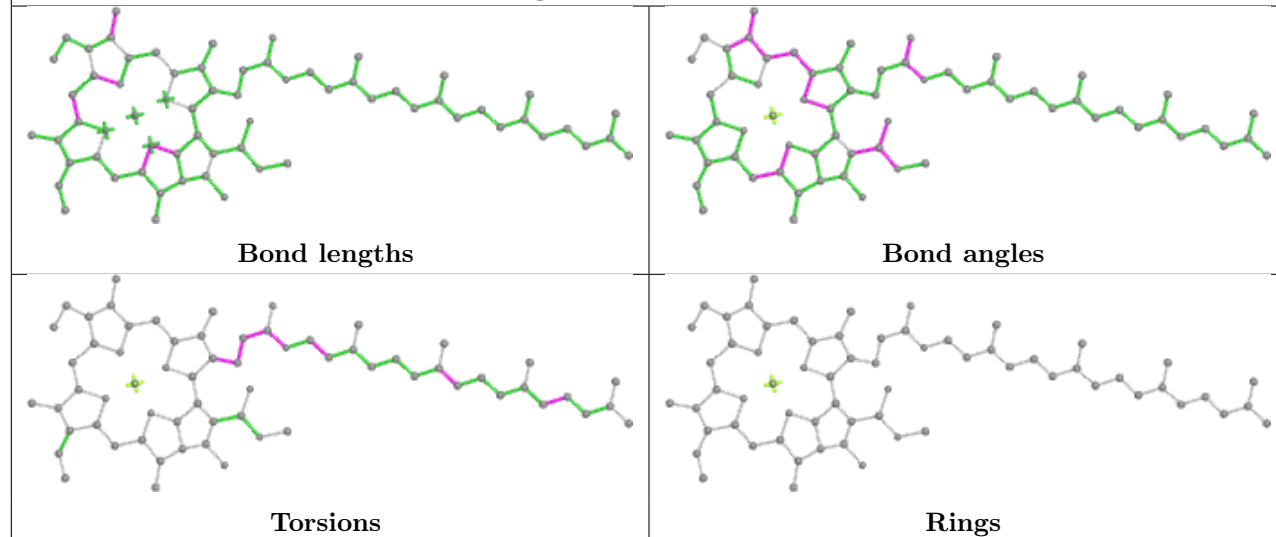
Bond angles

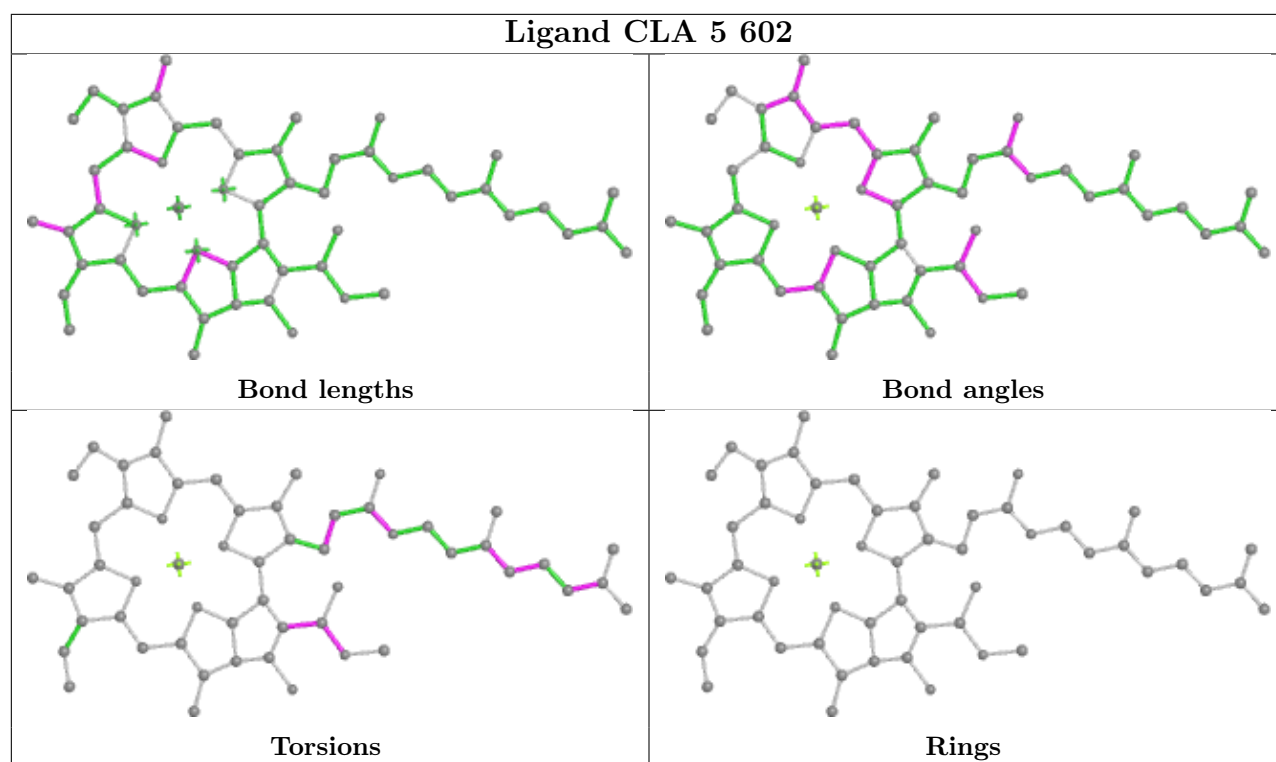


Torsions

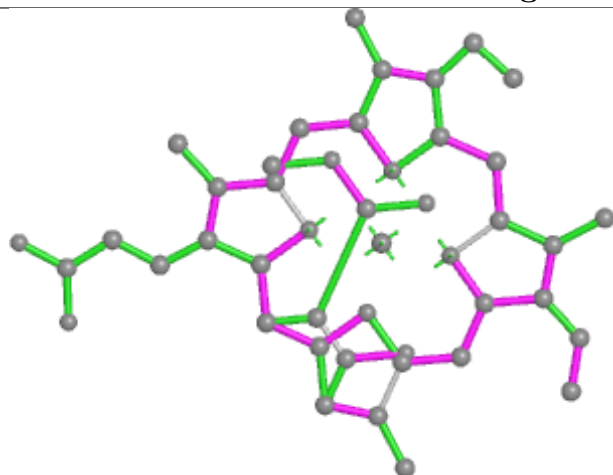


Rings

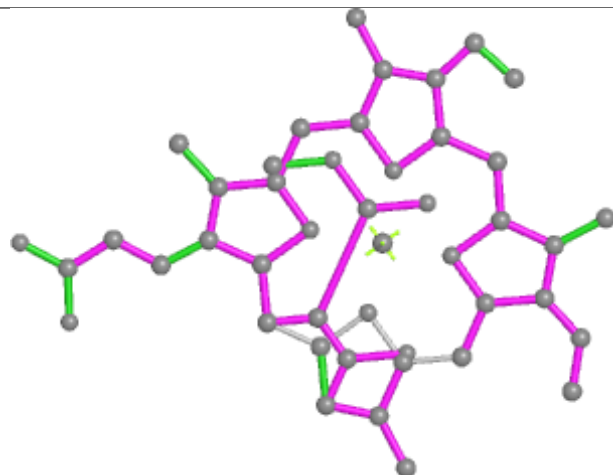
Ligand CLA 6 610**Ligand CLA D 404**



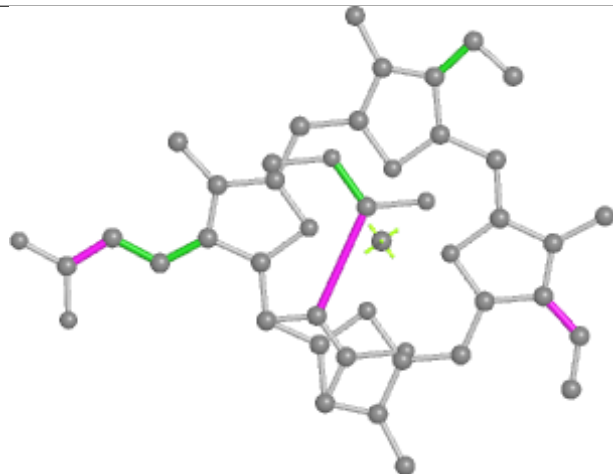
Ligand KC2 6 608



Bond lengths



Bond angles

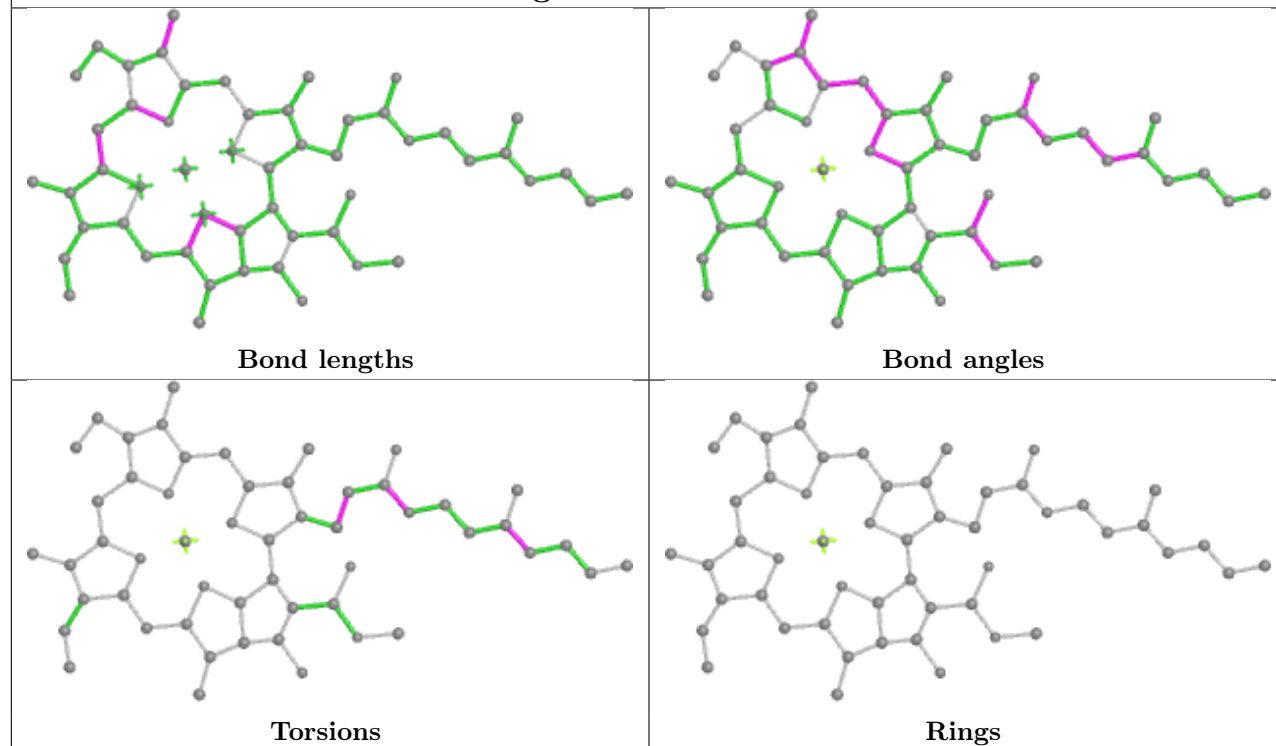


Torsions

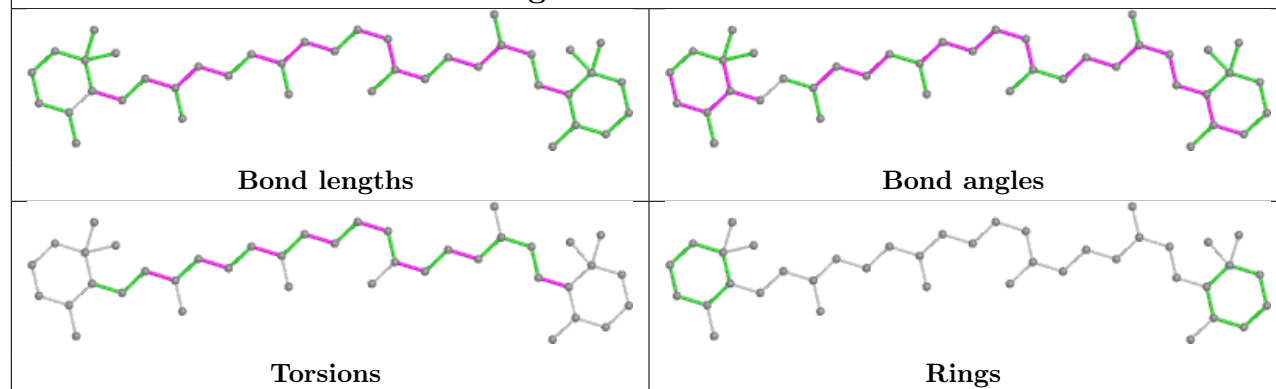


Rings

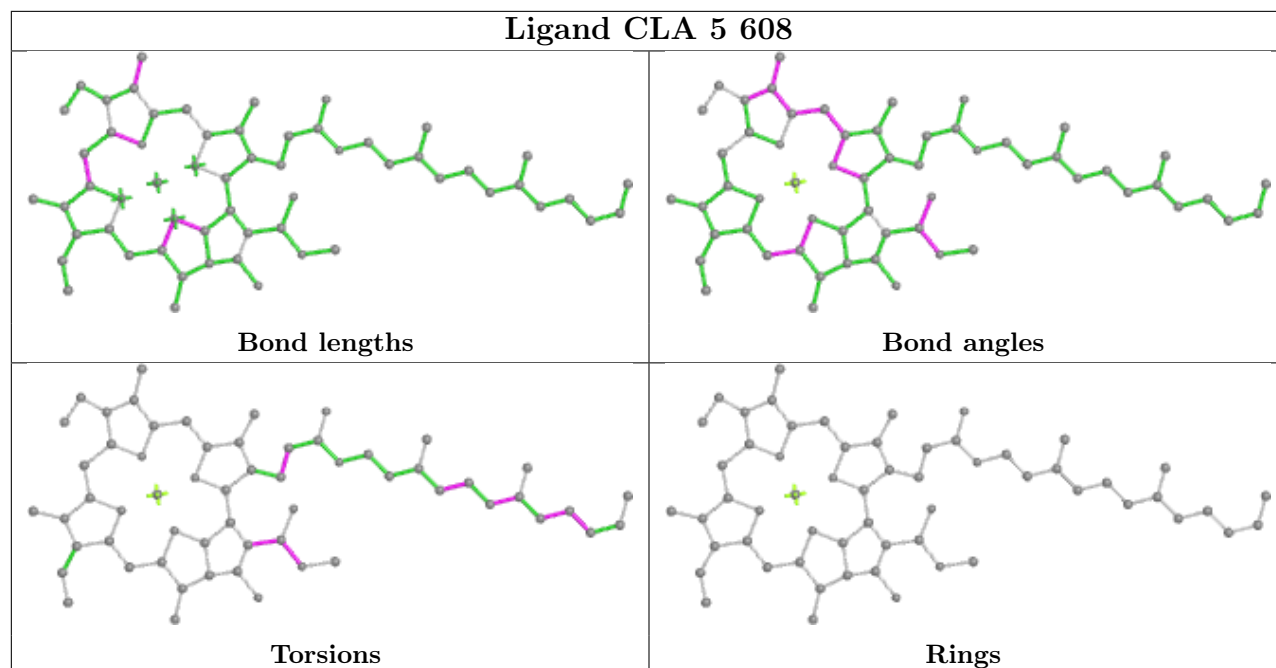
Ligand CLA P 609



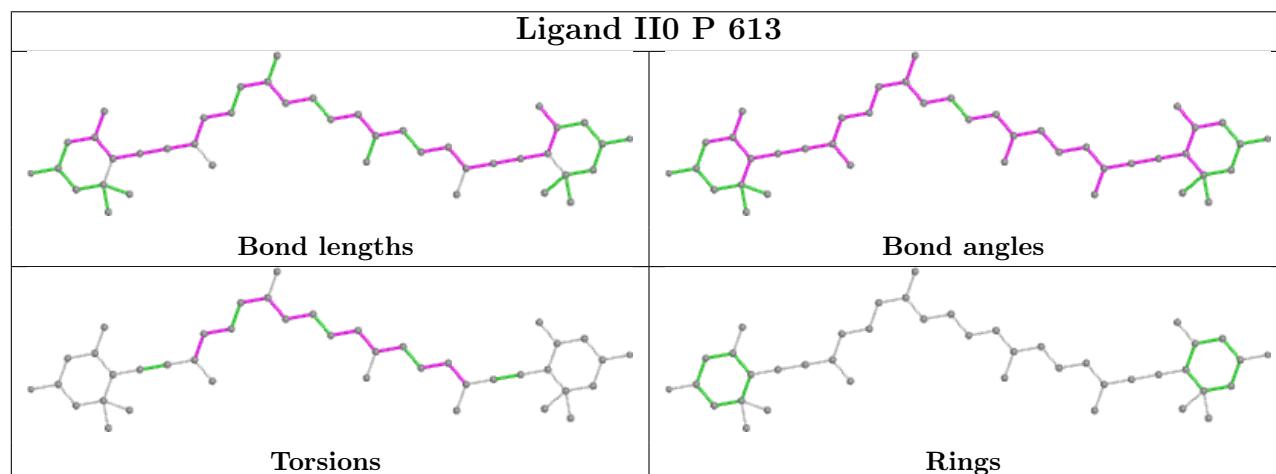
Ligand WVN c 518



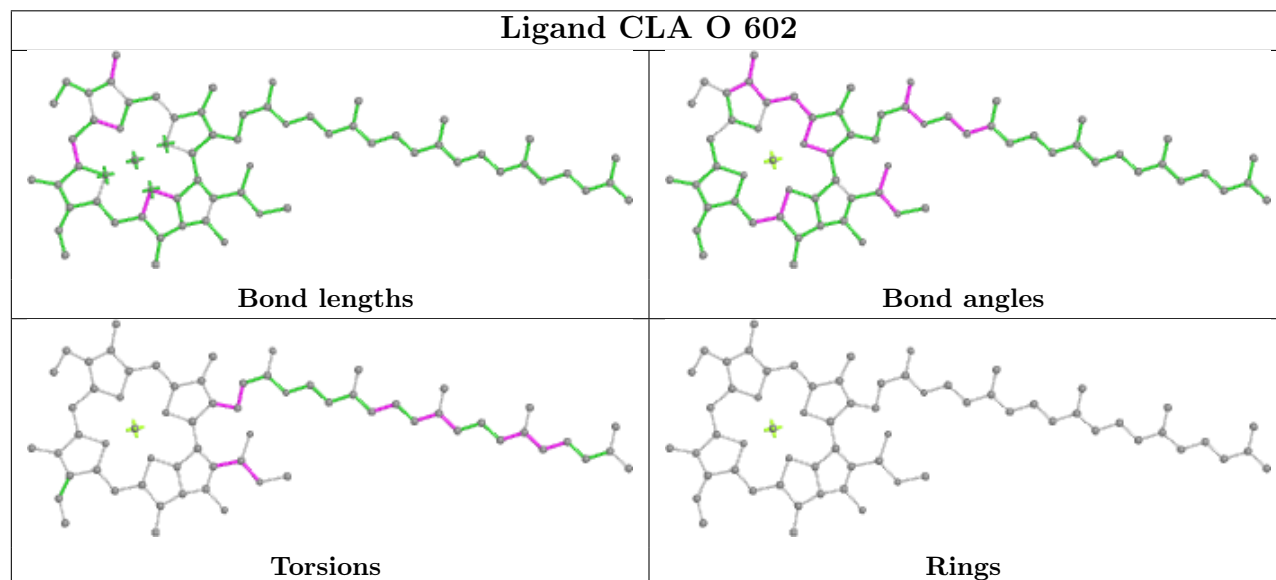
Ligand CLA 5 608

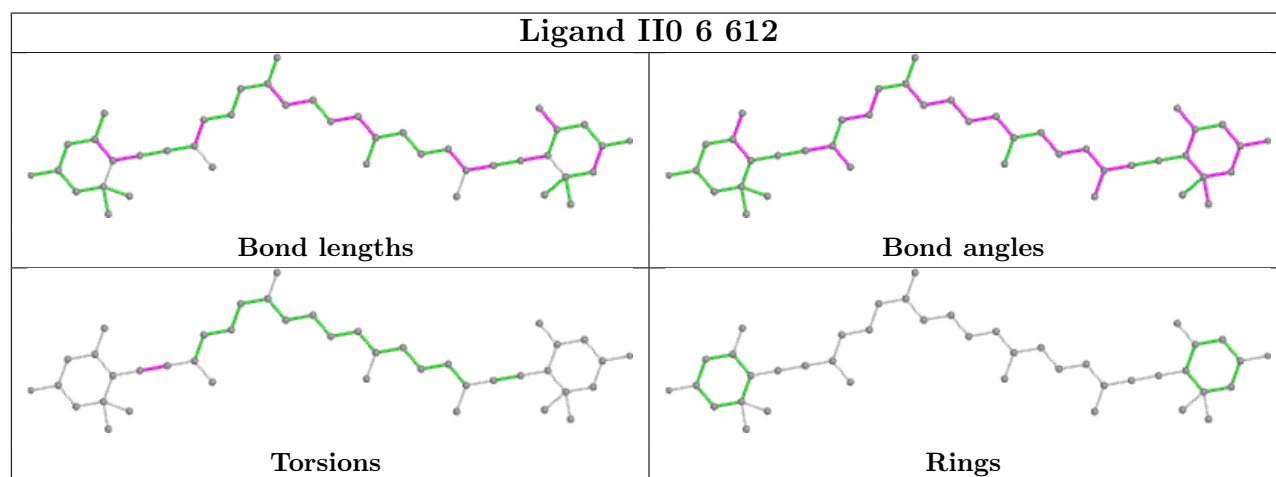
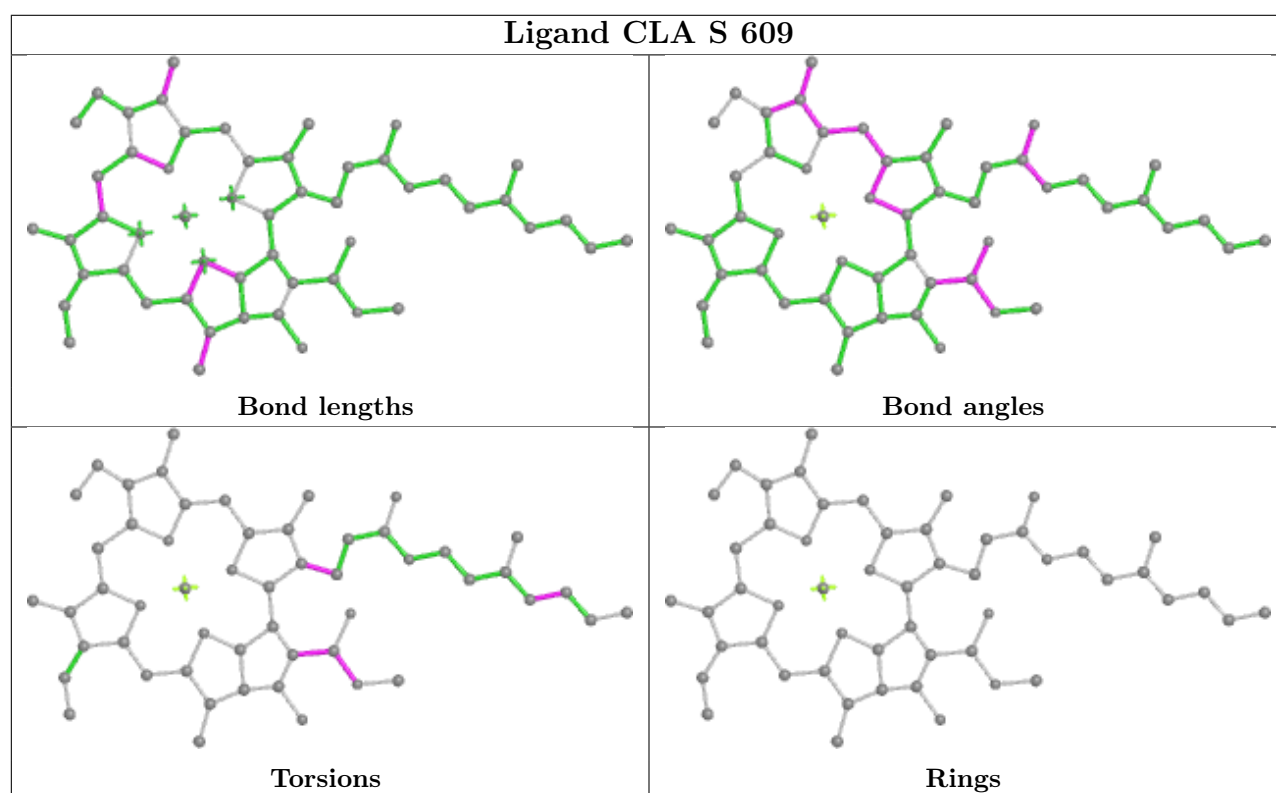
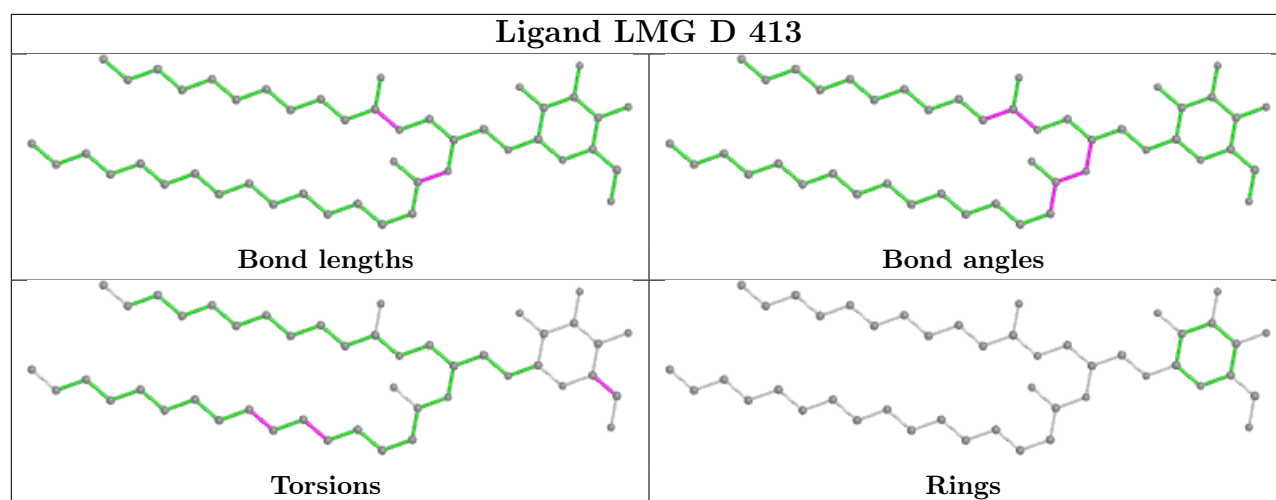


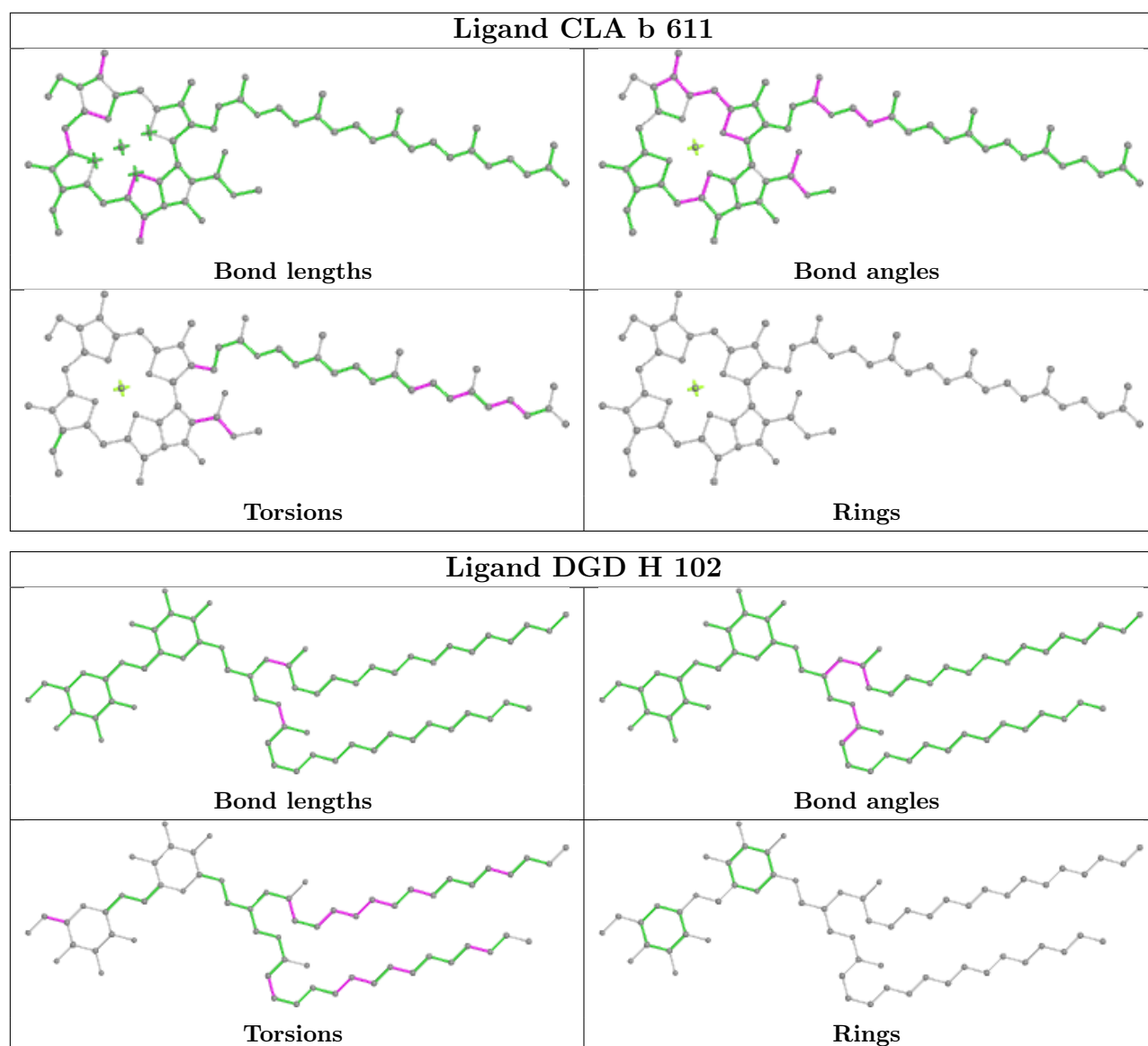
Ligand II0 P 613



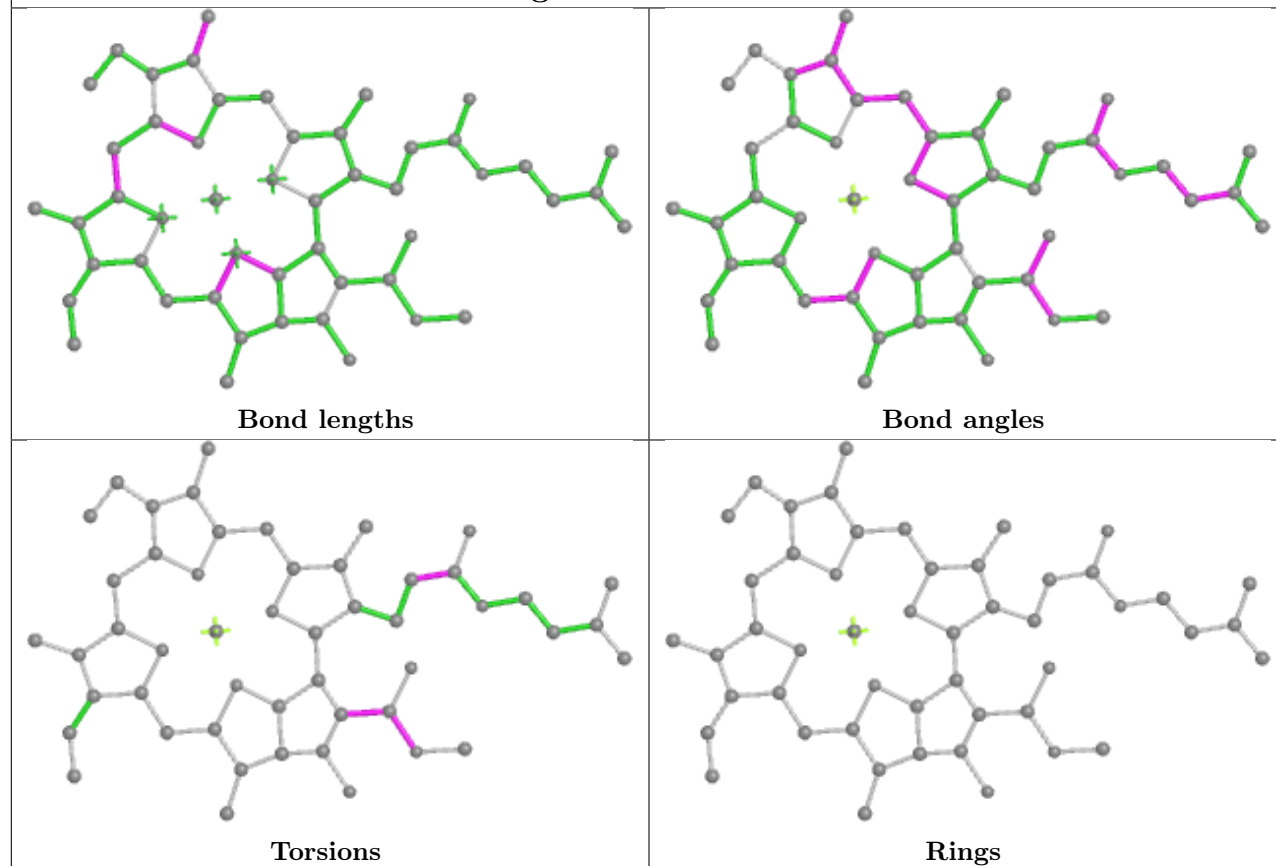
Ligand CLA O 602



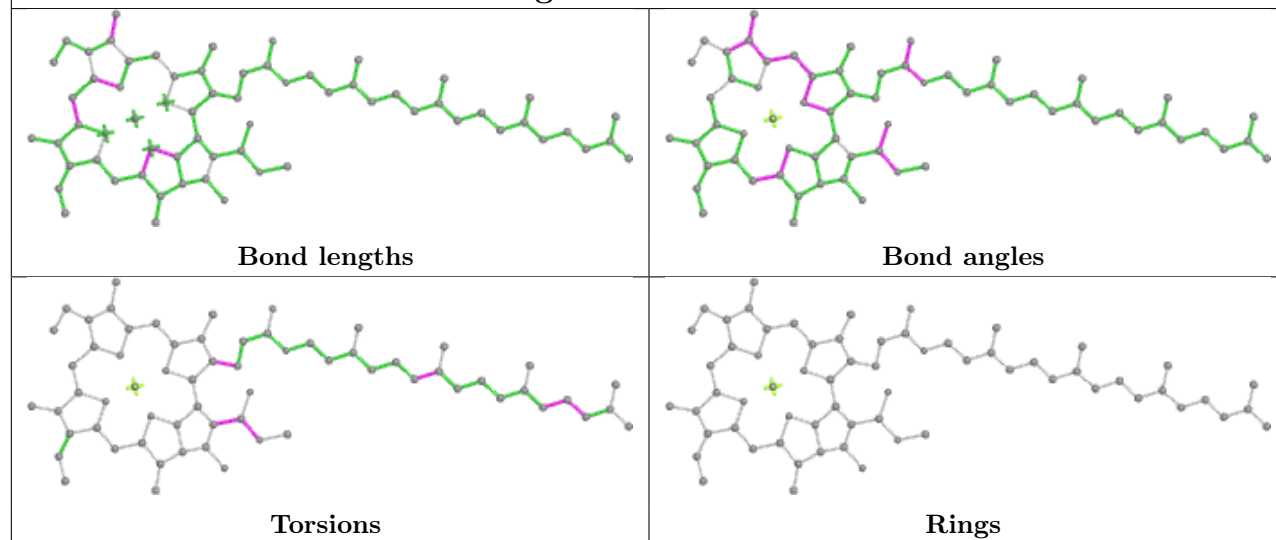




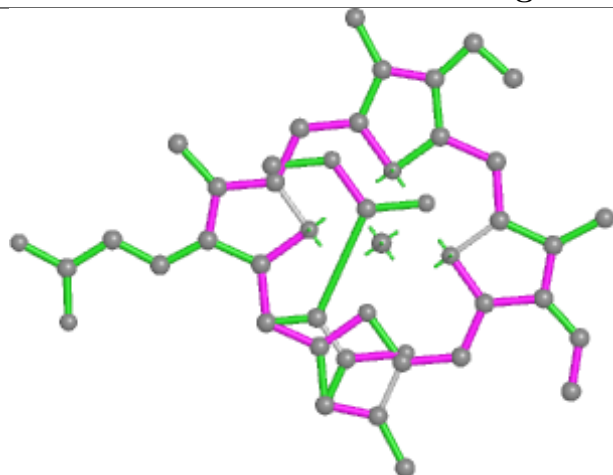
Ligand CLA N 606



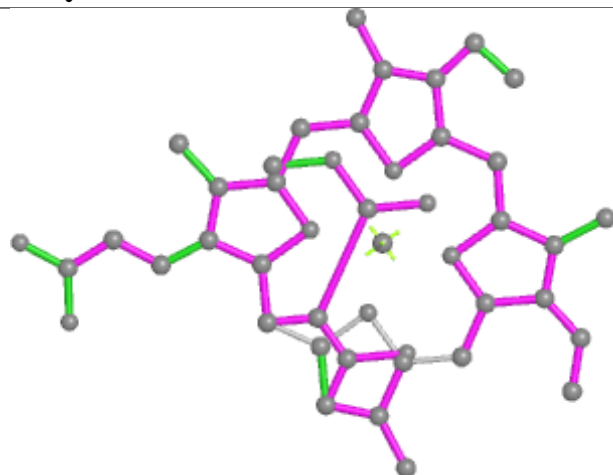
Ligand CLA b 609



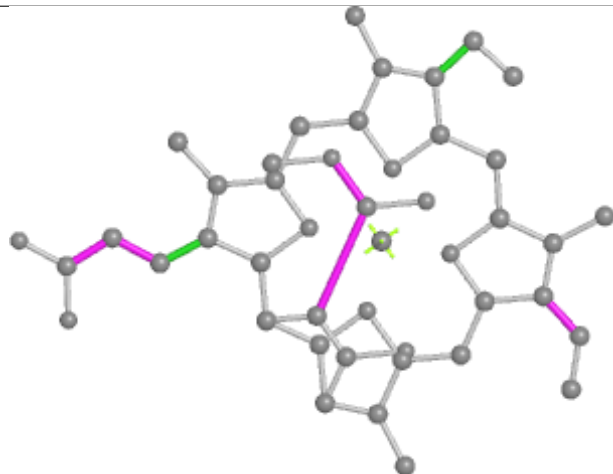
Ligand KC2 Q 309



Bond lengths



Bond angles

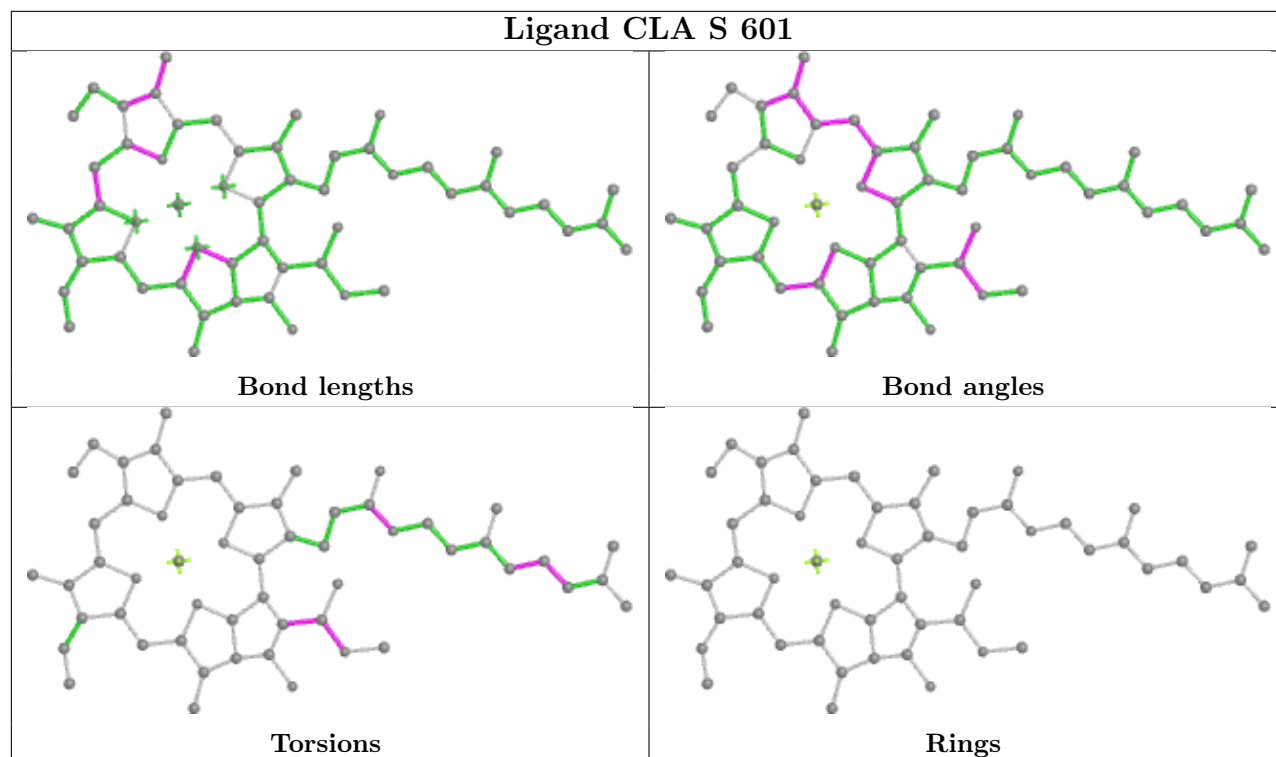


Torsions

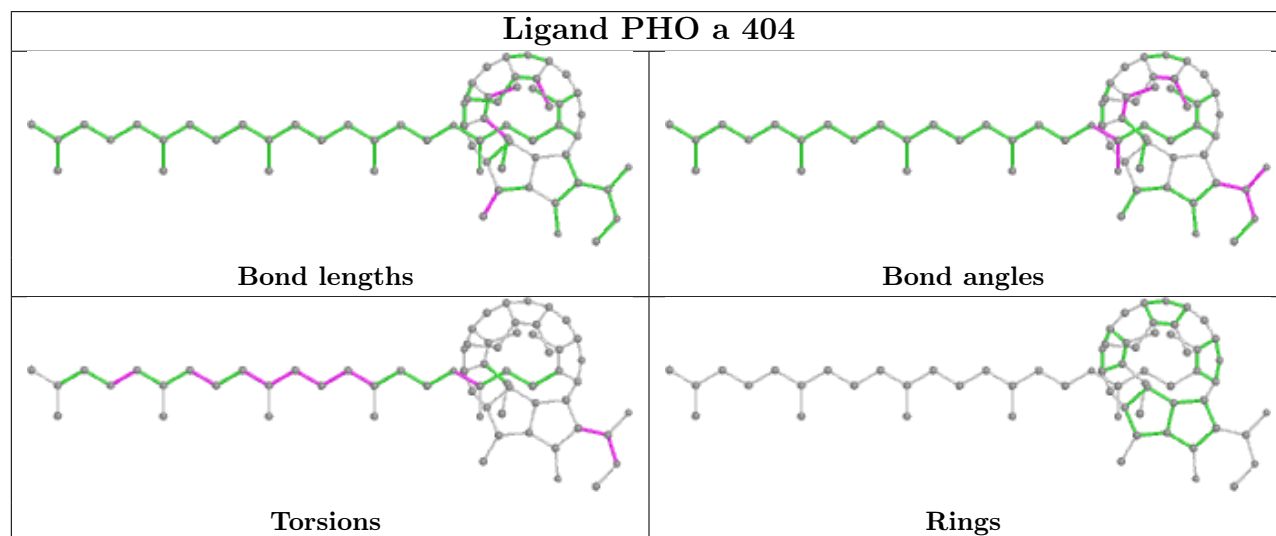


Rings

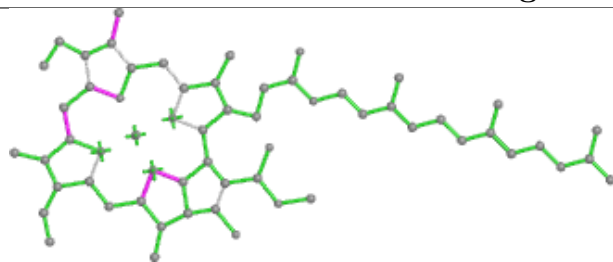
Ligand CLA S 601



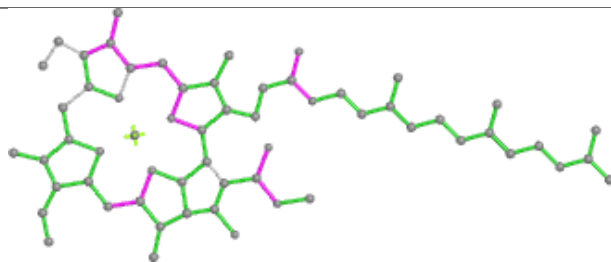
Ligand PHO a 404



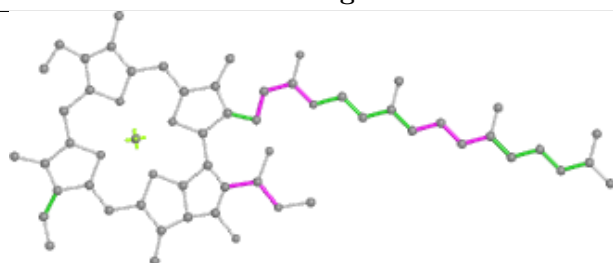
Ligand CLA c 506



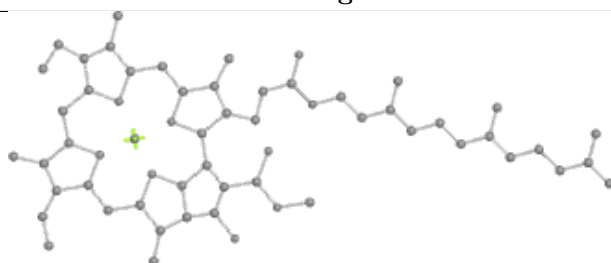
Bond lengths



Bond angles

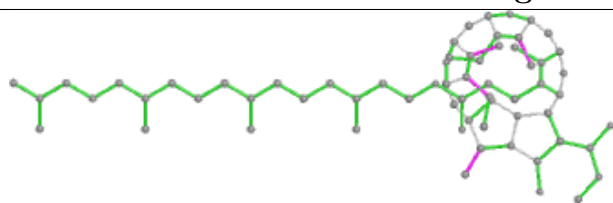


Torsions

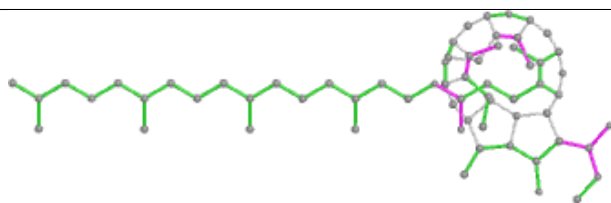


Rings

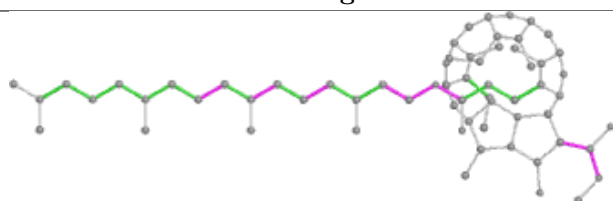
Ligand PHO d 403



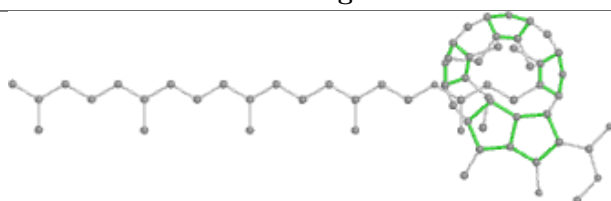
Bond lengths



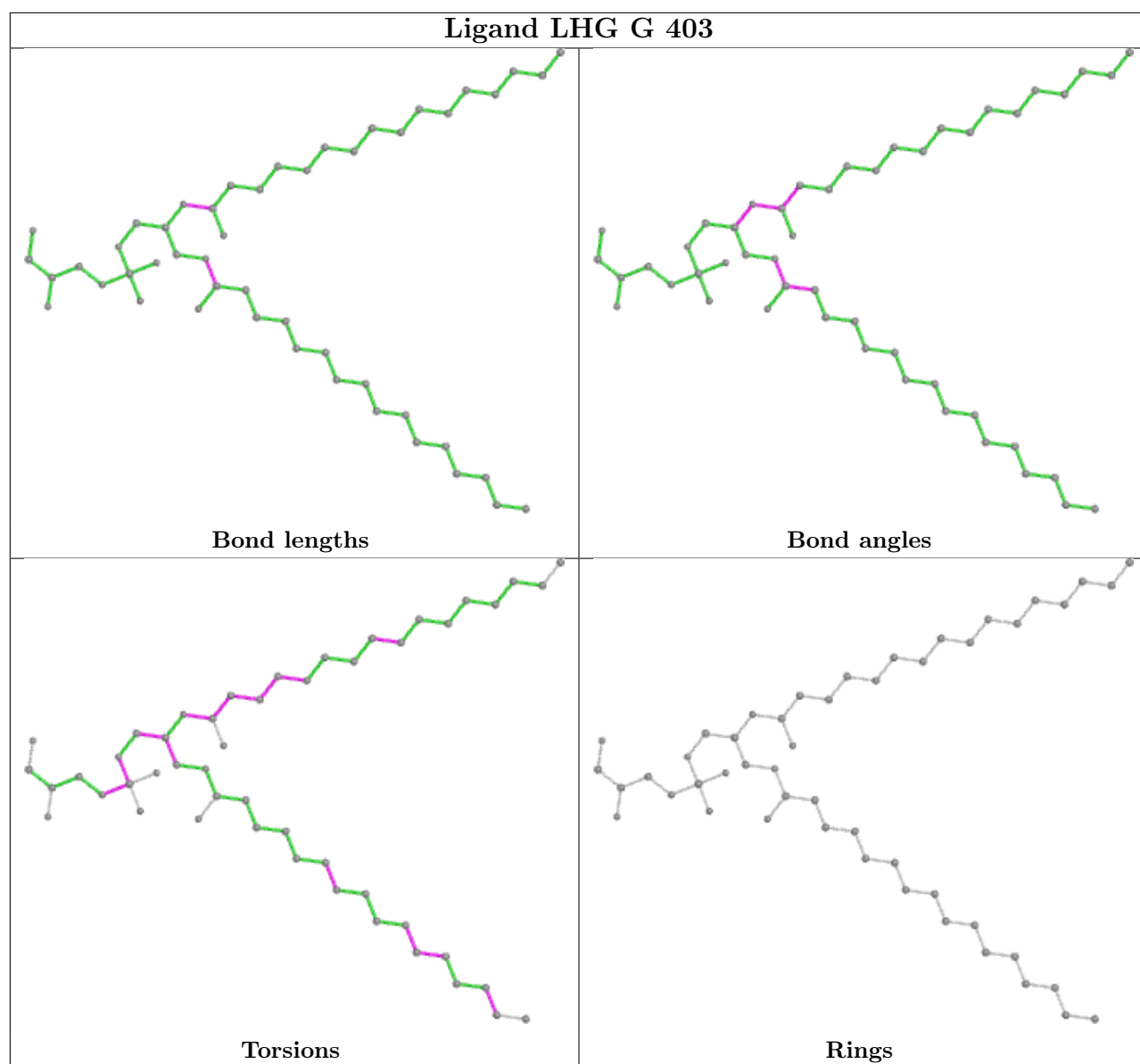
Bond angles



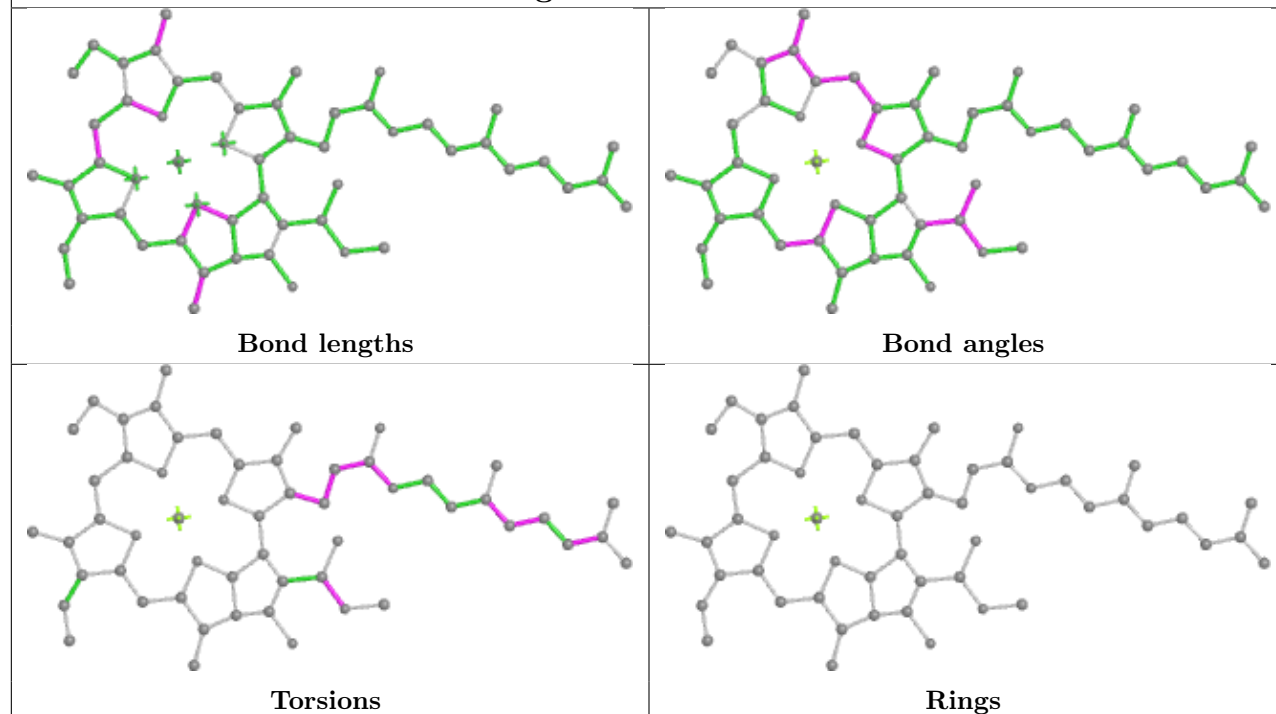
Torsions



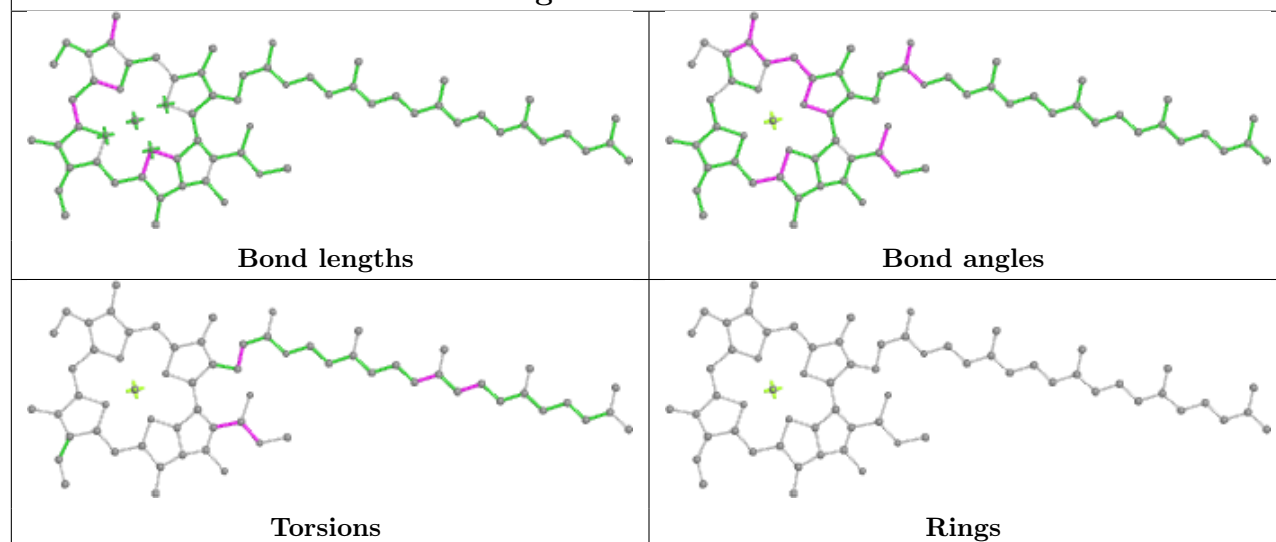
Rings

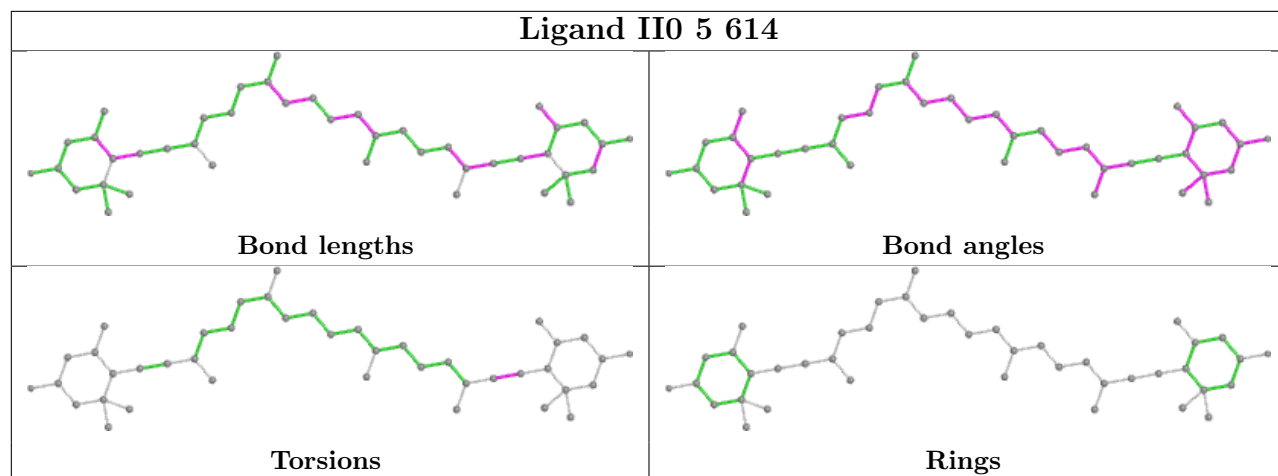
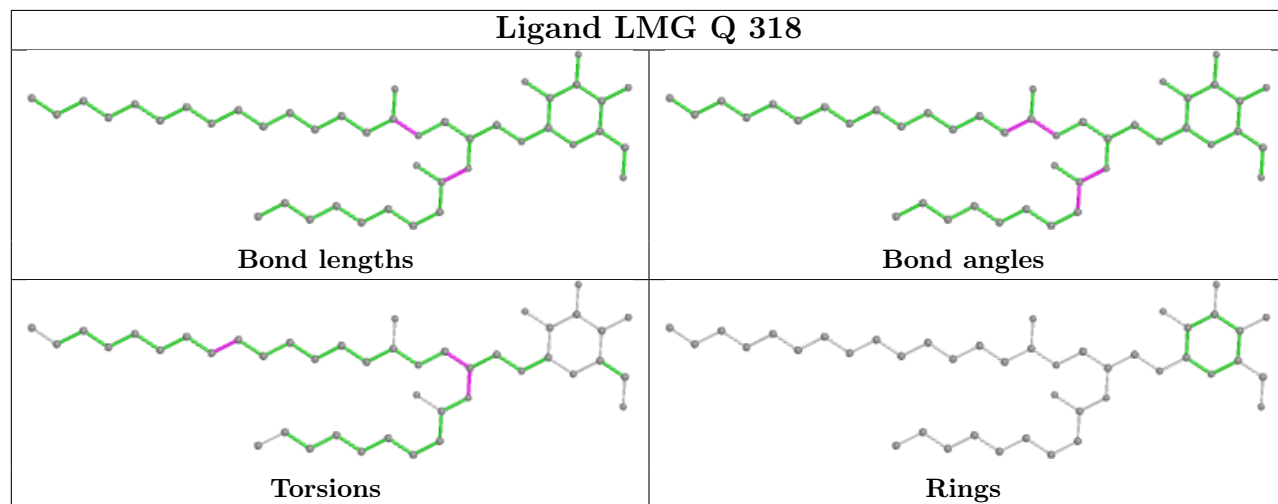


Ligand CLA S 605

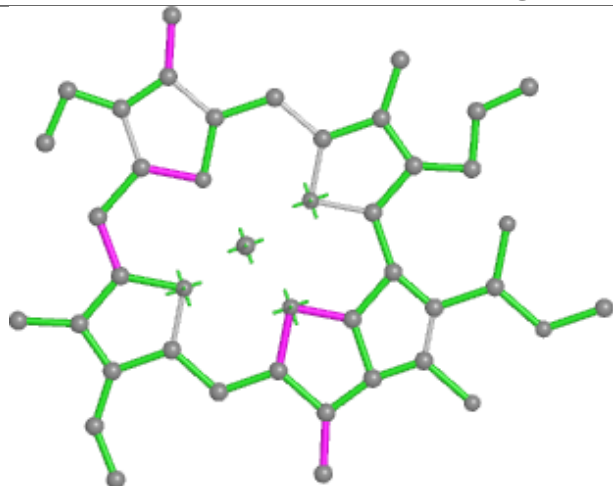


Ligand CLA b 606

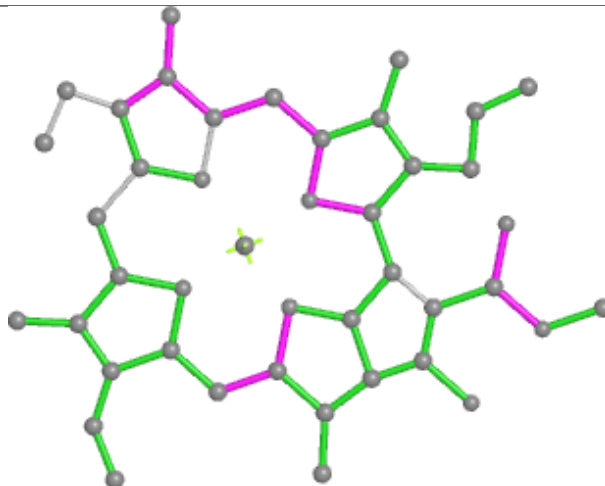


Ligand II0 5 614**Ligand LMG Q 318**

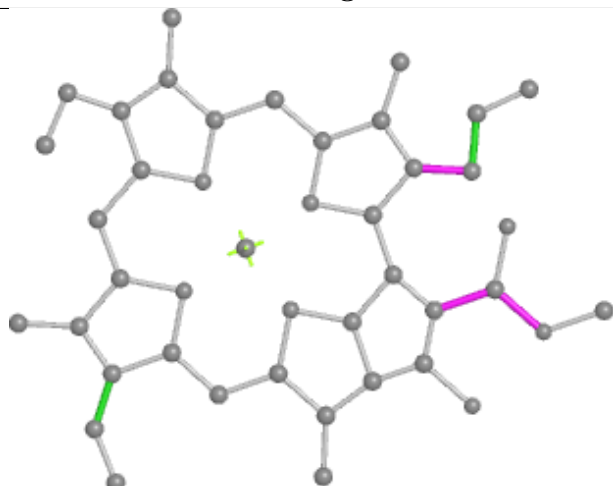
Ligand CLA R 307



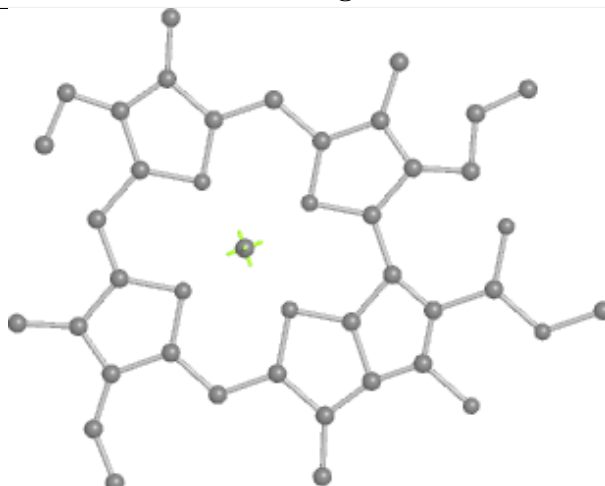
Bond lengths



Bond angles

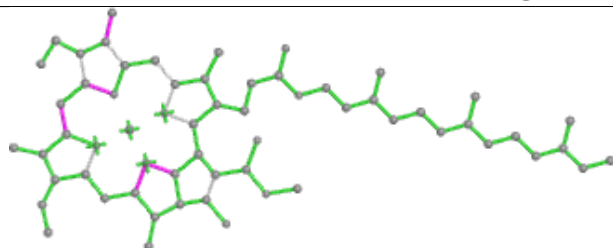


Torsions

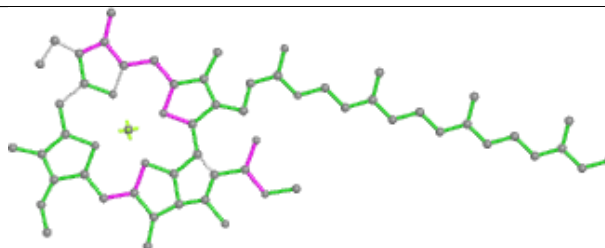


Rings

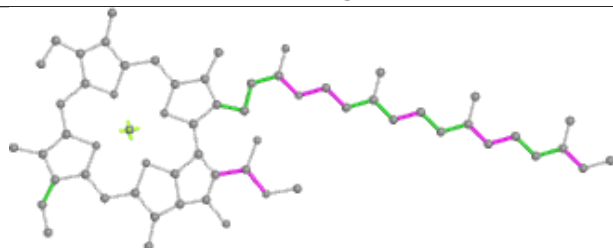
Ligand CLA d 406



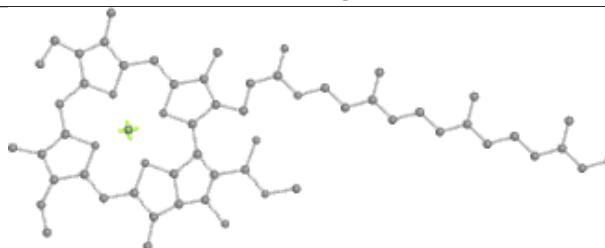
Bond lengths



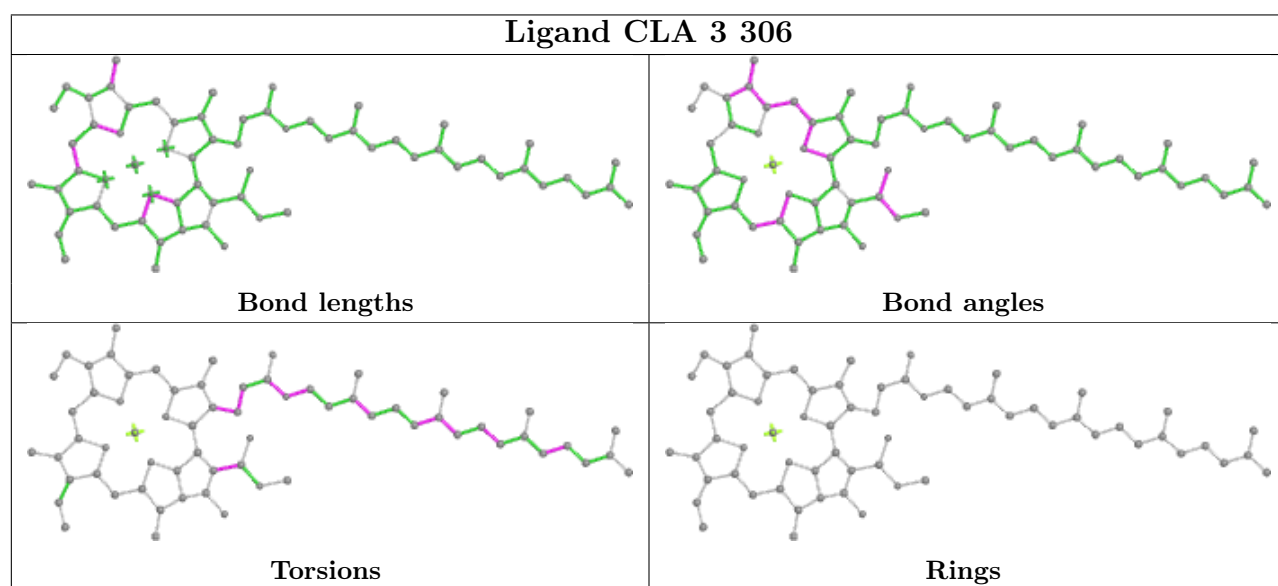
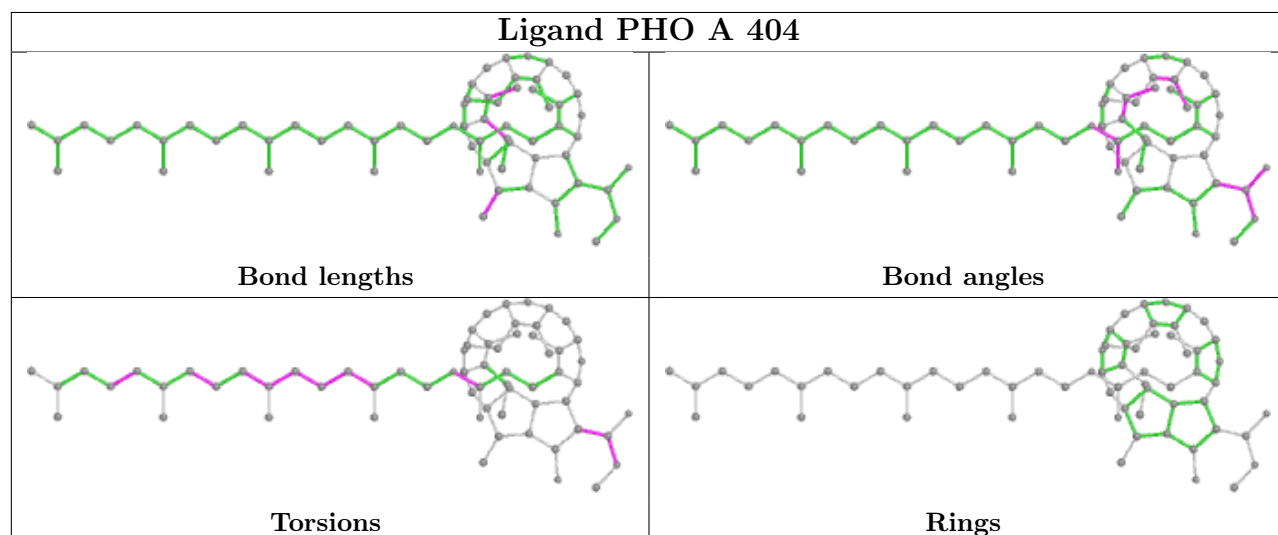
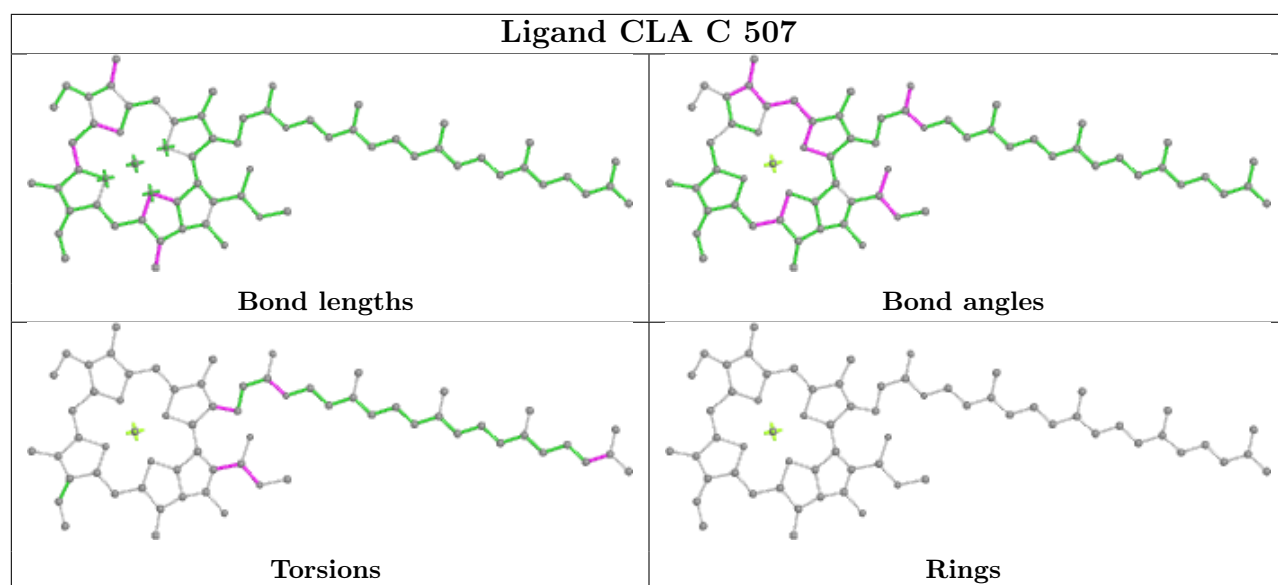
Bond angles

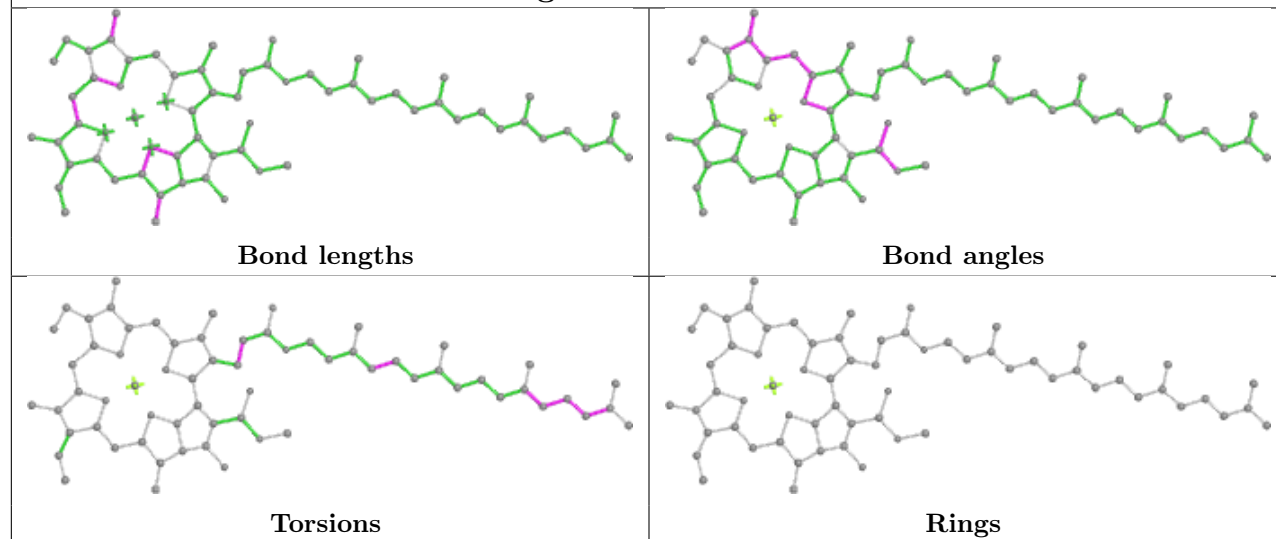
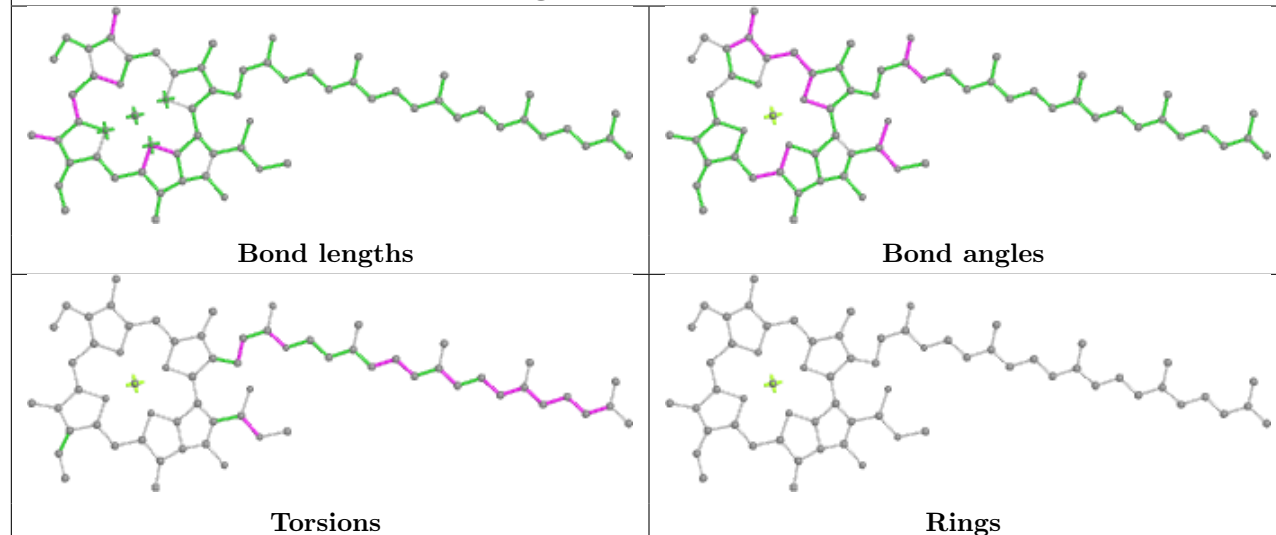
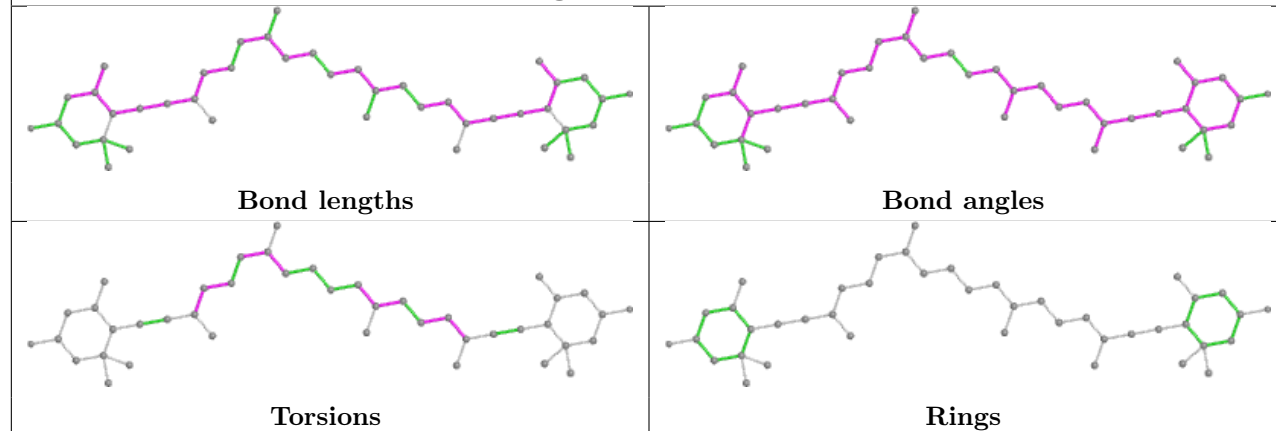


Torsions

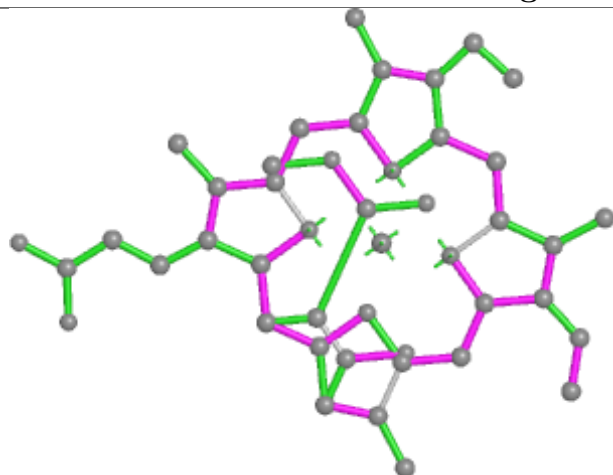


Rings

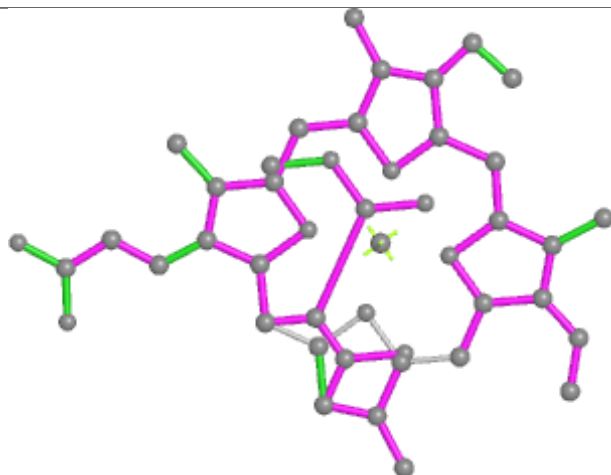


Ligand CLA c 509**Ligand CLA B 616****Ligand II0 1 617**

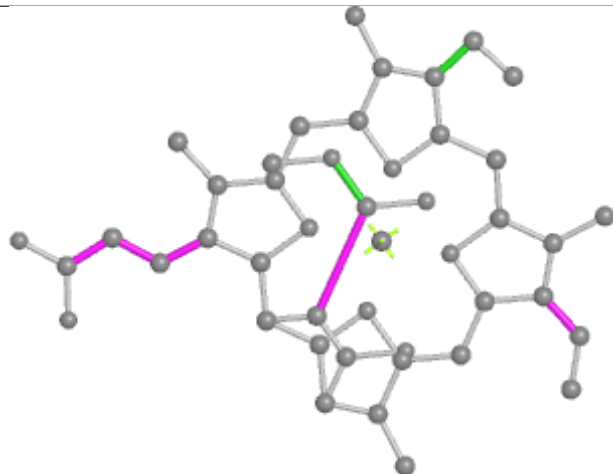
Ligand KC2 4 305



Bond lengths



Bond angles

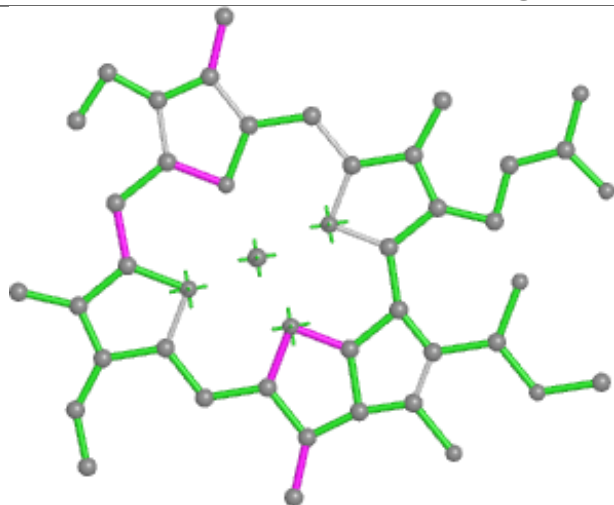


Torsions

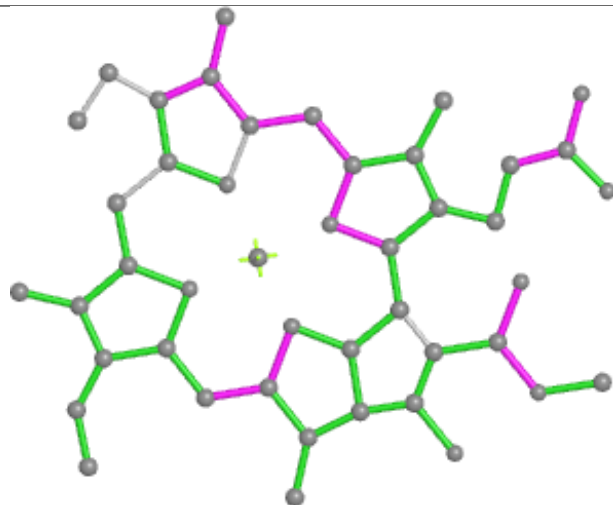


Rings

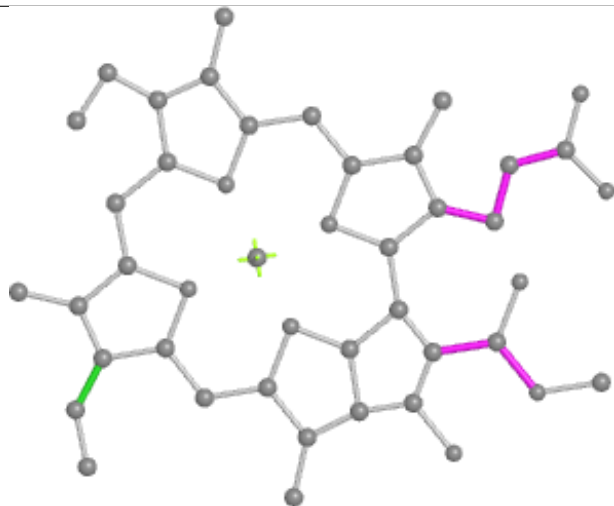
Ligand CLA P 611



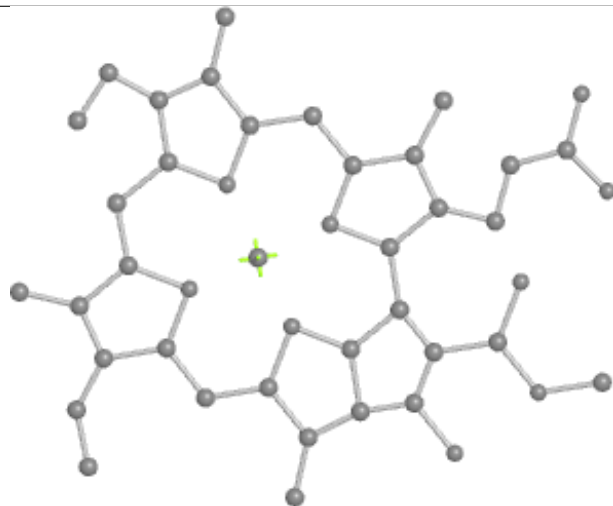
Bond lengths



Bond angles

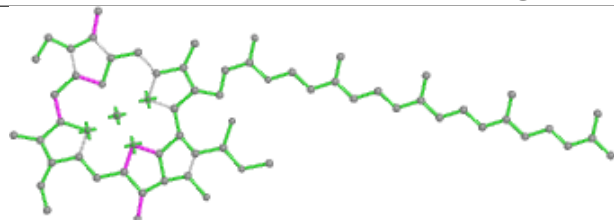


Torsions

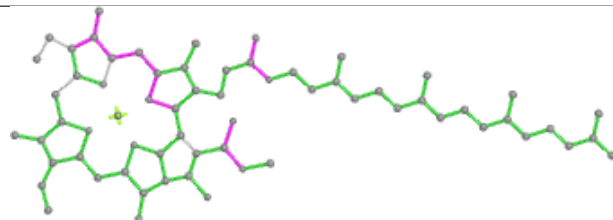


Rings

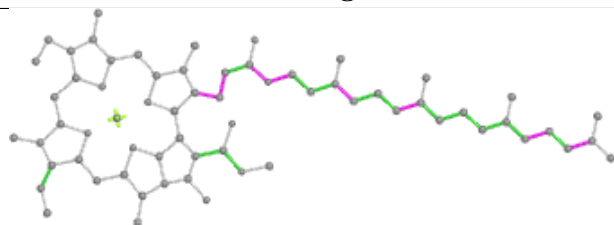
Ligand CLA C 510



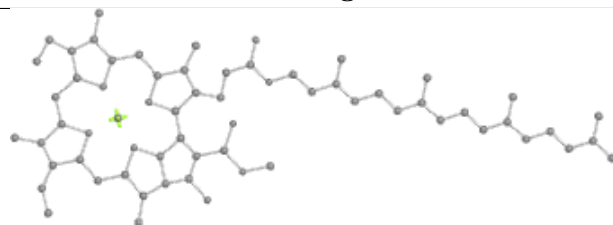
Bond lengths



Bond angles

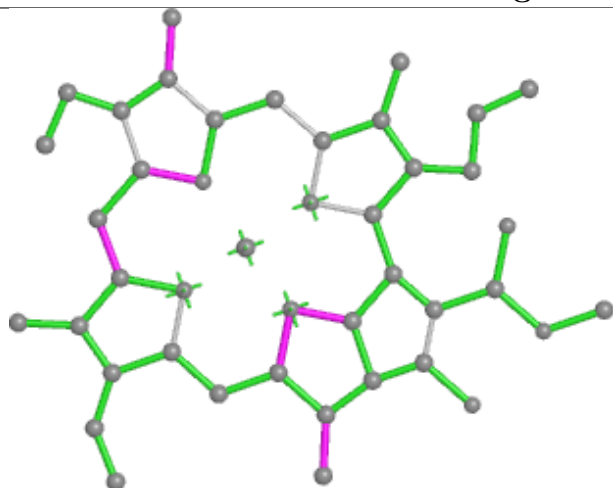


Torsions

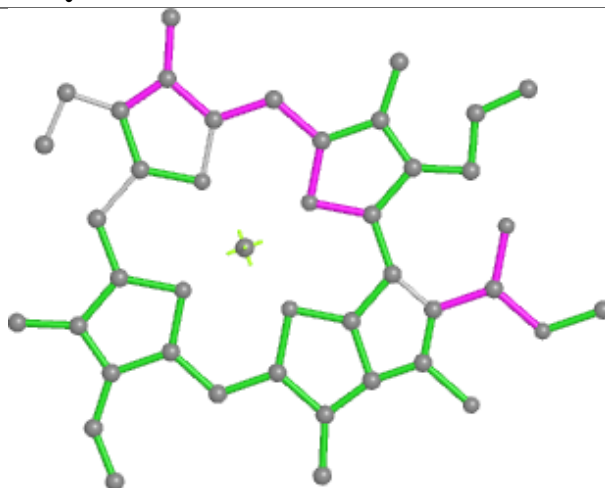


Rings

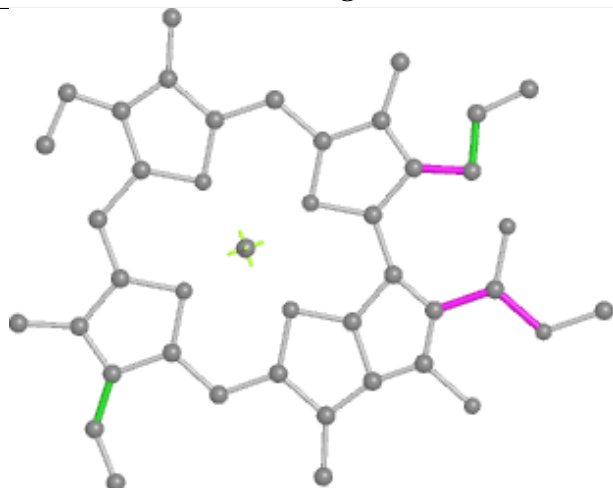
Ligand CLA Q 311



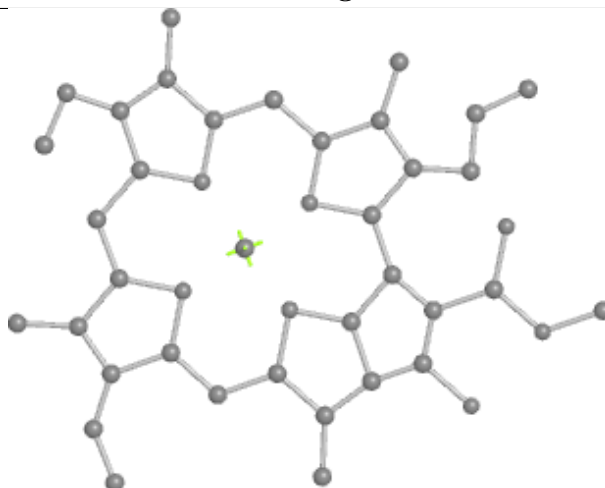
Bond lengths



Bond angles

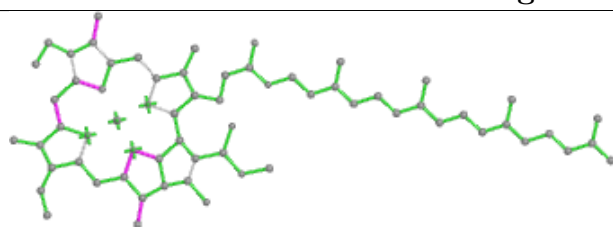


Torsions

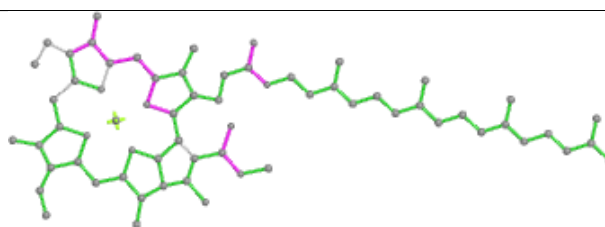


Rings

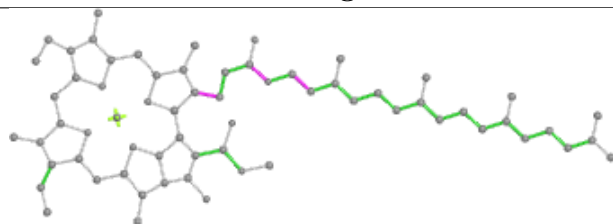
Ligand CLA d 405



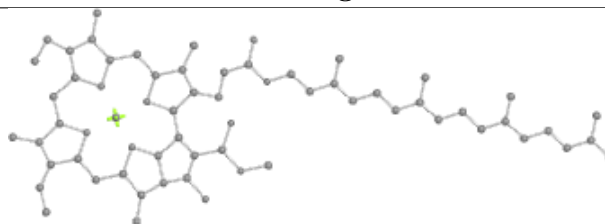
Bond lengths



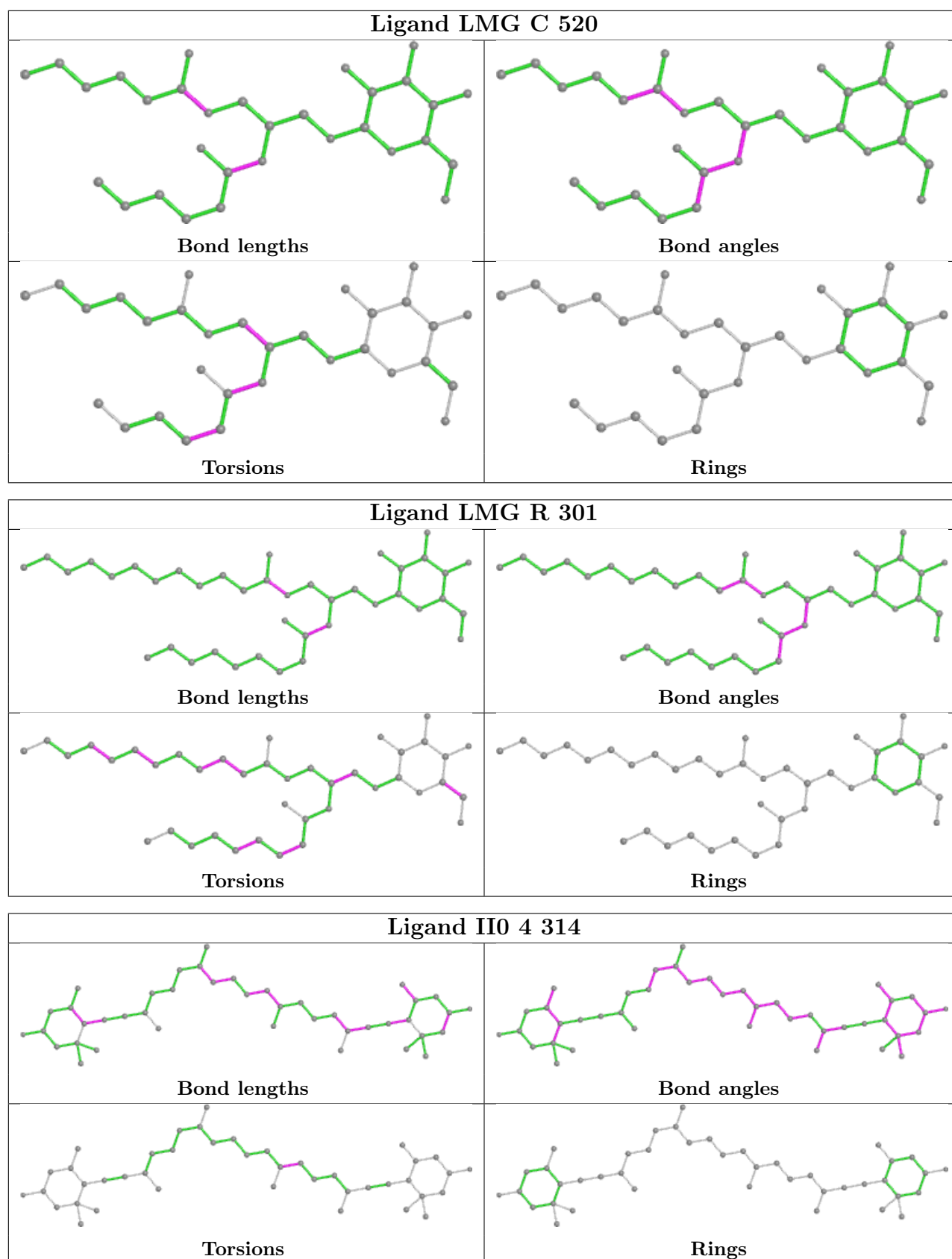
Bond angles

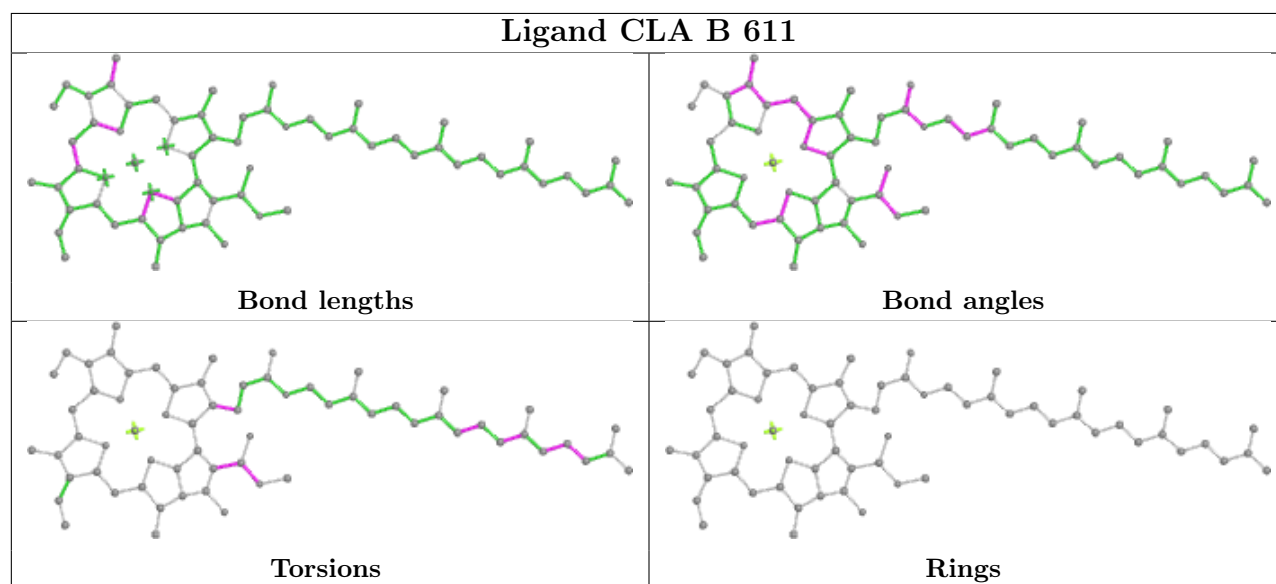
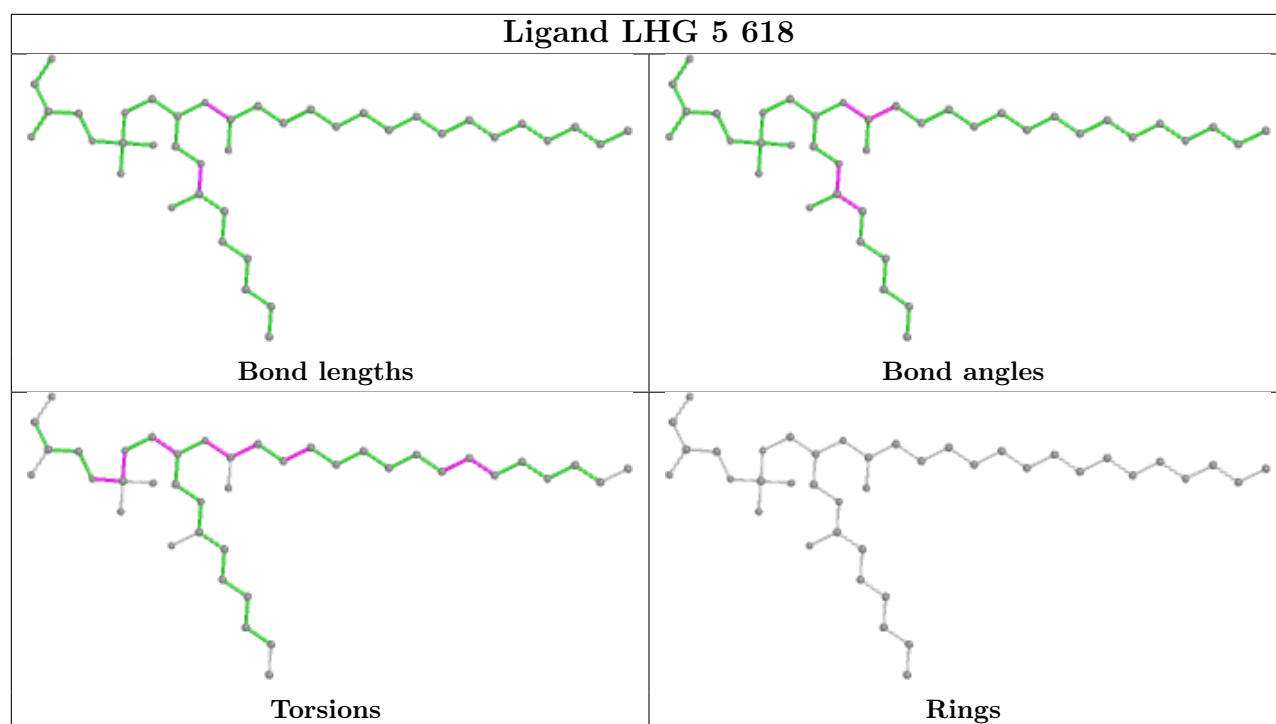


Torsions

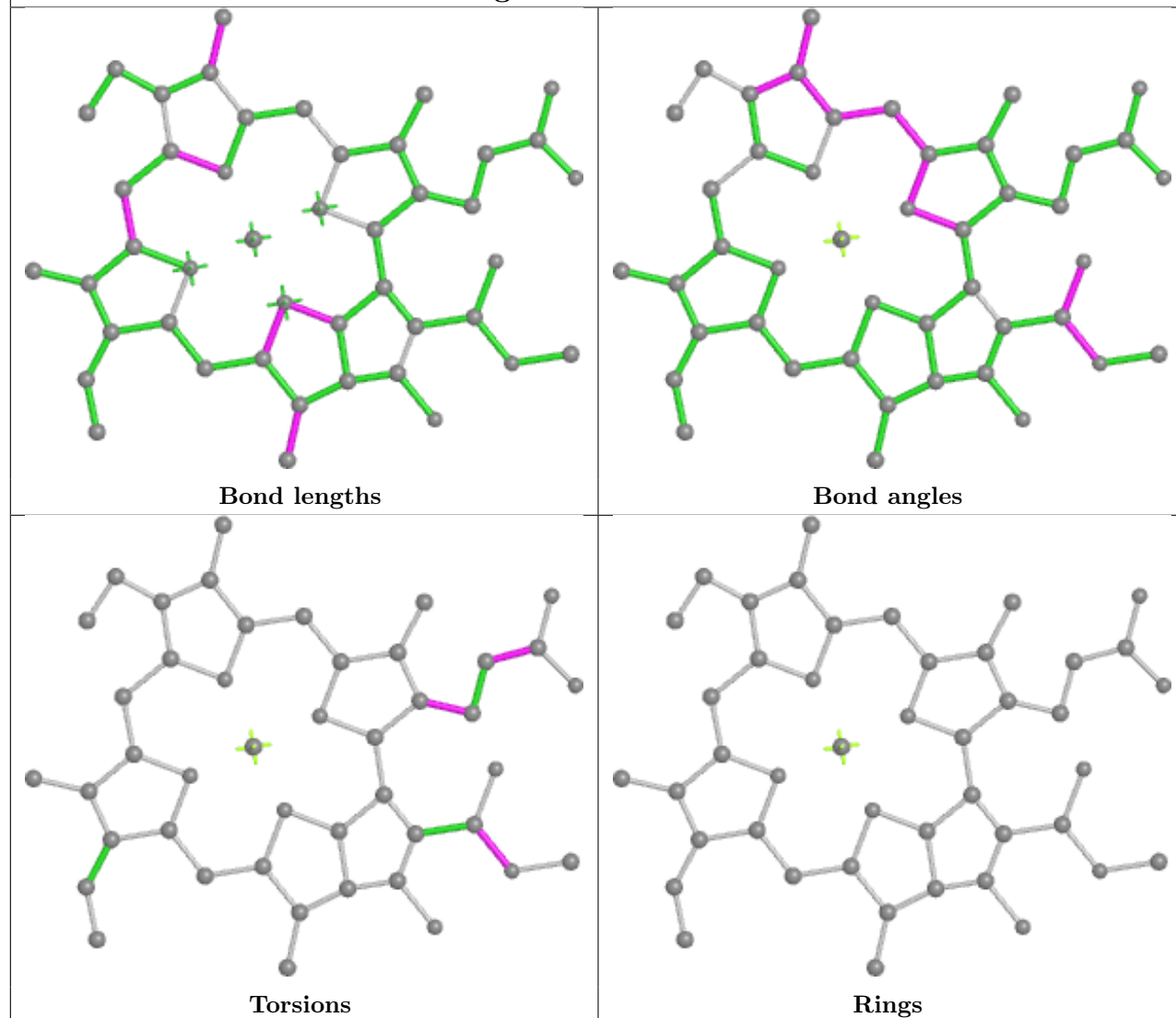


Rings

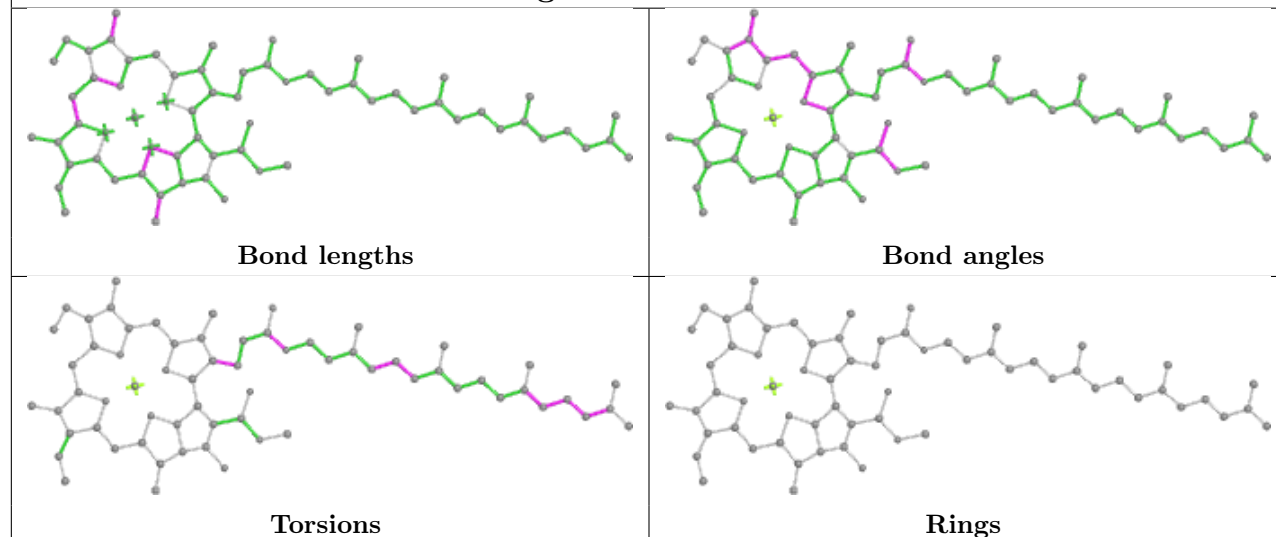




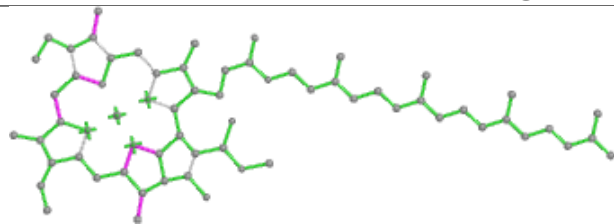
Ligand CLA 1 601



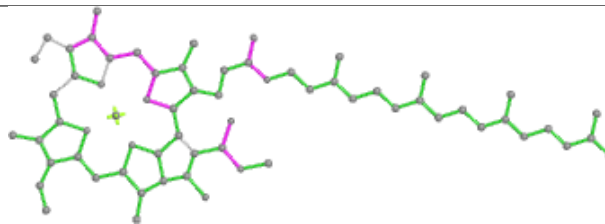
Ligand CLA c 514



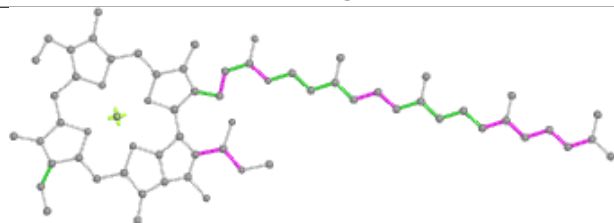
Ligand CLA S 604



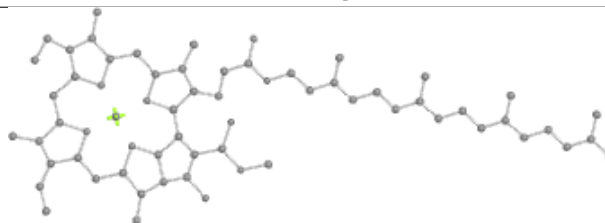
Bond lengths



Bond angles

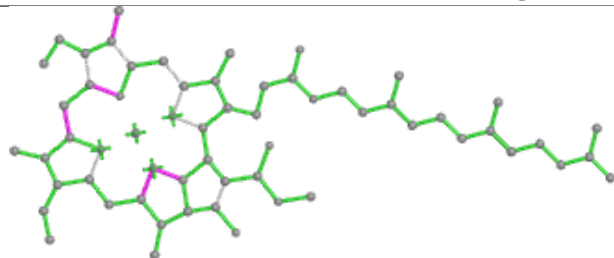


Torsions

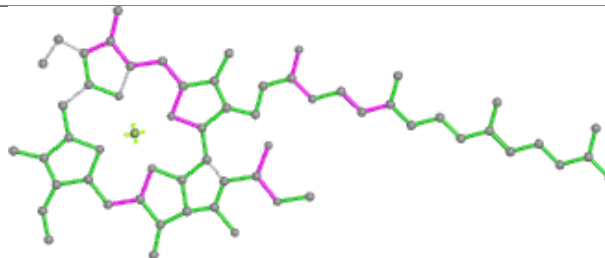


Rings

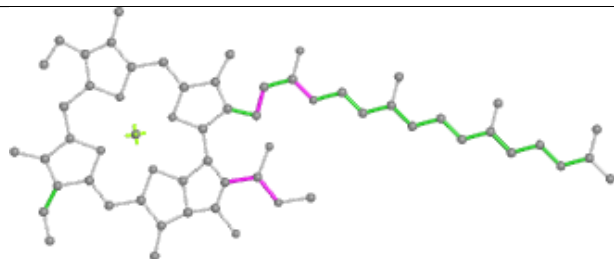
Ligand CLA N 602



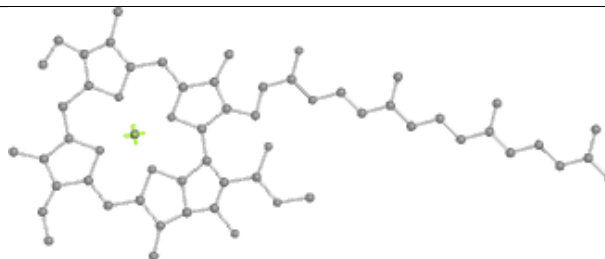
Bond lengths



Bond angles

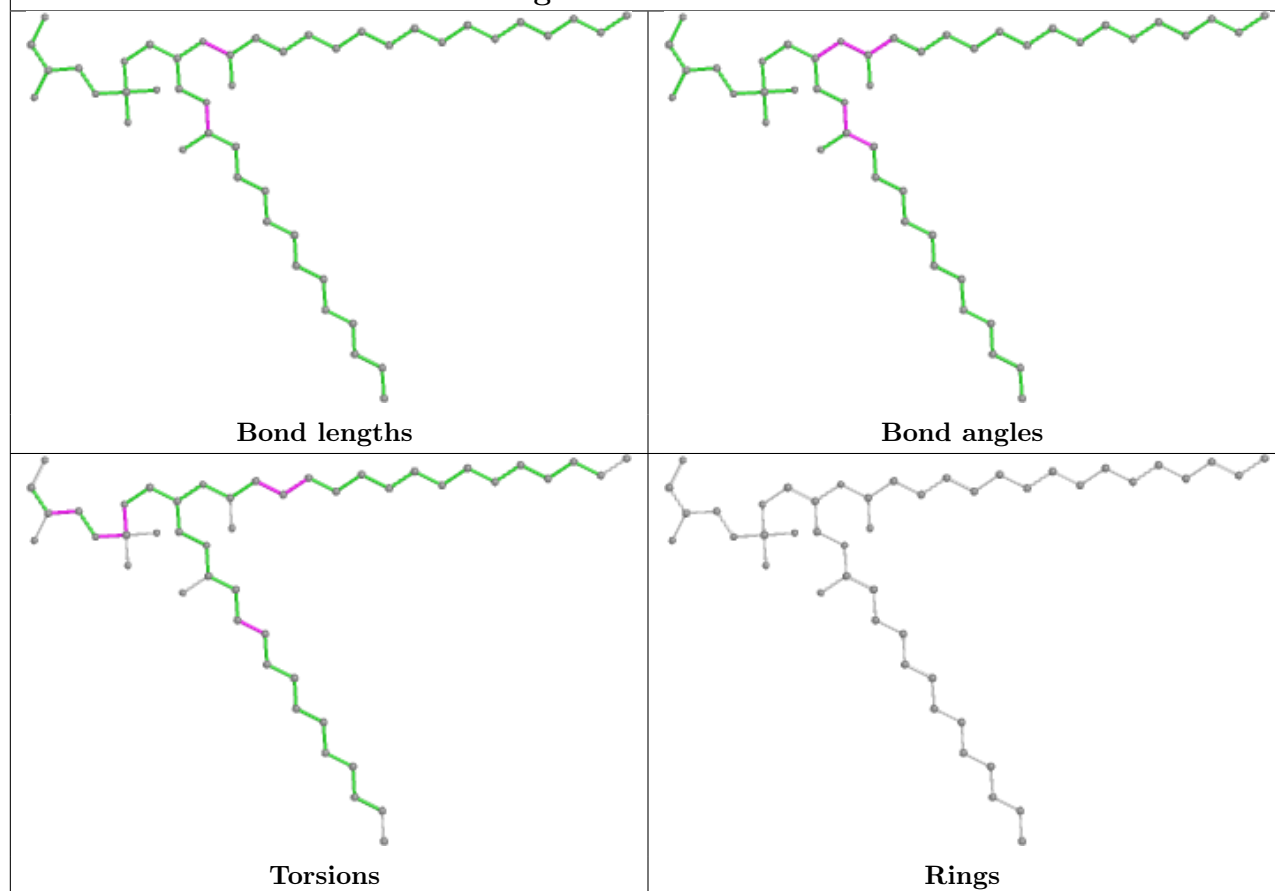


Torsions

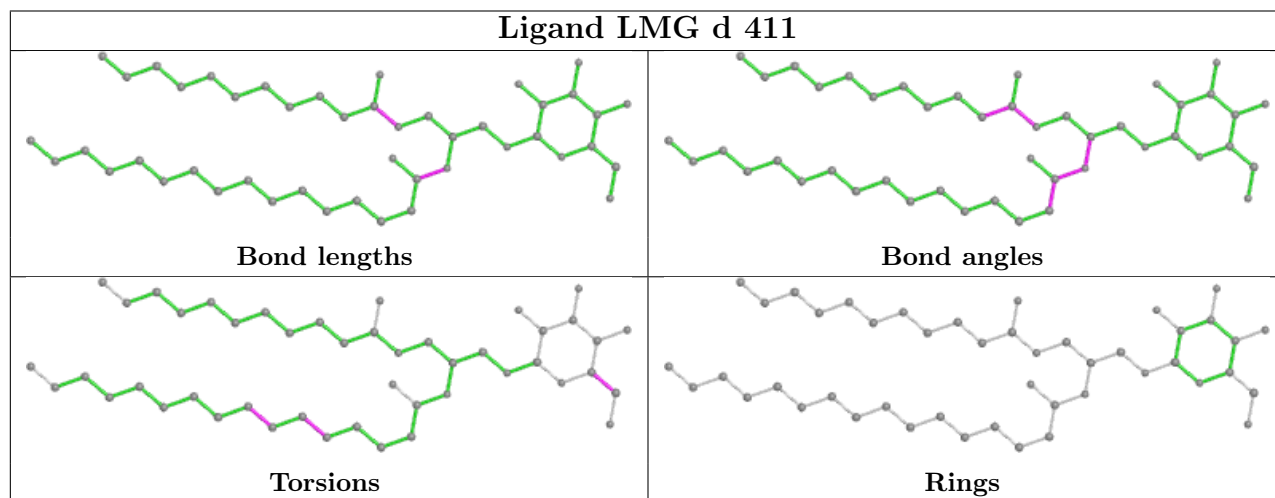


Rings

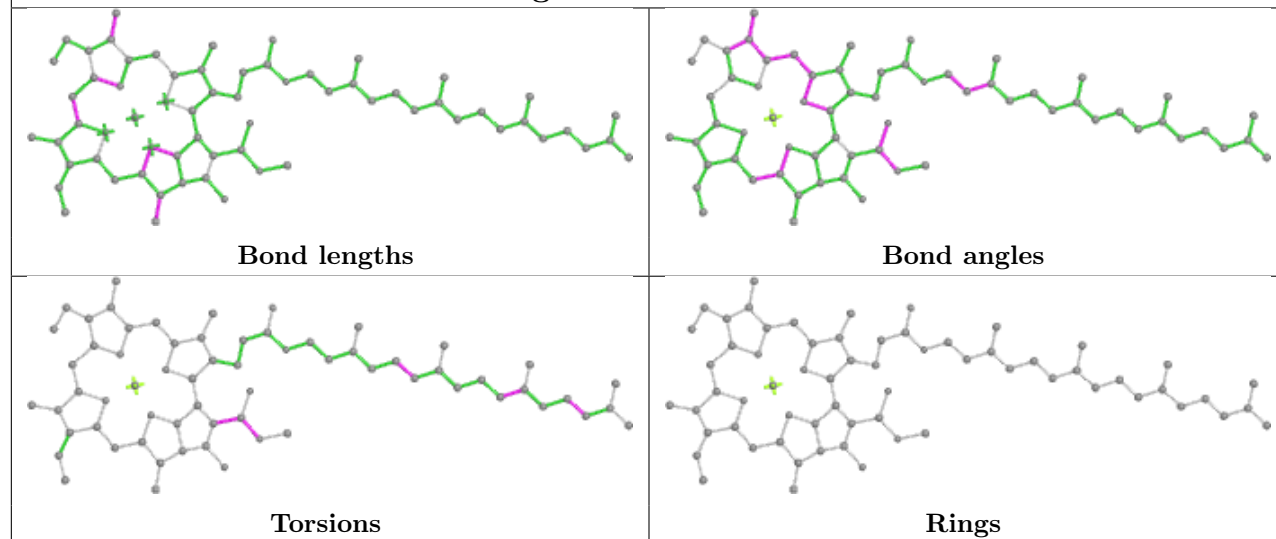
Ligand LHG 1 620



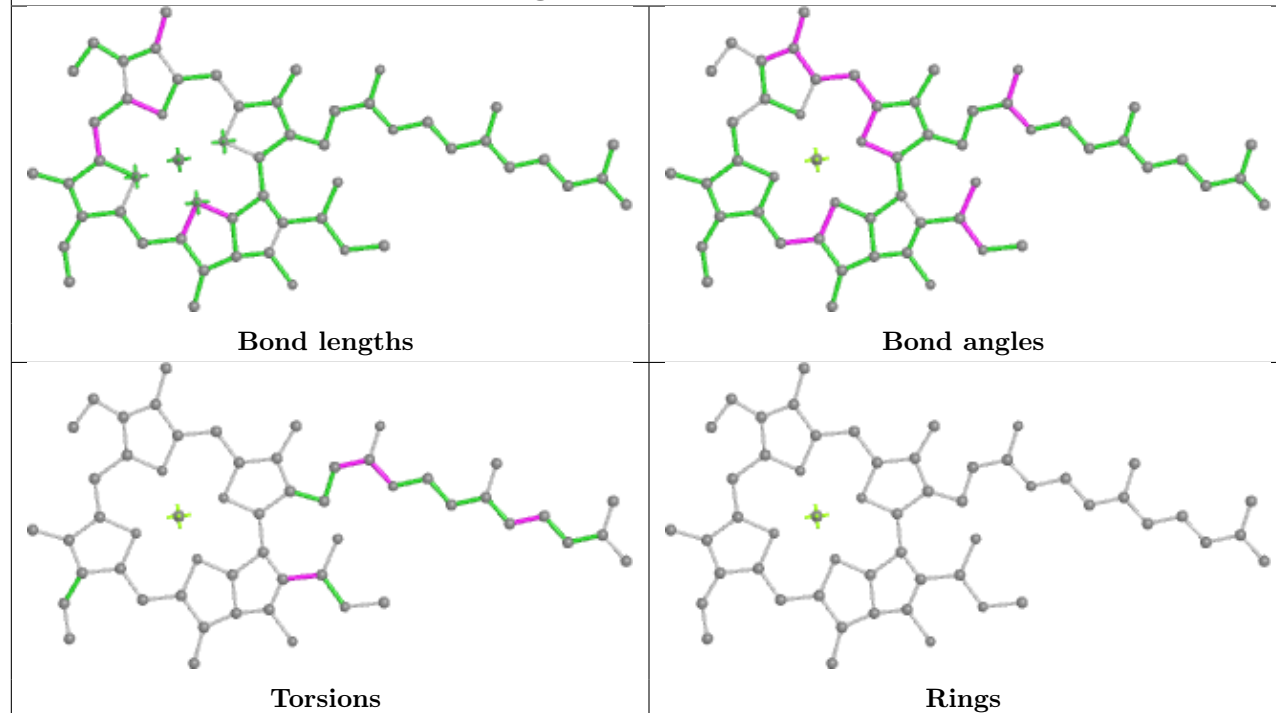
Ligand LMG d 411



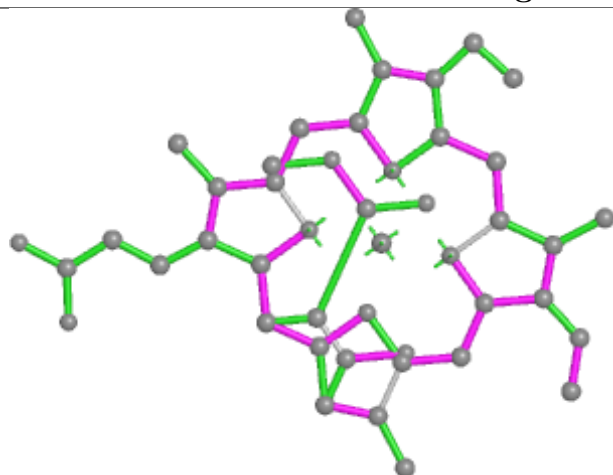
Ligand CLA B 605



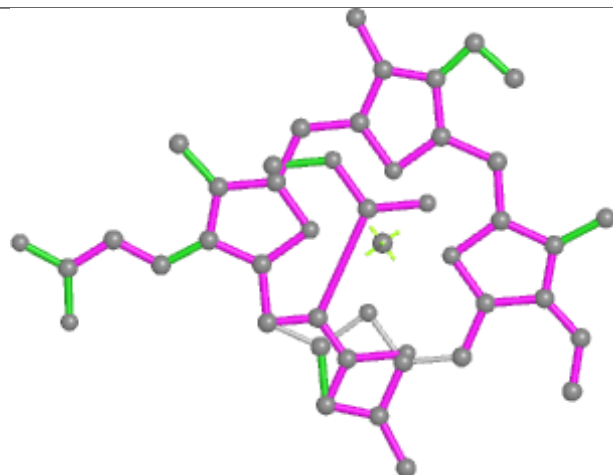
Ligand CLA R 302



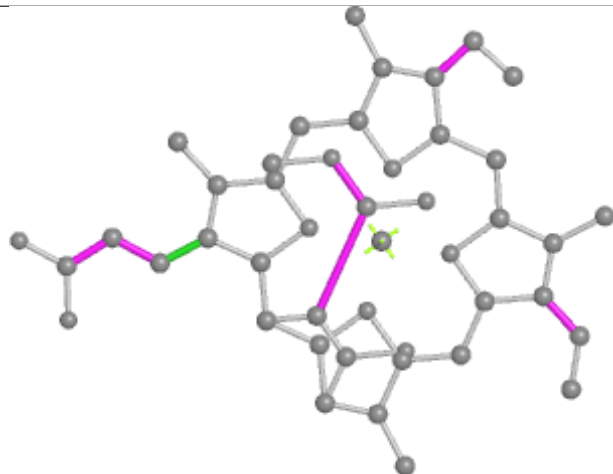
Ligand KC2 N 605



Bond lengths



Bond angles

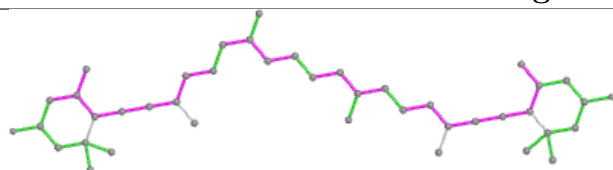


Torsions

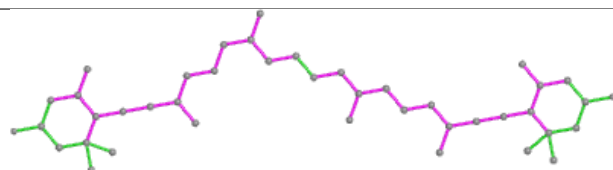


Rings

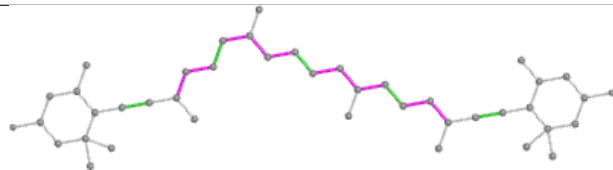
Ligand II0 3 311



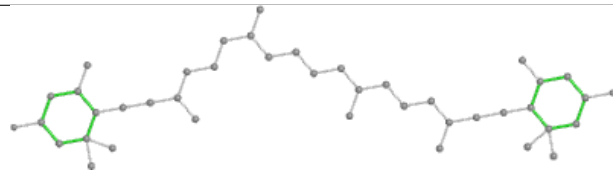
Bond lengths



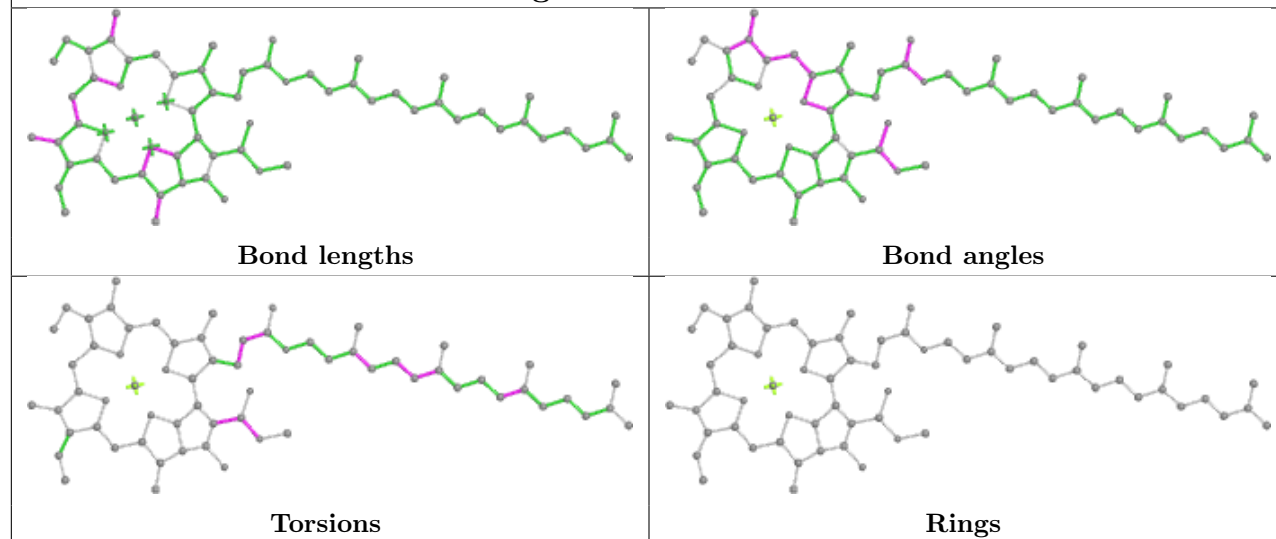
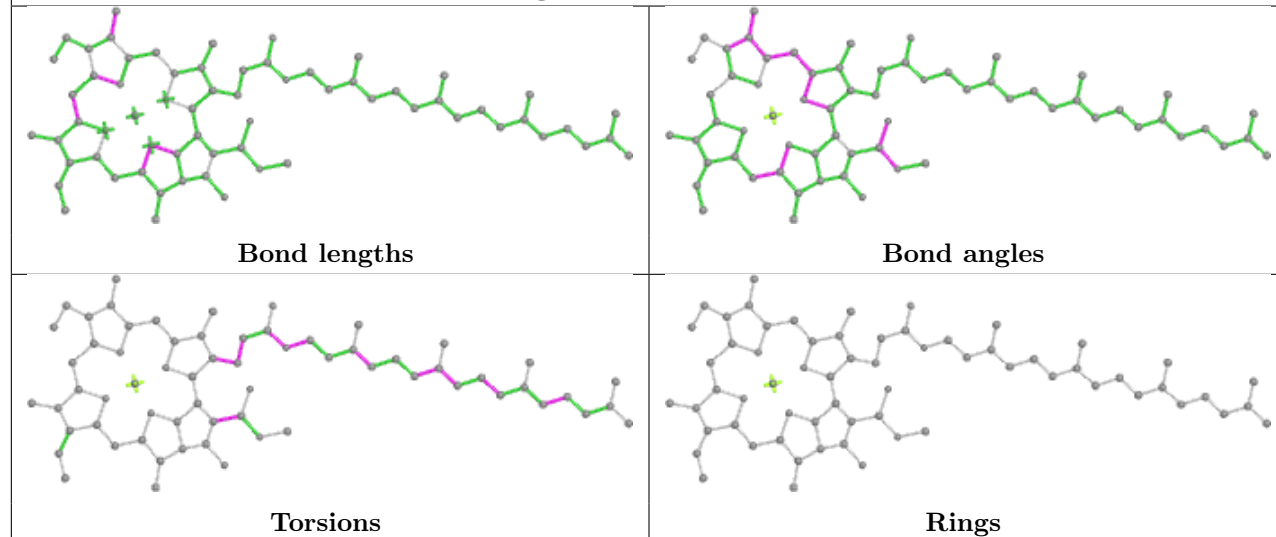
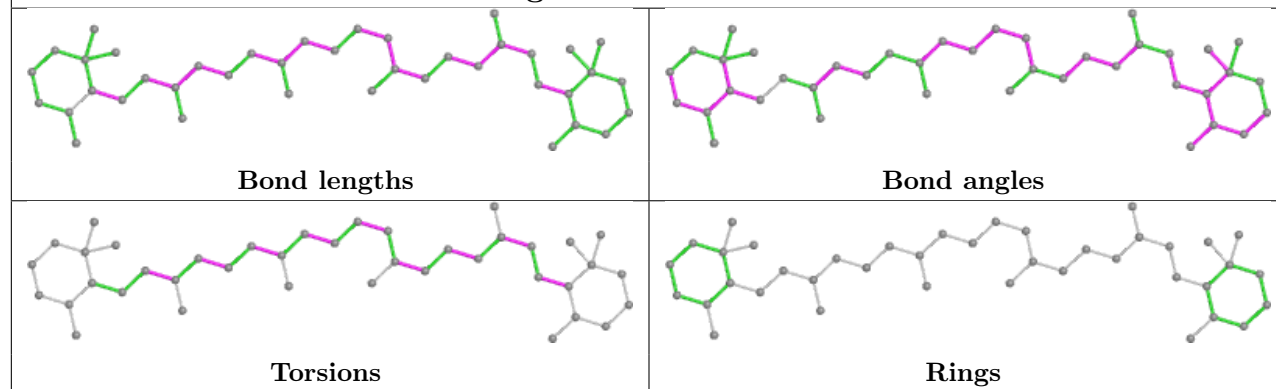
Bond angles



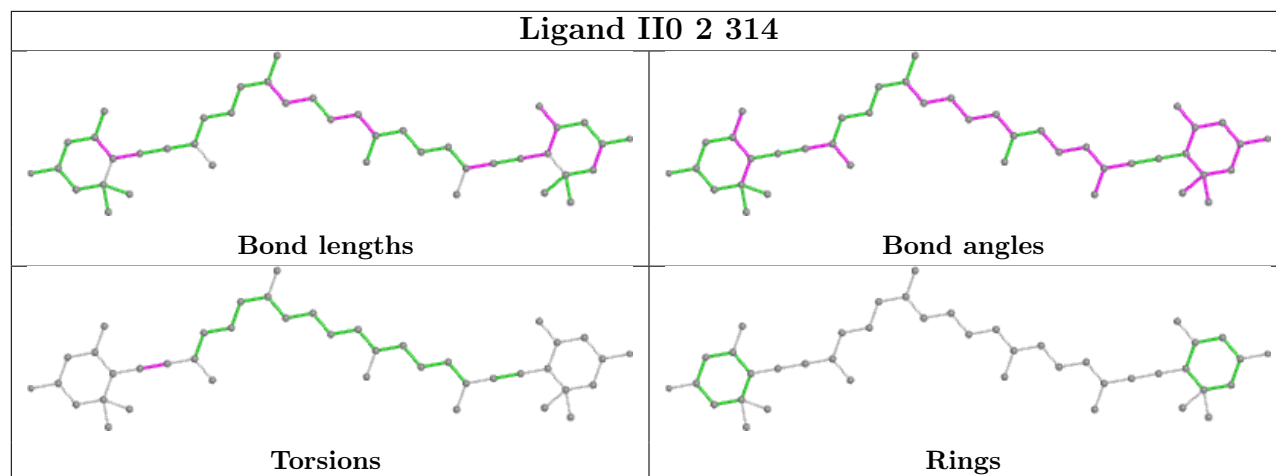
Torsions



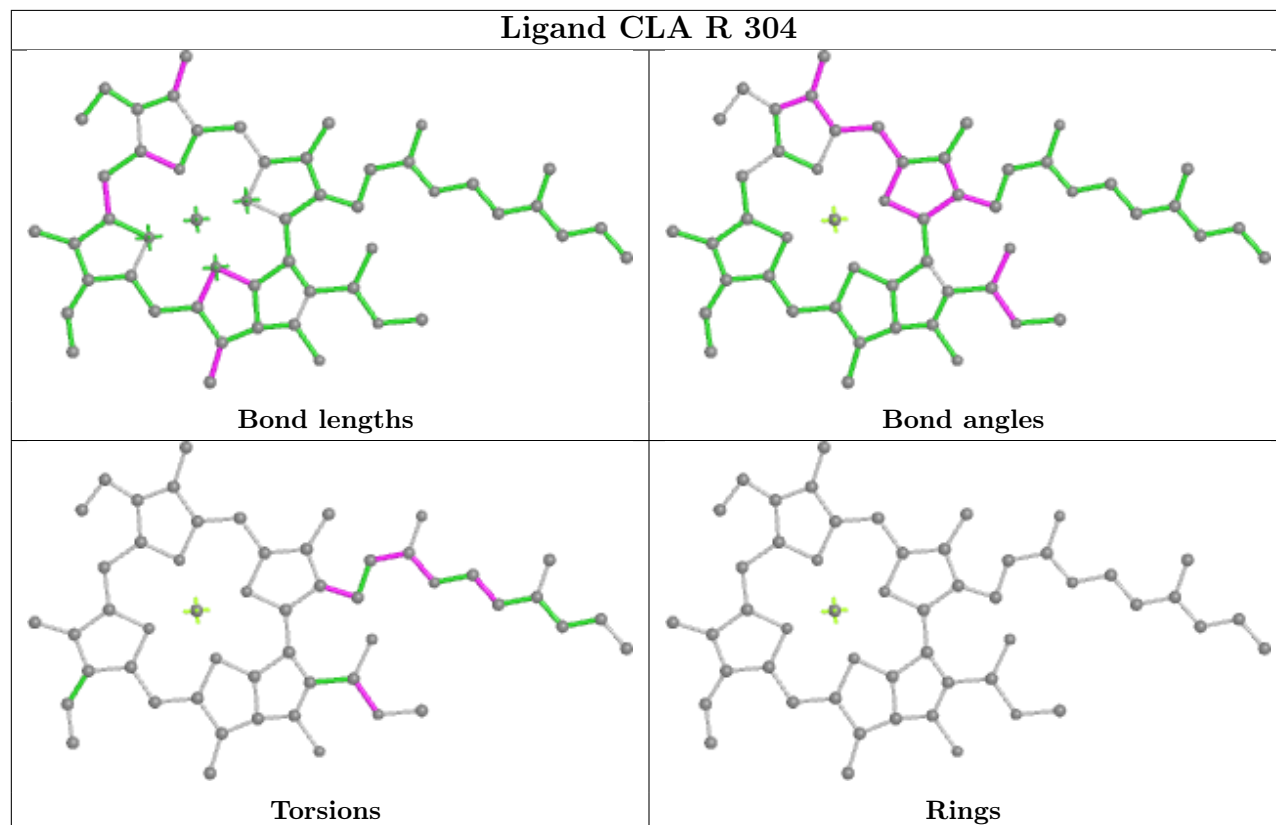
Rings

Ligand CLA C 503**Ligand CLA P 607****Ligand WVN b 617**

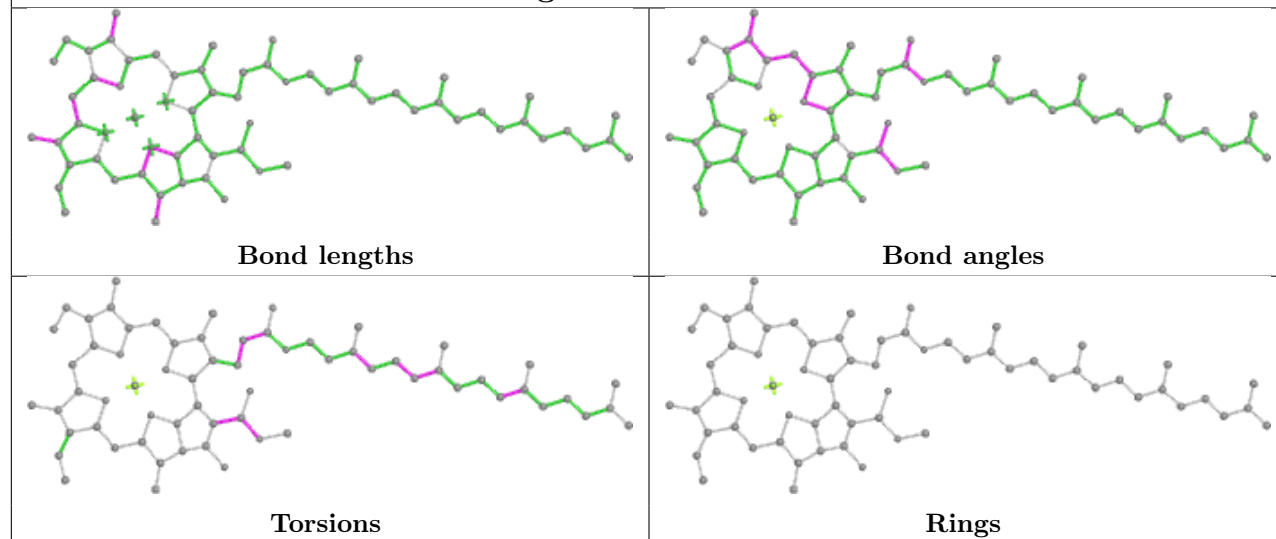
Ligand II0 2 314



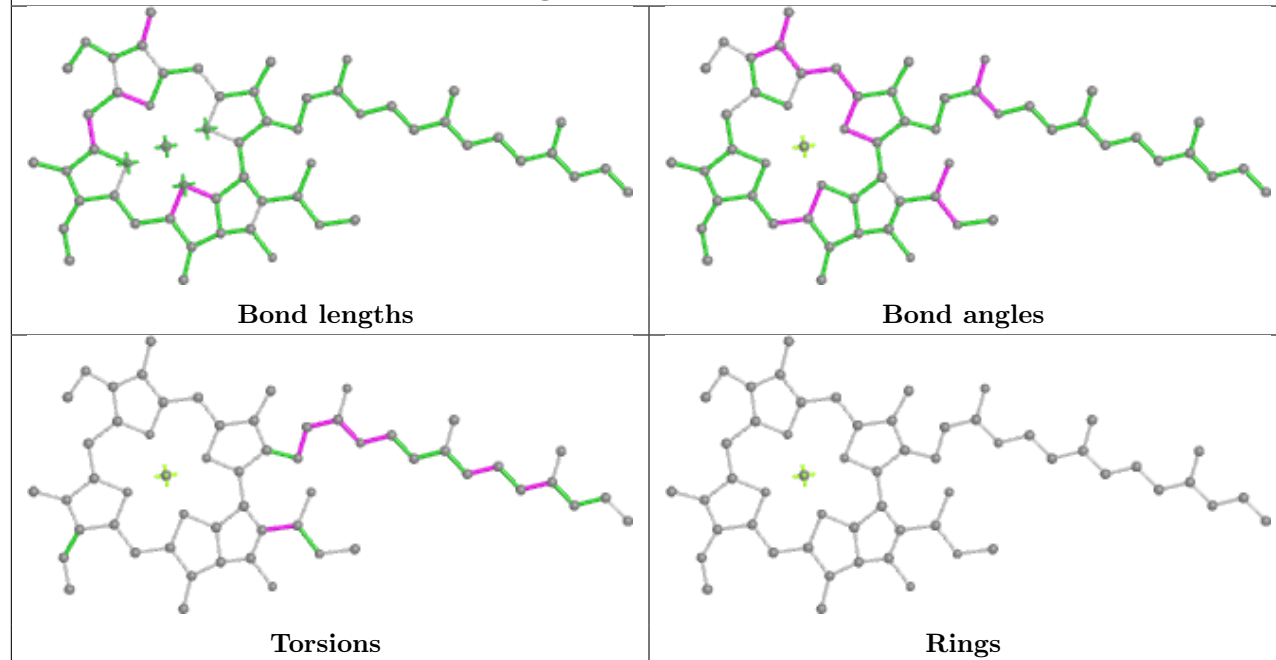
Ligand CLA R 304

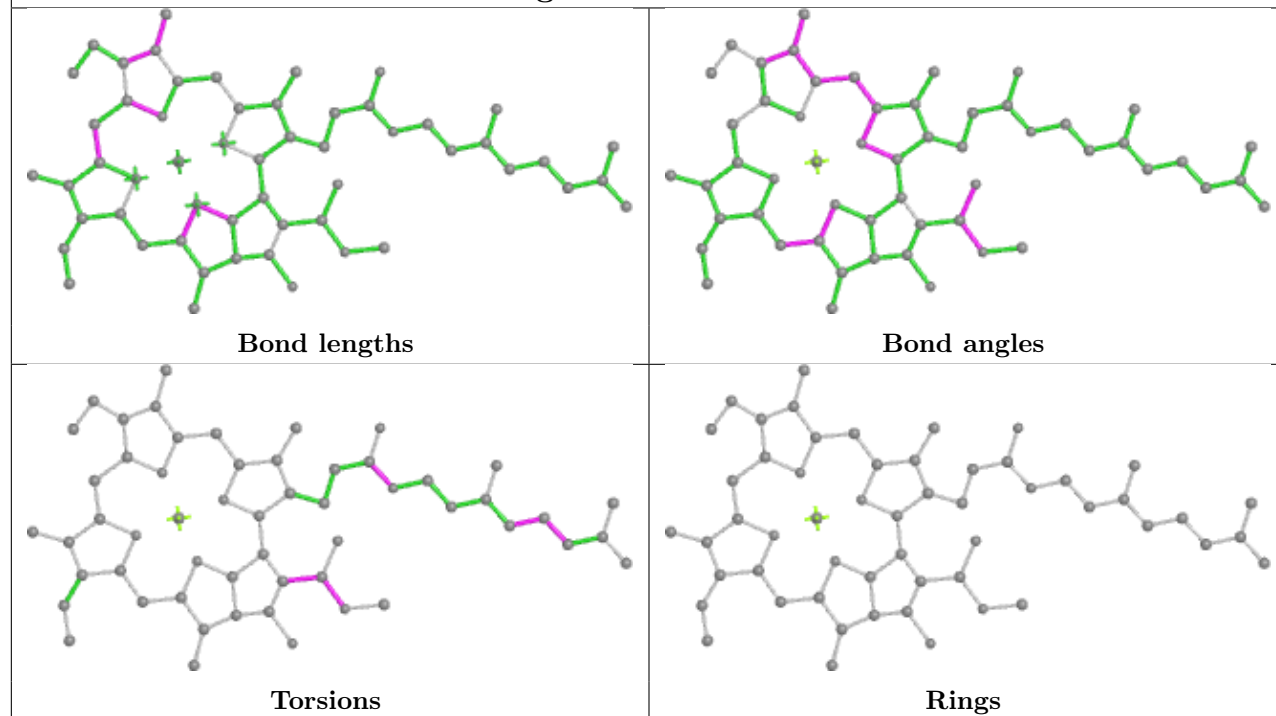
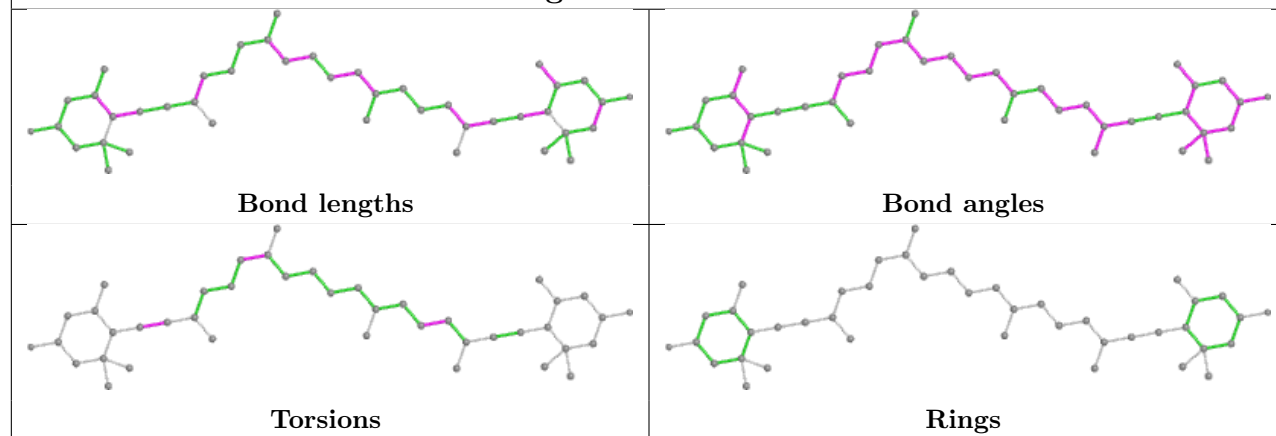


Ligand CLA c 504

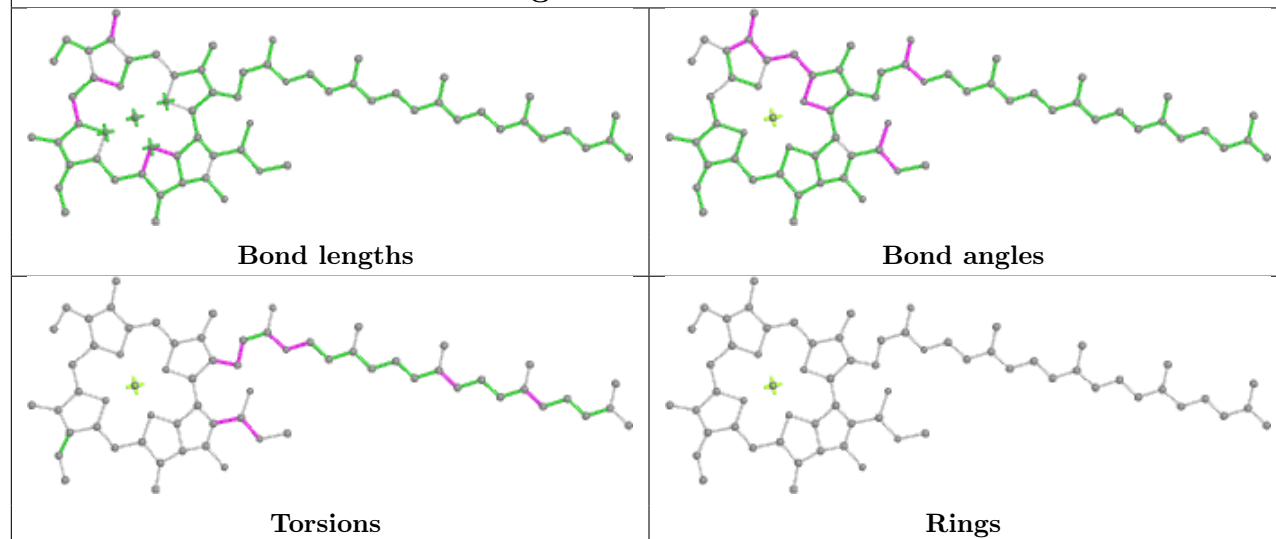


Ligand CLA 6 606

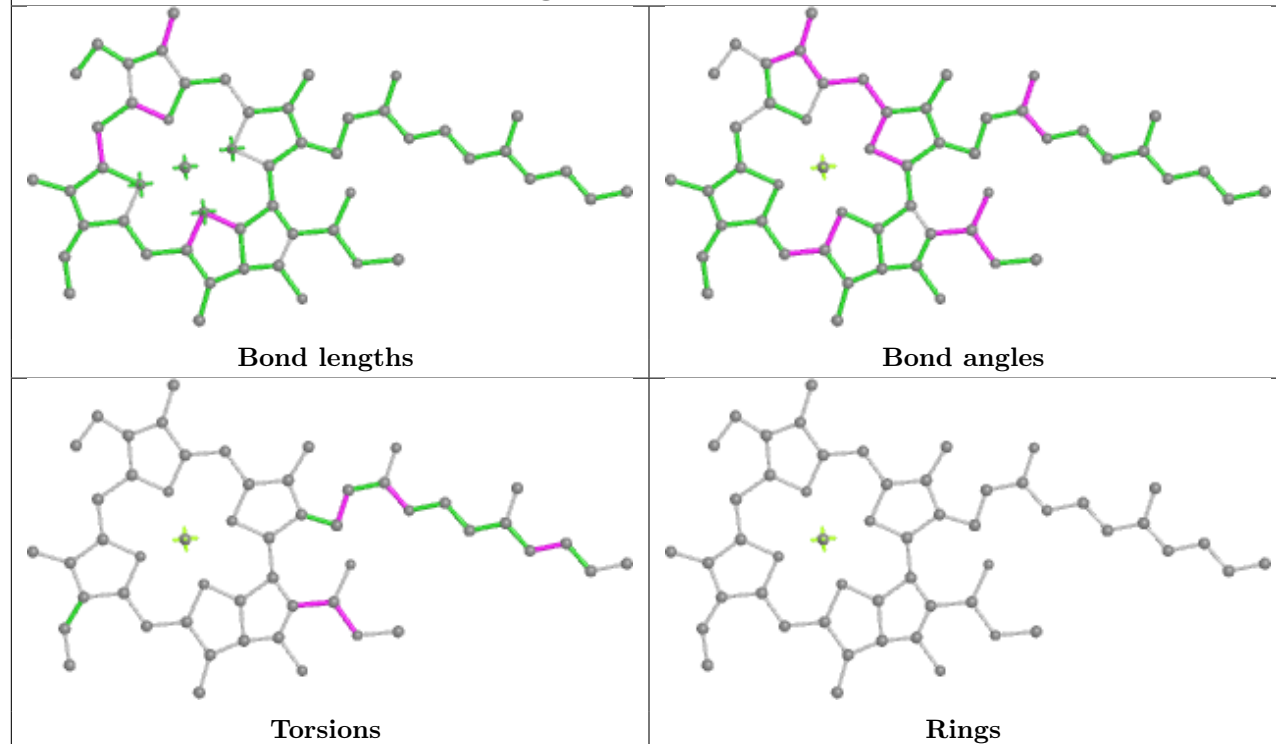


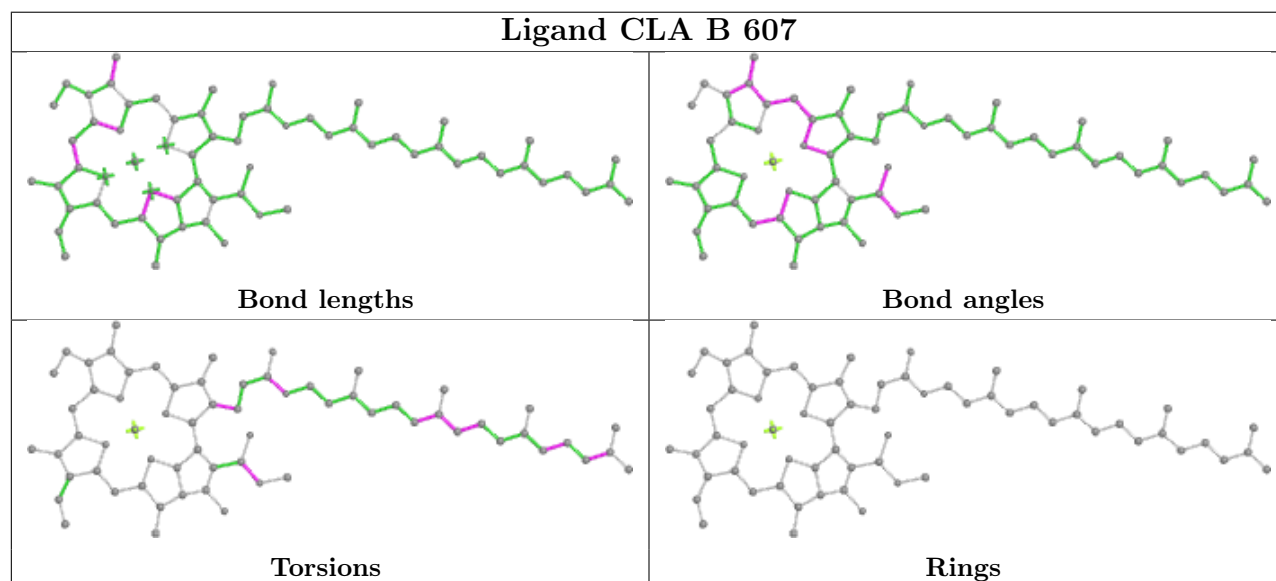
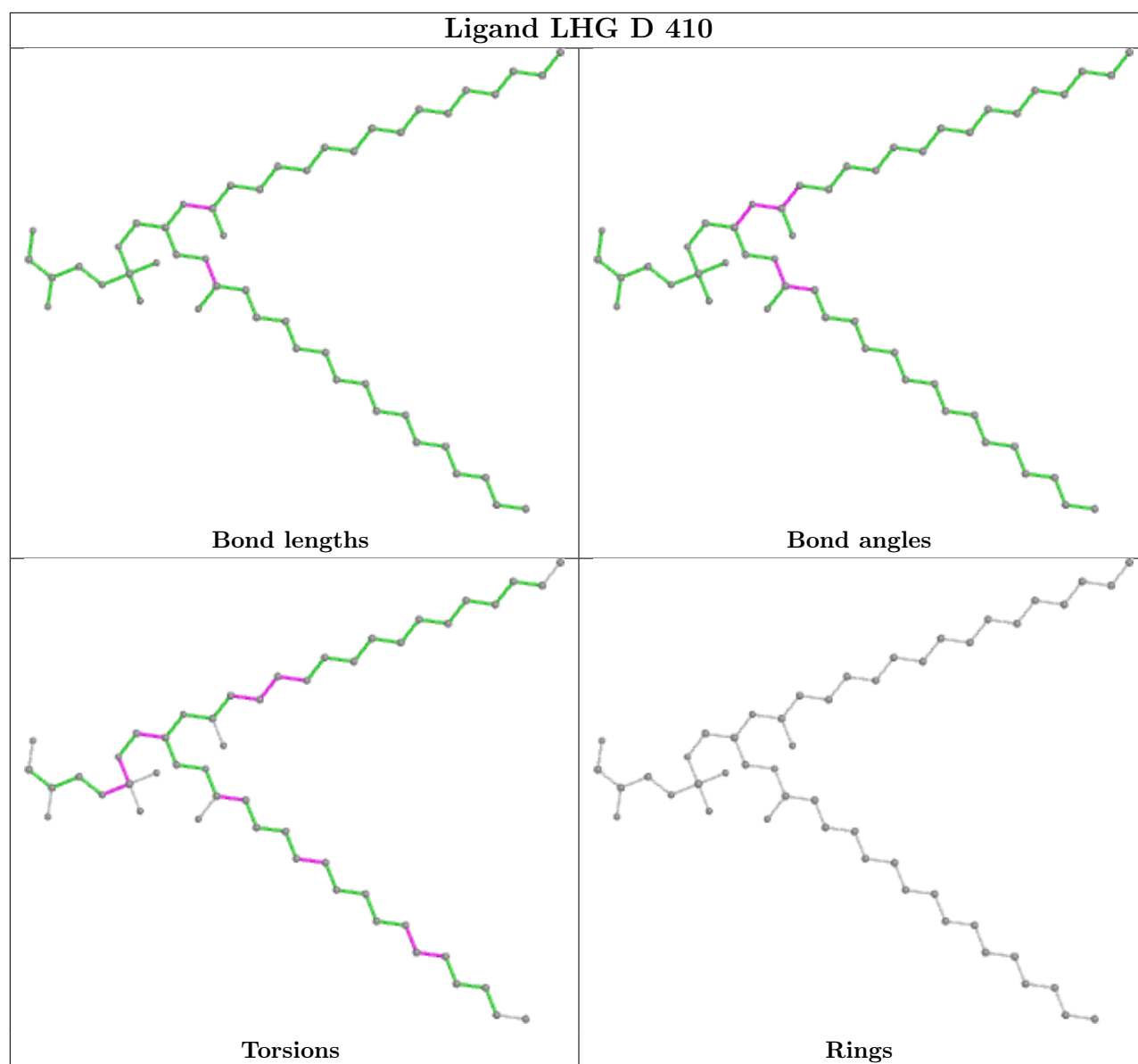
Ligand CLA 6 601**Ligand II0 N 618**

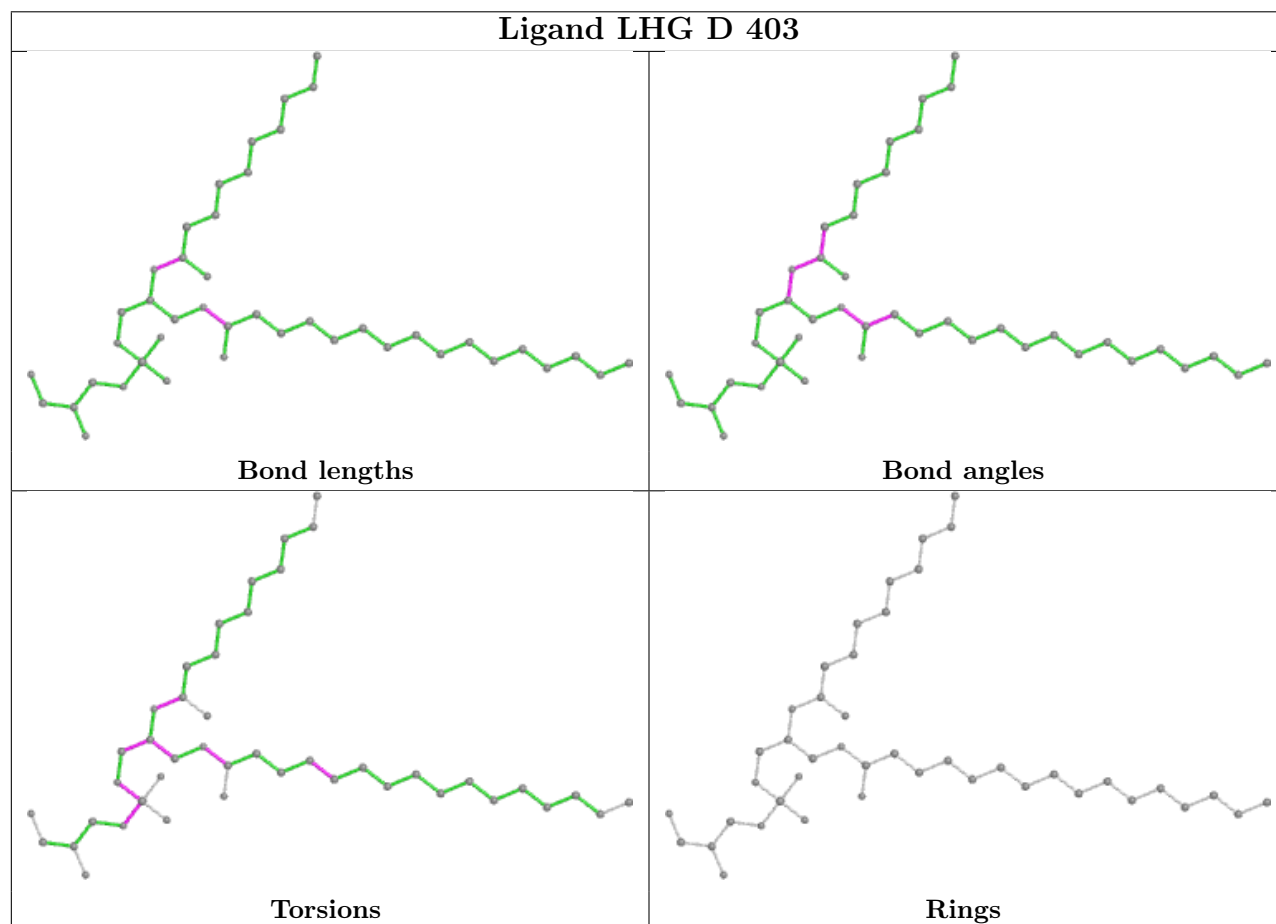
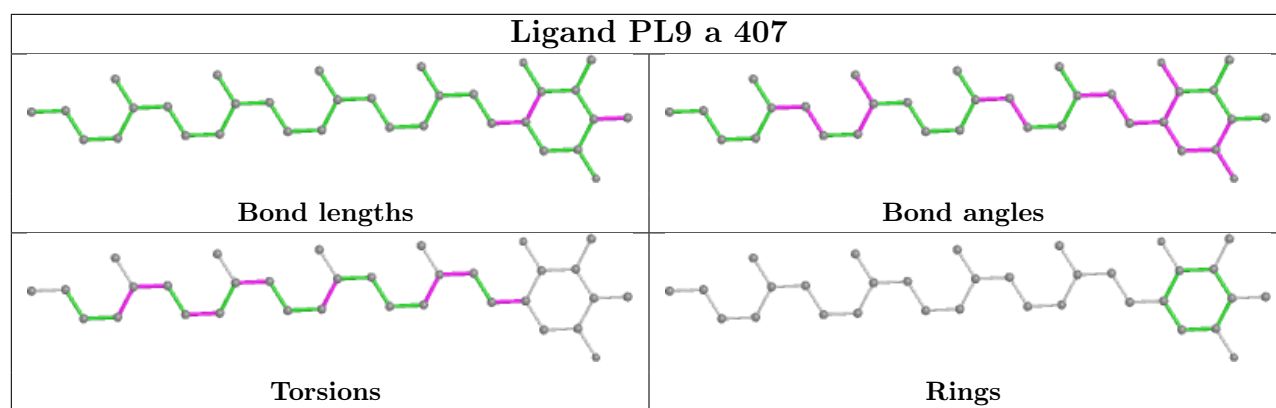
Ligand CLA R 306

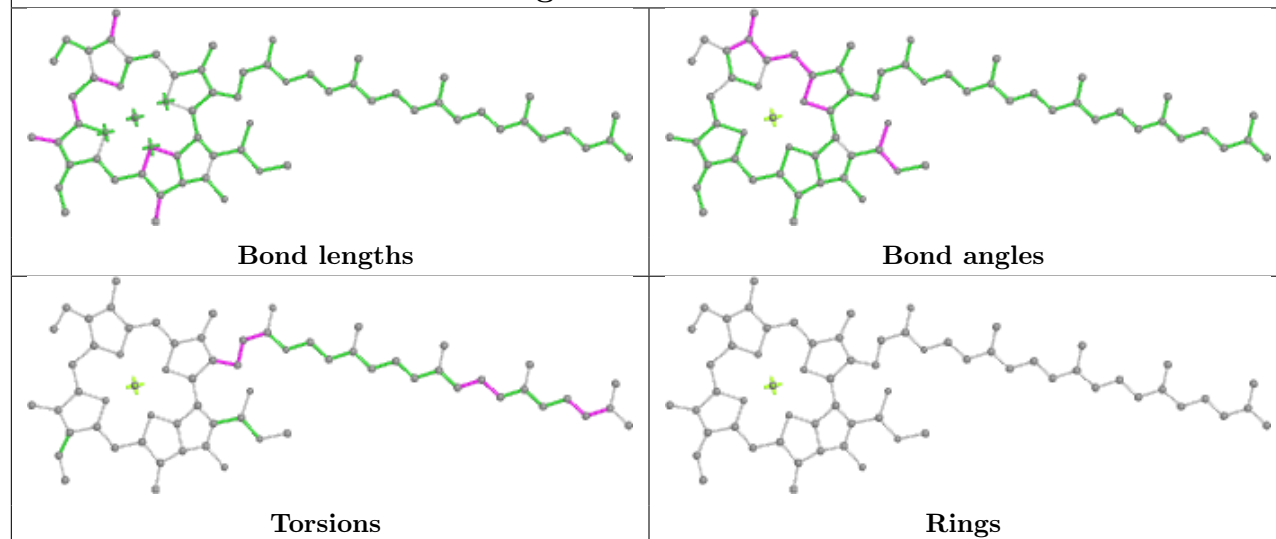
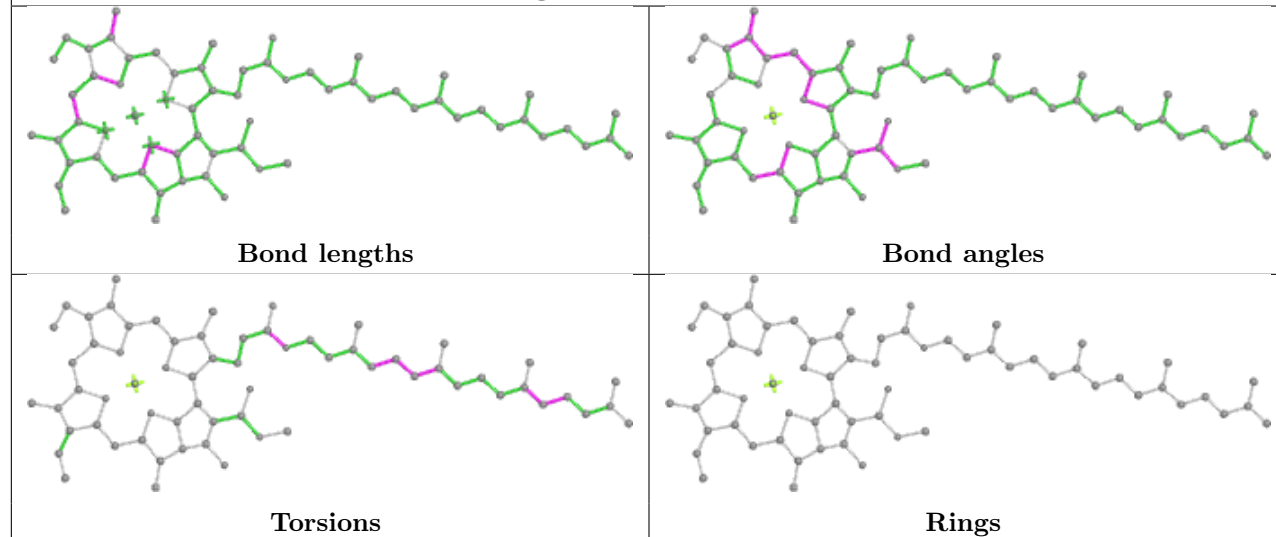


Ligand CLA c 515

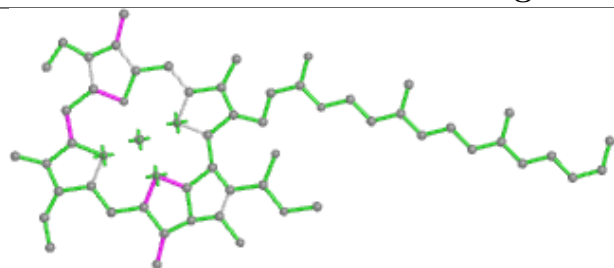




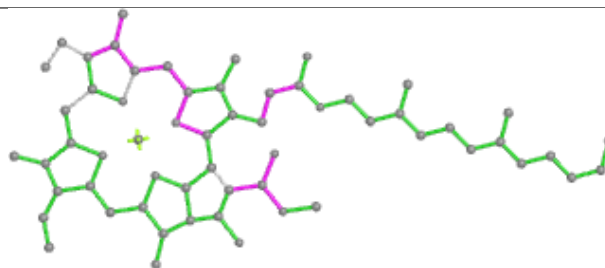


Ligand CLA 2 303**Ligand CLA P 606**

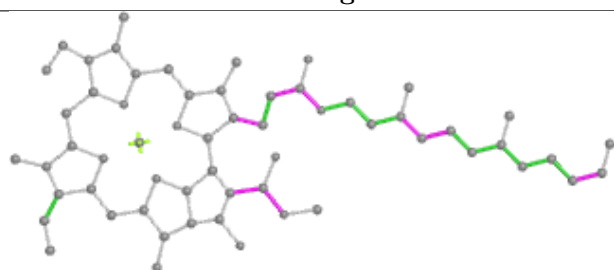
Ligand CLA B 604



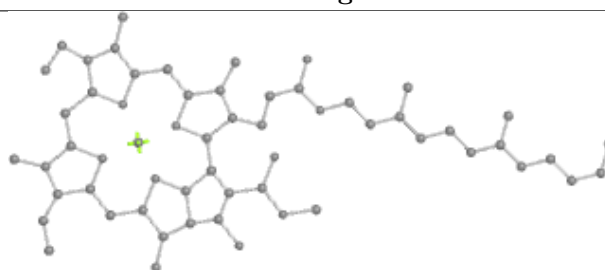
Bond lengths



Bond angles

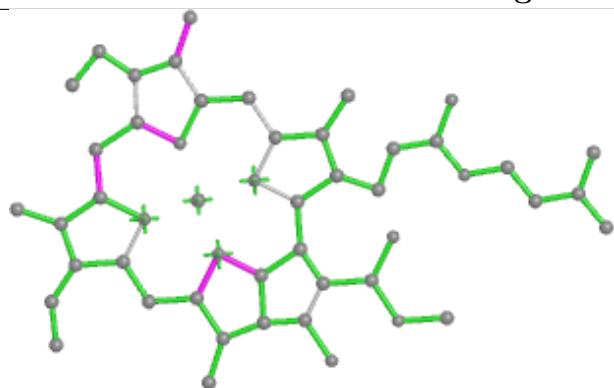


Torsions

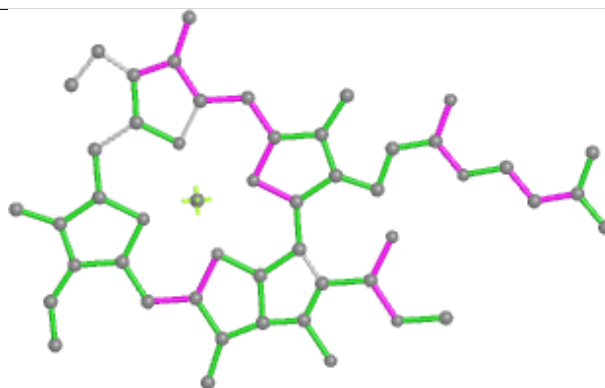


Rings

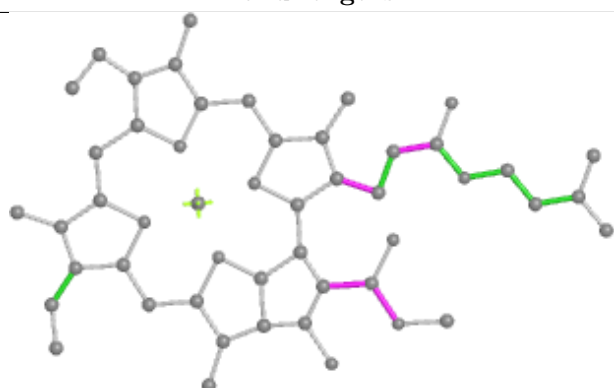
Ligand CLA B 601



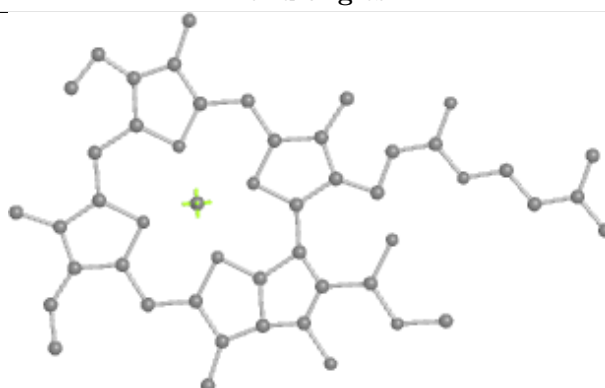
Bond lengths



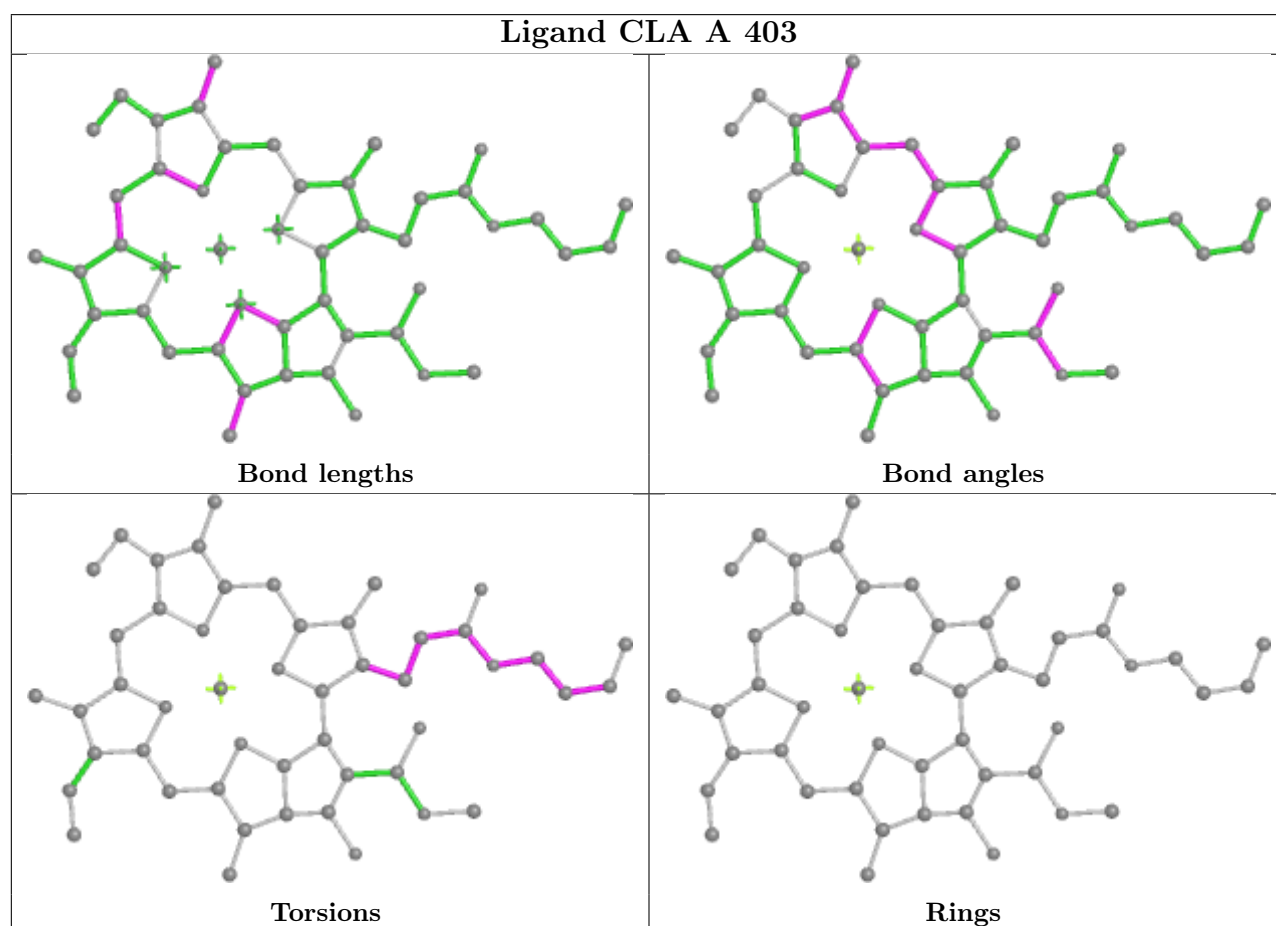
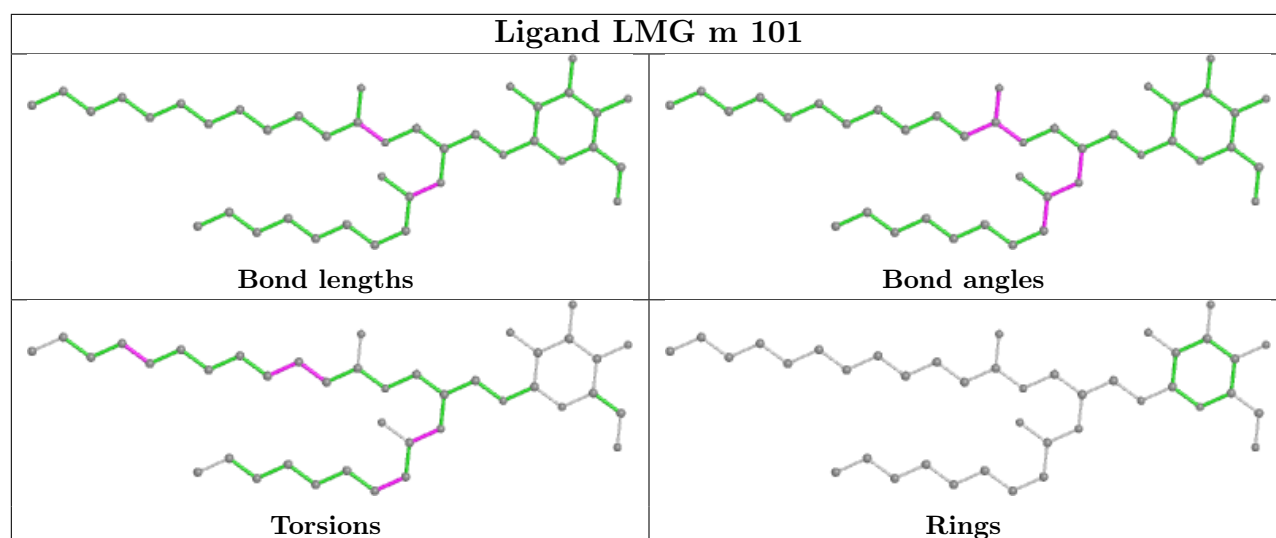
Bond angles



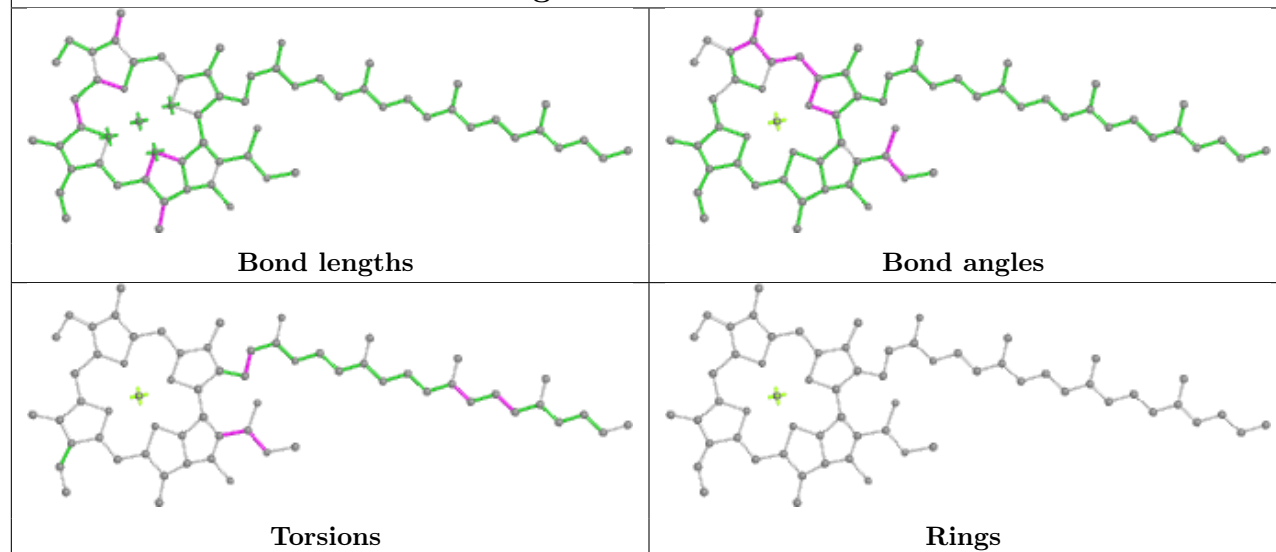
Torsions



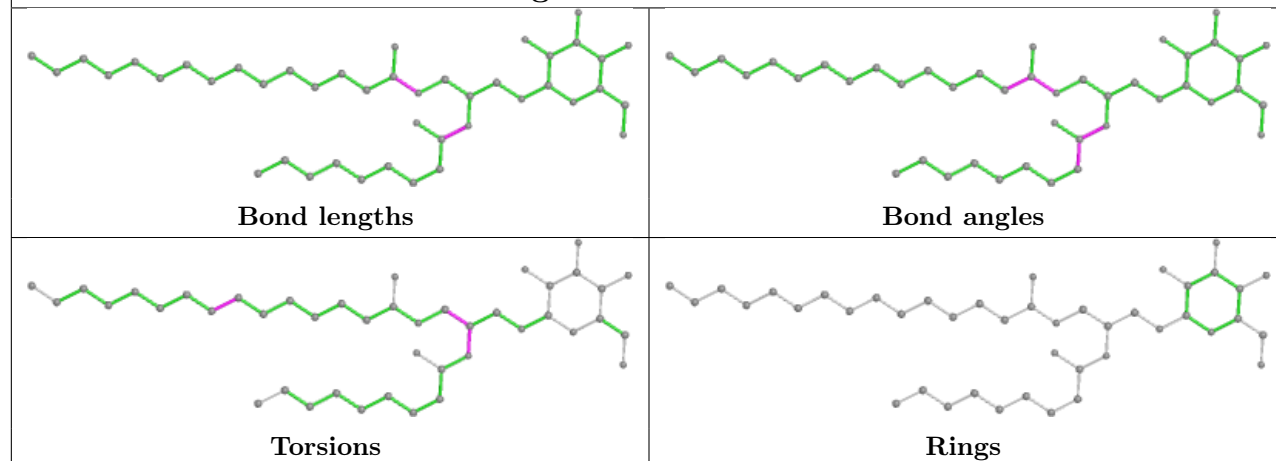
Rings



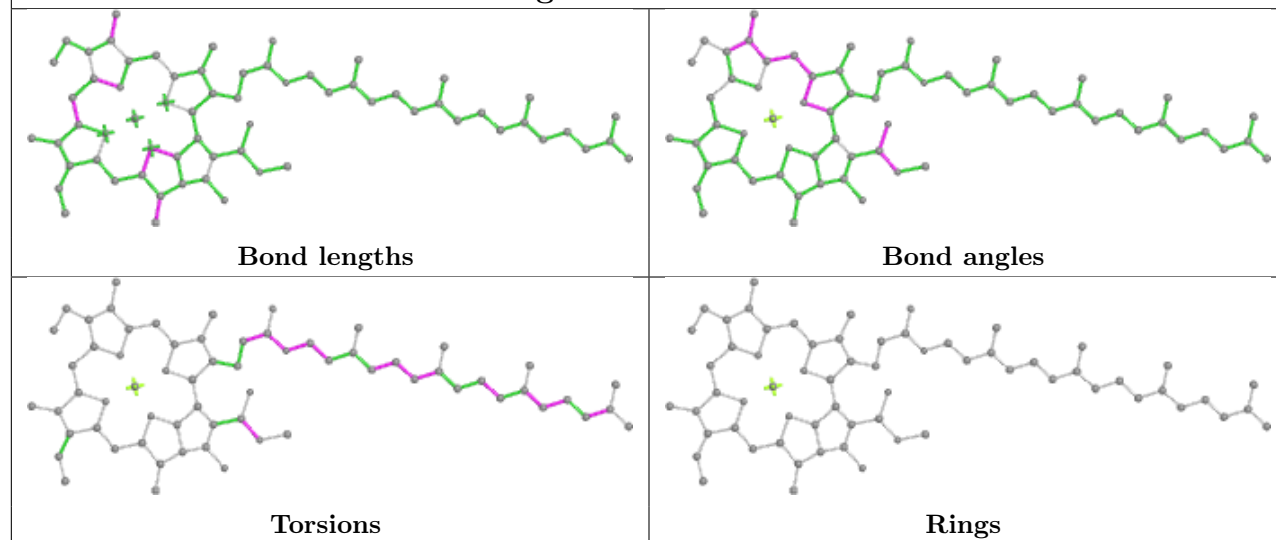
Ligand CLA P 604



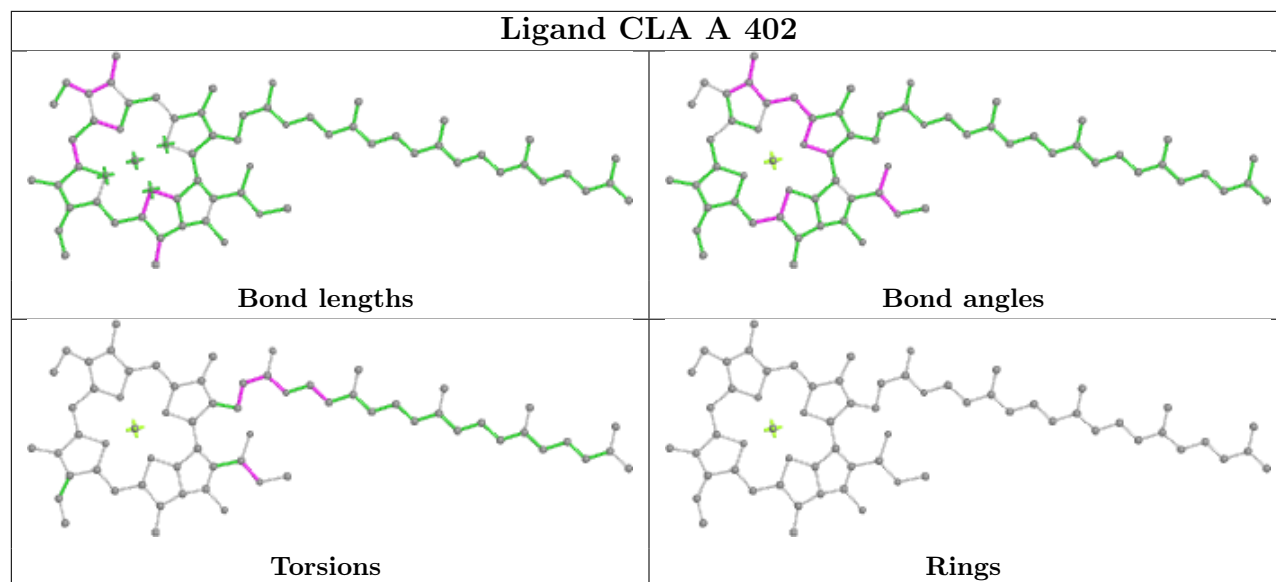
Ligand LMG 4 319



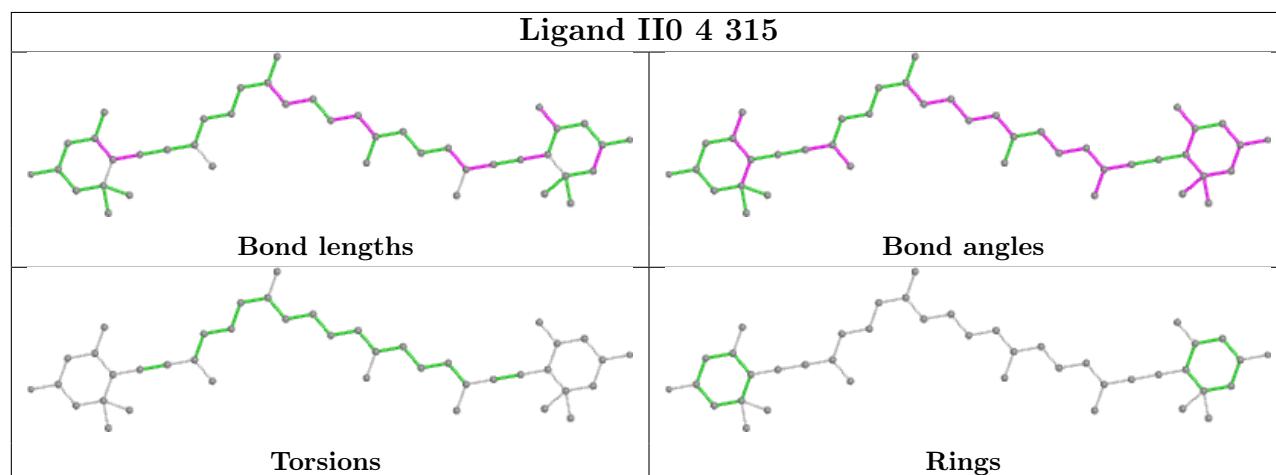
Ligand CLA 5 609



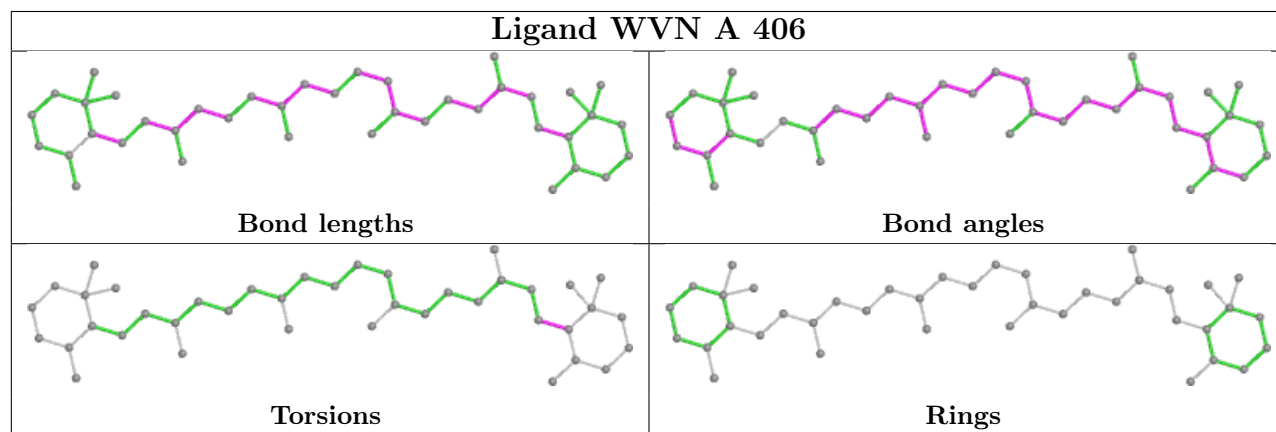
Ligand CLA A 402

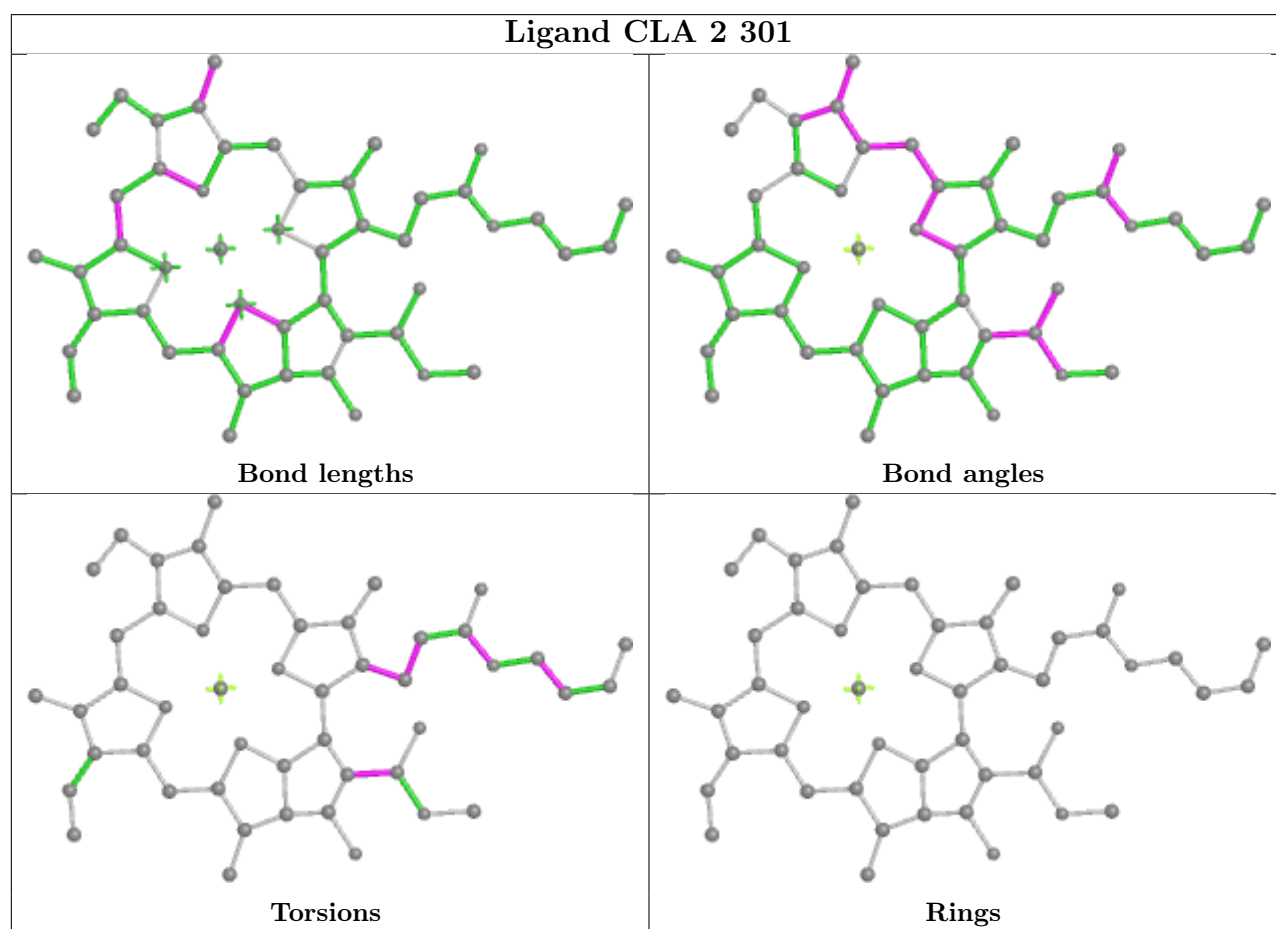
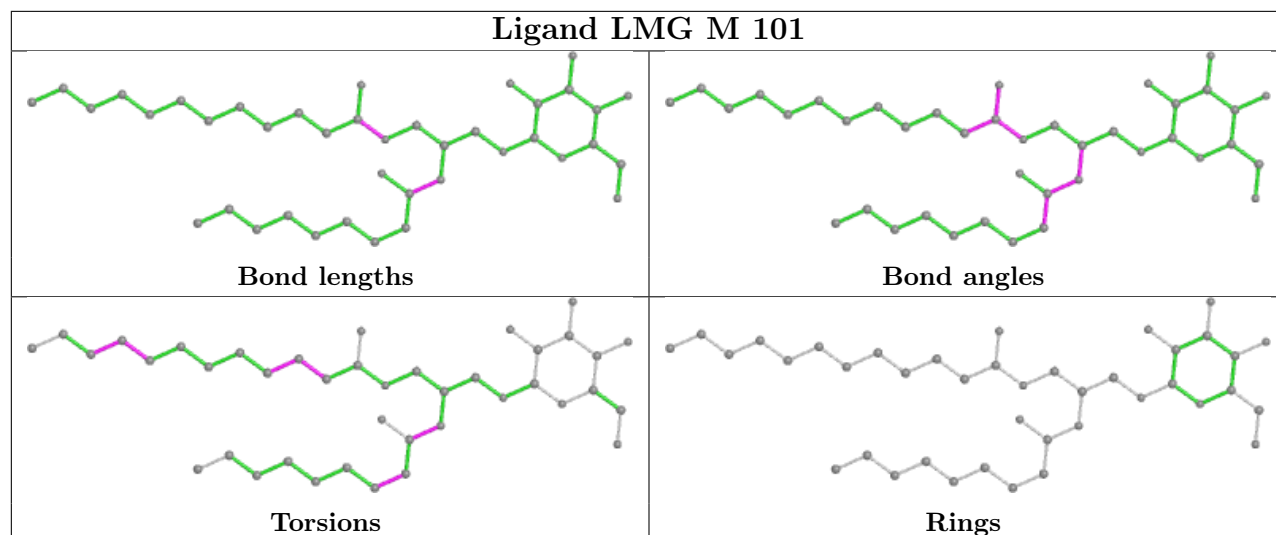


Ligand II0 4 315

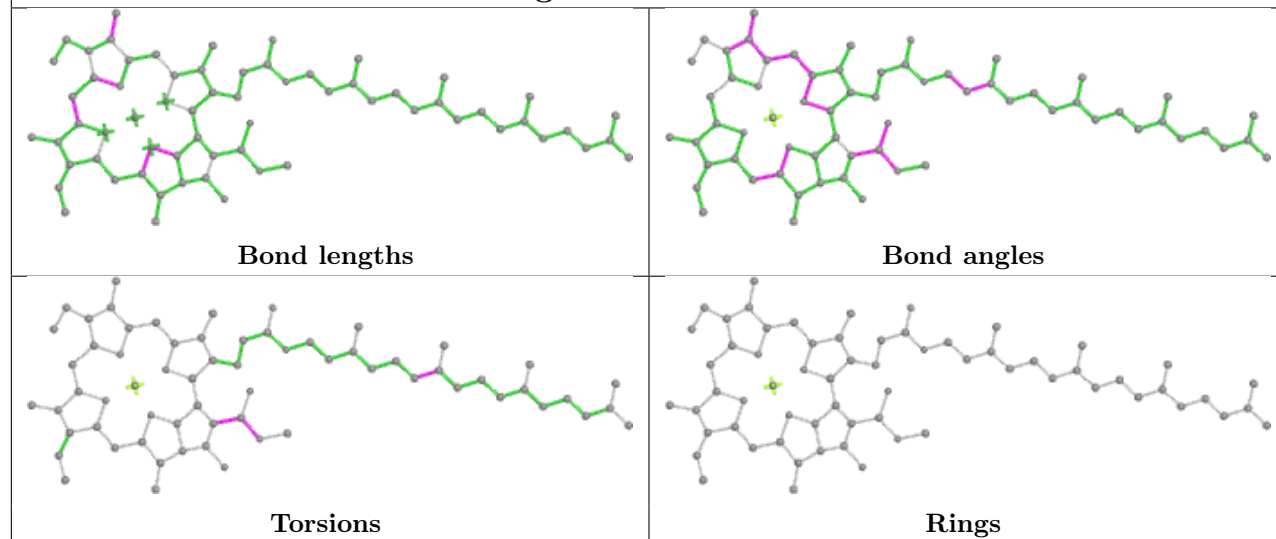


Ligand WVN A 406

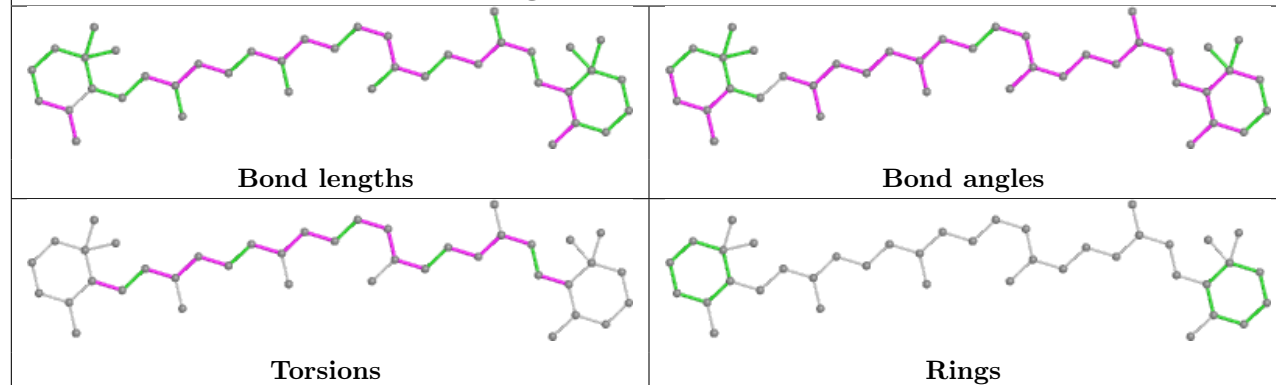




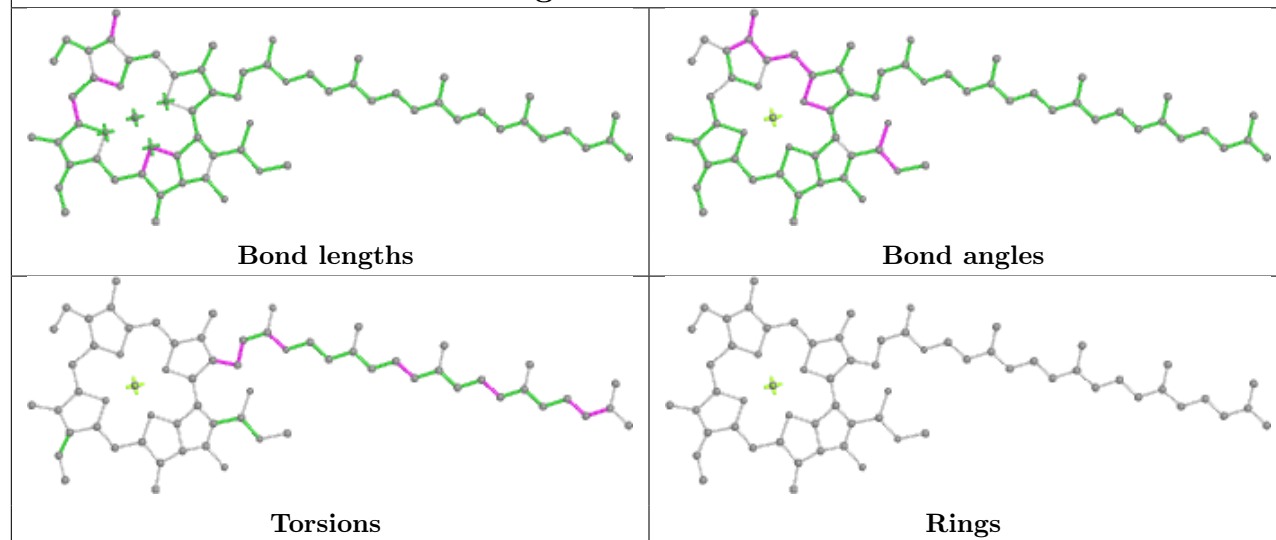
Ligand CLA b 602



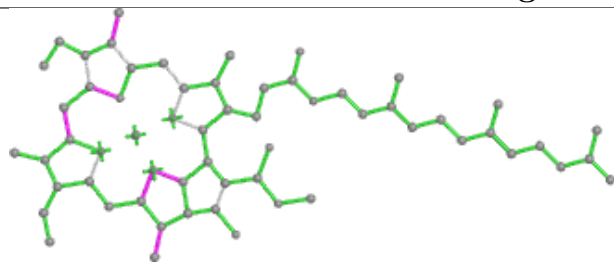
Ligand WVN C 516



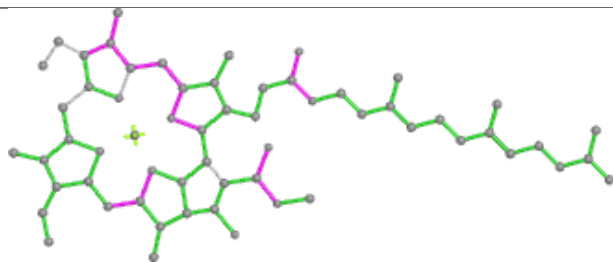
Ligand CLA b 615



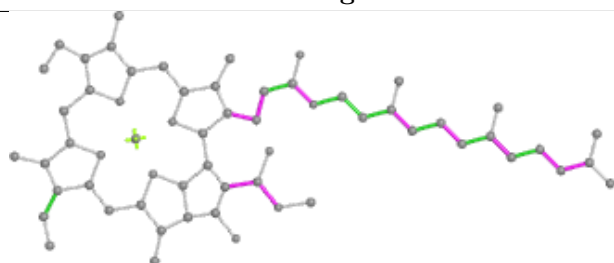
Ligand CLA 1 609



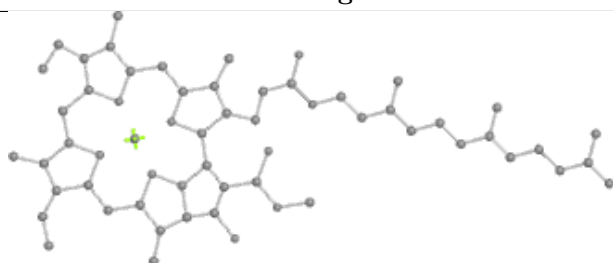
Bond lengths



Bond angles

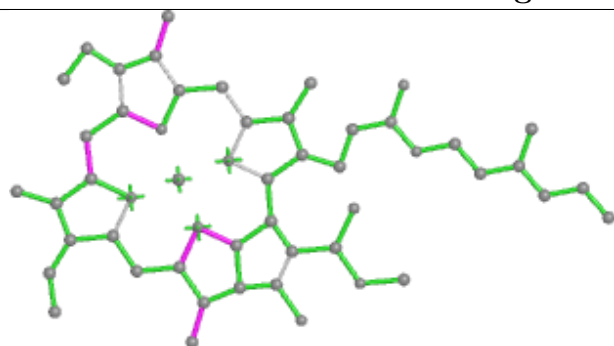


Torsions

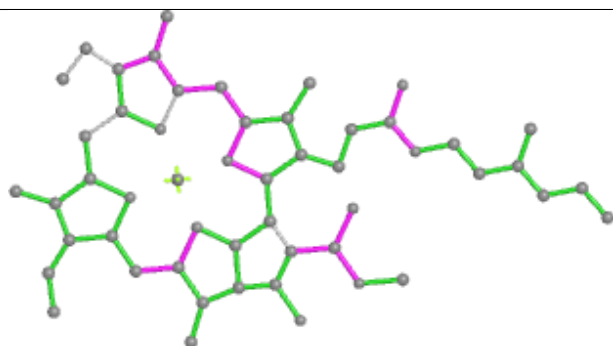


Rings

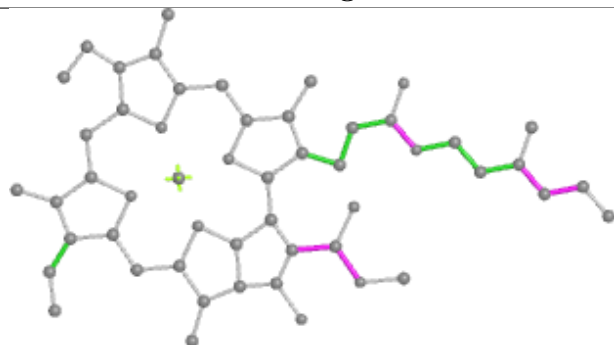
Ligand CLA C 514



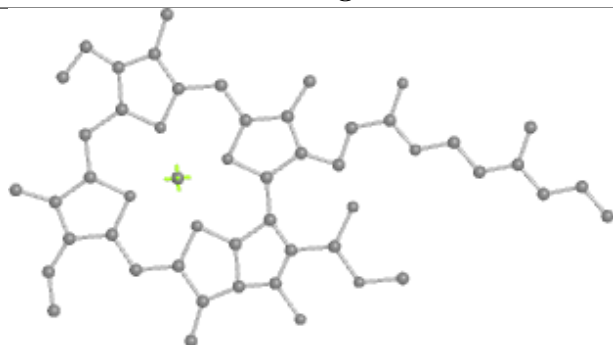
Bond lengths



Bond angles

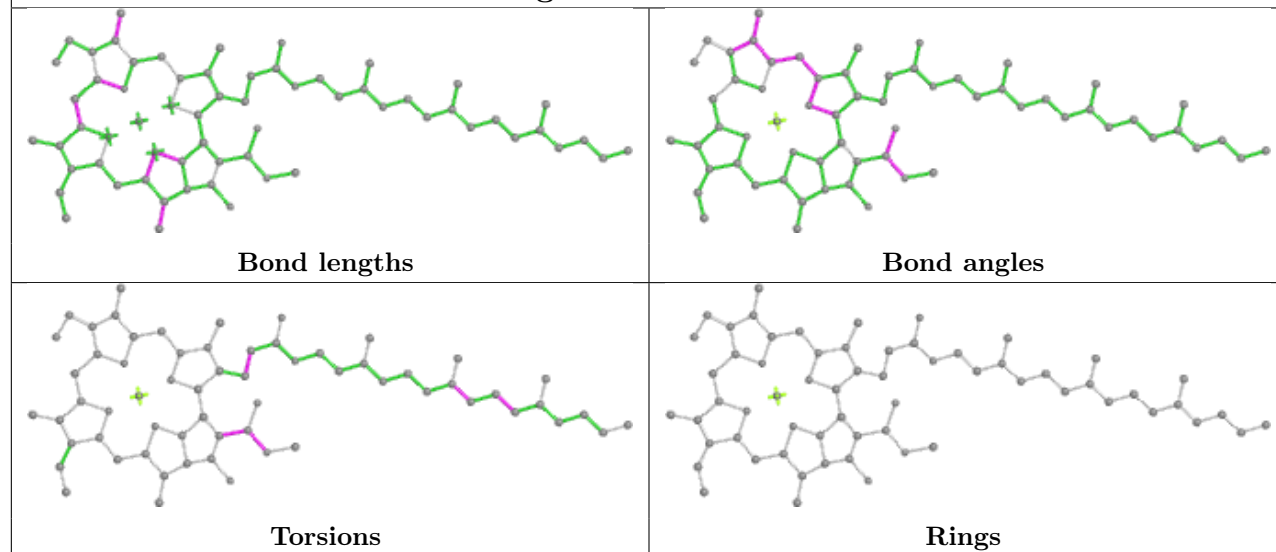


Torsions

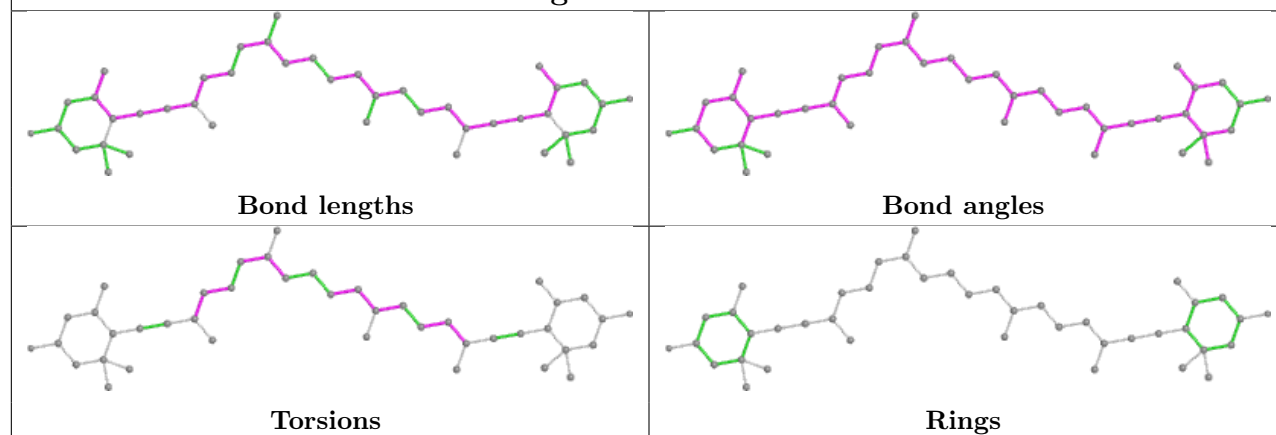


Rings

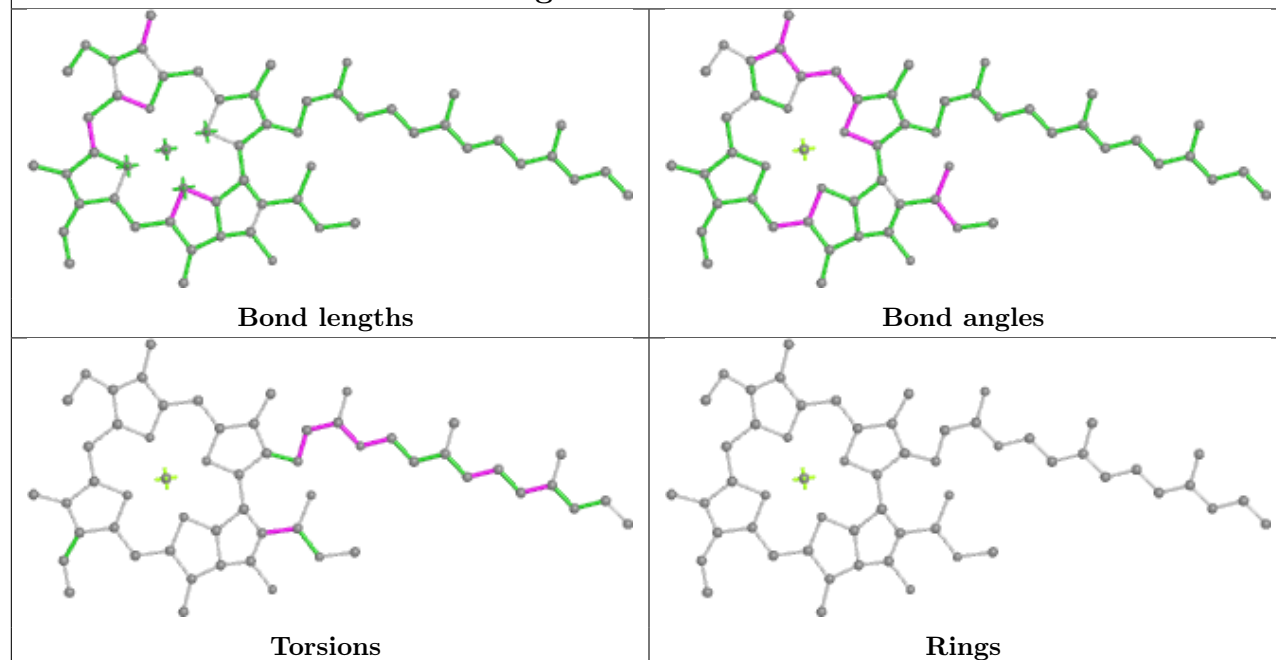
Ligand CLA 3 303



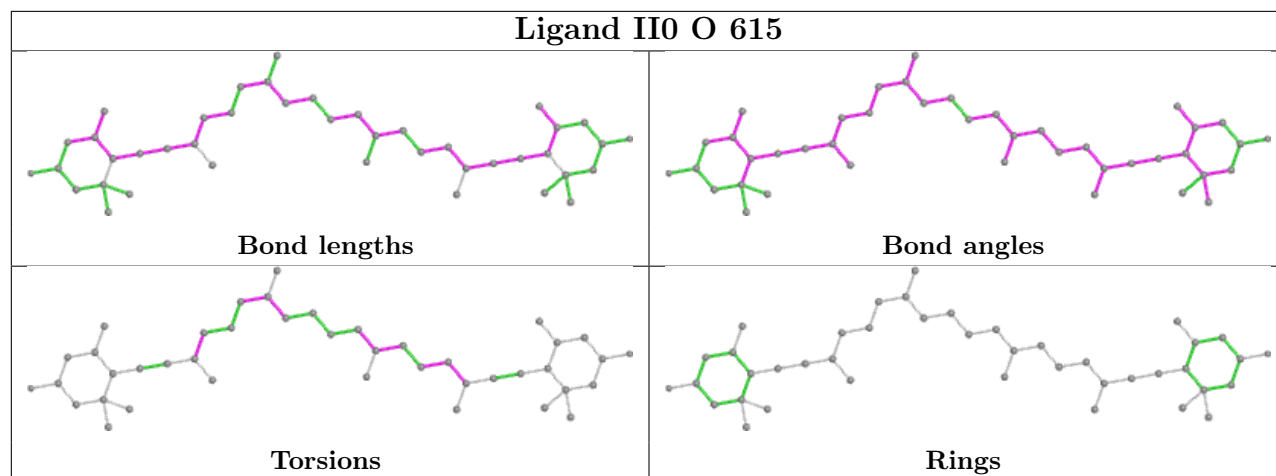
Ligand II0 1 616



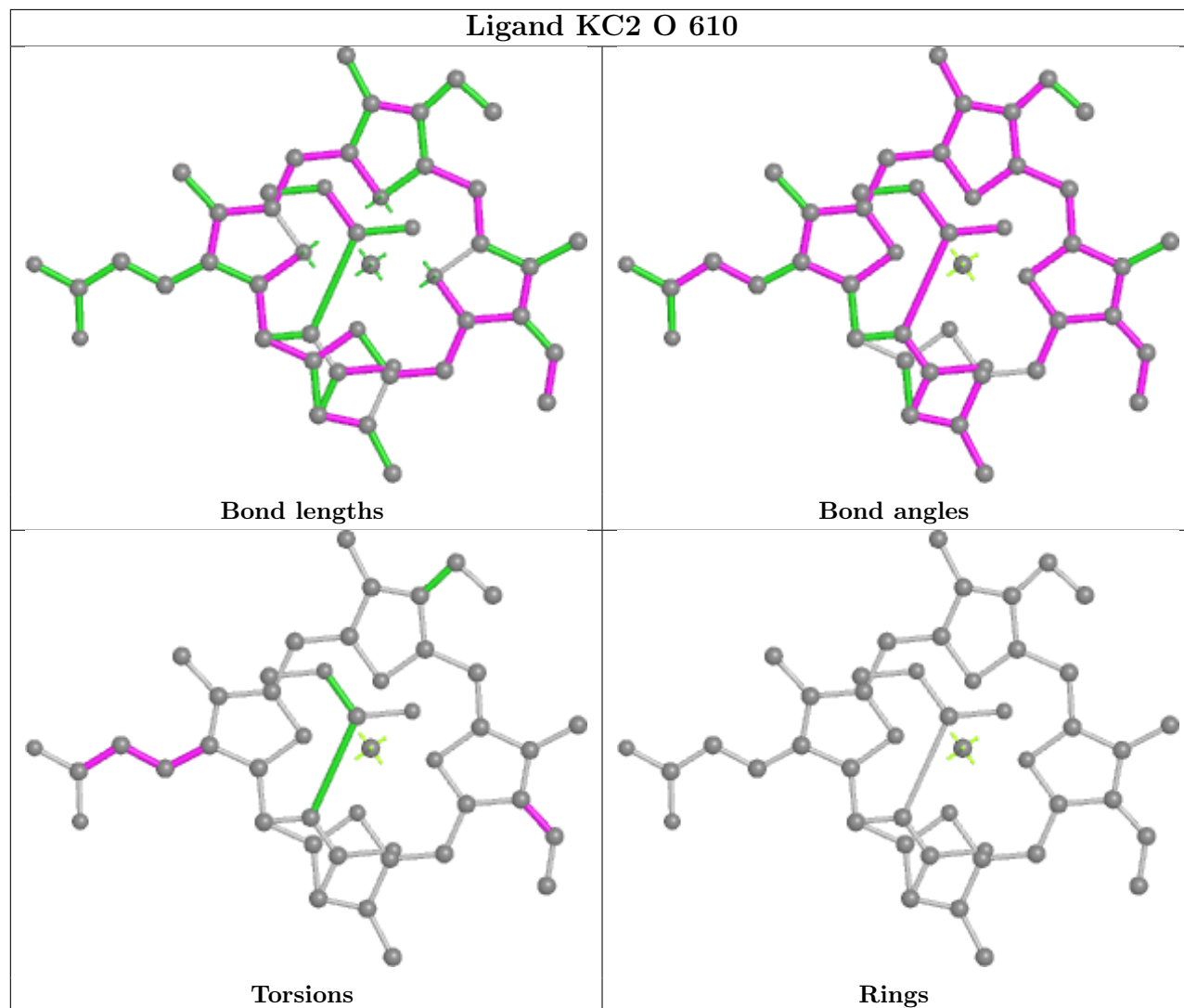
Ligand CLA S 606



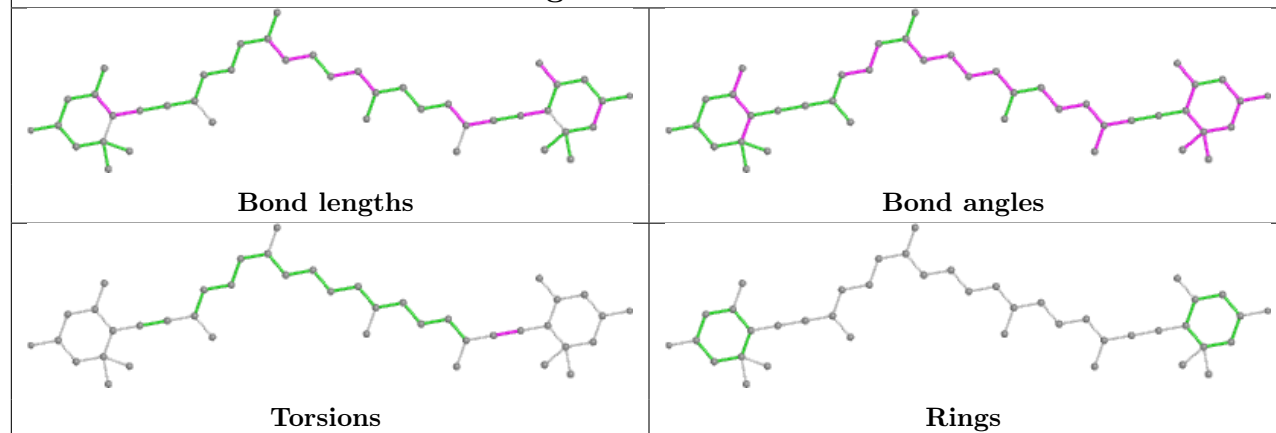
Ligand II0 O 615



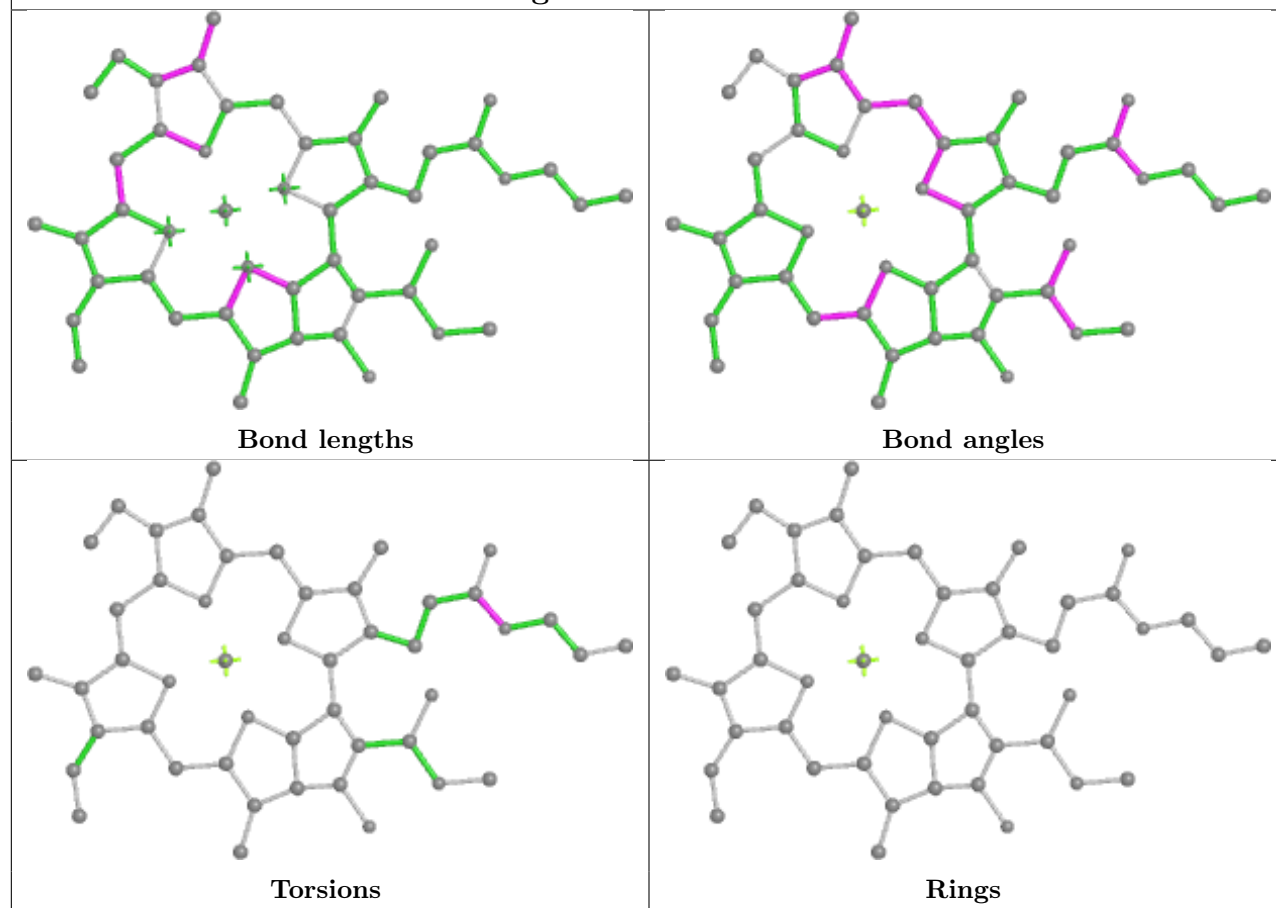
Ligand KC2 O 610



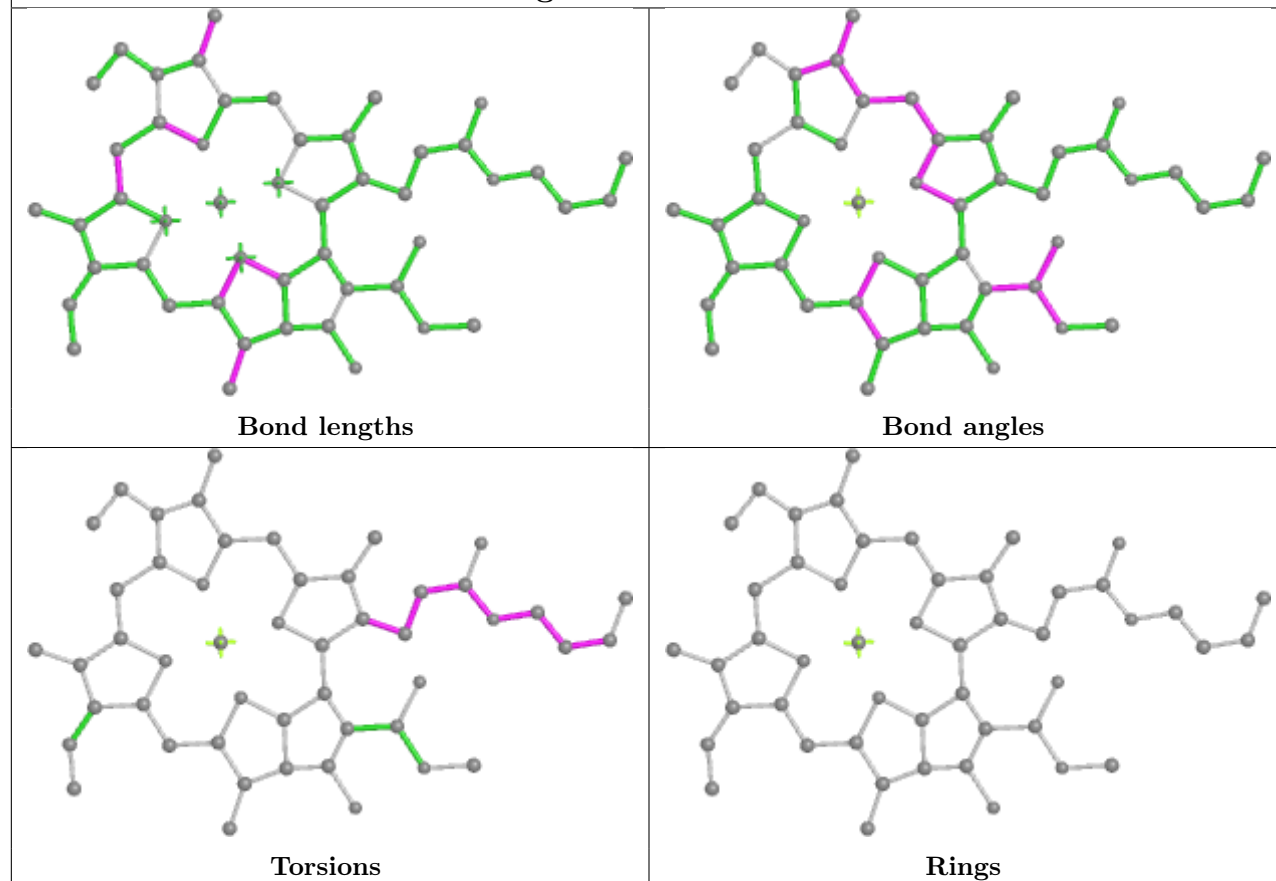
Ligand II0 R 315



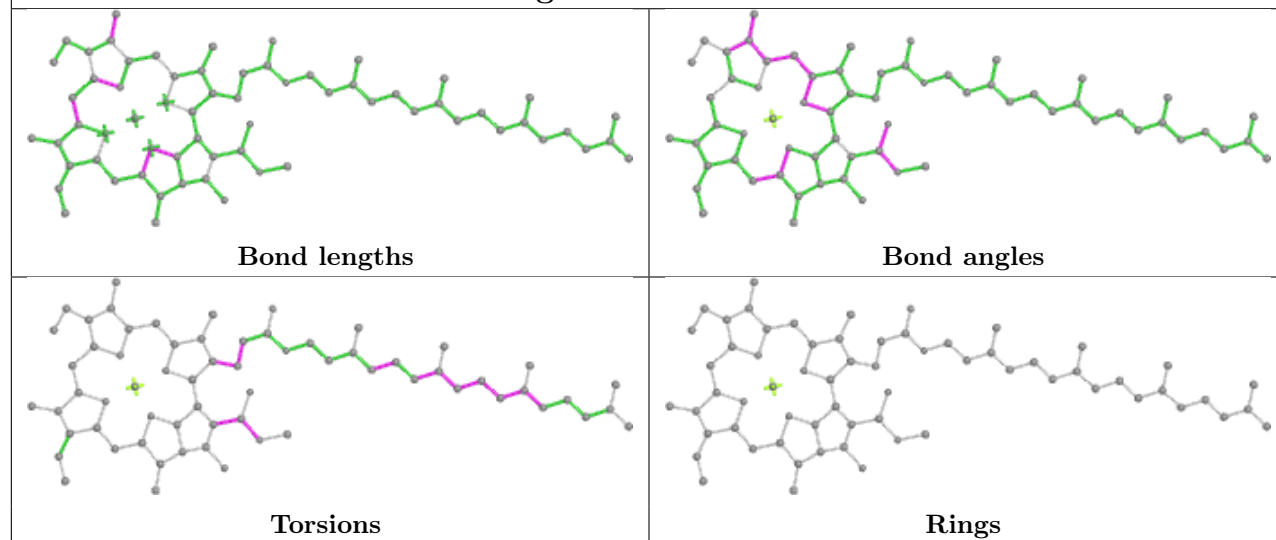
Ligand CLA O 607

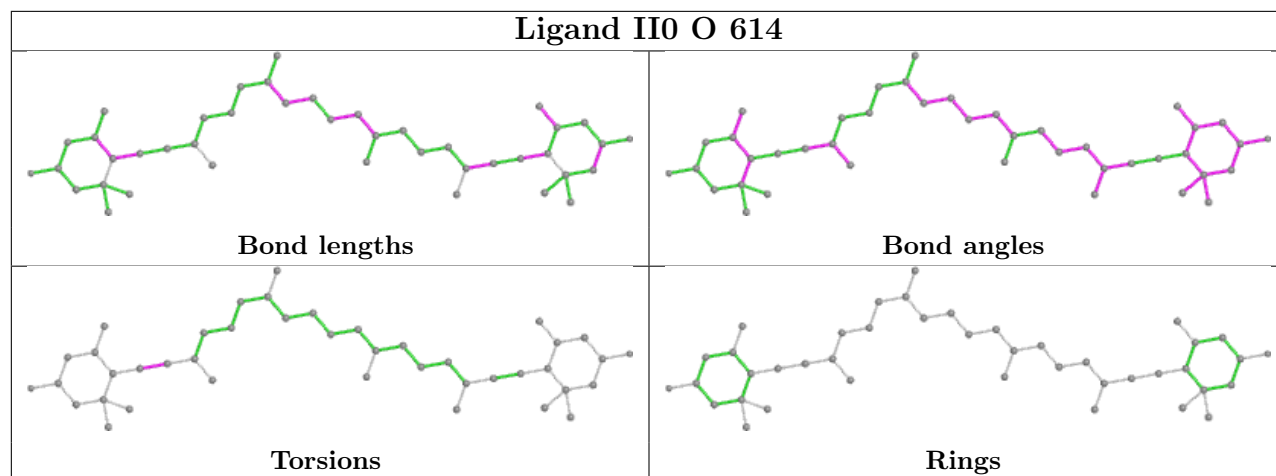
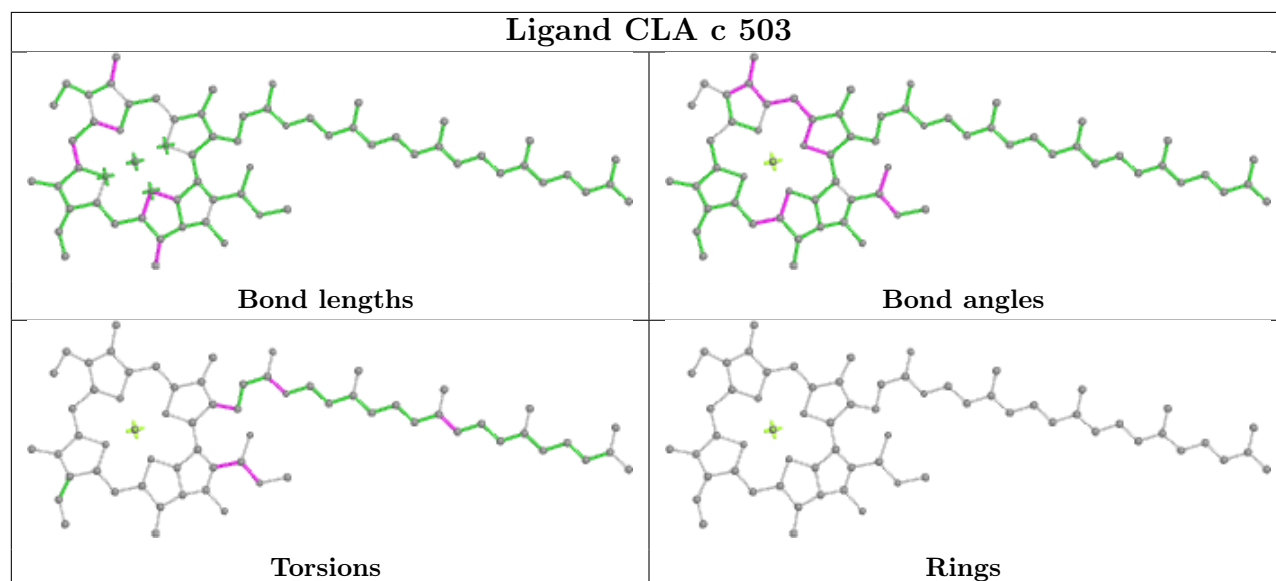


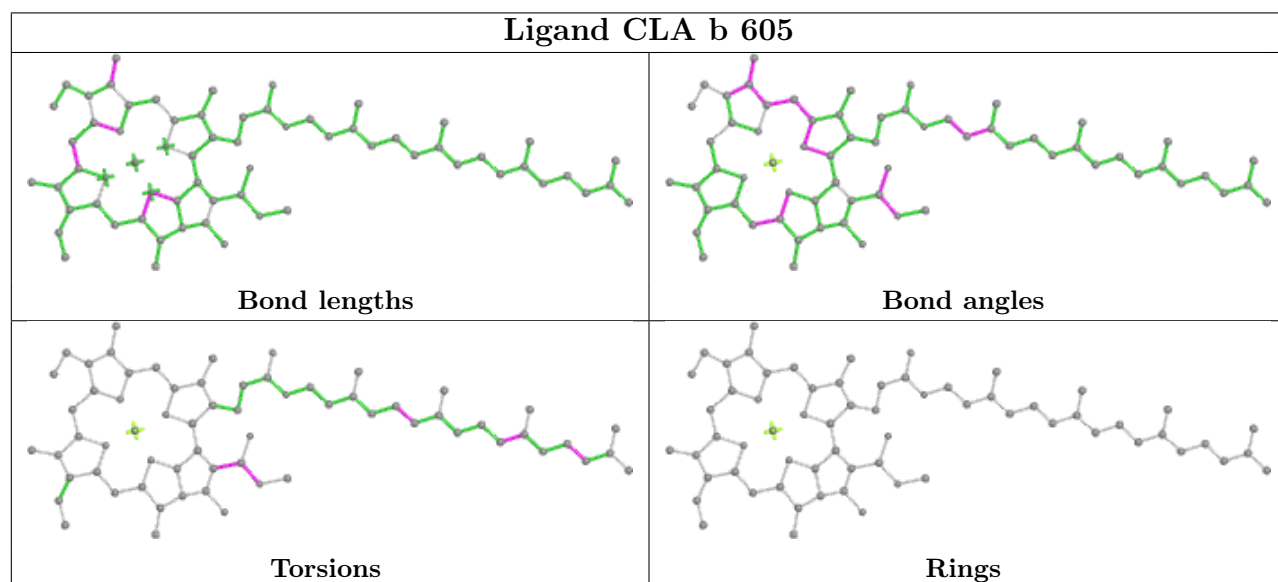
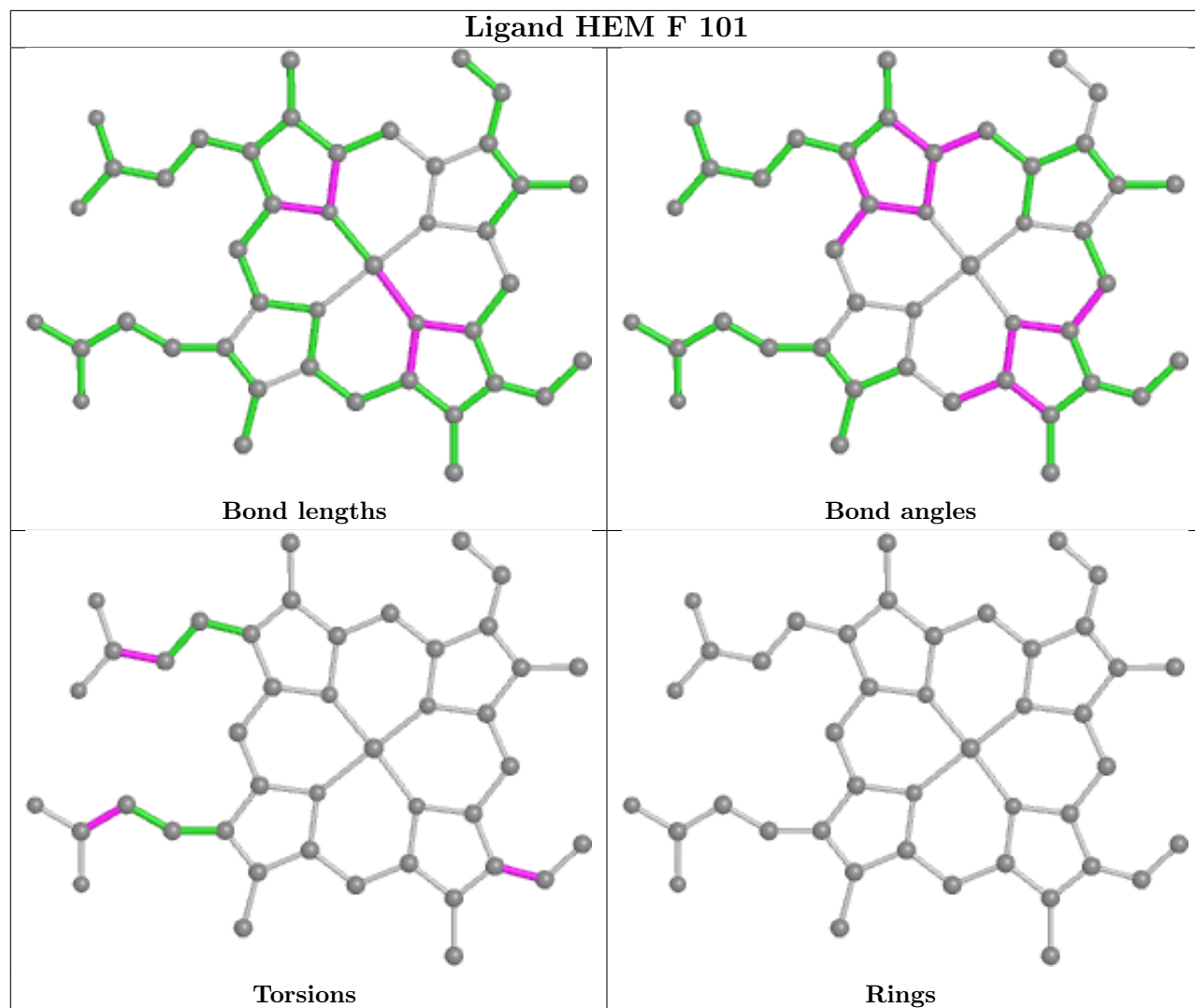
Ligand CLA a 403



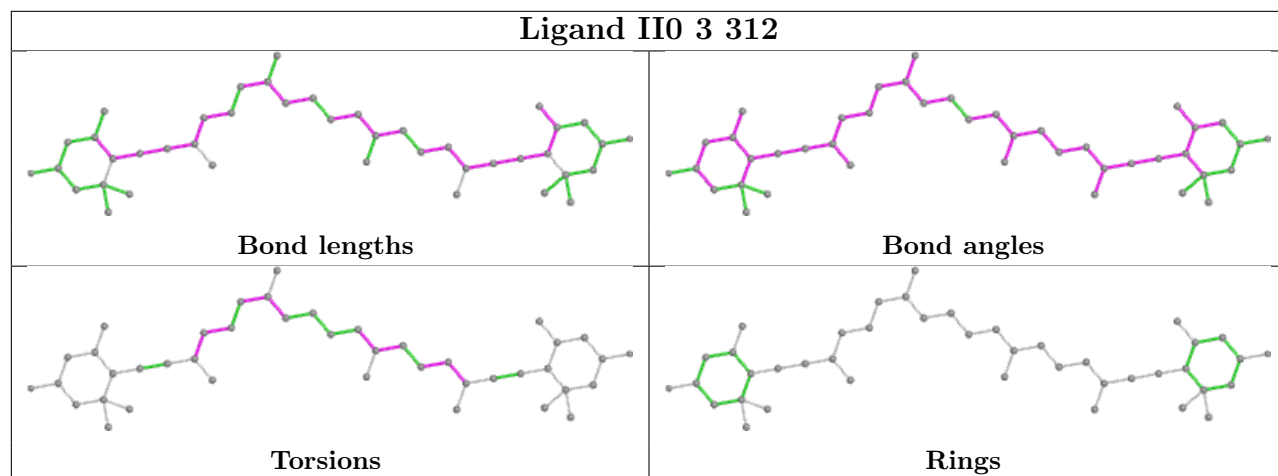
Ligand CLA 6 602



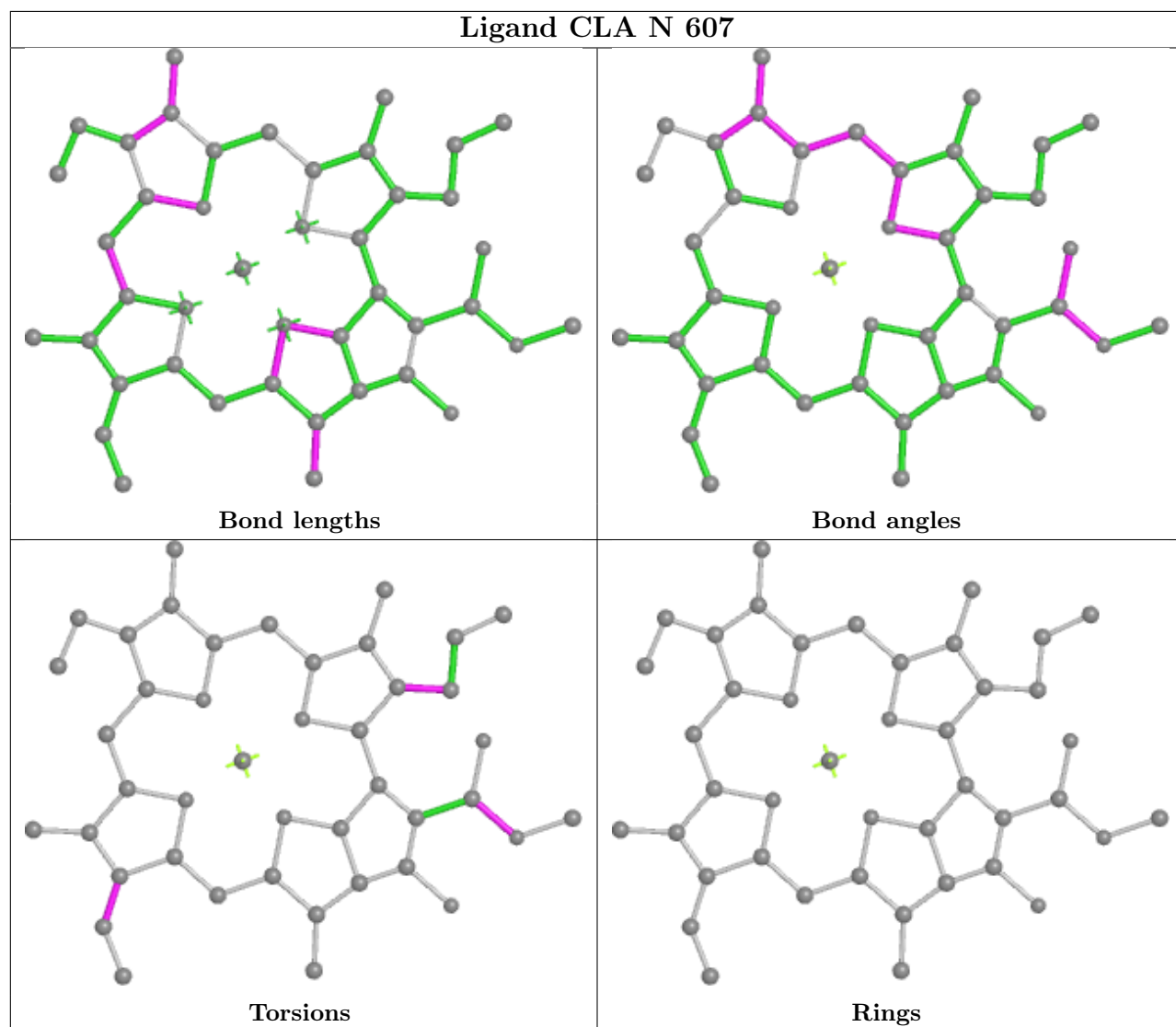
Ligand II0 O 614**Ligand CLA c 503**



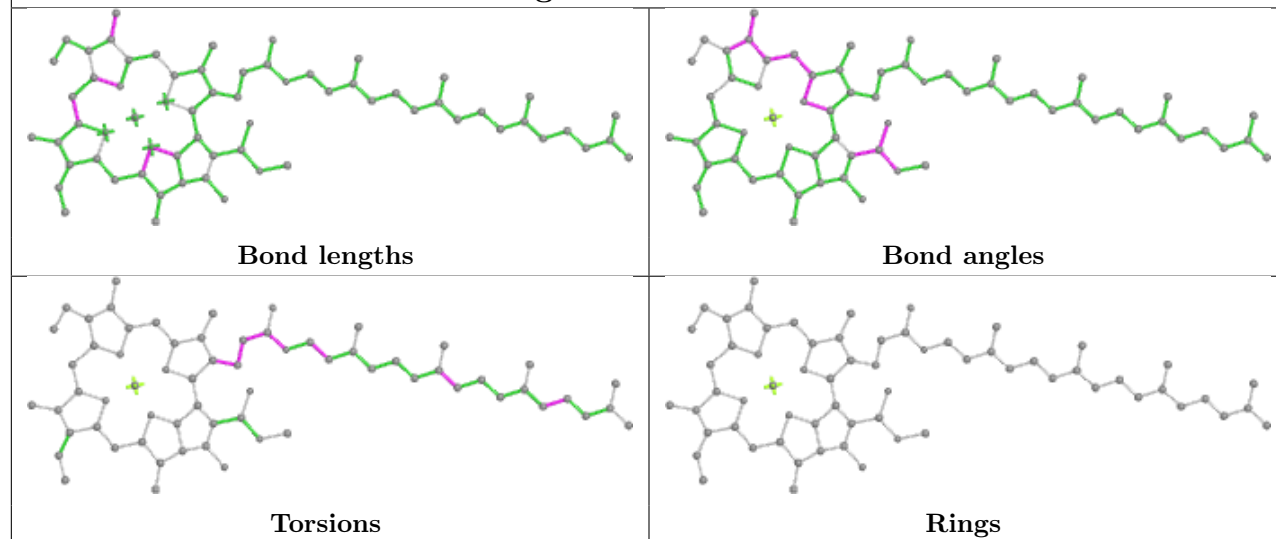
Ligand II0 3 312



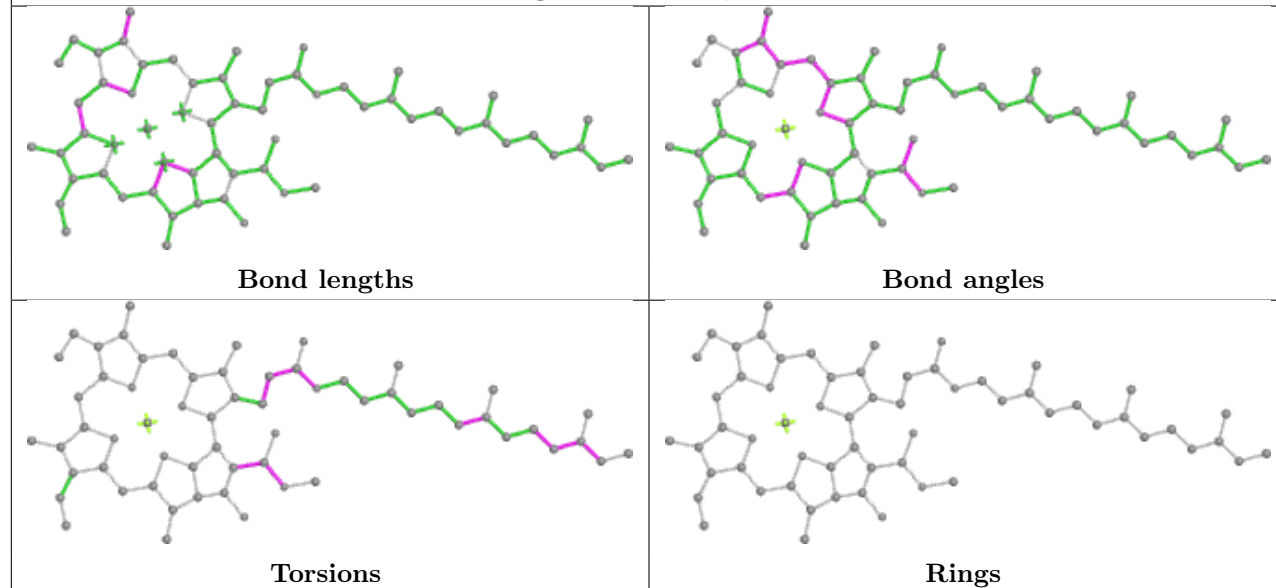
Ligand CLA N 607

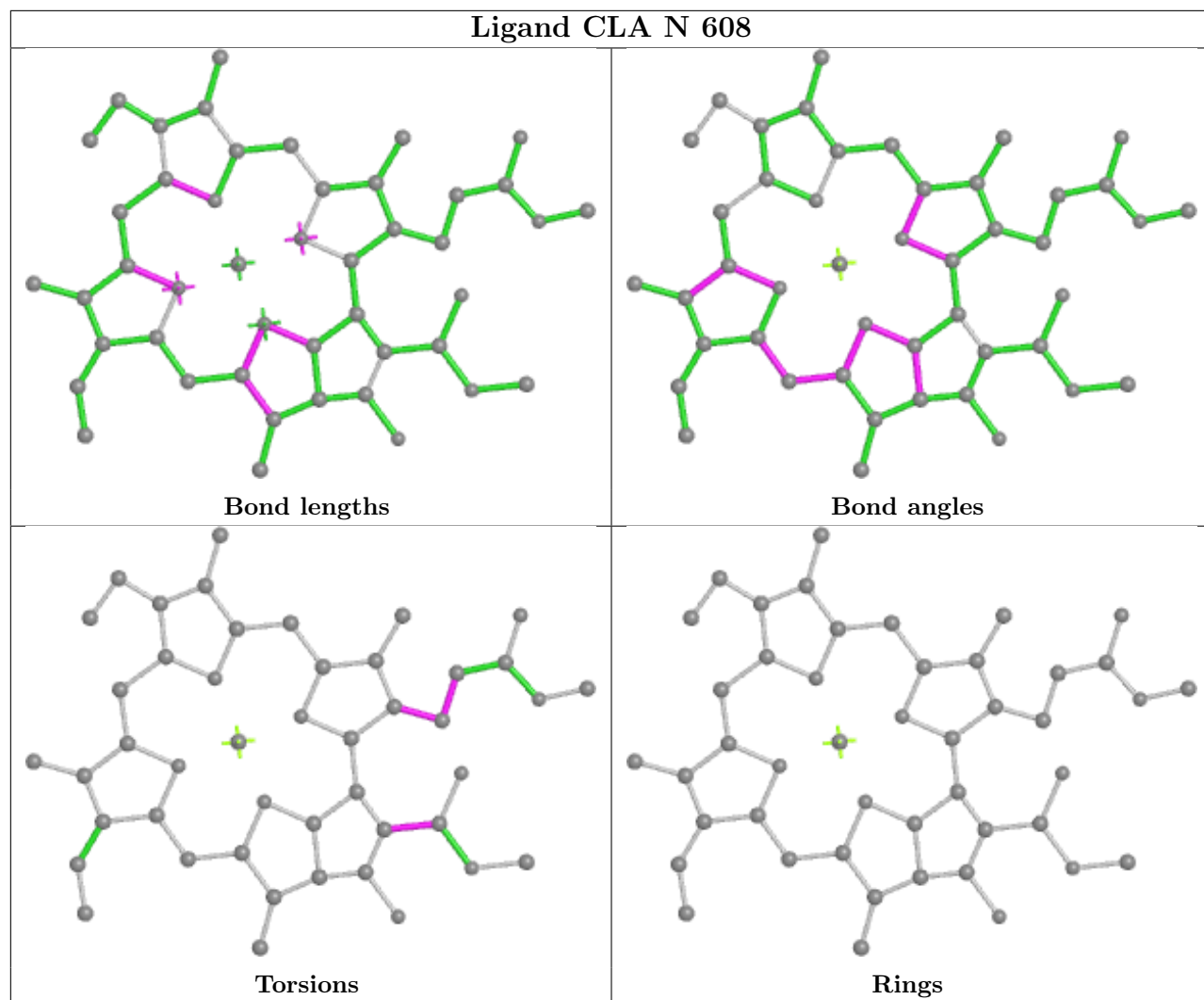


Ligand CLA d 402

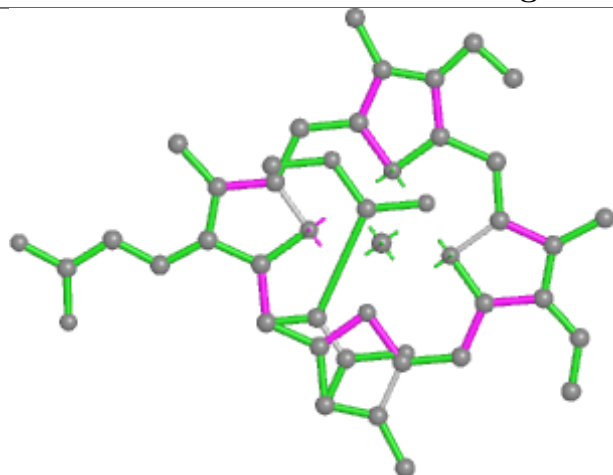


Ligand CLA Q 303

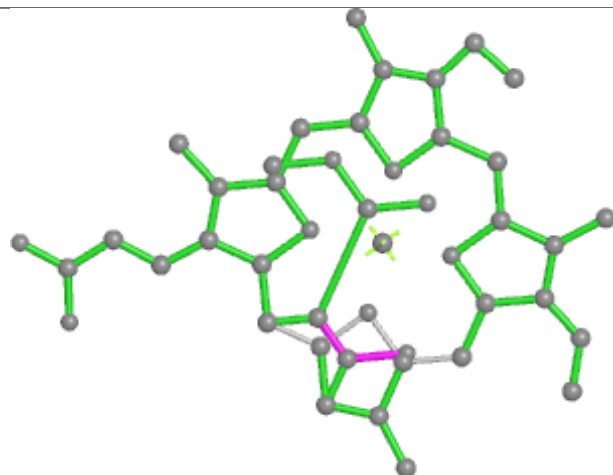




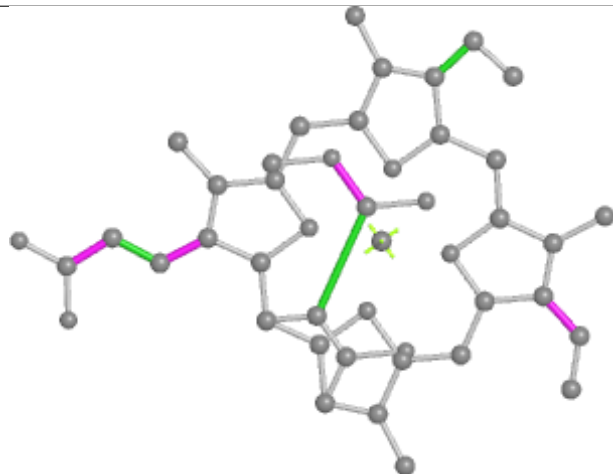
Ligand KC2 1 611



Bond lengths



Bond angles

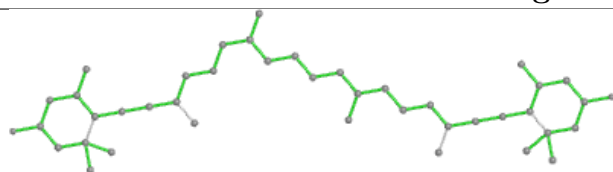


Torsions

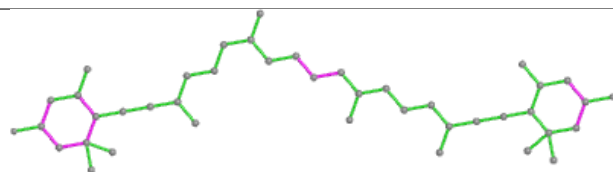


Rings

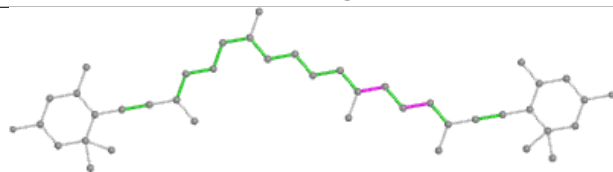
Ligand II0 2 320



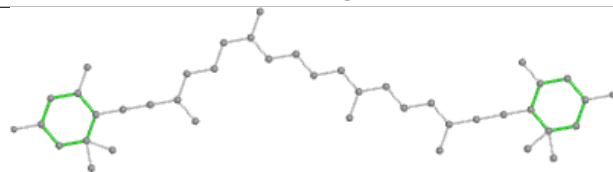
Bond lengths



Bond angles

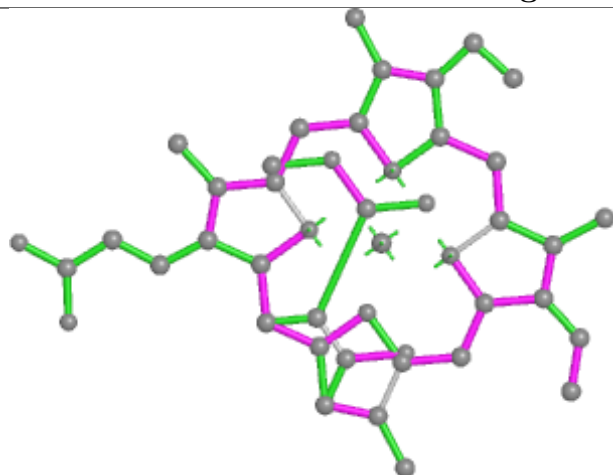


Torsions

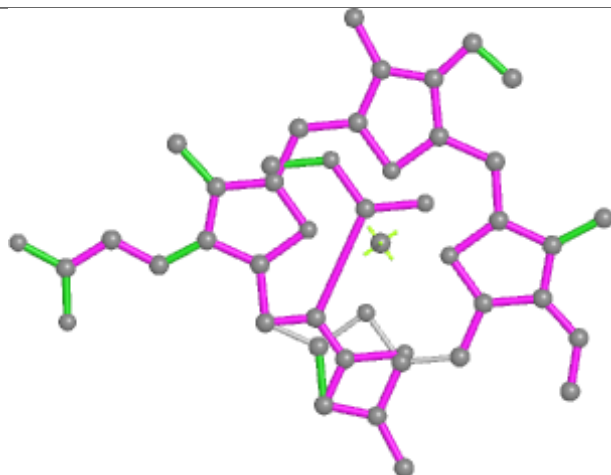


Rings

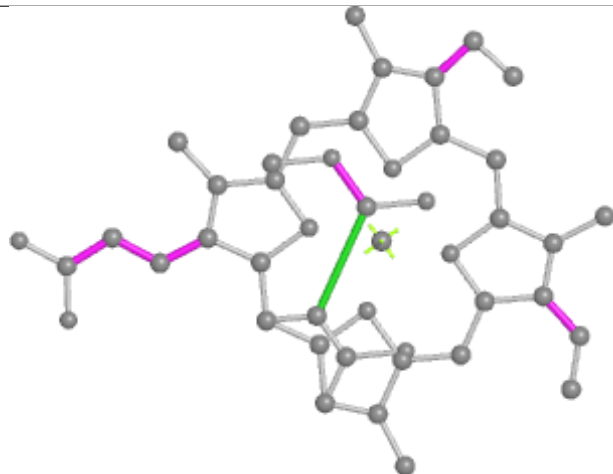
Ligand KC2 3 304



Bond lengths



Bond angles

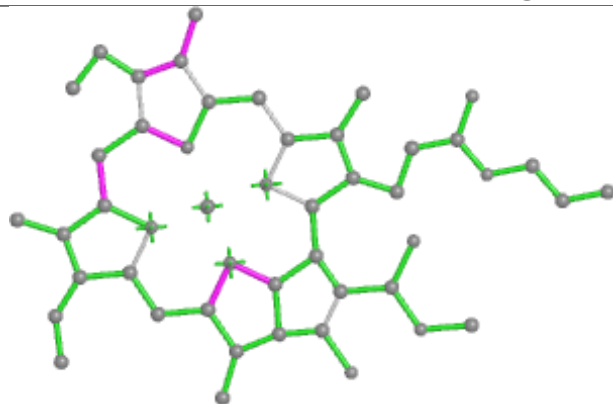


Torsions

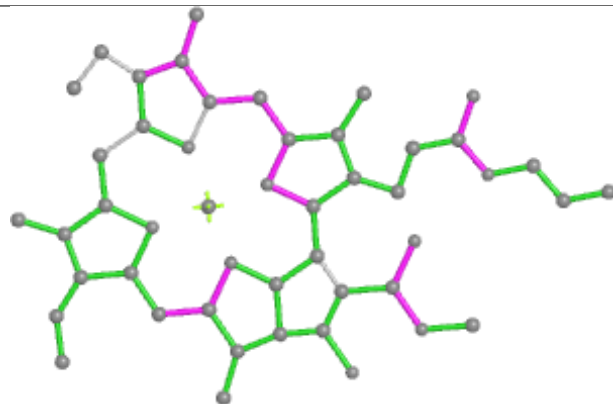


Rings

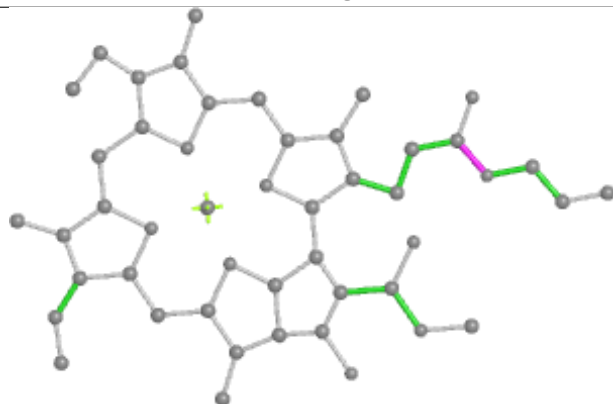
Ligand CLA 2 307



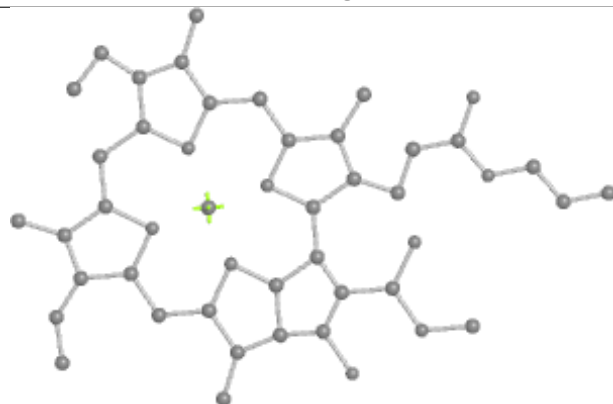
Bond lengths



Bond angles

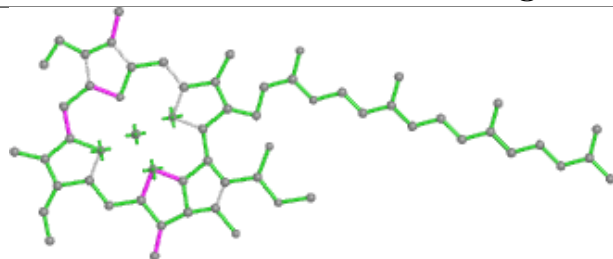


Torsions

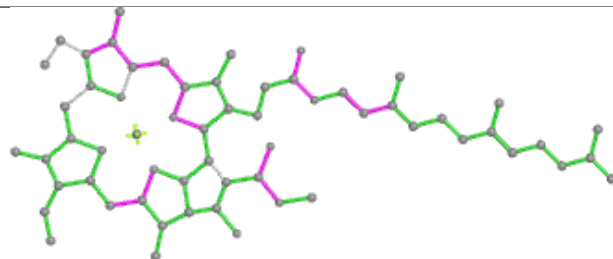


Rings

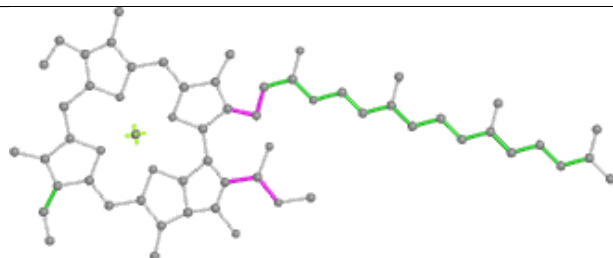
Ligand CLA 1 602



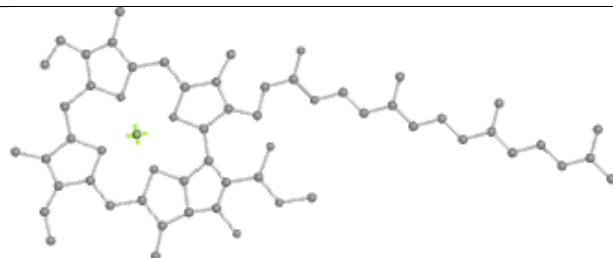
Bond lengths



Bond angles

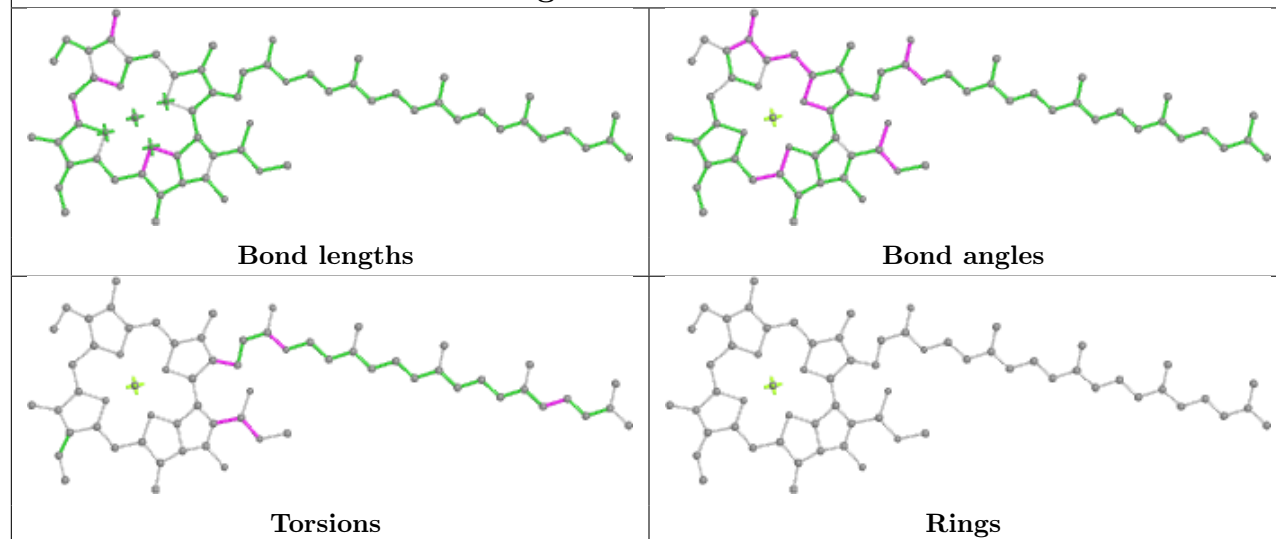


Torsions

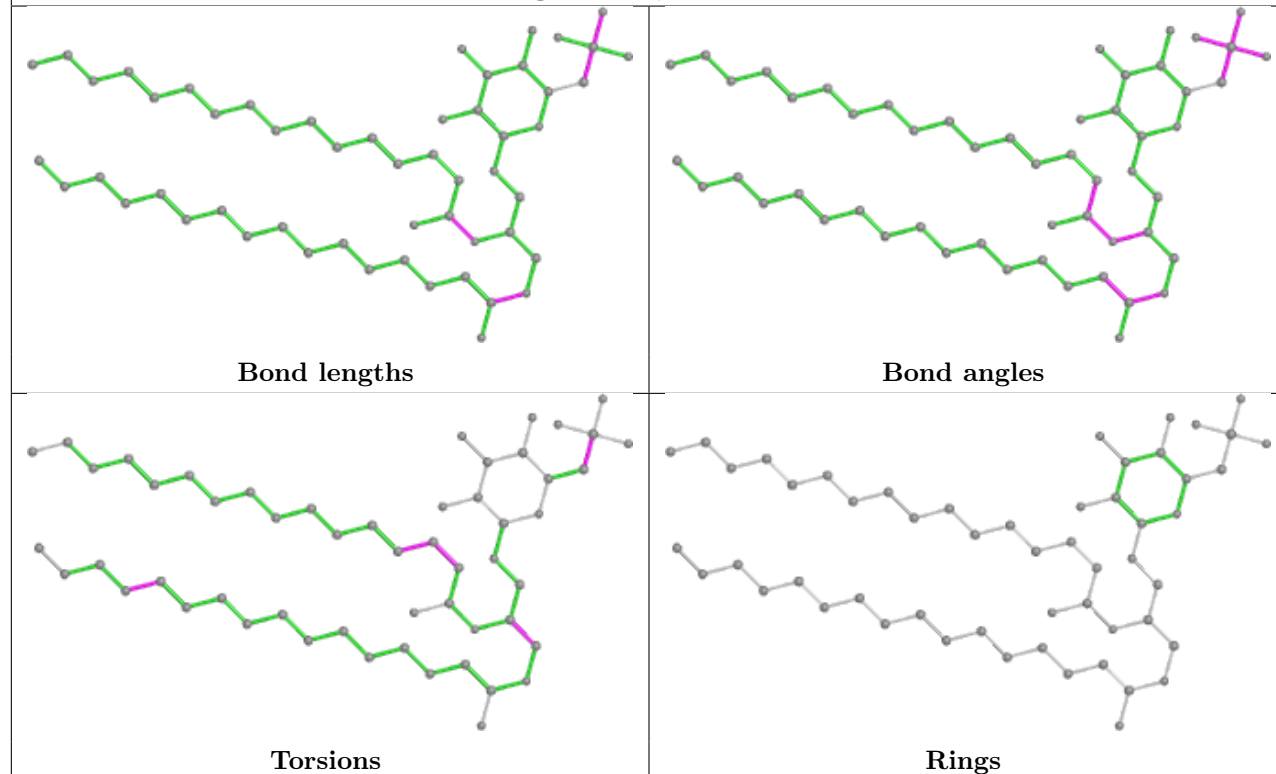


Rings

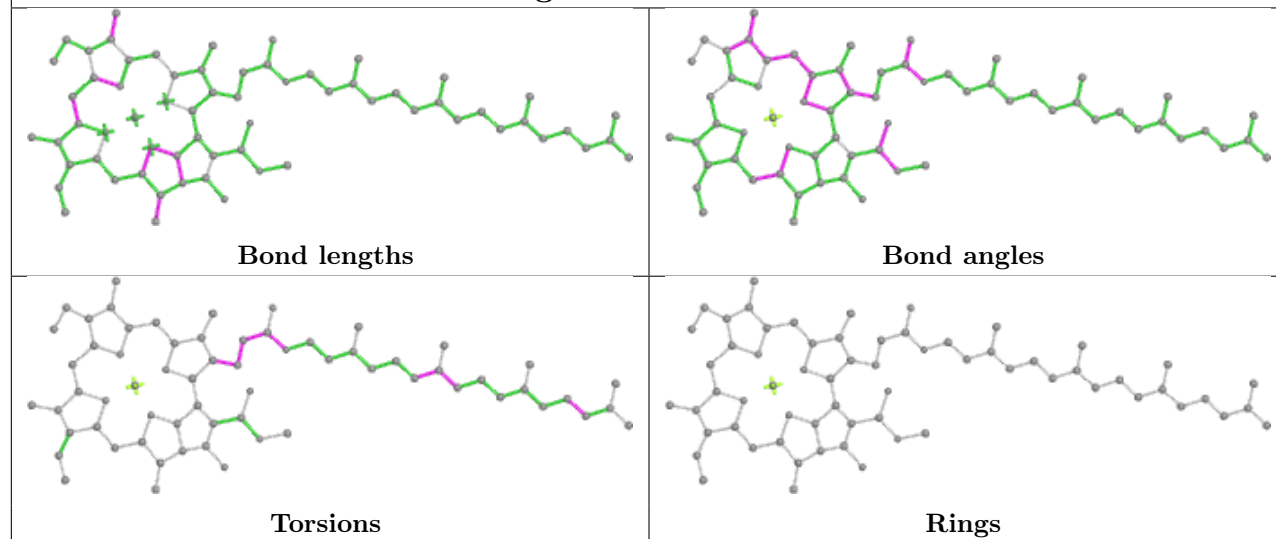
Ligand CLA c 508



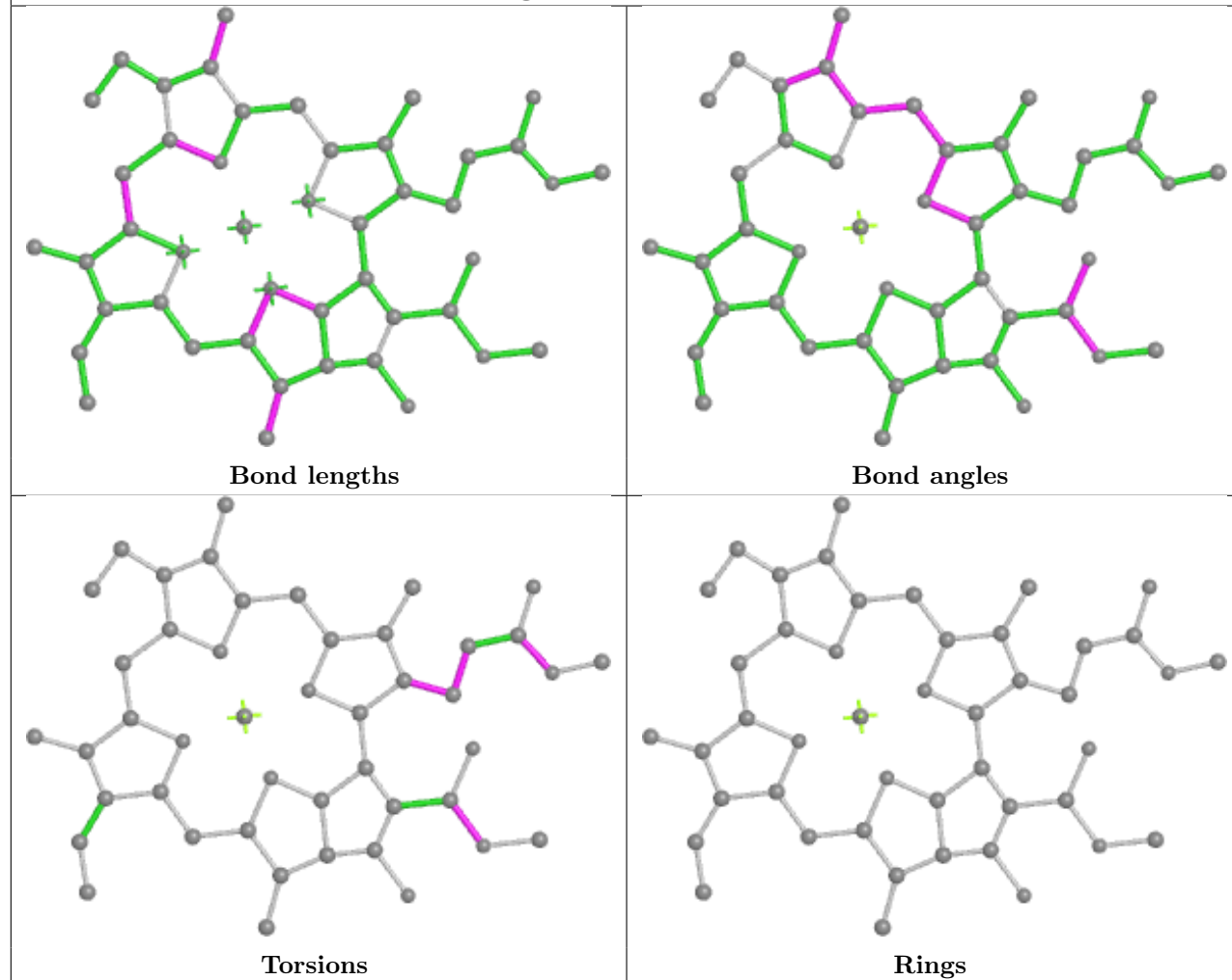
Ligand SQD D 401

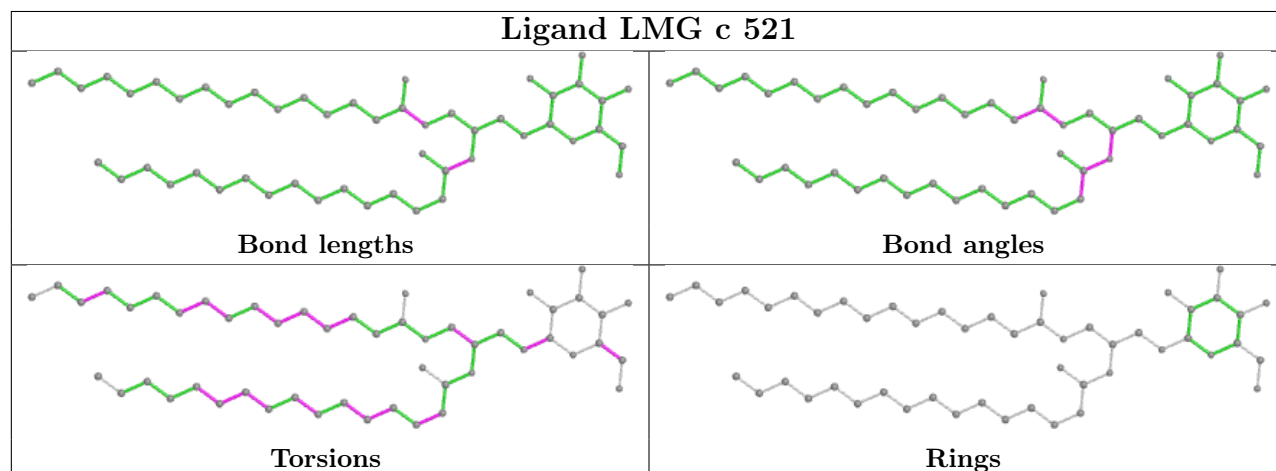
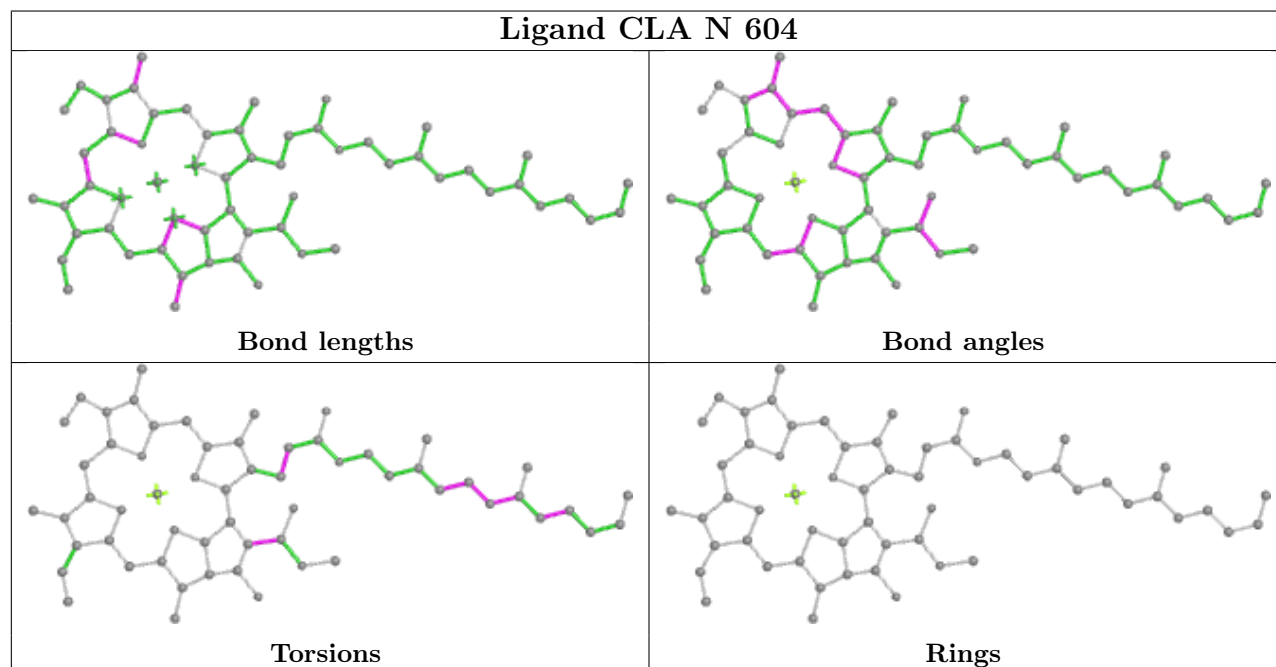
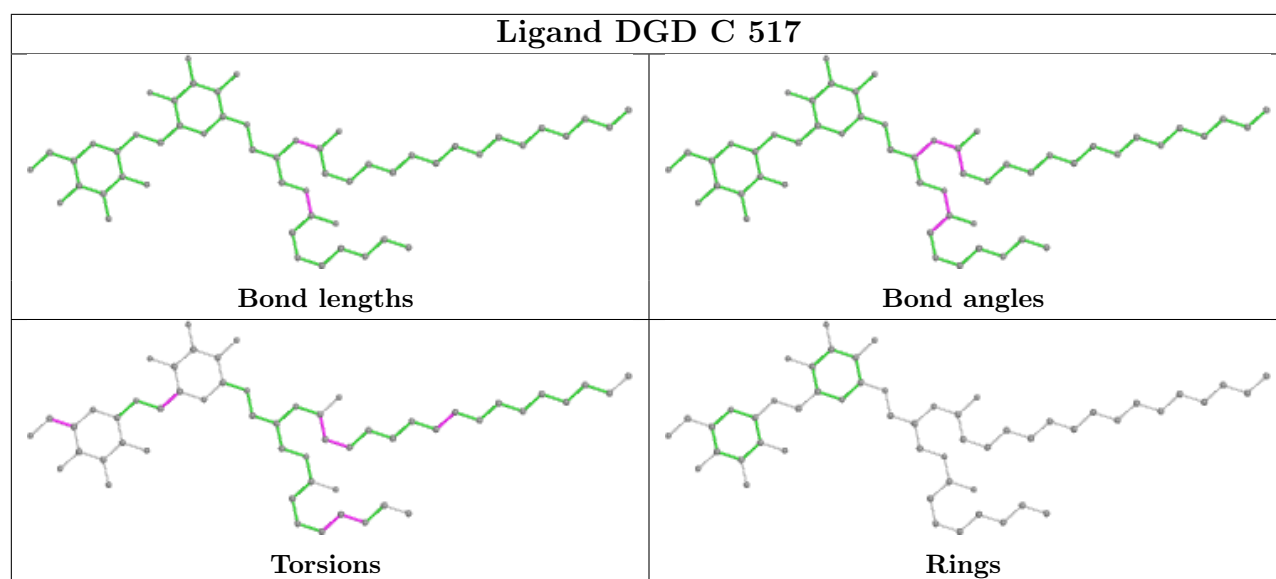


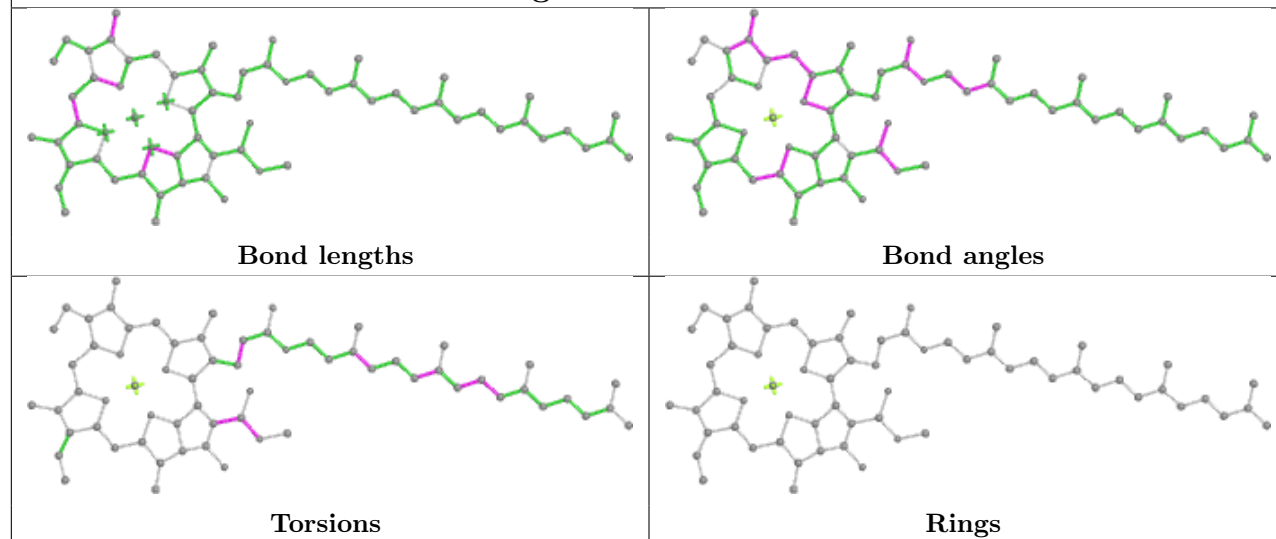
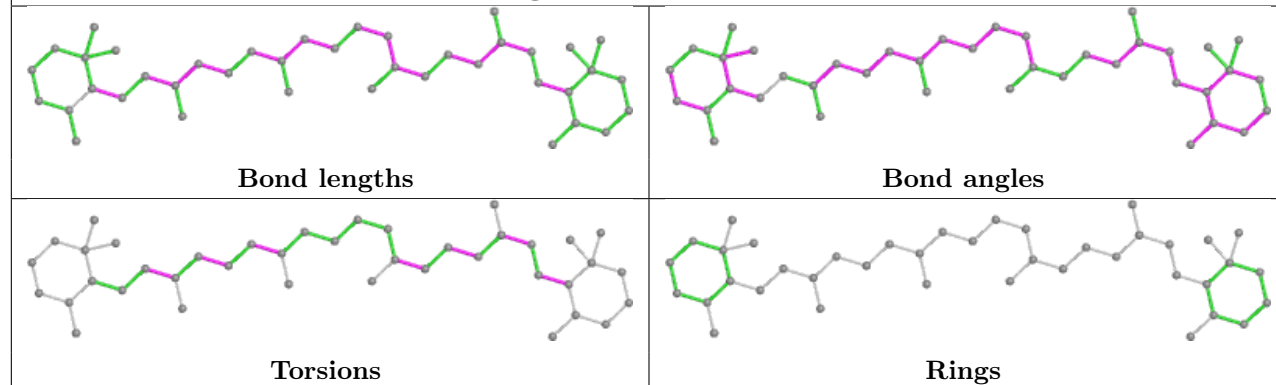
Ligand CLA b 612



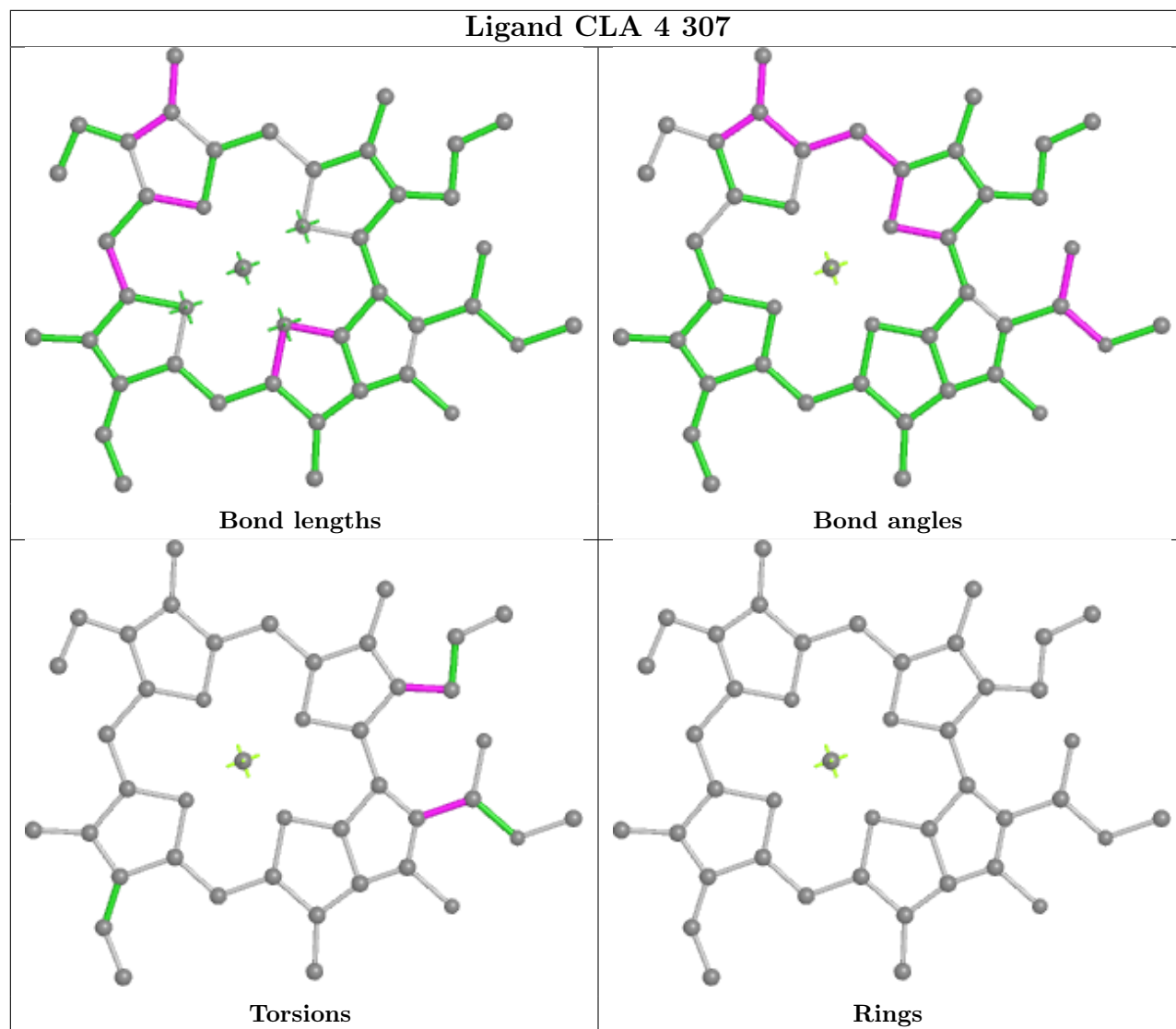
Ligand CLA 1 608

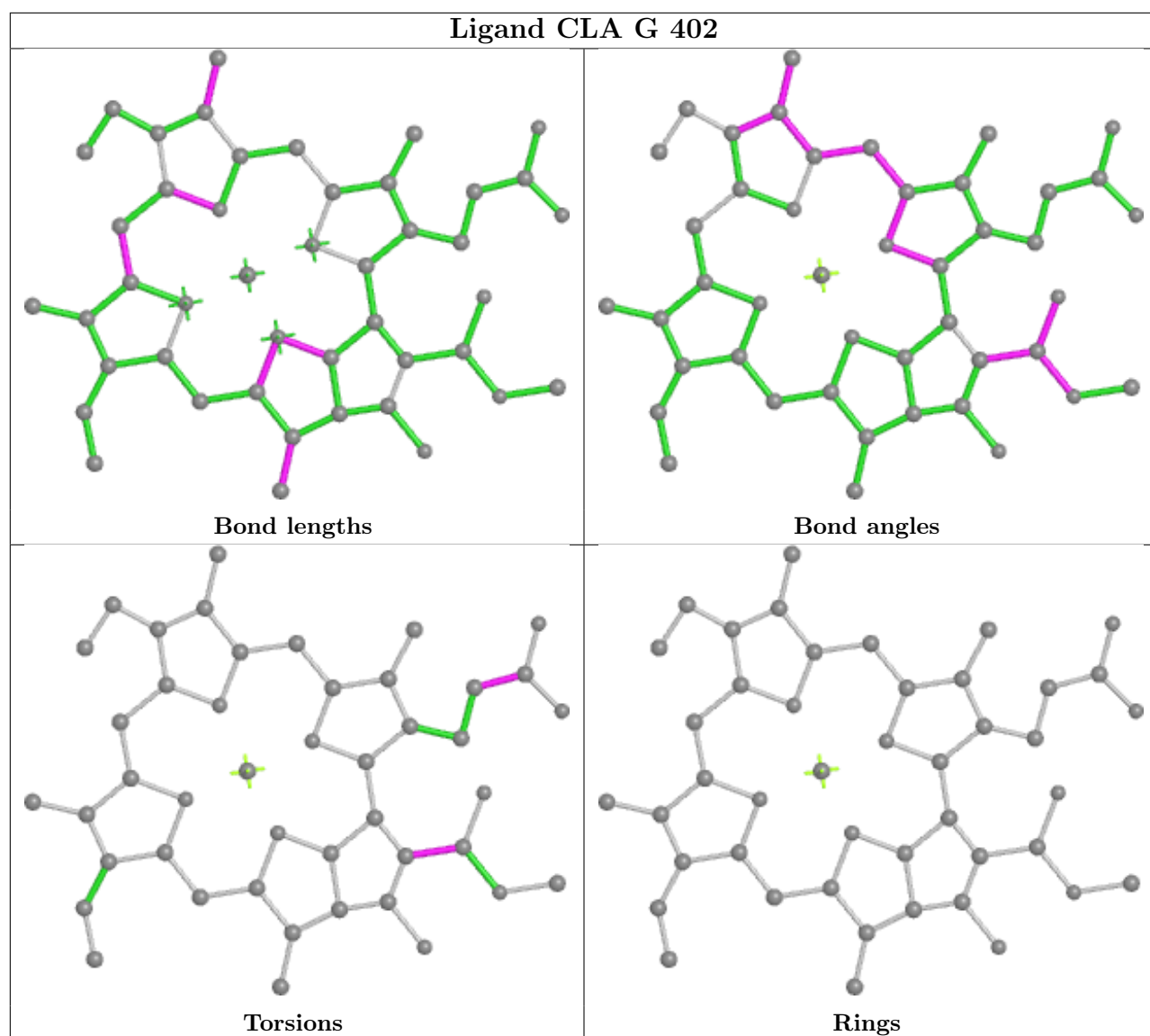




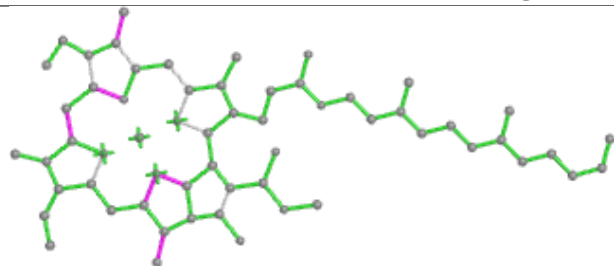
Ligand CLA B 606**Ligand WVN d 410**

Ligand CLA 4 307

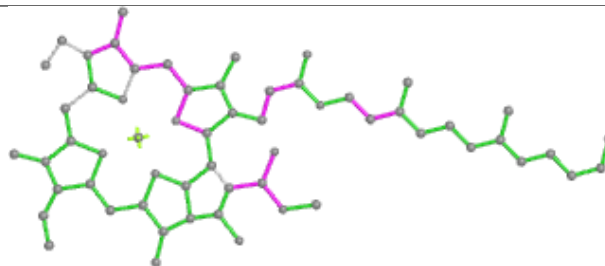




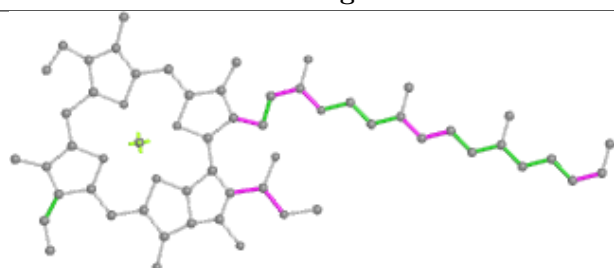
Ligand CLA b 604



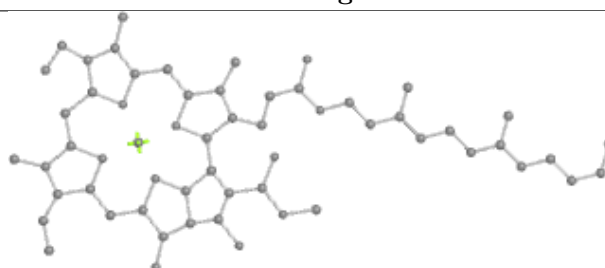
Bond lengths



Bond angles

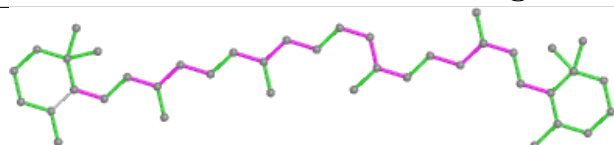


Torsions

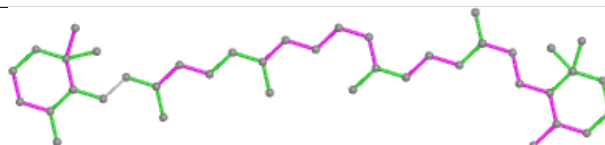


Rings

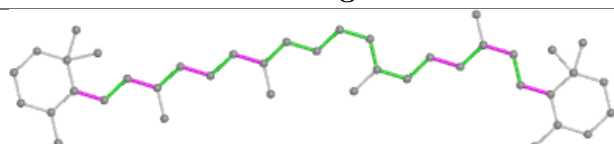
Ligand WVN 5 617



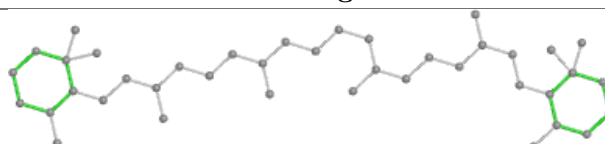
Bond lengths



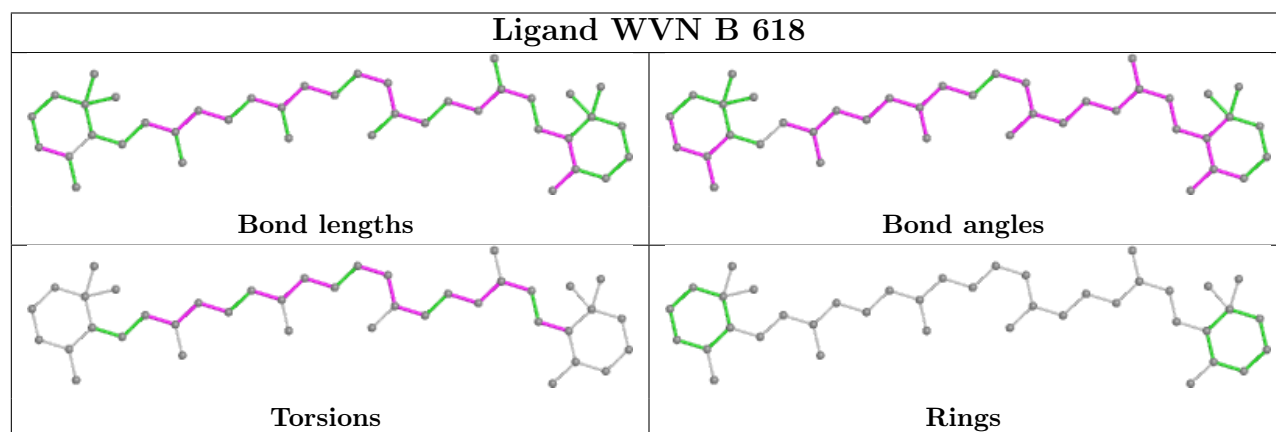
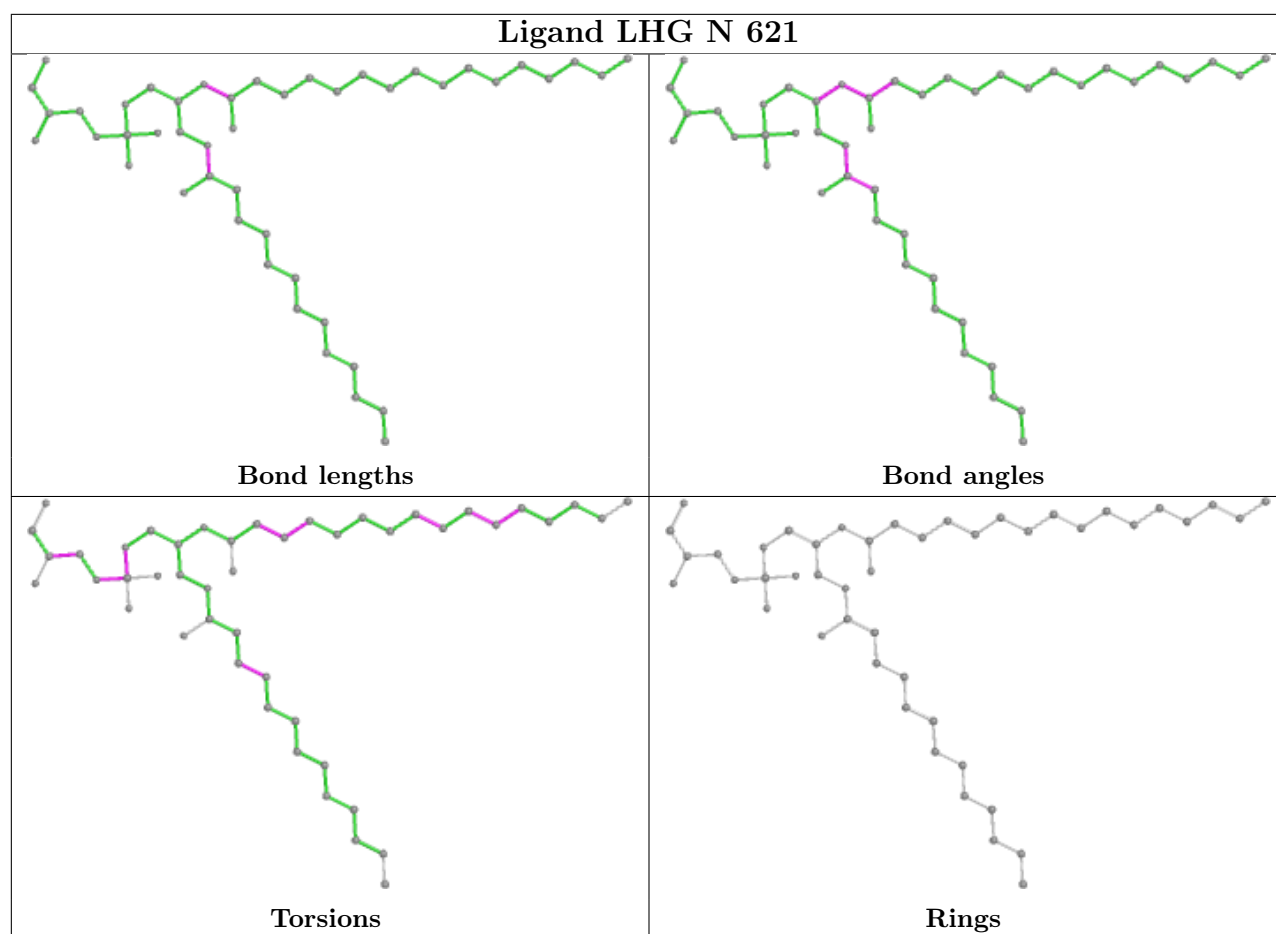
Bond angles

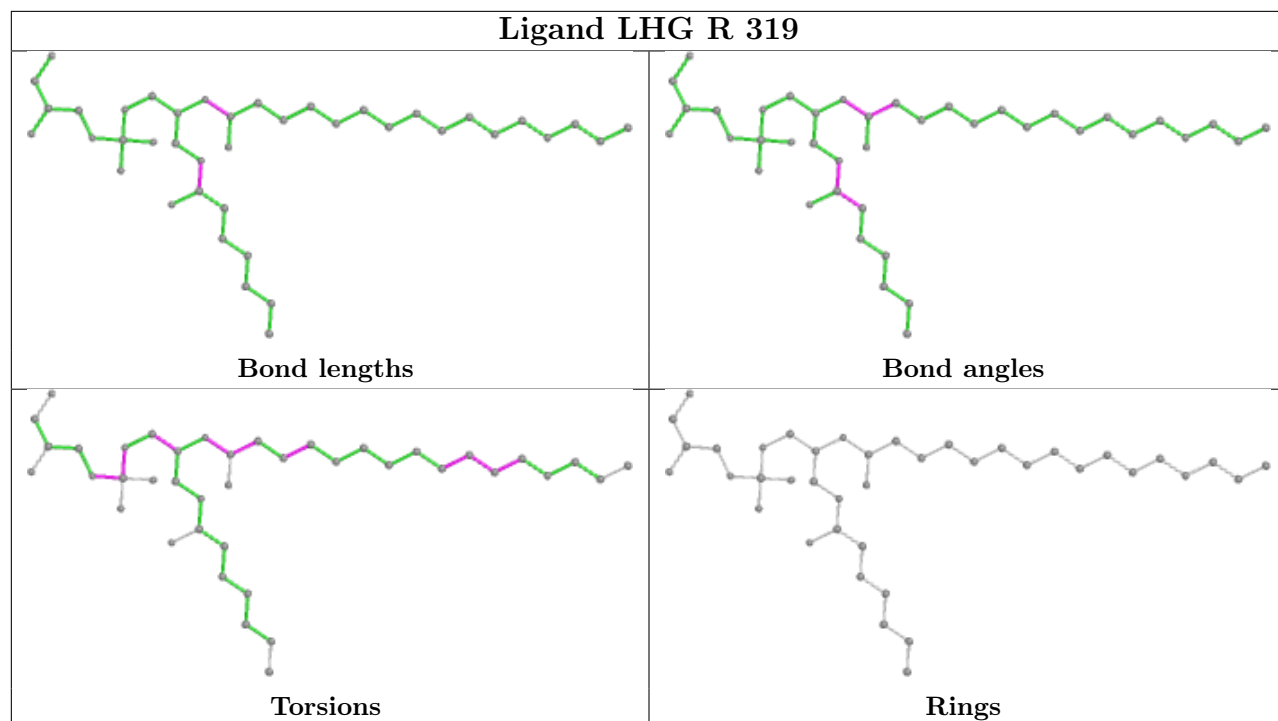


Torsions

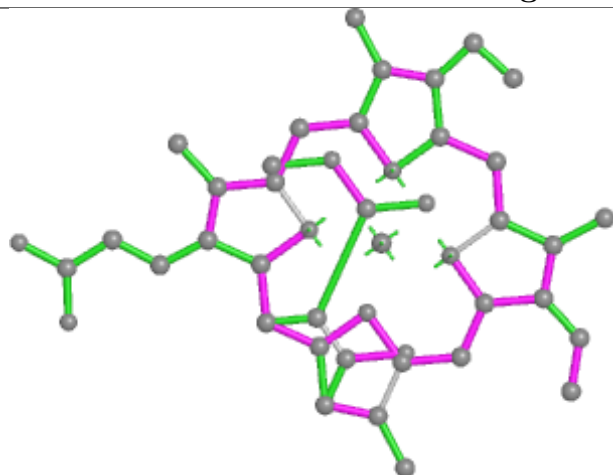


Rings

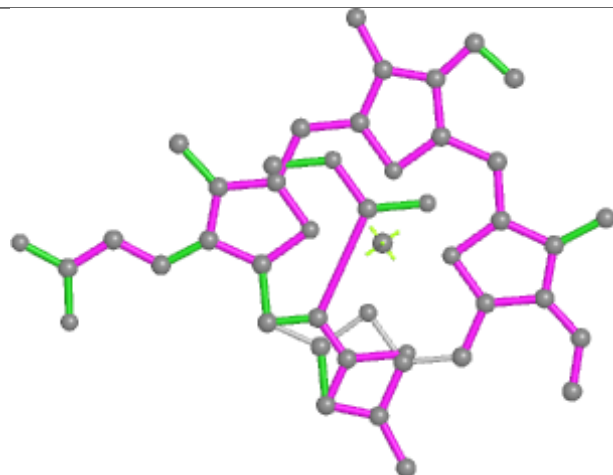




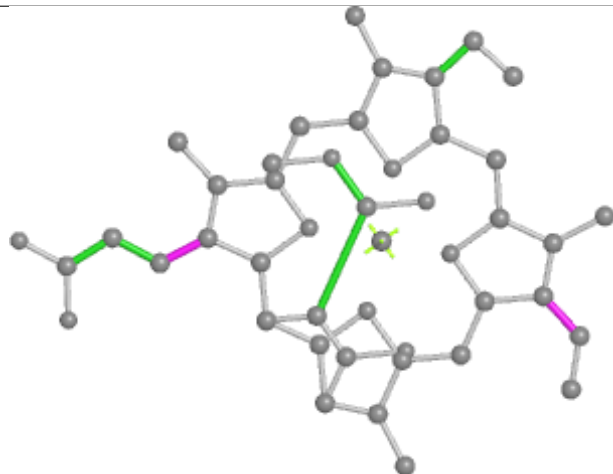
Ligand KC2 4 311



Bond lengths



Bond angles

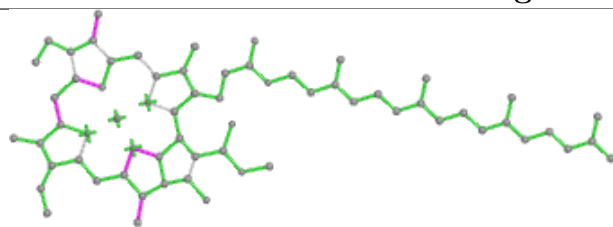


Torsions

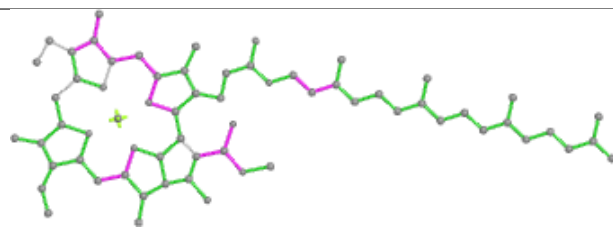


Rings

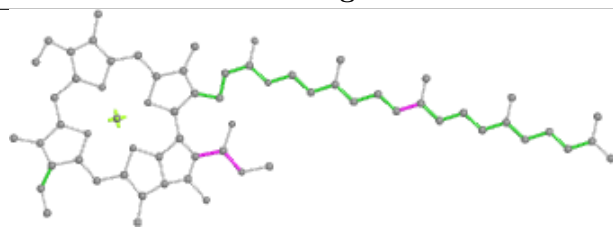
Ligand CLA B 602



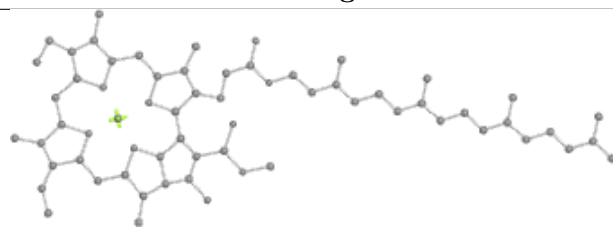
Bond lengths



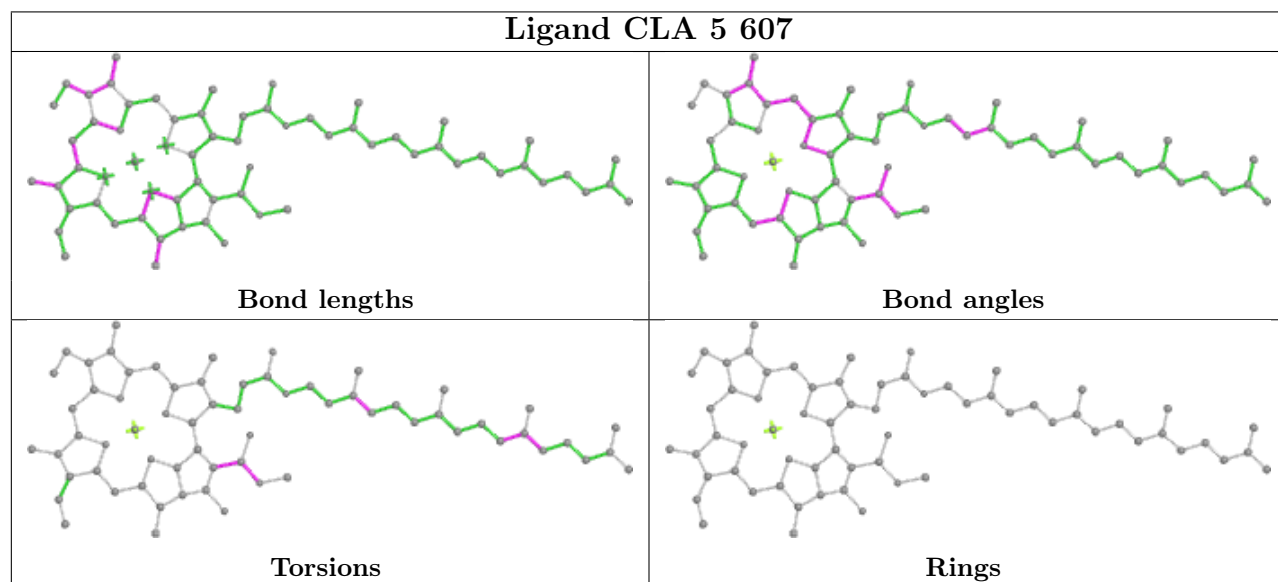
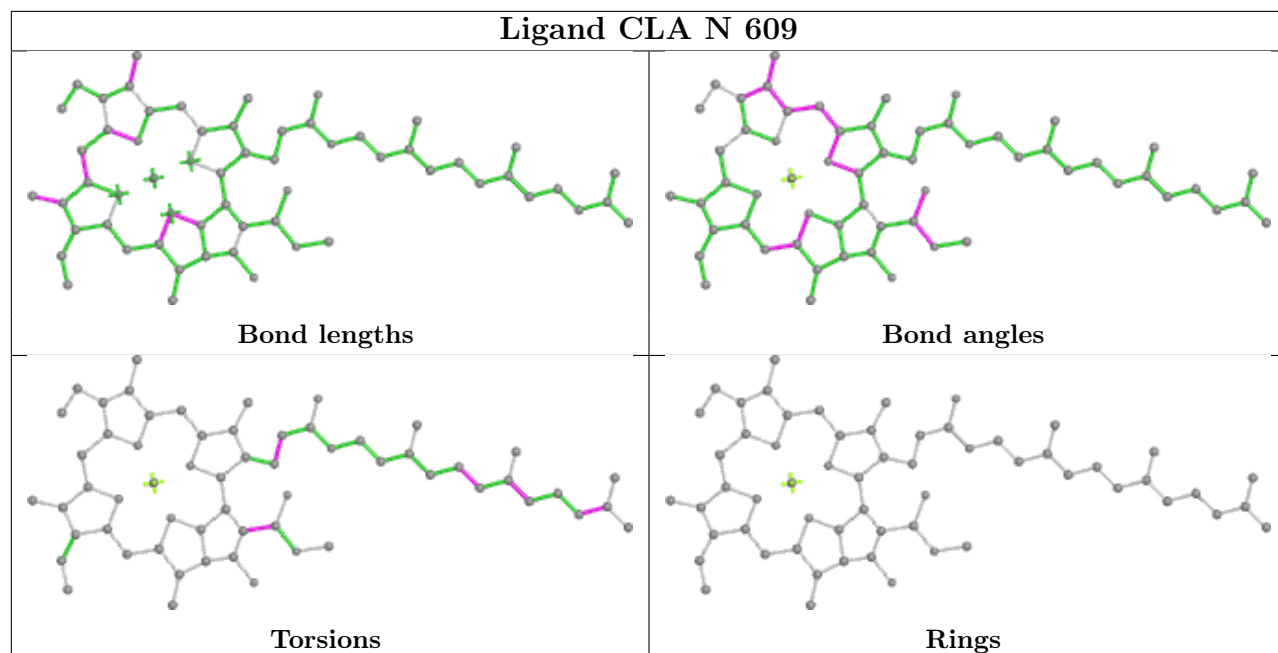
Bond angles



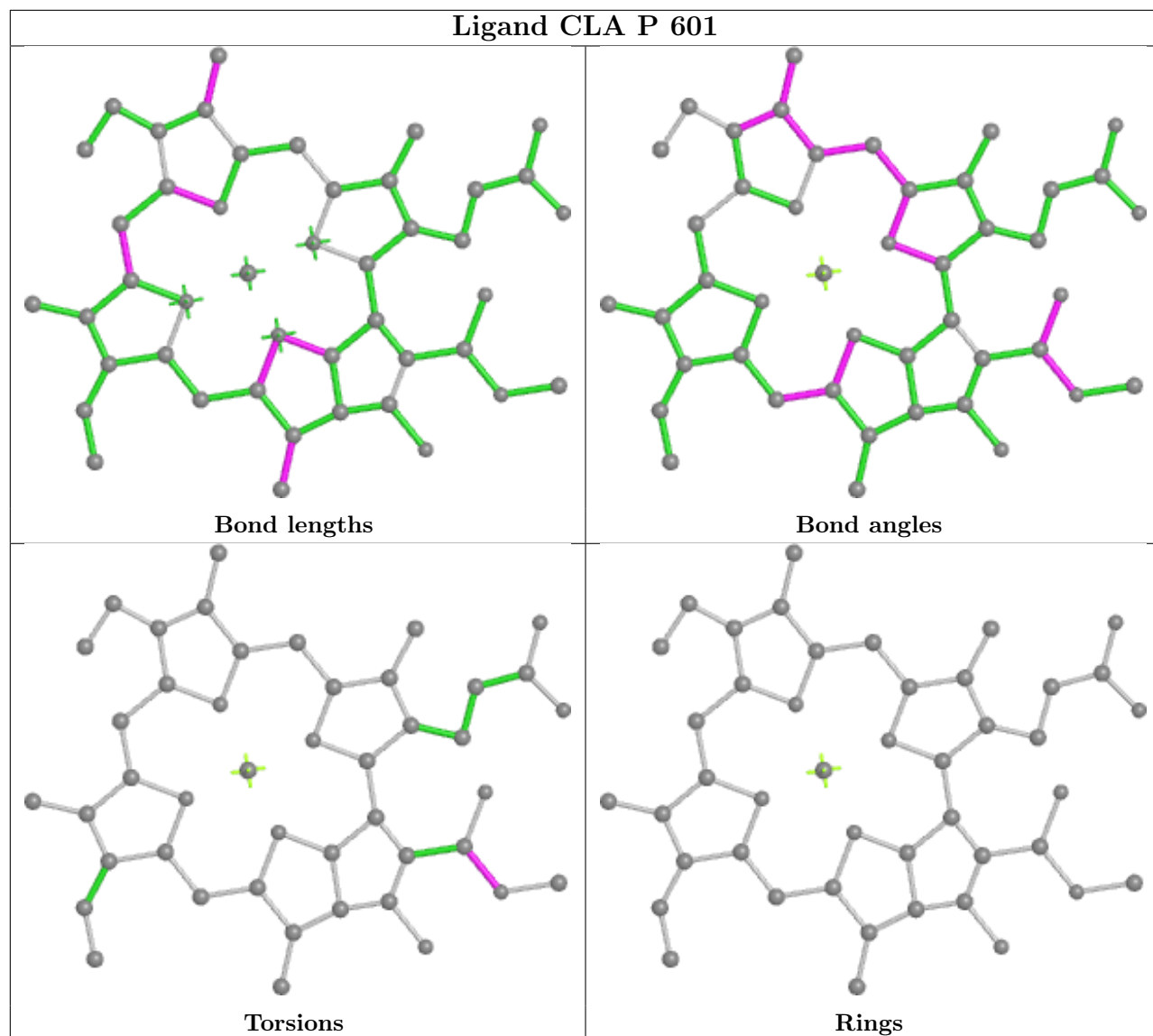
Torsions



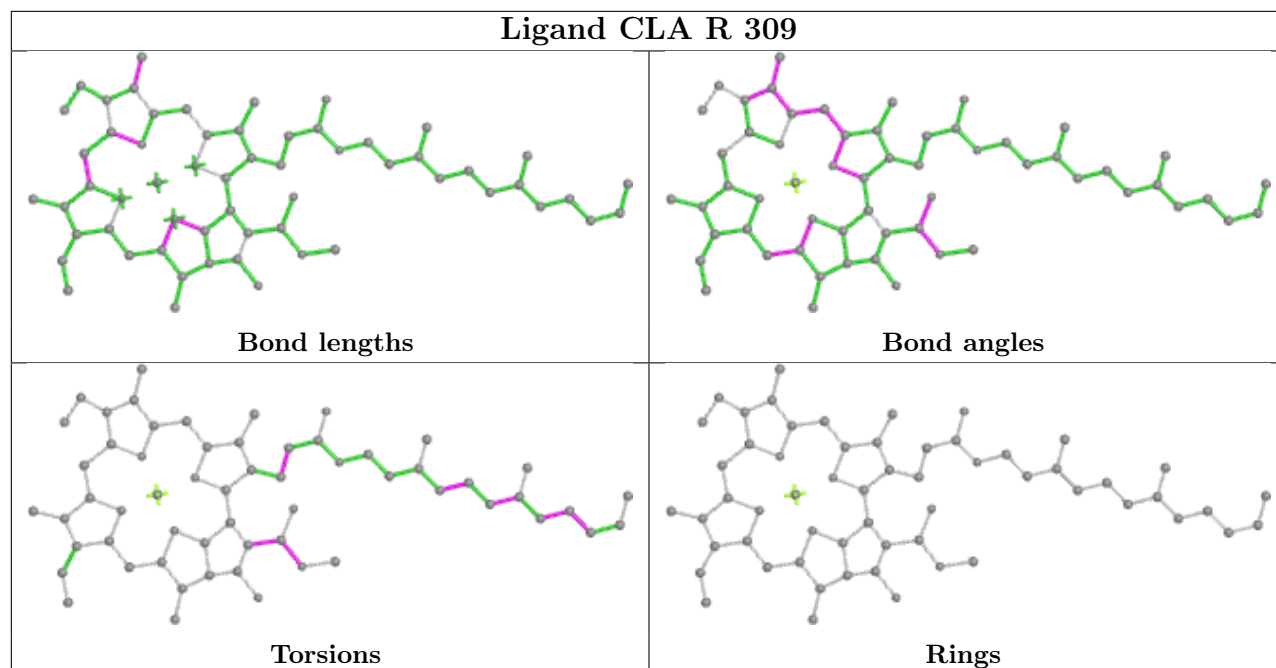
Rings



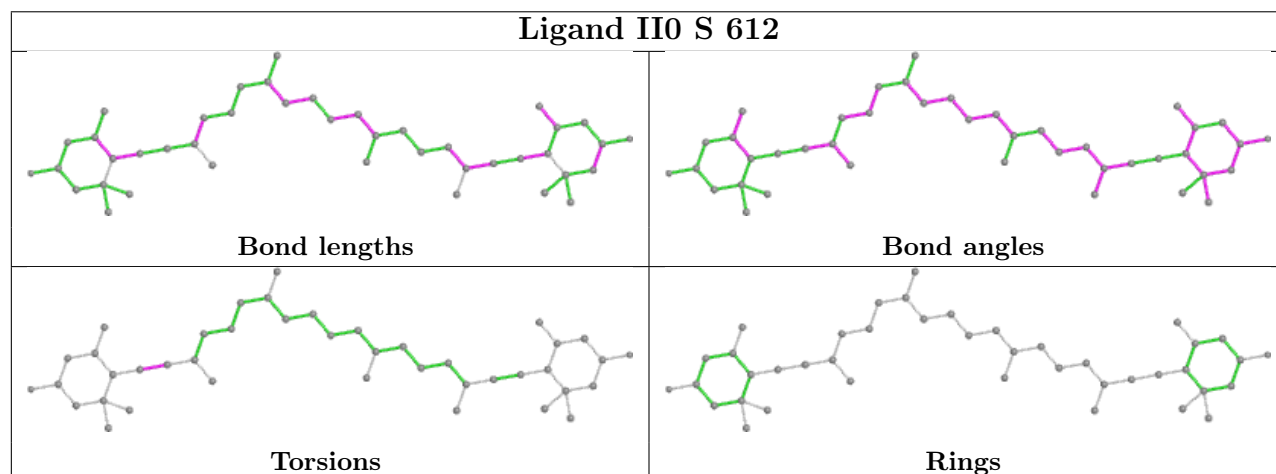
Ligand CLA P 601



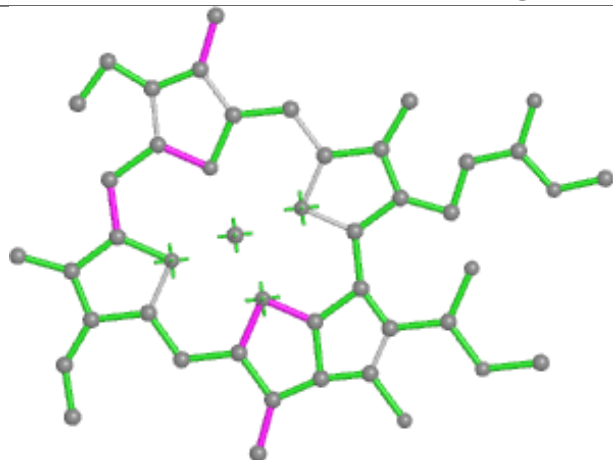
Ligand CLA R 309



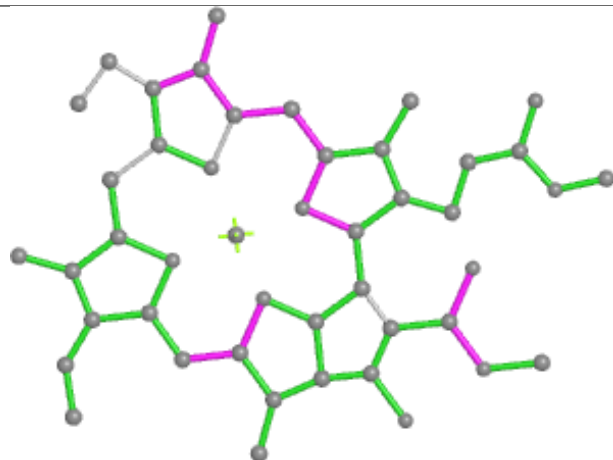
Ligand II0 S 612



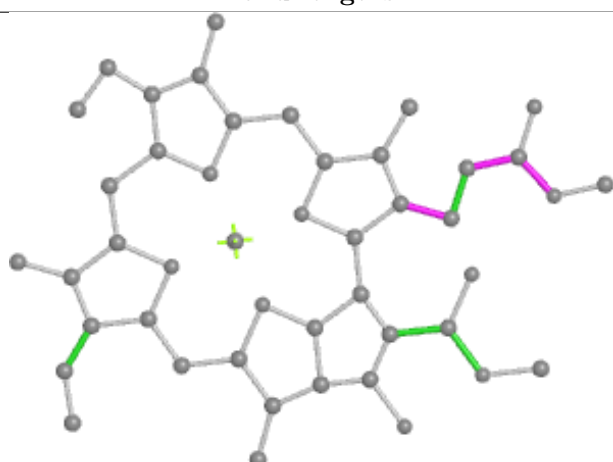
Ligand CLA R 313



Bond lengths



Bond angles

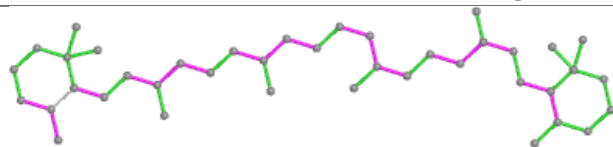


Torsions

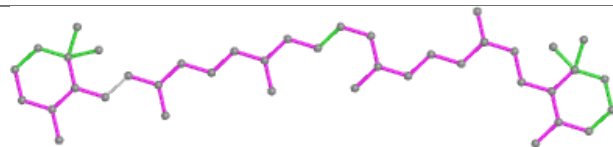


Rings

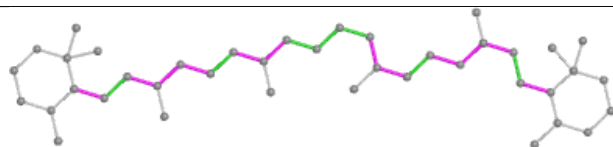
Ligand WVN 3 313



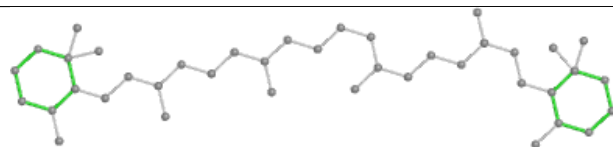
Bond lengths



Bond angles

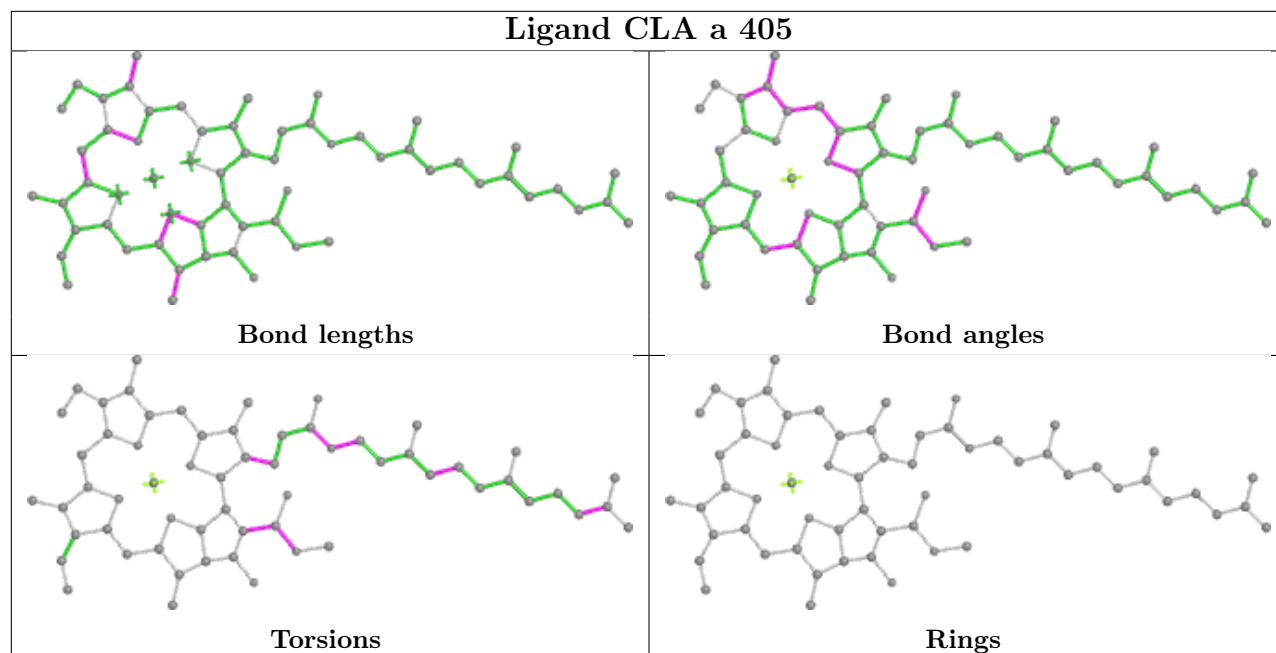


Torsions

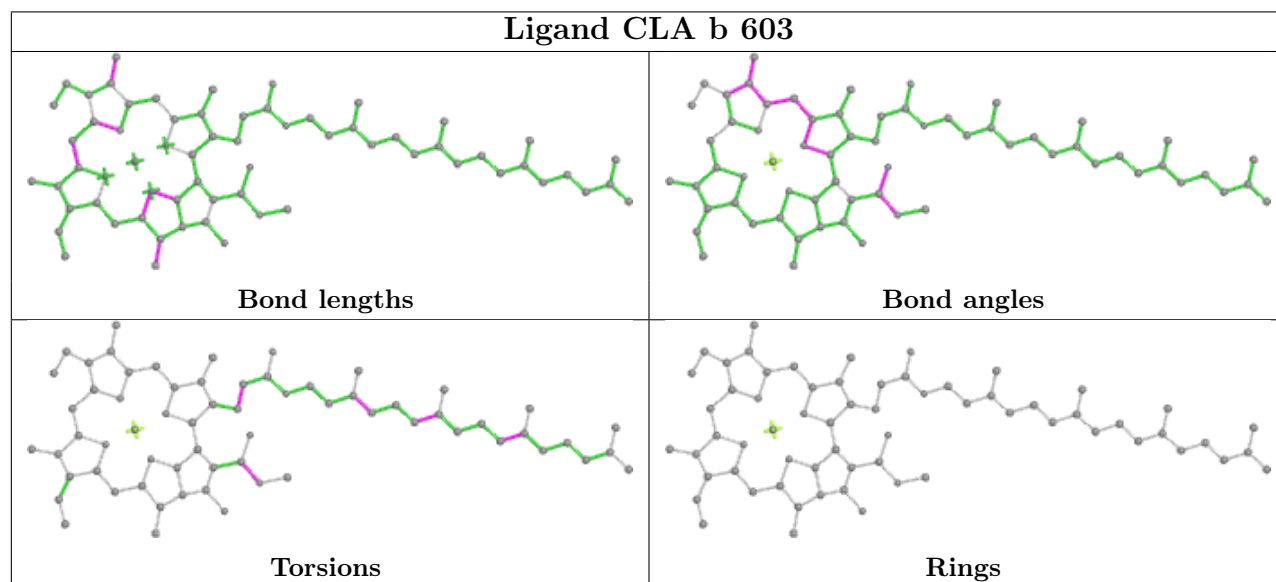


Rings

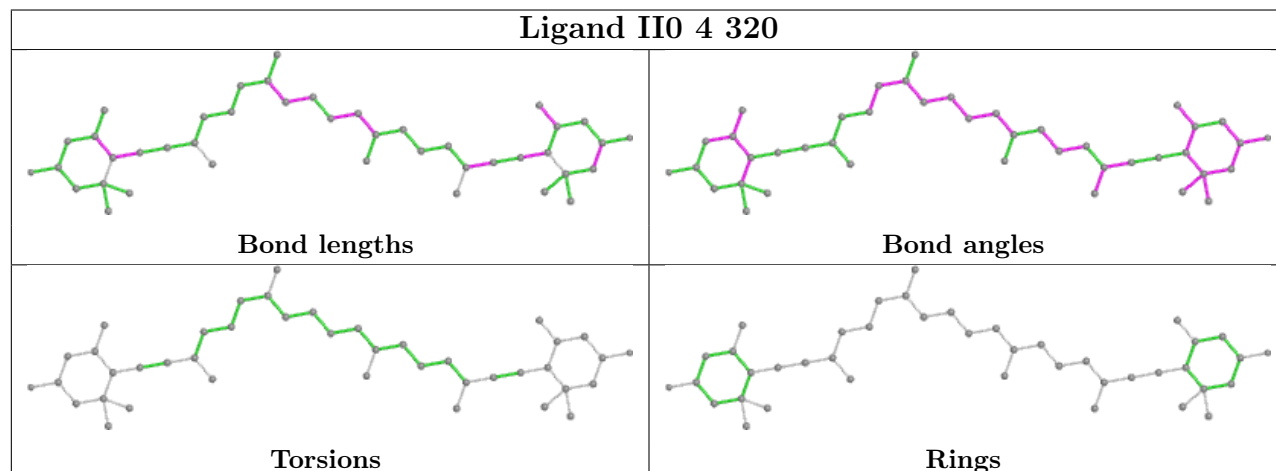
Ligand CLA a 405

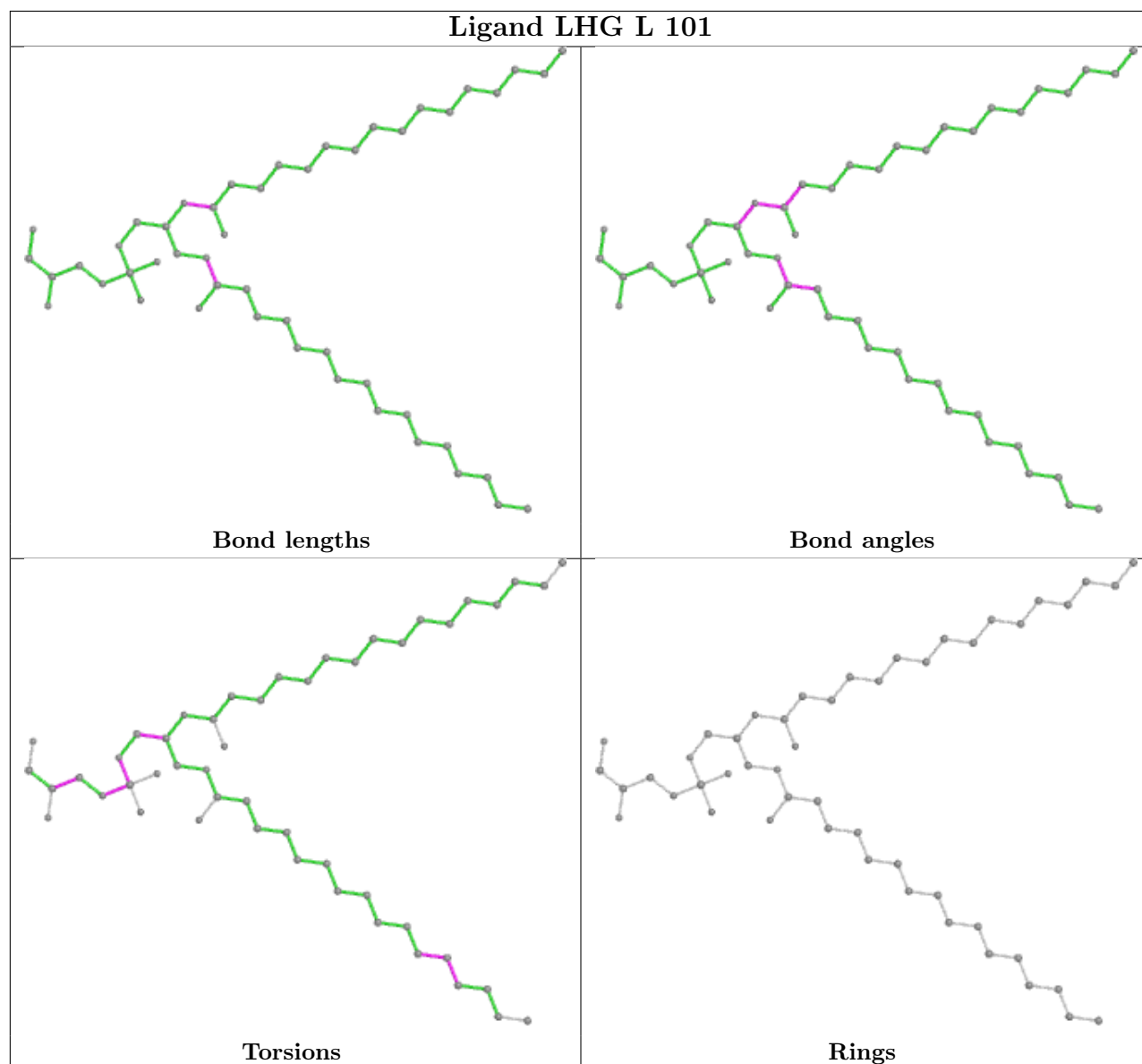
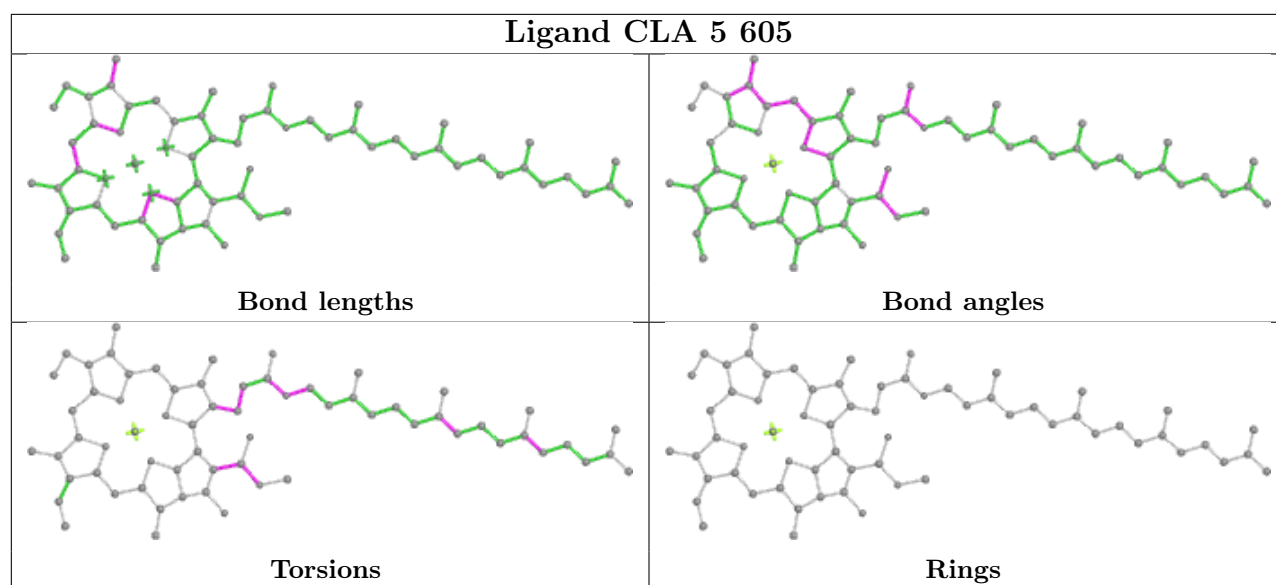


Ligand CLA b 603

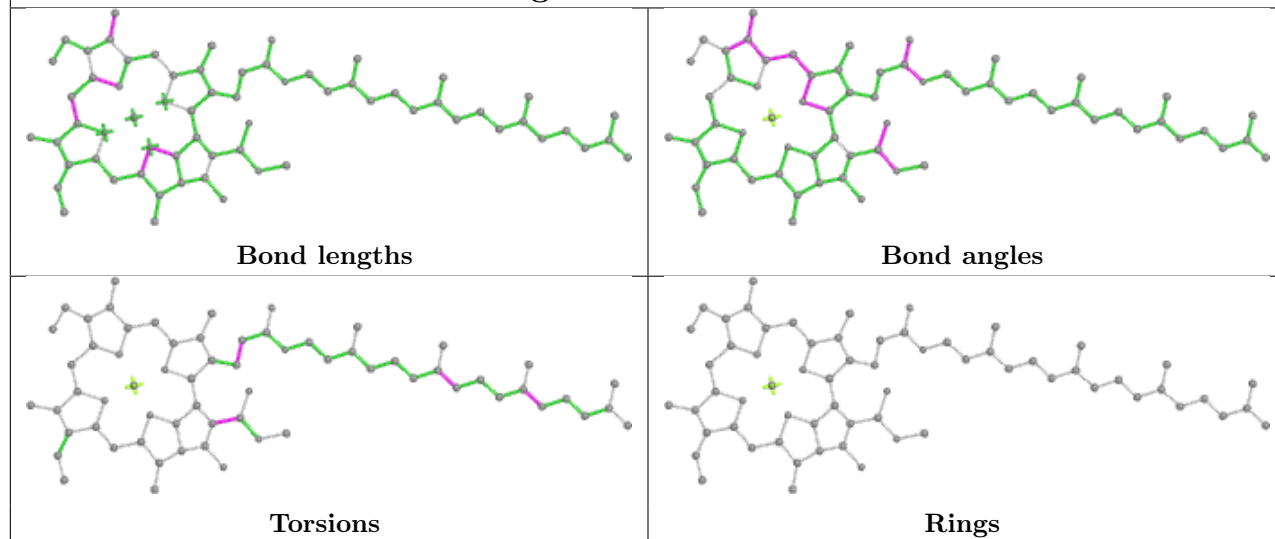


Ligand II0 4 320

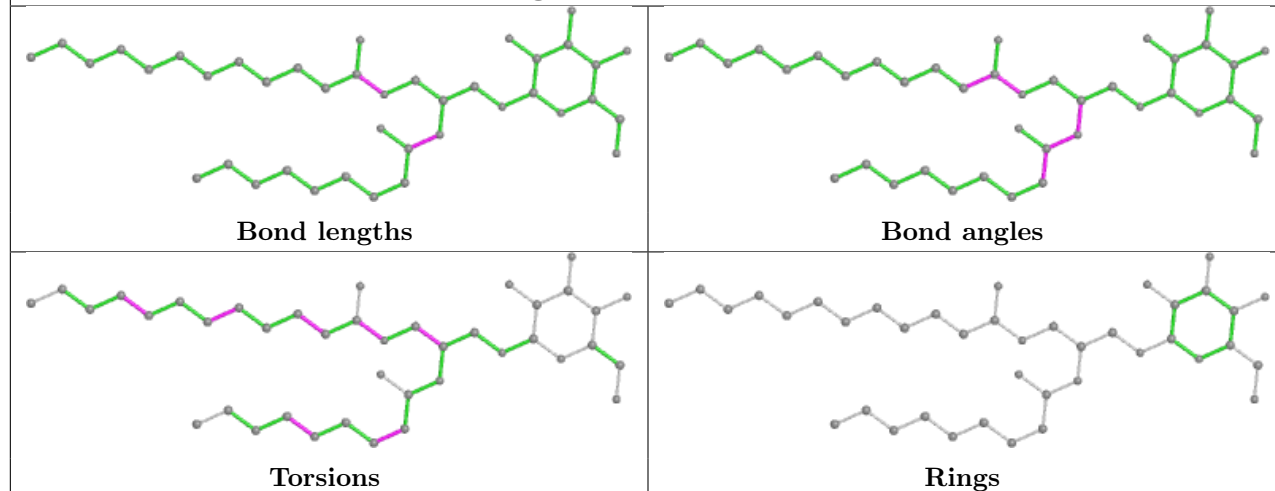




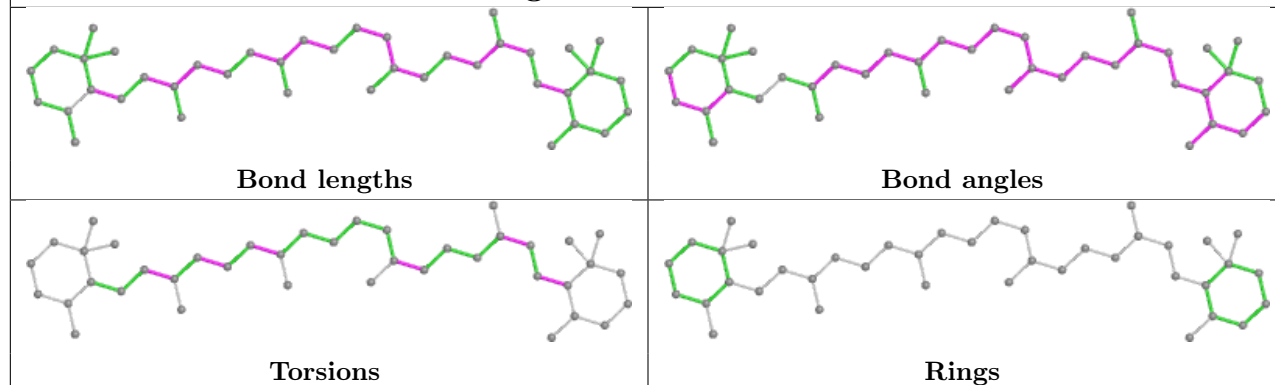
Ligand CLA B 608

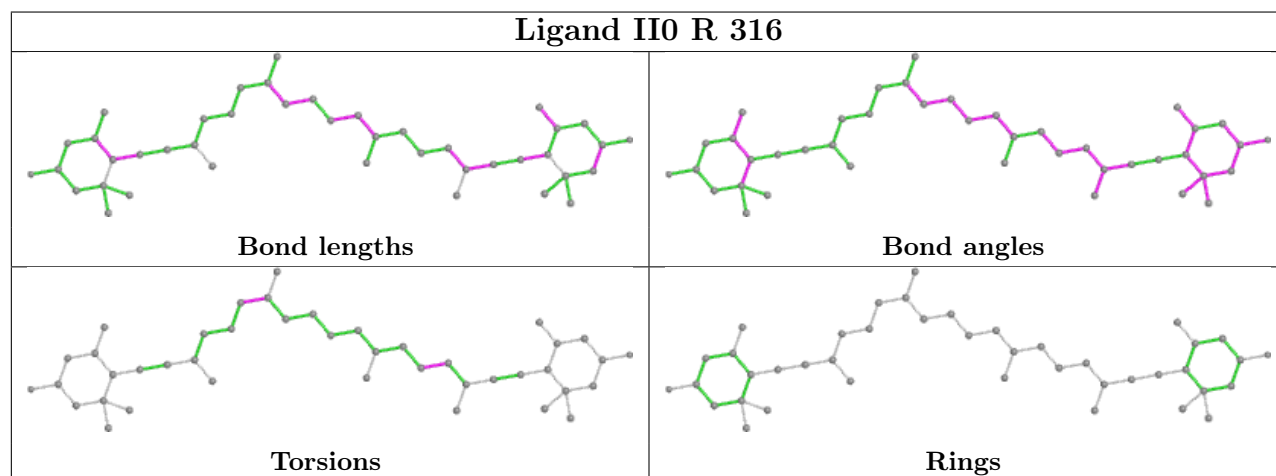
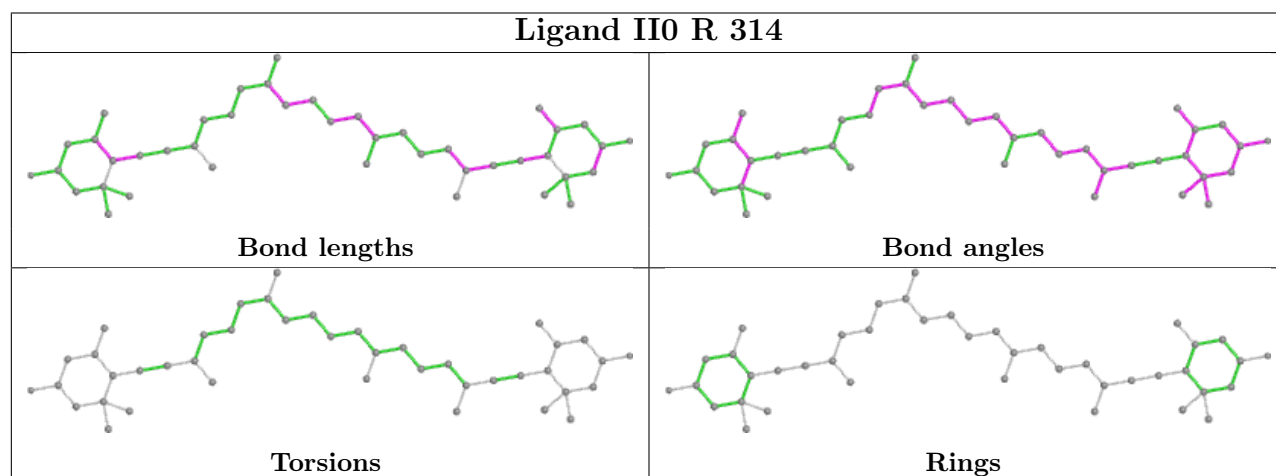
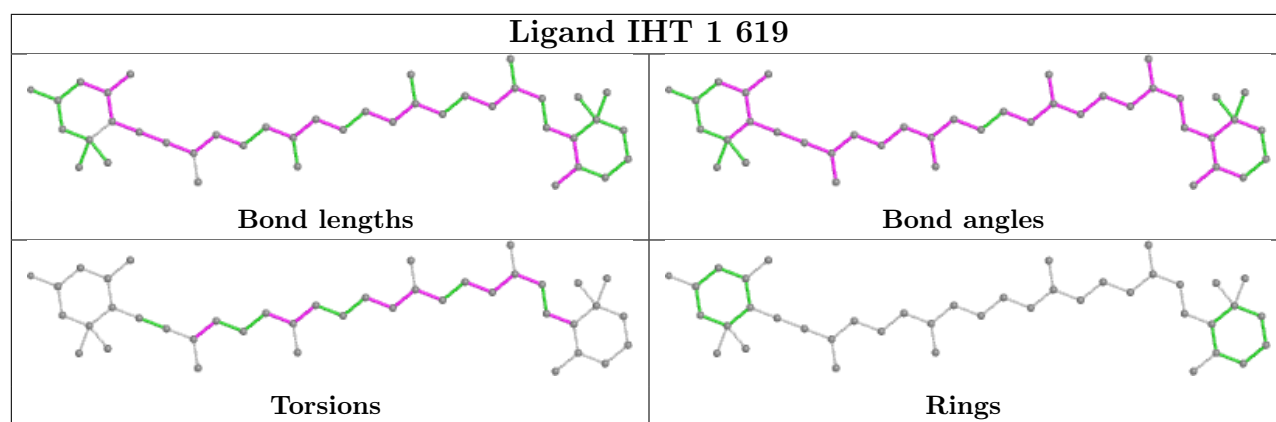


Ligand LMG d 404

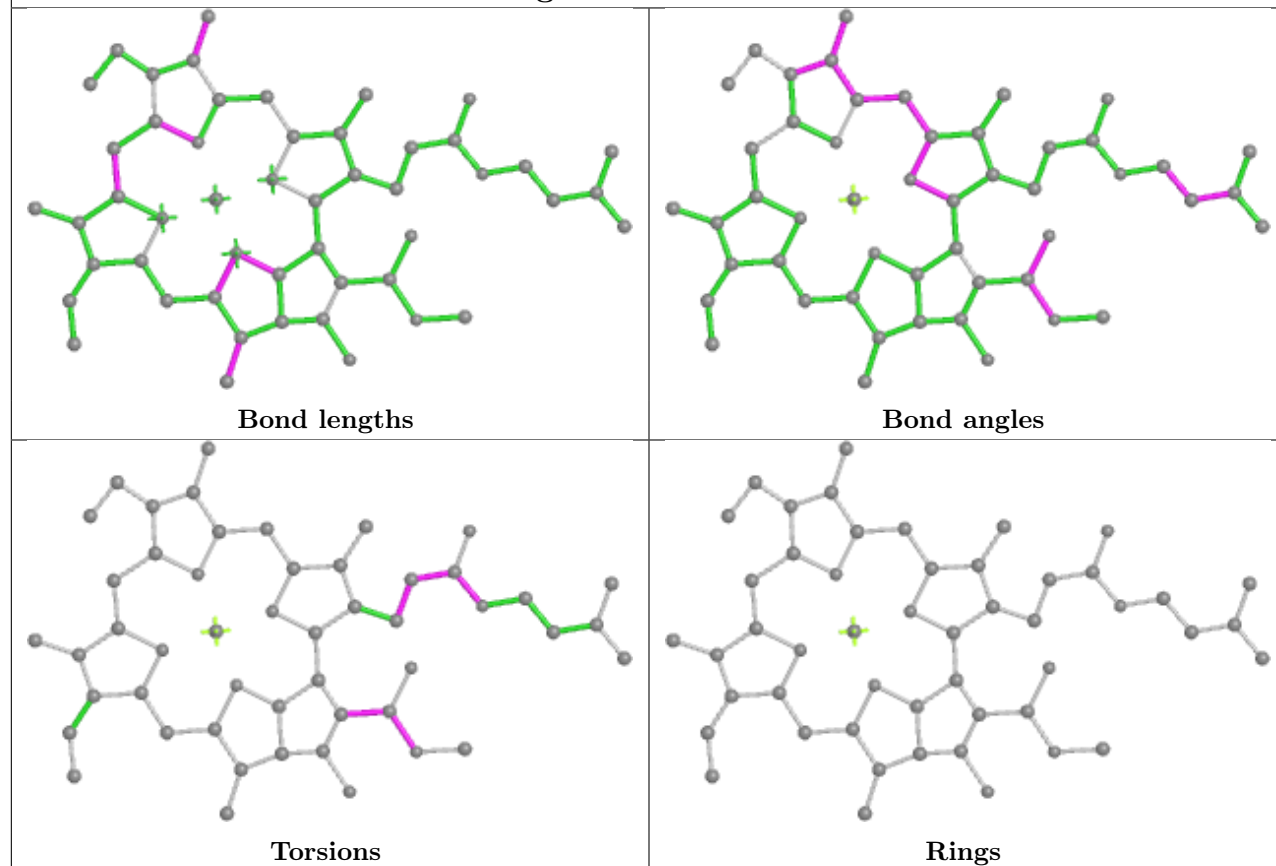


Ligand WVN b 618

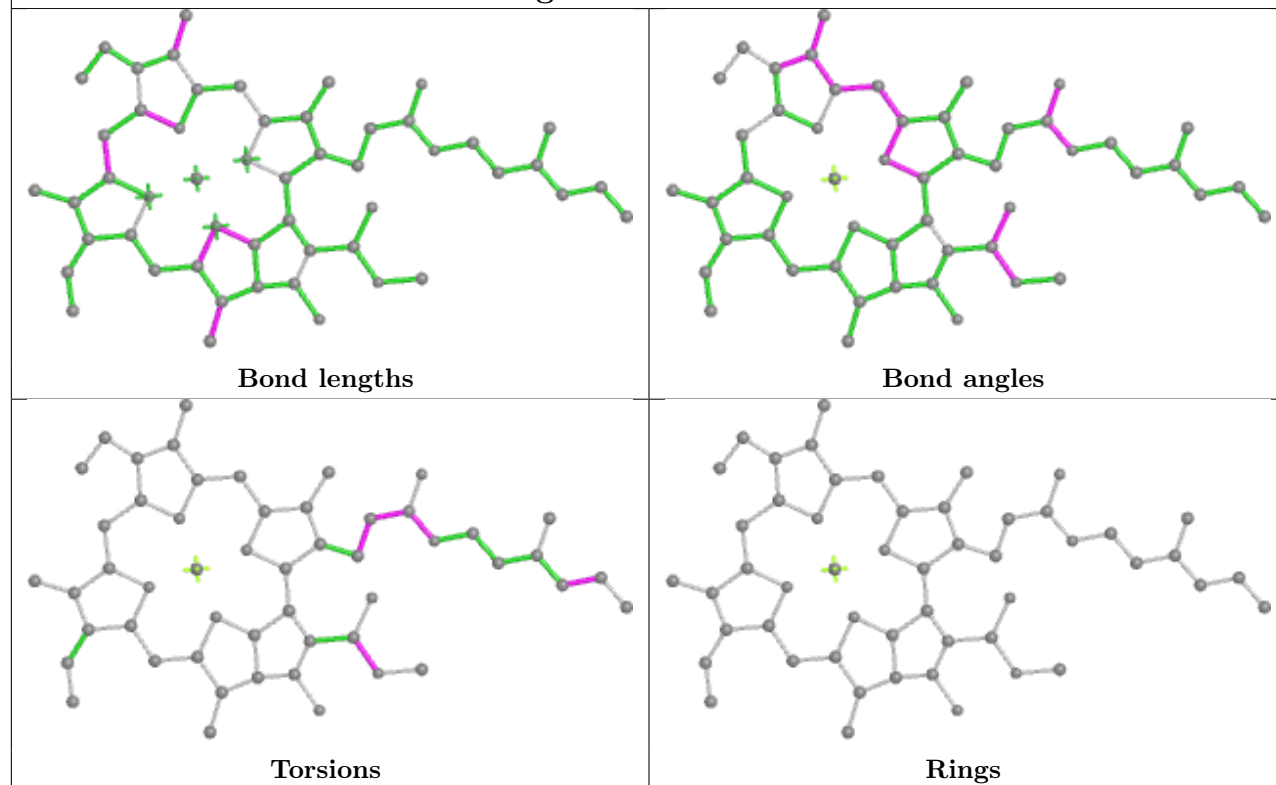


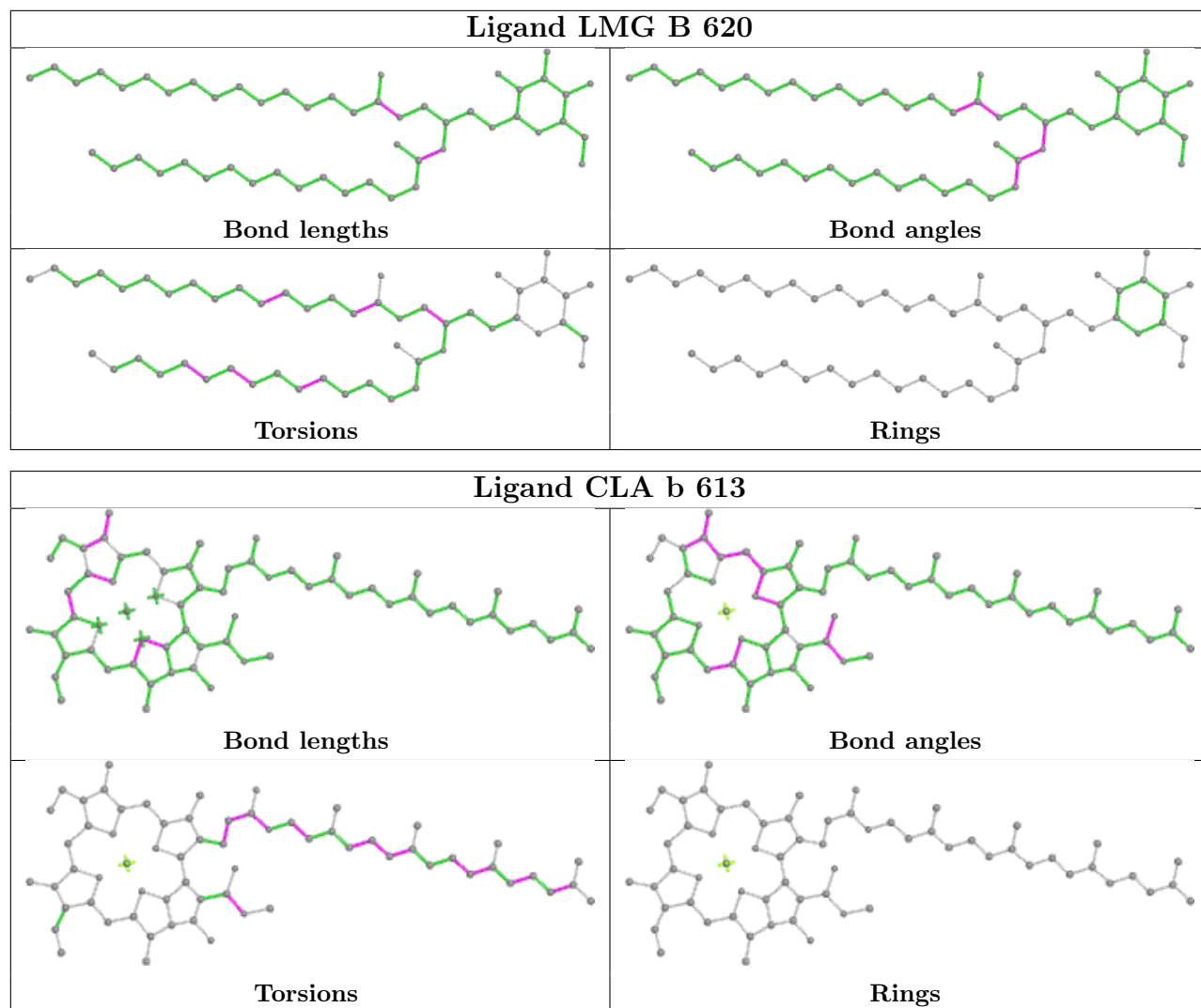


Ligand CLA 1 606

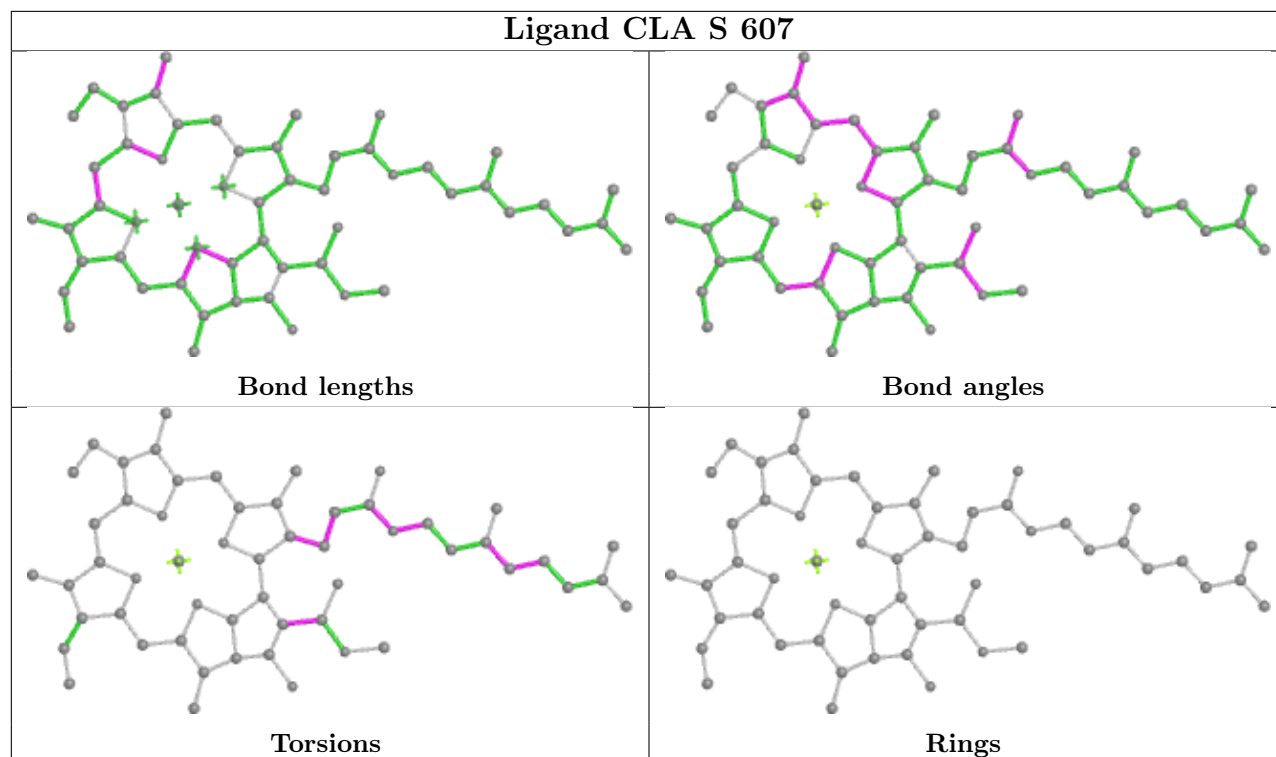


Ligand CLA 1 603

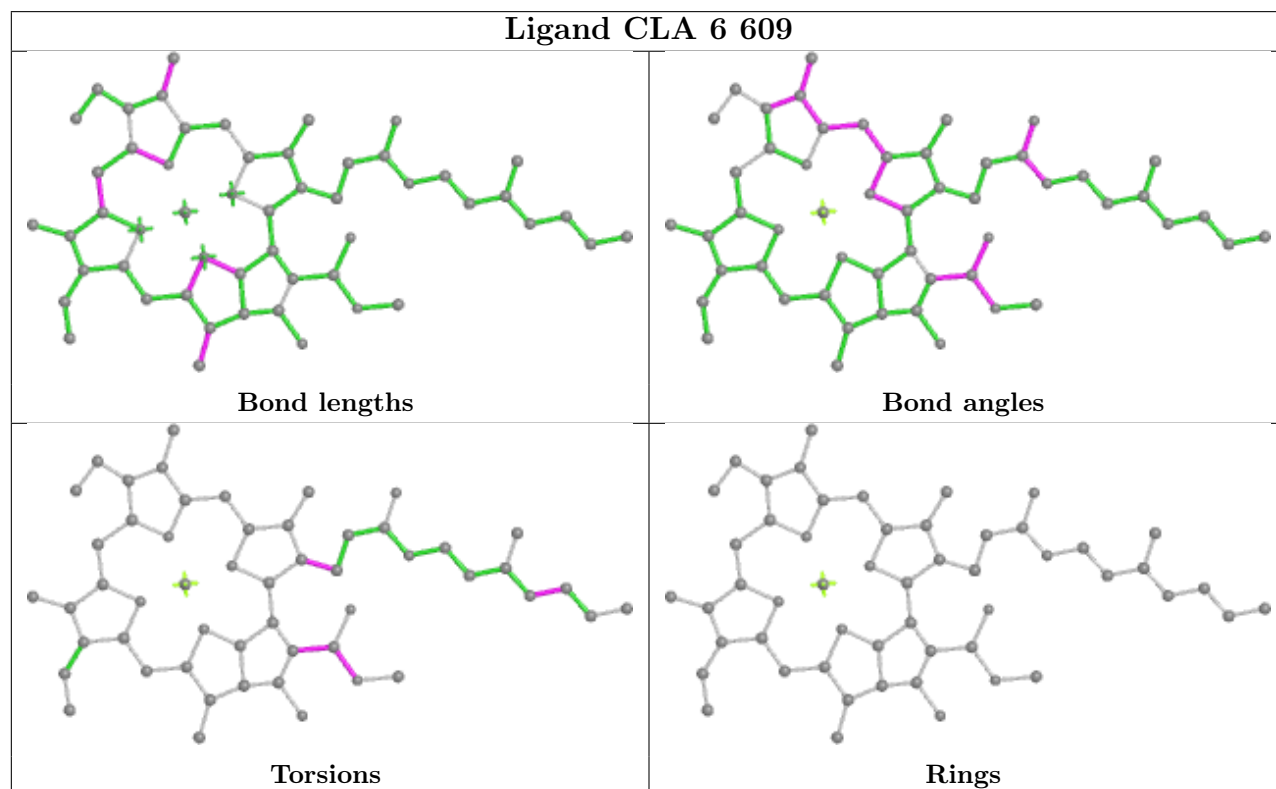




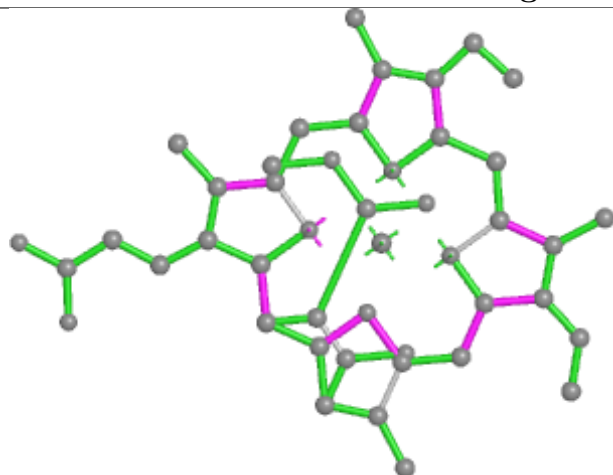
Ligand CLA S 607



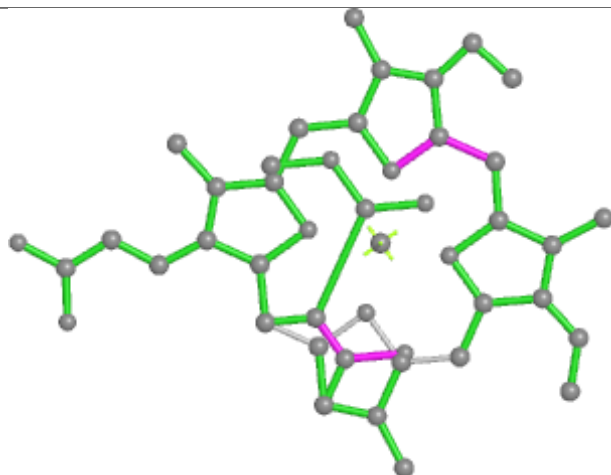
Ligand CLA 6 609



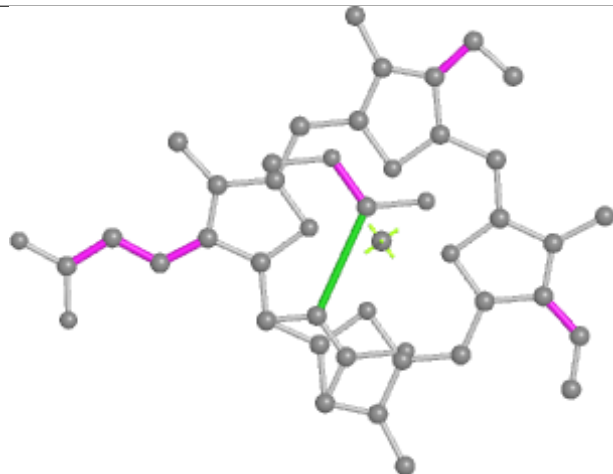
Ligand KC2 1 612



Bond lengths



Bond angles

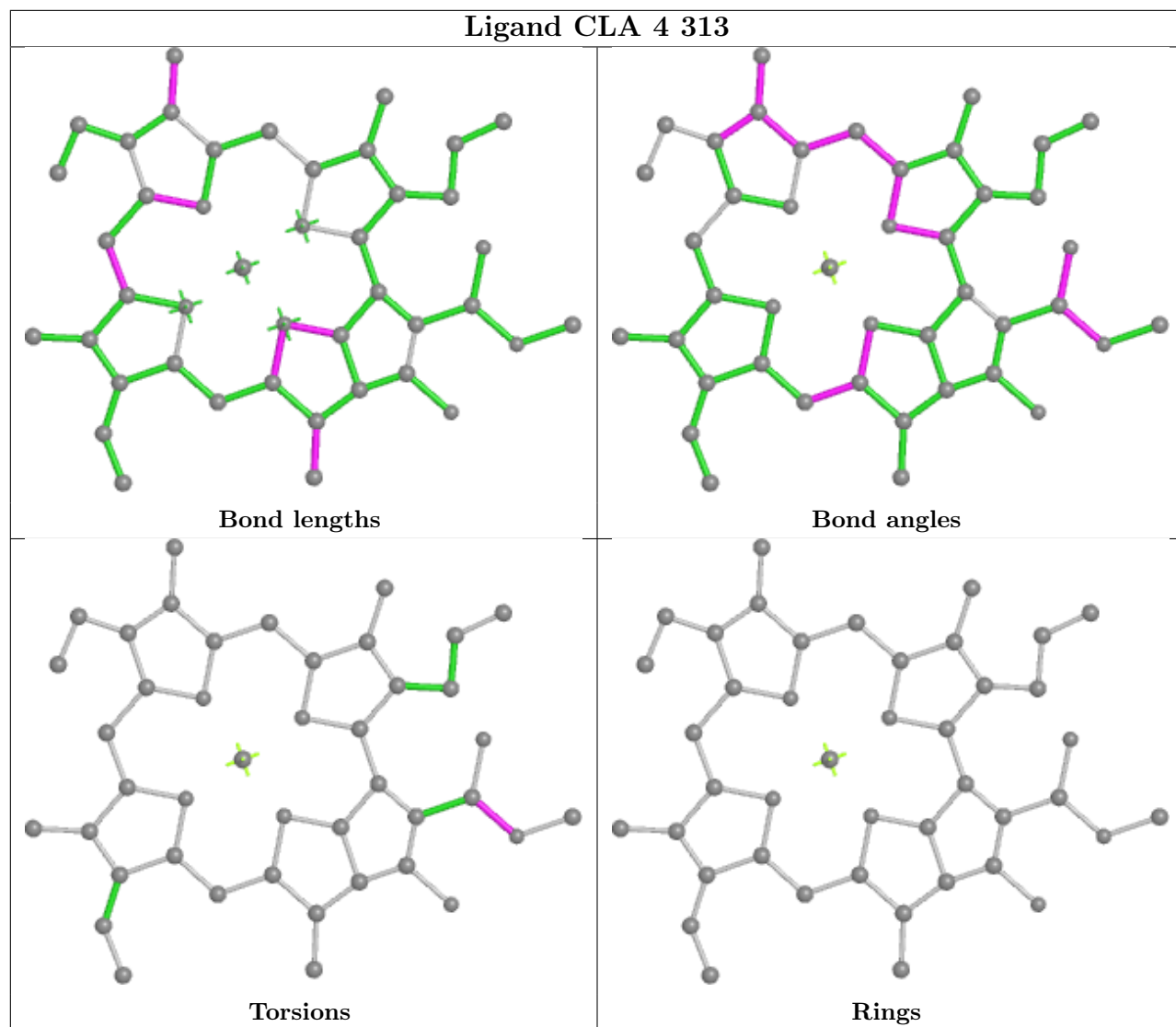


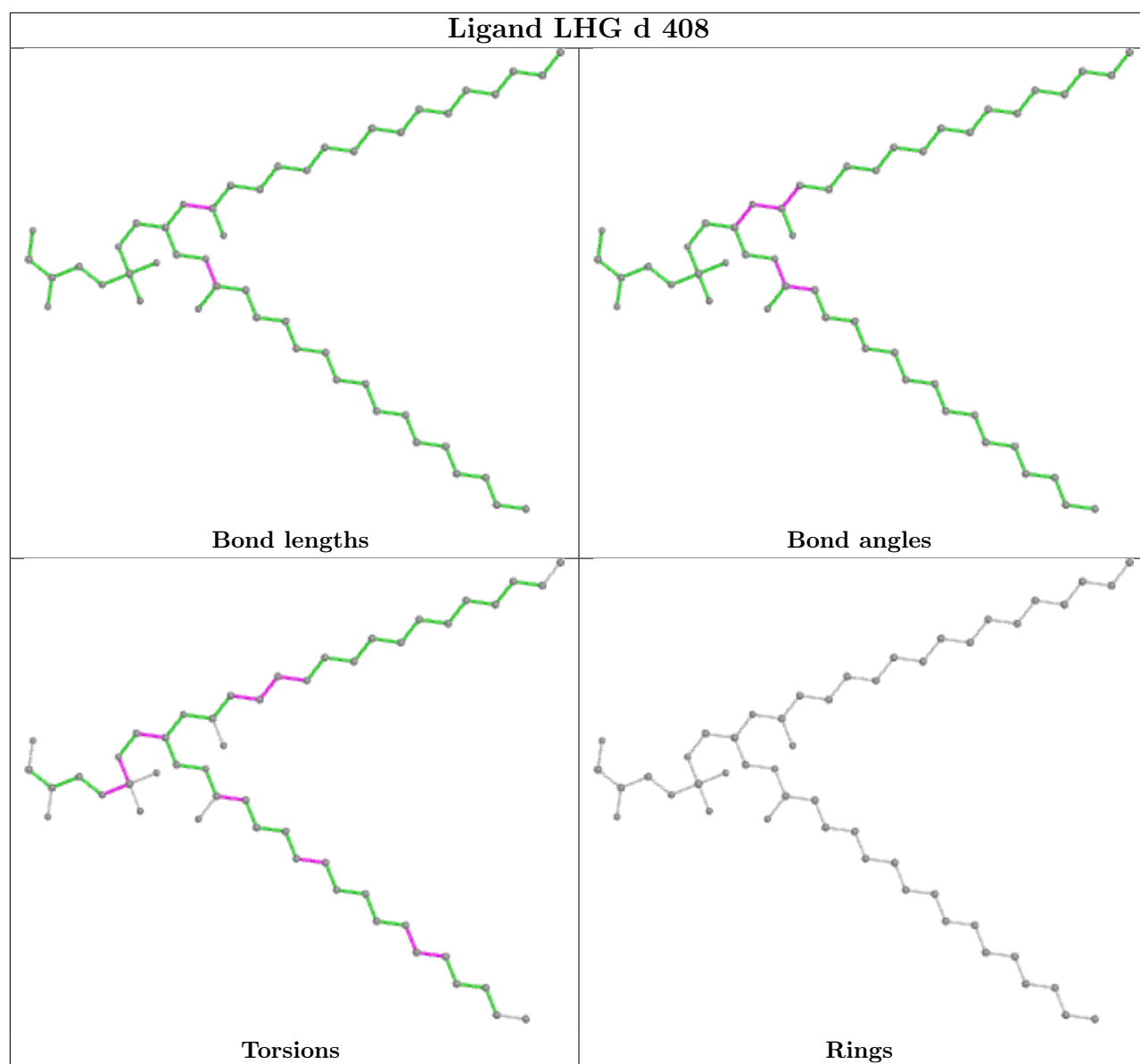
Torsions

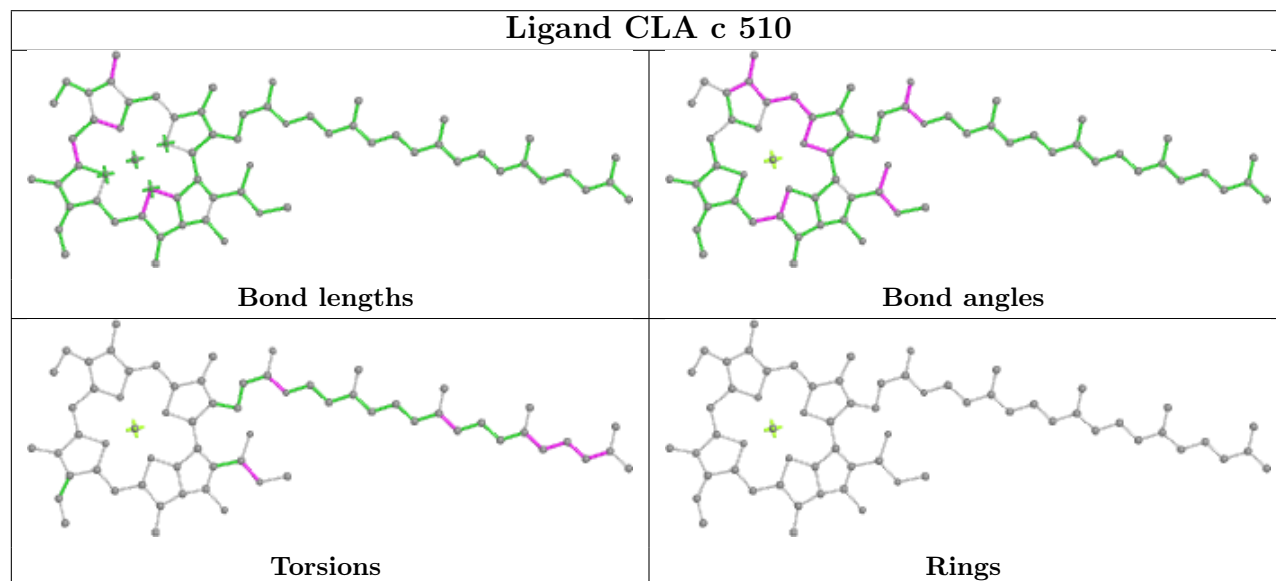
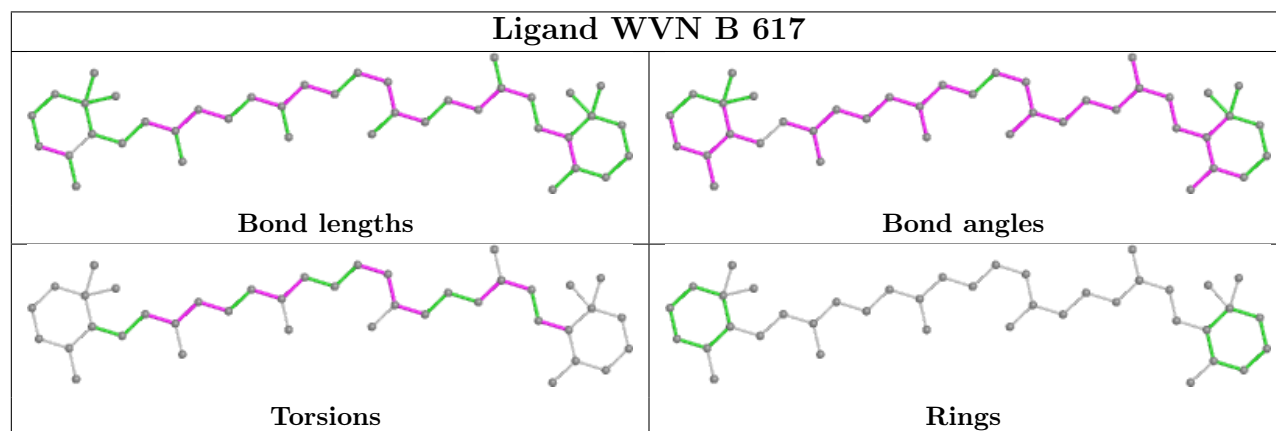
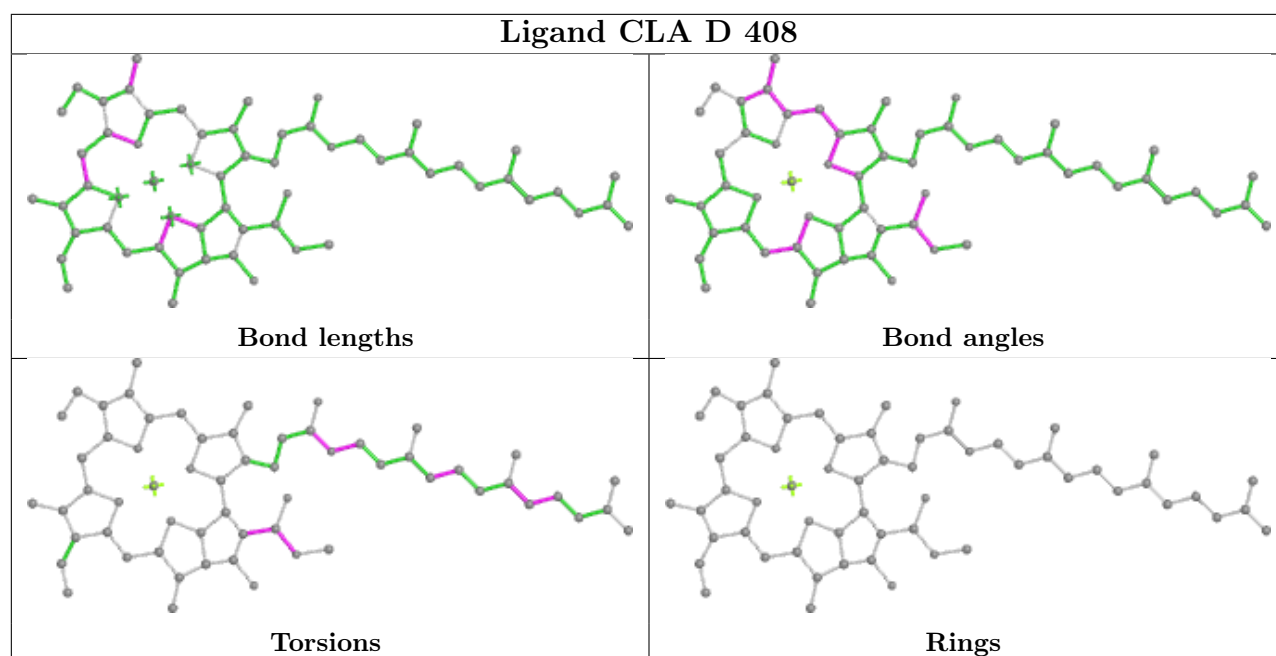


Rings

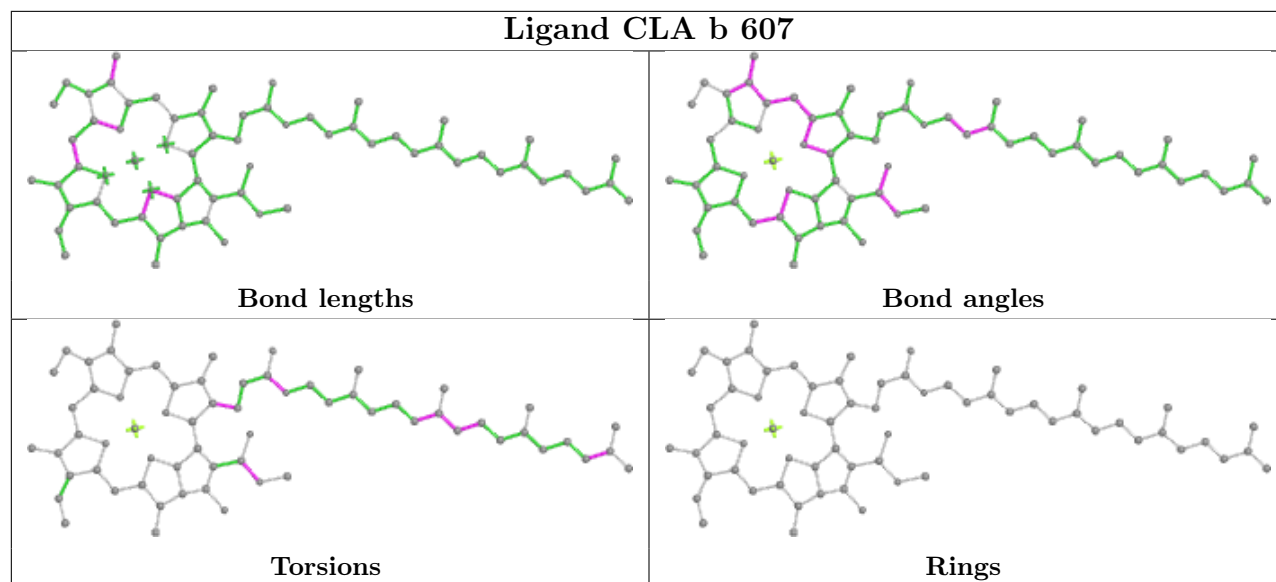
Ligand CLA 4 313



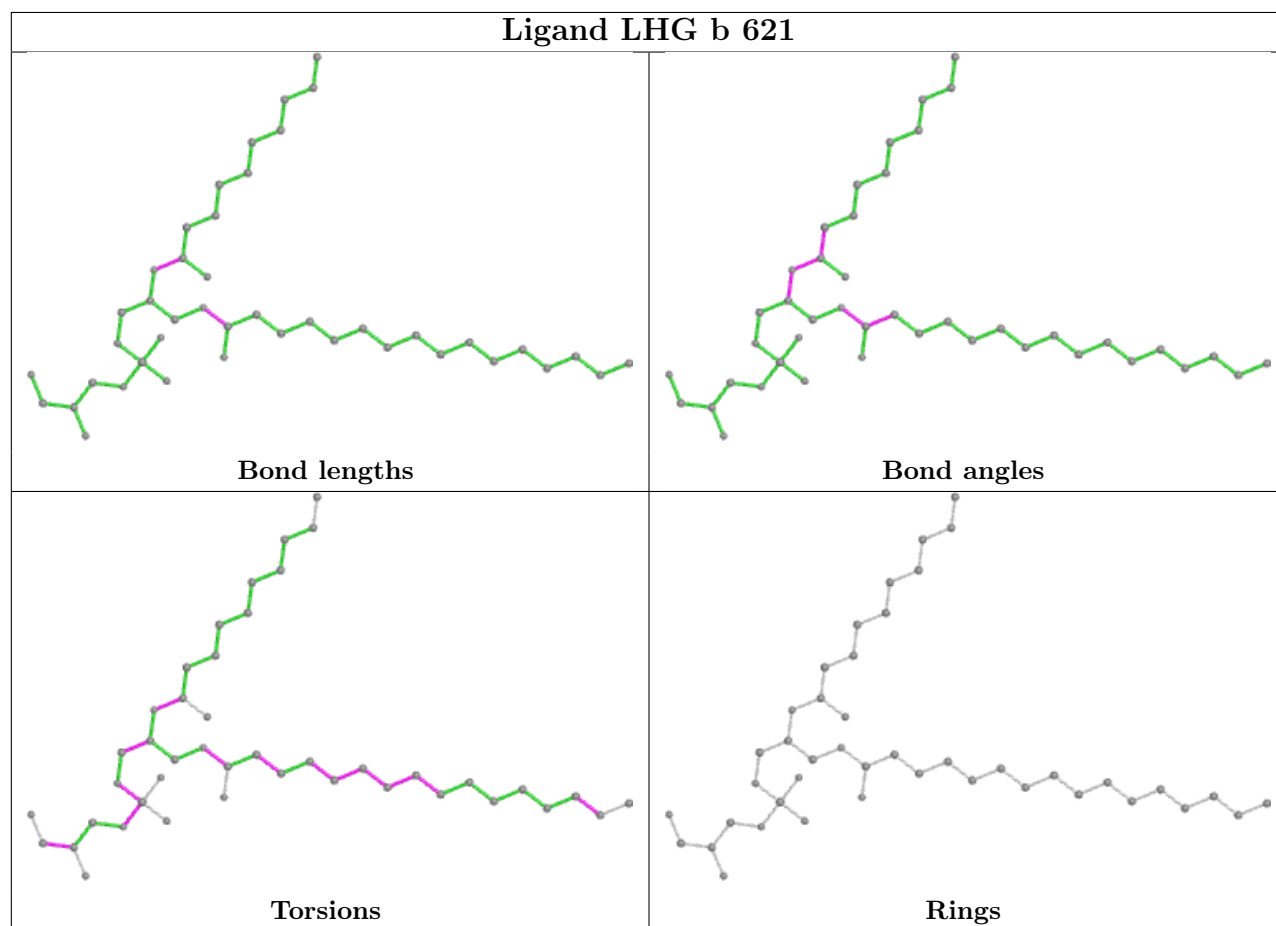




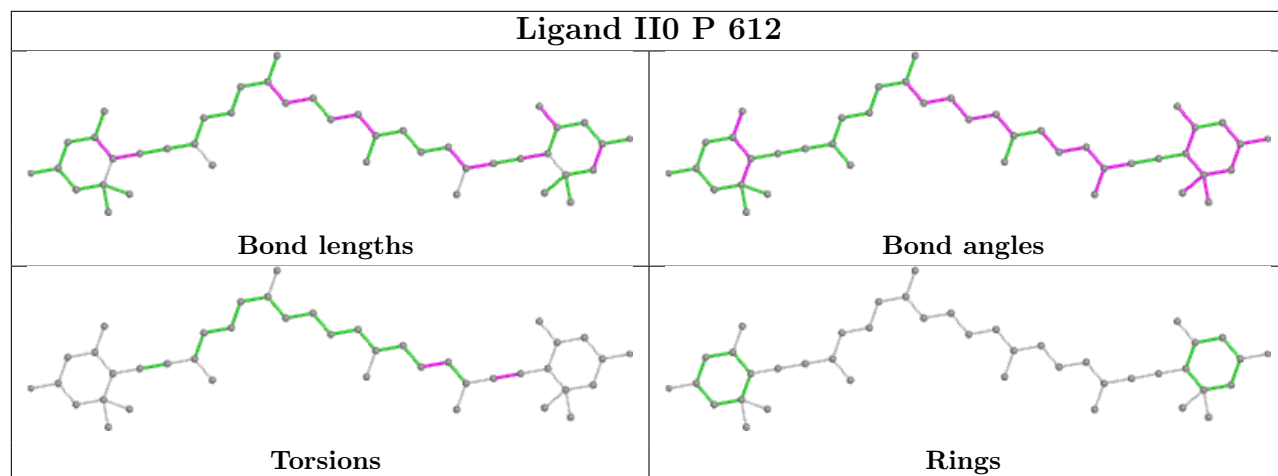
Ligand CLA b 607



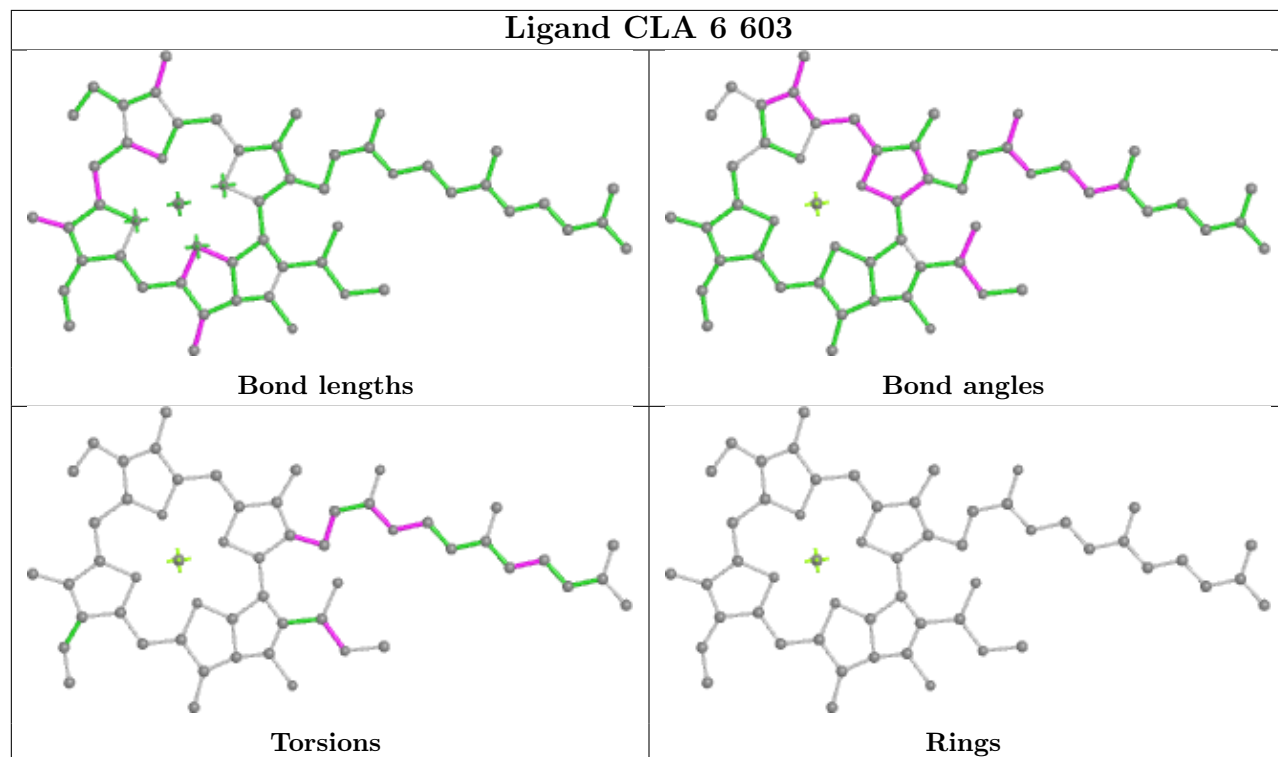
Ligand LHG b 621



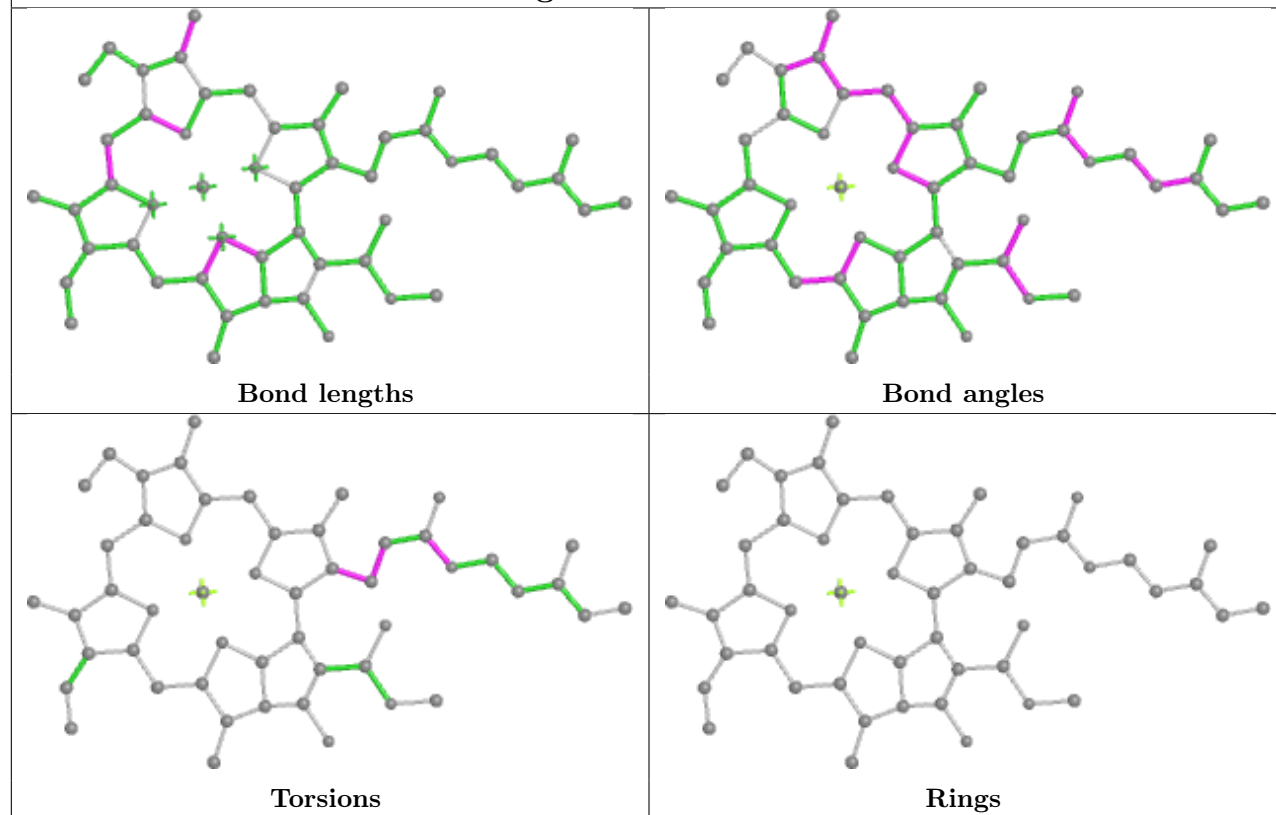
Ligand II0 P 612



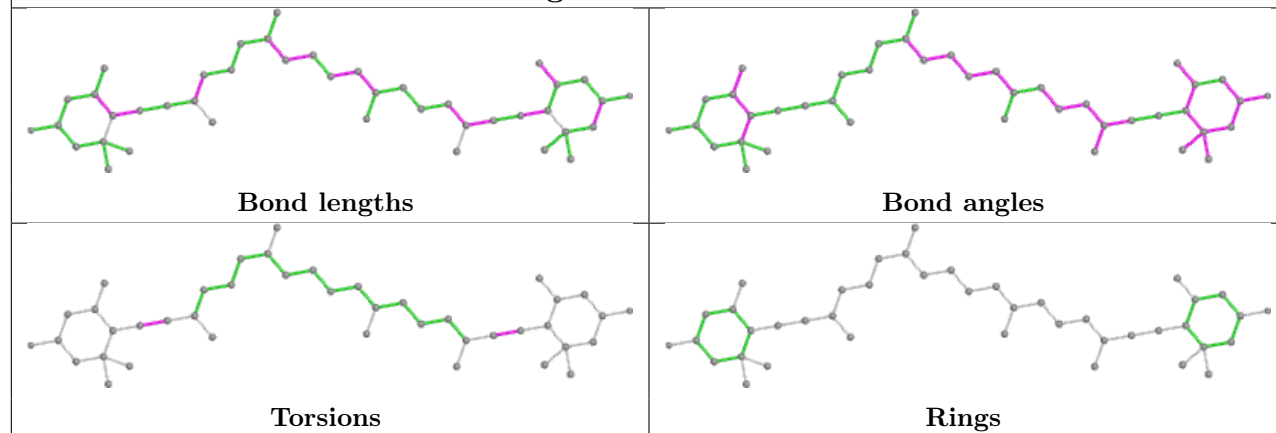
Ligand CLA 6 603

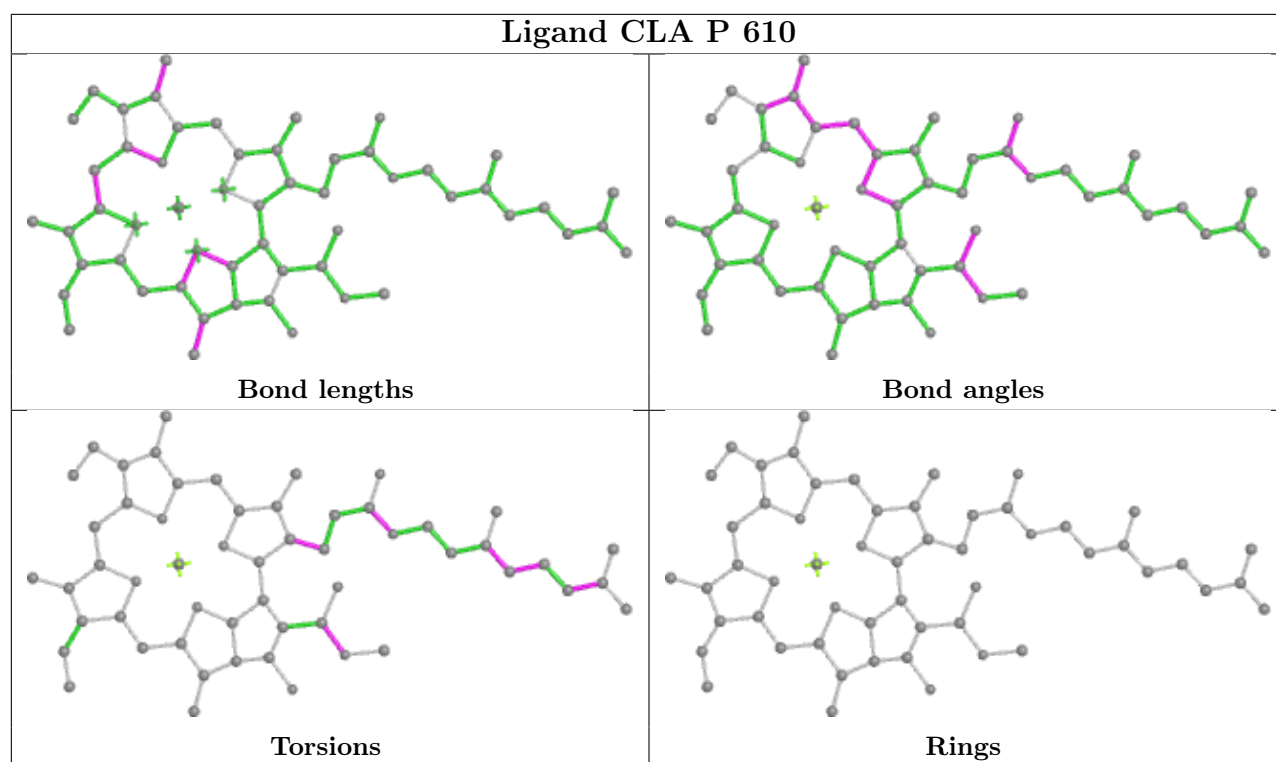


Ligand CLA 4 309

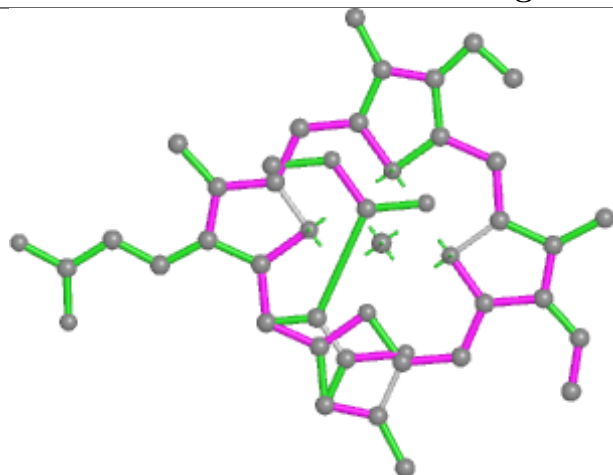


Ligand II0 O 613

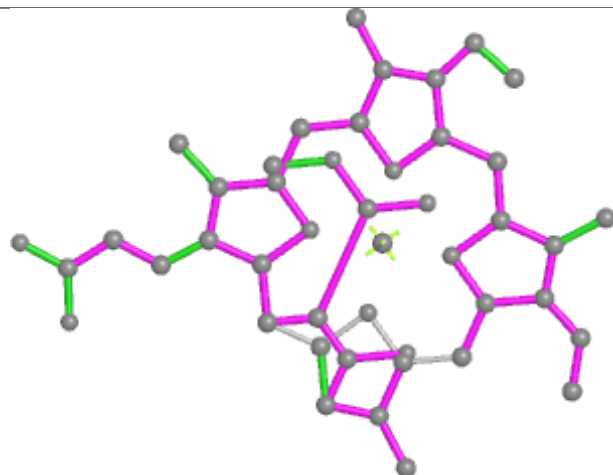




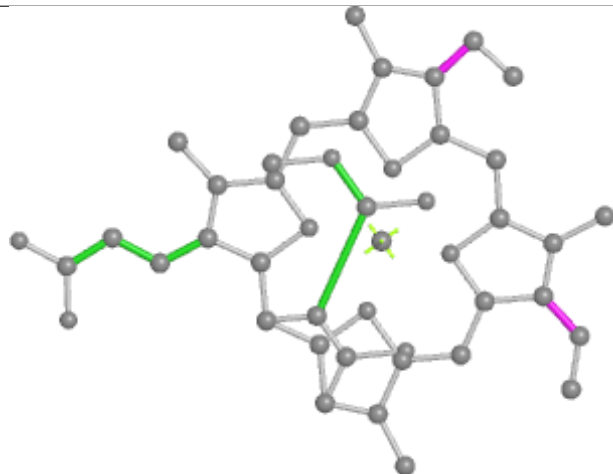
Ligand KC2 N 610



Bond lengths



Bond angles

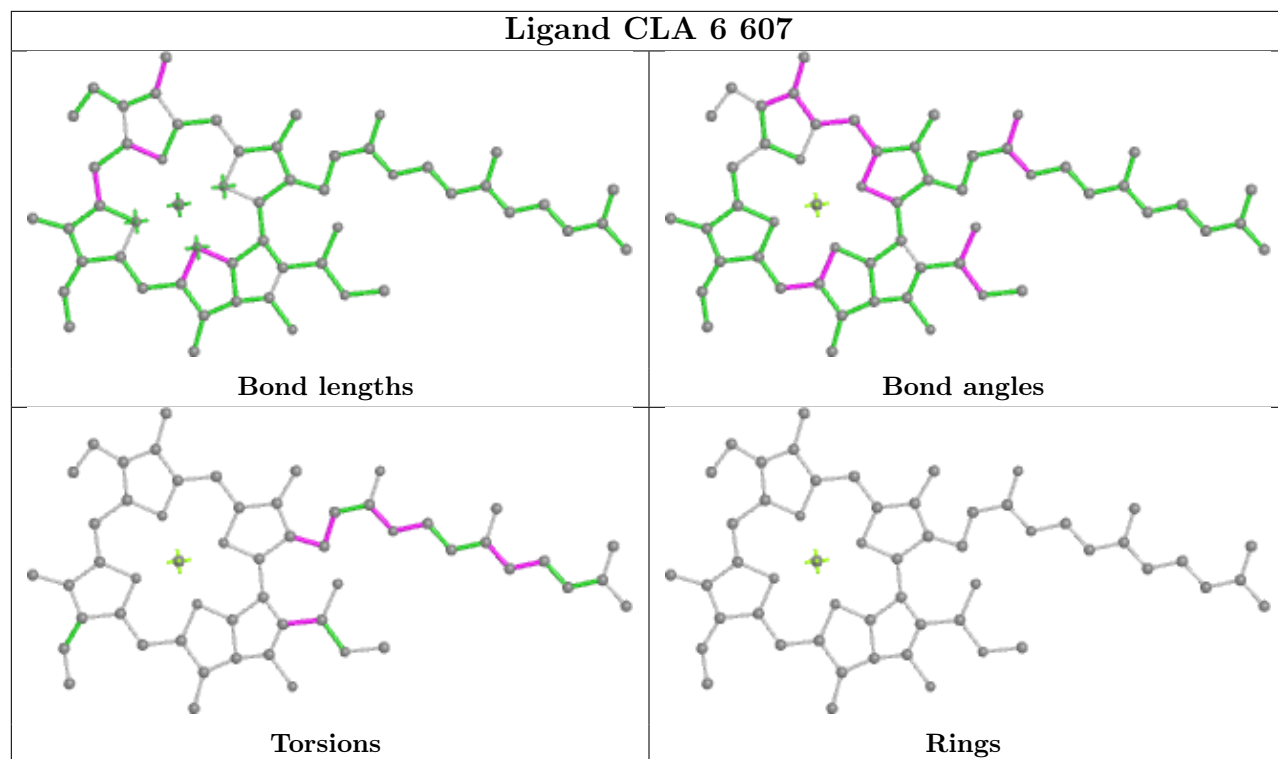


Torsions

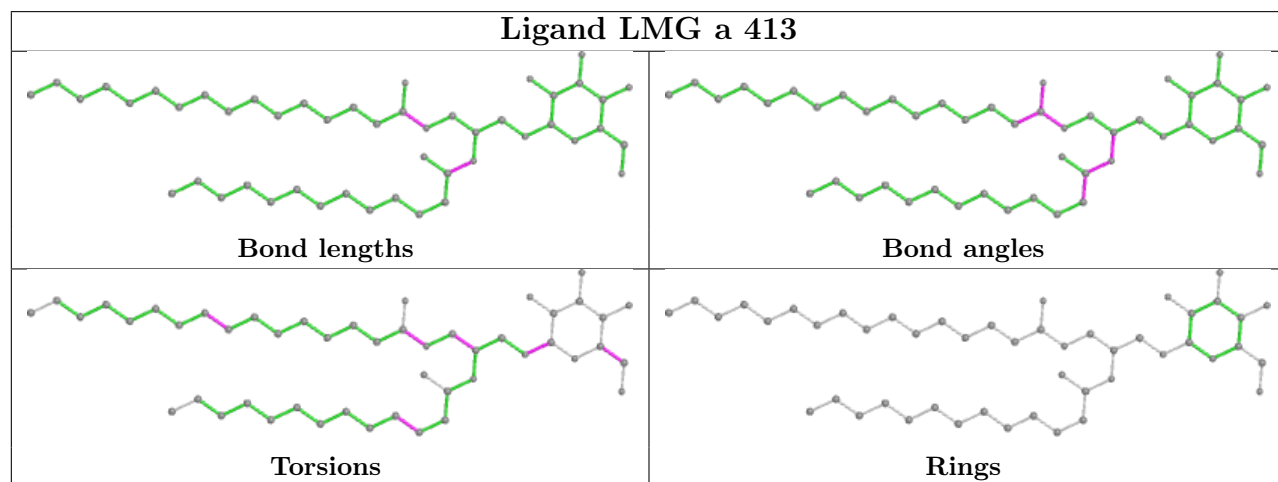


Rings

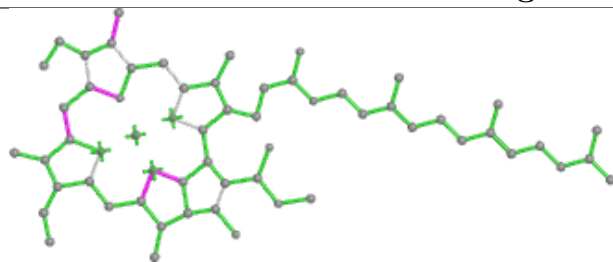
Ligand CLA 6 607



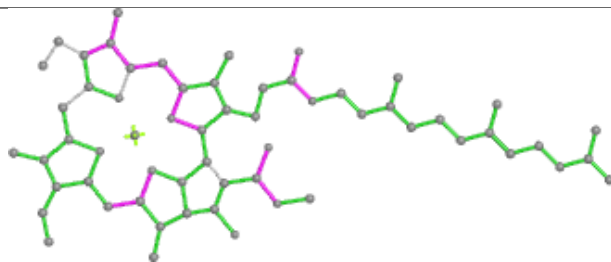
Ligand LMG a 413



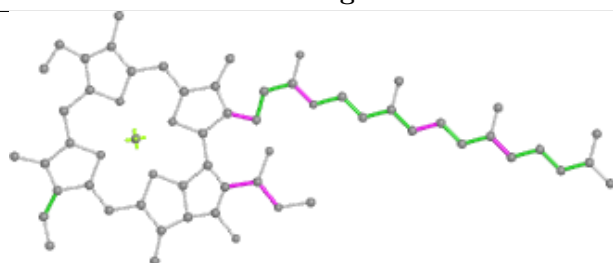
Ligand CLA b 614



Bond lengths



Bond angles

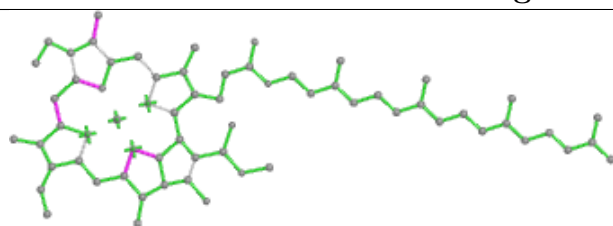


Torsions

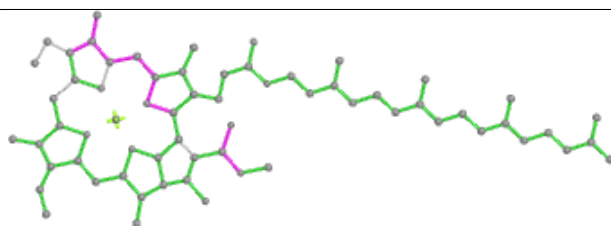


Rings

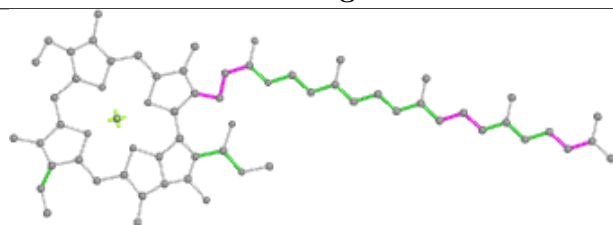
Ligand CLA O 603



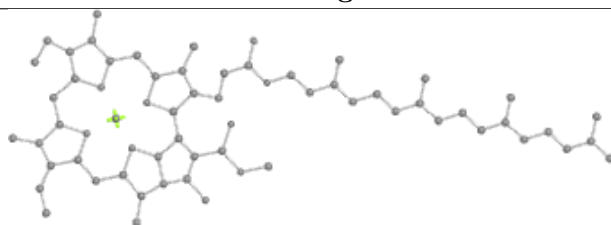
Bond lengths



Bond angles

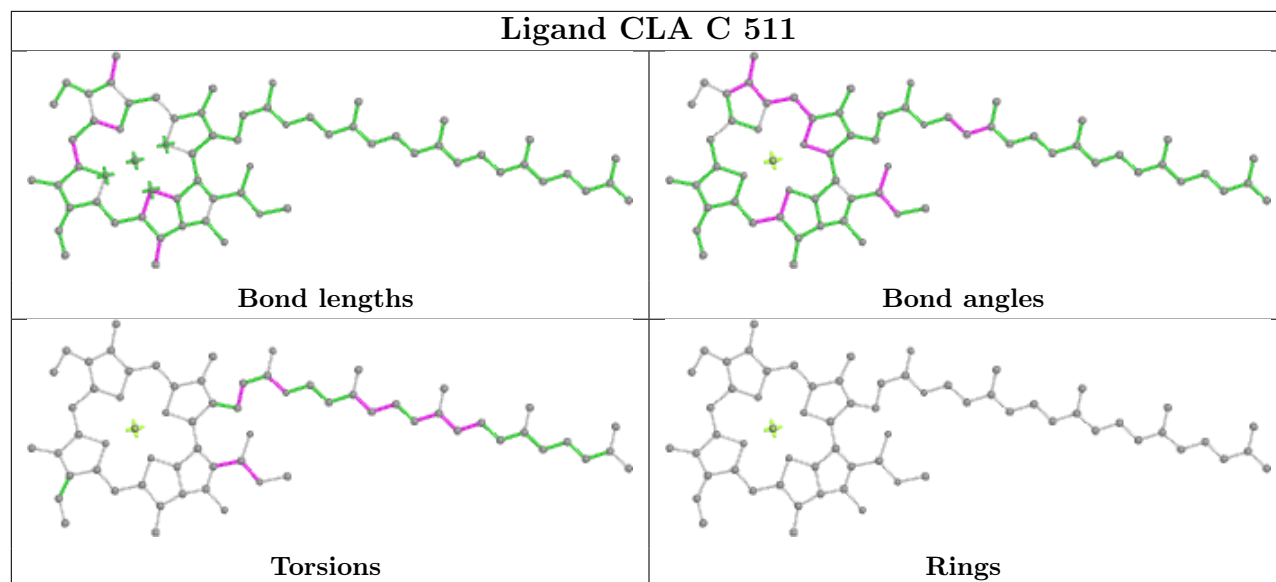


Torsions

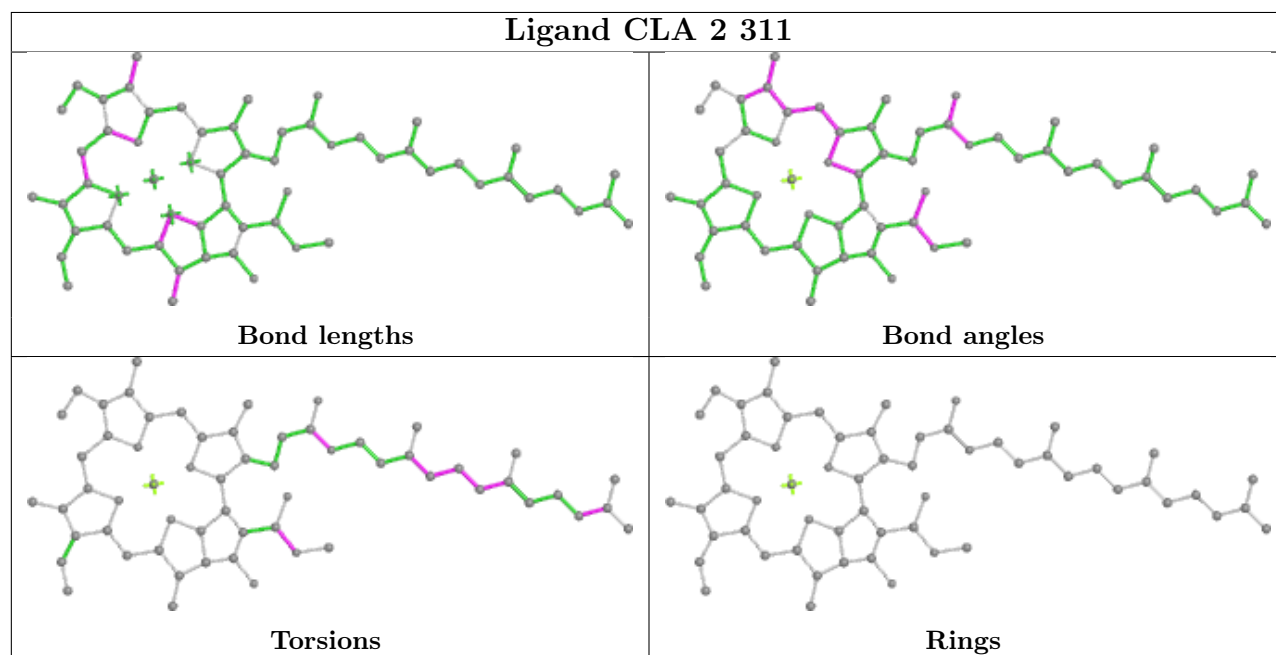


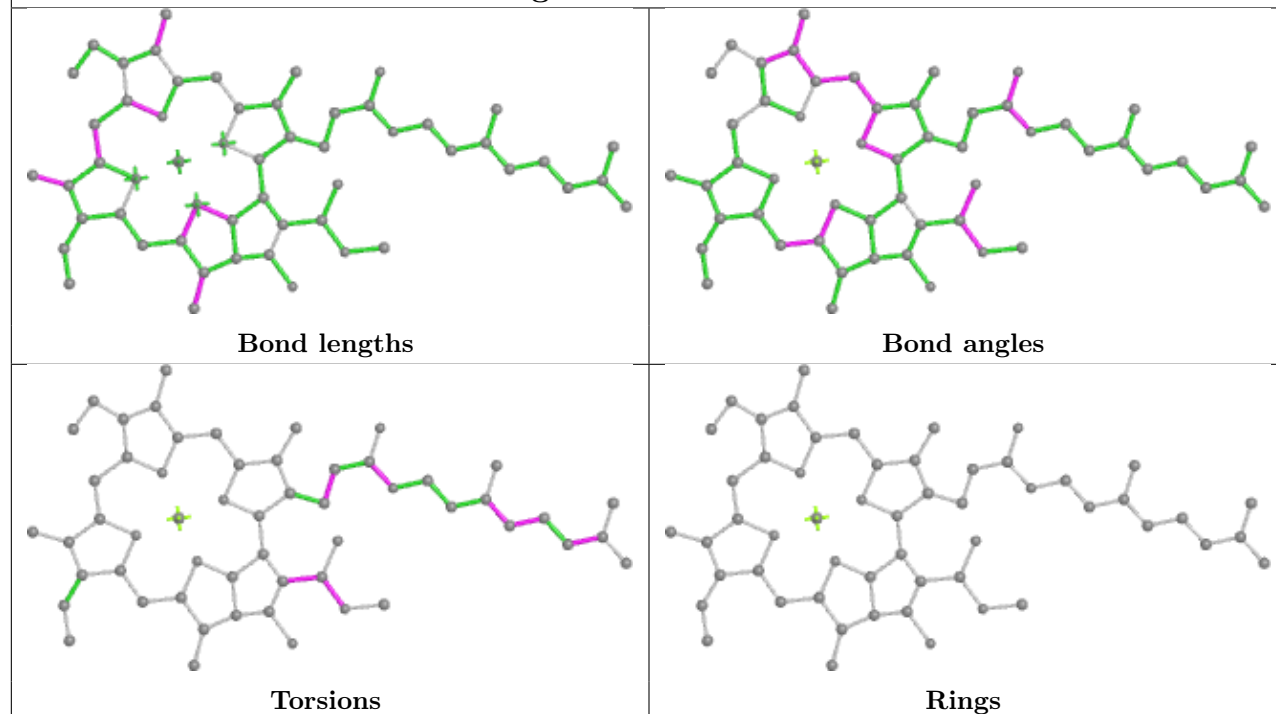
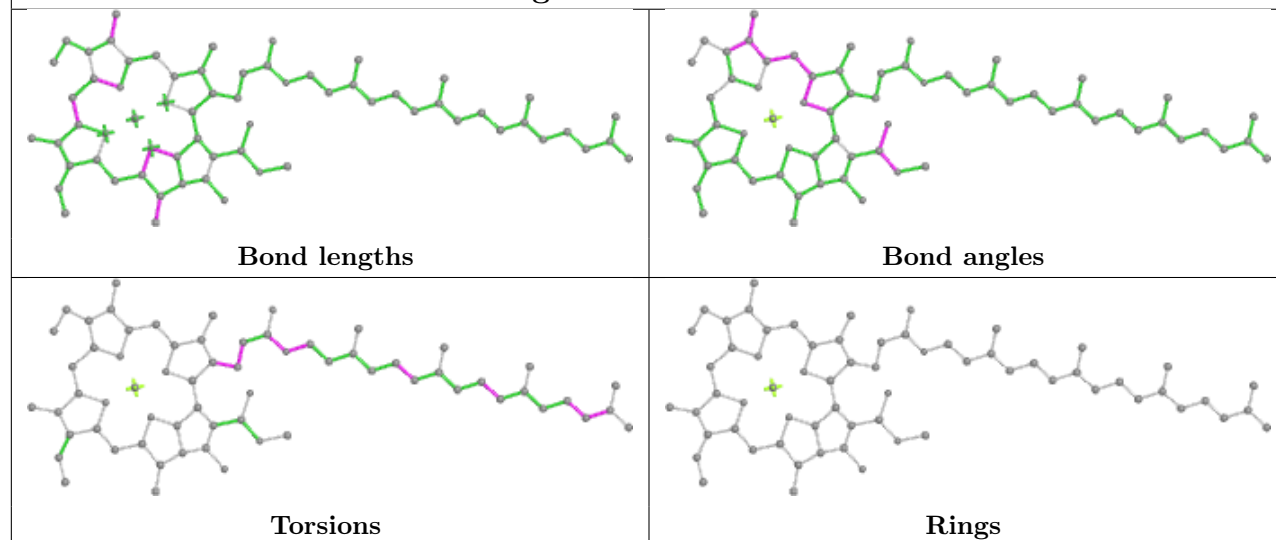
Rings

Ligand CLA C 511

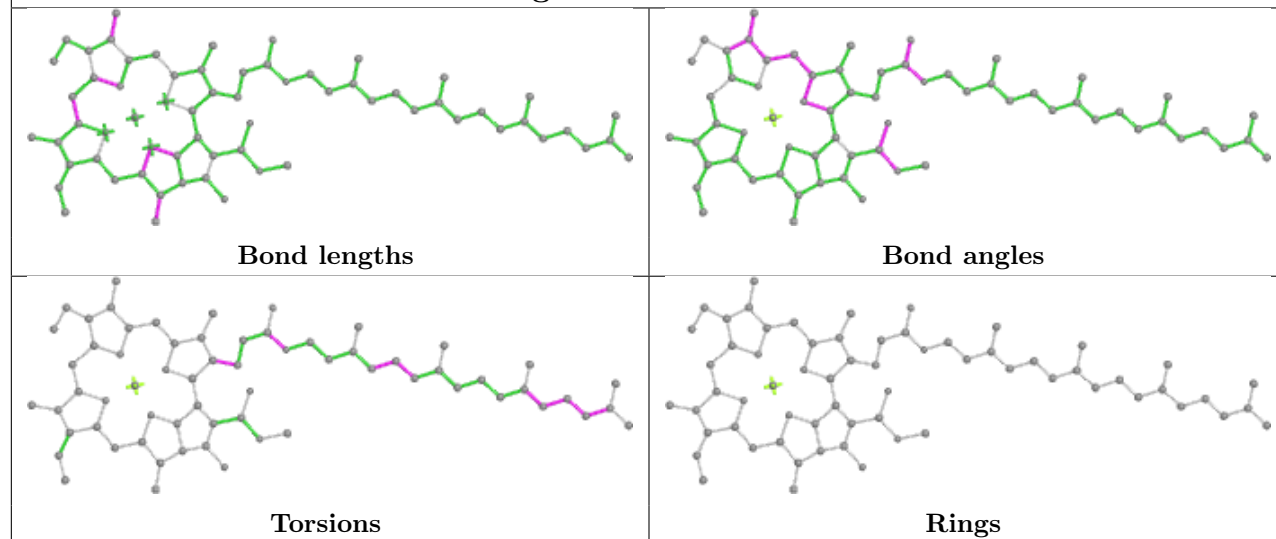


Ligand CLA 2 311

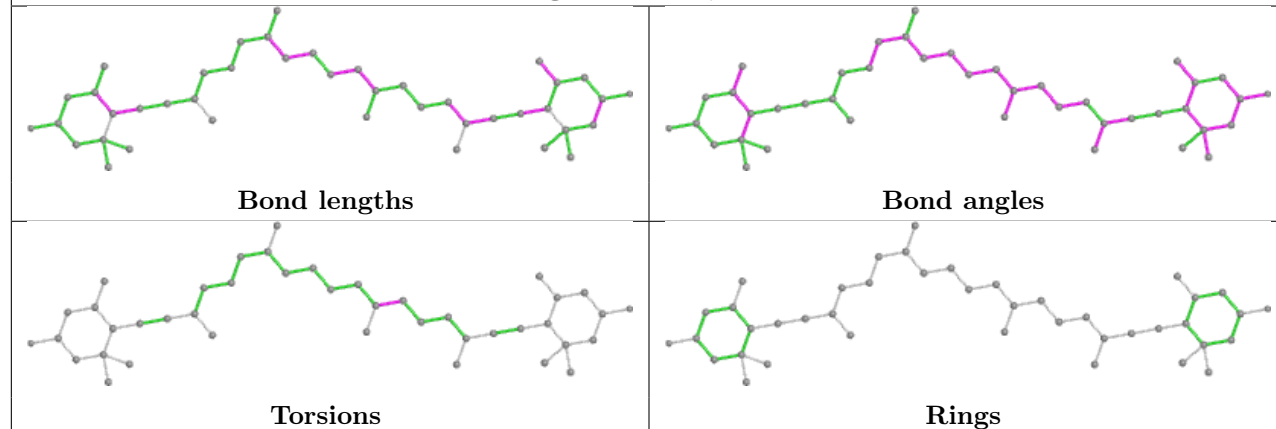


Ligand CLA R 303**Ligand CLA B 615**

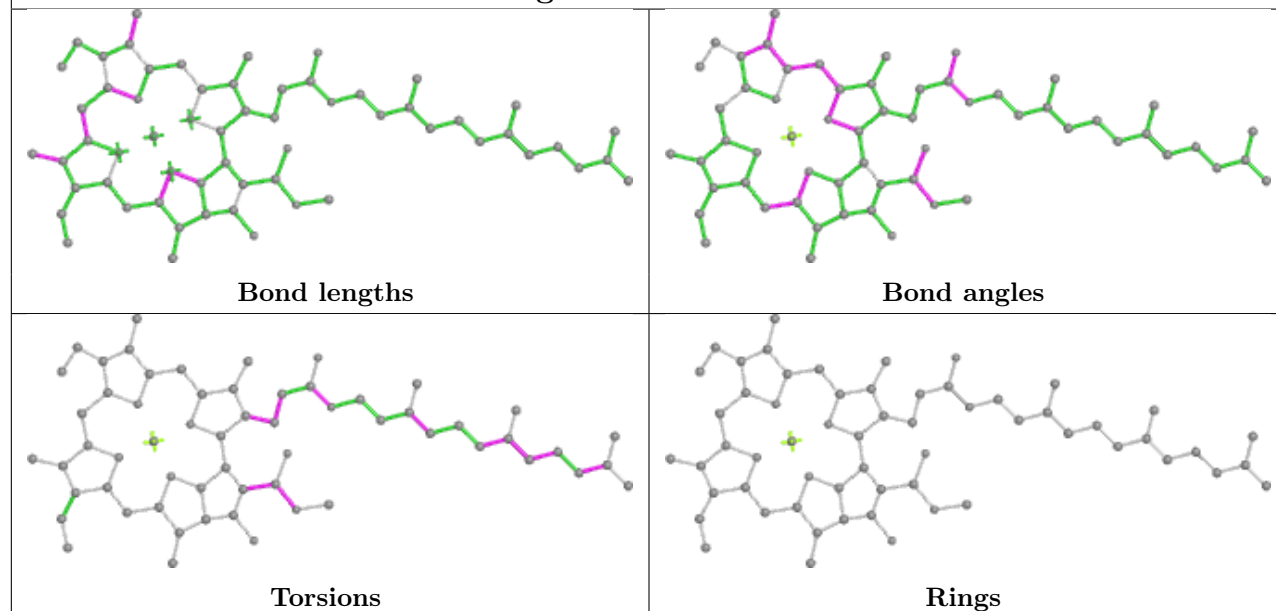
Ligand CLA C 513



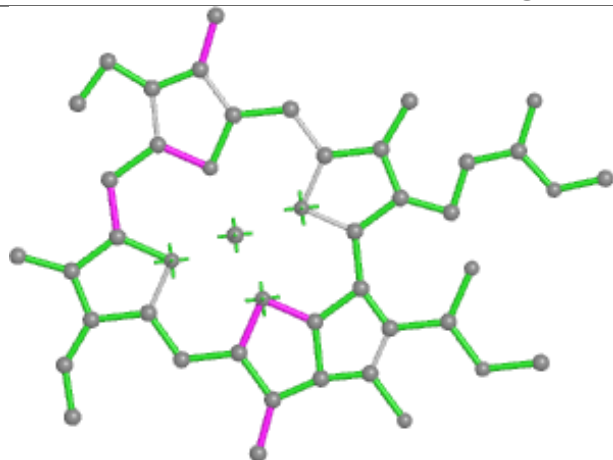
Ligand II0 Q 313



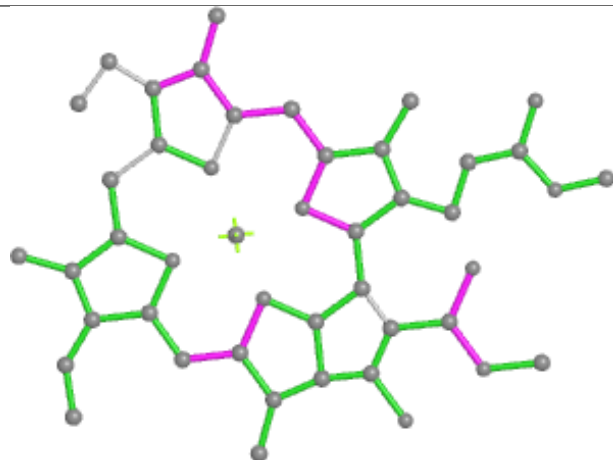
Ligand CLA 2 309



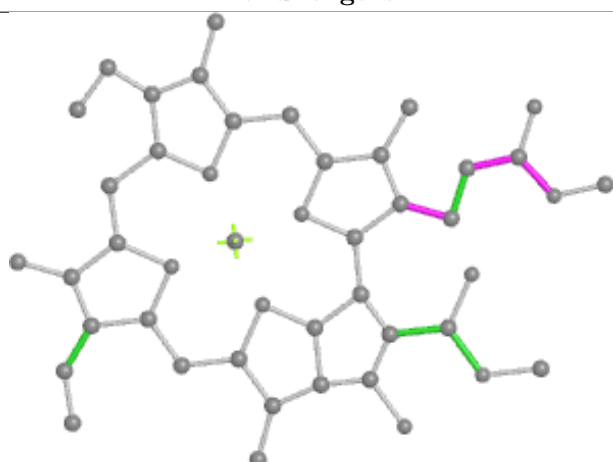
Ligand CLA 5 612



Bond lengths



Bond angles

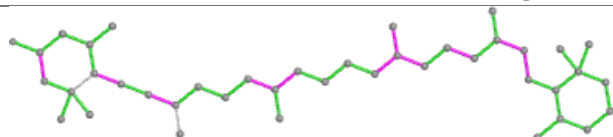


Torsions

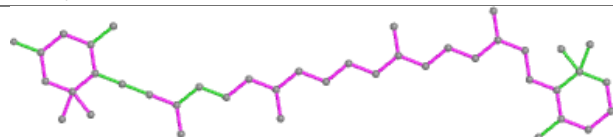


Rings

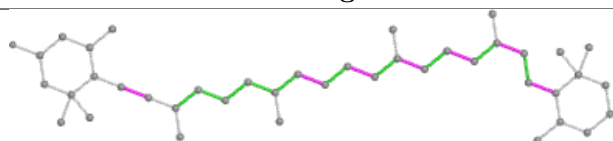
Ligand IHT Q 317



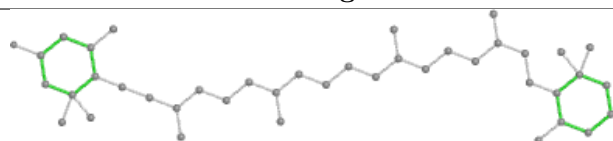
Bond lengths



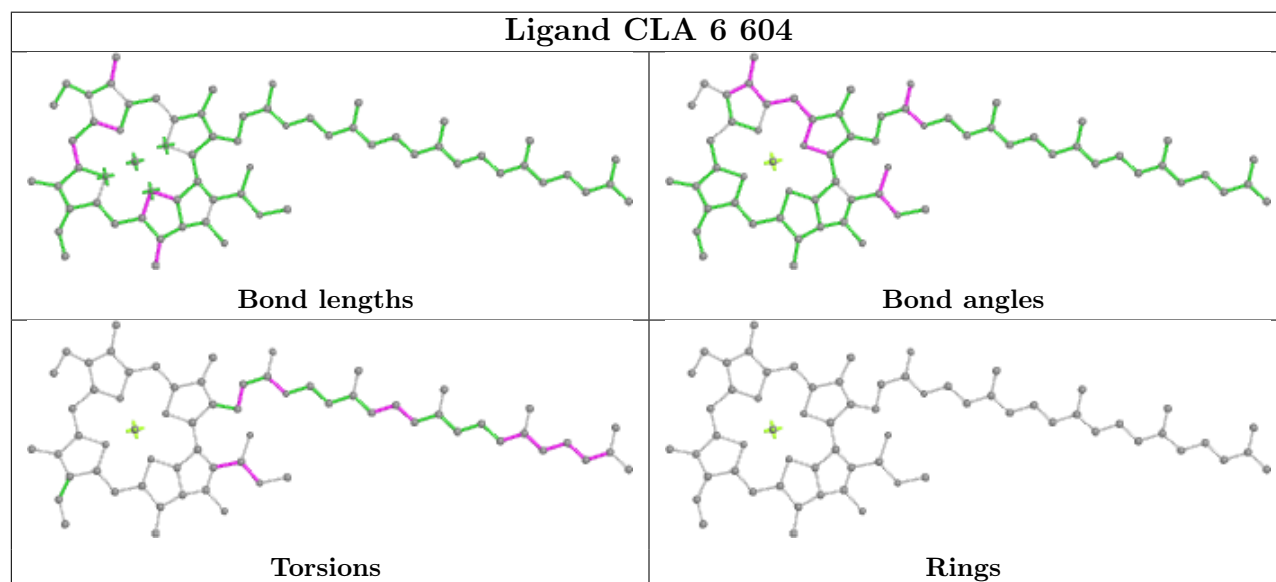
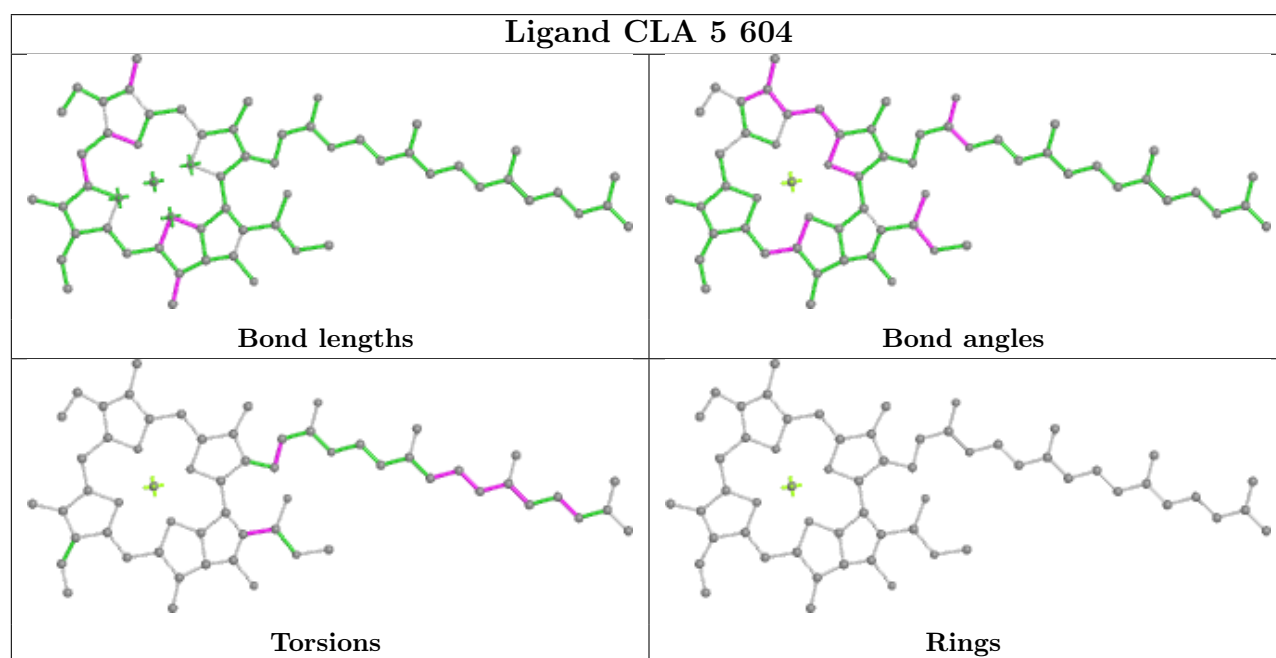
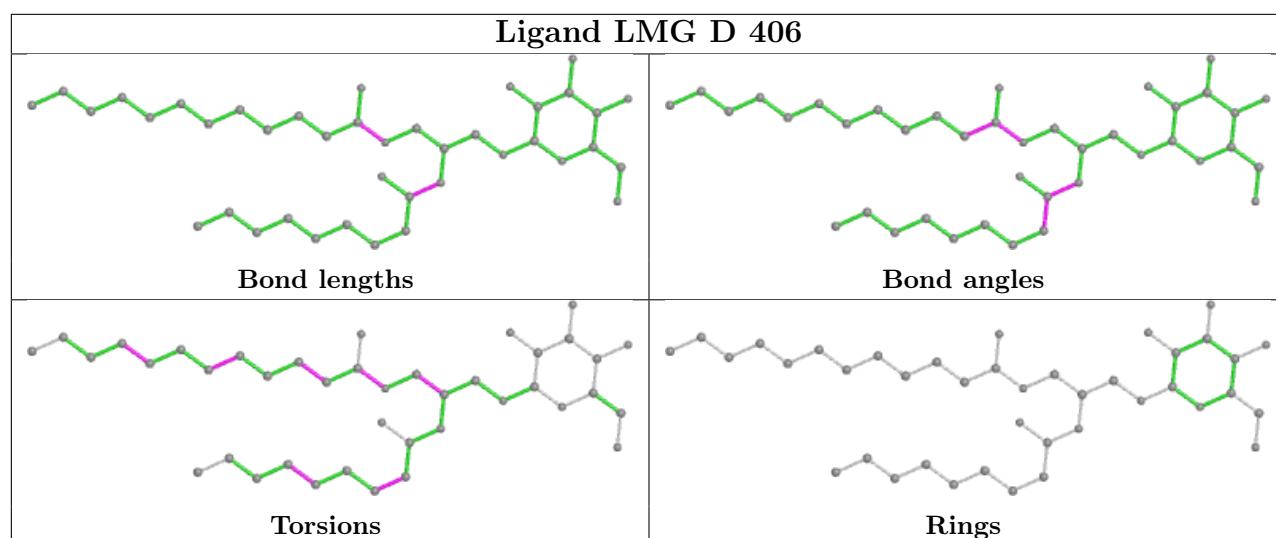
Bond angles



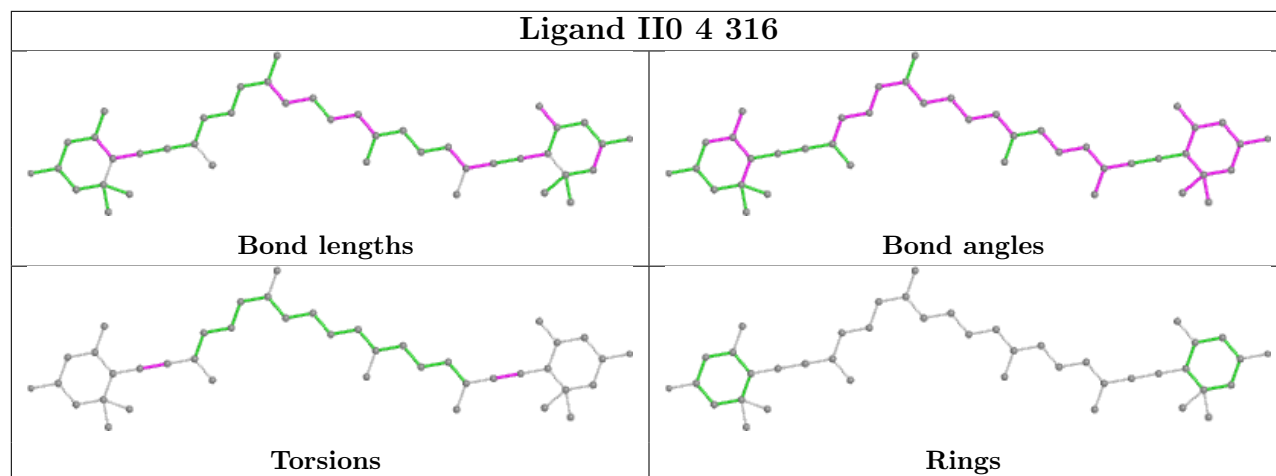
Torsions



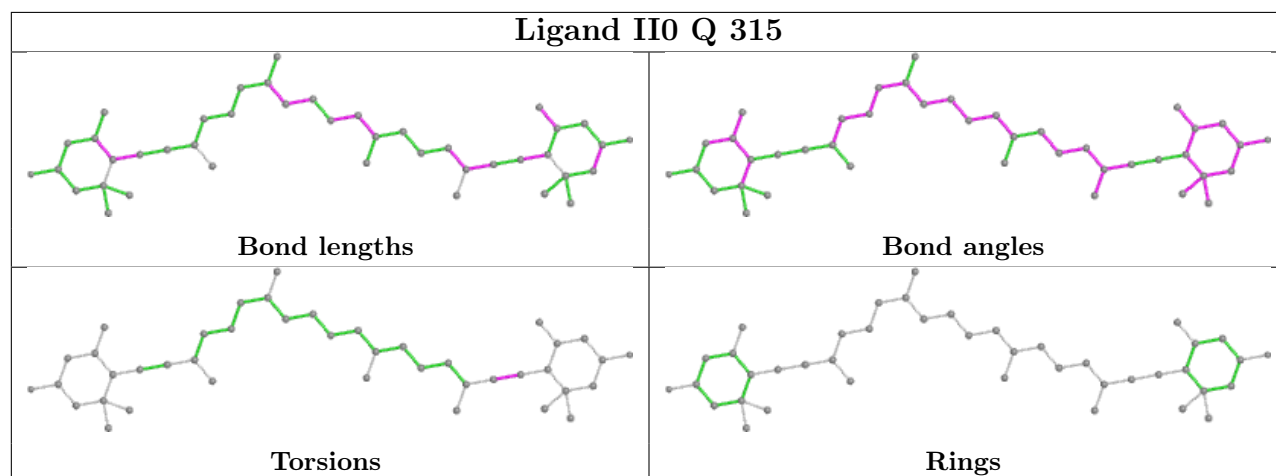
Rings

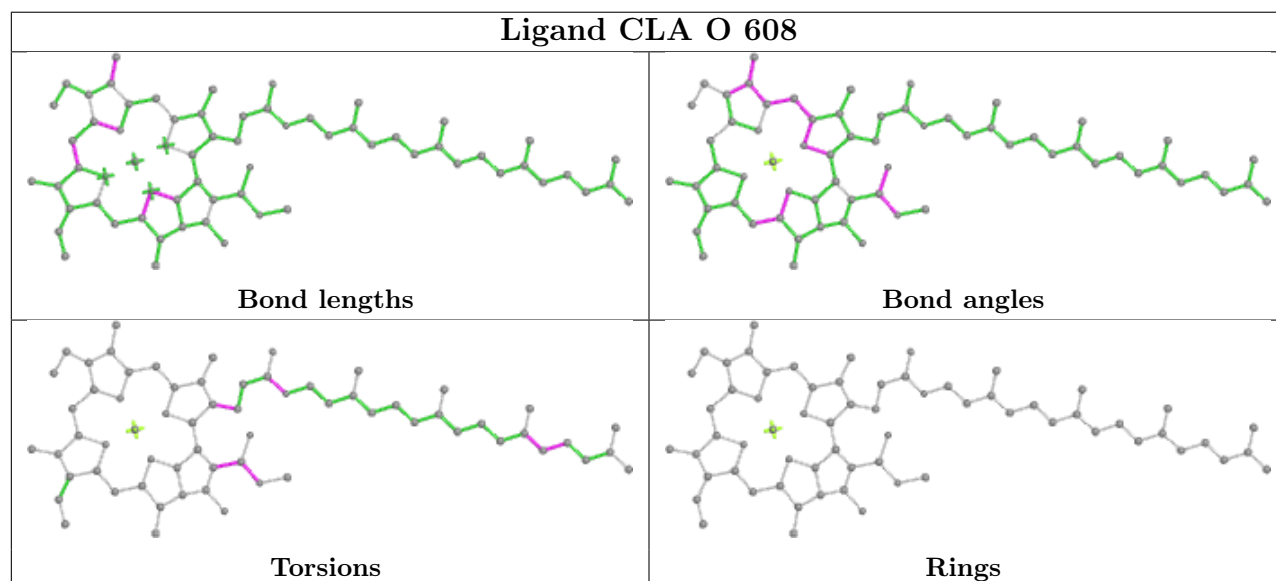
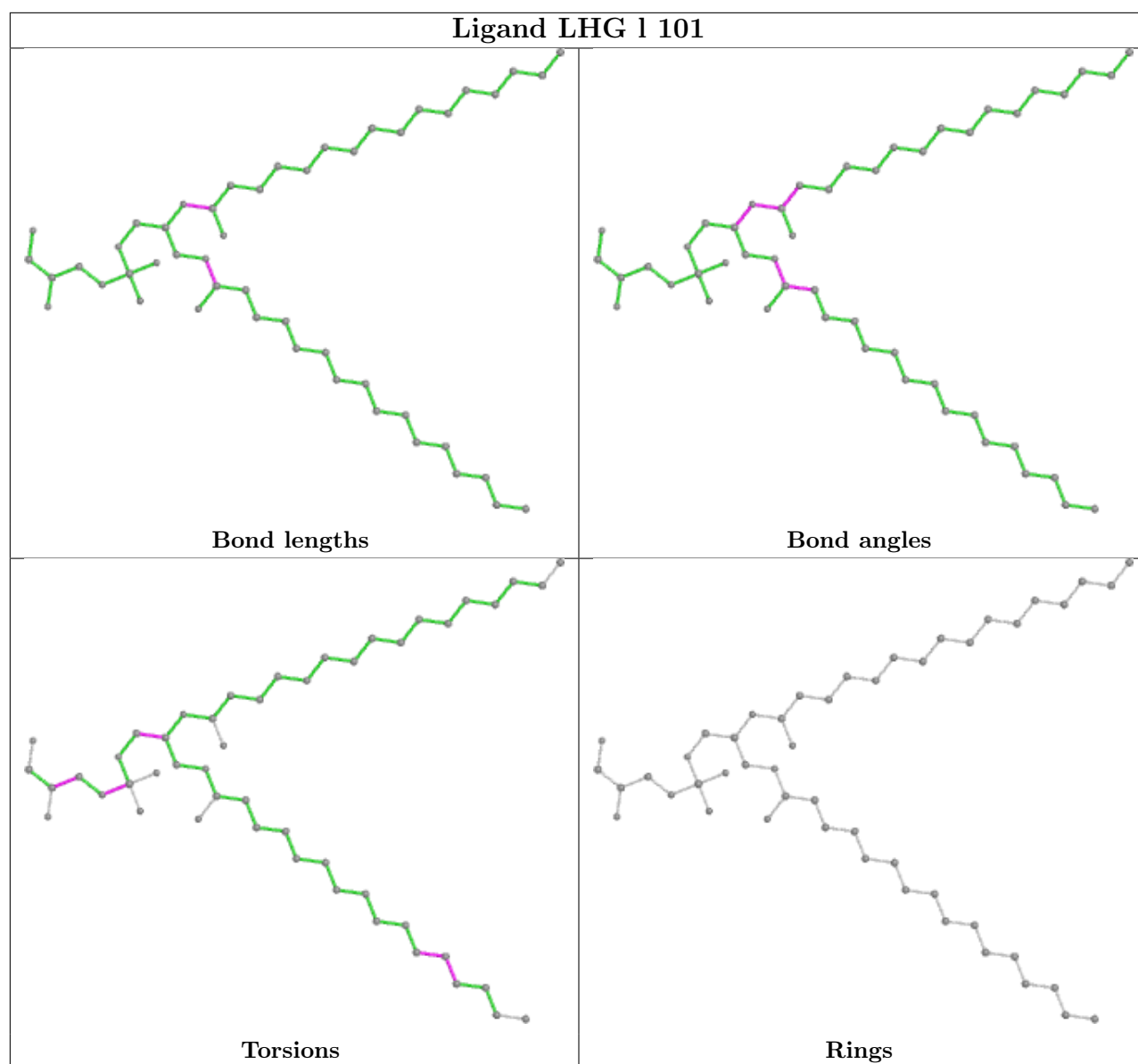


Ligand II0 4 316

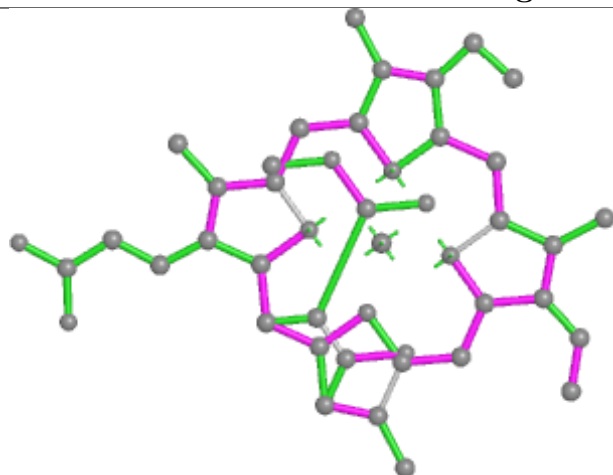


Ligand II0 Q 315

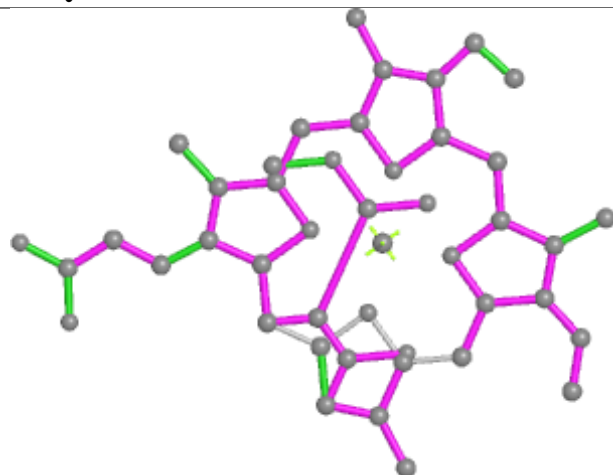




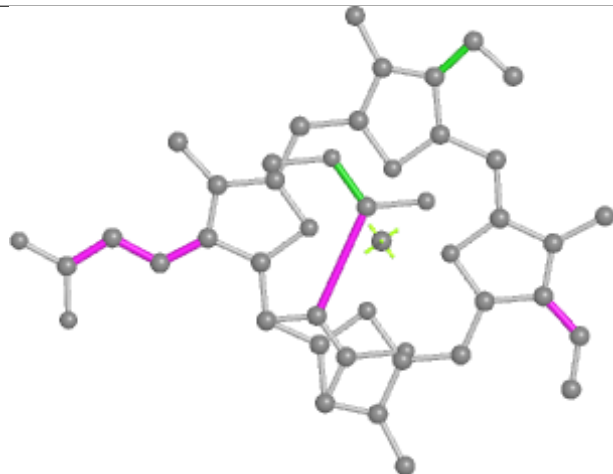
Ligand KC2 Q 304



Bond lengths



Bond angles

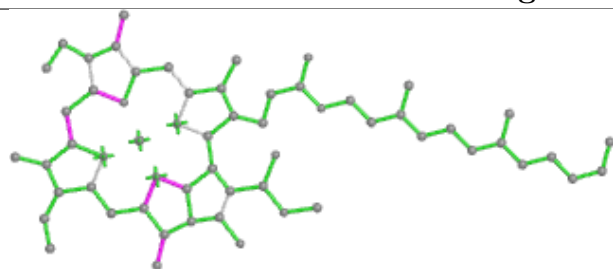


Torsions

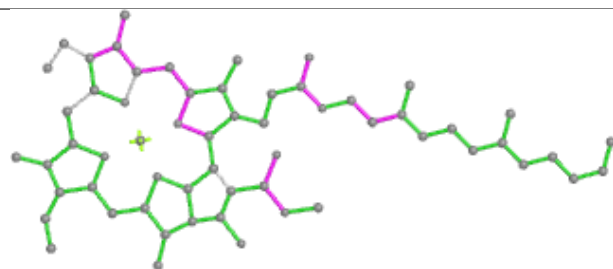


Rings

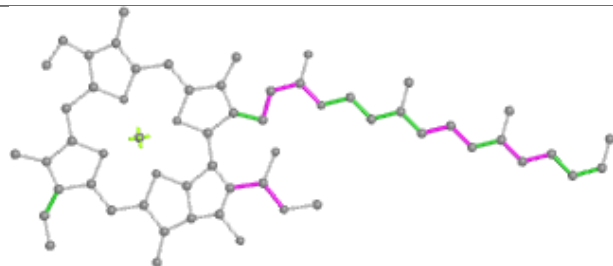
Ligand CLA 1 604



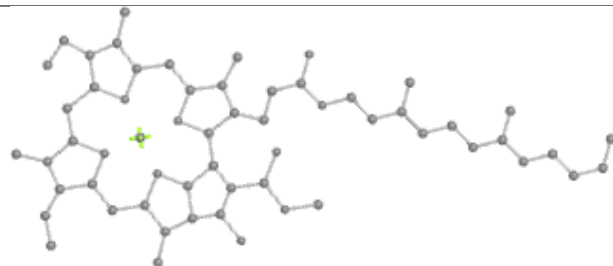
Bond lengths



Bond angles

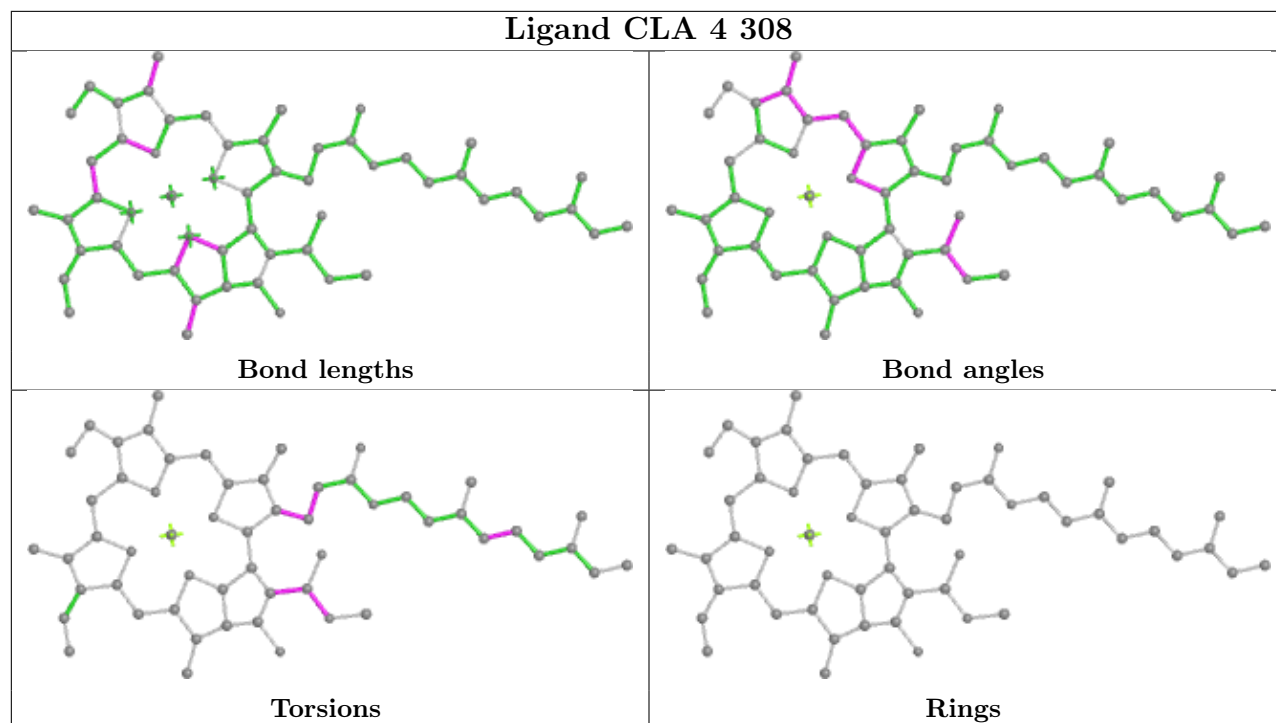


Torsions

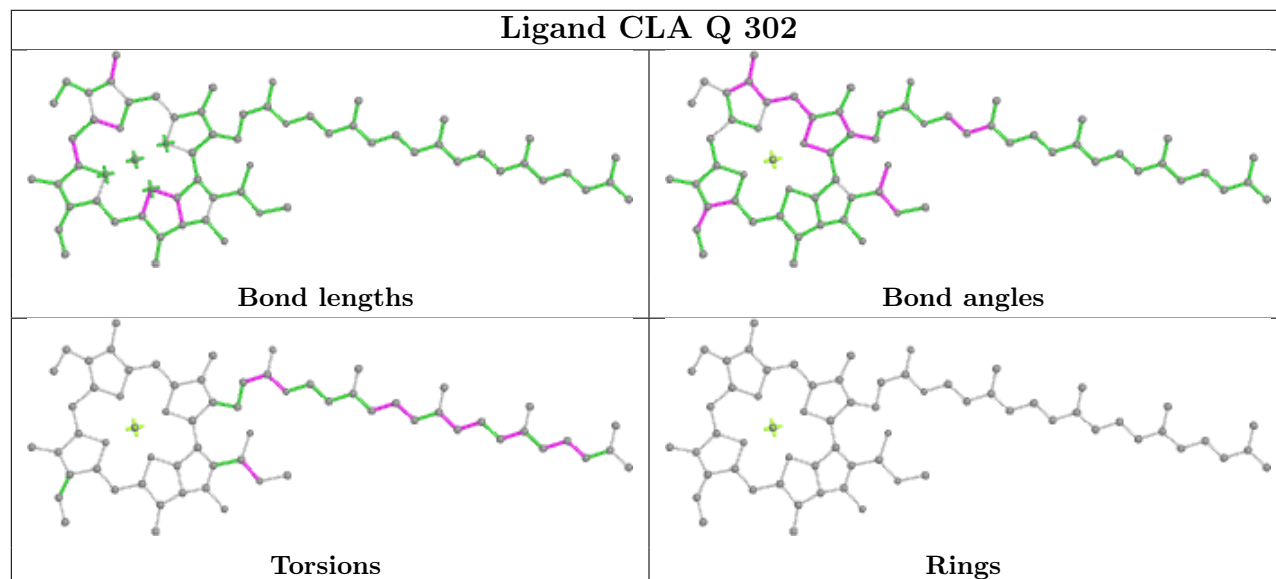


Rings

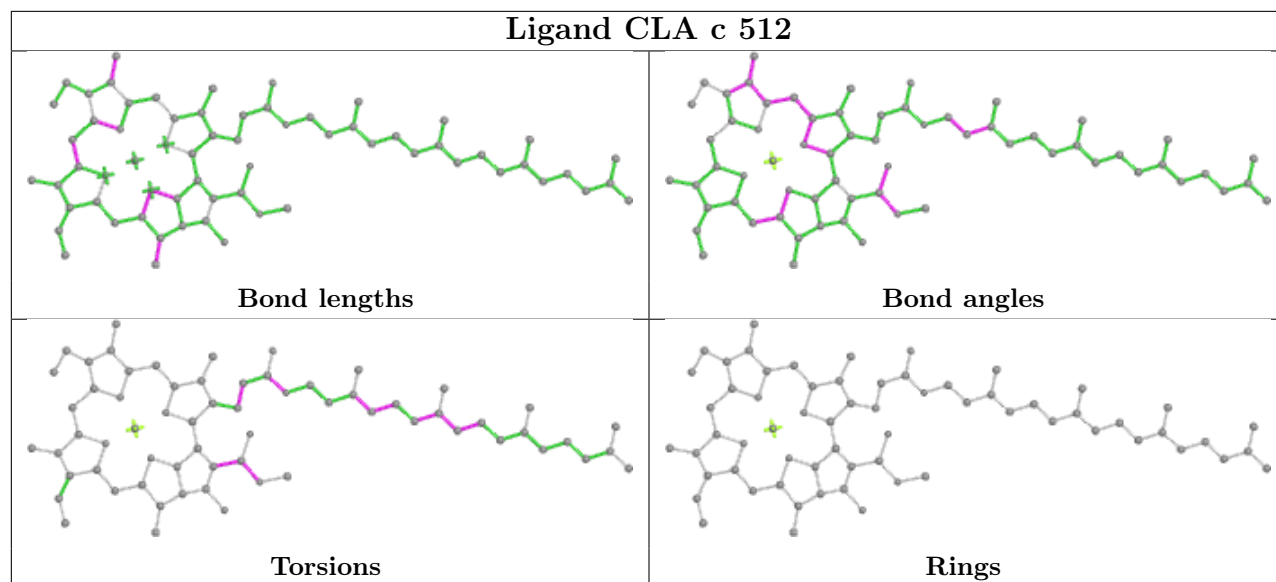
Ligand CLA 4 308



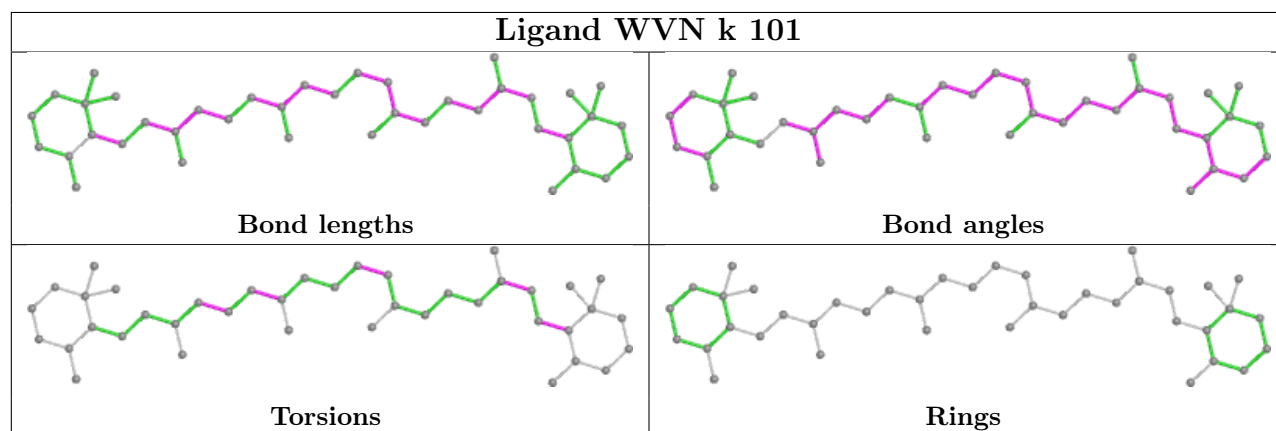
Ligand CLA Q 302



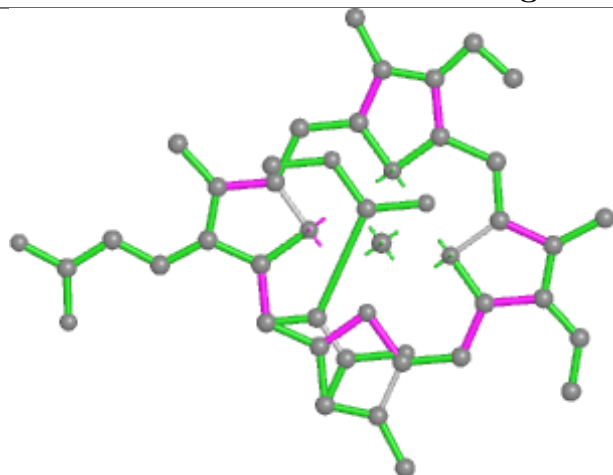
Ligand CLA c 512



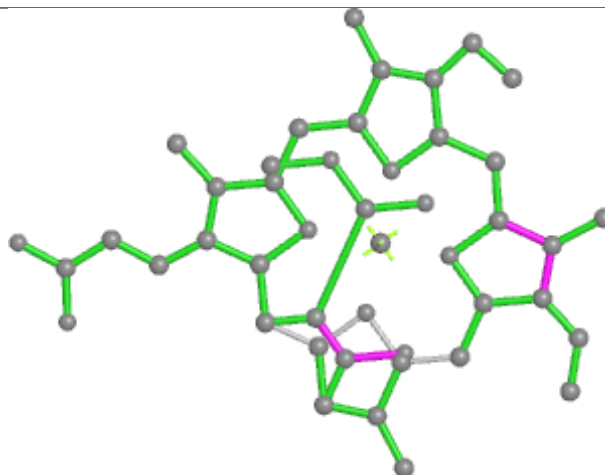
Ligand WVN k 101



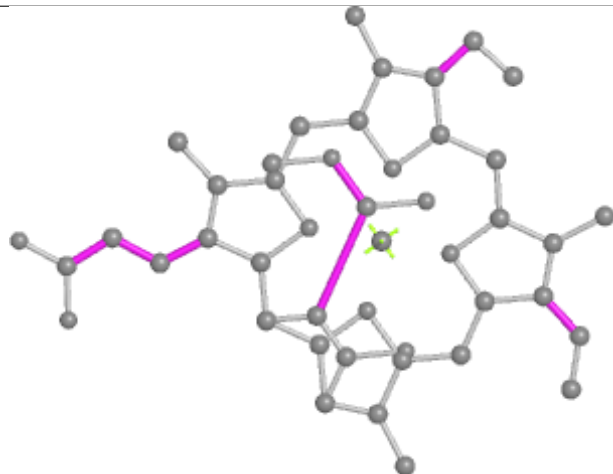
Ligand KC2 1 605



Bond lengths



Bond angles

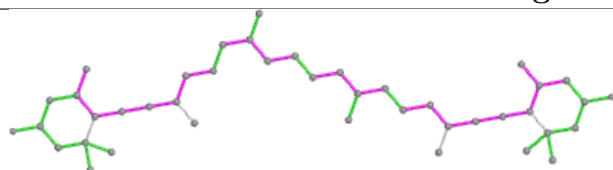


Torsions

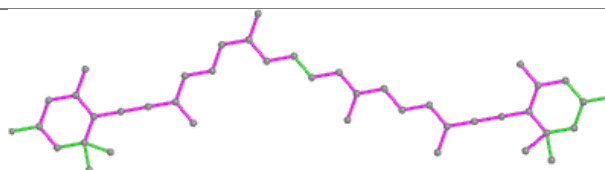


Rings

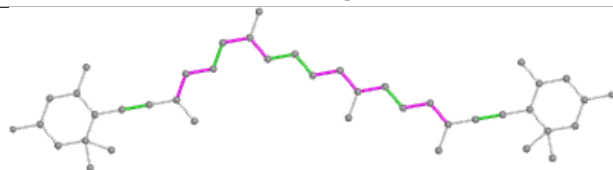
Ligand II0 1 618



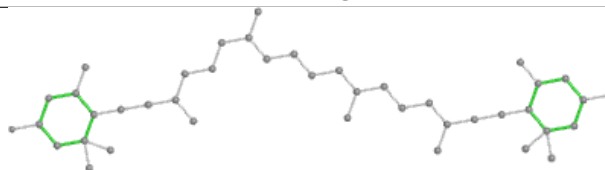
Bond lengths



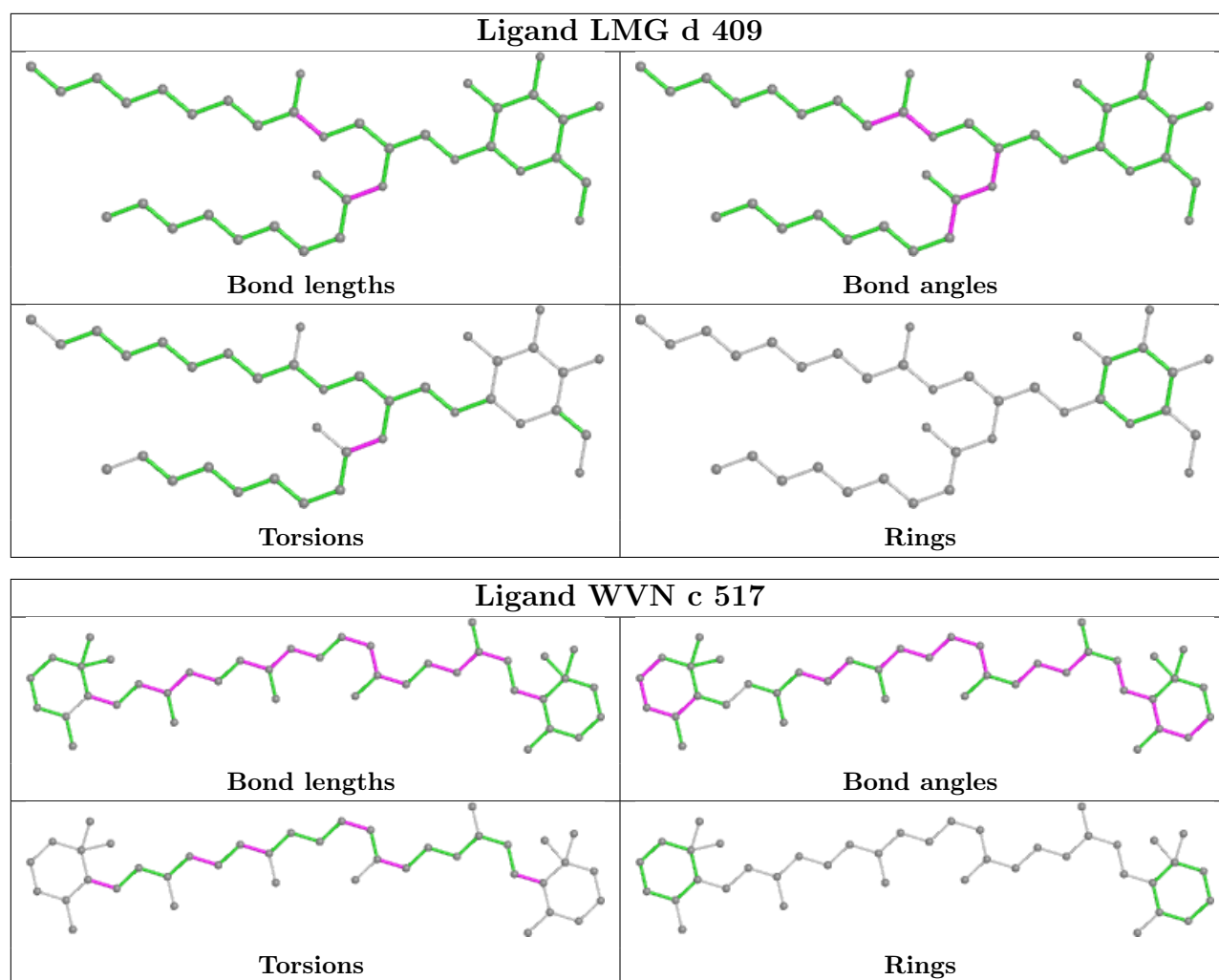
Bond angles



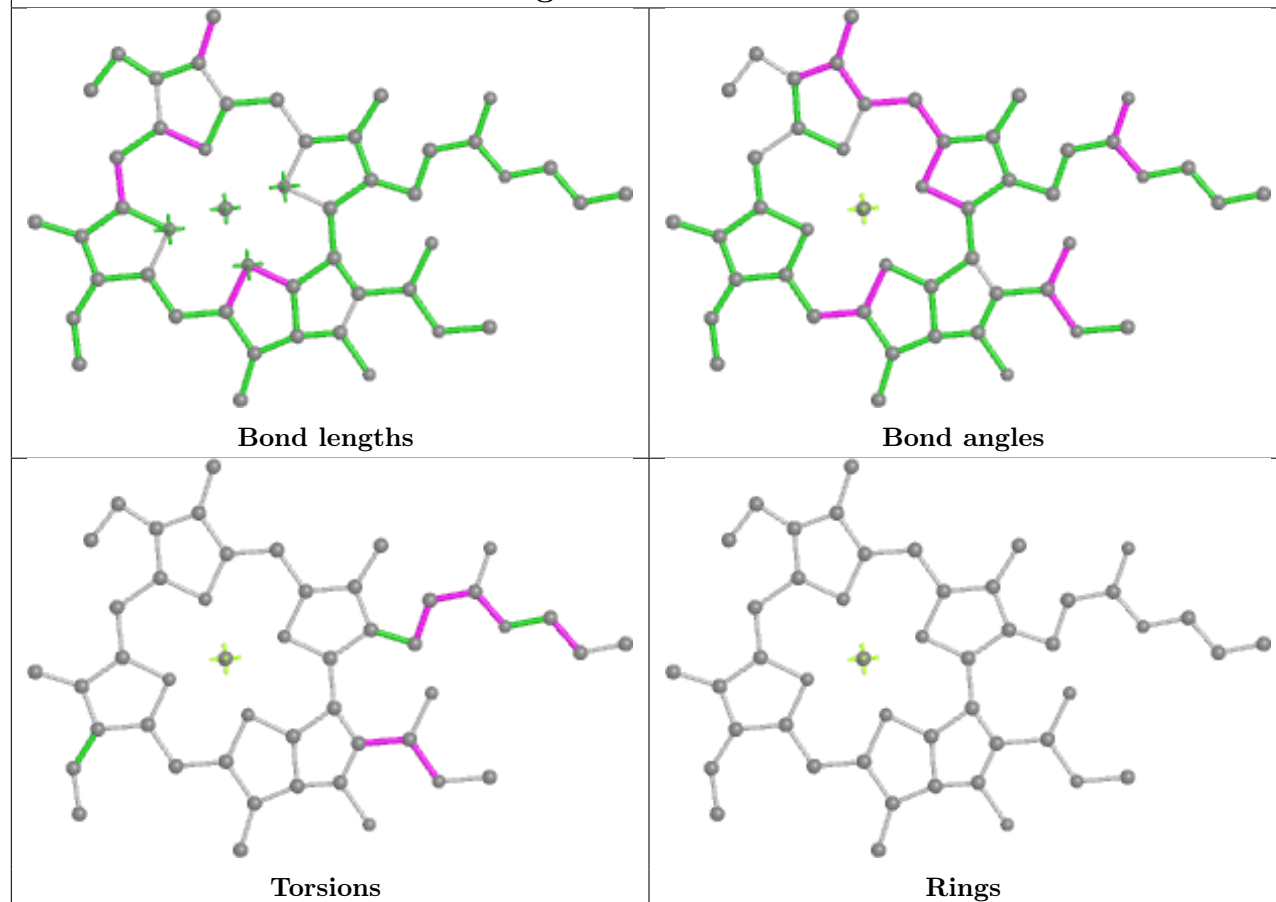
Torsions



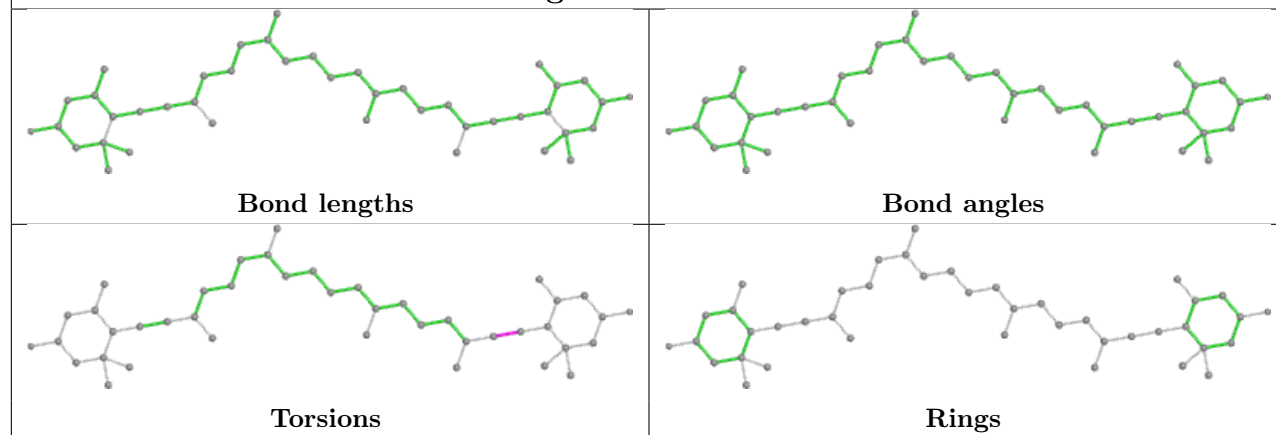
Rings



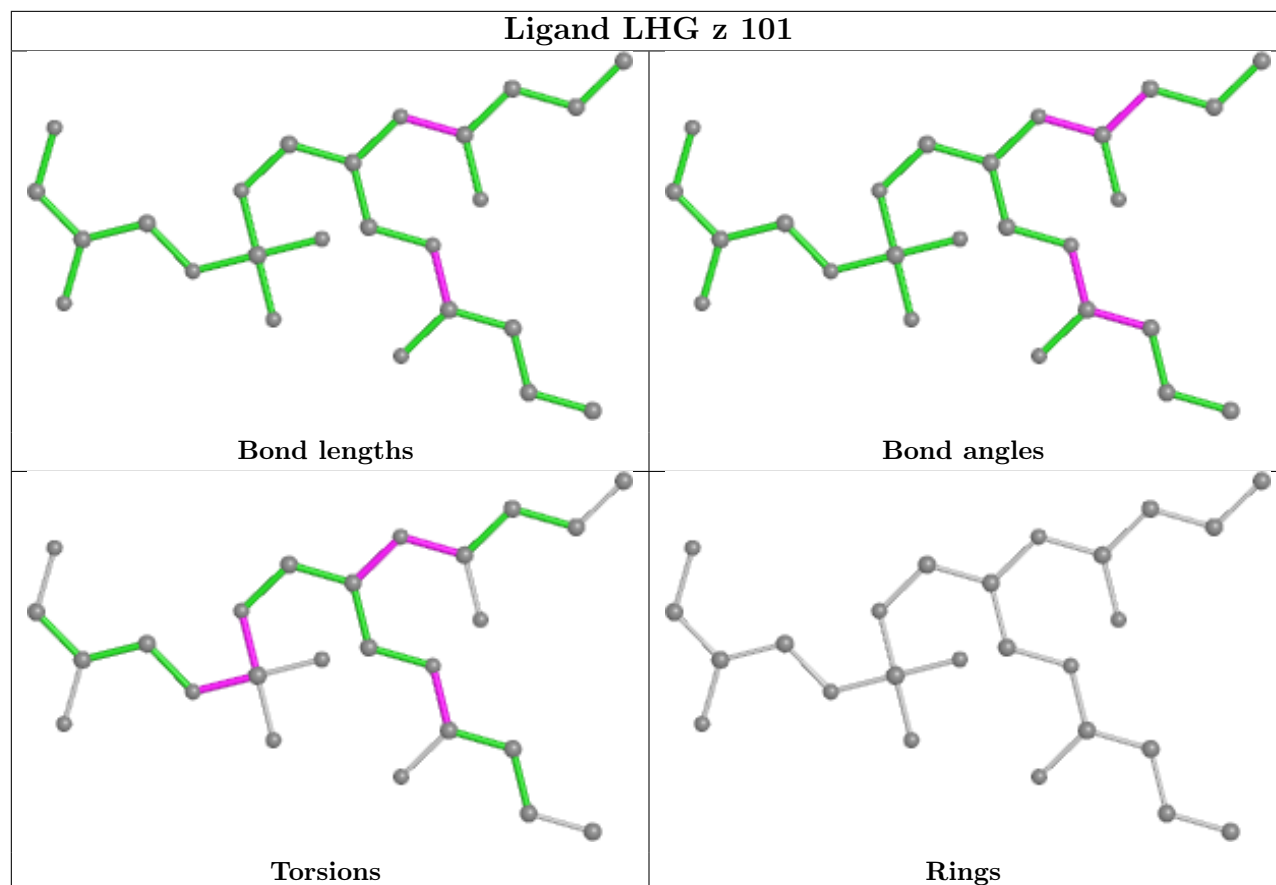
Ligand CLA 1 613



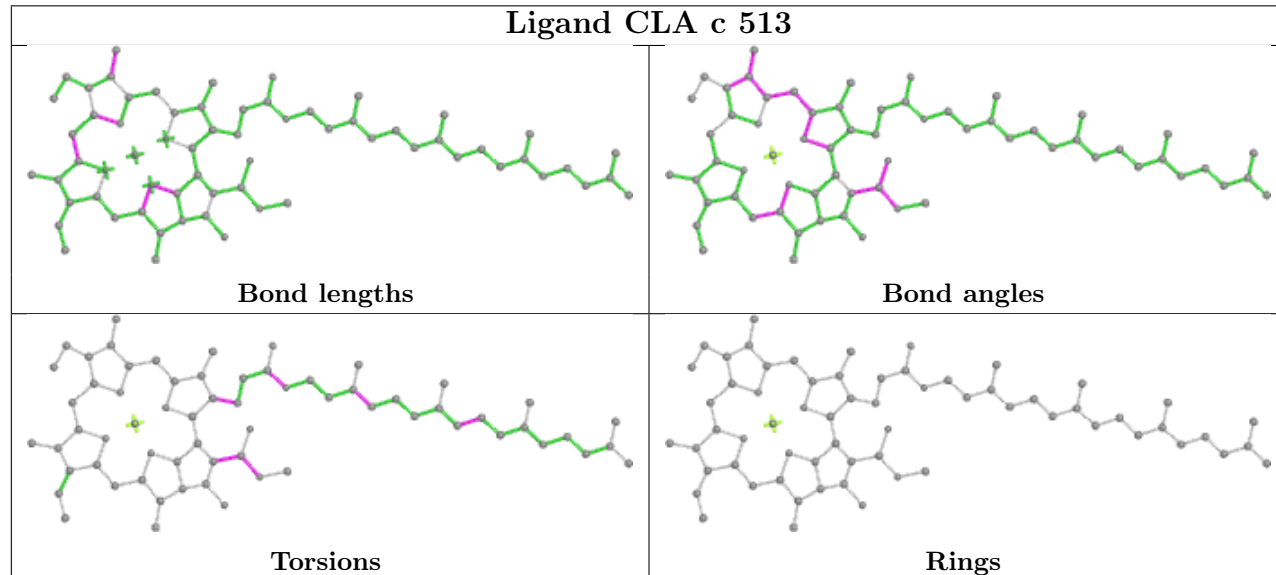
Ligand II0 O 618

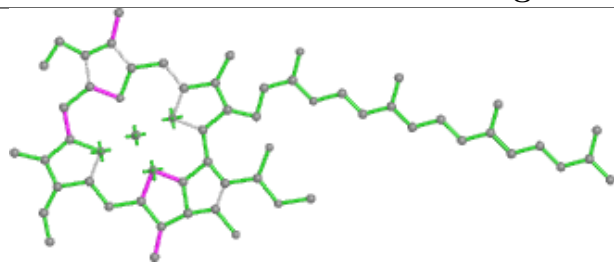


Ligand LHG z 101

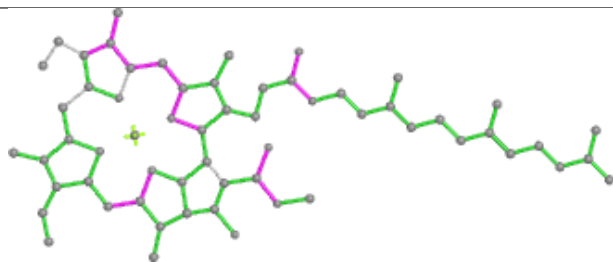


Ligand CLA c 513

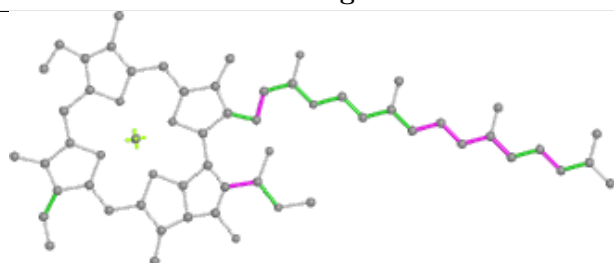


Ligand CLA R 305

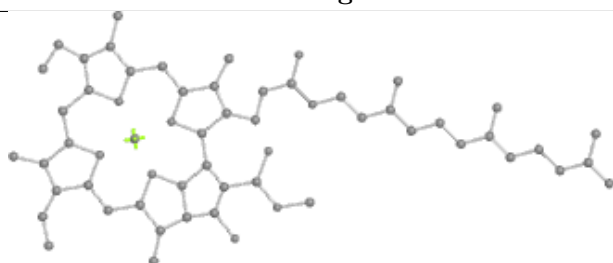
Bond lengths



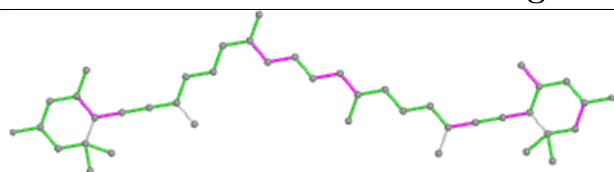
Bond angles



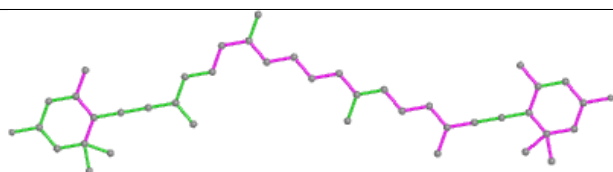
Torsions



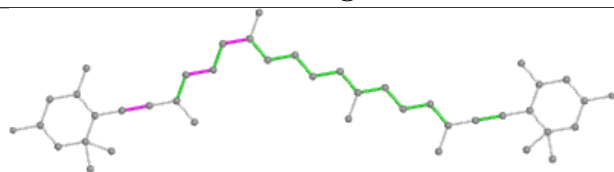
Rings

Ligand II0 N 615

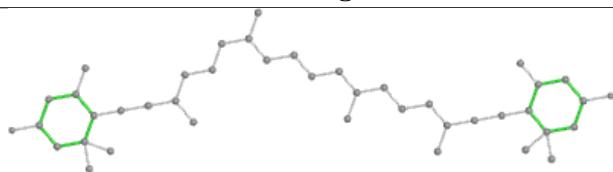
Bond lengths



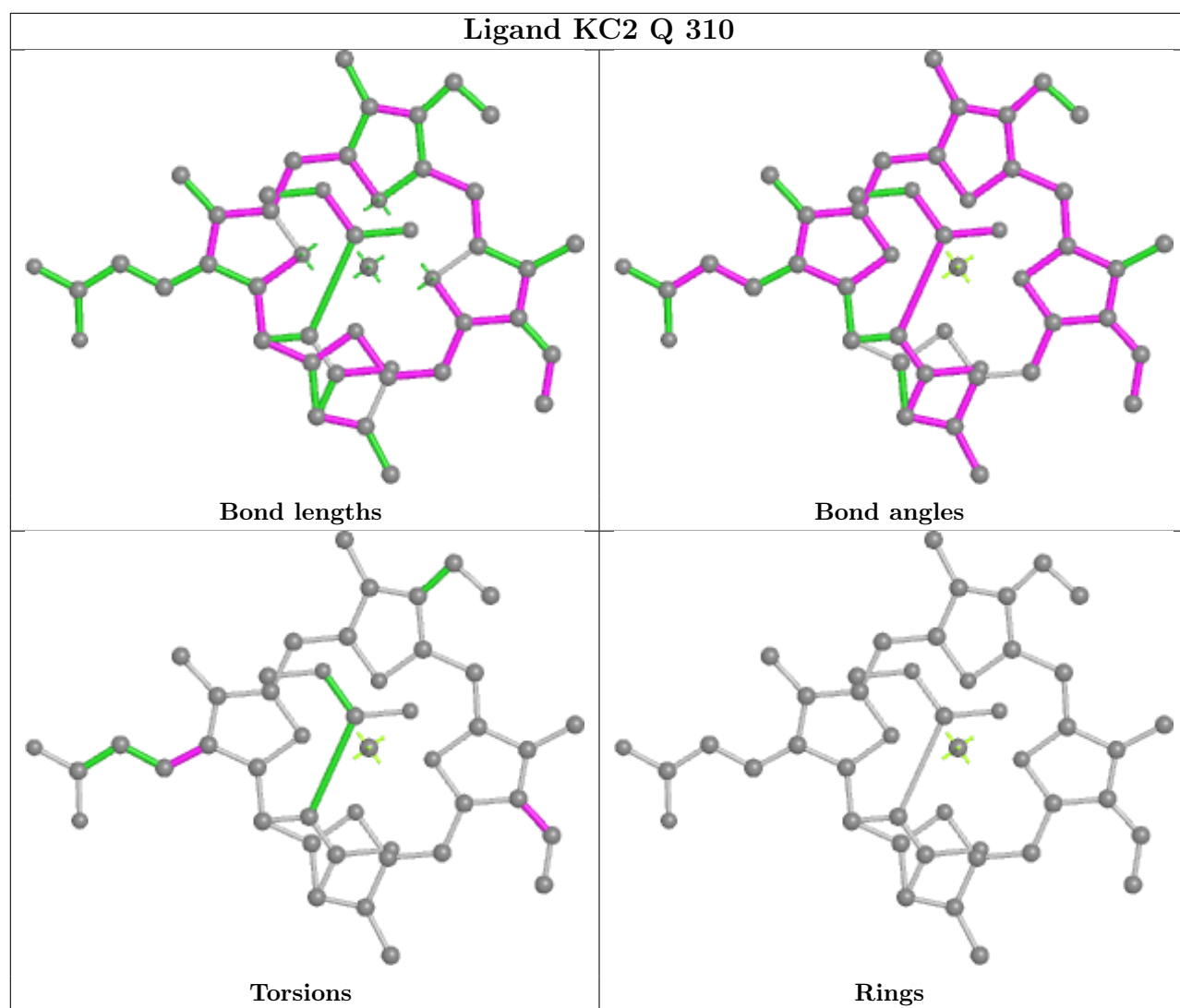
Bond angles



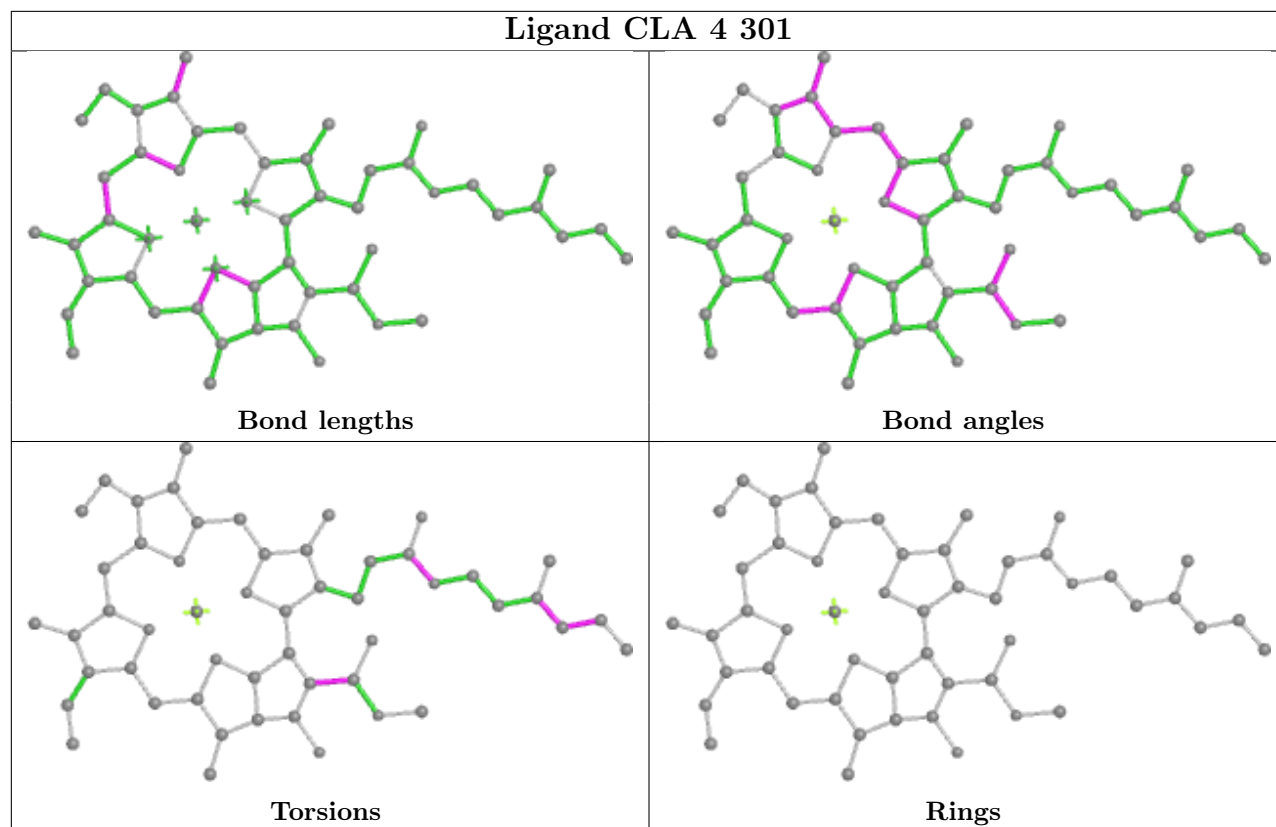
Torsions



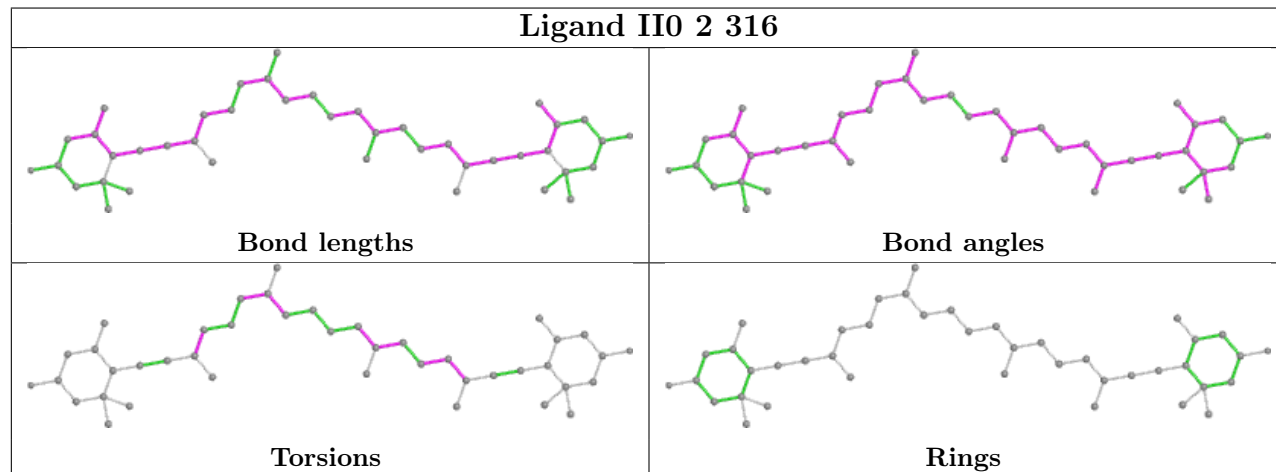
Rings



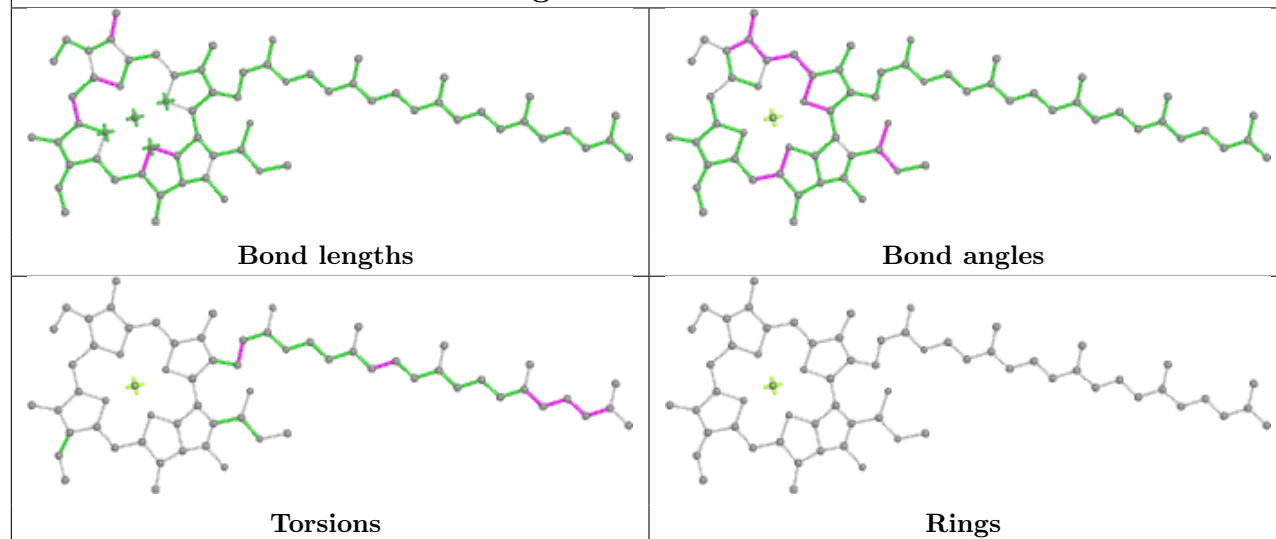
Ligand CLA 4 301



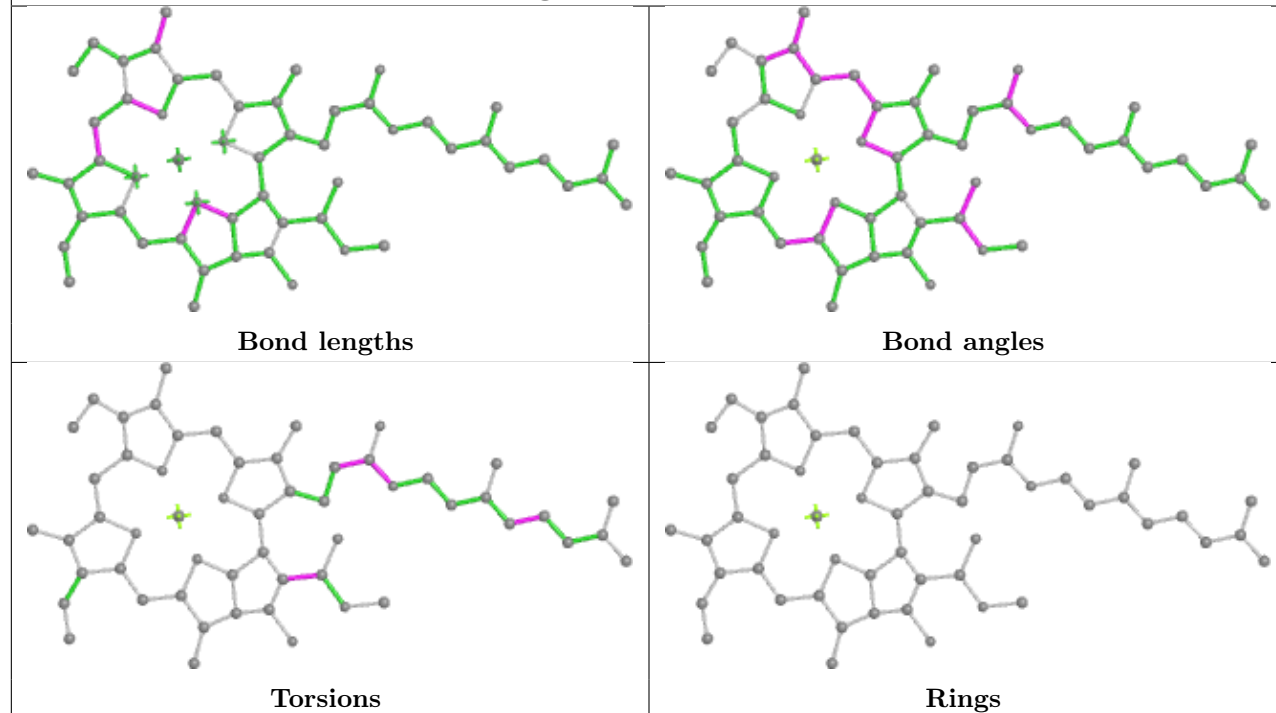
Ligand II0 2 316



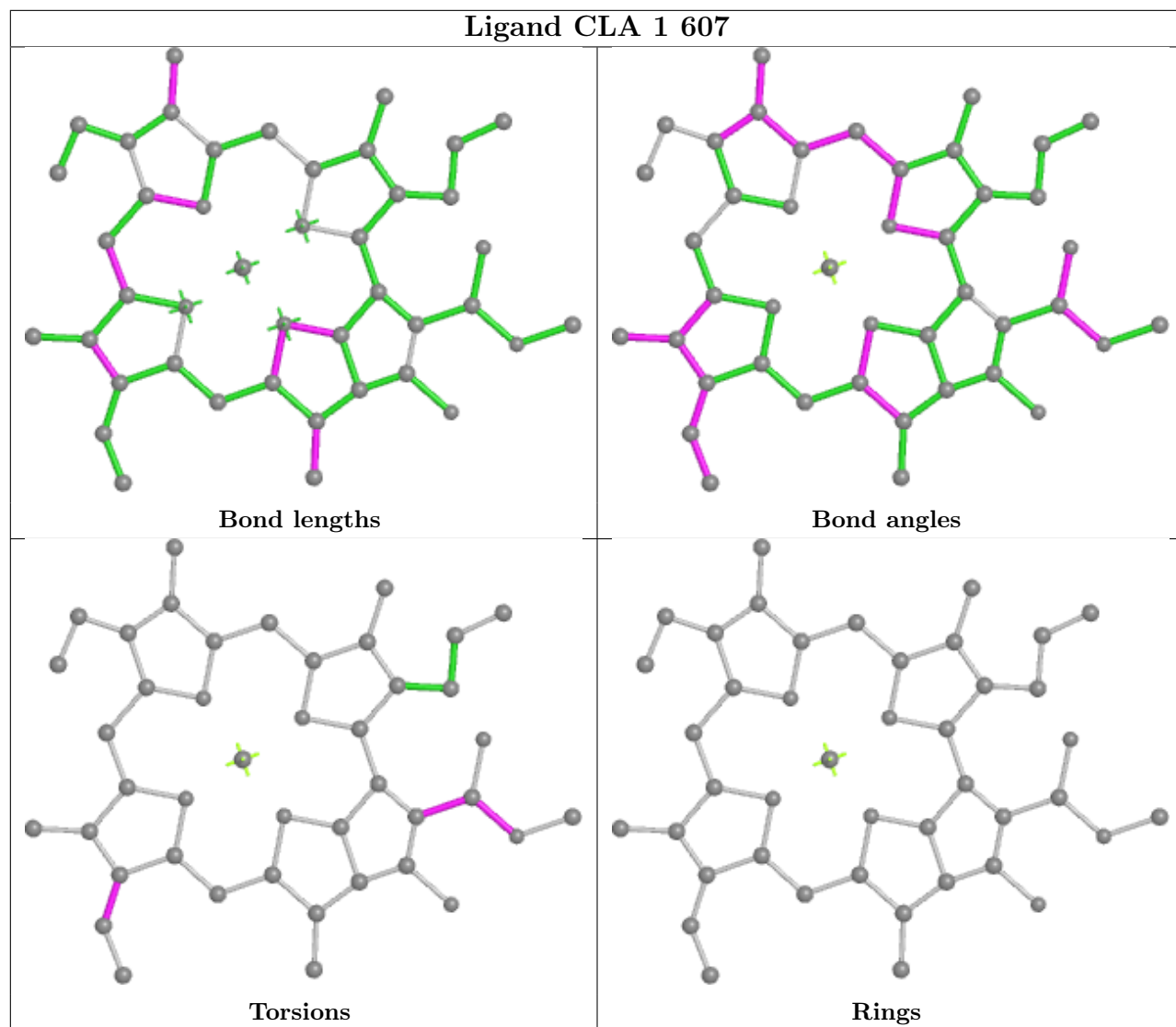
Ligand CLA C 508



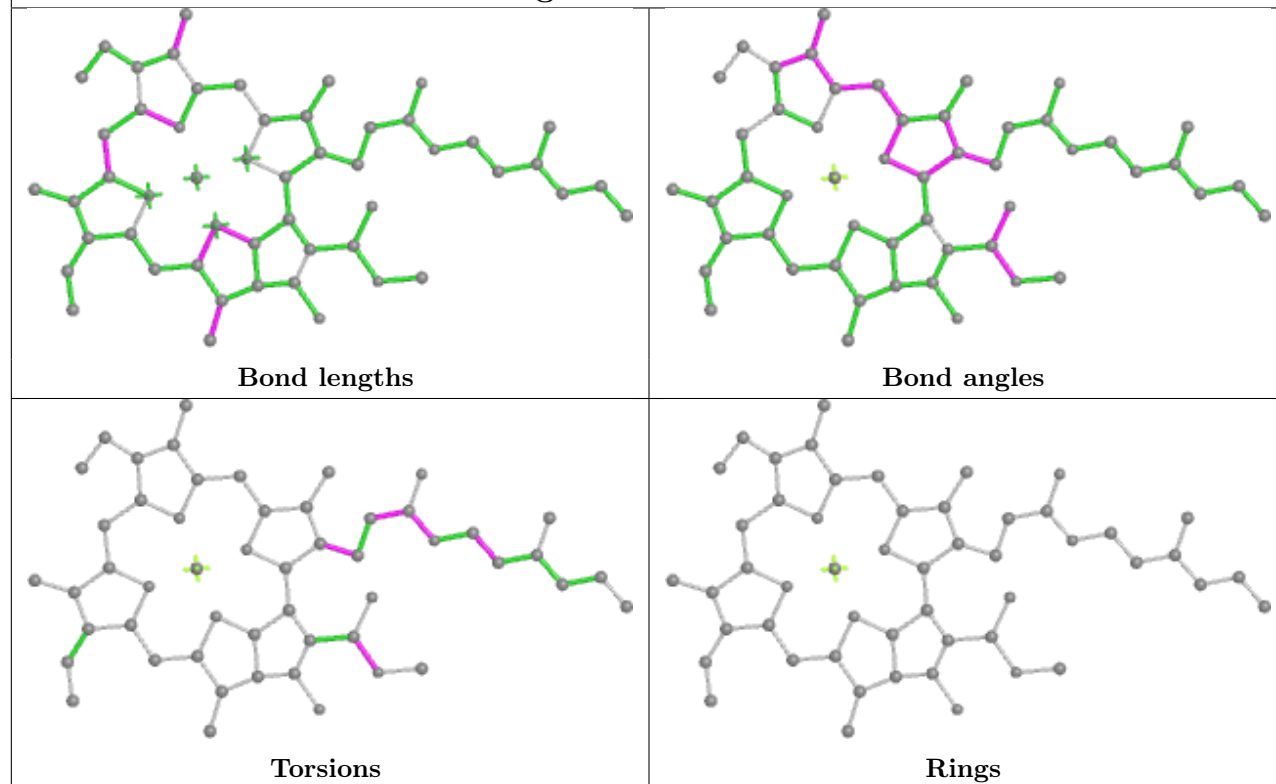
Ligand CLA 5 601



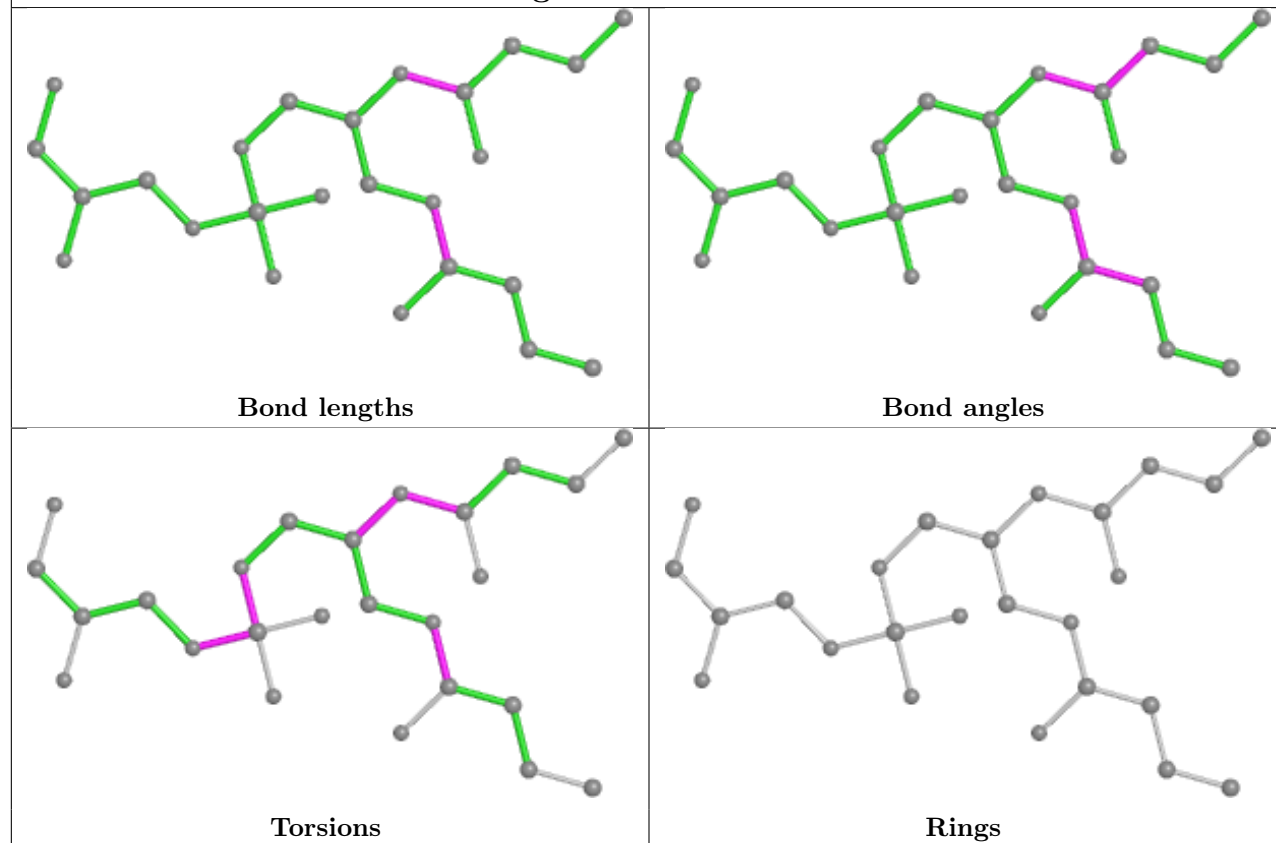
Ligand CLA 1 607

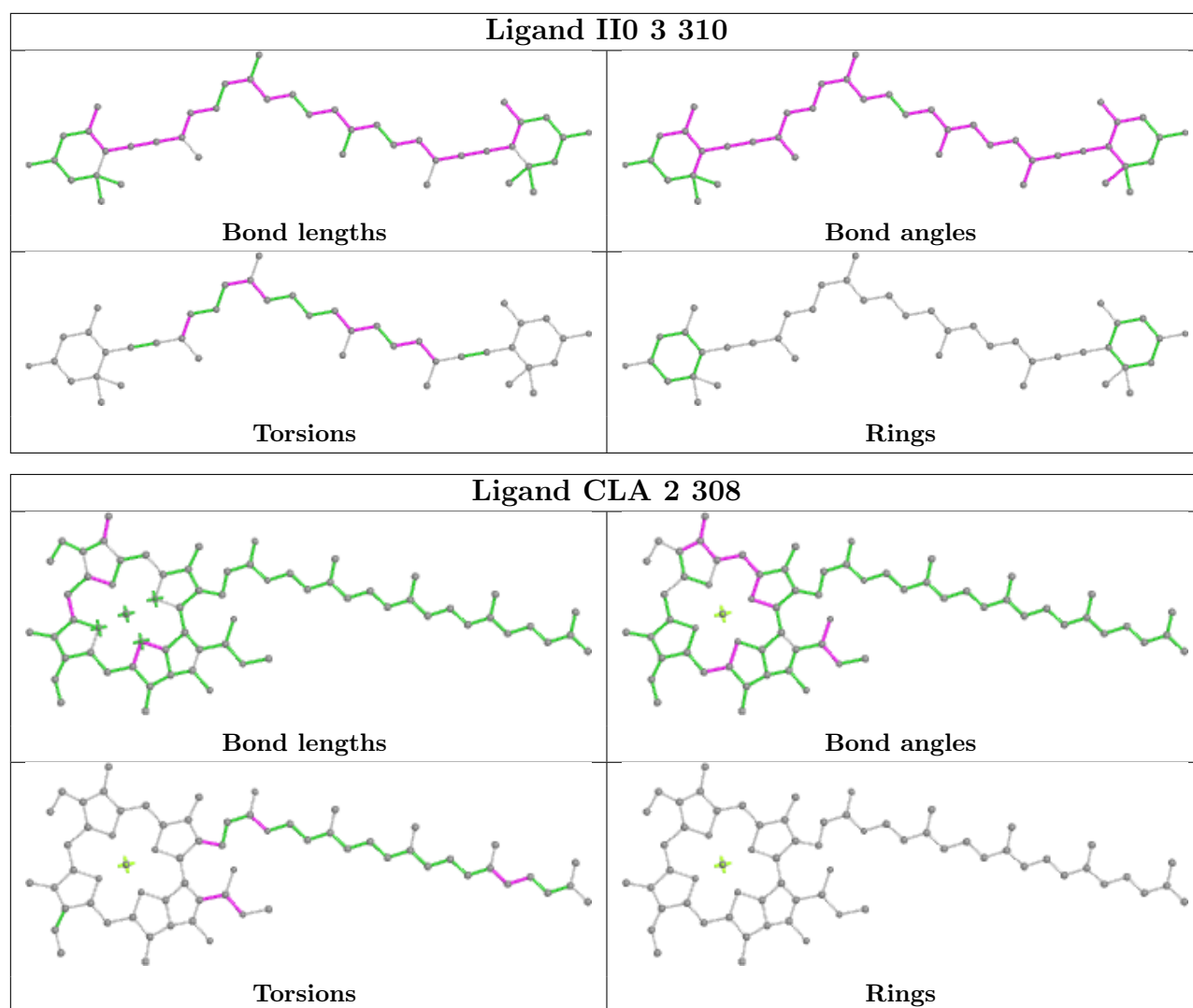


Ligand CLA 5 603

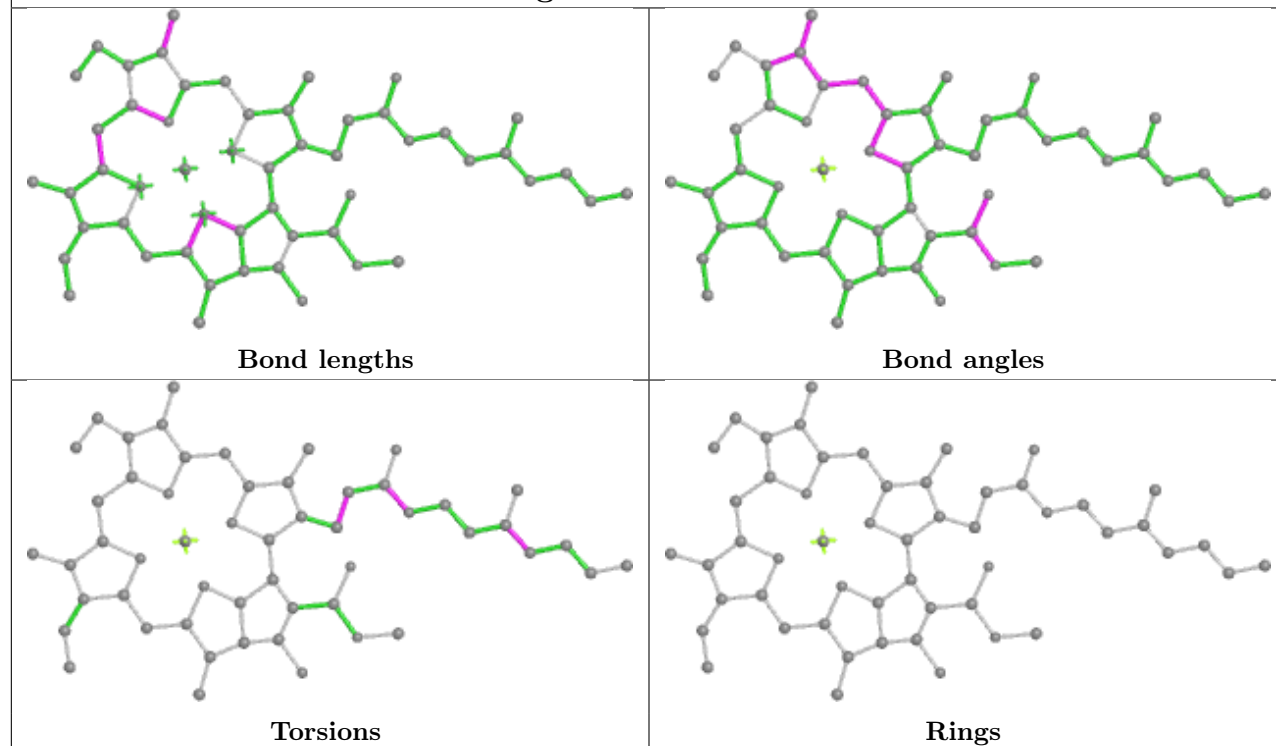


Ligand LHG Z 102

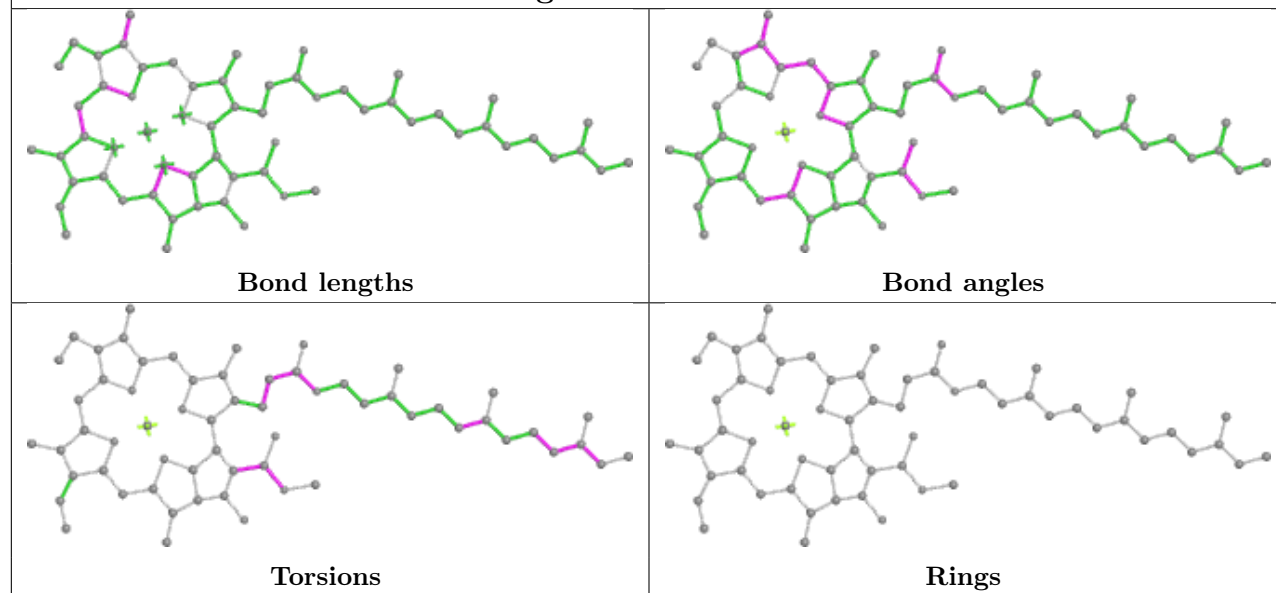




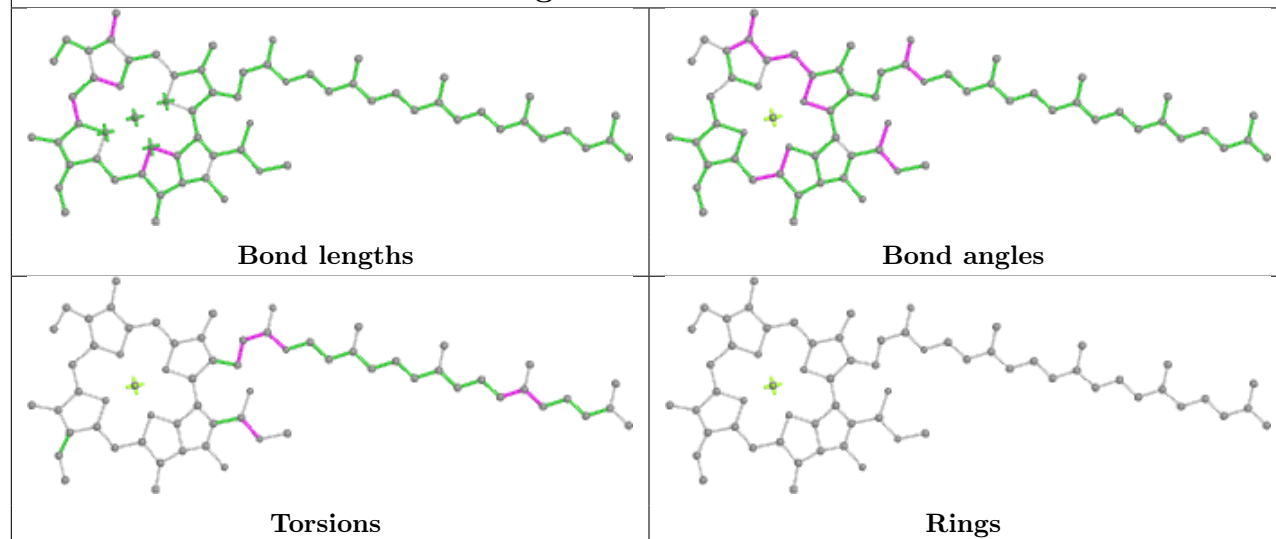
Ligand CLA 3 307



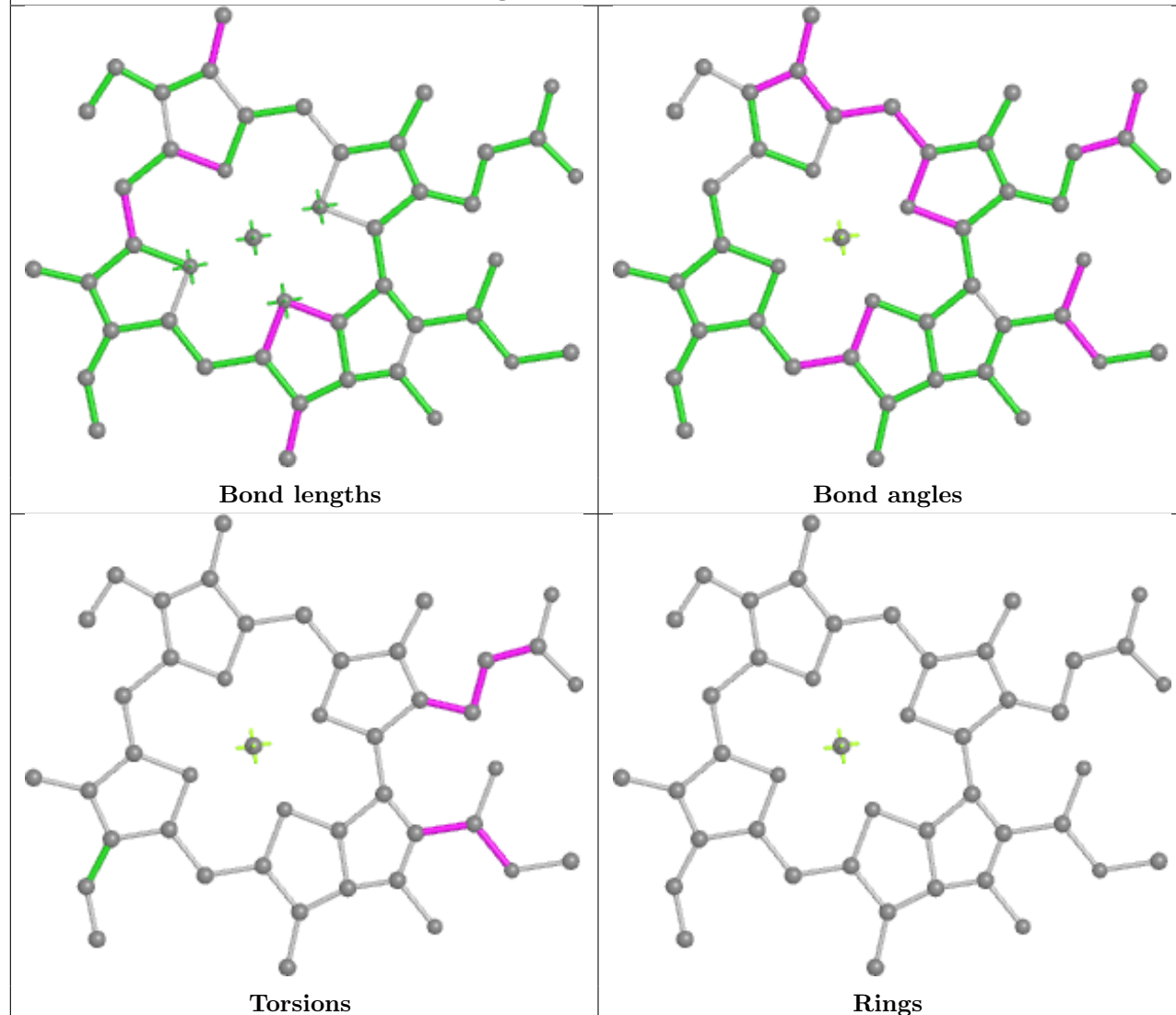
Ligand CLA 4 304

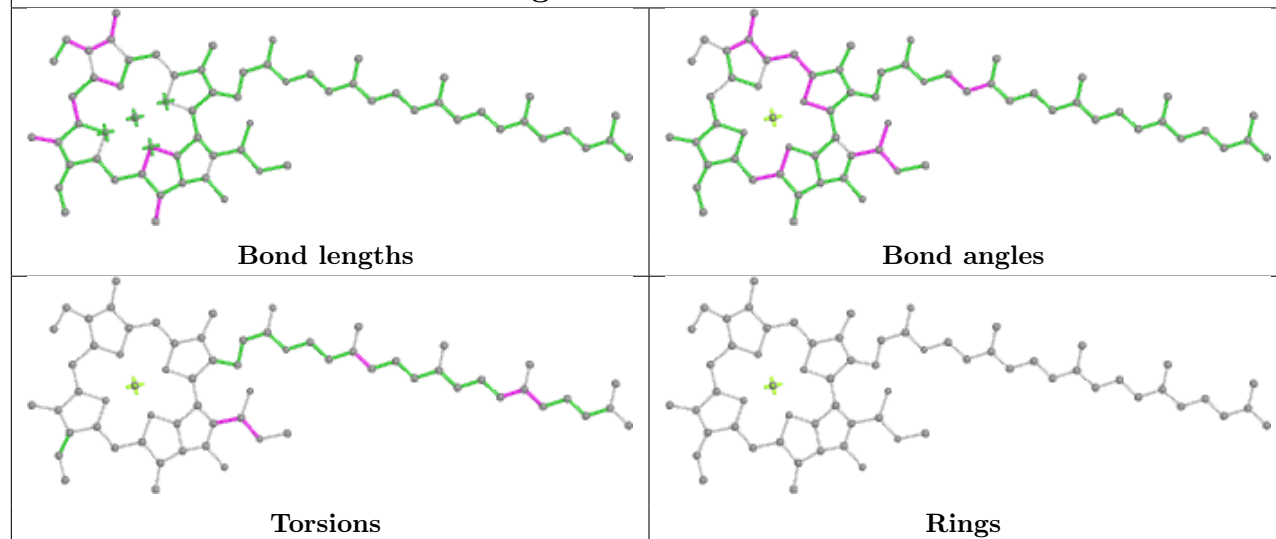
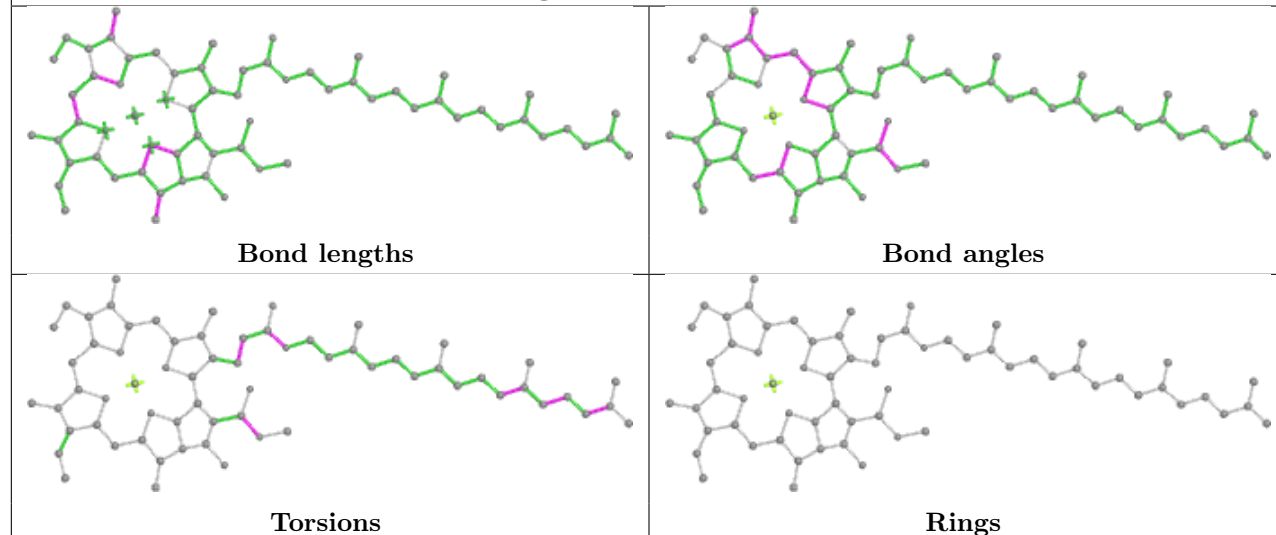
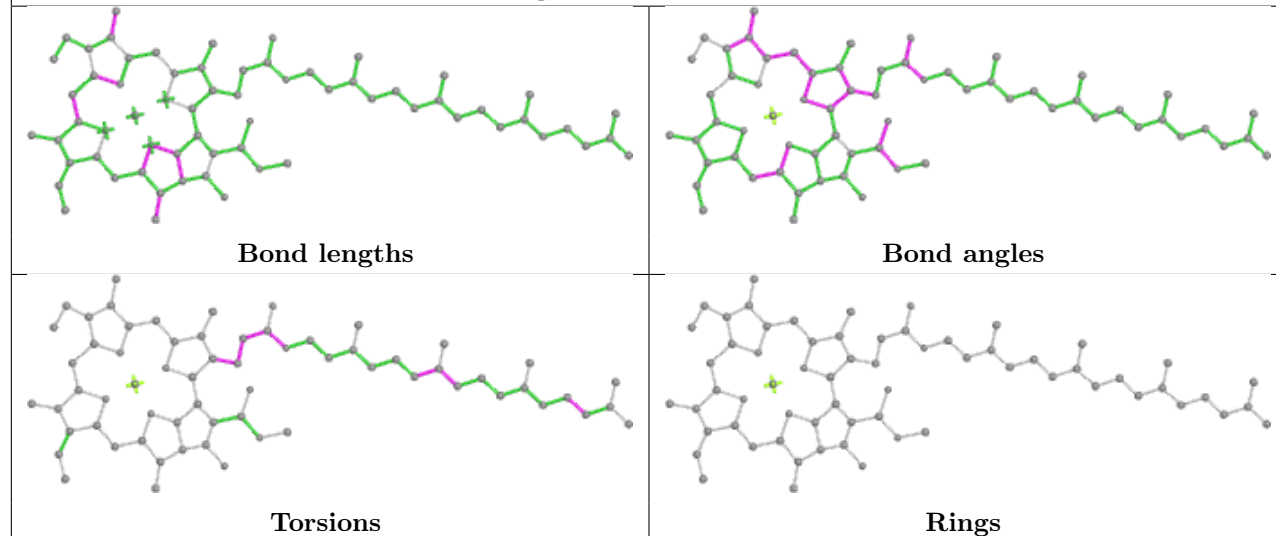


Ligand CLA b 610

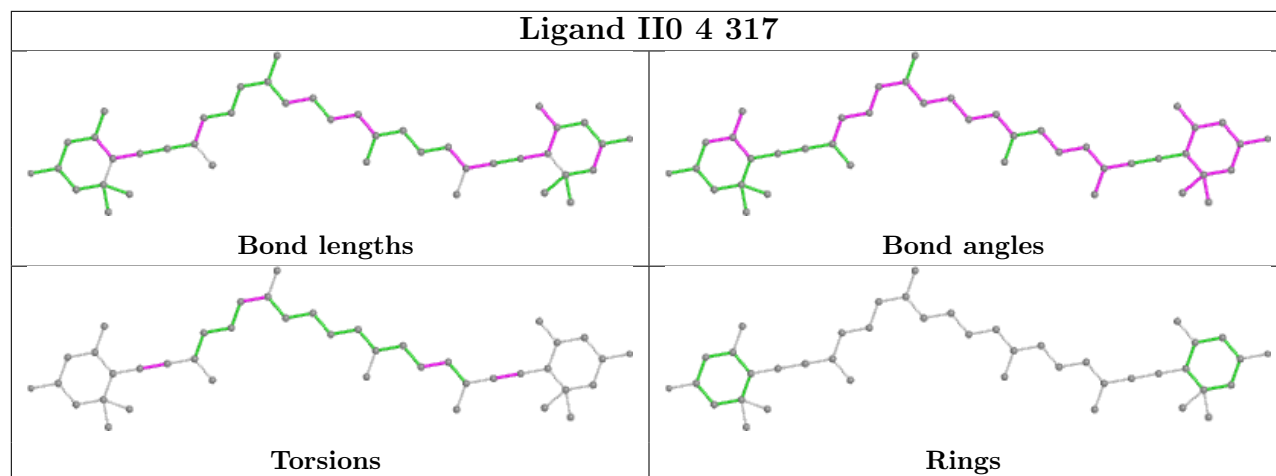


Ligand CLA 3 309

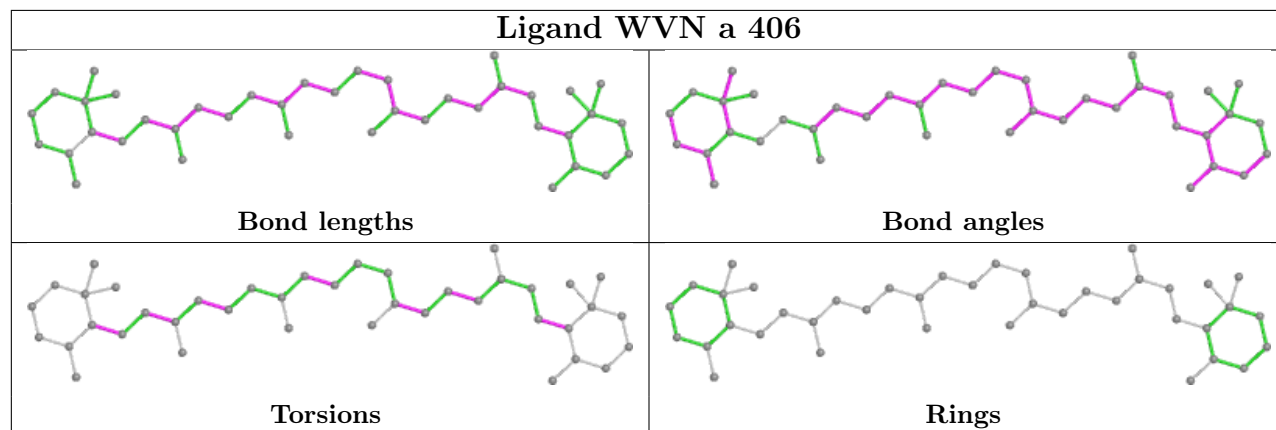


Ligand CLA R 308**Ligand CLA S 610****Ligand CLA B 612**

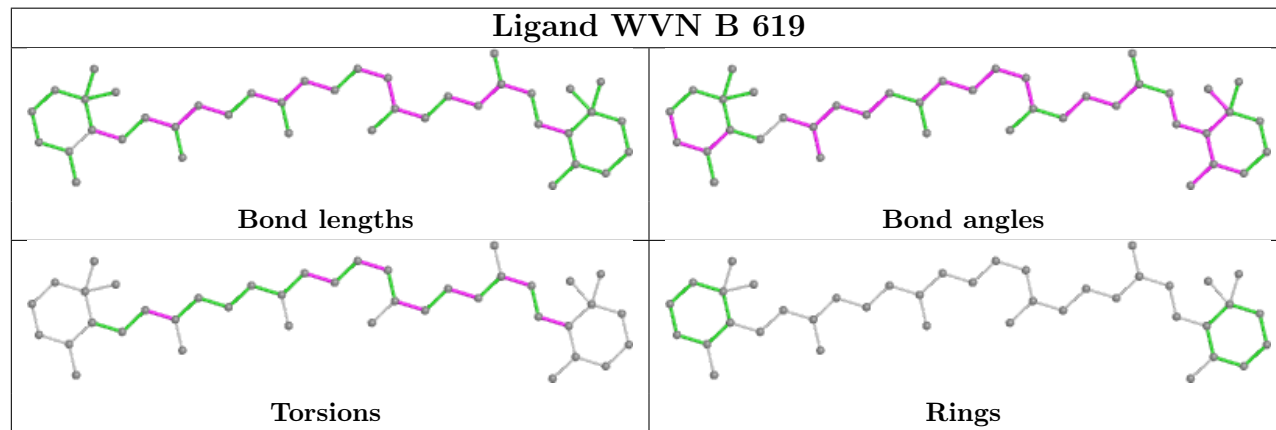
Ligand II0 4 317



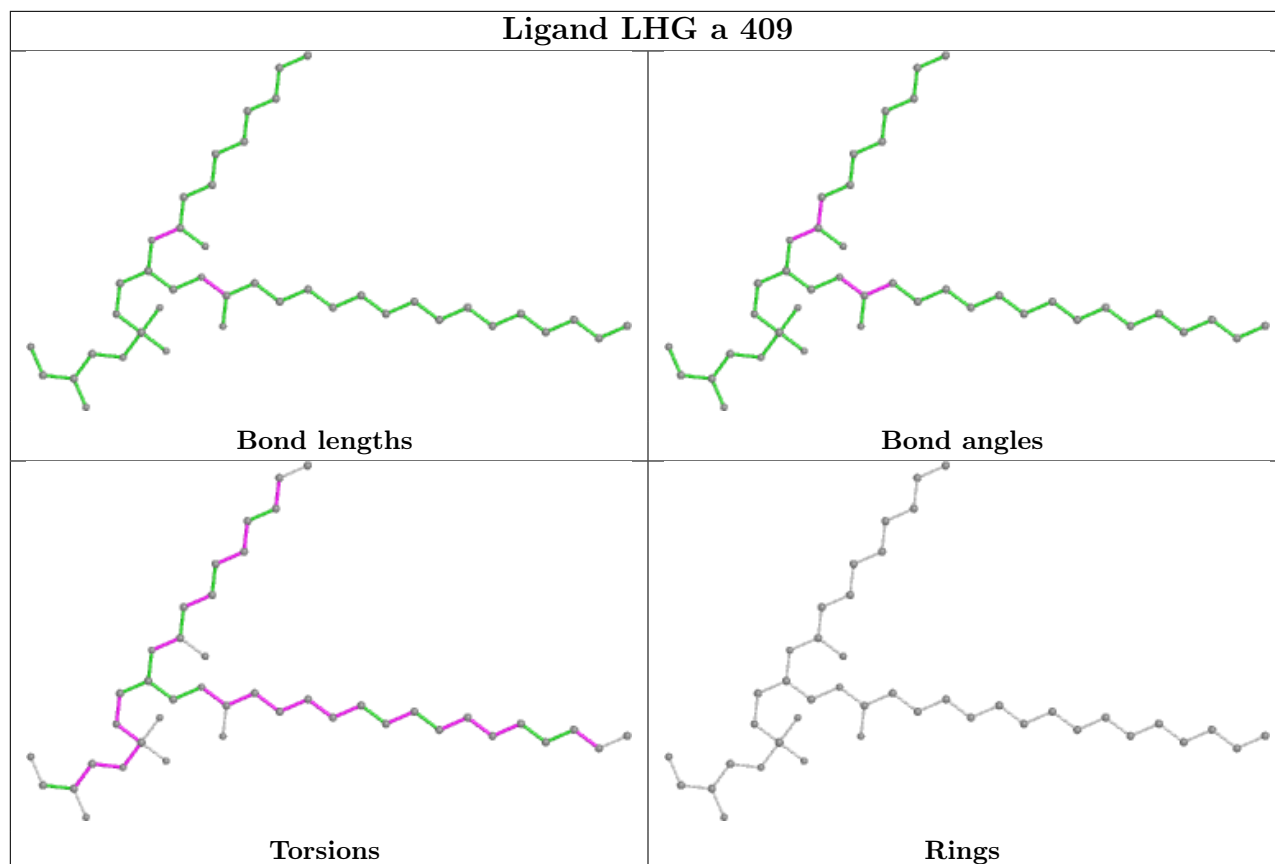
Ligand WVN a 406



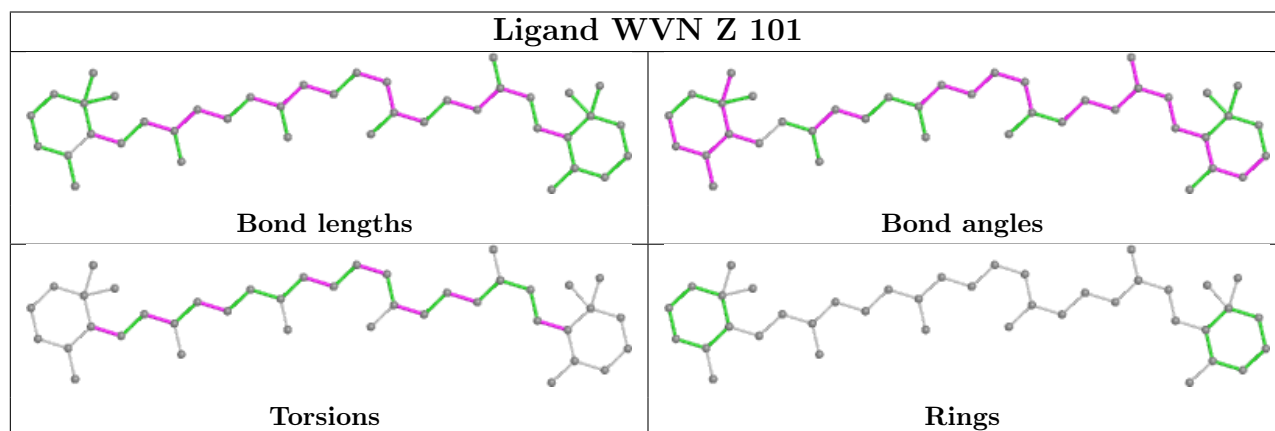
Ligand WVN B 619



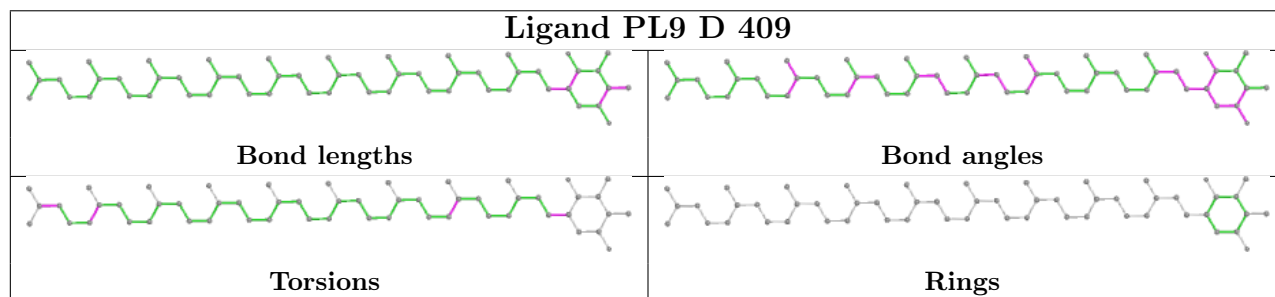
Ligand LHG a 409

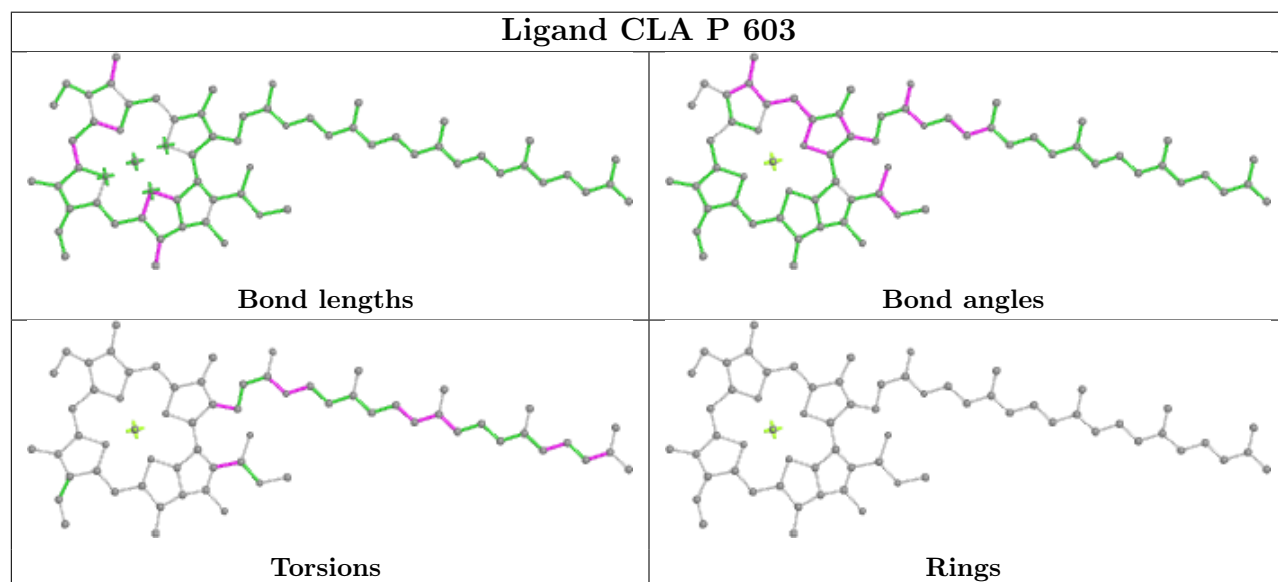
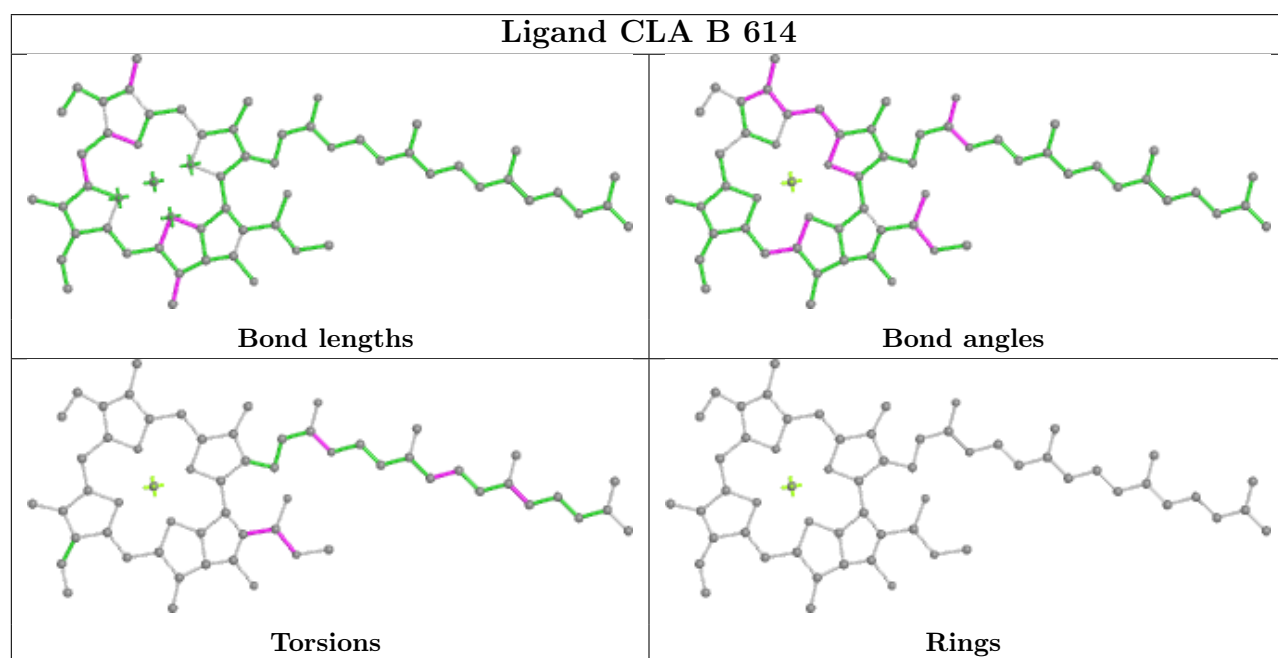
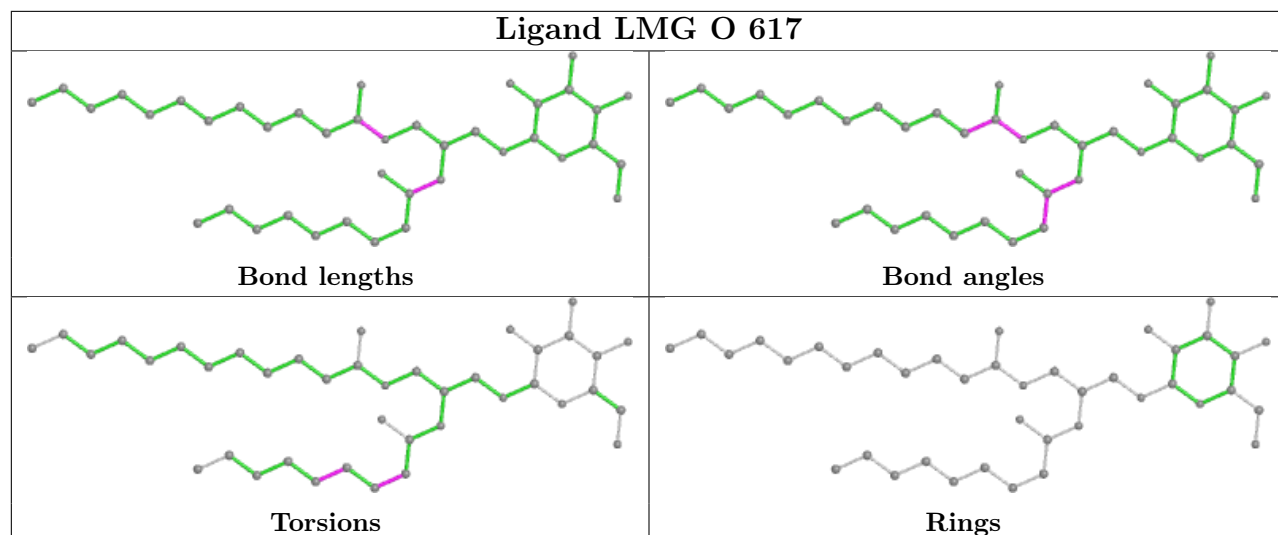


Ligand WVN Z 101

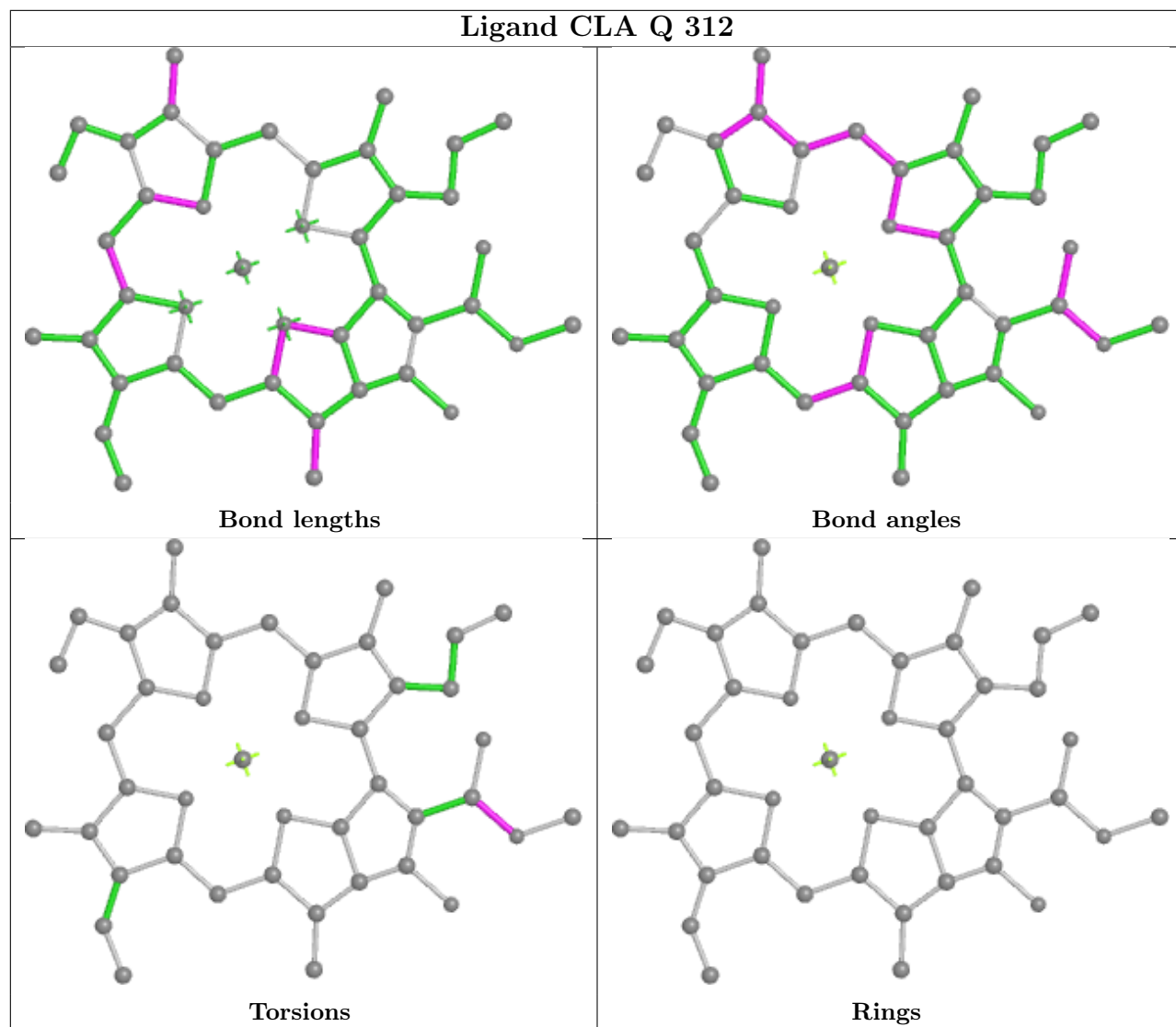


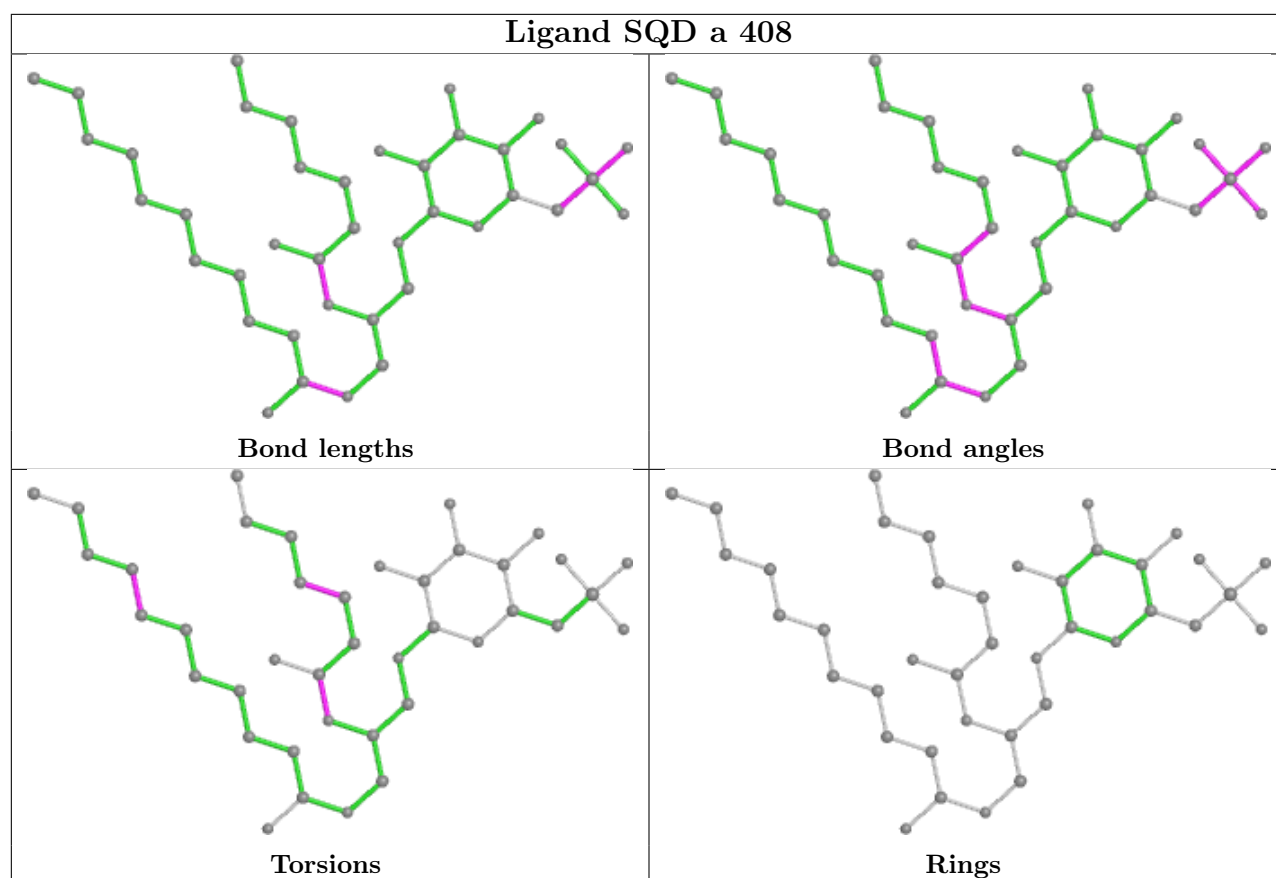
Ligand PL9 D 409



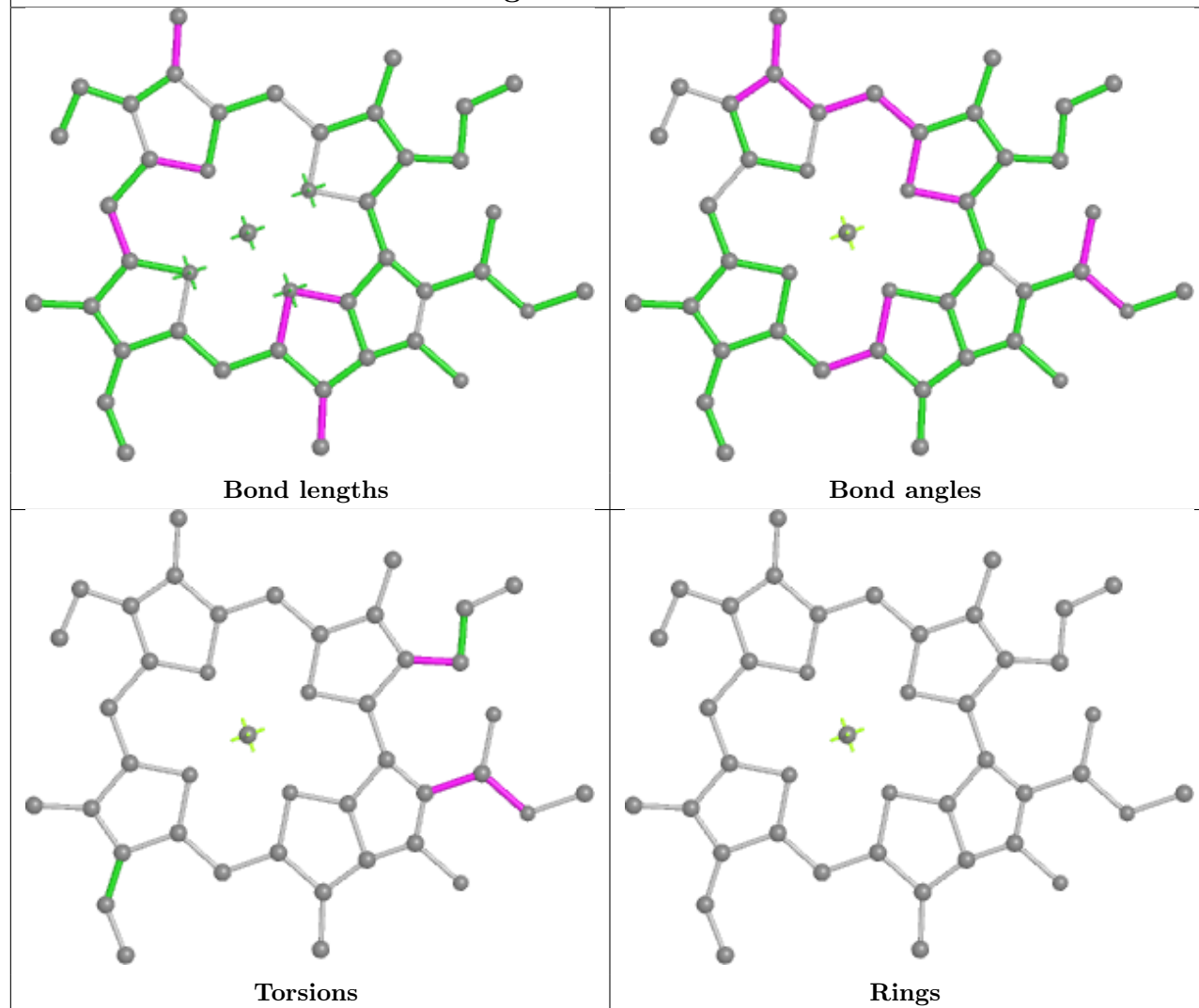


Ligand CLA Q 312

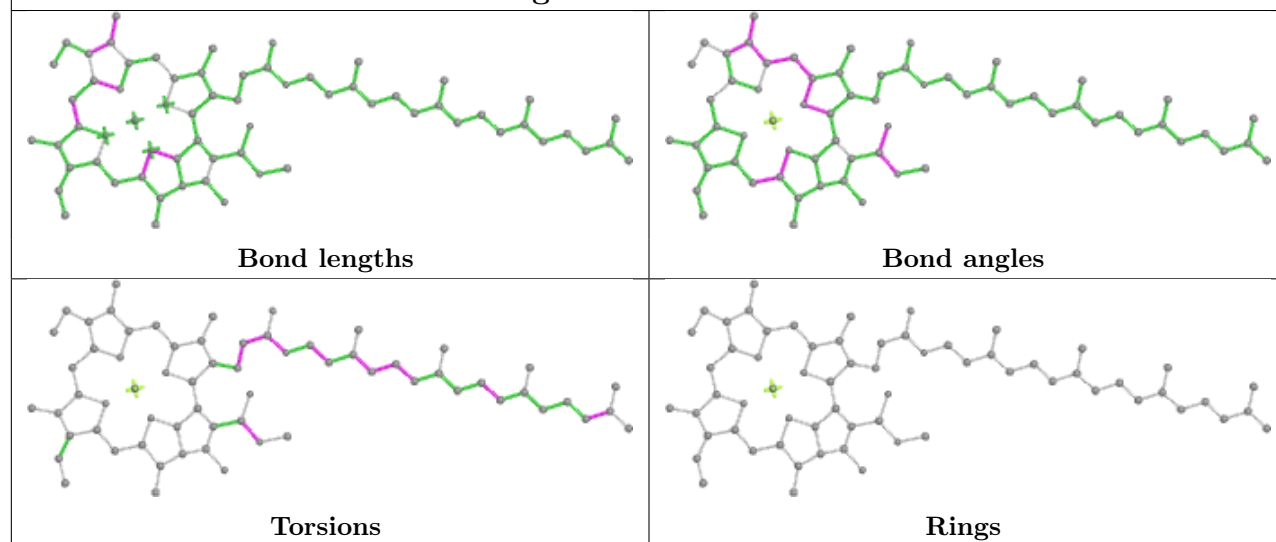


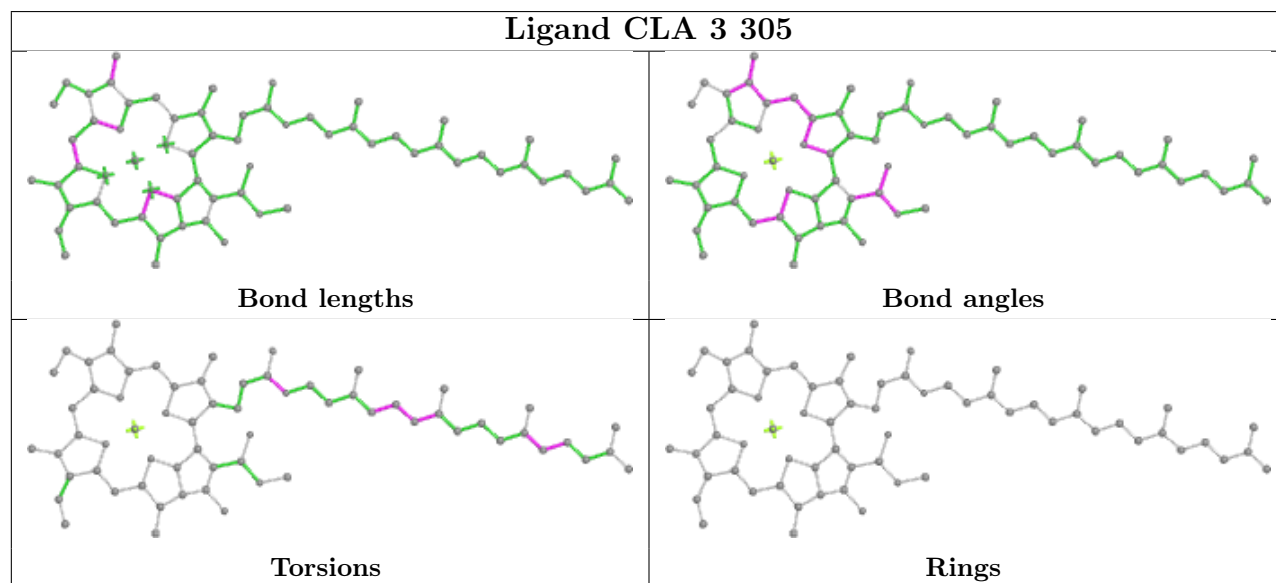
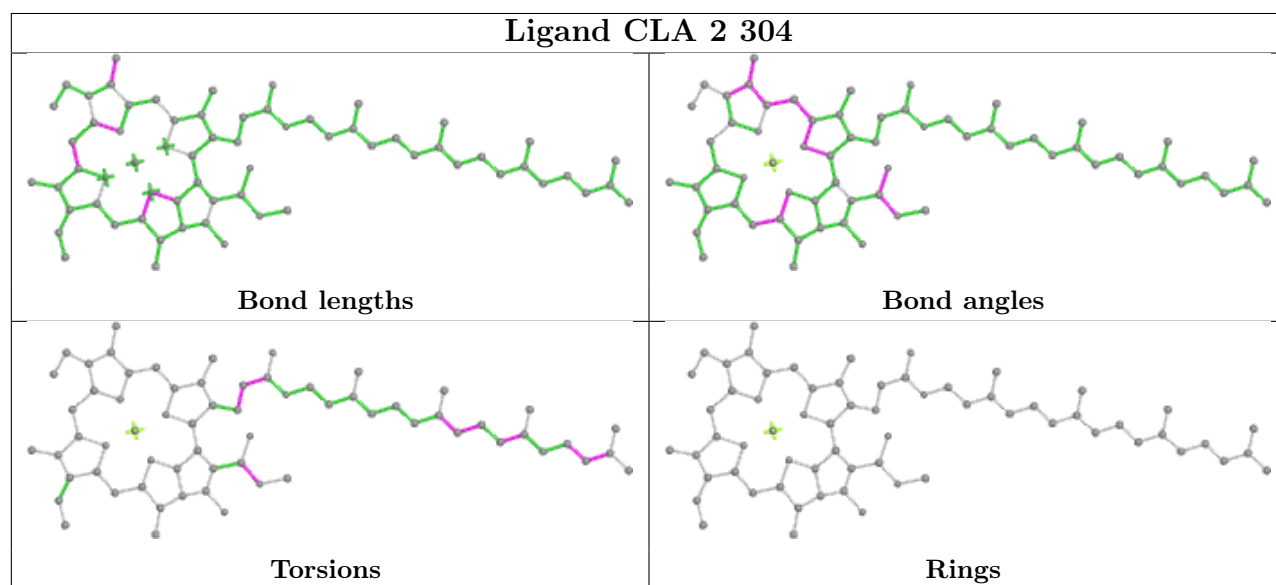
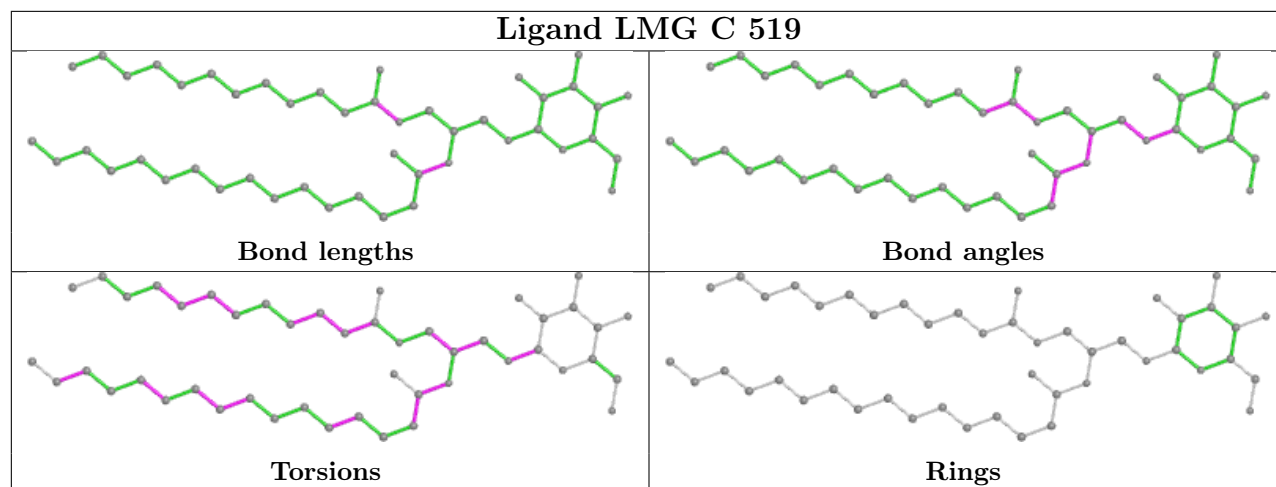


Ligand CLA 5 606

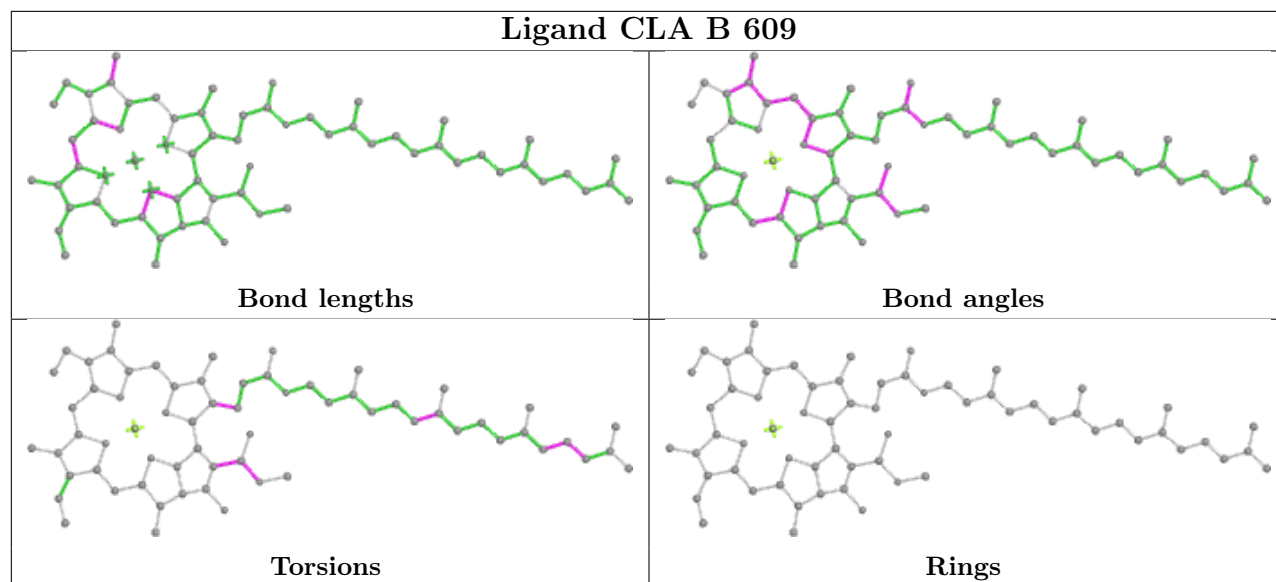


Ligand CLA B 613

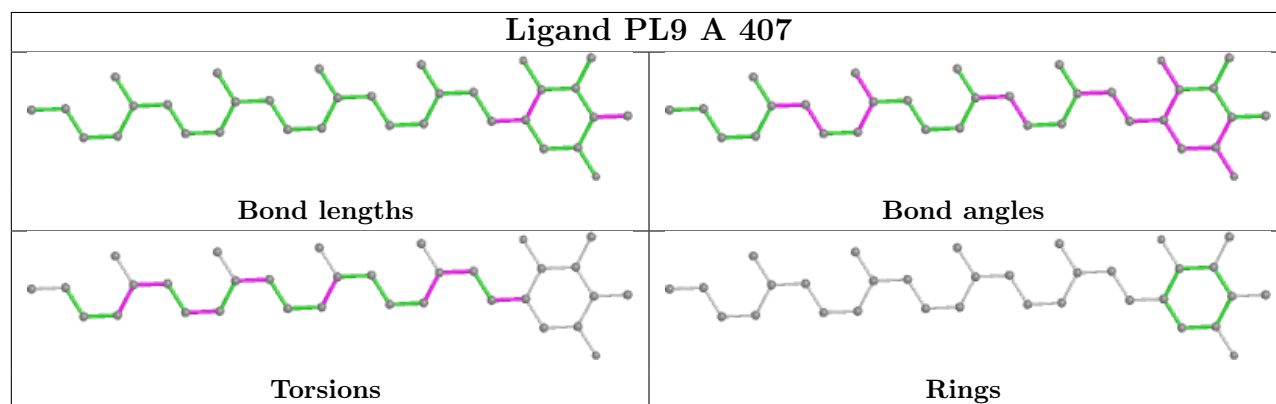




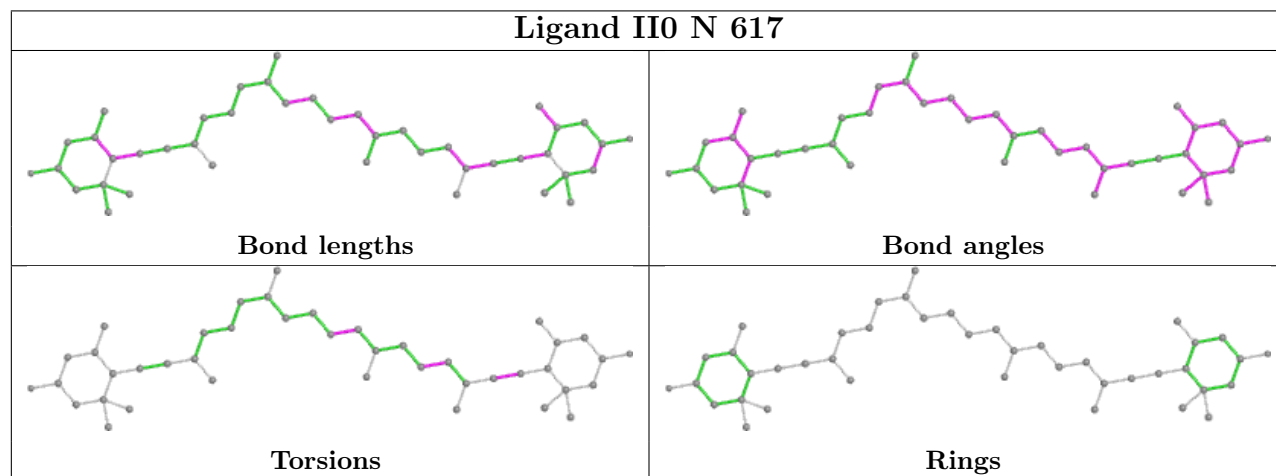
Ligand CLA B 609

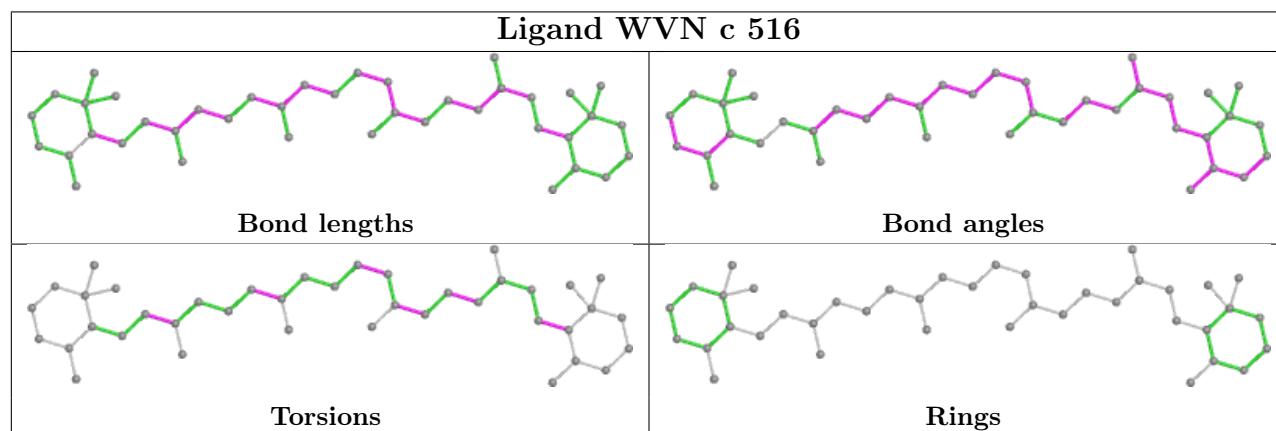
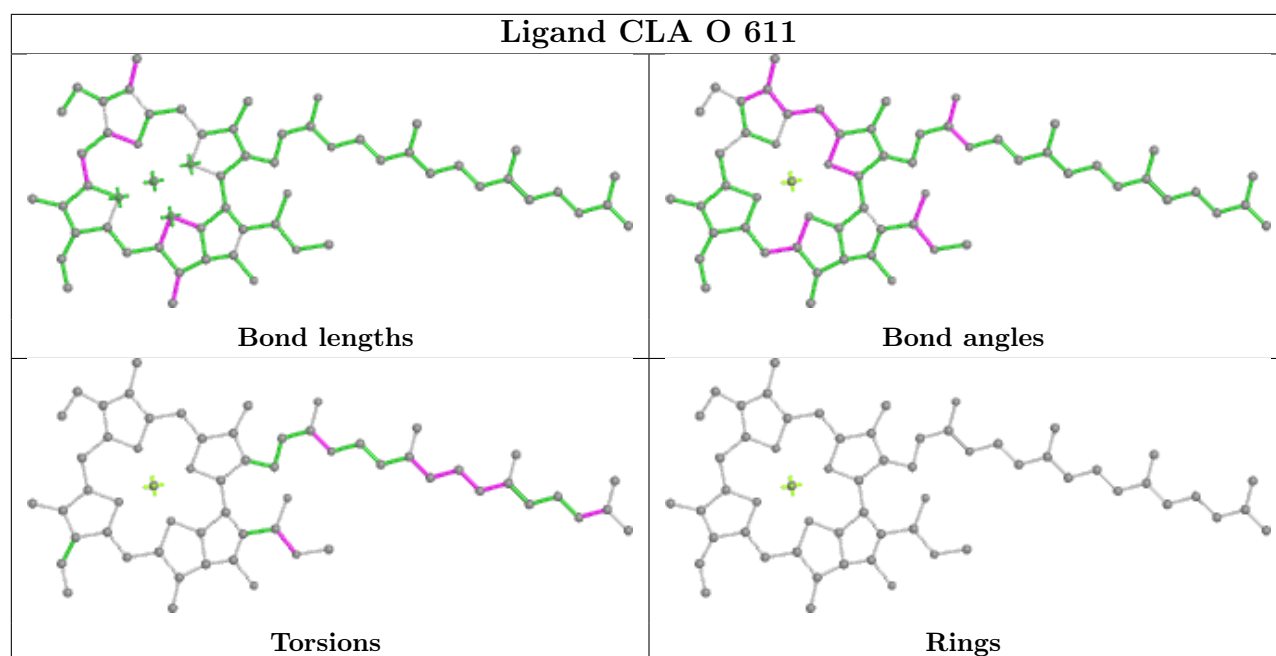


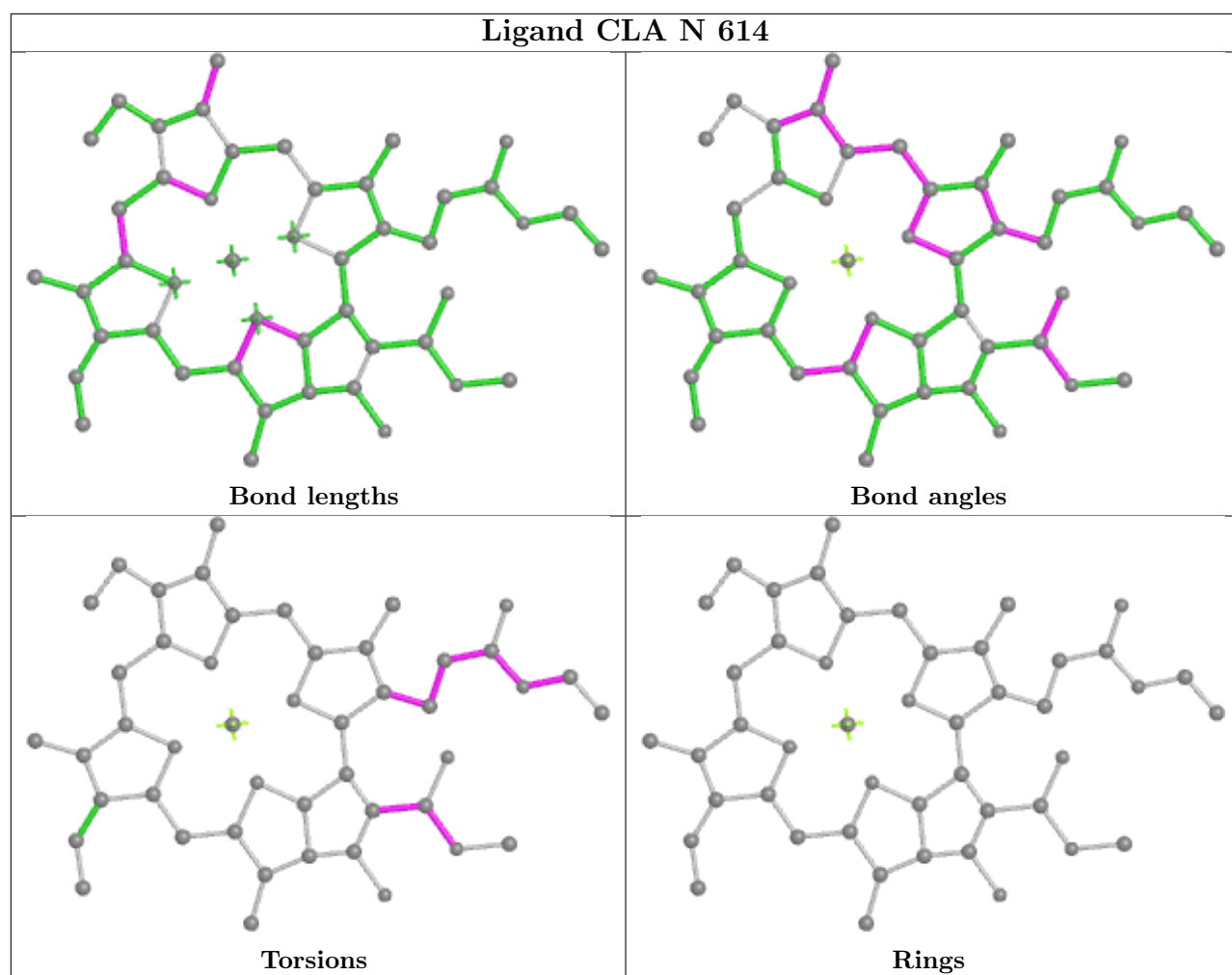
Ligand PL9 A 407



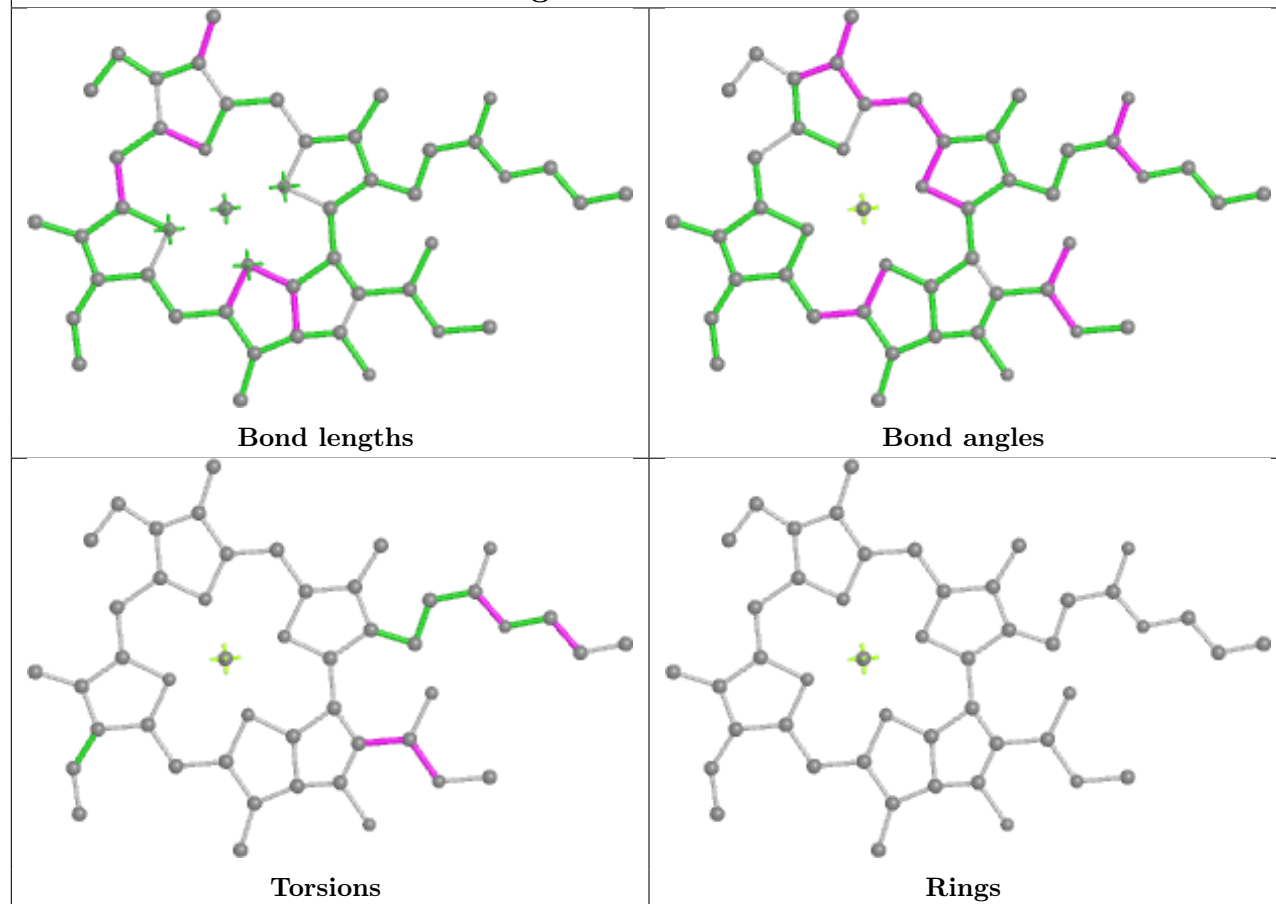
Ligand II0 N 617



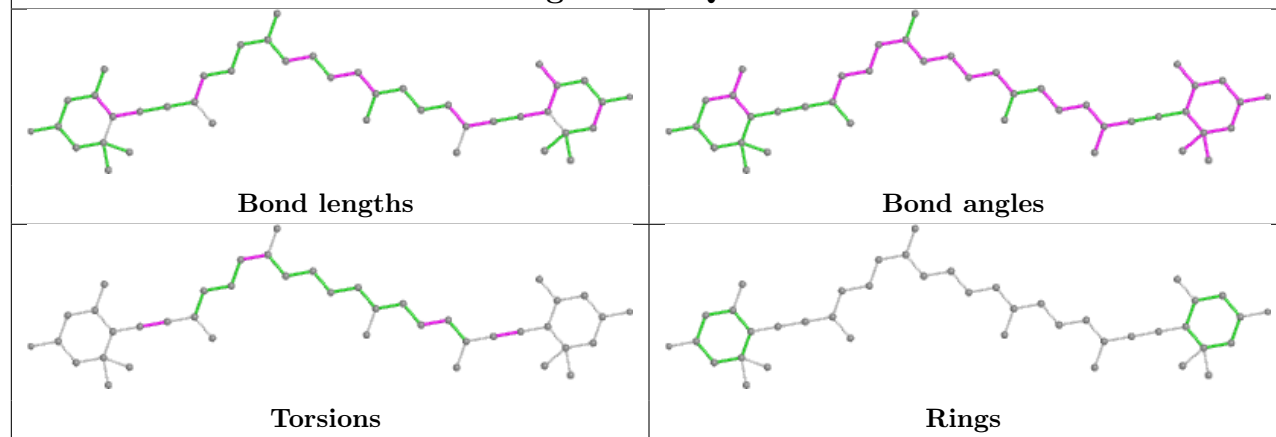




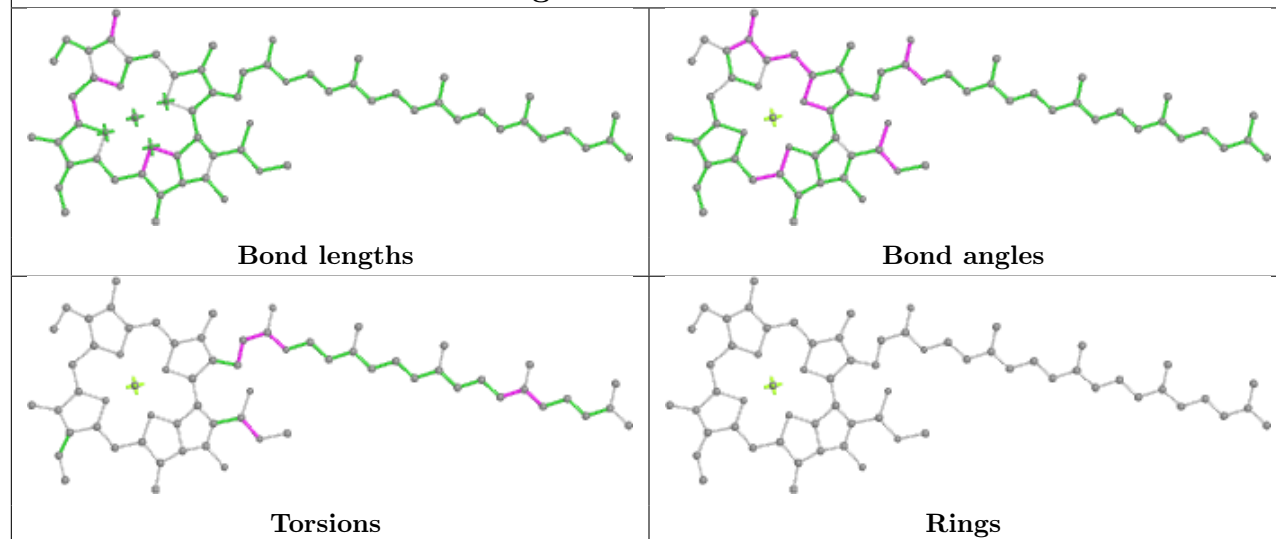
Ligand CLA N 613



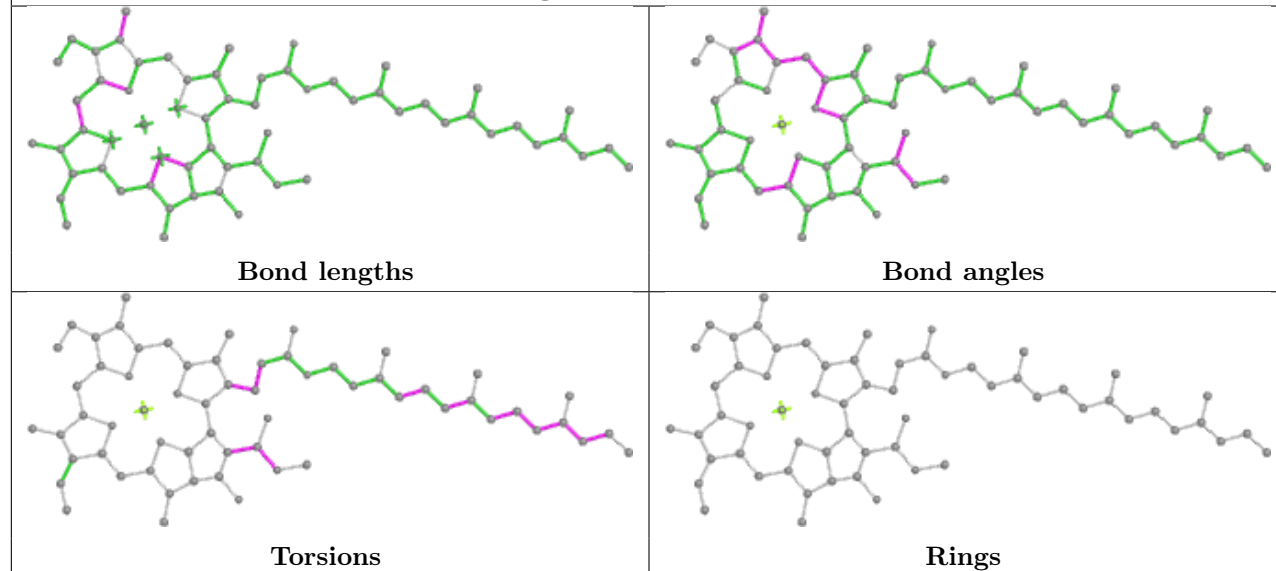
Ligand II0 Q 316



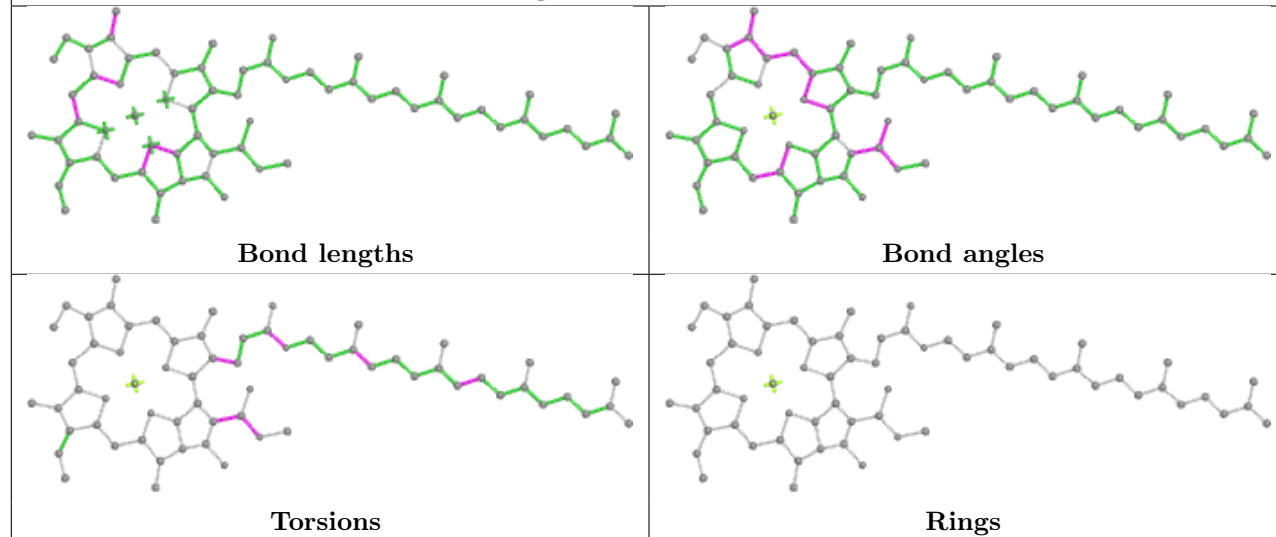
Ligand CLA B 610



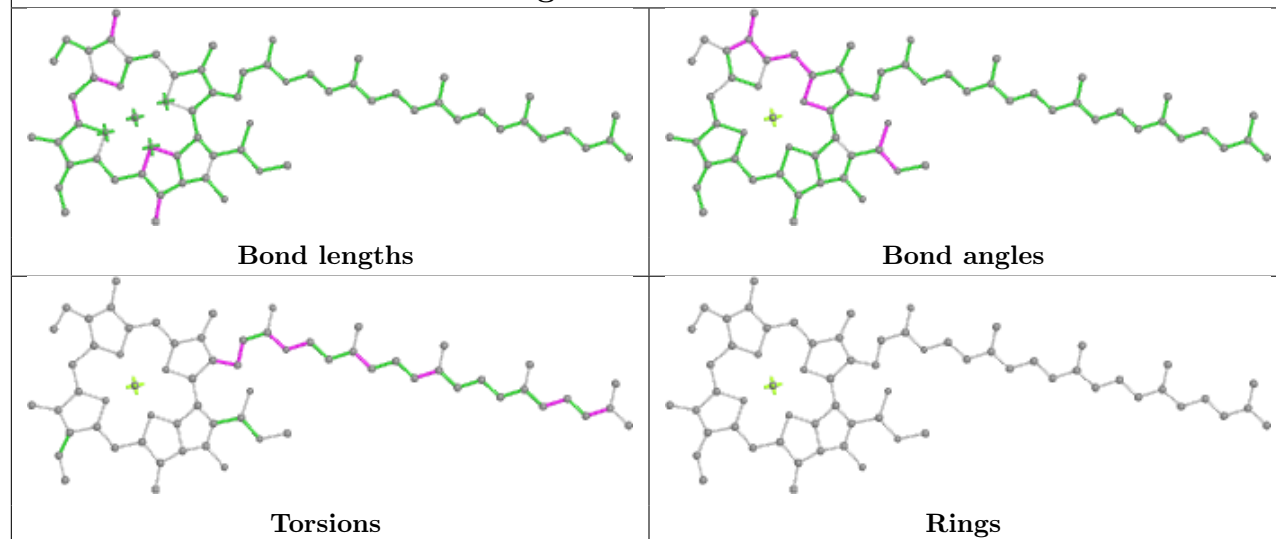
Ligand CLA 3 301



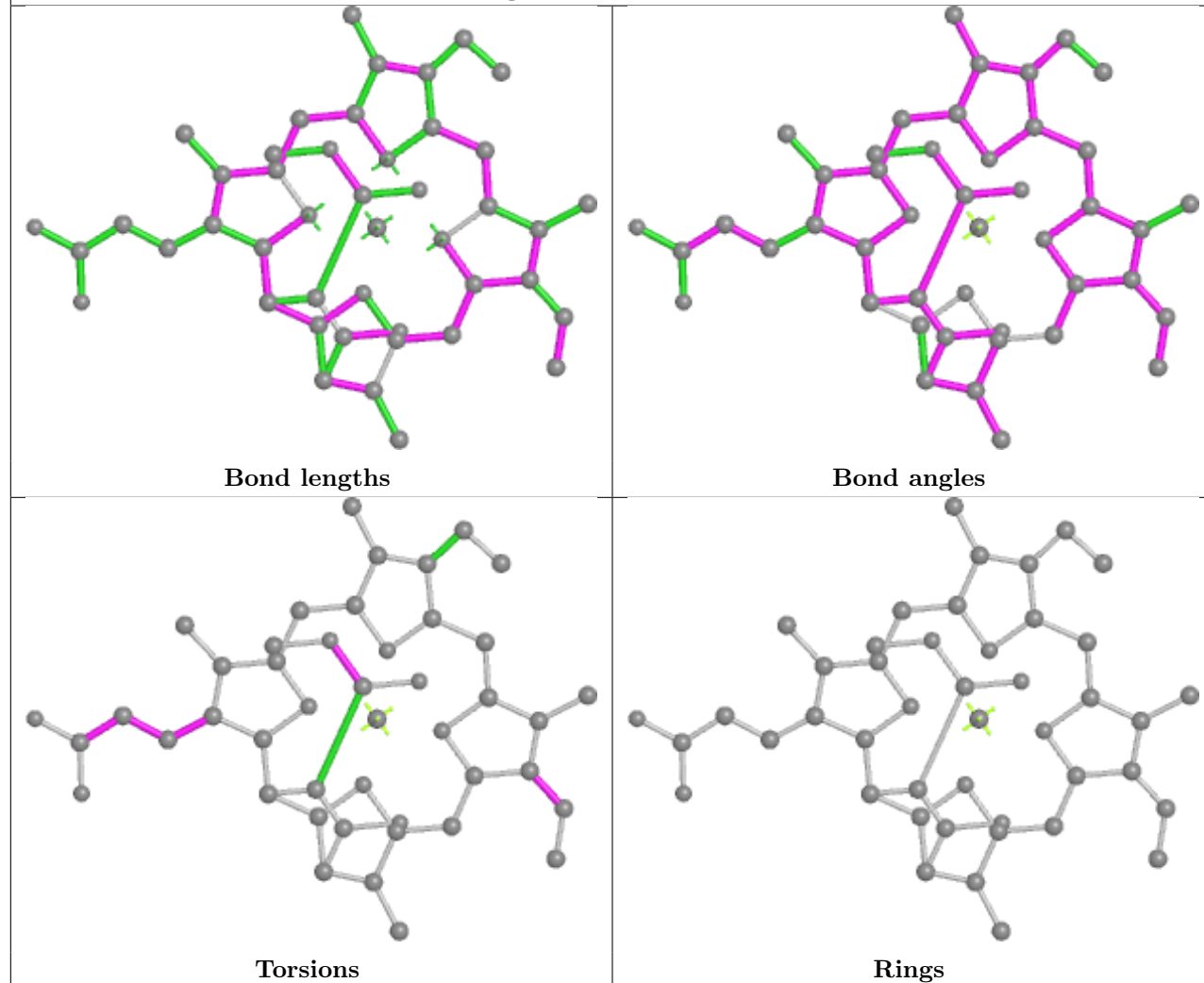
Ligand CLA C 512

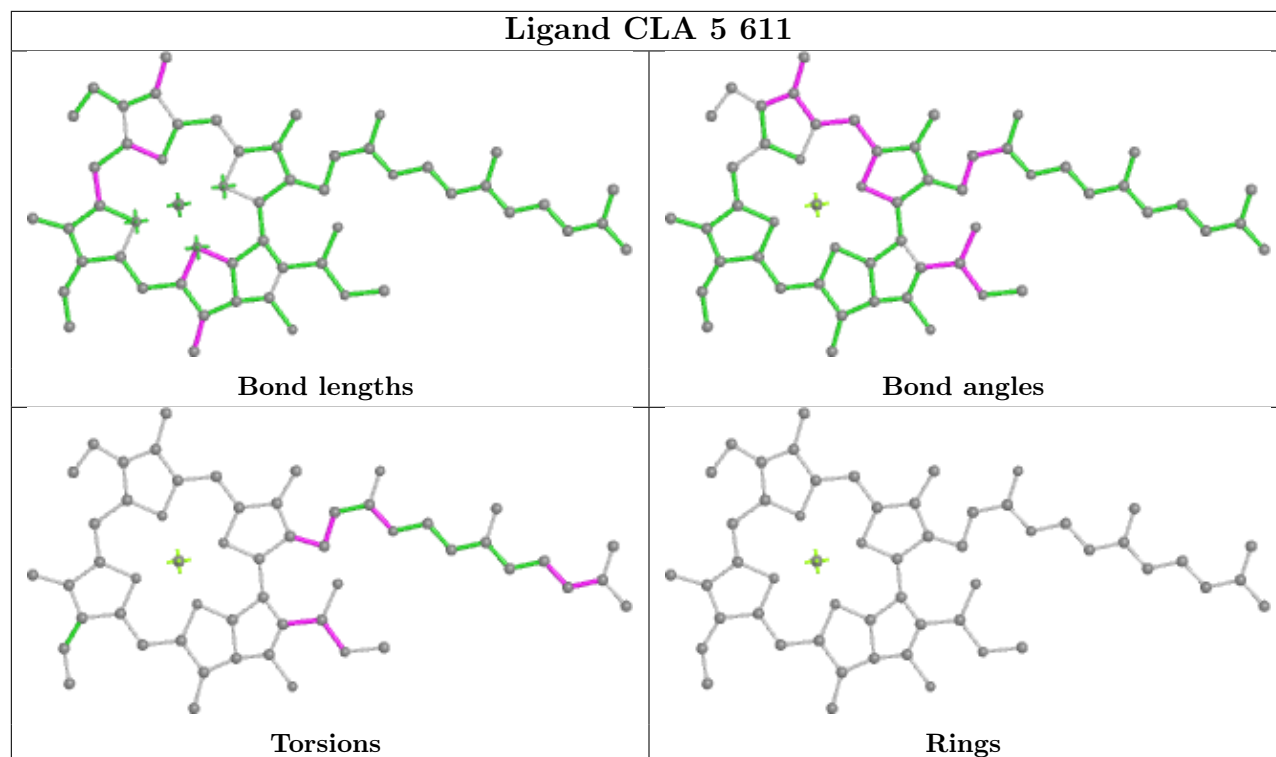
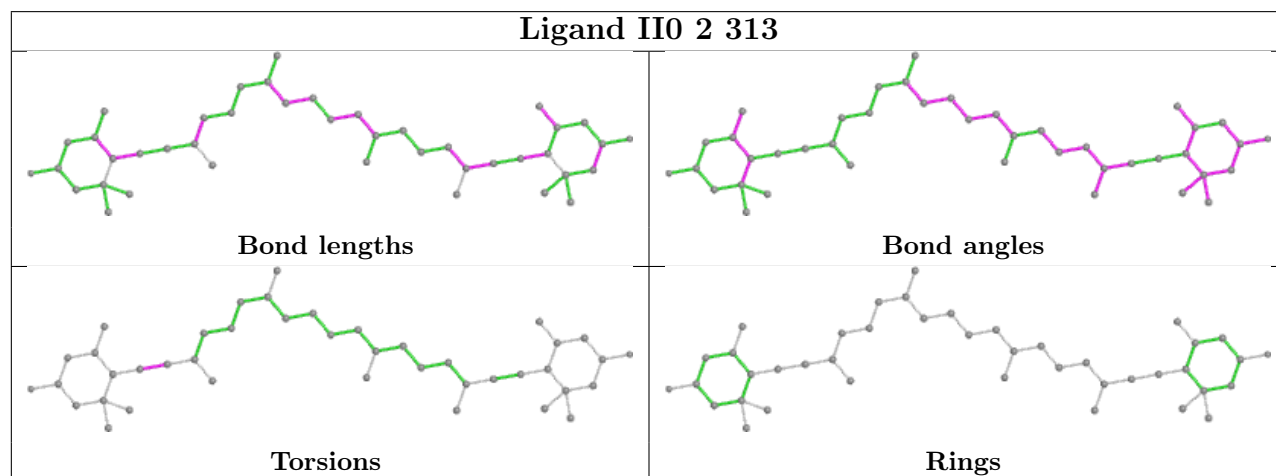


Ligand CLA c 511

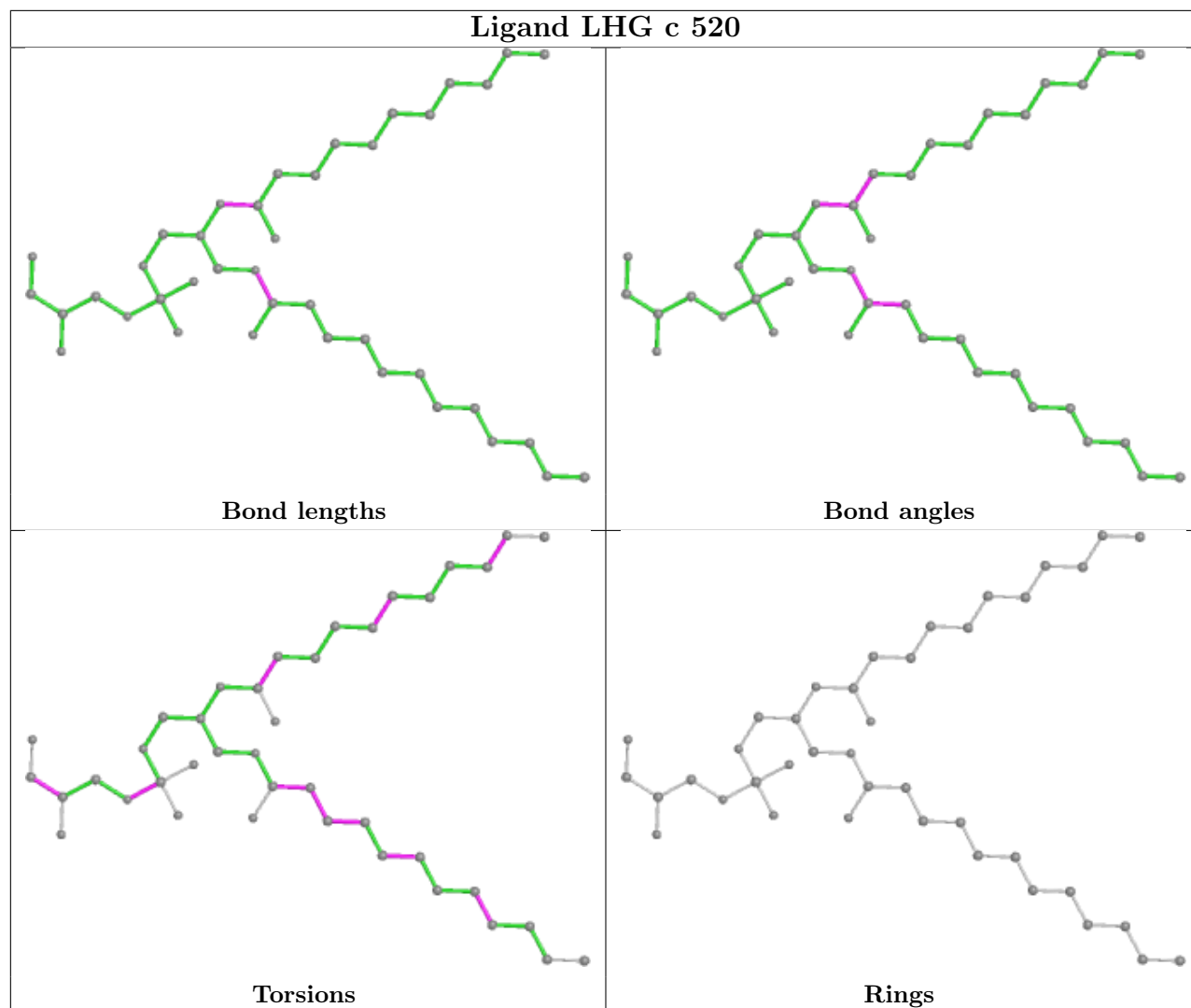


Ligand KC2 R 311

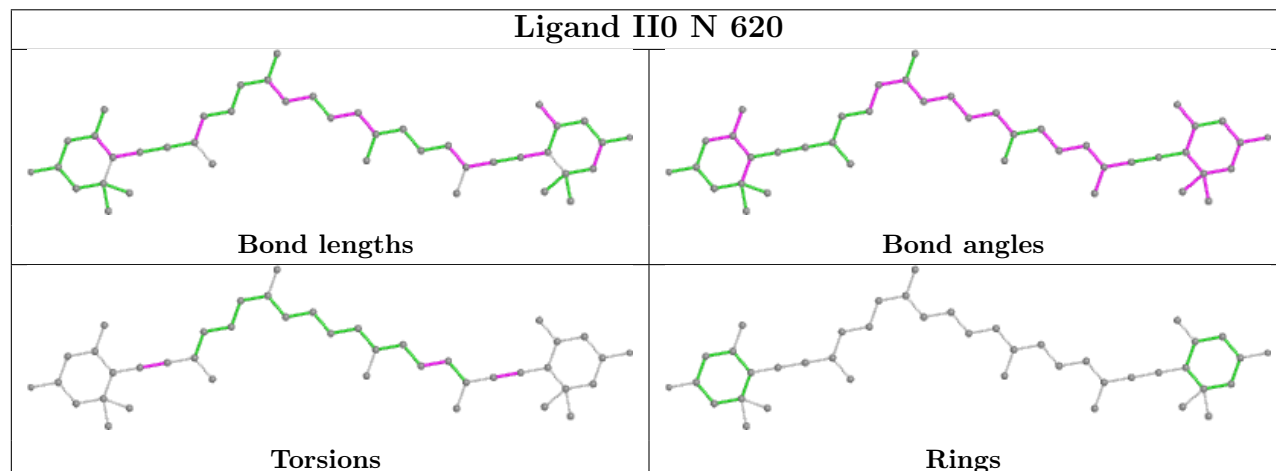


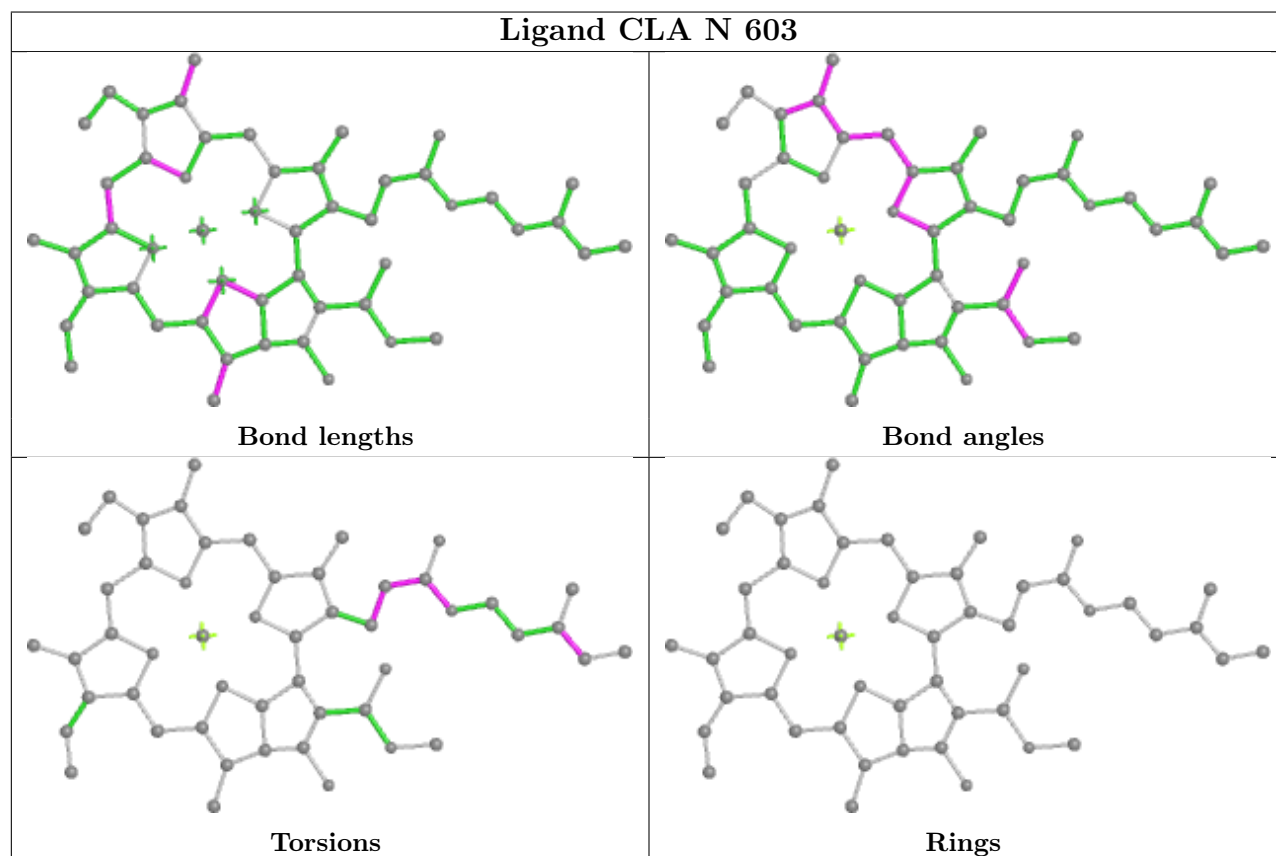
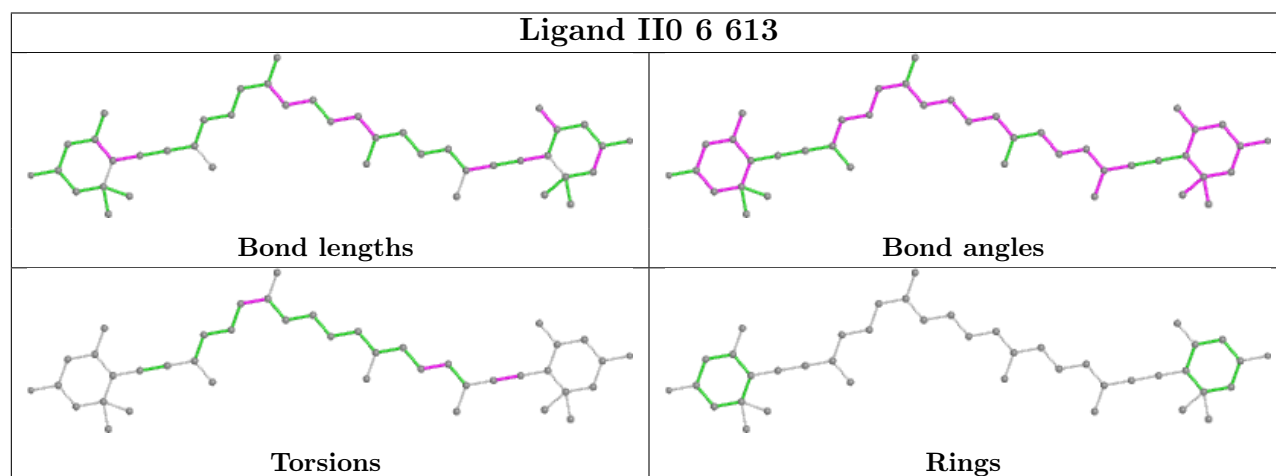
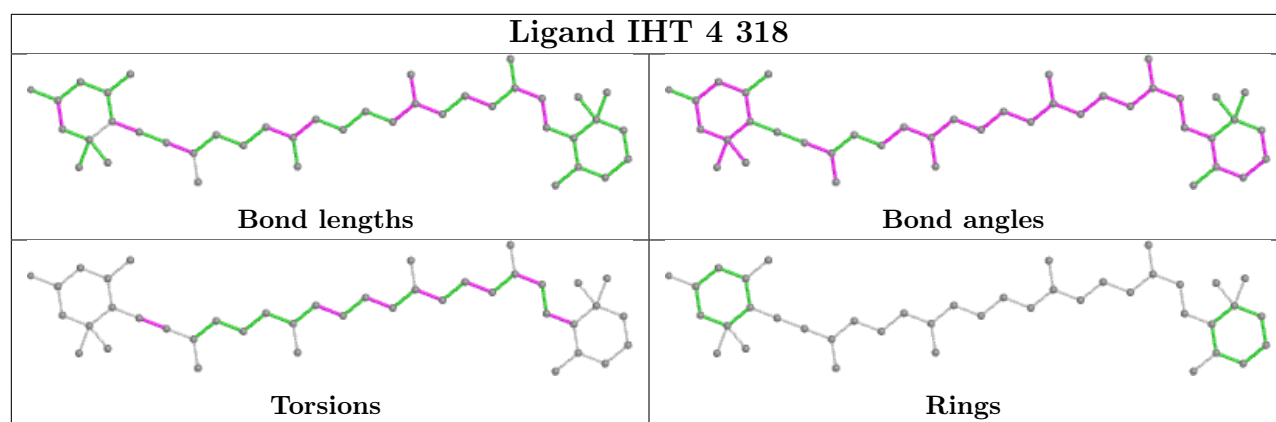
Ligand CLA 5 611**Ligand II0 2 313**

Ligand LHG c 520



Ligand II0 N 620





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

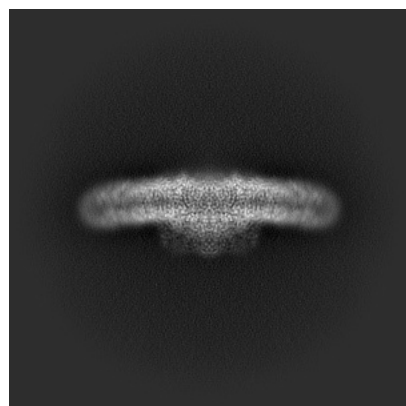
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62846. These allow visual inspection of the internal detail of the map and identification of artifacts.

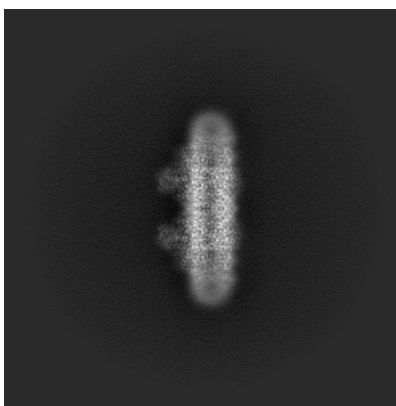
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

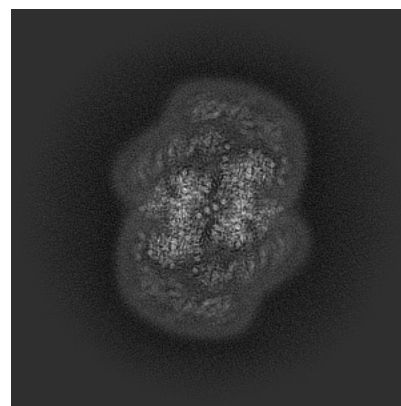
6.1.1 Primary map



X

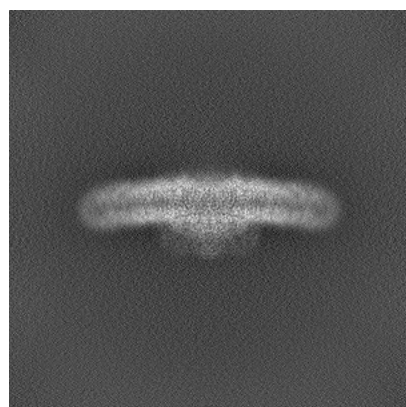


Y

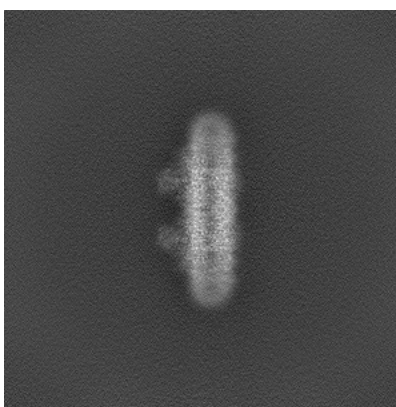


Z

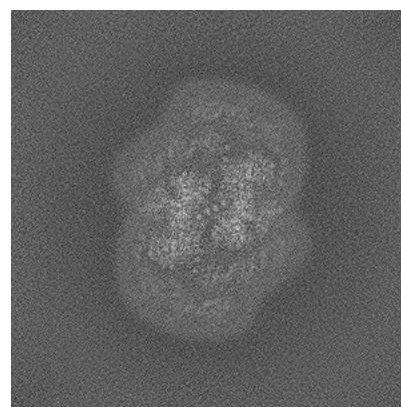
6.1.2 Raw map



X



Y

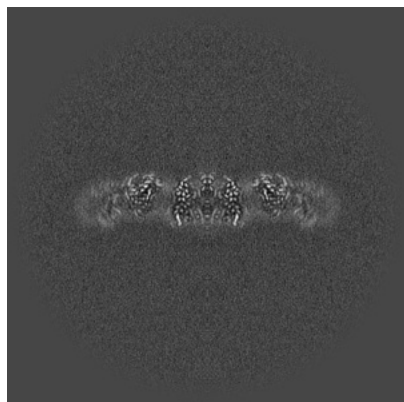


Z

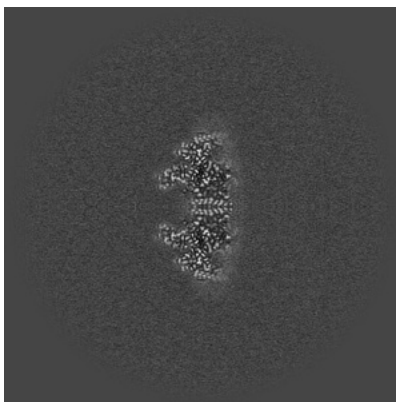
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

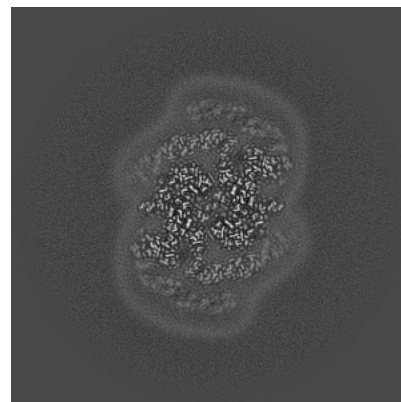
6.2.1 Primary map



X Index: 300

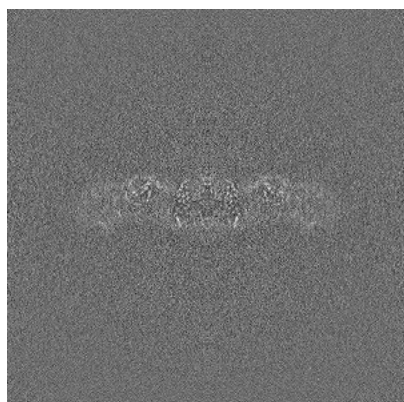


Y Index: 300

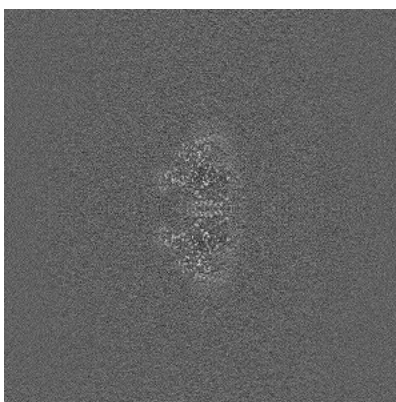


Z Index: 300

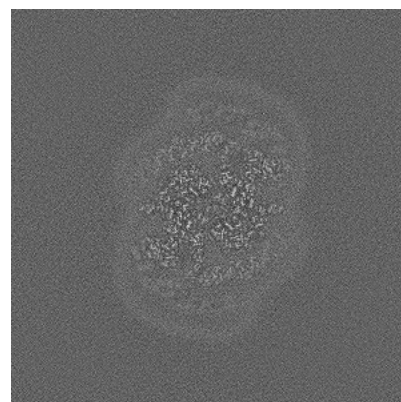
6.2.2 Raw map



X Index: 300



Y Index: 300

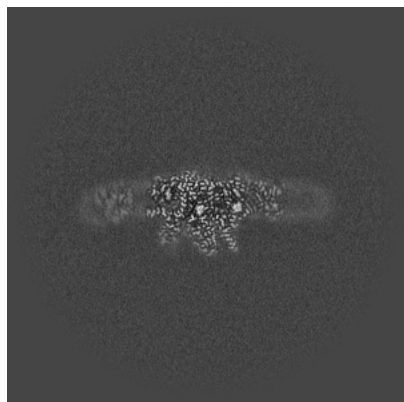


Z Index: 300

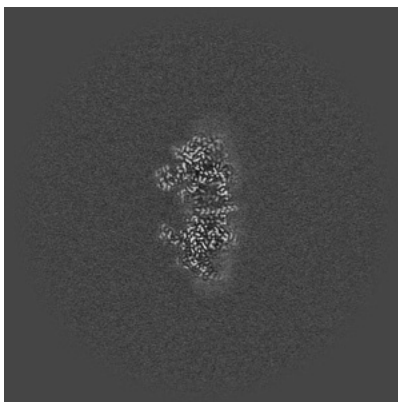
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

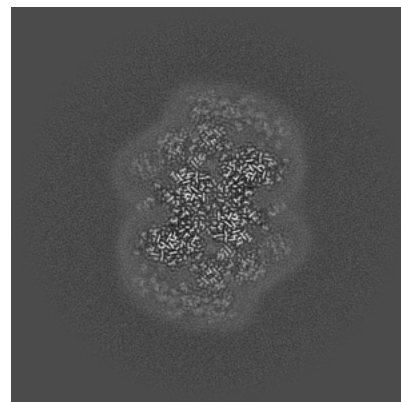
6.3.1 Primary map



X Index: 254

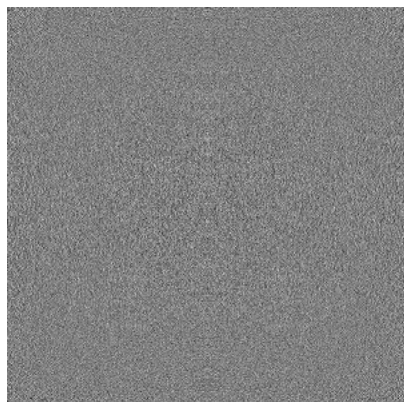


Y Index: 296

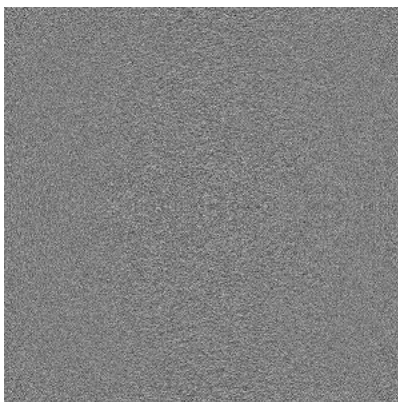


Z Index: 324

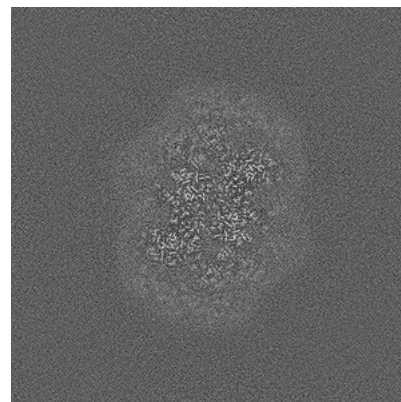
6.3.2 Raw map



X Index: 0



Y Index: 0

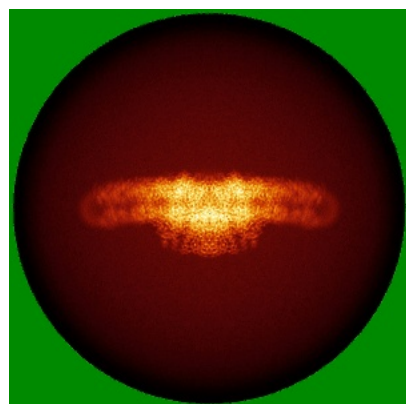


Z Index: 324

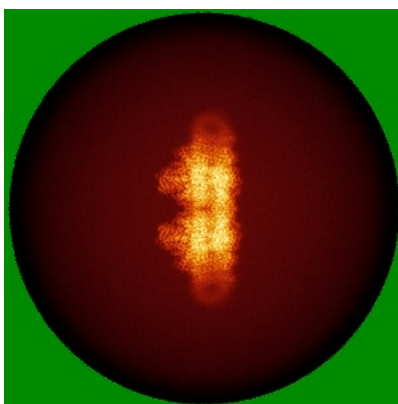
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

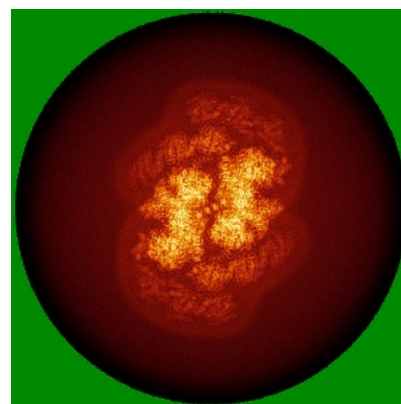
6.4.1 Primary map



X

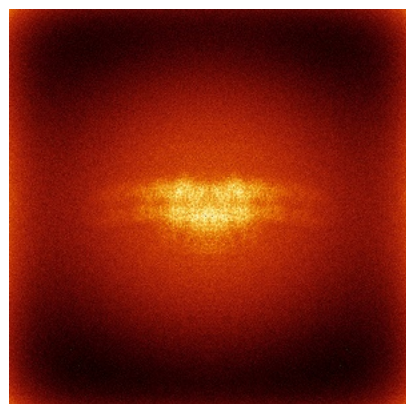


Y

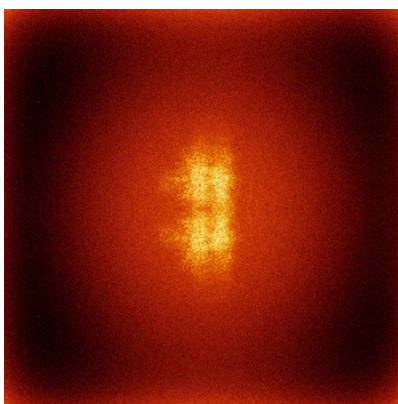


Z

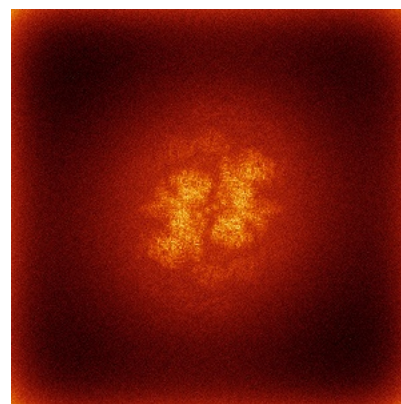
6.4.2 Raw map



X



Y

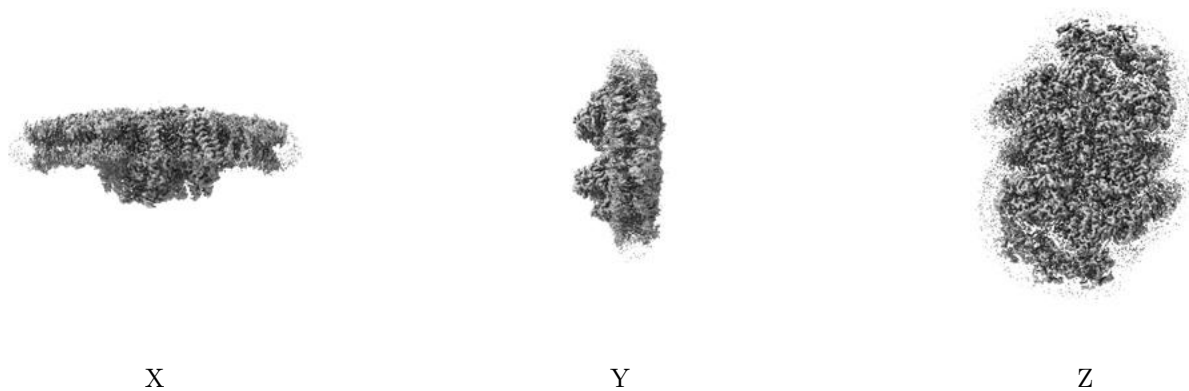


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

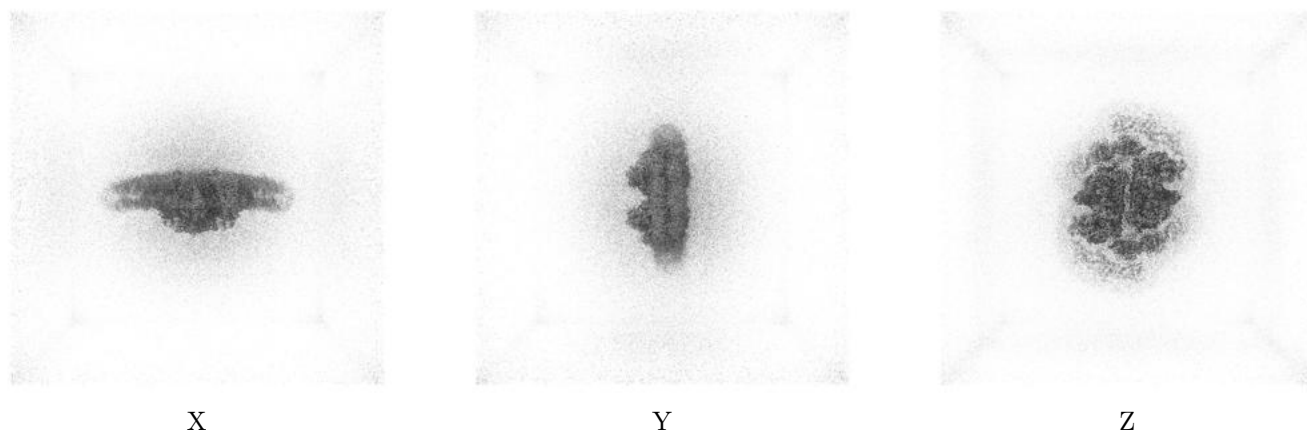
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

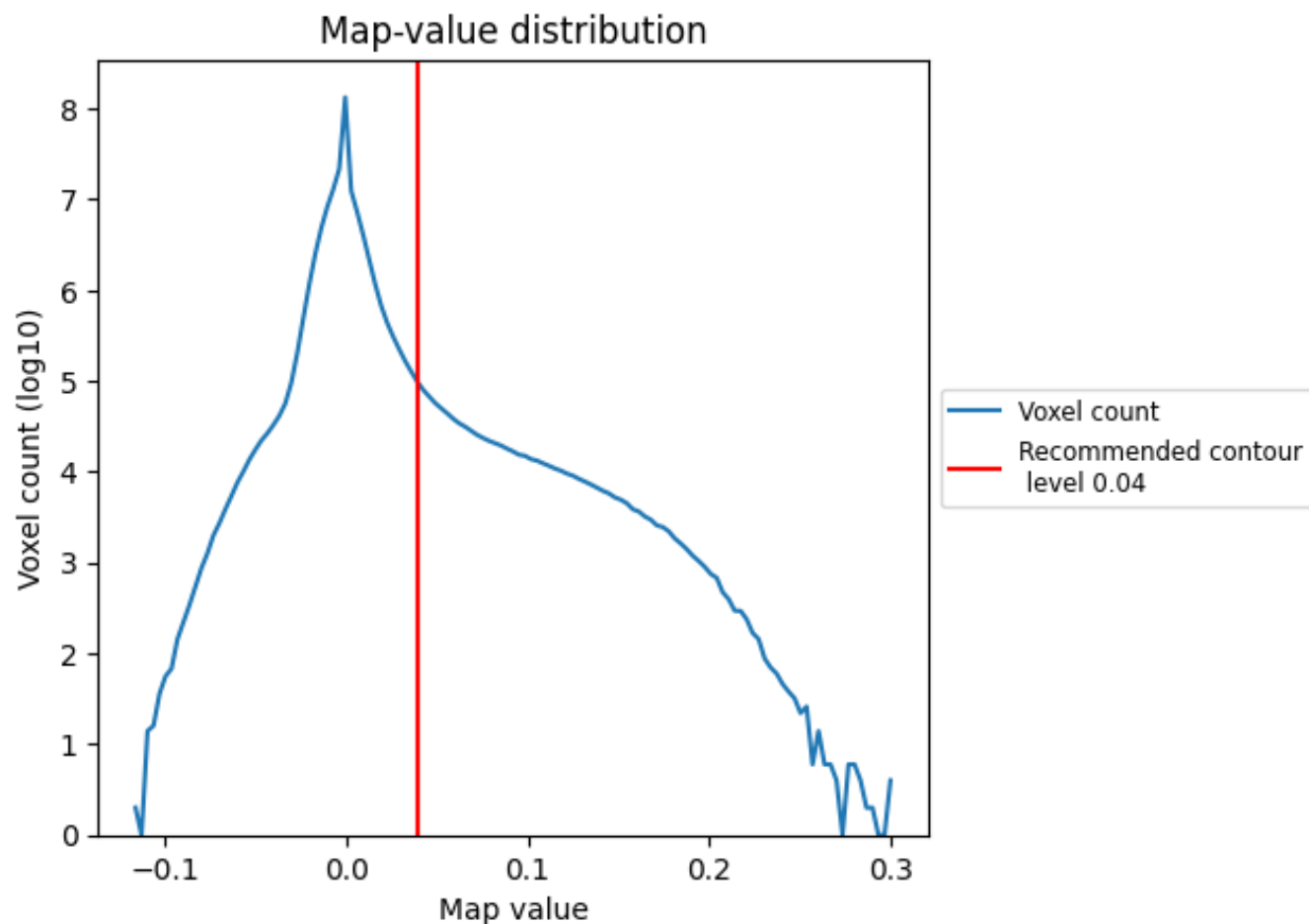
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

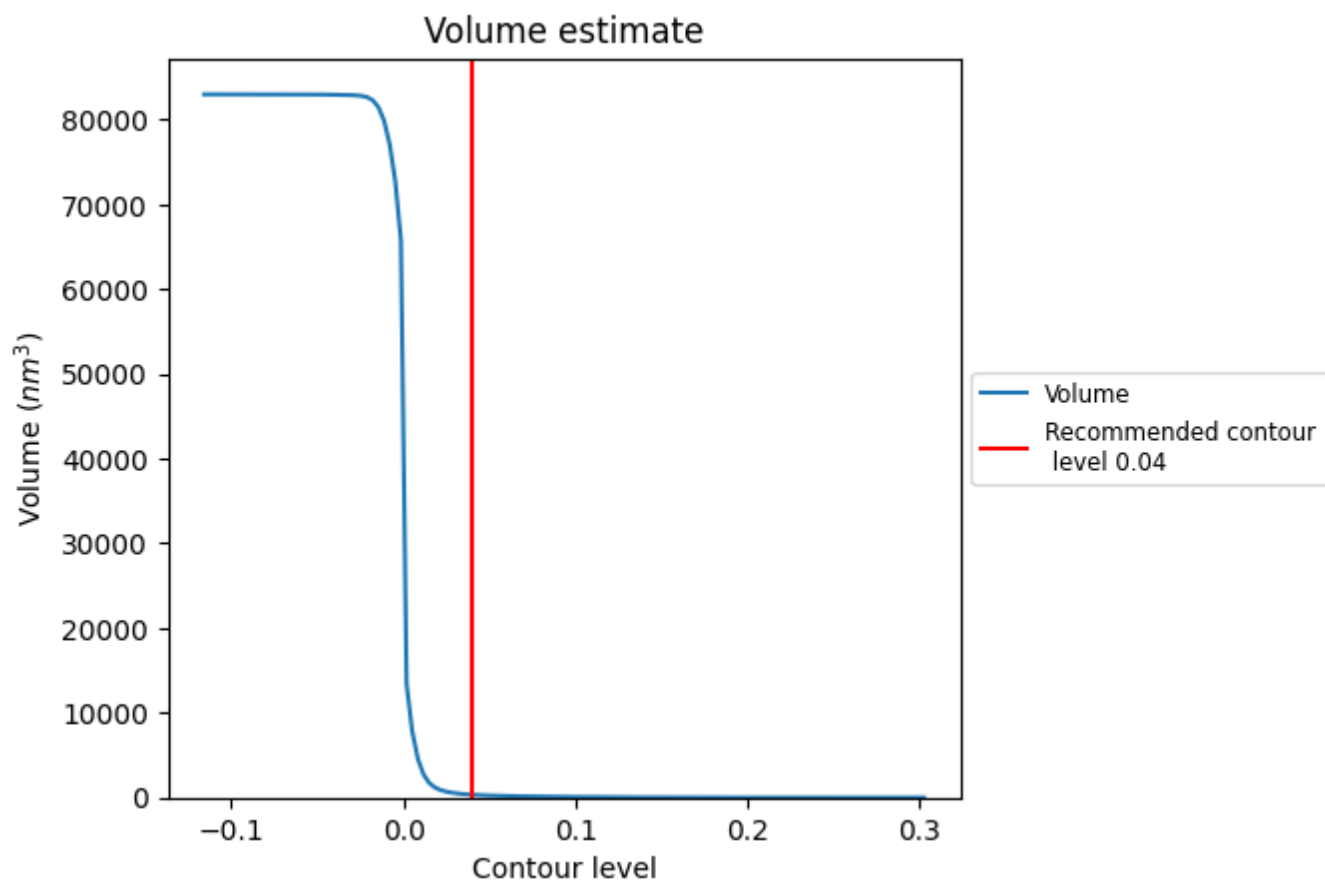
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

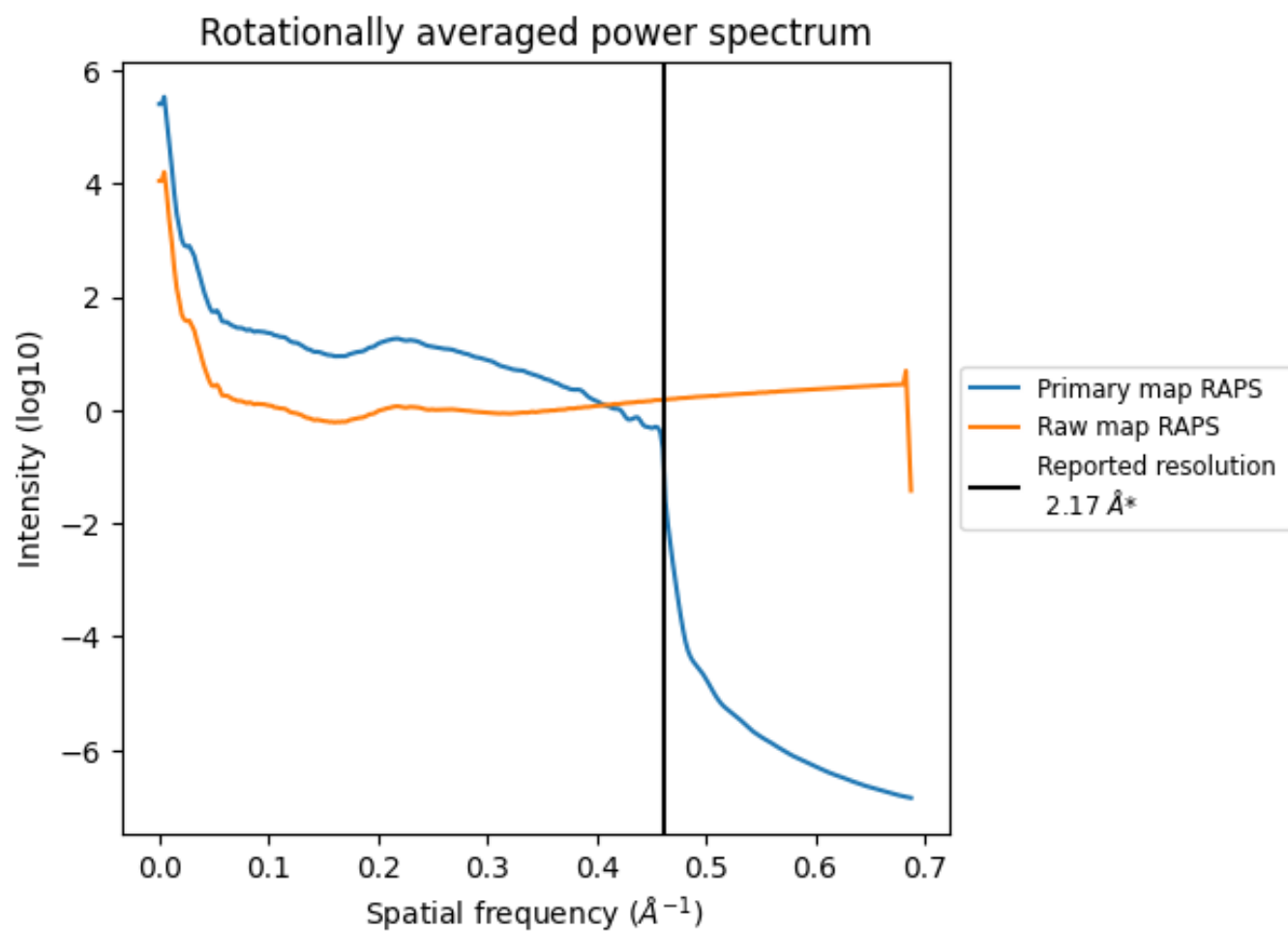
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 332 nm^3 ; this corresponds to an approximate mass of 300 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

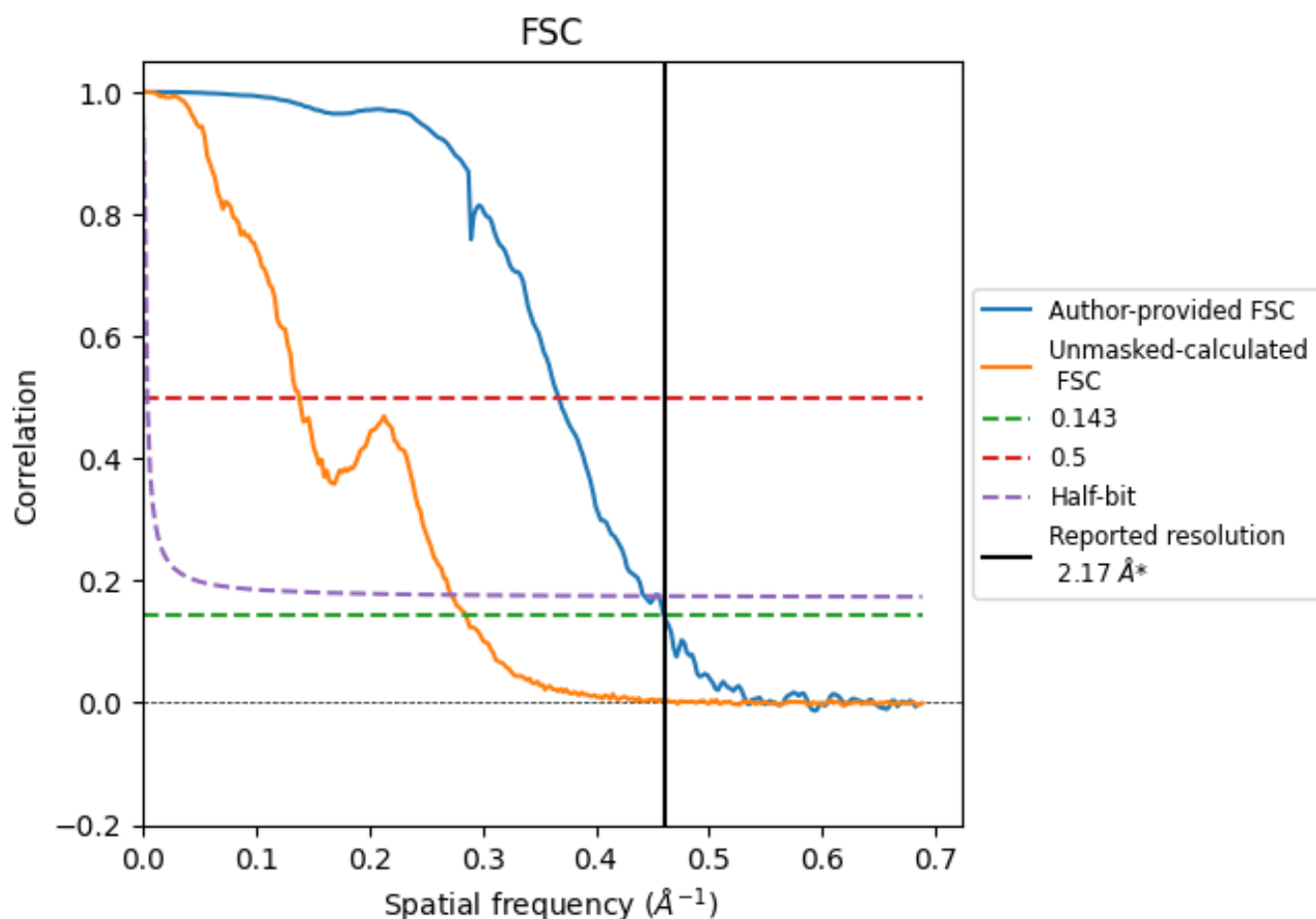


*Reported resolution corresponds to spatial frequency of 0.461 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.461 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.17	-	-
Author-provided FSC curve	2.17	2.72	2.26
Unmasked-calculated*	3.51	7.23	3.67

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.51 differs from the reported value 2.17 by more than 10 %

9 Map-model fit [i](#)

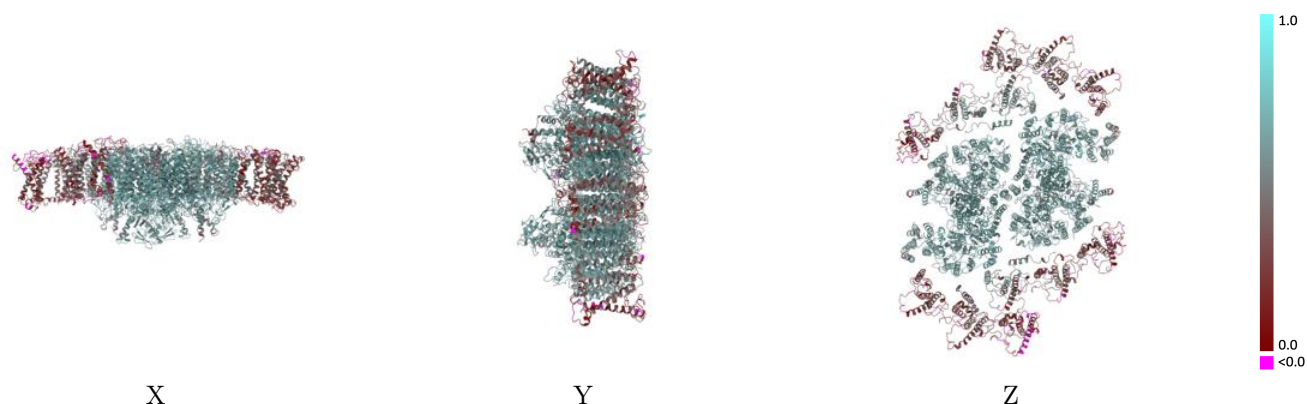
This section contains information regarding the fit between EMDB map EMD-62846 and PDB model 9L5V. Per-residue inclusion information can be found in section [3](#) on page [41](#).

9.1 Map-model overlay [i](#)



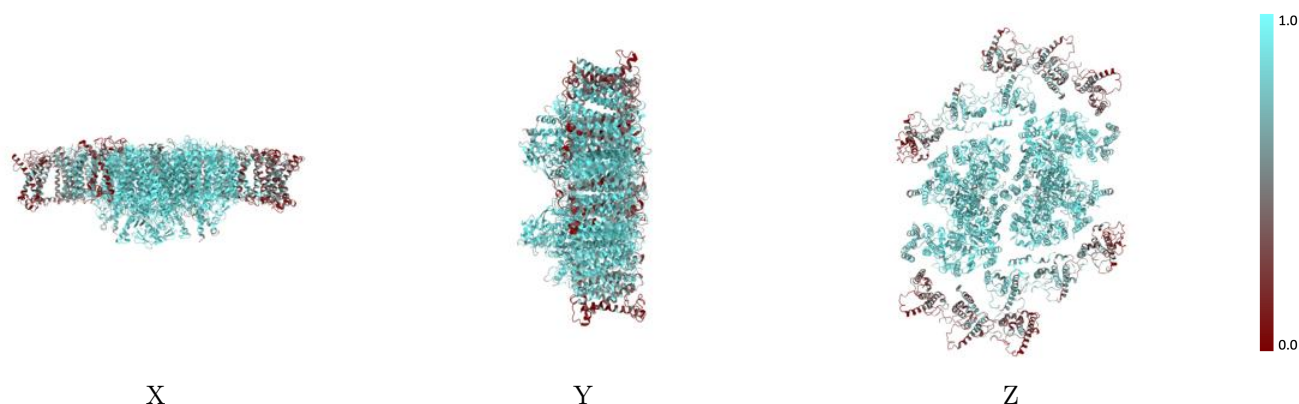
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



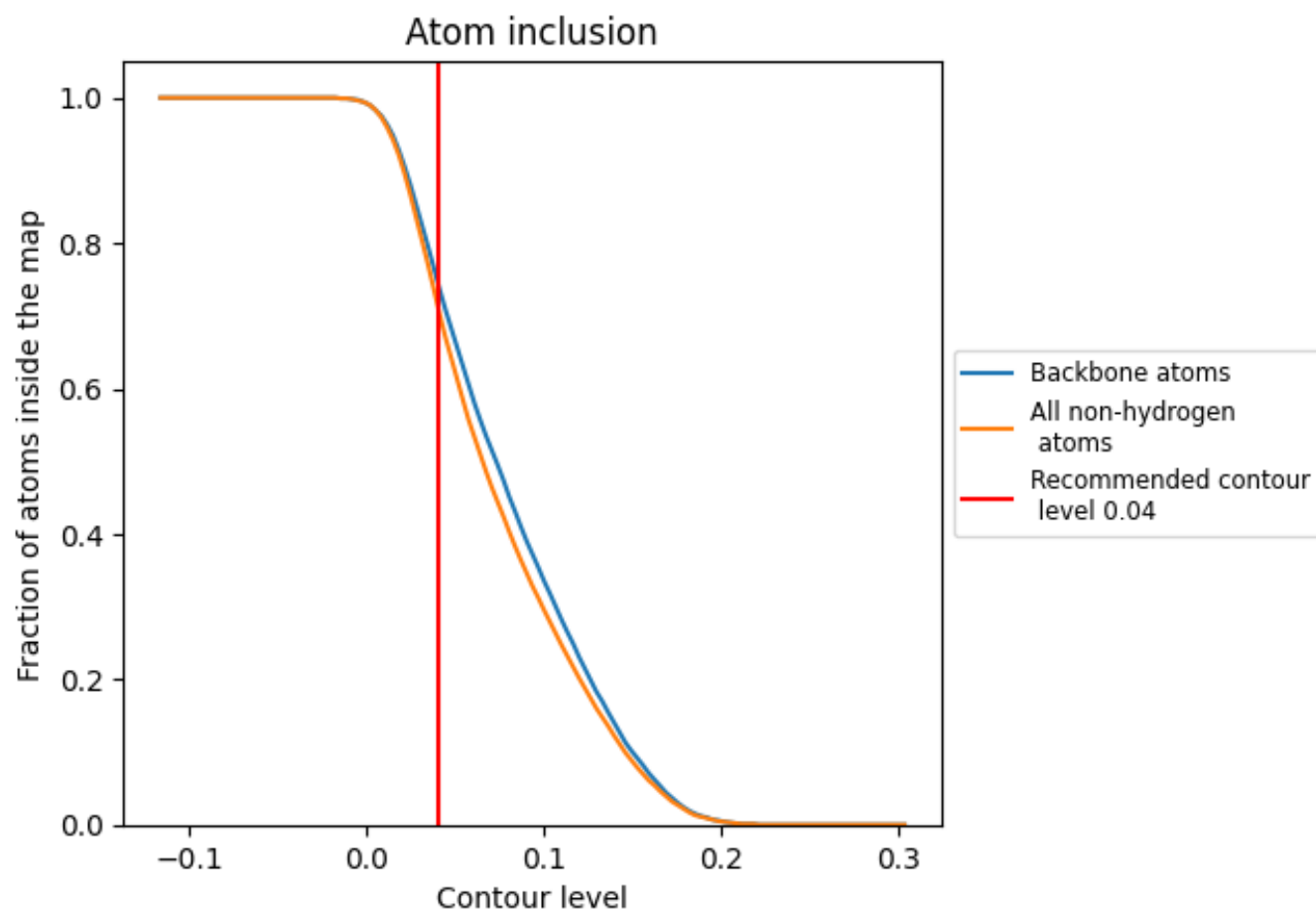
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

























The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7150	 0.5040
1	 0.2870	 0.2650
2	 0.6190	 0.3710
3	 0.7070	 0.4300
4	 0.3100	 0.2220
5	 0.3450	 0.2950
6	 0.2880	 0.2460
A	 0.9230	 0.6450
B	 0.9300	 0.6430
C	 0.8890	 0.6090
D	 0.9250	 0.6420
E	 0.7920	 0.5590
F	 0.7880	 0.5400
G	 0.6010	 0.4290
H	 0.9420	 0.6420
I	 0.9710	 0.6660
K	 0.8900	 0.6090
L	 0.9480	 0.6420
M	 0.8310	 0.6070
N	 0.2850	 0.2380
O	 0.7210	 0.4800
P	 0.7860	 0.5300
Q	 0.4000	 0.3430
R	 0.3820	 0.3370
S	 0.2910	 0.2520
T	 0.8830	 0.6370
W	 0.9120	 0.6400
X	 0.8830	 0.6240
Y	 0.6410	 0.5270
Z	 0.6820	 0.5240
a	 0.9040	 0.6330
b	 0.9240	 0.6350
c	 0.8840	 0.6080
d	 0.9310	 0.6470
e	 0.7980	 0.5510



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Chain	Atom inclusion	Q-score
f	 0.7860	 0.5430
g	 0.5930	 0.3990
h	 0.9230	 0.6210
i	 0.9790	 0.6720
k	 0.8550	 0.6000
l	 0.9650	 0.6580
m	 0.8250	 0.6040
t	 0.8910	 0.6410
w	 0.9290	 0.6520
x	 0.8750	 0.6250
y	 0.6540	 0.5320
z	 0.6410	 0.4730