



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 05:05 PM JST

PDB ID : 9XJ9 / pdb_00009xj9
EMDB ID : EMD-66932
Title : In situ structure of the PSI-LHCI-LHCII supercomplex from *Oryza sativa*
Authors : Li, J.; Elias, E.; Zhang, K.; Croce, R.; Zhu, J.
Deposited on : 2025-11-04
Resolution : 2.96 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.50

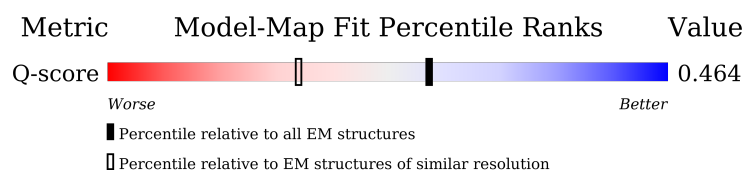
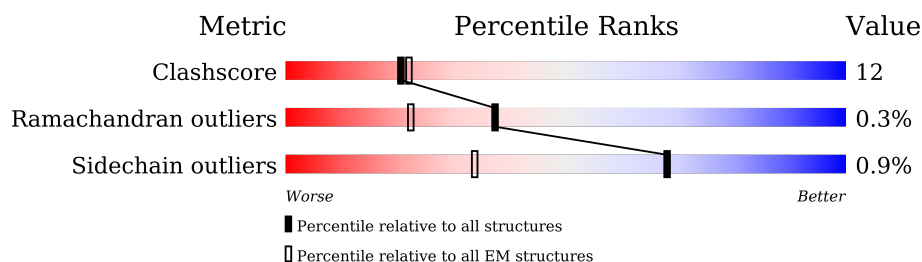
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 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.



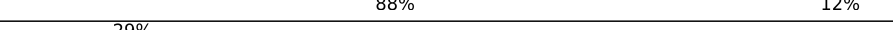
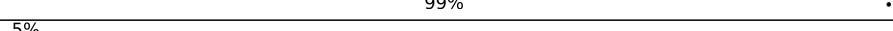
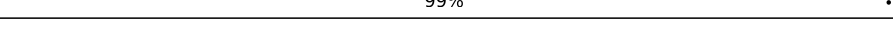
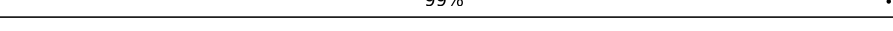
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13155 (2.46 - 3.46)

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	1	200	78% 22%
2	2	207	75% 24% •
3	3	222	80% 20%
4	4	198	75% 25%

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Mol	Chain	Length	Quality of chain
5	A	742	 74% 25% .
6	B	732	 74% 25% .
7	C	80	 79% 20% .
8	D	143	 82% 17% .
9	E	66	 85% 14% .
10	F	158	 76% 23% .
11	G	97	 82% 18%
12	H	93	 67% 27% 6%
13	I	30	 83% 17%
14	J	44	 70% 23% 7%
15	K	88	 72% 27% .
16	L	163	 80% 20% .
17	N	84	 88% 12%
18	O	92	 88% 12%
19	X	218	 29% 99% .
19	Z	218	 5% 99% .
20	Y	222	 . 99% .

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
22	CLA	1	307	X	-	-	-
22	CLA	1	317	X	-	-	-
22	CLA	1	318	X	-	-	-
22	CLA	2	304	X	-	-	-
22	CLA	2	307	X	-	-	-
22	CLA	2	318	X	-	-	-
22	CLA	3	309	X	-	-	-
22	CLA	3	310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	3	312	X	-	-	-
22	CLA	4	304	X	-	-	-
22	CLA	A	801	X	-	-	-
22	CLA	A	802	X	-	-	-
22	CLA	A	803	X	-	-	-
22	CLA	A	807	X	-	-	-
22	CLA	A	808	X	-	-	-
22	CLA	A	809	X	-	-	-
22	CLA	A	810	X	-	-	-
22	CLA	A	812	X	-	-	-
22	CLA	A	826	X	-	-	-
22	CLA	A	827	X	-	-	-
22	CLA	A	831	X	-	-	-
22	CLA	A	833	X	-	-	-
22	CLA	A	836	X	-	-	-
22	CLA	A	838	X	-	-	-
22	CLA	A	842	X	-	-	-
22	CLA	A	843	X	-	-	-
22	CLA	A	844	X	-	-	-
22	CLA	A	846	X	-	-	-
22	CLA	A	849	X	-	-	-
22	CLA	A	850	X	-	-	-
22	CLA	A	852	X	-	-	-
22	CLA	A	853	X	-	-	-
22	CLA	A	854	X	-	-	-
22	CLA	A	855	X	-	-	-
22	CLA	A	857	X	-	-	-
22	CLA	A	858	X	-	-	-
22	CLA	A	859	X	-	-	-
22	CLA	B	801	X	-	-	-
22	CLA	B	803	X	-	-	-
22	CLA	B	804	X	-	-	-
22	CLA	B	806	X	-	-	-
22	CLA	B	807	X	-	-	-
22	CLA	B	808	X	-	-	-
22	CLA	B	809	X	-	-	-
22	CLA	B	811	X	-	-	-
22	CLA	B	812	X	-	-	-
22	CLA	B	814	X	-	-	-
22	CLA	B	815	X	-	-	-
22	CLA	B	816	X	-	-	-
22	CLA	B	817	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	818	X	-	-	-
22	CLA	B	819	X	-	-	-
22	CLA	B	822	X	-	-	-
22	CLA	B	823	X	-	-	-
22	CLA	B	824	X	-	-	-
22	CLA	B	827	X	-	-	-
22	CLA	B	829	X	-	-	-
22	CLA	B	830	X	-	-	-
22	CLA	B	831	X	-	-	-
22	CLA	B	833	X	-	-	-
22	CLA	B	845	X	-	-	-
22	CLA	B	847	X	-	-	-
22	CLA	B	848	X	-	-	-
22	CLA	B	850	X	-	-	-
22	CLA	B	851	X	-	-	-
22	CLA	B	852	X	-	-	-
22	CLA	K	203	X	-	-	-
22	CLA	L	306	X	-	-	-
22	CLA	O	207	X	-	-	-
22	CLA	O	208	X	-	-	-
22	CLA	Y	311	X	-	-	-
30	CL0	A	825	X	-	-	-

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 43745 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 Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	200	Total	C	N	O	S	0	0
			1560	1013	258	283	6		

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	207	Total	C	N	O	S	0	0
			1612	1055	263	289	5		

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	222	Total	C	N	O	S	0	0
			1723	1134	276	307	6		

- Molecule 4 is a protein called Chlorophyll A-B binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	198	Total	C	N	O	S	0	0
			1570	1024	257	284	5		

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	742	Total	C	N	O	S	0	0
			5839	3824	992	1005	18		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	732	Total	C	N	O	S	0	0
			5856	3843	994	1006	13		

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			602	371	104	116	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	143	Total	C	N	O	S	0	0
			1128	726	197	202	3		

- Molecule 9 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	65	Total	C	N	O	S	0	0
			518	329	92	97			

- Molecule 10 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	158	Total	C	N	O	S	0	0
			1236	806	210	217	3		

- Molecule 11 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	97	Total	C	N	O	S	0	0
			760	492	128	139	1		

- Molecule 12 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	93	Total	C	N	O	S	0	0
			709	465	112	132			

- Molecule 13 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	30	Total	C	N	O	S	0	0
			232	160	35	36	1		

- Molecule 14 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	44	Total	C	N	O	S	0	0
			353	241	53	58	1		

- Molecule 15 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	88	Total	C	N	O	S	0	0
			620	392	107	117	4		

- Molecule 16 is a protein called Photosystem I reaction center subunit XI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	163	Total	C	N	O	S	0	0
			1223	809	194	218	2		

- Molecule 17 is a protein called Photosystem I reaction center subunit N, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	84	Total	C	N	O	S	0	0
			685	439	112	130	4		

- Molecule 18 is a protein called H0622F05.3 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	O	92	Total	C	N	O	0	0
			733	491	118	124		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	39	GLN	ARG	conflict	UNP Q01L93

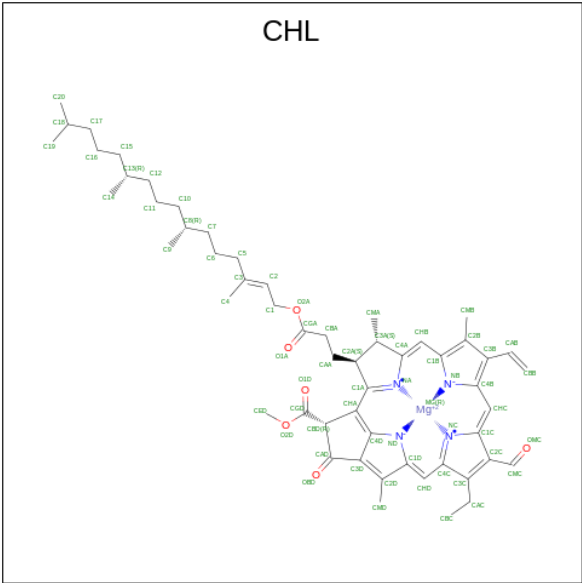
- Molecule 19 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	X	218	Total	C	N	O	0	0
			1094	658	218	218		
19	Z	218	Total	C	N	O	0	0
			1094	658	218	218		

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	Y	222	Total	C	N	O	0	0
			1112	669	222	221		

- Molecule 21 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



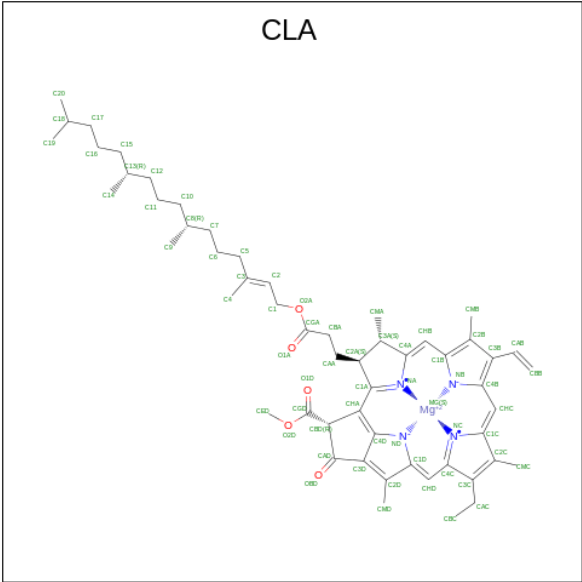
Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	X	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
21	X	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
21	X	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
21	X	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	X	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
21	X	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	Z	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
21	Z	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
21	Z	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	Z	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
21	Z	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
21	Z	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
22	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	1	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	2	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
22	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
22	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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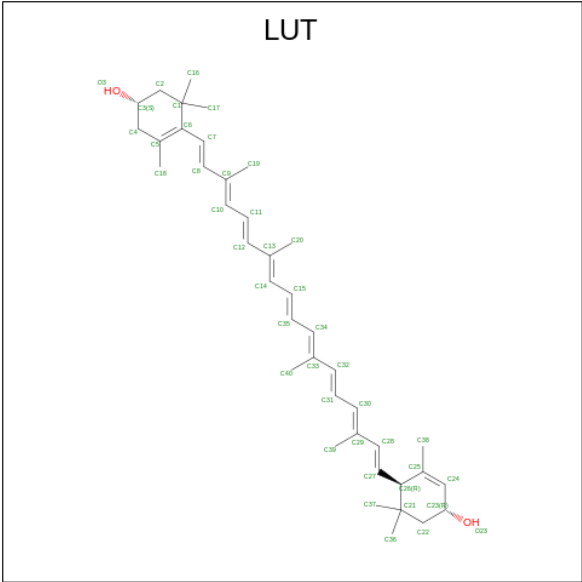
Mol	Chain	Residues	Atoms					AltConf
22	J	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	K	1	Total 44	C 34	Mg 1	N 4	O 5	0
22	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	K	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	N	1	Total 44	C 34	Mg 1	N 4	O 5	0
22	O	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	O	1	Total 64	C 54	Mg 1	N 4	O 5	0
22	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	O	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	X	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	X	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	X	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	X	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	X	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	X	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	X	1	Total 46	C 36	Mg 1	N 4	O 5	0

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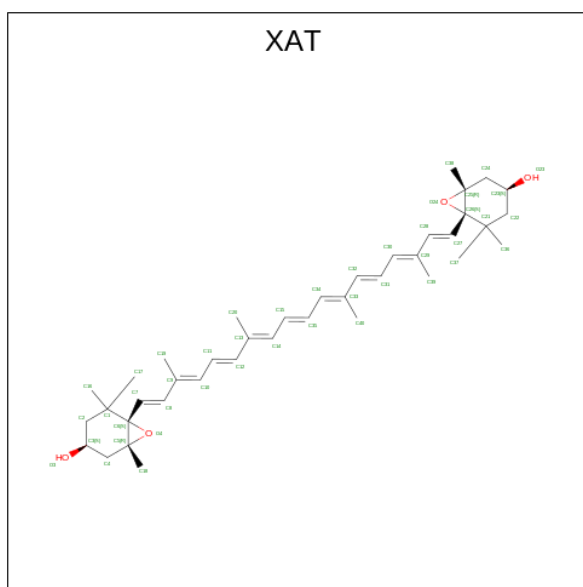
Mol	Chain	Residues	Atoms					AltConf
22	Y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 23 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



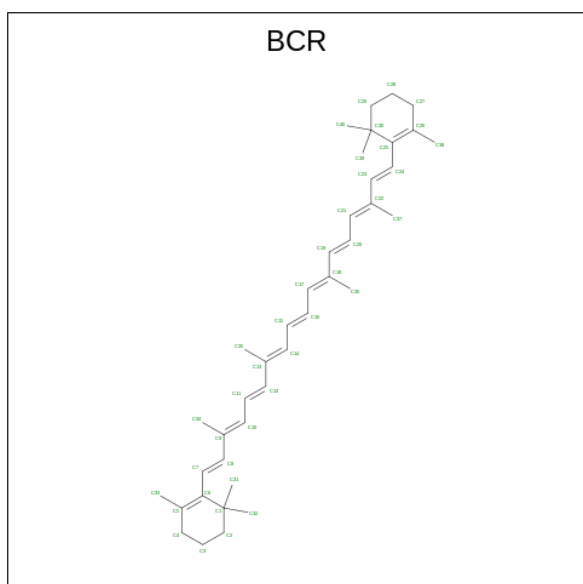
Mol	Chain	Residues	Atoms			AltConf
23	1	1	Total	C	O	0
			42	40	2	
23	2	1	Total	C	O	0
			42	40	2	
23	3	1	Total	C	O	0
			42	40	2	
23	4	1	Total	C	O	0
			42	40	2	
23	4	1	Total	C	O	0
			42	40	2	

- Molecule 24 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
24	1	1	Total	C	O	0
			44	40	4	
24	2	1	Total	C	O	0
			44	40	4	
24	3	1	Total	C	O	0
			44	40	4	
24	4	1	Total	C	O	0
			44	40	4	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



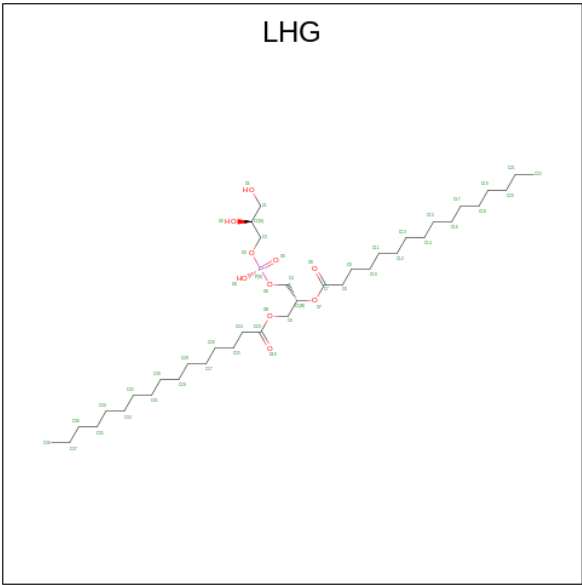
Mol	Chain	Residues	Atoms	AltConf
25	1	1	Total C 40 40	0
25	2	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	4	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 39 39	0
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 30 30	0
25	B	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	G	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	J	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
25	J	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	O	1	Total C 40 40	0
25	O	1	Total C 40 40	0

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



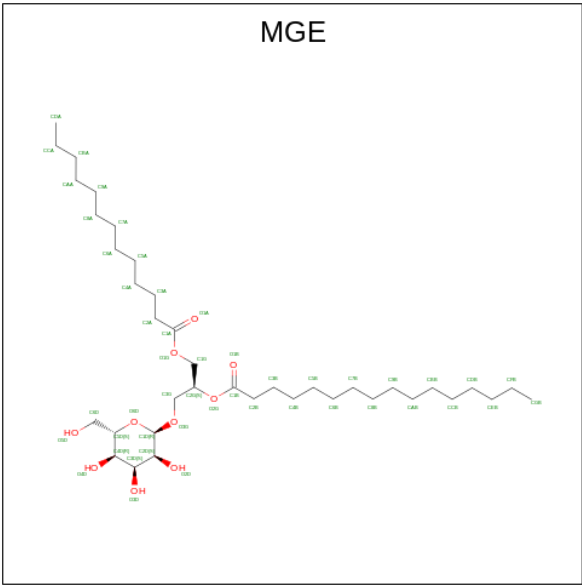
Mol	Chain	Residues	Atoms	AltConf
26	1	1	Total C O P 42 31 10 1	0
26	1	1	Total C O 29 25 4	0
26	1	1	Total C O 33 28 5	0

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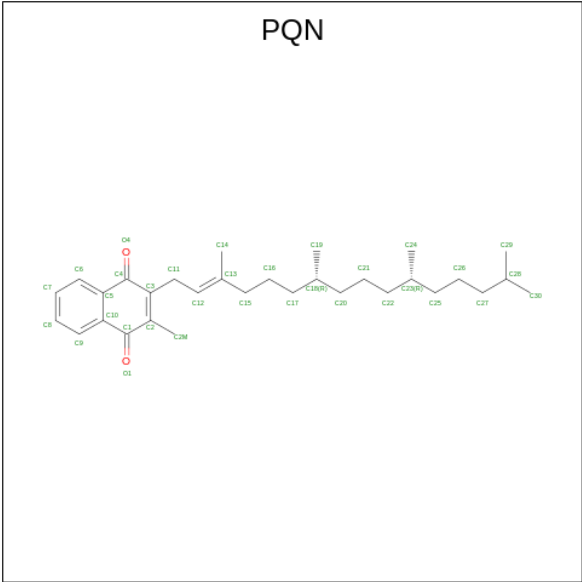
Mol	Chain	Residues	Atoms				AltConf
26	2	1	Total	C	O	P	0
			26	17	8	1	
26	2	1	Total	C	O	P	0
			29	20	8	1	
26	2	1	Total	C	O	P	0
			32	21	10	1	
26	2	1	Total	C	O	P	0
			36	27	8	1	
26	3	1	Total	C	O	P	0
			38	27	10	1	
26	4	1	Total	C	O	P	0
			29	20	8	1	
26	4	1	Total	C	O	P	0
			27	16	10	1	
26	4	1	Total	C	O	P	0
			36	27	8	1	
26	A	1	Total	C	O	P	0
			49	38	10	1	
26	A	1	Total	C	O	P	0
			24	15	8	1	
26	A	1	Total	C	O	P	0
			30	21	8	1	
26	A	1	Total	C	O	P	0
			33	22	10	1	
26	A	1	Total	C	O	P	0
			40	31	8	1	
26	B	1	Total	C	O	P	0
			30	19	10	1	
26	B	1	Total	C	O	P	0
			41	32	8	1	
26	F	1	Total	C	O	P	0
			31	22	8	1	
26	G	1	Total	C	O	P	0
			36	25	10	1	
26	G	1	Total	C	O	P	0
			25	16	8	1	
26	O	1	Total	C	O	P	0
			29	20	8	1	
26	O	1	Total	C	O	P	0
			28	19	8	1	
26	X	1	Total	C	O	P	0
			22	11	10	1	

- Molecule 27 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (CCD ID: MGE) (formula: C₃₈H₇₂O₁₀) (labeled as "Ligand of Interest" by depositor).



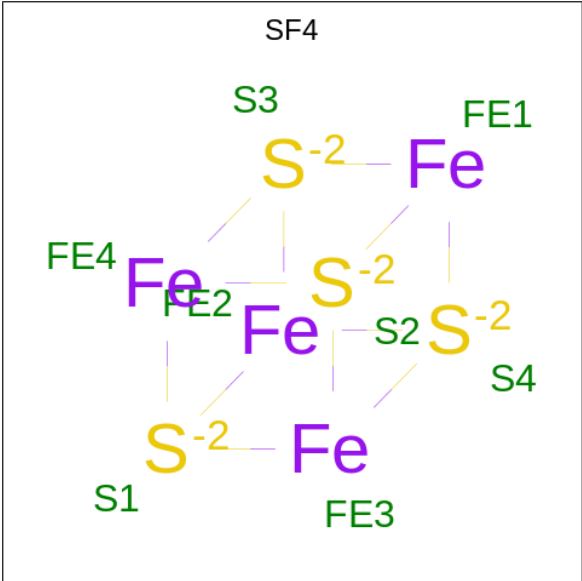
Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			37	27	10	
27	3	1	Total	C	O	0
			32	22	10	
27	3	1	Total	C	O	0
			26	16	10	
27	F	1	Total	C	O	0
			37	27	10	
27	F	1	Total	C	O	0
			28	18	10	
27	N	1	Total	C	O	0
			32	22	10	

- Molecule 28 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			33	31	2	
28	B	1	Total	C	O	0
			30	28	2	

- Molecule 29 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



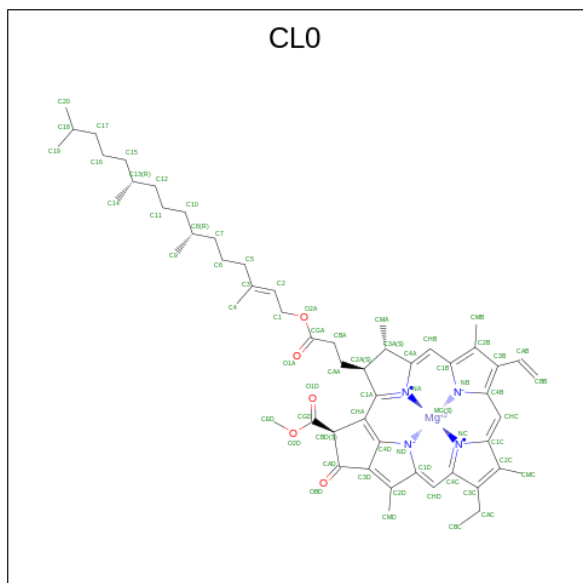
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	Fe	S	0
			8	4	4	

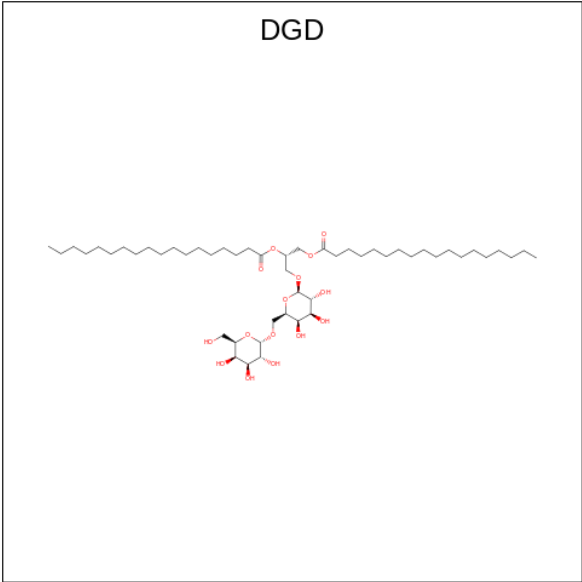
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Mol	Chain	Residues	Atoms			AltConf
29	C	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 30 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



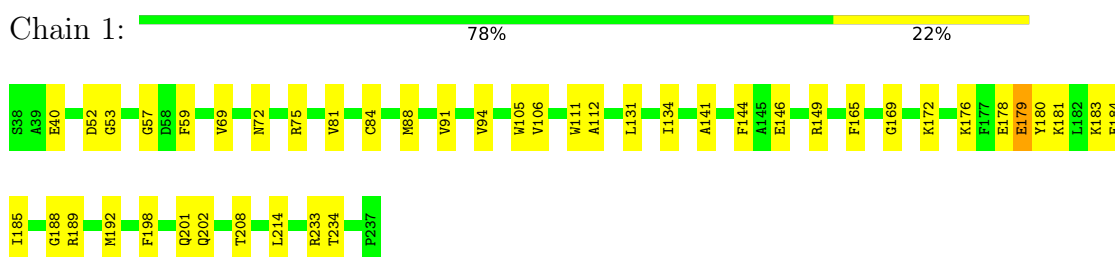


Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			59	44	15	
31	G	1	Total	C	O	0
			39	30	9	
31	J	1	Total	C	O	0
			58	43	15	
31	O	1	Total	C	O	0
			53	38	15	

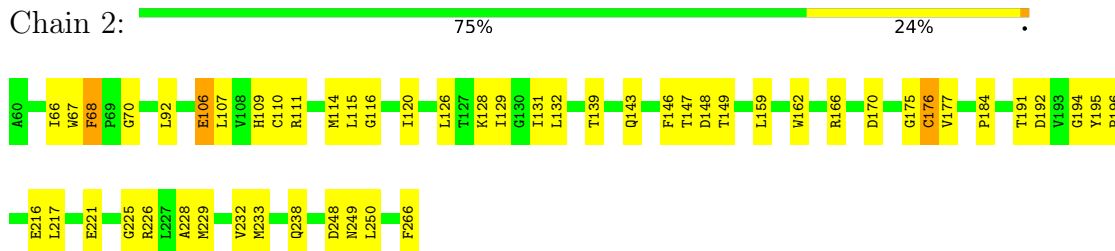
3 Residue-property plots

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.

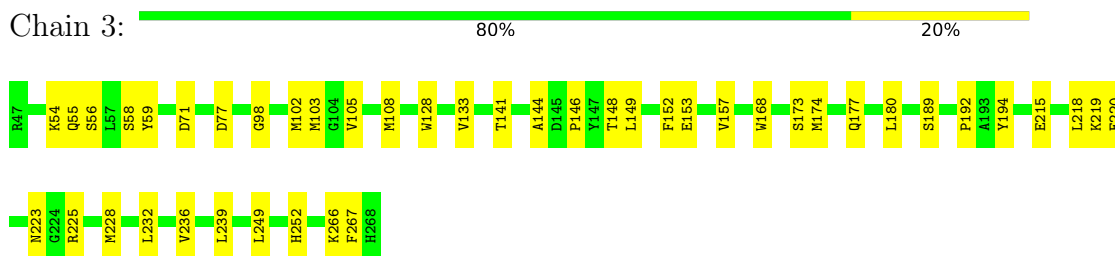
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



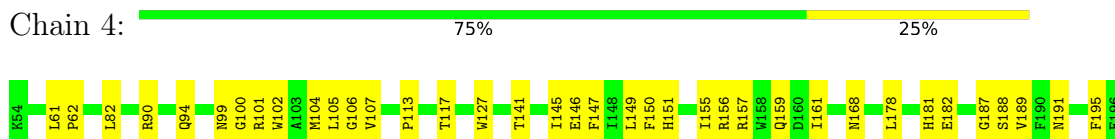
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



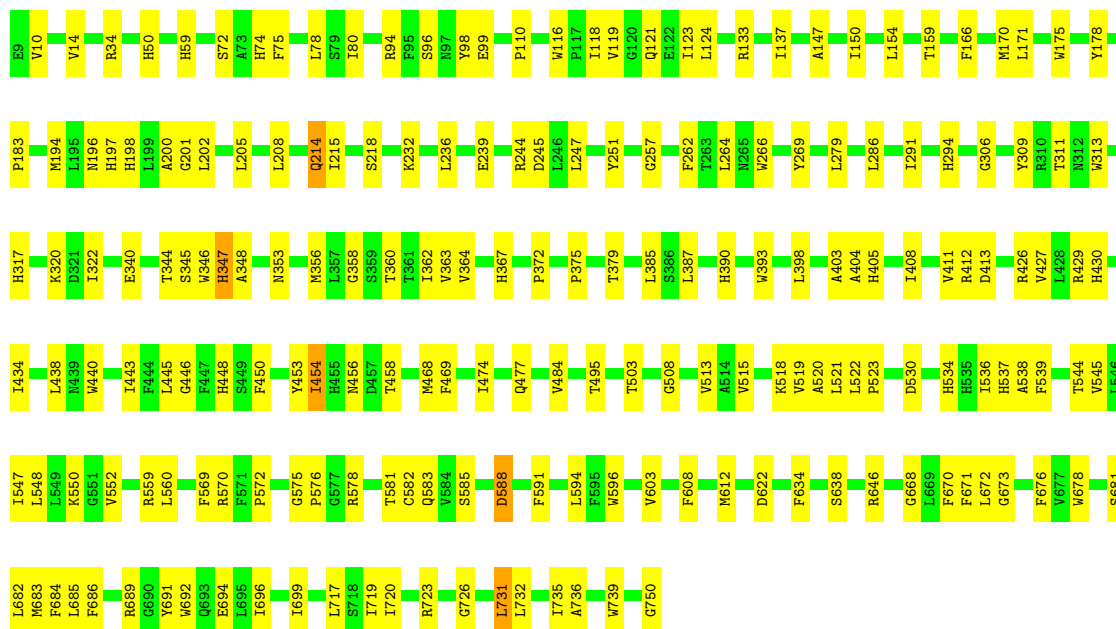
- Molecule 4: Chlorophyll A-B binding protein





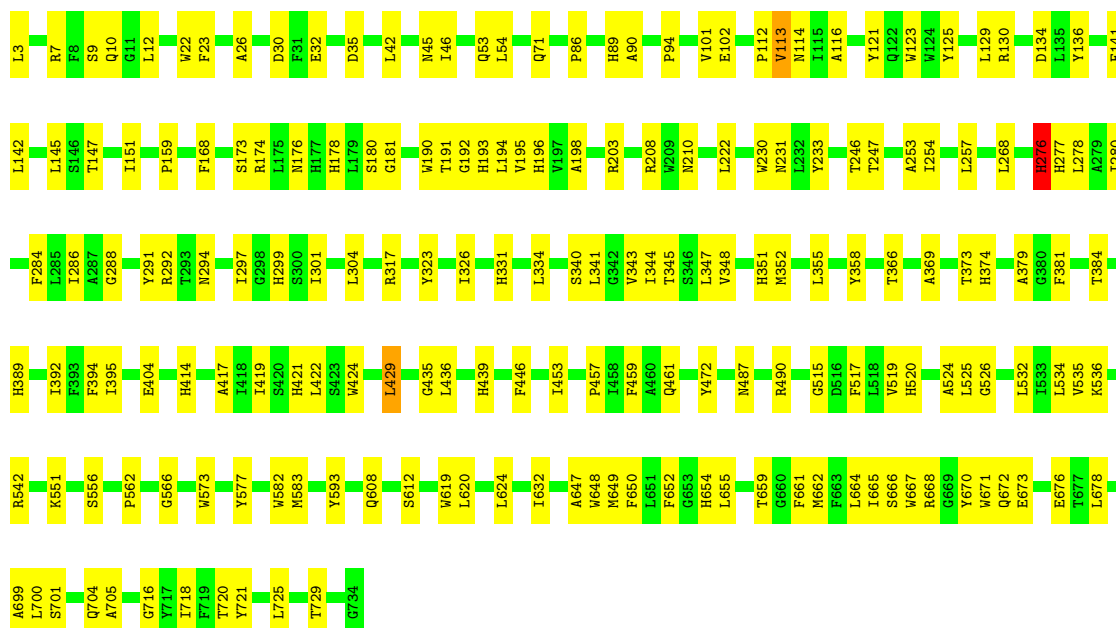
• Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

Chain A: 74% 25%



• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 74% 25%



• Molecule 7: Photosystem I iron-sulfur center

Chain C:  79% 20% .



- Molecule 8: Photosystem I reaction center subunit II, chloroplastic

Chain D:  82% 17% .



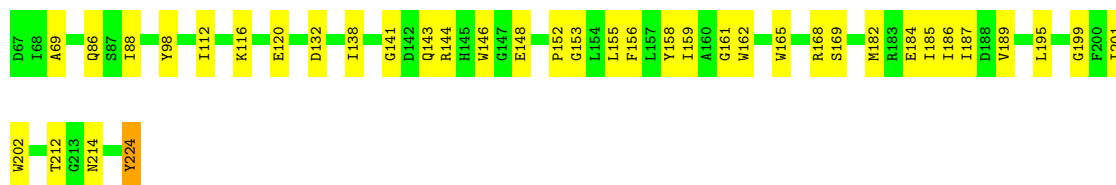
- Molecule 9: Photosystem I reaction center subunit IV

Chain E:  85% 14% .



- Molecule 10: Photosystem I reaction center subunit III

Chain F:  76% 23% .



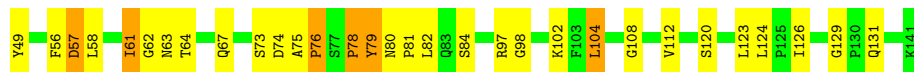
- Molecule 11: Photosystem I reaction center subunit V, chloroplastic

Chain G:  82% 18% .



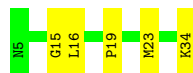
- Molecule 12: Photosystem I reaction center subunit VI, chloroplastic

Chain H:  67% 27% 6% .



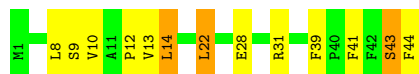
- Molecule 13: Photosystem I reaction center subunit VIII

Chain I:  83% 17% .



- Molecule 14: Photosystem I reaction center subunit IX

Chain J:  70% 23% 7%



- Molecule 15: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:  72% 27% .



- Molecule 16: Photosystem I reaction center subunit XI, chloroplastic

Chain L:  80% 20% .



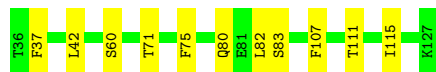
- Molecule 17: Photosystem I reaction center subunit N, chloroplastic

Chain N:  88% 12%

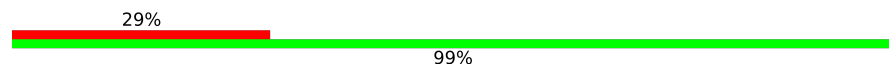


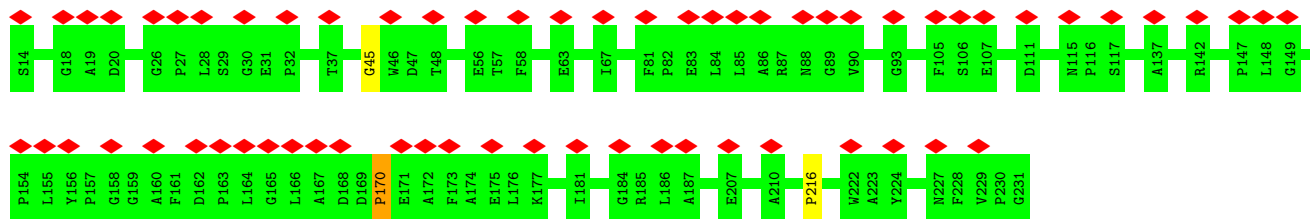
- Molecule 18: H0622F05.3 protein

Chain O:  88% 12%

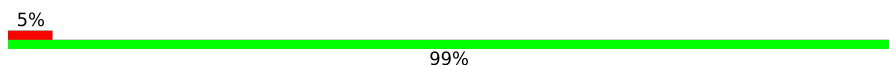


- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain X:  29% 99% .

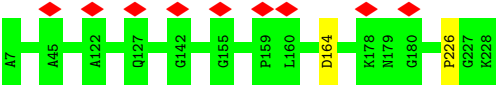


- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain Z:  5% 99% .



• Molecule 20: Chlorophyll a-b binding protein, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	124514	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 ($e^-/\text{\AA}^2$)	1.375	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.622	Depositor
Minimum map value	-0.191	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.018	Depositor
Map size ($\text{\AA}$)	419.84, 419.84, 419.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, MGE, XAT, CLA, PQN, CHL, CL0, SF4, DGD, LUT, LHG

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	1	0.30	0/1614	0.65	1/2203 (0.0%)
2	2	0.30	0/1670	0.67	2/2286 (0.1%)
3	3	0.28	0/1779	0.59	0/2419
4	4	0.27	0/1621	0.62	2/2214 (0.1%)
5	A	0.28	0/6037	0.55	6/8234 (0.1%)
6	B	0.27	0/6067	0.57	7/8285 (0.1%)
7	C	0.23	0/613	0.55	0/830
8	D	0.24	0/1157	0.53	0/1564
9	E	0.24	0/530	0.55	0/722
10	F	0.25	0/1265	0.56	1/1710 (0.1%)
11	G	0.29	0/780	0.69	0/1057
12	H	0.37	0/732	0.70	1/996 (0.1%)
13	I	0.36	0/238	0.84	0/324
14	J	0.35	0/364	0.70	0/495
15	K	0.23	0/626	0.56	0/847
16	L	0.26	0/1261	0.59	0/1726
17	N	0.19	0/701	0.49	0/939
18	O	0.26	0/762	0.65	0/1041
19	X	0.53	3/1109 (0.3%)	1.13	7/1547 (0.5%)
19	Z	0.17	0/1109	0.42	1/1547 (0.1%)
20	Y	0.17	0/1127	0.45	0/1571
All	All	0.28	3/31162 (0.0%)	0.61	28/42557 (0.1%)

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
6	B	0	1
7	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	D	0	1
14	J	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	X	216	PRO	CG-CD	-9.81	1.17	1.50
19	X	216	PRO	CB-CG	-8.18	1.08	1.49
19	X	170	PRO	CG-CD	-7.20	1.26	1.50

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	X	216	PRO	CB-CG-CD	23.09	179.97	106.10
19	X	216	PRO	N-CD-CG	-19.72	73.62	103.20
19	X	216	PRO	CA-CB-CG	-15.99	74.12	104.50
19	X	170	PRO	N-CD-CG	-14.10	82.05	103.20
19	X	170	PRO	CA-CB-CG	-10.22	85.08	104.50
19	X	170	PRO	N-CA-CB	-7.61	94.96	103.33
6	B	664	LEU	CA-C-N	-6.88	116.13	123.08
6	B	664	LEU	C-N-CA	-6.88	116.13	123.08
4	4	188	SER	CA-C-N	6.88	134.35	121.97
4	4	188	SER	C-N-CA	6.88	134.35	121.97
6	B	276	HIS	CA-CB-CG	6.71	120.52	113.80
12	H	81	PRO	N-CA-C	-6.65	104.29	113.53
6	B	276	HIS	CB-CA-C	6.53	121.02	109.65
2	2	184	PRO	CA-N-CD	-6.49	102.91	112.00
10	F	182	MET	CB-CG-SD	6.15	131.15	112.70
5	A	347	HIS	CA-C-N	5.99	132.98	121.54
5	A	347	HIS	C-N-CA	5.99	132.98	121.54
19	X	216	PRO	CA-N-CD	-5.91	103.73	112.00
1	1	179	GLU	CA-CB-CG	5.85	125.80	114.10
19	Z	55	PRO	CA-N-CD	-5.77	103.92	112.00
5	A	612	MET	CB-CG-SD	5.52	129.25	112.70
5	A	683	MET	CB-CG-SD	5.44	129.02	112.70
6	B	520	HIS	CB-CG-CD2	5.41	138.24	131.20
2	2	216	GLU	CA-CB-CG	5.27	124.64	114.10
6	B	159	PRO	CA-C-N	5.27	131.61	121.54
6	B	159	PRO	C-N-CA	5.27	131.61	121.54
5	A	454	ILE	CA-C-N	-5.08	114.16	122.54
5	A	454	ILE	C-N-CA	-5.08	114.16	122.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	B	276	HIS	Sidechain
7	C	26	LEU	Peptide
8	D	162	HIS	Peptide
14	J	41	PHE	Peptide

5.2 Too-close contacts

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	1	1560	0	1507	37	0
2	2	1612	0	1552	42	0
3	3	1723	0	1688	41	0
4	4	1570	0	1527	38	0
5	A	5839	0	5687	183	0
6	B	5856	0	5634	152	0
7	C	602	0	585	13	0
8	D	1128	0	1135	19	0
9	E	518	0	517	6	0
10	F	1236	0	1274	30	0
11	G	760	0	734	17	0
12	H	709	0	704	26	0
13	I	232	0	252	4	0
14	J	353	0	363	15	0
15	K	620	0	647	21	0
16	L	1223	0	1228	25	0
17	N	685	0	658	10	0
18	O	733	0	710	9	0
19	X	1094	0	618	1	0
19	Z	1094	0	618	1	0
20	Y	1112	0	618	1	0
21	1	89	0	60	2	0
21	2	188	0	127	11	0
21	3	97	0	67	3	0
21	4	177	0	111	5	0
21	X	281	0	188	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	Y	276	0	186	3	0
21	Z	280	0	186	5	0
22	1	614	0	477	30	0
22	2	544	0	437	21	0
22	3	628	0	508	24	0
22	4	487	0	352	17	0
22	A	2512	0	2384	161	0
22	B	2368	0	2303	159	0
22	F	92	0	66	4	0
22	G	143	0	111	11	0
22	H	41	0	29	0	0
22	J	41	0	28	1	0
22	K	191	0	151	9	0
22	L	155	0	138	16	0
22	N	44	0	30	0	0
22	O	258	0	224	6	0
22	X	322	0	230	4	0
22	Y	387	0	303	3	0
22	Z	368	0	264	0	0
23	1	42	0	56	4	0
23	2	42	0	56	4	0
23	3	42	0	56	5	0
23	4	84	0	112	9	0
24	1	44	0	56	4	0
24	2	44	0	56	9	0
24	3	44	0	56	7	0
24	4	44	0	56	5	0
25	1	40	0	56	6	0
25	2	40	0	56	12	0
25	3	40	0	56	2	0
25	4	40	0	56	1	0
25	A	239	0	333	34	0
25	B	310	0	431	44	0
25	F	40	0	56	6	0
25	G	40	0	56	4	0
25	I	40	0	56	5	0
25	J	80	0	112	11	0
25	K	40	0	56	5	0
25	L	160	0	223	12	0
25	O	80	0	112	9	0
26	1	104	0	147	4	0
26	2	123	0	135	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	3	38	0	46	3	0
26	4	92	0	96	5	0
26	A	176	0	215	29	0
26	B	71	0	86	10	0
26	F	31	0	35	3	0
26	G	61	0	65	2	0
26	O	57	0	60	2	0
26	X	22	0	16	0	0
27	1	37	0	43	3	0
27	3	58	0	58	3	0
27	F	65	0	70	3	0
27	N	32	0	34	2	0
28	A	33	0	46	4	0
28	B	30	0	37	7	0
29	A	8	0	0	0	0
29	C	16	0	0	2	0
30	A	65	0	71	4	0
31	B	59	0	79	4	0
31	G	39	0	47	9	0
31	J	58	0	77	0	0
31	O	53	0	64	4	0
All	All	43745	0	40906	1027	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 12.

All (1027) 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)
6:B:659:THR:O	6:B:662:MET:HB2	1.56	1.05
5:A:50:HIS:HE1	22:A:828:CLA:ND	1.55	1.03
22:1:303:CLA:HHB	31:G:201:DGD:HA22	1.45	0.97
5:A:198:HIS:HE1	22:A:838:CLA:ND	1.71	0.87
22:B:819:CLA:HAB	22:B:848:CLA:HHB	1.57	0.86
5:A:74:HIS:CE1	22:A:830:CLA:ND	2.45	0.85
22:2:318:CLA:HAC1	21:3:307:CHL:HBB2	1.59	0.85
22:B:812:CLA:HBA1	31:G:201:DGD:HB31	1.60	0.84
1:1:84:CYS:HB3	1:1:188:GLY:HA3	1.63	0.81
11:G:49:LEU:N	26:G:203:LHG:HO1	1.79	0.79
22:B:811:CLA:H71	31:G:201:DGD:HA41	1.66	0.78
10:F:187:ILE:HD11	14:J:14:LEU:HG	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:843:LHG:H342	22:B:849:CLA:HHD	1.66	0.77
6:B:178:HIS:HE1	22:B:803:CLA:ND	1.81	0.75
26:B:843:LHG:HC82	26:B:843:LHG:H272	1.69	0.74
10:F:159:ILE:O	10:F:162:TRP:HB3	1.88	0.74
15:K:101:THR:H	15:K:104:ASP:HB2	1.53	0.73
12:H:49:TYR:HB2	12:H:57:ASP:HB2	1.69	0.73
1:1:91:VAL:HG11	23:1:310:LUT:H12	1.70	0.72
26:F:301:LHG:H101	26:F:301:LHG:HC62	1.71	0.72
5:A:405:HIS:HE1	22:A:855:CLA:NA	1.88	0.71
27:3:305:MGE:C1G	26:A:822:LHG:HC92	2.19	0.71
22:4:304:CLA:HAB	24:4:320:XAT:H32	1.71	0.71
22:A:832:CLA:HMB3	22:A:833:CLA:HBB	1.73	0.70
22:A:844:CLA:H172	22:A:852:CLA:H12	1.73	0.70
3:3:103:MET:HB3	22:3:311:CLA:HBB2	1.73	0.69
1:1:201:GLN:HE21	22:1:307:CLA:C4D	1.99	0.69
5:A:175:TRP:NE1	26:A:822:LHG:O10	2.25	0.69
22:B:809:CLA:H2	22:B:816:CLA:H91	1.73	0.69
27:3:305:MGE:H1G1	26:A:822:LHG:HC92	1.75	0.68
21:Z:302:CHL:HBB2	21:Z:303:CHL:HBB1	1.75	0.68
6:B:355:LEU:HD13	22:B:807:CLA:HAA1	1.76	0.68
22:B:829:CLA:HAB	28:B:832:PQN:H151	1.76	0.68
25:3:303:BCR:H282	22:3:320:CLA:HAB	1.76	0.67
6:B:573:TRP:HE1	31:B:841:DGD:HB21	1.59	0.67
27:1:315:MGE:H5B2	22:G:205:CLA:ND	2.10	0.67
15:K:113:HIS:CD2	22:K:204:CLA:NC	2.62	0.66
6:B:373:THR:HG22	22:B:817:CLA:HAB	1.77	0.66
25:A:817:BCR:H10C	22:A:846:CLA:H101	1.77	0.66
22:A:804:CLA:HAB	25:A:817:BCR:H271	1.78	0.66
11:G:140:TYR:CG	22:G:205:CLA:HED1	2.30	0.66
22:B:802:CLA:HHD	25:B:840:BCR:H19C	1.76	0.66
2:2:166:ARG:NH1	22:2:322:CLA:OBD	2.28	0.66
25:B:835:BCR:H401	22:B:848:CLA:HMC1	1.78	0.66
26:2:314:LHG:C16	26:A:822:LHG:H111	2.26	0.65
22:B:816:CLA:H121	25:B:838:BCR:H15C	1.77	0.65
22:1:303:CLA:HMB2	31:G:201:DGD:HA42	1.77	0.65
26:2:314:LHG:C16	26:A:822:LHG:C10	2.74	0.65
26:A:823:LHG:HC81	22:A:856:CLA:HBA2	1.79	0.65
6:B:192:GLY:O	6:B:196:HIS:HB2	1.97	0.65
24:3:302:XAT:H28	22:3:312:CLA:HBB2	1.79	0.65
22:B:803:CLA:H2	22:B:847:CLA:H62	1.77	0.65
22:B:810:CLA:HMB1	25:G:202:BCR:H20C	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:116:TRP:HB3	25:J:101:BCR:H323	1.79	0.65
5:A:393:TRP:CD1	22:A:853:CLA:HAB	2.31	0.65
5:A:118:ILE:HG13	5:A:119:VAL:HG13	1.80	0.64
6:B:556:SER:HB3	31:B:841:DGD:HD2	1.80	0.64
6:B:347:LEU:O	6:B:351:HIS:HB2	1.97	0.64
6:B:429:LEU:HB3	6:B:525:LEU:HB2	1.80	0.63
10:F:159:ILE:HG23	22:F:305:CLA:HAA1	1.79	0.63
28:B:832:PQN:H221	25:B:839:BCR:H17C	1.79	0.63
22:1:308:CLA:HBC1	23:1:310:LUT:H182	1.80	0.63
4:4:234:LEU:HB2	23:4:319:LUT:H22	1.81	0.63
2:2:196:PRO:HB3	21:2:302:CHL:HBC2	1.80	0.63
22:A:810:CLA:H72	22:B:829:CLA:H43	1.80	0.63
22:A:832:CLA:HED1	17:N:92:ALA:HB2	1.81	0.63
22:1:303:CLA:CHB	31:G:201:DGD:HA22	2.27	0.62
22:B:850:CLA:HAB	22:B:851:CLA:HAA2	1.81	0.62
15:K:115:MET:HE1	22:K:205:CLA:HBB2	1.79	0.62
27:3:304:MGE:H4A1	27:3:304:MGE:H2B2	1.81	0.62
22:2:322:CLA:HBB2	22:4:304:CLA:HHD	1.81	0.62
16:L:110:PRO:HG3	22:L:307:CLA:HBB1	1.80	0.62
26:1:313:LHG:H112	22:1:317:CLA:HBC1	1.82	0.62
5:A:519:VAL:HG11	5:A:522:LEU:HD23	1.81	0.62
22:B:827:CLA:H71	25:F:302:BCR:H372	1.81	0.62
22:A:835:CLA:HBB2	22:A:838:CLA:HMA3	1.82	0.62
6:B:203:ARG:NH2	6:B:253:ALA:O	2.32	0.62
12:H:120:SER:HB3	12:H:123:LEU:HG	1.82	0.62
22:A:858:CLA:H13	25:I:101:BCR:H393	1.81	0.62
6:B:369:ALA:HB1	6:B:725:LEU:HD11	1.81	0.61
14:J:8:LEU:HA	14:J:13:VAL:HG11	1.82	0.61
6:B:45:ASN:ND2	22:B:833:CLA:OBD	2.34	0.61
6:B:700:LEU:HD21	28:B:832:PQN:H152	1.82	0.61
9:E:76:LYS:HE3	9:E:77:ARG:H	1.65	0.61
5:A:124:LEU:HD11	22:A:834:CLA:HBC3	1.82	0.61
5:A:560:LEU:O	8:D:128:ARG:NH2	2.34	0.61
12:H:75:ALA:O	12:H:76:PRO:C	2.43	0.60
14:J:43:SER:OG	14:J:44:PHE:N	2.33	0.60
5:A:363:VAL:HG11	22:A:844:CLA:H201	1.83	0.60
6:B:301:ILE:HG21	22:B:814:CLA:HBC2	1.82	0.60
3:3:266:LYS:O	5:A:244:ARG:NH1	2.34	0.60
6:B:422:LEU:HD13	6:B:532:LEU:HA	1.84	0.60
16:L:52:GLN:O	16:L:55:GLN:NE2	2.34	0.60
6:B:54:LEU:HD13	25:B:840:BCR:H401	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:4:322:LUT:H161	23:4:322:LUT:H8	1.83	0.60
5:A:552:VAL:HG11	25:A:817:BCR:HC31	1.83	0.60
25:J:101:BCR:H321	25:J:101:BCR:HC8	1.83	0.60
26:4:301:LHG:HC81	26:4:301:LHG:H262	1.84	0.60
7:C:27:GLU:OE1	8:D:176:ARG:NE	2.34	0.60
5:A:50:HIS:HD2	22:A:829:CLA:HAC1	1.67	0.59
22:A:837:CLA:HBC3	22:A:838:CLA:HAB	1.84	0.59
6:B:490:ARG:HD3	11:G:143:ASN:HD22	1.66	0.59
22:B:815:CLA:HMA1	25:B:838:BCR:H14C	1.84	0.59
25:B:834:BCR:H362	25:G:202:BCR:H393	1.85	0.59
3:3:249:LEU:HD13	23:3:301:LUT:H163	1.83	0.59
5:A:367:HIS:ND1	22:A:843:CLA:OBD	2.36	0.59
15:K:94:THR:OG1	15:K:100:PHE:O	2.21	0.59
6:B:178:HIS:CD2	22:B:803:CLA:NB	2.71	0.59
5:A:474:ILE:HD11	16:L:118:ARG:HH21	1.69	0.58
25:B:834:BCR:H381	25:B:836:BCR:H312	1.85	0.58
22:B:823:CLA:H12	25:B:844:BCR:HC42	1.85	0.58
10:F:152:PRO:HG3	14:J:39:PHE:HB2	1.85	0.58
12:H:56:PHE:CE2	12:H:58:LEU:HG	2.38	0.58
22:A:848:CLA:H3A	22:O:208:CLA:HBA1	1.86	0.58
25:B:844:BCR:H321	10:F:156:PHE:HB2	1.85	0.58
3:3:249:LEU:HD22	23:3:301:LUT:H172	1.84	0.58
5:A:495:THR:HG21	22:A:803:CLA:HMD1	1.86	0.58
6:B:668:ARG:HE	6:B:699:ALA:HB3	1.69	0.58
11:G:75:ARG:NH2	11:G:112:GLY:O	2.36	0.58
5:A:200:ALA:HB2	5:A:306:GLY:HA3	1.84	0.58
5:A:313:TRP:HD1	15:K:92:LEU:HD21	1.68	0.58
6:B:716:GLY:O	6:B:720:THR:OG1	2.17	0.58
23:2:310:LUT:H8	23:2:310:LUT:H171	1.86	0.57
22:A:831:CLA:HMB1	22:A:855:CLA:HBB2	1.85	0.57
5:A:445:LEU:HB3	5:A:539:PHE:HB2	1.86	0.57
3:3:180:LEU:HD11	25:3:303:BCR:H343	1.85	0.57
3:3:249:LEU:HB2	23:3:301:LUT:H22	1.86	0.57
2:2:111:ARG:NH2	2:2:194:GLY:O	2.37	0.57
26:A:824:LHG:H241	16:L:114:THR:HG22	1.85	0.57
25:1:312:BCR:HC21	11:G:68:PHE:HB3	1.85	0.57
12:H:82:LEU:C	12:H:84:SER:H	2.13	0.57
4:4:146:GLU:O	4:4:150:PHE:HB2	2.04	0.57
6:B:424:TRP:NE1	22:B:822:CLA:OBD	2.38	0.57
6:B:348:VAL:HG21	22:B:818:CLA:HHD	1.87	0.57
25:2:312:BCR:H403	21:2:321:CHL:C4A	2.26	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:202:LEU:HD13	22:A:838:CLA:HBB	1.87	0.57
5:A:594:LEU:HD21	22:A:855:CLA:HBC1	1.85	0.57
15:K:56:MET:HE1	15:K:117:VAL:HG23	1.86	0.57
1:1:189:ARG:NH2	22:1:317:CLA:O1D	2.38	0.56
5:A:538:ALA:HB2	22:A:806:CLA:HMA1	1.87	0.56
7:C:55:GLU:HB3	7:C:63:LEU:HD13	1.86	0.56
5:A:398:LEU:HD21	22:A:831:CLA:H142	1.88	0.56
22:A:810:CLA:H172	16:L:107:LEU:HD21	1.88	0.56
16:L:201:LEU:HG	22:L:307:CLA:HED3	1.88	0.56
4:4:195:PHE:HB2	22:4:311:CLA:HBA1	1.88	0.56
5:A:118:ILE:HB	25:J:101:BCR:H322	1.88	0.56
5:A:202:LEU:HD11	22:A:838:CLA:H11	1.88	0.56
6:B:26:ALA:HA	22:B:819:CLA:H42	1.86	0.56
4:4:61:LEU:HD12	4:4:62:PRO:HD2	1.86	0.56
26:2:313:LHG:H101	26:4:302:LHG:H251	1.88	0.56
14:J:12:PRO:HB2	25:J:101:BCR:H391	1.88	0.56
2:2:250:LEU:HB2	23:2:310:LUT:H24	1.87	0.56
25:2:312:BCR:H21C	21:2:321:CHL:H3A	1.87	0.56
5:A:411:VAL:HG21	5:A:569:PHE:HB2	1.88	0.56
25:A:818:BCR:H323	22:A:853:CLA:H11	1.88	0.56
6:B:86:PRO:O	6:B:116:ALA:N	2.36	0.56
6:B:358:TYR:OH	22:B:818:CLA:OBD	2.22	0.56
22:B:816:CLA:H192	22:B:831:CLA:H141	1.88	0.56
14:J:10:VAL:HG13	14:J:12:PRO:HD2	1.86	0.56
5:A:717:LEU:N	28:A:811:PQN:O4	2.39	0.55
22:B:846:CLA:HAC1	25:L:303:BCR:HC22	1.88	0.55
5:A:588:ASP:HA	5:A:591:PHE:HB3	1.88	0.55
22:X:304:CLA:HHC	22:X:304:CLA:HBB1	1.88	0.55
22:2:303:CLA:HHC	22:2:303:CLA:HBB1	1.88	0.55
6:B:317:ARG:NH1	6:B:404:GLU:O	2.40	0.55
22:B:803:CLA:H171	22:B:818:CLA:H93	1.87	0.55
12:H:97:ARG:NH1	16:L:152:GLU:OE2	2.39	0.55
2:2:250:LEU:HD13	23:2:310:LUT:H24	1.86	0.55
4:4:106:GLY:HA2	24:4:320:XAT:H181	1.87	0.55
6:B:168:PHE:O	6:B:174:ARG:NH2	2.33	0.55
7:C:17:CYS:HB3	29:C:102:SF4:S4	2.46	0.55
26:B:843:LHG:H152	22:B:849:CLA:HBC1	1.87	0.55
1:1:180:TYR:HB3	22:1:304:CLA:HBB	1.88	0.55
22:A:804:CLA:HHC	22:A:804:CLA:HBB1	1.89	0.55
22:1:317:CLA:H41	22:B:831:CLA:HBB2	1.88	0.55
5:A:266:TRP:CH2	22:A:842:CLA:HBB1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:842:CLA:CHD	22:A:843:CLA:HBB2	2.37	0.55
22:A:858:CLA:OBD	6:B:670:TYR:OH	2.21	0.55
22:O:209:CLA:HHC	22:O:209:CLA:HBB1	1.88	0.54
10:F:186:ILE:HG12	14:J:10:VAL:HG23	1.89	0.54
2:2:111:ARG:NH1	2:2:221:GLU:OE2	2.37	0.54
22:B:818:CLA:HBB1	22:B:818:CLA:HHC	1.90	0.54
22:B:824:CLA:HHC	22:B:824:CLA:HBB1	1.89	0.54
5:A:116:TRP:CB	25:J:101:BCR:H323	2.38	0.54
22:B:816:CLA:HBB1	22:B:816:CLA:HHC	1.89	0.54
22:G:206:CLA:HHC	22:G:206:CLA:HBB1	1.89	0.54
16:L:93:LEU:HB2	16:L:181:LYS:HB3	1.88	0.54
17:N:91:ARG:O	27:N:201:MGE:O4D	2.24	0.54
3:3:239:LEU:HD22	26:3:306:LHG:H282	1.89	0.54
5:A:445:LEU:HD13	5:A:539:PHE:HA	1.88	0.54
2:2:111:ARG:HA	2:2:114:MET:HE3	1.89	0.54
2:2:146:PHE:O	4:4:243:HIS:NE2	2.40	0.54
2:2:147:THR:OG1	2:2:148:ASP:N	2.41	0.54
6:B:649:MET:HA	6:B:652:PHE:HB3	1.90	0.54
22:A:812:CLA:HHC	22:A:812:CLA:HBB1	1.90	0.54
8:D:92:GLU:HG2	8:D:93:GLU:HG2	1.90	0.54
10:F:165:TRP:O	10:F:168:ARG:HB3	2.07	0.54
5:A:171:LEU:HD23	26:A:822:LHG:C31	2.37	0.54
22:B:808:CLA:HHC	22:B:808:CLA:HBB1	1.89	0.54
5:A:456:ASN:HD21	5:A:469:PHE:HB2	1.73	0.54
5:A:596:TRP:CH2	22:A:827:CLA:HAB	2.42	0.54
22:A:855:CLA:HHC	22:A:855:CLA:HBB1	1.90	0.54
22:B:813:CLA:HBA2	25:B:837:BCR:H14C	1.89	0.54
12:H:56:PHE:O	12:H:57:ASP:C	2.49	0.54
22:B:825:CLA:HAA2	22:G:205:CLA:HMA1	1.90	0.53
31:O:201:DGD:HA22	25:O:203:BCR:H292	1.89	0.53
5:A:596:TRP:HH2	22:A:827:CLA:HAB	1.74	0.53
6:B:136:TYR:CE1	26:B:843:LHG:HC92	2.43	0.53
1:1:75:ARG:NH2	31:G:201:DGD:O1B	2.38	0.53
5:A:171:LEU:HD23	26:A:822:LHG:H312	1.90	0.53
5:A:429:ARG:NH1	8:D:80:GLY:O	2.33	0.53
7:C:29:ILE:HD11	8:D:181:GLN:HE22	1.72	0.53
2:2:111:ARG:NE	21:2:302:CHL:OBD	2.35	0.53
2:2:166:ARG:NE	21:2:309:CHL:HMC	2.24	0.53
21:4:308:CHL:HHC	21:4:308:CHL:HBB1	1.90	0.53
20:Y:226:PRO:HD3	21:Z:303:CHL:HBA2	1.89	0.53
22:B:849:CLA:HMB3	22:B:850:CLA:HBB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:101:ARG:NH1	21:4:309:CHL:OBD	2.40	0.53
5:A:96:SER:O	17:N:88:ASN:ND2	2.41	0.53
6:B:389:HIS:HE1	22:B:819:CLA:NA	2.06	0.53
22:B:812:CLA:H93	25:B:834:BCR:HC22	1.91	0.53
4:4:191:ASN:OD1	23:4:319:LUT:O23	2.27	0.53
6:B:519:VAL:HG11	6:B:593:TYR:HB2	1.90	0.53
5:A:175:TRP:CD2	26:A:822:LHG:H252	2.44	0.53
22:A:809:CLA:HAC1	28:A:811:PQN:H171	1.90	0.53
8:D:63:GLY:N	8:D:65:VAL:O	2.42	0.53
5:A:98:TYR:OH	5:A:150:ILE:O	2.26	0.53
5:A:518:LYS:NZ	5:A:750:GLY:OXT	2.41	0.53
5:A:536:ILE:HD12	30:A:825:CL0:H63	1.91	0.53
22:A:853:CLA:H202	25:J:103:BCR:H19C	1.91	0.53
2:2:233:MET:HG2	24:2:311:XAT:H14	1.91	0.52
5:A:215:ILE:HD13	22:A:840:CLA:HBC2	1.90	0.52
25:O:203:BCR:HC31	26:O:205:LHG:HC41	1.91	0.52
1:1:192:MET:HG2	24:1:311:XAT:H15	1.91	0.52
4:4:205:GLU:HG3	22:4:311:CLA:C4B	2.40	0.52
6:B:53:GLN:HG2	22:B:847:CLA:H3A	1.92	0.52
1:1:189:ARG:HB3	22:1:317:CLA:HBC3	1.92	0.52
22:A:801:CLA:H102	28:B:832:PQN:H211	1.92	0.52
5:A:175:TRP:CZ2	26:A:822:LHG:C23	2.92	0.52
22:B:804:CLA:H192	25:B:835:BCR:H14C	1.90	0.52
22:B:849:CLA:HMB2	25:I:101:BCR:H313	1.90	0.52
21:1:316:CHL:HBB2	22:1:317:CLA:HHD	1.92	0.52
5:A:317:HIS:HB3	5:A:322:ILE:HD11	1.91	0.52
6:B:341:LEU:O	6:B:345:THR:OG1	2.24	0.52
6:B:718:ILE:HG23	22:B:817:CLA:HBB1	1.91	0.52
7:C:40:ALA:O	8:D:181:GLN:NE2	2.42	0.52
1:1:202:GLN:NE2	1:1:208:THR:O	2.42	0.52
22:B:852:CLA:NA	25:L:301:BCR:H393	2.25	0.52
5:A:364:VAL:HG22	22:A:844:CLA:H43	1.92	0.52
22:A:857:CLA:HBB1	22:L:306:CLA:H93	1.92	0.52
22:B:802:CLA:HHC	22:B:802:CLA:HBB1	1.91	0.52
22:B:807:CLA:HBA2	22:B:816:CLA:HBB2	1.91	0.52
12:H:74:ASP:OD1	12:H:74:ASP:N	2.38	0.52
5:A:159:THR:HG23	22:A:839:CLA:HBA1	1.92	0.52
5:A:175:TRP:CE2	26:A:822:LHG:C23	2.92	0.52
22:A:803:CLA:HMB2	22:A:852:CLA:C4A	2.30	0.52
1:1:183:LYS:HE2	22:1:306:CLA:HBD	1.92	0.52
2:2:159:LEU:HD23	25:2:312:BCR:H14C	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:857:CLA:H2	22:L:306:CLA:H43	1.91	0.52
1:1:149:ARG:NH2	22:1:303:CLA:O2D	2.44	0.51
26:2:316:LHG:HC81	17:N:103:PRO:HG3	1.92	0.51
5:A:194:MET:HB2	22:A:838:CLA:HBC2	1.91	0.51
5:A:550:LYS:HZ1	6:B:673:GLU:HB2	1.75	0.51
5:A:672:LEU:HD21	6:B:620:LEU:HD22	1.91	0.51
22:B:803:CLA:H72	22:B:814:CLA:H43	1.92	0.51
12:H:97:ARG:HG2	16:L:180:ALA:HB2	1.93	0.51
1:1:69:VAL:HB	1:1:72:ASN:HB2	1.92	0.51
2:2:225:GLY:O	2:2:229:MET:HG3	2.09	0.51
21:Y:304:CHL:HAB	21:Y:307:CHL:HMC	1.92	0.51
5:A:559:ARG:NH2	8:D:82:THR:O	2.44	0.51
30:A:825:CL0:H11	22:B:801:CLA:HMD1	1.92	0.51
4:4:151:HIS:HE1	22:4:316:CLA:ND	2.08	0.51
10:F:152:PRO:O	10:F:155:LEU:HB3	2.10	0.51
5:A:576:PRO:HD2	7:C:52:LYS:HG3	1.92	0.51
22:A:841:CLA:HHC	22:A:841:CLA:HBB1	1.92	0.51
22:B:817:CLA:H93	22:B:850:CLA:H12	1.93	0.51
6:B:389:HIS:HA	6:B:392:ILE:HD12	1.92	0.51
1:1:52:ASP:OD1	1:1:53:GLY:N	2.43	0.51
2:2:238:GLN:HE22	23:2:310:LUT:H222	1.75	0.51
24:2:311:XAT:H181	22:2:318:CLA:H142	1.92	0.51
5:A:198:HIS:CD2	22:A:838:CLA:NB	2.79	0.51
6:B:344:ILE:HB	22:B:808:CLA:H62	1.91	0.51
22:B:823:CLA:H92	22:F:305:CLA:HHB	1.93	0.51
5:A:175:TRP:CZ2	26:A:822:LHG:H242	2.46	0.51
5:A:578:ARG:NH2	8:D:130:GLU:OE2	2.42	0.51
22:A:846:CLA:H12	22:A:849:CLA:HBA2	1.92	0.51
22:B:811:CLA:H72	22:B:812:CLA:H72	1.92	0.51
22:O:208:CLA:HHC	22:O:208:CLA:HBB1	1.92	0.51
25:A:816:BCR:H23C	22:A:846:CLA:H171	1.93	0.51
25:B:840:BCR:H17C	25:B:840:BCR:H21C	1.92	0.51
12:H:112:VAL:HG21	13:I:16:LEU:HD12	1.93	0.51
16:L:113:LEU:HD12	22:L:307:CLA:HMB1	1.93	0.51
14:J:9:SER:HA	14:J:14:LEU:HD23	1.93	0.51
14:J:28:GLU:OE1	14:J:31:ARG:NH2	2.44	0.51
27:1:315:MGE:C5B	22:G:205:CLA:ND	2.71	0.50
21:2:302:CHL:HMA1	25:2:312:BCR:H19C	1.93	0.50
4:4:94:GLN:HG3	4:4:161:ILE:HG12	1.93	0.50
22:B:822:CLA:HMB1	25:B:844:BCR:H12C	1.92	0.50
25:B:839:BCR:H403	25:B:839:BCR:H23C	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:90:TRP:NE1	9:E:116:LYS:O	2.41	0.50
10:F:165:TRP:HE3	25:F:302:BCR:HC31	1.76	0.50
12:H:78:PRO:HG2	12:H:79:TYR:CZ	2.46	0.50
1:1:111:TRP:HZ2	22:1:320:CLA:HHD	1.75	0.50
2:2:176:CYS:SG	2:2:177:VAL:N	2.84	0.50
26:A:820:LHG:H341	22:A:831:CLA:H92	1.93	0.50
6:B:176:ASN:ND2	6:B:291:TYR:O	2.44	0.50
22:B:849:CLA:H2	25:I:101:BCR:HC42	1.93	0.50
22:B:849:CLA:H3A	22:B:850:CLA:HMB3	1.94	0.50
11:G:140:TYR:CD2	22:G:205:CLA:HED1	2.47	0.50
25:L:302:BCR:H342	25:L:304:BCR:H353	1.93	0.50
18:O:42:LEU:HB3	25:O:202:BCR:HC42	1.94	0.50
3:3:168:TRP:HA	3:3:192:PRO:HB3	1.93	0.50
5:A:583:GLN:HE21	6:B:667:TRP:HB2	1.77	0.50
22:A:827:CLA:H91	22:A:858:CLA:H102	1.93	0.50
6:B:125:TYR:O	6:B:130:ARG:NH1	2.45	0.50
4:4:113:PRO:O	4:4:117:THR:OG1	2.27	0.50
31:B:841:DGD:O5D	31:B:841:DGD:O4D	2.30	0.50
7:C:74:THR:HG23	7:C:79:LEU:HB2	1.94	0.50
2:2:238:GLN:HB3	2:2:249:ASN:HD22	1.76	0.50
21:2:302:CHL:HMB2	25:2:312:BCR:H15C	1.94	0.50
5:A:201:GLY:HA2	22:A:845:CLA:HBC1	1.93	0.50
15:K:94:THR:HG21	15:K:99:GLY:HA2	1.93	0.50
1:1:144:PHE:HD2	25:1:312:BCR:H352	1.77	0.50
3:3:105:VAL:HG11	23:3:301:LUT:H12	1.93	0.50
21:4:309:CHL:OMC	21:4:317:CHL:HMC	2.10	0.50
5:A:689:ARG:NH1	6:B:566:GLY:O	2.40	0.50
22:A:857:CLA:H52	22:L:306:CLA:H43	1.93	0.50
6:B:190:TRP:HD1	6:B:277:HIS:CG	2.29	0.50
22:B:805:CLA:HBB1	25:B:834:BCR:H382	1.93	0.50
9:E:117:VAL:HG12	9:E:123:SER:HB3	1.93	0.50
2:2:70:GLY:HA2	3:3:173:SER:HB2	1.94	0.50
4:4:203:GLU:HB3	22:4:312:CLA:HED2	1.92	0.50
5:A:264:LEU:O	15:K:124:LYS:NZ	2.45	0.50
22:A:857:CLA:H52	22:L:306:CLA:H11	1.94	0.50
6:B:136:TYR:CD2	26:B:843:LHG:HC5	2.46	0.50
3:3:144:ALA:HB3	3:3:149:LEU:HG	1.93	0.50
26:A:822:LHG:H272	22:A:836:CLA:CBB	2.42	0.50
22:A:846:CLA:H52	22:A:849:CLA:H51	1.94	0.50
6:B:134:ASP:OD2	6:B:208:ARG:NH1	2.44	0.50
6:B:700:LEU:HB3	6:B:704:GLN:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:212:THR:OG1	10:F:214:ASN:OD1	2.30	0.50
25:O:203:BCR:HC41	26:O:205:LHG:HC62	1.92	0.50
1:1:184:GLU:HA	22:1:304:CLA:HBB1	1.93	0.49
5:A:440:TRP:CE2	22:A:857:CLA:HAB	2.47	0.49
5:A:682:LEU:HA	5:A:685:LEU:HB2	1.94	0.49
6:B:457:PRO:HB3	6:B:517:PHE:HB2	1.94	0.49
10:F:88:ILE:HD12	10:F:112:ILE:HG23	1.93	0.49
2:2:191:THR:OG1	2:2:192:ASP:N	2.42	0.49
5:A:279:LEU:HD21	5:A:372:PRO:HD2	1.93	0.49
5:A:578:ARG:HH11	5:A:581:THR:HG21	1.76	0.49
5:A:622:ASP:OD1	5:A:622:ASP:N	2.44	0.49
6:B:395:ILE:HG23	6:B:551:LYS:HA	1.93	0.49
11:G:119:LEU:O	11:G:123:SER:OG	2.25	0.49
22:G:206:CLA:H72	22:G:207:CLA:HBB1	1.95	0.49
4:4:197:PRO:O	4:4:202:LYS:NZ	2.45	0.49
25:A:817:BCR:H12C	22:A:846:CLA:H8	1.95	0.49
25:F:302:BCR:H381	22:F:306:CLA:HBA1	1.94	0.49
1:1:233:ARG:NH1	1:1:234:THR:O	2.45	0.49
5:A:236:LEU:HB2	5:A:239:GLU:HG3	1.93	0.49
5:A:456:ASN:HA	5:A:468:MET:HG2	1.95	0.49
30:A:825:CL0:H7	22:B:845:CLA:HAB	1.94	0.49
22:A:859:CLA:H122	14:J:14:LEU:HD11	1.94	0.49
6:B:352:MET:HE2	22:B:808:CLA:HBA1	1.94	0.49
16:L:56:PRO:HB3	16:L:61:PRO:HA	1.95	0.49
17:N:112:LEU:O	17:N:116:LYS:N	2.45	0.49
6:B:194:LEU:HA	6:B:198:ALA:HB3	1.93	0.49
28:B:832:PQN:H142	25:B:839:BCR:H271	1.95	0.49
10:F:161:GLY:O	10:F:165:TRP:N	2.46	0.49
22:A:828:CLA:HHC	22:A:828:CLA:HBB1	1.94	0.49
2:2:128:LYS:NZ	2:2:248:ASP:OD1	2.37	0.49
5:A:684:PHE:HA	28:A:811:PQN:H9	1.93	0.49
23:4:322:LUT:H401	23:4:322:LUT:H35	1.57	0.49
5:A:118:ILE:HG23	5:A:119:VAL:HG22	1.95	0.49
5:A:438:LEU:HD21	5:A:545:VAL:HG12	1.95	0.49
5:A:572:PRO:HB3	5:A:719:ILE:HB	1.95	0.49
22:1:318:CLA:HMA2	22:1:318:CLA:H2	1.93	0.49
5:A:10:VAL:HG13	22:A:837:CLA:HED3	1.95	0.49
5:A:94:ARG:O	17:N:91:ARG:NH1	2.45	0.49
6:B:276:HIS:HB2	22:B:807:CLA:C4B	2.42	0.49
6:B:421:HIS:HB2	22:B:820:CLA:HAB	1.95	0.49
24:2:311:XAT:H161	24:2:311:XAT:H7	1.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:844:CLA:H8	22:A:854:CLA:H203	1.94	0.48
6:B:22:TRP:CG	6:B:704:GLN:HE22	2.31	0.48
6:B:71:GLN:NE2	22:B:849:CLA:O1D	2.37	0.48
22:B:833:CLA:ND	22:B:846:CLA:O1A	2.46	0.48
1:1:88:MET:HE1	22:1:304:CLA:HHC	1.95	0.48
25:2:312:BCR:H362	21:2:321:CHL:HBA2	1.95	0.48
4:4:141:THR:O	4:4:145:ILE:HG13	2.13	0.48
4:4:250:LEU:HD21	22:4:318:CLA:HAB	1.94	0.48
5:A:404:ALA:O	5:A:408:ILE:HG13	2.13	0.48
5:A:458:THR:HG23	22:B:851:CLA:HMC3	1.95	0.48
5:A:676:PHE:HD1	22:B:801:CLA:HAA1	1.78	0.48
6:B:439:HIS:HE1	22:B:823:CLA:NA	2.11	0.48
12:H:63:ASN:O	12:H:64:THR:C	2.56	0.48
2:2:175:GLY:O	2:2:177:VAL:N	2.46	0.48
26:2:314:LHG:C16	26:A:822:LHG:C11	2.91	0.48
22:A:857:CLA:H93	22:L:306:CLA:H102	1.96	0.48
6:B:384:THR:HG22	6:B:534:LEU:HD11	1.95	0.48
22:1:317:CLA:H41	22:1:317:CLA:H61	1.53	0.48
5:A:588:ASP:OD2	5:A:723:ARG:NH1	2.46	0.48
6:B:180:SER:HB3	6:B:288:GLY:HA3	1.95	0.48
22:B:822:CLA:H61	22:B:822:CLA:H102	1.77	0.48
16:L:158:ALA:HB2	16:L:174:GLN:HG3	1.95	0.48
4:4:187:GLY:N	22:4:311:CLA:OBD	2.39	0.48
6:B:414:HIS:HB2	6:B:417:ALA:HB3	1.96	0.48
2:2:229:MET:HE2	24:2:311:XAT:H203	1.95	0.48
3:3:102:MET:SD	3:3:223:ASN:HB3	2.54	0.48
22:3:317:CLA:HHC	22:3:317:CLA:HBB1	1.96	0.48
6:B:297:ILE:HG22	11:G:74:GLN:HE22	1.78	0.48
2:2:126:LEU:HA	2:2:129:ILE:HG12	1.96	0.48
3:3:218:LEU:HD12	22:3:308:CLA:HBB1	1.95	0.48
6:B:351:HIS:CD2	22:B:816:CLA:NC	2.82	0.48
10:F:189:VAL:HB	27:F:304:MGE:H2G	1.95	0.48
12:H:82:LEU:C	12:H:84:SER:N	2.70	0.48
15:K:55:ILE:O	15:K:59:THR:OG1	2.22	0.48
2:2:266:PHE:HE1	22:2:317:CLA:HBD	1.78	0.48
22:A:827:CLA:HAA1	6:B:655:LEU:HD13	1.95	0.48
22:A:836:CLA:H62	22:A:836:CLA:H41	1.61	0.48
6:B:9:SER:OG	31:B:841:DGD:O4E	2.32	0.48
22:2:308:CLA:HHC	22:2:308:CLA:HBB1	1.95	0.48
22:3:309:CLA:H61	22:3:309:CLA:H41	1.60	0.48
5:A:34:ARG:HH22	5:A:59:HIS:HA	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:846:CLA:H202	22:A:849:CLA:HAC2	1.96	0.48
6:B:582:TRP:HH2	22:B:801:CLA:HAB	1.79	0.48
12:H:124:LEU:HG	12:H:126:ILE:HG22	1.95	0.48
24:2:311:XAT:H201	24:2:311:XAT:H15	1.58	0.47
3:3:239:LEU:HD21	26:3:306:LHG:H151	1.96	0.47
5:A:50:HIS:HE1	22:A:828:CLA:C4D	2.23	0.47
5:A:403:ALA:HB1	5:A:548:LEU:HB3	1.94	0.47
5:A:570:ARG:HG3	5:A:720:ILE:HG21	1.94	0.47
22:A:838:CLA:H62	22:A:838:CLA:H41	1.58	0.47
22:A:846:CLA:CGA	22:A:850:CLA:HBB1	2.44	0.47
22:B:822:CLA:HAC2	22:B:827:CLA:H141	1.96	0.47
18:O:111:THR:O	18:O:115:ILE:HG13	2.13	0.47
1:1:112:ALA:HB1	1:1:131:LEU:HD13	1.96	0.47
3:3:174:MET:SD	3:3:174:MET:N	2.87	0.47
5:A:75:PHE:CE1	22:A:835:CLA:HBB1	2.47	0.47
5:A:456:ASN:OD1	5:A:469:PHE:N	2.44	0.47
6:B:394:PHE:O	6:B:542:ARG:NH1	2.46	0.47
22:B:815:CLA:H42	22:B:827:CLA:HBA1	1.96	0.47
27:1:315:MGE:H5B2	22:G:205:CLA:C4D	2.45	0.47
5:A:379:THR:HG21	5:A:515:VAL:HB	1.96	0.47
6:B:147:THR:O	6:B:151:ILE:HG13	2.15	0.47
10:F:132:ASP:OD1	10:F:132:ASP:N	2.46	0.47
10:F:185:ILE:HG13	10:F:186:ILE:HG13	1.96	0.47
25:K:201:BCR:HC8	22:K:204:CLA:HMC2	1.95	0.47
23:4:322:LUT:H31	23:4:322:LUT:H391	1.59	0.47
5:A:739:TRP:HB2	22:A:853:CLA:HBB1	1.96	0.47
22:A:859:CLA:H61	22:A:859:CLA:H41	1.70	0.47
6:B:102:GLU:OE2	12:H:131:GLN:N	2.43	0.47
6:B:136:TYR:CE2	26:B:843:LHG:HC5	2.49	0.47
6:B:276:HIS:CD2	6:B:280:ILE:HG12	2.50	0.47
22:B:831:CLA:H61	22:B:831:CLA:H41	1.54	0.47
25:B:840:BCR:H351	25:B:840:BCR:H15C	1.66	0.47
26:1:313:LHG:H202	22:4:316:CLA:HMA2	1.96	0.47
22:1:318:CLA:H11	22:B:831:CLA:HMC3	1.96	0.47
25:A:815:BCR:H351	25:A:815:BCR:H15C	1.77	0.47
25:A:819:BCR:H311	25:A:819:BCR:HC7	1.69	0.47
22:A:844:CLA:H41	22:A:844:CLA:H62	1.49	0.47
6:B:299:HIS:HB3	6:B:304:LEU:HD11	1.97	0.47
22:B:808:CLA:H201	22:B:809:CLA:H121	1.96	0.47
4:4:90:ARG:O	4:4:94:GLN:HG2	2.15	0.47
5:A:673:GLY:O	5:A:676:PHE:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:114:ASN:HD21	22:B:851:CLA:HMD1	1.80	0.47
8:D:158:VAL:HG21	12:H:58:LEU:HD11	1.95	0.47
8:D:185:SER:HB3	8:D:188:LYS:HG2	1.97	0.47
22:2:308:CLA:HED3	3:3:148:THR:HG23	1.97	0.47
3:3:108:MET:HE3	3:3:128:TRP:CD2	2.50	0.47
5:A:731:LEU:HD12	5:A:735:ILE:HD11	1.97	0.47
25:A:815:BCR:H311	22:A:854:CLA:H2	1.97	0.47
22:A:830:CLA:H41	22:A:854:CLA:H152	1.95	0.47
22:A:831:CLA:HBB	22:A:855:CLA:CBB	2.44	0.47
22:A:859:CLA:HED2	10:F:184:GLU:HA	1.97	0.47
6:B:30:ASP:HB2	22:B:819:CLA:HBA2	1.95	0.47
22:B:852:CLA:HAB	13:I:15:GLY:HA3	1.97	0.47
22:Y:314:CLA:HHC	22:Y:314:CLA:HBB1	1.95	0.47
1:1:106:VAL:HG21	1:1:202:GLN:HG2	1.97	0.47
1:1:141:ALA:HB1	25:1:312:BCR:H363	1.95	0.47
1:1:189:ARG:HA	1:1:192:MET:HE3	1.97	0.47
3:3:133:VAL:HG21	24:3:302:XAT:H382	1.97	0.47
5:A:194:MET:O	5:A:198:HIS:HB2	2.14	0.47
22:A:858:CLA:H191	22:B:830:CLA:H72	1.97	0.47
6:B:32:GLU:OE2	6:B:331:HIS:NE2	2.48	0.47
22:B:827:CLA:H93	22:B:828:CLA:HBC1	1.97	0.47
8:D:185:SER:OG	9:E:87:GLU:OE2	2.28	0.47
5:A:582:CYS:HB2	6:B:667:TRP:HB3	1.96	0.47
25:A:816:BCR:H20C	25:A:816:BCR:H361	1.65	0.47
6:B:292:ARG:NH1	11:G:78:VAL:O	2.48	0.47
22:B:807:CLA:HMD3	22:B:808:CLA:H141	1.96	0.47
21:Y:313:CHL:HBB	21:Z:305:CHL:HMB3	1.95	0.47
5:A:443:ILE:HA	22:A:858:CLA:CGA	2.45	0.47
5:A:678:TRP:O	5:A:681:SER:OG	2.18	0.47
15:K:74:SER:O	15:K:88:ARG:NH2	2.38	0.47
2:2:106:GLU:HB2	22:2:318:CLA:C1B	2.45	0.46
5:A:735:ILE:HD12	26:A:820:LHG:H383	1.97	0.46
25:A:817:BCR:H15C	22:A:852:CLA:O1A	2.14	0.46
7:C:23:THR:OG1	29:C:101:SF4:S3	2.73	0.46
1:1:146:GLU:OE2	22:1:303:CLA:C4A	2.60	0.46
5:A:387:LEU:HD11	22:A:854:CLA:HED3	1.97	0.46
3:3:220:GLU:OE1	22:3:316:CLA:NB	2.49	0.46
3:3:232:LEU:O	3:3:236:VAL:HG12	2.15	0.46
24:3:302:XAT:H371	22:3:312:CLA:HBB1	1.97	0.46
24:3:302:XAT:H30	22:3:310:CLA:HAC2	1.97	0.46
5:A:346:TRP:HB3	22:A:830:CLA:HAC1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:811:CLA:H71	31:G:201:DGD:C4A	2.41	0.46
4:4:204:LYS:HD3	22:4:313:CLA:HBA1	1.96	0.46
5:A:572:PRO:HD3	5:A:720:ILE:HD11	1.96	0.46
22:A:854:CLA:HBB1	22:A:854:CLA:HMB1	1.96	0.46
6:B:174:ARG:O	6:B:178:HIS:HB2	2.15	0.46
6:B:414:HIS:NE2	22:B:820:CLA:C4D	2.79	0.46
6:B:436:LEU:HD12	6:B:453:ILE:HB	1.98	0.46
22:B:803:CLA:H93	22:B:803:CLA:H62	1.76	0.46
15:K:113:HIS:CE1	25:K:201:BCR:H14C	2.50	0.46
18:O:107:PHE:O	18:O:111:THR:HG23	2.16	0.46
22:3:310:CLA:H122	22:A:835:CLA:HBC2	1.96	0.46
4:4:82:LEU:HD21	10:F:201:ILE:HD13	1.96	0.46
28:B:832:PQN:H111	28:B:832:PQN:H2M1	1.70	0.46
25:1:312:BCR:H20C	22:1:320:CLA:HBA1	1.97	0.46
21:1:316:CHL:HBB2	22:1:317:CLA:CHD	2.45	0.46
2:2:116:GLY:O	2:2:120:ILE:HG12	2.15	0.46
5:A:385:LEU:HA	5:A:608:PHE:HE2	1.81	0.46
25:A:816:BCR:H15C	25:A:816:BCR:H351	1.61	0.46
22:A:831:CLA:H112	22:A:831:CLA:H152	1.62	0.46
6:B:526:GLY:HA2	6:B:582:TRP:CZ3	2.50	0.46
1:1:178:GLU:HA	1:1:181:LYS:HE3	1.97	0.46
2:2:66:ILE:N	3:3:177:GLN:OE1	2.48	0.46
2:2:107:LEU:HD21	2:2:195:TYR:CZ	2.51	0.46
25:2:312:BCR:H272	22:2:320:CLA:NB	2.30	0.46
4:4:156:ARG:NE	21:4:309:CHL:OMC	2.37	0.46
25:A:814:BCR:H321	25:A:814:BCR:HC8	1.97	0.46
6:B:191:THR:HG21	6:B:278:LEU:HB2	1.98	0.46
6:B:334:LEU:HD11	22:B:819:CLA:HBB1	1.98	0.46
6:B:515:GLY:O	6:B:519:VAL:HG23	2.16	0.46
22:1:317:CLA:HBB1	22:1:317:CLA:H51	1.98	0.46
5:A:508:GLY:HA2	5:A:523:PRO:HB3	1.97	0.46
25:A:816:BCR:HC7	25:A:816:BCR:H331	1.70	0.46
15:K:113:HIS:CD2	22:K:204:CLA:ND	2.79	0.46
1:1:233:ARG:NH2	10:F:143:GLN:OE1	2.49	0.46
26:2:314:LHG:C16	26:A:822:LHG:H101	2.46	0.46
3:3:189:SER:OG	3:3:194:TYR:O	2.34	0.46
10:F:141:GLY:O	10:F:146:TRP:NE1	2.46	0.46
2:2:139:THR:O	2:2:143:GLN:NE2	2.48	0.46
2:2:166:ARG:HH21	21:2:309:CHL:HBC3	1.81	0.46
25:2:312:BCR:H12C	25:2:312:BCR:H341	1.97	0.46
3:3:54:LYS:HZ3	15:K:91:GLY:HA2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:56:SER:OG	3:3:71:ASP:O	2.33	0.46
5:A:99:GLU:OE1	5:A:232:LYS:NZ	2.49	0.46
5:A:214:GLN:HA	5:A:218:SER:HB2	1.98	0.46
6:B:173:SER:OG	22:B:802:CLA:O1D	2.29	0.46
6:B:181:GLY:HA3	22:B:803:CLA:HBB1	1.99	0.46
6:B:435:GLY:HA2	22:B:823:CLA:HMC3	1.98	0.46
22:B:852:CLA:C1A	25:L:301:BCR:H393	2.46	0.46
17:N:118:VAL:HG12	17:N:120:PHE:H	1.80	0.46
1:1:214:LEU:HD22	23:1:310:LUT:H42	1.98	0.45
5:A:175:TRP:CZ2	26:A:822:LHG:C24	2.99	0.45
5:A:175:TRP:CE2	26:A:822:LHG:H252	2.51	0.45
26:A:823:LHG:H182	22:A:849:CLA:H151	1.98	0.45
22:A:853:CLA:H41	22:A:853:CLA:H61	1.58	0.45
6:B:101:VAL:HG13	6:B:112:PRO:HD3	1.98	0.45
6:B:268:LEU:HD13	22:B:807:CLA:HMA2	1.98	0.45
6:B:343:VAL:HG21	22:B:816:CLA:H51	1.97	0.45
25:B:835:BCR:H402	22:B:847:CLA:H42	1.97	0.45
12:H:98:GLY:O	12:H:102:LYS:HG2	2.16	0.45
5:A:294:HIS:HE2	22:A:844:CLA:C2B	2.29	0.45
5:A:530:ASP:O	5:A:534:HIS:ND1	2.43	0.45
5:A:699:ILE:HD13	22:A:808:CLA:HMD1	1.98	0.45
22:A:840:CLA:H3A	22:A:840:CLA:HBA2	1.75	0.45
6:B:268:LEU:HD11	6:B:355:LEU:HB3	1.97	0.45
6:B:341:LEU:HD12	6:B:344:ILE:HD11	1.97	0.45
22:B:806:CLA:H92	22:B:806:CLA:H61	1.76	0.45
22:B:814:CLA:H52	22:B:814:CLA:H11	1.71	0.45
22:B:825:CLA:HED2	11:G:140:TYR:OH	2.16	0.45
26:B:843:LHG:H102	26:B:843:LHG:H131	1.31	0.45
10:F:187:ILE:HD11	14:J:14:LEU:CG	2.43	0.45
22:G:206:CLA:HBA1	22:G:206:CLA:H3A	1.67	0.45
5:A:408:ILE:HG21	22:A:855:CLA:HED3	1.98	0.45
22:A:846:CLA:H102	22:A:849:CLA:H62	1.99	0.45
15:K:126:ILE:HG22	31:O:201:DGD:HD61	1.98	0.45
16:L:140:VAL:O	16:L:144:MET:HG3	2.16	0.45
25:O:202:BCR:H15C	25:O:202:BCR:H351	1.75	0.45
2:2:131:ILE:HG22	2:2:132:LEU:HG	1.99	0.45
3:3:146:PRO:HA	3:3:149:LEU:HB2	1.98	0.45
5:A:405:HIS:HD1	5:A:408:ILE:HD12	1.81	0.45
5:A:570:ARG:NH1	26:A:820:LHG:O10	2.49	0.45
22:B:848:CLA:HHC	22:B:848:CLA:HBB1	1.98	0.45
17:N:111:ASP:OD1	17:N:111:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:314:LHG:H161	26:1:322:LHG:H271	1.99	0.45
22:1:321:CLA:HHC	22:1:321:CLA:HBB1	1.98	0.45
5:A:245:ASP:OD1	5:A:245:ASP:N	2.49	0.45
22:A:827:CLA:HBB2	22:A:858:CLA:HAA1	1.97	0.45
6:B:246:THR:OG1	6:B:247:THR:N	2.50	0.45
6:B:608:GLN:O	6:B:612:SER:CB	2.64	0.45
6:B:666:SER:OG	6:B:671:TRP:NE1	2.39	0.45
22:B:815:CLA:HBA2	22:B:828:CLA:HAA1	1.99	0.45
5:A:313:TRP:HH2	22:A:837:CLA:HHB	1.82	0.45
5:A:390:HIS:HE1	22:A:853:CLA:ND	2.14	0.45
25:A:818:BCR:H321	25:A:818:BCR:HC7	1.82	0.45
6:B:195:VAL:HG13	6:B:254:ILE:HG21	1.99	0.45
6:B:487:ASN:HB3	11:G:143:ASN:O	2.16	0.45
7:C:7:ILE:HB	8:D:181:GLN:HG2	1.99	0.45
23:3:301:LUT:H32	22:3:316:CLA:CBB	2.47	0.45
5:A:196:ASN:ND2	5:A:309:TYR:O	2.49	0.45
5:A:353:ASN:ND2	22:A:830:CLA:OBD	2.49	0.45
22:A:810:CLA:H61	22:A:810:CLA:H41	1.57	0.45
22:A:826:CLA:H51	22:A:826:CLA:H8	1.75	0.45
22:B:824:CLA:H93	22:B:824:CLA:H61	1.87	0.45
22:B:829:CLA:H111	22:B:830:CLA:H111	1.98	0.45
10:F:153:GLY:O	10:F:156:PHE:HB3	2.16	0.45
12:H:61:ILE:HD13	12:H:61:ILE:HA	1.71	0.45
22:2:318:CLA:H41	22:2:318:CLA:H61	1.68	0.45
4:4:127:TRP:HB2	24:4:320:XAT:H3	1.99	0.45
26:4:301:LHG:H281	26:4:301:LHG:H101	1.98	0.45
6:B:419:ILE:HD11	6:B:535:VAL:HG12	1.99	0.45
22:B:825:CLA:H3A	22:B:825:CLA:HBA2	1.58	0.45
22:J:102:CLA:HHC	22:J:102:CLA:HBB1	1.98	0.45
25:O:202:BCR:H361	25:O:202:BCR:H20C	1.71	0.45
22:4:316:CLA:HAC2	23:4:322:LUT:H7	1.99	0.45
5:A:257:GLY:O	5:A:269:TYR:OH	2.27	0.45
5:A:279:LEU:HD11	5:A:521:LEU:HD12	1.99	0.45
25:A:814:BCR:H331	22:A:839:CLA:HHB	1.98	0.45
26:A:823:LHG:H142	22:A:856:CLA:HBB1	1.99	0.45
26:B:843:LHG:H311	26:B:843:LHG:H282	1.54	0.45
1:1:178:GLU:HA	1:1:181:LYS:HB2	1.99	0.45
26:1:314:LHG:HC81	26:1:322:LHG:HC62	1.99	0.45
22:3:309:CLA:HBB1	22:3:309:CLA:H51	1.98	0.45
22:A:810:CLA:H191	16:L:103:HIS:HD2	1.82	0.45
22:B:809:CLA:HAC1	22:B:813:CLA:H72	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:837:BCR:H11C	25:B:837:BCR:H341	1.79	0.45
12:H:73:SER:HB2	16:L:81:SER:HB3	1.99	0.45
2:2:126:LEU:HB3	2:2:131:ILE:HB	1.98	0.44
26:2:314:LHG:C16	26:A:822:LHG:H102	2.47	0.44
3:3:54:LYS:NZ	15:K:90:SER:O	2.49	0.44
6:B:129:LEU:HD23	22:B:804:CLA:HED2	1.99	0.44
22:B:809:CLA:HMD2	22:B:812:CLA:HAC1	1.99	0.44
22:B:811:CLA:C4D	25:B:834:BCR:HC21	2.47	0.44
8:D:129:LYS:HE3	8:D:161:LEU:HD13	1.99	0.44
12:H:129:GLY:O	12:H:131:GLN:NE2	2.48	0.44
24:3:302:XAT:H391	24:3:302:XAT:H31	1.44	0.44
4:4:99:ASN:ND2	22:4:310:CLA:OBD	2.51	0.44
5:A:356:MET:O	5:A:360:THR:OG1	2.28	0.44
5:A:670:PHE:HZ	22:A:853:CLA:H111	1.82	0.44
25:A:816:BCR:H11C	25:A:816:BCR:H341	1.88	0.44
6:B:701:SER:O	6:B:705:ALA:N	2.42	0.44
22:B:808:CLA:H41	22:B:808:CLA:H61	1.56	0.44
22:B:818:CLA:H3A	22:B:818:CLA:HBA2	1.73	0.44
22:B:819:CLA:HMA1	22:B:847:CLA:HBC2	1.99	0.44
1:1:176:LYS:HA	1:1:179:GLU:HB3	1.99	0.44
5:A:14:VAL:HG12	5:A:183:PRO:HA	1.97	0.44
5:A:317:HIS:HA	22:A:847:CLA:HED1	2.00	0.44
5:A:544:THR:HA	5:A:547:ILE:HD12	1.98	0.44
5:A:691:TYR:HA	6:B:536:LYS:HZ1	1.81	0.44
6:B:90:ALA:HA	6:B:113:VAL:HG23	1.98	0.44
6:B:374:HIS:HB2	22:B:817:CLA:C1B	2.47	0.44
22:B:803:CLA:H2	22:B:847:CLA:H93	1.99	0.44
22:2:307:CLA:H142	22:2:307:CLA:H111	1.87	0.44
22:2:322:CLA:HMA1	26:4:302:LHG:H282	1.99	0.44
22:3:320:CLA:HHC	22:3:320:CLA:HBB1	2.00	0.44
4:4:107:VAL:HG11	23:4:319:LUT:H12	2.00	0.44
5:A:537:HIS:CE1	5:A:603:VAL:HG12	2.52	0.44
5:A:320:LYS:NZ	5:A:340:GLU:OE2	2.47	0.44
5:A:390:HIS:HE2	22:A:854:CLA:C2B	2.30	0.44
22:A:833:CLA:CHC	22:A:834:CLA:HMD2	2.48	0.44
6:B:294:ASN:HD21	11:G:98:ALA:HA	1.82	0.44
6:B:340:SER:HB3	22:B:814:CLA:H72	2.00	0.44
6:B:366:THR:HG23	6:B:729:THR:HB	1.98	0.44
25:B:837:BCR:H351	25:B:837:BCR:H15C	1.84	0.44
8:D:98:THR:HA	8:D:122:ASN:O	2.18	0.44
15:K:56:MET:HG2	22:K:204:CLA:C3D	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:L:302:BCR:H351	25:L:302:BCR:H15C	1.76	0.44
22:A:844:CLA:H203	22:A:852:CLA:HAA1	2.00	0.44
6:B:89:HIS:CE1	6:B:114:ASN:HD22	2.36	0.44
6:B:424:TRP:HZ3	22:B:828:CLA:HBC2	1.81	0.44
28:B:832:PQN:H172	25:B:839:BCR:H382	1.99	0.44
25:B:834:BCR:H341	25:B:834:BCR:H11C	1.74	0.44
22:1:321:CLA:C2D	27:F:303:MGE:H2B2	2.48	0.44
22:A:808:CLA:HBC2	25:B:844:BCR:H21C	1.99	0.44
25:A:817:BCR:H14C	22:A:849:CLA:H51	2.00	0.44
3:3:141:THR:O	3:3:141:THR:OG1	2.36	0.44
4:4:181:HIS:ND1	4:4:182:GLU:O	2.49	0.44
5:A:121:GLN:NE2	22:A:834:CLA:O1D	2.51	0.44
26:B:842:LHG:H131	26:F:301:LHG:H102	1.98	0.44
14:J:31:ARG:HE	25:J:101:BCR:H312	1.82	0.44
4:4:100:GLY:O	4:4:104:MET:HG3	2.18	0.44
4:4:216:PHE:CD2	24:4:320:XAT:H14	2.52	0.44
5:A:291:ILE:HG23	22:A:844:CLA:HMA3	2.00	0.44
5:A:578:ARG:HG2	7:C:49:VAL:HB	1.99	0.44
22:A:842:CLA:H102	25:K:201:BCR:HC21	1.99	0.44
6:B:472:TYR:HB3	10:F:69:ALA:HA	1.99	0.44
22:B:845:CLA:H152	22:B:845:CLA:H111	1.83	0.44
15:K:57:VAL:HG22	22:K:204:CLA:HBA2	2.00	0.44
25:1:312:BCR:H272	22:1:319:CLA:C1C	2.48	0.43
26:2:313:LHG:HC5	26:2:313:LHG:HC81	1.76	0.43
22:3:312:CLA:H143	22:3:312:CLA:H161	1.89	0.43
4:4:168:ASN:HB3	4:4:178:LEU:HB2	2.00	0.43
22:A:852:CLA:HBD	22:A:852:CLA:HBA2	2.00	0.43
26:B:843:LHG:H311	26:B:843:LHG:HC91	2.00	0.43
18:O:82:LEU:HD21	25:O:202:BCR:H24C	2.00	0.43
2:2:115:LEU:HB3	22:2:320:CLA:HBB2	2.00	0.43
22:3:312:CLA:H91	22:3:312:CLA:H112	1.88	0.43
5:A:411:VAL:HG23	5:A:412:ARG:HG3	1.99	0.43
22:A:827:CLA:HBB1	22:A:858:CLA:CHB	2.48	0.43
6:B:210:ASN:OD1	6:B:210:ASN:N	2.50	0.43
22:B:828:CLA:HHC	22:B:828:CLA:HBB1	2.00	0.43
15:K:51:ALA:O	15:K:55:ILE:HG13	2.18	0.43
22:2:318:CLA:H3A	22:2:318:CLA:HBA2	1.84	0.43
4:4:155:ILE:O	4:4:159:GLN:NE2	2.51	0.43
5:A:116:TRP:CZ2	27:N:201:MGE:H2D	2.53	0.43
5:A:585:SER:OG	5:A:588:ASP:OD1	2.22	0.43
22:B:823:CLA:H142	22:B:823:CLA:H111	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:162:TRP:CD1	10:F:199:GLY:HA3	2.53	0.43
12:H:104:LEU:HD13	12:H:104:LEU:HA	1.90	0.43
14:J:22:LEU:HD13	14:J:22:LEU:HA	1.85	0.43
16:L:125:GLN:OE1	16:L:125:GLN:N	2.47	0.43
22:L:306:CLA:H111	22:L:306:CLA:H72	1.87	0.43
4:4:205:GLU:HG3	22:4:311:CLA:NB	2.33	0.43
5:A:133:ARG:HD2	10:F:98:TYR:HE2	1.82	0.43
5:A:358:GLY:O	5:A:362:ILE:HG12	2.19	0.43
25:A:818:BCR:H343	22:A:853:CLA:H92	1.99	0.43
6:B:284:PHE:HE1	22:B:809:CLA:HHC	1.84	0.43
22:B:804:CLA:H13	22:B:804:CLA:H172	1.81	0.43
22:B:816:CLA:HHD	22:B:816:CLA:HAC1	1.77	0.43
22:B:829:CLA:H151	22:B:830:CLA:H161	2.00	0.43
7:C:5:VAL:HG22	7:C:67:VAL:HG22	2.00	0.43
7:C:9:ASP:HB2	9:E:107:ARG:HD3	1.99	0.43
10:F:116:LYS:O	10:F:120:GLU:HG2	2.18	0.43
23:4:322:LUT:H191	23:4:322:LUT:H11	1.65	0.43
22:A:807:CLA:H122	22:A:807:CLA:H51	2.00	0.43
22:A:809:CLA:H122	25:B:844:BCR:H363	2.00	0.43
22:B:803:CLA:H43	25:B:835:BCR:H19C	2.00	0.43
22:B:806:CLA:HAC2	22:B:807:CLA:H152	2.01	0.43
25:B:836:BCR:HC7	25:B:836:BCR:H331	1.69	0.43
22:F:306:CLA:HBA1	22:F:306:CLA:H3A	1.88	0.43
24:1:311:XAT:H361	24:1:311:XAT:H27	1.62	0.43
3:3:103:MET:HG3	22:3:312:CLA:H13	2.00	0.43
4:4:102:TRP:CE2	21:4:309:CHL:HED2	2.53	0.43
4:4:147:PHE:CD1	22:4:310:CLA:HBB2	2.53	0.43
5:A:575:GLY:HA2	6:B:562:PRO:HD3	2.01	0.43
22:A:810:CLA:H151	16:L:138:LEU:HD11	2.00	0.43
22:A:844:CLA:H111	22:A:844:CLA:H72	1.75	0.43
22:A:849:CLA:H162	22:A:849:CLA:H122	1.84	0.43
6:B:326:ILE:HD12	22:B:814:CLA:HMC2	2.01	0.43
25:B:837:BCR:H323	31:G:201:DGD:HB72	2.01	0.43
22:L:306:CLA:H2	22:L:306:CLA:H61	1.59	0.43
2:2:226:ARG:HB3	22:2:318:CLA:HBC3	2.00	0.43
5:A:732:LEU:HD22	22:A:809:CLA:HMA3	2.01	0.43
22:A:835:CLA:HED3	22:A:835:CLA:H2A	1.99	0.43
22:A:853:CLA:H111	22:A:853:CLA:H71	1.77	0.43
6:B:524:ALA:HB2	22:B:827:CLA:HMA1	2.00	0.43
22:B:818:CLA:H92	22:B:818:CLA:H62	1.85	0.43
1:1:40:GLU:HB2	1:1:59:PHE:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:304:CLA:H41	22:1:304:CLA:H62	1.70	0.43
24:3:302:XAT:H8	22:3:309:CLA:H71	2.00	0.43
23:4:322:LUT:H15	23:4:322:LUT:H201	1.65	0.43
5:A:427:VAL:HA	5:A:430:HIS:CE1	2.54	0.43
25:A:817:BCR:H361	25:A:817:BCR:H20C	1.81	0.43
6:B:582:TRP:CH2	22:B:801:CLA:HAB	2.52	0.43
25:B:839:BCR:H20C	25:B:839:BCR:H361	1.81	0.43
10:F:224:TYR:HD2	10:F:224:TYR:HA	1.67	0.43
26:F:301:LHG:H281	25:F:302:BCR:H14C	2.00	0.43
1:1:81:VAL:HG12	1:1:185:ILE:HD11	2.00	0.43
3:3:225:ARG:HA	3:3:228:MET:HE3	1.99	0.43
3:3:252:HIS:CG	22:3:318:CLA:HAA2	2.53	0.43
5:A:345:SER:OG	5:A:347:HIS:O	2.30	0.43
24:1:311:XAT:H391	24:1:311:XAT:H31	1.52	0.43
25:2:312:BCR:H24C	25:2:312:BCR:H371	1.78	0.43
4:4:157:ARG:NH1	22:4:310:CLA:O1D	2.40	0.43
6:B:141:PHE:HZ	22:B:804:CLA:H151	1.84	0.43
6:B:230:TRP:O	6:B:233:TYR:HB2	2.19	0.43
22:B:830:CLA:H61	22:B:830:CLA:H93	1.80	0.43
25:J:103:BCR:HC7	25:J:103:BCR:H331	1.68	0.43
22:K:203:CLA:H43	31:O:201:DGD:HA71	2.00	0.43
21:2:301:CHL:HBA1	26:2:316:LHG:H142	2.01	0.42
24:2:311:XAT:H11	24:2:311:XAT:H191	1.50	0.42
21:3:307:CHL:HED3	21:3:307:CHL:HBD	1.74	0.42
5:A:154:LEU:HD21	17:N:141:VAL:HG13	2.00	0.42
5:A:454:ILE:HG22	22:A:802:CLA:HBC2	2.01	0.42
25:A:819:BCR:H20C	25:A:819:BCR:H361	1.83	0.42
26:A:820:LHG:H272	26:A:820:LHG:H242	1.72	0.42
26:A:820:LHG:H161	22:A:828:CLA:HMB2	2.00	0.42
22:A:834:CLA:HBB1	22:A:853:CLA:H203	2.01	0.42
8:D:71:PRO:HA	12:H:56:PHE:HD2	1.84	0.42
10:F:158:TYR:HA	10:F:202:TRP:HE1	1.84	0.42
14:J:13:VAL:O	14:J:14:LEU:C	2.61	0.42
15:K:123:LEU:HB3	15:K:128:VAL:HB	2.00	0.42
25:K:201:BCR:H15C	25:K:201:BCR:H351	1.84	0.42
16:L:61:PRO:HG2	16:L:62:PHE:CE1	2.53	0.42
19:X:45:GLY:N	22:X:303:CLA:OBD	2.45	0.42
5:A:446:GLY:O	5:A:450:PHE:HB3	2.19	0.42
5:A:448:HIS:HB3	26:A:824:LHG:H322	2.01	0.42
6:B:672:GLN:O	6:B:676:GLU:HG3	2.19	0.42
25:J:103:BCR:H15C	25:J:103:BCR:H351	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:128:LYS:HD2	2:2:128:LYS:HA	1.86	0.42
24:3:302:XAT:H12	22:3:309:CLA:CBB	2.49	0.42
5:A:10:VAL:HG21	5:A:311:THR:HB	2.01	0.42
5:A:166:PHE:O	5:A:170:MET:HG2	2.19	0.42
5:A:503:THR:HG21	22:A:803:CLA:HMA2	2.02	0.42
22:A:832:CLA:HBB2	25:J:103:BCR:HC32	2.01	0.42
6:B:608:GLN:O	6:B:612:SER:HB2	2.18	0.42
22:B:814:CLA:H162	22:B:814:CLA:H122	1.83	0.42
12:H:78:PRO:HG2	12:H:79:TYR:CE2	2.54	0.42
2:2:162:TRP:CD1	25:2:312:BCR:H353	2.54	0.42
3:3:153:GLU:O	3:3:157:VAL:HG12	2.19	0.42
25:A:817:BCR:H11C	25:A:817:BCR:H341	1.91	0.42
7:C:26:LEU:HA	7:C:41:SER:O	2.18	0.42
11:G:85:GLN:N	11:G:88:LYS:O	2.52	0.42
24:1:311:XAT:H11	24:1:311:XAT:H191	1.77	0.42
5:A:634:PHE:O	5:A:638:SER:OG	2.35	0.42
5:A:736:ALA:HA	25:A:818:BCR:HC42	2.00	0.42
6:B:222:LEU:HD11	25:B:834:BCR:H391	2.01	0.42
22:K:203:CLA:HAA1	31:O:201:DGD:HG31	2.00	0.42
25:2:312:BCR:HC22	26:4:301:LHG:HC91	2.01	0.42
26:2:315:LHG:H262	22:2:318:CLA:HBC1	2.01	0.42
3:3:98:GLY:O	3:3:102:MET:HG3	2.19	0.42
5:A:205:LEU:HD22	25:A:814:BCR:H361	2.02	0.42
5:A:646:ARG:HA	6:B:632:ILE:HD12	2.00	0.42
22:B:808:CLA:H201	22:B:809:CLA:H102	2.00	0.42
22:B:825:CLA:C2D	22:G:205:CLA:HBB1	2.50	0.42
22:B:850:CLA:H72	22:B:850:CLA:H111	1.89	0.42
13:I:34:LYS:HA	13:I:34:LYS:HD2	1.72	0.42
16:L:90:VAL:HB	16:L:95:ARG:HD2	2.01	0.42
2:2:109:HIS:ND1	22:2:303:CLA:OBD	2.52	0.42
3:3:55:GLN:O	3:3:58:SER:OG	2.36	0.42
25:4:321:BCR:H351	25:4:321:BCR:H15C	1.83	0.42
22:A:809:CLA:H112	22:A:826:CLA:H121	2.00	0.42
25:A:816:BCR:H333	18:O:111:THR:HG21	2.01	0.42
22:A:846:CLA:H71	22:A:849:CLA:H62	2.02	0.42
6:B:381:PHE:HA	6:B:583:MET:HE2	2.02	0.42
22:B:811:CLA:H41	22:B:811:CLA:H61	1.53	0.42
22:B:827:CLA:H101	22:B:827:CLA:H62	1.92	0.42
25:B:834:BCR:H392	25:B:834:BCR:H24C	1.70	0.42
26:G:204:LHG:H241	22:G:206:CLA:HBC3	2.01	0.42
12:H:108:GLY:O	12:H:112:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:14:LEU:HD13	14:J:14:LEU:HA	1.88	0.42
15:K:63:MET:HG2	15:K:111:VAL:HB	2.02	0.42
15:K:106:LEU:HD23	15:K:106:LEU:HA	1.94	0.42
25:O:202:BCR:H341	25:O:202:BCR:H11C	1.58	0.42
1:1:165:PHE:HB3	22:1:304:CLA:HMD3	2.01	0.42
22:2:303:CLA:H3A	22:2:303:CLA:HBA2	1.75	0.42
5:A:247:LEU:O	5:A:251:TYR:N	2.43	0.42
5:A:340:GLU:O	5:A:344:THR:OG1	2.28	0.42
25:A:818:BCR:H391	22:B:822:CLA:HMA1	2.01	0.42
22:A:847:CLA:HMA1	22:A:848:CLA:HBD	2.02	0.42
22:B:833:CLA:HBA2	22:B:833:CLA:H3A	1.73	0.42
11:G:62:SER:OG	11:G:121:TRP:O	2.28	0.42
2:2:217:LEU:HD12	2:2:217:LEU:HA	1.92	0.42
5:A:150:ILE:HD11	22:A:839:CLA:HMA2	2.02	0.42
22:B:802:CLA:HAC1	25:B:840:BCR:H19C	2.02	0.42
25:B:840:BCR:H11C	25:B:840:BCR:H341	1.80	0.42
31:G:201:DGD:HB71	31:G:201:DGD:HBT2	1.79	0.42
25:G:202:BCR:H321	25:G:202:BCR:HC8	2.01	0.42
13:I:19:PRO:O	13:I:23:MET:HB2	2.20	0.42
16:L:177:ASP:OD1	16:L:178:GLY:N	2.53	0.42
22:O:208:CLA:H3A	22:O:208:CLA:HBA2	1.86	0.42
1:1:57:GLY:HA3	1:1:185:ILE:HG21	2.01	0.42
5:A:430:HIS:CE1	5:A:434:ILE:HD11	2.55	0.42
22:A:809:CLA:H92	22:A:826:CLA:H121	2.02	0.42
25:A:817:BCR:H403	25:A:817:BCR:H24C	1.75	0.42
22:A:854:CLA:H162	22:A:854:CLA:H122	1.75	0.42
6:B:439:HIS:HE1	22:B:823:CLA:C1A	2.32	0.42
25:I:101:BCR:H361	25:I:101:BCR:H20C	1.83	0.42
22:4:311:CLA:H3A	22:4:311:CLA:HBA2	1.81	0.41
5:A:262:PHE:HA	22:K:204:CLA:HBC3	2.02	0.41
5:A:539:PHE:HE1	22:A:858:CLA:HBA1	1.84	0.41
5:A:694:GLU:OE1	6:B:536:LYS:NZ	2.46	0.41
22:A:827:CLA:HBD	6:B:654:HIS:HB3	2.00	0.41
22:A:855:CLA:H193	22:A:855:CLA:H161	1.95	0.41
6:B:12:LEU:HD21	6:B:23:PHE:HB3	2.01	0.41
6:B:286:ILE:HD13	6:B:286:ILE:HA	1.91	0.41
22:B:827:CLA:H142	22:B:827:CLA:H112	1.88	0.41
25:L:302:BCR:H341	25:L:302:BCR:H11C	1.71	0.41
24:2:311:XAT:H11	24:2:311:XAT:H202	1.86	0.41
4:4:204:LYS:HE2	22:4:313:CLA:HBD	2.02	0.41
5:A:405:HIS:HE1	22:A:855:CLA:C1A	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:826:CLA:H41	22:A:826:CLA:H62	1.74	0.41
6:B:345:THR:HB	6:B:379:ALA:HB2	2.01	0.41
6:B:419:ILE:HD13	6:B:419:ILE:HA	1.87	0.41
6:B:620:LEU:HD12	6:B:624:LEU:HD12	2.02	0.41
6:B:647:ALA:O	6:B:650:PHE:HB3	2.20	0.41
25:B:835:BCR:H15C	25:B:835:BCR:H351	1.90	0.41
22:L:306:CLA:H143	22:L:306:CLA:H112	1.86	0.41
2:2:67:TRP:CD2	2:2:68:PHE:HB2	2.56	0.41
5:A:123:ILE:HG21	6:B:446:PHE:HA	2.02	0.41
5:A:426:ARG:O	5:A:430:HIS:ND1	2.42	0.41
5:A:681:SER:HB2	5:A:726:GLY:O	2.21	0.41
30:A:825:CL0:H41	30:A:825:CL0:H49	1.88	0.41
6:B:351:HIS:CE1	22:B:816:CLA:C1B	3.01	0.41
22:B:803:CLA:H3A	22:B:803:CLA:HBA1	1.57	0.41
22:B:815:CLA:C1B	25:B:838:BCR:H363	2.50	0.41
18:O:75:PHE:HB3	22:Y:311:CLA:H11	2.02	0.41
1:1:185:ILE:HD13	1:1:185:ILE:HA	1.94	0.41
22:1:303:CLA:HHC	22:1:303:CLA:HBB1	2.01	0.41
3:3:102:MET:CE	22:3:316:CLA:HHC	2.50	0.41
4:4:145:ILE:O	4:4:149:LEU:HD12	2.20	0.41
5:A:197:HIS:HB3	22:A:838:CLA:HBB1	2.02	0.41
5:A:477:GLN:H	26:A:821:LHG:HC81	1.84	0.41
22:B:822:CLA:H141	22:B:822:CLA:H161	1.91	0.41
25:2:312:BCR:HC7	25:2:312:BCR:H10C	1.87	0.41
4:4:225:VAL:HG23	4:4:226:THR:HG23	2.03	0.41
5:A:175:TRP:NE1	26:A:822:LHG:C23	2.84	0.41
5:A:484:VAL:HB	22:A:805:CLA:HED1	2.03	0.41
22:A:810:CLA:H152	25:L:301:BCR:H17C	2.03	0.41
6:B:10:GLN:N	6:B:35:ASP:OD2	2.54	0.41
22:B:807:CLA:H11	22:B:807:CLA:H51	1.79	0.41
22:B:829:CLA:H101	25:I:101:BCR:H382	2.01	0.41
10:F:138:ILE:N	10:F:148:GLU:OE1	2.43	0.41
25:O:203:BCR:H15C	25:O:203:BCR:H351	1.68	0.41
1:1:94:VAL:HG22	1:1:105:TRP:HB3	2.03	0.41
5:A:78:LEU:HD23	5:A:78:LEU:HA	1.94	0.41
5:A:559:ARG:HH21	8:D:83:GLY:HA2	1.85	0.41
22:A:812:CLA:H72	22:O:207:CLA:H91	2.01	0.41
22:A:812:CLA:CBB	22:A:849:CLA:HHB	2.51	0.41
22:A:838:CLA:HBB1	22:A:838:CLA:HHC	2.03	0.41
9:E:80:LYS:HD2	9:E:80:LYS:HA	1.87	0.41
12:H:67:GLN:HB3	16:L:159:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:K:201:BCR:H11C	25:K:201:BCR:H341	1.95	0.41
3:3:194:TYR:HB3	22:3:316:CLA:HED2	2.02	0.41
3:3:267:PHE:HE2	25:A:819:BCR:HC21	1.85	0.41
5:A:390:HIS:HE1	22:A:853:CLA:C1D	2.34	0.41
6:B:3:LEU:O	6:B:7:ARG:NH1	2.54	0.41
6:B:344:ILE:HD13	22:B:814:CLA:H61	2.03	0.41
6:B:619:TRP:CD2	22:B:845:CLA:H122	2.56	0.41
25:B:836:BCR:H20C	25:B:836:BCR:H361	1.92	0.41
16:L:55:GLN:HG3	18:O:37:PHE:HA	2.03	0.41
25:L:301:BCR:H323	22:L:306:CLA:H62	2.02	0.41
25:L:303:BCR:H11C	25:L:303:BCR:H341	1.97	0.41
3:3:215:GLU:HG2	3:3:219:LYS:HD2	2.03	0.41
5:A:147:ALA:HB2	5:A:375:PRO:HD2	2.02	0.41
25:A:819:BCR:H15C	25:A:819:BCR:H351	1.79	0.41
6:B:461:GLN:HG2	6:B:472:TYR:CZ	2.56	0.41
6:B:648:TRP:CE3	25:B:839:BCR:HC41	2.55	0.41
1:1:198:PHE:HE1	23:1:310:LUT:H163	1.86	0.41
2:2:166:ARG:HE	21:2:309:CHL:HMC	1.86	0.41
24:2:311:XAT:C13	22:2:319:CLA:HAB	2.50	0.41
26:3:306:LHG:HC62	26:3:306:LHG:H241	1.56	0.41
22:3:313:CLA:HHC	22:3:313:CLA:HBB1	2.03	0.41
4:4:216:PHE:CE1	24:4:320:XAT:H10	2.55	0.41
5:A:208:LEU:HG	22:A:840:CLA:HBB2	2.01	0.41
5:A:686:PHE:O	6:B:577:TYR:OH	2.36	0.41
5:A:717:LEU:HD21	28:A:811:PQN:H152	2.03	0.41
22:A:807:CLA:HAC2	22:A:857:CLA:HBC2	2.03	0.41
6:B:46:ILE:HA	6:B:46:ILE:HD13	1.83	0.41
6:B:94:PRO:HB2	22:B:852:CLA:HAA1	2.02	0.41
6:B:661:PHE:O	6:B:665:ILE:HG13	2.20	0.41
22:B:803:CLA:HHH	22:B:803:CLA:HAC2	1.88	0.41
22:B:806:CLA:H91	11:G:127:ILE:HG23	2.03	0.41
8:D:73:THR:HG23	8:D:121:PRO:HB2	2.03	0.41
25:G:202:BCR:H20C	25:G:202:BCR:H361	1.79	0.41
22:L:307:CLA:H3A	22:L:307:CLA:HBA2	1.82	0.41
22:X:301:CLA:HAC2	21:Y:307:CHL:HBC2	2.02	0.41
19:Z:131:GLN:HA	21:Z:302:CHL:HMA3	2.03	0.41
1:1:111:TRP:HH2	1:1:134:ILE:HG13	1.86	0.41
22:1:317:CLA:H62	22:1:318:CLA:H3A	2.03	0.41
2:2:148:ASP:OD1	2:2:149:THR:N	2.55	0.41
2:2:228:ALA:O	2:2:232:VAL:HG23	2.21	0.41
5:A:445:LEU:HG	22:A:806:CLA:HAB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:453:TYR:HE2	5:A:536:ILE:HG13	1.85	0.41
5:A:513:VAL:HG12	5:A:520:ALA:HB3	2.03	0.41
25:A:819:BCR:H392	25:A:819:BCR:H24C	1.74	0.41
22:A:827:CLA:H151	22:B:852:CLA:HBC3	2.03	0.41
6:B:193:HIS:HE1	22:B:804:CLA:C1A	2.34	0.41
22:B:804:CLA:H203	25:B:835:BCR:H16C	2.03	0.41
25:B:838:BCR:H15C	25:B:838:BCR:H351	1.84	0.41
22:B:851:CLA:H112	22:B:851:CLA:H151	1.77	0.41
8:D:141:SER:O	8:D:144:LYS:NZ	2.43	0.41
12:H:61:ILE:O	12:H:62:GLY:C	2.62	0.41
22:3:312:CLA:H141	21:3:314:CHL:HED3	2.02	0.40
4:4:217:LEU:O	4:4:221:VAL:HG23	2.22	0.40
5:A:72:SER:OG	5:A:178:TYR:HB2	2.20	0.40
5:A:96:SER:H	17:N:88:ASN:HD22	1.68	0.40
22:A:810:CLA:H18	22:L:306:CLA:HBB1	2.04	0.40
25:A:817:BCR:HC7	25:A:817:BCR:H321	1.89	0.40
6:B:323:TYR:HE2	11:G:85:GLN:HA	1.86	0.40
22:B:816:CLA:H41	22:B:816:CLA:H61	1.84	0.40
22:Y:311:CLA:H3A	22:Y:311:CLA:HBA1	1.76	0.40
25:1:312:BCR:H15C	25:1:312:BCR:H351	1.90	0.40
22:2:308:CLA:HAA2	3:3:152:PHE:CG	2.56	0.40
24:2:311:XAT:H31	24:2:311:XAT:H391	1.60	0.40
5:A:353:ASN:HD22	22:A:830:CLA:HMD1	1.87	0.40
25:A:815:BCR:H313	22:A:854:CLA:HAA2	2.03	0.40
6:B:42:LEU:O	6:B:46:ILE:HG12	2.21	0.40
25:B:837:BCR:H311	25:B:837:BCR:HC8	2.03	0.40
25:B:844:BCR:H20C	25:B:844:BCR:H361	1.86	0.40
10:F:169:SER:HB2	10:F:195:LEU:HD22	2.04	0.40
16:L:60:ASP:HA	16:L:61:PRO:HD3	1.89	0.40
25:L:301:BCR:H24C	25:L:301:BCR:H371	1.90	0.40
25:L:301:BCR:HC21	22:L:306:CLA:H62	2.04	0.40
18:O:60:SER:OG	18:O:71:THR:OG1	2.38	0.40
5:A:692:TRP:O	5:A:696:ILE:HG12	2.21	0.40
25:A:814:BCR:H361	25:A:814:BCR:H20C	1.93	0.40
25:A:818:BCR:H11C	25:A:818:BCR:HC8	1.91	0.40
6:B:280:ILE:HG23	6:B:284:PHE:CD2	2.56	0.40
6:B:347:LEU:HD12	6:B:347:LEU:HA	1.92	0.40
6:B:490:ARG:HD3	11:G:143:ASN:ND2	2.33	0.40
6:B:721:TYR:HB2	22:B:845:CLA:HED3	2.04	0.40
22:B:807:CLA:HHC	22:B:807:CLA:HBB1	2.03	0.40
22:B:815:CLA:CHB	22:B:828:CLA:HAA2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:169:GLY:O	1:1:172:LYS:HE2	2.22	0.40
3:3:59:TYR:OH	3:3:71:ASP:OD2	2.36	0.40
3:3:77:ASP:OD1	3:3:77:ASP:N	2.51	0.40
3:3:219:LYS:HE3	22:3:317:CLA:HAA2	2.04	0.40
5:A:286:LEU:HB2	5:A:291:ILE:HD11	2.03	0.40
5:A:668:GLY:O	5:A:671:PHE:HB3	2.21	0.40
22:A:850:CLA:H2	22:A:850:CLA:H61	1.89	0.40
6:B:459:PHE:HZ	25:F:302:BCR:H391	1.85	0.40
22:B:812:CLA:HMB2	22:B:831:CLA:C1D	2.52	0.40
22:B:852:CLA:HBA2	16:L:116:PRO:HG2	2.03	0.40
18:O:80:GLN:O	18:O:83:SER:OG	2.33	0.40
22:O:208:CLA:H3A	22:O:208:CLA:H11	2.03	0.40
21:Z:312:CHL:HBB1	21:Z:312:CHL:HHC	2.04	0.40
5:A:80:ILE:HG23	25:J:103:BCR:HC22	2.03	0.40
5:A:110:PRO:O	5:A:137:ILE:N	2.53	0.40
5:A:200:ALA:HB1	22:A:845:CLA:HBC3	2.02	0.40
5:A:393:TRP:HD1	22:A:853:CLA:HAB	1.81	0.40
22:A:829:CLA:O1A	22:A:836:CLA:ND	2.55	0.40
22:A:830:CLA:HHC	22:A:830:CLA:HBB1	2.03	0.40
22:A:833:CLA:H42	22:A:853:CLA:HMD2	2.03	0.40
22:A:844:CLA:HBB1	22:A:844:CLA:HMB1	2.02	0.40
6:B:86:PRO:HB3	6:B:121:TYR:CG	2.56	0.40
6:B:123:TRP:CH2	25:B:836:BCR:H391	2.57	0.40
6:B:142:LEU:HA	6:B:145:LEU:HB2	2.02	0.40
22:B:822:CLA:H142	25:F:302:BCR:H333	2.03	0.40
22:B:851:CLA:H151	22:B:851:CLA:H18	1.94	0.40
10:F:144:ARG:NE	27:F:303:MGE:O3D	2.55	0.40
16:L:108:VAL:HG21	16:L:197:ALA:HB3	2.04	0.40
25:L:303:BCR:H15C	25:L:303:BCR:H351	1.90	0.40
22:L:306:CLA:H141	22:L:306:CLA:H161	1.80	0.40
22:X:303:CLA:HBA1	22:X:303:CLA:H3A	1.90	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	1	198/200 (99%)	187 (94%)	11 (6%)	0	100	100
2	2	205/207 (99%)	187 (91%)	17 (8%)	1 (0%)	24	49
3	3	220/222 (99%)	207 (94%)	13 (6%)	0	100	100
4	4	196/198 (99%)	190 (97%)	5 (3%)	1 (0%)	24	49
5	A	740/742 (100%)	705 (95%)	34 (5%)	1 (0%)	48	72
6	B	730/732 (100%)	707 (97%)	23 (3%)	0	100	100
7	C	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
8	D	141/143 (99%)	133 (94%)	6 (4%)	2 (1%)	9	24
9	E	63/66 (96%)	57 (90%)	6 (10%)	0	100	100
10	F	156/158 (99%)	154 (99%)	2 (1%)	0	100	100
11	G	95/97 (98%)	89 (94%)	5 (5%)	1 (1%)	11	29
12	H	91/93 (98%)	77 (85%)	10 (11%)	4 (4%)	2	4
13	I	28/30 (93%)	28 (100%)	0	0	100	100
14	J	42/44 (96%)	36 (86%)	5 (12%)	1 (2%)	4	13
15	K	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
16	L	161/163 (99%)	153 (95%)	7 (4%)	1 (1%)	21	45
17	N	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
18	O	90/92 (98%)	81 (90%)	9 (10%)	0	100	100
19	X	216/218 (99%)	197 (91%)	19 (9%)	0	100	100
19	Z	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
20	Y	220/222 (99%)	202 (92%)	17 (8%)	1 (0%)	24	49
All	All	4054/4097 (99%)	3831 (94%)	210 (5%)	13 (0%)	37	59

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	176	CYS
4	4	189	VAL
5	A	348	ALA
8	D	163	PRO
12	H	76	PRO
14	J	43	SER
12	H	57	ASP

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Mol	Chain	Res	Type
20	Y	164	ASP
16	L	56	PRO
8	D	158	VAL
12	H	79	TYR
11	G	50	SER
12	H	78	PRO

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	1	162/162 (100%)	162 (100%)	0	100	100
2	2	165/165 (100%)	160 (97%)	5 (3%)	36	60
3	3	176/176 (100%)	176 (100%)	0	100	100
4	4	169/169 (100%)	168 (99%)	1 (1%)	78	89
5	A	602/602 (100%)	598 (99%)	4 (1%)	76	87
6	B	599/599 (100%)	594 (99%)	5 (1%)	73	85
7	C	69/70 (99%)	69 (100%)	0	100	100
8	D	121/121 (100%)	120 (99%)	1 (1%)	73	85
9	E	57/58 (98%)	57 (100%)	0	100	100
10	F	127/127 (100%)	125 (98%)	2 (2%)	55	75
11	G	81/81 (100%)	81 (100%)	0	100	100
12	H	76/76 (100%)	73 (96%)	3 (4%)	28	54
13	I	26/26 (100%)	26 (100%)	0	100	100
14	J	38/38 (100%)	36 (95%)	2 (5%)	20	45
15	K	64/64 (100%)	63 (98%)	1 (2%)	55	75
16	L	126/126 (100%)	125 (99%)	1 (1%)	73	85
17	N	73/73 (100%)	73 (100%)	0	100	100
18	O	77/77 (100%)	77 (100%)	0	100	100
19	X	16/165 (10%)	15 (94%)	1 (6%)	16	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	Z	16/165 (10%)	16 (100%)	0	100	100
20	Y	16/171 (9%)	16 (100%)	0	100	100
All	All	2856/3311 (86%)	2830 (99%)	26 (1%)	68	83

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	68	PHE
2	2	92	LEU
2	2	106	GLU
2	2	110	CYS
2	2	170	ASP
4	4	105	LEU
5	A	214	GLN
5	A	413	ASP
5	A	588	ASP
5	A	731	LEU
6	B	113	VAL
6	B	231	ASN
6	B	257	LEU
6	B	429	LEU
6	B	678	LEU
8	D	204	ASP
10	F	86	GLN
10	F	224	TYR
12	H	61	ILE
12	H	80	ASN
12	H	104	LEU
14	J	14	LEU
14	J	22	LEU
15	K	101	THR
16	L	91	SER
19	X	170	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	118	GLN
1	1	148	GLN
1	1	201	GLN

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Mol	Chain	Res	Type
1	1	225	ASN
2	2	102	ASN
2	2	133	ASN
2	2	186	ASN
2	2	249	ASN
4	4	163	ASN
4	4	236	GLN
5	A	222	ASN
5	A	353	ASN
5	A	455	HIS
5	A	636	GLN
6	B	114	ASN
6	B	158	GLN
6	B	229	GLN
6	B	276	HIS
6	B	506	ASN
6	B	520	HIS
6	B	603	GLN
8	D	181	GLN
8	D	182	ASN
10	F	136	HIS
11	G	114	ASN
11	G	126	HIS
11	G	143	ASN
12	H	83	GLN
18	O	68	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

286 ligands are modelled in this entry.

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
22	CLA	2	306	2	47,52,73	2.55	18 (38%)	56,88,113	3.49	26 (46%)
22	CLA	4	310	4	46,50,73	2.39	17 (36%)	55,85,113	3.26	27 (49%)
28	PQN	A	811	-	34,34,34	0.32	0	42,45,45	0.46	0
21	CHL	Z	302	-	51,55,74	2.21	18 (35%)	57,91,114	3.14	25 (43%)
22	CLA	O	210	-	45,49,73	2.62	18 (40%)	54,84,113	3.48	28 (51%)
21	CHL	1	301	1	47,51,74	2.21	17 (36%)	52,86,114	3.24	23 (44%)
22	CLA	A	830	5	54,58,73	2.46	18 (33%)	65,95,113	3.36	31 (47%)
22	CLA	B	820	6	49,53,73	2.34	18 (36%)	59,89,113	3.34	27 (45%)
26	LHG	X	314	22	21,21,48	0.35	0	22,26,54	0.50	0
22	CLA	B	807	6	65,71,73	1.94	13 (20%)	73,108,113	3.96	30 (41%)
22	CLA	2	318	2	65,69,73	2.18	19 (29%)	78,108,113	2.93	29 (37%)
26	LHG	2	316	-	35,35,48	0.41	0	39,40,54	0.52	1 (2%)
26	LHG	2	315	22	31,31,48	0.32	0	34,37,54	0.44	0
22	CLA	A	834	5	50,54,73	2.41	18 (36%)	60,90,113	3.24	28 (46%)
22	CLA	Z	306	-	50,54,73	2.50	19 (38%)	60,90,113	3.41	29 (48%)
22	CLA	B	816	6	69,73,73	2.22	20 (28%)	83,113,113	3.49	32 (38%)
22	CLA	K	203	-	64,68,73	2.21	19 (29%)	77,107,113	3.00	31 (40%)
21	CHL	Z	304	-	51,55,74	2.20	17 (33%)	57,91,114	3.12	22 (38%)
25	BCR	G	202	-	41,41,41	1.86	9 (21%)	56,56,56	2.57	21 (37%)
22	CLA	B	827	6	69,73,73	2.07	18 (26%)	83,113,113	2.82	33 (39%)
22	CLA	4	315	4	44,49,73	2.58	18 (40%)	52,84,113	3.51	25 (48%)
26	LHG	3	306	-	37,37,48	0.32	0	40,43,54	0.44	0
22	CLA	Y	309	-	50,54,73	2.51	20 (40%)	60,90,113	3.30	27 (45%)
22	CLA	B	846	6,22	50,54,73	2.45	19 (38%)	60,90,113	3.35	28 (46%)
21	CHL	Y	306	-	50,54,74	2.25	17 (34%)	56,90,114	3.17	20 (35%)
22	CLA	Z	313	-	50,54,73	2.52	20 (40%)	60,90,113	3.27	27 (45%)
22	CLA	B	847	-	69,73,73	2.12	19 (27%)	83,113,113	2.88	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	I	101	-	41,41,41	1.69	8 (19%)	56,56,56	1.80	14 (25%)
26	LHG	2	313	-	25,25,48	0.47	0	29,30,54	1.11	3 (10%)
22	CLA	A	833	5	69,73,73	2.13	20 (28%)	83,113,113	2.93	31 (37%)
26	LHG	A	820	-	48,48,48	0.27	0	51,54,54	0.38	0
22	CLA	Y	301	-	50,54,73	2.50	20 (40%)	60,90,113	3.29	28 (46%)
25	BCR	K	201	-	41,41,41	1.70	8 (19%)	56,56,56	1.76	13 (23%)
26	LHG	B	843	-	40,40,48	1.02	2 (5%)	43,45,54	1.08	2 (4%)
22	CLA	A	809	5	65,69,73	2.14	18 (27%)	78,108,113	2.95	30 (38%)
22	CLA	1	320	-	49,53,73	2.53	19 (38%)	59,89,113	3.31	27 (45%)
22	CLA	G	206	26	57,61,73	2.39	20 (35%)	68,98,113	3.20	28 (41%)
24	XAT	2	311	-	39,47,47	0.93	0	54,74,74	3.72	31 (57%)
22	CLA	B	818	6	69,73,73	2.07	19 (27%)	83,113,113	2.72	31 (37%)
29	SF4	C	102	7	0,12,12	-	-	-	-	-
22	CLA	A	837	5	46,50,73	2.53	18 (39%)	55,85,113	3.50	26 (47%)
22	CLA	B	829	-	69,73,73	2.12	19 (27%)	83,113,113	2.80	31 (37%)
25	BCR	L	302	-	41,41,41	1.72	9 (21%)	56,56,56	2.22	18 (32%)
22	CLA	4	314	4	43,48,73	2.58	20 (46%)	51,83,113	3.47	29 (56%)
22	CLA	B	853	6	56,60,73	2.36	20 (35%)	67,97,113	3.14	32 (47%)
21	CHL	Y	303	-	50,54,74	2.24	16 (32%)	56,90,114	3.20	21 (37%)
22	CLA	1	305	26	45,49,73	2.60	19 (42%)	54,84,113	3.44	28 (51%)
22	CLA	3	308	-	53,57,73	2.41	18 (33%)	62,93,113	3.38	28 (45%)
22	CLA	X	312	-	50,54,73	2.51	20 (40%)	60,90,113	3.30	27 (45%)
28	PQN	B	832	-	31,31,34	0.32	0	38,41,45	0.62	1 (2%)
22	CLA	1	319	-	52,56,73	2.42	19 (36%)	62,92,113	3.21	30 (48%)
22	CLA	A	802	5	69,73,73	2.13	18 (26%)	83,113,113	2.88	32 (38%)
22	CLA	1	309	-	46,50,73	2.52	19 (41%)	55,85,113	3.52	29 (52%)
25	BCR	B	840	-	30,30,41	2.15	8 (26%)	39,39,56	2.73	14 (35%)
25	BCR	A	818	-	40,40,41	1.57	7 (17%)	54,54,56	1.67	12 (22%)
22	CLA	Z	309	-	50,54,73	2.52	20 (40%)	60,90,113	3.32	26 (43%)
22	CLA	N	202	-	47,52,73	2.55	20 (42%)	56,88,113	3.34	25 (44%)
27	MGE	3	304	-	32,32,48	0.53	0	40,40,56	0.92	3 (7%)
25	BCR	O	203	-	41,41,41	1.79	8 (19%)	56,56,56	2.31	15 (26%)
21	CHL	Y	313	20	50,54,74	2.24	18 (36%)	56,90,114	3.20	20 (35%)
22	CLA	A	851	-	54,58,73	2.37	20 (37%)	65,95,113	3.23	30 (46%)
21	CHL	2	302	-	51,55,74	2.16	17 (33%)	57,91,114	3.03	21 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	4	312	-	49,53,73	2.50	19 (38%)	59,89,113	3.31	28 (47%)
22	CLA	A	803	5	60,64,73	2.21	18 (30%)	72,102,113	3.00	29 (40%)
25	BCR	A	816	-	41,41,41	1.69	9 (21%)	56,56,56	2.27	15 (26%)
22	CLA	X	311	26	50,54,73	2.51	20 (40%)	60,90,113	3.28	28 (46%)
31	DGD	J	104	-	59,59,67	0.94	3 (5%)	73,73,81	1.09	4 (5%)
22	CLA	Z	314	-	50,54,73	2.49	20 (40%)	60,90,113	3.28	27 (45%)
21	CHL	4	317	4	44,49,74	2.34	18 (40%)	48,84,114	3.35	21 (43%)
22	CLA	A	859	-	62,66,73	2.21	18 (29%)	74,104,113	3.06	30 (40%)
27	MGE	3	305	-	26,26,48	0.59	0	32,33,56	0.80	1 (3%)
31	DGD	B	841	-	60,60,67	0.89	2 (3%)	74,74,81	0.90	3 (4%)
25	BCR	B	844	-	41,41,41	1.69	9 (21%)	56,56,56	1.81	16 (28%)
22	CLA	A	831	5	69,73,73	2.10	18 (26%)	83,113,113	2.96	30 (36%)
22	CLA	H	201	12	45,49,73	2.61	20 (44%)	54,84,113	3.50	29 (53%)
21	CHL	4	307	-	48,53,74	2.22	16 (33%)	53,89,114	3.10	21 (39%)
21	CHL	X	306	-	51,55,74	2.22	17 (33%)	57,91,114	3.12	23 (40%)
25	BCR	2	312	-	41,41,41	1.64	8 (19%)	56,56,56	2.32	19 (33%)
22	CLA	2	308	2	56,60,73	2.38	20 (35%)	67,97,113	3.37	32 (47%)
22	CLA	Z	307	-	50,54,73	2.51	20 (40%)	60,90,113	3.30	26 (43%)
22	CLA	3	313	3	49,53,73	2.54	19 (38%)	59,89,113	3.35	26 (44%)
22	CLA	Y	310	-	50,54,73	2.52	20 (40%)	60,90,113	3.32	28 (46%)
21	CHL	Z	301	19	51,55,74	2.19	17 (33%)	57,91,114	3.17	21 (36%)
22	CLA	A	845	5	49,53,73	2.46	18 (36%)	59,89,113	3.44	30 (50%)
22	CLA	X	303	-	50,54,73	2.51	20 (40%)	60,90,113	3.29	27 (45%)
22	CLA	Y	314	-	50,54,73	2.51	20 (40%)	60,90,113	3.36	27 (45%)
25	BCR	B	835	-	41,41,41	1.71	8 (19%)	56,56,56	1.88	17 (30%)
31	DGD	G	201	-	39,39,67	1.04	2 (5%)	47,47,81	1.22	6 (12%)
22	CLA	B	803	6	69,73,73	2.18	20 (28%)	83,113,113	3.06	30 (36%)
22	CLA	4	311	4	49,53,73	2.50	19 (38%)	59,89,113	3.26	29 (49%)
22	CLA	Z	308	-	50,54,73	2.52	20 (40%)	60,90,113	3.30	28 (46%)
22	CLA	B	809	-	64,68,73	2.13	17 (26%)	77,107,113	2.86	31 (40%)
21	CHL	2	309	2	50,54,74	2.24	18 (36%)	56,90,114	3.19	21 (37%)
25	BCR	B	837	-	41,41,41	1.74	8 (19%)	56,56,56	2.11	19 (33%)
22	CLA	B	806	6	61,65,73	2.22	19 (31%)	73,103,113	3.02	29 (39%)
22	CLA	B	849	6	56,60,73	2.36	19 (33%)	67,97,113	3.22	32 (47%)
24	XAT	3	302	-	39,47,47	0.92	1 (2%)	54,74,74	4.13	25 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CHL	Z	305	-	51,55,74	2.22	17 (33%)	57,91,114	3.08	21 (36%)
22	CLA	A	847	5	46,50,73	2.49	17 (36%)	55,85,113	3.42	24 (43%)
26	LHG	4	303	-	35,35,48	0.34	0	38,40,54	0.45	0
22	CLA	A	838	5	69,73,73	2.19	18 (26%)	83,113,113	3.02	28 (33%)
21	CHL	2	301	-	54,58,74	2.13	16 (29%)	59,94,114	3.12	24 (40%)
22	CLA	3	311	-	49,53,73	2.50	19 (38%)	59,89,113	3.38	30 (50%)
22	CLA	3	317	-	47,52,73	2.57	19 (40%)	56,88,113	3.46	26 (46%)
22	CLA	3	319	3	49,53,73	2.53	20 (40%)	59,89,113	3.34	26 (44%)
22	CLA	L	307	-	49,53,73	2.50	20 (40%)	59,89,113	3.37	28 (47%)
22	CLA	1	304	1	57,61,73	2.33	19 (33%)	68,98,113	3.17	33 (48%)
22	CLA	B	845	-	69,73,73	2.06	16 (23%)	83,113,113	2.67	30 (36%)
22	CLA	Y	308	-	50,54,73	2.49	20 (40%)	60,90,113	3.34	30 (50%)
22	CLA	3	312	3	69,73,73	2.15	19 (27%)	83,113,113	2.94	32 (38%)
26	LHG	G	203	-	35,35,48	0.33	0	38,41,54	0.72	1 (2%)
21	CHL	Y	307	-	50,54,74	2.25	17 (34%)	56,90,114	3.15	22 (39%)
22	CLA	2	304	2	59,63,73	2.27	19 (32%)	71,101,113	2.96	32 (45%)
22	CLA	A	839	5	49,53,73	2.49	19 (38%)	59,89,113	3.32	26 (44%)
22	CLA	1	306	-	47,52,73	2.55	19 (40%)	56,88,113	3.37	26 (46%)
22	CLA	A	844	5	69,73,73	2.09	19 (27%)	83,113,113	2.87	29 (34%)
22	CLA	Y	312	-	50,54,73	2.53	20 (40%)	60,90,113	3.36	26 (43%)
25	BCR	B	838	-	41,41,41	1.67	13 (31%)	56,56,56	1.98	19 (33%)
22	CLA	3	316	3	49,53,73	2.50	20 (40%)	59,89,113	3.38	26 (44%)
21	CHL	X	307	-	50,54,74	2.25	17 (34%)	56,90,114	3.21	21 (37%)
25	BCR	F	302	-	41,41,41	1.70	9 (21%)	56,56,56	1.70	13 (23%)
22	CLA	A	808	5	69,73,73	2.10	19 (27%)	83,113,113	2.84	30 (36%)
21	CHL	Y	304	-	50,54,74	2.26	15 (30%)	56,90,114	3.16	21 (37%)
21	CHL	3	307	2	55,59,74	2.08	20 (36%)	60,95,114	3.18	24 (40%)
22	CLA	F	306	10	50,54,73	2.45	19 (38%)	60,90,113	3.28	28 (46%)
22	CLA	K	204	15	50,54,73	2.52	18 (36%)	60,90,113	3.21	26 (43%)
21	CHL	Z	303	-	50,54,74	2.26	19 (38%)	56,90,114	3.17	23 (41%)
22	CLA	B	828	6	51,55,73	2.39	19 (37%)	61,91,113	3.33	27 (44%)
22	CLA	B	848	-	61,65,73	2.23	19 (31%)	73,103,113	3.06	29 (39%)
22	CLA	B	851	6	69,73,73	2.03	17 (24%)	83,113,113	2.71	29 (34%)
23	LUT	1	310	-	42,43,43	1.63	8 (19%)	51,60,60	1.80	13 (25%)
29	SF4	C	101	7	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	O	207	-	68,72,73	2.11	19 (27%)	81,111,113	2.94	31 (38%)
25	BCR	O	202	-	41,41,41	1.59	8 (19%)	56,56,56	2.71	21 (37%)
22	CLA	3	320	-	45,50,73	2.54	19 (42%)	53,85,113	3.37	25 (47%)
22	CLA	A	841	-	50,54,73	2.45	19 (38%)	60,90,113	3.34	27 (45%)
22	CLA	A	827	-	69,73,73	2.00	19 (27%)	83,113,113	2.60	25 (30%)
22	CLA	G	207	11	49,53,73	2.50	20 (40%)	59,89,113	3.26	28 (47%)
26	LHG	1	322	-	32,32,48	0.29	0	34,34,54	0.56	0
22	CLA	2	303	2	49,53,73	2.45	19 (38%)	59,89,113	3.18	25 (42%)
22	CLA	A	854	5	69,73,73	2.03	18 (26%)	83,113,113	2.71	31 (37%)
22	CLA	B	831	26	69,73,73	2.10	18 (26%)	83,113,113	2.82	29 (34%)
22	CLA	A	801	5	64,68,73	2.17	19 (29%)	79,106,113	3.03	32 (40%)
22	CLA	L	305	16	49,53,73	2.49	19 (38%)	59,89,113	3.32	29 (49%)
22	CLA	1	317	1	61,65,73	2.24	19 (31%)	73,103,113	3.18	31 (42%)
22	CLA	Y	311	-	69,73,73	2.15	19 (27%)	83,113,113	2.91	31 (37%)
22	CLA	2	305	26	49,53,73	2.46	19 (38%)	59,89,113	3.35	28 (47%)
26	LHG	1	314	-	28,28,48	0.27	0	29,29,54	0.22	0
22	CLA	1	318	-	59,63,73	2.30	19 (32%)	71,101,113	3.05	28 (39%)
22	CLA	O	206	-	50,54,73	2.51	19 (38%)	60,90,113	3.25	26 (43%)
22	CLA	B	802	6	49,53,73	2.45	20 (40%)	59,89,113	3.50	28 (47%)
22	CLA	2	322	4	47,52,73	2.53	20 (42%)	56,88,113	3.32	26 (46%)
22	CLA	2	317	-	45,49,73	2.65	20 (44%)	54,84,113	3.45	28 (51%)
22	CLA	O	208	-	64,68,73	2.17	19 (29%)	77,107,113	3.07	29 (37%)
21	CHL	X	305	19	52,56,74	2.20	16 (30%)	58,92,114	3.13	22 (37%)
25	BCR	1	312	-	41,41,41	1.88	8 (19%)	56,56,56	2.50	14 (25%)
24	XAT	4	320	-	39,47,47	0.89	1 (2%)	54,74,74	2.63	19 (35%)
26	LHG	F	301	-	30,30,48	0.44	0	34,35,54	1.19	3 (8%)
22	CLA	A	812	26	59,63,73	2.30	19 (32%)	71,101,113	3.08	30 (42%)
22	CLA	B	817	-	62,66,73	2.16	19 (30%)	74,104,113	3.00	30 (40%)
22	CLA	A	856	5	55,59,73	2.32	19 (34%)	66,96,113	3.15	31 (46%)
22	CLA	A	853	5	69,73,73	2.09	20 (28%)	83,113,113	2.90	31 (37%)
26	LHG	A	821	-	23,23,48	0.49	0	27,28,54	0.71	1 (3%)
21	CHL	X	308	-	51,55,74	2.21	16 (31%)	57,91,114	3.16	21 (36%)
22	CLA	B	819	6	64,68,73	2.17	19 (29%)	77,107,113	2.81	31 (40%)
22	CLA	Z	310	-	50,54,73	2.51	20 (40%)	60,90,113	3.32	28 (46%)
22	CLA	A	857	5	60,64,73	2.26	19 (31%)	72,102,113	3.00	29 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CHL	X	309	-	50,54,74	2.25	17 (34%)	56,90,114	3.14	20 (35%)
22	CLA	A	840	5	49,53,73	2.51	19 (38%)	59,89,113	3.31	26 (44%)
22	CLA	A	846	-	69,73,73	2.13	19 (27%)	83,113,113	2.72	29 (34%)
22	CLA	B	804	6	69,73,73	2.06	19 (27%)	83,113,113	2.85	30 (36%)
22	CLA	B	824	6	64,68,73	2.23	20 (31%)	77,107,113	3.01	30 (38%)
22	CLA	G	205	-	49,53,73	2.53	19 (38%)	59,89,113	3.34	27 (45%)
25	BCR	L	303	-	41,41,41	1.68	9 (21%)	56,56,56	1.79	16 (28%)
22	CLA	A	832	5	51,55,73	2.46	19 (37%)	61,91,113	3.31	28 (45%)
26	LHG	4	301	-	28,28,48	0.36	0	31,33,54	0.60	1 (3%)
25	BCR	B	836	-	41,41,41	1.72	8 (19%)	56,56,56	1.82	15 (26%)
25	BCR	J	101	-	41,41,41	1.74	10 (24%)	56,56,56	1.88	19 (33%)
22	CLA	A	855	5	69,73,73	2.07	19 (27%)	83,113,113	2.72	31 (37%)
22	CLA	A	858	-	69,73,73	2.07	19 (27%)	83,113,113	3.00	29 (34%)
26	LHG	G	204	22	24,24,48	0.49	0	28,29,54	0.63	1 (3%)
31	DGD	O	201	-	54,54,67	0.95	2 (3%)	68,68,81	1.26	7 (10%)
22	CLA	A	805	-	54,58,73	2.33	19 (35%)	65,95,113	3.23	29 (44%)
22	CLA	B	825	-	50,54,73	2.46	20 (40%)	60,90,113	3.17	27 (45%)
25	BCR	A	817	-	41,41,41	1.67	8 (19%)	56,56,56	1.86	14 (25%)
27	MGE	N	201	-	32,32,48	0.59	0	40,40,56	0.77	1 (2%)
21	CHL	1	316	1	50,54,74	2.17	17 (34%)	56,90,114	3.11	20 (35%)
22	CLA	B	850	6	69,73,73	2.08	18 (26%)	83,113,113	2.85	31 (37%)
24	XAT	1	311	-	39,47,47	0.95	0	54,74,74	3.65	29 (53%)
26	LHG	A	823	22	32,32,48	0.29	0	35,38,54	0.39	0
25	BCR	A	814	-	41,41,41	1.64	9 (21%)	56,56,56	1.75	14 (25%)
22	CLA	B	808	6	69,73,73	2.15	19 (27%)	83,113,113	2.89	31 (37%)
22	CLA	4	316	4	45,49,73	2.55	18 (40%)	54,84,113	3.46	27 (50%)
22	CLA	3	309	3	63,67,73	2.23	19 (30%)	75,105,113	3.02	32 (42%)
25	BCR	J	103	-	41,41,41	1.69	9 (21%)	56,56,56	1.87	17 (30%)
21	CHL	4	309	-	50,54,74	2.18	18 (36%)	56,90,114	3.01	22 (39%)
22	CLA	3	318	3	49,53,73	2.47	20 (40%)	59,89,113	3.29	28 (47%)
22	CLA	A	810	-	69,73,73	2.07	19 (27%)	83,113,113	2.75	31 (37%)
22	CLA	A	829	5,22	54,58,73	2.36	20 (37%)	65,95,113	3.24	31 (47%)
22	CLA	X	313	-	50,54,73	2.51	20 (40%)	60,90,113	3.36	28 (46%)
22	CLA	X	304	-	50,54,73	2.75	22 (44%)	60,90,113	4.23	29 (48%)
22	CLA	A	836	5,22	64,68,73	2.21	19 (29%)	77,107,113	2.91	29 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	806	5	57,61,73	2.35	20 (35%)	68,98,113	3.11	30 (44%)
22	CLA	K	202	15	47,52,73	2.54	20 (42%)	56,88,113	3.29	25 (44%)
22	CLA	A	850	-	69,73,73	2.04	19 (27%)	83,113,113	2.82	31 (37%)
22	CLA	B	815	-	62,66,73	2.18	20 (32%)	74,104,113	2.93	29 (39%)
22	CLA	B	833	22	60,64,73	2.29	19 (31%)	72,102,113	3.12	32 (44%)
22	CLA	3	310	-	62,66,73	2.23	19 (30%)	74,104,113	2.99	28 (37%)
22	CLA	1	308	1	45,49,73	2.58	18 (40%)	54,84,113	3.53	29 (53%)
22	CLA	L	306	16	69,73,73	2.04	19 (27%)	83,113,113	2.92	31 (37%)
25	BCR	L	301	-	41,41,41	1.65	8 (19%)	56,56,56	1.83	17 (30%)
22	CLA	X	301	-	50,54,73	2.49	20 (40%)	60,90,113	3.29	27 (45%)
22	CLA	3	315	3	45,49,73	2.53	20 (44%)	54,84,113	3.26	27 (50%)
22	CLA	B	814	-	69,73,73	2.02	16 (23%)	83,113,113	3.00	34 (40%)
22	CLA	O	209	18	51,55,73	2.51	20 (39%)	61,91,113	3.32	27 (44%)
23	LUT	4	322	-	42,43,43	1.60	8 (19%)	51,60,60	3.12	17 (33%)
25	BCR	A	819	-	41,41,41	1.67	9 (21%)	56,56,56	1.91	16 (28%)
23	LUT	4	319	-	42,43,43	1.57	8 (19%)	51,60,60	1.61	12 (23%)
25	BCR	A	815	-	41,41,41	1.68	9 (21%)	56,56,56	1.86	16 (28%)
27	MGE	F	303	-	37,37,48	0.51	0	45,45,56	1.04	4 (8%)
21	CHL	3	314	-	50,54,74	2.15	18 (36%)	56,90,114	3.15	20 (35%)
25	BCR	L	304	-	41,41,41	1.68	8 (19%)	56,56,56	1.70	13 (23%)
26	LHG	A	824	-	39,39,48	0.39	0	43,44,54	0.74	1 (2%)
22	CLA	4	304	4	59,63,73	2.27	19 (32%)	71,101,113	3.05	29 (40%)
22	CLA	1	321	1	47,52,73	2.56	20 (42%)	56,88,113	3.29	26 (46%)
22	CLA	4	313	-	47,52,73	2.55	19 (40%)	56,88,113	3.43	26 (46%)
22	CLA	A	804	-	46,50,73	2.51	17 (36%)	55,85,113	3.50	29 (52%)
22	CLA	Y	302	-	50,54,73	2.52	20 (40%)	60,90,113	3.29	28 (46%)
22	CLA	B	811	6	60,64,73	2.24	19 (31%)	72,102,113	3.18	31 (43%)
22	CLA	2	307	2	64,68,73	2.18	19 (29%)	77,107,113	2.98	31 (40%)
22	CLA	B	852	6	59,63,73	2.29	20 (33%)	71,101,113	3.07	30 (42%)
22	CLA	B	812	6	63,67,73	2.18	19 (30%)	75,105,113	2.98	31 (41%)
21	CHL	4	308	-	48,53,74	2.25	18 (37%)	53,89,114	3.24	24 (45%)
21	CHL	Z	312	19	50,54,74	2.27	16 (32%)	56,90,114	3.15	23 (41%)
22	CLA	B	813	6	57,61,73	2.32	20 (35%)	68,98,113	3.02	31 (45%)
22	CLA	B	826	6	54,58,73	2.23	17 (31%)	65,95,113	3.35	30 (46%)
23	LUT	2	310	-	42,43,43	1.74	8 (19%)	51,60,60	2.01	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	MGE	1	315	-	37,37,48	0.57	0	45,45,56	1.06	3 (6%)
26	LHG	O	204	-	28,28,48	0.45	0	32,33,54	0.63	1 (3%)
22	CLA	1	307	1	59,63,73	2.26	19 (32%)	71,101,113	3.11	30 (42%)
22	CLA	A	807	5	65,69,73	2.15	20 (30%)	78,108,113	3.12	32 (41%)
22	CLA	B	801	-	59,63,73	2.15	15 (25%)	71,101,113	3.10	26 (36%)
21	CHL	Y	305	-	50,54,74	2.25	19 (38%)	56,90,114	3.16	22 (39%)
22	CLA	A	842	5	61,65,73	2.18	18 (29%)	72,102,113	3.01	28 (38%)
25	BCR	4	321	-	41,41,41	1.69	8 (19%)	56,56,56	1.81	14 (25%)
30	CL0	A	825	5	69,73,73	2.00	19 (27%)	83,113,113	2.68	28 (33%)
23	LUT	3	301	-	42,43,43	1.62	8 (19%)	51,60,60	1.46	11 (21%)
21	CHL	2	321	-	48,53,74	2.19	17 (35%)	53,89,114	3.23	23 (43%)
22	CLA	4	306	-	47,52,73	2.57	20 (42%)	56,88,113	3.28	26 (46%)
22	CLA	A	826	-	69,73,73	2.08	19 (27%)	83,113,113	2.94	28 (33%)
22	CLA	B	805	6	50,54,73	2.47	19 (38%)	60,90,113	3.29	26 (43%)
25	BCR	3	303	-	41,41,41	1.66	8 (19%)	56,56,56	1.73	13 (23%)
22	CLA	B	821	6	49,53,73	2.48	20 (40%)	59,89,113	3.33	28 (47%)
22	CLA	4	305	-	47,52,73	2.51	19 (40%)	56,88,113	3.42	28 (50%)
22	CLA	A	835	5	46,50,73	2.42	16 (34%)	55,85,113	3.30	25 (45%)
25	BCR	B	839	-	41,41,41	1.71	9 (21%)	56,56,56	1.90	15 (26%)
22	CLA	J	102	14	44,49,73	2.56	19 (43%)	52,84,113	3.45	26 (50%)
26	LHG	1	313	22	41,41,48	0.30	0	44,47,54	0.37	0
22	CLA	A	843	5	60,64,73	2.25	19 (31%)	72,102,113	3.10	29 (40%)
22	CLA	B	810	6	54,58,73	2.33	18 (33%)	65,95,113	3.26	29 (44%)
22	CLA	A	849	5	69,73,73	2.08	18 (26%)	83,113,113	2.84	30 (36%)
22	CLA	3	321	3	49,53,73	2.50	19 (38%)	59,89,113	3.27	27 (45%)
22	CLA	2	320	-	54,58,73	2.41	19 (35%)	65,95,113	3.12	33 (50%)
27	MGE	F	304	-	28,28,48	0.61	0	36,36,56	0.88	2 (5%)
22	CLA	A	828	5	43,48,73	2.71	21 (48%)	51,83,113	3.58	28 (54%)
22	CLA	A	848	5	49,53,73	2.47	19 (38%)	59,89,113	3.35	27 (45%)
26	LHG	2	314	-	28,28,48	0.45	0	32,33,54	0.83	2 (6%)
22	CLA	F	305	-	50,54,73	2.45	19 (38%)	60,90,113	3.27	26 (43%)
22	CLA	1	302	-	47,52,73	2.55	20 (42%)	56,88,113	3.32	25 (44%)
22	CLA	X	310	-	50,54,73	2.50	20 (40%)	60,90,113	3.34	28 (46%)
26	LHG	A	822	-	29,29,48	0.36	0	32,34,54	0.58	0
22	CLA	Z	311	-	50,54,73	2.51	20 (40%)	60,90,113	3.32	26 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LHG	4	302	-	26,26,48	0.36	0	29,32,54	0.62	0
26	LHG	B	842	22	29,29,48	0.32	0	32,35,54	0.49	0
29	SF4	A	813	5,6	0,12,12	-	-	-	-	-
22	CLA	4	318	4	50,54,73	2.53	20 (40%)	60,90,113	3.32	28 (46%)
22	CLA	A	852	-	65,69,73	2.17	19 (29%)	78,108,113	3.17	29 (37%)
21	CHL	X	302	-	51,55,74	2.22	19 (37%)	57,91,114	3.14	21 (36%)
22	CLA	B	823	6	65,69,73	2.15	19 (29%)	78,108,113	2.97	32 (41%)
22	CLA	B	822	6	69,73,73	2.07	19 (27%)	83,113,113	2.85	30 (36%)
26	LHG	O	205	-	27,27,48	0.46	0	31,32,54	0.60	1 (3%)
22	CLA	2	319	2	51,55,73	2.57	20 (39%)	61,91,113	3.50	29 (47%)
22	CLA	B	830	6	69,73,73	2.12	19 (27%)	83,113,113	2.92	33 (39%)
22	CLA	K	205	15	45,49,73	2.60	20 (44%)	54,84,113	3.48	30 (55%)
25	BCR	B	834	-	41,41,41	1.74	8 (19%)	56,56,56	2.03	17 (30%)
22	CLA	1	303	1	49,53,73	2.52	19 (38%)	59,89,113	3.38	31 (52%)

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
22	CLA	2	306	2	-	2/13/89/115	-
22	CLA	4	310	4	-	5/12/88/115	-
28	PQN	A	811	-	-	4/23/43/43	0/2/2/2
21	CHL	Z	302	-	-	1/19/95/117	-
22	CLA	O	210	-	-	2/10/86/115	-
21	CHL	1	301	1	-	11/14/90/117	-
22	CLA	A	830	5	-	3/21/97/115	-
22	CLA	B	820	6	-	3/15/91/115	-
26	LHG	X	314	22	-	3/25/25/53	-
22	CLA	B	807	6	1/1/15/20	12/39/111/115	-
22	CLA	2	318	2	1/1/14/20	13/35/111/115	-
26	LHG	2	316	-	-	2/37/37/53	-
26	LHG	2	315	22	-	10/36/36/53	-
22	CLA	A	834	5	-	8/17/93/115	-
22	CLA	Z	306	-	-	4/17/93/115	-
22	CLA	B	816	6	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	K	203	-	1/1/14/20	5/33/109/115	-
21	CHL	Z	304	-	-	7/19/95/117	-
25	BCR	G	202	-	-	8/29/63/63	0/2/2/2
22	CLA	B	827	6	1/1/15/20	11/39/115/115	-
22	CLA	4	315	4	-	3/10/86/115	-
26	LHG	3	306	-	-	12/42/42/53	-
22	CLA	Y	309	-	-	4/17/93/115	-
22	CLA	B	846	6,22	-	5/17/93/115	-
21	CHL	Y	306	-	-	7/17/93/117	-
22	CLA	Z	313	-	-	5/17/93/115	-
22	CLA	B	847	-	1/1/15/20	18/39/115/115	-
25	BCR	I	101	-	-	3/29/63/63	0/2/2/2
26	LHG	2	313	-	-	6/27/27/53	-
22	CLA	A	833	5	1/1/15/20	10/39/115/115	-
26	LHG	A	820	-	-	10/53/53/53	-
22	CLA	Y	301	-	-	1/17/93/115	-
25	BCR	K	201	-	-	2/29/63/63	0/2/2/2
26	LHG	B	843	-	-	21/44/44/53	-
22	CLA	A	809	5	1/1/14/20	13/35/111/115	-
22	CLA	1	320	-	-	2/15/91/115	-
22	CLA	G	206	26	-	10/25/101/115	-
24	XAT	2	311	-	-	5/31/93/93	0/4/4/4
22	CLA	B	818	6	1/1/15/20	12/39/115/115	-
29	SF4	C	102	7	-	-	0/6/5/5
22	CLA	A	837	5	-	4/12/88/115	-
22	CLA	B	829	-	1/1/15/20	10/39/115/115	-
25	BCR	L	302	-	-	4/29/63/63	0/2/2/2
22	CLA	4	314	4	-	0/8/84/115	-
22	CLA	B	853	6	-	10/24/100/115	-
21	CHL	Y	303	-	-	7/17/93/117	-
22	CLA	1	305	26	-	3/10/86/115	-
22	CLA	3	308	-	-	7/20/96/115	-
22	CLA	X	312	-	-	2/17/93/115	-
28	PQN	B	832	-	-	4/20/40/43	0/2/2/2
22	CLA	1	319	-	-	4/19/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	802	5	1/1/15/20	18/39/115/115	-
22	CLA	1	309	-	-	3/12/88/115	-
25	BCR	B	840	-	-	5/24/41/63	0/1/1/2
25	BCR	A	818	-	-	6/27/61/63	0/2/2/2
22	CLA	Z	309	-	-	4/17/93/115	-
22	CLA	N	202	-	-	2/13/89/115	-
27	MGE	3	304	-	-	5/27/47/63	0/1/1/1
25	BCR	O	203	-	-	4/29/63/63	0/2/2/2
21	CHL	Y	313	20	-	9/17/93/117	-
22	CLA	A	851	-	-	3/21/97/115	-
21	CHL	2	302	-	-	9/19/95/117	-
22	CLA	A	803	5	1/1/13/20	8/29/105/115	-
22	CLA	4	312	-	-	2/15/91/115	-
25	BCR	A	816	-	-	3/29/63/63	0/2/2/2
22	CLA	X	311	26	-	1/17/93/115	-
31	DGD	J	104	-	-	13/47/87/95	0/2/2/2
22	CLA	Z	314	-	-	5/17/93/115	-
21	CHL	4	317	4	-	6/10/86/117	-
22	CLA	A	859	-	1/1/13/20	13/31/107/115	-
27	MGE	3	305	-	-	11/20/40/63	0/1/1/1
31	DGD	B	841	-	-	11/48/88/95	0/2/2/2
25	BCR	B	844	-	-	3/29/63/63	0/2/2/2
22	CLA	A	831	5	1/1/15/20	12/39/115/115	-
22	CLA	H	201	12	-	2/10/86/115	-
21	CHL	4	307	-	-	11/15/91/117	-
21	CHL	X	306	-	-	8/19/95/117	-
25	BCR	2	312	-	-	8/29/63/63	0/2/2/2
22	CLA	2	308	2	-	7/24/100/115	-
22	CLA	Z	307	-	-	0/17/93/115	-
22	CLA	3	313	3	-	0/15/91/115	-
22	CLA	Y	310	-	-	5/17/93/115	-
21	CHL	Z	301	19	-	7/19/95/117	-
22	CLA	A	845	5	-	6/15/91/115	-
22	CLA	X	303	-	-	6/17/93/115	-
22	CLA	Y	314	-	-	2/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	B	835	-	-	4/29/63/63	0/2/2/2
22	CLA	B	803	6	1/1/15/20	19/39/115/115	-
22	CLA	4	311	4	-	7/15/91/115	-
22	CLA	Z	308	-	-	0/17/93/115	-
22	CLA	B	809	-	1/1/14/20	11/33/109/115	-
21	CHL	2	309	2	-	5/17/93/117	-
25	BCR	B	837	-	-	5/29/63/63	0/2/2/2
22	CLA	B	806	6	1/1/13/20	12/30/106/115	-
22	CLA	B	849	6	-	10/24/100/115	-
24	XAT	3	302	-	-	7/31/93/93	0/4/4/4
21	CHL	Z	305	-	-	9/19/95/117	-
22	CLA	A	847	5	-	2/12/88/115	-
26	LHG	4	303	-	-	1/39/39/53	-
22	CLA	A	838	5	1/1/15/20	21/39/115/115	-
21	CHL	2	301	-	-	9/22/98/117	-
22	CLA	3	311	-	-	6/15/91/115	-
22	CLA	3	317	-	-	3/13/89/115	-
22	CLA	3	319	3	-	4/15/91/115	-
22	CLA	L	307	-	-	5/15/91/115	-
22	CLA	1	304	1	-	8/25/101/115	-
22	CLA	B	845	-	1/1/15/20	17/39/115/115	-
22	CLA	Y	308	-	-	8/17/93/115	-
22	CLA	3	312	3	1/1/15/20	15/39/115/115	-
26	LHG	G	203	-	-	8/40/40/53	-
21	CHL	Y	307	-	-	7/17/93/117	-
22	CLA	2	304	2	1/1/13/20	7/27/103/115	-
22	CLA	A	839	5	-	6/15/91/115	-
22	CLA	1	306	-	-	4/13/89/115	-
22	CLA	A	844	5	1/1/15/20	9/39/115/115	-
22	CLA	Y	312	-	-	6/17/93/115	-
25	BCR	B	838	-	-	1/29/63/63	0/2/2/2
22	CLA	3	316	3	-	7/15/91/115	-
21	CHL	X	307	-	-	7/17/93/117	-
25	BCR	F	302	-	-	5/29/63/63	0/2/2/2
22	CLA	A	808	5	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CHL	Y	304	-	-	11/17/93/117	-
21	CHL	3	307	2	-	9/23/99/117	-
22	CLA	F	306	10	-	7/17/93/115	-
22	CLA	K	204	15	-	5/17/93/115	-
22	CLA	B	848	-	1/1/13/20	6/30/106/115	-
22	CLA	B	851	6	1/1/15/20	18/39/115/115	-
21	CHL	Z	303	-	-	9/17/93/117	-
22	CLA	B	828	6	-	5/18/94/115	-
23	LUT	1	310	-	-	2/29/67/67	0/2/2/2
31	DGD	G	201	-	-	5/33/53/95	0/1/1/2
22	CLA	O	207	-	1/1/14/20	10/38/114/115	-
25	BCR	O	202	-	-	3/29/63/63	0/2/2/2
29	SF4	C	101	7	-	-	0/6/5/5
22	CLA	3	320	-	-	2/11/87/115	-
22	CLA	A	841	-	-	1/17/93/115	-
22	CLA	A	827	-	1/1/15/20	13/39/115/115	-
22	CLA	G	207	11	-	6/15/91/115	-
26	LHG	1	322	-	-	5/34/34/53	-
22	CLA	2	303	2	-	6/15/91/115	-
22	CLA	B	831	26	1/1/15/20	19/39/115/115	-
22	CLA	A	854	5	1/1/15/20	11/39/115/115	-
22	CLA	A	801	5	1/1/13/20	10/32/108/115	-
22	CLA	L	305	16	-	4/15/91/115	-
22	CLA	1	317	1	1/1/13/20	14/30/106/115	-
22	CLA	Y	311	-	1/1/15/20	15/39/115/115	-
22	CLA	2	305	26	-	1/15/91/115	-
26	LHG	1	314	-	-	2/28/28/53	-
22	CLA	1	318	-	1/1/13/20	9/27/103/115	-
22	CLA	O	206	-	-	0/17/93/115	-
22	CLA	B	802	6	-	0/15/91/115	-
22	CLA	2	322	4	-	2/13/89/115	-
22	CLA	O	208	-	1/1/14/20	14/33/109/115	-
22	CLA	2	317	-	-	3/10/86/115	-
21	CHL	X	305	19	-	8/20/96/117	-
25	BCR	1	312	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	XAT	4	320	-	-	3/31/93/93	0/4/4/4
26	LHG	F	301	-	-	8/32/32/53	-
22	CLA	A	812	26	1/1/13/20	13/27/103/115	-
22	CLA	B	817	-	1/1/13/20	10/31/107/115	-
22	CLA	A	856	5	-	4/23/99/115	-
22	CLA	A	853	5	1/1/15/20	16/39/115/115	-
26	LHG	A	821	-	-	3/25/25/53	-
21	CHL	X	308	-	-	11/19/95/117	-
22	CLA	B	819	6	1/1/14/20	13/33/109/115	-
22	CLA	Z	310	-	-	0/17/93/115	-
22	CLA	A	857	5	1/1/13/20	4/29/105/115	-
21	CHL	X	309	-	-	10/17/93/117	-
22	CLA	A	846	-	1/1/15/20	12/39/115/115	-
22	CLA	B	804	6	1/1/15/20	13/39/115/115	-
22	CLA	B	824	6	1/1/14/20	7/33/109/115	-
22	CLA	A	840	5	-	5/15/91/115	-
22	CLA	G	205	-	-	8/15/91/115	-
25	BCR	L	303	-	-	2/29/63/63	0/2/2/2
22	CLA	A	832	5	-	1/18/94/115	-
26	LHG	4	301	-	-	8/32/32/53	-
25	BCR	B	836	-	-	4/29/63/63	0/2/2/2
25	BCR	J	101	-	-	4/29/63/63	0/2/2/2
22	CLA	A	855	5	1/1/15/20	7/39/115/115	-
22	CLA	A	858	-	1/1/15/20	13/39/115/115	-
26	LHG	G	204	22	-	1/26/26/53	-
31	DGD	O	201	-	-	11/42/82/95	0/2/2/2
22	CLA	A	805	-	-	6/21/97/115	-
22	CLA	B	825	-	-	5/17/93/115	-
25	BCR	A	817	-	-	4/29/63/63	0/2/2/2
27	MGE	N	201	-	-	7/26/46/63	0/1/1/1
21	CHL	1	316	1	-	8/17/93/117	-
22	CLA	B	850	6	1/1/15/20	18/39/115/115	-
24	XAT	1	311	-	-	11/31/93/93	0/4/4/4
26	LHG	A	823	22	-	1/36/36/53	-
25	BCR	A	814	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	808	6	1/1/15/20	13/39/115/115	-
22	CLA	4	316	4	-	3/10/86/115	-
22	CLA	3	309	3	1/1/13/20	14/32/108/115	-
25	BCR	J	103	-	-	4/29/63/63	0/2/2/2
21	CHL	4	309	-	-	11/17/93/117	-
22	CLA	A	810	-	1/1/15/20	18/39/115/115	-
22	CLA	3	318	3	-	4/15/91/115	-
22	CLA	A	829	5,22	-	10/21/97/115	-
22	CLA	X	313	-	-	9/17/93/115	-
22	CLA	X	304	-	-	7/17/93/115	-
22	CLA	A	836	5,22	1/1/14/20	6/33/109/115	-
22	CLA	A	806	5	-	10/25/101/115	-
22	CLA	K	202	15	-	7/13/89/115	-
22	CLA	A	850	-	1/1/15/20	11/39/115/115	-
22	CLA	B	815	-	1/1/13/20	15/31/107/115	-
22	CLA	B	833	22	1/1/13/20	13/29/105/115	-
22	CLA	3	310	-	1/1/13/20	19/31/107/115	-
22	CLA	1	308	1	-	3/10/86/115	-
22	CLA	L	306	16	1/1/15/20	21/39/115/115	-
25	BCR	L	301	-	-	7/29/63/63	0/2/2/2
22	CLA	X	301	-	-	0/17/93/115	-
22	CLA	3	315	3	-	6/10/86/115	-
22	CLA	B	814	-	1/1/15/20	10/39/115/115	-
22	CLA	O	209	18	-	4/18/94/115	-
23	LUT	4	322	-	-	3/29/67/67	0/2/2/2
25	BCR	A	819	-	-	4/29/63/63	0/2/2/2
23	LUT	4	319	-	-	0/29/67/67	0/2/2/2
25	BCR	A	815	-	-	3/29/63/63	0/2/2/2
27	MGE	F	303	-	-	14/32/52/63	0/1/1/1
21	CHL	3	314	-	-	6/17/93/117	-
25	BCR	L	304	-	-	0/29/63/63	0/2/2/2
26	LHG	A	824	-	-	8/41/41/53	-
22	CLA	4	304	4	1/1/13/20	7/27/103/115	-
22	CLA	1	321	1	-	2/13/89/115	-
22	CLA	4	313	-	-	4/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	804	-	-	4/12/88/115	-
22	CLA	Y	302	-	-	6/17/93/115	-
22	CLA	B	811	6	1/1/13/20	9/29/105/115	-
22	CLA	2	307	2	1/1/14/20	17/33/109/115	-
22	CLA	B	852	6	1/1/13/20	8/27/103/115	-
22	CLA	B	812	6	1/1/13/20	12/32/108/115	-
21	CHL	4	308	-	-	8/15/91/117	-
21	CHL	Z	312	19	-	7/17/93/117	-
22	CLA	B	813	6	-	11/25/101/115	-
22	CLA	B	826	6	-	8/21/97/115	-
23	LUT	2	310	-	-	4/29/67/67	0/2/2/2
27	MGE	1	315	-	-	15/32/52/63	0/1/1/1
26	LHG	O	204	-	-	4/30/30/53	-
22	CLA	1	307	1	1/1/13/20	9/27/103/115	-
22	CLA	A	807	5	1/1/14/20	17/35/111/115	-
22	CLA	B	801	-	1/1/13/20	10/27/103/115	-
30	CL0	A	825	5	1/1/15/20	10/39/115/115	-
22	CLA	A	842	5	1/1/12/20	7/29/105/115	-
21	CHL	Y	305	-	-	8/17/93/117	-
25	BCR	4	321	-	-	6/29/63/63	0/2/2/2
23	LUT	3	301	-	-	0/29/67/67	0/2/2/2
21	CHL	2	321	-	-	9/15/91/117	-
22	CLA	A	826	-	1/1/15/20	13/39/115/115	-
22	CLA	4	306	-	-	7/13/89/115	-
22	CLA	B	805	6	-	6/17/93/115	-
25	BCR	3	303	-	-	5/29/63/63	0/2/2/2
22	CLA	B	821	6	-	8/15/91/115	-
22	CLA	4	305	-	-	4/13/89/115	-
22	CLA	A	835	5	-	5/12/88/115	-
25	BCR	B	839	-	-	2/29/63/63	0/2/2/2
22	CLA	J	102	14	-	1/10/86/115	-
26	LHG	1	313	22	-	8/46/46/53	-
22	CLA	A	843	5	1/1/13/20	9/29/105/115	-
22	CLA	B	810	6	-	5/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	849	5	1/1/15/20	10/39/115/115	-
22	CLA	3	321	3	-	2/15/91/115	-
22	CLA	2	320	-	-	4/21/97/115	-
27	MGE	F	304	-	-	12/23/43/63	0/1/1/1
22	CLA	A	828	5	-	0/8/84/115	-
22	CLA	A	848	5	-	1/15/91/115	-
26	LHG	2	314	-	-	4/30/30/53	-
22	CLA	F	305	-	-	2/17/93/115	-
22	CLA	1	302	-	-	3/13/89/115	-
22	CLA	X	310	-	-	7/17/93/115	-
26	LHG	A	822	-	-	9/33/33/53	-
22	CLA	Z	311	-	-	4/17/93/115	-
26	LHG	4	302	-	-	14/31/31/53	-
26	LHG	B	842	22	-	6/34/34/53	-
29	SF4	A	813	5,6	-	-	0/6/5/5
22	CLA	A	852	-	1/1/14/20	16/35/111/115	-
22	CLA	4	318	4	-	8/17/93/115	-
21	CHL	X	302	-	-	7/19/95/117	-
22	CLA	B	823	6	1/1/14/20	12/35/111/115	-
22	CLA	B	822	6	1/1/15/20	9/39/115/115	-
26	LHG	O	205	-	-	3/29/29/53	-
22	CLA	2	319	2	-	5/17/93/115	-
22	CLA	B	830	6	1/1/15/20	17/39/115/115	-
22	CLA	K	205	15	-	2/10/86/115	-
25	BCR	B	834	-	-	5/29/63/63	0/2/2/2
22	CLA	1	303	1	-	6/15/91/115	-

All (4216) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	X	304	CLA	C1D-ND	10.04	1.50	1.37
22	3	317	CLA	C1D-ND	8.97	1.48	1.37
22	4	318	CLA	C1D-ND	8.90	1.48	1.37
22	Y	312	CLA	C1D-ND	8.87	1.48	1.37
22	A	830	CLA	C1D-ND	8.85	1.48	1.37
22	B	816	CLA	C1D-ND	8.83	1.48	1.37
22	2	308	CLA	C1D-ND	8.81	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	804	CLA	C1D-ND	8.80	1.48	1.37
22	B	803	CLA	C1D-ND	8.79	1.48	1.37
22	A	838	CLA	C1D-ND	8.79	1.48	1.37
22	K	204	CLA	C1D-ND	8.75	1.48	1.37
22	G	206	CLA	C1D-ND	8.74	1.48	1.37
22	3	312	CLA	C1D-ND	8.74	1.48	1.37
22	Y	314	CLA	C1D-ND	8.73	1.48	1.37
22	O	209	CLA	C1D-ND	8.73	1.48	1.37
22	2	306	CLA	C1D-ND	8.71	1.48	1.37
22	X	310	CLA	C1D-ND	8.71	1.48	1.37
22	Y	310	CLA	C1D-ND	8.71	1.48	1.37
22	B	833	CLA	C1D-ND	8.70	1.48	1.37
22	Y	311	CLA	C1D-ND	8.70	1.48	1.37
22	Z	311	CLA	C1D-ND	8.70	1.48	1.37
22	Z	306	CLA	C1D-ND	8.68	1.48	1.37
22	X	312	CLA	C1D-ND	8.68	1.48	1.37
22	Z	308	CLA	C1D-ND	8.68	1.48	1.37
22	X	313	CLA	C1D-ND	8.68	1.48	1.37
22	Z	307	CLA	C1D-ND	8.68	1.48	1.37
22	B	824	CLA	C1D-ND	8.68	1.48	1.37
22	X	303	CLA	C1D-ND	8.68	1.48	1.37
22	1	303	CLA	C1D-ND	8.68	1.48	1.37
22	2	317	CLA	C1D-ND	8.68	1.48	1.37
22	Y	302	CLA	C1D-ND	8.67	1.48	1.37
22	G	205	CLA	C1D-ND	8.65	1.48	1.37
22	Y	309	CLA	C1D-ND	8.64	1.48	1.37
22	Z	309	CLA	C1D-ND	8.64	1.48	1.37
22	A	837	CLA	C1D-ND	8.63	1.48	1.37
22	B	808	CLA	C1D-ND	8.63	1.48	1.37
22	Y	308	CLA	C1D-ND	8.63	1.48	1.37
22	X	301	CLA	C1D-ND	8.62	1.48	1.37
22	J	102	CLA	C1D-ND	8.62	1.48	1.37
22	2	322	CLA	C1D-ND	8.61	1.48	1.37
22	O	206	CLA	C1D-ND	8.61	1.48	1.37
22	X	311	CLA	C1D-ND	8.61	1.48	1.37
22	3	313	CLA	C1D-ND	8.61	1.48	1.37
22	3	308	CLA	C1D-ND	8.60	1.48	1.37
22	B	848	CLA	C1D-ND	8.59	1.48	1.37
22	Z	313	CLA	C1D-ND	8.59	1.48	1.37
22	3	319	CLA	C1D-ND	8.59	1.48	1.37
22	2	319	CLA	C1D-ND	8.59	1.48	1.37
22	2	318	CLA	C1D-ND	8.58	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	313	CLA	C1D-ND	8.58	1.48	1.37
22	1	306	CLA	C1D-ND	8.58	1.48	1.37
22	3	320	CLA	C1D-ND	8.58	1.48	1.37
22	O	208	CLA	C1D-ND	8.58	1.48	1.37
22	Z	310	CLA	C1D-ND	8.58	1.48	1.37
22	4	315	CLA	C1D-ND	8.57	1.48	1.37
22	A	802	CLA	C1D-ND	8.56	1.48	1.37
22	1	320	CLA	C1D-ND	8.56	1.48	1.37
22	1	302	CLA	C1D-ND	8.56	1.48	1.37
22	2	307	CLA	C1D-ND	8.55	1.48	1.37
22	A	832	CLA	C1D-ND	8.55	1.48	1.37
22	N	202	CLA	C1D-ND	8.54	1.48	1.37
22	K	205	CLA	C1D-ND	8.54	1.48	1.37
22	3	310	CLA	C1D-ND	8.54	1.48	1.37
22	A	812	CLA	C1D-ND	8.53	1.48	1.37
22	1	309	CLA	C1D-ND	8.52	1.48	1.37
22	Y	301	CLA	C1D-ND	8.52	1.48	1.37
22	O	210	CLA	C1D-ND	8.52	1.48	1.37
22	4	311	CLA	C1D-ND	8.52	1.48	1.37
22	Z	314	CLA	C1D-ND	8.51	1.48	1.37
22	1	318	CLA	C1D-ND	8.51	1.48	1.37
22	A	843	CLA	C1D-ND	8.50	1.48	1.37
22	B	849	CLA	C1D-ND	8.49	1.48	1.37
22	1	321	CLA	C1D-ND	8.49	1.48	1.37
22	4	305	CLA	C1D-ND	8.48	1.48	1.37
22	A	806	CLA	C1D-ND	8.48	1.48	1.37
22	1	305	CLA	C1D-ND	8.48	1.48	1.37
22	A	857	CLA	C1D-ND	8.48	1.48	1.37
22	B	805	CLA	C1D-ND	8.47	1.48	1.37
22	G	207	CLA	C1D-ND	8.47	1.48	1.37
22	3	311	CLA	C1D-ND	8.46	1.48	1.37
22	A	828	CLA	C1D-ND	8.46	1.48	1.37
22	B	852	CLA	C1D-ND	8.46	1.48	1.37
22	F	305	CLA	C1D-ND	8.46	1.48	1.37
22	1	304	CLA	C1D-ND	8.46	1.48	1.37
22	4	312	CLA	C1D-ND	8.45	1.48	1.37
22	1	307	CLA	C1D-ND	8.45	1.48	1.37
22	K	202	CLA	C1D-ND	8.44	1.48	1.37
22	A	836	CLA	C1D-ND	8.44	1.48	1.37
22	3	309	CLA	C1D-ND	8.43	1.48	1.37
22	A	841	CLA	C1D-ND	8.43	1.48	1.37
22	B	811	CLA	C1D-ND	8.43	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	839	CLA	C1D-ND	8.42	1.48	1.37
22	A	859	CLA	C1D-ND	8.41	1.48	1.37
22	A	833	CLA	C1D-ND	8.40	1.48	1.37
22	A	831	CLA	C1D-ND	8.39	1.48	1.37
22	H	201	CLA	C1D-ND	8.38	1.48	1.37
22	K	203	CLA	C1D-ND	8.37	1.48	1.37
22	B	806	CLA	C1D-ND	8.37	1.48	1.37
22	O	207	CLA	C1D-ND	8.36	1.48	1.37
22	3	316	CLA	C1D-ND	8.36	1.48	1.37
22	A	809	CLA	C1D-ND	8.36	1.48	1.37
22	A	840	CLA	C1D-ND	8.35	1.48	1.37
22	A	808	CLA	C1D-ND	8.35	1.48	1.37
22	B	853	CLA	C1D-ND	8.34	1.48	1.37
22	B	827	CLA	C1D-ND	8.34	1.48	1.37
22	F	306	CLA	C1D-ND	8.34	1.48	1.37
22	B	828	CLA	C1D-ND	8.34	1.48	1.37
22	L	305	CLA	C1D-ND	8.33	1.48	1.37
22	A	847	CLA	C1D-ND	8.33	1.48	1.37
22	2	320	CLA	C1D-ND	8.33	1.48	1.37
22	B	846	CLA	C1D-ND	8.33	1.48	1.37
22	1	319	CLA	C1D-ND	8.32	1.48	1.37
22	A	835	CLA	C1D-ND	8.31	1.48	1.37
22	B	804	CLA	C1D-ND	8.31	1.48	1.37
22	B	823	CLA	C1D-ND	8.30	1.48	1.37
22	A	805	CLA	C1D-ND	8.30	1.48	1.37
22	A	853	CLA	C1D-ND	8.30	1.48	1.37
22	B	831	CLA	C1D-ND	8.29	1.48	1.37
22	B	812	CLA	C1D-ND	8.28	1.48	1.37
22	A	801	CLA	C1D-ND	8.28	1.48	1.37
22	L	307	CLA	C1D-ND	8.26	1.47	1.37
22	A	807	CLA	C1D-ND	8.26	1.47	1.37
22	A	849	CLA	C1D-ND	8.25	1.47	1.37
22	4	306	CLA	C1D-ND	8.25	1.47	1.37
22	2	304	CLA	C1D-ND	8.24	1.47	1.37
22	A	845	CLA	C1D-ND	8.24	1.47	1.37
22	B	850	CLA	C1D-ND	8.24	1.47	1.37
22	B	809	CLA	C1D-ND	8.24	1.47	1.37
22	A	846	CLA	C1D-ND	8.24	1.47	1.37
22	B	821	CLA	C1D-ND	8.24	1.47	1.37
22	B	830	CLA	C1D-ND	8.23	1.47	1.37
22	B	829	CLA	C1D-ND	8.22	1.47	1.37
22	3	318	CLA	C1D-ND	8.21	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	829	CLA	C1D-ND	8.21	1.47	1.37
22	1	308	CLA	C1D-ND	8.21	1.47	1.37
22	4	314	CLA	C1D-ND	8.21	1.47	1.37
22	A	856	CLA	C1D-ND	8.17	1.47	1.37
22	3	321	CLA	C1D-ND	8.17	1.47	1.37
22	2	305	CLA	C1D-ND	8.16	1.47	1.37
22	B	825	CLA	C1D-ND	8.14	1.47	1.37
22	B	817	CLA	C1D-ND	8.13	1.47	1.37
22	A	852	CLA	C1D-ND	8.12	1.47	1.37
22	4	304	CLA	C1D-ND	8.11	1.47	1.37
22	B	810	CLA	C1D-ND	8.11	1.47	1.37
22	B	819	CLA	C1D-ND	8.09	1.47	1.37
22	A	858	CLA	C1D-ND	8.09	1.47	1.37
22	4	316	CLA	C1D-ND	8.09	1.47	1.37
22	A	851	CLA	C1D-ND	8.09	1.47	1.37
22	1	317	CLA	C1D-ND	8.08	1.47	1.37
22	B	813	CLA	C1D-ND	8.07	1.47	1.37
22	A	844	CLA	C1D-ND	8.07	1.47	1.37
22	B	847	CLA	C1D-ND	8.05	1.47	1.37
22	A	834	CLA	C1D-ND	8.04	1.47	1.37
22	A	810	CLA	C1D-ND	8.01	1.47	1.37
22	A	842	CLA	C1D-ND	8.01	1.47	1.37
22	A	850	CLA	C1D-ND	7.99	1.47	1.37
22	2	303	CLA	C1D-ND	7.96	1.47	1.37
22	A	855	CLA	C1D-ND	7.94	1.47	1.37
22	B	815	CLA	C1D-ND	7.94	1.47	1.37
22	A	848	CLA	C1D-ND	7.91	1.47	1.37
22	B	851	CLA	C1D-ND	7.91	1.47	1.37
22	B	822	CLA	C1D-ND	7.90	1.47	1.37
22	3	315	CLA	C1D-ND	7.86	1.47	1.37
22	A	803	CLA	C1D-ND	7.80	1.47	1.37
22	4	310	CLA	C1D-ND	7.69	1.47	1.37
22	L	306	CLA	C1D-ND	7.68	1.47	1.37
22	B	845	CLA	C1D-ND	7.62	1.47	1.37
22	B	802	CLA	C1D-ND	7.58	1.47	1.37
22	B	818	CLA	C1D-ND	7.55	1.47	1.37
22	B	814	CLA	C1D-ND	7.46	1.47	1.37
22	A	854	CLA	C1D-ND	7.02	1.46	1.37
22	A	826	CLA	C1D-ND	6.91	1.46	1.37
22	B	807	CLA	OBD-CAD	6.89	1.34	1.22
22	B	801	CLA	C1D-ND	6.82	1.46	1.37
22	A	827	CLA	C1D-ND	6.74	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	820	CLA	C1D-ND	6.73	1.46	1.37
25	B	840	BCR	C17-C18	6.44	1.44	1.35
30	A	825	CL0	C1D-ND	6.34	1.45	1.37
22	B	826	CLA	C1D-ND	6.29	1.45	1.37
22	A	826	CLA	CHC-C1C	5.53	1.49	1.38
25	1	312	BCR	C17-C18	5.48	1.43	1.35
22	X	304	CLA	O2D-CGD	5.43	1.46	1.33
22	B	831	CLA	O2D-CGD	5.37	1.46	1.33
22	3	316	CLA	O2D-CGD	5.33	1.46	1.33
22	1	303	CLA	O2D-CGD	5.29	1.46	1.33
22	A	808	CLA	O2D-CGD	5.25	1.46	1.33
22	3	318	CLA	O2D-CGD	5.25	1.46	1.33
22	2	320	CLA	O2D-CGD	5.24	1.46	1.33
22	3	311	CLA	O2D-CGD	5.23	1.46	1.33
22	A	826	CLA	O2D-CGD	5.23	1.46	1.33
25	G	202	BCR	C21-C22	5.22	1.42	1.35
22	X	310	CLA	O2D-CGD	5.22	1.45	1.33
21	Z	304	CHL	O2D-CGD	5.22	1.45	1.33
22	X	312	CLA	O2D-CGD	5.21	1.45	1.33
22	B	830	CLA	C3C-C2C	5.21	1.47	1.36
21	Y	305	CHL	O2D-CGD	5.21	1.45	1.33
22	Z	308	CLA	O2D-CGD	5.21	1.45	1.33
22	Y	310	CLA	O2D-CGD	5.20	1.45	1.33
22	Y	309	CLA	O2D-CGD	5.20	1.45	1.33
22	Z	311	CLA	O2D-CGD	5.20	1.45	1.33
22	Z	314	CLA	O2D-CGD	5.20	1.45	1.33
21	Y	303	CHL	O2D-CGD	5.20	1.45	1.33
21	Y	306	CHL	O2D-CGD	5.20	1.45	1.33
22	Z	307	CLA	O2D-CGD	5.20	1.45	1.33
21	Z	302	CHL	O2D-CGD	5.20	1.45	1.33
22	G	207	CLA	O2D-CGD	5.19	1.45	1.33
22	Z	313	CLA	O2D-CGD	5.19	1.45	1.33
22	Y	314	CLA	O2D-CGD	5.19	1.45	1.33
22	X	303	CLA	O2D-CGD	5.19	1.45	1.33
21	X	305	CHL	O2D-CGD	5.19	1.45	1.33
21	Y	313	CHL	O2D-CGD	5.19	1.45	1.33
21	X	306	CHL	O2D-CGD	5.19	1.45	1.33
22	2	319	CLA	O2D-CGD	5.19	1.45	1.33
22	2	304	CLA	O2D-CGD	5.19	1.45	1.33
22	Z	309	CLA	O2D-CGD	5.19	1.45	1.33
21	2	301	CHL	O2D-CGD	5.19	1.45	1.33
22	3	308	CLA	O2D-CGD	5.18	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Z	312	CHL	O2D-CGD	5.18	1.45	1.33
22	A	855	CLA	O2D-CGD	5.18	1.45	1.33
21	Y	304	CHL	O2D-CGD	5.18	1.45	1.33
21	X	302	CHL	O2D-CGD	5.18	1.45	1.33
22	X	301	CLA	O2D-CGD	5.18	1.45	1.33
21	Y	307	CHL	O2D-CGD	5.18	1.45	1.33
22	B	807	CLA	O2D-CGD	5.18	1.45	1.33
22	B	813	CLA	O2D-CGD	5.18	1.45	1.33
22	A	803	CLA	O2D-CGD	5.17	1.45	1.33
22	Z	310	CLA	O2D-CGD	5.17	1.45	1.33
21	X	309	CHL	O2D-CGD	5.17	1.45	1.33
22	1	304	CLA	O2D-CGD	5.17	1.45	1.33
22	4	312	CLA	O2D-CGD	5.17	1.45	1.33
22	4	311	CLA	O2D-CGD	5.17	1.45	1.33
22	3	312	CLA	O2D-CGD	5.17	1.45	1.33
22	X	311	CLA	O2D-CGD	5.17	1.45	1.33
22	B	801	CLA	CHC-C1C	5.17	1.49	1.38
22	1	320	CLA	O2D-CGD	5.17	1.45	1.33
22	F	306	CLA	O2D-CGD	5.16	1.45	1.33
21	Z	303	CHL	O2D-CGD	5.16	1.45	1.33
23	2	310	LUT	C30-C29	5.16	1.42	1.35
21	X	308	CHL	O2D-CGD	5.16	1.45	1.33
22	3	321	CLA	O2D-CGD	5.16	1.45	1.33
22	Y	311	CLA	O2D-CGD	5.16	1.45	1.33
22	Y	301	CLA	O2D-CGD	5.16	1.45	1.33
22	1	309	CLA	O2D-CGD	5.16	1.45	1.33
22	2	317	CLA	O2D-CGD	5.16	1.45	1.33
22	O	206	CLA	O2D-CGD	5.16	1.45	1.33
22	Y	302	CLA	O2D-CGD	5.15	1.45	1.33
22	O	210	CLA	O2D-CGD	5.15	1.45	1.33
21	Z	301	CHL	O2D-CGD	5.15	1.45	1.33
22	H	201	CLA	O2D-CGD	5.15	1.45	1.33
21	3	314	CHL	O2D-CGD	5.15	1.45	1.33
22	F	305	CLA	O2D-CGD	5.15	1.45	1.33
22	Y	308	CLA	O2D-CGD	5.15	1.45	1.33
22	B	833	CLA	O2D-CGD	5.15	1.45	1.33
22	3	319	CLA	O2D-CGD	5.15	1.45	1.33
22	A	842	CLA	O2D-CGD	5.15	1.45	1.33
22	2	307	CLA	O2D-CGD	5.14	1.45	1.33
22	O	209	CLA	O2D-CGD	5.14	1.45	1.33
22	X	313	CLA	O2D-CGD	5.14	1.45	1.33
22	B	812	CLA	O2D-CGD	5.14	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	319	CLA	O2D-CGD	5.14	1.45	1.33
22	Y	312	CLA	O2D-CGD	5.14	1.45	1.33
22	A	809	CLA	O2D-CGD	5.14	1.45	1.33
22	K	205	CLA	O2D-CGD	5.13	1.45	1.33
22	A	836	CLA	O2D-CGD	5.13	1.45	1.33
22	4	318	CLA	O2D-CGD	5.13	1.45	1.33
21	1	301	CHL	O2D-CGD	5.13	1.45	1.33
22	B	845	CLA	O2D-CGD	5.13	1.45	1.33
22	A	831	CLA	O2D-CGD	5.13	1.45	1.33
22	G	206	CLA	O2D-CGD	5.13	1.45	1.33
21	X	307	CHL	O2D-CGD	5.13	1.45	1.33
22	B	817	CLA	O2D-CGD	5.13	1.45	1.33
22	A	830	CLA	O2D-CGD	5.12	1.45	1.33
22	1	305	CLA	O2D-CGD	5.12	1.45	1.33
21	Z	305	CHL	O2D-CGD	5.12	1.45	1.33
22	3	310	CLA	O2D-CGD	5.12	1.45	1.33
22	B	829	CLA	O2D-CGD	5.11	1.45	1.33
22	K	204	CLA	O2D-CGD	5.11	1.45	1.33
21	2	309	CHL	O2D-CGD	5.11	1.45	1.33
22	2	318	CLA	O2D-CGD	5.11	1.45	1.33
22	B	808	CLA	O2D-CGD	5.11	1.45	1.33
22	B	853	CLA	O2D-CGD	5.11	1.45	1.33
22	O	207	CLA	O2D-CGD	5.10	1.45	1.33
22	A	846	CLA	O2D-CGD	5.10	1.45	1.33
22	A	848	CLA	O2D-CGD	5.09	1.45	1.33
22	A	833	CLA	O2D-CGD	5.09	1.45	1.33
22	B	819	CLA	O2D-CGD	5.09	1.45	1.33
22	B	849	CLA	O2D-CGD	5.09	1.45	1.33
22	B	846	CLA	O2D-CGD	5.09	1.45	1.33
22	B	852	CLA	O2D-CGD	5.09	1.45	1.33
22	L	307	CLA	O2D-CGD	5.09	1.45	1.33
22	B	816	CLA	O2D-CGD	5.08	1.45	1.33
22	4	310	CLA	O2D-CGD	5.08	1.45	1.33
25	1	312	BCR	C21-C22	5.08	1.42	1.35
22	3	313	CLA	O2D-CGD	5.08	1.45	1.33
22	A	849	CLA	O2D-CGD	5.07	1.45	1.33
22	1	308	CLA	C3A-C2A	-5.07	1.49	1.54
22	A	806	CLA	O2D-CGD	5.07	1.45	1.33
22	B	802	CLA	O2D-CGD	5.07	1.45	1.33
22	A	810	CLA	O2D-CGD	5.07	1.45	1.33
22	A	851	CLA	O2D-CGD	5.07	1.45	1.33
21	2	302	CHL	O2D-CGD	5.07	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	857	CLA	O2D-CGD	5.07	1.45	1.33
22	K	203	CLA	O2D-CGD	5.06	1.45	1.33
22	B	848	CLA	O2D-CGD	5.06	1.45	1.33
22	3	309	CLA	O2D-CGD	5.06	1.45	1.33
22	B	821	CLA	O2D-CGD	5.06	1.45	1.33
22	O	208	CLA	O2D-CGD	5.06	1.45	1.33
22	B	830	CLA	O2D-CGD	5.06	1.45	1.33
22	A	847	CLA	O2D-CGD	5.06	1.45	1.33
22	B	818	CLA	O2D-CGD	5.05	1.45	1.33
22	2	305	CLA	O2D-CGD	5.04	1.45	1.33
22	A	859	CLA	O2D-CGD	5.04	1.45	1.33
22	Z	306	CLA	O2D-CGD	5.04	1.45	1.33
22	A	844	CLA	O2D-CGD	5.03	1.45	1.33
22	4	304	CLA	O2D-CGD	5.03	1.45	1.33
22	4	316	CLA	O2D-CGD	5.03	1.45	1.33
22	A	854	CLA	O2D-CGD	5.03	1.45	1.33
22	B	801	CLA	O2D-CGD	5.02	1.45	1.33
22	A	852	CLA	O2D-CGD	5.02	1.45	1.33
22	B	816	CLA	CHB-C1B	5.02	1.50	1.39
22	A	843	CLA	O2D-CGD	5.01	1.45	1.33
21	1	301	CHL	C3D-C4D	-5.01	1.32	1.44
22	B	847	CLA	O2D-CGD	5.01	1.45	1.33
22	A	840	CLA	O2D-CGD	5.01	1.45	1.33
22	B	825	CLA	O2D-CGD	5.00	1.45	1.33
22	A	837	CLA	O2D-CGD	5.00	1.45	1.33
22	A	841	CLA	O2D-CGD	5.00	1.45	1.33
21	4	309	CHL	O2D-CGD	4.99	1.45	1.33
22	A	829	CLA	O2D-CGD	4.98	1.45	1.33
22	L	305	CLA	O2D-CGD	4.98	1.45	1.33
22	A	845	CLA	O2D-CGD	4.97	1.45	1.33
30	A	825	CL0	O2D-CGD	4.97	1.45	1.33
22	A	804	CLA	O2D-CGD	4.96	1.45	1.33
22	B	814	CLA	CHC-C1C	4.96	1.48	1.38
22	B	851	CLA	O2D-CGD	4.96	1.45	1.33
22	1	307	CLA	O2D-CGD	4.96	1.45	1.33
22	A	835	CLA	O2D-CGD	4.95	1.45	1.33
22	A	807	CLA	O2D-CGD	4.95	1.45	1.33
22	B	816	CLA	CHC-C1C	4.95	1.48	1.38
22	A	834	CLA	O2D-CGD	4.95	1.45	1.33
22	A	830	CLA	CHB-C1B	4.95	1.50	1.39
22	B	810	CLA	O2D-CGD	4.93	1.45	1.33
22	1	318	CLA	O2D-CGD	4.92	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	805	CLA	O2D-CGD	4.92	1.45	1.33
22	A	856	CLA	O2D-CGD	4.92	1.45	1.33
22	B	803	CLA	CHC-C1C	4.92	1.48	1.38
22	A	853	CLA	O2D-CGD	4.92	1.45	1.33
22	B	850	CLA	O2D-CGD	4.91	1.45	1.33
22	A	850	CLA	O2D-CGD	4.90	1.45	1.33
22	2	308	CLA	O2D-CGD	4.90	1.45	1.33
22	B	826	CLA	O2D-CGD	4.89	1.45	1.33
22	B	811	CLA	O2D-CGD	4.88	1.45	1.33
22	B	824	CLA	O2D-CGD	4.86	1.45	1.33
22	B	820	CLA	C3D-C4D	-4.86	1.33	1.44
22	B	827	CLA	O2D-CGD	4.86	1.45	1.33
22	A	801	CLA	O2D-CGD	4.85	1.45	1.33
22	B	818	CLA	C3D-C4D	-4.85	1.33	1.44
22	B	807	CLA	C4C-C3C	4.85	1.49	1.41
22	G	205	CLA	O2D-CGD	4.84	1.45	1.33
22	A	812	CLA	O2D-CGD	4.84	1.45	1.33
22	A	838	CLA	CHC-C1C	4.83	1.48	1.38
22	1	317	CLA	O2D-CGD	4.82	1.45	1.33
22	A	827	CLA	O2D-CGD	4.82	1.45	1.33
22	B	814	CLA	O2D-CGD	4.82	1.45	1.33
22	2	303	CLA	O2D-CGD	4.81	1.44	1.33
22	A	843	CLA	C3D-C4D	-4.81	1.33	1.44
22	B	804	CLA	O2D-CGD	4.81	1.44	1.33
22	B	823	CLA	O2D-CGD	4.81	1.44	1.33
22	B	803	CLA	O2D-CGD	4.79	1.44	1.33
21	2	302	CHL	C3D-C4D	-4.78	1.33	1.44
22	A	839	CLA	O2D-CGD	4.77	1.44	1.33
22	B	819	CLA	C3D-C4D	-4.77	1.33	1.44
22	2	319	CLA	CHB-C1B	4.77	1.50	1.39
22	B	829	CLA	C3D-C4D	-4.77	1.33	1.44
22	A	838	CLA	C3C-C2C	4.75	1.46	1.36
22	X	304	CLA	C3C-C2C	4.75	1.46	1.36
22	3	315	CLA	O2D-CGD	4.75	1.44	1.33
22	A	838	CLA	O2D-CGD	4.74	1.44	1.33
22	A	848	CLA	C3D-C4D	-4.74	1.33	1.44
22	L	306	CLA	O2D-CGD	4.74	1.44	1.33
22	B	803	CLA	C3C-C2C	4.74	1.46	1.36
22	A	851	CLA	C3D-C4D	-4.73	1.33	1.44
21	1	316	CHL	O2D-CGD	4.73	1.44	1.33
22	A	837	CLA	C3C-C2C	4.73	1.46	1.36
22	B	809	CLA	O2D-CGD	4.73	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	805	CLA	O2D-CGD	4.72	1.44	1.33
22	3	321	CLA	C3C-C2C	4.72	1.46	1.36
22	A	835	CLA	C3D-C4D	-4.72	1.33	1.44
22	A	832	CLA	O2D-CGD	4.71	1.44	1.33
22	A	858	CLA	O2D-CGD	4.70	1.44	1.33
22	B	845	CLA	CHC-C1C	4.70	1.48	1.38
22	B	829	CLA	CHC-C1C	4.69	1.48	1.38
21	4	317	CHL	C3A-C2A	-4.69	1.50	1.54
22	A	856	CLA	C3D-C4D	-4.69	1.33	1.44
22	A	802	CLA	O2D-CGD	4.68	1.44	1.33
22	B	848	CLA	C3D-C4D	-4.67	1.33	1.44
22	B	828	CLA	O2D-CGD	4.67	1.44	1.33
22	B	815	CLA	O2D-CGD	4.67	1.44	1.33
22	2	306	CLA	CHC-C1C	4.67	1.48	1.38
22	A	830	CLA	C3D-C4D	-4.66	1.33	1.44
22	B	820	CLA	O2D-CGD	4.66	1.44	1.33
22	A	802	CLA	C3C-C2C	4.66	1.46	1.36
22	J	102	CLA	O2D-CGD	4.66	1.45	1.30
21	4	309	CHL	C3D-C4D	-4.66	1.33	1.44
22	A	828	CLA	C3D-C4D	-4.65	1.33	1.44
22	B	822	CLA	C3D-C4D	-4.65	1.33	1.44
25	2	312	BCR	C10-C9	4.65	1.42	1.35
22	3	311	CLA	CHC-C1C	4.65	1.48	1.38
22	4	306	CLA	O2D-CGD	4.65	1.45	1.30
22	3	320	CLA	O2D-CGD	4.65	1.45	1.30
22	A	852	CLA	C3C-C2C	4.65	1.46	1.36
21	Y	304	CHL	C2C-C3C	4.65	1.46	1.36
22	3	317	CLA	O2D-CGD	4.65	1.45	1.30
21	4	308	CHL	C3D-C4D	-4.65	1.33	1.44
22	3	315	CLA	C3A-C2A	-4.64	1.50	1.54
22	4	315	CLA	C3D-C4D	-4.64	1.33	1.44
22	3	309	CLA	CHC-C1C	4.64	1.48	1.38
22	4	306	CLA	CHC-C1C	4.64	1.48	1.38
22	A	845	CLA	C3D-C4D	-4.64	1.33	1.44
22	G	206	CLA	C3C-C2C	4.64	1.46	1.36
22	Y	312	CLA	C3C-C2C	4.64	1.46	1.36
22	4	316	CLA	C3D-C4D	-4.63	1.33	1.44
22	B	827	CLA	C3D-C4D	-4.63	1.33	1.44
21	4	317	CHL	O2D-CGD	4.63	1.45	1.30
22	4	313	CLA	O2D-CGD	4.63	1.45	1.30
22	B	847	CLA	CHC-C1C	4.63	1.47	1.38
22	2	306	CLA	O2D-CGD	4.63	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	321	CLA	O2D-CGD	4.63	1.45	1.30
21	2	321	CHL	O2D-CGD	4.63	1.45	1.30
22	N	202	CLA	O2D-CGD	4.63	1.45	1.30
21	Z	302	CHL	C3D-C4D	-4.63	1.33	1.44
22	A	836	CLA	C3D-C4D	-4.63	1.33	1.44
22	4	314	CLA	O2D-CGD	4.62	1.45	1.30
22	4	315	CLA	O2D-CGD	4.62	1.45	1.30
21	4	308	CHL	O2D-CGD	4.62	1.45	1.30
22	A	851	CLA	CHC-C1C	4.62	1.47	1.38
21	3	314	CHL	C3D-C4D	-4.62	1.33	1.44
22	B	830	CLA	C3D-C4D	-4.62	1.33	1.44
22	1	302	CLA	O2D-CGD	4.62	1.45	1.30
22	K	202	CLA	O2D-CGD	4.62	1.45	1.30
21	Z	305	CHL	C2C-C3C	4.62	1.46	1.36
22	A	828	CLA	CHB-C1B	4.61	1.49	1.39
22	X	304	CLA	CHC-C1C	4.61	1.47	1.38
22	4	305	CLA	O2D-CGD	4.61	1.45	1.30
22	1	318	CLA	C3D-C4D	-4.61	1.33	1.44
22	A	807	CLA	C3D-C4D	-4.61	1.33	1.44
22	B	826	CLA	CHC-C1C	4.61	1.47	1.38
22	2	322	CLA	C3D-C4D	-4.61	1.33	1.44
21	4	317	CHL	C2C-C3C	4.61	1.46	1.36
22	A	846	CLA	C3C-C2C	4.61	1.46	1.36
22	O	209	CLA	C3C-C2C	4.61	1.46	1.36
22	4	312	CLA	C3D-C4D	-4.60	1.33	1.44
21	4	307	CHL	C3D-C4D	-4.60	1.33	1.44
22	L	307	CLA	CHC-C1C	4.60	1.47	1.38
22	B	815	CLA	CHC-C1C	4.60	1.47	1.38
22	A	828	CLA	O2D-CGD	4.60	1.45	1.30
22	A	846	CLA	C3D-C4D	-4.60	1.33	1.44
21	Z	312	CHL	C2C-C3C	4.60	1.46	1.36
22	K	204	CLA	CHC-C1C	4.60	1.47	1.38
22	3	321	CLA	C3D-C4D	-4.60	1.33	1.44
22	1	306	CLA	O2D-CGD	4.59	1.45	1.30
22	B	822	CLA	O2D-CGD	4.59	1.44	1.33
22	X	304	CLA	C4D-ND	4.59	1.43	1.37
21	4	307	CHL	O2D-CGD	4.59	1.45	1.30
21	2	309	CHL	C3D-C4D	-4.58	1.33	1.44
22	A	857	CLA	CHC-C1C	4.58	1.47	1.38
22	G	205	CLA	CHC-C1C	4.58	1.47	1.38
22	4	306	CLA	C3C-C2C	4.58	1.46	1.36
21	X	302	CHL	C2C-C3C	4.57	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	X	308	CHL	C3D-C4D	-4.57	1.33	1.44
22	4	305	CLA	CHC-C1C	4.57	1.47	1.38
22	2	319	CLA	CHC-C1C	4.57	1.47	1.38
21	Z	304	CHL	C3D-C4D	-4.57	1.33	1.44
21	Y	306	CHL	C2C-C3C	4.57	1.46	1.36
21	1	301	CHL	C2C-C3C	4.57	1.46	1.36
22	Z	314	CLA	C3C-C2C	4.56	1.46	1.36
22	A	852	CLA	C3D-C4D	-4.56	1.33	1.44
21	X	309	CHL	C2C-C3C	4.56	1.46	1.36
21	Y	303	CHL	C2C-C3C	4.56	1.46	1.36
22	3	320	CLA	C3C-C2C	4.56	1.46	1.36
22	B	825	CLA	C3D-C4D	-4.56	1.33	1.44
21	Y	305	CHL	C2C-C3C	4.56	1.46	1.36
22	A	857	CLA	C3D-C4D	-4.56	1.33	1.44
22	A	852	CLA	CHC-C1C	4.56	1.47	1.38
21	X	307	CHL	C2C-C3C	4.56	1.46	1.36
22	B	849	CLA	C3D-C4D	-4.56	1.33	1.44
21	Y	307	CHL	C2C-C3C	4.55	1.46	1.36
22	O	210	CLA	C3A-C2A	-4.55	1.50	1.54
22	2	322	CLA	O2D-CGD	4.55	1.45	1.30
22	4	306	CLA	C3D-C4D	-4.55	1.33	1.44
22	A	806	CLA	C3D-C4D	-4.55	1.33	1.44
22	B	802	CLA	O2A-CGA	4.55	1.46	1.30
22	B	847	CLA	C3D-C4D	-4.55	1.33	1.44
21	2	309	CHL	C2C-C3C	4.55	1.46	1.36
22	B	802	CLA	C3C-C2C	4.55	1.46	1.36
22	B	806	CLA	O2D-CGD	4.55	1.44	1.33
21	X	305	CHL	C2C-C3C	4.55	1.46	1.36
22	L	305	CLA	C3C-C2C	4.55	1.46	1.36
21	4	317	CHL	C3D-C4D	-4.55	1.33	1.44
22	1	302	CLA	C3D-C4D	-4.55	1.33	1.44
22	1	307	CLA	C3D-C4D	-4.55	1.33	1.44
22	Z	313	CLA	C3C-C2C	4.55	1.46	1.36
22	G	206	CLA	C3D-C4D	-4.55	1.33	1.44
22	A	832	CLA	C3C-C2C	4.55	1.46	1.36
22	X	311	CLA	C3C-C2C	4.55	1.46	1.36
22	B	847	CLA	C3C-C2C	4.55	1.46	1.36
22	X	313	CLA	C3C-C2C	4.54	1.46	1.36
22	3	311	CLA	C3D-C4D	-4.54	1.33	1.44
22	2	304	CLA	CHC-C1C	4.54	1.47	1.38
22	1	304	CLA	C3C-C2C	4.54	1.46	1.36
22	A	836	CLA	C3C-C2C	4.54	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Z	308	CLA	C3C-C2C	4.54	1.46	1.36
22	A	828	CLA	CHC-C1C	4.54	1.47	1.38
22	A	847	CLA	C3C-C2C	4.54	1.46	1.36
22	1	317	CLA	C3D-C4D	-4.54	1.33	1.44
22	2	308	CLA	C3D-C4D	-4.54	1.33	1.44
22	F	305	CLA	C3D-C4D	-4.54	1.33	1.44
22	Y	309	CLA	C3C-C2C	4.54	1.46	1.36
22	1	317	CLA	CHC-C1C	4.54	1.47	1.38
22	Y	302	CLA	C3C-C2C	4.54	1.46	1.36
22	X	303	CLA	C3C-C2C	4.54	1.46	1.36
22	A	831	CLA	C3D-C4D	-4.54	1.33	1.44
22	B	822	CLA	C3C-C2C	4.54	1.46	1.36
22	1	304	CLA	C3D-C4D	-4.54	1.33	1.44
22	B	852	CLA	C3D-C4D	-4.53	1.33	1.44
21	X	308	CHL	C2C-C3C	4.53	1.46	1.36
22	B	853	CLA	C3D-C4D	-4.53	1.33	1.44
22	A	812	CLA	CHC-C1C	4.53	1.47	1.38
22	2	320	CLA	C3C-C2C	4.53	1.46	1.36
22	4	318	CLA	C3C-C2C	4.53	1.46	1.36
22	B	853	CLA	C3C-C2C	4.53	1.46	1.36
21	Z	305	CHL	C3D-C4D	-4.53	1.34	1.44
22	A	840	CLA	C3C-C2C	4.53	1.46	1.36
22	H	201	CLA	C3C-C2C	4.53	1.46	1.36
22	L	306	CLA	C3C-C2C	4.53	1.46	1.36
22	3	313	CLA	C3C-C2C	4.53	1.46	1.36
22	A	829	CLA	CHC-C1C	4.53	1.47	1.38
21	Y	313	CHL	C3D-C4D	-4.52	1.34	1.44
22	2	319	CLA	C3C-C2C	4.52	1.45	1.36
22	O	206	CLA	C3C-C2C	4.52	1.46	1.36
22	B	828	CLA	C3D-C4D	-4.52	1.34	1.44
22	A	843	CLA	CHC-C1C	4.52	1.47	1.38
22	B	813	CLA	CHC-C1C	4.52	1.47	1.38
22	1	303	CLA	O2A-CGA	4.52	1.45	1.30
22	1	320	CLA	C3C-C2C	4.52	1.46	1.36
22	B	850	CLA	C3D-C4D	-4.52	1.34	1.44
22	K	205	CLA	C3C-C2C	4.52	1.46	1.36
21	Z	301	CHL	C2C-C3C	4.52	1.46	1.36
21	2	301	CHL	C3D-C4D	-4.52	1.34	1.44
22	K	203	CLA	CHC-C1C	4.52	1.47	1.38
21	Z	312	CHL	C3D-C4D	-4.52	1.34	1.44
22	A	805	CLA	C3D-C4D	-4.52	1.34	1.44
22	Z	307	CLA	C3C-C2C	4.51	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Z	310	CLA	C3C-C2C	4.51	1.46	1.36
21	Y	304	CHL	O2A-CGA	4.51	1.45	1.30
21	2	321	CHL	O2A-CGA	4.51	1.45	1.30
22	Z	306	CLA	C3C-C2C	4.51	1.46	1.36
22	B	813	CLA	C3D-C4D	-4.51	1.34	1.44
21	X	309	CHL	O2A-CGA	4.51	1.45	1.30
22	B	825	CLA	C3C-C2C	4.51	1.46	1.36
22	3	308	CLA	CHC-C1C	4.51	1.47	1.38
21	X	307	CHL	C3D-C4D	-4.51	1.34	1.44
22	B	821	CLA	C3C-C2C	4.51	1.46	1.36
22	1	309	CLA	C3C-C2C	4.51	1.46	1.36
21	Z	304	CHL	C2C-C3C	4.51	1.46	1.36
22	B	802	CLA	C3D-C4D	-4.51	1.34	1.44
22	B	806	CLA	C3D-C4D	-4.51	1.34	1.44
22	K	203	CLA	C3C-C2C	4.51	1.46	1.36
22	B	829	CLA	C3C-C2C	4.50	1.46	1.36
22	L	307	CLA	C3C-C2C	4.50	1.46	1.36
22	B	810	CLA	C3D-C4D	-4.50	1.34	1.44
22	B	812	CLA	C3D-C4D	-4.50	1.34	1.44
21	X	306	CHL	C2C-C3C	4.50	1.46	1.36
21	2	309	CHL	O2A-CGA	4.50	1.45	1.30
21	2	302	CHL	C2C-C3C	4.50	1.46	1.36
21	Y	305	CHL	O2A-CGA	4.50	1.45	1.30
22	2	303	CLA	O2A-CGA	4.50	1.45	1.30
22	2	320	CLA	C3D-C4D	-4.50	1.34	1.44
21	Y	313	CHL	O2A-CGA	4.50	1.45	1.30
21	Z	303	CHL	O2A-CGA	4.50	1.45	1.30
22	A	854	CLA	C3D-C4D	-4.50	1.34	1.44
22	1	321	CLA	O2A-CGA	4.50	1.45	1.30
22	3	321	CLA	O2A-CGA	4.50	1.45	1.30
21	Z	303	CHL	C3D-C4D	-4.50	1.34	1.44
22	A	801	CLA	C3D-C4D	-4.50	1.34	1.44
22	4	304	CLA	C3D-C4D	-4.50	1.34	1.44
22	Z	309	CLA	C3C-C2C	4.50	1.46	1.36
21	Z	305	CHL	CHD-C1D	4.50	1.47	1.38
22	3	312	CLA	CHC-C1C	4.50	1.47	1.38
22	F	306	CLA	CHC-C1C	4.50	1.47	1.38
22	A	855	CLA	C3C-C2C	4.49	1.46	1.36
22	3	313	CLA	O2A-CGA	4.49	1.45	1.30
21	Y	306	CHL	C3D-C4D	-4.49	1.34	1.44
21	Y	307	CHL	C3D-C4D	-4.49	1.34	1.44
21	Z	312	CHL	O2A-CGA	4.49	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	306	CLA	O2A-CGA	4.49	1.45	1.30
21	Z	302	CHL	C2C-C3C	4.49	1.46	1.36
22	1	318	CLA	C3C-C2C	4.49	1.46	1.36
22	G	206	CLA	CHC-C1C	4.49	1.47	1.38
21	X	309	CHL	C3D-C4D	-4.49	1.34	1.44
22	B	845	CLA	C3D-C4D	-4.49	1.34	1.44
22	G	205	CLA	O2A-CGA	4.49	1.45	1.30
21	X	306	CHL	C3D-C4D	-4.49	1.34	1.44
22	B	833	CLA	C3C-C2C	4.49	1.46	1.36
22	2	318	CLA	C3D-C4D	-4.49	1.34	1.44
22	A	840	CLA	O2A-CGA	4.49	1.45	1.30
21	2	321	CHL	C3D-C4D	-4.49	1.34	1.44
22	1	320	CLA	O2A-CGA	4.49	1.45	1.30
22	L	305	CLA	O2A-CGA	4.49	1.45	1.30
22	3	309	CLA	C3D-C4D	-4.49	1.34	1.44
21	4	309	CHL	O2A-CGA	4.49	1.45	1.30
22	N	202	CLA	O2A-CGA	4.49	1.45	1.30
21	Y	313	CHL	CHC-C1C	4.49	1.47	1.38
22	4	312	CLA	O2A-CGA	4.49	1.45	1.30
25	O	203	BCR	C14-C13	4.49	1.41	1.35
22	2	306	CLA	O2A-CGA	4.49	1.45	1.30
22	4	315	CLA	C3C-C2C	4.49	1.46	1.36
22	B	821	CLA	C3D-C4D	-4.48	1.34	1.44
21	4	307	CHL	O2A-CGA	4.48	1.45	1.30
22	3	317	CLA	O2A-CGA	4.48	1.45	1.30
21	Y	307	CHL	O2A-CGA	4.48	1.45	1.30
21	Y	303	CHL	O2A-CGA	4.48	1.45	1.30
22	3	319	CLA	O2A-CGA	4.48	1.45	1.30
22	Y	310	CLA	C3C-C2C	4.48	1.46	1.36
21	Z	303	CHL	C2C-C3C	4.48	1.46	1.36
22	A	833	CLA	C3D-C4D	-4.48	1.34	1.44
22	A	846	CLA	CHC-C1C	4.48	1.47	1.38
21	4	308	CHL	O2A-CGA	4.48	1.45	1.30
22	3	318	CLA	O2A-CGA	4.48	1.45	1.30
22	4	305	CLA	O2A-CGA	4.48	1.45	1.30
22	A	844	CLA	C3D-C4D	-4.48	1.34	1.44
22	1	319	CLA	C3C-C2C	4.48	1.46	1.36
21	3	314	CHL	O2A-CGA	4.48	1.45	1.30
22	3	311	CLA	O2A-CGA	4.48	1.45	1.30
22	3	319	CLA	C3C-C2C	4.48	1.46	1.36
22	X	312	CLA	C3C-C2C	4.48	1.46	1.36
22	H	201	CLA	CHC-C1C	4.48	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	302	CLA	O2A-CGA	4.48	1.45	1.30
21	Z	303	CHL	CHC-C1C	4.48	1.47	1.38
22	K	202	CLA	O2A-CGA	4.48	1.45	1.30
22	2	317	CLA	C3C-C2C	4.48	1.46	1.36
22	2	322	CLA	O2A-CGA	4.48	1.45	1.30
22	B	820	CLA	O2A-CGA	4.48	1.45	1.30
21	Y	304	CHL	C3D-C4D	-4.48	1.34	1.44
22	A	809	CLA	C3D-C4D	-4.48	1.34	1.44
22	3	316	CLA	O2A-CGA	4.47	1.45	1.30
22	F	305	CLA	C3C-C2C	4.47	1.46	1.36
21	X	307	CHL	O2A-CGA	4.47	1.45	1.30
22	B	821	CLA	O2A-CGA	4.47	1.45	1.30
22	4	311	CLA	C3D-C4D	-4.47	1.34	1.44
22	B	808	CLA	C3C-C2C	4.47	1.46	1.36
22	4	305	CLA	C3D-C4D	-4.47	1.34	1.44
22	4	311	CLA	CHC-C1C	4.47	1.47	1.38
22	A	806	CLA	C3C-C2C	4.47	1.46	1.36
22	Z	311	CLA	C3C-C2C	4.47	1.46	1.36
22	B	801	CLA	C3D-C4D	-4.47	1.34	1.44
22	B	824	CLA	C3D-C4D	-4.47	1.34	1.44
22	4	313	CLA	O2A-CGA	4.47	1.45	1.30
22	A	859	CLA	CHC-C1C	4.47	1.47	1.38
22	4	316	CLA	C3A-C2A	-4.47	1.50	1.54
22	K	204	CLA	C3D-C4D	-4.47	1.34	1.44
22	1	308	CLA	O2D-CGD	4.47	1.44	1.33
21	X	307	CHL	CHC-C1C	4.47	1.47	1.38
22	B	805	CLA	C3D-C4D	-4.47	1.34	1.44
21	4	308	CHL	C2C-C3C	4.47	1.46	1.36
22	Y	308	CLA	C3C-C2C	4.46	1.46	1.36
22	A	848	CLA	O2A-CGA	4.46	1.45	1.30
22	2	305	CLA	O2A-CGA	4.46	1.45	1.30
22	G	205	CLA	C3D-C4D	-4.46	1.34	1.44
22	G	207	CLA	O2A-CGA	4.46	1.45	1.30
22	A	839	CLA	O2A-CGA	4.46	1.45	1.30
22	X	310	CLA	C3C-C2C	4.46	1.46	1.36
22	1	320	CLA	C3D-C4D	-4.46	1.34	1.44
21	1	316	CHL	O2A-CGA	4.46	1.45	1.30
22	A	831	CLA	CHC-C1C	4.46	1.47	1.38
22	1	321	CLA	C3D-C4D	-4.46	1.34	1.44
22	1	306	CLA	O2A-CGA	4.46	1.45	1.30
22	A	854	CLA	C3C-C2C	4.46	1.46	1.36
21	Y	306	CHL	O2A-CGA	4.46	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	305	CLA	C3C-C2C	4.46	1.46	1.36
22	A	807	CLA	C3C-C2C	4.46	1.46	1.36
22	X	301	CLA	C3C-C2C	4.46	1.46	1.36
21	Z	301	CHL	C3D-C4D	-4.46	1.34	1.44
21	Y	305	CHL	C3D-C4D	-4.45	1.34	1.44
22	4	316	CLA	C3C-C2C	4.45	1.46	1.36
22	A	832	CLA	C3D-C4D	-4.45	1.34	1.44
22	B	846	CLA	C3D-C4D	-4.45	1.34	1.44
22	G	205	CLA	C3C-C2C	4.45	1.46	1.36
21	X	302	CHL	C3D-C4D	-4.45	1.34	1.44
22	A	847	CLA	C3D-C4D	-4.45	1.34	1.44
22	4	311	CLA	O2A-CGA	4.45	1.45	1.30
22	A	829	CLA	C3D-C4D	-4.45	1.34	1.44
22	B	808	CLA	C3D-C4D	-4.45	1.34	1.44
21	3	307	CHL	C3D-C4D	-4.45	1.34	1.44
22	2	305	CLA	C3D-C4D	-4.45	1.34	1.44
22	A	804	CLA	C3D-C4D	-4.45	1.34	1.44
22	4	313	CLA	C3C-C2C	4.45	1.46	1.36
21	1	316	CHL	C3D-C4D	-4.45	1.34	1.44
22	A	849	CLA	C3D-C4D	-4.44	1.34	1.44
22	B	824	CLA	C3C-C2C	4.44	1.46	1.36
22	K	203	CLA	C3D-C4D	-4.44	1.34	1.44
21	3	307	CHL	C2C-C3C	4.44	1.46	1.36
21	Y	313	CHL	C2C-C3C	4.44	1.46	1.36
22	A	855	CLA	C3D-C4D	-4.44	1.34	1.44
22	3	310	CLA	C3D-C4D	-4.44	1.34	1.44
21	4	307	CHL	C2C-C3C	4.44	1.46	1.36
22	K	202	CLA	C3C-C2C	4.44	1.46	1.36
22	B	849	CLA	C3C-C2C	4.44	1.46	1.36
22	3	308	CLA	C3C-C2C	4.44	1.46	1.36
22	A	840	CLA	C3D-C4D	-4.44	1.34	1.44
22	B	823	CLA	C3C-C2C	4.44	1.46	1.36
22	B	810	CLA	C3C-C2C	4.44	1.46	1.36
22	3	310	CLA	CHC-C1C	4.44	1.47	1.38
25	O	203	BCR	C17-C18	4.44	1.41	1.35
22	N	202	CLA	C3C-C2C	4.44	1.46	1.36
22	B	833	CLA	C3D-C4D	-4.44	1.34	1.44
22	1	321	CLA	CHC-C1C	4.43	1.47	1.38
22	L	307	CLA	C3D-C4D	-4.43	1.34	1.44
22	B	805	CLA	C3C-C2C	4.43	1.46	1.36
22	Y	301	CLA	C3D-C4D	-4.43	1.34	1.44
22	1	305	CLA	C3D-C4D	-4.43	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Y	303	CHL	C3D-C4D	-4.43	1.34	1.44
22	A	837	CLA	C3D-C4D	-4.43	1.34	1.44
21	X	305	CHL	C3D-C4D	-4.43	1.34	1.44
22	A	812	CLA	C3D-C4D	-4.43	1.34	1.44
22	B	815	CLA	C3C-C2C	4.43	1.46	1.36
22	Y	311	CLA	C3C-C2C	4.43	1.46	1.36
22	B	816	CLA	C3C-C2C	4.43	1.46	1.36
22	B	831	CLA	CHC-C1C	4.43	1.47	1.38
22	1	306	CLA	C3C-C2C	4.43	1.46	1.36
22	1	319	CLA	C3D-C4D	-4.43	1.34	1.44
22	3	309	CLA	C3C-C2C	4.43	1.46	1.36
21	2	301	CHL	C2C-C3C	4.42	1.46	1.36
22	2	304	CLA	C3D-C4D	-4.42	1.34	1.44
22	1	304	CLA	CHC-C1C	4.42	1.47	1.38
22	A	834	CLA	C3D-C4D	-4.42	1.34	1.44
21	2	309	CHL	CHC-C1C	4.42	1.47	1.38
22	1	305	CLA	CHC-C1C	4.42	1.47	1.38
22	B	815	CLA	C3D-C4D	-4.42	1.34	1.44
22	J	102	CLA	C3C-C2C	4.42	1.46	1.36
21	Z	302	CHL	CHC-C1C	4.42	1.47	1.38
22	Y	301	CLA	C3C-C2C	4.42	1.46	1.36
22	A	839	CLA	C3D-C4D	-4.41	1.34	1.44
22	1	321	CLA	C3C-C2C	4.41	1.46	1.36
22	B	828	CLA	C3C-C2C	4.41	1.46	1.36
22	1	308	CLA	C3D-C4D	-4.41	1.34	1.44
22	O	206	CLA	C3D-C4D	-4.41	1.34	1.44
22	2	317	CLA	CHC-C1C	4.41	1.47	1.38
22	3	315	CLA	C3D-C4D	-4.40	1.34	1.44
22	B	807	CLA	O2A-CGA	4.40	1.46	1.33
22	X	312	CLA	CHC-C1C	4.40	1.47	1.38
22	A	812	CLA	C3C-C2C	4.40	1.46	1.36
22	A	853	CLA	C3D-C4D	-4.40	1.34	1.44
22	K	205	CLA	C3D-C4D	-4.40	1.34	1.44
22	X	303	CLA	C3D-C4D	-4.40	1.34	1.44
22	A	848	CLA	C3C-C2C	4.40	1.46	1.36
22	A	851	CLA	C3C-C2C	4.40	1.46	1.36
22	A	833	CLA	CHC-C1C	4.40	1.47	1.38
22	2	322	CLA	C3C-C2C	4.40	1.46	1.36
22	H	201	CLA	C3D-C4D	-4.40	1.34	1.44
22	B	826	CLA	O2A-CGA	4.40	1.46	1.33
22	Y	314	CLA	C3C-C2C	4.40	1.46	1.36
21	X	306	CHL	CHC-C1C	4.40	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	308	CLA	C3C-C2C	4.40	1.46	1.36
22	3	313	CLA	C3D-C4D	-4.40	1.34	1.44
22	1	319	CLA	CHC-C1C	4.39	1.47	1.38
22	Y	310	CLA	CHC-C1C	4.39	1.47	1.38
22	B	823	CLA	CHC-C1C	4.39	1.47	1.38
22	A	843	CLA	C3C-C2C	4.39	1.46	1.36
22	Z	313	CLA	CHC-C1C	4.39	1.47	1.38
22	4	310	CLA	C3D-C4D	-4.39	1.34	1.44
22	1	309	CLA	CHC-C1C	4.39	1.47	1.38
21	X	302	CHL	CHC-C1C	4.39	1.47	1.38
22	Y	311	CLA	C3D-C4D	-4.39	1.34	1.44
22	2	308	CLA	C3C-C2C	4.39	1.46	1.36
22	B	809	CLA	C3D-C4D	-4.39	1.34	1.44
22	Z	307	CLA	CHC-C1C	4.39	1.47	1.38
22	3	321	CLA	CHC-C1C	4.38	1.47	1.38
22	A	803	CLA	C3D-C4D	-4.38	1.34	1.44
21	X	309	CHL	CHD-C1D	4.38	1.46	1.38
22	2	307	CLA	O2A-CGA	4.38	1.46	1.33
22	A	842	CLA	CHC-C1C	4.38	1.47	1.38
22	Y	302	CLA	CHC-C1C	4.38	1.47	1.38
22	B	819	CLA	C3C-C2C	4.38	1.46	1.36
22	A	806	CLA	CHC-C1C	4.38	1.47	1.38
22	2	303	CLA	C3C-C2C	4.38	1.46	1.36
22	B	804	CLA	C3D-C4D	-4.38	1.34	1.44
22	B	846	CLA	CHC-C1C	4.38	1.47	1.38
22	Z	310	CLA	CHC-C1C	4.38	1.47	1.38
22	Z	313	CLA	C3D-C4D	-4.38	1.34	1.44
22	G	207	CLA	C3C-C2C	4.38	1.46	1.36
22	2	319	CLA	C3D-C4D	-4.38	1.34	1.44
22	1	302	CLA	C3C-C2C	4.38	1.46	1.36
22	B	850	CLA	O2A-CGA	4.37	1.46	1.33
22	A	859	CLA	C3D-C4D	-4.37	1.34	1.44
22	A	856	CLA	C3C-C2C	4.37	1.46	1.36
22	3	312	CLA	C3D-C4D	-4.37	1.34	1.44
22	A	853	CLA	C3C-C2C	4.37	1.46	1.36
22	B	848	CLA	CHC-C1C	4.37	1.47	1.38
22	1	306	CLA	CHC-C1C	4.37	1.47	1.38
22	X	303	CLA	CHC-C1C	4.37	1.47	1.38
22	3	316	CLA	C3D-C4D	-4.37	1.34	1.44
22	A	802	CLA	C3D-C4D	-4.37	1.34	1.44
22	B	817	CLA	CHC-C1C	4.37	1.47	1.38
22	K	204	CLA	C3C-C2C	4.37	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	320	CLA	C3D-C4D	-4.37	1.34	1.44
22	L	307	CLA	O2A-CGA	4.37	1.45	1.30
22	X	311	CLA	CHC-C1C	4.37	1.47	1.38
22	X	313	CLA	CHC-C1C	4.37	1.47	1.38
22	A	842	CLA	C3D-C4D	-4.37	1.34	1.44
22	Z	309	CLA	C3D-C4D	-4.37	1.34	1.44
22	O	210	CLA	C3D-C4D	-4.37	1.34	1.44
22	A	834	CLA	CHC-C1C	4.36	1.47	1.38
22	L	306	CLA	CHC-C1C	4.36	1.47	1.38
22	3	318	CLA	C3D-C4D	-4.36	1.34	1.44
22	A	838	CLA	C3D-C4D	-4.36	1.34	1.44
22	1	317	CLA	O2A-CGA	4.36	1.46	1.33
22	B	804	CLA	CHC-C1C	4.36	1.47	1.38
21	X	305	CHL	CHC-C1C	4.36	1.47	1.38
22	4	314	CLA	C3C-C2C	4.36	1.46	1.36
22	2	317	CLA	C3D-C4D	-4.36	1.34	1.44
22	3	315	CLA	C3C-C2C	4.36	1.46	1.36
21	3	307	CHL	O2D-CGD	4.36	1.43	1.33
21	Y	304	CHL	CHC-C1C	4.35	1.47	1.38
22	2	320	CLA	O2A-CGA	4.35	1.46	1.33
22	J	102	CLA	C3D-C4D	-4.35	1.34	1.44
22	Z	314	CLA	C3D-C4D	-4.35	1.34	1.44
22	Z	308	CLA	CHC-C1C	4.35	1.47	1.38
22	Z	307	CLA	C3D-C4D	-4.35	1.34	1.44
22	3	308	CLA	C3D-C4D	-4.35	1.34	1.44
22	B	831	CLA	C3D-C4D	-4.35	1.34	1.44
22	A	801	CLA	C3C-C2C	4.35	1.46	1.36
22	Z	311	CLA	CHC-C1C	4.35	1.47	1.38
22	4	304	CLA	C3C-C2C	4.35	1.46	1.36
22	A	839	CLA	C3C-C2C	4.35	1.46	1.36
22	3	312	CLA	C3C-C2C	4.35	1.46	1.36
22	Y	302	CLA	C3D-C4D	-4.35	1.34	1.44
22	4	311	CLA	C3C-C2C	4.35	1.46	1.36
22	J	102	CLA	CHC-C1C	4.35	1.47	1.38
22	4	312	CLA	CHC-C1C	4.35	1.47	1.38
22	A	805	CLA	CHC-C1C	4.35	1.47	1.38
22	L	305	CLA	C3D-C4D	-4.35	1.34	1.44
22	A	844	CLA	O2A-CGA	4.35	1.46	1.33
22	Y	310	CLA	C3D-C4D	-4.34	1.34	1.44
21	2	309	CHL	CHD-C1D	4.34	1.46	1.38
21	X	308	CHL	CHC-C1C	4.34	1.47	1.38
22	N	202	CLA	CHC-C1C	4.34	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	303	CLA	C3D-C4D	-4.34	1.34	1.44
22	B	823	CLA	C3D-C4D	-4.34	1.34	1.44
22	A	808	CLA	C3D-C4D	-4.34	1.34	1.44
22	B	833	CLA	CHC-C1C	4.34	1.47	1.38
22	A	805	CLA	C3C-C2C	4.34	1.46	1.36
22	G	207	CLA	C3D-C4D	-4.34	1.34	1.44
22	N	202	CLA	C3D-C4D	-4.34	1.34	1.44
22	F	305	CLA	CHC-C1C	4.34	1.47	1.38
22	3	310	CLA	C3C-C2C	4.34	1.45	1.36
22	K	202	CLA	C3D-C4D	-4.34	1.34	1.44
22	1	317	CLA	C3C-C2C	4.34	1.45	1.36
21	Z	304	CHL	CHC-C1C	4.34	1.47	1.38
22	A	833	CLA	C3C-C2C	4.34	1.45	1.36
22	O	208	CLA	C3C-C2C	4.34	1.45	1.36
22	Y	312	CLA	CHC-C1C	4.34	1.47	1.38
21	Y	306	CHL	CHC-C1C	4.34	1.47	1.38
22	3	317	CLA	CHC-C1C	4.34	1.47	1.38
22	1	305	CLA	C3C-C2C	4.34	1.45	1.36
22	B	847	CLA	O2A-CGA	4.34	1.46	1.33
22	4	304	CLA	O2A-CGA	4.34	1.46	1.33
22	O	209	CLA	CHC-C1C	4.33	1.47	1.38
22	Y	309	CLA	C3D-C4D	-4.33	1.34	1.44
22	A	808	CLA	C3C-C2C	4.33	1.45	1.36
22	3	318	CLA	C3C-C2C	4.33	1.45	1.36
22	4	314	CLA	C3D-C4D	-4.33	1.34	1.44
22	B	845	CLA	O2A-CGA	4.33	1.46	1.33
22	B	851	CLA	C3D-C4D	-4.33	1.34	1.44
22	Y	314	CLA	C3D-C4D	-4.33	1.34	1.44
22	A	840	CLA	CHC-C1C	4.33	1.47	1.38
22	Z	309	CLA	CHC-C1C	4.33	1.47	1.38
22	X	311	CLA	C3D-C4D	-4.33	1.34	1.44
22	3	317	CLA	C3C-C2C	4.33	1.45	1.36
22	B	818	CLA	C3C-C2C	4.33	1.45	1.36
22	X	313	CLA	C3D-C4D	-4.33	1.34	1.44
22	O	210	CLA	C3C-C2C	4.33	1.45	1.36
22	O	207	CLA	C3D-C4D	-4.32	1.34	1.44
22	Y	309	CLA	CHC-C1C	4.32	1.47	1.38
22	B	852	CLA	C3C-C2C	4.32	1.45	1.36
21	1	316	CHL	C2C-C3C	4.32	1.46	1.36
22	1	303	CLA	C3D-C4D	-4.32	1.34	1.44
22	O	208	CLA	C3D-C4D	-4.32	1.34	1.44
22	L	305	CLA	CHC-C1C	4.32	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	827	CLA	C3C-C2C	4.32	1.45	1.36
22	Z	310	CLA	C3D-C4D	-4.32	1.34	1.44
22	B	833	CLA	O2A-CGA	4.32	1.46	1.33
22	B	849	CLA	O2A-CGA	4.32	1.46	1.33
22	Z	311	CLA	C3D-C4D	-4.32	1.34	1.44
22	B	811	CLA	C3D-C4D	-4.32	1.34	1.44
22	A	844	CLA	C3C-C2C	4.32	1.45	1.36
22	B	824	CLA	CHC-C1C	4.32	1.47	1.38
22	Z	308	CLA	C3D-C4D	-4.32	1.34	1.44
22	Y	314	CLA	CHC-C1C	4.32	1.47	1.38
22	Z	314	CLA	CHC-C1C	4.32	1.47	1.38
21	Y	304	CHL	CHD-C1D	4.32	1.46	1.38
22	4	318	CLA	CHC-C1C	4.32	1.47	1.38
22	B	806	CLA	C3C-C2C	4.32	1.45	1.36
22	A	838	CLA	O2A-CGA	4.31	1.45	1.33
22	B	853	CLA	O2A-CGA	4.31	1.45	1.33
22	O	209	CLA	C3D-C4D	-4.31	1.34	1.44
22	1	318	CLA	CHC-C1C	4.31	1.47	1.38
21	Z	312	CHL	CHD-C1D	4.31	1.46	1.38
22	A	857	CLA	C3C-C2C	4.31	1.45	1.36
22	1	302	CLA	CHC-C1C	4.31	1.47	1.38
21	Z	312	CHL	CHC-C1C	4.31	1.47	1.38
22	O	207	CLA	C3C-C2C	4.31	1.45	1.36
21	Y	306	CHL	CHD-C1D	4.31	1.46	1.38
22	X	301	CLA	CHC-C1C	4.31	1.47	1.38
22	1	309	CLA	C3D-C4D	-4.31	1.34	1.44
22	A	841	CLA	C3D-C4D	-4.31	1.34	1.44
21	4	307	CHL	CHD-C1D	4.31	1.46	1.38
22	B	805	CLA	CHC-C1C	4.30	1.47	1.38
22	Y	311	CLA	CHC-C1C	4.30	1.47	1.38
22	Y	311	CLA	O2A-CGA	4.30	1.45	1.33
22	A	841	CLA	C3C-C2C	4.30	1.45	1.36
21	Y	303	CHL	CHC-C1C	4.30	1.47	1.38
22	1	307	CLA	CHC-C1C	4.30	1.47	1.38
22	1	306	CLA	C3D-C4D	-4.30	1.34	1.44
22	A	827	CLA	CHC-C1C	4.30	1.47	1.38
21	Y	307	CHL	CHD-C1D	4.30	1.46	1.38
21	Z	301	CHL	CHC-C1C	4.30	1.47	1.38
22	A	857	CLA	O2A-CGA	4.29	1.45	1.33
22	1	303	CLA	C3C-C2C	4.29	1.45	1.36
22	A	803	CLA	CHC-C1C	4.29	1.47	1.38
22	2	308	CLA	CHC-C1C	4.29	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	X	307	CHL	CHD-C1D	4.29	1.46	1.38
21	Z	303	CHL	CHD-C1D	4.29	1.46	1.38
22	4	313	CLA	CHC-C1C	4.29	1.47	1.38
22	B	809	CLA	C3C-C2C	4.29	1.45	1.36
22	A	852	CLA	O2A-CGA	4.29	1.45	1.33
22	A	836	CLA	CHC-C1C	4.29	1.47	1.38
22	B	803	CLA	O2A-CGA	4.29	1.45	1.33
22	2	307	CLA	C3D-C4D	-4.29	1.34	1.44
22	O	210	CLA	CHC-C1C	4.29	1.47	1.38
22	1	319	CLA	O2A-CGA	4.29	1.45	1.33
22	X	310	CLA	CHC-C1C	4.28	1.47	1.38
31	B	841	DGD	O1G-C1A	4.28	1.45	1.33
22	Y	308	CLA	CHC-C1C	4.28	1.47	1.38
21	X	305	CHL	CHD-C1D	4.28	1.46	1.38
22	B	814	CLA	C3D-C4D	-4.28	1.34	1.44
22	A	845	CLA	C3C-C2C	4.28	1.45	1.36
22	A	805	CLA	O2A-CGA	4.28	1.45	1.33
22	B	826	CLA	CHB-C1B	4.28	1.49	1.39
22	B	803	CLA	C3D-C4D	-4.28	1.34	1.44
22	L	306	CLA	C3D-C4D	-4.28	1.34	1.44
22	X	301	CLA	C3D-C4D	-4.28	1.34	1.44
22	4	315	CLA	CHC-C1C	4.28	1.47	1.38
22	4	318	CLA	C3D-C4D	-4.27	1.34	1.44
22	A	810	CLA	C3D-C4D	-4.27	1.34	1.44
22	X	312	CLA	C3D-C4D	-4.27	1.34	1.44
21	X	302	CHL	CHD-C1D	4.27	1.46	1.38
22	A	803	CLA	C3C-C2C	4.27	1.45	1.36
22	B	831	CLA	C3C-C2C	4.27	1.45	1.36
22	H	201	CLA	C3A-C2A	-4.27	1.50	1.54
22	1	304	CLA	O2A-CGA	4.27	1.45	1.33
22	B	852	CLA	O2A-CGA	4.27	1.45	1.33
21	Y	305	CHL	CHD-C1D	4.27	1.46	1.38
22	B	825	CLA	CHC-C1C	4.27	1.47	1.38
22	A	846	CLA	O2A-CGA	4.27	1.45	1.33
22	A	859	CLA	O2A-CGA	4.27	1.45	1.33
22	A	807	CLA	CHC-C1C	4.27	1.47	1.38
22	4	313	CLA	C3D-C4D	-4.27	1.34	1.44
22	B	811	CLA	C3C-C2C	4.27	1.45	1.36
21	Y	305	CHL	CHC-C1C	4.26	1.47	1.38
22	A	836	CLA	O2A-CGA	4.26	1.45	1.33
22	4	304	CLA	CHC-C1C	4.26	1.47	1.38
21	1	301	CHL	CHD-C1D	4.26	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	319	CLA	CHC-C1C	4.26	1.47	1.38
21	4	309	CHL	CHC-C1C	4.26	1.47	1.38
21	X	308	CHL	CHD-C1D	4.26	1.46	1.38
22	A	850	CLA	CHC-C1C	4.26	1.47	1.38
22	3	313	CLA	CHC-C1C	4.26	1.47	1.38
22	A	803	CLA	O2A-CGA	4.26	1.45	1.33
22	3	319	CLA	C3D-C4D	-4.26	1.34	1.44
22	Y	308	CLA	C3D-C4D	-4.26	1.34	1.44
22	A	845	CLA	O2A-CGA	4.26	1.45	1.30
22	K	202	CLA	CHC-C1C	4.26	1.47	1.38
22	B	816	CLA	C4B-NB	-4.26	1.32	1.37
22	B	829	CLA	O2A-CGA	4.26	1.45	1.33
22	2	319	CLA	O2A-CGA	4.26	1.45	1.33
22	X	310	CLA	C3D-C4D	-4.26	1.34	1.44
31	J	104	DGD	O1G-C1A	4.25	1.45	1.33
31	J	104	DGD	O2G-C1B	4.25	1.46	1.34
21	X	305	CHL	O2A-CGA	4.25	1.45	1.33
22	4	310	CLA	C3C-C2C	4.25	1.45	1.36
22	A	802	CLA	CHC-C1C	4.25	1.47	1.38
22	3	316	CLA	CHC-C1C	4.25	1.47	1.38
22	A	859	CLA	C3C-C2C	4.25	1.45	1.36
22	O	209	CLA	O2A-CGA	4.25	1.45	1.33
30	A	825	CL0	C3D-C4D	-4.25	1.34	1.44
22	3	309	CLA	O2A-CGA	4.25	1.45	1.33
22	B	817	CLA	C3D-C4D	-4.25	1.34	1.44
22	A	849	CLA	C3C-C2C	4.25	1.45	1.36
22	F	306	CLA	C3C-C2C	4.25	1.45	1.36
30	A	825	CL0	C3C-C2C	4.25	1.45	1.36
22	Y	312	CLA	C3D-C4D	-4.25	1.34	1.44
22	B	821	CLA	CHC-C1C	4.24	1.47	1.38
22	A	832	CLA	O2A-CGA	4.24	1.45	1.33
22	A	856	CLA	O2A-CGA	4.24	1.45	1.33
22	2	306	CLA	C3D-C4D	-4.24	1.34	1.44
22	B	820	CLA	C3C-C2C	4.24	1.45	1.36
21	X	306	CHL	CHD-C1D	4.24	1.46	1.38
31	O	201	DGD	O1G-C1A	4.24	1.45	1.33
22	3	308	CLA	O2A-CGA	4.24	1.45	1.33
22	B	819	CLA	O2A-CGA	4.24	1.45	1.33
21	Y	307	CHL	CHC-C1C	4.24	1.47	1.38
22	4	312	CLA	C3C-C2C	4.24	1.45	1.36
22	Y	301	CLA	CHC-C1C	4.23	1.47	1.38
21	2	301	CHL	O2A-CGA	4.23	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	804	CLA	C3C-C2C	4.23	1.45	1.36
22	A	835	CLA	C3C-C2C	4.23	1.45	1.36
22	A	802	CLA	O2A-CGA	4.23	1.45	1.33
22	O	208	CLA	CHC-C1C	4.23	1.47	1.38
22	A	827	CLA	C3D-C4D	-4.23	1.34	1.44
22	F	306	CLA	C3D-C4D	-4.23	1.34	1.44
22	B	804	CLA	O2A-CGA	4.23	1.45	1.33
22	A	842	CLA	C3C-C2C	4.23	1.45	1.36
22	2	317	CLA	C3A-C2A	-4.23	1.50	1.54
21	4	308	CHL	CHD-C1D	4.22	1.46	1.38
22	2	305	CLA	CHC-C1C	4.22	1.47	1.38
22	B	812	CLA	C3C-C2C	4.22	1.45	1.36
22	A	808	CLA	CHC-C1C	4.22	1.47	1.38
22	2	319	CLA	C4B-NB	-4.22	1.32	1.37
22	A	810	CLA	O2A-CGA	4.22	1.45	1.33
22	A	850	CLA	O2A-CGA	4.22	1.45	1.33
22	A	858	CLA	C3D-C4D	-4.22	1.34	1.44
22	A	849	CLA	O2A-CGA	4.22	1.45	1.33
22	B	808	CLA	O2A-CGA	4.22	1.45	1.33
21	X	309	CHL	CHC-C1C	4.22	1.47	1.38
21	3	314	CHL	CHC-C1C	4.22	1.47	1.38
22	B	828	CLA	O2A-CGA	4.22	1.45	1.33
22	B	818	CLA	O2A-CGA	4.22	1.45	1.33
22	B	848	CLA	O2A-CGA	4.22	1.45	1.33
21	3	307	CHL	O2A-CGA	4.21	1.45	1.33
22	1	308	CLA	CHC-C1C	4.21	1.47	1.38
22	A	810	CLA	CHC-C1C	4.21	1.47	1.38
22	2	304	CLA	C3C-C2C	4.21	1.45	1.36
22	O	206	CLA	CHC-C1C	4.21	1.47	1.38
22	B	830	CLA	O2A-CGA	4.21	1.45	1.33
22	3	316	CLA	C3C-C2C	4.21	1.45	1.36
22	B	824	CLA	O2A-CGA	4.21	1.45	1.33
22	B	820	CLA	CHC-C1C	4.21	1.47	1.38
22	B	806	CLA	CHC-C1C	4.21	1.47	1.38
22	3	312	CLA	O2A-CGA	4.21	1.45	1.33
21	Z	301	CHL	CHD-C1D	4.21	1.46	1.38
21	Y	303	CHL	CHD-C1D	4.20	1.46	1.38
22	A	833	CLA	O2A-CGA	4.20	1.45	1.33
22	B	853	CLA	CHC-C1C	4.20	1.47	1.38
31	G	201	DGD	O1G-C1A	4.20	1.45	1.33
22	1	305	CLA	C3A-C2A	-4.20	1.50	1.54
22	A	850	CLA	C3D-C4D	-4.20	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Z	306	CLA	C3D-C4D	-4.20	1.34	1.44
22	B	814	CLA	C3C-C2C	4.20	1.45	1.36
22	A	855	CLA	O2A-CGA	4.20	1.45	1.33
22	2	322	CLA	CHC-C1C	4.19	1.47	1.38
22	B	809	CLA	CHC-C1C	4.19	1.47	1.38
22	A	830	CLA	CHC-C1C	4.19	1.47	1.38
22	O	207	CLA	O2A-CGA	4.19	1.45	1.33
22	B	826	CLA	C3D-C4D	-4.19	1.34	1.44
22	B	812	CLA	O2A-CGA	4.19	1.45	1.33
22	B	849	CLA	CHC-C1C	4.19	1.47	1.38
22	K	205	CLA	CHC-C1C	4.19	1.47	1.38
22	3	317	CLA	C3D-C4D	-4.19	1.34	1.44
21	2	302	CHL	CHD-C1D	4.19	1.46	1.38
22	Z	306	CLA	CHC-C1C	4.19	1.47	1.38
21	Z	304	CHL	CHD-C1D	4.18	1.46	1.38
22	B	822	CLA	CHC-C1C	4.18	1.47	1.38
21	4	309	CHL	CHD-C1D	4.18	1.46	1.38
22	A	842	CLA	O2A-CGA	4.18	1.45	1.33
22	A	834	CLA	C3C-C2C	4.18	1.45	1.36
22	A	854	CLA	CHC-C1C	4.17	1.47	1.38
21	2	301	CHL	CHD-C1D	4.17	1.46	1.38
22	1	320	CLA	CHC-C1C	4.17	1.47	1.38
22	O	207	CLA	CHC-C1C	4.17	1.47	1.38
22	2	304	CLA	O2A-CGA	4.17	1.45	1.33
22	A	804	CLA	CHC-C1C	4.17	1.47	1.38
22	B	831	CLA	O2A-CGA	4.17	1.45	1.33
22	A	837	CLA	CHC-C1C	4.17	1.47	1.38
21	Y	313	CHL	CHD-C1D	4.17	1.46	1.38
22	K	203	CLA	O2A-CGA	4.17	1.45	1.33
22	B	810	CLA	O2A-CGA	4.17	1.45	1.33
26	B	843	LHG	O7-C7	4.16	1.46	1.34
22	2	318	CLA	CHC-C1C	4.16	1.47	1.38
22	A	801	CLA	CHC-C1C	4.16	1.47	1.38
21	4	317	CHL	CHC-C1C	4.16	1.47	1.38
22	X	304	CLA	OBD-CAD	4.16	1.29	1.22
22	B	801	CLA	O2A-CGA	4.16	1.45	1.33
22	A	809	CLA	O2A-CGA	4.16	1.45	1.33
22	1	307	CLA	O2A-CGA	4.16	1.45	1.33
22	2	318	CLA	O2A-CGA	4.15	1.45	1.33
22	B	815	CLA	O2A-CGA	4.15	1.45	1.33
22	A	850	CLA	C3C-C2C	4.15	1.45	1.36
22	A	808	CLA	O2A-CGA	4.15	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	851	CLA	O2A-CGA	4.15	1.45	1.33
21	Z	302	CHL	CHD-C1D	4.15	1.46	1.38
22	G	207	CLA	CHC-C1C	4.15	1.46	1.38
22	3	310	CLA	O2A-CGA	4.15	1.45	1.33
22	A	829	CLA	O2A-CGA	4.15	1.45	1.33
21	Z	305	CHL	CHC-C1C	4.15	1.46	1.38
22	A	826	CLA	C3D-C4D	-4.14	1.34	1.44
22	A	826	CLA	CHC-C4B	4.14	1.48	1.39
22	A	853	CLA	O2A-CGA	4.14	1.45	1.33
22	A	806	CLA	O2A-CGA	4.14	1.45	1.33
22	B	808	CLA	CHC-C1C	4.14	1.46	1.38
22	K	204	CLA	CHB-C1B	4.14	1.48	1.39
22	A	858	CLA	C3C-C2C	4.14	1.45	1.36
22	G	206	CLA	O2A-CGA	4.14	1.45	1.33
22	A	853	CLA	CHC-C1C	4.14	1.46	1.38
22	A	812	CLA	O2A-CGA	4.14	1.45	1.33
21	2	321	CHL	CHD-C1D	4.14	1.46	1.38
22	B	809	CLA	O2A-CGA	4.13	1.45	1.33
22	B	817	CLA	O2A-CGA	4.13	1.45	1.33
22	3	318	CLA	CHC-C1C	4.13	1.46	1.38
30	A	825	CL0	O2A-CGA	4.13	1.45	1.33
22	B	811	CLA	CHC-C1C	4.13	1.46	1.38
30	A	825	CL0	CHC-C1C	4.13	1.46	1.38
22	L	306	CLA	O2A-CGA	4.13	1.45	1.33
22	A	801	CLA	O2A-CGA	4.13	1.45	1.33
26	B	843	LHG	O8-C23	4.12	1.45	1.33
22	B	813	CLA	O2A-CGA	4.12	1.45	1.33
22	A	851	CLA	O2A-CGA	4.12	1.45	1.33
22	2	307	CLA	CHC-C1C	4.12	1.46	1.38
21	2	321	CHL	C2C-C3C	4.12	1.45	1.36
22	A	856	CLA	CHC-C1C	4.12	1.46	1.38
22	2	303	CLA	CHC-C1C	4.12	1.46	1.38
22	A	847	CLA	CHC-C1C	4.12	1.46	1.38
21	3	307	CHL	CHC-C1C	4.12	1.46	1.38
22	A	826	CLA	O2A-CGA	4.12	1.45	1.33
22	A	831	CLA	C3C-C2C	4.12	1.45	1.36
22	A	858	CLA	CHC-C1C	4.11	1.46	1.38
22	2	306	CLA	C3C-C2C	4.11	1.45	1.36
22	A	843	CLA	O2A-CGA	4.11	1.45	1.33
22	Z	306	CLA	O2A-CGA	4.11	1.46	1.33
22	3	320	CLA	CHC-C1C	4.11	1.46	1.38
22	1	303	CLA	CHC-C1C	4.11	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	823	CLA	O2A-CGA	4.11	1.45	1.33
21	4	308	CHL	CHC-C1C	4.11	1.46	1.38
22	B	818	CLA	CHC-C1C	4.11	1.46	1.38
22	2	320	CLA	CHC-C1C	4.10	1.46	1.38
31	O	201	DGD	O2G-C1B	4.10	1.45	1.34
22	X	313	CLA	O2A-CGA	4.10	1.46	1.33
22	2	318	CLA	C3C-C2C	4.10	1.45	1.36
22	A	841	CLA	CHC-C1C	4.09	1.46	1.38
22	A	858	CLA	O2A-CGA	4.09	1.45	1.33
22	A	809	CLA	C3C-C2C	4.09	1.45	1.36
22	B	852	CLA	CHC-C1C	4.09	1.46	1.38
22	4	314	CLA	C3A-C2A	-4.09	1.50	1.54
31	B	841	DGD	O2G-C1B	4.09	1.45	1.34
25	1	312	BCR	C10-C9	4.09	1.41	1.35
22	B	806	CLA	O2A-CGA	4.09	1.45	1.33
25	G	202	BCR	C14-C13	4.08	1.41	1.35
22	A	807	CLA	O2A-CGA	4.08	1.45	1.33
21	3	314	CHL	C2C-C3C	4.08	1.45	1.36
22	B	826	CLA	C3C-C2C	4.08	1.45	1.36
21	2	301	CHL	CHC-C1C	4.08	1.46	1.38
22	B	816	CLA	O2A-CGA	4.07	1.45	1.33
22	1	318	CLA	O2A-CGA	4.07	1.45	1.33
22	2	307	CLA	C3C-C2C	4.07	1.45	1.36
22	B	813	CLA	C3C-C2C	4.07	1.45	1.36
22	A	839	CLA	CHC-C1C	4.07	1.46	1.38
21	1	316	CHL	CHD-C1D	4.07	1.46	1.38
22	Z	309	CLA	O2A-CGA	4.07	1.46	1.33
22	K	205	CLA	C3A-C2A	-4.07	1.50	1.54
22	B	850	CLA	CHC-C1C	4.07	1.46	1.38
22	B	816	CLA	C3D-C4D	-4.07	1.35	1.44
22	Y	302	CLA	O2A-CGA	4.07	1.46	1.33
22	Y	312	CLA	O2A-CGA	4.06	1.46	1.33
21	1	301	CHL	CHC-C1C	4.06	1.46	1.38
22	Y	309	CLA	O2A-CGA	4.06	1.45	1.33
21	X	306	CHL	O2A-CGA	4.06	1.45	1.33
22	Y	310	CLA	O2A-CGA	4.06	1.45	1.33
31	G	201	DGD	O2G-C1B	4.06	1.45	1.34
21	4	317	CHL	CHD-C1D	4.05	1.46	1.38
22	Z	311	CLA	O2A-CGA	4.05	1.45	1.33
21	X	308	CHL	O2A-CGA	4.05	1.45	1.33
22	X	310	CLA	O2A-CGA	4.05	1.45	1.33
21	X	302	CHL	O2A-CGA	4.05	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	811	CLA	O2A-CGA	4.05	1.45	1.33
22	4	314	CLA	CHC-C1C	4.05	1.46	1.38
21	Z	304	CHL	O2A-CGA	4.05	1.45	1.33
21	4	307	CHL	CHC-C1C	4.05	1.46	1.38
22	A	809	CLA	CHC-C1C	4.05	1.46	1.38
22	4	318	CLA	O2A-CGA	4.05	1.45	1.33
22	X	312	CLA	O2A-CGA	4.05	1.45	1.33
22	A	828	CLA	C3C-C2C	4.05	1.45	1.36
22	A	831	CLA	O2A-CGA	4.05	1.45	1.33
22	B	822	CLA	O2A-CGA	4.05	1.45	1.33
22	O	206	CLA	O2A-CGA	4.05	1.45	1.33
22	Y	308	CLA	O2A-CGA	4.04	1.45	1.33
22	B	805	CLA	O2A-CGA	4.04	1.45	1.33
22	A	829	CLA	C3C-C2C	4.04	1.45	1.36
22	3	311	CLA	C3C-C2C	4.04	1.45	1.36
22	Z	308	CLA	O2A-CGA	4.04	1.45	1.33
22	Y	314	CLA	O2A-CGA	4.04	1.45	1.33
21	Z	305	CHL	O2A-CGA	4.03	1.45	1.33
22	X	301	CLA	O2A-CGA	4.03	1.45	1.33
22	B	819	CLA	CHC-C1C	4.03	1.46	1.38
23	2	310	LUT	C34-C33	4.03	1.41	1.35
22	F	306	CLA	O2A-CGA	4.03	1.45	1.33
22	2	306	CLA	CHB-C1B	4.03	1.48	1.39
22	X	303	CLA	O2A-CGA	4.03	1.45	1.33
22	B	814	CLA	O2A-CGA	4.03	1.45	1.33
22	B	803	CLA	CHB-C1B	4.03	1.48	1.39
22	Z	307	CLA	O2A-CGA	4.03	1.45	1.33
22	Z	310	CLA	O2A-CGA	4.03	1.45	1.33
25	O	203	BCR	C21-C22	4.03	1.41	1.35
22	A	831	CLA	CHB-C1B	4.03	1.48	1.39
22	B	846	CLA	O2A-CGA	4.02	1.45	1.33
21	4	309	CHL	C2C-C3C	4.02	1.45	1.36
22	X	311	CLA	O2A-CGA	4.02	1.45	1.33
22	Z	313	CLA	O2A-CGA	4.02	1.45	1.33
25	B	840	BCR	C14-C13	4.02	1.41	1.35
22	2	308	CLA	O2A-CGA	4.02	1.45	1.33
22	B	848	CLA	C3C-C2C	4.02	1.45	1.36
21	Z	305	CHL	CHD-C4C	4.02	1.48	1.39
22	B	810	CLA	CHC-C1C	4.02	1.46	1.38
22	Z	314	CLA	O2A-CGA	4.02	1.45	1.33
22	B	827	CLA	O2A-CGA	4.01	1.45	1.33
22	A	841	CLA	O2A-CGA	4.01	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Y	301	CLA	O2A-CGA	4.01	1.45	1.33
21	Z	301	CHL	O2A-CGA	4.01	1.45	1.33
21	2	302	CHL	O2A-CGA	4.01	1.45	1.33
22	4	316	CLA	CHC-C1C	4.01	1.46	1.38
22	K	204	CLA	O2A-CGA	4.00	1.45	1.33
22	B	801	CLA	CHC-C4B	4.00	1.48	1.39
22	F	305	CLA	O2A-CGA	4.00	1.45	1.33
25	B	837	BCR	C14-C13	3.99	1.41	1.35
30	A	825	CL0	C1B-NB	-3.99	1.32	1.37
22	A	834	CLA	CHB-C1B	3.99	1.48	1.39
21	2	309	CHL	CHD-C4C	3.99	1.48	1.39
21	Z	302	CHL	O2A-CGA	3.98	1.45	1.33
25	L	302	BCR	C10-C9	3.98	1.41	1.35
22	X	304	CLA	O2A-CGA	3.97	1.45	1.33
23	2	310	LUT	C14-C13	3.97	1.41	1.35
22	B	850	CLA	C3C-C2C	3.97	1.45	1.36
22	A	834	CLA	O2A-CGA	3.96	1.45	1.33
22	B	825	CLA	O2A-CGA	3.96	1.45	1.33
21	X	309	CHL	CHD-C4C	3.96	1.48	1.39
22	B	802	CLA	CHC-C1C	3.96	1.46	1.38
22	B	817	CLA	C3C-C2C	3.96	1.45	1.36
21	Y	306	CHL	CHD-C4C	3.96	1.48	1.39
22	O	208	CLA	O2A-CGA	3.95	1.44	1.33
25	B	837	BCR	C10-C9	3.95	1.41	1.35
22	4	314	CLA	CHB-C1B	3.95	1.48	1.39
21	2	302	CHL	CHC-C1C	3.95	1.46	1.38
22	A	850	CLA	CHB-C1B	3.95	1.48	1.39
22	A	830	CLA	O2A-CGA	3.95	1.44	1.33
22	A	854	CLA	O2A-CGA	3.95	1.44	1.33
22	A	802	CLA	OBD-CAD	3.94	1.29	1.22
25	L	302	BCR	C21-C22	3.94	1.41	1.35
21	4	317	CHL	CHD-C4C	3.94	1.48	1.39
22	A	852	CLA	CHB-C1B	3.94	1.48	1.39
22	B	827	CLA	C3C-C2C	3.94	1.45	1.36
22	A	826	CLA	C3C-C2C	3.94	1.45	1.36
22	A	848	CLA	CHC-C1C	3.94	1.46	1.38
22	B	807	CLA	C3D-C4D	-3.93	1.35	1.44
21	Z	312	CHL	CHD-C4C	3.93	1.48	1.39
22	B	845	CLA	C3C-C2C	3.93	1.45	1.36
22	A	832	CLA	CHC-C1C	3.93	1.46	1.38
21	1	316	CHL	CHC-C1C	3.93	1.46	1.38
25	G	202	BCR	C17-C18	3.93	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	205	CLA	CHB-C1B	3.92	1.48	1.39
25	B	837	BCR	C17-C18	3.92	1.41	1.35
25	O	203	BCR	C10-C9	3.92	1.41	1.35
22	A	838	CLA	CHB-C1B	3.92	1.48	1.39
21	X	302	CHL	CHD-C4C	3.91	1.48	1.39
22	4	305	CLA	C3C-C2C	3.91	1.45	1.36
23	4	322	LUT	C30-C29	3.90	1.41	1.35
21	X	308	CHL	CHD-C4C	3.90	1.48	1.39
22	A	849	CLA	CHC-C1C	3.90	1.46	1.38
22	4	305	CLA	CHB-C1B	3.90	1.48	1.39
21	Z	303	CHL	CHD-C4C	3.90	1.48	1.39
22	4	310	CLA	CHC-C1C	3.89	1.46	1.38
25	G	202	BCR	C10-C9	3.89	1.40	1.35
21	X	307	CHL	CHD-C4C	3.89	1.48	1.39
21	Y	304	CHL	CHD-C4C	3.89	1.48	1.39
21	1	301	CHL	CHD-C4C	3.89	1.48	1.39
21	X	305	CHL	CHD-C4C	3.89	1.48	1.39
21	Y	307	CHL	CHD-C4C	3.89	1.48	1.39
21	Y	305	CHL	CHD-C4C	3.89	1.48	1.39
21	X	306	CHL	CHD-C4C	3.88	1.48	1.39
25	B	836	BCR	C10-C9	3.88	1.40	1.35
22	A	835	CLA	CHC-C1C	3.88	1.46	1.38
25	F	302	BCR	C8-C9	-3.87	1.37	1.45
21	4	308	CHL	CHD-C4C	3.86	1.48	1.39
22	3	318	CLA	CHB-C1B	3.86	1.48	1.39
22	B	807	CLA	CHB-C4A	-3.85	1.28	1.37
22	A	810	CLA	CHB-C1B	3.85	1.48	1.39
22	B	819	CLA	CHB-C1B	3.85	1.48	1.39
21	Y	303	CHL	CHD-C4C	3.85	1.48	1.39
22	B	807	CLA	CHC-C1C	3.84	1.46	1.38
21	Y	313	CHL	CHD-C4C	3.84	1.48	1.39
23	1	310	LUT	C14-C13	3.83	1.40	1.35
21	4	307	CHL	CHD-C4C	3.83	1.48	1.39
22	1	307	CLA	C3C-C2C	3.83	1.44	1.36
22	1	303	CLA	CHB-C1B	3.83	1.48	1.39
21	2	321	CHL	CHC-C1C	3.83	1.46	1.38
25	1	312	BCR	C14-C13	3.83	1.40	1.35
25	K	201	BCR	C10-C9	3.82	1.40	1.35
21	Z	301	CHL	CHD-C4C	3.82	1.48	1.39
21	Z	302	CHL	CHD-C4C	3.82	1.48	1.39
22	A	830	CLA	C3C-C2C	3.82	1.44	1.36
22	A	810	CLA	C3C-C2C	3.82	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	801	CLA	C3C-C2C	3.82	1.44	1.36
22	2	320	CLA	CHB-C1B	3.81	1.48	1.39
22	B	828	CLA	CHC-C1C	3.81	1.46	1.38
22	B	811	CLA	CHB-C1B	3.81	1.47	1.39
22	Y	310	CLA	CHB-C1B	3.81	1.47	1.39
22	A	845	CLA	CHB-C1B	3.80	1.47	1.39
21	Z	304	CHL	OBD-CAD	3.80	1.29	1.22
22	X	311	CLA	OBD-CAD	3.80	1.29	1.22
21	Z	304	CHL	CHD-C4C	3.80	1.47	1.39
21	2	302	CHL	CHD-C4C	3.80	1.47	1.39
22	Y	314	CLA	CHB-C1B	3.80	1.47	1.39
22	A	845	CLA	CHC-C1C	3.80	1.46	1.38
23	2	310	LUT	C10-C9	3.79	1.40	1.35
22	B	812	CLA	CHC-C1C	3.79	1.46	1.38
21	X	305	CHL	OBD-CAD	3.79	1.29	1.22
22	Y	311	CLA	OBD-CAD	3.79	1.29	1.22
21	4	309	CHL	CHD-C4C	3.79	1.47	1.39
22	Y	312	CLA	OBD-CAD	3.78	1.29	1.22
21	X	306	CHL	OBD-CAD	3.78	1.29	1.22
22	Y	302	CLA	OBD-CAD	3.78	1.29	1.22
22	O	209	CLA	OBD-CAD	3.78	1.29	1.22
22	G	206	CLA	CHB-C1B	3.78	1.47	1.39
25	B	840	BCR	C8-C9	-3.78	1.40	1.50
22	F	305	CLA	CHB-C1B	3.78	1.47	1.39
22	F	306	CLA	CHB-C1B	3.78	1.47	1.39
22	1	309	CLA	CHB-C1B	3.77	1.47	1.39
25	B	836	BCR	C14-C13	3.77	1.40	1.35
22	B	816	CLA	CHC-C4B	3.77	1.47	1.39
22	O	208	CLA	CHB-C1B	3.77	1.47	1.39
22	2	317	CLA	OBD-CAD	3.77	1.29	1.22
22	B	804	CLA	C3C-C2C	3.77	1.44	1.36
22	K	205	CLA	OBD-CAD	3.77	1.29	1.22
22	Z	310	CLA	OBD-CAD	3.77	1.29	1.22
22	1	320	CLA	CHB-C1B	3.77	1.47	1.39
21	X	307	CHL	OBD-CAD	3.77	1.29	1.22
22	B	851	CLA	OBD-CAD	3.76	1.29	1.22
22	3	320	CLA	OBD-CAD	3.76	1.29	1.22
25	A	816	BCR	C23-C22	-3.76	1.37	1.45
21	Y	303	CHL	OBD-CAD	3.76	1.29	1.22
22	O	206	CLA	OBD-CAD	3.76	1.29	1.22
22	H	201	CLA	CHB-C1B	3.76	1.47	1.39
22	A	827	CLA	C3D-C2D	3.76	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	827	CLA	CHC-C1C	3.76	1.46	1.38
22	X	312	CLA	OBD-CAD	3.76	1.29	1.22
22	3	321	CLA	OBD-CAD	3.76	1.29	1.22
22	3	310	CLA	CHB-C1B	3.76	1.47	1.39
22	Z	308	CLA	OBD-CAD	3.76	1.29	1.22
22	K	202	CLA	OBD-CAD	3.76	1.29	1.22
22	1	309	CLA	OBD-CAD	3.75	1.28	1.22
22	X	301	CLA	CHB-C1B	3.75	1.47	1.39
22	2	307	CLA	CHB-C1B	3.75	1.47	1.39
22	1	306	CLA	CHB-C1B	3.75	1.47	1.39
22	1	305	CLA	CHB-C1B	3.75	1.47	1.39
22	1	320	CLA	OBD-CAD	3.75	1.28	1.22
22	3	308	CLA	OBD-CAD	3.75	1.28	1.22
21	3	314	CHL	CHD-C1D	3.75	1.45	1.38
21	Y	305	CHL	OBD-CAD	3.75	1.28	1.22
22	Z	310	CLA	CHB-C1B	3.75	1.47	1.39
22	1	306	CLA	OBD-CAD	3.74	1.28	1.22
21	3	307	CHL	OBD-CAD	3.74	1.28	1.22
22	Z	308	CLA	CHB-C1B	3.74	1.47	1.39
22	1	302	CLA	CHB-C1B	3.74	1.47	1.39
22	H	201	CLA	OBD-CAD	3.74	1.28	1.22
22	2	320	CLA	OBD-CAD	3.74	1.28	1.22
22	X	313	CLA	OBD-CAD	3.74	1.28	1.22
22	O	210	CLA	OBD-CAD	3.74	1.28	1.22
21	2	301	CHL	CHD-C4C	3.73	1.47	1.39
22	Y	310	CLA	OBD-CAD	3.73	1.28	1.22
21	X	309	CHL	OBD-CAD	3.73	1.28	1.22
22	A	847	CLA	OBD-CAD	3.73	1.28	1.22
22	3	319	CLA	OBD-CAD	3.73	1.28	1.22
22	A	841	CLA	OBD-CAD	3.73	1.28	1.22
22	O	207	CLA	CHB-C1B	3.73	1.47	1.39
21	Y	304	CHL	OBD-CAD	3.73	1.28	1.22
25	B	834	BCR	C17-C18	3.73	1.40	1.35
22	B	819	CLA	OBD-CAD	3.73	1.28	1.22
22	3	315	CLA	CHC-C1C	3.73	1.46	1.38
22	A	858	CLA	C4B-NB	-3.73	1.33	1.37
25	B	836	BCR	C17-C18	3.73	1.40	1.35
21	Y	307	CHL	OBD-CAD	3.73	1.28	1.22
22	4	314	CLA	OBD-CAD	3.72	1.28	1.22
22	Z	309	CLA	OBD-CAD	3.72	1.28	1.22
22	Z	306	CLA	OBD-CAD	3.72	1.28	1.22
22	B	846	CLA	C3C-C2C	3.72	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Z	303	CHL	OBD-CAD	3.72	1.28	1.22
22	A	848	CLA	OBD-CAD	3.72	1.28	1.22
21	Z	301	CHL	OBD-CAD	3.72	1.28	1.22
21	Z	302	CHL	OBD-CAD	3.72	1.28	1.22
22	A	853	CLA	OBD-CAD	3.72	1.28	1.22
22	B	831	CLA	OBD-CAD	3.72	1.28	1.22
25	L	302	BCR	C17-C18	3.72	1.40	1.35
23	4	322	LUT	C10-C9	3.72	1.40	1.35
21	3	307	CHL	CHD-C1D	3.72	1.45	1.38
21	X	308	CHL	OBD-CAD	3.72	1.28	1.22
21	Y	306	CHL	OBD-CAD	3.72	1.28	1.22
21	Z	312	CHL	OBD-CAD	3.71	1.28	1.22
22	Z	311	CLA	OBD-CAD	3.71	1.28	1.22
22	1	308	CLA	OBD-CAD	3.71	1.28	1.22
22	L	306	CLA	OBD-CAD	3.71	1.28	1.22
22	2	307	CLA	OBD-CAD	3.71	1.28	1.22
22	X	304	CLA	CHC-C4B	3.71	1.47	1.39
22	Z	311	CLA	CHB-C1B	3.71	1.47	1.39
21	Z	305	CHL	OBD-CAD	3.71	1.28	1.22
22	B	811	CLA	OBD-CAD	3.71	1.28	1.22
22	3	309	CLA	CHB-C1B	3.71	1.47	1.39
22	B	826	CLA	OBD-CAD	3.71	1.28	1.22
22	Y	309	CLA	CHB-C1B	3.71	1.47	1.39
22	X	311	CLA	CHB-C1B	3.71	1.47	1.39
22	4	318	CLA	OBD-CAD	3.71	1.28	1.22
21	X	302	CHL	OBD-CAD	3.71	1.28	1.22
21	1	316	CHL	OBD-CAD	3.71	1.28	1.22
22	G	207	CLA	OBD-CAD	3.71	1.28	1.22
25	K	201	BCR	C21-C22	3.71	1.40	1.35
22	A	834	CLA	OBD-CAD	3.71	1.28	1.22
22	X	312	CLA	CHB-C1B	3.71	1.47	1.39
22	X	303	CLA	CHB-C1B	3.70	1.47	1.39
22	Y	308	CLA	OBD-CAD	3.70	1.28	1.22
22	4	306	CLA	OBD-CAD	3.70	1.28	1.22
22	Y	308	CLA	CHB-C1B	3.70	1.47	1.39
22	B	808	CLA	OBD-CAD	3.70	1.28	1.22
22	Z	314	CLA	OBD-CAD	3.70	1.28	1.22
22	A	804	CLA	CHB-C1B	3.70	1.47	1.39
22	B	814	CLA	CHC-C4B	3.70	1.47	1.39
22	Y	301	CLA	CHB-C1B	3.70	1.47	1.39
25	B	834	BCR	C14-C13	3.70	1.40	1.35
22	X	304	CLA	CHD-C1D	3.70	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	850	CLA	OBD-CAD	3.70	1.28	1.22
22	3	317	CLA	OBD-CAD	3.70	1.28	1.22
22	Y	314	CLA	OBD-CAD	3.70	1.28	1.22
22	4	313	CLA	OBD-CAD	3.70	1.28	1.22
22	K	202	CLA	CHB-C1B	3.69	1.47	1.39
22	B	833	CLA	CHB-C1B	3.69	1.47	1.39
22	3	312	CLA	OBD-CAD	3.69	1.28	1.22
22	4	315	CLA	OBD-CAD	3.69	1.28	1.22
22	Z	313	CLA	OBD-CAD	3.69	1.28	1.22
23	1	310	LUT	C30-C29	3.69	1.40	1.35
22	A	832	CLA	OBD-CAD	3.69	1.28	1.22
22	B	813	CLA	CHB-C1B	3.69	1.47	1.39
21	2	321	CHL	OBD-CAD	3.69	1.28	1.22
22	A	840	CLA	OBD-CAD	3.69	1.28	1.22
25	I	101	BCR	C10-C9	3.69	1.40	1.35
22	A	855	CLA	CHB-C1B	3.69	1.47	1.39
22	Y	309	CLA	OBD-CAD	3.69	1.28	1.22
21	4	317	CHL	OBD-CAD	3.69	1.28	1.22
21	2	321	CHL	CHD-C4C	3.68	1.47	1.39
22	Z	307	CLA	CHB-C1B	3.68	1.47	1.39
22	O	209	CLA	CHB-C1B	3.68	1.47	1.39
21	2	301	CHL	OBD-CAD	3.68	1.28	1.22
22	A	842	CLA	OBD-CAD	3.68	1.28	1.22
22	J	102	CLA	CHB-C1B	3.68	1.47	1.39
22	3	312	CLA	CHB-C1B	3.68	1.47	1.39
22	N	202	CLA	CHB-C1B	3.68	1.47	1.39
22	2	304	CLA	OBD-CAD	3.68	1.28	1.22
23	4	322	LUT	C34-C33	3.68	1.40	1.35
22	3	308	CLA	CHB-C1B	3.68	1.47	1.39
22	Y	302	CLA	CHB-C1B	3.67	1.47	1.39
21	4	307	CHL	OBD-CAD	3.67	1.28	1.22
22	A	844	CLA	CHC-C1C	3.67	1.46	1.38
22	K	203	CLA	OBD-CAD	3.67	1.28	1.22
22	4	310	CLA	CHB-C1B	3.67	1.47	1.39
25	B	834	BCR	C21-C22	3.67	1.40	1.35
22	Y	312	CLA	CHB-C1B	3.67	1.47	1.39
22	B	849	CLA	CHB-C1B	3.67	1.47	1.39
22	A	812	CLA	OBD-CAD	3.67	1.28	1.22
22	F	306	CLA	OBD-CAD	3.67	1.28	1.22
22	B	853	CLA	OBD-CAD	3.67	1.28	1.22
22	2	303	CLA	OBD-CAD	3.67	1.28	1.22
22	A	839	CLA	OBD-CAD	3.67	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	844	CLA	OBD-CAD	3.67	1.28	1.22
22	A	849	CLA	OBD-CAD	3.67	1.28	1.22
22	B	845	CLA	C1B-NB	-3.67	1.33	1.37
23	3	301	LUT	C34-C33	3.67	1.40	1.35
22	B	803	CLA	OBD-CAD	3.66	1.28	1.22
22	1	317	CLA	CHB-C1B	3.66	1.47	1.39
22	A	837	CLA	OBD-CAD	3.66	1.28	1.22
23	1	310	LUT	C34-C33	3.66	1.40	1.35
22	4	316	CLA	CHB-C1B	3.66	1.47	1.39
22	A	803	CLA	CHB-C1B	3.66	1.47	1.39
22	X	301	CLA	OBD-CAD	3.66	1.28	1.22
22	2	304	CLA	CHB-C1B	3.66	1.47	1.39
22	X	313	CLA	CHB-C1B	3.66	1.47	1.39
22	G	205	CLA	OBD-CAD	3.66	1.28	1.22
22	B	847	CLA	OBD-CAD	3.66	1.28	1.22
25	B	839	BCR	C21-C22	3.66	1.40	1.35
22	B	824	CLA	CHB-C1B	3.65	1.47	1.39
22	A	850	CLA	OBD-CAD	3.65	1.28	1.22
22	O	210	CLA	CHB-C1B	3.65	1.47	1.39
21	3	307	CHL	CHD-C4C	3.65	1.47	1.39
22	B	823	CLA	CHB-C1B	3.65	1.47	1.39
22	B	824	CLA	OBD-CAD	3.65	1.28	1.22
22	3	311	CLA	CHB-C1B	3.65	1.47	1.39
25	B	836	BCR	C21-C22	3.65	1.40	1.35
22	B	825	CLA	OBD-CAD	3.65	1.28	1.22
22	L	305	CLA	OBD-CAD	3.65	1.28	1.22
22	1	303	CLA	OBD-CAD	3.65	1.28	1.22
22	A	855	CLA	OBD-CAD	3.65	1.28	1.22
22	1	318	CLA	CHB-C1B	3.65	1.47	1.39
22	X	310	CLA	CHB-C1B	3.65	1.47	1.39
22	A	809	CLA	OBD-CAD	3.65	1.28	1.22
22	B	812	CLA	CHB-C1B	3.65	1.47	1.39
22	L	307	CLA	OBD-CAD	3.65	1.28	1.22
22	A	828	CLA	C3A-C2A	-3.64	1.51	1.54
22	O	206	CLA	CHB-C1B	3.64	1.47	1.39
22	3	313	CLA	OBD-CAD	3.64	1.28	1.22
22	B	848	CLA	CHB-C1B	3.64	1.47	1.39
22	3	313	CLA	CHB-C1B	3.64	1.47	1.39
22	4	318	CLA	CHB-C1B	3.64	1.47	1.39
22	3	315	CLA	CHB-C1B	3.64	1.47	1.39
22	A	802	CLA	CHB-C1B	3.63	1.47	1.39
22	1	307	CLA	CHB-C1B	3.63	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	317	CLA	CHB-C1B	3.63	1.47	1.39
25	B	834	BCR	C10-C9	3.63	1.40	1.35
25	L	304	BCR	C10-C9	3.63	1.40	1.35
22	X	310	CLA	OBD-CAD	3.63	1.28	1.22
25	J	101	BCR	C21-C22	3.63	1.40	1.35
22	J	102	CLA	OBD-CAD	3.63	1.28	1.22
22	A	852	CLA	C4B-NB	-3.63	1.33	1.37
22	3	317	CLA	CHB-C1B	3.63	1.47	1.39
22	A	849	CLA	CHB-C1B	3.63	1.47	1.39
22	A	858	CLA	MG-NA	-3.63	1.97	2.06
22	K	203	CLA	CHB-C1B	3.63	1.47	1.39
25	4	321	BCR	C21-C22	3.63	1.40	1.35
22	B	810	CLA	CHB-C1B	3.63	1.47	1.39
22	Z	309	CLA	CHB-C1B	3.62	1.47	1.39
22	4	312	CLA	CHB-C1B	3.62	1.47	1.39
22	L	307	CLA	CHB-C1B	3.62	1.47	1.39
22	X	304	CLA	C4D-CHA	3.62	1.51	1.38
22	Z	313	CLA	CHB-C1B	3.62	1.47	1.39
22	A	801	CLA	OBD-CAD	3.62	1.28	1.22
22	Z	307	CLA	OBD-CAD	3.62	1.28	1.22
25	B	838	BCR	C8-C9	-3.62	1.38	1.45
21	Z	312	CHL	CHC-C4B	3.62	1.47	1.39
22	B	816	CLA	OBD-CAD	3.62	1.28	1.22
25	L	302	BCR	C14-C13	3.62	1.40	1.35
22	B	828	CLA	CHB-C1B	3.62	1.47	1.39
22	A	854	CLA	C1B-NB	-3.62	1.33	1.37
22	B	814	CLA	OBD-CAD	3.61	1.28	1.22
22	1	321	CLA	CHB-C1B	3.61	1.47	1.39
22	1	321	CLA	OBD-CAD	3.61	1.28	1.22
22	B	830	CLA	OBD-CAD	3.61	1.28	1.22
22	1	305	CLA	OBD-CAD	3.61	1.28	1.22
22	B	845	CLA	OBD-CAD	3.61	1.28	1.22
22	Y	311	CLA	CHB-C1B	3.61	1.47	1.39
22	B	817	CLA	OBD-CAD	3.61	1.28	1.22
22	A	828	CLA	OBD-CAD	3.61	1.28	1.22
23	1	310	LUT	C10-C9	3.60	1.40	1.35
22	A	838	CLA	OBD-CAD	3.60	1.28	1.22
21	2	309	CHL	OBD-CAD	3.60	1.28	1.22
22	B	813	CLA	OBD-CAD	3.60	1.28	1.22
22	A	843	CLA	CHB-C1B	3.60	1.47	1.39
22	B	822	CLA	OBD-CAD	3.60	1.28	1.22
21	4	308	CHL	OBD-CAD	3.60	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	845	CLA	OBD-CAD	3.60	1.28	1.22
25	B	835	BCR	C10-C9	3.60	1.40	1.35
22	B	812	CLA	OBD-CAD	3.60	1.28	1.22
22	O	207	CLA	OBD-CAD	3.60	1.28	1.22
21	3	314	CHL	CHD-C4C	3.60	1.47	1.39
22	A	827	CLA	O2A-CGA	3.60	1.43	1.33
22	A	810	CLA	OBD-CAD	3.59	1.28	1.22
22	3	319	CLA	CHB-C1B	3.59	1.47	1.39
25	J	101	BCR	C17-C18	3.59	1.40	1.35
22	B	846	CLA	OBD-CAD	3.59	1.28	1.22
30	A	825	CL0	OBD-CAD	3.59	1.28	1.22
22	A	847	CLA	CHB-C1B	3.59	1.47	1.39
22	A	842	CLA	CHB-C1B	3.59	1.47	1.39
22	B	853	CLA	CHB-C1B	3.59	1.47	1.39
22	4	315	CLA	CHD-C1D	3.59	1.45	1.38
22	B	851	CLA	C3C-C2C	3.59	1.44	1.36
22	2	303	CLA	CHB-C1B	3.59	1.47	1.39
22	K	204	CLA	OBD-CAD	3.59	1.28	1.22
22	B	847	CLA	CHB-C1B	3.59	1.47	1.39
22	1	317	CLA	OBD-CAD	3.58	1.28	1.22
22	B	851	CLA	CHC-C1C	3.58	1.45	1.38
22	A	841	CLA	CHB-C1B	3.58	1.47	1.39
22	B	808	CLA	CHB-C1B	3.58	1.47	1.39
22	A	827	CLA	C4B-NB	-3.58	1.33	1.37
22	B	816	CLA	MG-NA	-3.58	1.97	2.06
22	4	313	CLA	CHB-C1B	3.58	1.47	1.39
22	B	827	CLA	CHB-C1B	3.58	1.47	1.39
22	A	859	CLA	OBD-CAD	3.58	1.28	1.22
22	2	322	CLA	CHB-C1B	3.58	1.47	1.39
22	B	817	CLA	CHB-C1B	3.58	1.47	1.39
22	B	805	CLA	OBD-CAD	3.57	1.28	1.22
25	B	839	BCR	C17-C18	3.57	1.40	1.35
21	1	316	CHL	CHD-C4C	3.57	1.47	1.39
25	A	817	BCR	C21-C22	3.57	1.40	1.35
22	X	303	CLA	OBD-CAD	3.57	1.28	1.22
22	A	832	CLA	CHB-C1B	3.57	1.47	1.39
21	4	309	CHL	OBD-CAD	3.57	1.28	1.22
22	Y	301	CLA	OBD-CAD	3.57	1.28	1.22
22	A	843	CLA	CHC-C4B	3.57	1.47	1.39
22	B	805	CLA	CHB-C1B	3.56	1.47	1.39
25	B	839	BCR	C14-C13	3.56	1.40	1.35
22	2	306	CLA	OBD-CAD	3.56	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	320	CLA	CHB-C1B	3.56	1.47	1.39
25	A	815	BCR	C8-C9	-3.55	1.38	1.45
22	3	318	CLA	OBD-CAD	3.55	1.28	1.22
22	A	809	CLA	CHB-C1B	3.55	1.47	1.39
22	B	806	CLA	CHB-C1B	3.55	1.47	1.39
23	3	301	LUT	C30-C29	3.55	1.40	1.35
22	3	315	CLA	OBD-CAD	3.55	1.28	1.22
22	1	304	CLA	C4B-NB	-3.55	1.33	1.37
22	G	207	CLA	CHB-C1B	3.55	1.47	1.39
22	Z	306	CLA	CHB-C1B	3.54	1.47	1.39
21	Z	303	CHL	CHC-C4B	3.54	1.47	1.39
22	B	813	CLA	CHC-C4B	3.54	1.47	1.39
21	Z	302	CHL	CHC-C4B	3.54	1.47	1.39
22	B	830	CLA	CHB-C1B	3.54	1.47	1.39
22	4	304	CLA	CHB-C1B	3.54	1.47	1.39
22	A	831	CLA	C4B-NB	-3.54	1.33	1.37
22	B	801	CLA	CHB-C1B	3.54	1.47	1.39
22	A	826	CLA	OBD-CAD	3.53	1.28	1.22
22	A	854	CLA	OBD-CAD	3.53	1.28	1.22
22	4	310	CLA	OBD-CAD	3.53	1.28	1.22
22	A	830	CLA	MG-NA	-3.53	1.97	2.06
22	B	833	CLA	OBD-CAD	3.53	1.28	1.22
22	B	806	CLA	OBD-CAD	3.53	1.28	1.22
22	B	804	CLA	CHB-C1B	3.52	1.47	1.39
22	2	305	CLA	CHB-C1B	3.52	1.47	1.39
22	B	830	CLA	CHC-C1C	3.52	1.45	1.38
23	4	322	LUT	C14-C13	3.52	1.40	1.35
22	B	803	CLA	C4B-NB	-3.52	1.33	1.37
22	A	837	CLA	CHB-C1B	3.52	1.47	1.39
22	4	304	CLA	OBD-CAD	3.52	1.28	1.22
22	2	308	CLA	CHB-C1B	3.52	1.47	1.39
22	A	840	CLA	CHB-C1B	3.52	1.47	1.39
22	4	316	CLA	OBD-CAD	3.52	1.28	1.22
22	B	849	CLA	OBD-CAD	3.52	1.28	1.22
22	B	803	CLA	CHC-C4B	3.51	1.47	1.39
25	B	838	BCR	C23-C22	-3.51	1.38	1.45
22	A	839	CLA	CHB-C1B	3.51	1.47	1.39
21	4	308	CHL	CHC-C4B	3.50	1.47	1.39
22	3	321	CLA	CHB-C1B	3.50	1.47	1.39
25	4	321	BCR	C17-C18	3.50	1.40	1.35
22	L	305	CLA	CHB-C1B	3.50	1.47	1.39
25	J	101	BCR	C14-C13	3.50	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	844	BCR	C23-C22	-3.50	1.38	1.45
22	B	810	CLA	OBD-CAD	3.50	1.28	1.22
22	N	202	CLA	OBD-CAD	3.50	1.28	1.22
22	2	308	CLA	OBD-CAD	3.50	1.28	1.22
22	2	318	CLA	CHB-C1B	3.49	1.47	1.39
22	B	845	CLA	CHB-C1B	3.49	1.47	1.39
25	K	201	BCR	C14-C13	3.49	1.40	1.35
25	J	103	BCR	C21-C22	3.49	1.40	1.35
22	2	319	CLA	OBD-CAD	3.49	1.28	1.22
25	B	837	BCR	C21-C22	3.49	1.40	1.35
22	B	847	CLA	CHC-C4B	3.49	1.47	1.39
22	A	828	CLA	C4B-NB	-3.49	1.33	1.37
22	3	316	CLA	C4B-NB	-3.48	1.33	1.37
22	K	204	CLA	C4B-NB	-3.48	1.33	1.37
21	Y	304	CHL	CHC-C4B	3.48	1.47	1.39
22	A	838	CLA	CHC-C4B	3.48	1.47	1.39
21	X	305	CHL	CHC-C4B	3.48	1.47	1.39
22	A	812	CLA	CHB-C1B	3.48	1.47	1.39
22	3	315	CLA	C4B-NB	-3.48	1.33	1.37
22	B	831	CLA	CHB-C1B	3.48	1.47	1.39
22	G	206	CLA	CHC-C4B	3.48	1.47	1.39
25	O	202	BCR	C10-C9	3.48	1.40	1.35
22	A	846	CLA	CHD-C1D	3.48	1.45	1.38
22	2	305	CLA	OBD-CAD	3.48	1.28	1.22
22	B	814	CLA	CHB-C1B	3.47	1.47	1.39
21	Y	303	CHL	CHC-C4B	3.47	1.47	1.39
22	A	829	CLA	OBD-CAD	3.47	1.28	1.22
22	A	806	CLA	CHD-C1D	3.47	1.45	1.38
25	K	201	BCR	C17-C18	3.47	1.40	1.35
21	X	302	CHL	CHC-C4B	3.47	1.47	1.39
25	A	816	BCR	C21-C22	3.47	1.40	1.35
22	A	848	CLA	CHB-C1B	3.47	1.47	1.39
22	2	318	CLA	OBD-CAD	3.47	1.28	1.22
22	L	306	CLA	CHB-C1B	3.46	1.47	1.39
21	X	307	CHL	CHC-C4B	3.46	1.47	1.39
23	3	301	LUT	C14-C13	3.46	1.40	1.35
25	B	839	BCR	C10-C9	3.46	1.40	1.35
21	3	307	CHL	CHC-C4B	3.46	1.47	1.39
25	I	101	BCR	C14-C13	3.46	1.40	1.35
22	A	808	CLA	CHB-C1B	3.46	1.47	1.39
25	J	103	BCR	C14-C13	3.46	1.40	1.35
22	B	848	CLA	CHC-C4B	3.46	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	206	CLA	OBD-CAD	3.46	1.28	1.22
21	X	306	CHL	CHC-C4B	3.46	1.47	1.39
21	X	308	CHL	CHC-C4B	3.46	1.47	1.39
22	Z	314	CLA	CHB-C1B	3.46	1.47	1.39
22	B	807	CLA	CHC-C4B	3.45	1.47	1.39
22	4	315	CLA	CHD-C4C	3.45	1.47	1.39
21	Y	313	CHL	CHC-C4B	3.45	1.47	1.39
22	A	851	CLA	CHC-C4B	3.45	1.47	1.39
22	3	309	CLA	OBD-CAD	3.45	1.28	1.22
25	L	304	BCR	C14-C13	3.44	1.40	1.35
22	A	844	CLA	C1B-NB	-3.44	1.33	1.37
22	4	305	CLA	CHC-C4B	3.44	1.47	1.39
22	A	846	CLA	CHD-C4C	3.44	1.47	1.39
25	J	101	BCR	C8-C9	-3.44	1.38	1.45
22	B	826	CLA	C4B-NB	-3.44	1.33	1.37
22	K	205	CLA	CHD-C4C	3.44	1.47	1.39
22	3	311	CLA	CHC-C4B	3.44	1.47	1.39
22	B	852	CLA	OBD-CAD	3.44	1.28	1.22
22	1	308	CLA	CHB-C1B	3.43	1.47	1.39
22	A	836	CLA	OBD-CAD	3.43	1.28	1.22
22	O	208	CLA	OBD-CAD	3.43	1.28	1.22
22	A	804	CLA	OBD-CAD	3.43	1.28	1.22
22	B	823	CLA	OBD-CAD	3.43	1.28	1.22
22	A	836	CLA	CHB-C1B	3.43	1.47	1.39
21	Z	304	CHL	CHC-C4B	3.43	1.47	1.39
22	B	809	CLA	CHB-C1B	3.43	1.47	1.39
22	A	802	CLA	CHC-C4B	3.42	1.47	1.39
25	I	101	BCR	C17-C18	3.42	1.40	1.35
25	A	816	BCR	C14-C13	3.42	1.40	1.35
25	O	202	BCR	C21-C22	3.42	1.40	1.35
22	A	830	CLA	C4B-NB	-3.42	1.33	1.37
22	A	838	CLA	C4B-NB	-3.42	1.33	1.37
22	A	829	CLA	CHD-C1D	3.42	1.45	1.38
22	1	317	CLA	CHC-C4B	3.42	1.47	1.39
22	2	320	CLA	CHD-C1D	3.41	1.45	1.38
22	B	815	CLA	OBD-CAD	3.41	1.28	1.22
25	B	835	BCR	C17-C18	3.41	1.40	1.35
23	3	301	LUT	C8-C9	-3.41	1.38	1.45
23	4	319	LUT	C34-C33	3.40	1.40	1.35
22	B	829	CLA	CHC-C4B	3.40	1.47	1.39
21	Y	305	CHL	CHC-C4B	3.40	1.47	1.39
22	A	801	CLA	CHB-C1B	3.40	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	310	CLA	OBD-CAD	3.40	1.28	1.22
22	A	857	CLA	CHB-C1B	3.40	1.47	1.39
25	J	103	BCR	C10-C9	3.40	1.40	1.35
22	4	305	CLA	OBD-CAD	3.40	1.28	1.22
22	A	859	CLA	CHB-C1B	3.40	1.47	1.39
22	B	821	CLA	OBD-CAD	3.40	1.28	1.22
25	3	303	BCR	C14-C13	3.40	1.40	1.35
22	A	835	CLA	CHB-C1B	3.39	1.47	1.39
21	Z	301	CHL	CHC-C4B	3.39	1.47	1.39
22	4	311	CLA	CHD-C1D	3.39	1.45	1.38
22	B	827	CLA	CHD-C1D	3.39	1.45	1.38
22	B	850	CLA	C4B-NB	-3.39	1.33	1.37
21	Y	307	CHL	CHC-C4B	3.39	1.47	1.39
22	1	304	CLA	CHC-C4B	3.39	1.47	1.39
22	A	812	CLA	CHC-C4B	3.39	1.47	1.39
25	L	301	BCR	C17-C18	3.39	1.40	1.35
22	B	809	CLA	OBD-CAD	3.39	1.28	1.22
22	B	818	CLA	C1B-NB	-3.39	1.33	1.37
22	1	319	CLA	OBD-CAD	3.39	1.28	1.22
22	4	304	CLA	C4B-NB	-3.39	1.33	1.37
25	L	304	BCR	C21-C22	3.38	1.40	1.35
22	B	818	CLA	OBD-CAD	3.38	1.28	1.22
25	L	301	BCR	C21-C22	3.38	1.40	1.35
25	J	101	BCR	C10-C9	3.38	1.40	1.35
22	A	830	CLA	OBD-CAD	3.38	1.28	1.22
22	O	206	CLA	CHD-C1D	3.38	1.44	1.38
22	3	321	CLA	CHC-C4B	3.38	1.47	1.39
25	4	321	BCR	C10-C9	3.37	1.40	1.35
21	Y	306	CHL	CHC-C4B	3.37	1.47	1.39
25	J	103	BCR	C17-C18	3.37	1.40	1.35
22	3	311	CLA	OBD-CAD	3.37	1.28	1.22
22	A	833	CLA	OBD-CAD	3.37	1.28	1.22
22	Z	314	CLA	CHD-C1D	3.37	1.44	1.38
25	L	304	BCR	C17-C18	3.37	1.40	1.35
22	4	315	CLA	CHB-C1B	3.37	1.47	1.39
22	1	308	CLA	CHD-C4C	3.37	1.46	1.39
21	X	309	CHL	CHC-C4B	3.36	1.47	1.39
25	A	814	BCR	C8-C9	-3.36	1.38	1.45
22	3	309	CLA	CHC-C4B	3.36	1.47	1.39
21	Y	313	CHL	OBD-CAD	3.36	1.28	1.22
22	B	821	CLA	CHB-C1B	3.36	1.46	1.39
22	F	306	CLA	CHC-C4B	3.36	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	844	CLA	CHD-C1D	3.36	1.44	1.38
22	A	808	CLA	OBD-CAD	3.36	1.28	1.22
22	2	306	CLA	CHC-C4B	3.36	1.46	1.39
22	B	825	CLA	CHD-C1D	3.36	1.44	1.38
22	Z	306	CLA	CHD-C1D	3.36	1.44	1.38
25	3	303	BCR	C23-C22	-3.36	1.38	1.45
25	B	840	BCR	C23-C22	-3.36	1.38	1.45
22	A	858	CLA	OBD-CAD	3.36	1.28	1.22
22	A	805	CLA	CHC-C4B	3.35	1.46	1.39
22	1	321	CLA	CHC-C4B	3.35	1.46	1.39
22	4	306	CLA	CHC-C4B	3.35	1.46	1.39
22	A	843	CLA	C4B-NB	-3.35	1.33	1.37
22	B	851	CLA	CHB-C1B	3.35	1.46	1.39
25	L	303	BCR	C8-C9	-3.35	1.38	1.45
22	B	819	CLA	CHD-C1D	3.35	1.44	1.38
22	B	851	CLA	C1B-NB	-3.35	1.33	1.37
22	4	306	CLA	CHD-C1D	3.35	1.44	1.38
22	B	829	CLA	C4B-NB	-3.35	1.33	1.37
22	B	802	CLA	CHB-C1B	3.34	1.46	1.39
22	A	852	CLA	CHC-C4B	3.34	1.46	1.39
22	4	312	CLA	CHC-C4B	3.34	1.46	1.39
22	A	826	CLA	C1B-NB	-3.34	1.33	1.37
22	1	307	CLA	OBD-CAD	3.34	1.28	1.22
22	A	806	CLA	CHB-C1B	3.34	1.46	1.39
25	2	312	BCR	C8-C9	-3.34	1.38	1.45
22	2	318	CLA	C4B-NB	-3.34	1.33	1.37
22	B	829	CLA	OBD-CAD	3.34	1.28	1.22
22	A	857	CLA	OBD-CAD	3.34	1.28	1.22
22	A	852	CLA	OBD-CAD	3.34	1.28	1.22
22	K	205	CLA	CHD-C1D	3.34	1.44	1.38
22	Z	313	CLA	CHD-C1D	3.34	1.44	1.38
25	A	816	BCR	C10-C9	3.33	1.40	1.35
22	2	308	CLA	CHD-C1D	3.33	1.44	1.38
22	A	833	CLA	CHB-C1B	3.33	1.46	1.39
22	A	831	CLA	OBD-CAD	3.33	1.28	1.22
22	A	807	CLA	CHB-C1B	3.33	1.46	1.39
22	B	852	CLA	CHB-C1B	3.33	1.46	1.39
22	Y	301	CLA	CHD-C1D	3.33	1.44	1.38
22	B	822	CLA	CHD-C4C	3.33	1.46	1.39
22	B	830	CLA	CHD-C1D	3.33	1.44	1.38
22	4	306	CLA	CHB-C1B	3.33	1.46	1.39
22	A	851	CLA	CHB-C1B	3.33	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	855	CLA	CHC-C1C	3.33	1.45	1.38
23	3	301	LUT	C10-C9	3.33	1.40	1.35
22	A	857	CLA	CHC-C4B	3.33	1.46	1.39
22	2	308	CLA	CHC-C4B	3.33	1.46	1.39
22	2	317	CLA	CHC-C4B	3.33	1.46	1.39
22	2	308	CLA	CHD-C4C	3.32	1.46	1.39
22	A	806	CLA	CHD-C4C	3.32	1.46	1.39
22	O	209	CLA	CHC-C4B	3.32	1.46	1.39
25	A	819	BCR	C23-C22	-3.32	1.38	1.45
25	F	302	BCR	C23-C22	-3.32	1.38	1.45
22	1	305	CLA	CHC-C4B	3.32	1.46	1.39
22	B	824	CLA	CHC-C4B	3.32	1.46	1.39
22	B	812	CLA	CHD-C1D	3.32	1.44	1.38
21	1	301	CHL	CHC-C4B	3.32	1.46	1.39
22	B	802	CLA	C3B-C4B	3.31	1.50	1.42
25	4	321	BCR	C14-C13	3.31	1.40	1.35
23	4	319	LUT	C14-C13	3.31	1.40	1.35
25	B	835	BCR	C14-C13	3.31	1.40	1.35
22	4	306	CLA	CHD-C4C	3.31	1.46	1.39
22	1	309	CLA	CHC-C4B	3.31	1.46	1.39
22	A	839	CLA	C4B-NB	-3.31	1.33	1.37
22	3	320	CLA	CHD-C1D	3.31	1.44	1.38
22	Y	310	CLA	CHC-C4B	3.31	1.46	1.39
22	2	322	CLA	CHC-C4B	3.30	1.46	1.39
22	B	853	CLA	CHD-C1D	3.30	1.44	1.38
22	A	836	CLA	CHD-C1D	3.30	1.44	1.38
25	A	818	BCR	C23-C22	-3.30	1.38	1.45
22	A	803	CLA	OBD-CAD	3.30	1.28	1.22
21	2	309	CHL	CHC-C4B	3.30	1.46	1.39
22	B	819	CLA	CHD-C4C	3.30	1.46	1.39
21	2	302	CHL	OBD-CAD	3.29	1.28	1.22
22	1	306	CLA	CHC-C4B	3.29	1.46	1.39
22	A	856	CLA	CHB-C1B	3.29	1.46	1.39
22	J	102	CLA	CHC-C4B	3.29	1.46	1.39
22	A	836	CLA	CHC-C4B	3.29	1.46	1.39
21	3	314	CHL	OBD-CAD	3.29	1.28	1.22
22	A	803	CLA	CHC-C4B	3.29	1.46	1.39
22	B	802	CLA	OBD-CAD	3.29	1.28	1.22
22	1	318	CLA	OBD-CAD	3.29	1.28	1.22
21	4	309	CHL	CHC-C4B	3.29	1.46	1.39
21	2	321	CHL	CHC-C4B	3.29	1.46	1.39
22	X	301	CLA	CHC-C4B	3.29	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	310	CLA	CHC-C4B	3.28	1.46	1.39
22	K	203	CLA	CHC-C4B	3.28	1.46	1.39
22	2	320	CLA	CHD-C4C	3.28	1.46	1.39
22	4	318	CLA	CHD-C1D	3.28	1.44	1.38
22	B	820	CLA	C3B-C4B	3.28	1.50	1.42
22	L	307	CLA	CHC-C4B	3.28	1.46	1.39
22	A	829	CLA	CHC-C4B	3.28	1.46	1.39
22	O	206	CLA	CHD-C4C	3.28	1.46	1.39
25	F	302	BCR	C17-C18	3.28	1.40	1.35
22	1	319	CLA	CHB-C1B	3.28	1.46	1.39
22	B	822	CLA	CHB-C1B	3.28	1.46	1.39
22	X	312	CLA	CHC-C4B	3.28	1.46	1.39
22	B	827	CLA	CHD-C4C	3.28	1.46	1.39
22	Z	314	CLA	CHD-C4C	3.28	1.46	1.39
22	B	850	CLA	CHB-C1B	3.27	1.46	1.39
25	L	303	BCR	C17-C18	3.27	1.40	1.35
22	X	303	CLA	CHC-C4B	3.27	1.46	1.39
22	B	818	CLA	CHB-C1B	3.27	1.46	1.39
22	4	318	CLA	CHD-C4C	3.27	1.46	1.39
25	A	818	BCR	C14-C13	3.27	1.40	1.35
22	A	855	CLA	C1B-NB	-3.27	1.33	1.37
22	B	845	CLA	C3B-C4B	3.27	1.50	1.42
22	Z	310	CLA	CHC-C4B	3.27	1.46	1.39
22	4	312	CLA	C4B-NB	-3.27	1.33	1.37
22	A	806	CLA	C4B-NB	-3.27	1.33	1.37
22	A	853	CLA	C4B-NB	-3.27	1.33	1.37
22	Y	311	CLA	CHD-C1D	3.27	1.44	1.38
22	Z	308	CLA	CHC-C4B	3.27	1.46	1.39
22	B	852	CLA	CHD-C1D	3.27	1.44	1.38
22	B	829	CLA	CHB-C1B	3.27	1.46	1.39
22	Y	302	CLA	CHD-C1D	3.26	1.44	1.38
22	2	304	CLA	CHC-C4B	3.26	1.46	1.39
22	Y	314	CLA	CHC-C4B	3.26	1.46	1.39
22	G	207	CLA	CHD-C1D	3.26	1.44	1.38
25	A	815	BCR	C21-C22	3.26	1.40	1.35
22	A	828	CLA	MG-NA	-3.26	1.98	2.06
22	B	853	CLA	CHD-C4C	3.26	1.46	1.39
22	B	817	CLA	C4B-NB	-3.26	1.33	1.37
22	B	846	CLA	CHD-C1D	3.26	1.44	1.38
21	3	314	CHL	CHC-C4B	3.26	1.46	1.39
22	K	205	CLA	CHB-C1B	3.26	1.46	1.39
22	1	319	CLA	CHD-C1D	3.26	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Z	307	CLA	CHC-C4B	3.25	1.46	1.39
22	X	304	CLA	C1B-NB	-3.25	1.33	1.37
22	B	825	CLA	CHD-C4C	3.25	1.46	1.39
22	1	319	CLA	CHD-C4C	3.25	1.46	1.39
22	4	311	CLA	CHD-C4C	3.25	1.46	1.39
22	A	805	CLA	OBD-CAD	3.25	1.28	1.22
22	2	303	CLA	CHC-C4B	3.25	1.46	1.39
21	2	301	CHL	CHC-C4B	3.25	1.46	1.39
22	A	801	CLA	CHD-C1D	3.25	1.44	1.38
22	N	202	CLA	CHC-C4B	3.25	1.46	1.39
22	A	839	CLA	CHD-C1D	3.25	1.44	1.38
25	A	818	BCR	C8-C9	-3.25	1.39	1.45
22	Y	301	CLA	CHD-C4C	3.24	1.46	1.39
22	A	832	CLA	CHD-C1D	3.24	1.44	1.38
22	Y	309	CLA	CHC-C4B	3.24	1.46	1.39
22	G	205	CLA	CHC-C4B	3.24	1.46	1.39
21	1	301	CHL	CHB-C1B	3.24	1.46	1.39
22	3	313	CLA	CHC-C4B	3.24	1.46	1.39
22	A	859	CLA	CHC-C4B	3.24	1.46	1.39
22	Z	309	CLA	CHD-C1D	3.24	1.44	1.38
22	B	804	CLA	OBD-CAD	3.24	1.28	1.22
22	X	311	CLA	CHC-C4B	3.24	1.46	1.39
22	1	302	CLA	CHD-C4C	3.24	1.46	1.39
25	B	844	BCR	C10-C9	3.24	1.40	1.35
22	F	305	CLA	OBD-CAD	3.24	1.28	1.22
25	L	301	BCR	C14-C13	3.24	1.40	1.35
22	B	815	CLA	CHC-C4B	3.24	1.46	1.39
25	A	817	BCR	C17-C18	3.24	1.40	1.35
22	A	802	CLA	C4B-NB	-3.24	1.33	1.37
22	A	845	CLA	CHD-C4C	3.24	1.46	1.39
22	Y	302	CLA	CHC-C4B	3.24	1.46	1.39
22	1	302	CLA	CHC-C4B	3.24	1.46	1.39
22	B	815	CLA	CHB-C1B	3.24	1.46	1.39
22	4	315	CLA	CHC-C4B	3.23	1.46	1.39
22	Y	311	CLA	CHD-C4C	3.23	1.46	1.39
22	Z	313	CLA	CHD-C4C	3.23	1.46	1.39
22	B	830	CLA	CHD-C4C	3.23	1.46	1.39
22	B	807	CLA	C3C-C2C	3.23	1.45	1.37
22	3	308	CLA	CHC-C4B	3.23	1.46	1.39
22	A	838	CLA	MG-NA	-3.23	1.98	2.06
21	Z	305	CHL	CHC-C4B	3.23	1.46	1.39
30	A	825	CL0	C4B-NB	-3.23	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	308	CLA	CHC-C4B	3.23	1.46	1.39
22	2	317	CLA	CHD-C1D	3.22	1.44	1.38
22	3	319	CLA	CHD-C1D	3.22	1.44	1.38
22	Y	312	CLA	CHD-C1D	3.22	1.44	1.38
22	B	833	CLA	CHC-C4B	3.22	1.46	1.39
22	B	818	CLA	CHC-C4B	3.22	1.46	1.39
22	B	808	CLA	CHD-C1D	3.22	1.44	1.38
22	K	202	CLA	CHD-C1D	3.22	1.44	1.38
22	3	312	CLA	CHC-C4B	3.22	1.46	1.39
22	Z	308	CLA	CHD-C1D	3.22	1.44	1.38
25	B	840	BCR	C21-C22	3.22	1.40	1.35
22	A	832	CLA	C4B-NB	-3.22	1.33	1.37
22	1	319	CLA	CHC-C4B	3.22	1.46	1.39
22	A	848	CLA	CHD-C1D	3.22	1.44	1.38
22	A	853	CLA	CHD-C4C	3.22	1.46	1.39
22	Z	311	CLA	CHD-C1D	3.22	1.44	1.38
22	1	307	CLA	CHC-C4B	3.22	1.46	1.39
22	B	831	CLA	CHC-C4B	3.21	1.46	1.39
22	B	821	CLA	CHC-C4B	3.21	1.46	1.39
22	Z	313	CLA	CHC-C4B	3.21	1.46	1.39
22	K	203	CLA	CHD-C4C	3.21	1.46	1.39
22	4	318	CLA	CHC-C4B	3.21	1.46	1.39
22	A	802	CLA	CHD-C1D	3.21	1.44	1.38
25	L	303	BCR	C23-C22	-3.21	1.39	1.45
22	Z	311	CLA	CHC-C4B	3.21	1.46	1.39
25	I	101	BCR	C21-C22	3.21	1.40	1.35
22	A	805	CLA	CHB-C1B	3.21	1.46	1.39
22	B	820	CLA	C1B-C2B	3.21	1.50	1.43
22	B	824	CLA	CHD-C1D	3.21	1.44	1.38
22	1	303	CLA	CHC-C4B	3.21	1.46	1.39
22	B	806	CLA	CHC-C4B	3.21	1.46	1.39
25	B	844	BCR	C14-C13	3.21	1.40	1.35
25	B	838	BCR	C12-C13	-3.21	1.39	1.45
22	1	302	CLA	CHD-C1D	3.21	1.44	1.38
22	Y	312	CLA	CHC-C4B	3.21	1.46	1.39
22	Y	309	CLA	CHD-C1D	3.21	1.44	1.38
25	3	303	BCR	C17-C18	3.21	1.40	1.35
22	B	831	CLA	C4B-NB	-3.21	1.33	1.37
22	3	316	CLA	OBD-CAD	3.21	1.28	1.22
21	Z	312	CHL	CHB-C1B	3.21	1.46	1.39
22	X	313	CLA	CHC-C4B	3.20	1.46	1.39
21	2	321	CHL	CHB-C1B	3.20	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	856	CLA	OBD-CAD	3.20	1.28	1.22
22	4	311	CLA	CHB-C1B	3.20	1.46	1.39
25	F	302	BCR	C12-C13	-3.20	1.39	1.45
22	H	201	CLA	CHD-C4C	3.20	1.46	1.39
22	Y	302	CLA	CHD-C4C	3.20	1.46	1.39
25	B	844	BCR	C17-C18	3.20	1.40	1.35
25	B	835	BCR	C21-C22	3.20	1.40	1.35
22	Z	309	CLA	CHC-C4B	3.20	1.46	1.39
22	X	303	CLA	CHD-C1D	3.20	1.44	1.38
22	3	321	CLA	CHD-C4C	3.20	1.46	1.39
22	1	321	CLA	CHD-C1D	3.19	1.44	1.38
22	X	310	CLA	CHD-C1D	3.19	1.44	1.38
22	F	305	CLA	CHC-C4B	3.19	1.46	1.39
22	A	833	CLA	CHD-C4C	3.19	1.46	1.39
22	A	853	CLA	CHD-C1D	3.19	1.44	1.38
22	A	810	CLA	CHC-C4B	3.19	1.46	1.39
22	B	845	CLA	CHC-C4B	3.19	1.46	1.39
22	A	855	CLA	C3D-C2D	3.19	1.47	1.39
22	Z	309	CLA	CHD-C4C	3.19	1.46	1.39
22	2	317	CLA	CHD-C4C	3.19	1.46	1.39
22	B	852	CLA	CHD-C4C	3.19	1.46	1.39
22	O	208	CLA	CHC-C4B	3.19	1.46	1.39
25	F	302	BCR	C21-C22	3.19	1.40	1.35
22	O	209	CLA	CHD-C1D	3.19	1.44	1.38
22	G	206	CLA	CHD-C1D	3.19	1.44	1.38
22	B	846	CLA	CHD-C4C	3.19	1.46	1.39
22	A	828	CLA	CHC-C4B	3.19	1.46	1.39
22	A	806	CLA	CHC-C4B	3.19	1.46	1.39
22	L	305	CLA	CHD-C4C	3.19	1.46	1.39
25	B	835	BCR	C23-C22	-3.19	1.39	1.45
22	G	207	CLA	CHD-C4C	3.19	1.46	1.39
22	A	858	CLA	CHB-C1B	3.19	1.46	1.39
22	A	829	CLA	CHD-C4C	3.19	1.46	1.39
22	B	846	CLA	CHB-C1B	3.19	1.46	1.39
22	H	201	CLA	CHC-C4B	3.19	1.46	1.39
22	A	835	CLA	OBD-CAD	3.18	1.28	1.22
21	X	306	CHL	CHB-C1B	3.18	1.46	1.39
22	A	846	CLA	CHC-C4B	3.18	1.46	1.39
22	B	849	CLA	CHC-C4B	3.18	1.46	1.39
22	B	824	CLA	CHD-C4C	3.18	1.46	1.39
22	A	837	CLA	CHD-C1D	3.18	1.44	1.38
23	4	319	LUT	C10-C9	3.18	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	312	CLA	OBD-CAD	3.18	1.28	1.22
22	A	844	CLA	CHD-C4C	3.18	1.46	1.39
22	A	846	CLA	C3D-C2D	3.18	1.47	1.39
22	X	313	CLA	CHD-C1D	3.18	1.44	1.38
22	Z	307	CLA	CHD-C1D	3.18	1.44	1.38
22	A	855	CLA	CHD-C1D	3.18	1.44	1.38
22	A	836	CLA	CHD-C4C	3.18	1.46	1.39
22	X	311	CLA	CHD-C1D	3.18	1.44	1.38
22	B	817	CLA	CHC-C4B	3.18	1.46	1.39
22	A	844	CLA	C3D-C2D	3.18	1.47	1.39
22	Z	306	CLA	CHD-C4C	3.18	1.46	1.39
22	X	312	CLA	CHD-C1D	3.18	1.44	1.38
22	Y	310	CLA	CHD-C1D	3.18	1.44	1.38
22	Y	312	CLA	CHD-C4C	3.18	1.46	1.39
25	A	814	BCR	C23-C22	-3.18	1.39	1.45
25	A	815	BCR	C17-C18	3.18	1.40	1.35
25	O	202	BCR	C17-C18	3.18	1.40	1.35
22	B	807	CLA	C3B-C4B	3.17	1.50	1.42
22	K	204	CLA	CHC-C4B	3.17	1.46	1.39
25	A	819	BCR	C8-C9	-3.17	1.39	1.45
25	B	838	BCR	C19-C18	-3.17	1.39	1.45
22	A	808	CLA	CHC-C4B	3.17	1.46	1.39
22	A	839	CLA	CHD-C4C	3.17	1.46	1.39
25	3	303	BCR	C8-C9	-3.17	1.39	1.45
22	X	313	CLA	CHD-C4C	3.17	1.46	1.39
22	Z	311	CLA	CHD-C4C	3.17	1.46	1.39
21	4	317	CHL	CHC-C4B	3.17	1.46	1.39
22	4	311	CLA	CHC-C4B	3.17	1.46	1.39
22	3	320	CLA	CHC-C4B	3.17	1.46	1.39
22	A	827	CLA	CHC-C4B	3.17	1.46	1.39
22	A	826	CLA	C3B-C4B	3.17	1.50	1.42
22	B	818	CLA	CHD-C1D	3.17	1.44	1.38
22	4	313	CLA	CHC-C4B	3.17	1.46	1.39
22	L	306	CLA	CHC-C4B	3.17	1.46	1.39
22	A	802	CLA	CHD-C4C	3.16	1.46	1.39
22	A	856	CLA	C4B-NB	-3.16	1.33	1.37
22	3	315	CLA	C3D-C2D	3.16	1.47	1.39
22	2	318	CLA	CHD-C1D	3.16	1.44	1.38
22	2	318	CLA	CHD-C4C	3.16	1.46	1.39
22	X	310	CLA	CHC-C4B	3.16	1.46	1.39
22	3	320	CLA	CHD-C4C	3.16	1.46	1.39
22	B	821	CLA	CHD-C4C	3.16	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	804	CLA	CHC-C4B	3.16	1.46	1.39
22	B	846	CLA	CHC-C4B	3.16	1.46	1.39
21	1	301	CHL	OBD-CAD	3.16	1.27	1.22
22	3	312	CLA	CHD-C1D	3.16	1.44	1.38
22	A	846	CLA	CHB-C1B	3.16	1.46	1.39
22	B	825	CLA	CHB-C1B	3.16	1.46	1.39
22	2	306	CLA	C4B-NB	-3.16	1.33	1.37
22	1	318	CLA	CHD-C4C	3.16	1.46	1.39
22	1	320	CLA	CHD-C1D	3.16	1.44	1.38
22	4	311	CLA	OBD-CAD	3.16	1.27	1.22
25	O	202	BCR	C14-C13	3.16	1.40	1.35
25	B	834	BCR	C23-C22	-3.16	1.39	1.45
25	B	844	BCR	C8-C9	-3.16	1.39	1.45
22	Z	307	CLA	CHD-C4C	3.16	1.46	1.39
22	Y	301	CLA	CHC-C4B	3.16	1.46	1.39
22	O	210	CLA	CHC-C4B	3.16	1.46	1.39
22	B	808	CLA	CHC-C4B	3.16	1.46	1.39
21	1	316	CHL	CHC-C4B	3.16	1.46	1.39
22	B	825	CLA	CHC-C4B	3.16	1.46	1.39
22	A	810	CLA	C3D-C2D	3.15	1.47	1.39
22	X	304	CLA	C3B-C4B	3.15	1.50	1.42
22	4	310	CLA	C4B-NB	-3.15	1.33	1.37
22	X	303	CLA	CHD-C4C	3.15	1.46	1.39
21	X	308	CHL	CHB-C1B	3.15	1.46	1.39
22	A	849	CLA	C3D-C2D	3.15	1.47	1.39
25	A	815	BCR	C14-C13	3.15	1.40	1.35
21	2	301	CHL	CHB-C1B	3.15	1.46	1.39
22	A	844	CLA	C4B-NB	-3.15	1.33	1.37
22	B	810	CLA	C1B-NB	-3.15	1.33	1.37
22	Y	309	CLA	CHD-C4C	3.15	1.46	1.39
22	B	829	CLA	CHD-C1D	3.15	1.44	1.38
22	A	807	CLA	OBD-CAD	3.15	1.27	1.22
22	B	805	CLA	CHD-C4C	3.15	1.46	1.39
22	G	206	CLA	CHD-C4C	3.15	1.46	1.39
22	A	844	CLA	MG-NA	-3.15	1.98	2.06
22	B	826	CLA	C3D-C2D	3.15	1.47	1.39
22	A	837	CLA	CHD-C4C	3.14	1.46	1.39
22	A	847	CLA	CHD-C4C	3.14	1.46	1.39
22	A	833	CLA	CHD-C1D	3.14	1.44	1.38
22	X	312	CLA	CHD-C4C	3.14	1.46	1.39
22	Z	308	CLA	CHD-C4C	3.14	1.46	1.39
22	A	854	CLA	C3D-C2D	3.14	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	829	CLA	CHD-C4C	3.14	1.46	1.39
22	3	316	CLA	CHB-C1B	3.14	1.46	1.39
22	O	206	CLA	CHC-C4B	3.14	1.46	1.39
22	3	319	CLA	CHC-C4B	3.14	1.46	1.39
22	A	854	CLA	CHB-C1B	3.14	1.46	1.39
22	1	318	CLA	CHC-C4B	3.14	1.46	1.39
25	3	303	BCR	C10-C9	3.14	1.39	1.35
22	A	848	CLA	CHC-C4B	3.14	1.46	1.39
22	3	316	CLA	CHC-C4B	3.14	1.46	1.39
22	L	305	CLA	CHD-C1D	3.14	1.44	1.38
21	X	309	CHL	CHB-C1B	3.14	1.46	1.39
22	B	823	CLA	CHC-C4B	3.14	1.46	1.39
21	Z	304	CHL	CHB-C1B	3.14	1.46	1.39
22	A	840	CLA	CHD-C1D	3.14	1.44	1.38
22	B	851	CLA	C3D-C2D	3.13	1.47	1.39
22	J	102	CLA	CHD-C1D	3.13	1.44	1.38
23	4	319	LUT	C30-C29	3.13	1.39	1.35
22	B	808	CLA	C1B-NB	-3.13	1.33	1.37
22	B	833	CLA	CHD-C4C	3.13	1.46	1.39
22	3	319	CLA	CHD-C4C	3.13	1.46	1.39
22	A	827	CLA	CHD-C1D	3.13	1.44	1.38
23	1	310	LUT	C8-C9	-3.13	1.39	1.45
22	2	322	CLA	C4B-NB	-3.13	1.33	1.37
22	B	851	CLA	CHD-C1D	3.13	1.44	1.38
22	Y	308	CLA	CHC-C4B	3.13	1.46	1.39
22	A	832	CLA	CHD-C4C	3.13	1.46	1.39
22	A	801	CLA	CHD-C4C	3.13	1.46	1.39
22	A	847	CLA	CHC-C4B	3.13	1.46	1.39
25	4	321	BCR	C8-C9	-3.13	1.39	1.45
22	B	806	CLA	CHD-C1D	3.12	1.44	1.38
22	A	856	CLA	CHD-C1D	3.12	1.44	1.38
22	K	202	CLA	CHD-C4C	3.12	1.46	1.39
22	Y	311	CLA	CHC-C4B	3.12	1.46	1.39
22	A	806	CLA	OBD-CAD	3.12	1.27	1.22
22	A	856	CLA	CHD-C4C	3.12	1.46	1.39
22	3	317	CLA	CHC-C4B	3.12	1.46	1.39
22	Z	310	CLA	CHD-C4C	3.12	1.46	1.39
22	Y	314	CLA	CHD-C1D	3.12	1.44	1.38
21	2	302	CHL	CHC-C4B	3.12	1.46	1.39
21	Y	304	CHL	CHB-C1B	3.12	1.46	1.39
22	O	209	CLA	CHD-C4C	3.12	1.46	1.39
22	Y	310	CLA	CHD-C4C	3.12	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	X	305	CHL	CHB-C1B	3.12	1.46	1.39
22	4	315	CLA	C1D-C2D	3.12	1.51	1.45
22	A	829	CLA	CHB-C1B	3.12	1.46	1.39
22	1	309	CLA	CHD-C4C	3.12	1.46	1.39
21	Y	307	CHL	CHB-C1B	3.12	1.46	1.39
22	B	825	CLA	C1B-NB	-3.12	1.34	1.37
25	L	301	BCR	C10-C9	3.12	1.39	1.35
22	1	303	CLA	CHD-C1D	3.12	1.44	1.38
22	3	309	CLA	CHD-C4C	3.12	1.46	1.39
22	X	311	CLA	CHD-C4C	3.12	1.46	1.39
22	A	852	CLA	MG-NA	-3.11	1.98	2.06
25	B	839	BCR	C8-C9	-3.11	1.39	1.45
25	L	301	BCR	C23-C22	-3.11	1.39	1.45
21	Y	303	CHL	CHB-C1B	3.11	1.46	1.39
25	A	819	BCR	C10-C9	3.11	1.39	1.35
22	A	812	CLA	C3B-C4B	3.11	1.50	1.42
21	4	309	CHL	CHB-C1B	3.11	1.46	1.39
22	B	849	CLA	C4B-NB	-3.11	1.34	1.37
25	A	815	BCR	C23-C22	-3.11	1.39	1.45
22	X	304	CLA	CHB-C1B	3.11	1.46	1.39
22	A	851	CLA	CHD-C4C	3.11	1.46	1.39
22	B	847	CLA	CHD-C4C	3.11	1.46	1.39
25	A	817	BCR	C23-C22	-3.11	1.39	1.45
22	A	857	CLA	CHD-C4C	3.11	1.46	1.39
25	I	101	BCR	C23-C22	-3.11	1.39	1.45
21	4	317	CHL	CHB-C1B	3.11	1.46	1.39
22	A	851	CLA	OBD-CAD	3.11	1.27	1.22
25	2	312	BCR	C23-C22	-3.11	1.39	1.45
22	B	812	CLA	CHD-C4C	3.11	1.46	1.39
22	A	849	CLA	CHD-C1D	3.10	1.44	1.38
22	A	840	CLA	CHD-C4C	3.10	1.46	1.39
22	B	853	CLA	CHC-C4B	3.10	1.46	1.39
22	A	804	CLA	CHD-C1D	3.10	1.44	1.38
25	A	819	BCR	C14-C13	3.10	1.39	1.35
22	A	831	CLA	CHC-C4B	3.10	1.46	1.39
22	B	822	CLA	CHD-C1D	3.10	1.44	1.38
22	Z	310	CLA	CHD-C1D	3.10	1.44	1.38
25	B	835	BCR	C19-C18	-3.10	1.39	1.45
22	3	318	CLA	CHC-C4B	3.10	1.46	1.39
22	O	207	CLA	CHC-C4B	3.10	1.46	1.39
22	2	304	CLA	CHD-C4C	3.10	1.46	1.39
22	Y	308	CLA	CHD-C1D	3.10	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	811	CLA	CHC-C4B	3.10	1.46	1.39
22	A	850	CLA	C4B-NB	-3.10	1.34	1.37
22	A	808	CLA	C3D-C2D	3.10	1.47	1.39
22	A	842	CLA	CHC-C4B	3.10	1.46	1.39
22	3	313	CLA	CHD-C1D	3.10	1.44	1.38
22	A	853	CLA	C3D-C2D	3.09	1.47	1.39
22	B	805	CLA	C4B-NB	-3.09	1.34	1.37
22	1	318	CLA	CHD-C1D	3.09	1.44	1.38
22	2	303	CLA	C3D-C2D	3.09	1.47	1.39
22	A	845	CLA	CHD-C1D	3.09	1.44	1.38
21	4	307	CHL	CHB-C1B	3.09	1.46	1.39
22	A	853	CLA	CHC-C4B	3.09	1.46	1.39
22	3	317	CLA	C3B-C4B	3.09	1.50	1.42
22	B	833	CLA	CHD-C1D	3.09	1.44	1.38
21	2	302	CHL	CHB-C1B	3.09	1.46	1.39
22	A	833	CLA	CHC-C4B	3.09	1.46	1.39
22	A	840	CLA	CHC-C4B	3.09	1.46	1.39
22	X	310	CLA	CHD-C4C	3.09	1.46	1.39
21	4	307	CHL	CHC-C4B	3.09	1.46	1.39
22	A	840	CLA	C4B-NB	-3.09	1.34	1.37
25	A	816	BCR	C8-C9	-3.09	1.39	1.45
22	B	827	CLA	C3D-C2D	3.09	1.47	1.39
22	K	205	CLA	C3D-C2D	3.09	1.47	1.39
25	A	814	BCR	C17-C18	3.09	1.39	1.35
22	A	804	CLA	CHD-C4C	3.09	1.46	1.39
22	O	210	CLA	CHD-C1D	3.08	1.44	1.38
25	A	817	BCR	C14-C13	3.08	1.39	1.35
22	A	856	CLA	CHC-C4B	3.08	1.46	1.39
22	Y	308	CLA	CHD-C4C	3.08	1.46	1.39
25	L	303	BCR	C21-C22	3.08	1.39	1.35
22	2	305	CLA	CHC-C4B	3.08	1.46	1.39
22	A	837	CLA	CHC-C4B	3.08	1.46	1.39
22	J	102	CLA	CHD-C4C	3.08	1.46	1.39
22	1	304	CLA	CHB-C1B	3.08	1.46	1.39
22	L	305	CLA	CHC-C4B	3.08	1.46	1.39
21	Y	306	CHL	CHB-C1B	3.08	1.46	1.39
25	L	303	BCR	C14-C13	3.08	1.39	1.35
22	L	307	CLA	CHD-C4C	3.08	1.46	1.39
22	A	806	CLA	C3D-C2D	3.08	1.47	1.39
22	A	857	CLA	CHD-C1D	3.08	1.44	1.38
22	B	805	CLA	CHD-C1D	3.08	1.44	1.38
25	B	839	BCR	C23-C22	-3.08	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	850	CLA	CHD-C1D	3.08	1.44	1.38
22	G	206	CLA	C3B-C4B	3.07	1.50	1.42
22	A	805	CLA	C4B-NB	-3.07	1.34	1.37
22	3	313	CLA	CHD-C4C	3.07	1.46	1.39
22	O	209	CLA	C3B-C4B	3.07	1.49	1.42
21	Z	302	CHL	CHB-C1B	3.07	1.46	1.39
22	A	803	CLA	C3D-C2D	3.07	1.47	1.39
21	X	302	CHL	CHB-C1B	3.07	1.46	1.39
22	B	805	CLA	CHC-C4B	3.07	1.46	1.39
22	Z	314	CLA	CHC-C4B	3.07	1.46	1.39
22	3	321	CLA	CHD-C1D	3.07	1.44	1.38
25	A	817	BCR	C8-C9	-3.07	1.39	1.45
22	B	808	CLA	C3B-C4B	3.07	1.49	1.42
22	A	807	CLA	CHC-C4B	3.07	1.46	1.39
30	A	825	CL0	C3D-C2D	3.07	1.47	1.39
22	B	803	CLA	MG-NA	-3.07	1.99	2.06
22	N	202	CLA	CHD-C1D	3.06	1.44	1.38
22	B	808	CLA	CHD-C4C	3.06	1.46	1.39
22	B	852	CLA	CHC-C4B	3.06	1.46	1.39
22	B	808	CLA	C3D-C2D	3.06	1.47	1.39
22	B	830	CLA	C3D-C2D	3.06	1.47	1.39
22	B	810	CLA	CHC-C4B	3.06	1.46	1.39
22	B	850	CLA	CHC-C4B	3.06	1.46	1.39
22	A	841	CLA	CHC-C4B	3.06	1.46	1.39
21	Z	303	CHL	CHB-C1B	3.06	1.46	1.39
22	B	804	CLA	CHC-C4B	3.06	1.46	1.39
22	X	301	CLA	CHD-C1D	3.06	1.44	1.38
22	K	202	CLA	CHC-C4B	3.06	1.46	1.39
22	A	854	CLA	CHC-C4B	3.06	1.46	1.39
25	L	304	BCR	C23-C22	-3.06	1.39	1.45
22	H	201	CLA	CHD-C1D	3.06	1.44	1.38
25	L	301	BCR	C8-C9	-3.06	1.39	1.45
21	Z	301	CHL	CHB-C1B	3.05	1.46	1.39
22	B	804	CLA	CHD-C1D	3.05	1.44	1.38
22	B	801	CLA	C3B-C4B	3.05	1.49	1.42
22	4	304	CLA	CHC-C4B	3.05	1.46	1.39
22	4	304	CLA	CHD-C1D	3.05	1.44	1.38
22	A	833	CLA	C4B-NB	-3.05	1.34	1.37
22	B	801	CLA	C1C-C2C	3.05	1.50	1.44
22	B	821	CLA	CHD-C1D	3.05	1.44	1.38
25	A	815	BCR	C12-C13	-3.05	1.39	1.45
22	A	847	CLA	CHD-C1D	3.05	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	X	304	CLA	C3D-C2D	3.05	1.47	1.39
22	B	822	CLA	CHC-C4B	3.04	1.46	1.39
22	K	203	CLA	CHD-C1D	3.04	1.44	1.38
21	Y	305	CHL	CHB-C1B	3.04	1.46	1.39
25	A	818	BCR	C21-C22	3.04	1.39	1.35
22	A	834	CLA	CHC-C4B	3.04	1.46	1.39
22	3	312	CLA	CHD-C4C	3.04	1.46	1.39
22	A	828	CLA	C4D-ND	3.04	1.41	1.37
22	1	320	CLA	CHC-C4B	3.04	1.46	1.39
25	J	103	BCR	C23-C22	-3.04	1.39	1.45
22	B	852	CLA	C3D-C2D	3.04	1.47	1.39
22	B	809	CLA	C4B-NB	-3.04	1.34	1.37
22	A	855	CLA	CHD-C4C	3.04	1.46	1.39
22	N	202	CLA	CHD-C4C	3.04	1.46	1.39
22	A	857	CLA	C4B-NB	-3.04	1.34	1.37
22	X	301	CLA	CHD-C4C	3.04	1.46	1.39
22	4	304	CLA	C3D-C2D	3.04	1.47	1.39
22	2	303	CLA	CHD-C1D	3.04	1.44	1.38
25	A	819	BCR	C17-C18	3.03	1.39	1.35
22	3	315	CLA	CHD-C1D	3.03	1.44	1.38
25	I	101	BCR	C8-C9	-3.03	1.39	1.45
25	L	303	BCR	C10-C9	3.03	1.39	1.35
21	Z	302	CHL	C3B-C4B	3.03	1.49	1.42
22	A	858	CLA	C1B-NB	-3.03	1.34	1.37
21	Z	312	CHL	C3B-C4B	3.03	1.49	1.42
22	1	304	CLA	OBD-CAD	3.03	1.27	1.22
21	3	314	CHL	CHB-C1B	3.03	1.46	1.39
21	Y	313	CHL	CHB-C1B	3.03	1.46	1.39
22	B	853	CLA	C3D-C2D	3.03	1.47	1.39
22	J	102	CLA	C3B-C4B	3.03	1.49	1.42
22	4	316	CLA	CHD-C4C	3.03	1.46	1.39
22	A	801	CLA	C3D-C2D	3.02	1.47	1.39
22	A	812	CLA	CHD-C1D	3.02	1.44	1.38
21	4	308	CHL	C3B-C4B	3.02	1.49	1.42
22	3	309	CLA	CHD-C1D	3.02	1.44	1.38
22	L	306	CLA	C3D-C2D	3.02	1.47	1.39
22	4	310	CLA	CHC-C4B	3.02	1.46	1.39
22	A	845	CLA	MG-NA	-3.02	1.99	2.06
22	Y	314	CLA	C3B-C4B	3.02	1.49	1.42
22	4	313	CLA	C4B-NB	-3.02	1.34	1.37
25	A	816	BCR	C17-C18	3.02	1.39	1.35
22	4	306	CLA	C3D-C2D	3.02	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	841	CLA	CHD-C1D	3.02	1.44	1.38
22	2	308	CLA	C3B-C4B	3.02	1.49	1.42
22	Z	306	CLA	CHC-C4B	3.02	1.46	1.39
22	B	815	CLA	C4B-NB	-3.02	1.34	1.37
25	J	103	BCR	C8-C9	-3.02	1.39	1.45
22	1	305	CLA	CHD-C1D	3.02	1.44	1.38
22	L	306	CLA	CHD-C4C	3.02	1.46	1.39
22	B	824	CLA	C3B-C4B	3.02	1.49	1.42
25	A	819	BCR	C21-C22	3.02	1.39	1.35
22	2	322	CLA	CHD-C1D	3.02	1.44	1.38
22	B	828	CLA	CHD-C4C	3.02	1.46	1.39
22	B	812	CLA	C3D-C2D	3.02	1.47	1.39
22	4	318	CLA	C3D-C2D	3.02	1.47	1.39
22	B	831	CLA	C3D-C2D	3.02	1.47	1.39
22	A	826	CLA	MG-NA	-3.02	1.99	2.06
22	A	807	CLA	CHD-C4C	3.01	1.46	1.39
22	G	207	CLA	C3D-C2D	3.01	1.47	1.39
22	B	809	CLA	CHC-C4B	3.01	1.46	1.39
22	B	820	CLA	CHB-C1B	3.01	1.46	1.39
22	B	823	CLA	C3D-C2D	3.01	1.47	1.39
22	B	820	CLA	CHD-C4C	3.01	1.46	1.39
22	A	808	CLA	CHD-C1D	3.01	1.44	1.38
22	A	830	CLA	CHC-C4B	3.01	1.46	1.39
22	1	321	CLA	CHD-C4C	3.01	1.46	1.39
22	1	308	CLA	CHD-C1D	3.01	1.44	1.38
22	Z	309	CLA	C3D-C2D	3.01	1.47	1.39
22	B	827	CLA	C4B-NB	-3.01	1.34	1.37
22	B	804	CLA	CHD-C4C	3.01	1.46	1.39
22	3	312	CLA	C4B-NB	-3.01	1.34	1.37
22	A	827	CLA	C1B-NB	-3.01	1.34	1.37
22	Y	314	CLA	CHD-C4C	3.01	1.46	1.39
25	B	844	BCR	C19-C18	-3.01	1.39	1.45
25	B	836	BCR	C23-C22	-3.00	1.39	1.45
22	2	317	CLA	C3B-C4B	3.00	1.49	1.42
22	Z	306	CLA	C3D-C2D	3.00	1.47	1.39
22	A	844	CLA	CHB-C1B	3.00	1.46	1.39
22	A	835	CLA	CHD-C4C	3.00	1.46	1.39
22	B	809	CLA	CHD-C4C	3.00	1.46	1.39
25	A	814	BCR	C14-C13	3.00	1.39	1.35
22	A	848	CLA	C1B-NB	-3.00	1.34	1.37
25	A	817	BCR	C12-C13	-3.00	1.39	1.45
22	B	818	CLA	CHD-C4C	3.00	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	308	CLA	C1D-C2D	3.00	1.51	1.45
22	2	320	CLA	CHC-C4B	3.00	1.46	1.39
22	Z	314	CLA	C3D-C2D	3.00	1.47	1.39
22	A	812	CLA	CHD-C4C	3.00	1.46	1.39
22	B	823	CLA	CHD-C1D	3.00	1.44	1.38
22	B	806	CLA	CHD-C4C	3.00	1.46	1.39
21	Z	312	CHL	C1D-C2D	3.00	1.51	1.45
22	A	836	CLA	C3B-C4B	3.00	1.49	1.42
22	B	813	CLA	CHD-C4C	3.00	1.46	1.39
22	3	311	CLA	C4B-NB	-2.99	1.34	1.37
22	B	846	CLA	C4B-NB	-2.99	1.34	1.37
22	Z	310	CLA	C3D-C2D	2.99	1.47	1.39
22	A	859	CLA	CHD-C4C	2.99	1.46	1.39
22	N	202	CLA	C3D-C2D	2.99	1.47	1.39
22	2	304	CLA	CHD-C1D	2.99	1.44	1.38
22	A	835	CLA	CHD-C1D	2.99	1.44	1.38
25	B	838	BCR	C14-C13	2.99	1.39	1.35
25	J	101	BCR	C23-C22	-2.99	1.39	1.45
22	F	306	CLA	C4B-NB	-2.99	1.34	1.37
21	X	307	CHL	CHB-C1B	2.99	1.46	1.39
22	B	801	CLA	C3D-C2D	2.99	1.47	1.39
22	B	817	CLA	C3D-C2D	2.99	1.47	1.39
22	A	842	CLA	C3D-C2D	2.99	1.47	1.39
23	2	310	LUT	C8-C9	-2.99	1.39	1.45
22	B	848	CLA	C4B-NB	-2.99	1.34	1.37
22	B	852	CLA	C4B-NB	-2.99	1.34	1.37
23	4	319	LUT	C8-C9	-2.99	1.39	1.45
22	Z	313	CLA	C3D-C2D	2.99	1.47	1.39
22	O	210	CLA	CHD-C4C	2.99	1.46	1.39
22	B	849	CLA	CHD-C1D	2.99	1.44	1.38
22	1	317	CLA	MG-NA	-2.99	1.99	2.06
22	A	850	CLA	CHC-C4B	2.99	1.46	1.39
22	A	851	CLA	C4B-NB	-2.99	1.34	1.37
22	1	303	CLA	CHD-C4C	2.99	1.46	1.39
22	1	302	CLA	OBD-CAD	2.99	1.27	1.22
22	X	311	CLA	C3D-C2D	2.99	1.47	1.39
22	A	854	CLA	C4B-NB	-2.99	1.34	1.37
22	2	318	CLA	C3D-C2D	2.99	1.47	1.39
22	Z	308	CLA	C3D-C2D	2.99	1.47	1.39
22	4	313	CLA	CHD-C4C	2.99	1.46	1.39
22	B	820	CLA	CHC-C4B	2.99	1.46	1.39
22	B	826	CLA	C3B-C4B	2.99	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	L	303	BCR	C12-C13	-2.99	1.39	1.45
22	B	846	CLA	C3D-C2D	2.99	1.47	1.39
22	3	320	CLA	C3D-C2D	2.98	1.47	1.39
22	1	319	CLA	C3D-C2D	2.98	1.47	1.39
22	1	321	CLA	C3B-C4B	2.98	1.49	1.42
22	A	801	CLA	C4B-NB	-2.98	1.34	1.37
22	O	207	CLA	C3D-C2D	2.98	1.47	1.39
22	A	839	CLA	CHC-C4B	2.98	1.46	1.39
22	B	826	CLA	MG-NA	-2.98	1.99	2.06
22	O	208	CLA	C3B-C4B	2.98	1.49	1.42
22	Y	311	CLA	C3D-C2D	2.98	1.47	1.39
22	K	205	CLA	CHC-C4B	2.98	1.46	1.39
22	4	313	CLA	CHD-C1D	2.98	1.44	1.38
22	A	831	CLA	MG-NA	-2.98	1.99	2.06
22	1	318	CLA	C4B-NB	-2.98	1.34	1.37
23	4	322	LUT	C8-C9	-2.98	1.39	1.45
22	2	319	CLA	CHC-C4B	2.98	1.46	1.39
21	1	316	CHL	CHB-C1B	2.98	1.46	1.39
22	B	813	CLA	CHD-C1D	2.97	1.44	1.38
21	2	309	CHL	C1D-C2D	2.97	1.51	1.45
25	A	818	BCR	C10-C9	2.97	1.39	1.35
22	A	858	CLA	C3D-C2D	2.97	1.47	1.39
21	X	309	CHL	C1D-C2D	2.97	1.51	1.45
22	4	314	CLA	CHC-C4B	2.97	1.46	1.39
30	A	825	CL0	CHB-C1B	2.97	1.46	1.39
22	2	306	CLA	C3B-C4B	2.97	1.49	1.42
22	A	840	CLA	C3D-C2D	2.97	1.47	1.39
22	B	851	CLA	CHD-C4C	2.97	1.46	1.39
22	2	320	CLA	C3D-C2D	2.97	1.47	1.39
22	B	809	CLA	CHD-C1D	2.97	1.44	1.38
22	B	815	CLA	CHD-C4C	2.97	1.46	1.39
22	2	317	CLA	C3D-C2D	2.97	1.47	1.39
22	A	808	CLA	CHD-C4C	2.97	1.46	1.39
22	4	314	CLA	C3D-C2D	2.97	1.47	1.39
22	B	804	CLA	C3D-C2D	2.97	1.47	1.39
22	B	818	CLA	C3B-C4B	2.97	1.49	1.42
22	3	316	CLA	C3D-C2D	2.97	1.47	1.39
21	Z	305	CHL	C3D-C2D	2.97	1.47	1.39
22	O	209	CLA	C3D-C2D	2.97	1.47	1.39
25	B	837	BCR	C23-C22	-2.96	1.39	1.45
30	A	825	CL0	CHC-C4B	2.96	1.46	1.39
22	A	809	CLA	CHD-C1D	2.96	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	849	CLA	CHD-C4C	2.96	1.46	1.39
22	B	850	CLA	CHD-C4C	2.96	1.46	1.39
22	B	809	CLA	C3D-C2D	2.96	1.47	1.39
22	A	839	CLA	C3D-C2D	2.96	1.47	1.39
22	Y	302	CLA	C3D-C2D	2.96	1.47	1.39
21	Z	305	CHL	CHB-C1B	2.96	1.46	1.39
22	2	305	CLA	CHD-C1D	2.96	1.44	1.38
22	A	802	CLA	C3D-C2D	2.96	1.47	1.39
22	B	813	CLA	C4B-NB	-2.96	1.34	1.37
22	B	805	CLA	C3D-C2D	2.96	1.47	1.39
22	A	807	CLA	MG-NA	-2.96	1.99	2.06
22	1	321	CLA	C3D-C2D	2.96	1.47	1.39
22	1	320	CLA	CHD-C4C	2.96	1.46	1.39
22	2	307	CLA	CHC-C4B	2.96	1.46	1.39
22	B	850	CLA	C3D-C2D	2.96	1.47	1.39
22	L	305	CLA	C3D-C2D	2.96	1.47	1.39
22	O	210	CLA	C3D-C2D	2.96	1.47	1.39
22	A	833	CLA	C3D-C2D	2.96	1.47	1.39
22	B	811	CLA	CHD-C4C	2.95	1.46	1.39
25	F	302	BCR	C14-C13	2.95	1.39	1.35
22	Z	307	CLA	C3D-C2D	2.95	1.47	1.39
22	2	319	CLA	MG-NA	-2.95	1.99	2.06
21	2	309	CHL	C3D-C2D	2.95	1.47	1.39
22	3	319	CLA	C3D-C2D	2.95	1.47	1.39
22	B	811	CLA	C4B-NB	-2.95	1.34	1.37
22	1	304	CLA	C3D-C2D	2.95	1.47	1.39
22	B	826	CLA	CHC-C4B	2.95	1.46	1.39
25	4	321	BCR	C23-C22	-2.95	1.39	1.45
22	X	310	CLA	C3D-C2D	2.95	1.47	1.39
22	1	307	CLA	C3D-C2D	2.95	1.47	1.39
22	B	827	CLA	OBD-CAD	2.95	1.27	1.22
22	1	318	CLA	C3D-C2D	2.95	1.47	1.39
21	Z	305	CHL	C1D-C2D	2.95	1.51	1.45
22	2	304	CLA	C4B-NB	-2.95	1.34	1.37
22	4	310	CLA	C3D-C2D	2.95	1.47	1.39
22	A	837	CLA	C3B-C4B	2.95	1.49	1.42
22	B	822	CLA	C3D-C2D	2.95	1.47	1.39
22	2	322	CLA	CHD-C4C	2.95	1.46	1.39
22	H	201	CLA	C3D-C2D	2.95	1.47	1.39
22	B	823	CLA	C4B-NB	-2.95	1.34	1.37
22	4	318	CLA	C1D-C2D	2.94	1.51	1.45
22	2	304	CLA	C3D-C2D	2.94	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Y	306	CHL	C1D-C2D	2.94	1.51	1.45
22	Z	311	CLA	C3D-C2D	2.94	1.47	1.39
25	B	835	BCR	C8-C9	-2.94	1.39	1.45
22	A	841	CLA	C3B-C4B	2.94	1.49	1.42
22	O	206	CLA	C3D-C2D	2.94	1.47	1.39
25	A	814	BCR	C12-C13	-2.94	1.39	1.45
22	3	317	CLA	CHD-C1D	2.94	1.44	1.38
22	B	848	CLA	C3B-C4B	2.94	1.49	1.42
22	K	203	CLA	C3D-C2D	2.94	1.47	1.39
22	2	307	CLA	CHD-C1D	2.94	1.44	1.38
22	A	835	CLA	C1B-NB	-2.94	1.34	1.37
22	A	809	CLA	CHD-C4C	2.94	1.45	1.39
22	B	823	CLA	CHD-C4C	2.94	1.45	1.39
22	2	318	CLA	CHC-C4B	2.94	1.46	1.39
25	A	814	BCR	C21-C22	2.94	1.39	1.35
22	1	302	CLA	C3D-C2D	2.93	1.47	1.39
22	A	826	CLA	C3D-C2D	2.93	1.47	1.39
22	A	808	CLA	C4B-NB	-2.93	1.34	1.37
22	A	848	CLA	CHD-C4C	2.93	1.45	1.39
22	B	816	CLA	C3B-C4B	2.93	1.49	1.42
22	2	307	CLA	CHD-C4C	2.93	1.45	1.39
22	1	302	CLA	C4B-NB	-2.93	1.34	1.37
22	O	207	CLA	CHD-C4C	2.93	1.45	1.39
22	Y	309	CLA	C3D-C2D	2.93	1.47	1.39
25	B	844	BCR	C21-C22	2.93	1.39	1.35
22	4	311	CLA	C3D-C2D	2.93	1.47	1.39
22	Y	314	CLA	C3D-C2D	2.93	1.47	1.39
22	2	322	CLA	OBD-CAD	2.93	1.27	1.22
22	1	308	CLA	C3D-C2D	2.93	1.47	1.39
22	1	306	CLA	C4B-NB	-2.93	1.34	1.37
22	X	312	CLA	C3D-C2D	2.93	1.47	1.39
22	1	320	CLA	C4B-NB	-2.93	1.34	1.37
22	A	841	CLA	C1B-NB	-2.93	1.34	1.37
21	Y	304	CHL	C3D-C2D	2.93	1.47	1.39
22	X	301	CLA	C3D-C2D	2.93	1.47	1.39
22	A	805	CLA	CHD-C4C	2.93	1.45	1.39
22	K	205	CLA	C1D-C2D	2.92	1.51	1.45
22	A	847	CLA	C3D-C2D	2.92	1.47	1.39
22	B	806	CLA	C4B-NB	-2.92	1.34	1.37
22	A	846	CLA	C1D-C2D	2.92	1.51	1.45
22	A	834	CLA	C4B-NB	-2.92	1.34	1.37
22	B	825	CLA	C3D-C2D	2.92	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	304	CLA	CHD-C4C	2.92	1.45	1.39
22	O	207	CLA	CHD-C1D	2.92	1.44	1.38
22	B	821	CLA	C3D-C2D	2.92	1.47	1.39
22	A	809	CLA	CHC-C4B	2.92	1.46	1.39
21	X	302	CHL	C3D-C2D	2.92	1.47	1.39
25	B	837	BCR	C8-C9	-2.92	1.39	1.45
22	Y	310	CLA	C3D-C2D	2.92	1.47	1.39
22	A	834	CLA	MG-NA	-2.92	1.99	2.06
22	K	202	CLA	C3D-C2D	2.92	1.47	1.39
22	4	316	CLA	CHC-C4B	2.92	1.46	1.39
22	1	307	CLA	CHD-C4C	2.92	1.45	1.39
22	3	308	CLA	CHD-C4C	2.92	1.45	1.39
22	A	838	CLA	C3B-C4B	2.92	1.49	1.42
22	1	303	CLA	C3D-C2D	2.92	1.47	1.39
22	3	308	CLA	C4B-NB	-2.92	1.34	1.37
22	B	850	CLA	MG-NA	-2.92	1.99	2.06
25	3	303	BCR	C21-C22	2.92	1.39	1.35
22	3	309	CLA	C4B-NB	-2.92	1.34	1.37
22	A	829	CLA	C3D-C2D	2.92	1.47	1.39
22	2	305	CLA	CHD-C4C	2.92	1.45	1.39
22	1	309	CLA	CHD-C1D	2.92	1.44	1.38
22	2	306	CLA	MG-NA	-2.92	1.99	2.06
22	G	205	CLA	CHD-C4C	2.91	1.45	1.39
22	1	304	CLA	C3B-C4B	2.91	1.49	1.42
22	B	848	CLA	C1B-NB	-2.91	1.34	1.37
22	K	203	CLA	C4B-NB	-2.91	1.34	1.37
22	X	313	CLA	C3D-C2D	2.91	1.47	1.39
22	B	827	CLA	C1D-C2D	2.91	1.51	1.45
30	A	825	CL0	CHD-C1D	2.91	1.44	1.38
22	K	205	CLA	C4B-NB	-2.91	1.34	1.37
22	B	849	CLA	C3D-C2D	2.91	1.47	1.39
21	X	308	CHL	C1D-C2D	2.91	1.51	1.45
22	3	316	CLA	C1B-NB	-2.91	1.34	1.37
21	Z	312	CHL	C3D-C2D	2.91	1.47	1.39
22	K	204	CLA	CHD-C1D	2.91	1.44	1.38
22	B	853	CLA	C4B-NB	-2.91	1.34	1.37
22	1	307	CLA	MG-NA	-2.91	1.99	2.06
25	G	202	BCR	C8-C9	-2.91	1.39	1.45
22	A	849	CLA	CHC-C4B	2.91	1.45	1.39
22	2	307	CLA	C3D-C2D	2.91	1.47	1.39
22	A	832	CLA	C3D-C2D	2.91	1.47	1.39
22	4	316	CLA	CHD-C1D	2.91	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	304	CLA	MG-NA	-2.91	1.99	2.06
22	A	845	CLA	C4B-NB	-2.91	1.34	1.37
22	3	309	CLA	C3D-C2D	2.90	1.47	1.39
22	B	801	CLA	MG-NA	-2.90	1.99	2.06
21	1	316	CHL	C3D-C2D	2.90	1.47	1.39
21	Y	305	CHL	C1D-C2D	2.90	1.51	1.45
22	3	313	CLA	C3D-C2D	2.90	1.47	1.39
22	2	303	CLA	C3B-C4B	2.90	1.49	1.42
22	1	306	CLA	CHD-C1D	2.90	1.44	1.38
22	B	847	CLA	CHD-C1D	2.90	1.44	1.38
22	B	847	CLA	MG-NA	-2.90	1.99	2.06
22	O	207	CLA	C4B-NB	-2.90	1.34	1.37
22	A	826	CLA	CHB-C1B	2.90	1.45	1.39
22	3	313	CLA	C3B-C4B	2.90	1.49	1.42
22	2	305	CLA	C3D-C2D	2.90	1.47	1.39
22	Y	312	CLA	C3D-C2D	2.90	1.47	1.39
22	3	316	CLA	CHD-C1D	2.90	1.44	1.38
22	F	305	CLA	CHD-C1D	2.90	1.44	1.38
21	Z	303	CHL	C3D-C2D	2.89	1.47	1.39
22	B	814	CLA	C1B-NB	-2.89	1.34	1.37
22	B	831	CLA	CHD-C1D	2.89	1.44	1.38
21	Z	303	CHL	C1D-C2D	2.89	1.51	1.45
22	Y	308	CLA	C3D-C2D	2.89	1.47	1.39
22	A	829	CLA	C1D-C2D	2.89	1.51	1.45
22	B	814	CLA	C3B-C4B	2.89	1.49	1.42
22	A	836	CLA	C3D-C2D	2.89	1.47	1.39
22	A	857	CLA	C3D-C2D	2.89	1.47	1.39
22	A	832	CLA	CHC-C4B	2.89	1.45	1.39
22	3	320	CLA	C3B-C4B	2.89	1.49	1.42
25	A	814	BCR	C19-C18	-2.89	1.39	1.45
22	H	201	CLA	C4B-NB	-2.89	1.34	1.37
22	A	856	CLA	C3D-C2D	2.89	1.47	1.39
22	A	841	CLA	CHD-C4C	2.89	1.45	1.39
22	X	303	CLA	C3D-C2D	2.89	1.47	1.39
22	Y	301	CLA	C1D-C2D	2.89	1.51	1.45
21	X	309	CHL	C3D-C2D	2.89	1.47	1.39
22	3	310	CLA	C4B-NB	-2.89	1.34	1.37
22	A	801	CLA	CHC-C4B	2.89	1.45	1.39
21	Y	304	CHL	C1D-C2D	2.89	1.51	1.45
25	K	201	BCR	C23-C22	-2.88	1.39	1.45
21	X	305	CHL	C1D-C2D	2.88	1.51	1.45
22	X	304	CLA	CHD-C4C	2.88	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	809	CLA	C3D-C2D	2.88	1.47	1.39
22	3	308	CLA	MG-NA	-2.88	1.99	2.06
22	Z	313	CLA	C1D-C2D	2.88	1.51	1.45
22	B	802	CLA	CHC-C4B	2.88	1.45	1.39
21	X	307	CHL	C3D-C2D	2.88	1.47	1.39
25	3	303	BCR	C19-C18	-2.88	1.39	1.45
21	X	307	CHL	C1D-C2D	2.88	1.51	1.45
21	X	302	CHL	C1D-C2D	2.88	1.51	1.45
22	1	306	CLA	CHD-C4C	2.88	1.45	1.39
22	A	833	CLA	C3B-C4B	2.88	1.49	1.42
22	A	804	CLA	C3B-C4B	2.88	1.49	1.42
22	B	828	CLA	CHC-C4B	2.88	1.45	1.39
22	1	305	CLA	CHD-C4C	2.88	1.45	1.39
21	X	305	CHL	C3D-C2D	2.88	1.47	1.39
22	A	812	CLA	C3D-C2D	2.88	1.47	1.39
21	2	309	CHL	CHB-C1B	2.88	1.45	1.39
22	A	847	CLA	C3B-C4B	2.88	1.49	1.42
22	B	825	CLA	C3B-C4B	2.88	1.49	1.42
22	G	207	CLA	CHC-C4B	2.88	1.45	1.39
22	A	806	CLA	C1D-C2D	2.88	1.51	1.45
22	A	834	CLA	CHD-C4C	2.88	1.45	1.39
22	A	858	CLA	CHD-C4C	2.88	1.45	1.39
22	Z	308	CLA	C1D-C2D	2.88	1.51	1.45
22	B	833	CLA	C3D-C2D	2.87	1.47	1.39
22	B	819	CLA	CHC-C4B	2.87	1.45	1.39
21	Y	307	CHL	C3D-C2D	2.87	1.47	1.39
25	L	303	BCR	C19-C18	-2.87	1.39	1.45
22	A	846	CLA	C1B-NB	-2.87	1.34	1.37
22	4	314	CLA	CHD-C4C	2.87	1.45	1.39
22	B	802	CLA	CHD-C1D	2.87	1.44	1.38
22	1	317	CLA	C3D-C2D	2.87	1.47	1.39
22	B	818	CLA	C3D-C2D	2.87	1.47	1.39
22	3	317	CLA	CHD-C4C	2.87	1.45	1.39
22	A	849	CLA	CHD-C4C	2.87	1.45	1.39
22	4	305	CLA	CHD-C4C	2.87	1.45	1.39
21	4	308	CHL	CHB-C1B	2.87	1.45	1.39
21	Z	301	CHL	C3D-C2D	2.87	1.46	1.39
21	Y	313	CHL	C3D-C2D	2.87	1.46	1.39
21	Y	305	CHL	C3D-C2D	2.87	1.46	1.39
21	4	317	CHL	C1D-C2D	2.87	1.51	1.45
21	4	317	CHL	C3D-C2D	2.87	1.46	1.39
22	A	849	CLA	C4B-NB	-2.86	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Y	312	CLA	C1D-C2D	2.86	1.51	1.45
22	A	843	CLA	CHD-C4C	2.86	1.45	1.39
22	A	852	CLA	C1B-NB	-2.86	1.34	1.37
22	Z	314	CLA	C1D-C2D	2.86	1.51	1.45
21	4	307	CHL	C1D-C2D	2.86	1.51	1.45
22	A	841	CLA	C3D-C2D	2.86	1.46	1.39
22	3	317	CLA	C4B-NB	-2.86	1.34	1.37
22	B	802	CLA	C1B-NB	-2.86	1.34	1.37
21	X	306	CHL	C3D-C2D	2.86	1.46	1.39
22	3	310	CLA	CHD-C4C	2.86	1.45	1.39
22	3	318	CLA	CHD-C1D	2.86	1.43	1.38
22	4	312	CLA	CHD-C1D	2.86	1.43	1.38
25	B	834	BCR	C8-C9	-2.86	1.39	1.45
22	1	307	CLA	CHD-C1D	2.86	1.43	1.38
22	2	307	CLA	C4B-NB	-2.86	1.34	1.37
22	3	310	CLA	CHD-C1D	2.86	1.43	1.38
22	1	317	CLA	C4B-NB	-2.86	1.34	1.37
22	A	833	CLA	C1B-NB	-2.86	1.34	1.37
22	1	305	CLA	C3D-C2D	2.85	1.46	1.39
22	1	309	CLA	C3D-C2D	2.85	1.46	1.39
22	B	808	CLA	C1D-C2D	2.85	1.51	1.45
25	2	312	BCR	C12-C13	-2.85	1.39	1.45
22	O	210	CLA	C4B-NB	-2.85	1.34	1.37
22	Y	301	CLA	C3D-C2D	2.85	1.46	1.39
22	A	803	CLA	C4B-NB	-2.85	1.34	1.37
22	B	806	CLA	C3D-C2D	2.85	1.46	1.39
22	Y	302	CLA	C1D-C2D	2.85	1.50	1.45
22	O	208	CLA	CHD-C4C	2.85	1.45	1.39
22	A	848	CLA	C3B-C4B	2.85	1.49	1.42
22	A	827	CLA	CHB-C1B	2.85	1.45	1.39
21	Y	306	CHL	C3D-C2D	2.85	1.46	1.39
22	A	807	CLA	CHD-C1D	2.85	1.43	1.38
21	Y	303	CHL	C3D-C2D	2.85	1.46	1.39
25	1	312	BCR	C23-C22	-2.85	1.39	1.45
22	Z	309	CLA	C1D-C2D	2.85	1.50	1.45
22	B	827	CLA	MG-NA	-2.85	1.99	2.06
22	4	312	CLA	C3D-C2D	2.85	1.46	1.39
22	A	851	CLA	C3D-C2D	2.85	1.46	1.39
22	G	205	CLA	C3D-C2D	2.85	1.46	1.39
22	B	831	CLA	CHD-C4C	2.85	1.45	1.39
22	3	315	CLA	CHC-C4B	2.84	1.45	1.39
21	Z	301	CHL	C1D-C2D	2.84	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	O	202	BCR	C8-C9	-2.84	1.39	1.45
25	A	819	BCR	C19-C18	-2.84	1.39	1.45
21	3	307	CHL	CHB-C1B	2.84	1.45	1.39
22	B	853	CLA	C1D-C2D	2.84	1.50	1.45
25	A	814	BCR	C10-C9	2.84	1.39	1.35
22	2	322	CLA	C3D-C2D	2.84	1.46	1.39
22	B	833	CLA	C4B-NB	-2.84	1.34	1.37
21	X	306	CHL	C1D-C2D	2.84	1.50	1.45
22	B	801	CLA	C1B-NB	-2.84	1.34	1.37
22	A	827	CLA	MG-NA	-2.84	1.99	2.06
22	A	859	CLA	C4B-NB	-2.84	1.34	1.37
25	A	815	BCR	C10-C9	2.83	1.39	1.35
30	A	825	CL0	MG-NA	-2.83	1.99	2.06
22	B	830	CLA	MG-NA	-2.83	1.99	2.06
22	L	305	CLA	C4B-NB	-2.83	1.34	1.37
22	Z	314	CLA	C4B-NB	-2.83	1.34	1.37
22	A	804	CLA	C3D-C2D	2.83	1.46	1.39
22	Z	306	CLA	C1D-C2D	2.83	1.50	1.45
22	3	311	CLA	CHD-C4C	2.83	1.45	1.39
22	B	828	CLA	CHD-C1D	2.83	1.43	1.38
22	2	320	CLA	C1D-C2D	2.83	1.50	1.45
21	X	308	CHL	C3D-C2D	2.83	1.46	1.39
22	1	304	CLA	CHD-C4C	2.83	1.45	1.39
22	A	828	CLA	C3B-C4B	2.83	1.49	1.42
22	O	206	CLA	C1D-C2D	2.83	1.50	1.45
22	B	822	CLA	C4B-NB	-2.83	1.34	1.37
22	L	307	CLA	CHD-C1D	2.83	1.43	1.38
21	2	321	CHL	C1D-C2D	2.83	1.50	1.45
22	B	824	CLA	C1D-C2D	2.83	1.50	1.45
22	B	810	CLA	CHD-C1D	2.82	1.43	1.38
22	Z	309	CLA	C4B-NB	-2.82	1.34	1.37
25	K	201	BCR	C8-C9	-2.82	1.39	1.45
22	A	833	CLA	MG-NA	-2.82	1.99	2.06
22	K	204	CLA	CHD-C4C	2.82	1.45	1.39
22	3	312	CLA	C1D-C2D	2.82	1.50	1.45
22	Y	310	CLA	C3B-C4B	2.82	1.49	1.42
22	F	306	CLA	CHD-C4C	2.82	1.45	1.39
22	F	305	CLA	CHD-C4C	2.82	1.45	1.39
22	3	315	CLA	CHD-C4C	2.82	1.45	1.39
22	A	848	CLA	C1D-C2D	2.82	1.50	1.45
22	4	305	CLA	C3B-C4B	2.82	1.49	1.42
22	A	807	CLA	C3B-C4B	2.82	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	318	CLA	CHD-C4C	2.82	1.45	1.39
22	X	311	CLA	C1D-C2D	2.81	1.50	1.45
22	4	305	CLA	C4B-NB	-2.81	1.34	1.37
22	A	803	CLA	CHD-C4C	2.81	1.45	1.39
22	3	320	CLA	C1D-C2D	2.81	1.50	1.45
22	G	205	CLA	CHD-C1D	2.81	1.43	1.38
22	J	102	CLA	C3D-C2D	2.81	1.46	1.39
22	1	318	CLA	MG-NA	-2.81	1.99	2.06
22	G	206	CLA	C1D-C2D	2.81	1.50	1.45
22	4	310	CLA	CHD-C1D	2.81	1.43	1.38
22	X	310	CLA	C4B-NB	-2.81	1.34	1.37
22	Y	311	CLA	C1D-C2D	2.81	1.50	1.45
22	2	305	CLA	C4B-NB	-2.81	1.34	1.37
22	A	854	CLA	CHD-C1D	2.81	1.43	1.38
22	A	809	CLA	C4B-NB	-2.81	1.34	1.37
22	Y	311	CLA	C4B-NB	-2.81	1.34	1.37
22	F	306	CLA	C3D-C2D	2.81	1.46	1.39
22	B	828	CLA	OBD-CAD	2.81	1.27	1.22
22	B	820	CLA	OBD-CAD	2.81	1.27	1.22
22	4	314	CLA	CHD-C1D	2.81	1.43	1.38
22	A	846	CLA	C3B-C4B	2.81	1.49	1.42
21	2	301	CHL	C3D-C2D	2.81	1.46	1.39
22	Y	302	CLA	C4B-NB	-2.81	1.34	1.37
22	3	308	CLA	C3D-C2D	2.81	1.46	1.39
22	N	202	CLA	C3B-C4B	2.81	1.49	1.42
22	1	317	CLA	C1D-C2D	2.80	1.50	1.45
23	4	319	LUT	C12-C13	-2.80	1.39	1.45
22	Z	311	CLA	C1D-C2D	2.80	1.50	1.45
22	F	305	CLA	C4B-NB	-2.80	1.34	1.37
21	4	307	CHL	C3D-C2D	2.80	1.46	1.39
21	Y	303	CHL	C1D-C2D	2.80	1.50	1.45
25	B	838	BCR	C17-C18	2.80	1.39	1.35
22	X	313	CLA	C1D-C2D	2.80	1.50	1.45
22	A	826	CLA	C1C-C2C	2.80	1.50	1.44
22	4	314	CLA	C4B-NB	-2.80	1.34	1.37
22	B	805	CLA	MG-NA	-2.80	1.99	2.06
22	O	209	CLA	C1D-C2D	2.80	1.50	1.45
22	Y	309	CLA	C1D-C2D	2.80	1.50	1.45
22	A	853	CLA	CHB-C1B	2.80	1.45	1.39
22	B	810	CLA	CHD-C4C	2.80	1.45	1.39
22	3	321	CLA	C3B-C4B	2.80	1.49	1.42
22	3	318	CLA	C3D-C2D	2.80	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	319	CLA	MG-NB	-2.80	2.00	2.05
22	B	813	CLA	C3D-C2D	2.80	1.46	1.39
22	B	802	CLA	CHD-C4C	2.80	1.45	1.39
22	X	304	CLA	MG-NA	-2.80	1.99	2.06
22	2	317	CLA	C1D-C2D	2.80	1.50	1.45
22	4	313	CLA	C3D-C2D	2.80	1.46	1.39
22	A	830	CLA	C3D-C2D	2.80	1.46	1.39
22	1	306	CLA	C3B-C4B	2.80	1.49	1.42
22	G	207	CLA	C4B-NB	-2.79	1.34	1.37
22	Y	309	CLA	C4B-NB	-2.79	1.34	1.37
22	1	306	CLA	C3D-C2D	2.79	1.46	1.39
22	B	821	CLA	C3B-C4B	2.79	1.49	1.42
23	4	319	LUT	C32-C33	-2.79	1.39	1.45
25	A	816	BCR	C19-C18	-2.79	1.39	1.45
21	4	308	CHL	C1D-C2D	2.79	1.50	1.45
22	3	313	CLA	C4B-NB	-2.79	1.34	1.37
22	A	851	CLA	CHD-C1D	2.79	1.43	1.38
22	B	847	CLA	C3B-C4B	2.79	1.49	1.42
22	X	301	CLA	C4B-NB	-2.79	1.34	1.37
22	B	804	CLA	C4B-NB	-2.79	1.34	1.37
22	Y	312	CLA	C4B-NB	-2.79	1.34	1.37
21	2	301	CHL	C1D-C2D	2.79	1.50	1.45
23	3	301	LUT	C12-C13	-2.79	1.40	1.45
25	B	836	BCR	C8-C9	-2.79	1.40	1.45
22	3	319	CLA	C1D-C2D	2.79	1.50	1.45
22	A	803	CLA	MG-NA	-2.79	1.99	2.06
22	B	810	CLA	MG-NA	-2.79	1.99	2.06
22	1	319	CLA	C4B-NB	-2.79	1.34	1.37
22	B	815	CLA	C3D-C2D	2.79	1.46	1.39
22	A	810	CLA	C1B-NB	-2.79	1.34	1.37
22	A	835	CLA	C4B-NB	-2.79	1.34	1.37
22	Z	311	CLA	C4B-NB	-2.79	1.34	1.37
22	1	317	CLA	CHD-C4C	2.79	1.45	1.39
22	1	305	CLA	C4B-NB	-2.79	1.34	1.37
22	Y	308	CLA	C4B-NB	-2.78	1.34	1.37
22	A	859	CLA	C3B-C4B	2.78	1.49	1.42
22	B	813	CLA	C1B-NB	-2.78	1.34	1.37
22	A	803	CLA	C1B-NB	-2.78	1.34	1.37
22	F	305	CLA	C3D-C2D	2.78	1.46	1.39
22	1	307	CLA	C4B-NB	-2.78	1.34	1.37
22	2	320	CLA	C4B-NB	-2.78	1.34	1.37
22	2	318	CLA	MG-NA	-2.78	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	315	CLA	C3D-C2D	2.78	1.46	1.39
22	B	851	CLA	C4B-NB	-2.78	1.34	1.37
22	A	809	CLA	C1B-NB	-2.78	1.34	1.37
22	B	825	CLA	C1D-C2D	2.78	1.50	1.45
22	B	812	CLA	C4B-NB	-2.78	1.34	1.37
22	B	831	CLA	MG-NA	-2.78	1.99	2.06
22	A	838	CLA	C3D-C2D	2.78	1.46	1.39
22	1	321	CLA	C4B-NB	-2.78	1.34	1.37
22	Y	310	CLA	C4B-NB	-2.78	1.34	1.37
25	2	312	BCR	C21-C22	2.78	1.39	1.35
22	3	317	CLA	C3D-C2D	2.78	1.46	1.39
22	1	302	CLA	C1D-C2D	2.78	1.50	1.45
22	1	308	CLA	C1D-C2D	2.78	1.50	1.45
22	Z	307	CLA	C1D-C2D	2.78	1.50	1.45
22	1	309	CLA	C4B-NB	-2.78	1.34	1.37
22	3	309	CLA	MG-NA	-2.78	1.99	2.06
22	B	824	CLA	C4B-NB	-2.78	1.34	1.37
22	Y	312	CLA	C3B-C4B	2.77	1.49	1.42
22	X	311	CLA	C4B-NB	-2.77	1.34	1.37
21	3	307	CHL	C1D-C2D	2.77	1.50	1.45
22	A	808	CLA	MG-NA	-2.77	1.99	2.06
22	A	850	CLA	C1B-NB	-2.77	1.34	1.37
22	B	819	CLA	C4B-NB	-2.77	1.34	1.37
22	K	202	CLA	C4B-NB	-2.77	1.34	1.37
22	L	306	CLA	C4B-NB	-2.77	1.34	1.37
22	A	842	CLA	CHD-C1D	2.77	1.43	1.38
22	4	315	CLA	C4B-NB	-2.77	1.34	1.37
22	A	842	CLA	CHD-C4C	2.77	1.45	1.39
22	2	303	CLA	CHD-C4C	2.77	1.45	1.39
21	1	301	CHL	C1D-C2D	2.77	1.50	1.45
22	B	846	CLA	C1D-C2D	2.77	1.50	1.45
22	O	208	CLA	CHD-C1D	2.77	1.43	1.38
22	A	859	CLA	C3D-C2D	2.77	1.46	1.39
22	B	828	CLA	MG-NA	-2.77	1.99	2.06
22	A	854	CLA	CHD-C4C	2.77	1.45	1.39
22	K	203	CLA	C1D-C2D	2.77	1.50	1.45
22	A	803	CLA	C3B-C4B	2.77	1.49	1.42
25	A	819	BCR	C12-C13	-2.77	1.40	1.45
22	1	317	CLA	CHD-C1D	2.76	1.43	1.38
22	B	820	CLA	C4B-NB	-2.76	1.34	1.37
22	1	304	CLA	CHD-C1D	2.76	1.43	1.38
22	3	310	CLA	C1B-NB	-2.76	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	815	BCR	C19-C18	-2.76	1.40	1.45
22	K	202	CLA	C1D-C2D	2.76	1.50	1.45
22	4	311	CLA	C1D-C2D	2.76	1.50	1.45
22	B	845	CLA	C3D-C2D	2.76	1.46	1.39
21	2	321	CHL	C3D-C2D	2.76	1.46	1.39
22	Z	310	CLA	C1D-C2D	2.76	1.50	1.45
22	K	204	CLA	C3D-C2D	2.76	1.46	1.39
22	4	316	CLA	MG-NA	-2.76	1.99	2.06
25	B	838	BCR	C10-C9	2.76	1.39	1.35
22	1	304	CLA	C1B-NB	-2.76	1.34	1.37
22	X	312	CLA	C4B-NB	-2.76	1.34	1.37
25	L	302	BCR	C23-C22	-2.76	1.40	1.45
22	1	302	CLA	C3B-C4B	2.76	1.49	1.42
22	B	815	CLA	C1B-NB	-2.76	1.34	1.37
22	A	859	CLA	MG-NA	-2.76	1.99	2.06
22	L	307	CLA	C3D-C2D	2.76	1.46	1.39
22	1	319	CLA	C1D-C2D	2.76	1.50	1.45
22	4	316	CLA	C4B-NB	-2.76	1.34	1.37
22	3	310	CLA	C3D-C2D	2.76	1.46	1.39
22	A	840	CLA	MG-NA	-2.76	1.99	2.06
22	B	851	CLA	MG-NA	-2.76	1.99	2.06
22	O	206	CLA	C3B-C4B	2.76	1.49	1.42
22	A	850	CLA	C3D-C2D	2.76	1.46	1.39
22	G	207	CLA	C1D-C2D	2.76	1.50	1.45
22	A	846	CLA	OBD-CAD	2.76	1.27	1.22
22	A	832	CLA	C1D-C2D	2.76	1.50	1.45
22	X	313	CLA	C3B-C4B	2.76	1.49	1.42
22	Z	310	CLA	C3B-C4B	2.76	1.49	1.42
22	B	810	CLA	C4B-NB	-2.76	1.34	1.37
22	A	810	CLA	MG-NA	-2.75	1.99	2.06
22	1	305	CLA	C3B-C4B	2.75	1.49	1.42
22	1	307	CLA	C3B-C4B	2.75	1.49	1.42
22	4	305	CLA	MG-NA	-2.75	1.99	2.06
22	A	847	CLA	C1B-NB	-2.75	1.34	1.37
22	X	313	CLA	C4B-NB	-2.75	1.34	1.37
22	3	316	CLA	C3B-C4B	2.75	1.49	1.42
22	B	848	CLA	MG-NA	-2.75	1.99	2.06
22	B	828	CLA	C3D-C2D	2.75	1.46	1.39
22	A	859	CLA	CHD-C1D	2.75	1.43	1.38
22	G	206	CLA	C3D-C2D	2.75	1.46	1.39
21	Y	313	CHL	C1D-C2D	2.75	1.50	1.45
22	X	303	CLA	C1D-C2D	2.75	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	810	CLA	CHD-C1D	2.75	1.43	1.38
22	1	303	CLA	C3B-C4B	2.75	1.49	1.42
22	B	824	CLA	C3D-C2D	2.75	1.46	1.39
22	3	316	CLA	CHD-C4C	2.75	1.45	1.39
22	2	319	CLA	C4D-ND	2.75	1.41	1.37
22	A	835	CLA	CHC-C4B	2.75	1.45	1.39
22	A	842	CLA	C4B-NB	-2.75	1.34	1.37
22	Y	314	CLA	C1D-C2D	2.75	1.50	1.45
22	A	847	CLA	MG-NA	-2.75	1.99	2.06
21	Y	307	CHL	C1D-C2D	2.75	1.50	1.45
22	B	820	CLA	CHD-C1D	2.75	1.43	1.38
22	3	316	CLA	MG-NA	-2.75	1.99	2.06
22	O	208	CLA	C3D-C2D	2.75	1.46	1.39
22	B	821	CLA	C4B-NB	-2.75	1.34	1.37
22	A	826	CLA	CHD-C4C	2.75	1.45	1.39
22	A	845	CLA	C3D-C2D	2.75	1.46	1.39
22	L	307	CLA	C4B-NB	-2.75	1.34	1.37
22	Z	313	CLA	C3B-C4B	2.75	1.49	1.42
22	X	312	CLA	C1D-C2D	2.74	1.50	1.45
30	A	825	CL0	CHB-C4A	-2.74	1.31	1.37
22	B	801	CLA	C4B-NB	-2.74	1.34	1.37
22	3	311	CLA	C3D-C2D	2.74	1.46	1.39
22	Y	310	CLA	C1D-C2D	2.74	1.50	1.45
22	H	201	CLA	C1D-C2D	2.74	1.50	1.45
22	N	202	CLA	C4B-NB	-2.74	1.34	1.37
22	A	835	CLA	C3D-C2D	2.74	1.46	1.39
22	1	318	CLA	C1B-NB	-2.74	1.34	1.37
22	Z	307	CLA	C4B-NB	-2.74	1.34	1.37
22	L	305	CLA	C1D-C2D	2.74	1.50	1.45
22	B	849	CLA	MG-NA	-2.74	1.99	2.06
22	Z	307	CLA	C3B-C4B	2.74	1.49	1.42
22	A	829	CLA	C4B-NB	-2.74	1.34	1.37
22	4	312	CLA	C3B-C4B	2.74	1.49	1.42
21	Z	304	CHL	C3D-C2D	2.74	1.46	1.39
25	G	202	BCR	C23-C22	-2.74	1.40	1.45
22	A	810	CLA	C4B-NB	-2.74	1.34	1.37
22	B	811	CLA	MG-NA	-2.74	1.99	2.06
22	B	822	CLA	C1D-C2D	2.74	1.50	1.45
22	Z	308	CLA	C3B-C4B	2.74	1.49	1.42
22	B	827	CLA	C1B-NB	-2.74	1.34	1.37
22	A	828	CLA	C3D-C2D	2.73	1.46	1.39
21	Z	302	CHL	C3D-C2D	2.73	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	312	CLA	CHD-C4C	2.73	1.45	1.39
22	4	306	CLA	C4B-NB	-2.73	1.34	1.37
22	A	833	CLA	C1D-C2D	2.73	1.50	1.45
22	A	829	CLA	C1B-NB	-2.73	1.34	1.37
22	A	846	CLA	C4B-NB	-2.73	1.34	1.37
22	A	841	CLA	C1D-C2D	2.73	1.50	1.45
25	F	302	BCR	C19-C18	-2.73	1.40	1.45
22	3	319	CLA	C3B-C4B	2.73	1.49	1.42
22	A	827	CLA	CHD-C4C	2.73	1.45	1.39
25	O	203	BCR	C23-C22	-2.73	1.40	1.45
22	B	847	CLA	C3D-C2D	2.73	1.46	1.39
22	4	306	CLA	MG-NA	-2.73	1.99	2.06
22	A	836	CLA	C1B-NB	-2.73	1.34	1.37
22	A	837	CLA	C3D-C2D	2.73	1.46	1.39
22	3	311	CLA	CHD-C1D	2.73	1.43	1.38
22	X	311	CLA	C3B-C4B	2.73	1.49	1.42
22	1	303	CLA	C4B-NB	-2.73	1.34	1.37
22	3	312	CLA	MG-NA	-2.73	1.99	2.06
22	Y	308	CLA	C1D-C2D	2.73	1.50	1.45
23	4	319	LUT	C28-C29	-2.72	1.40	1.45
22	3	310	CLA	C3B-C4B	2.72	1.49	1.42
22	A	845	CLA	C1D-C2D	2.72	1.50	1.45
22	X	303	CLA	C3B-C4B	2.72	1.49	1.42
22	A	843	CLA	CHD-C1D	2.72	1.43	1.38
22	A	807	CLA	C4B-NB	-2.72	1.34	1.37
22	B	817	CLA	MG-NA	-2.72	1.99	2.06
25	3	303	BCR	C12-C13	-2.72	1.40	1.45
22	4	318	CLA	C3B-C4B	2.72	1.49	1.42
22	2	319	CLA	C1B-NB	-2.72	1.34	1.37
22	1	308	CLA	C3B-C4B	2.72	1.49	1.42
22	3	309	CLA	C1D-C2D	2.72	1.50	1.45
22	Z	308	CLA	C4B-NB	-2.72	1.34	1.37
22	B	828	CLA	C3B-C4B	2.72	1.49	1.42
22	A	804	CLA	C4B-NB	-2.72	1.34	1.37
22	X	303	CLA	C4B-NB	-2.72	1.34	1.37
22	4	313	CLA	C3B-C4B	2.72	1.49	1.42
21	4	308	CHL	C3D-C2D	2.72	1.46	1.39
25	J	101	BCR	C12-C13	-2.72	1.40	1.45
22	B	833	CLA	C1D-C2D	2.72	1.50	1.45
22	O	210	CLA	MG-NA	-2.71	1.99	2.06
22	2	318	CLA	C1D-C2D	2.71	1.50	1.45
22	B	815	CLA	MG-NA	-2.71	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	318	CLA	C4B-NB	-2.71	1.34	1.37
22	3	312	CLA	C3D-C2D	2.71	1.46	1.39
22	A	843	CLA	C3D-C2D	2.71	1.46	1.39
22	K	204	CLA	MG-NA	-2.71	1.99	2.06
22	3	308	CLA	CHD-C1D	2.71	1.43	1.38
22	A	805	CLA	C3B-C4B	2.71	1.49	1.42
22	Z	306	CLA	C4B-NB	-2.71	1.34	1.37
22	X	312	CLA	C3B-C4B	2.71	1.49	1.42
22	Y	309	CLA	C3B-C4B	2.71	1.49	1.42
21	4	309	CHL	C3D-C2D	2.71	1.46	1.39
22	B	811	CLA	C3D-C2D	2.71	1.46	1.39
22	B	812	CLA	C1D-C2D	2.71	1.50	1.45
22	G	205	CLA	MG-NA	-2.71	1.99	2.06
22	4	316	CLA	C3D-C2D	2.71	1.46	1.39
22	Y	301	CLA	C4B-NB	-2.71	1.34	1.37
22	B	813	CLA	C3B-C4B	2.71	1.49	1.42
22	Z	311	CLA	C3B-C4B	2.71	1.49	1.42
22	B	816	CLA	C4D-ND	2.71	1.41	1.37
25	L	304	BCR	C8-C9	-2.71	1.40	1.45
22	2	306	CLA	C3D-C2D	2.71	1.46	1.39
25	A	817	BCR	C10-C9	2.71	1.39	1.35
22	A	846	CLA	MG-NA	-2.71	1.99	2.06
22	A	845	CLA	CHC-C4B	2.71	1.45	1.39
22	B	852	CLA	C1D-C2D	2.70	1.50	1.45
22	B	827	CLA	CHC-C4B	2.70	1.45	1.39
22	K	203	CLA	MG-NA	-2.70	1.99	2.06
22	A	804	CLA	C1B-NB	-2.70	1.34	1.37
22	A	831	CLA	C1B-NB	-2.70	1.34	1.37
22	B	823	CLA	C3B-C4B	2.70	1.49	1.42
22	B	803	CLA	C3D-C2D	2.70	1.46	1.39
22	4	306	CLA	C1D-C2D	2.70	1.50	1.45
22	1	303	CLA	MG-NA	-2.70	1.99	2.06
22	Y	301	CLA	C3B-C4B	2.70	1.49	1.42
22	1	306	CLA	MG-NA	-2.70	1.99	2.06
22	B	845	CLA	MG-NA	-2.70	1.99	2.06
22	A	830	CLA	CHD-C1D	2.70	1.43	1.38
22	B	849	CLA	C3B-C4B	2.70	1.49	1.42
22	A	851	CLA	C3B-C4B	2.70	1.49	1.42
22	J	102	CLA	C4B-NB	-2.70	1.34	1.37
22	A	832	CLA	MG-NA	-2.70	1.99	2.06
22	4	315	CLA	C3B-C4B	2.70	1.49	1.42
22	O	210	CLA	C3B-C4B	2.70	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	317	CLA	MG-NA	-2.69	1.99	2.06
22	A	838	CLA	CHD-C4C	2.69	1.45	1.39
22	2	305	CLA	C3B-C4B	2.69	1.49	1.42
22	A	805	CLA	C3D-C2D	2.69	1.46	1.39
22	A	805	CLA	CHD-C1D	2.69	1.43	1.38
22	B	828	CLA	C4B-NB	-2.69	1.34	1.37
22	3	313	CLA	C1D-C2D	2.69	1.50	1.45
22	A	837	CLA	C1D-C2D	2.69	1.50	1.45
22	Y	302	CLA	C3B-C4B	2.69	1.49	1.42
22	B	810	CLA	C3D-C2D	2.69	1.46	1.39
22	A	856	CLA	MG-NA	-2.69	1.99	2.06
22	A	839	CLA	C1D-C2D	2.69	1.50	1.45
22	4	311	CLA	C3B-C4B	2.69	1.49	1.42
22	B	815	CLA	C3B-C4B	2.69	1.49	1.42
22	B	829	CLA	C3D-C2D	2.69	1.46	1.39
22	G	206	CLA	MG-NA	-2.69	1.99	2.06
22	Z	309	CLA	MG-NA	-2.69	1.99	2.06
22	B	802	CLA	C4B-NB	-2.69	1.34	1.37
22	B	847	CLA	C4B-NB	-2.69	1.34	1.37
22	G	206	CLA	C4B-NB	-2.69	1.34	1.37
22	O	207	CLA	MG-NA	-2.69	1.99	2.06
22	B	825	CLA	MG-NA	-2.69	1.99	2.06
22	2	322	CLA	C3B-C4B	2.69	1.49	1.42
22	B	848	CLA	CHD-C4C	2.69	1.45	1.39
21	Y	305	CHL	C3B-C4B	2.69	1.49	1.42
22	3	321	CLA	C3D-C2D	2.69	1.46	1.39
22	X	301	CLA	C3B-C4B	2.68	1.49	1.42
22	B	829	CLA	MG-NA	-2.68	1.99	2.06
21	Z	304	CHL	C1D-C2D	2.68	1.50	1.45
22	3	320	CLA	C1B-NB	-2.68	1.34	1.37
22	B	821	CLA	C1D-C2D	2.68	1.50	1.45
22	A	842	CLA	MG-NA	-2.68	1.99	2.06
22	B	824	CLA	MG-NA	-2.68	1.99	2.06
22	A	837	CLA	C4B-NB	-2.68	1.34	1.37
30	A	825	CL0	CHD-C4C	2.68	1.45	1.39
22	1	318	CLA	C3B-C4B	2.68	1.49	1.42
22	1	309	CLA	C1D-C2D	2.68	1.50	1.45
22	O	208	CLA	C4B-NB	-2.68	1.34	1.37
22	F	306	CLA	C3B-C4B	2.68	1.49	1.42
22	3	313	CLA	MG-NA	-2.68	1.99	2.06
23	3	301	LUT	C28-C29	-2.68	1.40	1.45
22	3	320	CLA	C4B-NB	-2.68	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	828	CLA	C1B-NB	-2.68	1.34	1.37
22	A	849	CLA	MG-NA	-2.68	1.99	2.06
22	A	810	CLA	C3B-C4B	2.68	1.49	1.42
22	Z	310	CLA	C4B-NB	-2.68	1.34	1.37
25	B	844	BCR	C12-C13	-2.68	1.40	1.45
21	Z	302	CHL	C1D-C2D	2.68	1.50	1.45
22	X	310	CLA	C1D-C2D	2.67	1.50	1.45
22	2	303	CLA	C4B-NB	-2.67	1.34	1.37
22	G	205	CLA	C4B-NB	-2.67	1.34	1.37
22	B	846	CLA	MG-NA	-2.67	1.99	2.06
22	K	204	CLA	C1B-C2B	2.67	1.49	1.43
21	X	306	CHL	C3B-C4B	2.67	1.49	1.42
22	2	308	CLA	C4B-NB	-2.67	1.34	1.37
22	B	833	CLA	MG-NA	-2.67	1.99	2.06
22	B	848	CLA	C3D-C2D	2.67	1.46	1.39
22	4	304	CLA	MG-NA	-2.67	1.99	2.06
22	A	804	CLA	MG-NA	-2.67	1.99	2.06
22	J	102	CLA	C1D-C2D	2.67	1.50	1.45
22	B	809	CLA	MG-NA	-2.67	1.99	2.06
22	2	318	CLA	C1B-NB	-2.67	1.34	1.37
22	L	306	CLA	MG-NA	-2.67	1.99	2.06
22	B	814	CLA	C4B-NB	-2.67	1.34	1.37
22	4	314	CLA	C1B-C2B	2.67	1.49	1.43
22	B	808	CLA	MG-NA	-2.67	1.99	2.06
22	2	307	CLA	MG-NA	-2.67	1.99	2.06
22	B	811	CLA	CHD-C1D	2.67	1.43	1.38
22	4	316	CLA	C1B-NB	-2.67	1.34	1.37
22	A	810	CLA	CHD-C4C	2.66	1.45	1.39
22	A	853	CLA	MG-NA	-2.66	1.99	2.06
22	1	309	CLA	C3B-C4B	2.66	1.49	1.42
22	N	202	CLA	C1D-C2D	2.66	1.50	1.45
22	O	206	CLA	C4B-NB	-2.66	1.34	1.37
25	A	818	BCR	C12-C13	-2.66	1.40	1.45
22	3	319	CLA	C4B-NB	-2.66	1.34	1.37
22	B	814	CLA	CHD-C4C	2.66	1.45	1.39
22	B	830	CLA	C1B-NB	-2.66	1.34	1.37
22	O	208	CLA	C1B-NB	-2.66	1.34	1.37
22	Z	309	CLA	C3B-C4B	2.66	1.49	1.42
22	H	201	CLA	C1B-C2B	2.66	1.49	1.43
22	Y	308	CLA	C3B-C4B	2.66	1.49	1.42
22	F	305	CLA	C3B-C4B	2.66	1.49	1.42
23	1	310	LUT	C12-C13	-2.66	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	314	CLA	MG-NA	-2.66	2.00	2.06
21	Z	301	CHL	C3B-C4B	2.66	1.49	1.42
21	2	302	CHL	C3D-C2D	2.66	1.46	1.39
22	3	311	CLA	MG-NA	-2.66	2.00	2.06
22	4	305	CLA	C3D-C2D	2.66	1.46	1.39
22	B	805	CLA	C1D-C2D	2.65	1.50	1.45
25	B	834	BCR	C19-C18	-2.65	1.40	1.45
22	A	857	CLA	C1D-C2D	2.65	1.50	1.45
22	X	310	CLA	C3B-C4B	2.65	1.49	1.42
22	1	321	CLA	C1D-C2D	2.65	1.50	1.45
22	4	318	CLA	MG-NA	-2.65	2.00	2.06
22	B	852	CLA	MG-NA	-2.65	2.00	2.06
25	4	321	BCR	C12-C13	-2.65	1.40	1.45
21	3	314	CHL	C3D-C2D	2.65	1.46	1.39
21	Z	303	CHL	C3B-C4B	2.65	1.49	1.42
22	A	831	CLA	C1B-C2B	2.65	1.49	1.43
22	A	812	CLA	MG-NA	-2.65	2.00	2.06
22	B	819	CLA	C1B-NB	-2.65	1.34	1.37
22	B	830	CLA	C4B-NB	-2.65	1.34	1.37
22	A	850	CLA	CHD-C4C	2.65	1.45	1.39
25	A	817	BCR	C19-C18	-2.65	1.40	1.45
22	B	830	CLA	C1D-C2D	2.65	1.50	1.45
21	X	308	CHL	C3B-C4B	2.65	1.49	1.42
22	Z	313	CLA	C4B-NB	-2.65	1.34	1.37
22	A	812	CLA	C1D-C2D	2.65	1.50	1.45
22	B	815	CLA	CHD-C1D	2.65	1.43	1.38
22	3	318	CLA	C4B-NB	-2.65	1.34	1.37
25	L	301	BCR	C12-C13	-2.64	1.40	1.45
22	B	806	CLA	C1D-C2D	2.64	1.50	1.45
22	Z	306	CLA	C3B-C4B	2.64	1.49	1.42
22	2	303	CLA	C1B-NB	-2.64	1.34	1.37
22	B	806	CLA	C3B-C4B	2.64	1.49	1.42
21	X	305	CHL	C3B-C4B	2.64	1.49	1.42
22	B	802	CLA	MG-NA	-2.64	2.00	2.06
21	Y	313	CHL	C3B-C4B	2.64	1.48	1.42
22	B	802	CLA	C4C-C3C	2.64	1.49	1.45
22	A	859	CLA	C1B-NB	-2.64	1.34	1.37
22	O	208	CLA	MG-NA	-2.64	2.00	2.06
21	Y	303	CHL	C3B-C4B	2.64	1.48	1.42
21	2	302	CHL	C1D-C2D	2.64	1.50	1.45
22	A	830	CLA	C1B-C2B	2.64	1.49	1.43
22	2	317	CLA	C1B-NB	-2.64	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	312	CLA	C1B-NB	-2.64	1.34	1.37
22	B	812	CLA	CHC-C4B	2.64	1.45	1.39
22	A	848	CLA	C3D-C2D	2.64	1.46	1.39
21	3	307	CHL	C3D-C2D	2.64	1.46	1.39
22	A	834	CLA	C3D-C2D	2.64	1.46	1.39
22	A	802	CLA	C1D-C2D	2.64	1.50	1.45
22	3	318	CLA	C3B-C4B	2.64	1.48	1.42
22	A	803	CLA	CHD-C1D	2.64	1.43	1.38
25	O	202	BCR	C19-C18	-2.64	1.40	1.45
22	4	310	CLA	CHD-C4C	2.64	1.45	1.39
22	2	308	CLA	MG-NA	-2.64	2.00	2.06
22	2	304	CLA	C1B-NB	-2.63	1.34	1.37
25	L	304	BCR	C19-C18	-2.63	1.40	1.45
21	Y	304	CHL	C3B-C4B	2.63	1.48	1.42
22	A	828	CLA	CHD-C4C	2.63	1.45	1.39
22	L	306	CLA	CHD-C1D	2.63	1.43	1.38
22	A	858	CLA	CHC-C4B	2.63	1.45	1.39
30	A	825	CL0	C3B-C4B	2.63	1.48	1.42
22	B	802	CLA	C1C-C2C	2.63	1.49	1.44
22	A	831	CLA	CHD-C4C	2.63	1.45	1.39
22	A	805	CLA	C1B-NB	-2.63	1.34	1.37
22	B	833	CLA	C3B-C4B	2.63	1.48	1.42
22	O	207	CLA	C3B-C4B	2.63	1.48	1.42
22	F	305	CLA	MG-NA	-2.63	2.00	2.06
21	2	301	CHL	C3B-C4B	2.63	1.48	1.42
22	A	801	CLA	MG-NA	-2.63	2.00	2.06
22	A	809	CLA	MG-NA	-2.63	2.00	2.06
22	3	312	CLA	C3B-C4B	2.63	1.48	1.42
22	A	841	CLA	C4B-NB	-2.63	1.34	1.37
22	3	318	CLA	C1B-C2B	2.63	1.49	1.43
25	L	301	BCR	C19-C18	-2.63	1.40	1.45
21	Z	304	CHL	C3B-C4B	2.63	1.48	1.42
22	4	313	CLA	MG-NA	-2.63	2.00	2.06
22	4	313	CLA	C1B-NB	-2.62	1.34	1.37
22	Y	311	CLA	C3B-C4B	2.62	1.48	1.42
22	A	837	CLA	C1B-NB	-2.62	1.34	1.37
22	A	841	CLA	MG-NA	-2.62	2.00	2.06
22	B	831	CLA	C1B-NB	-2.62	1.34	1.37
22	A	840	CLA	C3B-C4B	2.62	1.48	1.42
22	4	311	CLA	C4B-NB	-2.62	1.34	1.37
22	Y	311	CLA	MG-NA	-2.62	2.00	2.06
22	2	307	CLA	C1B-C2B	2.62	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	817	CLA	CHD-C4C	2.62	1.45	1.39
22	A	836	CLA	MG-NA	-2.62	2.00	2.06
25	B	839	BCR	C12-C13	-2.62	1.40	1.45
22	A	834	CLA	C1B-NB	-2.62	1.34	1.37
22	B	814	CLA	MG-NA	-2.62	2.00	2.06
22	A	828	CLA	C1B-C2B	2.62	1.49	1.43
22	Z	306	CLA	C1B-C2B	2.62	1.49	1.43
22	A	808	CLA	C3B-C4B	2.62	1.48	1.42
22	B	845	CLA	CHD-C4C	2.62	1.45	1.39
22	B	814	CLA	C1C-C2C	2.61	1.49	1.44
22	A	812	CLA	C4B-NB	-2.61	1.34	1.37
22	1	319	CLA	MG-NA	-2.61	2.00	2.06
22	X	312	CLA	C1B-C2B	2.61	1.49	1.43
22	B	803	CLA	C3B-C4B	2.61	1.48	1.42
22	O	207	CLA	C1B-C2B	2.61	1.49	1.43
22	3	315	CLA	MG-NA	-2.61	2.00	2.06
22	A	836	CLA	C4B-NB	-2.61	1.34	1.37
22	L	305	CLA	MG-NA	-2.61	2.00	2.06
22	Y	310	CLA	MG-NA	-2.61	2.00	2.06
21	Y	307	CHL	C3B-C4B	2.61	1.48	1.42
22	4	311	CLA	MG-NA	-2.61	2.00	2.06
22	A	836	CLA	C1D-C2D	2.61	1.50	1.45
22	B	845	CLA	CHD-C1D	2.61	1.43	1.38
22	2	319	CLA	C3D-C2D	2.61	1.46	1.39
22	A	804	CLA	C1D-C2D	2.61	1.50	1.45
22	Y	314	CLA	C4B-NB	-2.61	1.34	1.37
22	Y	302	CLA	MG-NA	-2.61	2.00	2.06
21	X	302	CHL	C3B-C4B	2.61	1.48	1.42
22	A	844	CLA	C1D-C2D	2.61	1.50	1.45
22	3	308	CLA	C3B-C4B	2.61	1.48	1.42
22	3	309	CLA	C3B-C4B	2.61	1.48	1.42
22	1	308	CLA	C4B-NB	-2.60	1.34	1.37
22	A	807	CLA	C3D-C2D	2.60	1.46	1.39
22	4	306	CLA	C3B-C4B	2.60	1.48	1.42
22	B	819	CLA	C3D-C2D	2.60	1.46	1.39
21	Y	306	CHL	C3B-C4B	2.60	1.48	1.42
22	F	306	CLA	CHD-C1D	2.60	1.43	1.38
22	A	849	CLA	C1B-C2B	2.60	1.49	1.43
22	3	316	CLA	C1C-C2C	2.60	1.49	1.44
22	L	307	CLA	C3B-C4B	2.60	1.48	1.42
22	A	806	CLA	MG-NA	-2.60	2.00	2.06
22	4	305	CLA	CHD-C1D	2.60	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	305	CLA	C1B-NB	-2.60	1.34	1.37
22	Y	314	CLA	MG-NA	-2.60	2.00	2.06
22	3	311	CLA	C3B-C4B	2.60	1.48	1.42
22	3	308	CLA	C1D-C2D	2.60	1.50	1.45
22	B	853	CLA	MG-NA	-2.60	2.00	2.06
22	H	201	CLA	MG-NA	-2.59	2.00	2.06
23	3	301	LUT	C32-C33	-2.59	1.40	1.45
22	4	311	CLA	C1B-NB	-2.59	1.34	1.37
22	Y	310	CLA	C1B-C2B	2.59	1.49	1.43
22	1	302	CLA	MG-NA	-2.59	2.00	2.06
22	B	830	CLA	CHC-C4B	2.59	1.45	1.39
22	A	843	CLA	OBD-CAD	2.59	1.26	1.22
22	B	806	CLA	C1B-C2B	2.59	1.49	1.43
22	A	831	CLA	C3D-C2D	2.59	1.46	1.39
22	1	318	CLA	C1D-C2D	2.59	1.50	1.45
22	1	320	CLA	C1B-C2B	2.59	1.49	1.43
22	Z	313	CLA	MG-NA	-2.59	2.00	2.06
22	B	820	CLA	MG-NA	-2.59	2.00	2.06
22	A	812	CLA	C1B-NB	-2.59	1.34	1.37
22	L	307	CLA	MG-NA	-2.59	2.00	2.06
22	1	320	CLA	C3B-C4B	2.59	1.48	1.42
22	B	810	CLA	C3B-C4B	2.59	1.48	1.42
22	2	305	CLA	C1B-NB	-2.59	1.34	1.37
25	2	312	BCR	C14-C13	2.59	1.39	1.35
22	A	851	CLA	C1B-NB	-2.59	1.34	1.37
22	A	858	CLA	CHD-C1D	2.59	1.43	1.38
22	L	307	CLA	C1D-C2D	2.58	1.50	1.45
22	B	811	CLA	C3B-C4B	2.58	1.48	1.42
22	1	320	CLA	C3D-C2D	2.58	1.46	1.39
22	A	858	CLA	C4C-C3C	2.58	1.49	1.45
22	3	315	CLA	C1B-NB	-2.58	1.34	1.37
22	B	808	CLA	C4B-NB	-2.58	1.34	1.37
22	A	830	CLA	CHD-C4C	2.58	1.45	1.39
21	4	309	CHL	C1D-C2D	2.58	1.50	1.45
22	K	204	CLA	C3B-C4B	2.58	1.48	1.42
21	3	314	CHL	C1D-C2D	2.58	1.50	1.45
22	G	207	CLA	C1B-NB	-2.58	1.34	1.37
22	4	312	CLA	MG-NA	-2.58	2.00	2.06
22	2	304	CLA	C3B-C4B	2.58	1.48	1.42
25	B	838	BCR	C21-C22	2.58	1.39	1.35
22	Z	310	CLA	C1B-C2B	2.58	1.49	1.43
22	G	205	CLA	C1D-C2D	2.58	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	801	CLA	C1D-C2D	2.58	1.50	1.45
22	2	303	CLA	MG-NA	-2.58	2.00	2.06
22	X	311	CLA	C1B-C2B	2.58	1.49	1.43
22	X	303	CLA	MG-NA	-2.58	2.00	2.06
22	4	304	CLA	C1D-C2D	2.58	1.50	1.45
22	Z	311	CLA	MG-NA	-2.58	2.00	2.06
22	3	317	CLA	C1B-NB	-2.58	1.34	1.37
22	4	310	CLA	C1B-NB	-2.58	1.34	1.37
22	A	847	CLA	C4B-NB	-2.58	1.34	1.37
22	B	812	CLA	C1B-NB	-2.58	1.34	1.37
22	4	310	CLA	MG-NA	-2.58	2.00	2.06
22	2	320	CLA	MG-NA	-2.57	2.00	2.06
22	B	802	CLA	C1B-C2B	2.57	1.49	1.43
21	2	302	CHL	C4B-NB	-2.57	1.34	1.37
22	B	819	CLA	C1D-C2D	2.57	1.50	1.45
22	B	803	CLA	CHD-C4C	2.57	1.45	1.39
21	X	309	CHL	C3B-C4B	2.57	1.48	1.42
22	Z	314	CLA	MG-NA	-2.57	2.00	2.06
22	2	307	CLA	C1D-C2D	2.57	1.50	1.45
22	1	303	CLA	C1D-C2D	2.57	1.50	1.45
22	3	320	CLA	MG-NA	-2.57	2.00	2.06
22	A	805	CLA	MG-NA	-2.57	2.00	2.06
22	O	209	CLA	C4B-NB	-2.57	1.34	1.37
22	A	828	CLA	CHD-C1D	2.57	1.43	1.38
22	1	308	CLA	MG-NA	-2.57	2.00	2.06
25	J	103	BCR	C12-C13	-2.57	1.40	1.45
22	G	205	CLA	C1B-C2B	2.57	1.49	1.43
22	3	317	CLA	C1D-C2D	2.57	1.50	1.45
22	2	305	CLA	MG-NA	-2.57	2.00	2.06
22	A	829	CLA	C3B-C4B	2.57	1.48	1.42
22	X	301	CLA	MG-NA	-2.57	2.00	2.06
21	1	316	CHL	C1B-C2B	2.57	1.49	1.43
22	B	822	CLA	MG-NA	-2.57	2.00	2.06
21	2	301	CHL	C1B-C2B	2.57	1.49	1.43
22	O	209	CLA	MG-NA	-2.57	2.00	2.06
22	Y	309	CLA	C1B-C2B	2.57	1.49	1.43
22	B	846	CLA	C3B-C4B	2.56	1.48	1.42
22	1	305	CLA	MG-NA	-2.56	2.00	2.06
22	O	206	CLA	MG-NA	-2.56	2.00	2.06
22	X	301	CLA	C1D-C2D	2.56	1.50	1.45
22	B	813	CLA	MG-NA	-2.56	2.00	2.06
21	X	307	CHL	C3B-C4B	2.56	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	803	CLA	C1B-NB	-2.56	1.34	1.37
22	2	318	CLA	C3B-C4B	2.56	1.48	1.42
21	3	307	CHL	C3B-C4B	2.56	1.48	1.42
22	B	812	CLA	C1B-C2B	2.56	1.49	1.43
22	A	848	CLA	MG-NA	-2.56	2.00	2.06
22	Z	310	CLA	MG-NA	-2.56	2.00	2.06
22	B	847	CLA	C1D-C2D	2.56	1.50	1.45
22	A	853	CLA	C1D-C2D	2.56	1.50	1.45
22	A	856	CLA	C1B-NB	-2.56	1.34	1.37
22	2	308	CLA	C3D-C2D	2.56	1.46	1.39
22	X	313	CLA	MG-NA	-2.56	2.00	2.06
22	1	309	CLA	C1B-C2B	2.56	1.49	1.43
22	B	809	CLA	C1B-NB	-2.56	1.34	1.37
22	A	838	CLA	C1B-NB	-2.55	1.34	1.37
25	I	101	BCR	C19-C18	-2.55	1.40	1.45
22	B	802	CLA	C3D-C2D	2.55	1.46	1.39
22	3	310	CLA	MG-NA	-2.55	2.00	2.06
22	A	834	CLA	CHD-C1D	2.55	1.43	1.38
22	B	846	CLA	C1B-NB	-2.55	1.34	1.37
22	1	321	CLA	MG-NA	-2.55	2.00	2.06
21	Z	305	CHL	C1B-NB	-2.55	1.34	1.37
22	A	809	CLA	C3B-C4B	2.55	1.48	1.42
21	Z	305	CHL	C4C-C3C	2.55	1.49	1.45
21	2	309	CHL	C3B-C4B	2.55	1.48	1.42
22	G	206	CLA	C1B-C2B	2.55	1.49	1.43
22	1	321	CLA	C1B-NB	-2.55	1.34	1.37
22	A	807	CLA	C1B-C2B	2.55	1.49	1.43
22	B	821	CLA	C1B-NB	-2.55	1.34	1.37
22	Z	306	CLA	MG-NA	-2.55	2.00	2.06
22	B	849	CLA	C1D-C2D	2.55	1.50	1.45
22	B	828	CLA	C1B-C2B	2.54	1.49	1.43
22	2	322	CLA	C1D-C2D	2.54	1.50	1.45
22	A	830	CLA	C4D-ND	2.54	1.41	1.37
22	A	827	CLA	OBD-CAD	2.54	1.26	1.22
22	A	854	CLA	MG-NA	-2.54	2.00	2.06
22	A	843	CLA	C3B-C4B	2.54	1.48	1.42
22	A	843	CLA	MG-NA	-2.54	2.00	2.06
22	A	840	CLA	C1D-C2D	2.54	1.50	1.45
21	X	306	CHL	C1B-C2B	2.54	1.49	1.43
25	B	837	BCR	C19-C18	-2.54	1.40	1.45
22	A	847	CLA	C1D-C2D	2.54	1.50	1.45
22	B	811	CLA	C1D-C2D	2.54	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	F	302	BCR	C10-C9	2.54	1.39	1.35
22	2	317	CLA	C4B-NB	-2.54	1.34	1.37
22	Z	309	CLA	C1B-C2B	2.54	1.49	1.43
22	A	837	CLA	MG-NA	-2.54	2.00	2.06
22	K	202	CLA	MG-NA	-2.54	2.00	2.06
22	1	309	CLA	MG-NA	-2.54	2.00	2.06
22	A	806	CLA	C3B-C4B	2.54	1.48	1.42
22	A	857	CLA	MG-NA	-2.54	2.00	2.06
25	J	103	BCR	C19-C18	-2.54	1.40	1.45
22	4	304	CLA	C1B-NB	-2.54	1.34	1.37
22	B	833	CLA	C1B-C2B	2.54	1.49	1.43
22	2	307	CLA	C3B-C4B	2.54	1.48	1.42
22	B	803	CLA	CHD-C1D	2.54	1.43	1.38
22	X	311	CLA	MG-NA	-2.54	2.00	2.06
22	Z	307	CLA	C1B-C2B	2.54	1.49	1.43
22	X	301	CLA	C1B-C2B	2.54	1.49	1.43
22	3	311	CLA	C1B-C2B	2.53	1.49	1.43
22	A	855	CLA	C4B-NB	-2.53	1.34	1.37
22	4	313	CLA	C1D-C2D	2.53	1.50	1.45
22	A	838	CLA	CHD-C1D	2.53	1.43	1.38
22	B	853	CLA	C1B-NB	-2.53	1.34	1.37
22	B	828	CLA	C1D-C2D	2.53	1.50	1.45
22	1	317	CLA	C3B-C4B	2.53	1.48	1.42
22	B	811	CLA	C1B-C2B	2.53	1.49	1.43
22	Y	302	CLA	C1B-C2B	2.53	1.49	1.43
22	A	830	CLA	C3B-C4B	2.53	1.48	1.42
22	A	838	CLA	C1D-C2D	2.53	1.50	1.45
22	A	832	CLA	C3B-C4B	2.53	1.48	1.42
21	Y	304	CHL	C1B-C2B	2.53	1.49	1.43
22	B	806	CLA	MG-NA	-2.53	2.00	2.06
22	2	308	CLA	C1B-NB	-2.53	1.34	1.37
25	J	101	BCR	C19-C18	-2.53	1.40	1.45
22	B	848	CLA	CHD-C1D	2.53	1.43	1.38
22	N	202	CLA	C1B-C2B	2.53	1.49	1.43
22	Z	308	CLA	MG-NA	-2.53	2.00	2.06
22	O	207	CLA	C1D-C2D	2.53	1.50	1.45
22	3	319	CLA	C1B-C2B	2.53	1.49	1.43
22	F	306	CLA	MG-NA	-2.53	2.00	2.06
22	Y	312	CLA	C1B-C2B	2.53	1.49	1.43
22	Z	311	CLA	C1B-C2B	2.53	1.49	1.43
22	O	206	CLA	C1B-NB	-2.53	1.34	1.37
21	Y	303	CHL	C1B-C2B	2.53	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	317	CLA	MG-NA	-2.52	2.00	2.06
22	B	823	CLA	MG-NA	-2.52	2.00	2.06
22	A	801	CLA	C1B-C2B	2.52	1.49	1.43
22	A	829	CLA	MG-NA	-2.52	2.00	2.06
22	X	312	CLA	MG-NA	-2.52	2.00	2.06
21	Z	305	CHL	C3B-C4B	2.52	1.48	1.42
22	A	851	CLA	C1C-C2C	2.52	1.49	1.44
22	A	855	CLA	MG-NA	-2.52	2.00	2.06
22	A	855	CLA	C4C-C3C	2.52	1.49	1.45
22	X	310	CLA	C1B-C2B	2.52	1.49	1.43
22	O	210	CLA	C1D-C2D	2.52	1.50	1.45
22	J	102	CLA	MG-NA	-2.52	2.00	2.06
22	J	102	CLA	C1B-NB	-2.52	1.34	1.37
22	B	829	CLA	C1D-C2D	2.51	1.50	1.45
21	4	317	CHL	C1B-C2B	2.51	1.49	1.43
22	A	845	CLA	C1B-NB	-2.51	1.34	1.37
22	O	209	CLA	C1B-NB	-2.51	1.34	1.37
22	G	207	CLA	MG-NA	-2.51	2.00	2.06
22	Y	311	CLA	C1B-NB	-2.51	1.34	1.37
22	B	831	CLA	C3B-C4B	2.51	1.48	1.42
22	B	818	CLA	C4B-NB	-2.51	1.34	1.37
22	B	804	CLA	C1B-NB	-2.51	1.34	1.37
22	B	822	CLA	C1B-NB	-2.51	1.34	1.37
22	O	208	CLA	C1D-C2D	2.51	1.50	1.45
21	Z	301	CHL	C1B-C2B	2.51	1.49	1.43
22	A	852	CLA	C1B-C2B	2.51	1.49	1.43
22	K	202	CLA	C3B-C4B	2.51	1.48	1.42
22	A	850	CLA	CHD-C1D	2.51	1.43	1.38
22	3	319	CLA	MG-NA	-2.51	2.00	2.06
22	Y	309	CLA	MG-NA	-2.51	2.00	2.06
22	L	307	CLA	C1B-C2B	2.51	1.49	1.43
21	X	308	CHL	C1B-C2B	2.51	1.49	1.43
22	A	835	CLA	MG-NA	-2.51	2.00	2.06
22	X	313	CLA	C1B-C2B	2.51	1.49	1.43
22	Y	308	CLA	C1B-C2B	2.51	1.49	1.43
22	A	806	CLA	C1B-NB	-2.51	1.34	1.37
22	A	832	CLA	C1B-NB	-2.51	1.34	1.37
21	Y	307	CHL	C1B-C2B	2.51	1.49	1.43
22	3	321	CLA	C4B-NB	-2.50	1.34	1.37
22	3	321	CLA	C1D-C2D	2.50	1.50	1.45
25	O	202	BCR	C12-C13	-2.50	1.40	1.45
21	Y	307	CHL	C4C-C3C	2.50	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	811	CLA	C1B-NB	-2.50	1.34	1.37
22	1	306	CLA	C1B-NB	-2.50	1.34	1.37
21	X	302	CHL	C1B-C2B	2.50	1.49	1.43
22	Y	314	CLA	C1B-C2B	2.50	1.49	1.43
22	Z	308	CLA	C1B-C2B	2.50	1.49	1.43
22	1	306	CLA	C1D-C2D	2.50	1.50	1.45
25	B	839	BCR	C19-C18	-2.50	1.40	1.45
22	4	312	CLA	C1B-NB	-2.50	1.34	1.37
22	A	851	CLA	MG-NA	-2.50	2.00	2.06
22	Y	312	CLA	MG-NA	-2.50	2.00	2.06
22	B	804	CLA	C1D-C2D	2.50	1.50	1.45
25	O	202	BCR	C23-C22	-2.50	1.40	1.45
22	A	831	CLA	CHD-C1D	2.50	1.43	1.38
22	Z	307	CLA	MG-NA	-2.50	2.00	2.06
22	A	849	CLA	C1D-C2D	2.50	1.50	1.45
22	B	825	CLA	C4B-NB	-2.50	1.34	1.37
22	2	306	CLA	CHD-C4C	2.50	1.44	1.39
22	1	305	CLA	C1B-C2B	2.49	1.49	1.43
22	B	805	CLA	C1B-C2B	2.49	1.49	1.43
22	Z	314	CLA	C3B-C4B	2.49	1.48	1.42
22	K	205	CLA	MG-NA	-2.49	2.00	2.06
21	X	305	CHL	C1B-C2B	2.49	1.49	1.43
22	1	302	CLA	C1B-C2B	2.49	1.49	1.43
22	Y	311	CLA	C1B-C2B	2.49	1.49	1.43
22	A	801	CLA	C1B-NB	-2.49	1.34	1.37
22	Y	308	CLA	MG-NA	-2.49	2.00	2.06
22	1	320	CLA	C1B-NB	-2.49	1.34	1.37
22	B	852	CLA	C3B-C4B	2.49	1.48	1.42
22	B	849	CLA	C1B-C2B	2.49	1.49	1.43
22	A	845	CLA	C1B-C2B	2.49	1.49	1.43
22	A	840	CLA	C1B-NB	-2.49	1.34	1.37
22	3	321	CLA	C1B-NB	-2.49	1.34	1.37
22	F	305	CLA	C1B-NB	-2.49	1.34	1.37
22	A	842	CLA	C1B-C2B	2.49	1.49	1.43
22	K	202	CLA	C1B-NB	-2.49	1.34	1.37
22	N	202	CLA	MG-NA	-2.49	2.00	2.06
22	A	839	CLA	C1B-C2B	2.49	1.49	1.43
22	K	202	CLA	C1B-C2B	2.49	1.49	1.43
22	Y	314	CLA	C1B-NB	-2.49	1.34	1.37
22	A	856	CLA	C1D-C2D	2.49	1.50	1.45
21	4	317	CHL	C3B-C4B	2.48	1.48	1.42
22	4	316	CLA	C3B-C4B	2.48	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	803	CLA	C1D-C2D	2.48	1.50	1.45
22	B	817	CLA	CHD-C1D	2.48	1.43	1.38
22	A	808	CLA	C1B-NB	-2.48	1.34	1.37
22	O	208	CLA	C1B-C2B	2.48	1.49	1.43
22	O	210	CLA	C1B-C2B	2.48	1.49	1.43
22	A	859	CLA	C1D-C2D	2.48	1.50	1.45
22	1	307	CLA	C1B-C2B	2.48	1.49	1.43
22	4	315	CLA	MG-NA	-2.48	2.00	2.06
22	A	830	CLA	C1D-C2D	2.48	1.50	1.45
22	L	305	CLA	C3B-C4B	2.48	1.48	1.42
22	1	307	CLA	C1D-C2D	2.48	1.50	1.45
22	1	320	CLA	C1D-C2D	2.48	1.50	1.45
22	3	318	CLA	MG-NA	-2.48	2.00	2.06
22	3	313	CLA	C1B-NB	-2.48	1.34	1.37
21	Z	304	CHL	C1B-C2B	2.48	1.49	1.43
22	A	835	CLA	C3B-C4B	2.48	1.48	1.42
21	2	321	CHL	C1B-C2B	2.48	1.49	1.43
22	4	315	CLA	C1B-C2B	2.48	1.49	1.43
22	4	318	CLA	C1B-C2B	2.48	1.49	1.43
21	Y	306	CHL	C1B-C2B	2.47	1.49	1.43
22	B	822	CLA	C3B-C4B	2.47	1.48	1.42
22	4	312	CLA	C1C-C2C	2.47	1.49	1.44
22	A	807	CLA	C1B-NB	-2.47	1.34	1.37
22	2	319	CLA	CHD-C4C	2.47	1.44	1.39
21	Y	305	CHL	C1B-C2B	2.47	1.49	1.43
22	B	819	CLA	MG-NA	-2.47	2.00	2.06
25	G	202	BCR	C12-C13	-2.47	1.40	1.45
22	2	322	CLA	MG-NA	-2.47	2.00	2.06
22	A	851	CLA	C1D-C2D	2.47	1.50	1.45
21	Y	313	CHL	C1B-C2B	2.47	1.49	1.43
22	B	823	CLA	C1B-C2B	2.47	1.49	1.43
22	B	804	CLA	MG-NA	-2.47	2.00	2.06
23	4	322	LUT	C32-C33	-2.47	1.40	1.45
21	X	309	CHL	C4C-C3C	2.47	1.49	1.45
22	Y	301	CLA	C1B-C2B	2.47	1.49	1.43
22	3	316	CLA	C1D-C2D	2.47	1.50	1.45
21	Y	306	CHL	C4C-C3C	2.46	1.49	1.45
22	Y	301	CLA	C4C-C3C	2.46	1.49	1.45
22	4	305	CLA	C1B-NB	-2.46	1.34	1.37
23	4	322	LUT	C12-C13	-2.46	1.40	1.45
22	2	306	CLA	C1B-NB	-2.46	1.34	1.37
22	A	808	CLA	C1D-C2D	2.46	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	301	CHL	C3D-C2D	2.46	1.45	1.39
22	Y	301	CLA	C1B-NB	-2.46	1.34	1.37
22	4	304	CLA	C1B-C2B	2.46	1.49	1.43
22	1	320	CLA	MG-NA	-2.46	2.00	2.06
25	L	304	BCR	C12-C13	-2.46	1.40	1.45
22	A	809	CLA	C1D-C2D	2.46	1.50	1.45
22	B	822	CLA	C1B-C2B	2.46	1.49	1.43
22	2	319	CLA	C1D-C2D	2.46	1.50	1.45
22	B	812	CLA	MG-NA	-2.46	2.00	2.06
22	A	849	CLA	C3B-C4B	2.46	1.48	1.42
22	A	828	CLA	C1B-NB	-2.45	1.34	1.37
22	O	210	CLA	C1B-NB	-2.45	1.34	1.37
22	A	852	CLA	C3B-C4B	2.45	1.48	1.42
22	4	313	CLA	C1B-C2B	2.45	1.49	1.43
22	A	834	CLA	C1B-C2B	2.45	1.49	1.43
22	F	306	CLA	C1B-C2B	2.45	1.49	1.43
25	B	840	BCR	C10-C9	2.45	1.41	1.35
22	2	320	CLA	C1B-C2B	2.45	1.49	1.43
22	B	809	CLA	C1D-C2D	2.45	1.50	1.45
22	B	813	CLA	C1B-C2B	2.45	1.49	1.43
22	X	303	CLA	C1B-C2B	2.45	1.49	1.43
22	4	314	CLA	C3B-C4B	2.45	1.48	1.42
22	4	306	CLA	C1B-NB	-2.45	1.34	1.37
22	A	842	CLA	C1B-NB	-2.45	1.34	1.37
22	F	305	CLA	C1B-C2B	2.45	1.49	1.43
25	K	201	BCR	C19-C18	-2.45	1.40	1.45
22	L	306	CLA	C1B-C2B	2.45	1.49	1.43
22	B	849	CLA	C1B-NB	-2.45	1.34	1.37
22	4	305	CLA	C1D-C2D	2.45	1.50	1.45
22	B	823	CLA	C1B-NB	-2.44	1.34	1.37
22	2	320	CLA	C1B-NB	-2.44	1.34	1.37
22	A	802	CLA	C3B-C4B	2.44	1.48	1.42
21	X	309	CHL	C1B-C2B	2.44	1.49	1.43
22	Y	301	CLA	MG-NA	-2.44	2.00	2.06
22	A	839	CLA	MG-NA	-2.44	2.00	2.06
22	Z	313	CLA	C1B-C2B	2.44	1.49	1.43
22	1	306	CLA	C1B-C2B	2.44	1.49	1.43
22	A	827	CLA	CHB-C4A	-2.44	1.31	1.37
22	K	203	CLA	C1B-C2B	2.44	1.49	1.43
22	B	824	CLA	C1B-NB	-2.44	1.34	1.37
22	B	851	CLA	CHC-C4B	2.44	1.44	1.39
22	B	817	CLA	C1B-NB	-2.44	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	203	CLA	C3B-C4B	2.44	1.48	1.42
21	4	309	CHL	C1B-NB	-2.44	1.34	1.37
21	1	316	CHL	C4B-NB	-2.44	1.34	1.37
22	X	310	CLA	MG-NA	-2.44	2.00	2.06
25	B	834	BCR	C12-C13	-2.44	1.40	1.45
25	B	835	BCR	C12-C13	-2.44	1.40	1.45
23	1	310	LUT	C32-C33	-2.43	1.40	1.45
22	B	805	CLA	C3B-C4B	2.43	1.48	1.42
21	4	307	CHL	C1B-C2B	2.43	1.49	1.43
22	3	317	CLA	C1B-C2B	2.43	1.49	1.43
22	B	846	CLA	C1C-C2C	2.43	1.49	1.44
22	3	321	CLA	C1B-C2B	2.43	1.49	1.43
22	A	852	CLA	C3D-C2D	2.43	1.45	1.39
22	3	308	CLA	C1B-C2B	2.43	1.49	1.43
22	2	319	CLA	C1B-C2B	2.43	1.49	1.43
22	B	804	CLA	C1B-C2B	2.43	1.49	1.43
22	1	303	CLA	C1B-C2B	2.43	1.49	1.43
21	1	301	CHL	C3B-C4B	2.43	1.48	1.42
22	1	320	CLA	C4C-C3C	2.43	1.49	1.45
22	A	840	CLA	C1B-C2B	2.43	1.49	1.43
22	J	102	CLA	C1B-C2B	2.43	1.49	1.43
21	Y	304	CHL	C4C-C3C	2.43	1.49	1.45
22	3	319	CLA	C1B-NB	-2.42	1.34	1.37
22	B	818	CLA	MG-NA	-2.42	2.00	2.06
22	B	805	CLA	C1B-NB	-2.42	1.34	1.37
22	B	820	CLA	C3D-C2D	2.42	1.45	1.39
25	4	321	BCR	C19-C18	-2.42	1.40	1.45
22	1	319	CLA	C3B-C4B	2.42	1.48	1.42
21	Z	303	CHL	C1B-C2B	2.42	1.49	1.43
22	Z	306	CLA	C1B-NB	-2.42	1.34	1.37
22	A	857	CLA	C3B-C4B	2.42	1.48	1.42
22	A	853	CLA	C1B-NB	-2.42	1.34	1.37
22	Z	313	CLA	C1B-NB	-2.42	1.34	1.37
22	O	209	CLA	C1B-C2B	2.42	1.48	1.43
22	G	205	CLA	C3B-C4B	2.42	1.48	1.42
21	4	317	CHL	C4C-C3C	2.42	1.49	1.45
22	3	309	CLA	C1B-C2B	2.42	1.48	1.43
25	B	840	BCR	C12-C13	-2.41	1.40	1.45
25	I	101	BCR	C12-C13	-2.41	1.40	1.45
22	Y	302	CLA	C1B-NB	-2.41	1.34	1.37
22	3	310	CLA	C1D-C2D	2.41	1.50	1.45
22	B	816	CLA	C3D-C2D	2.41	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	313	CLA	C1B-C2B	2.41	1.48	1.43
22	1	308	CLA	C1B-C2B	2.41	1.48	1.43
22	B	831	CLA	C1B-C2B	2.41	1.48	1.43
21	X	307	CHL	C1B-C2B	2.41	1.48	1.43
22	F	306	CLA	C1B-NB	-2.41	1.34	1.37
22	A	843	CLA	C1B-NB	-2.41	1.34	1.37
22	3	312	CLA	C1B-C2B	2.41	1.48	1.43
22	2	304	CLA	MG-NA	-2.41	2.00	2.06
22	1	304	CLA	C1C-C2C	2.41	1.49	1.44
22	1	319	CLA	C1B-NB	-2.41	1.34	1.37
22	G	206	CLA	C1B-NB	-2.41	1.34	1.37
22	B	804	CLA	C3B-C4B	2.41	1.48	1.42
22	A	807	CLA	C1D-C2D	2.41	1.50	1.45
22	4	315	CLA	C1B-NB	-2.41	1.34	1.37
23	1	310	LUT	C28-C29	-2.41	1.40	1.45
25	2	312	BCR	C17-C18	2.41	1.39	1.35
22	1	305	CLA	C1B-NB	-2.41	1.34	1.37
22	1	308	CLA	C1B-NB	-2.40	1.34	1.37
22	Z	314	CLA	C1B-NB	-2.40	1.34	1.37
21	Z	312	CHL	C1B-C2B	2.40	1.48	1.43
21	X	305	CHL	C4C-C3C	2.40	1.49	1.45
22	G	205	CLA	C1B-NB	-2.40	1.34	1.37
22	A	842	CLA	C3B-C4B	2.40	1.48	1.42
22	4	312	CLA	C1B-C2B	2.40	1.48	1.43
23	2	310	LUT	C28-C29	-2.40	1.40	1.45
22	A	832	CLA	C1B-C2B	2.40	1.48	1.43
22	B	823	CLA	C1D-C2D	2.40	1.50	1.45
22	B	814	CLA	C3D-C2D	2.40	1.45	1.39
22	B	812	CLA	C4C-C3C	2.40	1.49	1.45
22	X	303	CLA	C1B-NB	-2.40	1.34	1.37
22	B	830	CLA	C4C-C3C	2.40	1.49	1.45
22	A	826	CLA	CHD-C1D	2.40	1.43	1.38
22	A	837	CLA	C1B-C2B	2.40	1.48	1.43
22	B	847	CLA	C1B-NB	-2.40	1.34	1.37
22	B	824	CLA	C1B-C2B	2.39	1.48	1.43
22	L	307	CLA	C1B-NB	-2.39	1.34	1.37
22	K	204	CLA	C1D-C2D	2.39	1.50	1.45
22	A	848	CLA	C4B-NB	-2.39	1.34	1.37
22	Z	314	CLA	C1B-C2B	2.39	1.48	1.43
22	B	826	CLA	C1D-C2D	2.39	1.50	1.45
21	Y	305	CHL	C4C-C3C	2.39	1.49	1.45
22	X	304	CLA	C1B-C2B	2.39	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	X	301	CLA	C1B-NB	-2.38	1.34	1.37
22	Z	309	CLA	C1B-NB	-2.38	1.34	1.37
22	2	306	CLA	CHD-C1D	2.38	1.43	1.38
22	A	858	CLA	C3B-C4B	2.38	1.48	1.42
22	A	852	CLA	CHD-C4C	2.38	1.44	1.39
22	B	806	CLA	C1B-NB	-2.38	1.34	1.37
22	H	201	CLA	C1B-NB	-2.38	1.34	1.37
21	X	307	CHL	C4C-C3C	2.38	1.49	1.45
21	X	308	CHL	C4C-C3C	2.38	1.49	1.45
22	A	837	CLA	C4C-C3C	2.38	1.49	1.45
25	B	836	BCR	C19-C18	-2.38	1.40	1.45
22	3	308	CLA	C1B-NB	-2.38	1.34	1.37
22	2	307	CLA	C1B-NB	-2.38	1.34	1.37
21	1	301	CHL	C1B-C2B	2.37	1.48	1.43
22	1	302	CLA	C1B-NB	-2.37	1.34	1.37
25	G	202	BCR	C20-C19	2.37	1.40	1.34
22	4	316	CLA	C1B-C2B	2.37	1.48	1.43
25	1	312	BCR	C8-C9	-2.37	1.40	1.45
22	3	311	CLA	C1D-C2D	2.37	1.50	1.45
21	4	309	CHL	C3B-C4B	2.37	1.48	1.42
22	1	317	CLA	C1B-C2B	2.37	1.48	1.43
22	B	830	CLA	C3B-C4B	2.37	1.48	1.42
21	2	321	CHL	C3B-C4B	2.37	1.48	1.42
25	A	816	BCR	C11-C12	2.37	1.40	1.34
22	3	318	CLA	C1B-NB	-2.37	1.34	1.37
22	L	306	CLA	C1B-NB	-2.37	1.34	1.37
22	A	850	CLA	MG-NA	-2.37	2.00	2.06
22	B	807	CLA	C1C-C2C	2.37	1.49	1.44
22	2	322	CLA	C1B-C2B	2.36	1.48	1.43
22	X	313	CLA	C1B-NB	-2.36	1.34	1.37
22	A	844	CLA	CHC-C4B	2.36	1.44	1.39
25	K	201	BCR	C12-C13	-2.36	1.40	1.45
21	Z	302	CHL	C1B-C2B	2.36	1.48	1.43
22	X	310	CLA	C1B-NB	-2.36	1.34	1.37
22	B	848	CLA	C1D-C2D	2.36	1.50	1.45
22	O	207	CLA	C1B-NB	-2.36	1.34	1.37
22	B	815	CLA	C1D-C2D	2.36	1.50	1.45
21	3	314	CHL	C3B-C4B	2.36	1.48	1.42
22	N	202	CLA	C1B-NB	-2.36	1.34	1.37
21	3	314	CHL	C1B-NB	-2.36	1.34	1.37
22	B	852	CLA	C1B-C2B	2.36	1.48	1.43
25	L	302	BCR	C19-C18	-2.36	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	322	CLA	C1B-NB	-2.35	1.34	1.37
22	A	835	CLA	C1D-C2D	2.35	1.50	1.45
22	B	821	CLA	MG-NA	-2.35	2.00	2.06
21	X	302	CHL	C4C-C3C	2.35	1.49	1.45
22	Y	310	CLA	C1B-NB	-2.35	1.34	1.37
22	4	310	CLA	C3B-C4B	2.35	1.48	1.42
22	A	854	CLA	C3B-C4B	2.35	1.48	1.42
22	O	206	CLA	C4C-C3C	2.35	1.49	1.45
21	2	302	CHL	C1B-C2B	2.35	1.48	1.43
22	B	816	CLA	MG-ND	2.35	2.10	2.05
22	A	834	CLA	C3B-C4B	2.35	1.48	1.42
22	1	317	CLA	C1B-NB	-2.35	1.34	1.37
22	3	315	CLA	C1B-C2B	2.35	1.48	1.43
22	K	203	CLA	C1B-NB	-2.35	1.34	1.37
22	A	809	CLA	C1B-C2B	2.35	1.48	1.43
21	1	316	CHL	C1D-C2D	2.35	1.50	1.45
22	2	308	CLA	C1B-C2B	2.35	1.48	1.43
21	Y	313	CHL	C1B-NB	-2.35	1.34	1.37
22	1	309	CLA	C1B-NB	-2.35	1.34	1.37
22	Y	309	CLA	C1B-NB	-2.35	1.34	1.37
21	1	301	CHL	C4C-C3C	2.34	1.49	1.45
21	Y	303	CHL	C4C-C3C	2.34	1.49	1.45
22	B	802	CLA	C1D-C2D	2.34	1.49	1.45
22	B	833	CLA	C1B-NB	-2.34	1.34	1.37
22	4	305	CLA	C1B-C2B	2.34	1.48	1.43
22	F	305	CLA	C1D-C2D	2.34	1.49	1.45
22	A	855	CLA	C3B-C4B	2.34	1.48	1.42
22	A	858	CLA	C1D-C2D	2.34	1.49	1.45
22	K	205	CLA	C1B-NB	-2.34	1.34	1.37
22	4	310	CLA	C1B-C2B	2.34	1.48	1.43
21	Z	301	CHL	C4C-C3C	2.34	1.49	1.45
22	A	849	CLA	C1B-NB	-2.34	1.34	1.37
22	A	807	CLA	C1C-C2C	2.34	1.49	1.44
23	2	310	LUT	C12-C13	-2.33	1.40	1.45
22	Z	307	CLA	C1B-NB	-2.33	1.34	1.37
22	3	311	CLA	C1C-C2C	2.33	1.49	1.44
22	B	829	CLA	C3B-C4B	2.33	1.48	1.42
22	A	808	CLA	C1B-C2B	2.33	1.48	1.43
22	B	848	CLA	OBD-CAD	2.33	1.26	1.22
22	B	809	CLA	C3B-C4B	2.33	1.48	1.42
22	B	820	CLA	C4C-C3C	2.33	1.49	1.45
22	Y	308	CLA	C1B-NB	-2.33	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Z	311	CLA	C1B-NB	-2.33	1.34	1.37
22	A	853	CLA	CHB-C4A	-2.33	1.32	1.37
22	B	850	CLA	C1B-C2B	2.33	1.48	1.43
22	B	830	CLA	C1B-C2B	2.33	1.48	1.43
21	4	308	CHL	C4C-C3C	2.33	1.49	1.45
22	2	303	CLA	C1B-C2B	2.33	1.48	1.43
22	O	206	CLA	C1B-C2B	2.33	1.48	1.43
22	L	306	CLA	C3B-C4B	2.33	1.48	1.42
22	Z	308	CLA	C1B-NB	-2.33	1.34	1.37
21	2	301	CHL	C4C-C3C	2.33	1.49	1.45
22	Y	312	CLA	C4C-C3C	2.33	1.49	1.45
22	2	306	CLA	C1B-C2B	2.33	1.48	1.43
23	2	310	LUT	C32-C33	-2.32	1.41	1.45
21	Z	312	CHL	C4C-C3C	2.32	1.49	1.45
22	B	819	CLA	C4C-C3C	2.32	1.49	1.45
22	Z	310	CLA	C1B-NB	-2.32	1.34	1.37
22	4	318	CLA	C1B-NB	-2.32	1.34	1.37
21	4	308	CHL	C1B-C2B	2.32	1.48	1.43
22	2	304	CLA	C1D-C2D	2.32	1.49	1.45
25	1	312	BCR	C12-C13	-2.32	1.41	1.45
22	B	813	CLA	C1D-C2D	2.32	1.49	1.45
22	B	817	CLA	C3B-C4B	2.32	1.48	1.42
21	X	306	CHL	C4C-C3C	2.32	1.49	1.45
22	X	312	CLA	C1B-NB	-2.32	1.34	1.37
25	B	836	BCR	C12-C13	-2.32	1.41	1.45
22	1	305	CLA	C1D-C2D	2.31	1.49	1.45
22	4	316	CLA	C1D-C2D	2.31	1.49	1.45
22	B	847	CLA	C1B-C2B	2.31	1.48	1.43
22	B	850	CLA	C1D-C2D	2.31	1.49	1.45
22	1	307	CLA	C1B-NB	-2.31	1.34	1.37
22	3	311	CLA	C1B-NB	-2.31	1.34	1.37
22	2	319	CLA	CHD-C1D	2.31	1.42	1.38
22	A	805	CLA	C1D-C2D	2.31	1.49	1.45
22	B	850	CLA	C1B-NB	-2.31	1.34	1.37
22	2	320	CLA	C3B-C4B	2.30	1.48	1.42
22	B	853	CLA	C3B-C4B	2.30	1.48	1.42
22	K	205	CLA	C3B-C4B	2.30	1.48	1.42
22	A	806	CLA	C4C-C3C	2.30	1.49	1.45
22	B	829	CLA	C1B-NB	-2.30	1.35	1.37
22	A	838	CLA	C1C-C2C	2.30	1.49	1.44
22	X	311	CLA	C1B-NB	-2.30	1.35	1.37
22	2	305	CLA	C1B-C2B	2.30	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Y	312	CLA	C1B-NB	-2.30	1.35	1.37
25	L	302	BCR	C8-C9	-2.30	1.41	1.45
22	A	853	CLA	C3B-C4B	2.30	1.48	1.42
22	1	319	CLA	C1B-C2B	2.30	1.48	1.43
22	B	816	CLA	C1B-C2B	2.29	1.48	1.43
21	2	309	CHL	C1B-C2B	2.29	1.48	1.43
22	B	820	CLA	C1C-C2C	2.29	1.49	1.44
22	2	319	CLA	C3B-C4B	2.29	1.48	1.42
22	A	833	CLA	C1B-C2B	2.29	1.48	1.43
22	3	318	CLA	C1D-C2D	2.29	1.49	1.45
22	A	840	CLA	C4C-C3C	2.29	1.49	1.45
22	Z	306	CLA	C4C-C3C	2.29	1.49	1.45
25	L	302	BCR	C12-C13	-2.29	1.41	1.45
22	A	855	CLA	CHC-C4B	2.29	1.44	1.39
21	2	321	CHL	C4C-C3C	2.28	1.49	1.45
22	A	832	CLA	C4C-C3C	2.28	1.49	1.45
22	A	843	CLA	C1D-C2D	2.28	1.49	1.45
22	4	304	CLA	C1C-C2C	2.28	1.49	1.44
22	4	315	CLA	C4C-C3C	2.28	1.49	1.45
22	A	839	CLA	C1B-NB	-2.28	1.35	1.37
22	A	843	CLA	C1C-C2C	2.28	1.49	1.44
22	B	821	CLA	C1B-C2B	2.28	1.48	1.43
22	A	858	CLA	C1B-C2B	2.28	1.48	1.43
22	4	304	CLA	C3B-C4B	2.28	1.48	1.42
21	4	307	CHL	C1B-NB	-2.28	1.35	1.37
21	2	302	CHL	C4C-C3C	2.28	1.49	1.45
22	A	831	CLA	C3B-C4B	2.28	1.48	1.42
22	X	313	CLA	C4C-C3C	2.27	1.49	1.45
22	1	321	CLA	C1B-C2B	2.27	1.48	1.43
22	B	810	CLA	C1D-C2D	2.27	1.49	1.45
22	A	827	CLA	MG-NB	-2.27	2.01	2.05
22	Z	313	CLA	C4C-C3C	2.27	1.48	1.45
21	3	307	CHL	C4C-C3C	2.27	1.48	1.45
22	B	826	CLA	CHD-C4C	2.26	1.44	1.39
22	4	314	CLA	C1B-NB	-2.26	1.35	1.37
22	2	318	CLA	C1B-C2B	2.26	1.48	1.43
21	Z	302	CHL	C4C-C3C	2.26	1.48	1.45
21	3	307	CHL	C1B-C2B	2.26	1.48	1.43
22	X	304	CLA	C4C-C3C	2.26	1.48	1.45
22	3	309	CLA	C1B-NB	-2.26	1.35	1.37
22	B	827	CLA	C1B-C2B	2.25	1.48	1.43
22	A	857	CLA	C1C-C2C	2.25	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	853	CLA	C1B-C2B	2.25	1.48	1.43
22	B	852	CLA	C1B-NB	-2.25	1.35	1.37
22	1	317	CLA	C1C-C2C	2.25	1.48	1.44
22	A	850	CLA	C3B-C4B	2.25	1.48	1.42
21	3	314	CHL	C1B-C2B	2.25	1.48	1.43
22	A	842	CLA	C1D-C2D	2.25	1.49	1.45
21	2	309	CHL	CHB-C4A	-2.25	1.32	1.37
22	F	306	CLA	C1C-C2C	2.25	1.48	1.44
22	B	850	CLA	C3B-C4B	2.25	1.48	1.42
22	A	844	CLA	C3B-C4B	2.25	1.48	1.42
21	3	307	CHL	C4B-NB	-2.25	1.35	1.37
22	L	306	CLA	C1C-C2C	2.25	1.48	1.44
21	3	307	CHL	CHB-C4A	-2.24	1.32	1.37
22	A	857	CLA	C1B-C2B	2.24	1.48	1.43
22	A	802	CLA	C1B-C2B	2.24	1.48	1.43
22	F	306	CLA	C1D-C2D	2.24	1.49	1.45
22	B	848	CLA	C1B-C2B	2.24	1.48	1.43
22	B	827	CLA	C3B-C4B	2.24	1.48	1.42
22	2	320	CLA	C4C-C3C	2.24	1.48	1.45
23	4	322	LUT	C28-C29	-2.24	1.41	1.45
25	J	101	BCR	C2-C3	-2.24	1.47	1.52
22	B	845	CLA	C4B-NB	-2.24	1.35	1.37
30	A	825	CL0	MG-NB	-2.24	2.01	2.05
22	X	304	CLA	C1C-C2C	2.24	1.48	1.44
21	Z	304	CHL	C4C-C3C	2.24	1.48	1.45
22	B	821	CLA	C4C-C3C	2.24	1.48	1.45
22	2	317	CLA	C1B-C2B	2.23	1.48	1.43
21	4	308	CHL	CHB-C4A	-2.23	1.32	1.37
22	B	826	CLA	C1B-C2B	2.23	1.48	1.43
21	4	308	CHL	C1B-NB	-2.23	1.35	1.37
22	H	201	CLA	C4C-C3C	2.23	1.48	1.45
22	1	304	CLA	C1D-C2D	2.23	1.49	1.45
25	B	837	BCR	C12-C13	-2.23	1.41	1.45
22	A	856	CLA	C3B-C4B	2.23	1.48	1.42
22	X	310	CLA	C4C-C3C	2.23	1.48	1.45
25	B	839	BCR	C29-C28	-2.23	1.47	1.52
22	4	312	CLA	C1D-C2D	2.23	1.49	1.45
25	O	203	BCR	C8-C9	-2.23	1.41	1.45
22	A	803	CLA	C1B-C2B	2.23	1.48	1.43
22	Z	314	CLA	C4C-C3C	2.23	1.48	1.45
22	B	816	CLA	C3B-C2B	2.22	1.48	1.41
22	2	308	CLA	C4C-C3C	2.22	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	307	CLA	C4C-C3C	2.22	1.48	1.45
22	B	851	CLA	C1D-C2D	2.22	1.49	1.45
21	2	309	CHL	C4C-C3C	2.22	1.48	1.45
22	4	318	CLA	C4C-C3C	2.22	1.48	1.45
22	B	826	CLA	CHD-C1D	2.22	1.42	1.38
22	B	851	CLA	C3B-C4B	2.22	1.48	1.42
22	B	846	CLA	C1B-C2B	2.22	1.48	1.43
22	A	855	CLA	C1D-C2D	2.22	1.49	1.45
21	1	301	CHL	C4B-NB	-2.22	1.35	1.37
22	Y	311	CLA	C4C-C3C	2.22	1.48	1.45
22	A	827	CLA	C1C-C2C	2.22	1.48	1.44
22	A	846	CLA	CHB-C4A	-2.22	1.32	1.37
22	B	803	CLA	C1C-C2C	2.21	1.48	1.44
22	A	810	CLA	C1B-C2B	2.21	1.48	1.43
25	1	312	BCR	C19-C18	-2.21	1.41	1.45
22	X	311	CLA	C4C-C3C	2.21	1.48	1.45
22	K	204	CLA	C1B-NB	-2.21	1.35	1.37
22	3	320	CLA	C4C-C3C	2.21	1.48	1.45
22	3	309	CLA	C1C-C2C	2.21	1.48	1.44
22	2	306	CLA	C1D-C2D	2.21	1.49	1.45
22	B	812	CLA	C3B-C4B	2.21	1.47	1.42
22	Z	308	CLA	C4C-C3C	2.21	1.48	1.45
22	4	314	CLA	C1D-C2D	2.21	1.49	1.45
22	A	808	CLA	C1C-C2C	2.21	1.48	1.44
22	Y	310	CLA	C4C-C3C	2.20	1.48	1.45
22	B	852	CLA	C4C-C3C	2.20	1.48	1.45
22	A	854	CLA	CHB-C4A	-2.20	1.32	1.37
22	Z	310	CLA	C4C-C3C	2.20	1.48	1.45
22	Z	307	CLA	C1C-C2C	2.20	1.48	1.44
22	A	844	CLA	CHB-C4A	-2.20	1.32	1.37
22	1	305	CLA	C1C-C2C	2.20	1.48	1.44
22	A	812	CLA	C1B-C2B	2.20	1.48	1.43
22	B	816	CLA	C1D-C2D	2.19	1.49	1.45
21	X	302	CHL	C2C-C1C	2.19	1.49	1.44
22	4	305	CLA	C1C-C2C	2.19	1.48	1.44
22	Z	309	CLA	C4C-C3C	2.19	1.48	1.45
22	A	852	CLA	C3B-C2B	2.19	1.48	1.41
22	A	802	CLA	C4C-C3C	2.19	1.48	1.45
21	2	301	CHL	C1B-NB	-2.19	1.35	1.37
22	B	822	CLA	C4C-C3C	2.19	1.48	1.45
21	4	307	CHL	C3B-C4B	2.19	1.47	1.42
22	A	850	CLA	C1B-C2B	2.19	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	851	CLA	C1B-C2B	2.19	1.48	1.43
22	G	207	CLA	C3B-C4B	2.19	1.47	1.42
21	Z	305	CHL	CHB-C4A	-2.19	1.32	1.37
21	Z	303	CHL	C4C-C3C	2.19	1.48	1.45
22	1	302	CLA	C4C-C3C	2.19	1.48	1.45
22	X	312	CLA	C1C-C2C	2.18	1.48	1.44
22	2	317	CLA	C4C-C3C	2.18	1.48	1.45
22	B	819	CLA	C1B-C2B	2.18	1.48	1.43
22	B	818	CLA	C1D-C2D	2.18	1.49	1.45
22	A	802	CLA	C1C-C2C	2.18	1.48	1.44
21	1	316	CHL	C3B-C4B	2.18	1.47	1.42
22	L	306	CLA	C1D-C2D	2.18	1.49	1.45
21	2	321	CHL	C1B-NB	-2.18	1.35	1.37
22	X	303	CLA	C4C-C3C	2.18	1.48	1.45
25	L	303	BCR	C29-C28	-2.18	1.47	1.52
22	Y	309	CLA	C4C-C3C	2.18	1.48	1.45
22	3	320	CLA	C1B-C2B	2.18	1.48	1.43
31	J	104	DGD	O5D-C1E	2.18	1.43	1.40
22	A	826	CLA	CHB-C4A	-2.18	1.32	1.37
21	Y	313	CHL	C4C-C3C	2.17	1.48	1.45
22	B	828	CLA	C4C-C3C	2.17	1.48	1.45
22	B	847	CLA	C1C-C2C	2.17	1.48	1.44
22	B	817	CLA	C1C-C2C	2.17	1.48	1.44
22	B	815	CLA	C1B-C2B	2.17	1.48	1.43
22	B	801	CLA	MG-NB	-2.17	2.01	2.05
22	J	102	CLA	C1C-C2C	2.17	1.48	1.44
22	1	318	CLA	C1B-C2B	2.17	1.48	1.43
22	B	803	CLA	C1B-C2B	2.17	1.48	1.43
24	4	320	XAT	O4-C5	-2.17	1.43	1.46
22	J	102	CLA	C4C-C3C	2.17	1.48	1.45
21	4	307	CHL	C4C-C3C	2.17	1.48	1.45
22	1	304	CLA	CHB-C4A	-2.17	1.32	1.37
22	L	305	CLA	C1B-C2B	2.17	1.48	1.43
21	Z	302	CHL	C1B-NB	-2.17	1.35	1.37
21	4	309	CHL	C4C-C3C	2.17	1.48	1.45
22	3	310	CLA	C1C-C2C	2.17	1.48	1.44
25	O	203	BCR	C19-C18	-2.17	1.41	1.45
22	G	206	CLA	C4C-C3C	2.17	1.48	1.45
22	B	804	CLA	C1C-C2C	2.17	1.48	1.44
21	4	309	CHL	C1B-C2B	2.17	1.48	1.43
22	1	303	CLA	C1B-NB	-2.17	1.35	1.37
22	A	828	CLA	C1D-C2D	2.17	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	818	BCR	C17-C16	-2.17	1.38	1.44
22	X	303	CLA	C1C-C2C	2.17	1.48	1.44
22	3	321	CLA	C4C-C3C	2.17	1.48	1.45
22	X	304	CLA	C4B-NB	-2.16	1.35	1.37
22	Y	308	CLA	C4C-C3C	2.16	1.48	1.45
22	1	321	CLA	C4C-C3C	2.16	1.48	1.45
22	B	817	CLA	C1B-C2B	2.16	1.48	1.43
22	X	304	CLA	C3D-CAD	2.16	1.52	1.45
21	2	321	CHL	MG-NA	-2.16	2.01	2.06
22	A	857	CLA	C1B-NB	-2.16	1.35	1.37
22	3	318	CLA	C1C-C2C	2.16	1.48	1.44
22	Y	302	CLA	C4C-C3C	2.16	1.48	1.45
25	A	816	BCR	C2-C3	-2.16	1.47	1.52
22	A	843	CLA	C1B-C2B	2.16	1.48	1.43
21	3	307	CHL	C1B-NB	-2.16	1.35	1.37
22	2	317	CLA	C1C-C2C	2.16	1.48	1.44
22	X	312	CLA	C4C-C3C	2.15	1.48	1.45
21	3	314	CHL	C2C-C1C	2.15	1.49	1.44
22	A	829	CLA	C1C-C2C	2.15	1.48	1.44
21	4	317	CHL	C1B-NB	-2.15	1.35	1.37
22	B	810	CLA	C1B-C2B	2.15	1.48	1.43
22	A	801	CLA	C4C-C3C	2.15	1.48	1.45
22	K	205	CLA	C1B-C2B	2.15	1.48	1.43
22	F	305	CLA	C1C-C2C	2.15	1.48	1.44
22	X	301	CLA	C1C-C2C	2.15	1.48	1.44
22	G	207	CLA	C1B-C2B	2.15	1.48	1.43
22	A	804	CLA	C1B-C2B	2.15	1.48	1.43
22	A	833	CLA	C1C-C2C	2.15	1.48	1.44
21	3	307	CHL	MG-NA	-2.15	2.01	2.06
22	A	834	CLA	C1D-C2D	2.15	1.49	1.45
22	Z	310	CLA	C1C-C2C	2.15	1.48	1.44
22	B	817	CLA	C1D-C2D	2.15	1.49	1.45
22	A	836	CLA	C1B-C2B	2.15	1.48	1.43
22	A	848	CLA	C4C-C3C	2.15	1.48	1.45
22	4	306	CLA	C1C-C2C	2.15	1.48	1.44
22	K	203	CLA	C1C-C2C	2.15	1.48	1.44
21	2	309	CHL	C4B-NB	-2.14	1.35	1.37
21	Z	305	CHL	C1B-C2B	2.14	1.48	1.43
22	Y	302	CLA	C1C-C2C	2.14	1.48	1.44
21	Y	307	CHL	C1B-NB	-2.14	1.35	1.37
22	B	818	CLA	CHB-C4A	-2.14	1.32	1.37
21	1	316	CHL	C4C-C3C	2.14	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	805	CLA	C1C-C2C	2.14	1.48	1.44
22	A	850	CLA	C1C-C2C	2.14	1.48	1.44
21	X	306	CHL	C2C-C1C	2.14	1.49	1.44
22	3	313	CLA	C4C-C3C	2.14	1.48	1.45
22	A	826	CLA	C4B-NB	-2.14	1.35	1.37
22	H	201	CLA	C3B-C4B	2.14	1.47	1.42
22	Z	307	CLA	C4C-C3C	2.14	1.48	1.45
21	4	309	CHL	CHB-C4A	-2.14	1.32	1.37
22	A	845	CLA	C3B-C4B	2.14	1.47	1.42
22	Z	313	CLA	C1C-C2C	2.14	1.48	1.44
22	4	313	CLA	C4C-C3C	2.14	1.48	1.45
22	3	318	CLA	C4C-C3C	2.13	1.48	1.45
22	A	807	CLA	C4C-C3C	2.13	1.48	1.45
22	N	202	CLA	C1C-C2C	2.13	1.48	1.44
22	Z	308	CLA	C1C-C2C	2.13	1.48	1.44
25	B	838	BCR	C11-C10	-2.13	1.36	1.43
22	A	854	CLA	C1C-C2C	2.13	1.48	1.44
22	Z	311	CLA	C1C-C2C	2.13	1.48	1.44
22	B	825	CLA	CHB-C4A	-2.13	1.32	1.37
22	N	202	CLA	C4C-C3C	2.13	1.48	1.45
22	4	306	CLA	C1B-C2B	2.13	1.48	1.43
22	3	310	CLA	C1B-C2B	2.13	1.48	1.43
22	1	321	CLA	C1C-C2C	2.13	1.48	1.44
22	A	846	CLA	C4C-C3C	2.13	1.48	1.45
21	X	307	CHL	C2C-C1C	2.13	1.49	1.44
25	B	838	BCR	C29-C28	-2.13	1.47	1.52
22	A	810	CLA	C1C-C2C	2.12	1.48	1.44
22	A	847	CLA	C1B-C2B	2.12	1.48	1.43
22	B	815	CLA	C1C-C2C	2.12	1.48	1.44
22	X	311	CLA	C1C-C2C	2.12	1.48	1.44
22	A	828	CLA	MG-ND	2.12	2.10	2.05
22	2	303	CLA	C1C-C2C	2.12	1.48	1.44
22	4	311	CLA	C1B-C2B	2.12	1.48	1.43
21	X	309	CHL	C1B-NB	-2.12	1.35	1.37
22	4	310	CLA	C1C-C2C	2.12	1.48	1.44
22	2	304	CLA	C1C-C2C	2.12	1.48	1.44
22	G	207	CLA	C4C-C3C	2.12	1.48	1.45
22	A	801	CLA	C4B-C3B	2.12	1.48	1.43
22	G	205	CLA	C1C-C2C	2.12	1.48	1.44
22	Y	308	CLA	C1C-C2C	2.11	1.48	1.44
22	A	839	CLA	C3B-C4B	2.11	1.47	1.42
21	Z	301	CHL	C1B-NB	-2.11	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	314	CLA	C1C-C2C	2.11	1.48	1.44
22	B	816	CLA	C1C-C2C	2.11	1.48	1.44
22	3	319	CLA	C4C-C3C	2.11	1.48	1.45
22	B	806	CLA	C4C-C3C	2.11	1.48	1.45
22	Y	314	CLA	C4C-C3C	2.11	1.48	1.45
25	B	838	BCR	C15-C14	-2.11	1.36	1.43
21	Z	302	CHL	CHB-C4A	-2.11	1.32	1.37
22	B	849	CLA	C1C-C2C	2.11	1.48	1.44
21	Y	305	CHL	C2C-C1C	2.11	1.49	1.44
22	1	303	CLA	C4C-C3C	2.11	1.48	1.45
21	Y	303	CHL	C2C-C1C	2.11	1.49	1.44
22	B	829	CLA	C1C-C2C	2.11	1.48	1.44
22	B	807	CLA	C3A-C2A	-2.11	1.48	1.54
21	Y	306	CHL	C2C-C1C	2.11	1.49	1.44
22	A	850	CLA	C4C-C3C	2.11	1.48	1.45
22	2	305	CLA	C1C-C2C	2.11	1.48	1.44
22	A	852	CLA	C1C-C2C	2.11	1.48	1.44
25	B	840	BCR	C29-C28	-2.11	1.47	1.52
22	Y	314	CLA	C1C-C2C	2.11	1.48	1.44
22	A	826	CLA	C1D-C2D	2.11	1.49	1.45
22	1	309	CLA	C1C-C2C	2.11	1.48	1.44
22	1	318	CLA	C4C-C3C	2.10	1.48	1.45
22	Z	311	CLA	C4C-C3C	2.10	1.48	1.45
22	Y	310	CLA	C1C-C2C	2.10	1.48	1.44
25	F	302	BCR	C11-C10	-2.10	1.36	1.43
21	Z	302	CHL	C2C-C1C	2.10	1.49	1.44
22	2	307	CLA	C4C-C3C	2.10	1.48	1.45
21	4	317	CHL	C4B-NB	-2.10	1.35	1.37
21	1	301	CHL	C1B-NB	-2.10	1.35	1.37
22	A	852	CLA	CHD-C1D	2.10	1.42	1.38
25	G	202	BCR	C19-C18	-2.10	1.41	1.45
21	Y	305	CHL	C1B-NB	-2.10	1.35	1.37
30	A	825	CL0	C1C-C2C	2.10	1.48	1.44
22	A	831	CLA	C1D-C2D	2.10	1.49	1.45
22	3	317	CLA	C4C-C3C	2.10	1.48	1.45
22	Y	309	CLA	C1C-C2C	2.10	1.48	1.44
22	X	310	CLA	C1C-C2C	2.09	1.48	1.44
22	2	305	CLA	C1D-C2D	2.09	1.49	1.45
21	Z	303	CHL	C2C-C1C	2.09	1.49	1.44
22	1	307	CLA	C4C-C3C	2.09	1.48	1.45
22	K	202	CLA	C1C-C2C	2.09	1.48	1.44
22	X	301	CLA	C4C-C3C	2.09	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	301	CHL	MG-NA	-2.09	2.01	2.06
21	Y	313	CHL	CHB-C4A	-2.09	1.32	1.37
22	1	309	CLA	C4C-C3C	2.09	1.48	1.45
25	A	815	BCR	C11-C10	-2.09	1.37	1.43
22	3	315	CLA	C4C-C3C	2.09	1.48	1.45
22	A	829	CLA	C1B-C2B	2.09	1.48	1.43
21	X	307	CHL	CHB-C4A	-2.08	1.32	1.37
22	2	303	CLA	C1D-C2D	2.08	1.49	1.45
22	B	823	CLA	C1C-C2C	2.08	1.48	1.44
22	O	209	CLA	C4C-C3C	2.08	1.48	1.45
22	A	806	CLA	C1C-C2C	2.08	1.48	1.44
21	4	309	CHL	C1D-ND	-2.08	1.35	1.37
22	B	829	CLA	C1B-C2B	2.08	1.48	1.43
22	A	859	CLA	C1B-C2B	2.08	1.48	1.43
22	G	206	CLA	C1C-C2C	2.08	1.48	1.44
22	4	318	CLA	C1C-C2C	2.08	1.48	1.44
22	B	813	CLA	C1C-C2C	2.08	1.48	1.44
22	Z	309	CLA	C1C-C2C	2.08	1.48	1.44
21	Z	304	CHL	C2C-C1C	2.08	1.49	1.44
22	1	319	CLA	C1C-C2C	2.08	1.48	1.44
21	Z	303	CHL	CHB-C4A	-2.08	1.32	1.37
22	B	811	CLA	C1C-C2C	2.07	1.48	1.44
21	4	308	CHL	MG-NA	-2.07	2.01	2.06
25	J	103	BCR	C2-C3	-2.07	1.47	1.52
22	X	304	CLA	C1D-C2D	2.07	1.49	1.45
22	2	304	CLA	C4C-C3C	2.07	1.48	1.45
25	J	101	BCR	C29-C28	-2.07	1.47	1.52
22	2	322	CLA	C1C-C2C	2.07	1.48	1.44
22	B	824	CLA	C1C-C2C	2.07	1.48	1.44
22	K	205	CLA	C1C-C2C	2.07	1.48	1.44
25	B	844	BCR	C20-C21	-2.07	1.37	1.43
22	3	316	CLA	CHB-C4A	-2.07	1.32	1.37
22	K	202	CLA	C4C-C3C	2.07	1.48	1.45
22	A	839	CLA	C4C-C3C	2.07	1.48	1.45
22	4	314	CLA	C4C-C3C	2.06	1.48	1.45
22	X	313	CLA	C1C-C2C	2.06	1.48	1.44
22	O	207	CLA	C1C-C2C	2.06	1.48	1.44
22	3	321	CLA	MG-NA	-2.06	2.01	2.06
21	2	302	CHL	CHB-C4A	-2.06	1.32	1.37
22	3	316	CLA	C1B-C2B	2.06	1.48	1.43
22	B	807	CLA	MG-NA	-2.06	2.01	2.06
22	4	311	CLA	C4C-C3C	2.06	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	856	CLA	C1B-C2B	2.06	1.48	1.43
22	Y	312	CLA	C1C-C2C	2.06	1.48	1.44
22	B	853	CLA	C1C-C2C	2.06	1.48	1.44
22	3	315	CLA	C3B-C4B	2.06	1.47	1.42
22	Y	301	CLA	C1C-C2C	2.05	1.48	1.44
21	X	302	CHL	C1B-NB	-2.05	1.35	1.37
22	H	201	CLA	C1C-C2C	2.05	1.48	1.44
22	B	848	CLA	C1C-C2C	2.05	1.48	1.44
21	Z	303	CHL	MG-NA	-2.05	2.01	2.06
21	Z	303	CHL	C1B-NB	-2.05	1.35	1.37
22	B	853	CLA	C4C-C3C	2.05	1.48	1.45
25	A	819	BCR	C29-C28	-2.05	1.47	1.52
25	B	838	BCR	C20-C21	-2.05	1.37	1.43
22	O	209	CLA	C1C-C2C	2.04	1.48	1.44
22	2	318	CLA	C4C-C3C	2.04	1.48	1.45
22	L	305	CLA	C1C-C2C	2.04	1.48	1.44
21	Y	313	CHL	C4B-NB	-2.04	1.35	1.37
25	O	203	BCR	C12-C13	-2.04	1.41	1.45
22	A	841	CLA	C4C-C3C	2.04	1.48	1.45
22	A	841	CLA	C1B-C2B	2.04	1.48	1.43
22	A	844	CLA	C4C-C3C	2.04	1.48	1.45
21	Z	304	CHL	C1B-NB	-2.04	1.35	1.37
22	B	825	CLA	C4C-C3C	2.04	1.48	1.45
22	A	848	CLA	C1C-C2C	2.04	1.48	1.44
22	B	819	CLA	C3B-C4B	2.04	1.47	1.42
22	B	831	CLA	C1D-C2D	2.04	1.49	1.45
21	3	307	CHL	C1D-ND	-2.03	1.35	1.37
22	A	836	CLA	C4C-C3C	2.03	1.48	1.45
22	B	816	CLA	MG-NB	-2.03	2.01	2.05
22	A	856	CLA	C1C-C2C	2.03	1.48	1.44
22	K	205	CLA	C4C-C3C	2.03	1.48	1.45
21	Y	305	CHL	CHB-C4A	-2.03	1.32	1.37
22	B	825	CLA	C1C-C2C	2.03	1.48	1.44
22	3	320	CLA	C1C-C2C	2.03	1.48	1.44
22	B	805	CLA	C4C-C3C	2.03	1.48	1.45
22	G	207	CLA	C1C-C2C	2.03	1.48	1.44
22	3	312	CLA	C1C-C2C	2.03	1.48	1.44
22	A	803	CLA	C1C-C2C	2.03	1.48	1.44
22	O	208	CLA	C1C-C2C	2.03	1.48	1.44
21	Y	306	CHL	C1B-NB	-2.03	1.35	1.37
22	A	806	CLA	C1B-C2B	2.03	1.48	1.43
21	3	314	CHL	CHB-C4A	-2.03	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	821	CLA	C1C-C2C	2.03	1.48	1.44
22	A	855	CLA	CMB-C2B	-2.02	1.46	1.50
21	X	305	CHL	C2C-C1C	2.02	1.48	1.44
25	B	838	BCR	C16-C17	-2.02	1.37	1.43
24	3	302	XAT	O24-C25	-2.02	1.43	1.46
21	X	309	CHL	CHB-C4A	-2.02	1.32	1.37
22	Z	314	CLA	C1C-C2C	2.02	1.48	1.44
21	Z	312	CHL	C2C-C1C	2.02	1.48	1.44
22	3	319	CLA	C1C-C2C	2.02	1.48	1.44
22	A	833	CLA	C4C-C3C	2.02	1.48	1.45
22	4	306	CLA	C4C-C3C	2.02	1.48	1.45
21	4	317	CHL	MG-NA	-2.02	2.01	2.06
22	B	852	CLA	C1C-C2C	2.02	1.48	1.44
22	A	853	CLA	C1B-C2B	2.02	1.48	1.43
21	3	314	CHL	MG-NA	-2.02	2.01	2.06
21	1	316	CHL	CHB-C4A	-2.02	1.32	1.37
22	B	833	CLA	C1C-C2C	2.02	1.48	1.44
21	Z	301	CHL	C2C-C1C	2.02	1.48	1.44
22	A	812	CLA	C1C-C2C	2.02	1.48	1.44
22	A	828	CLA	C4C-C3C	2.02	1.48	1.45
21	X	308	CHL	CHB-C4A	-2.02	1.32	1.37
21	Y	305	CHL	CMC-C2C	2.02	1.49	1.45
22	A	853	CLA	C1C-C2C	2.01	1.48	1.44
22	B	824	CLA	C4C-C3C	2.01	1.48	1.45
21	2	302	CHL	MG-NA	-2.01	2.01	2.06
22	B	815	CLA	C4C-C3C	2.01	1.48	1.45
22	1	306	CLA	C1C-C2C	2.01	1.48	1.44
21	X	302	CHL	CMC-C2C	2.01	1.49	1.45
25	L	302	BCR	C8-C7	2.01	1.39	1.33
22	A	829	CLA	CHB-C4A	-2.01	1.32	1.37
22	2	308	CLA	C1C-C2C	2.01	1.48	1.44
22	3	315	CLA	C1C-C2C	2.01	1.48	1.44
21	2	309	CHL	MG-NA	-2.01	2.01	2.06
22	1	302	CLA	C1C-C2C	2.01	1.48	1.44
22	B	813	CLA	CHB-C4A	-2.01	1.32	1.37
22	L	307	CLA	C1C-C2C	2.01	1.48	1.44
21	X	306	CHL	CMC-C2C	2.01	1.49	1.45
25	2	312	BCR	C20-C19	2.01	1.39	1.34
25	A	814	BCR	C15-C14	-2.00	1.37	1.43
21	Y	307	CHL	CHB-C4A	-2.00	1.32	1.37
22	A	827	CLA	C3B-C4B	2.00	1.47	1.42
22	A	851	CLA	C4C-C3C	2.00	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	808	CLA	C4C-C3C	2.00	1.48	1.45
22	B	818	CLA	C4C-C3C	2.00	1.48	1.45
21	X	302	CHL	CHB-C4A	-2.00	1.32	1.37
22	A	805	CLA	CHB-C4A	-2.00	1.32	1.37
22	B	808	CLA	C1C-C2C	2.00	1.48	1.44
22	A	810	CLA	C1D-C2D	2.00	1.49	1.45
22	B	803	CLA	C3B-C2B	2.00	1.48	1.41
22	3	315	CLA	C1D-C2D	2.00	1.49	1.45
22	2	322	CLA	C4C-C3C	2.00	1.48	1.45

All (6469) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	X	304	CLA	C4D-CHA-C1A	-18.66	98.54	121.25
22	B	807	CLA	C1D-C2D-C3D	-17.44	102.03	110.84
22	B	807	CLA	C2B-C1B-NB	15.81	120.83	110.23
22	B	816	CLA	C1D-ND-C4D	-12.50	97.45	106.33
22	B	814	CLA	C1D-ND-C4D	-11.29	98.32	106.33
22	A	826	CLA	C2B-C1B-NB	11.27	117.78	110.23
21	3	307	CHL	C2B-C1B-NB	11.03	117.63	110.23
21	Y	313	CHL	C2B-C1B-NB	10.97	117.59	110.23
21	4	308	CHL	C2B-C1B-NB	10.96	117.58	110.23
22	B	820	CLA	C2B-C1B-NB	10.94	117.57	110.23
24	1	311	XAT	C27-C28-C29	-10.89	108.63	125.53
24	3	302	XAT	O24-C25-C24	10.89	121.56	113.38
21	2	309	CHL	C2B-C1B-NB	10.88	117.53	110.23
22	A	853	CLA	C2B-C1B-NB	10.76	117.44	110.23
21	X	307	CHL	C2B-C1B-NB	10.71	117.41	110.23
21	Z	302	CHL	C2B-C1B-NB	10.58	117.33	110.23
21	Y	305	CHL	C2B-C1B-NB	10.57	117.32	110.23
22	B	803	CLA	C1D-ND-C4D	-10.55	98.84	106.33
21	Z	303	CHL	C2B-C1B-NB	10.54	117.30	110.23
21	Y	306	CHL	C2B-C1B-NB	10.51	117.28	110.23
22	1	317	CLA	C1D-ND-C4D	-10.50	98.88	106.33
21	X	302	CHL	C2B-C1B-NB	10.49	117.26	110.23
21	X	309	CHL	C2B-C1B-NB	10.45	117.24	110.23
22	4	305	CLA	C1D-ND-C4D	-10.44	98.92	106.33
21	4	317	CHL	C2B-C1B-NB	10.44	117.23	110.23
21	Z	301	CHL	C2B-C1B-NB	10.44	117.23	110.23
21	X	305	CHL	C2B-C1B-NB	10.43	117.23	110.23
21	Y	307	CHL	C2B-C1B-NB	10.42	117.22	110.23
21	Z	305	CHL	C2B-C1B-NB	10.39	117.20	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Y	303	CHL	C2B-C1B-NB	10.38	117.19	110.23
21	Y	304	CHL	C2B-C1B-NB	10.36	117.17	110.23
22	2	319	CLA	C1D-ND-C4D	-10.35	98.99	106.33
22	G	205	CLA	C1D-ND-C4D	-10.34	98.99	106.33
21	X	308	CHL	C2B-C1B-NB	10.34	117.17	110.23
21	Z	304	CHL	C2B-C1B-NB	10.31	117.14	110.23
22	3	308	CLA	C1D-ND-C4D	-10.30	99.02	106.33
22	A	852	CLA	C1D-ND-C4D	-10.29	99.02	106.33
21	2	301	CHL	C2B-C1B-NB	10.26	117.11	110.23
22	A	838	CLA	C1D-ND-C4D	-10.25	99.05	106.33
24	3	302	XAT	C40-C33-C34	-10.23	108.59	122.92
22	B	811	CLA	C1D-ND-C4D	-10.22	99.07	106.33
22	A	834	CLA	C1D-ND-C4D	-10.22	99.07	106.33
21	Z	312	CHL	C2B-C1B-NB	10.22	117.08	110.23
22	A	830	CLA	C1D-ND-C4D	-10.20	99.09	106.33
21	1	316	CHL	C2B-C1B-NB	10.17	117.05	110.23
21	X	306	CHL	C2B-C1B-NB	10.14	117.03	110.23
22	O	208	CLA	C1D-ND-C4D	-10.09	99.16	106.33
22	A	802	CLA	C1D-ND-C4D	-10.07	99.18	106.33
22	B	802	CLA	C1D-ND-C4D	-10.07	99.18	106.33
22	A	829	CLA	C2B-C1B-NB	10.05	116.97	110.23
22	1	308	CLA	C1D-ND-C4D	-10.00	99.23	106.33
22	2	306	CLA	C1D-ND-C4D	-9.99	99.24	106.33
22	B	830	CLA	C2C-C1C-NC	9.98	119.33	109.97
22	A	828	CLA	C1D-ND-C4D	-9.96	99.26	106.33
22	L	307	CLA	C1D-ND-C4D	-9.95	99.27	106.33
22	A	803	CLA	C1D-ND-C4D	-9.93	99.28	106.33
24	1	311	XAT	O24-C25-C38	9.90	126.92	115.06
22	A	831	CLA	C1D-ND-C4D	-9.88	99.32	106.33
22	A	858	CLA	C2B-C1B-NB	9.86	116.84	110.23
22	1	309	CLA	C1D-ND-C4D	-9.84	99.35	106.33
22	3	309	CLA	C1D-ND-C4D	-9.83	99.35	106.33
22	3	311	CLA	C1D-ND-C4D	-9.80	99.37	106.33
22	G	206	CLA	C1D-ND-C4D	-9.79	99.38	106.33
21	3	314	CHL	C2B-C1B-NB	9.76	116.77	110.23
21	2	321	CHL	C2B-C1B-NB	9.76	116.77	110.23
22	A	858	CLA	C1D-ND-C4D	-9.75	99.41	106.33
22	X	304	CLA	C4D-C3D-CAD	9.70	119.53	108.10
22	B	848	CLA	C1D-ND-C4D	-9.70	99.45	106.33
22	O	209	CLA	C1D-ND-C4D	-9.69	99.45	106.33
22	2	308	CLA	C1D-ND-C4D	-9.69	99.45	106.33
21	1	301	CHL	C2B-C1B-NB	9.67	116.71	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Y	310	CLA	C1D-ND-C4D	-9.66	99.47	106.33
22	B	802	CLA	C2B-C1B-NB	9.66	116.71	110.23
22	A	855	CLA	C2C-C1C-NC	9.65	119.01	109.97
22	B	805	CLA	C1D-ND-C4D	-9.64	99.48	106.33
22	F	306	CLA	C1D-ND-C4D	-9.63	99.49	106.33
22	B	849	CLA	C1D-ND-C4D	-9.62	99.50	106.33
22	B	846	CLA	C2B-C1B-NB	9.62	116.68	110.23
22	A	844	CLA	C2B-C1B-NB	9.61	116.68	110.23
22	K	203	CLA	C1D-ND-C4D	-9.61	99.51	106.33
22	1	306	CLA	C1D-ND-C4D	-9.60	99.51	106.33
22	B	810	CLA	C1D-ND-C4D	-9.59	99.52	106.33
22	L	306	CLA	C1D-ND-C4D	-9.57	99.54	106.33
24	3	302	XAT	C32-C33-C34	9.56	133.61	118.94
22	A	833	CLA	C1D-ND-C4D	-9.56	99.55	106.33
22	A	847	CLA	C1D-ND-C4D	-9.56	99.55	106.33
22	B	801	CLA	C1D-ND-C4D	-9.54	99.56	106.33
22	4	311	CLA	C2B-C1B-NB	9.53	116.62	110.23
22	Z	310	CLA	C1D-ND-C4D	-9.52	99.57	106.33
21	4	309	CHL	C2B-C1B-NB	9.52	116.61	110.23
22	B	824	CLA	C1D-ND-C4D	-9.51	99.58	106.33
22	3	313	CLA	C1D-ND-C4D	-9.50	99.59	106.33
22	A	807	CLA	C1D-ND-C4D	-9.50	99.59	106.33
22	A	859	CLA	C1D-ND-C4D	-9.50	99.59	106.33
22	B	822	CLA	C2B-C1B-NB	9.50	116.60	110.23
22	A	830	CLA	C2C-C1C-NC	9.49	118.86	109.97
22	A	805	CLA	C2B-C1B-NB	9.48	116.59	110.23
22	1	302	CLA	C1D-ND-C4D	-9.47	99.61	106.33
22	K	204	CLA	C1D-ND-C4D	-9.47	99.61	106.33
22	B	833	CLA	C1D-ND-C4D	-9.46	99.61	106.33
22	Y	314	CLA	C1D-ND-C4D	-9.46	99.62	106.33
22	H	201	CLA	C1D-ND-C4D	-9.44	99.63	106.33
22	3	317	CLA	C1D-ND-C4D	-9.43	99.63	106.33
22	X	313	CLA	C1D-ND-C4D	-9.43	99.64	106.33
22	A	812	CLA	C1D-ND-C4D	-9.43	99.64	106.33
21	4	307	CHL	C2B-C1B-NB	9.42	116.55	110.23
22	4	314	CLA	C1D-ND-C4D	-9.42	99.64	106.33
22	3	312	CLA	C1D-ND-C4D	-9.42	99.65	106.33
22	A	840	CLA	C1D-ND-C4D	-9.41	99.65	106.33
22	A	842	CLA	C1D-ND-C4D	-9.40	99.66	106.33
22	A	845	CLA	C1D-ND-C4D	-9.40	99.66	106.33
22	J	102	CLA	C1D-ND-C4D	-9.40	99.66	106.33
22	B	828	CLA	C1D-ND-C4D	-9.39	99.66	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	815	CLA	C1D-ND-C4D	-9.39	99.66	106.33
22	Z	313	CLA	C1D-ND-C4D	-9.39	99.67	106.33
22	Z	309	CLA	C1D-ND-C4D	-9.37	99.68	106.33
22	2	308	CLA	CMD-C2D-C1D	9.36	141.20	124.71
22	A	836	CLA	C1D-ND-C4D	-9.36	99.69	106.33
22	1	304	CLA	C2B-C1B-NB	9.35	116.50	110.23
22	A	837	CLA	C1D-ND-C4D	-9.34	99.70	106.33
22	1	303	CLA	C1D-ND-C4D	-9.34	99.70	106.33
22	B	806	CLA	C1D-ND-C4D	-9.34	99.70	106.33
22	2	317	CLA	C1D-ND-C4D	-9.33	99.71	106.33
21	1	301	CHL	CMD-C2D-C1D	9.32	141.14	124.71
22	X	304	CLA	C2B-C1B-NB	9.32	116.48	110.23
22	1	307	CLA	C1D-ND-C4D	-9.30	99.73	106.33
22	O	210	CLA	C1D-ND-C4D	-9.29	99.74	106.33
22	X	301	CLA	C1D-ND-C4D	-9.29	99.74	106.33
22	A	850	CLA	C1D-ND-C4D	-9.28	99.74	106.33
22	A	832	CLA	C1D-ND-C4D	-9.28	99.75	106.33
22	B	831	CLA	C1D-ND-C4D	-9.27	99.75	106.33
22	4	313	CLA	C1D-ND-C4D	-9.26	99.75	106.33
22	Y	312	CLA	C1D-ND-C4D	-9.26	99.76	106.33
22	A	809	CLA	C1D-ND-C4D	-9.26	99.76	106.33
22	Z	311	CLA	C1D-ND-C4D	-9.25	99.76	106.33
22	X	303	CLA	C1D-ND-C4D	-9.25	99.76	106.33
24	3	302	XAT	C31-C30-C29	-9.25	114.11	127.31
22	A	851	CLA	C1D-ND-C4D	-9.25	99.77	106.33
22	A	804	CLA	C1D-ND-C4D	-9.25	99.77	106.33
22	A	841	CLA	C1D-ND-C4D	-9.23	99.77	106.33
22	X	312	CLA	C1D-ND-C4D	-9.23	99.78	106.33
22	A	826	CLA	C1D-ND-C4D	-9.23	99.78	106.33
22	1	318	CLA	C1D-ND-C4D	-9.23	99.78	106.33
22	Z	308	CLA	C1D-ND-C4D	-9.23	99.78	106.33
22	2	319	CLA	C2C-C1C-NC	9.23	118.62	109.97
22	F	305	CLA	C1D-ND-C4D	-9.22	99.78	106.33
22	4	316	CLA	C1D-ND-C4D	-9.22	99.79	106.33
22	Y	309	CLA	C1D-ND-C4D	-9.21	99.80	106.33
22	1	321	CLA	C1D-ND-C4D	-9.20	99.80	106.33
22	A	806	CLA	C2B-C1B-NB	9.20	116.40	110.23
22	X	311	CLA	C1D-ND-C4D	-9.20	99.80	106.33
22	4	318	CLA	C1D-ND-C4D	-9.20	99.80	106.33
22	Z	307	CLA	C1D-ND-C4D	-9.20	99.80	106.33
22	3	310	CLA	C1D-ND-C4D	-9.20	99.80	106.33
22	3	315	CLA	C2C-C1C-NC	9.20	118.59	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	812	CLA	C2C-C1C-NC	9.19	118.59	109.97
21	2	302	CHL	C2B-C1B-NB	9.19	116.40	110.23
22	1	304	CLA	C1D-ND-C4D	-9.19	99.80	106.33
22	Y	311	CLA	C1D-ND-C4D	-9.18	99.81	106.33
22	4	315	CLA	CMD-C2D-C1D	9.18	140.89	124.71
22	1	305	CLA	C1D-ND-C4D	-9.18	99.81	106.33
22	A	843	CLA	C1D-ND-C4D	-9.18	99.81	106.33
22	A	808	CLA	C1D-ND-C4D	-9.17	99.82	106.33
22	Y	302	CLA	C1D-ND-C4D	-9.16	99.83	106.33
22	A	859	CLA	C2B-C1B-NB	9.16	116.37	110.23
22	B	823	CLA	C1D-ND-C4D	-9.15	99.83	106.33
22	4	312	CLA	C1D-ND-C4D	-9.14	99.84	106.33
22	N	202	CLA	C1D-ND-C4D	-9.13	99.85	106.33
22	A	801	CLA	C2B-C1B-NB	9.13	116.35	110.23
22	B	813	CLA	C1D-ND-C4D	-9.13	99.85	106.33
22	B	851	CLA	C2C-C1C-NC	9.12	118.52	109.97
22	3	321	CLA	C1D-ND-C4D	-9.12	99.85	106.33
22	2	318	CLA	C1D-ND-C4D	-9.12	99.86	106.33
22	B	821	CLA	C1D-ND-C4D	-9.11	99.86	106.33
22	A	851	CLA	C2B-C1B-NB	9.11	116.34	110.23
22	Y	308	CLA	C1D-ND-C4D	-9.11	99.87	106.33
22	4	304	CLA	C1D-ND-C4D	-9.09	99.88	106.33
22	B	829	CLA	C2B-C1B-NB	9.09	116.33	110.23
22	K	205	CLA	C2B-C1B-NB	9.09	116.33	110.23
22	2	307	CLA	C1D-ND-C4D	-9.09	99.88	106.33
22	4	315	CLA	C1D-ND-C4D	-9.07	99.89	106.33
22	B	815	CLA	C2B-C1B-NB	9.06	116.31	110.23
22	L	305	CLA	C1D-ND-C4D	-9.06	99.90	106.33
22	3	320	CLA	C1D-ND-C4D	-9.05	99.91	106.33
22	B	828	CLA	C2C-C1C-NC	9.05	118.45	109.97
22	B	808	CLA	C1D-ND-C4D	-9.05	99.91	106.33
22	B	847	CLA	C1D-ND-C4D	-9.04	99.91	106.33
22	B	826	CLA	CMD-C2D-C1D	9.03	140.62	124.71
22	A	848	CLA	CMD-C2D-C1D	9.02	140.62	124.71
22	A	839	CLA	C2B-C1B-NB	9.02	116.28	110.23
22	4	315	CLA	C2B-C1B-NB	9.02	116.28	110.23
22	A	810	CLA	C1D-ND-C4D	-9.01	99.93	106.33
22	4	310	CLA	C2C-C1C-NC	9.01	118.42	109.97
25	B	840	BCR	C16-C15-C14	9.01	141.94	123.47
22	Y	301	CLA	C1D-ND-C4D	-9.00	99.94	106.33
22	A	846	CLA	C2B-C1B-NB	9.00	116.27	110.23
22	O	206	CLA	C1D-ND-C4D	-9.00	99.94	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	826	CLA	C2B-C1B-NB	9.00	116.27	110.23
22	A	848	CLA	C1D-ND-C4D	-9.00	99.94	106.33
22	3	319	CLA	C1D-ND-C4D	-9.00	99.94	106.33
22	3	316	CLA	C1D-ND-C4D	-9.00	99.94	106.33
22	2	304	CLA	C1D-ND-C4D	-9.00	99.94	106.33
22	A	857	CLA	C1D-ND-C4D	-8.98	99.95	106.33
22	B	821	CLA	C2B-C1B-NB	8.98	116.25	110.23
22	A	854	CLA	C2B-C1B-NB	8.98	116.25	110.23
22	A	833	CLA	C2B-C1B-NB	8.97	116.24	110.23
22	3	318	CLA	C1D-ND-C4D	-8.97	99.97	106.33
22	B	852	CLA	C2B-C1B-NB	8.96	116.24	110.23
22	2	322	CLA	C1D-ND-C4D	-8.96	99.97	106.33
22	A	812	CLA	C2B-C1B-NB	8.94	116.23	110.23
22	1	308	CLA	C2B-C1B-NB	8.93	116.22	110.23
22	B	817	CLA	C1D-ND-C4D	-8.93	99.99	106.33
22	A	807	CLA	C2B-C1B-NB	8.92	116.21	110.23
22	2	320	CLA	C1D-ND-C4D	-8.92	100.00	106.33
22	3	316	CLA	C2B-C1B-NB	8.91	116.21	110.23
24	3	302	XAT	C35-C34-C33	8.90	140.02	127.31
22	4	306	CLA	C2B-C1B-NB	8.90	116.20	110.23
24	3	302	XAT	C15-C35-C34	-8.90	105.25	123.47
22	A	827	CLA	C2B-C1B-NB	8.89	116.19	110.23
22	4	306	CLA	C1D-ND-C4D	-8.89	100.02	106.33
22	K	202	CLA	C1D-ND-C4D	-8.88	100.02	106.33
22	X	310	CLA	C1D-ND-C4D	-8.88	100.03	106.33
22	A	808	CLA	C2B-C1B-NB	8.88	116.19	110.23
30	A	825	CL0	C2B-C1B-NB	8.88	116.18	110.23
22	Z	306	CLA	C2B-C1B-NB	8.88	116.18	110.23
22	A	837	CLA	C2B-C1B-NB	8.87	116.18	110.23
22	B	822	CLA	C1D-ND-C4D	-8.87	100.03	106.33
22	B	827	CLA	C1D-ND-C4D	-8.85	100.05	106.33
22	A	806	CLA	C1D-ND-C4D	-8.84	100.05	106.33
22	A	857	CLA	C2B-C1B-NB	8.84	116.16	110.23
22	A	856	CLA	C2B-C1B-NB	8.84	116.16	110.23
22	A	828	CLA	C2C-C1C-NC	8.82	118.24	109.97
22	1	320	CLA	C2C-C1C-NC	8.82	118.23	109.97
22	B	816	CLA	CHD-C4C-C3C	-8.80	111.91	124.84
22	B	829	CLA	C1D-ND-C4D	-8.79	100.09	106.33
22	2	305	CLA	C2B-C1B-NB	8.79	116.12	110.23
22	3	319	CLA	C2B-C1B-NB	8.79	116.12	110.23
22	B	801	CLA	CHD-C4C-C3C	-8.79	111.93	124.84
24	2	311	XAT	C11-C10-C9	-8.78	114.78	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	825	CLA	C2B-C1B-NB	8.78	116.12	110.23
22	B	853	CLA	C1D-ND-C4D	-8.78	100.10	106.33
22	1	319	CLA	C1D-ND-C4D	-8.77	100.11	106.33
22	B	845	CLA	C1D-ND-C4D	-8.77	100.11	106.33
22	B	823	CLA	C2B-C1B-NB	8.77	116.11	110.23
22	4	318	CLA	C2B-C1B-NB	8.76	116.11	110.23
22	A	844	CLA	C2C-C1C-NC	8.76	118.18	109.97
22	2	308	CLA	C2B-C1B-NB	8.75	116.10	110.23
22	B	846	CLA	C1D-ND-C4D	-8.75	100.12	106.33
22	Z	306	CLA	C2C-C1C-NC	8.75	118.17	109.97
22	Z	314	CLA	C1D-ND-C4D	-8.74	100.13	106.33
22	B	804	CLA	C2B-C1B-NB	8.74	116.09	110.23
22	1	319	CLA	C2B-C1B-NB	8.73	116.09	110.23
22	L	305	CLA	C2B-C1B-NB	8.73	116.09	110.23
22	1	320	CLA	C1D-ND-C4D	-8.73	100.13	106.33
23	4	322	LUT	C15-C35-C34	8.73	141.35	123.47
22	X	310	CLA	C2B-C1B-NB	8.73	116.08	110.23
22	B	850	CLA	C2B-C1B-NB	8.72	116.08	110.23
22	B	816	CLA	C4A-NA-C1A	8.72	110.63	106.71
22	B	809	CLA	C1D-ND-C4D	-8.71	100.15	106.33
22	4	314	CLA	C2C-C1C-NC	8.70	118.12	109.97
22	B	831	CLA	C2B-C1B-NB	8.70	116.06	110.23
22	A	850	CLA	C2C-C1C-NC	8.70	118.12	109.97
22	3	317	CLA	C2B-C1B-NB	8.70	116.06	110.23
22	Z	314	CLA	C2B-C1B-NB	8.69	116.06	110.23
22	1	303	CLA	C2C-C1C-NC	8.69	118.11	109.97
22	4	313	CLA	C2C-C1C-NC	8.69	118.11	109.97
22	B	804	CLA	C1D-ND-C4D	-8.69	100.17	106.33
22	Y	311	CLA	C2B-C1B-NB	8.68	116.05	110.23
22	A	849	CLA	C2C-C1C-NC	8.68	118.11	109.97
22	4	316	CLA	C2C-C1C-NC	8.67	118.10	109.97
22	B	847	CLA	C2B-C1B-NB	8.67	116.05	110.23
22	A	805	CLA	C1D-ND-C4D	-8.67	100.18	106.33
22	A	832	CLA	C2C-C1C-NC	8.67	118.09	109.97
22	A	839	CLA	C1D-ND-C4D	-8.66	100.18	106.33
22	A	804	CLA	C2C-C1C-NC	8.66	118.08	109.97
22	3	318	CLA	C2C-C1C-NC	8.66	118.08	109.97
22	B	810	CLA	C2C-C1C-NC	8.65	118.08	109.97
22	B	808	CLA	C2C-C1C-NC	8.65	118.07	109.97
22	A	836	CLA	C2B-C1B-NB	8.64	116.03	110.23
22	B	830	CLA	C1D-ND-C4D	-8.64	100.20	106.33
22	O	207	CLA	C1D-ND-C4D	-8.63	100.20	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	845	CLA	C2C-C1C-NC	8.63	118.05	109.97
22	B	802	CLA	C2C-C1C-NC	8.62	118.04	109.97
22	4	313	CLA	C2B-C1B-NB	8.62	116.01	110.23
22	B	850	CLA	C1D-ND-C4D	-8.61	100.22	106.33
22	B	806	CLA	C2B-C1B-NB	8.61	116.01	110.23
22	Y	312	CLA	C2B-C1B-NB	8.61	116.01	110.23
22	3	312	CLA	CMD-C2D-C1D	8.60	139.88	124.71
22	2	317	CLA	C2B-C1B-NB	8.59	115.99	110.23
22	B	852	CLA	C1D-ND-C4D	-8.59	100.23	106.33
22	A	837	CLA	C2C-C1C-NC	8.59	118.02	109.97
21	4	308	CHL	CMD-C2D-C1D	8.58	139.84	124.71
22	Z	313	CLA	C2B-C1B-NB	8.58	115.98	110.23
22	A	843	CLA	C2B-C1B-NB	8.57	115.98	110.23
22	A	835	CLA	C2C-C1C-NC	8.57	118.00	109.97
22	1	321	CLA	C2B-C1B-NB	8.56	115.97	110.23
22	X	310	CLA	C2C-C1C-NC	8.56	117.99	109.97
22	O	209	CLA	C2B-C1B-NB	8.55	115.97	110.23
22	B	819	CLA	CMD-C2D-C1D	8.55	139.78	124.71
22	Z	309	CLA	C2B-C1B-NB	8.55	115.96	110.23
22	4	304	CLA	C2B-C1B-NB	8.54	115.96	110.23
22	2	303	CLA	C2C-C1C-NC	8.54	117.97	109.97
22	2	318	CLA	C2B-C1B-NB	8.54	115.96	110.23
21	2	321	CHL	CMD-C2D-C1D	8.54	139.76	124.71
22	Z	306	CLA	C1D-ND-C4D	-8.53	100.27	106.33
21	3	307	CHL	CMD-C2D-C1D	8.53	139.75	124.71
22	A	801	CLA	C2C-C1C-NC	8.53	117.96	109.97
22	B	805	CLA	C2B-C1B-NB	8.52	115.95	110.23
22	A	848	CLA	C2C-C1C-NC	8.52	117.96	109.97
22	G	206	CLA	CMD-C2D-C1D	8.52	139.73	124.71
21	2	302	CHL	CMD-C2D-C1D	8.52	139.73	124.71
22	X	313	CLA	C2B-C1B-NB	8.52	115.94	110.23
21	3	314	CHL	CMD-C2D-C1D	8.52	139.72	124.71
21	X	308	CHL	CMD-C2D-C1D	8.51	139.72	124.71
22	3	320	CLA	C2C-C1C-NC	8.51	117.94	109.97
22	Y	312	CLA	C2C-C1C-NC	8.50	117.94	109.97
22	3	317	CLA	C2C-C1C-NC	8.50	117.93	109.97
22	3	308	CLA	C2B-C1B-NB	8.49	115.93	110.23
22	1	320	CLA	CMD-C2D-C1D	8.49	139.67	124.71
22	O	207	CLA	C2C-C1C-NC	8.48	117.92	109.97
22	Y	308	CLA	C2B-C1B-NB	8.48	115.92	110.23
22	B	816	CLA	C3C-C4C-NC	8.48	120.08	110.57
22	Z	311	CLA	C2B-C1B-NB	8.48	115.92	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	827	CLA	C2C-C1C-NC	8.48	117.91	109.97
22	O	208	CLA	C2C-C1C-NC	8.47	117.91	109.97
22	G	207	CLA	C2C-C1C-NC	8.47	117.90	109.97
22	A	837	CLA	CMD-C2D-C1D	8.46	139.62	124.71
22	A	839	CLA	C2C-C1C-NC	8.46	117.90	109.97
22	O	206	CLA	C2C-C1C-NC	8.46	117.90	109.97
22	B	819	CLA	C1D-ND-C4D	-8.46	100.33	106.33
22	Y	308	CLA	C2C-C1C-NC	8.46	117.89	109.97
22	X	303	CLA	C2B-C1B-NB	8.45	115.90	110.23
22	B	824	CLA	CMD-C2D-C1D	8.45	139.61	124.71
22	K	202	CLA	C2C-C1C-NC	8.45	117.89	109.97
22	B	816	CLA	C2C-C1C-NC	8.44	117.88	109.97
22	Y	314	CLA	C2C-C1C-NC	8.44	117.88	109.97
22	3	313	CLA	C2B-C1B-NB	8.44	115.89	110.23
22	A	840	CLA	C2B-C1B-NB	8.43	115.89	110.23
22	A	849	CLA	C2B-C1B-NB	8.43	115.88	110.23
22	A	845	CLA	CMD-C2D-C1D	8.42	139.55	124.71
22	O	210	CLA	C2B-C1B-NB	8.41	115.87	110.23
22	A	846	CLA	C1D-ND-C4D	-8.40	100.36	106.33
21	4	307	CHL	CMD-C2D-C1D	8.40	139.51	124.71
22	Y	301	CLA	CMD-C2D-C1D	8.39	139.51	124.71
22	K	205	CLA	C1D-ND-C4D	-8.39	100.38	106.33
22	A	841	CLA	C2C-C1C-NC	8.39	117.83	109.97
22	Y	301	CLA	C2C-C1C-NC	8.38	117.83	109.97
22	N	202	CLA	C2C-C1C-NC	8.38	117.83	109.97
22	4	311	CLA	C1D-ND-C4D	-8.38	100.38	106.33
22	3	321	CLA	C2B-C1B-NB	8.38	115.85	110.23
22	Z	307	CLA	C2B-C1B-NB	8.38	115.85	110.23
22	X	304	CLA	C2A-C1A-CHA	-8.38	109.21	123.86
22	N	202	CLA	C2B-C1B-NB	8.37	115.84	110.23
22	3	319	CLA	C2C-C1C-NC	8.37	117.81	109.97
22	2	303	CLA	C2B-C1B-NB	8.37	115.84	110.23
22	L	306	CLA	C2B-C1B-NB	8.36	115.84	110.23
22	A	847	CLA	C2C-C1C-NC	8.36	117.81	109.97
22	3	312	CLA	C2B-C1B-NB	8.36	115.84	110.23
22	B	812	CLA	C1D-ND-C4D	-8.36	100.40	106.33
22	B	817	CLA	C2B-C1B-NB	8.36	115.83	110.23
22	O	207	CLA	C2B-C1B-NB	8.35	115.83	110.23
21	Y	306	CHL	CMD-C2D-C1D	8.35	139.42	124.71
22	Z	308	CLA	C2B-C1B-NB	8.34	115.82	110.23
21	Z	302	CHL	CMD-C2D-C1D	8.34	139.41	124.71
22	1	307	CLA	C2B-C1B-NB	8.34	115.82	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	321	CLA	CMD-C2D-C1D	8.33	139.40	124.71
22	X	312	CLA	C2B-C1B-NB	8.33	115.82	110.23
22	B	801	CLA	C3C-C4C-NC	8.33	119.91	110.57
22	Y	309	CLA	C2B-C1B-NB	8.33	115.81	110.23
21	Y	305	CHL	CMD-C2D-C1D	8.33	139.39	124.71
22	A	807	CLA	C2C-C1C-NC	8.32	117.77	109.97
21	2	309	CHL	CMD-C2D-C1D	8.32	139.37	124.71
21	X	306	CHL	CMD-C2D-C1D	8.32	139.37	124.71
22	Y	312	CLA	CMD-C2D-C1D	8.31	139.37	124.71
22	B	824	CLA	C2B-C1B-NB	8.31	115.80	110.23
22	A	849	CLA	C1D-ND-C4D	-8.31	100.43	106.33
22	B	825	CLA	C1D-ND-C4D	-8.31	100.43	106.33
21	Z	301	CHL	CMD-C2D-C1D	8.30	139.35	124.71
22	X	311	CLA	C2B-C1B-NB	8.30	115.80	110.23
21	X	305	CHL	CMD-C2D-C1D	8.30	139.33	124.71
22	Y	311	CLA	C2C-C1C-NC	8.30	117.74	109.97
22	A	842	CLA	C2B-C1B-NB	8.29	115.79	110.23
22	B	833	CLA	C2B-C1B-NB	8.29	115.79	110.23
22	B	811	CLA	C2C-C1C-NC	8.29	117.74	109.97
22	2	303	CLA	C1D-ND-C4D	-8.29	100.45	106.33
24	2	311	XAT	C7-C8-C9	-8.28	112.68	125.53
21	4	317	CHL	CMD-C2D-C1D	8.28	139.31	124.71
21	Y	303	CHL	CMD-C2D-C1D	8.28	139.31	124.71
21	Z	312	CHL	CMD-C2D-C1D	8.28	139.31	124.71
22	2	322	CLA	C2C-C1C-NC	8.28	117.73	109.97
22	B	849	CLA	C2C-C1C-NC	8.28	117.73	109.97
22	X	301	CLA	C2B-C1B-NB	8.28	115.78	110.23
22	Y	309	CLA	C2C-C1C-NC	8.28	117.73	109.97
22	3	320	CLA	C2B-C1B-NB	8.28	115.78	110.23
21	X	309	CHL	CMD-C2D-C1D	8.27	139.29	124.71
22	Y	302	CLA	C2B-C1B-NB	8.27	115.78	110.23
21	Z	303	CHL	CMD-C2D-C1D	8.27	139.28	124.71
22	Z	314	CLA	C2C-C1C-NC	8.26	117.71	109.97
22	Z	308	CLA	C2C-C1C-NC	8.26	117.71	109.97
22	2	320	CLA	C2C-C1C-NC	8.25	117.70	109.97
22	B	829	CLA	CMD-C2D-C1D	8.25	139.25	124.71
22	J	102	CLA	C2B-C1B-NB	8.25	115.76	110.23
22	Z	310	CLA	C2B-C1B-NB	8.24	115.76	110.23
22	Z	311	CLA	C2C-C1C-NC	8.24	117.69	109.97
22	Y	301	CLA	C2B-C1B-NB	8.24	115.76	110.23
22	G	207	CLA	C1D-ND-C4D	-8.24	100.48	106.33
22	A	843	CLA	CMD-C2D-C1D	8.24	139.23	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	K	203	CLA	C2B-C1B-NB	8.24	115.75	110.23
22	1	309	CLA	C2B-C1B-NB	8.24	115.75	110.23
22	4	312	CLA	C2B-C1B-NB	8.23	115.75	110.23
22	A	805	CLA	CMD-C2D-C1D	8.23	139.21	124.71
22	L	307	CLA	C2B-C1B-NB	8.23	115.75	110.23
22	X	301	CLA	C2C-C1C-NC	8.22	117.68	109.97
22	A	856	CLA	C1D-ND-C4D	-8.22	100.49	106.33
22	B	828	CLA	CMD-C2D-C1D	8.22	139.21	124.71
21	X	307	CHL	CMD-C2D-C1D	8.22	139.20	124.71
22	3	316	CLA	C2C-C1C-NC	8.22	117.67	109.97
22	2	322	CLA	C2B-C1B-NB	8.21	115.74	110.23
22	A	841	CLA	CMD-C2D-C1D	8.21	139.18	124.71
22	J	102	CLA	C2C-C1C-NC	8.21	117.66	109.97
22	A	809	CLA	C2C-C1C-NC	8.21	117.66	109.97
22	B	852	CLA	C2C-C1C-NC	8.21	117.66	109.97
21	2	301	CHL	CMD-C2D-C1D	8.20	139.17	124.71
22	4	305	CLA	CMD-C2D-C1D	8.20	139.17	124.71
22	X	303	CLA	CMD-C2D-C1D	8.20	139.16	124.71
22	F	305	CLA	C2C-C1C-NC	8.19	117.65	109.97
21	Y	304	CHL	CMD-C2D-C1D	8.19	139.16	124.71
22	3	309	CLA	C2B-C1B-NB	8.19	115.72	110.23
21	Z	305	CHL	CMD-C2D-C1D	8.19	139.15	124.71
22	2	305	CLA	C1D-ND-C4D	-8.19	100.52	106.33
22	3	313	CLA	C2C-C1C-NC	8.19	117.64	109.97
22	X	303	CLA	C2C-C1C-NC	8.19	117.64	109.97
22	A	801	CLA	C1D-ND-C4D	-8.18	100.52	106.33
22	B	833	CLA	CMD-C2D-C1D	8.18	139.13	124.71
21	Z	304	CHL	CMD-C2D-C1D	8.18	139.13	124.71
22	1	317	CLA	CMD-C2D-C1D	8.18	139.13	124.71
22	1	305	CLA	C2B-C1B-NB	8.18	115.72	110.23
22	A	829	CLA	C1D-ND-C4D	-8.18	100.52	106.33
22	O	209	CLA	C2C-C1C-NC	8.18	117.64	109.97
22	X	313	CLA	C2C-C1C-NC	8.18	117.63	109.97
22	B	847	CLA	CMD-C2D-C1D	8.18	139.13	124.71
22	A	838	CLA	C2C-C1C-NC	8.18	117.63	109.97
22	J	102	CLA	CMD-C2D-C1D	8.17	139.12	124.71
22	B	811	CLA	CMD-C2D-C1D	8.17	139.12	124.71
22	B	821	CLA	C2C-C1C-NC	8.17	117.63	109.97
22	X	311	CLA	C2C-C1C-NC	8.17	117.63	109.97
22	B	849	CLA	C2B-C1B-NB	8.17	115.71	110.23
22	A	859	CLA	CMD-C2D-C1D	8.17	139.10	124.71
30	A	825	CL0	C2C-C1C-NC	8.16	117.62	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	310	CLA	C2C-C1C-NC	8.16	117.62	109.97
22	A	835	CLA	CMD-C2D-C1D	8.16	139.10	124.71
22	B	848	CLA	C2B-C1B-NB	8.16	115.70	110.23
22	1	302	CLA	C2C-C1C-NC	8.16	117.62	109.97
22	Z	307	CLA	C2C-C1C-NC	8.16	117.62	109.97
22	Z	310	CLA	C2C-C1C-NC	8.16	117.61	109.97
22	2	304	CLA	C2B-C1B-NB	8.15	115.70	110.23
22	Y	302	CLA	C2C-C1C-NC	8.15	117.61	109.97
22	O	206	CLA	C2B-C1B-NB	8.15	115.70	110.23
22	1	309	CLA	C2C-C1C-NC	8.15	117.61	109.97
22	Y	310	CLA	C2C-C1C-NC	8.15	117.60	109.97
22	B	848	CLA	CMD-C2D-C1D	8.15	139.07	124.71
24	4	320	XAT	O4-C5-C4	8.14	119.50	113.38
22	Z	309	CLA	C2C-C1C-NC	8.14	117.60	109.97
22	O	206	CLA	CMD-C2D-C1D	8.14	139.06	124.71
22	4	318	CLA	C2C-C1C-NC	8.14	117.59	109.97
22	1	302	CLA	C2B-C1B-NB	8.14	115.69	110.23
22	Y	314	CLA	C2B-C1B-NB	8.14	115.69	110.23
22	2	305	CLA	C2C-C1C-NC	8.13	117.59	109.97
22	X	312	CLA	C2C-C1C-NC	8.13	117.59	109.97
22	A	829	CLA	CMD-C2D-C1D	8.13	139.04	124.71
22	B	816	CLA	CMD-C2D-C1D	8.13	139.04	124.71
22	B	819	CLA	C2C-C1C-NC	8.13	117.59	109.97
22	A	856	CLA	C2C-C1C-NC	8.13	117.58	109.97
21	4	309	CHL	CMD-C2D-C1D	8.13	139.03	124.71
21	3	307	CHL	C2C-C3C-C4C	-8.13	100.70	106.49
22	2	308	CLA	C2C-C1C-NC	8.12	117.58	109.97
22	1	317	CLA	C2B-C1B-NB	8.12	115.67	110.23
22	A	858	CLA	C2C-C1C-NC	8.12	117.58	109.97
22	B	825	CLA	CMD-C2D-C1D	8.12	139.02	124.71
22	O	208	CLA	C2B-C1B-NB	8.11	115.67	110.23
22	3	308	CLA	CMD-C2D-C1D	8.11	139.01	124.71
22	2	319	CLA	CMD-C2D-C1D	8.11	139.01	124.71
22	L	307	CLA	CMD-C2D-C1D	8.11	139.00	124.71
22	3	317	CLA	CMD-C2D-C1D	8.10	138.99	124.71
22	Y	310	CLA	C2B-C1B-NB	8.09	115.66	110.23
22	B	853	CLA	CMD-C2D-C1D	8.09	138.97	124.71
22	A	847	CLA	C2B-C1B-NB	8.09	115.66	110.23
22	F	306	CLA	C2B-C1B-NB	8.09	115.66	110.23
22	A	808	CLA	C2C-C1C-NC	8.09	117.55	109.97
22	H	201	CLA	CMD-C2D-C1D	8.09	138.97	124.71
22	X	313	CLA	CMD-C2D-C1D	8.08	138.96	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2	320	CLA	CMD-C2D-C1D	8.08	138.96	124.71
22	A	804	CLA	C2B-C1B-NB	8.08	115.65	110.23
22	4	311	CLA	CMD-C2D-C1D	8.08	138.95	124.71
22	4	318	CLA	CMD-C2D-C1D	8.08	138.95	124.71
22	A	853	CLA	C1D-ND-C4D	-8.07	100.60	106.33
21	Y	307	CHL	CMD-C2D-C1D	8.07	138.94	124.71
22	K	205	CLA	C2C-C1C-NC	8.07	117.53	109.97
22	1	306	CLA	C2C-C1C-NC	8.07	117.53	109.97
21	Y	313	CHL	CMD-C2D-C1D	8.07	138.93	124.71
22	G	206	CLA	C2C-C1C-NC	8.06	117.53	109.97
22	A	831	CLA	C2C-C1C-NC	8.06	117.52	109.97
22	O	208	CLA	CMD-C2D-C1D	8.06	138.92	124.71
22	A	848	CLA	C2B-C1B-NB	8.06	115.64	110.23
22	1	308	CLA	CMD-C2D-C1D	8.06	138.91	124.71
22	Y	308	CLA	CMD-C2D-C1D	8.06	138.91	124.71
22	3	311	CLA	C2B-C1B-NB	8.06	115.63	110.23
22	Y	314	CLA	CMD-C2D-C1D	8.05	138.91	124.71
22	K	205	CLA	CMD-C2D-C1D	8.05	138.91	124.71
25	A	816	BCR	C16-C15-C14	8.05	139.97	123.47
22	2	322	CLA	CMD-C2D-C1D	8.05	138.90	124.71
22	A	804	CLA	CMD-C2D-C1D	8.05	138.90	124.71
22	A	835	CLA	C1D-ND-C4D	-8.05	100.62	106.33
22	1	309	CLA	CMD-C2D-C1D	8.05	138.90	124.71
22	K	202	CLA	CMD-C2D-C1D	8.05	138.90	124.71
22	B	833	CLA	C2C-C1C-NC	8.04	117.51	109.97
22	B	822	CLA	CMD-C2D-C1D	8.04	138.88	124.71
22	B	818	CLA	C2B-C1B-NB	8.04	115.62	110.23
22	B	809	CLA	C2C-C1C-NC	8.04	117.50	109.97
22	A	809	CLA	C2B-C1B-NB	8.04	115.62	110.23
21	X	302	CHL	CMD-C2D-C1D	8.03	138.87	124.71
22	2	307	CLA	C2B-C1B-NB	8.03	115.62	110.23
22	Z	313	CLA	C2C-C1C-NC	8.03	117.50	109.97
22	3	312	CLA	C2C-C1C-NC	8.03	117.50	109.97
22	3	320	CLA	CMD-C2D-C1D	8.03	138.86	124.71
22	Z	311	CLA	CMD-C2D-C1D	8.03	138.86	124.71
22	A	841	CLA	C2B-C1B-NB	8.03	115.61	110.23
22	H	201	CLA	C2B-C1B-NB	8.02	115.61	110.23
22	Y	310	CLA	CMD-C2D-C1D	8.02	138.85	124.71
22	Z	314	CLA	CMD-C2D-C1D	8.02	138.85	124.71
22	2	317	CLA	C2C-C1C-NC	8.02	117.48	109.97
22	B	824	CLA	C2C-C1C-NC	8.02	117.48	109.97
22	Y	311	CLA	CMD-C2D-C1D	8.02	138.84	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Z	307	CLA	CMD-C2D-C1D	8.01	138.84	124.71
22	G	206	CLA	C2B-C1B-NB	8.01	115.60	110.23
22	Z	308	CLA	CMD-C2D-C1D	8.01	138.83	124.71
22	B	808	CLA	CMD-C2D-C1D	8.01	138.83	124.71
22	B	806	CLA	C2C-C1C-NC	8.01	117.47	109.97
22	B	801	CLA	C2B-C1B-NB	8.01	115.60	110.23
22	1	306	CLA	C2B-C1B-NB	8.00	115.60	110.23
22	2	317	CLA	CMD-C2D-C1D	8.00	138.82	124.71
22	2	307	CLA	C2C-C1C-NC	8.00	117.47	109.97
22	2	318	CLA	C2C-C1C-NC	8.00	117.47	109.97
22	X	310	CLA	CMD-C2D-C1D	8.00	138.81	124.71
22	B	814	CLA	C2B-C1B-NB	8.00	115.59	110.23
22	B	853	CLA	C2C-C1C-NC	8.00	117.46	109.97
22	Y	302	CLA	CMD-C2D-C1D	7.99	138.80	124.71
22	A	810	CLA	C2C-C1C-NC	7.99	117.46	109.97
22	Z	313	CLA	CMD-C2D-C1D	7.99	138.80	124.71
22	Y	309	CLA	CMD-C2D-C1D	7.99	138.79	124.71
22	1	318	CLA	C2C-C1C-NC	7.99	117.45	109.97
22	1	321	CLA	C2C-C1C-NC	7.98	117.45	109.97
22	O	209	CLA	CMD-C2D-C1D	7.98	138.78	124.71
22	4	310	CLA	C1D-ND-C4D	-7.98	100.67	106.33
22	A	857	CLA	CMD-C2D-C1D	7.98	138.77	124.71
22	3	313	CLA	CMD-C2D-C1D	7.98	138.77	124.71
22	A	839	CLA	CMD-C2D-C1D	7.98	138.77	124.71
22	A	812	CLA	CMD-C2D-C1D	7.97	138.77	124.71
22	A	852	CLA	C2B-C1B-NB	7.97	115.58	110.23
22	Z	306	CLA	CMD-C2D-C1D	7.97	138.76	124.71
22	A	832	CLA	CMD-C2D-C1D	7.97	138.75	124.71
22	B	821	CLA	CMD-C2D-C1D	7.97	138.75	124.71
22	L	305	CLA	C2C-C1C-NC	7.97	117.44	109.97
22	A	835	CLA	C2B-C1B-NB	7.97	115.57	110.23
22	1	302	CLA	CMD-C2D-C1D	7.96	138.75	124.71
22	X	312	CLA	CMD-C2D-C1D	7.96	138.73	124.71
22	3	310	CLA	C2B-C1B-NB	7.95	115.56	110.23
22	B	826	CLA	CHD-C4C-C3C	-7.95	113.16	124.84
22	G	207	CLA	CMD-C2D-C1D	7.94	138.72	124.71
22	F	306	CLA	C2C-C1C-NC	7.94	117.41	109.97
22	G	205	CLA	CMD-C2D-C1D	7.94	138.71	124.71
22	B	825	CLA	C2C-C1C-NC	7.94	117.41	109.97
22	A	803	CLA	C2B-C1B-NB	7.93	115.55	110.23
22	B	809	CLA	C2B-C1B-NB	7.93	115.55	110.23
22	3	319	CLA	CMD-C2D-C1D	7.93	138.69	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	846	CLA	CMD-C2D-C1D	7.93	138.68	124.71
22	4	313	CLA	CMD-C2D-C1D	7.92	138.68	124.71
22	Z	309	CLA	CMD-C2D-C1D	7.92	138.68	124.71
22	A	803	CLA	C2C-C1C-NC	7.92	117.39	109.97
22	B	853	CLA	C2B-C1B-NB	7.92	115.54	110.23
22	B	818	CLA	C2C-C1C-NC	7.92	117.39	109.97
22	3	309	CLA	CMD-C2D-C1D	7.92	138.67	124.71
22	1	318	CLA	C2B-C1B-NB	7.92	115.54	110.23
25	O	203	BCR	C16-C15-C14	7.91	139.68	123.47
22	K	202	CLA	C2B-C1B-NB	7.91	115.53	110.23
22	B	826	CLA	C2C-C1C-NC	7.90	117.37	109.97
22	2	306	CLA	C2C-C1C-NC	7.90	117.37	109.97
22	L	305	CLA	CMD-C2D-C1D	7.90	138.63	124.71
22	3	311	CLA	CMD-C2D-C1D	7.90	138.63	124.71
22	4	304	CLA	C2C-C1C-NC	7.90	117.37	109.97
22	A	833	CLA	CMD-C2D-C1D	7.89	138.62	124.71
22	4	315	CLA	C2C-C1C-NC	7.89	117.36	109.97
22	B	852	CLA	CMD-C2D-C1D	7.89	138.62	124.71
22	K	204	CLA	C2C-C1C-NC	7.89	117.36	109.97
22	B	813	CLA	C2B-C1B-NB	7.88	115.52	110.23
22	B	823	CLA	C2C-C1C-NC	7.88	117.35	109.97
22	B	822	CLA	C2C-C1C-NC	7.87	117.35	109.97
22	2	318	CLA	CMD-C2D-C1D	7.87	138.58	124.71
22	A	805	CLA	C2C-C1C-NC	7.87	117.34	109.97
22	B	806	CLA	CMD-C2D-C1D	7.87	138.58	124.71
22	2	307	CLA	CMD-C2D-C1D	7.87	138.58	124.71
22	A	840	CLA	C2C-C1C-NC	7.87	117.34	109.97
22	Z	310	CLA	CMD-C2D-C1D	7.86	138.56	124.71
22	1	306	CLA	CMD-C2D-C1D	7.85	138.55	124.71
22	4	316	CLA	C2B-C1B-NB	7.85	115.50	110.23
22	A	831	CLA	CMD-C2D-C1D	7.85	138.54	124.71
22	B	803	CLA	CMD-C2D-C1D	7.84	138.53	124.71
22	A	853	CLA	CMD-C2D-C1D	7.84	138.53	124.71
22	B	812	CLA	CMD-C2D-C1D	7.84	138.52	124.71
22	B	803	CLA	C3C-C4C-NC	7.83	119.36	110.57
22	O	210	CLA	C2C-C1C-NC	7.83	117.31	109.97
22	A	827	CLA	C2C-C1C-NC	7.83	117.31	109.97
22	A	838	CLA	CMD-C2D-C1D	7.82	138.50	124.71
22	H	201	CLA	C2C-C1C-NC	7.82	117.30	109.97
23	4	322	LUT	C35-C15-C14	7.82	139.49	123.47
22	1	318	CLA	CMD-C2D-C1D	7.82	138.49	124.71
22	A	852	CLA	CHD-C4C-C3C	-7.82	113.35	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	828	CLA	C2B-C1B-NB	7.81	115.47	110.23
22	3	321	CLA	C2C-C1C-NC	7.81	117.29	109.97
22	A	802	CLA	C2B-C1B-NB	7.81	115.47	110.23
21	2	301	CHL	C2C-C3C-C4C	-7.80	100.93	106.49
22	3	310	CLA	CMD-C2D-C1D	7.80	138.46	124.71
22	4	312	CLA	C2C-C1C-NC	7.80	117.28	109.97
22	A	832	CLA	C2B-C1B-NB	7.80	115.46	110.23
22	G	205	CLA	C2C-C1C-NC	7.80	117.28	109.97
22	A	856	CLA	CMD-C2D-C1D	7.80	138.45	124.71
23	4	322	LUT	C7-C8-C9	7.80	138.01	126.23
22	1	319	CLA	CMD-C2D-C1D	7.79	138.45	124.71
25	O	202	BCR	C24-C23-C22	7.79	138.01	126.23
22	A	855	CLA	C1D-ND-C4D	-7.79	100.80	106.33
22	1	321	CLA	CMD-C2D-C1D	7.79	138.44	124.71
22	X	311	CLA	CMD-C2D-C1D	7.79	138.44	124.71
22	B	810	CLA	C2B-C1B-NB	7.79	115.45	110.23
22	K	203	CLA	CMD-C2D-C1D	7.78	138.43	124.71
22	A	833	CLA	C2C-C1C-NC	7.78	117.26	109.97
22	F	305	CLA	CMD-C2D-C1D	7.78	138.42	124.71
22	B	807	CLA	C2C-C1C-NC	7.78	117.26	109.97
22	A	807	CLA	CMD-C2D-C1D	7.78	138.42	124.71
22	A	806	CLA	C2C-C1C-NC	7.78	117.26	109.97
22	N	202	CLA	CMD-C2D-C1D	7.77	138.41	124.71
22	1	307	CLA	CMD-C2D-C1D	7.77	138.40	124.71
22	A	830	CLA	CMD-C2D-C1D	7.77	138.40	124.71
22	B	827	CLA	CMD-C2D-C1D	7.76	138.40	124.71
22	B	811	CLA	C2B-C1B-NB	7.76	115.44	110.23
22	A	851	CLA	CMD-C2D-C1D	7.76	138.39	124.71
22	2	305	CLA	O2D-CGD-CBD	7.76	125.06	111.27
22	L	306	CLA	C2C-C1C-NC	7.75	117.23	109.97
22	3	318	CLA	C2B-C1B-NB	7.75	115.43	110.23
22	F	305	CLA	C2B-C1B-NB	7.75	115.43	110.23
22	A	806	CLA	CMD-C2D-C1D	7.75	138.37	124.71
22	2	306	CLA	C2B-C1B-NB	7.74	115.42	110.23
22	B	803	CLA	C2C-C1C-NC	7.73	117.22	109.97
22	B	803	CLA	C2B-C1B-NB	7.73	115.42	110.23
22	B	805	CLA	CMD-C2D-C1D	7.73	138.34	124.71
22	1	319	CLA	C2C-C1C-NC	7.73	117.21	109.97
22	A	836	CLA	CMD-C2D-C1D	7.73	138.33	124.71
22	A	809	CLA	CMD-C2D-C1D	7.73	138.33	124.71
22	A	802	CLA	CMD-C2D-C1D	7.73	138.33	124.71
22	B	831	CLA	C2C-C1C-NC	7.72	117.21	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	807	CLA	C4C-NC-C1C	-7.72	99.85	106.27
22	1	305	CLA	C2C-C1C-NC	7.72	117.21	109.97
22	4	305	CLA	C2B-C1B-NB	7.71	115.40	110.23
22	G	207	CLA	C2B-C1B-NB	7.71	115.40	110.23
22	A	854	CLA	C2C-C1C-NC	7.71	117.19	109.97
22	A	846	CLA	CMD-C2D-C1D	7.70	138.29	124.71
21	Y	313	CHL	C2C-C3C-C4C	-7.70	101.00	106.49
22	1	303	CLA	CMD-C2D-C1D	7.70	138.28	124.71
22	1	320	CLA	C2B-C1B-NB	7.69	115.39	110.23
22	2	306	CLA	CMD-C2D-C1D	7.69	138.26	124.71
21	2	309	CHL	C2C-C3C-C4C	-7.68	101.01	106.49
22	A	834	CLA	C2C-C1C-NC	7.68	117.17	109.97
22	B	847	CLA	C2C-C1C-NC	7.68	117.17	109.97
22	X	301	CLA	CMD-C2D-C1D	7.67	138.23	124.71
22	K	203	CLA	C2C-C1C-NC	7.66	117.15	109.97
22	4	306	CLA	CMD-C2D-C1D	7.66	138.22	124.71
22	B	830	CLA	CMD-C2D-C1D	7.66	138.22	124.71
22	B	830	CLA	C2B-C1B-NB	7.66	115.37	110.23
22	4	316	CLA	CMD-C2D-C1D	7.66	138.21	124.71
22	4	310	CLA	C2B-C1B-NB	7.65	115.36	110.23
22	A	852	CLA	C2C-C1C-NC	7.65	117.14	109.97
22	A	802	CLA	C2C-C1C-NC	7.65	117.14	109.97
22	3	315	CLA	C1D-ND-C4D	-7.64	100.91	106.33
22	1	308	CLA	C2C-C1C-NC	7.64	117.13	109.97
22	A	847	CLA	CMD-C2D-C1D	7.63	138.16	124.71
22	B	815	CLA	CMD-C2D-C1D	7.63	138.16	124.71
22	B	820	CLA	CMD-C2D-C1D	7.63	138.16	124.71
22	B	818	CLA	C1D-ND-C4D	-7.62	100.92	106.33
22	3	315	CLA	C2B-C1B-NB	7.62	115.34	110.23
22	A	801	CLA	CMD-C2D-C1D	7.61	138.13	124.71
22	B	850	CLA	C2C-C1C-NC	7.61	117.11	109.97
22	B	817	CLA	C2C-C1C-NC	7.61	117.10	109.97
21	Y	304	CHL	C2C-C3C-C4C	-7.60	101.07	106.49
22	B	827	CLA	C2B-C1B-NB	7.60	115.33	110.23
22	O	207	CLA	CMD-C2D-C1D	7.60	138.11	124.71
24	2	311	XAT	O4-C5-C4	7.60	119.09	113.38
21	Z	302	CHL	C2C-C3C-C4C	-7.60	101.07	106.49
22	B	804	CLA	CMD-C2D-C1D	7.59	138.09	124.71
22	B	812	CLA	C2B-C1B-NB	7.59	115.32	110.23
22	B	848	CLA	C2C-C1C-NC	7.58	117.08	109.97
22	1	303	CLA	C2B-C1B-NB	7.58	115.31	110.23
22	B	849	CLA	CMD-C2D-C1D	7.58	138.06	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	810	CLA	CMD-C2D-C1D	7.57	138.06	124.71
22	O	210	CLA	CMD-C2D-C1D	7.57	138.06	124.71
21	1	301	CHL	C2C-C3C-C4C	-7.56	101.10	106.49
22	K	204	CLA	CMD-C2D-C1D	7.56	138.03	124.71
22	B	813	CLA	C2C-C1C-NC	7.55	117.05	109.97
22	A	844	CLA	C1D-ND-C4D	-7.55	100.97	106.33
21	2	321	CHL	C2C-C3C-C4C	-7.55	101.11	106.49
21	1	316	CHL	C2C-C3C-C4C	-7.54	101.11	106.49
22	A	853	CLA	C2C-C1C-NC	7.54	117.03	109.97
22	A	840	CLA	CMD-C2D-C1D	7.54	137.99	124.71
22	3	318	CLA	CMD-C2D-C1D	7.53	137.98	124.71
22	A	836	CLA	C2C-C1C-NC	7.52	117.02	109.97
22	A	838	CLA	C2B-C1B-NB	7.52	115.27	110.23
22	A	854	CLA	C1D-ND-C4D	-7.51	101.00	106.33
22	A	842	CLA	C2C-C1C-NC	7.50	117.00	109.97
21	Z	304	CHL	C2C-C3C-C4C	-7.49	101.15	106.49
25	1	312	BCR	C15-C16-C17	7.49	138.82	123.47
22	A	838	CLA	C3C-C4C-NC	7.49	118.97	110.57
22	B	809	CLA	CMD-C2D-C1D	7.49	137.91	124.71
21	Z	301	CHL	C2C-C3C-C4C	-7.49	101.15	106.49
22	B	805	CLA	C2C-C1C-NC	7.48	116.98	109.97
22	A	852	CLA	C3C-C4C-NC	7.48	118.96	110.57
22	B	851	CLA	C2B-C1B-NB	7.47	115.24	110.23
22	A	826	CLA	CHD-C4C-C3C	-7.47	113.86	124.84
21	Y	307	CHL	C2C-C3C-C4C	-7.46	101.17	106.49
22	A	834	CLA	CMD-C2D-C1D	7.46	137.86	124.71
22	A	852	CLA	CMD-C2D-C1D	7.46	137.86	124.71
21	X	308	CHL	C2C-C3C-C4C	-7.46	101.17	106.49
22	3	308	CLA	C2C-C1C-NC	7.45	116.95	109.97
22	4	311	CLA	C2C-C1C-NC	7.45	116.95	109.97
25	1	312	BCR	C7-C8-C9	7.44	137.48	126.23
21	4	308	CHL	C2C-C3C-C4C	-7.44	101.19	106.49
22	B	845	CLA	C2B-C1B-NB	7.43	115.22	110.23
22	4	312	CLA	CMD-C2D-C1D	7.43	137.81	124.71
22	A	812	CLA	C2C-C1C-NC	7.42	116.92	109.97
22	F	306	CLA	CMD-C2D-C1D	7.40	137.76	124.71
21	4	317	CHL	C2C-C3C-C4C	-7.40	101.21	106.49
22	3	316	CLA	CMD-C2D-C1D	7.40	137.75	124.71
22	A	859	CLA	C2C-C1C-NC	7.39	116.89	109.97
22	A	843	CLA	C2C-C1C-NC	7.38	116.89	109.97
22	3	309	CLA	C2C-C1C-NC	7.37	116.88	109.97
22	A	846	CLA	C2C-C1C-NC	7.37	116.88	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	X	305	CHL	C2C-C3C-C4C	-7.36	101.24	106.49
22	1	305	CLA	CMD-C2D-C1D	7.36	137.68	124.71
21	Y	303	CHL	C2C-C3C-C4C	-7.35	101.25	106.49
22	B	818	CLA	CMD-C2D-C1D	7.34	137.65	124.71
21	Z	312	CHL	C2C-C3C-C4C	-7.34	101.26	106.49
22	A	829	CLA	C2C-C1C-NC	7.34	116.84	109.97
22	A	857	CLA	C2C-C1C-NC	7.34	116.84	109.97
22	L	307	CLA	C2C-C1C-NC	7.33	116.84	109.97
22	A	831	CLA	C2B-C1B-NB	7.32	115.14	110.23
22	G	205	CLA	C2B-C1B-NB	7.32	115.14	110.23
21	X	307	CHL	C2C-C3C-C4C	-7.32	101.27	106.49
22	A	851	CLA	C2C-C1C-NC	7.31	116.82	109.97
22	4	304	CLA	CMD-C2D-C1D	7.31	137.59	124.71
22	B	813	CLA	CMD-C2D-C1D	7.31	137.59	124.71
22	X	304	CLA	CMD-C2D-C1D	7.30	137.57	124.71
22	B	804	CLA	C2C-C1C-NC	7.29	116.81	109.97
22	2	319	CLA	C3C-C4C-NC	7.29	118.53	110.57
22	4	314	CLA	C2B-C1B-NB	7.27	115.11	110.23
22	1	304	CLA	C2C-C1C-NC	7.26	116.77	109.97
22	A	844	CLA	CMD-C2D-C1D	7.26	137.50	124.71
22	2	306	CLA	C3C-C4C-NC	7.24	118.69	110.57
22	2	304	CLA	CMD-C2D-C1D	7.24	137.47	124.71
22	A	830	CLA	C4A-NA-C1A	7.24	109.96	106.71
22	B	826	CLA	C3C-C4C-NC	7.22	118.67	110.57
22	1	307	CLA	C2C-C1C-NC	7.21	116.72	109.97
21	Y	306	CHL	C2C-C3C-C4C	-7.19	101.37	106.49
22	B	851	CLA	C1D-ND-C4D	-7.18	101.23	106.33
22	4	305	CLA	C2C-C1C-NC	7.18	116.70	109.97
22	B	803	CLA	CHD-C4C-C3C	-7.18	114.29	124.84
21	1	316	CHL	CMD-C2D-C1D	7.18	137.36	124.71
22	L	306	CLA	O2D-CGD-CBD	7.17	124.01	111.27
21	4	309	CHL	C2C-C3C-C4C	-7.17	101.38	106.49
22	A	849	CLA	CMD-C2D-C1D	7.17	137.35	124.71
22	4	306	CLA	C2C-C1C-NC	7.16	116.68	109.97
22	B	850	CLA	CMD-C2D-C1D	7.15	137.31	124.71
22	A	845	CLA	C2B-C1B-NB	7.14	115.02	110.23
22	B	846	CLA	C2C-C1C-NC	7.14	116.66	109.97
21	X	302	CHL	C2C-C3C-C4C	-7.14	101.40	106.49
22	2	305	CLA	CMD-C2D-C1D	7.13	137.28	124.71
22	2	304	CLA	C2C-C1C-NC	7.13	116.65	109.97
22	B	817	CLA	CHD-C4C-C3C	-7.13	114.36	124.84
22	B	802	CLA	CMD-C2D-C1D	7.12	137.27	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	815	CLA	C2C-C1C-NC	7.12	116.64	109.97
21	Z	303	CHL	C2C-C3C-C4C	-7.11	101.42	106.49
22	B	820	CLA	C2C-C1C-NC	7.11	116.63	109.97
22	3	311	CLA	C2C-C1C-NC	7.11	116.63	109.97
22	B	820	CLA	C1D-ND-C4D	-7.10	101.29	106.33
24	1	311	XAT	C38-C25-C26	-7.10	110.36	122.26
22	A	801	CLA	C1B-C2B-C3B	-7.10	100.29	107.03
24	4	320	XAT	O24-C25-C24	7.08	118.70	113.38
21	Z	305	CHL	C2C-C3C-C4C	-7.08	101.44	106.49
21	Y	305	CHL	C2C-C3C-C4C	-7.07	101.45	106.49
22	1	304	CLA	CMD-C2D-C1D	7.07	137.17	124.71
22	B	823	CLA	CMD-C2D-C1D	7.07	137.17	124.71
22	X	304	CLA	C2C-C1C-NC	7.07	116.59	109.97
21	2	302	CHL	C2C-C3C-C4C	-7.06	101.45	106.49
22	K	204	CLA	C2B-C1B-NB	7.06	114.97	110.23
22	A	828	CLA	CMD-C2D-C1D	7.06	137.16	124.71
22	B	814	CLA	CMD-C2D-C1D	7.05	137.14	124.71
21	X	309	CHL	C2C-C3C-C4C	-7.05	101.47	106.49
25	O	203	BCR	C7-C8-C9	7.05	136.88	126.23
22	B	817	CLA	CMD-C2D-C1D	7.05	137.13	124.71
22	A	838	CLA	CHD-C4C-C3C	-7.03	114.50	124.84
22	B	817	CLA	C3C-C4C-NC	7.03	118.46	110.57
24	1	311	XAT	C31-C30-C29	-7.03	117.28	127.31
22	A	850	CLA	C3C-C4C-NC	7.02	118.44	110.57
22	A	808	CLA	CMD-C2D-C1D	7.01	137.07	124.71
21	X	306	CHL	C2C-C3C-C4C	-6.98	101.51	106.49
22	Z	306	CLA	O2D-CGD-CBD	6.97	123.66	111.27
22	2	306	CLA	CHD-C4C-C3C	-6.97	114.59	124.84
24	3	302	XAT	C27-C28-C29	-6.96	114.73	125.53
22	A	827	CLA	C1D-ND-C4D	-6.93	101.41	106.33
22	A	810	CLA	C2B-C1B-NB	6.92	114.87	110.23
22	A	842	CLA	CMD-C2D-C1D	6.89	136.86	124.71
22	A	826	CLA	C3C-C4C-NC	6.86	118.26	110.57
22	A	858	CLA	CMD-C2D-C1D	6.85	136.79	124.71
22	A	850	CLA	C2B-C1B-NB	6.84	114.82	110.23
22	B	851	CLA	CMD-C2D-C1D	6.84	136.77	124.71
21	4	307	CHL	C2C-C3C-C4C	-6.82	101.63	106.49
22	A	827	CLA	C3C-C4C-NC	6.81	118.21	110.57
22	2	320	CLA	C2B-C1B-NB	6.81	114.80	110.23
30	A	825	CL0	C3C-C4C-NC	6.79	118.19	110.57
22	1	317	CLA	C2C-C1C-NC	6.79	116.33	109.97
22	4	310	CLA	C3C-C4C-NC	6.79	118.19	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	834	CLA	C2B-C1B-NB	6.79	114.78	110.23
22	A	854	CLA	C3C-C4C-NC	6.78	118.17	110.57
24	3	302	XAT	O4-C5-C4	6.77	118.46	113.38
22	4	314	CLA	CMD-C2D-C1D	6.76	136.63	124.71
22	3	308	CLA	CHD-C4C-C3C	-6.76	114.90	124.84
22	A	843	CLA	C3C-C4C-NC	6.74	118.14	110.57
22	A	853	CLA	C3B-C2B-C1B	-6.72	99.05	107.16
22	B	807	CLA	C3B-C2B-C1B	-6.72	99.05	107.16
22	F	306	CLA	C3C-C4C-NC	6.69	118.08	110.57
22	B	808	CLA	C2B-C1B-NB	6.68	114.71	110.23
22	A	831	CLA	C3C-C4C-NC	6.67	118.06	110.57
22	B	845	CLA	C3C-C4C-NC	6.66	118.04	110.57
22	A	850	CLA	CMD-C2D-C1D	6.66	136.46	124.71
22	A	828	CLA	C3C-C4C-NC	6.66	118.04	110.57
22	B	820	CLA	C3B-C2B-C1B	-6.65	99.13	107.16
22	B	845	CLA	C2C-C1C-NC	6.65	116.20	109.97
22	B	816	CLA	CHC-C4B-NB	-6.61	117.26	124.26
22	B	814	CLA	C3C-C4C-NC	6.60	117.97	110.57
22	B	829	CLA	C2C-C1C-NC	6.59	116.14	109.97
22	L	306	CLA	CMD-C2D-C1D	6.58	136.31	124.71
22	3	318	CLA	C3C-C4C-NC	6.58	117.95	110.57
22	3	310	CLA	C3C-C4C-NC	6.58	117.95	110.57
22	4	314	CLA	C3C-C4C-NC	6.57	117.94	110.57
22	2	303	CLA	C3C-C4C-NC	6.57	117.94	110.57
22	A	810	CLA	C3C-C4C-NC	6.56	117.93	110.57
22	3	316	CLA	C3C-C4C-NC	6.56	117.93	110.57
22	B	814	CLA	C2C-C1C-NC	6.55	116.11	109.97
25	2	312	BCR	C16-C15-C14	6.54	136.88	123.47
22	A	831	CLA	CHD-C4C-C3C	-6.54	115.23	124.84
22	3	315	CLA	C3C-C4C-NC	6.52	117.88	110.57
22	A	842	CLA	C3C-C4C-NC	6.52	117.88	110.57
22	A	855	CLA	CMD-C2D-C1D	6.52	136.20	124.71
22	F	305	CLA	C3C-C4C-NC	6.50	117.87	110.57
22	B	845	CLA	CHD-C4C-C3C	-6.50	115.28	124.84
22	1	320	CLA	C3C-C4C-NC	6.50	117.86	110.57
22	B	845	CLA	CMD-C2D-C1D	6.48	136.13	124.71
22	B	816	CLA	C2D-C1D-ND	6.47	114.87	110.10
22	B	848	CLA	C3C-C4C-NC	6.46	117.82	110.57
22	4	312	CLA	C3C-C4C-NC	6.45	117.81	110.57
22	A	842	CLA	CHD-C4C-C3C	-6.45	115.36	124.84
22	B	831	CLA	C3C-C4C-NC	6.44	117.80	110.57
22	A	805	CLA	C3C-C4C-NC	6.41	117.77	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	L	302	BCR	C7-C8-C9	6.41	135.91	126.23
22	B	802	CLA	C3C-C4C-NC	6.40	117.75	110.57
22	B	848	CLA	CHD-C4C-C3C	-6.40	115.44	124.84
22	B	820	CLA	O2D-CGD-CBD	6.38	122.61	111.27
22	A	849	CLA	C3C-C4C-NC	6.37	117.72	110.57
22	A	841	CLA	C3C-C4C-NC	6.37	117.72	110.57
22	B	808	CLA	O2D-CGD-CBD	6.36	122.58	111.27
22	B	826	CLA	C3B-C2B-C1B	-6.36	99.48	107.16
22	1	305	CLA	C3C-C4C-NC	6.35	117.70	110.57
22	B	826	CLA	O2D-CGD-CBD	6.35	122.55	111.27
22	3	317	CLA	C3C-C4C-NC	6.35	117.69	110.57
22	B	823	CLA	C3C-C4C-NC	6.33	117.67	110.57
22	B	826	CLA	C4A-NA-C1A	6.33	109.55	106.71
22	F	305	CLA	CHD-C4C-C3C	-6.33	115.54	124.84
22	2	307	CLA	C3C-C4C-NC	6.33	117.67	110.57
22	1	306	CLA	C3C-C4C-NC	6.32	117.66	110.57
22	A	808	CLA	C3C-C4C-NC	6.32	117.66	110.57
22	B	807	CLA	C4A-NA-C1A	-6.32	103.86	106.71
24	1	311	XAT	O4-C5-C4	6.32	118.13	113.38
22	A	854	CLA	CHD-C4C-C3C	-6.32	115.55	124.84
22	1	304	CLA	C3C-C4C-NC	6.31	117.64	110.57
22	A	826	CLA	C3B-C2B-C1B	-6.30	99.55	107.16
21	3	307	CHL	CHD-C1D-ND	-6.30	118.66	124.45
22	1	317	CLA	CHD-C4C-C3C	-6.30	115.58	124.84
22	4	316	CLA	C3C-C4C-NC	6.29	117.63	110.57
22	B	830	CLA	C3C-C4C-NC	6.29	117.62	110.57
22	2	305	CLA	C3C-C4C-NC	6.28	117.62	110.57
22	4	305	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
22	4	313	CLA	C3C-C4C-NC	6.28	117.61	110.57
22	L	306	CLA	C3C-C4C-NC	6.28	117.61	110.57
22	B	831	CLA	CMD-C2D-C1D	6.27	135.76	124.71
22	K	204	CLA	C3C-C4C-NC	6.26	117.59	110.57
22	A	805	CLA	CHD-C4C-C3C	-6.26	115.63	124.84
22	O	207	CLA	C3C-C4C-NC	6.26	117.59	110.57
21	3	314	CHL	CHD-C1D-ND	-6.26	118.70	124.45
22	A	837	CLA	C3C-C4C-NC	6.26	117.59	110.57
22	A	804	CLA	O2D-CGD-CBD	6.25	122.38	111.27
22	A	826	CLA	CMD-C2D-C1D	6.25	135.73	124.71
22	B	819	CLA	C2B-C1B-NB	6.25	114.42	110.23
22	O	207	CLA	CHD-C4C-C3C	-6.25	115.66	124.84
22	B	808	CLA	C3C-C4C-NC	6.24	117.57	110.57
22	2	303	CLA	CMD-C2D-C1D	6.24	135.71	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	311	CLA	C3C-C4C-NC	6.24	117.57	110.57
22	B	809	CLA	C3C-C4C-NC	6.24	117.57	110.57
22	1	304	CLA	CHD-C4C-C3C	-6.24	115.67	124.84
22	A	843	CLA	CHD-C4C-C3C	-6.23	115.69	124.84
22	N	202	CLA	C3C-C4C-NC	6.23	117.55	110.57
21	Z	303	CHL	CHD-C1D-ND	-6.22	118.73	124.45
22	A	830	CLA	C3C-C4C-NC	6.21	117.53	110.57
22	3	316	CLA	CHD-C4C-C3C	-6.21	115.72	124.84
22	2	319	CLA	CHD-C4C-C3C	-6.20	115.29	124.98
22	O	208	CLA	C3C-C4C-NC	6.20	117.53	110.57
22	Y	308	CLA	C3C-C4C-NC	6.19	117.52	110.57
24	2	311	XAT	C31-C30-C29	-6.19	118.47	127.31
21	2	309	CHL	CHD-C1D-ND	-6.19	118.77	124.45
22	2	322	CLA	C3C-C4C-NC	6.19	117.51	110.57
22	A	848	CLA	C3C-C4C-NC	6.19	117.51	110.57
22	A	807	CLA	O2D-CGD-CBD	6.18	122.26	111.27
22	F	306	CLA	CHD-C4C-C3C	-6.18	115.76	124.84
22	4	312	CLA	CHD-C4C-C3C	-6.17	115.77	124.84
22	3	310	CLA	CHD-C4C-C3C	-6.17	115.77	124.84
22	B	849	CLA	C3C-C4C-NC	6.17	117.49	110.57
22	B	847	CLA	C3C-C4C-NC	6.17	117.49	110.57
25	B	840	BCR	C15-C16-C17	6.15	136.08	123.47
22	A	835	CLA	C3C-C4C-NC	6.15	117.47	110.57
24	2	311	XAT	O24-C25-C24	6.15	118.00	113.38
22	B	815	CLA	C3C-C4C-NC	6.15	117.47	110.57
22	4	310	CLA	CMD-C2D-C1D	6.15	135.55	124.71
22	2	305	CLA	CHD-C4C-C3C	-6.15	115.81	124.84
22	B	809	CLA	CHD-C4C-C3C	-6.14	115.81	124.84
21	4	317	CHL	CHD-C1D-ND	-6.14	118.81	124.45
22	X	310	CLA	C3C-C4C-NC	6.14	117.46	110.57
22	B	814	CLA	O2D-CGD-CBD	6.14	122.17	111.27
22	H	201	CLA	C3C-C4C-NC	6.14	117.45	110.57
22	B	831	CLA	CHD-C4C-C3C	-6.14	115.82	124.84
22	X	301	CLA	C3C-C4C-NC	6.12	117.44	110.57
22	3	315	CLA	CMD-C2D-C1D	6.12	135.50	124.71
22	3	311	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
30	A	825	CL0	CHD-C4C-C3C	-6.11	115.86	124.84
22	A	850	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
22	A	812	CLA	C3C-C4C-NC	6.10	117.41	110.57
22	1	317	CLA	C3C-C4C-NC	6.10	117.41	110.57
22	B	850	CLA	C3B-C2B-C1B	-6.09	99.81	107.16
22	1	303	CLA	C3C-C4C-NC	6.09	117.40	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	307	CLA	C3C-C4C-NC	6.09	117.40	110.57
22	1	303	CLA	O2D-CGD-CBD	6.09	122.08	111.27
21	X	306	CHL	CHD-C1D-ND	-6.08	118.86	124.45
22	A	808	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
22	K	202	CLA	C3C-C4C-NC	6.08	117.39	110.57
22	B	810	CLA	C3C-C4C-NC	6.08	117.39	110.57
22	X	312	CLA	C3C-C4C-NC	6.08	117.39	110.57
22	A	835	CLA	CHD-C4C-C3C	-6.08	115.91	124.84
22	O	208	CLA	CHD-C4C-C3C	-6.07	115.91	124.84
22	Z	310	CLA	C3C-C4C-NC	6.07	117.38	110.57
21	Z	312	CHL	CHD-C1D-ND	-6.07	118.88	124.45
22	A	827	CLA	C3B-C2B-C1B	-6.07	99.84	107.16
22	4	304	CLA	C3C-C4C-NC	6.06	117.37	110.57
24	2	311	XAT	C38-C25-C26	-6.06	112.10	122.26
22	B	816	CLA	C1D-CHD-C4C	-6.06	112.99	126.06
21	4	307	CHL	CHD-C1D-ND	-6.06	118.89	124.45
22	A	858	CLA	C3B-C2B-C1B	-6.05	99.85	107.16
22	A	828	CLA	CHD-C4C-C3C	-6.05	115.94	124.84
22	Z	307	CLA	C3C-C4C-NC	6.05	117.36	110.57
22	Y	309	CLA	C3C-C4C-NC	6.05	117.35	110.57
22	A	809	CLA	C3C-C4C-NC	6.04	117.34	110.57
22	A	828	CLA	C4A-NA-C1A	6.04	109.42	106.71
25	G	202	BCR	C23-C22-C21	6.03	128.20	118.94
22	B	829	CLA	C3B-C2B-C1B	-6.03	99.88	107.16
22	J	102	CLA	C3C-C4C-NC	6.03	117.33	110.57
22	A	859	CLA	CHD-C4C-C3C	-6.03	115.98	124.84
22	A	853	CLA	CHD-C4C-C3C	-6.02	115.99	124.84
22	3	312	CLA	C3C-C4C-NC	6.02	117.32	110.57
22	3	317	CLA	CHD-C4C-C3C	-6.02	116.00	124.84
21	X	308	CHL	CHD-C1D-ND	-6.02	118.92	124.45
22	4	316	CLA	CHD-C4C-C3C	-6.02	116.00	124.84
22	3	308	CLA	C3C-C4C-NC	6.02	117.32	110.57
22	4	305	CLA	C3C-C4C-NC	6.02	117.32	110.57
22	X	311	CLA	C3C-C4C-NC	6.01	117.31	110.57
22	B	814	CLA	CHD-C4C-C3C	-6.01	116.01	124.84
22	A	801	CLA	C3C-C4C-NC	6.01	117.31	110.57
22	A	803	CLA	CMD-C2D-C1D	6.00	135.29	124.71
22	1	307	CLA	C3C-C4C-NC	6.00	117.30	110.57
22	Y	312	CLA	C3C-C4C-NC	6.00	117.30	110.57
22	B	810	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
22	A	810	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
22	B	828	CLA	C3C-C4C-NC	5.99	117.29	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	X	307	CHL	CHD-C1D-ND	-5.99	118.95	124.45
22	A	839	CLA	C3B-C2B-C1B	-5.98	99.94	107.16
22	1	306	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
22	A	802	CLA	C3C-C4C-NC	5.98	117.28	110.57
22	B	804	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
22	B	811	CLA	C3C-C4C-NC	5.97	117.27	110.57
22	O	209	CLA	C3C-C4C-NC	5.97	117.27	110.57
22	G	207	CLA	C3C-C4C-NC	5.97	117.27	110.57
22	A	803	CLA	C3C-C4C-NC	5.97	117.27	110.57
22	A	859	CLA	C3C-C4C-NC	5.97	117.27	110.57
22	B	823	CLA	CHD-C4C-C3C	-5.97	116.07	124.84
22	4	314	CLA	CHD-C4C-C3C	-5.96	116.07	124.84
22	B	821	CLA	C3C-C4C-NC	5.96	117.26	110.57
22	B	806	CLA	C3C-C4C-NC	5.96	117.25	110.57
22	A	841	CLA	O2D-CGD-CBD	5.96	121.86	111.27
21	Y	306	CHL	CHD-C1D-ND	-5.96	118.98	124.45
22	G	205	CLA	C3C-C4C-NC	5.95	117.24	110.57
22	1	309	CLA	C3C-C4C-NC	5.95	117.24	110.57
22	A	857	CLA	C3B-C2B-C1B	-5.94	99.99	107.16
22	2	304	CLA	C3C-C4C-NC	5.94	117.23	110.57
22	A	832	CLA	C3C-C4C-NC	5.94	117.23	110.57
24	3	302	XAT	C31-C32-C33	-5.94	109.74	126.42
22	Z	306	CLA	C3C-C4C-NC	5.94	117.23	110.57
30	A	825	CL0	CMD-C2D-C1D	5.94	135.17	124.71
22	4	310	CLA	CHD-C4C-C3C	-5.94	116.12	124.84
22	A	841	CLA	CHD-C4C-C3C	-5.94	116.12	124.84
21	X	302	CHL	CHD-C1D-ND	-5.93	119.00	124.45
21	Y	304	CHL	CHD-C1D-ND	-5.93	119.00	124.45
22	B	820	CLA	C3C-C4C-NC	5.93	117.22	110.57
22	A	843	CLA	C3B-C2B-C1B	-5.93	100.00	107.16
22	L	305	CLA	C3C-C4C-NC	5.93	117.22	110.57
21	Z	305	CHL	CHD-C1D-ND	-5.93	119.01	124.45
22	A	834	CLA	C3C-C4C-NC	5.92	117.22	110.57
22	X	303	CLA	C3C-C4C-NC	5.92	117.22	110.57
22	Z	311	CLA	C3C-C4C-NC	5.92	117.22	110.57
22	A	839	CLA	C3C-C4C-NC	5.92	117.21	110.57
22	3	319	CLA	C3C-C4C-NC	5.92	117.21	110.57
24	2	311	XAT	O24-C25-C38	5.92	122.15	115.06
21	3	314	CHL	C2C-C3C-C4C	-5.92	102.27	106.49
22	Z	308	CLA	C3C-C4C-NC	5.92	117.21	110.57
22	2	319	CLA	C4A-NA-C1A	5.92	109.37	106.71
22	A	829	CLA	C3B-C2B-C1B	-5.91	100.02	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	807	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
22	G	206	CLA	C3C-C4C-NC	5.91	117.20	110.57
21	Y	305	CHL	CHD-C1D-ND	-5.91	119.02	124.45
21	Y	303	CHL	CHD-C1D-ND	-5.91	119.03	124.45
21	3	307	CHL	C3B-C2B-C1B	-5.90	100.04	107.16
21	1	316	CHL	C3B-C2B-C1B	-5.90	100.04	107.16
21	X	305	CHL	CHD-C1D-ND	-5.90	119.03	124.45
22	B	804	CLA	C3C-C4C-NC	5.90	117.19	110.57
22	Y	314	CLA	C3C-C4C-NC	5.90	117.19	110.57
22	L	305	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
22	A	809	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
22	A	857	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
22	A	834	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
22	O	210	CLA	C3C-C4C-NC	5.89	117.18	110.57
22	B	812	CLA	C3C-C4C-NC	5.89	117.17	110.57
22	A	855	CLA	O2D-CGD-CBD	5.88	121.72	111.27
22	Y	302	CLA	C3C-C4C-NC	5.88	117.17	110.57
22	A	810	CLA	CMD-C2D-C1D	5.88	135.08	124.71
22	A	855	CLA	C3C-C4C-NC	5.88	117.16	110.57
22	A	857	CLA	C3C-C4C-NC	5.88	117.16	110.57
22	3	313	CLA	C3C-C4C-NC	5.88	117.16	110.57
22	A	851	CLA	C3C-C4C-NC	5.87	117.16	110.57
22	A	828	CLA	C2B-C1B-NB	5.87	114.17	110.23
24	4	320	XAT	C26-C27-C28	-5.87	113.57	125.99
22	B	818	CLA	C3C-C4C-NC	5.87	117.16	110.57
22	A	826	CLA	C2C-C1C-NC	5.87	115.47	109.97
30	A	825	CL0	C1D-ND-C4D	-5.87	102.17	106.33
22	A	856	CLA	C3C-C4C-NC	5.87	117.15	110.57
21	Y	313	CHL	CHD-C1D-ND	-5.86	119.07	124.45
22	Y	310	CLA	C3C-C4C-NC	5.86	117.14	110.57
22	2	307	CLA	CHD-C4C-C3C	-5.86	116.23	124.84
22	B	813	CLA	C3C-C4C-NC	5.85	117.14	110.57
22	1	321	CLA	C3C-C4C-NC	5.85	117.13	110.57
22	A	853	CLA	C3C-C4C-NC	5.85	117.13	110.57
22	3	320	CLA	C3C-C4C-NC	5.85	117.13	110.57
22	X	301	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
22	Y	308	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
22	X	313	CLA	C3C-C4C-NC	5.84	117.12	110.57
22	A	840	CLA	C3C-C4C-NC	5.84	117.12	110.57
22	1	305	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
21	4	308	CHL	CHD-C1D-ND	-5.83	119.10	124.45
22	G	205	CLA	CHD-C4C-C3C	-5.83	116.27	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	X	309	CHL	CHD-C1D-ND	-5.83	119.10	124.45
22	B	829	CLA	C3C-C4C-NC	5.82	117.10	110.57
22	2	317	CLA	C3C-C4C-NC	5.82	117.10	110.57
22	B	811	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
21	Z	301	CHL	CHD-C1D-ND	-5.81	119.11	124.45
22	A	805	CLA	C3B-C2B-C1B	-5.81	100.15	107.16
22	Y	301	CLA	C3C-C4C-NC	5.81	117.08	110.57
22	A	856	CLA	CHD-C4C-C3C	-5.81	116.31	124.84
21	2	309	CHL	C3B-C2B-C1B	-5.80	100.17	107.16
22	K	205	CLA	CHD-C4C-C3C	-5.79	116.32	124.84
22	A	849	CLA	CHD-C4C-C3C	-5.79	116.33	124.84
22	Z	309	CLA	C3C-C4C-NC	5.78	117.06	110.57
22	A	807	CLA	C3C-C4C-NC	5.78	117.05	110.57
22	1	319	CLA	C3C-C4C-NC	5.78	117.05	110.57
22	X	313	CLA	O2D-CGD-CBD	5.78	121.53	111.27
22	H	201	CLA	CHD-C4C-C3C	-5.77	116.35	124.84
22	A	858	CLA	CAC-C3C-C4C	5.77	132.30	124.81
21	1	301	CHL	CHD-C1D-ND	-5.77	119.15	124.45
22	A	851	CLA	C3B-C2B-C1B	-5.77	100.19	107.16
22	Z	314	CLA	C3C-C4C-NC	5.77	117.05	110.57
22	3	318	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
22	B	825	CLA	C3C-C4C-NC	5.77	117.04	110.57
22	2	303	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
22	B	815	CLA	CHD-C4C-C3C	-5.76	116.38	124.84
22	B	817	CLA	C3B-C2B-C1B	-5.76	100.21	107.16
21	X	307	CHL	C3B-C2B-C1B	-5.75	100.22	107.16
22	B	831	CLA	C3B-C2B-C1B	-5.75	100.22	107.16
22	B	850	CLA	C3C-C4C-NC	5.75	117.02	110.57
22	1	309	CLA	O2D-CGD-CBD	5.74	121.47	111.27
22	B	852	CLA	C3C-C4C-NC	5.74	117.00	110.57
22	B	833	CLA	CHD-C4C-C3C	-5.73	116.41	124.84
22	N	202	CLA	CHD-C4C-C3C	-5.73	116.41	124.84
22	B	853	CLA	C3C-C4C-NC	5.73	117.00	110.57
22	B	833	CLA	C3C-C4C-NC	5.73	116.99	110.57
22	K	203	CLA	C3C-C4C-NC	5.72	116.99	110.57
22	3	321	CLA	C3C-C4C-NC	5.72	116.99	110.57
22	A	812	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
22	A	804	CLA	C3C-C4C-NC	5.72	116.98	110.57
22	G	207	CLA	O2D-CGD-CBD	5.72	121.43	111.27
22	B	846	CLA	C3B-C2B-C1B	-5.72	100.26	107.16
22	2	304	CLA	CHD-C4C-C3C	-5.72	116.44	124.84
22	K	202	CLA	CHD-C4C-C3C	-5.71	116.44	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	849	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
22	A	839	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
22	4	318	CLA	C3C-C4C-NC	5.71	116.98	110.57
22	A	804	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
22	3	312	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
22	K	205	CLA	C3C-C4C-NC	5.71	116.97	110.57
22	2	322	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
22	1	304	CLA	C3B-C2B-C1B	-5.70	100.28	107.16
22	4	313	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
22	3	309	CLA	C3C-C4C-NC	5.70	116.96	110.57
22	X	312	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
22	A	847	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
22	Z	313	CLA	C3C-C4C-NC	5.69	116.96	110.57
22	O	209	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
21	2	301	CHL	CHD-C1D-ND	-5.69	119.22	124.45
21	2	321	CHL	CHD-C1D-ND	-5.68	119.24	124.45
22	4	304	CLA	C3B-C2B-C1B	-5.68	100.31	107.16
22	Z	307	CLA	CHD-C4C-C3C	-5.68	116.50	124.84
22	B	810	CLA	O2D-CGD-CBD	5.67	121.35	111.27
22	Y	311	CLA	C3C-C4C-NC	5.67	116.93	110.57
21	Y	313	CHL	C3B-C2B-C1B	-5.67	100.32	107.16
22	K	205	CLA	C3B-C2B-C1B	-5.67	100.32	107.16
24	2	311	XAT	C40-C33-C34	-5.67	114.98	122.92
23	4	322	LUT	C8-C9-C10	5.67	127.64	118.94
22	A	845	CLA	C1C-C2C-C3C	-5.67	101.00	106.96
22	A	852	CLA	C3B-C2B-C1B	-5.67	100.32	107.16
21	Z	302	CHL	CHD-C1D-ND	-5.67	119.25	124.45
22	Y	314	CLA	O2D-CGD-CBD	5.67	121.34	111.27
22	X	310	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
21	2	302	CHL	CHD-C1D-ND	-5.66	119.25	124.45
22	B	824	CLA	C3C-C4C-NC	5.66	116.92	110.57
22	X	311	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
22	A	806	CLA	C3B-C2B-C1B	-5.66	100.33	107.16
22	X	304	CLA	C3C-C4C-NC	5.66	116.92	110.57
22	O	210	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
22	B	807	CLA	CMD-C2D-C1D	5.65	135.29	118.85
22	B	814	CLA	C2D-C1D-ND	5.65	114.27	110.10
23	4	322	LUT	C32-C33-C34	5.64	127.60	118.94
24	2	311	XAT	C26-C27-C28	-5.64	114.06	125.99
22	B	852	CLA	C3B-C2B-C1B	-5.64	100.35	107.16
22	G	207	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
22	A	827	CLA	CHD-C4C-C3C	-5.63	116.57	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Y	314	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
22	O	206	CLA	C3C-C4C-NC	5.62	116.88	110.57
22	Z	311	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
22	A	829	CLA	O2D-CGD-CBD	5.62	121.25	111.27
24	1	311	XAT	C28-C29-C30	5.62	127.56	118.94
22	B	829	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
22	1	317	CLA	CHD-C1D-ND	-5.61	119.30	124.45
22	B	806	CLA	C3B-C2B-C1B	-5.61	100.39	107.16
22	B	801	CLA	C2C-C1C-NC	5.61	115.23	109.97
22	3	315	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
22	B	822	CLA	C3B-C2B-C1B	-5.61	100.39	107.16
25	1	312	BCR	C21-C20-C19	5.61	140.72	123.22
24	2	311	XAT	C15-C14-C13	-5.61	119.30	127.31
24	1	311	XAT	C15-C35-C34	-5.61	111.98	123.47
22	3	311	CLA	C3B-C2B-C1B	-5.60	100.40	107.16
22	A	829	CLA	C3C-C4C-NC	5.60	116.85	110.57
22	A	856	CLA	C3B-C2B-C1B	-5.60	100.40	107.16
22	B	803	CLA	O2D-CGD-CBD	5.60	121.21	111.27
21	Z	304	CHL	CHD-C1D-ND	-5.59	119.32	124.45
22	L	306	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
22	4	304	CLA	CHD-C4C-C3C	-5.59	116.63	124.84
21	Z	303	CHL	C3B-C2B-C1B	-5.59	100.42	107.16
22	A	844	CLA	C3C-C4C-NC	5.59	116.83	110.57
22	4	311	CLA	C3C-C4C-NC	5.58	116.83	110.57
22	A	848	CLA	CHD-C1D-ND	-5.58	119.33	124.45
22	Y	309	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
24	3	302	XAT	C6-C7-C8	-5.58	114.19	125.99
22	1	318	CLA	C3C-C4C-NC	5.58	116.83	110.57
22	1	319	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
22	K	203	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
22	1	319	CLA	C3B-C2B-C1B	-5.58	100.43	107.16
22	B	847	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
22	A	806	CLA	C3C-C4C-NC	5.57	116.82	110.57
22	B	805	CLA	C3C-C4C-NC	5.57	116.82	110.57
22	B	815	CLA	C3B-C2B-C1B	-5.57	100.43	107.16
22	X	303	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
25	O	202	BCR	C8-C9-C10	5.57	127.49	118.94
22	K	205	CLA	O2D-CGD-CBD	5.57	121.17	111.27
22	3	309	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
22	3	319	CLA	CHD-C4C-C3C	-5.57	116.66	124.84
22	A	801	CLA	CHD-C4C-C3C	-5.57	116.66	124.84
22	Y	311	CLA	O2D-CGD-CBD	5.57	121.16	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	302	CHL	C3B-C2B-C1B	-5.56	100.44	107.16
22	O	207	CLA	O2D-CGD-CBD	5.56	121.15	111.27
22	Z	308	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
22	B	851	CLA	C3C-C4C-NC	5.55	116.80	110.57
23	4	322	LUT	C30-C31-C32	5.55	140.54	123.22
22	2	320	CLA	C3C-C4C-NC	5.55	116.79	110.57
22	A	845	CLA	CHD-C4C-C3C	-5.54	116.69	124.84
22	K	203	CLA	O2D-CGD-CBD	5.54	121.11	111.27
22	3	313	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
22	A	830	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
21	Y	306	CHL	C3B-C2B-C1B	-5.53	100.49	107.16
22	A	833	CLA	C3C-C4C-NC	5.53	116.77	110.57
21	X	302	CHL	C3B-C2B-C1B	-5.53	100.49	107.16
22	Z	310	CLA	CHD-C4C-C3C	-5.53	116.72	124.84
22	B	825	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
22	2	319	CLA	C1C-C2C-C3C	-5.52	102.01	107.07
22	B	847	CLA	C3B-C2B-C1B	-5.52	100.50	107.16
22	H	201	CLA	C3B-C2B-C1B	-5.52	100.50	107.16
22	4	306	CLA	C3B-C2B-C1B	-5.51	100.50	107.16
22	1	303	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
22	1	309	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
22	A	801	CLA	C3B-C4B-NB	5.51	113.93	110.23
22	J	102	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
22	B	804	CLA	O2D-CGD-CBD	5.51	121.06	111.27
22	Y	312	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
22	1	302	CLA	C3C-C4C-NC	5.51	116.75	110.57
22	3	308	CLA	C3B-C2B-C1B	-5.51	100.51	107.16
22	B	823	CLA	O2D-CGD-CBD	5.50	121.05	111.27
22	A	837	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
22	A	829	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
22	Y	302	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
22	2	308	CLA	O2D-CGD-CBD	5.50	121.03	111.27
22	X	304	CLA	O2D-CGD-CBD	5.50	121.03	111.27
22	A	802	CLA	C3B-C2B-C1B	-5.50	100.53	107.16
22	L	306	CLA	C3B-C2B-C1B	-5.49	100.53	107.16
22	1	308	CLA	CHD-C1D-ND	-5.49	119.41	124.45
22	B	801	CLA	C3B-C2B-C1B	-5.49	100.53	107.16
22	A	851	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
25	O	202	BCR	C10-C11-C12	5.49	140.35	123.22
21	Y	304	CHL	C3B-C2B-C1B	-5.49	100.54	107.16
21	Y	305	CHL	C3B-C2B-C1B	-5.49	100.54	107.16
22	B	850	CLA	O2D-CGD-CBD	5.49	121.02	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	820	CLA	CHD-C4C-C3C	-5.49	116.78	124.84
22	B	821	CLA	CHD-C4C-C3C	-5.49	116.78	124.84
21	Z	304	CHL	C3B-C2B-C1B	-5.48	100.54	107.16
22	4	311	CLA	C3B-C2B-C1B	-5.48	100.54	107.16
22	A	828	CLA	CHC-C4B-NB	-5.48	118.45	124.26
22	A	836	CLA	C3C-C4C-NC	5.48	116.72	110.57
22	A	847	CLA	C3C-C4C-NC	5.48	116.72	110.57
21	1	316	CHL	C3C-C4C-NC	5.48	116.72	110.57
22	B	852	CLA	CHD-C4C-C3C	-5.48	116.79	124.84
22	1	318	CLA	O2D-CGD-CBD	5.48	121.00	111.27
22	1	307	CLA	CHD-C4C-C3C	-5.48	116.79	124.84
25	G	202	BCR	C21-C20-C19	5.47	140.30	123.22
21	Y	307	CHL	C3B-C2B-C1B	-5.47	100.55	107.16
21	Y	307	CHL	CHD-C1D-ND	-5.47	119.43	124.45
22	B	828	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
22	B	804	CLA	C3B-C2B-C1B	-5.47	100.56	107.16
22	4	306	CLA	C3C-C4C-NC	5.47	116.70	110.57
22	3	316	CLA	C3B-C2B-C1B	-5.47	100.56	107.16
22	A	845	CLA	O2D-CGD-CBD	5.47	120.98	111.27
24	2	311	XAT	C15-C35-C34	-5.46	112.28	123.47
22	2	318	CLA	C3C-C4C-NC	5.46	116.70	110.57
22	B	810	CLA	C1C-C2C-C3C	-5.46	101.22	106.96
21	4	309	CHL	CHD-C1D-ND	-5.46	119.44	124.45
22	K	203	CLA	C3B-C2B-C1B	-5.46	100.57	107.16
21	X	305	CHL	C3B-C2B-C1B	-5.46	100.57	107.16
22	B	806	CLA	CHD-C4C-C3C	-5.46	116.82	124.84
22	B	811	CLA	O2D-CGD-CBD	5.46	120.97	111.27
22	B	830	CLA	CHD-C4C-C3C	-5.46	116.82	124.84
21	Z	304	CHL	C3C-C4C-NC	5.46	116.69	110.57
22	B	850	CLA	CHD-C4C-C3C	-5.45	116.82	124.84
25	O	203	BCR	C12-C13-C14	5.45	127.31	118.94
22	3	312	CLA	C3B-C2B-C1B	-5.45	100.58	107.16
21	3	307	CHL	C3C-C4C-NC	5.45	116.69	110.57
22	B	808	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
21	3	314	CHL	CHD-C4C-C3C	-5.45	116.83	124.84
22	1	317	CLA	O2D-CGD-CBD	5.45	120.95	111.27
21	Z	302	CHL	C3C-C4C-NC	5.45	116.68	110.57
22	A	844	CLA	O2D-CGD-CBD	5.45	120.95	111.27
22	X	313	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
22	4	315	CLA	C3B-C2B-C1B	-5.45	100.59	107.16
25	O	202	BCR	C37-C22-C21	-5.44	115.30	122.92
21	2	321	CHL	C3C-C4C-NC	5.44	116.67	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	831	CLA	C3B-C2B-C1B	-5.44	100.59	107.16
22	A	807	CLA	C3B-C2B-C1B	-5.44	100.59	107.16
22	A	808	CLA	C3B-C2B-C1B	-5.44	100.60	107.16
21	X	308	CHL	C3B-C2B-C1B	-5.44	100.60	107.16
21	Y	303	CHL	C3B-C2B-C1B	-5.43	100.60	107.16
22	B	853	CLA	CHD-C4C-C3C	-5.43	116.85	124.84
22	B	833	CLA	O2D-CGD-CBD	5.43	120.92	111.27
22	B	803	CLA	C3B-C2B-C1B	-5.43	100.61	107.16
21	4	317	CHL	C3B-C2B-C1B	-5.43	100.61	107.16
21	Y	303	CHL	C3C-C4C-NC	5.42	116.65	110.57
22	B	802	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
21	Z	301	CHL	C3B-C2B-C1B	-5.42	100.62	107.16
22	1	320	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
22	1	321	CLA	CHD-C4C-C3C	-5.42	116.88	124.84
22	2	317	CLA	CHD-C4C-C3C	-5.42	116.88	124.84
22	B	851	CLA	CHD-C4C-C3C	-5.42	116.88	124.84
22	B	807	CLA	O2D-CGD-CBD	5.42	120.89	111.27
22	B	801	CLA	CMC-C2C-C1C	5.41	133.28	125.04
21	Y	313	CHL	C3C-C4C-NC	5.41	116.64	110.57
23	1	310	LUT	C1-C6-C5	-5.41	114.99	122.61
22	Y	310	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
22	Z	313	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
21	X	309	CHL	C3B-C2B-C1B	-5.41	100.63	107.16
22	2	322	CLA	C3B-C2B-C1B	-5.41	100.63	107.16
22	B	805	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
22	4	318	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
22	B	824	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
22	B	846	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
22	1	305	CLA	O2D-CGD-CBD	5.40	120.86	111.27
22	B	823	CLA	C3B-C2B-C1B	-5.40	100.65	107.16
22	G	206	CLA	CHD-C4C-C3C	-5.39	116.91	124.84
22	A	833	CLA	O2D-CGD-CBD	5.39	120.84	111.27
22	Z	314	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
21	Z	305	CHL	O2D-CGD-CBD	5.38	120.83	111.27
22	B	846	CLA	CMC-C2C-C1C	5.38	133.24	125.04
25	O	202	BCR	C34-C9-C10	-5.38	115.39	122.92
22	3	320	CLA	CHD-C4C-C3C	-5.37	116.95	124.84
22	B	805	CLA	C3B-C2B-C1B	-5.37	100.68	107.16
21	Y	307	CHL	C3C-C4C-NC	5.37	116.59	110.57
22	Y	311	CLA	C3B-C2B-C1B	-5.37	100.68	107.16
22	H	201	CLA	O2D-CGD-CBD	5.37	120.80	111.27
22	X	310	CLA	C3B-C2B-C1B	-5.36	100.69	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	307	CLA	CAC-C3C-C4C	5.36	131.76	124.81
22	F	306	CLA	C3B-C2B-C1B	-5.36	100.69	107.16
22	4	313	CLA	C3B-C2B-C1B	-5.36	100.69	107.16
21	Z	301	CHL	C3C-C4C-NC	5.36	116.58	110.57
21	X	306	CHL	C3B-C2B-C1B	-5.36	100.69	107.16
22	A	859	CLA	C3B-C2B-C1B	-5.36	100.69	107.16
22	Y	311	CLA	CHD-C4C-C3C	-5.36	116.97	124.84
22	A	840	CLA	C3B-C2B-C1B	-5.36	100.70	107.16
22	Z	306	CLA	C3B-C2B-C1B	-5.36	100.70	107.16
22	3	309	CLA	C3B-C2B-C1B	-5.36	100.70	107.16
22	L	307	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
22	A	842	CLA	C3B-C2B-C1B	-5.35	100.70	107.16
22	B	849	CLA	O2D-CGD-CBD	5.35	120.77	111.27
22	2	308	CLA	C3C-C4C-NC	5.35	116.57	110.57
22	Z	309	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
22	A	803	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
24	2	311	XAT	C6-C7-C8	5.34	137.29	125.99
21	Y	304	CHL	C3C-C4C-NC	5.34	116.56	110.57
22	B	822	CLA	C3C-C4C-NC	5.34	116.56	110.57
22	O	207	CLA	C3B-C2B-C1B	-5.34	100.72	107.16
22	B	813	CLA	C3B-C2B-C1B	-5.33	100.72	107.16
25	2	312	BCR	C10-C11-C12	5.33	139.86	123.22
22	4	312	CLA	C3B-C2B-C1B	-5.33	100.72	107.16
22	Z	314	CLA	C3B-C2B-C1B	-5.33	100.72	107.16
22	1	308	CLA	C3B-C2B-C1B	-5.33	100.73	107.16
21	X	305	CHL	C3C-C4C-NC	5.32	116.53	110.57
22	A	832	CLA	O2D-CGD-CBD	5.31	120.71	111.27
22	1	317	CLA	C3B-C2B-C1B	-5.31	100.75	107.16
22	Z	309	CLA	C3B-C2B-C1B	-5.31	100.75	107.16
22	A	847	CLA	O2D-CGD-CBD	5.30	120.69	111.27
21	2	302	CHL	C3C-C4C-NC	5.30	116.52	110.57
21	X	307	CHL	C3C-C4C-NC	5.30	116.51	110.57
22	A	855	CLA	C2B-C1B-NB	5.30	113.78	110.23
22	4	318	CLA	C3B-C2B-C1B	-5.29	100.77	107.16
21	4	308	CHL	C3B-C2B-C1B	-5.29	100.77	107.16
22	B	833	CLA	C3B-C2B-C1B	-5.29	100.78	107.16
22	3	319	CLA	C3B-C2B-C1B	-5.29	100.78	107.16
22	Y	312	CLA	C3B-C2B-C1B	-5.29	100.78	107.16
21	X	302	CHL	C3C-C4C-NC	5.29	116.50	110.57
22	Z	306	CLA	CHD-C4C-C3C	-5.28	117.07	124.84
22	X	312	CLA	C3B-C2B-C1B	-5.28	100.78	107.16
24	1	311	XAT	C18-C5-C6	-5.28	113.41	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	846	CLA	C3C-C4C-NC	5.28	116.49	110.57
21	2	301	CHL	C3C-C4C-NC	5.28	116.49	110.57
22	Z	311	CLA	C3B-C2B-C1B	-5.28	100.79	107.16
22	B	830	CLA	C1C-C2C-C3C	-5.27	101.41	106.96
22	Y	308	CLA	C3B-C2B-C1B	-5.27	100.80	107.16
22	Z	307	CLA	C3B-C2B-C1B	-5.27	100.80	107.16
22	A	844	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
22	B	821	CLA	C3B-C2B-C1B	-5.27	100.80	107.16
22	B	849	CLA	C3B-C2B-C1B	-5.27	100.80	107.16
22	L	307	CLA	C3B-C2B-C1B	-5.27	100.80	107.16
21	Y	306	CHL	C3C-C4C-NC	5.27	116.48	110.57
22	A	849	CLA	C3B-C2B-C1B	-5.27	100.81	107.16
22	A	858	CLA	C3C-C4C-NC	5.26	116.47	110.57
22	B	819	CLA	C3C-C4C-NC	5.26	116.47	110.57
21	2	301	CHL	C3B-C2B-C1B	-5.26	100.81	107.16
21	X	308	CHL	C3C-C4C-NC	5.26	116.47	110.57
22	A	840	CLA	O2D-CGD-CBD	5.26	120.61	111.27
22	Y	309	CLA	C3B-C2B-C1B	-5.26	100.81	107.16
22	A	846	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
21	1	301	CHL	C3B-C2B-C1B	-5.26	100.82	107.16
22	X	311	CLA	C3B-C2B-C1B	-5.26	100.82	107.16
23	2	310	LUT	C15-C35-C34	5.26	134.24	123.47
22	4	311	CLA	CHD-C4C-C3C	-5.25	117.12	124.84
21	X	307	CHL	O2D-CGD-CBD	5.25	120.60	111.27
21	3	314	CHL	C3C-C4C-NC	5.25	116.46	110.57
21	Y	305	CHL	C3C-C4C-NC	5.25	116.46	110.57
22	L	305	CLA	O2D-CGD-CBD	5.25	120.59	111.27
22	B	846	CLA	C3C-C4C-NC	5.25	116.45	110.57
22	1	305	CLA	C3B-C2B-C1B	-5.24	100.83	107.16
22	B	822	CLA	CHD-C1D-ND	-5.24	119.64	124.45
22	O	210	CLA	C3B-C2B-C1B	-5.24	100.83	107.16
22	A	832	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
22	2	318	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
21	3	314	CHL	C3D-C2D-C1D	-5.24	98.68	105.83
25	L	302	BCR	C16-C15-C14	5.24	134.20	123.47
22	1	309	CLA	C3B-C2B-C1B	-5.24	100.84	107.16
22	B	802	CLA	C3B-C2B-C1B	-5.24	100.84	107.16
22	X	301	CLA	C3B-C2B-C1B	-5.23	100.85	107.16
24	4	320	XAT	C18-C5-C6	-5.23	113.50	122.26
22	1	321	CLA	C3B-C2B-C1B	-5.23	100.85	107.16
22	3	315	CLA	C3B-C2B-C1B	-5.22	100.86	107.16
22	3	321	CLA	C3B-C2B-C1B	-5.22	100.86	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	856	CLA	O2D-CGD-CBD	5.22	120.54	111.27
22	2	305	CLA	C3B-C2B-C1B	-5.22	100.86	107.16
22	X	313	CLA	C3B-C2B-C1B	-5.22	100.86	107.16
22	2	318	CLA	C3B-C2B-C1B	-5.22	100.87	107.16
22	4	318	CLA	O2D-CGD-CBD	5.22	120.53	111.27
22	B	813	CLA	CHD-C4C-C3C	-5.21	117.17	124.84
21	X	302	CHL	O2D-CGD-CBD	5.21	120.53	111.27
22	Z	313	CLA	C3B-C2B-C1B	-5.21	100.87	107.16
22	A	848	CLA	CHD-C4C-C3C	-5.21	117.18	124.84
22	L	305	CLA	C3B-C2B-C1B	-5.21	100.88	107.16
21	4	307	CHL	C3C-C4C-NC	5.20	116.40	110.57
22	2	320	CLA	CHD-C4C-C3C	-5.20	117.20	124.84
21	X	306	CHL	C3C-C4C-NC	5.20	116.40	110.57
22	X	304	CLA	C3B-C2B-C1B	-5.20	100.89	107.16
22	B	816	CLA	C3B-C2B-C1B	-5.19	100.89	107.16
22	1	317	CLA	C3D-C4D-ND	5.19	118.64	110.24
22	A	806	CLA	O2D-CGD-CBD	5.19	120.50	111.27
21	Z	302	CHL	C3B-C2B-C1B	-5.19	100.90	107.16
25	G	202	BCR	C15-C16-C17	5.19	134.10	123.47
25	L	302	BCR	C34-C9-C10	-5.19	115.66	122.92
22	Z	310	CLA	C3B-C2B-C1B	-5.18	100.90	107.16
22	Y	302	CLA	C3B-C2B-C1B	-5.18	100.91	107.16
22	X	303	CLA	C3B-C2B-C1B	-5.18	100.91	107.16
22	3	321	CLA	O2D-CGD-CBD	5.17	120.46	111.27
22	A	833	CLA	C3B-C2B-C1B	-5.17	100.92	107.16
22	1	318	CLA	CHD-C4C-C3C	-5.17	117.25	124.84
21	3	307	CHL	C3D-C2D-C1D	-5.16	98.78	105.83
24	2	311	XAT	C32-C33-C34	5.16	126.86	118.94
22	Z	308	CLA	C3B-C2B-C1B	-5.16	100.93	107.16
22	A	858	CLA	CHB-C4A-NA	5.16	131.64	124.51
25	1	312	BCR	C20-C21-C22	5.16	134.67	127.31
22	1	302	CLA	C3B-C2B-C1B	-5.15	100.94	107.16
21	Y	303	CHL	O2D-CGD-CBD	5.15	120.42	111.27
22	A	846	CLA	CHD-C1D-ND	-5.15	119.72	124.45
22	B	848	CLA	C3B-C2B-C1B	-5.15	100.94	107.16
21	4	308	CHL	C3C-C4C-NC	5.15	116.35	110.57
22	N	202	CLA	C3B-C2B-C1B	-5.15	100.95	107.16
21	Z	303	CHL	C3C-C4C-NC	5.15	116.34	110.57
22	B	852	CLA	O2D-CGD-CBD	5.14	120.41	111.27
22	4	315	CLA	CHD-C1D-ND	-5.14	119.73	124.45
22	X	304	CLA	CHA-C1A-NA	5.14	138.17	126.40
22	1	308	CLA	CHD-C4C-C3C	-5.14	117.28	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	206	CLA	CHD-C4C-C3C	-5.14	117.29	124.84
21	Z	312	CHL	C3C-C4C-NC	5.13	116.33	110.57
22	A	812	CLA	C3B-C2B-C1B	-5.13	100.96	107.16
22	2	308	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
22	A	848	CLA	O2D-CGD-CBD	5.13	120.38	111.27
22	B	847	CLA	O2D-CGD-CBD	5.13	120.38	111.27
22	A	836	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
21	1	301	CHL	C3C-C4C-NC	5.13	116.32	110.57
22	2	307	CLA	C3B-C2B-C1B	-5.13	100.97	107.16
22	K	204	CLA	C3B-C2B-C1B	-5.13	100.97	107.16
22	B	853	CLA	C3B-C2B-C1B	-5.12	100.97	107.16
21	3	314	CHL	C3B-C2B-C1B	-5.12	100.98	107.16
22	4	306	CLA	CHD-C4C-C3C	-5.12	117.32	124.84
22	A	806	CLA	CHD-C4C-C3C	-5.12	117.32	124.84
21	4	307	CHL	C3B-C2B-C1B	-5.11	100.99	107.16
22	A	840	CLA	CHD-C4C-C3C	-5.11	117.33	124.84
22	A	851	CLA	O2D-CGD-CBD	5.11	120.34	111.27
21	Y	307	CHL	O2D-CGD-CBD	5.10	120.33	111.27
22	1	302	CLA	CHD-C4C-C3C	-5.10	117.34	124.84
22	Y	310	CLA	C3B-C2B-C1B	-5.10	101.00	107.16
22	A	844	CLA	C3B-C4B-NB	5.10	115.24	110.52
22	G	205	CLA	C3B-C2B-C1B	-5.10	101.01	107.16
21	3	314	CHL	C2D-C1D-ND	5.09	113.86	110.10
22	B	812	CLA	CHD-C4C-C3C	-5.09	117.36	124.84
21	Z	305	CHL	C3B-C2B-C1B	-5.09	101.02	107.16
22	A	838	CLA	C3B-C2B-C1B	-5.09	101.02	107.16
22	1	307	CLA	C3B-C2B-C1B	-5.09	101.02	107.16
22	3	313	CLA	C3B-C2B-C1B	-5.08	101.02	107.16
22	Z	310	CLA	O2D-CGD-CBD	5.08	120.30	111.27
21	3	307	CHL	C2D-C1D-ND	5.08	113.85	110.10
21	2	321	CHL	C3B-C2B-C1B	-5.08	101.03	107.16
22	A	854	CLA	CMD-C2D-C1D	5.08	133.66	124.71
22	1	306	CLA	C3B-C2B-C1B	-5.07	101.04	107.16
24	3	302	XAT	C18-C5-C6	-5.07	113.76	122.26
21	X	309	CHL	C3C-C4C-NC	5.06	116.25	110.57
24	4	320	XAT	C38-C25-C26	-5.06	113.77	122.26
22	2	303	CLA	C3B-C2B-C1B	-5.06	101.05	107.16
22	B	818	CLA	CHD-C4C-C3C	-5.05	117.42	124.84
25	B	837	BCR	C24-C23-C22	5.05	133.86	126.23
22	B	805	CLA	O2D-CGD-CBD	5.05	120.24	111.27
22	A	837	CLA	C3B-C2B-C1B	-5.04	101.08	107.16
22	A	847	CLA	C1C-C2C-C3C	-5.04	101.66	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	F	302	BCR	C16-C15-C14	5.04	133.79	123.47
22	2	306	CLA	C3B-C2B-C1B	-5.04	101.08	107.16
21	Z	312	CHL	C3B-C2B-C1B	-5.04	101.08	107.16
22	A	853	CLA	CHD-C1D-ND	-5.03	119.83	124.45
22	3	317	CLA	C3B-C2B-C1B	-5.03	101.09	107.16
22	Z	308	CLA	O2D-CGD-CBD	5.03	120.21	111.27
21	4	309	CHL	C3C-C4C-NC	5.03	116.21	110.57
22	B	822	CLA	CHD-C4C-C3C	-5.03	117.44	124.84
22	4	316	CLA	O2D-CGD-CBD	5.03	120.20	111.27
22	B	826	CLA	CHC-C4B-NB	-5.02	118.94	124.26
22	B	814	CLA	C3B-C2B-C1B	-5.02	101.10	107.16
22	A	843	CLA	O2D-CGD-CBD	5.02	120.19	111.27
22	B	827	CLA	O2D-CGD-CBD	5.02	120.18	111.27
22	A	833	CLA	CHD-C4C-C3C	-5.01	117.47	124.84
25	G	202	BCR	C24-C23-C22	-5.01	118.66	126.23
22	Y	301	CLA	C3B-C2B-C1B	-5.01	101.11	107.16
22	Y	301	CLA	CHD-C4C-C3C	-5.01	117.47	124.84
22	2	308	CLA	C3B-C2B-C1B	-5.01	101.12	107.16
21	Z	312	CHL	O2D-CGD-CBD	5.01	120.16	111.27
21	Z	305	CHL	C3C-C4C-NC	5.00	116.18	110.57
21	X	305	CHL	O2D-CGD-CBD	5.00	120.16	111.27
22	B	817	CLA	O2D-CGD-CBD	5.00	120.16	111.27
22	O	210	CLA	O2D-CGD-CBD	5.00	120.16	111.27
22	A	802	CLA	C4D-CHA-C1A	-5.00	115.16	121.25
22	A	852	CLA	O2D-CGD-CBD	5.00	120.16	111.27
22	4	315	CLA	C3C-C4C-NC	5.00	116.18	110.57
22	B	851	CLA	C1C-C2C-C3C	-5.00	101.70	106.96
21	X	308	CHL	O2D-CGD-CBD	5.00	120.15	111.27
21	Y	304	CHL	O2D-CGD-CBD	4.99	120.14	111.27
21	X	306	CHL	O2D-CGD-CBD	4.99	120.14	111.27
21	Y	306	CHL	O2D-CGD-CBD	4.99	120.14	111.27
22	2	319	CLA	C1D-CHD-C4C	-4.99	115.29	126.06
22	3	317	CLA	CHC-C4B-NB	-4.99	118.97	124.26
22	A	804	CLA	C1C-C2C-C3C	-4.99	101.71	106.96
22	G	206	CLA	C3B-C2B-C1B	-4.99	101.14	107.16
22	4	305	CLA	C3B-C2B-C1B	-4.98	101.15	107.16
22	1	308	CLA	C3D-C4D-ND	4.98	118.30	110.24
25	2	312	BCR	C11-C10-C9	4.98	134.42	127.31
22	B	845	CLA	CHC-C4B-NB	-4.98	118.98	124.26
22	B	811	CLA	C3B-C2B-C1B	-4.98	101.15	107.16
22	A	826	CLA	CMC-C2C-C1C	4.98	132.62	125.04
22	X	301	CLA	O2D-CGD-CBD	4.97	120.11	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	316	CLA	CMC-C2C-C1C	4.97	132.60	125.04
22	3	318	CLA	C3B-C2B-C1B	-4.96	101.17	107.16
22	F	305	CLA	C3B-C2B-C1B	-4.96	101.17	107.16
24	1	311	XAT	C11-C10-C9	-4.96	120.23	127.31
22	1	320	CLA	C3B-C2B-C1B	-4.96	101.18	107.16
22	A	834	CLA	C3D-C4D-ND	4.95	118.25	110.24
21	2	309	CHL	C3C-C4C-NC	4.95	116.12	110.57
22	K	202	CLA	C3B-C2B-C1B	-4.95	101.19	107.16
22	B	816	CLA	CHB-C1B-NB	-4.95	119.02	124.26
22	4	310	CLA	C3B-C2B-C1B	-4.95	101.19	107.16
22	B	810	CLA	C4D-CHA-C1A	-4.95	115.23	121.25
22	B	808	CLA	CHC-C4B-NB	-4.95	119.02	124.26
22	3	319	CLA	O2D-CGD-CBD	4.95	120.06	111.27
22	O	209	CLA	C3B-C2B-C1B	-4.94	101.20	107.16
22	3	313	CLA	O2D-CGD-CBD	4.94	120.04	111.27
21	X	309	CHL	O2D-CGD-CBD	4.93	120.03	111.27
22	A	845	CLA	CHD-C1D-ND	-4.93	119.92	124.45
21	1	316	CHL	CHD-C1D-ND	-4.93	119.92	124.45
21	4	317	CHL	C3C-C4C-NC	4.93	116.10	110.57
21	2	309	CHL	O2D-CGD-CBD	4.93	120.02	111.27
22	Y	312	CLA	O2D-CGD-CBD	4.93	120.02	111.27
22	J	102	CLA	C3B-C2B-C1B	-4.92	101.22	107.16
22	2	306	CLA	C4A-NA-C1A	4.92	108.92	106.71
22	K	204	CLA	O2D-CGD-CBD	4.92	120.01	111.27
22	B	853	CLA	O2D-CGD-CBD	4.92	120.01	111.27
23	4	322	LUT	C39-C29-C30	-4.92	116.03	122.92
21	1	316	CHL	O2D-CGD-CBD	4.92	120.01	111.27
22	B	824	CLA	C3B-C2B-C1B	-4.92	101.23	107.16
22	B	802	CLA	C3D-C4D-ND	4.91	118.19	110.24
22	K	204	CLA	CHD-C4C-C3C	-4.91	117.62	124.84
22	1	308	CLA	C3C-C4C-NC	4.91	116.08	110.57
22	Y	309	CLA	O2D-CGD-CBD	4.91	119.99	111.27
22	B	816	CLA	C2B-C1B-NB	4.91	113.52	110.23
21	4	309	CHL	C3B-C2B-C1B	-4.91	101.24	107.16
22	A	855	CLA	CHD-C4C-C3C	-4.90	117.63	124.84
22	A	838	CLA	CHC-C4B-NB	-4.90	119.07	124.26
22	3	309	CLA	O2D-CGD-CBD	4.90	119.98	111.27
22	O	208	CLA	C3B-C2B-C1B	-4.90	101.24	107.16
22	2	304	CLA	C3B-C2B-C1B	-4.90	101.25	107.16
22	2	319	CLA	C2B-C1B-NB	4.90	113.52	110.23
22	A	803	CLA	C3B-C2B-C1B	-4.90	101.25	107.16
22	4	304	CLA	O2D-CGD-CBD	4.90	119.97	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	827	CLA	C3C-C4C-NC	4.90	116.06	110.57
21	Z	301	CHL	O2D-CGD-CBD	4.89	119.97	111.27
22	A	844	CLA	C3B-C2B-C1B	-4.89	101.25	107.16
25	B	838	BCR	C7-C8-C9	4.89	133.63	126.23
22	2	306	CLA	CHC-C4B-NB	-4.89	119.08	124.26
22	Y	302	CLA	O2D-CGD-CBD	4.89	119.95	111.27
22	B	814	CLA	C4D-CHA-C1A	-4.89	115.30	121.25
22	Z	311	CLA	O2D-CGD-CBD	4.88	119.95	111.27
22	4	314	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
22	A	802	CLA	CHD-C4C-C3C	-4.88	117.66	124.84
25	B	835	BCR	C15-C16-C17	4.88	133.47	123.47
22	2	307	CLA	O2D-CGD-CBD	4.88	119.94	111.27
22	B	801	CLA	O2D-CGD-CBD	4.88	119.94	111.27
22	A	807	CLA	C1C-C2C-C3C	-4.88	101.83	106.96
26	F	301	LHG	O7-C7-C8	4.88	122.01	111.50
22	2	319	CLA	C4C-C3C-C2C	-4.88	102.60	107.07
22	Z	307	CLA	O2D-CGD-CBD	4.87	119.92	111.27
22	Y	301	CLA	O2D-CGD-CBD	4.87	119.92	111.27
25	1	312	BCR	C16-C15-C14	4.87	133.45	123.47
22	A	854	CLA	C3B-C2B-C1B	-4.87	101.29	107.16
22	B	816	CLA	O2D-CGD-CBD	4.87	119.92	111.27
22	B	827	CLA	CHD-C4C-C3C	-4.87	117.69	124.84
22	Y	314	CLA	C3B-C2B-C1B	-4.87	101.29	107.16
22	2	317	CLA	C3B-C2B-C1B	-4.86	101.29	107.16
22	A	845	CLA	C3D-C4D-ND	4.86	118.11	110.24
22	B	812	CLA	O2D-CGD-CBD	4.86	119.91	111.27
22	O	206	CLA	O2D-CGD-CBD	4.86	119.90	111.27
22	B	814	CLA	C3D-C4D-ND	4.86	118.10	110.24
22	O	208	CLA	O2D-CGD-CBD	4.86	119.90	111.27
22	A	850	CLA	O2D-CGD-CBD	4.86	119.90	111.27
22	X	311	CLA	O2D-CGD-CBD	4.86	119.90	111.27
22	K	205	CLA	CHD-C1D-ND	-4.86	119.99	124.45
22	2	317	CLA	O2D-CGD-CBD	4.85	119.89	111.27
25	B	838	BCR	C34-C9-C8	4.85	125.72	118.08
22	B	812	CLA	C1C-C2C-C3C	-4.85	101.85	106.96
22	4	316	CLA	C3B-C2B-C1B	-4.85	101.30	107.16
22	B	819	CLA	CHD-C4C-C3C	-4.85	117.71	124.84
22	A	836	CLA	C3D-C4D-ND	4.85	118.09	110.24
31	O	201	DGD	C1E-O6E-C5E	4.85	123.21	113.69
22	B	807	CLA	C4D-CHA-C1A	-4.85	115.35	121.25
22	B	805	CLA	C3D-C4D-ND	4.85	118.08	110.24
22	A	836	CLA	C3B-C2B-C1B	-4.84	101.32	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	308	CLA	C1C-C2C-C3C	-4.84	101.87	106.96
22	A	831	CLA	O2D-CGD-CBD	4.84	119.87	111.27
22	B	802	CLA	C1C-C2C-C3C	-4.84	101.87	106.96
25	B	838	BCR	C16-C15-C14	4.84	133.38	123.47
21	Y	313	CHL	O2D-CGD-CBD	4.83	119.86	111.27
22	3	321	CLA	CHD-C4C-C3C	-4.83	117.74	124.84
22	K	203	CLA	C3D-C4D-ND	4.83	118.06	110.24
22	Z	314	CLA	O2D-CGD-CBD	4.83	119.86	111.27
21	2	321	CHL	C3D-C2D-C1D	-4.83	99.24	105.83
22	4	316	CLA	C1C-C2C-C3C	-4.83	101.88	106.96
22	B	820	CLA	CAC-C3C-C4C	4.83	131.07	124.81
22	3	310	CLA	C3B-C2B-C1B	-4.82	101.34	107.16
30	A	825	CL0	C3B-C2B-C1B	-4.82	101.34	107.16
22	B	828	CLA	C1C-C2C-C3C	-4.82	101.89	106.96
22	3	315	CLA	C1C-C2C-C3C	-4.82	101.89	106.96
22	A	847	CLA	C3D-C4D-ND	4.82	118.03	110.24
21	Y	313	CHL	C3D-C2D-C1D	-4.82	99.26	105.83
22	B	827	CLA	C1C-C2C-C3C	-4.82	101.89	106.96
22	B	809	CLA	C3B-C2B-C1B	-4.81	101.35	107.16
22	3	316	CLA	C1C-C2C-C3C	-4.81	101.90	106.96
22	3	309	CLA	C3D-C4D-ND	4.81	118.02	110.24
24	3	302	XAT	C38-C25-C26	-4.81	114.20	122.26
22	B	853	CLA	CHD-C1D-ND	-4.81	120.04	124.45
23	4	322	LUT	C40-C33-C34	-4.80	116.19	122.92
22	4	310	CLA	C1C-C2C-C3C	-4.80	101.91	106.96
22	A	830	CLA	C1C-C2C-C3C	-4.80	101.91	106.96
22	4	305	CLA	C3D-C4D-ND	4.80	118.01	110.24
21	Z	301	CHL	C3D-C2D-C1D	-4.80	99.28	105.83
21	2	301	CHL	C3D-C2D-C1D	-4.80	99.29	105.83
22	A	845	CLA	C3C-C4C-NC	4.79	115.94	110.57
22	A	839	CLA	O2D-CGD-CBD	4.79	119.78	111.27
22	A	809	CLA	C3B-C2B-C1B	-4.79	101.38	107.16
21	4	317	CHL	C3D-C2D-C1D	-4.79	99.29	105.83
22	B	801	CLA	C4D-CHA-C1A	-4.79	115.42	121.25
22	A	830	CLA	CHC-C4B-NB	-4.78	119.19	124.26
25	G	202	BCR	C12-C13-C14	4.78	126.28	118.94
22	1	318	CLA	C3B-C2B-C1B	-4.78	101.39	107.16
22	G	206	CLA	O2D-CGD-CBD	4.78	119.76	111.27
21	1	316	CHL	CMB-C2B-C1B	4.77	132.64	125.37
22	O	208	CLA	C1C-C2C-C3C	-4.77	101.94	106.96
22	B	813	CLA	C3D-C4D-ND	4.77	117.96	110.24
22	A	826	CLA	C4D-CHA-C1A	-4.77	115.45	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	308	CLA	O2D-CGD-CBD	4.77	119.74	111.27
22	B	807	CLA	CHB-C4A-NA	4.77	131.10	124.51
22	Z	309	CLA	O2D-CGD-CBD	4.77	119.74	111.27
22	A	832	CLA	C3B-C2B-C1B	-4.77	101.41	107.16
23	4	322	LUT	C19-C9-C10	-4.76	116.25	122.92
22	X	304	CLA	CHB-C4A-NA	4.76	131.10	124.51
24	3	302	XAT	C30-C31-C32	4.76	138.08	123.22
22	4	315	CLA	CHD-C4C-C3C	-4.76	117.84	124.84
22	L	305	CLA	CHD-C1D-ND	-4.76	120.08	124.45
21	Y	303	CHL	C3D-C2D-C1D	-4.76	99.34	105.83
22	A	802	CLA	C3D-C4D-ND	4.75	117.93	110.24
22	2	308	CLA	C6-C5-C3	-4.75	106.85	114.62
22	A	848	CLA	C3D-C4D-ND	4.75	117.92	110.24
24	1	311	XAT	O4-C5-C18	4.75	120.75	115.06
21	4	307	CHL	C3D-C2D-C1D	-4.75	99.35	105.83
22	Y	308	CLA	O2D-CGD-CBD	4.75	119.70	111.27
22	O	206	CLA	C3B-C2B-C1B	-4.75	101.43	107.16
21	Y	305	CHL	C3D-C2D-C1D	-4.74	99.36	105.83
21	4	309	CHL	CAC-C3C-C4C	4.74	130.96	124.81
22	B	848	CLA	C3D-C2D-C1D	-4.74	99.37	105.83
21	2	301	CHL	O2D-CGD-CBD	4.74	119.69	111.27
22	A	803	CLA	C3D-C4D-ND	4.73	117.90	110.24
23	2	310	LUT	C30-C31-C32	4.73	137.99	123.22
25	B	839	BCR	C15-C16-C17	4.73	133.17	123.47
22	B	825	CLA	CHD-C1D-ND	-4.73	120.11	124.45
25	B	834	BCR	C34-C9-C10	-4.73	116.30	122.92
22	O	210	CLA	C4D-CHA-C1A	-4.73	115.49	121.25
21	Z	302	CHL	O2D-CGD-CBD	4.73	119.67	111.27
25	4	321	BCR	C16-C15-C14	4.73	133.16	123.47
22	4	315	CLA	C3D-C4D-ND	4.72	117.88	110.24
22	2	320	CLA	C3D-C4D-ND	4.72	117.88	110.24
21	Z	304	CHL	O2D-CGD-CBD	4.72	119.66	111.27
22	2	308	CLA	CHD-C1D-ND	-4.72	120.12	124.45
22	B	819	CLA	C3D-C4D-ND	4.72	117.87	110.24
22	B	846	CLA	CAC-C3C-C4C	4.72	130.93	124.81
22	G	206	CLA	C3D-C4D-ND	4.72	117.87	110.24
22	Z	313	CLA	C3D-C4D-ND	4.72	117.87	110.24
22	1	302	CLA	C3D-C4D-ND	4.71	117.86	110.24
22	F	305	CLA	O2D-CGD-CBD	4.71	119.64	111.27
22	O	207	CLA	C1C-C2C-C3C	-4.71	102.01	106.96
22	O	209	CLA	C3D-C4D-ND	4.71	117.85	110.24
25	A	816	BCR	C35-C13-C14	-4.70	116.34	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	829	CLA	C3D-C4D-ND	4.70	117.84	110.24
21	X	305	CHL	C3D-C2D-C1D	-4.70	99.42	105.83
21	X	302	CHL	C3D-C2D-C1D	-4.70	99.42	105.83
22	A	803	CLA	O2D-CGD-CBD	4.70	119.61	111.27
22	X	312	CLA	O2D-CGD-CBD	4.70	119.61	111.27
25	A	815	BCR	C16-C15-C14	4.70	133.09	123.47
22	X	304	CLA	CHB-C1B-NB	-4.69	119.29	124.26
22	G	207	CLA	C3B-C2B-C1B	-4.69	101.50	107.16
22	B	807	CLA	C3C-C4C-NC	4.69	118.28	112.30
22	3	308	CLA	C3D-C4D-ND	4.69	117.83	110.24
22	B	812	CLA	C3B-C2B-C1B	-4.69	101.50	107.16
24	1	311	XAT	C35-C15-C14	4.69	133.08	123.47
22	B	816	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
22	B	827	CLA	CHD-C1D-ND	-4.69	120.14	124.45
22	B	808	CLA	C1C-C2C-C3C	-4.69	102.03	106.96
21	Y	306	CHL	C3D-C2D-C1D	-4.68	99.44	105.83
22	3	321	CLA	C4D-CHA-C1A	-4.68	115.55	121.25
25	I	101	BCR	C37-C22-C21	-4.68	116.36	122.92
22	Y	310	CLA	C3D-C4D-ND	4.68	117.81	110.24
22	L	306	CLA	C3D-C4D-ND	4.68	117.81	110.24
22	A	802	CLA	O2D-CGD-CBD	4.68	119.58	111.27
25	A	816	BCR	C19-C18-C17	4.68	126.12	118.94
22	L	307	CLA	O2D-CGD-CBD	4.68	119.58	111.27
22	A	836	CLA	O2D-CGD-CBD	4.68	119.58	111.27
22	2	308	CLA	C3D-C4D-ND	4.68	117.80	110.24
22	B	821	CLA	CHD-C1D-ND	-4.67	120.16	124.45
22	A	833	CLA	C3D-C4D-ND	4.67	117.80	110.24
22	B	849	CLA	C3D-C4D-ND	4.67	117.80	110.24
22	A	843	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
21	2	302	CHL	C3D-C2D-C1D	-4.67	99.46	105.83
22	B	811	CLA	C1C-C2C-C3C	-4.67	102.05	106.96
22	X	310	CLA	O2D-CGD-CBD	4.67	119.57	111.27
22	B	813	CLA	C4D-CHA-C1A	-4.67	115.57	121.25
22	Y	310	CLA	O2D-CGD-CBD	4.67	119.56	111.27
21	4	317	CHL	C3B-C4B-NB	4.67	114.84	110.52
22	G	206	CLA	C4D-CHA-C1A	-4.67	115.57	121.25
22	2	319	CLA	O2D-CGD-CBD	4.67	119.56	111.27
22	A	842	CLA	O2D-CGD-CBD	4.67	119.56	111.27
22	2	306	CLA	C1D-CHD-C4C	-4.67	115.99	126.06
22	A	848	CLA	C1C-C2C-C3C	-4.67	102.05	106.96
21	X	306	CHL	C3D-C2D-C1D	-4.66	99.46	105.83
22	Z	306	CLA	C1C-C2C-C3C	-4.66	102.06	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	840	CLA	C3D-C4D-ND	4.66	117.77	110.24
22	B	824	CLA	CHC-C4B-NB	-4.66	119.33	124.26
22	A	836	CLA	C4D-CHA-C1A	-4.66	115.58	121.25
22	A	845	CLA	C4D-CHA-C1A	-4.66	115.58	121.25
22	3	320	CLA	C1C-C2C-C3C	-4.66	102.06	106.96
22	2	318	CLA	O2D-CGD-CBD	4.65	119.54	111.27
22	B	801	CLA	C2D-C1D-ND	4.65	113.53	110.10
22	A	805	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
21	Y	304	CHL	C3D-C2D-C1D	-4.65	99.48	105.83
22	G	205	CLA	C3D-C4D-ND	4.65	117.76	110.24
22	A	804	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
22	Y	314	CLA	C1C-C2C-C3C	-4.65	102.07	106.96
22	H	201	CLA	CHD-C1D-ND	-4.65	120.18	124.45
22	A	830	CLA	C2B-C1B-NB	4.65	113.35	110.23
22	A	846	CLA	C3D-C4D-ND	4.65	117.76	110.24
22	3	320	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
22	B	818	CLA	O2D-CGD-CBD	4.65	119.52	111.27
21	Z	303	CHL	O2D-CGD-CBD	4.65	119.52	111.27
22	1	303	CLA	C3B-C2B-C1B	-4.64	101.56	107.16
22	A	832	CLA	C3D-C4D-ND	4.64	117.75	110.24
22	4	306	CLA	C3D-C4D-ND	4.64	117.75	110.24
21	Z	303	CHL	C3D-C2D-C1D	-4.64	99.50	105.83
22	B	827	CLA	C3D-C4D-ND	4.64	117.74	110.24
22	A	809	CLA	O2D-CGD-CBD	4.64	119.51	111.27
22	A	834	CLA	C3B-C2B-C1B	-4.63	101.57	107.16
22	A	830	CLA	CHC-C1C-C2C	-4.63	113.86	126.73
22	2	320	CLA	C1C-C2C-C3C	-4.63	102.09	106.96
21	X	307	CHL	C3D-C2D-C1D	-4.63	99.51	105.83
21	X	309	CHL	C3D-C2D-C1D	-4.63	99.51	105.83
22	B	816	CLA	C3D-C4D-ND	4.63	117.72	110.24
22	3	308	CLA	O2D-CGD-CBD	4.63	119.49	111.27
22	B	827	CLA	C3B-C2B-C1B	-4.63	101.58	107.16
22	A	806	CLA	CHD-C1D-ND	-4.62	120.20	124.45
22	4	304	CLA	C3D-C4D-ND	4.62	117.72	110.24
22	Z	309	CLA	C3D-C4D-ND	4.62	117.72	110.24
22	B	810	CLA	C3B-C2B-C1B	-4.62	101.58	107.16
22	B	846	CLA	O2D-CGD-CBD	4.62	119.47	111.27
22	B	824	CLA	C3D-C4D-ND	4.62	117.71	110.24
21	Z	312	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
22	3	318	CLA	O2D-CGD-CBD	4.62	119.47	111.27
22	G	205	CLA	C1C-C2C-C3C	-4.61	102.11	106.96
21	Y	313	CHL	CHD-C4C-C3C	-4.61	118.06	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	318	CLA	C3D-C4D-ND	4.61	117.70	110.24
22	A	806	CLA	C3D-C4D-ND	4.61	117.70	110.24
22	B	828	CLA	C3B-C2B-C1B	-4.61	101.60	107.16
22	2	303	CLA	O2D-CGD-CBD	4.61	119.46	111.27
22	O	209	CLA	O2D-CGD-CBD	4.60	119.45	111.27
22	L	307	CLA	C3D-C4D-ND	4.60	117.69	110.24
22	G	207	CLA	C1C-C2C-C3C	-4.60	102.12	106.96
22	K	202	CLA	C1C-C2C-C3C	-4.60	102.12	106.96
22	2	320	CLA	CHD-C1D-ND	-4.60	120.22	124.45
21	4	308	CHL	C3D-C2D-C1D	-4.60	99.55	105.83
22	A	841	CLA	CHD-C1D-ND	-4.60	120.22	124.45
22	B	807	CLA	C4C-C3C-C2C	-4.60	101.18	105.92
22	A	850	CLA	C3B-C2B-C1B	-4.60	101.61	107.16
22	1	305	CLA	C4D-CHA-C1A	-4.59	115.66	121.25
22	A	835	CLA	C1C-C2C-C3C	-4.59	102.13	106.96
22	1	319	CLA	O2D-CGD-CBD	4.59	119.43	111.27
22	A	830	CLA	C1D-CHD-C4C	-4.59	116.15	126.06
25	O	203	BCR	C35-C13-C14	-4.59	116.50	122.92
23	4	322	LUT	C28-C29-C30	4.59	125.98	118.94
22	B	817	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
25	B	834	BCR	C7-C8-C9	4.58	133.16	126.23
22	A	801	CLA	C1C-C2C-C3C	-4.58	102.14	106.96
22	B	819	CLA	C4D-CHA-C1A	-4.58	115.67	121.25
22	B	846	CLA	CHD-C1D-ND	-4.58	120.25	124.45
21	2	309	CHL	C3D-C2D-C1D	-4.58	99.58	105.83
22	A	812	CLA	CHC-C4B-NB	-4.58	119.41	124.26
22	2	304	CLA	O2D-CGD-CBD	4.58	119.40	111.27
22	B	833	CLA	C3D-C4D-ND	4.57	117.64	110.24
22	L	307	CLA	CHD-C1D-ND	-4.57	120.25	124.45
21	Y	303	CHL	CHD-C4C-C3C	-4.57	118.12	124.84
22	B	848	CLA	CHC-C4B-NB	-4.57	119.42	124.26
22	1	303	CLA	C1C-C2C-C3C	-4.57	102.15	106.96
22	B	803	CLA	C3D-C4D-ND	4.57	117.62	110.24
22	2	318	CLA	C3D-C4D-ND	4.57	117.62	110.24
22	A	846	CLA	C3B-C2B-C1B	-4.57	101.65	107.16
22	A	855	CLA	CHC-C1C-C2C	-4.56	114.06	126.73
21	X	308	CHL	C3D-C2D-C1D	-4.56	99.61	105.83
22	A	839	CLA	C1C-C2C-C3C	-4.56	102.16	106.96
22	B	826	CLA	C1D-CHD-C4C	-4.56	116.22	126.06
22	K	205	CLA	C1C-C2C-C3C	-4.56	102.16	106.96
21	3	314	CHL	O2D-CGD-CBD	4.56	119.36	111.27
22	A	832	CLA	C1C-C2C-C3C	-4.55	102.17	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	839	CLA	CHD-C1D-ND	-4.55	120.27	124.45
21	Z	302	CHL	CHD-C4C-C3C	-4.55	118.15	124.84
22	H	201	CLA	C3D-C4D-ND	4.55	117.60	110.24
22	K	203	CLA	CHD-C1D-ND	-4.55	120.27	124.45
22	Z	313	CLA	CHD-C1D-ND	-4.55	120.27	124.45
22	1	302	CLA	C1C-C2C-C3C	-4.55	102.17	106.96
22	2	308	CLA	C1C-C2C-C3C	-4.55	102.17	106.96
22	3	319	CLA	C1C-C2C-C3C	-4.55	102.17	106.96
22	A	849	CLA	C1C-C2C-C3C	-4.55	102.18	106.96
22	B	853	CLA	C3D-C4D-ND	4.55	117.59	110.24
22	B	811	CLA	C3D-C4D-ND	4.54	117.59	110.24
22	Z	310	CLA	C3D-C4D-ND	4.54	117.59	110.24
22	4	318	CLA	C3D-C4D-ND	4.54	117.58	110.24
22	4	315	CLA	C1C-C2C-C3C	-4.54	102.18	106.96
22	3	313	CLA	C3D-C4D-ND	4.54	117.58	110.24
22	B	812	CLA	CHD-C1D-ND	-4.54	120.28	124.45
21	1	316	CHL	C3D-C2D-C1D	-4.54	99.64	105.83
22	2	317	CLA	C3D-C4D-ND	4.54	117.58	110.24
22	B	831	CLA	C3D-C4D-ND	4.54	117.58	110.24
22	A	855	CLA	C1C-C2C-C3C	-4.54	102.19	106.96
22	1	309	CLA	C3D-C4D-ND	4.54	117.58	110.24
22	B	822	CLA	C3D-C4D-ND	4.54	117.58	110.24
22	A	854	CLA	O2D-CGD-CBD	4.54	119.33	111.27
22	A	801	CLA	O2D-CGD-CBD	4.54	119.33	111.27
22	O	206	CLA	C1C-C2C-C3C	-4.53	102.19	106.96
22	1	319	CLA	CHD-C1D-ND	-4.53	120.29	124.45
22	3	308	CLA	CHD-C1D-ND	-4.53	120.29	124.45
22	2	319	CLA	C3B-C2B-C1B	-4.53	101.69	107.16
22	Y	311	CLA	C1C-C2C-C3C	-4.53	102.19	106.96
24	2	311	XAT	O4-C5-C18	4.53	120.49	115.06
22	4	318	CLA	CHD-C1D-ND	-4.53	120.29	124.45
22	A	852	CLA	C4D-CHA-C1A	-4.53	115.74	121.25
22	A	856	CLA	C1C-C2C-C3C	-4.53	102.20	106.96
21	Z	302	CHL	C3D-C2D-C1D	-4.52	99.66	105.83
22	Z	314	CLA	C1C-C2C-C3C	-4.52	102.20	106.96
22	3	318	CLA	C1C-C2C-C3C	-4.52	102.20	106.96
22	A	829	CLA	CHD-C1D-ND	-4.52	120.30	124.45
21	Z	305	CHL	C3D-C2D-C1D	-4.52	99.66	105.83
22	2	303	CLA	C1C-C2C-C3C	-4.52	102.20	106.96
22	B	833	CLA	C1C-C2C-C3C	-4.52	102.20	106.96
22	Y	301	CLA	C3D-C4D-ND	4.52	117.55	110.24
22	Z	311	CLA	C1C-C2C-C3C	-4.52	102.21	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	826	CLA	CHD-C1D-ND	-4.52	120.30	124.45
22	Z	313	CLA	O2D-CGD-CBD	4.52	119.29	111.27
25	L	304	BCR	C34-C9-C10	-4.52	116.60	122.92
22	O	206	CLA	C3D-C4D-ND	4.52	117.54	110.24
22	A	833	CLA	C1C-C2C-C3C	-4.51	102.21	106.96
22	X	310	CLA	C1C-C2C-C3C	-4.51	102.21	106.96
22	A	849	CLA	O2D-CGD-CBD	4.51	119.28	111.27
22	1	309	CLA	CHD-C1D-ND	-4.51	120.31	124.45
22	Z	314	CLA	CHD-C1D-ND	-4.51	120.31	124.45
22	A	828	CLA	C3D-C4D-ND	4.51	117.53	110.24
22	A	845	CLA	C3B-C2B-C1B	-4.51	101.72	107.16
27	1	315	MGE	C1D-O6D-C5D	4.51	122.54	113.69
25	J	103	BCR	C34-C9-C10	-4.51	116.61	122.92
22	A	858	CLA	CHC-C1C-C2C	-4.51	114.21	126.73
22	1	309	CLA	C1C-C2C-C3C	-4.51	102.22	106.96
22	B	849	CLA	C1C-C2C-C3C	-4.51	102.22	106.96
22	4	306	CLA	C4D-CHA-C1A	-4.50	115.77	121.25
22	G	206	CLA	CHC-C4B-NB	-4.50	119.49	124.26
21	Z	304	CHL	CHD-C4C-C3C	-4.50	118.22	124.84
22	4	314	CLA	C1C-C2C-C3C	-4.50	102.22	106.96
22	Z	308	CLA	C3D-C4D-ND	4.50	117.52	110.24
22	Y	312	CLA	C1C-C2C-C3C	-4.50	102.22	106.96
22	K	204	CLA	C3D-C4D-ND	4.50	117.52	110.24
22	A	844	CLA	CHD-C1D-ND	-4.50	120.32	124.45
22	B	810	CLA	C3D-C4D-ND	4.50	117.52	110.24
22	X	313	CLA	C3D-C4D-ND	4.50	117.52	110.24
21	Y	307	CHL	C3D-C2D-C1D	-4.50	99.69	105.83
24	4	320	XAT	C35-C34-C33	-4.50	120.89	127.31
22	B	830	CLA	CHD-C1D-ND	-4.50	120.32	124.45
22	B	853	CLA	C1C-C2C-C3C	-4.49	102.23	106.96
22	B	852	CLA	CHD-C1D-ND	-4.49	120.32	124.45
22	2	320	CLA	C3B-C2B-C1B	-4.49	101.74	107.16
22	A	838	CLA	C4A-NA-C1A	4.49	108.73	106.71
22	A	849	CLA	CHD-C1D-ND	-4.49	120.33	124.45
25	1	312	BCR	C34-C9-C8	4.49	125.16	118.08
22	Y	311	CLA	C3D-C4D-ND	4.49	117.50	110.24
21	Z	301	CHL	CHD-C4C-C3C	-4.49	118.24	124.84
23	4	322	LUT	C12-C13-C14	4.49	125.83	118.94
22	A	828	CLA	C1D-CHD-C4C	-4.49	116.37	126.06
22	X	303	CLA	C3D-C4D-ND	4.49	117.50	110.24
22	2	304	CLA	C3D-C4D-ND	4.49	117.50	110.24
22	J	102	CLA	C3D-C4D-ND	4.49	117.50	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	805	CLA	CHD-C1D-ND	-4.49	120.33	124.45
22	B	824	CLA	C1C-C2C-C3C	-4.49	102.24	106.96
22	1	302	CLA	CHD-C1D-ND	-4.49	120.33	124.45
22	Z	308	CLA	C1C-C2C-C3C	-4.48	102.24	106.96
22	B	823	CLA	C3D-C4D-ND	4.48	117.49	110.24
22	2	308	CLA	CHC-C4B-NB	-4.48	119.51	124.26
22	K	204	CLA	CHC-C4B-NB	-4.48	119.51	124.26
21	Y	305	CHL	O2D-CGD-CBD	4.48	119.23	111.27
22	B	811	CLA	CHD-C1D-ND	-4.48	120.34	124.45
22	4	312	CLA	O2D-CGD-CBD	4.48	119.23	111.27
21	Y	313	CHL	C3B-C4B-NB	4.48	114.67	110.52
22	3	320	CLA	C3D-C4D-ND	4.48	117.48	110.24
22	B	828	CLA	CHD-C1D-ND	-4.48	120.34	124.45
25	G	202	BCR	C19-C18-C17	4.48	125.81	118.94
22	G	207	CLA	CHD-C1D-ND	-4.47	120.34	124.45
22	1	306	CLA	C3D-C4D-ND	4.47	117.48	110.24
22	3	311	CLA	O2D-CGD-CBD	4.47	119.22	111.27
24	1	311	XAT	C30-C31-C32	4.47	137.18	123.22
22	4	311	CLA	CHD-C1D-ND	-4.47	120.34	124.45
21	Y	303	CHL	C2D-C1D-ND	4.47	113.40	110.10
22	B	851	CLA	O2D-CGD-CBD	4.47	119.21	111.27
22	A	847	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
22	Y	302	CLA	C3D-C4D-ND	4.47	117.47	110.24
22	A	842	CLA	C3D-C4D-ND	4.47	117.47	110.24
22	3	312	CLA	C1C-C2C-C3C	-4.47	102.26	106.96
22	Y	308	CLA	C1C-C2C-C3C	-4.47	102.26	106.96
24	4	320	XAT	C6-C7-C8	-4.47	116.55	125.99
22	L	305	CLA	C3D-C4D-ND	4.47	117.46	110.24
22	B	802	CLA	O2D-CGD-CBD	4.47	119.20	111.27
25	O	202	BCR	C12-C13-C14	4.47	125.79	118.94
22	F	305	CLA	C1C-C2C-C3C	-4.46	102.26	106.96
22	X	303	CLA	O2D-CGD-CBD	4.46	119.20	111.27
22	A	828	CLA	C3B-C2B-C1B	-4.46	101.78	107.16
22	A	859	CLA	CHD-C1D-ND	-4.46	120.36	124.45
22	B	803	CLA	C4A-NA-C1A	4.46	108.71	106.71
22	L	305	CLA	C1C-C2C-C3C	-4.46	102.27	106.96
25	1	312	BCR	C16-C17-C18	4.46	133.67	127.31
22	A	838	CLA	C3D-C4D-ND	4.46	117.45	110.24
25	B	840	BCR	C12-C13-C14	4.46	125.78	118.94
25	G	202	BCR	C36-C18-C17	-4.46	116.68	122.92
22	O	209	CLA	C1C-C2C-C3C	-4.45	102.27	106.96
22	A	833	CLA	CHD-C1D-ND	-4.45	120.36	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	311	XAT	C35-C34-C33	-4.45	120.96	127.31
22	2	319	CLA	C2D-C1D-ND	4.45	113.38	110.10
22	B	808	CLA	C3D-C4D-ND	4.45	117.43	110.24
22	B	830	CLA	C3D-C4D-ND	4.45	117.43	110.24
22	B	822	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
22	Y	302	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
22	B	815	CLA	C3D-C4D-ND	4.45	117.43	110.24
22	1	321	CLA	C3D-C4D-ND	4.45	117.43	110.24
21	4	309	CHL	C3D-C2D-C1D	-4.45	99.76	105.83
25	B	837	BCR	C30-C25-C26	-4.45	116.35	122.61
22	Y	311	CLA	CHD-C1D-ND	-4.45	120.37	124.45
22	1	307	CLA	C3D-C4D-ND	4.44	117.43	110.24
22	1	319	CLA	C3D-C4D-ND	4.44	117.42	110.24
22	Y	309	CLA	C3D-C4D-ND	4.44	117.42	110.24
22	4	315	CLA	C4D-CHA-C1A	-4.44	115.85	121.25
22	Z	311	CLA	C3D-C4D-ND	4.44	117.42	110.24
22	A	852	CLA	C1D-CHD-C4C	-4.44	116.48	126.06
21	2	301	CHL	C3B-C4B-NB	4.44	114.63	110.52
22	2	305	CLA	C1C-C2C-C3C	-4.44	102.29	106.96
22	3	311	CLA	C4D-CHA-C1A	-4.44	115.85	121.25
21	Z	301	CHL	C2D-C1D-ND	4.44	113.37	110.10
22	N	202	CLA	C1C-C2C-C3C	-4.44	102.29	106.96
22	X	312	CLA	C3D-C4D-ND	4.43	117.41	110.24
22	X	303	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
22	X	311	CLA	C3D-C4D-ND	4.43	117.41	110.24
22	2	319	CLA	CHC-C4B-NB	-4.43	119.56	124.26
22	X	301	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
22	B	825	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
24	1	311	XAT	C31-C32-C33	4.43	138.86	126.42
22	A	833	CLA	CHC-C4B-NB	-4.43	119.57	124.26
22	K	203	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
22	3	309	CLA	CHD-C1D-ND	-4.43	120.39	124.45
22	3	321	CLA	C3D-C4D-ND	4.43	117.40	110.24
22	2	319	CLA	CHC-C1C-C2C	-4.43	114.43	126.73
21	X	302	CHL	CHD-C4C-C3C	-4.43	118.33	124.84
22	A	833	CLA	C4D-CHA-C1A	-4.43	115.86	121.25
22	Z	309	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
22	O	206	CLA	CHD-C1D-ND	-4.43	120.39	124.45
22	A	803	CLA	C4D-CHA-C1A	-4.42	115.86	121.25
22	A	830	CLA	C3D-C4D-ND	4.42	117.39	110.24
22	B	851	CLA	CAC-C3C-C4C	4.42	130.55	124.81
22	B	821	CLA	C3D-C4D-ND	4.42	117.39	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	209	CLA	CHC-C4B-NB	-4.42	119.58	124.26
22	O	208	CLA	C3D-C4D-ND	4.42	117.39	110.24
22	4	318	CLA	C1C-C2C-C3C	-4.42	102.31	106.96
22	B	828	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
21	1	316	CHL	CHD-C4C-C3C	-4.42	118.34	124.84
22	Y	314	CLA	C3D-C4D-ND	4.42	117.39	110.24
22	J	102	CLA	C1C-C2C-C3C	-4.42	102.31	106.96
22	2	306	CLA	C2D-C1D-ND	4.42	113.36	110.10
21	1	301	CHL	C3D-C2D-C1D	-4.42	99.81	105.83
21	Z	303	CHL	CHD-C4C-C3C	-4.42	118.35	124.84
22	A	837	CLA	C3D-C4D-ND	4.42	117.38	110.24
22	4	304	CLA	C1C-C2C-C3C	-4.41	102.31	106.96
22	4	313	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
22	1	317	CLA	C4D-CHA-C1A	-4.41	115.88	121.25
22	B	847	CLA	CHD-C1D-ND	-4.41	120.40	124.45
22	A	808	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
22	1	304	CLA	CHC-C4B-NB	-4.41	119.59	124.26
22	B	806	CLA	C3D-C4D-ND	4.41	117.37	110.24
22	Y	309	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
22	1	317	CLA	C3D-C2D-C1D	-4.41	99.82	105.83
22	Z	307	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
22	3	309	CLA	C4D-CHA-C1A	-4.41	115.89	121.25
22	4	314	CLA	C3D-C4D-ND	4.41	117.36	110.24
22	Y	301	CLA	CHD-C1D-ND	-4.40	120.41	124.45
22	B	833	CLA	CHD-C1D-ND	-4.40	120.41	124.45
22	B	845	CLA	O2D-CGD-CBD	4.40	119.09	111.27
22	A	851	CLA	CHD-C1D-ND	-4.40	120.41	124.45
22	B	802	CLA	CHC-C4B-NB	-4.40	119.60	124.26
22	1	304	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
22	B	847	CLA	C3D-C4D-ND	4.40	117.35	110.24
21	4	317	CHL	C2D-C1D-ND	4.40	113.34	110.10
21	X	307	CHL	CHD-C4C-C3C	-4.40	118.38	124.84
22	A	847	CLA	CHD-C1D-ND	-4.40	120.42	124.45
22	B	815	CLA	CHD-C1D-ND	-4.40	120.42	124.45
21	2	321	CHL	C3B-C4B-NB	4.39	114.59	110.52
22	A	812	CLA	C3D-C4D-ND	4.39	117.35	110.24
22	A	834	CLA	C4D-CHA-C1A	-4.39	115.90	121.25
21	X	306	CHL	CHD-C4C-C3C	-4.39	118.38	124.84
22	3	320	CLA	CHD-C1D-ND	-4.39	120.42	124.45
22	4	311	CLA	O2D-CGD-CBD	4.39	119.07	111.27
22	Z	307	CLA	C3D-C4D-ND	4.39	117.34	110.24
22	Z	313	CLA	C1C-C2C-C3C	-4.39	102.34	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	L	302	BCR	C12-C13-C14	4.39	125.68	118.94
22	B	825	CLA	C3B-C2B-C1B	-4.39	101.86	107.16
21	Y	313	CHL	C2D-C1D-ND	4.39	113.34	110.10
22	B	846	CLA	C3D-C4D-ND	4.39	117.33	110.24
22	3	308	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
22	Z	314	CLA	C3D-C4D-ND	4.38	117.33	110.24
22	Z	309	CLA	CHD-C1D-ND	-4.38	120.43	124.45
22	2	322	CLA	C1C-C2C-C3C	-4.38	102.35	106.96
22	Y	312	CLA	C3D-C4D-ND	4.38	117.33	110.24
22	4	316	CLA	C3D-C4D-ND	4.38	117.33	110.24
22	X	312	CLA	C1C-C2C-C3C	-4.38	102.35	106.96
22	2	322	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
22	A	810	CLA	CAC-C3C-C4C	4.38	130.49	124.81
22	2	317	CLA	CHD-C1D-ND	-4.38	120.43	124.45
22	Y	301	CLA	C1C-C2C-C3C	-4.38	102.36	106.96
21	X	302	CHL	C2D-C1D-ND	4.38	113.33	110.10
22	1	303	CLA	C3D-C4D-ND	4.38	117.32	110.24
22	3	311	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
22	A	837	CLA	CHC-C4B-NB	-4.38	119.62	124.26
22	O	210	CLA	C3D-C4D-ND	4.37	117.31	110.24
22	Y	310	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
22	B	811	CLA	C3D-C2D-C1D	-4.37	99.86	105.83
22	A	808	CLA	C3D-C4D-ND	4.37	117.31	110.24
22	B	830	CLA	O2D-CGD-CBD	4.37	119.03	111.27
22	O	208	CLA	CHC-C4B-NB	-4.37	119.63	124.26
22	3	308	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
22	2	318	CLA	CHD-C1D-ND	-4.37	120.44	124.45
22	O	208	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
21	X	305	CHL	CHD-C4C-C3C	-4.37	118.42	124.84
22	A	859	CLA	C3D-C4D-ND	4.37	117.30	110.24
22	A	844	CLA	CHC-C1C-C2C	-4.37	114.60	126.73
22	B	818	CLA	C1C-C2C-C3C	-4.37	102.37	106.96
22	2	306	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
22	A	828	CLA	C1C-C2C-C3C	-4.36	102.37	106.96
22	A	857	CLA	C3D-C4D-ND	4.36	117.30	110.24
22	X	301	CLA	C3D-C4D-ND	4.36	117.30	110.24
30	A	825	CL0	O2D-CGD-CBD	4.36	119.02	111.27
22	O	209	CLA	CHD-C1D-ND	-4.36	120.45	124.45
22	A	851	CLA	C3D-C4D-ND	4.36	117.29	110.24
22	1	319	CLA	C1C-C2C-C3C	-4.36	102.37	106.96
22	A	858	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
25	B	840	BCR	C19-C18-C17	4.36	125.63	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	X	313	CLA	C1C-C2C-C3C	-4.36	102.38	106.96
22	K	205	CLA	C3D-C4D-ND	4.36	117.29	110.24
25	G	202	BCR	C34-C9-C10	-4.36	116.82	122.92
22	G	206	CLA	C1C-C2C-C3C	-4.36	102.38	106.96
22	X	311	CLA	C1C-C2C-C3C	-4.35	102.38	106.96
22	Z	310	CLA	C1C-C2C-C3C	-4.35	102.38	106.96
22	A	803	CLA	C1C-C2C-C3C	-4.35	102.38	106.96
22	2	317	CLA	C1C-C2C-C3C	-4.35	102.38	106.96
22	1	307	CLA	C4D-CHA-C1A	-4.35	115.95	121.25
22	G	205	CLA	C4D-CHA-C1A	-4.35	115.95	121.25
22	A	809	CLA	C3D-C4D-ND	4.35	117.27	110.24
22	B	818	CLA	C4D-CHA-C1A	-4.35	115.96	121.25
22	B	846	CLA	C1C-C2C-C3C	-4.35	102.38	106.96
22	A	852	CLA	C4-C3-C5	4.35	122.58	115.27
22	3	308	CLA	C2D-C1D-ND	4.35	113.31	110.10
21	Y	305	CHL	CHD-C4C-C3C	-4.35	118.45	124.84
22	Z	310	CLA	CHD-C1D-ND	-4.34	120.46	124.45
21	Z	304	CHL	C3D-C2D-C1D	-4.34	99.90	105.83
22	A	851	CLA	C3D-C2D-C1D	-4.34	99.90	105.83
22	B	850	CLA	CAA-C2A-C3A	-4.34	100.89	112.78
22	J	102	CLA	CHC-C4B-NB	-4.34	119.66	124.26
21	2	301	CHL	C2D-C1D-ND	4.34	113.30	110.10
22	B	852	CLA	C3D-C4D-ND	4.34	117.26	110.24
22	B	803	CLA	C4C-C3C-C2C	-4.34	100.57	106.90
22	B	808	CLA	CHD-C1D-ND	-4.34	120.47	124.45
22	X	313	CLA	CHD-C1D-ND	-4.34	120.47	124.45
22	A	841	CLA	CHC-C4B-NB	-4.34	119.67	124.26
22	4	305	CLA	C2D-C1D-ND	4.34	113.30	110.10
22	3	313	CLA	C1C-C2C-C3C	-4.33	102.40	106.96
21	3	307	CHL	CHD-C4C-C3C	-4.33	118.47	124.84
22	B	830	CLA	C3B-C2B-C1B	-4.33	101.93	107.16
22	A	804	CLA	C3D-C4D-ND	4.33	117.24	110.24
22	B	801	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
21	2	302	CHL	CHD-C4C-C3C	-4.33	118.48	124.84
22	A	810	CLA	O2D-CGD-CBD	4.33	118.96	111.27
21	Y	304	CHL	CHD-C4C-C3C	-4.33	118.48	124.84
22	A	837	CLA	CHD-C1D-ND	-4.33	120.48	124.45
22	X	303	CLA	CHD-C1D-ND	-4.33	120.48	124.45
21	X	306	CHL	C2D-C1D-ND	4.33	113.29	110.10
25	A	817	BCR	C34-C9-C10	-4.32	116.87	122.92
22	3	312	CLA	C4D-CHA-C1A	-4.32	115.99	121.25
22	A	841	CLA	C3D-C4D-ND	4.32	117.23	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	X	305	CHL	C2D-C1D-ND	4.32	113.29	110.10
21	Z	312	CHL	CHD-C4C-C3C	-4.32	118.49	124.84
21	2	321	CHL	C2D-C1D-ND	4.32	113.29	110.10
25	B	837	BCR	C16-C15-C14	4.32	132.33	123.47
22	L	307	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
22	B	803	CLA	CHC-C4B-NB	-4.32	119.68	124.26
22	A	831	CLA	C4D-CHA-C1A	-4.32	115.99	121.25
22	B	824	CLA	CHD-C1D-ND	-4.32	120.49	124.45
25	B	840	BCR	C16-C17-C18	4.32	133.47	127.31
21	2	321	CHL	CHD-C4C-C3C	-4.31	118.50	124.84
22	A	832	CLA	CHD-C1D-ND	-4.31	120.49	124.45
22	B	821	CLA	C1C-C2C-C3C	-4.31	102.42	106.96
22	B	819	CLA	CAC-C3C-C4C	4.31	130.41	124.81
22	1	309	CLA	C4D-CHA-C1A	-4.31	116.00	121.25
22	A	858	CLA	C3D-C4D-ND	4.31	117.22	110.24
21	Z	303	CHL	C2D-C1D-ND	4.31	113.28	110.10
22	X	304	CLA	C1C-C2C-C3C	-4.31	102.42	106.96
22	B	831	CLA	O2D-CGD-CBD	4.31	118.93	111.27
22	A	837	CLA	O2D-CGD-CBD	4.31	118.93	111.27
25	B	839	BCR	C37-C22-C21	-4.31	116.89	122.92
22	4	312	CLA	C1C-C2C-C3C	-4.31	102.43	106.96
22	L	306	CLA	C1C-C2C-C3C	-4.31	102.43	106.96
21	X	308	CHL	CHD-C4C-C3C	-4.31	118.51	124.84
21	4	309	CHL	O2D-CGD-CBD	4.31	118.92	111.27
22	3	312	CLA	C3D-C4D-ND	4.31	117.20	110.24
25	1	312	BCR	C34-C9-C10	-4.30	116.90	122.92
22	B	804	CLA	CAC-C3C-C4C	4.30	130.39	124.81
22	B	852	CLA	C1C-C2C-C3C	-4.30	102.43	106.96
22	3	316	CLA	C4D-CHA-C1A	-4.30	116.01	121.25
25	A	816	BCR	C10-C11-C12	4.30	136.64	123.22
21	2	302	CHL	CMB-C2B-C1B	4.30	131.92	125.37
22	A	827	CLA	O2D-CGD-CBD	4.30	118.91	111.27
22	Y	308	CLA	CHD-C1D-ND	-4.30	120.51	124.45
22	Y	314	CLA	CHC-C4B-NB	-4.30	119.71	124.26
22	A	837	CLA	C1C-C2C-C3C	-4.29	102.44	106.96
22	A	804	CLA	CHD-C1D-ND	-4.29	120.51	124.45
22	B	803	CLA	C2D-C1D-ND	4.29	113.27	110.10
21	Z	305	CHL	C3B-C4B-NB	4.29	114.50	110.52
22	3	317	CLA	C3D-C2D-C1D	-4.29	99.97	105.83
22	3	319	CLA	C3D-C4D-ND	4.29	117.18	110.24
22	A	851	CLA	C1C-C2C-C3C	-4.29	102.44	106.96
22	B	822	CLA	O2D-CGD-CBD	4.29	118.89	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	847	CLA	C4D-CHA-C1A	-4.29	116.03	121.25
22	A	852	CLA	C3D-C4D-ND	4.29	117.18	110.24
21	4	307	CHL	CHD-C4C-C3C	-4.29	118.54	124.84
22	A	857	CLA	CHD-C1D-ND	-4.29	120.51	124.45
22	3	311	CLA	C3D-C4D-ND	4.29	117.17	110.24
25	B	837	BCR	C34-C9-C10	-4.29	116.92	122.92
21	Y	305	CHL	C2D-C1D-ND	4.29	113.26	110.10
21	3	307	CHL	C1D-ND-C4D	-4.29	103.29	106.33
22	4	306	CLA	CHD-C1D-ND	-4.29	120.51	124.45
22	1	317	CLA	C2D-C1D-ND	4.29	113.26	110.10
22	B	819	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
22	4	313	CLA	C3D-C4D-ND	4.28	117.17	110.24
22	2	319	CLA	C3D-C4D-ND	4.28	117.17	110.24
22	B	820	CLA	C3D-C4D-ND	4.28	117.16	110.24
22	A	841	CLA	C3B-C2B-C1B	-4.28	101.99	107.16
22	2	308	CLA	C4D-CHA-C1A	-4.28	116.04	121.25
22	A	828	CLA	CHC-C1C-C2C	-4.28	114.84	126.73
22	1	321	CLA	C1C-C2C-C3C	-4.28	102.46	106.96
22	L	307	CLA	C4D-CHA-C1A	-4.28	116.04	121.25
22	3	321	CLA	C1C-C2C-C3C	-4.28	102.46	106.96
21	2	321	CHL	CAC-C3C-C4C	4.27	130.36	124.81
22	A	810	CLA	C3B-C2B-C1B	-4.27	102.00	107.16
22	3	316	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
22	4	305	CLA	C3D-C2D-C1D	-4.27	100.01	105.83
22	A	838	CLA	C3D-C2D-C1D	-4.27	100.01	105.83
22	B	804	CLA	CMC-C2C-C1C	4.26	131.53	125.04
22	B	830	CLA	CHC-C1C-C2C	-4.26	114.89	126.73
22	2	304	CLA	C4D-CHA-C1A	-4.26	116.06	121.25
22	3	309	CLA	C1C-C2C-C3C	-4.26	102.47	106.96
22	2	320	CLA	O2D-CGD-CBD	4.26	118.84	111.27
22	4	305	CLA	C4D-CHA-C1A	-4.26	116.06	121.25
21	X	309	CHL	C3B-C4B-NB	4.26	114.47	110.52
22	A	841	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
22	K	202	CLA	CHD-C1D-ND	-4.26	120.54	124.45
22	F	306	CLA	C3D-C4D-ND	4.26	117.13	110.24
22	1	320	CLA	C1C-C2C-C3C	-4.26	102.48	106.96
22	N	202	CLA	C3D-C4D-ND	4.26	117.12	110.24
22	3	310	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
22	B	825	CLA	C3D-C4D-ND	4.25	117.12	110.24
22	A	804	CLA	CHC-C4B-NB	-4.25	119.75	124.26
22	A	855	CLA	C3B-C4B-NB	4.25	114.46	110.52
22	A	848	CLA	C3B-C2B-C1B	-4.25	102.03	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Y	312	CLA	CHD-C1D-ND	-4.25	120.55	124.45
22	Z	308	CLA	CHD-C1D-ND	-4.25	120.55	124.45
25	O	202	BCR	C7-C8-C9	-4.25	119.81	126.23
22	1	309	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
22	K	202	CLA	C3D-C4D-ND	4.25	117.11	110.24
22	3	318	CLA	C3D-C4D-ND	4.25	117.11	110.24
22	B	809	CLA	O2D-CGD-CBD	4.25	118.81	111.27
22	Z	311	CLA	CHD-C1D-ND	-4.24	120.55	124.45
22	B	814	CLA	C3D-C2D-C1D	-4.24	100.04	105.83
25	A	816	BCR	C36-C18-C17	-4.24	116.98	122.92
22	A	831	CLA	C3D-C4D-ND	4.24	117.10	110.24
22	A	835	CLA	C3B-C2B-C1B	-4.24	102.04	107.16
22	1	307	CLA	C3D-C2D-C1D	-4.24	100.05	105.83
22	1	305	CLA	C3D-C4D-ND	4.24	117.09	110.24
21	Y	306	CHL	CHD-C4C-C3C	-4.24	118.61	124.84
22	2	307	CLA	C3D-C4D-ND	4.24	117.09	110.24
22	B	825	CLA	O2D-CGD-CBD	4.23	118.79	111.27
22	O	210	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
25	B	834	BCR	C8-C9-C10	4.23	125.44	118.94
22	A	801	CLA	CHB-C4A-NA	4.23	130.36	124.51
22	B	821	CLA	O2D-CGD-CBD	4.23	118.79	111.27
22	3	319	CLA	CHD-C1D-ND	-4.23	120.56	124.45
25	B	844	BCR	C15-C16-C17	4.23	132.14	123.47
22	B	802	CLA	CHD-C1D-ND	-4.23	120.57	124.45
22	A	858	CLA	C4A-NA-C1A	4.23	108.61	106.71
22	3	313	CLA	CHD-C1D-ND	-4.23	120.57	124.45
25	L	302	BCR	C35-C13-C14	-4.23	117.00	122.92
22	1	304	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
22	A	839	CLA	C3D-C4D-ND	4.23	117.07	110.24
22	Y	308	CLA	C3D-C4D-ND	4.23	117.07	110.24
22	B	806	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
22	1	304	CLA	C3D-C4D-ND	4.22	117.07	110.24
22	A	805	CLA	CHD-C1D-ND	-4.22	120.57	124.45
22	B	802	CLA	C4A-NA-C1A	4.22	108.61	106.71
22	1	318	CLA	C1C-C2C-C3C	-4.22	102.52	106.96
22	A	849	CLA	C3D-C4D-ND	4.22	117.07	110.24
22	B	830	CLA	C3B-C4B-NB	4.22	114.43	110.52
22	A	810	CLA	C3D-C4D-ND	4.22	117.06	110.24
22	A	830	CLA	CAC-C3C-C4C	4.22	130.28	124.81
22	B	806	CLA	C4D-CHA-C1A	-4.22	116.11	121.25
22	N	202	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
22	A	858	CLA	O2D-CGD-CBD	4.22	118.77	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	835	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
22	A	809	CLA	C1C-C2C-C3C	-4.22	102.52	106.96
22	A	812	CLA	O2D-CGD-CBD	4.22	118.76	111.27
25	2	312	BCR	C36-C18-C17	-4.22	117.02	122.92
21	1	316	CHL	C2D-C1D-ND	4.22	113.21	110.10
22	A	807	CLA	C3D-C4D-ND	4.22	117.06	110.24
22	B	809	CLA	C3D-C4D-ND	4.21	117.06	110.24
22	Y	302	CLA	CHD-C1D-ND	-4.21	120.58	124.45
22	B	850	CLA	C4D-CHA-C1A	-4.21	116.12	121.25
22	A	851	CLA	C4D-CHA-C1A	-4.21	116.12	121.25
22	A	852	CLA	C2D-C1D-ND	4.21	113.21	110.10
25	O	202	BCR	C35-C13-C14	-4.21	117.02	122.92
21	1	301	CHL	O2D-CGD-CBD	4.21	118.75	111.27
22	3	310	CLA	O2D-CGD-CBD	4.21	118.75	111.27
21	Y	307	CHL	CHD-C4C-C3C	-4.21	118.66	124.84
22	A	831	CLA	C3D-C2D-C1D	-4.21	100.09	105.83
22	Y	309	CLA	CHD-C1D-ND	-4.21	120.59	124.45
23	2	310	LUT	C31-C30-C29	4.20	133.31	127.31
25	J	103	BCR	C16-C15-C14	4.20	132.08	123.47
22	K	204	CLA	C1D-CHD-C4C	-4.20	117.00	126.06
24	1	311	XAT	C6-C7-C8	-4.20	117.11	125.99
22	A	850	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
22	A	836	CLA	CHC-C4B-NB	-4.20	119.81	124.26
22	B	803	CLA	C3D-C2D-C1D	-4.20	100.10	105.83
22	Y	310	CLA	CHD-C1D-ND	-4.20	120.60	124.45
22	A	838	CLA	O2D-CGD-CBD	4.19	118.72	111.27
21	X	307	CHL	C2D-C1D-ND	4.19	113.19	110.10
22	A	829	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
22	1	308	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
23	4	322	LUT	C20-C13-C14	-4.19	117.05	122.92
30	A	825	CL0	C1C-C2C-C3C	-4.19	102.55	106.96
22	A	831	CLA	C1D-CHD-C4C	-4.19	117.02	126.06
22	O	207	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
23	4	322	LUT	C10-C11-C12	4.19	136.29	123.22
21	4	309	CHL	CHD-C4C-C3C	-4.19	118.68	124.84
22	B	829	CLA	CHD-C1D-ND	-4.19	120.61	124.45
21	Y	304	CHL	C2D-C1D-ND	4.18	113.19	110.10
22	A	859	CLA	C4-C3-C5	4.18	122.31	115.27
22	A	857	CLA	C3D-C2D-C1D	-4.18	100.12	105.83
22	A	830	CLA	O2D-CGD-CBD	4.18	118.69	111.27
22	B	821	CLA	C3D-C2D-C1D	-4.18	100.13	105.83
22	A	850	CLA	C2D-C1D-ND	4.18	113.18	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	O	203	BCR	C34-C9-C10	-4.17	117.08	122.92
22	A	807	CLA	C3D-C2D-C1D	-4.17	100.13	105.83
22	B	812	CLA	C3D-C4D-ND	4.17	116.99	110.24
21	1	301	CHL	CHD-C4C-C3C	-4.17	118.71	124.84
22	A	859	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
22	1	320	CLA	O2D-CGD-CBD	4.17	118.67	111.27
22	3	316	CLA	CHC-C4B-NB	-4.17	119.85	124.26
22	Z	307	CLA	CHD-C1D-ND	-4.17	120.63	124.45
31	J	104	DGD	O2G-C1B-C2B	4.16	120.47	111.50
22	3	313	CLA	CHC-C4B-NB	-4.16	119.85	124.26
21	Z	312	CHL	C2D-C1D-ND	4.16	113.17	110.10
22	A	830	CLA	CHB-C1B-NB	-4.16	119.85	124.26
21	1	301	CHL	C3B-C4B-NB	4.16	114.38	110.52
21	4	307	CHL	C2D-C1D-ND	4.16	113.17	110.10
22	A	858	CLA	CHB-C1B-NB	-4.16	119.85	124.26
22	B	828	CLA	O2D-CGD-CBD	4.16	118.66	111.27
22	2	307	CLA	C3D-C2D-C1D	-4.16	100.16	105.83
22	A	856	CLA	CHD-C1D-ND	-4.16	120.63	124.45
21	2	301	CHL	CHD-C4C-C3C	-4.16	118.73	124.84
22	B	826	CLA	CHC-C1C-C2C	-4.16	115.19	126.73
21	4	308	CHL	CHD-C4C-C3C	-4.15	118.73	124.84
22	3	310	CLA	C1C-C2C-C3C	-4.15	102.59	106.96
22	A	827	CLA	C3D-C4D-ND	4.15	116.96	110.24
22	B	850	CLA	C3D-C4D-ND	4.15	116.96	110.24
21	Y	307	CHL	C3B-C4B-NB	4.15	114.37	110.52
22	4	312	CLA	C3D-C2D-C1D	-4.15	100.16	105.83
22	A	836	CLA	CHD-C1D-ND	-4.15	120.64	124.45
22	2	306	CLA	C3D-C4D-ND	4.15	116.95	110.24
22	B	813	CLA	C1C-C2C-C3C	-4.15	102.59	106.96
22	B	816	CLA	C4D-CHA-C1A	-4.15	116.20	121.25
22	3	318	CLA	C4D-CHA-C1A	-4.15	116.20	121.25
22	3	315	CLA	O2D-CGD-CBD	4.15	118.64	111.27
22	B	806	CLA	CHD-C1D-ND	-4.15	120.64	124.45
22	O	208	CLA	C2D-C1D-ND	4.15	113.16	110.10
22	3	310	CLA	C3D-C4D-ND	4.14	116.94	110.24
22	B	809	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
22	A	858	CLA	C2D-C1D-ND	4.14	113.16	110.10
22	X	312	CLA	CHD-C1D-ND	-4.14	120.65	124.45
21	2	309	CHL	CHD-C4C-C3C	-4.14	118.75	124.84
22	B	811	CLA	C2D-C1D-ND	4.14	113.16	110.10
21	3	314	CHL	C1D-ND-C4D	-4.14	103.39	106.33
22	2	318	CLA	C1C-C2C-C3C	-4.14	102.60	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	852	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
22	X	311	CLA	CHD-C1D-ND	-4.14	120.65	124.45
22	4	304	CLA	CHD-C1D-ND	-4.14	120.65	124.45
25	B	840	BCR	C35-C13-C14	-4.14	117.12	122.92
22	B	828	CLA	C3D-C4D-ND	4.14	116.93	110.24
22	A	838	CLA	C2D-C1D-ND	4.14	113.15	110.10
22	1	320	CLA	C4D-CHA-C1A	-4.14	116.21	121.25
22	A	801	CLA	CHD-C1D-ND	-4.14	120.65	124.45
22	B	851	CLA	CHC-C1C-C2C	-4.14	115.24	126.73
22	2	318	CLA	C3D-C2D-C1D	-4.14	100.19	105.83
22	4	312	CLA	C4D-CHA-C1A	-4.14	116.22	121.25
22	B	804	CLA	CHD-C1D-ND	-4.14	120.65	124.45
22	B	847	CLA	C1C-C2C-C3C	-4.14	102.61	106.96
22	B	814	CLA	CMC-C2C-C1C	4.13	131.34	125.04
22	1	306	CLA	C1C-C2C-C3C	-4.13	102.61	106.96
22	A	826	CLA	C3D-C4D-ND	4.13	116.92	110.24
22	Y	308	CLA	C3D-C2D-C1D	-4.13	100.19	105.83
22	A	834	CLA	C1C-C2C-C3C	-4.13	102.61	106.96
22	A	854	CLA	C1C-C2C-C3C	-4.13	102.61	106.96
22	B	801	CLA	C1D-CHD-C4C	-4.13	117.15	126.06
22	B	822	CLA	C3D-C2D-C1D	-4.13	100.19	105.83
22	2	317	CLA	CHC-C4B-NB	-4.13	119.89	124.26
22	B	823	CLA	C1C-C2C-C3C	-4.13	102.61	106.96
22	B	807	CLA	CHB-C1B-C2B	-4.13	115.58	127.24
22	Z	306	CLA	CHD-C1D-ND	-4.13	120.66	124.45
22	A	802	CLA	C3D-C2D-C1D	-4.13	100.20	105.83
22	L	306	CLA	CHD-C1D-ND	-4.13	120.66	124.45
22	1	318	CLA	C4D-CHA-C1A	-4.13	116.23	121.25
22	4	311	CLA	C4D-CHA-C1A	-4.13	116.23	121.25
22	B	833	CLA	C4D-CHA-C1A	-4.13	116.23	121.25
22	3	312	CLA	CHD-C1D-ND	-4.13	120.66	124.45
22	F	305	CLA	C3D-C4D-ND	4.13	116.91	110.24
21	Z	301	CHL	C3B-C4B-NB	4.12	114.34	110.52
22	3	321	CLA	CHD-C1D-ND	-4.12	120.66	124.45
22	X	313	CLA	C4D-CHA-C1A	-4.12	116.23	121.25
22	H	201	CLA	C3D-C2D-C1D	-4.12	100.20	105.83
22	B	804	CLA	C3D-C4D-ND	4.12	116.91	110.24
22	A	853	CLA	C1C-C2C-C3C	-4.12	102.62	106.96
22	K	203	CLA	C4D-CHA-C1A	-4.12	116.23	121.25
21	X	308	CHL	C3B-C4B-NB	4.12	114.34	110.52
22	A	841	CLA	C1C-C2C-C3C	-4.12	102.62	106.96
22	4	312	CLA	C3D-C4D-ND	4.12	116.91	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	X	302	CHL	C3B-C4B-NB	4.12	114.34	110.52
22	A	847	CLA	CHC-C4B-NB	-4.12	119.90	124.26
22	2	322	CLA	C3D-C4D-ND	4.12	116.90	110.24
22	1	307	CLA	O2D-CGD-CBD	4.12	118.58	111.27
25	3	303	BCR	C34-C9-C10	-4.12	117.16	122.92
22	X	310	CLA	C3D-C4D-ND	4.12	116.90	110.24
22	1	321	CLA	C4D-CHA-C1A	-4.11	116.24	121.25
21	Y	305	CHL	C3B-C4B-NB	4.11	114.33	110.52
21	Y	306	CHL	C3B-C4B-NB	4.11	114.33	110.52
21	Y	303	CHL	C3B-C4B-NB	4.11	114.33	110.52
22	1	318	CLA	CHD-C1D-ND	-4.11	120.67	124.45
22	1	307	CLA	CHD-C1D-ND	-4.11	120.68	124.45
22	F	306	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
22	1	320	CLA	C3D-C4D-ND	4.11	116.89	110.24
22	A	812	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
22	A	807	CLA	C4D-CHA-C1A	-4.11	116.25	121.25
21	Y	306	CHL	C2D-C1D-ND	4.11	113.13	110.10
22	F	305	CLA	C3D-C2D-C1D	-4.11	100.23	105.83
22	A	852	CLA	C3D-C2D-C1D	-4.11	100.23	105.83
22	X	304	CLA	O2D-CGD-O1D	-4.11	115.81	123.84
22	O	208	CLA	CHD-C1D-ND	-4.11	120.68	124.45
25	O	202	BCR	C19-C18-C17	4.10	125.24	118.94
22	A	857	CLA	O2D-CGD-CBD	4.10	118.56	111.27
22	B	809	CLA	C3D-C2D-C1D	-4.10	100.23	105.83
22	G	205	CLA	C3D-C2D-C1D	-4.10	100.23	105.83
25	L	304	BCR	C37-C22-C21	-4.10	117.18	122.92
22	O	208	CLA	C4D-CHA-C1A	-4.10	116.26	121.25
22	A	805	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
22	A	831	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
22	A	856	CLA	C3D-C4D-ND	4.10	116.87	110.24
22	A	854	CLA	C3D-C4D-ND	4.10	116.87	110.24
22	A	855	CLA	C3D-C4D-ND	4.10	116.87	110.24
22	3	316	CLA	O2D-CGD-CBD	4.10	118.55	111.27
22	B	847	CLA	C4D-CHA-C1A	-4.10	116.26	121.25
22	A	806	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
21	4	307	CHL	C3B-C4B-NB	4.10	114.31	110.52
22	2	303	CLA	C3D-C4D-ND	4.10	116.86	110.24
22	3	320	CLA	CHC-C4B-NB	-4.09	119.92	124.26
25	A	814	BCR	C37-C22-C21	-4.09	117.19	122.92
22	N	202	CLA	CHD-C1D-ND	-4.09	120.69	124.45
22	B	829	CLA	O2D-CGD-CBD	4.09	118.54	111.27
22	J	102	CLA	C4D-CHA-C1A	-4.09	116.27	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	809	CLA	CHD-C1D-ND	-4.09	120.69	124.45
22	G	206	CLA	CHD-C1D-ND	-4.09	120.69	124.45
25	I	101	BCR	C15-C16-C17	4.09	131.86	123.47
22	B	853	CLA	C4D-CHA-C1A	-4.09	116.27	121.25
25	A	814	BCR	C34-C9-C10	-4.09	117.19	122.92
22	2	308	CLA	CMD-C2D-C3D	-4.09	118.20	127.61
22	A	835	CLA	CHD-C1D-ND	-4.09	120.69	124.45
22	A	838	CLA	C1D-CHD-C4C	-4.09	117.23	126.06
22	A	853	CLA	C3D-C2D-C1D	-4.09	100.25	105.83
22	A	807	CLA	CHD-C1D-ND	-4.09	120.70	124.45
22	Y	301	CLA	CAC-C3C-C4C	4.09	130.12	124.81
22	1	302	CLA	C3D-C2D-C1D	-4.09	100.25	105.83
22	2	319	CLA	C3D-C2D-C1D	-4.09	100.25	105.83
22	Y	310	CLA	C4D-CHA-C1A	-4.09	116.28	121.25
22	A	846	CLA	C1C-C2C-C3C	-4.08	102.66	106.96
22	3	313	CLA	C3D-C2D-C1D	-4.08	100.26	105.83
22	4	311	CLA	C3D-C4D-ND	4.08	116.84	110.24
22	B	803	CLA	CHB-C1B-NB	-4.08	119.94	124.26
22	3	316	CLA	C3D-C4D-ND	4.08	116.84	110.24
21	4	307	CHL	CMB-C2B-C1B	4.08	131.58	125.37
22	A	839	CLA	C3D-C2D-C1D	-4.08	100.26	105.83
22	B	848	CLA	C3D-C4D-ND	4.08	116.83	110.24
22	A	836	CLA	C1C-C2C-C3C	-4.08	102.67	106.96
22	A	804	CLA	C3D-C2D-C1D	-4.08	100.27	105.83
22	Y	314	CLA	C3D-C2D-C1D	-4.07	100.27	105.83
22	A	857	CLA	C1C-C2C-C3C	-4.07	102.67	106.96
25	A	815	BCR	C37-C22-C21	-4.07	117.22	122.92
22	X	310	CLA	CHD-C1D-ND	-4.07	120.71	124.45
25	L	302	BCR	C37-C22-C21	-4.07	117.22	122.92
24	2	311	XAT	C8-C9-C10	4.07	125.19	118.94
22	B	852	CLA	C3D-C2D-C1D	-4.07	100.28	105.83
22	A	812	CLA	CHD-C1D-ND	-4.07	120.72	124.45
22	A	826	CLA	C1C-C2C-C3C	-4.07	102.68	106.96
22	B	812	CLA	C3B-C4B-NB	4.07	114.29	110.52
22	1	321	CLA	CHC-C4B-NB	-4.07	119.95	124.26
22	4	310	CLA	C4D-CHA-C1A	-4.07	116.30	121.25
22	B	829	CLA	C4D-CHA-C1A	-4.07	116.30	121.25
22	3	309	CLA	C3D-C2D-C1D	-4.07	100.28	105.83
22	B	818	CLA	CHC-C4B-NB	-4.07	119.95	124.26
22	G	205	CLA	CHD-C1D-ND	-4.06	120.72	124.45
25	O	203	BCR	C37-C22-C21	-4.06	117.23	122.92
22	L	305	CLA	C3D-C2D-C1D	-4.06	100.29	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Y	314	CLA	CHD-C1D-ND	-4.06	120.72	124.45
22	B	801	CLA	CMD-C2D-C1D	4.06	131.87	124.71
22	Z	310	CLA	C3D-C2D-C1D	-4.06	100.29	105.83
22	Y	314	CLA	C4D-CHA-C1A	-4.06	116.31	121.25
22	Z	307	CLA	C3D-C2D-C1D	-4.06	100.29	105.83
22	1	317	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
22	A	850	CLA	C3D-C2D-C1D	-4.06	100.30	105.83
25	G	202	BCR	C35-C13-C14	-4.06	117.24	122.92
22	B	803	CLA	CAC-C3C-C2C	4.06	134.47	127.53
22	A	832	CLA	CHC-C4B-NB	-4.06	119.96	124.26
25	O	203	BCR	C34-C9-C8	4.05	124.47	118.08
21	X	305	CHL	C3B-C4B-NB	4.05	114.28	110.52
22	A	831	CLA	CHB-C1B-NB	-4.05	119.97	124.26
22	B	848	CLA	C2D-C1D-ND	4.05	113.09	110.10
22	B	806	CLA	C3D-C2D-C1D	-4.05	100.30	105.83
22	X	313	CLA	C3D-C2D-C1D	-4.05	100.30	105.83
24	3	302	XAT	O4-C5-C18	4.05	119.91	115.06
25	2	312	BCR	C35-C13-C14	-4.05	117.25	122.92
22	3	317	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
22	4	306	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
22	1	304	CLA	C4D-CHA-C1A	-4.05	116.32	121.25
22	B	807	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
25	3	303	BCR	C16-C15-C14	4.05	131.76	123.47
22	4	313	CLA	C3D-C2D-C1D	-4.04	100.31	105.83
22	K	202	CLA	C3D-C2D-C1D	-4.04	100.31	105.83
25	A	817	BCR	C37-C22-C21	-4.04	117.26	122.92
21	Z	302	CHL	C2D-C1D-ND	4.04	113.08	110.10
22	B	805	CLA	C3D-C2D-C1D	-4.04	100.32	105.83
21	Y	304	CHL	C3B-C4B-NB	4.04	114.26	110.52
21	4	308	CHL	C3B-C4B-NB	4.04	114.26	110.52
24	2	311	XAT	C11-C12-C13	-4.04	115.07	126.42
25	A	819	BCR	C37-C22-C21	-4.04	117.27	122.92
22	Y	312	CLA	C3D-C2D-C1D	-4.04	100.32	105.83
22	A	850	CLA	CAC-C3C-C4C	4.04	130.05	124.81
22	4	315	CLA	CMD-C2D-C3D	-4.04	118.33	127.61
25	L	301	BCR	C37-C22-C21	-4.04	117.27	122.92
22	A	808	CLA	C3D-C2D-C1D	-4.04	100.32	105.83
22	A	844	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
22	B	818	CLA	C3D-C4D-ND	4.03	116.77	110.24
22	B	815	CLA	C3D-C2D-C1D	-4.03	100.33	105.83
21	X	309	CHL	CHD-C4C-C3C	-4.03	118.91	124.84
22	B	833	CLA	C3D-C2D-C1D	-4.03	100.33	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	O	202	BCR	C15-C16-C17	4.03	131.73	123.47
22	B	846	CLA	C4D-CHA-C1A	-4.03	116.34	121.25
22	F	306	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
22	K	203	CLA	C3D-C2D-C1D	-4.03	100.33	105.83
31	G	201	DGD	O2G-C1B-C2B	4.03	120.18	111.50
22	X	310	CLA	C3D-C2D-C1D	-4.03	100.34	105.83
22	A	803	CLA	C2D-C1D-ND	4.03	113.07	110.10
22	A	832	CLA	C3D-C2D-C1D	-4.03	100.34	105.83
22	B	819	CLA	C3B-C2B-C1B	-4.02	102.30	107.16
22	A	810	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
22	X	312	CLA	C4D-CHA-C1A	-4.02	116.35	121.25
22	1	303	CLA	C3D-C2D-C1D	-4.02	100.34	105.83
22	3	317	CLA	C3D-C4D-ND	4.02	116.74	110.24
22	A	840	CLA	C4D-CHA-C1A	-4.02	116.36	121.25
22	B	802	CLA	C4D-CHA-C1A	-4.02	116.36	121.25
22	B	851	CLA	C3B-C4B-NB	4.02	114.24	110.52
22	2	320	CLA	C4D-CHA-C1A	-4.02	116.36	121.25
22	B	845	CLA	C4D-CHA-C1A	-4.02	116.36	121.25
21	Z	312	CHL	C1D-ND-C4D	-4.02	103.48	106.33
22	G	207	CLA	C3D-C4D-ND	4.02	116.74	110.24
22	Z	306	CLA	C3D-C4D-ND	4.02	116.74	110.24
22	K	204	CLA	CHC-C1C-C2C	-4.02	115.57	126.73
22	4	310	CLA	O2D-CGD-CBD	4.02	118.40	111.27
22	A	845	CLA	C3B-C4B-NB	4.02	114.24	110.52
21	4	308	CHL	C2D-C1D-ND	4.02	113.06	110.10
22	B	808	CLA	C3D-C2D-C1D	-4.01	100.35	105.83
22	K	205	CLA	C3D-C2D-C1D	-4.01	100.35	105.83
21	3	314	CHL	C3B-C4B-NB	4.01	114.24	110.52
25	A	817	BCR	C38-C26-C25	4.01	129.03	124.53
24	3	302	XAT	C35-C15-C14	4.01	131.69	123.47
22	A	848	CLA	CMD-C2D-C3D	-4.01	118.39	127.61
22	3	311	CLA	CMC-C2C-C1C	4.01	131.15	125.04
22	A	855	CLA	C4D-CHA-C1A	-4.01	116.37	121.25
22	4	304	CLA	C3D-C2D-C1D	-4.01	100.36	105.83
22	B	849	CLA	C3D-C2D-C1D	-4.01	100.36	105.83
22	A	838	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
22	1	306	CLA	C4D-CHA-C1A	-4.01	116.37	121.25
25	O	202	BCR	C36-C18-C17	-4.01	117.31	122.92
25	B	836	BCR	C37-C22-C21	-4.01	117.31	122.92
25	L	301	BCR	C38-C26-C25	4.00	129.03	124.53
22	B	816	CLA	CAC-C3C-C2C	4.00	134.38	127.53
22	B	845	CLA	C3D-C4D-ND	4.00	116.72	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	843	LHG	O7-C7-C8	4.00	120.12	111.50
22	G	207	CLA	C3D-C2D-C1D	-4.00	100.37	105.83
22	Y	302	CLA	C4D-CHA-C1A	-4.00	116.38	121.25
22	3	315	CLA	C3D-C4D-ND	4.00	116.71	110.24
22	B	807	CLA	C4D-C3D-CAD	4.00	112.81	108.10
22	Z	311	CLA	C3D-C2D-C1D	-4.00	100.38	105.83
25	B	836	BCR	C34-C9-C10	-4.00	117.33	122.92
22	A	829	CLA	C3D-C4D-ND	4.00	116.70	110.24
22	A	850	CLA	C3D-C4D-ND	3.99	116.70	110.24
22	A	856	CLA	C3D-C2D-C1D	-3.99	100.38	105.83
22	A	810	CLA	C4D-CHA-C1A	-3.99	116.39	121.25
22	Y	309	CLA	C3D-C2D-C1D	-3.99	100.39	105.83
22	Z	310	CLA	C4D-CHA-C1A	-3.99	116.39	121.25
22	A	854	CLA	CAA-C2A-C3A	-3.99	101.86	112.78
22	1	319	CLA	C4D-CHA-C1A	-3.99	116.40	121.25
21	Z	303	CHL	C1D-ND-C4D	-3.99	103.50	106.33
22	2	303	CLA	CHC-C4B-NB	-3.98	120.04	124.26
22	A	846	CLA	O2D-CGD-CBD	3.98	118.35	111.27
22	Z	308	CLA	C3D-C2D-C1D	-3.98	100.40	105.83
22	A	802	CLA	CHD-C1D-ND	-3.98	120.80	124.45
22	A	809	CLA	CHD-C1D-ND	-3.98	120.80	124.45
25	B	834	BCR	C16-C15-C14	3.98	131.63	123.47
22	2	307	CLA	CHD-C1D-ND	-3.98	120.80	124.45
22	B	818	CLA	C3B-C2B-C1B	-3.98	102.36	107.16
22	A	844	CLA	C3D-C4D-ND	3.98	116.68	110.24
22	O	209	CLA	C3D-C2D-C1D	-3.98	100.40	105.83
22	X	311	CLA	C3D-C2D-C1D	-3.98	100.40	105.83
22	Y	311	CLA	C3D-C2D-C1D	-3.98	100.40	105.83
22	1	306	CLA	C3D-C2D-C1D	-3.98	100.40	105.83
22	4	314	CLA	C3D-C2D-C1D	-3.98	100.40	105.83
22	G	206	CLA	C3D-C2D-C1D	-3.98	100.40	105.83
22	Y	310	CLA	C3D-C2D-C1D	-3.98	100.40	105.83
22	B	816	CLA	C4C-C3C-C2C	-3.98	101.10	106.90
22	F	305	CLA	C4D-CHA-C1A	-3.98	116.41	121.25
21	X	308	CHL	C2D-C1D-ND	3.98	113.03	110.10
22	4	305	CLA	CHC-C4B-NB	-3.98	120.05	124.26
22	A	858	CLA	CHD-C1D-ND	-3.97	120.80	124.45
22	3	320	CLA	C3D-C2D-C1D	-3.97	100.41	105.83
22	A	843	CLA	C3D-C4D-ND	3.97	116.67	110.24
22	B	812	CLA	CHC-C1C-C2C	-3.97	115.69	126.73
22	B	849	CLA	C4D-CHA-C1A	-3.97	116.41	121.25
22	2	317	CLA	C3D-C2D-C1D	-3.97	100.41	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	826	CLA	CMD-C2D-C3D	-3.97	118.48	127.61
22	O	207	CLA	CHD-C1D-ND	-3.97	120.81	124.45
25	K	201	BCR	C34-C9-C10	-3.97	117.36	122.92
25	A	817	BCR	C16-C15-C14	3.97	131.60	123.47
22	1	305	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
22	B	804	CLA	C3D-C2D-C1D	-3.97	100.42	105.83
22	O	207	CLA	C3D-C4D-ND	3.97	116.65	110.24
22	Z	309	CLA	C3D-C2D-C1D	-3.96	100.42	105.83
22	4	305	CLA	C1D-CHD-C4C	-3.96	117.51	126.06
21	X	306	CHL	C3B-C4B-NB	3.96	114.19	110.52
21	Z	304	CHL	C3B-C4B-NB	3.96	114.19	110.52
22	Y	302	CLA	C3D-C2D-C1D	-3.96	100.42	105.83
22	A	801	CLA	C3D-C4D-ND	3.96	116.64	110.24
22	3	317	CLA	CHC-C1C-C2C	-3.96	115.74	126.73
25	2	312	BCR	C37-C22-C21	-3.96	117.38	122.92
22	A	855	CLA	CAC-C3C-C4C	3.96	129.94	124.81
25	G	202	BCR	C20-C21-C22	3.96	132.96	127.31
22	B	819	CLA	CHD-C1D-ND	-3.96	120.82	124.45
22	A	827	CLA	C1C-C2C-C3C	-3.96	102.80	106.96
22	B	819	CLA	CMD-C2D-C3D	-3.96	118.51	127.61
22	3	317	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
21	Y	303	CHL	C1D-ND-C4D	-3.95	103.53	106.33
25	B	834	BCR	C1-C6-C5	-3.95	117.04	122.61
22	1	318	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
22	B	824	CLA	O2D-CGD-CBD	3.95	118.29	111.27
22	A	807	CLA	C4A-NA-C1A	3.95	108.48	106.71
22	A	858	CLA	CHC-C4B-NB	-3.95	120.07	124.26
22	A	859	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
22	A	837	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
22	O	210	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
22	A	807	CLA	CMB-C2B-C1B	3.95	131.39	125.37
22	A	829	CLA	C4D-CHA-C1A	-3.95	116.44	121.25
22	A	809	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
22	F	306	CLA	C2D-C1D-ND	3.95	113.01	110.10
22	3	319	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
22	B	803	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
21	X	306	CHL	C1D-ND-C4D	-3.95	103.53	106.33
22	A	842	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
22	A	801	CLA	C3D-C2D-C1D	-3.95	100.45	105.83
22	3	310	CLA	C4D-CHA-C1A	-3.95	116.45	121.25
22	Z	309	CLA	C4D-CHA-C1A	-3.95	116.45	121.25
22	2	307	CLA	CAC-C3C-C4C	3.95	129.93	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	850	CLA	CAC-C3C-C4C	3.95	129.93	124.81
22	A	859	CLA	O2D-CGD-CBD	3.94	118.28	111.27
22	3	313	CLA	C4D-CHA-C1A	-3.94	116.45	121.25
23	2	310	LUT	C19-C9-C10	-3.94	117.40	122.92
22	B	822	CLA	C3B-C4B-NB	3.94	114.17	110.52
22	4	305	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
22	A	831	CLA	C2D-C1D-ND	3.93	113.00	110.10
22	A	840	CLA	CHD-C1D-ND	-3.93	120.84	124.45
22	B	853	CLA	C3D-C2D-C1D	-3.93	100.46	105.83
22	4	318	CLA	C3D-C2D-C1D	-3.93	100.46	105.83
22	X	303	CLA	C4D-CHA-C1A	-3.93	116.46	121.25
22	X	301	CLA	C3D-C2D-C1D	-3.93	100.47	105.83
22	B	827	CLA	C3B-C4B-NB	3.93	114.16	110.52
22	B	827	CLA	CAC-C3C-C4C	3.93	129.91	124.81
22	A	802	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
21	Y	307	CHL	C2D-C1D-ND	3.93	113.00	110.10
22	Z	308	CLA	C4D-CHA-C1A	-3.93	116.47	121.25
22	X	312	CLA	C3D-C2D-C1D	-3.93	100.47	105.83
22	L	307	CLA	C2D-C1D-ND	3.92	113.00	110.10
22	X	301	CLA	CHD-C1D-ND	-3.92	120.85	124.45
22	Y	301	CLA	C4D-CHA-C1A	-3.92	116.48	121.25
22	B	812	CLA	CAC-C3C-C4C	3.92	129.90	124.81
22	A	830	CLA	C3B-C2B-C1B	-3.92	102.43	107.16
22	A	807	CLA	CAA-CBA-CGA	-3.92	101.80	113.25
22	B	851	CLA	C3B-C2B-C1B	-3.92	102.43	107.16
22	4	305	CLA	CHD-C1D-ND	-3.92	120.85	124.45
22	O	209	CLA	C4D-CHA-C1A	-3.92	116.48	121.25
22	A	833	CLA	C3D-C2D-C1D	-3.92	100.49	105.83
23	4	319	LUT	C19-C9-C8	3.91	124.24	118.08
22	B	816	CLA	CHB-C4A-NA	3.91	129.92	124.51
22	1	319	CLA	C3D-C2D-C1D	-3.91	100.49	105.83
25	K	201	BCR	C37-C22-C21	-3.91	117.45	122.92
22	B	828	CLA	C4D-CHA-C1A	-3.91	116.49	121.25
25	A	819	BCR	C16-C15-C14	3.91	131.48	123.47
21	2	309	CHL	C2D-C1D-ND	3.91	112.98	110.10
22	H	201	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
22	A	854	CLA	C4D-CHA-C1A	-3.91	116.49	121.25
22	X	303	CLA	C3D-C2D-C1D	-3.91	100.50	105.83
21	4	317	CHL	C1D-ND-C4D	-3.91	103.56	106.33
22	1	321	CLA	C3D-C2D-C1D	-3.91	100.50	105.83
24	2	311	XAT	C12-C13-C14	3.91	124.93	118.94
25	4	321	BCR	C37-C22-C21	-3.90	117.45	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	210	CLA	CHD-C1D-ND	-3.90	120.87	124.45
22	B	808	CLA	O2A-CGA-CBA	3.90	124.16	111.91
22	A	853	CLA	C3D-C4D-ND	3.90	116.55	110.24
22	3	320	CLA	C4D-CHA-C1A	-3.90	116.50	121.25
22	X	304	CLA	CHC-C4B-NB	-3.90	120.13	124.26
22	Z	313	CLA	C3D-C2D-C1D	-3.90	100.51	105.83
22	Z	306	CLA	C4D-CHA-C1A	-3.90	116.50	121.25
22	L	306	CLA	C2D-C1D-ND	3.90	112.98	110.10
22	A	848	CLA	C4D-CHA-C1A	-3.90	116.50	121.25
25	A	819	BCR	C38-C26-C25	3.90	128.91	124.53
22	2	318	CLA	CHC-C4B-NB	-3.90	120.13	124.26
22	1	306	CLA	CHC-C4B-NB	-3.90	120.13	124.26
22	G	205	CLA	C2D-C1D-ND	3.90	112.97	110.10
22	B	848	CLA	C1C-C2C-C3C	-3.89	102.86	106.96
21	X	309	CHL	C2D-C1D-ND	3.89	112.97	110.10
22	B	828	CLA	CHC-C1C-C2C	-3.89	115.92	126.73
22	4	313	CLA	CHC-C4B-NB	-3.89	120.14	124.26
22	4	318	CLA	C4D-CHA-C1A	-3.89	116.51	121.25
22	4	311	CLA	C3D-C2D-C1D	-3.89	100.52	105.83
21	1	316	CHL	CHB-C1B-NB	-3.89	120.14	124.26
22	B	846	CLA	C3D-C2D-C1D	-3.89	100.53	105.83
22	B	824	CLA	C3D-C2D-C1D	-3.89	100.53	105.83
22	A	829	CLA	C3D-C2D-C1D	-3.89	100.53	105.83
22	4	306	CLA	CHB-C4A-NA	3.89	129.88	124.51
22	3	312	CLA	C3D-C2D-C1D	-3.89	100.53	105.83
22	B	823	CLA	C3D-C2D-C1D	-3.89	100.53	105.83
22	B	816	CLA	C1C-C2C-C3C	-3.88	102.87	106.96
21	X	302	CHL	C1D-ND-C4D	-3.88	103.58	106.33
22	B	804	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
22	3	311	CLA	C2D-C1D-ND	3.88	112.96	110.10
22	A	846	CLA	C3D-C2D-C1D	-3.88	100.54	105.83
26	2	313	LHG	O7-C7-C8	3.88	119.86	111.50
22	B	848	CLA	C1D-CHD-C4C	-3.88	117.70	126.06
22	A	840	CLA	C3D-C2D-C1D	-3.87	100.55	105.83
22	A	806	CLA	C3D-C2D-C1D	-3.87	100.55	105.83
22	B	827	CLA	CHC-C1C-C2C	-3.87	115.98	126.73
22	A	826	CLA	O2D-CGD-CBD	3.87	118.15	111.27
22	3	308	CLA	C4D-CHA-C1A	-3.87	116.54	121.25
22	Y	311	CLA	C4D-CHA-C1A	-3.87	116.54	121.25
22	A	803	CLA	CHC-C4B-NB	-3.87	120.16	124.26
22	Z	314	CLA	C4D-CHA-C1A	-3.87	116.54	121.25
25	4	321	BCR	C34-C9-C10	-3.87	117.50	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Z	305	CHL	CHD-C4C-C3C	-3.87	119.15	124.84
22	L	306	CLA	C3D-C2D-C1D	-3.87	100.55	105.83
22	1	309	CLA	C2D-C1D-ND	3.87	112.95	110.10
22	1	303	CLA	CHC-C4B-NB	-3.87	120.17	124.26
22	B	848	CLA	CHD-C1D-ND	-3.86	120.90	124.45
25	A	819	BCR	C33-C5-C6	3.86	128.87	124.53
25	J	101	BCR	C37-C22-C21	-3.86	117.51	122.92
22	Y	312	CLA	C4D-CHA-C1A	-3.86	116.55	121.25
25	B	837	BCR	C37-C22-C23	3.86	124.16	118.08
22	L	307	CLA	CAC-C3C-C4C	3.86	129.82	124.81
22	4	311	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
22	A	826	CLA	CMB-C2B-C3B	3.86	135.94	126.59
25	J	103	BCR	C37-C22-C21	-3.86	117.52	122.92
22	Z	306	CLA	C3D-C2D-C1D	-3.86	100.56	105.83
22	Z	314	CLA	C3D-C2D-C1D	-3.86	100.56	105.83
21	X	307	CHL	C1D-ND-C4D	-3.86	103.59	106.33
21	Z	304	CHL	C2D-C1D-ND	3.86	112.95	110.10
22	4	304	CLA	C4D-CHA-C1A	-3.86	116.56	121.25
22	J	102	CLA	CHD-C1D-ND	-3.86	120.91	124.45
21	1	316	CHL	C3B-C4B-NB	3.85	114.09	110.52
22	3	319	CLA	C4D-CHA-C1A	-3.85	116.56	121.25
22	A	804	CLA	C4D-CHA-C1A	-3.85	116.56	121.25
22	4	305	CLA	CMC-C2C-C1C	3.85	130.91	125.04
25	B	840	BCR	C37-C22-C21	-3.85	117.53	122.92
22	Z	307	CLA	C4D-CHA-C1A	-3.85	116.56	121.25
22	2	305	CLA	C3D-C4D-ND	3.85	116.47	110.24
25	B	844	BCR	C38-C26-C25	3.85	128.85	124.53
22	3	308	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
22	4	312	CLA	CMC-C2C-C1C	3.85	130.90	125.04
21	Z	301	CHL	C1D-ND-C4D	-3.85	103.60	106.33
22	2	322	CLA	C4D-CHA-C1A	-3.85	116.57	121.25
22	B	825	CLA	C4D-CHA-C1A	-3.85	116.57	121.25
22	A	832	CLA	C3B-C4B-NB	3.85	114.08	110.52
22	A	838	CLA	CHD-C1D-ND	-3.85	120.92	124.45
22	A	838	CLA	CHB-C4A-NA	3.85	129.83	124.51
21	X	308	CHL	C1D-ND-C4D	-3.85	103.60	106.33
22	H	201	CLA	C4D-CHA-C1A	-3.85	116.57	121.25
22	Z	311	CLA	C4D-CHA-C1A	-3.85	116.57	121.25
22	B	812	CLA	C3D-C2D-C1D	-3.84	100.59	105.83
22	2	307	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
22	B	814	CLA	CHB-C4A-NA	3.84	129.83	124.51
22	A	803	CLA	C3D-C2D-C1D	-3.84	100.59	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	830	CLA	C3D-C2D-C1D	-3.84	100.59	105.83
22	Y	309	CLA	C4D-CHA-C1A	-3.84	116.57	121.25
22	2	308	CLA	C3D-C2D-C1D	-3.84	100.59	105.83
22	X	311	CLA	C4D-CHA-C1A	-3.84	116.58	121.25
22	1	303	CLA	CHD-C1D-ND	-3.84	120.93	124.45
22	B	849	CLA	CHD-C1D-ND	-3.84	120.93	124.45
22	A	812	CLA	C4D-CHA-C1A	-3.84	116.58	121.25
22	Z	313	CLA	C4D-CHA-C1A	-3.84	116.58	121.25
22	B	816	CLA	CHC-C1C-C2C	-3.84	116.08	126.73
22	2	304	CLA	CAC-C3C-C4C	3.84	129.79	124.81
22	O	206	CLA	C4D-CHA-C1A	-3.84	116.58	121.25
22	2	317	CLA	C4D-CHA-C1A	-3.83	116.58	121.25
22	X	301	CLA	C4D-CHA-C1A	-3.83	116.58	121.25
22	B	850	CLA	C3D-C2D-C1D	-3.83	100.60	105.83
21	2	321	CHL	CHB-C4A-NA	3.83	129.81	124.51
22	4	316	CLA	C4D-CHA-C1A	-3.83	116.58	121.25
22	2	303	CLA	C4D-CHA-C1A	-3.83	116.59	121.25
22	A	834	CLA	O2D-CGD-CBD	3.83	118.07	111.27
21	X	305	CHL	C1D-ND-C4D	-3.83	103.61	106.33
22	L	306	CLA	C4D-CHA-C1A	-3.82	116.60	121.25
22	A	849	CLA	C3D-C2D-C1D	-3.82	100.61	105.83
21	2	301	CHL	CAC-C3C-C4C	3.82	129.77	124.81
22	B	826	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
21	Z	302	CHL	C1D-ND-C4D	-3.82	103.62	106.33
22	1	321	CLA	CHD-C1D-ND	-3.82	120.94	124.45
25	A	816	BCR	C34-C9-C10	-3.82	117.57	122.92
25	A	816	BCR	C37-C22-C21	-3.82	117.57	122.92
22	A	826	CLA	C3D-C2D-C1D	-3.82	100.62	105.83
22	1	302	CLA	C4D-CHA-C1A	-3.82	116.60	121.25
21	4	308	CHL	C1D-ND-C4D	-3.82	103.62	106.33
22	B	848	CLA	C4D-CHA-C1A	-3.82	116.60	121.25
22	1	305	CLA	C3D-C2D-C1D	-3.82	100.62	105.83
22	A	847	CLA	C3D-C2D-C1D	-3.82	100.62	105.83
22	A	829	CLA	CHB-C4A-NA	3.82	129.79	124.51
22	B	813	CLA	O2D-CGD-CBD	3.82	118.05	111.27
21	2	309	CHL	C3B-C4B-NB	3.81	114.05	110.52
25	A	819	BCR	C34-C9-C10	-3.81	117.58	122.92
22	A	845	CLA	CHC-C1C-C2C	-3.81	116.14	126.73
25	O	202	BCR	C37-C22-C23	3.81	124.08	118.08
22	B	831	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
25	O	202	BCR	C16-C15-C14	3.81	131.28	123.47
22	4	312	CLA	CHC-C4B-NB	-3.81	120.22	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	303	CLA	C4D-CHA-C1A	-3.81	116.61	121.25
22	4	314	CLA	C4D-CHA-C1A	-3.81	116.61	121.25
25	L	303	BCR	C37-C22-C21	-3.81	117.59	122.92
22	4	313	CLA	CHC-C1C-C2C	-3.80	116.16	126.73
22	A	810	CLA	CMC-C2C-C1C	3.80	130.83	125.04
22	2	307	CLA	C4D-CHA-C1A	-3.80	116.62	121.25
22	3	317	CLA	C4A-NA-C1A	3.80	108.42	106.71
22	1	308	CLA	C2D-C1D-ND	3.80	112.91	110.10
22	X	304	CLA	C1D-ND-C4D	-3.80	103.64	106.33
22	O	206	CLA	CHC-C4B-NB	-3.80	120.23	124.26
22	4	310	CLA	C3D-C4D-ND	3.80	116.38	110.24
22	J	102	CLA	C3D-C2D-C1D	-3.80	100.65	105.83
22	A	845	CLA	CBC-CAC-C3C	-3.79	101.97	112.43
21	3	307	CHL	CAC-C3C-C4C	3.79	129.73	124.81
21	Z	312	CHL	C3B-C4B-NB	3.79	114.03	110.52
25	B	835	BCR	C34-C9-C10	-3.79	117.61	122.92
22	A	805	CLA	C3D-C4D-ND	3.79	116.37	110.24
22	B	817	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
21	4	309	CHL	C3B-C4B-NB	3.79	114.03	110.52
25	2	312	BCR	C12-C13-C14	3.79	124.76	118.94
22	B	828	CLA	CHC-C4B-NB	-3.79	120.25	124.26
22	A	844	CLA	C3D-C2D-C1D	-3.79	100.66	105.83
22	1	306	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
22	3	311	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
22	1	318	CLA	CHC-C4B-NB	-3.79	120.25	124.26
22	3	317	CLA	CHD-C1D-ND	-3.79	120.97	124.45
22	A	842	CLA	CHD-C1D-ND	-3.79	120.97	124.45
22	A	834	CLA	C2D-C1D-ND	3.79	112.89	110.10
22	B	828	CLA	C3B-C4B-NB	3.79	114.03	110.52
22	K	204	CLA	C4C-C3C-C2C	-3.79	101.38	106.90
21	X	307	CHL	C3B-C4B-NB	3.78	114.03	110.52
24	2	311	XAT	C18-C5-C6	-3.78	115.92	122.26
22	A	828	CLA	C4D-CHA-C1A	-3.78	116.64	121.25
22	4	316	CLA	CHD-C1D-ND	-3.78	120.98	124.45
22	3	310	CLA	C1D-CHD-C4C	-3.78	117.90	126.06
22	A	808	CLA	CHD-C1D-ND	-3.78	120.98	124.45
22	A	842	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
22	A	859	CLA	CHC-C4B-NB	-3.78	120.25	124.26
22	Y	310	CLA	CHC-C4B-NB	-3.78	120.26	124.26
22	B	805	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
22	3	311	CLA	CAC-C3C-C4C	3.78	129.71	124.81
22	A	843	CLA	C4C-C3C-C2C	-3.78	101.39	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	302	CLA	CHC-C4B-NB	-3.78	120.26	124.26
22	B	802	CLA	C3D-C2D-C1D	-3.78	100.68	105.83
21	1	316	CHL	CHB-C4A-NA	3.77	129.73	124.51
22	O	206	CLA	C3D-C2D-C1D	-3.77	100.68	105.83
25	F	302	BCR	C37-C22-C21	-3.77	117.64	122.92
22	B	850	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
21	2	302	CHL	O2D-CGD-CBD	3.77	117.97	111.27
22	Z	306	CLA	CHC-C1C-C2C	-3.77	116.25	126.73
22	B	817	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
22	A	841	CLA	CHC-C1C-C2C	-3.77	116.26	126.73
22	A	837	CLA	CHC-C1C-C2C	-3.77	116.26	126.73
22	B	807	CLA	CMB-C2B-C3B	3.77	135.71	126.59
22	3	311	CLA	CHD-C1D-ND	-3.77	120.99	124.45
21	Z	304	CHL	C1D-ND-C4D	-3.77	103.66	106.33
22	A	840	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
22	B	820	CLA	CMB-C2B-C1B	3.77	131.10	125.37
22	K	204	CLA	C3D-C2D-C1D	-3.76	100.69	105.83
25	L	301	BCR	C34-C9-C10	-3.76	117.65	122.92
21	4	317	CHL	CHD-C4C-C3C	-3.76	119.31	124.84
21	Z	302	CHL	C3B-C4B-NB	3.76	114.01	110.52
22	B	831	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
22	2	322	CLA	CHD-C1D-ND	-3.76	121.00	124.45
22	A	835	CLA	C3D-C4D-ND	3.76	116.32	110.24
22	2	306	CLA	C4C-C3C-C2C	-3.76	101.42	106.90
22	3	312	CLA	O2D-CGD-CBD	3.76	117.95	111.27
22	A	845	CLA	C3D-C2D-C1D	-3.76	100.70	105.83
22	B	826	CLA	CAC-C3C-C4C	3.76	129.68	124.81
22	A	850	CLA	C1D-CHD-C4C	-3.76	117.96	126.06
22	G	205	CLA	CHB-C1B-NB	-3.75	120.28	124.26
22	A	834	CLA	C1D-CHD-C4C	-3.75	117.96	126.06
22	B	801	CLA	C4C-C3C-C2C	-3.75	101.43	106.90
25	L	304	BCR	C15-C16-C17	3.75	131.16	123.47
22	A	842	CLA	C2D-C1D-ND	3.75	112.87	110.10
22	Y	301	CLA	C3D-C2D-C1D	-3.75	100.71	105.83
25	I	101	BCR	C34-C9-C10	-3.75	117.67	122.92
21	Y	305	CHL	C1D-ND-C4D	-3.75	103.67	106.33
22	1	320	CLA	CHC-C1C-C2C	-3.75	116.32	126.73
25	A	818	BCR	C37-C22-C21	-3.75	117.67	122.92
22	3	316	CLA	CHD-C1D-ND	-3.75	121.01	124.45
25	O	202	BCR	C21-C20-C19	3.75	134.91	123.22
22	4	316	CLA	C3D-C2D-C1D	-3.75	100.72	105.83
22	B	827	CLA	C3D-C2D-C1D	-3.74	100.72	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Z	303	CHL	C3B-C4B-NB	3.74	113.99	110.52
22	B	818	CLA	C4-C3-C5	3.74	121.57	115.27
22	A	810	CLA	C3D-C2D-C1D	-3.74	100.72	105.83
22	2	318	CLA	CAC-C3C-C4C	3.74	129.67	124.81
22	A	852	CLA	CAC-C3C-C2C	3.74	133.93	127.53
22	A	829	CLA	CMC-C2C-C1C	3.74	130.73	125.04
22	B	812	CLA	CMB-C2B-C1B	3.74	131.06	125.37
22	B	846	CLA	CHB-C4A-NA	3.74	129.68	124.51
21	Y	306	CHL	C1D-ND-C4D	-3.74	103.68	106.33
22	2	306	CLA	CHC-C1C-C2C	-3.74	116.35	126.73
22	F	306	CLA	C4D-CHA-C1A	-3.74	116.70	121.25
22	G	205	CLA	O2D-CGD-CBD	3.74	117.91	111.27
21	2	301	CHL	C1D-ND-C4D	-3.74	103.68	106.33
22	A	842	CLA	C4D-CHA-C1A	-3.73	116.70	121.25
21	4	309	CHL	C2D-C1D-ND	3.73	112.86	110.10
22	Y	312	CLA	CHC-C4B-NB	-3.73	120.31	124.26
22	B	817	CLA	C2D-C1D-ND	3.73	112.86	110.10
22	4	313	CLA	C1D-CHD-C4C	-3.73	118.00	126.06
22	A	838	CLA	C4C-C3C-C2C	-3.73	101.46	106.90
22	A	852	CLA	C4A-NA-C1A	3.73	108.38	106.71
23	2	310	LUT	C40-C33-C34	-3.73	117.70	122.92
22	A	830	CLA	C3D-C2D-C1D	-3.73	100.74	105.83
22	B	825	CLA	C3D-C2D-C1D	-3.73	100.74	105.83
22	A	806	CLA	CAC-C3C-C4C	3.73	129.65	124.81
22	B	807	CLA	CMC-C2C-C1C	3.73	130.71	125.04
22	A	835	CLA	C3B-C4B-NB	3.73	113.97	110.52
22	4	314	CLA	CHB-C1B-NB	-3.72	120.32	124.26
21	1	301	CHL	CMD-C2D-C3D	-3.72	119.06	127.61
22	A	851	CLA	CMC-C2C-C1C	3.72	130.71	125.04
22	G	207	CLA	CHC-C1C-C2C	-3.72	116.40	126.73
22	A	849	CLA	C3B-C4B-NB	3.72	113.97	110.52
21	Y	304	CHL	C1D-ND-C4D	-3.72	103.69	106.33
22	B	818	CLA	CHD-C1D-ND	-3.72	121.04	124.45
25	A	815	BCR	C34-C9-C10	-3.72	117.72	122.92
22	A	837	CLA	C4D-CHA-C1A	-3.71	116.73	121.25
22	A	857	CLA	C4D-CHA-C1A	-3.71	116.73	121.25
25	B	836	BCR	C15-C16-C17	3.71	131.08	123.47
22	4	314	CLA	C2D-C1D-ND	3.71	112.84	110.10
23	1	310	LUT	C39-C29-C30	-3.71	117.73	122.92
22	N	202	CLA	CHC-C4B-NB	-3.71	120.33	124.26
22	4	315	CLA	C3D-C2D-C1D	-3.71	100.77	105.83
25	L	303	BCR	C34-C9-C8	3.71	123.92	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	F	302	BCR	C34-C9-C10	-3.71	117.73	122.92
22	B	810	CLA	C3D-C2D-C1D	-3.70	100.78	105.83
22	1	303	CLA	CHB-C4A-NA	3.70	129.63	124.51
22	2	322	CLA	CHC-C4B-NB	-3.70	120.34	124.26
22	A	858	CLA	CHD-C4C-C3C	-3.70	119.40	124.84
22	A	805	CLA	CHC-C4B-NB	-3.70	120.34	124.26
22	B	847	CLA	C3D-C2D-C1D	-3.70	100.78	105.83
22	A	853	CLA	C4-C3-C5	3.70	121.50	115.27
22	F	305	CLA	CHD-C1D-ND	-3.70	121.05	124.45
22	3	312	CLA	CHB-C1B-NB	-3.70	120.34	124.26
22	B	805	CLA	C4D-CHA-C1A	-3.70	116.75	121.25
22	A	859	CLA	C4D-CHA-C1A	-3.69	116.75	121.25
22	B	807	CLA	C2A-C1A-CHA	-3.69	117.40	123.86
22	A	812	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
22	3	312	CLA	CHB-C4A-NA	3.69	129.62	124.51
22	A	858	CLA	C4C-C3C-C2C	-3.69	101.52	106.90
22	B	825	CLA	CHC-C4B-NB	-3.69	120.35	124.26
21	2	321	CHL	C1D-ND-C4D	-3.69	103.72	106.33
22	A	804	CLA	CHC-C1C-C2C	-3.69	116.49	126.73
22	X	310	CLA	C4D-CHA-C1A	-3.69	116.76	121.25
22	B	803	CLA	C4D-CHA-C1A	-3.68	116.77	121.25
31	O	201	DGD	O2G-C1B-C2B	3.68	119.44	111.50
22	A	843	CLA	C1D-CHD-C4C	-3.68	118.11	126.06
22	A	858	CLA	C4D-CHA-C1A	-3.68	116.77	121.25
21	Z	305	CHL	C2D-C1D-ND	3.68	112.82	110.10
22	B	817	CLA	C3D-C4D-ND	3.68	116.19	110.24
22	3	311	CLA	CMB-C2B-C1B	3.68	130.97	125.37
22	A	852	CLA	C4C-C3C-C2C	-3.68	101.53	106.90
21	2	302	CHL	C3B-C4B-NB	3.68	113.93	110.52
23	1	310	LUT	C1-C6-C7	3.68	126.19	115.78
25	A	815	BCR	C34-C9-C8	3.68	123.87	118.08
22	2	304	CLA	C3D-C2D-C1D	-3.68	100.81	105.83
22	2	305	CLA	C1D-CHD-C4C	-3.68	118.13	126.06
21	Y	313	CHL	C1D-ND-C4D	-3.67	103.72	106.33
22	4	306	CLA	C3D-C2D-C1D	-3.67	100.82	105.83
22	3	310	CLA	CHC-C4B-NB	-3.67	120.37	124.26
22	1	320	CLA	CHB-C1B-NB	-3.67	120.37	124.26
22	B	852	CLA	CAC-C3C-C4C	3.67	129.57	124.81
22	A	853	CLA	CHB-C4A-NA	3.67	129.59	124.51
22	A	850	CLA	CHC-C1C-C2C	-3.67	116.55	126.73
25	J	103	BCR	C35-C13-C14	-3.67	117.79	122.92
22	B	806	CLA	O2D-CGD-CBD	3.67	117.78	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	811	CLA	C4-C3-C5	3.67	121.44	115.27
22	O	206	CLA	CHC-C1C-C2C	-3.67	116.55	126.73
22	A	806	CLA	C4D-CHA-C1A	-3.66	116.79	121.25
22	Z	306	CLA	C3B-C4B-NB	3.66	113.91	110.52
22	A	830	CLA	CMB-C2B-C1B	3.66	130.95	125.37
22	A	809	CLA	CHC-C1C-C2C	-3.66	116.56	126.73
22	A	805	CLA	O2D-CGD-CBD	3.66	117.78	111.27
21	4	317	CHL	CAA-C2A-C3A	-3.66	107.56	116.10
24	1	311	XAT	C39-C29-C28	-3.66	112.31	118.08
22	A	845	CLA	CMB-C2B-C1B	3.66	130.94	125.37
25	3	303	BCR	C37-C22-C21	-3.66	117.80	122.92
25	K	201	BCR	C35-C13-C14	-3.66	117.80	122.92
22	3	312	CLA	CHC-C4B-NB	-3.66	120.39	124.26
25	G	202	BCR	C16-C15-C14	3.66	130.96	123.47
22	A	807	CLA	CHB-C4A-NA	3.65	129.57	124.51
25	B	839	BCR	C36-C18-C17	-3.65	117.81	122.92
21	3	307	CHL	C3B-C4B-NB	3.65	113.90	110.52
22	B	823	CLA	CHD-C1D-ND	-3.65	121.10	124.45
22	1	307	CLA	CHC-C4B-NB	-3.65	120.39	124.26
22	3	318	CLA	C3D-C2D-C1D	-3.65	100.85	105.83
22	B	845	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
22	Y	312	CLA	CHC-C1C-C2C	-3.65	116.59	126.73
22	B	845	CLA	C4C-C3C-C2C	-3.65	101.58	106.90
22	3	321	CLA	C3D-C2D-C1D	-3.65	100.85	105.83
23	2	310	LUT	C32-C33-C34	3.65	124.54	118.94
22	B	807	CLA	CHC-C4B-NB	-3.65	120.40	124.26
22	4	314	CLA	CHC-C1C-C2C	-3.65	116.60	126.73
22	N	202	CLA	C4D-CHA-C1A	-3.65	116.81	121.25
22	A	831	CLA	C4A-NA-C1A	3.65	108.34	106.71
22	3	310	CLA	C2D-C1D-ND	3.64	112.79	110.10
22	1	320	CLA	CMD-C2D-C3D	-3.64	119.23	127.61
22	A	843	CLA	CHD-C1D-ND	-3.64	121.11	124.45
24	2	311	XAT	C31-C32-C33	-3.64	116.19	126.42
21	Z	305	CHL	CAC-C3C-C4C	3.64	129.53	124.81
22	A	838	CLA	CAC-C3C-C2C	3.64	133.76	127.53
25	B	837	BCR	C37-C22-C21	-3.64	117.82	122.92
22	A	802	CLA	C2D-C1D-ND	3.64	112.79	110.10
22	B	803	CLA	CHD-C1D-ND	-3.64	121.11	124.45
22	2	304	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
22	L	305	CLA	C4D-CHA-C1A	-3.64	116.82	121.25
22	B	826	CLA	C3D-C2D-C1D	-3.64	100.86	105.83
25	A	815	BCR	C12-C13-C14	3.64	124.52	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	834	CLA	C3D-C2D-C1D	-3.64	100.87	105.83
22	A	848	CLA	CHC-C4B-NB	-3.64	120.41	124.26
22	A	801	CLA	CHC-C1C-C2C	-3.64	116.63	126.73
25	A	817	BCR	C36-C18-C17	-3.64	117.83	122.92
22	1	304	CLA	CHD-C1D-ND	-3.63	121.11	124.45
22	X	310	CLA	CHC-C1C-C2C	-3.63	116.64	126.73
22	2	305	CLA	C4D-CHA-C1A	-3.63	116.83	121.25
22	1	307	CLA	C4C-C3C-C2C	-3.63	101.60	106.90
22	L	306	CLA	CHB-C4A-NA	3.63	129.54	124.51
22	B	831	CLA	C3D-C2D-C1D	-3.63	100.87	105.83
22	A	801	CLA	CHB-C1B-NB	-3.63	120.41	124.26
22	B	802	CLA	C2D-C1D-ND	3.63	112.78	110.10
21	X	309	CHL	CAC-C3C-C4C	3.63	129.52	124.81
22	A	802	CLA	C1-C2-C3	-3.63	119.76	126.04
21	2	302	CHL	C2D-C1D-ND	3.63	112.78	110.10
22	B	850	CLA	CMB-C2B-C1B	3.63	130.90	125.37
25	2	312	BCR	C30-C25-C24	3.63	126.05	115.78
22	4	316	CLA	CHC-C1C-C2C	-3.63	116.65	126.73
21	4	308	CHL	CHB-C4A-NA	3.63	129.53	124.51
24	4	320	XAT	O24-C25-C38	3.63	119.40	115.06
22	1	308	CLA	C4D-CHA-C1A	-3.63	116.83	121.25
22	1	318	CLA	CHC-C1C-C2C	-3.63	116.65	126.73
22	1	307	CLA	CAA-C2A-C3A	-3.63	102.85	112.78
22	B	849	CLA	CHC-C4B-NB	-3.63	120.42	124.26
24	3	302	XAT	C15-C14-C13	-3.63	122.14	127.31
22	1	304	CLA	C2D-C1D-ND	3.63	112.78	110.10
22	B	851	CLA	C3D-C2D-C1D	-3.63	100.88	105.83
22	G	207	CLA	C4D-CHA-C1A	-3.63	116.84	121.25
24	3	302	XAT	C10-C11-C12	-3.62	111.91	123.22
22	A	839	CLA	C3B-C4B-NB	3.62	113.88	110.52
22	4	314	CLA	CMB-C2B-C1B	3.62	130.89	125.37
22	1	303	CLA	CHC-C1C-C2C	-3.62	116.67	126.73
22	4	312	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
22	A	847	CLA	CHC-C1C-C2C	-3.62	116.67	126.73
22	B	808	CLA	C4D-CHA-C1A	-3.62	116.84	121.25
21	3	314	CHL	C1C-C2C-C3C	-3.62	104.24	107.11
22	B	815	CLA	C4-C3-C5	3.62	121.36	115.27
22	Y	301	CLA	CHC-C1C-C2C	-3.62	116.68	126.73
22	O	207	CLA	CHC-C1C-C2C	-3.62	116.68	126.73
22	Y	314	CLA	CHC-C1C-C2C	-3.62	116.68	126.73
21	2	309	CHL	C1D-ND-C4D	-3.62	103.77	106.33
21	4	308	CHL	CAC-C3C-C4C	3.62	129.50	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	X	303	CLA	CHC-C4B-NB	-3.62	120.43	124.26
22	Y	308	CLA	CHC-C1C-C2C	-3.62	116.69	126.73
22	2	305	CLA	C3D-C2D-C1D	-3.62	100.90	105.83
22	1	304	CLA	O2D-CGD-CBD	3.62	117.69	111.27
22	A	826	CLA	C2D-C1D-ND	3.61	112.77	110.10
22	A	849	CLA	CHC-C1C-C2C	-3.61	116.69	126.73
22	B	808	CLA	CHC-C1C-C2C	-3.61	116.69	126.73
22	B	821	CLA	CHC-C4B-NB	-3.61	120.43	124.26
22	K	202	CLA	C4D-CHA-C1A	-3.61	116.85	121.25
22	3	311	CLA	CHB-C4A-NA	3.61	129.51	124.51
22	B	819	CLA	CHC-C1C-C2C	-3.61	116.70	126.73
25	B	837	BCR	C35-C13-C14	-3.61	117.86	122.92
22	K	202	CLA	CHC-C1C-C2C	-3.61	116.70	126.73
22	A	828	CLA	CHB-C1B-NB	-3.61	120.43	124.26
22	1	307	CLA	C2D-C1D-ND	3.61	112.77	110.10
22	Z	306	CLA	CHB-C1B-NB	-3.61	120.44	124.26
22	A	835	CLA	CHC-C1C-C2C	-3.61	116.71	126.73
25	B	837	BCR	C8-C9-C10	3.61	124.48	118.94
22	3	318	CLA	CHC-C1C-C2C	-3.61	116.71	126.73
22	O	208	CLA	CHC-C1C-C2C	-3.61	116.71	126.73
22	A	852	CLA	CHB-C1B-NB	-3.61	120.44	124.26
21	4	307	CHL	C1D-ND-C4D	-3.61	103.77	106.33
22	B	823	CLA	CHC-C4B-NB	-3.61	120.44	124.26
22	B	801	CLA	C3D-C4D-ND	3.60	116.07	110.24
25	A	816	BCR	C21-C20-C19	3.60	134.46	123.22
25	1	312	BCR	C35-C13-C14	-3.60	117.88	122.92
22	B	829	CLA	C4C-C3C-C2C	-3.60	101.65	106.90
22	3	320	CLA	CHC-C1C-C2C	-3.60	116.73	126.73
21	X	307	CHL	CAC-C3C-C4C	3.60	129.48	124.81
22	A	829	CLA	CAC-C3C-C4C	3.60	129.48	124.81
25	B	835	BCR	C38-C26-C25	3.60	128.57	124.53
22	A	831	CLA	CHC-C1C-C2C	-3.60	116.73	126.73
25	B	835	BCR	C19-C18-C17	3.60	124.47	118.94
25	I	101	BCR	C38-C26-C25	3.60	128.57	124.53
25	G	202	BCR	C8-C9-C10	3.60	124.47	118.94
22	3	311	CLA	CHB-C1B-NB	-3.60	120.45	124.26
22	4	313	CLA	CHD-C1D-ND	-3.60	121.15	124.45
22	A	838	CLA	CHC-C1C-C2C	-3.60	116.74	126.73
22	A	840	CLA	CHC-C4B-NB	-3.60	120.45	124.26
22	A	835	CLA	O2D-CGD-CBD	3.59	117.66	111.27
22	B	814	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
21	Y	307	CHL	CAC-C3C-C4C	3.59	129.47	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	810	CLA	CHC-C1C-C2C	-3.59	116.75	126.73
22	1	306	CLA	C2D-C1D-ND	3.59	112.75	110.10
22	B	848	CLA	O2D-CGD-CBD	3.59	117.65	111.27
22	B	817	CLA	CMC-C2C-C1C	3.59	130.51	125.04
22	A	840	CLA	CHC-C1C-C2C	-3.59	116.75	126.73
22	B	824	CLA	C4D-CHA-C1A	-3.59	116.88	121.25
25	2	312	BCR	C1-C6-C5	-3.59	117.56	122.61
22	K	204	CLA	C4D-CHA-C1A	-3.59	116.88	121.25
22	O	208	CLA	C1D-CHD-C4C	-3.59	118.32	126.06
22	B	817	CLA	CHD-C1D-ND	-3.59	121.16	124.45
22	A	805	CLA	C1D-CHD-C4C	-3.59	118.32	126.06
22	2	322	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
22	Y	311	CLA	CHC-C1C-C2C	-3.58	116.77	126.73
25	B	844	BCR	C34-C9-C10	-3.58	117.90	122.92
22	3	313	CLA	CHC-C1C-C2C	-3.58	116.78	126.73
21	2	301	CHL	CHB-C4A-NA	3.58	129.47	124.51
22	4	313	CLA	C4D-CHA-C1A	-3.58	116.89	121.25
22	L	306	CLA	CMB-C2B-C1B	3.58	130.82	125.37
22	F	305	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
22	A	805	CLA	C2D-C1D-ND	3.58	112.74	110.10
22	3	319	CLA	CHC-C1C-C2C	-3.58	116.79	126.73
22	A	830	CLA	C1-C2-C3	-3.58	120.96	126.75
22	A	827	CLA	CHB-C4A-NA	3.58	129.46	124.51
22	3	317	CLA	C2D-C1D-ND	3.58	112.74	110.10
22	3	315	CLA	CHC-C1C-C2C	-3.57	116.80	126.73
22	2	320	CLA	C3D-C2D-C1D	-3.57	100.95	105.83
25	A	818	BCR	C34-C9-C10	-3.57	117.92	122.92
25	B	835	BCR	C36-C18-C17	-3.57	117.92	122.92
22	1	319	CLA	CHB-C4A-NA	3.57	129.45	124.51
22	B	805	CLA	C3B-C4B-NB	3.57	113.83	110.52
23	3	301	LUT	C39-C29-C30	-3.57	117.92	122.92
22	Z	306	CLA	CHB-C4A-NA	3.57	129.45	124.51
25	B	838	BCR	C1-C6-C5	-3.57	117.59	122.61
22	B	810	CLA	CHD-C1D-ND	-3.57	121.17	124.45
22	A	855	CLA	C3D-C2D-C1D	-3.57	100.96	105.83
22	A	802	CLA	C4C-C3C-C2C	-3.57	101.70	106.90
22	A	856	CLA	C4D-CHA-C1A	-3.57	116.91	121.25
22	B	815	CLA	C4C-C3C-C2C	-3.57	101.70	106.90
22	A	855	CLA	CHC-C4B-NB	-3.56	120.48	124.26
22	B	829	CLA	C3D-C2D-C1D	-3.56	100.97	105.83
22	1	306	CLA	CHC-C1C-C2C	-3.56	116.83	126.73
22	A	807	CLA	CHB-C1B-NB	-3.56	120.48	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	304	CLA	C1D-CHD-C4C	-3.56	118.37	126.06
22	A	854	CLA	C4C-C3C-C2C	-3.56	101.70	106.90
22	3	312	CLA	CHC-C1C-C2C	-3.56	116.84	126.73
22	A	836	CLA	C3D-C2D-C1D	-3.56	100.97	105.83
21	2	321	CHL	CHB-C1B-NB	-3.56	120.49	124.26
22	A	809	CLA	CAC-C3C-C4C	3.56	129.43	124.81
22	2	307	CLA	CHC-C1C-C2C	-3.56	116.84	126.73
25	B	838	BCR	C37-C22-C21	-3.56	117.94	122.92
22	B	826	CLA	C4C-C3C-C2C	-3.56	101.71	106.90
22	4	311	CLA	CHC-C4B-NB	-3.56	120.49	124.26
22	B	811	CLA	CHC-C4B-NB	-3.56	120.49	124.26
22	2	305	CLA	O2D-CGD-O1D	-3.56	116.89	123.84
25	L	303	BCR	C34-C9-C10	-3.56	117.94	122.92
22	B	804	CLA	C4D-CHA-C1A	-3.56	116.92	121.25
22	L	307	CLA	C4C-C3C-C2C	-3.56	101.72	106.90
21	Y	305	CHL	CHB-C4A-NA	3.55	129.43	124.51
25	B	839	BCR	C34-C9-C10	-3.55	117.94	122.92
22	B	830	CLA	CAC-C3C-C2C	3.55	133.61	127.53
22	O	207	CLA	C1D-CHD-C4C	-3.55	118.39	126.06
22	A	854	CLA	CMB-C2B-C3B	3.55	135.19	126.59
22	4	315	CLA	CAC-C3C-C4C	3.55	129.42	124.81
21	Z	304	CHL	CAC-C3C-C4C	3.55	129.42	124.81
22	A	808	CLA	C4D-CHA-C1A	-3.55	116.93	121.25
22	A	848	CLA	C3D-C2D-C1D	-3.55	100.98	105.83
22	A	849	CLA	CHB-C1B-NB	-3.55	120.50	124.26
22	B	851	CLA	CHD-C1D-ND	-3.55	121.19	124.45
22	2	304	CLA	CHD-C1D-ND	-3.55	121.19	124.45
22	B	807	CLA	C11-C10-C8	-3.55	104.45	115.92
22	1	320	CLA	CHC-C4B-NB	-3.55	120.50	124.26
22	G	205	CLA	CHB-C4A-NA	3.55	129.42	124.51
22	A	853	CLA	O2D-CGD-CBD	3.55	117.57	111.27
22	1	306	CLA	CHD-C1D-ND	-3.55	121.19	124.45
22	N	202	CLA	CHC-C1C-C2C	-3.55	116.88	126.73
22	A	855	CLA	C4C-C3C-C2C	-3.55	101.73	106.90
22	4	310	CLA	CHC-C1C-C2C	-3.55	116.88	126.73
22	A	827	CLA	C4C-C3C-C2C	-3.55	101.73	106.90
21	Y	306	CHL	CAC-C3C-C4C	3.54	129.41	124.81
30	A	825	CL0	C3D-C4D-ND	3.54	115.97	110.24
22	Z	314	CLA	CHC-C1C-C2C	-3.54	116.89	126.73
22	A	859	CLA	C2D-C1D-ND	3.54	112.71	110.10
22	A	810	CLA	CHC-C4B-NB	-3.54	120.51	124.26
22	B	803	CLA	CHB-C4A-NA	3.54	129.41	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	306	CLA	C1D-CHD-C4C	-3.54	118.42	126.06
25	A	819	BCR	C35-C13-C14	-3.54	117.97	122.92
25	J	101	BCR	C7-C8-C9	3.54	131.58	126.23
22	H	201	CLA	CHB-C1B-NB	-3.54	120.51	124.26
22	K	204	CLA	CHB-C1B-NB	-3.54	120.51	124.26
22	A	843	CLA	C2D-C1D-ND	3.54	112.71	110.10
22	X	304	CLA	CMD-C2D-C3D	-3.54	119.48	127.61
22	A	843	CLA	C4D-CHA-C1A	-3.54	116.94	121.25
22	L	307	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
22	Z	311	CLA	CHC-C1C-C2C	-3.53	116.92	126.73
22	A	834	CLA	CMB-C2B-C1B	3.53	130.75	125.37
22	B	820	CLA	C4C-C3C-C2C	-3.53	101.75	106.90
22	Z	309	CLA	CHC-C4B-NB	-3.53	120.52	124.26
22	A	835	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
23	4	319	LUT	C39-C29-C30	-3.53	117.98	122.92
22	B	850	CLA	CHB-C4A-NA	3.53	129.39	124.51
21	1	316	CHL	CAC-C3C-C4C	3.53	129.39	124.81
22	B	814	CLA	CAC-C3C-C4C	3.53	129.39	124.81
25	A	815	BCR	C35-C13-C14	-3.53	117.98	122.92
22	A	834	CLA	CHC-C1C-C2C	-3.53	116.93	126.73
22	B	808	CLA	C3B-C4B-NB	3.53	113.79	110.52
25	A	817	BCR	C19-C18-C17	3.53	124.35	118.94
22	A	804	CLA	C1D-CHD-C4C	-3.53	118.45	126.06
22	A	843	CLA	CAC-C3C-C4C	3.53	129.38	124.81
22	A	809	CLA	C3B-C4B-NB	3.53	113.79	110.52
22	B	810	CLA	CHC-C4B-NB	-3.53	120.53	124.26
25	B	834	BCR	C35-C13-C14	-3.52	117.99	122.92
22	B	831	CLA	C4-C3-C5	3.52	121.20	115.27
25	J	101	BCR	C34-C9-C10	-3.52	117.99	122.92
21	Y	313	CHL	CAC-C3C-C4C	3.52	129.38	124.81
22	Z	310	CLA	CHC-C4B-NB	-3.52	120.53	124.26
22	A	840	CLA	C4C-C3C-C2C	-3.52	101.77	106.90
25	F	302	BCR	C38-C26-C25	3.52	128.48	124.53
30	A	825	CL0	C4D-CHA-C1A	-3.52	116.96	121.25
22	Z	313	CLA	CHC-C4B-NB	-3.52	120.53	124.26
22	4	310	CLA	C1D-CHD-C4C	-3.52	118.47	126.06
25	B	839	BCR	C19-C18-C17	3.52	124.34	118.94
22	1	305	CLA	CHC-C4B-NB	-3.52	120.53	124.26
22	2	308	CLA	CHC-C1C-C2C	-3.52	116.96	126.73
22	B	819	CLA	O2D-CGD-CBD	3.52	117.52	111.27
22	Y	309	CLA	CHC-C1C-C2C	-3.52	116.96	126.73
22	2	320	CLA	CHC-C1C-C2C	-3.52	116.96	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	810	CLA	C1D-CHD-C4C	-3.52	118.47	126.06
22	A	841	CLA	C2D-C1D-ND	3.52	112.69	110.10
22	B	811	CLA	CHC-C1C-C2C	-3.51	116.97	126.73
22	3	317	CLA	CHB-C4A-NA	3.51	129.37	124.51
22	Z	309	CLA	CHC-C1C-C2C	-3.51	116.98	126.73
22	A	858	CLA	C3B-C4B-NB	3.51	113.77	110.52
22	A	838	CLA	C4D-CHA-C1A	-3.51	116.98	121.25
25	L	302	BCR	C36-C18-C17	-3.51	118.01	122.92
22	A	840	CLA	CHB-C4A-NA	3.51	129.36	124.51
21	X	308	CHL	CAC-C3C-C4C	3.51	129.36	124.81
25	K	201	BCR	C38-C26-C25	3.51	128.47	124.53
22	2	319	CLA	C4D-CHA-C1A	-3.51	116.98	121.25
22	A	834	CLA	CHD-C1D-ND	-3.50	121.23	124.45
22	2	318	CLA	C1D-CHD-C4C	-3.50	118.50	126.06
22	Y	302	CLA	CHC-C1C-C2C	-3.50	117.00	126.73
22	B	852	CLA	CHC-C1C-C2C	-3.50	117.00	126.73
22	3	310	CLA	CHC-C1C-C2C	-3.50	117.00	126.73
22	G	205	CLA	CHC-C1C-C2C	-3.50	117.00	126.73
22	3	315	CLA	CMB-C2B-C1B	3.50	130.70	125.37
22	Z	308	CLA	CHC-C1C-C2C	-3.50	117.00	126.73
21	X	305	CHL	CAC-C3C-C4C	3.50	129.35	124.81
22	B	850	CLA	CHD-C1D-ND	-3.50	121.24	124.45
25	B	844	BCR	C37-C22-C21	-3.50	118.02	122.92
22	X	313	CLA	CHC-C1C-C2C	-3.50	117.01	126.73
22	3	312	CLA	CMD-C2D-C3D	-3.50	119.57	127.61
22	3	312	CLA	C4-C3-C5	3.50	121.16	115.27
22	B	851	CLA	CMC-C2C-C1C	3.50	130.36	125.04
22	A	842	CLA	CMB-C2B-C1B	3.50	130.69	125.37
22	A	851	CLA	C1-C2-C3	-3.50	121.09	126.75
25	B	840	BCR	C38-C26-C25	3.50	128.45	124.53
22	A	837	CLA	C4C-C3C-C2C	-3.50	101.80	106.90
22	A	807	CLA	CHC-C1C-C2C	-3.49	117.02	126.73
22	F	305	CLA	CHC-C4B-NB	-3.49	120.56	124.26
23	2	310	LUT	C1-C6-C7	3.49	125.66	115.78
21	Z	301	CHL	CHB-C4A-NA	3.49	129.34	124.51
25	4	321	BCR	C36-C18-C17	-3.49	118.03	122.92
22	B	831	CLA	C4D-CHA-C1A	-3.49	117.00	121.25
22	A	808	CLA	CHB-C4A-NA	3.49	129.34	124.51
22	A	828	CLA	CAC-C3C-C4C	3.49	129.34	124.81
22	B	827	CLA	C4D-CHA-C1A	-3.49	117.00	121.25
25	G	202	BCR	C37-C22-C23	-3.49	112.58	118.08
22	O	207	CLA	CHB-C1B-NB	-3.49	120.56	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Z	307	CLA	CHC-C4B-NB	-3.49	120.56	124.26
22	2	308	CLA	CAC-C3C-C4C	3.49	129.34	124.81
22	B	819	CLA	C3B-C4B-NB	3.49	113.75	110.52
22	3	319	CLA	CHB-C1B-NB	-3.49	120.56	124.26
22	A	834	CLA	CHB-C1B-NB	-3.49	120.56	124.26
22	B	823	CLA	C4D-CHA-C1A	-3.49	117.00	121.25
22	X	301	CLA	CHC-C1C-C2C	-3.49	117.05	126.73
22	3	309	CLA	C2D-C1D-ND	3.49	112.67	110.10
21	Z	302	CHL	CAC-C3C-C4C	3.49	129.33	124.81
22	B	809	CLA	CHC-C1C-C2C	-3.49	117.05	126.73
22	X	303	CLA	CHC-C1C-C2C	-3.49	117.05	126.73
22	4	314	CLA	C1D-CHD-C4C	-3.48	118.54	126.06
22	B	809	CLA	C1D-CHD-C4C	-3.48	118.54	126.06
22	3	316	CLA	C2D-C1D-ND	3.48	112.67	110.10
22	Z	308	CLA	CHC-C4B-NB	-3.48	120.57	124.26
21	2	302	CHL	CHB-C4A-NA	3.48	129.33	124.51
22	H	201	CLA	C2D-C1D-ND	3.48	112.67	110.10
22	B	805	CLA	CHC-C1C-C2C	-3.48	117.06	126.73
22	2	307	CLA	CHB-C1B-NB	-3.48	120.57	124.26
22	A	831	CLA	C1-C2-C3	-3.48	120.02	126.04
22	2	307	CLA	C2D-C1D-ND	3.48	112.67	110.10
22	1	320	CLA	C4C-C3C-C2C	-3.48	101.83	106.90
22	X	311	CLA	CHC-C1C-C2C	-3.48	117.06	126.73
22	1	320	CLA	C3D-C2D-C1D	-3.48	101.08	105.83
22	Y	301	CLA	CHC-C4B-NB	-3.48	120.58	124.26
22	O	209	CLA	CHC-C1C-C2C	-3.48	117.07	126.73
22	J	102	CLA	CHC-C1C-C2C	-3.48	117.07	126.73
21	3	307	CHL	CHB-C4A-NA	3.48	129.32	124.51
21	Z	312	CHL	C3D-C4D-ND	3.48	115.86	110.24
22	A	809	CLA	C1D-CHD-C4C	-3.47	118.56	126.06
30	A	825	CL0	C4C-C3C-C2C	-3.47	101.83	106.90
21	X	307	CHL	CHB-C4A-NA	3.47	129.32	124.51
22	B	815	CLA	C1C-C2C-C3C	-3.47	103.30	106.96
22	A	838	CLA	CHB-C1B-NB	-3.47	120.58	124.26
22	2	317	CLA	CHC-C1C-C2C	-3.47	117.09	126.73
22	O	207	CLA	C4D-CHA-C1A	-3.47	117.02	121.25
21	X	309	CHL	C1D-ND-C4D	-3.47	103.87	106.33
25	B	838	BCR	C37-C22-C23	3.47	123.55	118.08
22	A	846	CLA	CHC-C4B-NB	-3.47	120.58	124.26
22	A	854	CLA	C3B-C4B-NB	3.47	113.73	110.52
21	2	301	CHL	CHB-C1B-NB	-3.47	120.58	124.26
22	4	311	CLA	CAC-C3C-C4C	3.47	129.31	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	841	DGD	O2G-C1B-C2B	3.47	118.97	111.50
21	X	302	CHL	CAC-C3C-C4C	3.47	129.31	124.81
22	3	310	CLA	CHD-C1D-ND	-3.47	121.27	124.45
25	O	202	BCR	C33-C5-C6	3.46	128.42	124.53
22	B	813	CLA	CHB-C1B-NB	-3.46	120.59	124.26
22	Z	309	CLA	CHB-C1B-NB	-3.46	120.59	124.26
22	A	842	CLA	C4C-C3C-C2C	-3.46	101.85	106.90
22	3	319	CLA	CHC-C4B-NB	-3.46	120.59	124.26
22	4	318	CLA	CHC-C1C-C2C	-3.46	117.11	126.73
22	Z	307	CLA	CHC-C1C-C2C	-3.46	117.11	126.73
22	B	824	CLA	CAA-C2A-C3A	-3.46	103.30	112.78
22	4	318	CLA	CHC-C4B-NB	-3.46	120.59	124.26
22	B	831	CLA	C4C-C3C-C2C	-3.46	101.85	106.90
22	B	847	CLA	CHC-C1C-C2C	-3.46	117.11	126.73
22	B	830	CLA	C4C-C3C-C2C	-3.46	101.85	106.90
22	B	825	CLA	CHC-C1C-C2C	-3.46	117.12	126.73
22	X	310	CLA	CHB-C1B-NB	-3.46	120.60	124.26
22	A	807	CLA	C1D-CHD-C4C	-3.46	118.60	126.06
22	A	830	CLA	CHB-C4A-NA	3.46	129.29	124.51
22	O	210	CLA	CHC-C4B-NB	-3.46	120.60	124.26
22	B	833	CLA	CHC-C1C-C2C	-3.46	117.13	126.73
22	1	309	CLA	CHC-C1C-C2C	-3.46	117.13	126.73
22	A	839	CLA	CHC-C1C-C2C	-3.46	117.13	126.73
22	A	840	CLA	CAC-C3C-C4C	3.46	129.29	124.81
22	B	805	CLA	C2D-C1D-ND	3.45	112.65	110.10
22	B	849	CLA	CHB-C1B-NB	-3.45	120.60	124.26
22	Y	310	CLA	CHC-C1C-C2C	-3.45	117.14	126.73
22	B	851	CLA	C3D-C4D-ND	3.45	115.83	110.24
22	B	804	CLA	CHB-C4A-NA	3.45	129.29	124.51
22	A	842	CLA	CHB-C1B-NB	-3.45	120.60	124.26
22	Z	313	CLA	CHC-C1C-C2C	-3.45	117.14	126.73
22	B	823	CLA	C1D-CHD-C4C	-3.45	118.61	126.06
22	B	824	CLA	CHB-C4A-NA	3.45	129.28	124.51
22	A	812	CLA	C4C-C3C-C2C	-3.45	101.87	106.90
22	1	309	CLA	CHB-C1B-NB	-3.45	120.61	124.26
22	X	301	CLA	CHC-C4B-NB	-3.45	120.61	124.26
25	K	201	BCR	C36-C18-C17	-3.45	118.09	122.92
22	4	313	CLA	C2D-C1D-ND	3.45	112.64	110.10
22	G	206	CLA	CHC-C1C-C2C	-3.45	117.16	126.73
22	2	305	CLA	CHC-C1C-C2C	-3.44	117.16	126.73
22	F	305	CLA	CHC-C1C-C2C	-3.44	117.16	126.73
21	2	309	CHL	CAC-C3C-C4C	3.44	129.28	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	808	CLA	O2D-CGD-CBD	3.44	117.39	111.27
25	K	201	BCR	C15-C16-C17	3.44	130.53	123.47
22	2	307	CLA	C4C-C3C-C2C	-3.44	101.88	106.90
22	L	306	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
22	X	313	CLA	CHC-C4B-NB	-3.44	120.61	124.26
22	A	848	CLA	CHC-C1C-C2C	-3.44	117.17	126.73
22	L	305	CLA	CHC-C1C-C2C	-3.44	117.17	126.73
22	Z	310	CLA	CHC-C1C-C2C	-3.44	117.17	126.73
22	B	849	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
22	K	205	CLA	CHC-C1C-C2C	-3.44	117.18	126.73
22	3	315	CLA	C3D-C2D-C1D	-3.44	101.14	105.83
22	3	311	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
22	1	305	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
22	B	807	CLA	C1-C2-C3	-3.44	120.10	126.04
22	4	313	CLA	CHB-C4A-NA	3.44	129.26	124.51
21	4	317	CHL	CHB-C1B-NB	-3.43	120.62	124.26
21	3	307	CHL	O2D-CGD-CBD	3.43	117.37	111.27
22	A	803	CLA	CHB-C4A-NA	3.43	129.26	124.51
22	X	312	CLA	CHC-C1C-C2C	-3.43	117.19	126.73
22	A	809	CLA	C4D-CHA-C1A	-3.43	117.07	121.25
22	B	811	CLA	C4D-CHA-C1A	-3.43	117.07	121.25
21	Z	302	CHL	CHB-C4A-NA	3.43	129.26	124.51
22	Y	314	CLA	C1D-CHD-C4C	-3.43	118.65	126.06
25	A	818	BCR	C17-C16-C15	3.43	132.45	124.81
22	B	823	CLA	CHB-C4A-NA	3.43	129.26	124.51
25	I	101	BCR	C36-C18-C17	-3.43	118.11	122.92
22	1	302	CLA	CHC-C1C-C2C	-3.43	117.20	126.73
25	B	834	BCR	C38-C26-C25	3.43	128.38	124.53
22	B	802	CLA	C3B-C4B-NB	3.43	113.70	110.52
22	B	816	CLA	C1-C2-C3	-3.43	120.11	126.04
22	A	850	CLA	C4C-C3C-C2C	-3.43	101.90	106.90
25	A	819	BCR	C2-C1-C6	3.43	115.76	110.48
22	Z	311	CLA	CHC-C4B-NB	-3.43	120.63	124.26
30	A	825	CL0	CHC-C1C-C2C	-3.43	117.21	126.73
21	Z	301	CHL	CAC-C3C-C4C	3.43	129.26	124.81
22	B	817	CLA	C4C-C3C-C2C	-3.43	101.90	106.90
25	A	819	BCR	C36-C18-C17	-3.43	118.12	122.92
22	A	847	CLA	C1D-CHD-C4C	-3.43	118.66	126.06
22	G	206	CLA	CHB-C1B-NB	-3.43	120.63	124.26
22	2	307	CLA	C3B-C4B-NB	3.43	113.69	110.52
22	A	842	CLA	CHB-C4A-NA	3.42	129.25	124.51
22	A	845	CLA	CMD-C2D-C3D	-3.42	119.74	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	304	CLA	CAC-C3C-C4C	3.42	129.25	124.81
22	A	808	CLA	C2D-C1D-ND	3.42	112.63	110.10
22	A	802	CLA	CAC-C3C-C4C	3.42	129.25	124.81
22	O	206	CLA	C3B-C4B-NB	3.42	113.69	110.52
22	A	846	CLA	C4D-CHA-C1A	-3.42	117.08	121.25
25	B	839	BCR	C30-C25-C26	-3.42	117.79	122.61
22	B	820	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
21	Y	303	CHL	CHB-C4A-NA	3.42	129.24	124.51
21	2	309	CHL	C3D-C4D-ND	3.42	115.77	110.24
22	2	308	CLA	C1-C2-C3	-3.42	120.13	126.04
22	2	303	CLA	CHC-C1C-C2C	-3.42	117.23	126.73
22	3	321	CLA	CMD-C2D-C3D	-3.42	119.75	127.61
25	B	834	BCR	C37-C22-C21	-3.42	118.13	122.92
22	1	317	CLA	CAA-C2A-C1A	-3.42	100.77	111.97
22	F	306	CLA	CHB-C1B-NB	-3.42	120.64	124.26
22	B	821	CLA	C4D-CHA-C1A	-3.42	117.09	121.25
21	Z	303	CHL	C3D-C4D-ND	3.42	115.77	110.24
22	3	309	CLA	C4-C3-C5	3.42	121.02	115.27
22	2	303	CLA	C3D-C2D-C1D	-3.42	101.17	105.83
22	3	318	CLA	CHD-C1D-ND	-3.42	121.31	124.45
25	4	321	BCR	C35-C13-C14	-3.42	118.14	122.92
22	O	210	CLA	CHC-C1C-C2C	-3.42	117.24	126.73
22	2	303	CLA	CHB-C4A-NA	3.42	129.24	124.51
22	A	842	CLA	C1D-CHD-C4C	-3.42	118.69	126.06
22	A	843	CLA	C1C-C2C-C3C	-3.42	103.37	106.96
22	G	206	CLA	C1D-CHD-C4C	-3.41	118.69	126.06
22	B	814	CLA	CHC-C4B-NB	-3.41	120.64	124.26
22	4	310	CLA	CHB-C4A-NA	3.41	129.23	124.51
22	1	318	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
22	B	821	CLA	CHC-C1C-C2C	-3.41	117.25	126.73
21	X	302	CHL	CHB-C4A-NA	3.41	129.23	124.51
23	1	310	LUT	C19-C9-C10	-3.41	118.14	122.92
25	A	814	BCR	C15-C16-C17	3.41	130.46	123.47
21	Y	307	CHL	C1D-ND-C4D	-3.41	103.91	106.33
21	1	301	CHL	CAC-C3C-C4C	3.41	129.24	124.81
22	A	841	CLA	C4C-C3C-C2C	-3.41	101.93	106.90
23	4	319	LUT	C19-C9-C10	-3.41	118.15	122.92
22	B	828	CLA	C2D-C1D-ND	3.41	112.62	110.10
22	N	202	CLA	C2D-C1D-ND	3.41	112.62	110.10
22	Z	310	CLA	C2D-C1D-ND	3.41	112.62	110.10
25	L	301	BCR	C16-C15-C14	3.41	130.46	123.47
22	Z	309	CLA	CHB-C4A-NA	3.41	129.23	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	852	CLA	O2A-CGA-CBA	3.41	122.61	111.91
22	B	829	CLA	CMD-C2D-C3D	-3.41	119.77	127.61
22	H	201	CLA	CHC-C1C-C2C	-3.41	117.26	126.73
22	B	815	CLA	CAC-C3C-C4C	3.41	129.23	124.81
22	X	301	CLA	C1D-CHD-C4C	-3.41	118.71	126.06
30	A	825	CL0	CMB-C2B-C3B	3.41	134.84	126.59
22	Y	301	CLA	CMD-C2D-C3D	-3.41	119.78	127.61
22	B	802	CLA	CHC-C1C-C2C	-3.41	117.27	126.73
22	J	102	CLA	C1D-CHD-C4C	-3.40	118.71	126.06
22	2	307	CLA	CHB-C4A-NA	3.40	129.22	124.51
21	Y	305	CHL	CAC-C3C-C4C	3.40	129.23	124.81
22	1	306	CLA	CHB-C1B-NB	-3.40	120.66	124.26
22	B	845	CLA	C3B-C2B-C1B	-3.40	103.06	107.16
25	A	818	BCR	C38-C26-C25	3.40	128.35	124.53
21	4	317	CHL	CHB-C4A-NA	3.40	129.22	124.51
25	L	302	BCR	C10-C11-C12	3.40	133.83	123.22
25	B	837	BCR	C12-C13-C14	3.40	124.16	118.94
22	G	205	CLA	C4A-NA-C1A	3.40	108.23	106.71
25	A	815	BCR	C38-C26-C25	3.40	128.35	124.53
22	3	308	CLA	CHC-C1C-C2C	-3.40	117.28	126.73
22	B	805	CLA	CHB-C1B-NB	-3.40	120.66	124.26
22	1	307	CLA	O2A-CGA-CBA	3.40	122.58	111.91
30	A	825	CL0	CHC-C4B-NB	-3.40	120.66	124.26
22	A	844	CLA	C4C-C3C-C2C	-3.40	101.94	106.90
22	A	844	CLA	CHB-C4A-NA	3.40	129.21	124.51
22	3	315	CLA	C1D-CHD-C4C	-3.40	118.73	126.06
22	A	832	CLA	C4D-CHA-C1A	-3.40	117.11	121.25
25	J	103	BCR	C12-C13-C14	3.40	124.16	118.94
21	Y	307	CHL	CHB-C4A-NA	3.40	129.21	124.51
22	4	310	CLA	C3D-C2D-C1D	-3.40	101.19	105.83
22	K	203	CLA	C2D-C1D-ND	3.40	112.61	110.10
22	B	833	CLA	C1D-CHD-C4C	-3.40	118.73	126.06
22	1	320	CLA	C3B-C4B-NB	3.40	113.67	110.52
22	2	318	CLA	CHC-C1C-C2C	-3.40	117.30	126.73
22	O	210	CLA	CHB-C1B-NB	-3.39	120.66	124.26
22	A	850	CLA	C4A-NA-C1A	3.39	108.23	106.71
22	Y	310	CLA	C2D-C1D-ND	3.39	112.61	110.10
22	1	303	CLA	CAC-C3C-C4C	3.39	129.21	124.81
22	2	306	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
22	B	847	CLA	CHB-C4A-NA	3.39	129.20	124.51
22	A	837	CLA	C3B-C4B-NB	3.39	113.66	110.52
22	4	313	CLA	CHB-C1B-NB	-3.39	120.67	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	K	205	CLA	CAA-C2A-C3A	-3.39	108.18	116.10
22	B	831	CLA	CHC-C1C-C2C	-3.39	117.31	126.73
22	B	824	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
22	A	826	CLA	C4-C3-C5	3.39	120.97	115.27
22	1	320	CLA	CHD-C1D-ND	-3.39	121.34	124.45
21	3	314	CHL	CHB-C4A-NA	3.39	129.20	124.51
22	Y	309	CLA	CHB-C1B-NB	-3.39	120.67	124.26
22	X	301	CLA	CHB-C1B-NB	-3.39	120.67	124.26
22	Y	309	CLA	CHC-C4B-NB	-3.39	120.67	124.26
22	A	849	CLA	CMB-C2B-C1B	3.39	130.53	125.37
22	B	829	CLA	CAC-C3C-C4C	3.39	129.20	124.81
22	A	840	CLA	CHB-C1B-NB	-3.39	120.67	124.26
22	1	317	CLA	C1-C2-C3	-3.39	120.19	126.04
21	Y	306	CHL	CHB-C4A-NA	3.39	129.19	124.51
22	A	832	CLA	CHC-C1C-C2C	-3.39	117.33	126.73
22	X	310	CLA	C3B-C4B-NB	3.38	113.66	110.52
21	2	302	CHL	C1C-C2C-C3C	-3.38	104.43	107.11
22	B	803	CLA	CHC-C1C-C2C	-3.38	117.33	126.73
22	3	317	CLA	C4C-C3C-C2C	-3.38	101.97	106.90
22	B	815	CLA	CHC-C4B-NB	-3.38	120.68	124.26
22	B	820	CLA	C3B-C4B-NB	3.38	113.65	110.52
22	X	312	CLA	CHC-C4B-NB	-3.38	120.68	124.26
21	X	309	CHL	CHB-C4A-NA	3.38	129.19	124.51
22	B	828	CLA	CHB-C1B-NB	-3.38	120.68	124.26
22	B	820	CLA	CMD-C2D-C3D	-3.38	119.84	127.61
22	2	320	CLA	C3B-C4B-NB	3.38	113.65	110.52
22	Z	314	CLA	C3B-C4B-NB	3.38	113.65	110.52
22	3	317	CLA	CHB-C1B-NB	-3.38	120.68	124.26
24	4	320	XAT	O4-C5-C18	3.38	119.10	115.06
22	1	303	CLA	C1D-CHD-C4C	-3.37	118.78	126.06
21	X	308	CHL	CHB-C4A-NA	3.37	129.18	124.51
22	B	814	CLA	C4C-C3C-C2C	-3.37	101.98	106.90
22	2	318	CLA	C3B-C4B-NB	3.37	113.64	110.52
22	B	824	CLA	CMD-C2D-C3D	-3.37	119.85	127.61
25	B	834	BCR	C12-C13-C14	3.37	124.12	118.94
22	A	842	CLA	CHC-C1C-C2C	-3.37	117.36	126.73
22	1	309	CLA	CHC-C4B-NB	-3.37	120.69	124.26
22	X	304	CLA	CHD-C4C-C3C	-3.37	119.88	124.84
22	A	847	CLA	C2D-C1D-ND	3.37	112.59	110.10
22	F	306	CLA	C4C-C3C-C2C	-3.37	101.98	106.90
25	A	817	BCR	C15-C16-C17	3.37	130.38	123.47
22	G	206	CLA	CMD-C2D-C3D	-3.37	119.86	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	210	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
22	4	310	CLA	CHB-C1B-NB	-3.37	120.69	124.26
22	4	310	CLA	C3B-C4B-NB	3.37	113.64	110.52
22	X	311	CLA	CHC-C4B-NB	-3.37	120.69	124.26
22	4	311	CLA	CHC-C1C-C2C	-3.37	117.37	126.73
22	A	851	CLA	CAC-C3C-C4C	3.37	129.18	124.81
22	B	818	CLA	CAC-C3C-C4C	3.37	129.18	124.81
21	X	308	CHL	C3D-C4D-ND	3.37	115.69	110.24
25	B	835	BCR	C37-C22-C21	-3.37	118.21	122.92
22	B	823	CLA	C2D-C1D-ND	3.37	112.58	110.10
21	4	307	CHL	C1C-C2C-C3C	-3.37	104.44	107.11
22	4	318	CLA	C3B-C4B-NB	3.37	113.64	110.52
22	F	306	CLA	CHD-C1D-ND	-3.37	121.36	124.45
22	B	806	CLA	CHB-C1B-NB	-3.37	120.69	124.26
22	1	304	CLA	O2A-CGA-CBA	3.37	122.47	111.91
22	A	809	CLA	CHB-C4A-NA	3.36	129.16	124.51
21	4	307	CHL	CHB-C1B-NB	-3.36	120.69	124.26
22	X	312	CLA	CHB-C1B-NB	-3.36	120.69	124.26
22	3	319	CLA	C3B-C4B-NB	3.36	113.64	110.52
22	B	828	CLA	CHB-C4A-NA	3.36	129.16	124.51
23	4	319	LUT	C11-C10-C9	3.36	132.11	127.31
25	A	817	BCR	C34-C9-C8	3.36	123.38	118.08
22	O	207	CLA	CHC-C4B-NB	-3.36	120.70	124.26
22	3	313	CLA	C1D-CHD-C4C	-3.36	118.80	126.06
25	1	312	BCR	C12-C13-C14	3.36	124.10	118.94
22	B	853	CLA	O2A-CGA-CBA	3.36	122.46	111.91
22	3	318	CLA	CHB-C1B-NB	-3.36	120.70	124.26
22	B	822	CLA	CAC-C3C-C4C	3.36	129.17	124.81
22	B	815	CLA	C2D-C1D-ND	3.36	112.58	110.10
25	B	836	BCR	C35-C13-C14	-3.36	118.22	122.92
22	A	833	CLA	CHB-C1B-NB	-3.36	120.70	124.26
22	Z	306	CLA	CHC-C4B-NB	-3.36	120.70	124.26
22	2	322	CLA	CHC-C1C-C2C	-3.36	117.40	126.73
22	B	822	CLA	CHC-C1C-C2C	-3.36	117.40	126.73
22	2	307	CLA	C1D-CHD-C4C	-3.36	118.81	126.06
22	Y	302	CLA	CHC-C4B-NB	-3.36	120.70	124.26
22	B	849	CLA	CHC-C1C-C2C	-3.36	117.41	126.73
22	A	830	CLA	C4D-CHA-C1A	-3.36	117.16	121.25
25	L	304	BCR	C35-C13-C14	-3.35	118.22	122.92
22	B	849	CLA	C2D-C1D-ND	3.35	112.58	110.10
22	Z	311	CLA	CHB-C1B-NB	-3.35	120.71	124.26
22	4	314	CLA	C3B-C4B-NB	3.35	113.63	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	831	CLA	CHB-C1B-NB	-3.35	120.71	124.26
22	Y	312	CLA	CHB-C1B-NB	-3.35	120.71	124.26
22	B	845	CLA	CHC-C1C-C2C	-3.35	117.42	126.73
22	4	304	CLA	CMC-C2C-C1C	3.35	130.15	125.04
22	A	855	CLA	C1D-CHD-C4C	-3.35	118.83	126.06
22	B	833	CLA	CHB-C1B-NB	-3.35	120.71	124.26
22	B	853	CLA	C4-C3-C5	3.35	120.91	115.27
22	B	830	CLA	C4D-CHA-C1A	-3.35	117.17	121.25
22	Y	308	CLA	C4D-CHA-C1A	-3.35	117.17	121.25
22	4	312	CLA	CHD-C1D-ND	-3.35	121.37	124.45
22	O	208	CLA	CHB-C1B-NB	-3.35	120.71	124.26
22	X	310	CLA	CHC-C4B-NB	-3.35	120.71	124.26
22	4	315	CLA	C3B-C4B-NB	3.35	113.62	110.52
25	B	835	BCR	C35-C13-C14	-3.35	118.23	122.92
25	B	836	BCR	C1-C6-C7	3.35	125.25	115.78
22	B	806	CLA	CAC-C3C-C4C	3.35	129.15	124.81
22	A	856	CLA	CHB-C4A-NA	3.35	129.14	124.51
22	O	209	CLA	C2D-C1D-ND	3.35	112.57	110.10
23	4	319	LUT	C39-C29-C28	3.35	123.35	118.08
22	B	830	CLA	CMB-C2B-C1B	3.35	130.47	125.37
22	3	313	CLA	C2D-C1D-ND	3.34	112.57	110.10
22	4	316	CLA	C1D-CHD-C4C	-3.34	118.84	126.06
22	4	306	CLA	CMA-C3A-C4A	-3.34	102.78	111.77
25	J	103	BCR	C38-C26-C25	3.34	128.28	124.53
22	B	851	CLA	C4D-CHA-C1A	-3.34	117.18	121.25
22	4	318	CLA	CHB-C1B-NB	-3.34	120.72	124.26
22	A	809	CLA	CHC-C4B-NB	-3.34	120.72	124.26
21	X	307	CHL	C3D-C4D-ND	3.34	115.65	110.24
25	B	836	BCR	C16-C15-C14	3.34	130.32	123.47
25	J	101	BCR	C16-C15-C14	3.34	130.32	123.47
22	H	201	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
22	B	829	CLA	C1D-CHD-C4C	-3.34	118.85	126.06
22	Y	311	CLA	CHB-C1B-NB	-3.34	120.72	124.26
22	1	321	CLA	CHC-C1C-C2C	-3.34	117.45	126.73
22	A	806	CLA	CHC-C1C-C2C	-3.34	117.45	126.73
21	Z	304	CHL	CHB-C4A-NA	3.34	129.13	124.51
25	L	302	BCR	C38-C26-C25	3.34	128.28	124.53
22	F	306	CLA	CHC-C1C-C2C	-3.34	117.45	126.73
22	A	837	CLA	CMD-C2D-C3D	-3.34	119.93	127.61
22	4	314	CLA	CHD-C1D-ND	-3.34	121.39	124.45
21	Z	312	CHL	CAC-C3C-C4C	3.34	129.14	124.81
22	3	312	CLA	C1D-CHD-C4C	-3.34	118.86	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Y	313	CHL	CHB-C1B-NB	-3.34	120.72	124.26
22	1	305	CLA	CHB-C1B-NB	-3.34	120.72	124.26
22	A	807	CLA	CHC-C4B-NB	-3.34	120.72	124.26
21	X	306	CHL	C3D-C4D-ND	3.34	115.64	110.24
21	Z	304	CHL	C3D-C4D-ND	3.34	115.64	110.24
22	Y	311	CLA	CHC-C4B-NB	-3.34	120.72	124.26
21	X	305	CHL	CHB-C4A-NA	3.34	129.12	124.51
22	4	311	CLA	CHB-C4A-NA	3.34	129.12	124.51
31	O	201	DGD	O6E-C5E-C4E	3.34	115.75	109.69
25	L	303	BCR	C30-C25-C24	3.33	125.21	115.78
22	B	813	CLA	CMC-C2C-C1C	3.33	130.12	125.04
22	G	207	CLA	C3B-C4B-NB	3.33	113.61	110.52
22	Y	301	CLA	C3B-C4B-NB	3.33	113.61	110.52
22	2	320	CLA	CMB-C2B-C1B	3.33	130.44	125.37
22	A	803	CLA	CHC-C1C-C2C	-3.33	117.47	126.73
22	G	205	CLA	CHC-C4B-NB	-3.33	120.73	124.26
22	4	316	CLA	C3B-C4B-NB	3.33	113.61	110.52
21	4	317	CHL	C3D-C4D-ND	3.33	115.63	110.24
22	1	320	CLA	C1D-CHD-C4C	-3.33	118.87	126.06
30	A	825	CL0	O2A-CGA-CBA	3.33	122.36	111.91
22	A	840	CLA	CMB-C2B-C1B	3.33	130.44	125.37
22	K	202	CLA	C3B-C4B-NB	3.33	113.60	110.52
22	B	812	CLA	C4D-CHA-C1A	-3.33	117.20	121.25
22	2	304	CLA	C1D-CHD-C4C	-3.33	118.88	126.06
22	Y	302	CLA	CHB-C1B-NB	-3.33	120.73	124.26
21	3	307	CHL	C3D-C4D-ND	3.33	115.62	110.24
22	A	808	CLA	CHC-C1C-C2C	-3.33	117.49	126.73
22	B	802	CLA	CHB-C1B-NB	-3.33	120.73	124.26
22	B	847	CLA	CHC-C4B-NB	-3.33	120.73	124.26
22	X	313	CLA	CHB-C1B-NB	-3.33	120.73	124.26
22	B	811	CLA	C1D-CHD-C4C	-3.33	118.88	126.06
22	2	304	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
22	B	824	CLA	CHC-C1C-C2C	-3.33	117.49	126.73
22	A	837	CLA	CHB-C1B-NB	-3.33	120.73	124.26
22	B	831	CLA	C2D-C1D-ND	3.33	112.56	110.10
22	A	856	CLA	CHC-C1C-C2C	-3.33	117.49	126.73
22	A	808	CLA	C1D-CHD-C4C	-3.33	118.88	126.06
22	1	307	CLA	C3B-C4B-NB	3.33	113.60	110.52
22	B	805	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
22	B	823	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
22	A	841	CLA	C1D-CHD-C4C	-3.32	118.89	126.06
22	N	202	CLA	C1D-CHD-C4C	-3.32	118.89	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	805	CLA	CHB-C4A-NA	3.32	129.11	124.51
22	Z	310	CLA	CHB-C1B-NB	-3.32	120.74	124.26
22	B	813	CLA	C3D-C2D-C1D	-3.32	101.30	105.83
22	B	805	CLA	C1D-CHD-C4C	-3.32	118.89	126.06
22	B	811	CLA	CHB-C1B-NB	-3.32	120.74	124.26
22	X	310	CLA	CHB-C4A-NA	3.32	129.11	124.51
22	A	845	CLA	C1D-CHD-C4C	-3.32	118.89	126.06
22	O	209	CLA	C1D-CHD-C4C	-3.32	118.89	126.06
22	B	801	CLA	CHB-C4A-NA	3.32	129.10	124.51
22	A	841	CLA	C3B-C4B-NB	3.32	113.60	110.52
22	H	201	CLA	C3B-C4B-NB	3.32	113.60	110.52
22	1	305	CLA	C4C-C3C-C2C	-3.32	102.06	106.90
22	B	821	CLA	CAC-C3C-C4C	3.32	129.12	124.81
21	4	317	CHL	CAC-C3C-C4C	3.32	129.12	124.81
22	3	318	CLA	CAC-C3C-C4C	3.32	129.12	124.81
22	Y	308	CLA	CHB-C1B-NB	-3.32	120.75	124.26
21	X	306	CHL	CAC-C3C-C4C	3.32	129.11	124.81
22	L	306	CLA	CHB-C1B-NB	-3.31	120.75	124.26
22	B	810	CLA	C1D-CHD-C4C	-3.31	118.91	126.06
21	X	302	CHL	C3D-C4D-ND	3.31	115.60	110.24
24	2	311	XAT	C20-C13-C14	-3.31	118.28	122.92
21	1	301	CHL	C1D-ND-C4D	-3.31	103.98	106.33
22	B	823	CLA	CHB-C1B-NB	-3.31	120.75	124.26
22	Y	308	CLA	C1D-CHD-C4C	-3.31	118.91	126.06
22	3	309	CLA	CHB-C1B-NB	-3.31	120.75	124.26
22	Y	310	CLA	C1D-CHD-C4C	-3.31	118.91	126.06
22	1	304	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
22	A	804	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
22	Y	314	CLA	C2D-C1D-ND	3.31	112.54	110.10
22	O	210	CLA	C1D-CHD-C4C	-3.31	118.92	126.06
30	A	825	CL0	CHB-C4A-NA	3.31	129.09	124.51
22	A	810	CLA	CHC-C1C-C2C	-3.31	117.54	126.73
22	B	849	CLA	CHB-C4A-NA	3.31	129.09	124.51
22	3	320	CLA	C3B-C4B-NB	3.31	113.58	110.52
22	A	812	CLA	CHC-C1C-C2C	-3.31	117.55	126.73
22	A	832	CLA	C1D-CHD-C4C	-3.31	118.92	126.06
22	A	859	CLA	C1D-CHD-C4C	-3.31	118.93	126.06
22	A	836	CLA	CHC-C1C-C2C	-3.31	117.55	126.73
22	3	310	CLA	C4C-C3C-C2C	-3.31	102.08	106.90
22	A	827	CLA	CMB-C2B-C1B	3.30	130.40	125.37
25	B	837	BCR	C1-C6-C5	-3.30	117.96	122.61
22	2	318	CLA	C4D-CHA-C1A	-3.30	117.23	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	3	301	LUT	C19-C9-C10	-3.30	118.30	122.92
22	1	321	CLA	CHB-C4A-NA	3.30	129.08	124.51
21	Y	307	CHL	CHB-C1B-NB	-3.30	120.76	124.26
22	A	848	CLA	C3B-C4B-NB	3.30	113.58	110.52
22	1	303	CLA	C3B-C4B-NB	3.30	113.58	110.52
22	B	811	CLA	C3B-C4B-NB	3.30	113.58	110.52
22	F	306	CLA	CHC-C4B-NB	-3.30	120.76	124.26
22	A	805	CLA	C4C-C3C-C2C	-3.30	102.09	106.90
22	2	303	CLA	C1D-CHD-C4C	-3.30	118.94	126.06
22	B	851	CLA	C1D-CHD-C4C	-3.30	118.94	126.06
22	A	839	CLA	CHB-C1B-NB	-3.30	120.77	124.26
22	Y	311	CLA	CAC-C3C-C4C	3.30	129.09	124.81
22	A	850	CLA	C4D-CHA-C1A	-3.30	117.24	121.25
22	Y	308	CLA	CHC-C4B-NB	-3.30	120.77	124.26
25	K	201	BCR	C16-C15-C14	3.30	130.23	123.47
22	B	823	CLA	CHC-C1C-C2C	-3.30	117.57	126.73
21	4	308	CHL	C3D-C4D-ND	3.30	115.57	110.24
22	1	304	CLA	CHB-C4A-NA	3.30	129.07	124.51
22	A	812	CLA	C1D-CHD-C4C	-3.30	118.95	126.06
22	1	307	CLA	CHC-C1C-C2C	-3.29	117.58	126.73
25	B	836	BCR	C36-C18-C17	-3.29	118.31	122.92
27	F	303	MGE	C3G-O3G-C1D	3.29	120.17	113.74
22	1	305	CLA	CHD-C1D-ND	-3.29	121.43	124.45
22	Z	309	CLA	C3B-C4B-NB	3.29	113.57	110.52
22	A	857	CLA	C1D-CHD-C4C	-3.29	118.95	126.06
22	2	306	CLA	CHB-C4A-NA	3.29	129.06	124.51
22	1	321	CLA	C1D-CHD-C4C	-3.29	118.96	126.06
21	1	316	CHL	C1D-ND-C4D	-3.29	104.00	106.33
22	4	304	CLA	C3B-C4B-NB	3.29	113.57	110.52
22	A	831	CLA	CHC-C4B-NB	-3.29	120.77	124.26
22	Z	307	CLA	C1D-CHD-C4C	-3.29	118.96	126.06
22	B	809	CLA	CMB-C2B-C1B	3.29	130.38	125.37
22	4	315	CLA	CHC-C1C-C2C	-3.29	117.60	126.73
22	A	859	CLA	CHC-C1C-C2C	-3.29	117.60	126.73
30	A	825	CL0	C3D-C2D-C1D	-3.29	101.34	105.83
22	A	851	CLA	C2D-C1D-ND	3.29	112.53	110.10
22	B	847	CLA	CAC-C3C-C4C	3.29	129.08	124.81
22	Y	302	CLA	CHB-C4A-NA	3.29	129.06	124.51
22	F	305	CLA	CHB-C1B-NB	-3.29	120.78	124.26
22	2	303	CLA	C4C-C3C-C2C	-3.29	102.11	106.90
22	B	803	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
22	X	313	CLA	C2D-C1D-ND	3.29	112.53	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	207	CLA	CHB-C4A-NA	3.29	129.06	124.51
25	B	844	BCR	C37-C22-C23	3.29	123.25	118.08
22	A	810	CLA	CAA-CBA-CGA	-3.28	103.65	113.25
22	X	304	CLA	CAC-C3C-C4C	3.28	129.07	124.81
30	A	825	CL0	C1D-CHD-C4C	-3.28	118.97	126.06
22	3	315	CLA	C4D-CHA-C1A	-3.28	117.25	121.25
22	B	848	CLA	C4C-C3C-C2C	-3.28	102.11	106.90
22	O	210	CLA	C2D-C1D-ND	3.28	112.52	110.10
22	Z	311	CLA	C1D-CHD-C4C	-3.28	118.97	126.06
22	Z	308	CLA	CHB-C1B-NB	-3.28	120.78	124.26
22	B	812	CLA	CHB-C1B-NB	-3.28	120.78	124.26
22	1	320	CLA	CHB-C4A-NA	3.28	129.05	124.51
22	4	314	CLA	C4C-C3C-C2C	-3.28	102.11	106.90
21	2	321	CHL	CMB-C2B-C1B	3.28	130.37	125.37
22	3	316	CLA	CHB-C4A-NA	3.28	129.05	124.51
22	1	302	CLA	CAC-C3C-C4C	3.28	129.06	124.81
22	B	850	CLA	C4C-C3C-C2C	-3.28	102.12	106.90
21	Z	303	CHL	CAC-C3C-C4C	3.28	129.06	124.81
22	A	810	CLA	C2D-C1D-ND	3.28	112.52	110.10
21	Y	304	CHL	CHB-C4A-NA	3.28	129.04	124.51
22	A	833	CLA	C4-C3-C5	3.28	120.78	115.27
22	A	837	CLA	CHB-C4A-NA	3.28	129.04	124.51
22	1	318	CLA	C1-C2-C3	-3.28	120.38	126.04
22	2	322	CLA	C2D-C1D-ND	3.28	112.52	110.10
22	A	840	CLA	C2D-C1D-ND	3.28	112.52	110.10
22	X	312	CLA	C1D-CHD-C4C	-3.28	118.99	126.06
22	1	306	CLA	C4C-C3C-C2C	-3.28	102.12	106.90
22	G	206	CLA	CHB-C4A-NA	3.28	129.04	124.51
22	Y	311	CLA	C3B-C4B-NB	3.28	113.55	110.52
22	3	308	CLA	CHB-C1B-NB	-3.27	120.79	124.26
22	Y	312	CLA	C3B-C4B-NB	3.27	113.55	110.52
22	A	844	CLA	C4A-NA-C1A	3.27	108.18	106.71
22	2	320	CLA	CMD-C2D-C3D	-3.27	120.09	127.61
22	N	202	CLA	CHB-C1B-NB	-3.27	120.79	124.26
22	B	850	CLA	C1D-CHD-C4C	-3.27	119.00	126.06
22	B	853	CLA	CHC-C1C-C2C	-3.27	117.64	126.73
21	Y	303	CHL	CHB-C1B-NB	-3.27	120.79	124.26
22	B	848	CLA	CHC-C1C-C2C	-3.27	117.64	126.73
25	J	101	BCR	C1-C6-C7	3.27	125.03	115.78
22	B	847	CLA	CMD-C2D-C3D	-3.27	120.09	127.61
22	A	805	CLA	CHC-C1C-C2C	-3.27	117.65	126.73
22	B	810	CLA	C2D-C1D-ND	3.27	112.51	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	810	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
22	1	305	CLA	CHC-C1C-C2C	-3.27	117.65	126.73
22	L	307	CLA	CHC-C1C-C2C	-3.27	117.65	126.73
22	4	304	CLA	CHB-C1B-NB	-3.27	120.80	124.26
22	A	845	CLA	CHB-C1B-NB	-3.27	120.80	124.26
22	L	307	CLA	CHB-C1B-NB	-3.27	120.80	124.26
22	B	814	CLA	CHD-C1D-ND	-3.27	121.45	124.45
21	Z	305	CHL	C1D-ND-C4D	-3.27	104.02	106.33
25	G	202	BCR	C38-C26-C25	3.27	128.19	124.53
25	B	844	BCR	C7-C8-C9	3.26	131.17	126.23
22	A	846	CLA	CHC-C1C-C2C	-3.26	117.66	126.73
22	1	306	CLA	CHB-C4A-NA	3.26	129.03	124.51
22	Y	309	CLA	C1D-CHD-C4C	-3.26	119.02	126.06
22	3	318	CLA	C1D-CHD-C4C	-3.26	119.02	126.06
25	A	816	BCR	C1-C6-C7	3.26	125.01	115.78
22	1	302	CLA	C1D-CHD-C4C	-3.26	119.02	126.06
22	A	812	CLA	CAC-C3C-C4C	3.26	129.04	124.81
22	3	308	CLA	CHC-C4B-NB	-3.26	120.81	124.26
22	Z	308	CLA	C1D-CHD-C4C	-3.26	119.03	126.06
24	2	311	XAT	C37-C21-C36	-3.26	102.56	107.37
22	2	308	CLA	C1D-CHD-C4C	-3.26	119.03	126.06
21	Z	302	CHL	C3D-C4D-ND	3.26	115.51	110.24
22	B	845	CLA	C3D-C2D-C1D	-3.26	101.39	105.83
21	4	309	CHL	C1D-ND-C4D	-3.26	104.02	106.33
22	B	806	CLA	CHC-C1C-C2C	-3.26	117.68	126.73
22	L	306	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
22	A	835	CLA	C4D-CHA-C1A	-3.26	117.29	121.25
22	A	857	CLA	CMB-C2B-C1B	3.26	130.33	125.37
22	2	305	CLA	C3B-C4B-NB	3.26	113.53	110.52
22	B	852	CLA	C1D-CHD-C4C	-3.25	119.04	126.06
22	B	826	CLA	C1-C2-C3	-3.25	121.49	126.75
25	2	312	BCR	C2-C1-C6	3.25	115.49	110.48
22	X	313	CLA	CHB-C4A-NA	3.25	129.01	124.51
22	A	837	CLA	C1D-CHD-C4C	-3.25	119.04	126.06
22	4	314	CLA	CAC-C3C-C4C	3.25	129.03	124.81
22	3	318	CLA	C3B-C4B-NB	3.25	113.53	110.52
22	X	313	CLA	C3B-C4B-NB	3.25	113.53	110.52
22	O	210	CLA	CHB-C4A-NA	3.25	129.01	124.51
21	Y	303	CHL	CAC-C3C-C4C	3.25	129.03	124.81
22	B	831	CLA	CHC-C4B-NB	-3.25	120.81	124.26
22	X	311	CLA	C1D-CHD-C4C	-3.25	119.04	126.06
22	A	833	CLA	C3B-C4B-NB	3.25	113.53	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	833	CLA	CHB-C4A-NA	3.25	129.01	124.51
22	1	303	CLA	C2D-C1D-ND	3.25	112.50	110.10
22	A	831	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
22	X	311	CLA	CHB-C1B-NB	-3.25	120.82	124.26
22	B	820	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
22	X	303	CLA	C1D-CHD-C4C	-3.25	119.05	126.06
21	Y	306	CHL	C3D-C4D-ND	3.25	115.49	110.24
22	B	833	CLA	C2D-C1D-ND	3.25	112.50	110.10
22	B	850	CLA	CHC-C1C-C2C	-3.25	117.71	126.73
22	B	813	CLA	C1D-CHD-C4C	-3.25	119.05	126.06
22	Y	312	CLA	C1D-CHD-C4C	-3.25	119.05	126.06
22	B	833	CLA	CHC-C4B-NB	-3.25	120.82	124.26
21	Y	304	CHL	C3D-C4D-ND	3.25	115.49	110.24
22	1	308	CLA	C3B-C4B-NB	3.25	113.53	110.52
22	A	847	CLA	C3B-C4B-NB	3.25	113.53	110.52
22	B	809	CLA	C4C-C3C-C2C	-3.25	102.17	106.90
22	A	835	CLA	CHC-C4B-NB	-3.25	120.82	124.26
22	3	319	CLA	CHB-C4A-NA	3.25	129.00	124.51
22	B	801	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
22	2	306	CLA	CHB-C1B-NB	-3.24	120.82	124.26
22	A	832	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
22	Z	314	CLA	CHB-C4A-NA	3.24	129.00	124.51
22	A	801	CLA	C4D-CHA-C1A	-3.24	117.30	121.25
22	B	820	CLA	CHD-C1D-ND	-3.24	121.47	124.45
25	B	835	BCR	C37-C22-C23	3.24	123.19	118.08
22	B	810	CLA	CHB-C4A-NA	3.24	129.00	124.51
22	Y	310	CLA	CHB-C1B-NB	-3.24	120.83	124.26
22	B	813	CLA	CAC-C3C-C4C	3.24	129.02	124.81
22	2	304	CLA	O2A-CGA-CBA	3.24	122.08	111.91
21	Y	305	CHL	CHB-C1B-NB	-3.24	120.83	124.26
22	2	305	CLA	CHC-C4B-NB	-3.24	120.83	124.26
22	4	312	CLA	CHB-C1B-NB	-3.24	120.83	124.26
22	B	801	CLA	CHC-C4B-NB	-3.24	120.83	124.26
22	A	839	CLA	CHB-C4A-NA	3.24	128.99	124.51
22	A	802	CLA	C2A-C1A-CHA	-3.24	118.19	123.86
22	B	821	CLA	C2D-C1D-ND	3.24	112.49	110.10
22	A	840	CLA	C1D-CHD-C4C	-3.24	119.07	126.06
22	B	808	CLA	C4-C3-C5	3.24	120.72	115.27
22	K	202	CLA	C1D-CHD-C4C	-3.24	119.08	126.06
22	O	207	CLA	C4A-NA-C1A	3.24	108.16	106.71
22	X	310	CLA	C1D-CHD-C4C	-3.24	119.08	126.06
24	4	320	XAT	C24-C23-C22	-3.24	104.53	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Y	308	CLA	C3B-C4B-NB	3.23	113.52	110.52
22	4	313	CLA	C4A-NA-C1A	3.23	108.16	106.71
22	3	309	CLA	O2A-CGA-CBA	3.23	122.06	111.91
21	Z	305	CHL	CHB-C4A-NA	3.23	128.98	124.51
22	3	318	CLA	C4C-C3C-C2C	-3.23	102.18	106.90
22	1	319	CLA	CMB-C2B-C1B	3.23	130.29	125.37
22	1	320	CLA	CMB-C2B-C1B	3.23	130.29	125.37
25	G	202	BCR	C37-C22-C21	-3.23	118.40	122.92
22	Z	311	CLA	C3B-C4B-NB	3.23	113.51	110.52
22	A	852	CLA	CHC-C1C-C2C	-3.23	117.75	126.73
22	3	315	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
22	A	801	CLA	CAC-C3C-C4C	3.23	129.00	124.81
22	A	849	CLA	C4D-CHA-C1A	-3.23	117.32	121.25
22	A	803	CLA	C1D-CHD-C4C	-3.23	119.09	126.06
22	Z	306	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
22	K	203	CLA	CHC-C1C-C2C	-3.23	117.76	126.73
21	Z	301	CHL	CHB-C1B-NB	-3.23	120.84	124.26
22	B	802	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
21	X	305	CHL	C3D-C4D-ND	3.23	115.46	110.24
22	F	306	CLA	O2D-CGD-CBD	3.23	117.00	111.27
22	X	301	CLA	C2D-C1D-ND	3.23	112.48	110.10
22	2	307	CLA	CMB-C2B-C1B	3.23	130.28	125.37
22	B	818	CLA	CHC-C1C-C2C	-3.23	117.77	126.73
22	B	804	CLA	C3B-C4B-NB	3.23	113.51	110.52
22	1	320	CLA	CAC-C3C-C4C	3.23	129.00	124.81
22	A	856	CLA	C1D-CHD-C4C	-3.23	119.10	126.06
22	4	310	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
22	A	807	CLA	C2D-C1D-ND	3.22	112.48	110.10
22	X	304	CLA	CGD-CBD-CAD	-3.22	100.30	110.73
22	Y	308	CLA	C2D-C1D-ND	3.22	112.48	110.10
21	2	309	CHL	CHB-C4A-NA	3.22	128.97	124.51
22	2	308	CLA	CHB-C4A-NA	3.22	128.97	124.51
22	A	803	CLA	CHD-C1D-ND	-3.22	121.49	124.45
22	4	305	CLA	CAC-C3C-C4C	3.22	128.99	124.81
22	1	319	CLA	CHC-C1C-C2C	-3.22	117.78	126.73
22	B	824	CLA	O2A-CGA-CBA	3.22	122.01	111.91
24	3	302	XAT	C28-C29-C30	3.22	123.88	118.94
22	Z	309	CLA	CAC-C3C-C4C	3.22	128.99	124.81
22	F	306	CLA	CHB-C4A-NA	3.22	128.96	124.51
22	O	207	CLA	C3B-C4B-NB	3.22	113.50	110.52
22	Z	308	CLA	C3B-C4B-NB	3.22	113.50	110.52
22	G	207	CLA	CMB-C2B-C1B	3.22	130.27	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	838	BCR	C30-C25-C24	3.22	124.88	115.78
22	A	854	CLA	C1D-CHD-C4C	-3.22	119.12	126.06
22	1	321	CLA	CAC-C3C-C4C	3.22	128.98	124.81
22	1	307	CLA	C1D-CHD-C4C	-3.22	119.12	126.06
22	Z	310	CLA	CAC-C3C-C4C	3.22	128.98	124.81
22	Y	310	CLA	CAC-C3C-C4C	3.21	128.98	124.81
22	1	302	CLA	C2D-C1D-ND	3.21	112.47	110.10
22	4	304	CLA	C2D-C1D-ND	3.21	112.47	110.10
22	Y	302	CLA	C1D-CHD-C4C	-3.21	119.12	126.06
22	3	317	CLA	C3B-C4B-NB	3.21	113.50	110.52
25	L	301	BCR	C35-C13-C14	-3.21	118.42	122.92
22	Z	306	CLA	CAC-C3C-C4C	3.21	128.98	124.81
22	J	102	CLA	CMD-C2D-C3D	-3.21	120.22	127.61
22	4	315	CLA	CHC-C4B-NB	-3.21	120.86	124.26
25	J	103	BCR	C1-C6-C7	3.21	124.86	115.78
21	1	301	CHL	C3D-C4D-ND	3.21	115.43	110.24
21	Z	305	CHL	C3D-C4D-ND	3.21	115.43	110.24
22	B	807	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
22	K	204	CLA	CAC-C3C-C4C	3.21	128.98	124.81
25	B	839	BCR	C30-C25-C24	3.21	124.86	115.78
25	A	815	BCR	C36-C18-C17	-3.21	118.43	122.92
25	2	312	BCR	C1-C6-C7	3.21	124.86	115.78
22	A	829	CLA	C1-C2-C3	-3.21	121.56	126.75
22	A	841	CLA	CAC-C3C-C4C	3.21	128.97	124.81
22	G	206	CLA	C2D-C1D-ND	3.21	112.47	110.10
21	X	305	CHL	CHB-C1B-NB	-3.21	120.86	124.26
22	O	207	CLA	CMB-C2B-C1B	3.21	130.26	125.37
22	4	318	CLA	CHB-C4A-NA	3.21	128.95	124.51
22	B	829	CLA	C1C-C2C-C3C	-3.21	103.58	106.96
22	Y	311	CLA	C1D-CHD-C4C	-3.21	119.14	126.06
21	Z	301	CHL	C3D-C4D-ND	3.21	115.43	110.24
22	2	322	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
22	1	307	CLA	CHB-C1B-NB	-3.21	120.86	124.26
22	A	852	CLA	CHC-C4B-NB	-3.21	120.86	124.26
22	A	833	CLA	CHC-C1C-C2C	-3.21	117.83	126.73
22	4	312	CLA	C4C-C3C-C2C	-3.21	102.23	106.90
22	A	844	CLA	CMB-C2B-C3B	3.21	134.35	126.59
22	B	825	CLA	CMD-C2D-C3D	-3.20	120.24	127.61
22	F	305	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
22	A	845	CLA	CAA-C2A-C1A	-3.20	101.48	111.97
22	B	830	CLA	CMC-C2C-C3C	3.20	134.81	126.12
24	1	311	XAT	C26-C27-C28	3.20	132.77	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	849	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
22	X	304	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
22	4	313	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
22	Z	307	CLA	CHB-C1B-NB	-3.20	120.87	124.26
22	B	804	CLA	C1D-CHD-C4C	-3.20	119.15	126.06
22	1	308	CLA	CHC-C1C-C2C	-3.20	117.84	126.73
22	A	848	CLA	CAC-C3C-C4C	3.20	128.96	124.81
22	B	810	CLA	CHB-C1B-NB	-3.20	120.87	124.26
22	B	815	CLA	CHC-C1C-C2C	-3.20	117.84	126.73
22	A	803	CLA	CHB-C1B-NB	-3.20	120.87	124.26
22	A	832	CLA	CHB-C1B-NB	-3.20	120.87	124.26
25	A	819	BCR	C19-C18-C17	3.20	123.85	118.94
22	A	833	CLA	CAC-C3C-C4C	3.20	128.96	124.81
22	O	206	CLA	CMD-C2D-C3D	-3.20	120.26	127.61
21	Y	303	CHL	C3D-C4D-ND	3.20	115.41	110.24
22	3	309	CLA	C1D-CHD-C4C	-3.20	119.16	126.06
22	G	205	CLA	C1D-CHD-C4C	-3.20	119.16	126.06
25	B	838	BCR	C34-C9-C10	-3.20	118.44	122.92
22	2	317	CLA	CAC-C3C-C4C	3.20	128.96	124.81
22	B	822	CLA	CHB-C4A-NA	3.19	128.93	124.51
22	1	302	CLA	CHB-C1B-NB	-3.19	120.88	124.26
22	B	821	CLA	C4C-C3C-C2C	-3.19	102.24	106.90
22	3	316	CLA	C1D-CHD-C4C	-3.19	119.17	126.06
22	3	313	CLA	C4C-C3C-C2C	-3.19	102.24	106.90
22	B	831	CLA	CHB-C4A-NA	3.19	128.93	124.51
22	B	852	CLA	C4D-CHA-C1A	-3.19	117.36	121.25
22	B	808	CLA	C3B-C2B-C1B	-3.19	103.31	107.16
21	2	302	CHL	CHB-C1B-NB	-3.19	120.88	124.26
22	L	305	CLA	C2D-C1D-ND	3.19	112.46	110.10
22	3	321	CLA	CHC-C1C-C2C	-3.19	117.87	126.73
25	B	844	BCR	C36-C18-C17	-3.19	118.45	122.92
22	B	809	CLA	C2D-C1D-ND	3.19	112.45	110.10
21	Y	306	CHL	CHB-C1B-NB	-3.19	120.88	124.26
22	B	806	CLA	CHB-C4A-NA	3.19	128.92	124.51
22	3	315	CLA	CAA-C2A-C3A	-3.19	108.66	116.10
22	O	206	CLA	CAC-C3C-C4C	3.19	128.95	124.81
22	2	317	CLA	C1D-CHD-C4C	-3.19	119.18	126.06
22	F	305	CLA	C2D-C1D-ND	3.19	112.45	110.10
25	2	312	BCR	C21-C20-C19	3.19	133.17	123.22
22	X	303	CLA	C3B-C4B-NB	3.19	113.47	110.52
22	L	307	CLA	CHC-C4B-NB	-3.19	120.88	124.26
22	A	849	CLA	CAC-C3C-C4C	3.19	128.95	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	851	CLA	CHB-C4A-NA	3.19	128.92	124.51
21	Y	305	CHL	C3D-C4D-ND	3.19	115.39	110.24
22	Y	302	CLA	C3B-C4B-NB	3.19	113.47	110.52
22	N	202	CLA	CAC-C3C-C4C	3.19	128.94	124.81
22	K	205	CLA	C4D-CHA-C1A	-3.19	117.37	121.25
22	Y	314	CLA	CHB-C1B-NB	-3.19	120.88	124.26
25	J	103	BCR	C36-C18-C17	-3.19	118.46	122.92
22	2	308	CLA	C3B-C4B-NB	3.19	113.47	110.52
22	2	307	CLA	C4A-NA-C1A	3.19	108.14	106.71
22	3	321	CLA	CHC-C4B-NB	-3.18	120.89	124.26
22	4	311	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
22	A	855	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
22	3	315	CLA	CHB-C4A-NA	3.18	128.91	124.51
22	N	202	CLA	C3B-C4B-NB	3.18	113.47	110.52
22	A	836	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
22	B	818	CLA	C3D-C2D-C1D	-3.18	101.49	105.83
22	H	201	CLA	CAC-C3C-C4C	3.18	128.94	124.81
22	4	315	CLA	CHB-C1B-NB	-3.18	120.89	124.26
21	4	307	CHL	C3D-C4D-ND	3.18	115.38	110.24
22	A	826	CLA	CHB-C4A-NA	3.18	128.91	124.51
22	B	808	CLA	CHB-C4A-NA	3.18	128.91	124.51
22	B	817	CLA	CHB-C4A-NA	3.18	128.91	124.51
21	X	309	CHL	C3D-C4D-ND	3.18	115.38	110.24
22	4	312	CLA	CAC-C3C-C4C	3.18	128.94	124.81
22	Y	312	CLA	CMD-C2D-C3D	-3.18	120.30	127.61
22	B	830	CLA	C1-C2-C3	-3.18	120.55	126.04
22	1	318	CLA	CAC-C3C-C4C	3.18	128.93	124.81
22	2	320	CLA	C1-C2-C3	-3.18	121.61	126.75
22	3	319	CLA	C1D-CHD-C4C	-3.18	119.20	126.06
21	4	307	CHL	CHB-C4A-NA	3.18	128.91	124.51
22	4	315	CLA	CHB-C4A-NA	3.18	128.91	124.51
22	1	308	CLA	CHC-C4B-NB	-3.18	120.89	124.26
22	B	805	CLA	CHC-C4B-NB	-3.18	120.89	124.26
22	B	813	CLA	CHD-C1D-ND	-3.18	121.54	124.45
22	A	855	CLA	CHD-C1D-ND	-3.17	121.54	124.45
21	X	308	CHL	CHB-C1B-NB	-3.17	120.90	124.26
22	3	320	CLA	C1D-CHD-C4C	-3.17	119.21	126.06
22	B	830	CLA	CHC-C4B-NB	-3.17	120.90	124.26
25	3	303	BCR	C37-C22-C23	3.17	123.07	118.08
22	A	859	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
25	J	101	BCR	C30-C25-C24	3.17	124.75	115.78
22	A	852	CLA	CHB-C4A-NA	3.17	128.90	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	804	CLA	CHB-C1B-NB	-3.17	120.90	124.26
22	X	312	CLA	C3B-C4B-NB	3.17	113.45	110.52
22	Y	311	CLA	O2A-CGA-CBA	3.17	121.85	111.91
22	O	207	CLA	C2D-C1D-ND	3.17	112.44	110.10
25	B	839	BCR	C34-C9-C8	3.17	123.07	118.08
22	B	818	CLA	C1-O2A-CGA	3.17	124.75	116.44
25	I	101	BCR	C19-C18-C17	3.17	123.80	118.94
21	X	306	CHL	CHB-C4A-NA	3.17	128.89	124.51
22	2	306	CLA	C4D-CHA-C1A	-3.17	117.40	121.25
22	3	315	CLA	C3B-C4B-NB	3.16	113.45	110.52
22	B	828	CLA	CMB-C2B-C1B	3.16	130.19	125.37
22	G	206	CLA	CMB-C2B-C1B	3.16	130.19	125.37
22	X	303	CLA	CMD-C2D-C3D	-3.16	120.33	127.61
22	2	317	CLA	C2D-C1D-ND	3.16	112.44	110.10
22	Z	309	CLA	C1D-CHD-C4C	-3.16	119.23	126.06
22	A	808	CLA	CHB-C1B-NB	-3.16	120.91	124.26
22	3	311	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
22	A	859	CLA	CHB-C4A-NA	3.16	128.89	124.51
22	Y	311	CLA	CHB-C4A-NA	3.16	128.89	124.51
22	B	810	CLA	C3B-C4B-NB	3.16	113.45	110.52
21	2	301	CHL	C3D-C4D-ND	3.16	115.35	110.24
25	B	840	BCR	C21-C20-C19	3.16	133.07	123.22
22	2	318	CLA	C2D-C1D-ND	3.16	112.43	110.10
22	A	812	CLA	CHB-C4A-NA	3.16	128.88	124.51
22	B	804	CLA	CHC-C1C-C2C	-3.16	117.96	126.73
22	O	210	CLA	C3B-C4B-NB	3.16	113.44	110.52
22	A	835	CLA	CAC-C3C-C4C	3.16	128.90	124.81
22	B	822	CLA	CHB-C1B-NB	-3.15	120.92	124.26
21	X	302	CHL	CHB-C1B-NB	-3.15	120.92	124.26
22	Z	313	CLA	C1D-CHD-C4C	-3.15	119.25	126.06
22	X	313	CLA	CAC-C3C-C4C	3.15	128.90	124.81
22	A	804	CLA	C2D-C1D-ND	3.15	112.43	110.10
22	X	313	CLA	C1D-CHD-C4C	-3.15	119.26	126.06
22	B	808	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
22	A	810	CLA	C4-C3-C5	3.15	120.57	115.27
22	B	849	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
22	Z	310	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
22	L	305	CLA	C3B-C4B-NB	3.15	113.44	110.52
22	2	305	CLA	O1D-CGD-CBD	-3.15	118.04	124.48
22	J	102	CLA	CHB-C1B-NB	-3.15	120.92	124.26
22	A	843	CLA	CHB-C4A-NA	3.15	128.87	124.51
22	B	814	CLA	C1D-CHD-C4C	-3.15	119.26	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	317	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
22	N	202	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
22	K	202	CLA	CHB-C1B-NB	-3.15	120.92	124.26
22	A	848	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
25	3	303	BCR	C35-C13-C14	-3.15	118.52	122.92
21	Y	304	CHL	CHB-C1B-NB	-3.15	120.93	124.26
25	G	202	BCR	C1-C6-C5	-3.15	118.18	122.61
21	Z	303	CHL	CHB-C4A-NA	3.15	128.86	124.51
25	L	302	BCR	C19-C18-C17	3.15	123.77	118.94
22	K	205	CLA	CHB-C4A-NA	3.14	128.86	124.51
22	A	829	CLA	CMD-C2D-C3D	-3.14	120.38	127.61
22	4	318	CLA	C1D-CHD-C4C	-3.14	119.28	126.06
22	A	827	CLA	C1-C2-C3	-3.14	120.61	126.04
21	Z	304	CHL	CHB-C1B-NB	-3.14	120.93	124.26
22	B	817	CLA	CHC-C1C-C2C	-3.14	118.00	126.73
22	Y	309	CLA	C3B-C4B-NB	3.14	113.43	110.52
22	B	802	CLA	CMB-C2B-C1B	3.14	130.15	125.37
25	B	837	BCR	C1-C6-C7	3.14	124.67	115.78
25	L	303	BCR	C7-C8-C9	3.14	130.98	126.23
21	X	306	CHL	CHB-C1B-NB	-3.14	120.93	124.26
22	G	206	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
22	A	808	CLA	C3B-C4B-NB	3.14	113.43	110.52
22	X	301	CLA	C3B-C4B-NB	3.14	113.43	110.52
22	B	806	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
21	X	309	CHL	CHB-C1B-NB	-3.14	120.93	124.26
24	2	311	XAT	C19-C9-C10	-3.14	118.53	122.92
22	4	312	CLA	C2D-C1D-ND	3.14	112.42	110.10
22	Y	312	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
25	L	303	BCR	C33-C5-C6	3.14	128.05	124.53
22	A	830	CLA	C2D-C1D-ND	3.14	112.42	110.10
22	X	311	CLA	C4C-C3C-C2C	-3.14	102.33	106.90
22	4	305	CLA	CHC-C1C-C2C	-3.14	118.02	126.73
22	K	203	CLA	CHB-C1B-NB	-3.14	120.94	124.26
22	1	309	CLA	C3B-C4B-NB	3.14	113.42	110.52
22	B	819	CLA	C1D-CHD-C4C	-3.14	119.29	126.06
22	3	313	CLA	CHB-C1B-NB	-3.14	120.94	124.26
22	2	305	CLA	C4C-C3C-C2C	-3.14	102.33	106.90
22	3	317	CLA	CAC-C3C-C4C	3.13	128.88	124.81
22	A	831	CLA	CHD-C1D-ND	-3.13	121.57	124.45
31	G	201	DGD	O1G-C1A-C2A	3.13	121.74	111.91
22	O	206	CLA	C1D-CHD-C4C	-3.13	119.30	126.06
25	L	304	BCR	C36-C18-C17	-3.13	118.53	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Y	307	CHL	C3D-C4D-ND	3.13	115.31	110.24
22	3	321	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
22	B	810	CLA	C1-C2-C3	-3.13	121.68	126.75
22	L	306	CLA	CHC-C1C-C2C	-3.13	118.03	126.73
22	4	305	CLA	CHB-C1B-NB	-3.13	120.94	124.26
21	Y	313	CHL	CHB-C4A-NA	3.13	128.84	124.51
22	N	202	CLA	CHB-C4A-NA	3.13	128.84	124.51
24	1	311	XAT	C24-C23-C22	-3.13	104.73	110.77
22	A	808	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
22	B	818	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
22	1	308	CLA	CHB-C1B-NB	-3.13	120.94	124.26
22	3	318	CLA	CHC-C4B-NB	-3.13	120.94	124.26
22	L	305	CLA	CHB-C4A-NA	3.13	128.84	124.51
22	B	805	CLA	CAC-C3C-C4C	3.13	128.87	124.81
22	2	318	CLA	C4-C3-C5	3.13	120.53	115.27
25	A	814	BCR	C30-C25-C24	3.13	124.63	115.78
22	B	824	CLA	CHB-C1B-NB	-3.13	120.95	124.26
22	2	304	CLA	CMC-C2C-C1C	3.13	129.80	125.04
22	B	821	CLA	CHB-C4A-NA	3.13	128.83	124.51
21	4	309	CHL	CHB-C4A-NA	3.12	128.83	124.51
22	B	820	CLA	C2A-C1A-CHA	-3.12	118.40	123.86
22	A	854	CLA	CHC-C1C-C2C	-3.12	118.05	126.73
22	B	833	CLA	C3B-C4B-NB	3.12	113.41	110.52
22	Z	307	CLA	C2D-C1D-ND	3.12	112.41	110.10
22	A	809	CLA	C4C-C3C-C2C	-3.12	102.34	106.90
22	O	209	CLA	C4C-C3C-C2C	-3.12	102.34	106.90
22	B	812	CLA	CHB-C4A-NA	3.12	128.83	124.51
25	A	816	BCR	C1-C6-C5	-3.12	118.22	122.61
22	Z	313	CLA	C3B-C4B-NB	3.12	113.41	110.52
22	4	316	CLA	CHB-C1B-NB	-3.12	120.95	124.26
22	B	852	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
22	Y	308	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
21	Y	313	CHL	C3D-C4D-ND	3.12	115.28	110.24
22	A	853	CLA	CHC-C1C-C2C	-3.12	118.06	126.73
22	A	828	CLA	CHB-C4A-NA	3.12	128.83	124.51
22	Y	312	CLA	CHB-C4A-NA	3.12	128.83	124.51
22	Y	310	CLA	C3B-C4B-NB	3.12	113.41	110.52
21	4	308	CHL	CHB-C1B-NB	-3.12	120.95	124.26
22	B	849	CLA	CMB-C2B-C1B	3.12	130.12	125.37
22	X	311	CLA	C3B-C4B-NB	3.12	113.41	110.52
21	Z	305	CHL	C1C-C2C-C3C	-3.12	104.64	107.11
22	A	809	CLA	CHB-C1B-NB	-3.12	120.96	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	307	CLA	C1-C2-C3	-3.12	120.65	126.04
22	A	858	CLA	C1C-C2C-C3C	-3.12	103.68	106.96
22	2	303	CLA	CHB-C1B-NB	-3.12	120.96	124.26
22	A	809	CLA	C2D-C1D-ND	3.12	112.40	110.10
22	3	309	CLA	CHC-C1C-C2C	-3.12	118.08	126.73
22	B	846	CLA	C3B-C4B-NB	3.12	113.41	110.52
22	1	305	CLA	C2D-C1D-ND	3.11	112.40	110.10
22	Z	309	CLA	C2D-C1D-ND	3.11	112.40	110.10
22	2	306	CLA	CAC-C3C-C4C	3.11	128.85	124.81
21	X	307	CHL	CHB-C1B-NB	-3.11	120.96	124.26
22	K	203	CLA	C1D-CHD-C4C	-3.11	119.35	126.06
25	A	819	BCR	C12-C13-C14	3.11	123.71	118.94
22	Y	309	CLA	C2D-C1D-ND	3.11	112.39	110.10
22	2	307	CLA	CHC-C4B-NB	-3.11	120.97	124.26
22	A	808	CLA	O2A-CGA-CBA	3.11	121.66	111.91
22	K	204	CLA	C2D-C1D-ND	3.11	112.39	110.10
22	J	102	CLA	CHB-C4A-NA	3.11	128.81	124.51
22	A	844	CLA	C4D-CHA-C1A	-3.11	117.47	121.25
22	B	845	CLA	CAC-C3C-C4C	3.11	128.84	124.81
22	B	823	CLA	C3B-C4B-NB	3.11	113.40	110.52
22	A	835	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
22	Y	309	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
25	B	836	BCR	C1-C6-C5	-3.11	118.24	122.61
22	A	857	CLA	C2D-C1D-ND	3.10	112.39	110.10
22	4	313	CLA	C3B-C4B-NB	3.10	113.39	110.52
22	Z	311	CLA	C2D-C1D-ND	3.10	112.39	110.10
25	A	814	BCR	C1-C6-C5	-3.10	118.24	122.61
25	G	202	BCR	C10-C11-C12	3.10	132.90	123.22
22	4	306	CLA	CAC-C3C-C4C	3.10	128.84	124.81
22	4	313	CLA	CAC-C3C-C4C	3.10	128.84	124.81
22	B	848	CLA	CHB-C1B-NB	-3.10	120.97	124.26
25	3	303	BCR	C1-C6-C7	3.10	124.55	115.78
22	A	808	CLA	CHC-C4B-NB	-3.10	120.97	124.26
22	A	828	CLA	C3D-C2D-C1D	-3.10	101.60	105.83
22	A	827	CLA	CMD-C2D-C1D	3.10	130.18	124.71
22	A	833	CLA	C2D-C1D-ND	3.10	112.39	110.10
22	A	836	CLA	C1D-CHD-C4C	-3.10	119.38	126.06
22	B	828	CLA	C1D-CHD-C4C	-3.10	119.38	126.06
22	G	206	CLA	C4-C3-C5	3.10	120.48	115.27
22	A	827	CLA	CAC-C3C-C4C	3.09	128.82	124.81
22	Y	309	CLA	CAC-C3C-C4C	3.09	128.82	124.81
22	O	209	CLA	CHB-C4A-NA	3.09	128.79	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Z	311	CLA	CHB-C4A-NA	3.09	128.79	124.51
21	4	309	CHL	C3D-C4D-ND	3.09	115.24	110.24
22	4	304	CLA	C1D-CHD-C4C	-3.09	119.38	126.06
22	B	851	CLA	C4A-NA-C1A	3.09	108.10	106.71
22	3	308	CLA	CHB-C4A-NA	3.09	128.79	124.51
22	Z	310	CLA	C3B-C4B-NB	3.09	113.39	110.52
22	Z	314	CLA	CHB-C1B-NB	-3.09	120.98	124.26
22	A	832	CLA	C2D-C1D-ND	3.09	112.38	110.10
22	X	313	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
25	L	301	BCR	C36-C18-C17	-3.09	118.59	122.92
22	X	312	CLA	C2D-C1D-ND	3.09	112.38	110.10
22	Z	308	CLA	C2D-C1D-ND	3.09	112.38	110.10
22	A	803	CLA	CAC-C3C-C4C	3.09	128.82	124.81
22	X	310	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
22	1	303	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
25	B	835	BCR	C20-C21-C22	3.09	131.72	127.31
22	B	828	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
22	A	812	CLA	C2D-C1D-ND	3.09	112.38	110.10
22	Z	307	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
22	L	307	CLA	CMB-C2B-C1B	3.09	130.07	125.37
22	1	305	CLA	CHB-C4A-NA	3.09	128.78	124.51
22	K	204	CLA	C1C-C2C-C3C	-3.09	103.71	106.96
22	Y	312	CLA	C2D-C1D-ND	3.09	112.38	110.10
22	A	803	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
22	Z	310	CLA	C1D-CHD-C4C	-3.09	119.40	126.06
22	1	302	CLA	C3B-C4B-NB	3.09	113.38	110.52
22	3	313	CLA	C3B-C4B-NB	3.09	113.38	110.52
22	Y	314	CLA	C3B-C4B-NB	3.09	113.38	110.52
22	B	833	CLA	CMD-C2D-C3D	-3.08	120.52	127.61
22	A	836	CLA	CAC-C3C-C4C	3.08	128.81	124.81
22	4	311	CLA	CMD-C2D-C3D	-3.08	120.52	127.61
22	O	209	CLA	C3B-C4B-NB	3.08	113.38	110.52
22	X	303	CLA	CHB-C1B-NB	-3.08	120.99	124.26
22	O	210	CLA	C4C-C3C-C2C	-3.08	102.40	106.90
22	2	308	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
22	B	808	CLA	C1D-CHD-C4C	-3.08	119.41	126.06
22	A	853	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
22	A	839	CLA	C1D-CHD-C4C	-3.08	119.41	126.06
22	F	306	CLA	CAC-C3C-C4C	3.08	128.81	124.81
22	Y	310	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
22	B	826	CLA	O2A-CGA-CBA	3.08	121.57	111.91
22	X	312	CLA	C4C-C3C-C2C	-3.08	102.41	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	X	311	CLA	C2D-C1D-ND	3.08	112.37	110.10
22	Z	313	CLA	C2D-C1D-ND	3.08	112.37	110.10
22	A	854	CLA	C1-C2-C3	-3.08	120.72	126.04
22	1	318	CLA	C3B-C4B-NB	3.08	113.37	110.52
23	4	322	LUT	C1-C6-C7	3.08	124.49	115.78
22	B	813	CLA	C4-C3-C5	3.08	120.45	115.27
25	A	818	BCR	C33-C5-C6	3.08	127.98	124.53
22	B	847	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
25	J	101	BCR	C2-C1-C6	3.08	115.22	110.48
22	1	307	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
22	1	307	CLA	CMC-C2C-C1C	3.08	129.72	125.04
30	A	825	CL0	C1-C2-C3	-3.07	120.72	126.04
22	2	319	CLA	CHB-C1B-NB	-3.07	121.00	124.26
22	4	304	CLA	O2A-CGA-CBA	3.07	121.56	111.91
22	1	321	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
25	J	101	BCR	C35-C13-C14	-3.07	118.62	122.92
22	1	305	CLA	CAC-C3C-C4C	3.07	128.80	124.81
22	G	207	CLA	C1D-CHD-C4C	-3.07	119.43	126.06
22	A	849	CLA	O2A-CGA-CBA	3.07	121.55	111.91
25	L	303	BCR	C15-C16-C17	3.07	129.77	123.47
21	Y	304	CHL	CAC-C3C-C4C	3.07	128.80	124.81
22	3	315	CLA	CHB-C1B-NB	-3.07	121.00	124.26
22	B	809	CLA	CHB-C4A-NA	3.07	128.76	124.51
22	A	806	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
22	A	841	CLA	C4D-CHA-C1A	-3.07	117.51	121.25
22	X	301	CLA	CHB-C4A-NA	3.07	128.76	124.51
21	2	321	CHL	C3D-C4D-ND	3.07	115.21	110.24
22	A	855	CLA	C1-C2-C3	-3.07	120.73	126.04
22	A	832	CLA	CAC-C3C-C4C	3.07	128.79	124.81
22	B	814	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
22	A	827	CLA	C4-C3-C5	3.07	120.44	115.27
22	B	815	CLA	C1D-CHD-C4C	-3.07	119.44	126.06
21	Z	312	CHL	CHB-C4A-NA	3.07	128.76	124.51
22	A	812	CLA	C1-C2-C3	-3.07	120.73	126.04
22	4	314	CLA	CAA-C2A-C3A	-3.07	108.94	116.10
24	2	311	XAT	C24-C23-C22	3.07	116.70	110.77
22	Z	314	CLA	CAC-C3C-C4C	3.07	128.79	124.81
25	3	303	BCR	C1-C6-C5	-3.07	118.29	122.61
22	J	102	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
22	X	301	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
22	B	853	CLA	CMD-C2D-C3D	-3.07	120.56	127.61
22	4	314	CLA	C4A-NA-C1A	3.07	108.08	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Y	314	CLA	CHB-C4A-NA	3.07	128.75	124.51
21	1	301	CHL	C2D-C1D-ND	3.07	112.36	110.10
23	4	322	LUT	C1-C6-C5	-3.07	118.29	122.61
22	B	829	CLA	CAA-C2A-C3A	-3.07	104.38	112.78
22	4	304	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
22	2	308	CLA	CHB-C1B-NB	-3.07	121.01	124.26
22	A	843	CLA	CHC-C4B-NB	-3.07	121.01	124.26
22	B	850	CLA	CHB-C1B-NB	-3.07	121.01	124.26
22	B	809	CLA	C4D-CHA-C1A	-3.06	117.52	121.25
21	4	308	CHL	CHC-C4B-NB	-3.06	121.01	124.26
22	Y	308	CLA	CAC-C3C-C4C	3.06	128.78	124.81
22	B	826	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
25	J	101	BCR	C30-C25-C26	-3.06	118.30	122.61
22	H	201	CLA	C1D-CHD-C4C	-3.06	119.45	126.06
25	B	839	BCR	C23-C22-C21	3.06	123.64	118.94
22	A	849	CLA	CHB-C4A-NA	3.06	128.75	124.51
22	B	846	CLA	CHC-C4B-NB	-3.06	121.02	124.26
23	3	301	LUT	C15-C35-C34	3.06	129.75	123.47
24	2	311	XAT	C28-C29-C30	3.06	123.64	118.94
21	4	307	CHL	CAC-C3C-C4C	3.06	128.78	124.81
22	A	843	CLA	C1-C2-C3	-3.06	120.75	126.04
25	1	312	BCR	C2-C1-C6	3.06	115.19	110.48
22	L	305	CLA	C1D-CHD-C4C	-3.06	119.46	126.06
21	X	309	CHL	C1C-C2C-C3C	-3.06	104.69	107.11
22	Y	301	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
22	Z	314	CLA	CMD-C2D-C3D	-3.06	120.58	127.61
22	3	308	CLA	C4A-NA-C1A	3.06	108.08	106.71
22	A	829	CLA	CHC-C1C-C2C	-3.06	118.23	126.73
22	Y	308	CLA	CHB-C4A-NA	3.06	128.74	124.51
22	A	801	CLA	C1D-CHD-C4C	-3.06	119.46	126.06
25	L	301	BCR	C29-C30-C25	3.06	115.19	110.48
22	Z	307	CLA	CHB-C4A-NA	3.06	128.74	124.51
22	1	318	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
22	4	318	CLA	CMD-C2D-C3D	-3.06	120.58	127.61
22	Z	313	CLA	CHB-C1B-NB	-3.06	121.02	124.26
22	B	822	CLA	O2A-CGA-CBA	3.06	121.50	111.91
22	B	852	CLA	C3B-C4B-NB	3.06	113.35	110.52
22	B	806	CLA	C2D-C1D-ND	3.06	112.36	110.10
22	K	205	CLA	C1D-CHD-C4C	-3.06	119.47	126.06
22	1	317	CLA	CMC-C2C-C1C	3.05	129.69	125.04
22	A	832	CLA	CHB-C4A-NA	3.05	128.73	124.51
22	B	824	CLA	C3B-C4B-NB	3.05	113.35	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	318	CLA	C2D-C1D-ND	3.05	112.35	110.10
22	B	845	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
22	1	309	CLA	CHB-C4A-NA	3.05	128.73	124.51
22	2	322	CLA	CHB-C4A-NA	3.05	128.73	124.51
22	1	309	CLA	C1D-CHD-C4C	-3.05	119.48	126.06
22	1	308	CLA	CHB-C4A-NA	3.05	128.73	124.51
22	Z	307	CLA	C3B-C4B-NB	3.05	113.34	110.52
22	O	209	CLA	CHB-C1B-NB	-3.05	121.03	124.26
22	2	305	CLA	CHD-C1D-ND	-3.05	121.65	124.45
22	K	205	CLA	CMB-C2B-C1B	3.05	130.01	125.37
22	B	846	CLA	CHB-C1B-NB	-3.05	121.03	124.26
22	X	303	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
31	J	104	DGD	O1G-C1A-C2A	3.05	121.47	111.91
22	B	828	CLA	C4A-NA-C1A	3.05	108.08	106.71
22	X	311	CLA	CHB-C4A-NA	3.04	128.72	124.51
22	B	802	CLA	CAC-C3C-C4C	3.04	128.76	124.81
22	B	845	CLA	C4-C3-C5	3.04	120.39	115.27
22	B	827	CLA	C1D-CHD-C4C	-3.04	119.49	126.06
25	L	303	BCR	C30-C25-C26	-3.04	118.33	122.61
22	B	818	CLA	CHB-C4A-NA	3.04	128.72	124.51
22	X	312	CLA	CHB-C4A-NA	3.04	128.72	124.51
21	4	308	CHL	CMD-C2D-C3D	-3.04	120.61	127.61
22	A	834	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
22	A	806	CLA	C1D-CHD-C4C	-3.04	119.50	126.06
22	A	851	CLA	CMB-C2B-C1B	3.04	130.00	125.37
22	A	841	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
22	A	839	CLA	C4D-CHA-C1A	-3.04	117.55	121.25
25	J	101	BCR	C1-C6-C5	-3.04	118.33	122.61
22	H	201	CLA	CHB-C4A-NA	3.04	128.71	124.51
22	A	839	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
22	B	818	CLA	CAA-CBA-CGA	-3.04	104.38	113.25
30	A	825	CL0	CAC-C3C-C4C	3.04	128.75	124.81
25	B	844	BCR	C34-C9-C8	3.04	122.86	118.08
22	B	849	CLA	C6-C5-C3	-3.04	109.66	114.62
25	A	814	BCR	C36-C18-C17	-3.04	118.67	122.92
22	A	828	CLA	C4C-C3C-C2C	-3.03	102.47	106.90
22	A	827	CLA	CHC-C1C-C2C	-3.03	118.30	126.73
22	4	306	CLA	C4C-C3C-C2C	-3.03	102.47	106.90
22	2	304	CLA	CHC-C1C-C2C	-3.03	118.30	126.73
21	3	314	CHL	C3D-C4D-ND	3.03	115.14	110.24
22	Y	309	CLA	CHB-C4A-NA	3.03	128.71	124.51
22	1	317	CLA	C2A-C1A-CHA	-3.03	118.56	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	321	CLA	CHB-C4A-NA	3.03	128.70	124.51
22	B	847	CLA	O2A-CGA-CBA	3.03	121.42	111.91
25	4	321	BCR	C33-C5-C6	3.03	127.93	124.53
22	X	310	CLA	CAC-C3C-C4C	3.03	128.74	124.81
22	A	831	CLA	CHB-C4A-NA	3.03	128.70	124.51
22	A	839	CLA	CAC-C3C-C4C	3.03	128.74	124.81
25	L	304	BCR	C16-C15-C14	3.03	129.68	123.47
22	B	821	CLA	C3B-C4B-NB	3.03	113.32	110.52
22	B	819	CLA	C3D-C2D-C1D	-3.03	101.70	105.83
22	A	827	CLA	C1D-CHD-C4C	-3.03	119.53	126.06
22	O	208	CLA	C1-C2-C3	-3.03	120.81	126.04
22	A	842	CLA	C3B-C4B-NB	3.03	113.32	110.52
22	3	316	CLA	C4C-C3C-C2C	-3.03	102.49	106.90
22	L	305	CLA	C4C-C3C-C2C	-3.03	102.49	106.90
22	Z	308	CLA	C4C-C3C-C2C	-3.03	102.49	106.90
22	Z	308	CLA	CAC-C3C-C4C	3.03	128.74	124.81
22	A	857	CLA	CMC-C2C-C1C	3.03	129.65	125.04
22	O	208	CLA	C4-C3-C5	3.03	120.36	115.27
22	A	826	CLA	CHB-C1B-C2B	-3.03	118.69	127.24
22	G	205	CLA	CMB-C2B-C1B	3.03	129.98	125.37
22	A	833	CLA	CMC-C2C-C1C	3.03	129.65	125.04
22	Y	310	CLA	CHB-C4A-NA	3.02	128.69	124.51
21	1	316	CHL	C3D-C4D-ND	3.02	115.13	110.24
22	3	310	CLA	CAC-C3C-C4C	3.02	128.73	124.81
22	4	306	CLA	CHC-C1C-C2C	-3.02	118.33	126.73
22	A	857	CLA	CHB-C4A-NA	3.02	128.69	124.51
22	J	102	CLA	CAC-C3C-C4C	3.02	128.73	124.81
22	1	304	CLA	C4-C3-C5	3.02	120.35	115.27
22	F	305	CLA	CHB-C4A-NA	3.02	128.69	124.51
22	A	857	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
25	I	101	BCR	C35-C13-C14	-3.02	118.69	122.92
21	2	302	CHL	C1D-ND-C4D	-3.02	104.19	106.33
22	B	813	CLA	CHC-C4B-NB	-3.02	121.06	124.26
27	3	304	MGE	C1D-O6D-C5D	3.02	119.62	113.69
22	B	823	CLA	C1-C2-C3	-3.02	120.82	126.04
22	Z	306	CLA	CMD-C2D-C3D	-3.02	120.67	127.61
22	B	848	CLA	CMC-C2C-C1C	3.02	129.64	125.04
22	B	833	CLA	CHB-C4A-NA	3.02	128.69	124.51
22	A	856	CLA	CMB-C2B-C1B	3.02	129.97	125.37
22	A	836	CLA	C2A-C1A-CHA	-3.02	118.58	123.86
22	B	801	CLA	C1-C2-C3	-3.02	120.82	126.04
22	2	317	CLA	C4C-C3C-C2C	-3.02	102.50	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	840	CLA	C3B-C4B-NB	3.02	113.31	110.52
22	X	310	CLA	C2D-C1D-ND	3.02	112.33	110.10
22	B	802	CLA	CMC-C2C-C1C	3.02	129.63	125.04
22	A	801	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
22	B	819	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
22	A	810	CLA	CHB-C4A-NA	3.02	128.68	124.51
22	B	820	CLA	C1D-CHD-C4C	-3.02	119.55	126.06
21	X	308	CHL	CMD-C2D-C3D	-3.02	120.68	127.61
22	Z	306	CLA	C4C-C3C-C2C	-3.01	102.50	106.90
22	Z	309	CLA	C4C-C3C-C2C	-3.01	102.50	106.90
22	Y	301	CLA	CHB-C1B-NB	-3.01	121.07	124.26
22	3	320	CLA	C4C-C3C-C2C	-3.01	102.50	106.90
22	Y	301	CLA	C1D-CHD-C4C	-3.01	119.56	126.06
22	G	207	CLA	CHB-C4A-NA	3.01	128.68	124.51
22	K	202	CLA	CHB-C4A-NA	3.01	128.68	124.51
22	B	852	CLA	C1-C2-C3	-3.01	120.83	126.04
22	B	806	CLA	C1D-CHD-C4C	-3.01	119.56	126.06
22	A	806	CLA	CHB-C4A-NA	3.01	128.68	124.51
22	Y	302	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
22	B	822	CLA	C4D-CHA-C1A	-3.01	117.58	121.25
22	K	205	CLA	CMD-C2D-C3D	-3.01	120.69	127.61
22	Z	313	CLA	CMD-C2D-C3D	-3.01	120.69	127.61
22	3	319	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
22	A	844	CLA	C1D-CHD-C4C	-3.01	119.56	126.06
22	A	836	CLA	CMD-C2D-C3D	-3.01	120.69	127.61
22	J	102	CLA	C2D-C1D-ND	3.01	112.32	110.10
25	J	101	BCR	C36-C18-C17	-3.01	118.71	122.92
22	K	202	CLA	CHC-C4B-NB	-3.01	121.07	124.26
22	Y	311	CLA	C2D-C1D-ND	3.01	112.32	110.10
22	1	318	CLA	CHB-C4A-NA	3.01	128.67	124.51
22	3	313	CLA	CHB-C4A-NA	3.01	128.67	124.51
22	B	805	CLA	CHB-C4A-NA	3.01	128.67	124.51
22	3	311	CLA	CHC-C4B-NB	-3.01	121.08	124.26
22	K	202	CLA	C2D-C1D-ND	3.01	112.32	110.10
22	B	831	CLA	CHD-C1D-ND	-3.01	121.69	124.45
22	L	307	CLA	CHB-C4A-NA	3.01	128.67	124.51
22	4	316	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
22	K	202	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
22	Z	310	CLA	CHB-C4A-NA	3.00	128.67	124.51
22	A	855	CLA	CAA-C2A-C3A	-3.00	104.55	112.78
22	1	309	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
22	1	319	CLA	C4C-C3C-C2C	-3.00	102.52	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	837	CLA	C2D-C1D-ND	3.00	112.32	110.10
30	A	825	CL0	O2D-CGD-O1D	-3.00	117.97	123.84
22	A	836	CLA	C3B-C4B-NB	3.00	113.30	110.52
22	B	833	CLA	C1-C2-C3	-3.00	120.85	126.04
22	2	305	CLA	CHB-C4A-NA	3.00	128.66	124.51
22	3	315	CLA	CAC-C3C-C4C	3.00	128.70	124.81
22	2	304	CLA	CHC-C4B-NB	-3.00	121.08	124.26
22	2	319	CLA	CMD-C2D-C3D	-3.00	120.71	127.61
22	K	202	CLA	CMB-C2B-C1B	3.00	129.94	125.37
22	B	813	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
25	4	321	BCR	C12-C13-C14	3.00	123.54	118.94
22	Z	306	CLA	CMB-C2B-C1B	3.00	129.94	125.37
22	A	858	CLA	O2A-CGA-CBA	3.00	121.32	111.91
24	4	320	XAT	C35-C15-C14	-3.00	117.33	123.47
22	B	819	CLA	O2A-CGA-CBA	3.00	121.32	111.91
22	A	850	CLA	CHB-C4A-NA	3.00	128.66	124.51
22	A	832	CLA	CAA-C2A-C3A	-3.00	104.57	112.78
23	3	301	LUT	C39-C29-C28	3.00	122.80	118.08
21	1	301	CHL	CHB-C4A-NA	3.00	128.66	124.51
25	4	321	BCR	C30-C25-C24	3.00	124.26	115.78
22	3	320	CLA	CMD-C2D-C3D	-3.00	120.72	127.61
22	1	307	CLA	CHB-C4A-NA	3.00	128.66	124.51
22	A	856	CLA	C4-C3-C5	3.00	119.41	115.98
22	Z	306	CLA	C1D-CHD-C4C	-3.00	119.59	126.06
22	B	825	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
22	A	827	CLA	C4D-CHA-C1A	-2.99	117.61	121.25
25	G	202	BCR	C1-C6-C7	2.99	124.25	115.78
22	X	313	CLA	CMD-C2D-C3D	-2.99	120.73	127.61
22	A	857	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
22	A	850	CLA	CMC-C2C-C1C	2.99	129.60	125.04
21	Y	306	CHL	C1C-C2C-C3C	-2.99	104.74	107.11
22	Z	314	CLA	C1D-CHD-C4C	-2.99	119.60	126.06
22	B	820	CLA	CHB-C1B-NB	-2.99	121.09	124.26
22	2	317	CLA	C3B-C4B-NB	2.99	113.29	110.52
22	3	308	CLA	CMB-C2B-C1B	2.99	129.93	125.37
22	A	859	CLA	CMD-C2D-C3D	-2.99	120.73	127.61
22	B	845	CLA	C1-C2-C3	-2.99	120.87	126.04
24	4	320	XAT	C4-C3-C2	-2.99	105.00	110.77
21	X	306	CHL	C1C-C2C-C3C	-2.99	104.74	107.11
22	Y	310	CLA	CMD-C2D-C3D	-2.99	120.74	127.61
22	3	317	CLA	C4D-CHA-C1A	-2.99	117.61	121.25
22	4	318	CLA	C4C-C3C-C2C	-2.99	102.54	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	304	CLA	CHC-C1C-C2C	-2.99	118.43	126.73
25	A	818	BCR	C34-C9-C8	2.99	122.79	118.08
22	B	848	CLA	CAC-C3C-C4C	2.99	128.69	124.81
22	2	319	CLA	CHB-C4A-NA	2.99	128.64	124.51
25	B	835	BCR	C24-C25-C26	2.99	128.70	121.46
22	A	806	CLA	CHC-C4B-NB	-2.99	121.09	124.26
22	A	854	CLA	C3D-C2D-C1D	-2.99	101.75	105.83
21	Y	305	CHL	C1C-C2C-C3C	-2.99	104.74	107.11
22	B	853	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
22	K	203	CLA	CMB-C2B-C1B	2.99	129.92	125.37
22	B	847	CLA	C1D-CHD-C4C	-2.99	119.62	126.06
22	Y	311	CLA	CMD-C2D-C3D	-2.99	120.75	127.61
22	Z	314	CLA	C4C-C3C-C2C	-2.99	102.55	106.90
22	4	318	CLA	CAC-C3C-C4C	2.98	128.68	124.81
22	1	317	CLA	O2A-CGA-CBA	2.98	121.28	111.91
22	Z	313	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
22	X	311	CLA	CAC-C3C-C4C	2.98	128.68	124.81
22	B	849	CLA	C3B-C4B-NB	2.98	113.28	110.52
22	B	808	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
22	Z	311	CLA	CMD-C2D-C3D	-2.98	120.76	127.61
22	2	318	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
25	O	202	BCR	C29-C30-C25	2.98	115.07	110.48
25	B	836	BCR	C12-C13-C14	2.98	123.51	118.94
22	A	828	CLA	CMB-C2B-C1B	2.98	129.91	125.37
31	B	841	DGD	O1G-C1A-C2A	2.98	121.26	111.91
22	A	834	CLA	C3B-C4B-NB	2.98	113.28	110.52
25	A	814	BCR	C34-C9-C8	2.98	122.77	118.08
22	B	811	CLA	CMB-C2B-C1B	2.98	129.91	125.37
22	A	804	CLA	C3B-C4B-NB	2.98	113.28	110.52
22	O	208	CLA	C3B-C4B-NB	2.98	113.28	110.52
22	Z	308	CLA	CMD-C2D-C3D	-2.98	120.76	127.61
22	Y	302	CLA	CMD-C2D-C3D	-2.98	120.77	127.61
25	A	818	BCR	C35-C13-C14	-2.98	118.75	122.92
22	2	317	CLA	CMD-C2D-C3D	-2.98	120.77	127.61
22	B	846	CLA	CMD-C2D-C3D	-2.98	120.77	127.61
25	1	312	BCR	C38-C26-C25	2.98	127.87	124.53
22	3	320	CLA	C2D-C1D-ND	2.98	112.30	110.10
22	3	316	CLA	CAC-C3C-C4C	2.98	128.67	124.81
22	Z	307	CLA	CAC-C3C-C4C	2.98	128.67	124.81
22	2	322	CLA	CHB-C1B-NB	-2.97	121.11	124.26
22	Z	311	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
22	2	304	CLA	CHB-C4A-NA	2.97	128.62	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Z	311	CLA	CAC-C3C-C4C	2.97	128.67	124.81
22	B	821	CLA	C1D-CHD-C4C	-2.97	119.64	126.06
22	2	304	CLA	C3B-C4B-NB	2.97	113.27	110.52
22	1	303	CLA	C4A-NA-C1A	2.97	108.04	106.71
22	X	304	CLA	OBD-CAD-C3D	2.97	135.67	128.52
22	A	846	CLA	CHB-C4A-NA	2.97	128.62	124.51
25	A	814	BCR	C7-C8-C9	2.97	130.72	126.23
22	1	302	CLA	CHB-C4A-NA	2.97	128.62	124.51
22	3	309	CLA	CHB-C4A-NA	2.97	128.62	124.51
22	K	202	CLA	CMD-C2D-C3D	-2.97	120.78	127.61
22	X	312	CLA	CMD-C2D-C3D	-2.97	120.78	127.61
22	B	852	CLA	O2A-CGA-CBA	2.97	121.22	111.91
22	B	820	CLA	C4D-CHA-C1A	-2.97	117.64	121.25
22	4	305	CLA	CMD-C2D-C3D	-2.97	120.78	127.61
22	4	306	CLA	CHC-C4B-NB	-2.97	121.11	124.26
21	X	307	CHL	CMB-C2B-C1B	2.97	129.89	125.37
22	4	310	CLA	CAC-C3C-C4C	2.97	128.66	124.81
21	2	302	CHL	CBB-CAB-C3B	-2.97	112.86	127.62
25	4	321	BCR	C15-C16-C17	2.97	129.55	123.47
22	G	207	CLA	CAC-C3C-C4C	2.97	128.66	124.81
22	4	312	CLA	CHB-C4A-NA	2.97	128.61	124.51
22	A	846	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
22	A	833	CLA	C1D-CHD-C4C	-2.97	119.66	126.06
22	3	319	CLA	CMB-C2B-C1B	2.97	129.89	125.37
22	1	321	CLA	CHB-C1B-NB	-2.97	121.12	124.26
22	2	304	CLA	C2D-C1D-ND	2.96	112.29	110.10
25	2	312	BCR	C24-C23-C22	-2.96	121.76	126.23
25	K	201	BCR	C12-C13-C14	2.96	123.49	118.94
22	A	841	CLA	CMD-C2D-C3D	-2.96	120.80	127.61
22	A	851	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
22	O	206	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
22	B	811	CLA	O1D-CGD-CBD	-2.96	118.42	124.48
22	Y	302	CLA	C2D-C1D-ND	2.96	112.29	110.10
22	K	204	CLA	CMB-C2B-C1B	2.96	129.88	125.37
22	Y	302	CLA	CAC-C3C-C4C	2.96	128.65	124.81
22	A	807	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	B	809	CLA	CAC-C3C-C4C	2.96	128.65	124.81
22	A	856	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
22	B	818	CLA	CMD-C2D-C3D	-2.96	120.81	127.61
22	Y	314	CLA	CMD-C2D-C3D	-2.96	120.81	127.61
22	X	303	CLA	C2D-C1D-ND	2.96	112.28	110.10
22	2	320	CLA	O2A-CGA-CBA	2.96	121.19	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	302	CHL	CMD-C2D-C3D	-2.96	120.81	127.61
22	4	304	CLA	CHB-C4A-NA	2.96	128.60	124.51
25	B	834	BCR	C36-C18-C17	-2.96	118.78	122.92
22	B	817	CLA	CAC-C3C-C4C	2.96	128.65	124.81
22	A	831	CLA	CMB-C2B-C1B	2.96	129.87	125.37
22	B	808	CLA	CMD-C2D-C3D	-2.96	120.81	127.61
22	O	209	CLA	CMD-C2D-C3D	-2.96	120.81	127.61
22	A	804	CLA	CMD-C2D-C3D	-2.96	120.81	127.61
22	1	308	CLA	CMA-C3A-C2A	-2.96	109.20	116.10
22	2	322	CLA	CAC-C3C-C4C	2.96	128.65	124.81
21	Z	302	CHL	CHB-C1B-NB	-2.96	121.13	124.26
22	B	801	CLA	O2A-CGA-CBA	2.96	121.18	111.91
22	Y	309	CLA	CMD-C2D-C3D	-2.96	120.82	127.61
22	A	850	CLA	CHB-C1B-NB	-2.95	121.13	124.26
22	L	307	CLA	C3B-C4B-NB	2.95	113.26	110.52
25	L	301	BCR	C1-C6-C7	2.95	124.14	115.78
22	K	202	CLA	CAC-C3C-C4C	2.95	128.64	124.81
22	3	321	CLA	CHB-C1B-NB	-2.95	121.13	124.26
22	A	851	CLA	CHC-C4B-NB	-2.95	121.13	124.26
22	H	201	CLA	CMB-C2B-C1B	2.95	129.86	125.37
22	A	807	CLA	C3B-C4B-NB	2.95	113.25	110.52
22	A	835	CLA	CMD-C2D-C3D	-2.95	120.83	127.61
22	B	852	CLA	CHB-C4A-NA	2.95	128.59	124.51
22	A	850	CLA	C3B-C4B-NB	2.95	113.25	110.52
22	H	201	CLA	CMD-C2D-C3D	-2.95	120.83	127.61
22	X	303	CLA	CHB-C4A-NA	2.95	128.59	124.51
22	K	205	CLA	C3B-C4B-NB	2.95	113.25	110.52
22	A	832	CLA	CMB-C2B-C1B	2.95	129.86	125.37
22	3	319	CLA	C2D-C1D-ND	2.95	112.28	110.10
25	K	201	BCR	C19-C18-C17	2.95	123.46	118.94
22	A	828	CLA	C2D-C1D-ND	2.95	112.28	110.10
22	B	830	CLA	C1D-CHD-C4C	-2.95	119.70	126.06
22	A	804	CLA	CHB-C4A-NA	2.95	128.59	124.51
22	K	203	CLA	CHB-C4A-NA	2.95	128.59	124.51
22	B	804	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
22	Z	313	CLA	CHB-C4A-NA	2.95	128.59	124.51
25	B	834	BCR	C37-C22-C23	2.94	122.72	118.08
22	A	807	CLA	O2A-CGA-CBA	2.94	121.15	111.91
22	F	305	CLA	C3B-C4B-NB	2.94	113.25	110.52
22	J	102	CLA	C3B-C4B-NB	2.94	113.25	110.52
22	3	310	CLA	CHB-C4A-NA	2.94	128.58	124.51
22	X	310	CLA	CMD-C2D-C3D	-2.94	120.84	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	820	CLA	CHC-C1C-C2C	-2.94	118.56	126.73
21	X	302	CHL	C1C-C2C-C3C	-2.94	104.78	107.11
22	Y	314	CLA	CAC-C3C-C4C	2.94	128.63	124.81
21	4	308	CHL	CMB-C2B-C1B	2.94	129.85	125.37
22	B	822	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
22	A	853	CLA	C1-C2-C3	-2.94	120.96	126.04
22	B	831	CLA	CAC-C3C-C4C	2.94	128.63	124.81
25	L	304	BCR	C12-C13-C14	2.94	123.45	118.94
22	2	320	CLA	CAC-C3C-C4C	2.94	128.62	124.81
22	A	830	CLA	CMD-C2D-C3D	-2.94	120.85	127.61
22	A	851	CLA	CHB-C1B-NB	-2.94	121.14	124.26
21	2	309	CHL	CMB-C2B-C1B	2.94	129.85	125.37
21	Z	303	CHL	CMB-C2B-C1B	2.94	129.85	125.37
22	3	309	CLA	CHC-C4B-NB	-2.94	121.15	124.26
21	1	301	CHL	CHB-C1B-NB	-2.94	121.15	124.26
22	4	318	CLA	C2D-C1D-ND	2.94	112.27	110.10
22	Z	307	CLA	CMD-C2D-C3D	-2.94	120.86	127.61
22	4	311	CLA	C3B-C4B-NB	2.94	113.24	110.52
22	B	812	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
22	F	306	CLA	CMC-C2C-C1C	2.93	129.51	125.04
21	Z	303	CHL	CHB-C1B-NB	-2.93	121.15	124.26
22	3	319	CLA	CMD-C2D-C3D	-2.93	120.86	127.61
22	A	849	CLA	C1D-CHD-C4C	-2.93	119.73	126.06
22	3	320	CLA	CAC-C3C-C4C	2.93	128.62	124.81
22	B	812	CLA	CMD-C2D-C3D	-2.93	120.87	127.61
22	4	311	CLA	C1D-CHD-C4C	-2.93	119.74	126.06
22	3	318	CLA	C2D-C1D-ND	2.93	112.26	110.10
22	B	827	CLA	CMD-C2D-C3D	-2.93	120.88	127.61
22	Z	308	CLA	CHB-C4A-NA	2.93	128.56	124.51
22	A	808	CLA	CMC-C2C-C1C	2.93	129.50	125.04
22	B	805	CLA	CMB-C2B-C1B	2.93	129.83	125.37
22	B	853	CLA	C3B-C4B-NB	2.93	113.23	110.52
25	B	844	BCR	C19-C18-C17	2.93	123.43	118.94
22	Y	308	CLA	CMD-C2D-C3D	-2.93	120.88	127.61
23	1	310	LUT	C39-C29-C28	2.93	122.69	118.08
22	B	810	CLA	C4A-NA-C1A	2.92	108.02	106.71
22	3	311	CLA	CHC-C1C-C2C	-2.92	118.61	126.73
22	A	833	CLA	CMD-C2D-C3D	-2.92	120.89	127.61
22	B	806	CLA	C3B-C4B-NB	2.92	113.23	110.52
22	2	318	CLA	CHB-C4A-NA	2.92	128.56	124.51
22	Z	313	CLA	CAC-C3C-C4C	2.92	128.60	124.81
22	B	813	CLA	CHC-C1C-C2C	-2.92	118.61	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	858	CLA	C1D-CHD-C4C	-2.92	119.75	126.06
22	B	802	CLA	C1D-CHD-C4C	-2.92	119.75	126.06
22	B	822	CLA	CMD-C2D-C3D	-2.92	120.89	127.61
22	Z	309	CLA	CMD-C2D-C3D	-2.92	120.89	127.61
22	4	314	CLA	CHB-C4A-NA	2.92	128.55	124.51
22	Z	310	CLA	CMB-C2B-C1B	2.92	129.82	125.37
22	A	808	CLA	CAC-C3C-C4C	2.92	128.60	124.81
22	X	312	CLA	CAC-C3C-C4C	2.92	128.60	124.81
25	A	815	BCR	C33-C5-C6	2.92	127.81	124.53
22	B	824	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
22	B	846	CLA	C1D-CHD-C4C	-2.92	119.76	126.06
22	A	855	CLA	O2A-CGA-CBA	2.92	121.07	111.91
22	B	816	CLA	C4D-C3D-CAD	2.92	111.54	108.10
22	A	836	CLA	C1-C2-C3	-2.92	121.00	126.04
22	G	207	CLA	CMD-C2D-C3D	-2.92	120.90	127.61
22	A	832	CLA	CMD-C2D-C3D	-2.92	120.90	127.61
22	B	813	CLA	CHB-C4A-NA	2.92	128.55	124.51
22	4	305	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
22	A	843	CLA	CHC-C1C-C2C	-2.92	118.63	126.73
22	B	819	CLA	CMB-C2B-C1B	2.92	129.81	125.37
22	O	207	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
22	B	828	CLA	CMD-C2D-C3D	-2.91	120.91	127.61
22	B	830	CLA	CHB-C4A-NA	2.91	128.54	124.51
21	3	314	CHL	CHB-C1B-NB	-2.91	121.17	124.26
22	1	317	CLA	CHC-C4B-NB	-2.91	121.17	124.26
25	O	202	BCR	C2-C1-C6	2.91	114.97	110.48
21	2	301	CHL	CMB-C2B-C1B	2.91	129.81	125.37
22	G	207	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
22	A	805	CLA	C1-C2-C3	-2.91	122.04	126.75
22	A	849	CLA	CHC-C4B-NB	-2.91	121.18	124.26
22	K	204	CLA	C3B-C4B-NB	2.91	113.21	110.52
22	2	320	CLA	C1D-CHD-C4C	-2.91	119.78	126.06
22	A	832	CLA	O2A-CGA-CBA	2.91	121.03	111.91
22	B	806	CLA	CMB-C2B-C1B	2.91	129.80	125.37
22	3	312	CLA	O2A-CGA-CBA	2.91	121.03	111.91
25	J	103	BCR	C1-C6-C5	-2.91	118.52	122.61
22	B	831	CLA	CMB-C2B-C1B	2.91	129.79	125.37
22	O	210	CLA	CAA-C2A-C3A	-2.91	109.32	116.10
21	Z	302	CHL	CMD-C2D-C3D	-2.91	120.93	127.61
22	1	319	CLA	CHB-C1B-NB	-2.91	121.18	124.26
21	2	302	CHL	C3D-C4D-ND	2.91	114.94	110.24
25	B	836	BCR	C19-C18-C17	2.90	123.40	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	X	305	CHL	CMB-C2B-C1B	2.90	129.79	125.37
22	A	834	CLA	CHC-C4B-NB	-2.90	121.18	124.26
25	B	838	BCR	C30-C25-C26	-2.90	118.53	122.61
22	A	844	CLA	CAC-C3C-C4C	2.90	128.58	124.81
22	B	833	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
22	A	846	CLA	C1D-CHD-C4C	-2.90	119.80	126.06
22	A	834	CLA	CHB-C4A-NA	2.90	128.53	124.51
22	B	811	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
22	B	806	CLA	CHC-C4B-NB	-2.90	121.19	124.26
22	1	304	CLA	CMC-C2C-C1C	2.90	129.46	125.04
22	3	312	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
22	K	203	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
22	B	852	CLA	CMB-C2B-C1B	2.90	129.78	125.37
22	3	318	CLA	CHB-C4A-NA	2.90	128.52	124.51
21	4	317	CHL	CMB-C2B-C1B	2.90	129.78	125.37
25	L	303	BCR	C37-C22-C23	2.90	122.64	118.08
22	B	821	CLA	CHB-C1B-NB	-2.90	121.19	124.26
22	4	316	CLA	CHB-C4A-NA	2.90	128.52	124.51
22	2	320	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
22	B	815	CLA	C4D-CHA-C1A	-2.90	117.72	121.25
22	O	210	CLA	CAC-C3C-C4C	2.90	128.57	124.81
22	1	304	CLA	O2A-CGA-O1A	-2.90	116.28	123.59
22	B	847	CLA	CHB-C1B-NB	-2.90	121.19	124.26
22	B	801	CLA	CAC-C3C-C2C	2.89	132.48	127.53
22	3	312	CLA	CMB-C2B-C1B	2.89	129.78	125.37
22	A	830	CLA	C3B-C4B-NB	2.89	113.20	110.52
22	Y	314	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
22	A	839	CLA	CMD-C2D-C3D	-2.89	120.96	127.61
22	4	306	CLA	CMD-C2D-C3D	-2.89	120.96	127.61
21	Y	303	CHL	CMB-C2B-C1B	2.89	129.77	125.37
21	Z	301	CHL	CMB-C2B-C1B	2.89	129.77	125.37
22	3	309	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
21	Z	304	CHL	CMD-C2D-C3D	-2.89	120.96	127.61
22	A	812	CLA	CMD-C2D-C3D	-2.89	120.96	127.61
22	L	307	CLA	CAA-CBA-CGA	-2.89	104.83	112.51
22	2	306	CLA	CHD-C1D-ND	-2.89	121.80	124.45
22	3	313	CLA	CMD-C2D-C3D	-2.89	120.97	127.61
22	F	306	CLA	CMB-C2B-C1B	2.89	129.77	125.37
22	B	848	CLA	CHB-C4A-NA	2.89	128.51	124.51
22	B	830	CLA	CHB-C1B-NB	-2.89	121.20	124.26
22	4	313	CLA	CMD-C2D-C3D	-2.89	120.97	127.61
21	Y	303	CHL	C1C-C2C-C3C	-2.89	104.82	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	810	CLA	C3B-C4B-NB	2.89	113.19	110.52
22	1	308	CLA	CMD-C2D-C3D	-2.89	120.97	127.61
22	3	308	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
22	B	825	CLA	C3B-C4B-NB	2.89	113.19	110.52
22	B	811	CLA	CAC-C3C-C4C	2.89	128.55	124.81
25	L	301	BCR	C34-C9-C8	2.89	122.62	118.08
22	4	316	CLA	CHC-C4B-NB	-2.88	121.20	124.26
22	Y	310	CLA	CAA-C2A-C3A	-2.88	104.88	112.78
22	1	306	CLA	C3B-C4B-NB	2.88	113.19	110.52
22	1	319	CLA	C1D-CHD-C4C	-2.88	119.84	126.06
22	Y	311	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
21	1	316	CHL	C1C-C2C-C3C	-2.88	104.83	107.11
22	B	810	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
22	B	804	CLA	C2D-C1D-ND	2.88	112.23	110.10
22	A	845	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	B	828	CLA	CAC-C3C-C4C	2.88	128.55	124.81
22	1	302	CLA	CMD-C2D-C3D	-2.88	120.99	127.61
22	B	829	CLA	CHB-C4A-NA	2.88	128.49	124.51
22	B	827	CLA	C4-C3-C5	2.88	120.11	115.27
25	B	839	BCR	C29-C30-C25	2.88	114.91	110.48
22	O	208	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
22	O	208	CLA	C4A-NA-C1A	2.88	108.00	106.71
21	2	321	CHL	CMD-C2D-C3D	-2.88	121.00	127.61
22	4	314	CLA	CHC-C4B-NB	-2.87	121.21	124.26
22	1	321	CLA	CMD-C2D-C3D	-2.87	121.00	127.61
22	Z	309	CLA	CMB-C2B-C1B	2.87	129.75	125.37
22	2	317	CLA	CHB-C4A-NA	2.87	128.49	124.51
22	B	811	CLA	CMD-C2D-C3D	-2.87	121.01	127.61
21	3	307	CHL	CHB-C1B-NB	-2.87	121.22	124.26
22	B	827	CLA	CHB-C4A-NA	2.87	128.48	124.51
21	Y	307	CHL	CMB-C2B-C1B	2.87	129.74	125.37
22	4	316	CLA	CMB-C2B-C1B	2.87	129.74	125.37
22	1	304	CLA	C1-C2-C3	-2.87	121.08	126.04
22	A	842	CLA	C4A-NA-C1A	2.87	108.00	106.71
25	A	814	BCR	C1-C6-C7	2.87	123.89	115.78
22	A	810	CLA	CAA-C2A-C3A	-2.87	104.92	112.78
21	X	308	CHL	CMB-C2B-C1B	2.87	129.74	125.37
22	4	305	CLA	CHB-C4A-NA	2.87	128.48	124.51
22	A	802	CLA	O2A-CGA-CBA	2.87	120.91	111.91
22	A	804	CLA	CAC-C3C-C4C	2.87	128.53	124.81
22	B	825	CLA	C1D-CHD-C4C	-2.87	119.87	126.06
22	3	308	CLA	O2A-CGA-CBA	2.87	120.91	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	317	CLA	CMD-C2D-C3D	-2.87	121.02	127.61
22	B	811	CLA	CHB-C4A-NA	2.87	128.48	124.51
22	1	306	CLA	CMD-C2D-C3D	-2.87	121.02	127.61
22	B	853	CLA	C1D-CHD-C4C	-2.87	119.88	126.06
22	L	307	CLA	C1D-CHD-C4C	-2.87	119.88	126.06
22	A	853	CLA	C1D-CHD-C4C	-2.86	119.88	126.06
21	Y	307	CHL	C1C-C2C-C3C	-2.86	104.84	107.11
22	B	801	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
25	L	303	BCR	C35-C13-C14	-2.86	118.91	122.92
22	A	809	CLA	CAA-C2A-C3A	-2.86	104.94	112.78
22	X	303	CLA	CAC-C3C-C4C	2.86	128.52	124.81
25	O	202	BCR	C11-C10-C9	-2.86	123.23	127.31
22	2	303	CLA	CAC-C3C-C4C	2.86	128.52	124.81
22	1	319	CLA	CMD-C2D-C3D	-2.86	121.04	127.61
22	Y	308	CLA	CMB-C2B-C1B	2.86	129.72	125.37
21	2	309	CHL	CMD-C2D-C3D	-2.86	121.04	127.61
22	3	309	CLA	CMD-C2D-C3D	-2.86	121.04	127.61
22	O	209	CLA	O2A-CGA-CBA	2.86	120.87	111.91
22	1	317	CLA	CMD-C2D-C3D	-2.86	121.05	127.61
22	A	838	CLA	CMB-C2B-C1B	2.86	129.72	125.37
22	1	317	CLA	CHB-C1B-NB	-2.86	121.23	124.26
22	G	205	CLA	CMD-C2D-C3D	-2.86	121.05	127.61
22	L	307	CLA	CMD-C2D-C3D	-2.86	121.05	127.61
22	A	841	CLA	CHB-C4A-NA	2.85	128.46	124.51
21	Y	304	CHL	CMB-C2B-C1B	2.85	129.72	125.37
22	B	847	CLA	CMB-C2B-C1B	2.85	129.72	125.37
22	A	831	CLA	C3B-C4B-NB	2.85	113.16	110.52
22	A	807	CLA	CAC-C3C-C4C	2.85	128.51	124.81
22	1	318	CLA	CMD-C2D-C3D	-2.85	121.06	127.61
22	4	312	CLA	C3B-C4B-NB	2.85	113.16	110.52
22	1	309	CLA	CMD-C2D-C3D	-2.85	121.06	127.61
22	4	316	CLA	CMD-C2D-C3D	-2.85	121.06	127.61
25	F	302	BCR	C36-C18-C17	-2.85	118.93	122.92
22	K	205	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
22	B	827	CLA	CBC-CAC-C3C	-2.85	104.58	112.43
22	1	306	CLA	CAC-C3C-C4C	2.85	128.50	124.81
25	A	818	BCR	C37-C22-C23	2.85	122.56	118.08
25	4	321	BCR	C19-C18-C17	2.85	123.31	118.94
21	X	302	CHL	CMB-C2B-C1B	2.85	129.70	125.37
25	B	838	BCR	C35-C13-C14	-2.85	118.94	122.92
25	B	834	BCR	C10-C11-C12	2.85	132.10	123.22
22	Y	312	CLA	CAC-C3C-C4C	2.85	128.50	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	318	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
22	B	814	CLA	C1-C2-C3	-2.84	121.12	126.04
22	L	305	CLA	CMD-C2D-C3D	-2.84	121.07	127.61
25	B	835	BCR	C12-C13-C14	2.84	123.30	118.94
22	O	208	CLA	CMC-C2C-C1C	2.84	129.37	125.04
22	O	207	CLA	C1-C2-C3	-2.84	121.13	126.04
22	A	806	CLA	CMD-C2D-C3D	-2.84	121.08	127.61
22	B	824	CLA	C2D-C1D-ND	2.84	112.20	110.10
21	X	306	CHL	CMB-C2B-C1B	2.84	129.69	125.37
22	4	312	CLA	CHC-C1C-C2C	-2.84	118.84	126.73
22	A	843	CLA	CHB-C1B-NB	-2.84	121.25	124.26
22	1	321	CLA	CMB-C2B-C1B	2.84	129.69	125.37
25	J	101	BCR	C34-C9-C8	2.84	122.55	118.08
22	A	807	CLA	CMC-C2C-C1C	2.84	129.36	125.04
22	B	808	CLA	O2A-C1-C2	2.84	116.09	108.64
22	2	320	CLA	CHB-C1B-NB	-2.84	121.25	124.26
22	1	321	CLA	C2D-C1D-ND	2.84	112.19	110.10
22	A	845	CLA	CHB-C4A-NA	2.84	128.43	124.51
22	B	809	CLA	C3B-C4B-NB	2.84	113.15	110.52
22	B	829	CLA	CHC-C1C-C2C	-2.84	118.85	126.73
22	A	857	CLA	CAC-C3C-C4C	2.84	128.49	124.81
22	B	823	CLA	CMB-C2B-C1B	2.84	129.69	125.37
23	2	310	LUT	C28-C29-C30	2.83	123.29	118.94
22	B	850	CLA	C2A-C3A-C4A	-2.83	97.29	101.87
22	A	810	CLA	CMB-C2B-C1B	2.83	129.69	125.37
22	1	306	CLA	C4A-NA-C1A	2.83	107.98	106.71
24	2	311	XAT	C35-C34-C33	2.83	131.35	127.31
24	3	302	XAT	O24-C25-C38	2.83	118.45	115.06
22	X	313	CLA	CMB-C2B-C1B	2.83	129.68	125.37
22	A	857	CLA	CMD-C2D-C3D	-2.83	121.10	127.61
22	B	852	CLA	CMD-C2D-C3D	-2.83	121.10	127.61
22	B	852	CLA	CHB-C1B-NB	-2.83	121.26	124.26
22	Y	302	CLA	CMB-C2B-C1B	2.83	129.68	125.37
22	B	821	CLA	CMD-C2D-C3D	-2.83	121.10	127.61
22	B	806	CLA	CMD-C2D-C3D	-2.83	121.10	127.61
22	B	815	CLA	CHB-C4A-NA	2.83	128.43	124.51
22	A	852	CLA	C3B-C4B-NB	2.83	113.14	110.52
22	B	813	CLA	CMD-C2D-C3D	-2.83	121.11	127.61
22	1	302	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
22	4	315	CLA	C2A-C1A-CHA	-2.83	118.91	123.86
22	3	310	CLA	C3B-C4B-NB	2.83	113.14	110.52
22	A	846	CLA	C3B-C4B-NB	2.83	113.14	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	846	CLA	CHC-C1C-C2C	-2.83	118.87	126.73
22	1	303	CLA	CHB-C1B-NB	-2.83	121.26	124.26
22	2	318	CLA	CHB-C1B-NB	-2.83	121.26	124.26
22	B	827	CLA	C2A-C1A-CHA	-2.83	118.91	123.86
22	X	310	CLA	CMB-C2B-C1B	2.83	129.68	125.37
22	A	845	CLA	C2D-C1D-ND	2.83	112.19	110.10
22	2	322	CLA	CMB-C2B-C1B	2.83	129.67	125.37
22	B	822	CLA	C2D-C1D-ND	2.83	112.19	110.10
22	3	318	CLA	CMB-C2B-C1B	2.83	129.67	125.37
21	Y	305	CHL	CMB-C2B-C1B	2.83	129.67	125.37
22	A	851	CLA	C1D-CHD-C4C	-2.82	119.96	126.06
22	Y	309	CLA	CMB-C2B-C1B	2.82	129.67	125.37
22	4	315	CLA	CMB-C2B-C1B	2.82	129.67	125.37
22	B	833	CLA	O2A-CGA-CBA	2.82	120.77	111.91
22	B	814	CLA	O2A-CGA-CBA	2.82	120.77	111.91
22	4	316	CLA	C2D-C1D-ND	2.82	112.18	110.10
22	3	316	CLA	CHB-C1B-NB	-2.82	121.27	124.26
25	B	837	BCR	C36-C18-C17	-2.82	118.98	122.92
22	K	203	CLA	C4-C3-C5	2.82	120.01	115.27
22	B	849	CLA	CAC-C3C-C4C	2.82	128.47	124.81
22	B	815	CLA	CHB-C1B-NB	-2.82	121.28	124.26
22	A	829	CLA	C3B-C4B-NB	2.82	113.13	110.52
21	4	307	CHL	CMD-C2D-C3D	-2.82	121.14	127.61
22	3	308	CLA	CMD-C2D-C3D	-2.82	121.14	127.61
22	A	854	CLA	CAA-CBA-CGA	-2.82	105.02	113.25
22	A	802	CLA	CMB-C2B-C1B	2.82	129.66	125.37
22	B	818	CLA	C3B-C4B-NB	2.82	113.13	110.52
22	1	303	CLA	CMB-C2B-C1B	2.82	129.66	125.37
24	4	320	XAT	C10-C11-C12	-2.81	114.43	123.22
21	Y	306	CHL	CMD-C2D-C3D	-2.81	121.14	127.61
22	A	803	CLA	C1-C2-C3	-2.81	121.18	126.04
22	A	859	CLA	CAC-C3C-C4C	2.81	128.46	124.81
22	A	805	CLA	CMB-C2B-C1B	2.81	129.65	125.37
22	4	316	CLA	CAA-C2A-C3A	-2.81	109.53	116.10
22	K	203	CLA	C1-C2-C3	-2.81	121.18	126.04
22	Z	310	CLA	CMD-C2D-C3D	-2.81	121.14	127.61
25	L	303	BCR	C36-C18-C17	-2.81	118.98	122.92
22	A	858	CLA	C4-C3-C5	2.81	120.00	115.27
22	B	806	CLA	O2A-CGA-CBA	2.81	120.73	111.91
25	L	301	BCR	C1-C6-C5	-2.81	118.65	122.61
22	A	845	CLA	C2A-C1A-CHA	-2.81	118.94	123.86
22	A	856	CLA	CAC-C3C-C4C	2.81	128.46	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	822	CLA	C1-C2-C3	-2.81	121.18	126.04
23	3	301	LUT	C40-C33-C34	-2.81	118.99	122.92
22	A	853	CLA	CMD-C2D-C3D	-2.81	121.15	127.61
22	A	856	CLA	CMD-C2D-C3D	-2.81	121.15	127.61
22	B	820	CLA	C3D-C2D-C1D	-2.81	102.00	105.83
22	1	309	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
22	B	812	CLA	C4-C3-C5	2.81	120.00	115.27
22	F	306	CLA	O2A-CGA-CBA	2.81	123.33	112.23
22	K	205	CLA	CBB-CAB-C3B	-2.81	113.65	127.62
22	3	319	CLA	CAC-C3C-C4C	2.81	128.45	124.81
22	3	309	CLA	CMC-C2C-C1C	2.81	129.32	125.04
22	A	843	CLA	CMC-C2C-C1C	2.81	129.32	125.04
25	A	819	BCR	C24-C25-C26	2.81	128.26	121.46
22	1	317	CLA	C1D-CHD-C4C	-2.81	120.00	126.06
22	B	810	CLA	CMD-C2D-C3D	-2.81	121.16	127.61
22	B	825	CLA	CHB-C4A-NA	2.81	128.39	124.51
22	X	311	CLA	CMD-C2D-C3D	-2.81	121.16	127.61
22	4	306	CLA	C1D-CHD-C4C	-2.81	120.00	126.06
21	Z	304	CHL	CMB-C2B-C1B	2.81	129.64	125.37
21	Z	312	CHL	CMD-C2D-C3D	-2.80	121.16	127.61
22	B	825	CLA	CAC-C3C-C4C	2.80	128.45	124.81
21	X	306	CHL	CMD-C2D-C3D	-2.80	121.16	127.61
22	A	833	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
22	A	846	CLA	CMD-C2D-C3D	-2.80	121.17	127.61
22	X	313	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
22	B	833	CLA	CMB-C2B-C1B	2.80	129.64	125.37
22	Z	311	CLA	CMB-C2B-C1B	2.80	129.64	125.37
22	3	318	CLA	CMD-C2D-C3D	-2.80	121.17	127.61
22	A	851	CLA	CHB-C4A-NA	2.80	128.38	124.51
24	1	311	XAT	C40-C33-C34	-2.80	119.00	122.92
22	O	207	CLA	O2A-CGA-CBA	2.80	120.70	111.91
22	A	846	CLA	C2A-C1A-CHA	-2.80	118.96	123.86
21	2	321	CHL	C1C-C2C-C3C	-2.80	104.89	107.11
22	B	830	CLA	CMD-C2D-C3D	-2.80	121.18	127.61
25	F	302	BCR	C33-C5-C6	2.80	127.67	124.53
22	Z	314	CLA	CHC-C4B-NB	-2.80	121.30	124.26
21	4	309	CHL	CMD-C2D-C3D	-2.80	121.18	127.61
22	A	854	CLA	CHB-C4A-NA	2.80	128.38	124.51
25	B	837	BCR	C38-C26-C25	2.79	127.67	124.53
22	A	851	CLA	CHC-C1C-C2C	-2.79	118.97	126.73
22	2	303	CLA	CMB-C2B-C1B	2.79	129.62	125.37
22	O	206	CLA	CHB-C4A-NA	2.79	128.37	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	X	309	CHL	CMD-C2D-C3D	-2.79	121.19	127.61
21	Z	305	CHL	CMD-C2D-C3D	-2.79	121.19	127.61
24	3	302	XAT	C4-C3-C2	-2.79	105.38	110.77
22	B	826	CLA	CHD-C1D-ND	-2.79	121.89	124.45
21	3	307	CHL	CMB-C2B-C1B	2.79	129.62	125.37
22	1	305	CLA	CMB-C2B-C1B	2.79	129.62	125.37
22	X	312	CLA	CMB-C2B-C1B	2.79	129.62	125.37
22	X	304	CLA	CHC-C1C-C2C	-2.79	118.98	126.73
22	O	208	CLA	CMD-C2D-C3D	-2.79	121.19	127.61
22	K	203	CLA	C3B-C4B-NB	2.79	113.10	110.52
22	B	813	CLA	CMB-C2B-C1B	2.79	129.62	125.37
22	O	208	CLA	CHB-C4A-NA	2.79	128.37	124.51
25	A	817	BCR	C30-C25-C26	-2.79	118.69	122.61
22	B	815	CLA	CMB-C2B-C1B	2.79	129.62	125.37
22	A	842	CLA	CAC-C3C-C4C	2.79	128.43	124.81
22	A	846	CLA	CAC-C3C-C4C	2.79	128.43	124.81
22	A	847	CLA	CMD-C2D-C3D	-2.79	121.21	127.61
22	A	856	CLA	C3B-C4B-NB	2.79	113.10	110.52
22	1	309	CLA	CMB-C2B-C1B	2.78	129.61	125.37
22	2	308	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
22	B	815	CLA	O2A-CGA-CBA	2.78	120.64	111.91
22	B	816	CLA	O2A-CGA-CBA	2.78	120.64	111.91
22	A	809	CLA	CMD-C2D-C3D	-2.78	121.21	127.61
22	A	809	CLA	C4A-NA-C1A	2.78	107.96	106.71
22	G	205	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
22	1	305	CLA	C3B-C4B-NB	2.78	113.09	110.52
22	A	842	CLA	CHC-C4B-NB	-2.78	121.31	124.26
25	L	304	BCR	C8-C9-C10	2.78	123.21	118.94
22	A	806	CLA	C1-C2-C3	-2.78	121.23	126.04
25	O	203	BCR	C36-C18-C17	-2.78	119.03	122.92
21	Z	303	CHL	CMD-C2D-C3D	-2.78	121.22	127.61
22	A	839	CLA	C2D-C1D-ND	2.78	112.15	110.10
22	2	318	CLA	CMD-C2D-C3D	-2.78	121.22	127.61
22	K	203	CLA	CMD-C2D-C3D	-2.78	121.23	127.61
22	4	310	CLA	CMC-C2C-C1C	2.78	129.27	125.04
22	A	828	CLA	CMD-C2D-C3D	-2.78	121.23	127.61
22	1	317	CLA	CHC-C1C-C2C	-2.77	119.02	126.73
24	3	302	XAT	C19-C9-C8	2.77	122.45	118.08
22	K	204	CLA	CMD-C2D-C3D	-2.77	121.23	127.61
22	B	814	CLA	CHB-C1B-NB	-2.77	121.32	124.26
22	Z	306	CLA	O1D-CGD-CBD	-2.77	118.81	124.48
22	3	312	CLA	C2D-C1D-ND	2.77	112.15	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2	310	LUT	C20-C13-C14	-2.77	119.04	122.92
22	2	322	CLA	CMD-C2D-C3D	-2.77	121.24	127.61
27	F	303	MGE	O6D-C1D-O3G	2.77	116.54	109.97
25	L	302	BCR	C1-C6-C5	-2.77	118.71	122.61
22	B	852	CLA	CHC-C4B-NB	-2.77	121.32	124.26
22	B	804	CLA	CMB-C2B-C1B	2.77	129.59	125.37
22	A	834	CLA	CMD-C2D-C3D	-2.77	121.24	127.61
30	A	825	CL0	CGD-CBD-CAD	2.77	119.70	110.73
22	1	319	CLA	O2A-CGA-CBA	2.77	120.60	111.91
21	Z	312	CHL	CHB-C1B-NB	-2.77	121.33	124.26
22	4	304	CLA	C4-C3-C5	2.77	119.93	115.27
21	X	305	CHL	CMD-C2D-C3D	-2.77	121.25	127.61
22	4	310	CLA	CHC-C4B-NB	-2.77	121.33	124.26
22	A	804	CLA	CMC-C2C-C1C	2.77	129.25	125.04
22	A	833	CLA	CMB-C2B-C1B	2.77	129.58	125.37
25	A	815	BCR	C1-C6-C5	-2.77	118.72	122.61
22	A	854	CLA	C4-C3-C5	2.77	119.92	115.27
21	4	308	CHL	C1C-C2C-C3C	-2.77	104.92	107.11
22	B	811	CLA	C1-C2-C3	-2.76	121.26	126.04
22	A	832	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
24	2	311	XAT	C36-C21-C26	2.76	117.51	110.05
22	2	305	CLA	CHB-C1B-NB	-2.76	121.33	124.26
21	Y	305	CHL	CMD-C2D-C3D	-2.76	121.26	127.61
22	A	802	CLA	C1D-CHD-C4C	-2.76	120.10	126.06
22	B	814	CLA	C4-C3-C5	2.76	119.92	115.27
22	4	306	CLA	CMB-C2B-C1B	2.76	129.58	125.37
22	2	307	CLA	CMD-C2D-C3D	-2.76	121.26	127.61
22	1	307	CLA	CMB-C2B-C1B	2.76	129.58	125.37
22	L	306	CLA	C3B-C4B-NB	2.76	113.08	110.52
22	X	304	CLA	CMB-C2B-C1B	2.76	129.57	125.37
22	A	805	CLA	CAC-C3C-C4C	2.76	128.39	124.81
22	3	309	CLA	CMB-C2B-C1B	2.76	129.57	125.37
22	A	846	CLA	C1-C2-C3	-2.76	121.27	126.04
22	A	859	CLA	C3B-C4B-NB	2.76	113.08	110.52
22	4	306	CLA	CHB-C1B-NB	-2.76	121.34	124.26
22	3	316	CLA	CHC-C1C-C2C	-2.76	119.07	126.73
22	B	811	CLA	CMC-C2C-C1C	2.76	129.24	125.04
22	B	821	CLA	CMB-C2B-C1B	2.76	129.57	125.37
22	X	301	CLA	CMB-C2B-C1B	2.76	129.57	125.37
22	3	320	CLA	CHB-C4A-NA	2.76	128.32	124.51
22	A	856	CLA	CMC-C2C-C1C	2.76	129.24	125.04
22	B	847	CLA	C4-C3-C5	2.76	119.91	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Y	311	CLA	CMB-C2B-C1B	2.76	129.57	125.37
21	2	309	CHL	CHB-C1B-NB	-2.76	121.34	124.26
22	A	854	CLA	O2A-CGA-CBA	2.75	120.55	111.91
22	2	304	CLA	C1-C2-C3	-2.75	121.28	126.04
31	O	201	DGD	O6E-C1E-C2E	2.75	116.18	110.35
25	O	203	BCR	C16-C17-C18	2.75	131.24	127.31
22	2	303	CLA	C3B-C4B-NB	2.75	113.07	110.52
22	B	824	CLA	CAA-CBA-CGA	-2.75	105.21	113.25
22	B	814	CLA	CMB-C2B-C1B	2.75	129.56	125.37
21	X	307	CHL	CMD-C2D-C3D	-2.75	121.28	127.61
22	A	858	CLA	CMB-C2B-C1B	2.75	129.56	125.37
22	3	313	CLA	CAC-C3C-C4C	2.75	128.38	124.81
22	B	824	CLA	CAC-C3C-C4C	2.75	128.38	124.81
22	A	812	CLA	O2A-CGA-CBA	2.75	120.54	111.91
22	1	308	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
22	K	204	CLA	CHB-C4A-NA	2.75	128.31	124.51
24	2	311	XAT	C27-C28-C29	2.75	129.80	125.53
22	B	831	CLA	O2A-CGA-CBA	2.75	120.53	111.91
21	Y	306	CHL	CMB-C2B-C1B	2.75	129.56	125.37
22	1	305	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
22	B	853	CLA	CHB-C4A-NA	2.75	128.31	124.51
22	A	805	CLA	CMD-C2D-C3D	-2.75	121.29	127.61
25	A	817	BCR	C35-C13-C14	-2.75	119.07	122.92
22	1	308	CLA	CMC-C2C-C1C	2.75	129.22	125.04
22	K	203	CLA	O2A-CGA-CBA	2.75	120.53	111.91
22	A	843	CLA	CMD-C2D-C3D	-2.75	121.30	127.61
22	1	317	CLA	C3B-C4B-NB	2.75	113.06	110.52
22	X	301	CLA	CMD-C2D-C3D	-2.75	121.30	127.61
22	3	313	CLA	CMB-C2B-C1B	2.74	129.55	125.37
22	A	812	CLA	CHB-C1B-NB	-2.74	121.35	124.26
22	O	210	CLA	CMB-C2B-C1B	2.74	129.54	125.37
22	2	317	CLA	CAA-C2A-C3A	-2.74	109.70	116.10
22	2	318	CLA	CMC-C2C-C1C	2.74	129.21	125.04
22	A	827	CLA	C3D-C2D-C1D	-2.74	102.09	105.83
22	2	320	CLA	CHB-C4A-NA	2.74	128.30	124.51
22	X	301	CLA	CAC-C3C-C4C	2.74	128.37	124.81
31	O	201	DGD	O1G-C1A-C2A	2.74	120.51	111.91
22	A	830	CLA	CHD-C1D-ND	-2.74	121.94	124.45
22	1	303	CLA	O1D-CGD-CBD	-2.74	118.88	124.48
22	A	801	CLA	O2A-CGA-CBA	2.74	120.50	111.91
22	A	837	CLA	CMB-C2B-C1B	2.74	129.54	125.37
22	L	306	CLA	O1D-CGD-CBD	-2.74	118.88	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	K	203	CLA	CHC-C4B-NB	-2.74	121.36	124.26
22	O	207	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
22	B	850	CLA	C1-C2-C3	-2.74	121.31	126.04
25	B	838	BCR	C33-C5-C6	2.74	127.60	124.53
22	B	808	CLA	C2D-C1D-ND	2.74	112.12	110.10
22	F	305	CLA	CMD-C2D-C3D	-2.74	121.32	127.61
25	J	103	BCR	C8-C9-C10	2.73	123.14	118.94
22	B	851	CLA	CHC-C4B-NB	-2.73	121.36	124.26
22	B	805	CLA	CMD-C2D-C3D	-2.73	121.33	127.61
22	1	308	CLA	CMB-C2B-C1B	2.73	129.53	125.37
22	B	824	CLA	CMB-C2B-C1B	2.73	129.53	125.37
22	A	829	CLA	CHC-C4B-NB	-2.73	121.37	124.26
22	B	827	CLA	CHB-C1B-NB	-2.73	121.37	124.26
22	1	308	CLA	C1D-CHD-C4C	-2.73	120.17	126.06
22	B	812	CLA	O2A-CGA-CBA	2.73	120.47	111.91
22	O	208	CLA	CAC-C3C-C4C	2.73	128.35	124.81
22	B	848	CLA	C1-C2-C3	-2.73	121.33	126.04
22	B	823	CLA	CAC-C3C-C4C	2.73	128.35	124.81
22	A	849	CLA	C2D-C1D-ND	2.73	112.11	110.10
22	B	828	CLA	O2A-CGA-CBA	2.73	120.47	111.91
22	1	317	CLA	CHB-C4A-NA	2.73	128.28	124.51
22	B	826	CLA	CMB-C2B-C1B	2.73	129.52	125.37
22	2	303	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
22	1	308	CLA	CBC-CAC-C3C	-2.73	104.92	112.43
22	1	317	CLA	C4-C3-C5	2.72	119.86	115.27
22	B	813	CLA	C1-C2-C3	-2.72	121.33	126.04
22	1	318	CLA	CHB-C1B-NB	-2.72	121.37	124.26
22	B	804	CLA	O2A-CGA-CBA	2.72	120.45	111.91
22	A	831	CLA	CMD-C2D-C3D	-2.72	121.35	127.61
22	A	806	CLA	C4-C3-C5	2.72	119.85	115.27
21	X	305	CHL	O2A-CGA-CBA	2.72	120.45	111.91
25	A	815	BCR	C19-C18-C17	2.72	123.12	118.94
21	3	314	CHL	CMB-C2B-C1B	2.72	129.51	125.37
22	N	202	CLA	CMB-C2B-C1B	2.72	129.51	125.37
21	Y	303	CHL	CMD-C2D-C3D	-2.72	121.36	127.61
22	Y	311	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
22	B	803	CLA	CMD-C2D-C3D	-2.72	121.36	127.61
22	O	206	CLA	CHB-C1B-NB	-2.72	121.38	124.26
22	B	802	CLA	CHB-C4A-NA	2.72	128.27	124.51
22	1	303	CLA	CMD-C2D-C3D	-2.72	121.36	127.61
22	3	308	CLA	C3B-C4B-NB	2.72	113.04	110.52
21	Y	304	CHL	CMD-C2D-C3D	-2.72	121.36	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	802	CLA	CHC-C1C-C2C	-2.72	119.18	126.73
22	A	829	CLA	C1D-CHD-C4C	-2.72	120.20	126.06
22	A	833	CLA	O2A-CGA-CBA	2.72	120.43	111.91
22	Y	311	CLA	C1-C2-C3	-2.72	121.34	126.04
22	Y	314	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
22	A	810	CLA	CHB-C1B-NB	-2.71	121.38	124.26
22	4	315	CLA	C1D-CHD-C4C	-2.71	120.20	126.06
21	Y	307	CHL	CMD-C2D-C3D	-2.71	121.37	127.61
21	Z	301	CHL	CMD-C2D-C3D	-2.71	121.37	127.61
22	A	810	CLA	CHD-C1D-ND	-2.71	121.96	124.45
25	2	312	BCR	C30-C25-C26	-2.71	118.79	122.61
21	X	305	CHL	C1C-C2C-C3C	-2.71	104.96	107.11
25	B	844	BCR	C35-C13-C14	-2.71	119.12	122.92
22	B	852	CLA	C2D-C1D-ND	2.71	112.10	110.10
22	G	205	CLA	C3B-C4B-NB	2.71	113.03	110.52
22	A	852	CLA	CHD-C1D-ND	-2.71	121.97	124.45
22	A	807	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
22	A	803	CLA	C3B-C4B-NB	2.71	113.03	110.52
22	B	845	CLA	CHB-C4A-NA	2.71	128.25	124.51
22	Z	314	CLA	CMB-C2B-C1B	2.70	129.49	125.37
22	Y	312	CLA	CMB-C2B-C1B	2.70	129.49	125.37
22	1	317	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
21	4	317	CHL	CMD-C2D-C3D	-2.70	121.40	127.61
22	L	305	CLA	CHC-C4B-NB	-2.70	121.40	124.26
22	A	809	CLA	CMB-C2B-C1B	2.70	129.48	125.37
22	Z	307	CLA	CMB-C2B-C1B	2.70	129.48	125.37
22	A	807	CLA	C1-C2-C3	-2.70	121.37	126.04
25	B	834	BCR	C15-C16-C17	2.70	129.00	123.47
22	A	827	CLA	CMC-C2C-C1C	2.70	129.15	125.04
22	A	829	CLA	CHB-C1B-NB	-2.70	121.40	124.26
22	A	801	CLA	CMD-C2D-C3D	-2.70	121.41	127.61
22	B	823	CLA	C4-C3-C5	2.70	119.81	115.27
23	1	310	LUT	C40-C33-C34	-2.70	119.14	122.92
25	O	203	BCR	C11-C10-C9	2.70	131.16	127.31
21	2	302	CHL	CAC-C3C-C4C	2.70	128.31	124.81
22	B	817	CLA	CHB-C1B-NB	-2.70	121.40	124.26
21	1	301	CHL	C1C-C2C-C3C	-2.70	104.97	107.11
22	1	306	CLA	CMB-C2B-C1B	2.70	129.47	125.37
22	3	309	CLA	C3B-C4B-NB	2.70	113.02	110.52
22	Y	301	CLA	CHB-C4A-NA	2.69	128.24	124.51
22	B	803	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
22	B	851	CLA	O2A-CGA-CBA	2.69	120.36	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	302	CLA	CMB-C2B-C1B	2.69	129.47	125.37
21	Z	312	CHL	C1C-C2C-C3C	-2.69	104.98	107.11
22	A	806	CLA	C2A-C1A-CHA	-2.69	119.15	123.86
22	A	803	CLA	CMC-C2C-C1C	2.69	129.14	125.04
22	A	807	CLA	CMD-C2D-C3D	-2.69	121.42	127.61
22	O	208	CLA	CMB-C2B-C1B	2.69	129.47	125.37
22	B	812	CLA	C1D-CHD-C4C	-2.69	120.25	126.06
22	L	305	CLA	CMB-C2B-C1B	2.69	129.47	125.37
22	B	851	CLA	C1-C2-C3	-2.69	121.39	126.04
25	F	302	BCR	C1-C6-C5	-2.69	118.83	122.61
22	1	309	CLA	CAC-C3C-C4C	2.69	128.30	124.81
22	3	309	CLA	C2A-C1A-CHA	-2.69	119.16	123.86
22	B	846	CLA	CMB-C2B-C1B	2.69	129.46	125.37
22	2	319	CLA	CHD-C1D-ND	-2.69	121.98	124.45
22	B	853	CLA	C2D-C1D-ND	2.69	112.08	110.10
22	1	318	CLA	C4-C3-C5	2.68	119.79	115.27
22	A	834	CLA	CAC-C3C-C4C	2.68	128.29	124.81
31	O	201	DGD	O6D-C5D-C6D	2.68	112.08	106.67
21	X	307	CHL	C1C-C2C-C3C	-2.68	104.98	107.11
21	Z	303	CHL	C1C-C2C-C3C	-2.68	104.98	107.11
25	L	301	BCR	C12-C13-C14	2.68	123.06	118.94
22	A	801	CLA	CMB-C2B-C1B	2.68	129.45	125.37
22	A	856	CLA	C1-C2-C3	-2.68	121.41	126.04
22	3	318	CLA	C4A-NA-C1A	2.68	107.91	106.71
25	B	837	BCR	C15-C16-C17	2.68	128.96	123.47
25	L	301	BCR	C15-C16-C17	2.68	128.96	123.47
22	A	803	CLA	O2A-CGA-CBA	2.68	120.32	111.91
24	2	311	XAT	C17-C1-C16	-2.68	103.42	107.37
22	A	851	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
22	3	321	CLA	CAC-C3C-C4C	2.68	128.29	124.81
22	A	840	CLA	CMD-C2D-C3D	-2.68	121.45	127.61
22	B	845	CLA	O2A-CGA-CBA	2.68	120.31	111.91
22	A	835	CLA	CHB-C4A-NA	2.68	128.22	124.51
22	B	847	CLA	CMC-C2C-C1C	2.68	129.12	125.04
22	B	850	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
25	A	816	BCR	C16-C17-C18	2.68	131.13	127.31
22	4	315	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
22	3	316	CLA	C3B-C4B-NB	2.68	113.00	110.52
22	A	806	CLA	C3B-C4B-NB	2.68	113.00	110.52
21	3	307	CHL	O2A-CGA-CBA	2.68	120.31	111.91
25	A	816	BCR	C23-C22-C21	2.68	123.05	118.94
21	Z	312	CHL	CMB-C2B-C1B	2.68	129.45	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	X	311	CLA	CMB-C2B-C1B	2.68	129.45	125.37
21	3	307	CHL	CMD-C2D-C3D	-2.68	121.46	127.61
22	B	827	CLA	C1-C2-C3	-2.68	121.41	126.04
25	B	834	BCR	C24-C25-C26	2.68	127.94	121.46
23	2	310	LUT	C39-C29-C30	-2.67	119.18	122.92
22	A	805	CLA	O2A-CGA-CBA	2.67	120.30	111.91
22	B	813	CLA	C2D-C1D-ND	2.67	112.07	110.10
22	A	802	CLA	CMD-C2D-C3D	-2.67	121.47	127.61
21	2	301	CHL	O2A-CGA-CBA	2.67	120.29	111.91
22	A	809	CLA	CMC-C2C-C1C	2.67	129.11	125.04
22	2	308	CLA	C2A-C1A-CHA	-2.67	119.19	123.86
22	A	829	CLA	C4C-C3C-C2C	-2.67	103.00	106.90
22	A	847	CLA	C4C-C3C-C2C	-2.67	103.00	106.90
22	A	856	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
22	B	804	CLA	CMD-C2D-C3D	-2.67	121.47	127.61
22	1	319	CLA	C2D-C1D-ND	2.67	112.07	110.10
21	Z	302	CHL	CMB-C2B-C1B	2.67	129.43	125.37
22	B	817	CLA	C4-C3-C5	2.67	119.76	115.27
22	3	310	CLA	CMC-C2C-C1C	2.67	129.10	125.04
22	A	838	CLA	CMD-C2D-C3D	-2.67	121.48	127.61
22	A	857	CLA	CHB-C1B-NB	-2.67	121.43	124.26
22	1	305	CLA	CMC-C2C-C1C	2.67	129.10	125.04
22	A	830	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
22	X	304	CLA	C3B-C4B-NB	2.67	112.99	110.52
22	B	827	CLA	CMC-C2C-C1C	2.67	129.10	125.04
22	A	829	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
22	1	304	CLA	CBA-CAA-C2A	2.67	121.73	113.86
22	3	310	CLA	CMD-C2D-C3D	-2.67	121.48	127.61
22	Y	310	CLA	CMB-C2B-C1B	2.67	129.43	125.37
23	4	319	LUT	C10-C11-C12	-2.67	114.90	123.22
22	B	830	CLA	C2D-C1D-ND	2.67	112.07	110.10
22	L	305	CLA	CHB-C1B-NB	-2.66	121.44	124.26
22	A	804	CLA	CHB-C1B-NB	-2.66	121.44	124.26
25	A	816	BCR	C34-C9-C8	2.66	122.27	118.08
25	B	840	BCR	C36-C18-C17	-2.66	119.19	122.92
22	A	859	CLA	CHB-C1B-NB	-2.66	121.44	124.26
22	3	312	CLA	C3B-C4B-NB	2.66	112.98	110.52
22	1	318	CLA	O2A-CGA-CBA	2.66	120.26	111.91
22	2	305	CLA	CAC-C3C-C4C	2.66	128.26	124.81
22	Z	308	CLA	CMB-C2B-C1B	2.66	129.42	125.37
21	1	301	CHL	C2A-C1A-CHA	-2.66	119.20	123.86
22	4	311	CLA	CHB-C1B-NB	-2.66	121.44	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	L	304	BCR	C38-C26-C25	2.66	127.52	124.53
22	A	805	CLA	C4D-CHA-C1A	-2.66	118.01	121.25
22	B	815	CLA	CMD-C2D-C3D	-2.66	121.50	127.61
22	O	210	CLA	CMD-C2D-C3D	-2.66	121.50	127.61
22	L	306	CLA	CAC-C3C-C4C	2.66	128.26	124.81
22	3	311	CLA	CMD-C2D-C3D	-2.66	121.50	127.61
22	Z	314	CLA	C2D-C1D-ND	2.66	112.06	110.10
22	B	816	CLA	CMD-C2D-C3D	-2.66	121.50	127.61
22	3	321	CLA	C3B-C4B-NB	2.66	112.98	110.52
22	3	310	CLA	C1-C2-C3	-2.66	121.45	126.04
25	2	312	BCR	C40-C30-C25	2.66	114.61	110.30
22	N	202	CLA	CMD-C2D-C3D	-2.66	121.50	127.61
22	3	312	CLA	CAC-C3C-C4C	2.66	128.26	124.81
22	A	844	CLA	CHC-C4B-NB	-2.66	121.45	124.26
22	2	318	CLA	CMB-C2B-C1B	2.66	129.41	125.37
25	A	815	BCR	C7-C8-C9	2.66	130.25	126.23
21	Y	304	CHL	C1C-C2C-C3C	-2.65	105.01	107.11
22	B	807	CLA	C3B-C4B-NB	2.65	112.98	110.52
22	O	206	CLA	C2D-C1D-ND	2.65	112.06	110.10
22	A	806	CLA	O2A-CGA-CBA	2.65	120.23	111.91
22	3	321	CLA	CMB-C2B-C1B	2.65	129.41	125.37
22	B	819	CLA	C4-C3-C5	2.65	119.73	115.27
22	A	847	CLA	CHB-C4A-NA	2.65	128.18	124.51
22	B	845	CLA	O1D-CGD-CBD	-2.65	119.06	124.48
25	A	814	BCR	C35-C13-C14	-2.65	119.21	122.92
22	F	306	CLA	C4A-NA-C1A	2.65	107.90	106.71
25	3	303	BCR	C12-C13-C14	2.65	123.01	118.94
22	1	319	CLA	CAC-C3C-C4C	2.65	128.25	124.81
22	3	309	CLA	CAC-C3C-C4C	2.65	128.25	124.81
22	B	813	CLA	O2A-CGA-CBA	2.65	120.22	111.91
21	Z	301	CHL	C1C-C2C-C3C	-2.65	105.01	107.11
21	4	317	CHL	C1C-C2C-C3C	-2.65	105.01	107.11
22	4	310	CLA	C4A-NA-C1A	2.65	107.90	106.71
21	Z	312	CHL	CHC-C4B-NB	-2.65	121.45	124.26
22	B	820	CLA	CHC-C4B-NB	-2.65	121.45	124.26
22	A	850	CLA	CHC-C4B-NB	-2.65	121.46	124.26
22	4	313	CLA	CMB-C2B-C1B	2.65	129.40	125.37
25	B	844	BCR	C24-C25-C26	2.64	127.87	121.46
22	A	808	CLA	C1-C2-C3	-2.64	121.47	126.04
25	B	840	BCR	C10-C11-C12	2.64	131.46	123.22
25	G	202	BCR	C7-C8-C9	2.64	130.23	126.23
21	2	301	CHL	CMD-C2D-C3D	-2.64	121.54	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	307	CLA	CMD-C2D-C3D	-2.64	121.54	127.61
30	A	825	CL0	CMC-C2C-C1C	2.64	129.06	125.04
22	2	308	CLA	C2D-C1D-ND	2.64	112.05	110.10
25	B	839	BCR	C35-C13-C14	-2.64	119.23	122.92
22	B	848	CLA	CMD-C2D-C3D	-2.64	121.54	127.61
22	A	853	CLA	CMB-C2B-C1B	2.64	129.39	125.37
22	G	206	CLA	C3B-C4B-NB	2.64	112.96	110.52
25	B	834	BCR	C33-C5-C6	2.64	127.49	124.53
22	A	853	CLA	C4D-CHA-C1A	-2.64	118.04	121.25
22	B	853	CLA	CAC-C3C-C4C	2.64	128.23	124.81
22	B	809	CLA	CHC-C4B-NB	-2.64	121.47	124.26
22	3	318	CLA	CMC-C2C-C1C	2.64	129.05	125.04
21	Z	304	CHL	C1C-C2C-C3C	-2.64	105.02	107.11
22	B	814	CLA	CHC-C1C-C2C	-2.64	119.41	126.73
22	B	804	CLA	C1-C2-C3	-2.63	121.49	126.04
31	B	841	DGD	C2G-O2G-C1B	-2.63	111.31	117.79
22	2	317	CLA	CHB-C1B-NB	-2.63	121.47	124.26
22	1	321	CLA	CMC-C2C-C1C	2.63	129.05	125.04
22	3	312	CLA	C4A-NA-C1A	2.63	107.89	106.71
22	A	853	CLA	CAC-C3C-C4C	2.63	128.23	124.81
22	1	302	CLA	CMC-C2C-C1C	2.63	129.05	125.04
22	3	310	CLA	CHB-C1B-NB	-2.63	121.47	124.26
25	B	835	BCR	C34-C9-C8	2.63	122.22	118.08
22	K	203	CLA	CMC-C2C-C1C	2.63	129.05	125.04
22	Y	314	CLA	CMC-C2C-C1C	2.63	129.04	125.04
22	B	809	CLA	C1-C2-C3	-2.63	121.50	126.04
22	B	818	CLA	CMC-C2C-C1C	2.63	129.04	125.04
22	Y	314	CLA	CMB-C2B-C1B	2.63	129.37	125.37
25	A	816	BCR	C11-C12-C13	2.63	133.80	126.42
22	B	849	CLA	CMD-C2D-C3D	-2.63	121.57	127.61
23	1	310	LUT	C35-C15-C14	2.63	128.86	123.47
22	2	303	CLA	CHD-C1D-ND	-2.63	122.04	124.45
22	G	206	CLA	C1-C2-C3	-2.63	121.50	126.04
22	4	305	CLA	CBC-CAC-C3C	-2.63	105.19	112.43
22	A	848	CLA	CHB-C4A-NA	2.63	128.14	124.51
22	A	836	CLA	CHB-C4A-NA	2.63	128.14	124.51
22	2	308	CLA	CMB-C2B-C1B	2.62	129.37	125.37
22	A	812	CLA	CMB-C2B-C1B	2.62	129.37	125.37
22	G	207	CLA	CHB-C1B-NB	-2.62	121.48	124.26
22	B	812	CLA	C4A-NA-C1A	2.62	107.89	106.71
22	B	830	CLA	O2A-CGA-CBA	2.62	120.13	111.91
21	3	314	CHL	CMD-C2D-C3D	-2.62	121.59	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	I	101	BCR	C33-C5-C6	2.62	127.47	124.53
22	1	302	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
22	B	824	CLA	C1-C2-C3	-2.62	121.52	126.04
23	2	310	LUT	C7-C6-C5	-2.62	115.12	121.46
22	2	318	CLA	O2A-CGA-CBA	2.62	120.12	111.91
22	3	317	CLA	CMB-C2B-C1B	2.62	129.35	125.37
22	A	809	CLA	C1-C2-C3	-2.61	121.52	126.04
22	A	844	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
25	B	838	BCR	C16-C17-C18	2.61	131.04	127.31
22	A	851	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
22	1	305	CLA	CAA-C2A-C3A	-2.61	110.00	116.10
22	1	319	CLA	C3B-C4B-NB	2.61	112.94	110.52
22	B	818	CLA	C1D-CHD-C4C	-2.61	120.42	126.06
21	X	309	CHL	CMB-C2B-C1B	2.61	129.34	125.37
22	J	102	CLA	CMB-C2B-C1B	2.61	129.34	125.37
22	B	809	CLA	O2A-CGA-CBA	2.61	120.09	111.91
25	2	312	BCR	C24-C25-C26	-2.61	115.14	121.46
22	A	843	CLA	CMB-C2B-C1B	2.61	129.34	125.37
22	A	835	CLA	CMC-C2C-C1C	2.61	129.01	125.04
25	B	837	BCR	C20-C21-C22	2.61	131.03	127.31
22	B	831	CLA	C1-C2-C3	-2.60	121.54	126.04
23	1	310	LUT	C11-C10-C9	2.60	131.03	127.31
22	4	304	CLA	CHC-C4B-NB	-2.60	121.50	124.26
25	3	303	BCR	C36-C18-C17	-2.60	119.28	122.92
21	X	308	CHL	C1C-C2C-C3C	-2.60	105.05	107.11
22	B	822	CLA	C4-C3-C5	2.60	119.65	115.27
22	A	849	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
22	4	306	CLA	CMC-C2C-C1C	2.60	129.00	125.04
22	A	835	CLA	C2D-C1D-ND	2.60	112.02	110.10
25	A	819	BCR	C34-C9-C8	2.60	122.17	118.08
22	L	306	CLA	C1D-CHD-C4C	-2.60	120.45	126.06
22	A	802	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
21	2	321	CHL	C4A-NA-C1A	2.60	107.87	106.71
22	B	824	CLA	CMC-C2C-C1C	2.60	128.99	125.04
22	A	853	CLA	CAA-CBA-CGA	-2.60	105.67	113.25
22	K	203	CLA	CAC-C3C-C4C	2.60	128.18	124.81
22	L	306	CLA	O2A-CGA-CBA	2.59	120.05	111.91
22	1	304	CLA	CHC-C1C-C2C	-2.59	119.52	126.73
22	Y	301	CLA	C2D-C1D-ND	2.59	112.02	110.10
22	1	307	CLA	C4-C3-C5	2.59	119.63	115.27
22	B	845	CLA	CHD-C1D-ND	-2.59	122.07	124.45
22	H	201	CLA	O2D-CGD-O1D	-2.59	118.77	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	207	CLA	C2D-C1D-ND	2.59	112.01	110.10
22	B	826	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
25	B	836	BCR	C38-C26-C25	2.59	127.44	124.53
25	A	816	BCR	C12-C13-C14	2.59	122.91	118.94
22	A	856	CLA	O2A-CGA-CBA	2.59	120.03	111.91
21	Z	302	CHL	CHC-C4B-NB	-2.59	121.52	124.26
22	B	831	CLA	C3B-C4B-NB	2.59	112.92	110.52
22	A	851	CLA	CMD-C2D-C3D	-2.59	121.66	127.61
22	L	305	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
21	2	321	CHL	OMC-CMC-C2C	-2.59	119.84	125.69
22	B	803	CLA	CBC-CAC-C3C	2.59	119.56	112.43
21	4	307	CHL	O2D-CGD-O1D	-2.59	118.22	124.09
22	A	836	CLA	CHB-C1B-NB	-2.59	121.52	124.26
22	B	850	CLA	O2A-CGA-CBA	2.59	120.02	111.91
22	3	321	CLA	C2A-C1A-CHA	-2.58	119.34	123.86
22	F	306	CLA	C3B-C4B-NB	2.58	112.91	110.52
22	B	848	CLA	CMB-C2B-C1B	2.58	129.30	125.37
22	B	827	CLA	O2A-CGA-CBA	2.58	120.02	111.91
22	A	847	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
22	A	804	CLA	C4C-C3C-C2C	-2.58	103.13	106.90
25	L	302	BCR	C34-C9-C8	2.58	122.15	118.08
22	A	859	CLA	CBA-CAA-C2A	-2.58	106.24	113.86
22	O	209	CLA	CMB-C2B-C1B	2.58	129.30	125.37
22	K	205	CLA	C2D-C1D-ND	2.58	112.01	110.10
22	A	805	CLA	CBA-CAA-C2A	-2.58	106.24	113.86
22	G	207	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
22	B	845	CLA	CMC-C2C-C1C	2.58	128.97	125.04
22	A	829	CLA	O2A-CGA-CBA	2.58	120.01	111.91
22	B	849	CLA	O2A-CGA-CBA	2.58	120.00	111.91
22	A	828	CLA	O2D-CGD-O1D	-2.58	118.23	124.09
22	B	853	CLA	CHB-C1B-NB	-2.58	121.53	124.26
22	2	307	CLA	O2A-CGA-CBA	2.58	120.00	111.91
24	3	302	XAT	C24-C23-C22	-2.58	105.80	110.77
22	1	305	CLA	CMD-C2D-C3D	-2.57	121.69	127.61
25	B	844	BCR	C11-C10-C9	2.57	130.98	127.31
22	B	816	CLA	CHD-C1D-ND	-2.57	122.09	124.45
22	A	843	CLA	C4-C3-C5	2.57	119.60	115.27
23	4	319	LUT	C40-C33-C34	-2.57	119.32	122.92
22	3	315	CLA	CHD-C1D-ND	-2.57	122.09	124.45
22	B	811	CLA	C4A-NA-C1A	2.57	107.86	106.71
21	X	302	CHL	CMD-C2D-C3D	-2.57	121.70	127.61
22	A	801	CLA	CMB-C2B-C3B	2.57	130.25	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	206	CLA	CAC-C3C-C4C	2.57	128.14	124.81
22	A	836	CLA	C2D-C1D-ND	2.56	111.99	110.10
22	1	307	CLA	O2A-CGA-O1A	-2.56	117.12	123.59
22	3	315	CLA	CMA-C3A-C2A	-2.56	110.11	116.10
22	A	833	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
22	2	304	CLA	CMD-C2D-C3D	-2.56	121.72	127.61
22	B	846	CLA	C2D-C1D-ND	2.56	111.99	110.10
22	L	307	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
22	3	312	CLA	C1-C2-C3	-2.56	121.61	126.04
22	B	827	CLA	CHC-C4B-NB	-2.56	121.55	124.26
24	1	311	XAT	C19-C9-C10	-2.56	119.34	122.92
25	B	844	BCR	C33-C5-C6	2.56	127.40	124.53
22	B	818	CLA	C2A-C1A-CHA	-2.56	119.39	123.86
22	3	321	CLA	C1D-CHD-C4C	-2.56	120.54	126.06
22	B	816	CLA	C4-C3-C5	2.56	119.57	115.27
22	Y	311	CLA	CMC-C2C-C1C	2.56	128.93	125.04
22	A	831	CLA	CAC-C3C-C4C	2.55	128.12	124.81
22	4	311	CLA	CMB-C2B-C1B	2.55	129.26	125.37
22	A	834	CLA	CBC-CAC-C3C	-2.55	105.39	112.43
22	A	856	CLA	CHB-C1B-NB	-2.55	121.55	124.26
22	2	308	CLA	CMC-C2C-C1C	2.55	128.93	125.04
22	3	320	CLA	CHB-C1B-NB	-2.55	121.56	124.26
25	F	302	BCR	C35-C13-C14	-2.55	119.35	122.92
22	X	310	CLA	C4A-NA-C1A	2.55	107.85	106.71
22	Y	312	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
22	B	850	CLA	CMC-C2C-C1C	2.55	128.92	125.04
22	B	820	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	A	852	CLA	C4-C3-C2	-2.55	117.14	123.68
22	A	831	CLA	CMC-C2C-C1C	2.55	128.92	125.04
22	4	312	CLA	CMB-C2B-C1B	2.55	129.25	125.37
25	J	101	BCR	C37-C22-C23	2.55	122.09	118.08
22	O	208	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
22	K	205	CLA	CAC-C3C-C4C	2.55	128.12	124.81
26	G	203	LHG	O7-C5-C4	2.55	117.62	108.40
22	K	203	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
22	B	847	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
22	4	318	CLA	CMB-C2B-C1B	2.54	129.25	125.37
22	A	852	CLA	CMB-C2B-C3B	2.54	132.75	126.59
22	3	310	CLA	O2A-CGA-CBA	2.54	119.89	111.91
31	J	104	DGD	C1E-O6E-C5E	2.54	118.68	113.69
25	B	834	BCR	C19-C18-C17	2.54	122.84	118.94
22	O	207	CLA	CMD-C2D-C3D	-2.54	121.77	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	812	CLA	C3B-C4B-NB	2.54	112.87	110.52
22	2	322	CLA	C3B-C4B-NB	2.54	112.87	110.52
22	4	315	CLA	CMC-C2C-C1C	2.54	128.90	125.04
22	A	855	CLA	CED-O2D-CGD	2.54	121.67	115.94
22	A	828	CLA	CMC-C2C-C1C	2.53	128.90	125.04
22	F	305	CLA	CMB-C2B-C1B	2.53	129.23	125.37
22	L	306	CLA	CMC-C2C-C1C	2.53	128.90	125.04
22	B	827	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
25	A	814	BCR	C30-C25-C26	-2.53	119.05	122.61
22	B	847	CLA	C2D-C1D-ND	2.53	111.97	110.10
23	4	319	LUT	C35-C15-C14	2.53	128.66	123.47
22	A	853	CLA	CMC-C2C-C1C	2.53	128.89	125.04
22	G	206	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
22	A	828	CLA	C3B-C4B-NB	2.53	112.86	110.52
22	O	207	CLA	CMC-C2C-C1C	2.53	128.89	125.04
22	A	805	CLA	CMC-C2C-C1C	2.53	128.89	125.04
22	2	305	CLA	CMC-C2C-C1C	2.53	128.89	125.04
25	3	303	BCR	C30-C25-C24	2.53	122.92	115.78
22	B	833	CLA	CAC-C3C-C4C	2.53	128.09	124.81
22	B	817	CLA	CMB-C2B-C1B	2.53	129.22	125.37
24	1	311	XAT	C8-C9-C10	2.52	122.81	118.94
22	2	307	CLA	CMC-C2C-C1C	2.52	128.88	125.04
22	1	319	CLA	CMC-C2C-C1C	2.52	128.88	125.04
22	H	201	CLA	CMA-C3A-C2A	-2.52	110.22	116.10
21	Y	313	CHL	CMD-C2D-C3D	-2.52	121.82	127.61
22	2	305	CLA	CMD-C2D-C3D	-2.52	121.82	127.61
22	B	810	CLA	C4C-C3C-C2C	-2.52	103.23	106.90
22	K	204	CLA	CHD-C1D-ND	-2.52	122.14	124.45
22	A	806	CLA	CMC-C2C-C1C	2.52	128.87	125.04
22	X	312	CLA	CMC-C2C-C1C	2.52	128.87	125.04
22	L	306	CLA	CAA-C2A-C3A	-2.52	105.89	112.78
22	X	301	CLA	CMC-C2C-C1C	2.51	128.87	125.04
22	A	844	CLA	CMD-C2D-C3D	-2.51	121.83	127.61
22	Z	306	CLA	C4A-NA-C1A	2.51	107.84	106.71
22	B	833	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
22	2	306	CLA	CMD-C2D-C3D	-2.51	121.83	127.61
22	A	849	CLA	C1-C2-C3	-2.51	121.70	126.04
22	4	306	CLA	C2D-C1D-ND	2.51	111.95	110.10
22	A	826	CLA	C1-C2-C3	-2.51	121.70	126.04
22	A	806	CLA	CHB-C1B-NB	-2.51	121.60	124.26
22	A	850	CLA	CHD-C1D-ND	-2.51	122.15	124.45
25	L	302	BCR	C15-C16-C17	2.51	128.61	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	848	CLA	CMC-C2C-C1C	2.51	128.86	125.04
22	Z	306	CLA	C2D-C1D-ND	2.51	111.95	110.10
22	A	840	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
22	2	303	CLA	CMC-C2C-C1C	2.51	128.86	125.04
22	A	857	CLA	CHC-C4B-NB	-2.51	121.60	124.26
22	A	806	CLA	C2D-C1D-ND	2.51	111.95	110.10
25	B	840	BCR	C34-C9-C8	2.51	120.14	114.60
25	4	321	BCR	C30-C25-C26	-2.51	119.08	122.61
22	B	829	CLA	CHC-C4B-NB	-2.51	121.61	124.26
21	Z	305	CHL	O2D-CGD-O1D	-2.50	118.94	123.84
22	B	809	CLA	CMD-C2D-C3D	-2.50	121.86	127.61
22	G	205	CLA	CMC-C2C-C1C	2.50	128.85	125.04
22	A	856	CLA	C2D-C1D-ND	2.50	111.95	110.10
22	A	833	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
22	B	830	CLA	CAA-CBA-CGA	-2.50	105.95	113.25
22	A	837	CLA	CAC-C3C-C4C	2.50	128.05	124.81
22	A	830	CLA	CMC-C2C-C1C	2.50	128.85	125.04
22	B	807	CLA	O2A-C1-C2	2.50	115.20	108.64
22	X	303	CLA	CMB-C2B-C1B	2.50	129.18	125.37
21	Z	305	CHL	CHB-C1B-NB	-2.50	121.61	124.26
22	2	319	CLA	CMC-C2C-C1C	2.50	128.84	125.04
22	B	853	CLA	CMB-C2B-C1B	2.50	129.17	125.37
22	2	308	CLA	O2A-CGA-CBA	2.50	119.74	111.91
22	B	829	CLA	C4-C3-C5	2.50	119.47	115.27
22	N	202	CLA	CMC-C2C-C1C	2.50	128.84	125.04
25	A	817	BCR	C24-C25-C26	2.50	127.51	121.46
22	4	310	CLA	CMB-C2B-C1B	2.49	129.17	125.37
23	4	322	LUT	C35-C34-C33	-2.49	123.75	127.31
22	A	855	CLA	CMB-C2B-C1B	2.49	129.17	125.37
25	L	301	BCR	C19-C18-C17	2.49	122.77	118.94
22	B	808	CLA	C6-C7-C8	-2.49	107.86	115.92
22	A	801	CLA	CHC-C4B-NB	-2.49	121.62	124.26
22	O	209	CLA	CAC-C3C-C4C	2.49	128.04	124.81
22	A	854	CLA	CHB-C1B-C2B	-2.49	120.20	127.24
22	1	319	CLA	CHC-C4B-NB	-2.49	121.62	124.26
21	X	307	CHL	O2D-CGD-O1D	-2.49	118.97	123.84
22	4	314	CLA	CMC-C2C-C1C	2.49	128.83	125.04
22	B	816	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
25	A	818	BCR	C24-C25-C26	2.49	127.49	121.46
22	A	834	CLA	C2A-C1A-CHA	-2.49	119.51	123.86
25	L	304	BCR	C19-C18-C17	2.49	122.76	118.94
21	X	302	CHL	O2D-CGD-O1D	-2.49	118.97	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	X	310	CLA	CBA-CAA-C2A	-2.49	106.52	113.86
25	B	839	BCR	C29-C28-C27	-2.49	105.82	111.38
22	A	845	CLA	CAA-CBA-CGA	-2.49	105.91	112.51
22	B	809	CLA	CMC-C2C-C1C	2.49	128.82	125.04
22	2	304	CLA	O2A-CGA-O1A	-2.49	117.32	123.59
22	K	205	CLA	CMC-C2C-C1C	2.49	128.82	125.04
22	A	854	CLA	CHC-C4B-NB	-2.48	121.63	124.26
22	A	808	CLA	CED-O2D-CGD	2.48	121.56	115.94
22	B	850	CLA	C2D-C1D-ND	2.48	111.93	110.10
22	B	846	CLA	CMA-C3A-C4A	-2.48	105.10	111.77
22	A	834	CLA	C4A-NA-C1A	2.48	107.82	106.71
22	A	852	CLA	CMD-C2D-C3D	-2.48	121.90	127.61
24	4	320	XAT	C38-C25-C24	2.48	117.07	114.28
22	Z	311	CLA	CMC-C2C-C1C	2.48	128.82	125.04
24	1	311	XAT	C7-C8-C9	2.48	129.38	125.53
25	L	301	BCR	C27-C26-C25	-2.48	119.13	122.73
22	B	808	CLA	O1D-CGD-CBD	-2.48	119.41	124.48
22	2	319	CLA	O2A-CGA-CBA	2.48	119.69	111.91
22	J	102	CLA	CMC-C2C-C1C	2.48	128.81	125.04
25	B	836	BCR	C2-C1-C6	2.48	114.30	110.48
22	B	805	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
31	J	104	DGD	O6D-C5D-C6D	2.48	111.67	106.67
22	A	859	CLA	CMC-C2C-C1C	2.48	128.81	125.04
22	B	807	CLA	C4-C3-C5	2.48	119.44	115.27
22	A	803	CLA	C2A-C1A-CHA	-2.47	119.53	123.86
24	3	302	XAT	C8-C9-C10	-2.47	115.15	118.94
23	3	301	LUT	C20-C13-C14	-2.47	119.46	122.92
30	A	825	CL0	CHB-C1B-C2B	-2.47	120.26	127.24
22	B	804	CLA	CHC-C4B-NB	-2.47	121.64	124.26
22	Z	307	CLA	CMC-C2C-C1C	2.47	128.80	125.04
22	A	857	CLA	O2A-CGA-CBA	2.47	119.65	111.91
21	Y	303	CHL	O2D-CGD-O1D	-2.47	119.01	123.84
22	2	317	CLA	CMC-C2C-C1C	2.47	128.80	125.04
22	B	849	CLA	C4-C3-C5	2.47	119.42	115.27
25	4	321	BCR	C7-C6-C5	2.47	127.44	121.46
22	A	849	CLA	CMC-C2C-C1C	2.47	128.79	125.04
22	Z	310	CLA	CMC-C2C-C1C	2.46	128.79	125.04
21	3	307	CHL	CAA-C2A-C3A	-2.46	106.03	112.78
22	Y	310	CLA	CMC-C2C-C1C	2.46	128.79	125.04
25	J	101	BCR	C12-C13-C14	2.46	122.72	118.94
22	Y	301	CLA	CMC-C2C-C1C	2.46	128.79	125.04
22	A	844	CLA	CMC-C2C-C3C	2.46	132.80	126.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	311	XAT	C15-C14-C13	-2.46	123.80	127.31
22	A	858	CLA	CHC-C1C-NC	2.46	127.94	124.20
22	A	830	CLA	C5-C3-C4	2.46	120.04	114.60
21	Z	302	CHL	C1C-C2C-C3C	-2.46	105.16	107.11
22	1	309	CLA	CMC-C2C-C1C	2.46	128.78	125.04
22	F	305	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
22	A	842	CLA	O2A-CGA-CBA	2.46	119.62	111.91
22	1	303	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
22	Z	310	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
22	A	844	CLA	O2A-CGA-CBA	2.45	119.61	111.91
22	A	847	CLA	C2A-C1A-CHA	-2.45	119.57	123.86
25	O	203	BCR	C38-C26-C25	2.45	127.28	124.53
22	A	802	CLA	CHC-C4B-NB	-2.45	121.66	124.26
22	A	855	CLA	C2D-C1D-ND	2.45	111.91	110.10
22	B	823	CLA	O2A-CGA-CBA	2.45	119.60	111.91
22	K	202	CLA	CMC-C2C-C1C	2.45	128.77	125.04
22	A	859	CLA	C4-C3-C2	-2.45	117.39	123.68
22	A	836	CLA	C4-C3-C5	2.45	119.39	115.27
21	Z	312	CHL	C2A-C1A-CHA	-2.45	119.58	123.86
25	I	101	BCR	C23-C22-C21	2.45	122.70	118.94
22	B	845	CLA	C3B-C4B-NB	2.45	112.78	110.52
22	A	844	CLA	CHB-C1B-C2B	-2.45	120.33	127.24
22	A	853	CLA	CHB-C1B-C2B	-2.45	120.33	127.24
22	4	305	CLA	C3B-C4B-NB	2.44	112.78	110.52
22	1	308	CLA	C4C-C3C-C2C	-2.44	103.33	106.90
22	A	838	CLA	O2A-CGA-CBA	2.44	119.58	111.91
22	B	849	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
22	A	826	CLA	O2A-CGA-CBA	2.44	119.58	111.91
25	F	302	BCR	C24-C25-C26	2.44	127.37	121.46
22	Z	309	CLA	CMC-C2C-C1C	2.44	128.75	125.04
22	3	311	CLA	CMA-C3A-C4A	-2.44	105.22	111.77
22	A	853	CLA	CHB-C1B-NB	-2.44	121.68	124.26
22	B	849	CLA	CMC-C2C-C1C	2.44	128.75	125.04
22	F	306	CLA	CMD-C2D-C3D	-2.43	122.01	127.61
22	3	321	CLA	C2D-C1D-ND	2.43	111.90	110.10
22	B	853	CLA	CMC-C2C-C1C	2.43	128.75	125.04
22	4	312	CLA	CMD-C2D-C3D	-2.43	122.02	127.61
22	A	843	CLA	O2A-CGA-CBA	2.43	119.54	111.91
22	4	318	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
22	A	850	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
23	1	310	LUT	C20-C13-C14	-2.43	119.52	122.92
22	A	831	CLA	O2A-CGA-CBA	2.43	119.54	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	814	BCR	C19-C18-C17	2.43	122.67	118.94
22	A	853	CLA	C3B-C4B-NB	2.43	112.77	110.52
25	L	303	BCR	C16-C15-C14	2.43	128.45	123.47
30	A	825	CL0	C4-C3-C5	2.43	119.36	115.27
22	B	817	CLA	C4D-CHA-C1A	-2.43	118.29	121.25
22	X	304	CLA	CMC-C2C-C1C	2.43	128.74	125.04
22	B	823	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
22	3	312	CLA	CMC-C2C-C1C	2.43	128.74	125.04
22	A	849	CLA	CMD-C2D-C3D	-2.43	122.03	127.61
22	A	850	CLA	O2A-CGA-CBA	2.43	119.53	111.91
22	B	815	CLA	C3B-C4B-NB	2.43	112.77	110.52
22	Z	308	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
22	A	838	CLA	C1-C2-C3	-2.43	121.85	126.04
21	2	301	CHL	C1C-C2C-C3C	-2.43	105.19	107.11
22	B	822	CLA	C2A-C1A-CHA	-2.43	119.62	123.86
25	J	103	BCR	C15-C16-C17	2.43	128.44	123.47
22	Y	308	CLA	CMC-C2C-C1C	2.42	128.73	125.04
22	B	817	CLA	CHC-C4B-NB	-2.42	121.69	124.26
25	2	312	BCR	C20-C19-C18	2.42	133.22	126.42
22	A	845	CLA	CMC-C2C-C1C	2.42	128.73	125.04
22	4	310	CLA	C2D-C1D-ND	2.42	111.89	110.10
22	2	322	CLA	CMC-C2C-C1C	2.42	128.73	125.04
22	B	827	CLA	C4C-C3C-C2C	-2.42	103.37	106.90
22	B	825	CLA	CHB-C1B-C2B	-2.42	120.39	127.24
22	4	304	CLA	CMD-C2D-C3D	-2.42	122.04	127.61
23	1	310	LUT	C35-C34-C33	2.42	130.77	127.31
22	3	315	CLA	CMC-C2C-C1C	2.42	128.73	125.04
22	G	207	CLA	CMC-C2C-C1C	2.42	128.73	125.04
22	A	846	CLA	C2D-C1D-ND	2.42	111.89	110.10
22	A	845	CLA	CHC-C4B-NB	-2.42	121.69	124.26
22	1	321	CLA	C3B-C4B-NB	2.42	112.76	110.52
22	A	801	CLA	C2D-C1D-ND	2.42	111.89	110.10
22	B	846	CLA	C4C-C3C-C2C	-2.42	103.37	106.90
22	B	802	CLA	CMD-C2D-C3D	-2.42	122.05	127.61
25	B	839	BCR	C21-C20-C19	2.42	130.76	123.22
22	A	853	CLA	O2A-CGA-CBA	2.42	119.50	111.91
22	B	826	CLA	C1D-ND-C4D	-2.42	104.62	106.33
22	G	206	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
22	B	851	CLA	CAA-C2A-C3A	-2.42	106.16	112.78
23	1	310	LUT	C15-C35-C34	2.42	128.43	123.47
22	A	801	CLA	CMC-C2C-C1C	2.42	128.72	125.04
22	A	839	CLA	CMC-C2C-C1C	2.42	128.72	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Y	301	CLA	CMB-C2B-C1B	2.42	129.05	125.37
22	4	305	CLA	CMB-C2B-C1B	2.41	129.05	125.37
22	A	852	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
25	J	103	BCR	C19-C18-C17	2.41	122.65	118.94
22	A	842	CLA	CMC-C2C-C1C	2.41	128.71	125.04
23	2	310	LUT	C1-C6-C5	-2.41	119.22	122.61
22	A	846	CLA	CHB-C1B-C2B	-2.41	120.42	127.24
22	B	808	CLA	CAC-C3C-C4C	2.41	127.94	124.81
22	B	804	CLA	C4-C3-C5	2.41	119.33	115.27
22	B	829	CLA	CHB-C1B-NB	-2.41	121.71	124.26
22	A	828	CLA	CAA-C2A-C3A	-2.41	110.47	116.10
22	X	311	CLA	CMC-C2C-C1C	2.41	128.71	125.04
22	B	817	CLA	C4A-NA-C1A	2.41	107.79	106.71
26	B	843	LHG	O8-C23-C24	2.41	119.47	111.91
22	1	303	CLA	CMC-C2C-C1C	2.41	128.71	125.04
22	B	851	CLA	C4C-C3C-C2C	-2.41	103.39	106.90
22	B	853	CLA	CHC-C4B-NB	-2.41	121.71	124.26
22	B	826	CLA	O1D-CGD-CBD	-2.41	119.56	124.48
21	Y	307	CHL	O2D-CGD-O1D	-2.41	119.13	123.84
22	A	836	CLA	O2A-CGA-CBA	2.41	119.46	111.91
22	A	831	CLA	C7-C6-C5	-2.41	106.83	113.36
22	A	826	CLA	C4C-C3C-C2C	-2.40	103.39	106.90
22	A	855	CLA	C4-C3-C5	2.40	119.32	115.27
22	A	801	CLA	C4B-C3B-C2B	-2.40	104.75	107.03
31	G	201	DGD	C2G-O2G-C1B	-2.40	111.87	117.79
22	B	816	CLA	CHD-C4C-NC	2.40	127.99	124.20
26	A	824	LHG	O4-P-O5	2.40	120.09	110.68
22	B	850	CLA	CMD-C2D-C3D	-2.40	122.09	127.61
25	B	840	BCR	C20-C19-C18	2.40	133.16	126.42
21	X	305	CHL	O2D-CGD-O1D	-2.40	119.14	123.84
22	A	857	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
22	A	834	CLA	CMC-C2C-C1C	2.40	128.69	125.04
21	Y	304	CHL	O2D-CGD-O1D	-2.40	119.15	123.84
22	L	305	CLA	CAC-C3C-C4C	2.40	127.92	124.81
22	A	848	CLA	C2A-C1A-CHA	-2.40	119.67	123.86
26	O	205	LHG	O4-P-O5	2.40	120.06	110.68
22	Z	313	CLA	CMB-C2B-C1B	2.40	129.02	125.37
25	A	819	BCR	C4-C5-C6	-2.40	119.25	122.73
25	B	834	BCR	C24-C23-C22	2.39	129.85	126.23
22	A	839	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
22	1	317	CLA	CMB-C2B-C1B	2.39	129.01	125.37
22	K	205	CLA	O1D-CGD-CBD	-2.39	119.59	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	320	XAT	C19-C9-C8	2.39	121.84	118.08
22	B	822	CLA	CHC-C4B-NB	-2.39	121.73	124.26
25	A	819	BCR	C7-C6-C5	2.39	127.25	121.46
25	3	303	BCR	C24-C23-C22	2.39	129.85	126.23
22	B	812	CLA	CHC-C4B-NB	-2.39	121.73	124.26
22	2	306	CLA	C3B-C4B-NB	2.39	112.73	110.52
22	B	807	CLA	CAA-C2A-C1A	2.39	119.80	111.97
22	A	835	CLA	OBD-CAD-C3D	-2.39	122.77	128.52
21	1	301	CHL	CMB-C2B-C1B	2.39	129.01	125.37
25	1	312	BCR	C37-C22-C21	-2.39	119.58	122.92
27	F	304	MGE	C1D-C2D-C3D	2.39	114.97	110.00
22	A	828	CLA	CMA-C3A-C2A	-2.39	110.53	116.10
25	K	201	BCR	C24-C25-C26	2.39	127.25	121.46
22	4	311	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
22	B	848	CLA	O2A-CGA-CBA	2.39	119.40	111.91
25	J	103	BCR	C24-C25-C26	2.39	127.24	121.46
27	3	304	MGE	C2G-O2G-C1B	2.39	123.67	117.79
22	A	838	CLA	C4-C3-C5	2.39	119.28	115.27
22	Y	311	CLA	C4-C3-C5	2.39	119.28	115.27
25	A	818	BCR	C19-C18-C17	-2.39	119.50	124.81
22	G	207	CLA	C4A-NA-C1A	2.38	107.78	106.71
25	L	303	BCR	C7-C6-C5	2.38	127.24	121.46
22	4	318	CLA	CMC-C2C-C1C	2.38	128.67	125.04
22	2	319	CLA	CMB-C2B-C1B	2.38	129.00	125.37
22	2	305	CLA	C2D-C1D-ND	2.38	111.86	110.10
22	Z	308	CLA	CMC-C2C-C1C	2.38	128.67	125.04
22	4	316	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
22	B	852	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
22	Y	309	CLA	CMC-C2C-C1C	2.38	128.67	125.04
22	B	801	CLA	CMB-C2B-C1B	2.38	129.00	125.37
22	B	849	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
22	A	808	CLA	CMB-C2B-C1B	2.38	128.99	125.37
25	B	840	BCR	C24-C25-C26	2.38	127.22	121.46
25	2	312	BCR	C37-C22-C23	2.38	121.82	118.08
23	3	301	LUT	C11-C10-C9	2.38	130.70	127.31
25	B	837	BCR	C10-C11-C12	2.38	130.63	123.22
22	A	849	CLA	C4-C3-C5	2.38	119.27	115.27
22	A	827	CLA	CAA-CBA-CGA	-2.38	106.31	113.25
22	B	826	CLA	CHD-C4C-NC	2.38	127.95	124.20
22	2	320	CLA	C2D-C1D-ND	2.38	111.86	110.10
22	K	204	CLA	C4A-NA-C1A	2.38	107.77	106.71
25	A	815	BCR	C24-C25-C26	2.37	127.22	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2	307	CLA	C4-C3-C5	2.37	119.27	115.27
22	3	321	CLA	O2D-CGD-O1D	-2.37	119.19	123.84
22	B	812	CLA	C2D-C1D-ND	2.37	111.85	110.10
22	B	850	CLA	C3B-C4B-NB	2.37	112.72	110.52
26	2	314	LHG	O4-P-O5	2.37	119.98	110.68
22	1	308	CLA	CAC-C3C-C4C	2.37	127.89	124.81
22	B	853	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
22	B	833	CLA	CMC-C2C-C1C	2.37	128.65	125.04
22	B	853	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
26	F	301	LHG	O4-P-O5	2.37	119.97	110.68
22	X	301	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
21	Y	306	CHL	O2D-CGD-O1D	-2.37	119.20	123.84
22	A	843	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
22	A	827	CLA	O2A-CGA-CBA	2.37	119.34	111.91
22	K	204	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
22	2	318	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
21	Z	312	CHL	O2D-CGD-O1D	-2.37	119.21	123.84
25	L	302	BCR	C24-C25-C26	2.37	127.19	121.46
21	1	316	CHL	O2D-CGD-O1D	-2.37	119.21	123.84
21	X	306	CHL	O2D-CGD-O1D	-2.37	119.21	123.84
22	B	851	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
25	A	819	BCR	C37-C22-C23	2.36	121.80	118.08
22	O	210	CLA	CMC-C2C-C1C	2.36	128.64	125.04
22	B	804	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
22	B	823	CLA	CMC-C2C-C1C	2.36	128.64	125.04
22	B	806	CLA	C4-C3-C5	2.36	119.25	115.27
22	B	824	CLA	C4-C3-C5	2.36	119.25	115.27
22	Y	309	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
22	B	852	CLA	CMC-C2C-C1C	2.36	128.64	125.04
22	3	313	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
21	Z	303	CHL	C2A-C1A-CHA	-2.36	119.73	123.86
22	B	810	CLA	C5-C3-C4	2.36	119.82	114.60
26	2	316	LHG	O4-P-O5	2.36	119.92	110.68
22	A	802	CLA	CHB-C1B-NB	-2.36	121.76	124.26
21	Y	313	CHL	CMB-C2B-C3B	2.36	132.30	126.59
22	2	306	CLA	CMC-C2C-C1C	2.36	128.63	125.04
22	X	313	CLA	CMC-C2C-C1C	2.36	128.63	125.04
22	K	203	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
22	X	310	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
22	K	205	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
22	A	853	CLA	C2D-C1D-ND	2.36	111.84	110.10
22	A	850	CLA	CMB-C2B-C1B	2.36	128.96	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	X	309	CHL	O2D-CGD-O1D	-2.35	119.24	123.84
22	A	854	CLA	CHD-C1D-ND	-2.35	122.29	124.45
22	1	319	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
22	B	801	CLA	CHD-C4C-NC	2.35	127.91	124.20
22	4	306	CLA	C3B-C4B-NB	2.35	112.70	110.52
26	G	204	LHG	O4-P-O5	2.35	119.89	110.68
25	J	103	BCR	C29-C30-C25	2.35	114.10	110.48
22	Y	302	CLA	CMC-C2C-C1C	2.35	128.62	125.04
22	A	808	CLA	C4A-NA-C1A	2.35	107.76	106.71
22	A	806	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
26	2	313	LHG	O4-P-O5	2.35	119.88	110.68
22	2	304	CLA	C4-C3-C5	2.35	119.22	115.27
26	A	821	LHG	O4-P-O5	2.35	119.87	110.68
22	X	310	CLA	CMC-C2C-C1C	2.35	128.61	125.04
22	A	809	CLA	CBA-CAA-C2A	2.35	120.79	113.86
22	3	316	CLA	CED-O2D-CGD	2.35	121.24	115.94
22	2	317	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
22	Z	311	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
22	B	812	CLA	CMC-C2C-C1C	2.34	128.61	125.04
25	J	101	BCR	C15-C16-C17	2.34	128.28	123.47
22	4	310	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
22	Y	302	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
22	4	316	CLA	CAC-C3C-C4C	2.34	127.85	124.81
22	A	807	CLA	O1D-CGD-CBD	-2.34	119.69	124.48
21	4	309	CHL	OMC-CMC-C2C	-2.34	120.39	125.69
22	A	810	CLA	O2A-CGA-CBA	2.34	119.25	111.91
22	A	853	CLA	C6-C7-C8	-2.34	108.35	115.92
21	Z	304	CHL	C2A-C1A-CHA	-2.34	119.77	123.86
22	B	803	CLA	C6-C5-C3	-2.34	107.32	113.45
22	A	859	CLA	C1-C2-C3	-2.34	122.00	126.04
22	2	308	CLA	C4-C3-C5	2.34	119.20	115.27
22	B	813	CLA	CED-O2D-CGD	2.34	121.22	115.94
22	3	310	CLA	C4A-NA-C1A	2.34	107.76	106.71
22	Z	307	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
22	3	316	CLA	CMD-C2D-C3D	-2.34	122.24	127.61
22	B	825	CLA	CMC-C2C-C1C	2.34	128.60	125.04
22	B	804	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
22	B	849	CLA	C1-C2-C3	-2.34	122.00	126.04
22	X	303	CLA	CMC-C2C-C1C	2.33	128.59	125.04
25	B	835	BCR	C33-C5-C6	2.33	127.15	124.53
21	3	307	CHL	O2D-CGD-O1D	-2.33	119.28	123.84
22	Z	314	CLA	CMC-C2C-C1C	2.33	128.59	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	803	CLA	CBC-CAC-C3C	-2.33	106.00	112.43
21	3	307	CHL	C1C-C2C-C3C	-2.33	105.27	107.11
22	X	311	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
22	B	811	CLA	O2A-CGA-CBA	2.33	119.21	111.91
22	Z	313	CLA	CMC-C2C-C1C	2.33	128.58	125.04
22	3	312	CLA	CED-O2D-CGD	2.33	121.20	115.94
22	B	819	CLA	C2A-C1A-CHA	-2.32	119.79	123.86
27	F	303	MGE	O3G-C3G-C2G	-2.32	105.29	110.90
21	Z	304	CHL	C4D-CHA-C1A	-2.32	118.42	121.25
22	1	319	CLA	CMA-C3A-C4A	-2.32	105.53	111.77
22	H	201	CLA	CAA-C2A-C3A	-2.32	110.68	116.10
21	X	308	CHL	O2D-CGD-O1D	-2.32	119.30	123.84
22	A	850	CLA	C1-C2-C3	-2.32	122.03	126.04
24	2	311	XAT	C39-C29-C30	-2.32	119.67	122.92
22	O	207	CLA	C4-C3-C5	2.32	119.18	115.27
22	B	806	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
22	B	831	CLA	CMC-C2C-C1C	2.32	128.57	125.04
22	B	811	CLA	CAA-CBA-CGA	-2.32	106.47	113.25
22	A	802	CLA	C3B-C4B-NB	2.32	112.67	110.52
22	A	851	CLA	O2A-CGA-CBA	2.32	119.19	111.91
22	B	816	CLA	C3D-C4D-CHA	-2.32	107.42	112.72
22	B	845	CLA	CBC-CAC-C3C	-2.32	106.05	112.43
22	A	836	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
25	B	838	BCR	C11-C10-C9	2.32	130.62	127.31
22	4	304	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
22	A	829	CLA	CMA-C3A-C4A	-2.31	105.56	111.77
22	B	823	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
21	2	309	CHL	O2D-CGD-O1D	-2.31	119.32	123.84
22	X	312	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
26	O	204	LHG	O4-P-O5	2.31	119.72	110.68
22	4	304	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
21	Z	301	CHL	O2D-CGD-O1D	-2.31	119.32	123.84
22	B	813	CLA	C3B-C4B-NB	2.31	112.66	110.52
22	3	309	CLA	C1-C2-C3	-2.31	122.05	126.04
25	A	818	BCR	C7-C6-C5	2.31	127.05	121.46
28	B	832	PQN	C2M-C2-C3	-2.31	120.64	124.40
24	1	311	XAT	C20-C13-C14	-2.31	119.69	122.92
22	B	819	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
25	L	302	BCR	C33-C5-C6	2.31	127.12	124.53
22	Z	314	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
25	B	838	BCR	C12-C13-C14	2.30	122.47	118.94
22	O	206	CLA	O2D-CGD-O1D	-2.30	119.34	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	847	CLA	CHB-C1B-NB	-2.30	121.82	124.26
21	Z	302	CHL	O2D-CGD-O1D	-2.30	119.34	123.84
22	G	207	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
21	4	309	CHL	CMB-C2B-C1B	2.30	128.87	125.37
22	A	804	CLA	CMB-C2B-C1B	2.30	128.87	125.37
22	1	304	CLA	CHB-C1B-NB	-2.30	121.82	124.26
22	3	308	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
22	3	319	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
22	A	803	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
22	B	822	CLA	CMC-C2C-C1C	2.30	128.54	125.04
22	3	318	CLA	CED-O2D-CGD	2.30	121.13	115.94
22	B	851	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
22	3	309	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
22	B	822	CLA	C1D-CHD-C4C	-2.29	121.11	126.06
22	B	814	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
22	B	810	CLA	O2A-CGA-CBA	2.29	119.11	111.91
22	Z	309	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
22	A	845	CLA	C4A-NA-C1A	2.29	107.74	106.71
25	B	839	BCR	C33-C5-C6	2.29	127.10	124.53
22	B	846	CLA	C2A-C1A-CHA	-2.29	119.85	123.86
21	Y	313	CHL	O2D-CGD-O1D	-2.29	119.36	123.84
21	4	309	CHL	CHB-C1B-NB	-2.29	121.83	124.26
22	B	821	CLA	CAA-C2A-C1A	2.29	119.48	111.97
22	1	304	CLA	CED-O2D-CGD	2.29	121.12	115.94
25	L	304	BCR	C24-C25-C26	2.29	127.01	121.46
22	B	818	CLA	CHB-C1B-C2B	-2.29	120.77	127.24
23	4	319	LUT	C20-C13-C14	-2.29	119.72	122.92
23	3	301	LUT	C3-C4-C5	2.29	116.41	111.85
22	A	827	CLA	CHB-C1B-C2B	-2.28	120.78	127.24
25	B	844	BCR	C29-C30-C25	2.28	114.00	110.48
22	Y	308	CLA	C4A-NA-C1A	2.28	107.73	106.71
22	B	809	CLA	CHB-C1B-NB	-2.28	121.84	124.26
22	Y	309	CLA	O2A-CGA-CBA	2.28	121.25	112.23
22	2	305	CLA	CGD-CBD-CAD	2.28	118.12	110.73
22	K	205	CLA	CHB-C1B-NB	-2.28	121.84	124.26
25	A	819	BCR	C15-C16-C17	2.28	128.15	123.47
22	B	827	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
22	B	833	CLA	C4-C3-C5	2.28	119.10	115.27
22	O	206	CLA	CMB-C2B-C1B	2.28	128.84	125.37
22	A	812	CLA	C4-C3-C5	2.28	119.10	115.27
22	Y	301	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
22	X	304	CLA	CAD-C3D-C2D	-2.28	129.81	140.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	L	303	BCR	C12-C13-C14	2.28	122.43	118.94
22	2	322	CLA	O2D-CGD-O1D	-2.28	118.92	124.09
22	1	320	CLA	C4A-NA-C1A	2.28	107.73	106.71
22	B	817	CLA	O2A-CGA-CBA	2.28	119.05	111.91
25	O	202	BCR	C28-C27-C26	-2.27	110.02	114.08
22	4	313	CLA	O2D-CGD-O1D	-2.27	118.92	124.09
22	G	207	CLA	CHC-C4B-NB	-2.27	121.85	124.26
22	B	820	CLA	CHB-C1B-C2B	-2.27	120.82	127.24
22	A	855	CLA	C3B-C2B-C1B	-2.27	104.42	107.16
22	B	823	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
22	A	842	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
22	A	833	CLA	C1-C2-C3	-2.27	122.12	126.04
27	N	201	MGE	C1D-O6D-C5D	2.27	118.14	113.69
22	4	316	CLA	CMC-C2C-C1C	2.27	128.49	125.04
22	A	850	CLA	C16-C15-C13	-2.27	108.59	115.92
22	B	845	CLA	C2D-C1D-ND	2.27	111.77	110.10
22	B	819	CLA	CMC-C2C-C1C	2.27	128.49	125.04
22	B	822	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
24	2	311	XAT	C35-C15-C14	2.26	128.11	123.47
25	O	203	BCR	C19-C18-C17	2.26	122.42	118.94
22	A	831	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
22	L	305	CLA	CMC-C2C-C1C	2.26	128.48	125.04
22	B	820	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
22	A	802	CLA	CAA-C2A-C1A	-2.26	104.57	111.97
25	G	202	BCR	C23-C24-C25	2.26	133.55	127.20
25	A	818	BCR	C12-C13-C14	2.26	122.41	118.94
25	F	302	BCR	C12-C13-C14	2.26	122.40	118.94
22	A	826	CLA	C1D-CHD-C4C	-2.26	121.19	126.06
25	B	838	BCR	C29-C28-C27	-2.25	106.34	111.38
22	2	304	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
22	B	808	CLA	CBA-CAA-C2A	2.25	120.52	113.86
22	B	833	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
22	1	321	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
22	Y	301	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
22	B	807	CLA	CBC-CAC-C3C	-2.25	108.04	113.82
22	B	829	CLA	C3B-C4B-NB	2.25	112.60	110.52
21	X	306	CHL	C2A-C1A-CHA	-2.25	119.92	123.86
22	2	307	CLA	C1-C2-C3	-2.25	122.15	126.04
22	B	815	CLA	C1-C2-C3	-2.25	122.15	126.04
21	Z	304	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
21	2	301	CHL	O1D-CGD-CBD	-2.25	119.88	124.48
22	B	803	CLA	O2A-CGA-CBA	2.25	118.96	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	827	CLA	C2D-C1D-ND	2.25	111.76	110.10
22	A	844	CLA	C1-C2-C3	-2.25	122.16	126.04
23	2	310	LUT	C15-C14-C13	2.25	130.52	127.31
22	B	812	CLA	C1-C2-C3	-2.25	122.16	126.04
31	G	201	DGD	C3D-C4D-C5D	2.25	113.27	109.77
22	B	816	CLA	CMB-C2B-C1B	2.25	128.79	125.37
22	A	829	CLA	C5-C3-C4	2.25	119.56	114.60
22	3	316	CLA	CMB-C2B-C1B	2.25	128.79	125.37
21	Y	305	CHL	O2D-CGD-O1D	-2.25	119.45	123.84
22	L	307	CLA	O2D-CGD-O1D	-2.25	119.45	123.84
24	1	311	XAT	C37-C21-C36	-2.24	104.06	107.37
22	1	319	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
22	B	805	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
25	3	303	BCR	C30-C25-C26	-2.24	119.46	122.61
26	F	301	LHG	O7-C7-O9	-2.24	118.29	123.70
22	2	305	CLA	CMB-C2B-C1B	2.24	128.78	125.37
31	G	201	DGD	C6D-C5D-C4D	-2.24	108.94	113.07
22	B	831	CLA	CED-O2D-CGD	2.24	121.00	115.94
22	B	821	CLA	CMC-C2C-C1C	2.24	128.45	125.04
22	2	304	CLA	CMB-C2B-C3B	2.24	132.01	126.59
22	1	306	CLA	O2D-CGD-O1D	-2.24	119.01	124.09
25	B	837	BCR	C7-C8-C9	2.24	129.61	126.23
22	A	829	CLA	CMB-C2B-C3B	2.24	132.00	126.59
24	1	311	XAT	C32-C33-C34	2.24	122.37	118.94
22	O	206	CLA	C2A-C1A-CHA	-2.24	119.95	123.86
22	B	807	CLA	CAC-C3C-C4C	2.23	129.19	125.61
22	1	318	CLA	C2A-C1A-CHA	-2.23	119.95	123.86
25	A	817	BCR	C27-C26-C25	-2.23	119.49	122.73
22	1	320	CLA	CED-O2D-CGD	2.23	120.99	115.94
22	O	210	CLA	C2A-C1A-CHA	-2.23	119.95	123.85
22	A	841	CLA	C4A-NA-C1A	2.23	107.71	106.71
22	B	845	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
26	2	314	LHG	O7-C5-C6	2.23	116.48	108.40
22	A	805	CLA	CHB-C1B-C2B	-2.23	120.94	127.24
22	B	819	CLA	C1-O2A-CGA	2.23	122.30	116.44
22	A	848	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
22	4	312	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
22	2	319	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
25	L	302	BCR	C29-C30-C25	2.23	113.91	110.48
25	L	301	BCR	C24-C25-C26	2.23	126.86	121.46
22	A	854	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
22	B	828	CLA	O2D-CGD-O1D	-2.23	119.48	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	306	CLA	CHC-C4B-NB	-2.23	121.90	124.26
24	2	311	XAT	C10-C11-C12	2.23	130.16	123.22
22	B	829	CLA	O2A-CGA-CBA	2.23	118.89	111.91
22	A	846	CLA	O2A-CGA-CBA	2.22	118.89	111.91
22	A	858	CLA	CBB-CAB-C3B	-2.22	116.56	127.62
22	3	313	CLA	C2A-C1A-CHA	-2.22	119.97	123.86
22	B	845	CLA	CHB-C1B-C2B	-2.22	120.96	127.24
22	B	847	CLA	C4A-NA-C1A	2.22	107.70	106.71
22	O	207	CLA	CAC-C3C-C4C	2.22	127.69	124.81
22	A	841	CLA	CHB-C1B-NB	-2.22	121.91	124.26
22	A	802	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
22	B	852	CLA	C4-C3-C5	2.22	119.01	115.27
22	B	829	CLA	CBB-CAB-C3B	-2.22	116.57	127.62
22	1	304	CLA	C2A-C3A-C4A	-2.22	98.29	101.87
22	B	846	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
22	B	817	CLA	O1D-CGD-CBD	-2.22	119.95	124.48
22	A	810	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
22	A	803	CLA	CMB-C2B-C1B	2.21	128.74	125.37
22	3	311	CLA	C3B-C4B-NB	2.21	112.57	110.52
23	4	322	LUT	C31-C30-C29	-2.21	124.15	127.31
22	B	826	CLA	C3D-C4D-ND	2.21	113.82	110.24
22	A	801	CLA	C4A-NA-C1A	2.21	107.70	106.71
21	3	314	CHL	O2D-CGD-O1D	-2.21	119.51	123.84
25	G	202	BCR	C24-C25-C26	2.21	126.82	121.46
22	B	806	CLA	CMC-C2C-C1C	2.21	128.41	125.04
22	H	201	CLA	CMC-C2C-C1C	2.21	128.41	125.04
22	K	202	CLA	O2D-CGD-O1D	-2.21	119.07	124.09
21	Y	303	CHL	CAA-C2A-C3A	-2.21	106.72	112.78
22	A	802	CLA	CMC-C2C-C1C	2.21	128.41	125.04
22	B	847	CLA	C3B-C4B-NB	2.21	112.56	110.52
22	B	827	CLA	CMB-C2B-C1B	2.21	128.73	125.37
22	B	829	CLA	C2D-C1D-ND	2.21	111.73	110.10
21	2	301	CHL	CHC-C4B-NB	-2.21	121.92	124.26
22	A	857	CLA	C1-C2-C3	-2.21	122.22	126.04
22	B	826	CLA	C5-C3-C4	2.21	119.48	114.60
22	B	802	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
25	I	101	BCR	C34-C9-C8	2.21	121.55	118.08
21	Y	313	CHL	C1C-C2C-C3C	-2.21	105.36	107.11
22	B	830	CLA	C4-C3-C5	2.21	118.98	115.27
22	B	817	CLA	C3B-C4B-NB	2.21	112.56	110.52
22	3	319	CLA	CMC-C2C-C1C	2.21	128.40	125.04
25	L	301	BCR	C23-C22-C21	2.21	122.33	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	311	CLA	C2D-C1D-ND	2.21	111.73	110.10
22	A	810	CLA	CED-O2D-CGD	2.20	120.92	115.94
21	X	307	CHL	C2A-C1A-CHA	-2.20	120.00	123.86
30	A	825	CL0	O2A-CGA-O1A	-2.20	118.03	123.59
22	A	828	CLA	CHD-C1D-ND	-2.20	122.43	124.45
22	A	801	CLA	C4-C3-C5	2.20	118.98	115.27
21	1	301	CHL	C4D-CHA-C1A	-2.20	118.57	121.25
22	A	854	CLA	CMC-C2C-C1C	2.20	128.40	125.04
22	B	815	CLA	CMC-C2C-C1C	2.20	128.40	125.04
22	J	102	CLA	O2D-CGD-O1D	-2.20	119.08	124.09
21	2	309	CHL	C2A-C1A-CHA	-2.20	120.01	123.86
22	2	320	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
25	A	817	BCR	C29-C30-C25	2.20	113.87	110.48
22	B	830	CLA	C4A-NA-C1A	2.20	107.70	106.71
22	1	303	CLA	CED-O2D-CGD	2.20	120.92	115.94
24	1	311	XAT	C16-C1-C2	-2.20	105.16	108.98
25	O	202	BCR	C7-C6-C5	2.20	126.79	121.46
21	4	309	CHL	C1C-C2C-C3C	-2.20	105.37	107.11
22	B	814	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
21	4	308	CHL	CAA-C2A-C3A	-2.20	106.75	112.78
22	A	859	CLA	O2A-CGA-CBA	2.20	118.81	111.91
25	B	844	BCR	C1-C6-C5	-2.20	119.52	122.61
23	4	319	LUT	C7-C8-C9	2.20	129.56	126.23
22	1	309	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
22	A	855	CLA	CMC-C2C-C3C	2.20	132.09	126.12
22	X	304	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
22	B	818	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
22	A	812	CLA	CMC-C2C-C1C	2.20	128.39	125.04
25	A	814	BCR	C37-C22-C23	2.20	121.54	118.08
21	Z	303	CHL	O2D-CGD-O1D	-2.20	119.54	123.84
22	1	308	CLA	C2A-C1A-CHA	-2.20	120.02	123.85
25	J	101	BCR	C19-C18-C17	2.20	122.31	118.94
22	A	848	CLA	C2D-C1D-ND	2.20	111.72	110.10
25	B	837	BCR	C19-C18-C17	2.19	122.31	118.94
25	B	838	BCR	C36-C18-C17	-2.19	119.85	122.92
22	2	303	CLA	C2D-C1D-ND	2.19	111.72	110.10
21	2	301	CHL	OMC-CMC-C2C	-2.19	120.73	125.69
27	3	305	MGE	C2G-O2G-C1B	2.19	123.19	117.79
22	B	807	CLA	CMC-C2C-C3C	-2.19	126.58	129.92
25	F	302	BCR	C37-C22-C23	2.19	121.53	118.08
22	B	819	CLA	CED-O2D-CGD	2.19	120.89	115.94
22	3	315	CLA	C2D-C1D-ND	2.19	111.72	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	829	CLA	CHB-C1B-C2B	-2.19	121.05	127.24
24	4	320	XAT	O24-C25-C26	-2.19	57.15	58.96
22	A	856	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
25	A	815	BCR	C37-C22-C23	2.19	121.53	118.08
23	1	310	LUT	C19-C9-C8	2.19	121.53	118.08
22	3	320	CLA	O2D-CGD-O1D	-2.19	119.12	124.09
22	2	320	CLA	CHC-C4B-NB	-2.19	121.94	124.26
22	B	853	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
24	4	320	XAT	C20-C13-C12	2.19	121.53	118.08
22	B	809	CLA	C4A-NA-C1A	2.19	107.69	106.71
22	K	203	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
22	X	303	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
25	1	312	BCR	C24-C25-C26	2.19	126.76	121.46
22	B	817	CLA	C1-C2-C3	-2.19	122.26	126.04
22	B	829	CLA	C1-C2-C3	-2.19	122.26	126.04
22	B	808	CLA	O2A-CGA-O1A	-2.19	118.08	123.59
22	2	306	CLA	CMB-C2B-C1B	2.19	128.70	125.37
24	4	320	XAT	O4-C5-C6	-2.19	57.15	58.96
22	A	857	CLA	C6-C5-C3	-2.19	107.72	113.45
22	A	849	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
22	2	320	CLA	CMC-C2C-C1C	2.19	128.37	125.04
22	A	848	CLA	C1D-CHD-C4C	-2.18	121.34	126.06
21	X	308	CHL	C2A-C1A-CHA	-2.18	120.04	123.86
22	O	209	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
22	B	848	CLA	C3B-C4B-NB	2.18	112.54	110.52
21	Z	302	CHL	C4D-CHA-C1A	-2.18	118.59	121.25
22	3	320	CLA	CMC-C2C-C1C	2.18	128.36	125.04
25	K	201	BCR	C37-C22-C23	2.18	121.51	118.08
22	4	310	CLA	CHD-C1D-ND	-2.18	122.45	124.45
21	4	317	CHL	O2D-CGD-O1D	-2.18	119.14	124.09
22	G	205	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
21	2	301	CHL	CED-O2D-CGD	2.18	120.86	115.94
22	B	813	CLA	C4A-NA-C1A	-2.18	105.73	106.71
26	2	313	LHG	O7-C7-O9	-2.18	118.44	123.70
22	A	808	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
22	A	827	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
25	O	203	BCR	C24-C25-C26	2.18	126.73	121.46
22	Y	308	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
22	2	306	CLA	O2D-CGD-O1D	-2.18	119.15	124.09
22	A	843	CLA	CBB-CAB-C3B	-2.17	116.80	127.62
27	F	304	MGE	C1D-O6D-C5D	2.17	117.96	113.69
22	A	826	CLA	CHC-C4B-NB	-2.17	121.96	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	837	CLA	C4A-NA-C1A	2.17	107.68	106.71
22	B	814	CLA	C4A-NA-C1A	2.17	107.68	106.71
25	O	202	BCR	C4-C5-C6	-2.17	119.58	122.73
22	3	310	CLA	C4-C3-C5	2.17	118.93	115.27
22	A	826	CLA	CHD-C4C-NC	2.17	127.63	124.20
22	B	853	CLA	C1-C2-C3	-2.17	122.29	126.04
22	A	804	CLA	CBC-CAC-C3C	-2.17	106.45	112.43
30	A	825	CL0	C3B-C4B-NB	2.17	112.53	110.52
25	A	814	BCR	C24-C25-C26	-2.17	116.21	121.46
22	A	805	CLA	C5-C3-C4	2.17	119.39	114.60
22	B	825	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
22	B	816	CLA	CBA-CAA-C2A	-2.17	107.47	113.86
22	A	854	CLA	C11-C10-C8	-2.17	108.92	115.92
25	I	101	BCR	C12-C13-C14	2.17	122.27	118.94
25	L	301	BCR	C28-C27-C26	-2.17	110.21	114.08
22	1	321	CLA	O2D-CGD-O1D	-2.17	119.17	124.09
22	3	320	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
22	A	826	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
22	F	305	CLA	CMC-C2C-C1C	2.16	128.34	125.04
22	L	305	CLA	C4A-NA-C1A	2.16	107.68	106.71
22	Z	306	CLA	O2A-CGA-CBA	2.16	120.78	112.23
22	X	313	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
22	2	319	CLA	C4D-C3D-CAD	2.16	110.64	108.10
22	A	812	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
22	A	850	CLA	C4-C3-C5	2.16	118.91	115.27
21	2	309	CHL	CHB-C1B-C2B	-2.16	121.13	127.24
22	2	320	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
22	1	304	CLA	CHB-C1B-C2B	-2.16	121.14	127.24
23	3	301	LUT	C19-C9-C8	2.16	121.48	118.08
21	Z	312	CHL	C4D-CHA-C1A	-2.16	118.62	121.25
21	3	307	CHL	CHC-C4B-NB	-2.16	121.97	124.26
22	H	201	CLA	CHC-C4B-NB	-2.16	121.97	124.26
22	3	311	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
22	A	810	CLA	C1-C2-C3	-2.15	122.32	126.04
21	3	307	CHL	CHB-C1B-C2B	-2.15	121.16	127.24
22	Z	310	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
22	2	320	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
22	B	831	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
22	2	319	CLA	C3B-C4B-NB	2.15	112.51	110.52
25	O	203	BCR	C11-C12-C13	2.15	132.46	126.42
22	H	201	CLA	C2A-C1A-CHA	-2.15	120.10	123.85
22	B	848	CLA	C4-C3-C5	2.15	118.89	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Z	301	CHL	O2A-CGA-CBA	2.15	120.73	112.23
22	2	304	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
22	B	830	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
25	L	302	BCR	C2-C1-C6	2.15	113.79	110.48
22	A	830	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
25	B	836	BCR	C24-C25-C26	2.15	126.66	121.46
22	Z	308	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
22	A	846	CLA	C4-C3-C5	2.15	118.88	115.27
25	B	836	BCR	C34-C9-C8	2.14	121.46	118.08
21	2	321	CHL	O2D-CGD-O1D	-2.14	119.22	124.09
22	B	809	CLA	CBB-CAB-C3B	-2.14	116.96	127.62
22	B	829	CLA	CMB-C2B-C3B	2.14	131.78	126.59
21	4	308	CHL	C2A-C1A-CHA	-2.14	120.11	123.86
22	A	842	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
21	Z	305	CHL	CHB-C1B-C2B	-2.14	121.19	127.24
22	B	803	CLA	CMB-C2B-C3B	2.14	131.77	126.59
22	B	819	CLA	CHC-C4B-NB	-2.14	121.99	124.26
22	L	306	CLA	C1-C2-C3	-2.14	122.34	126.04
22	A	846	CLA	CMC-C2C-C1C	2.14	128.30	125.04
22	X	313	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
21	Z	302	CHL	O2A-CGA-CBA	2.14	120.67	112.23
23	3	301	LUT	C32-C33-C34	2.14	122.22	118.94
22	1	304	CLA	CMB-C2B-C1B	2.14	128.62	125.37
22	A	850	CLA	C11-C12-C13	-2.13	109.02	115.92
22	A	851	CLA	C3B-C4B-NB	2.13	112.50	110.52
22	B	807	CLA	CHC-C1C-C2C	-2.13	120.80	126.73
25	J	101	BCR	C29-C30-C25	2.13	113.77	110.48
22	1	306	CLA	CMC-C2C-C1C	2.13	128.29	125.04
22	B	815	CLA	O2D-CGD-CBD	2.13	115.06	111.27
22	3	315	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
25	A	815	BCR	C29-C30-C25	2.13	113.77	110.48
25	B	835	BCR	C30-C25-C24	-2.13	109.75	115.78
22	B	802	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
22	3	315	CLA	CHC-C4B-NB	-2.13	122.00	124.26
22	A	829	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
22	3	312	CLA	CBA-CAA-C2A	-2.13	107.57	113.86
22	A	851	CLA	C5-C3-C4	2.13	119.31	114.60
22	B	819	CLA	CHB-C4A-NA	2.13	127.46	124.51
27	1	315	MGE	C7B-C6B-C5B	-2.13	103.61	114.42
23	4	319	LUT	C31-C30-C29	2.13	130.35	127.31
22	A	837	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
22	A	826	CLA	C4A-NA-C1A	2.13	107.66	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	826	CLA	CED-O2D-CGD	2.13	120.75	115.94
25	B	835	BCR	C1-C6-C5	-2.13	119.62	122.61
22	Y	314	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
22	A	836	CLA	CMB-C2B-C1B	2.13	128.61	125.37
22	A	839	CLA	CMB-C2B-C1B	2.13	128.61	125.37
22	3	311	CLA	C2A-C1A-CHA	-2.13	120.14	123.86
22	Z	314	CLA	O2A-CGA-CBA	2.12	120.63	112.23
22	B	849	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
22	3	317	CLA	O2D-CGD-O1D	-2.12	119.27	124.09
22	B	806	CLA	O2A-C1-C2	2.12	114.21	108.64
22	A	802	CLA	CHB-C4A-NA	2.12	127.45	124.51
22	A	809	CLA	CAA-C2A-C1A	2.12	118.92	111.97
22	B	812	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
25	B	835	BCR	C7-C8-C9	2.12	129.44	126.23
21	1	301	CHL	OMC-CMC-C2C	-2.12	120.90	125.69
22	B	826	CLA	CHB-C4A-NA	2.12	127.44	124.51
22	4	314	CLA	O2D-CGD-O1D	-2.12	119.28	124.09
21	4	308	CHL	C4D-CHA-C1A	-2.12	118.67	121.25
22	B	803	CLA	C3B-C4B-NB	2.12	112.48	110.52
22	A	848	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
22	4	313	CLA	O2A-CGA-O1A	-2.12	118.02	123.30
22	A	856	CLA	CHC-C4B-NB	-2.12	122.02	124.26
22	2	319	CLA	CAC-C3C-C4C	2.12	128.26	125.04
22	B	833	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
22	B	809	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
22	1	317	CLA	O2A-C1-C2	2.12	114.20	108.64
25	B	838	BCR	C24-C25-C26	-2.12	116.33	121.46
22	B	821	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
22	X	303	CLA	C2A-C1A-CHA	-2.12	120.16	123.86
22	Z	306	CLA	CMC-C2C-C1C	2.12	128.26	125.04
22	4	311	CLA	CMC-C2C-C1C	2.11	128.26	125.04
22	2	304	CLA	CHB-C1B-NB	-2.11	122.02	124.26
22	4	314	CLA	CMA-C3A-C2A	-2.11	111.17	116.10
22	A	838	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
25	L	303	BCR	C19-C18-C17	2.11	122.18	118.94
21	Z	302	CHL	C2A-C1A-CHA	-2.11	120.17	123.86
22	4	305	CLA	C2A-C1A-CHA	-2.11	120.17	123.86
22	B	819	CLA	CHB-C1B-NB	-2.11	122.02	124.26
22	Z	310	CLA	O2A-CGA-CBA	2.11	120.57	112.23
22	4	311	CLA	O2A-CGA-CBA	2.11	120.80	114.03
22	Z	313	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
21	Z	303	CHL	C4D-CHA-C1A	-2.11	118.68	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	850	CLA	CHC-C4B-NB	-2.11	122.03	124.26
22	B	851	CLA	CMB-C2B-C1B	2.11	128.58	125.37
22	2	322	CLA	C2A-C1A-CHA	-2.11	120.18	123.86
25	L	304	BCR	C1-C6-C5	-2.10	119.65	122.61
25	B	844	BCR	C30-C25-C24	-2.10	109.83	115.78
22	1	305	CLA	C2A-C1A-CHA	-2.10	120.18	123.85
22	4	306	CLA	O2D-CGD-O1D	-2.10	119.31	124.09
21	Y	304	CHL	C2A-C1A-CHA	-2.10	120.18	123.86
22	1	309	CLA	C4A-NA-C1A	2.10	107.65	106.71
22	B	829	CLA	CMC-C2C-C1C	2.10	128.24	125.04
22	A	856	CLA	CBB-CAB-C3B	-2.10	117.17	127.62
22	B	818	CLA	C5-C3-C2	-2.10	116.87	121.12
22	X	304	CLA	CHA-C4D-ND	2.10	136.89	132.50
22	1	309	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
22	2	320	CLA	CED-O2D-CGD	2.10	120.68	115.94
22	N	202	CLA	O2D-CGD-O1D	-2.10	119.33	124.09
22	A	854	CLA	CAC-C3C-C2C	2.10	131.12	127.53
22	B	830	CLA	C2A-C1A-CHA	-2.10	120.19	123.86
25	I	101	BCR	C27-C26-C25	-2.09	119.69	122.73
22	B	814	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
22	O	209	CLA	CMC-C2C-C1C	2.09	128.23	125.04
22	G	205	CLA	CAC-C3C-C4C	2.09	127.53	124.81
22	2	307	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
22	4	311	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
22	B	813	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
22	B	847	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
22	4	315	CLA	C2D-C1D-ND	2.09	111.64	110.10
22	A	833	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
22	Y	308	CLA	CED-O2D-CGD	2.09	120.66	115.94
22	B	823	CLA	CAA-CBA-CGA	-2.09	107.15	113.25
25	F	302	BCR	C19-C18-C17	2.09	122.15	118.94
31	G	201	DGD	O1G-C1A-O1A	-2.09	118.32	123.59
21	2	321	CHL	C4D-CHA-C1A	-2.09	118.71	121.25
22	A	857	CLA	C3B-C4B-NB	2.09	112.45	110.52
25	2	312	BCR	C2-C3-C4	-2.09	106.71	111.38
22	L	306	CLA	C11-C10-C8	-2.09	109.17	115.92
22	B	803	CLA	O1D-CGD-CBD	-2.09	120.22	124.48
22	1	320	CLA	C4D-C3D-CAD	2.09	110.55	108.10
21	Z	305	CHL	O1D-CGD-CBD	-2.09	120.22	124.48
22	A	859	CLA	CMB-C2B-C1B	2.09	128.54	125.37
22	Y	311	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
22	B	808	CLA	CHB-C1B-NB	-2.08	122.05	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	805	CLA	CHB-C1B-NB	-2.08	122.05	124.26
24	1	311	XAT	O24-C25-C26	-2.08	57.23	58.96
22	1	320	CLA	C2D-C1D-ND	2.08	111.64	110.10
26	4	301	LHG	O7-C5-C4	2.08	115.94	108.40
22	3	311	CLA	CED-O2D-CGD	2.08	120.64	115.94
25	L	304	BCR	C33-C5-C6	2.08	126.86	124.53
21	Y	305	CHL	C4D-CHA-C1A	-2.08	118.72	121.25
22	Y	310	CLA	O2A-CGA-CBA	2.08	120.45	112.23
22	B	810	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
22	B	823	CLA	C6-C5-C3	-2.08	108.01	113.45
22	A	855	CLA	CMD-C2D-C3D	-2.08	122.84	127.61
22	2	318	CLA	C1-C2-C3	-2.08	122.45	126.04
22	4	305	CLA	C4A-NA-C1A	2.08	107.64	106.71
22	A	841	CLA	O1D-CGD-CBD	-2.08	120.24	124.48
22	B	822	CLA	O2D-CGD-O1D	-2.07	119.78	123.84
22	B	826	CLA	CHB-C1B-C2B	-2.07	121.38	127.24
22	3	308	CLA	CAC-C3C-C2C	2.07	131.08	127.53
25	J	103	BCR	C37-C22-C23	2.07	121.34	118.08
22	B	814	CLA	C1-O2A-CGA	2.07	121.88	116.44
22	4	318	CLA	C2A-C1A-CHA	-2.07	120.24	123.86
22	K	205	CLA	CHB-C1B-C2B	-2.07	121.39	127.24
25	3	303	BCR	C20-C21-C22	2.07	130.26	127.31
22	Y	308	CLA	CBA-CAA-C2A	-2.07	107.75	113.86
22	3	318	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
22	B	825	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
22	A	804	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
22	3	309	CLA	CAA-C2A-C1A	-2.07	105.20	111.97
22	B	809	CLA	C6-C7-C8	-2.07	109.24	115.92
22	X	311	CLA	C2A-C1A-CHA	-2.07	120.25	123.86
25	F	302	BCR	C4-C5-C6	-2.07	119.73	122.73
21	3	314	CHL	CED-O2D-CGD	2.07	120.61	115.94
22	B	848	CLA	C6-C5-C3	-2.07	108.04	113.45
22	B	821	CLA	O2A-CGA-CBA	2.06	120.66	114.03
22	B	818	CLA	C7-C6-C5	-2.06	107.75	113.36
25	L	303	BCR	C24-C25-C26	-2.06	116.46	121.46
23	2	310	LUT	C12-C13-C14	2.06	122.11	118.94
22	A	802	CLA	C2A-C3A-C4A	-2.06	98.54	101.87
22	A	806	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
21	4	307	CHL	C4D-CHA-C1A	-2.06	118.74	121.25
22	A	841	CLA	O2A-CGA-CBA	2.06	120.38	112.23
21	4	317	CHL	C2A-C1A-CHA	-2.06	120.25	123.85
22	2	320	CLA	O2A-CGA-O1A	-2.06	118.39	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	829	CLA	C1-O2A-CGA	2.06	121.84	116.44
22	A	804	CLA	C4A-NA-C1A	2.06	107.63	106.71
22	A	840	CLA	CMA-C3A-C4A	-2.06	106.25	111.77
23	4	319	LUT	C35-C34-C33	2.06	130.24	127.31
25	I	101	BCR	C24-C25-C26	2.05	126.44	121.46
22	L	306	CLA	CMA-C3A-C4A	-2.05	106.25	111.77
22	4	311	CLA	CHB-C1B-C2B	-2.05	121.43	127.24
24	4	320	XAT	C39-C29-C28	2.05	121.31	118.08
22	Y	302	CLA	C2A-C1A-CHA	-2.05	120.27	123.86
22	A	830	CLA	CED-O2D-CGD	2.05	120.58	115.94
22	4	305	CLA	O2D-CGD-O1D	-2.05	119.43	124.09
22	1	304	CLA	CAC-C3C-C2C	2.05	131.04	127.53
22	3	311	CLA	O2A-CGA-CBA	2.05	120.63	114.03
22	B	825	CLA	O2A-CGA-CBA	2.05	120.34	112.23
22	B	833	CLA	CAA-CBA-CGA	-2.05	107.25	113.25
22	B	818	CLA	CMB-C2B-C3B	2.05	131.56	126.59
22	2	307	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
22	B	801	CLA	CHB-C1B-NB	-2.05	122.08	124.26
22	4	310	CLA	CED-O2D-CGD	2.05	120.58	115.94
22	1	303	CLA	C2A-C1A-CHA	-2.05	120.27	123.86
22	B	852	CLA	C2A-C1A-CHA	-2.05	120.28	123.86
25	B	839	BCR	C11-C10-C9	2.05	130.23	127.31
25	B	836	BCR	C7-C6-C5	-2.05	116.50	121.46
22	A	853	CLA	CMB-C2B-C3B	2.05	131.55	126.59
21	X	302	CHL	C2A-C1A-CHA	-2.05	120.28	123.86
22	X	312	CLA	C2A-C1A-CHA	-2.05	120.28	123.86
22	B	801	CLA	C4-C3-C5	2.05	118.71	115.27
22	B	853	CLA	C2A-C1A-CHA	-2.05	120.28	123.86
22	J	102	CLA	C2A-C1A-CHA	-2.05	120.28	123.86
22	B	810	CLA	CMC-C2C-C1C	2.04	128.15	125.04
22	L	305	CLA	C2A-C1A-CHA	-2.04	120.28	123.86
21	4	308	CHL	CHB-C1B-C2B	-2.04	121.46	127.24
22	4	304	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
22	4	312	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
22	A	832	CLA	CMC-C2C-C1C	2.04	128.15	125.04
21	4	307	CHL	CAA-C2A-C3A	-2.04	107.19	112.78
22	Y	312	CLA	C4A-NA-C1A	2.04	107.62	106.71
21	2	321	CHL	CBA-CAA-C2A	-2.04	107.84	113.86
22	B	814	CLA	C6-C5-C3	-2.04	108.10	113.45
22	A	835	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
22	Y	310	CLA	CED-O2D-CGD	2.04	120.56	115.94
22	A	844	CLA	O1D-CGD-CBD	-2.04	120.31	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	306	CLA	CED-O2D-CGD	2.04	120.55	115.94
25	4	321	BCR	C34-C9-C8	2.04	121.29	118.08
24	1	311	XAT	C10-C11-C12	-2.04	116.85	123.22
23	1	310	LUT	C2-C3-C4	-2.04	107.51	110.30
22	B	815	CLA	C2A-C1A-CHA	-2.04	120.29	123.86
22	A	854	CLA	C2D-C1D-ND	2.04	111.61	110.10
22	2	308	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
22	B	819	CLA	C4D-C3D-CAD	2.04	110.50	108.10
21	4	309	CHL	C4D-CHA-C1A	-2.04	118.77	121.25
27	3	304	MGE	O6D-C1D-O3G	2.04	114.80	109.97
22	2	320	CLA	C5-C3-C4	2.04	119.10	114.60
22	Y	302	CLA	O2A-CGA-CBA	2.04	120.28	112.23
22	B	812	CLA	CED-O2D-CGD	2.04	120.54	115.94
22	Y	311	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
21	X	306	CHL	C4D-CHA-C1A	-2.03	118.77	121.25
21	Y	307	CHL	C4D-CHA-C1A	-2.03	118.78	121.25
22	A	845	CLA	C4C-C3C-C2C	-2.03	103.93	106.90
22	3	309	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
22	A	812	CLA	C2A-C1A-CHA	-2.03	120.31	123.86
22	X	311	CLA	O2A-CGA-CBA	2.03	120.25	112.23
25	B	837	BCR	C27-C26-C25	-2.03	119.78	122.73
22	B	827	CLA	CBA-CAA-C2A	2.03	119.85	113.86
21	2	302	CHL	O2A-CGA-CBA	2.03	120.25	112.23
25	B	838	BCR	C8-C9-C10	-2.03	115.83	118.94
24	3	302	XAT	O4-C5-C6	-2.03	57.28	58.96
22	1	303	CLA	O2A-CGA-CBA	2.03	120.54	114.03
25	A	817	BCR	C21-C20-C19	2.03	129.54	123.22
21	Y	305	CHL	CED-O2D-CGD	2.03	120.52	115.94
22	L	307	CLA	CED-O2D-CGD	2.03	120.52	115.94
22	3	321	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
22	3	308	CLA	CMC-C2C-C1C	2.03	128.12	125.04
22	2	317	CLA	CMB-C2B-C1B	2.02	128.45	125.37
22	Z	308	CLA	O2A-CGA-CBA	2.02	120.23	112.23
22	4	314	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
22	Z	313	CLA	C2A-C1A-CHA	-2.02	120.32	123.86
25	L	302	BCR	C23-C22-C21	2.02	122.05	118.94
22	2	304	CLA	C6-C5-C3	-2.02	108.15	113.45
22	1	304	CLA	C3B-C4B-NB	2.02	112.39	110.52
22	B	817	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
22	A	855	CLA	CHB-C4A-NA	2.02	127.31	124.51
25	J	101	BCR	C7-C6-C5	-2.02	116.57	121.46
21	4	309	CHL	CHB-C1B-C2B	-2.02	121.53	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	J	101	BCR	C24-C23-C22	2.02	129.29	126.23
25	J	103	BCR	C2-C1-C6	2.02	113.59	110.48
25	A	815	BCR	C4-C5-C6	-2.02	119.80	122.73
21	X	306	CHL	O2A-CGA-CBA	2.02	120.21	112.23
22	B	826	CLA	CHB-C1B-NB	-2.02	122.12	124.26
22	X	301	CLA	O2A-CGA-CBA	2.02	120.20	112.23
22	O	207	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
25	J	103	BCR	C7-C6-C5	-2.02	116.58	121.46
22	B	845	CLA	C4-C3-C2	-2.02	118.50	123.68
22	K	205	CLA	CHC-C4B-NB	-2.02	122.12	124.26
23	3	301	LUT	C35-C15-C14	2.02	127.60	123.47
21	Z	302	CHL	CHB-C1B-C2B	-2.02	121.55	127.24
25	4	321	BCR	C24-C25-C26	-2.01	116.58	121.46
22	A	801	CLA	O2D-CGD-O1D	-2.01	119.90	123.84
31	O	201	DGD	C2G-O2G-C1B	-2.01	112.83	117.79
25	B	835	BCR	C10-C11-C12	2.01	129.50	123.22
22	A	858	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
22	A	848	CLA	O2A-CGA-CBA	2.01	120.50	114.03
21	Y	307	CHL	O2A-CGA-CBA	2.01	120.50	114.03
21	1	301	CHL	CAA-C2A-C3A	-2.01	109.23	114.26
22	3	317	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
22	2	317	CLA	C2A-C1A-CHA	-2.01	120.34	123.85
21	X	305	CHL	C2A-C1A-CHA	-2.01	120.34	123.86
22	A	855	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
21	Z	303	CHL	CHB-C1B-C2B	-2.01	121.55	127.24
22	B	851	CLA	CAA-CBA-CGA	-2.01	107.37	113.25
27	1	315	MGE	O6D-C1D-O3G	2.01	114.74	109.97
22	A	808	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
27	F	303	MGE	O3G-C1D-C2D	2.01	111.44	108.30
25	B	838	BCR	C20-C21-C22	2.01	130.18	127.31
25	K	201	BCR	C29-C30-C25	2.01	113.57	110.48
21	4	308	CHL	O2D-CGD-O1D	-2.01	119.53	124.09
22	A	846	CLA	CMB-C2B-C3B	2.01	131.45	126.59
25	O	203	BCR	C1-C6-C5	-2.01	119.79	122.61
22	4	318	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
22	1	304	CLA	CMD-C2D-C3D	-2.01	123.00	127.61
22	B	850	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
22	Y	308	CLA	O2A-CGA-CBA	2.00	120.15	112.23
22	L	305	CLA	O2A-CGA-CBA	2.00	120.47	114.03
21	1	316	CHL	CMD-C2D-C3D	-2.00	123.00	127.61
22	Y	301	CLA	O2A-CGA-CBA	2.00	120.15	112.23
25	I	101	BCR	C21-C20-C19	2.00	129.47	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	814	CLA	C4D-C3D-CAD	2.00	110.46	108.10
22	1	319	CLA	CBB-CAB-C3B	-2.00	117.65	127.62
22	B	825	CLA	CAA-CBA-CGA	-2.00	107.40	113.25
22	A	801	CLA	CMA-C3A-C4A	-2.00	106.39	111.77
22	B	830	CLA	CED-O2D-CGD	2.00	120.47	115.94
22	4	314	CLA	C2A-C1A-CHA	-2.00	120.36	123.85
22	4	312	CLA	CED-O2D-CGD	2.00	120.47	115.94
22	A	807	CLA	C4-C3-C5	2.00	118.64	115.27
22	3	312	CLA	C4D-C3D-CAD	2.00	110.46	108.10
22	F	305	CLA	O2A-CGA-CBA	2.00	120.14	112.23
22	A	830	CLA	CHC-C1C-NC	2.00	127.24	124.20
22	A	839	CLA	CMB-C2B-C3B	2.00	131.43	126.59
24	3	302	XAT	C39-C29-C28	-2.00	114.92	118.08
25	K	201	BCR	C33-C5-C6	2.00	126.77	124.53

All (72) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	1	307	CLA	C8
22	1	317	CLA	C8
22	1	318	CLA	C8
22	2	304	CLA	C8
22	2	307	CLA	C8
22	2	318	CLA	C8
22	3	309	CLA	C8
22	3	310	CLA	C8
22	3	312	CLA	C8
22	4	304	CLA	C8
22	A	801	CLA	C8
22	A	802	CLA	C8
22	A	803	CLA	C8
22	A	807	CLA	C8
22	A	808	CLA	C8
22	A	809	CLA	C8
22	A	810	CLA	C8
22	A	812	CLA	C8
22	A	826	CLA	C8
22	A	827	CLA	C8
22	A	831	CLA	C8
22	A	833	CLA	C8
22	A	836	CLA	C8
22	A	838	CLA	C8

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Mol	Chain	Res	Type	Atom
22	A	842	CLA	C8
22	A	843	CLA	C8
22	A	844	CLA	C8
22	A	846	CLA	C8
22	A	849	CLA	C8
22	A	850	CLA	C8
22	A	852	CLA	C8
22	A	853	CLA	C8
22	A	854	CLA	C8
22	A	855	CLA	C8
22	A	857	CLA	C8
22	A	858	CLA	C8
22	A	859	CLA	C8
22	B	801	CLA	C8
22	B	803	CLA	C8
22	B	804	CLA	C8
22	B	806	CLA	C8
22	B	807	CLA	C8
22	B	808	CLA	C8
22	B	809	CLA	C8
22	B	811	CLA	C8
22	B	812	CLA	C8
22	B	814	CLA	C8
22	B	815	CLA	C8
22	B	816	CLA	C8
22	B	817	CLA	C8
22	B	818	CLA	C8
22	B	819	CLA	C8
22	B	822	CLA	C8
22	B	823	CLA	C8
22	B	824	CLA	C8
22	B	827	CLA	C8
22	B	829	CLA	C8
22	B	830	CLA	C8
22	B	831	CLA	C8
22	B	833	CLA	C8
22	B	845	CLA	C8
22	B	847	CLA	C8
22	B	848	CLA	C8
22	B	850	CLA	C8
22	B	851	CLA	C8
22	B	852	CLA	C8

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Mol	Chain	Res	Type	Atom
22	K	203	CLA	C8
22	L	306	CLA	C8
22	O	207	CLA	C8
22	O	208	CLA	C8
22	Y	311	CLA	C8
30	A	825	CL0	CBD

All (2014) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	1	301	CHL	C1A-C2A-CAA-CBA
21	1	301	CHL	C3A-C2A-CAA-CBA
21	1	301	CHL	C1C-C2C-CMC-OMC
21	1	301	CHL	C3C-C2C-CMC-OMC
21	1	301	CHL	CBD-CGD-O2D-CED
21	2	301	CHL	C1C-C2C-CMC-OMC
21	2	301	CHL	C3C-C2C-CMC-OMC
21	2	302	CHL	C1A-C2A-CAA-CBA
21	2	302	CHL	C3A-C2A-CAA-CBA
21	2	302	CHL	C2B-C3B-CAB-CBB
21	2	302	CHL	C4B-C3B-CAB-CBB
21	2	302	CHL	CBD-CGD-O2D-CED
21	2	321	CHL	C1C-C2C-CMC-OMC
21	2	321	CHL	C3C-C2C-CMC-OMC
21	3	307	CHL	C1C-C2C-CMC-OMC
21	3	307	CHL	C3C-C2C-CMC-OMC
21	3	307	CHL	CBD-CGD-O2D-CED
21	4	307	CHL	C2B-C3B-CAB-CBB
21	4	307	CHL	C4B-C3B-CAB-CBB
21	4	307	CHL	C3C-C2C-CMC-OMC
21	4	308	CHL	C3C-C2C-CMC-OMC
21	4	309	CHL	C1A-C2A-CAA-CBA
21	4	309	CHL	C3A-C2A-CAA-CBA
21	4	309	CHL	C2B-C3B-CAB-CBB
21	4	309	CHL	C4B-C3B-CAB-CBB
21	4	309	CHL	C1C-C2C-CMC-OMC
21	4	309	CHL	C3C-C2C-CMC-OMC
21	X	305	CHL	C3C-C2C-CMC-OMC
21	X	306	CHL	C2A-CAA-CBA-CGA
21	X	308	CHL	C2A-CAA-CBA-CGA
21	X	308	CHL	C3C-C2C-CMC-OMC
21	X	309	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
21	X	309	CHL	C3C-C2C-CMC-OMC
21	Y	303	CHL	C3C-C2C-CMC-OMC
21	Y	304	CHL	C1C-C2C-CMC-OMC
21	Y	304	CHL	C3C-C2C-CMC-OMC
21	Y	307	CHL	C3C-C2C-CMC-OMC
21	Y	313	CHL	C1A-C2A-CAA-CBA
21	Y	313	CHL	C3A-C2A-CAA-CBA
21	Y	313	CHL	C3C-C2C-CMC-OMC
21	Z	301	CHL	C3C-C2C-CMC-OMC
21	Z	305	CHL	C2A-CAA-CBA-CGA
21	Z	305	CHL	C1C-C2C-CMC-OMC
21	Z	305	CHL	C3C-C2C-CMC-OMC
21	Z	312	CHL	C3C-C2C-CMC-OMC
22	1	303	CLA	C1A-C2A-CAA-CBA
22	1	303	CLA	CHA-CBD-CGD-O1D
22	1	303	CLA	CHA-CBD-CGD-O2D
22	1	304	CLA	CBD-CGD-O2D-CED
22	1	304	CLA	C2-C3-C5-C6
22	1	304	CLA	C4-C3-C5-C6
22	1	317	CLA	CHA-CBD-CGD-O1D
22	1	317	CLA	CHA-CBD-CGD-O2D
22	1	317	CLA	C2-C3-C5-C6
22	1	317	CLA	C4-C3-C5-C6
22	2	303	CLA	C3A-C2A-CAA-CBA
22	2	307	CLA	CHA-CBD-CGD-O1D
22	2	307	CLA	CHA-CBD-CGD-O2D
22	2	318	CLA	C1A-C2A-CAA-CBA
22	2	318	CLA	C3A-C2A-CAA-CBA
22	2	318	CLA	C2B-C3B-CAB-CBB
22	2	318	CLA	C4B-C3B-CAB-CBB
22	2	318	CLA	C2-C3-C5-C6
22	2	318	CLA	C4-C3-C5-C6
22	3	308	CLA	C2B-C3B-CAB-CBB
22	3	308	CLA	C4B-C3B-CAB-CBB
22	3	309	CLA	C2B-C3B-CAB-CBB
22	3	309	CLA	C4B-C3B-CAB-CBB
22	3	309	CLA	C4-C3-C5-C6
22	3	310	CLA	CBD-CGD-O2D-CED
22	3	312	CLA	C2-C3-C5-C6
22	3	312	CLA	C4-C3-C5-C6
22	3	315	CLA	CBD-CGD-O2D-CED
22	3	316	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	3	316	CLA	C3A-C2A-CAA-CBA
22	3	316	CLA	C2B-C3B-CAB-CBB
22	3	316	CLA	C4B-C3B-CAB-CBB
22	4	306	CLA	C1A-C2A-CAA-CBA
22	4	306	CLA	C4B-C3B-CAB-CBB
22	4	310	CLA	C1A-C2A-CAA-CBA
22	4	310	CLA	C3A-C2A-CAA-CBA
22	4	311	CLA	C1A-C2A-CAA-CBA
22	4	311	CLA	C3A-C2A-CAA-CBA
22	4	312	CLA	CHA-CBD-CGD-O1D
22	4	312	CLA	CHA-CBD-CGD-O2D
22	4	315	CLA	C1A-C2A-CAA-CBA
22	4	318	CLA	CHA-CBD-CGD-O1D
22	4	318	CLA	CHA-CBD-CGD-O2D
22	A	801	CLA	CBD-CGD-O2D-CED
22	A	803	CLA	C1A-C2A-CAA-CBA
22	A	805	CLA	CBD-CGD-O2D-CED
22	A	808	CLA	C14-C13-C15-C16
22	A	809	CLA	C1A-C2A-CAA-CBA
22	A	810	CLA	C1A-C2A-CAA-CBA
22	A	810	CLA	C2-C3-C5-C6
22	A	810	CLA	C4-C3-C5-C6
22	A	812	CLA	CHA-CBD-CGD-O1D
22	A	812	CLA	CHA-CBD-CGD-O2D
22	A	812	CLA	CAD-CBD-CGD-O1D
22	A	826	CLA	C2-C3-C5-C6
22	A	826	CLA	C4-C3-C5-C6
22	A	827	CLA	C1A-C2A-CAA-CBA
22	A	829	CLA	C1A-C2A-CAA-CBA
22	A	833	CLA	CHA-CBD-CGD-O1D
22	A	833	CLA	CHA-CBD-CGD-O2D
22	A	834	CLA	C2B-C3B-CAB-CBB
22	A	834	CLA	C4B-C3B-CAB-CBB
22	A	835	CLA	CBD-CGD-O2D-CED
22	A	837	CLA	C1A-C2A-CAA-CBA
22	A	838	CLA	C2-C3-C5-C6
22	A	838	CLA	C4-C3-C5-C6
22	A	839	CLA	C1A-C2A-CAA-CBA
22	A	839	CLA	C3A-C2A-CAA-CBA
22	A	840	CLA	C3A-C2A-CAA-CBA
22	A	842	CLA	C4B-C3B-CAB-CBB
22	A	843	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	A	843	CLA	C3A-C2A-CAA-CBA
22	A	844	CLA	C2-C3-C5-C6
22	A	844	CLA	C4-C3-C5-C6
22	A	847	CLA	C3A-C2A-CAA-CBA
22	A	849	CLA	C1A-C2A-CAA-CBA
22	A	850	CLA	CHA-CBD-CGD-O1D
22	A	850	CLA	CHA-CBD-CGD-O2D
22	A	851	CLA	C2B-C3B-CAB-CBB
22	A	851	CLA	C4B-C3B-CAB-CBB
22	A	852	CLA	C1A-C2A-CAA-CBA
22	A	852	CLA	C2-C1-O2A-CGA
22	A	852	CLA	CHA-CBD-CGD-O1D
22	A	852	CLA	CHA-CBD-CGD-O2D
22	A	852	CLA	C4-C3-C5-C6
22	A	853	CLA	CBD-CGD-O2D-CED
22	A	853	CLA	C2-C3-C5-C6
22	A	853	CLA	C4-C3-C5-C6
22	A	854	CLA	C1A-C2A-CAA-CBA
22	A	856	CLA	C4-C3-C5-C6
22	A	857	CLA	C2B-C3B-CAB-CBB
22	A	857	CLA	C4B-C3B-CAB-CBB
22	A	858	CLA	C4B-C3B-CAB-CBB
22	A	858	CLA	CBD-CGD-O2D-CED
22	B	801	CLA	CBD-CGD-O2D-CED
22	B	803	CLA	C1A-C2A-CAA-CBA
22	B	803	CLA	C3A-C2A-CAA-CBA
22	B	805	CLA	C1A-C2A-CAA-CBA
22	B	806	CLA	CBD-CGD-O2D-CED
22	B	808	CLA	C1A-C2A-CAA-CBA
22	B	808	CLA	C3A-C2A-CAA-CBA
22	B	809	CLA	C4B-C3B-CAB-CBB
22	B	809	CLA	CHA-CBD-CGD-O1D
22	B	809	CLA	CHA-CBD-CGD-O2D
22	B	809	CLA	CBD-CGD-O2D-CED
22	B	813	CLA	CHA-CBD-CGD-O1D
22	B	813	CLA	CHA-CBD-CGD-O2D
22	B	814	CLA	C2B-C3B-CAB-CBB
22	B	814	CLA	C4B-C3B-CAB-CBB
22	B	815	CLA	C4-C3-C5-C6
22	B	817	CLA	C2B-C3B-CAB-CBB
22	B	817	CLA	C4B-C3B-CAB-CBB
22	B	819	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	B	821	CLA	C1A-C2A-CAA-CBA
22	B	821	CLA	C3A-C2A-CAA-CBA
22	B	822	CLA	CBD-CGD-O2D-CED
22	B	824	CLA	CBD-CGD-O2D-CED
22	B	825	CLA	C3A-C2A-CAA-CBA
22	B	828	CLA	CBD-CGD-O2D-CED
22	B	829	CLA	C2B-C3B-CAB-CBB
22	B	829	CLA	C4B-C3B-CAB-CBB
22	B	831	CLA	C1A-C2A-CAA-CBA
22	B	831	CLA	CHA-CBD-CGD-O1D
22	B	831	CLA	CHA-CBD-CGD-O2D
22	B	831	CLA	CBD-CGD-O2D-CED
22	B	833	CLA	C2A-CAA-CBA-CGA
22	B	845	CLA	C2A-CAA-CBA-CGA
22	B	845	CLA	CHA-CBD-CGD-O1D
22	B	845	CLA	CHA-CBD-CGD-O2D
22	B	845	CLA	CBD-CGD-O2D-CED
22	B	846	CLA	C4B-C3B-CAB-CBB
22	B	847	CLA	C1A-C2A-CAA-CBA
22	B	847	CLA	C3A-C2A-CAA-CBA
22	B	850	CLA	C1A-C2A-CAA-CBA
22	B	851	CLA	C1A-C2A-CAA-CBA
22	B	853	CLA	C1A-C2A-CAA-CBA
22	B	853	CLA	C4B-C3B-CAB-CBB
22	B	853	CLA	C2-C3-C5-C6
22	B	853	CLA	C4-C3-C5-C6
22	G	205	CLA	C4B-C3B-CAB-CBB
22	G	205	CLA	CHA-CBD-CGD-O1D
22	G	205	CLA	CHA-CBD-CGD-O2D
22	G	205	CLA	CAD-CBD-CGD-O1D
22	G	206	CLA	C2-C3-C5-C6
22	G	206	CLA	C4-C3-C5-C6
22	G	207	CLA	C2B-C3B-CAB-CBB
22	G	207	CLA	C4B-C3B-CAB-CBB
22	G	207	CLA	CHA-CBD-CGD-O1D
22	G	207	CLA	CHA-CBD-CGD-O2D
22	K	203	CLA	C1A-C2A-CAA-CBA
22	K	203	CLA	C2B-C3B-CAB-CBB
22	K	203	CLA	C4B-C3B-CAB-CBB
22	K	204	CLA	C1A-C2A-CAA-CBA
22	K	204	CLA	C3A-C2A-CAA-CBA
22	K	205	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	K	205	CLA	C4B-C3B-CAB-CBB
22	L	305	CLA	C2B-C3B-CAB-CBB
22	L	305	CLA	C4B-C3B-CAB-CBB
22	L	306	CLA	C2B-C3B-CAB-CBB
22	L	306	CLA	C4B-C3B-CAB-CBB
22	L	307	CLA	C2B-C3B-CAB-CBB
22	L	307	CLA	C4B-C3B-CAB-CBB
22	O	208	CLA	C1A-C2A-CAA-CBA
22	O	208	CLA	C3A-C2A-CAA-CBA
22	O	209	CLA	C1A-C2A-CAA-CBA
22	X	304	CLA	C1A-C2A-CAA-CBA
22	X	304	CLA	CAD-CBD-CGD-O1D
22	Y	314	CLA	CHA-CBD-CGD-O1D
22	Y	314	CLA	CHA-CBD-CGD-O2D
22	Z	309	CLA	C1A-C2A-CAA-CBA
22	Z	313	CLA	CHA-CBD-CGD-O1D
22	Z	313	CLA	CHA-CBD-CGD-O2D
22	Z	314	CLA	C1A-C2A-CAA-CBA
23	2	310	LUT	C7-C8-C9-C19
23	2	310	LUT	C29-C30-C31-C32
24	1	311	XAT	O4-C6-C7-C8
24	1	311	XAT	C7-C8-C9-C10
24	1	311	XAT	C7-C8-C9-C19
24	1	311	XAT	C13-C14-C15-C35
24	1	311	XAT	C21-C26-C27-C28
24	2	311	XAT	C1-C6-C7-C8
24	3	302	XAT	C27-C28-C29-C30
24	3	302	XAT	C27-C28-C29-C39
24	4	320	XAT	C27-C28-C29-C30
24	4	320	XAT	C27-C28-C29-C39
25	1	312	BCR	C36-C18-C19-C20
25	2	312	BCR	C7-C8-C9-C10
25	2	312	BCR	C7-C8-C9-C34
25	2	312	BCR	C36-C18-C19-C20
25	4	321	BCR	C37-C22-C23-C24
25	A	817	BCR	C21-C22-C23-C24
25	A	817	BCR	C37-C22-C23-C24
25	A	817	BCR	C23-C24-C25-C26
25	A	817	BCR	C23-C24-C25-C30
25	A	819	BCR	C23-C24-C25-C26
25	A	819	BCR	C23-C24-C25-C30
25	B	834	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
25	B	835	BCR	C23-C24-C25-C26
25	B	835	BCR	C23-C24-C25-C30
25	G	202	BCR	C37-C22-C23-C24
25	G	202	BCR	C22-C23-C24-C25
25	J	101	BCR	C7-C8-C9-C34
25	J	103	BCR	C7-C8-C9-C10
25	L	301	BCR	C7-C8-C9-C34
25	O	203	BCR	C11-C12-C13-C14
25	O	203	BCR	C11-C12-C13-C35
26	1	313	LHG	C4-O6-P-O5
26	1	313	LHG	O10-C23-O8-C6
26	1	313	LHG	C24-C23-O8-C6
26	2	313	LHG	O9-C7-O7-C5
26	2	313	LHG	C8-C7-O7-C5
26	2	315	LHG	C3-O3-P-O5
26	2	315	LHG	C3-O3-P-O6
26	2	315	LHG	C4-O6-P-O4
26	3	306	LHG	O10-C23-O8-C6
26	3	306	LHG	C24-C23-O8-C6
26	4	301	LHG	C4-O6-P-O5
26	4	302	LHG	C3-O3-P-O5
26	4	302	LHG	O10-C23-O8-C6
26	4	302	LHG	C24-C23-O8-C6
26	A	820	LHG	O2-C2-C3-O3
26	A	820	LHG	C3-O3-P-O5
26	A	820	LHG	C3-O3-P-O6
26	A	822	LHG	C5-C4-O6-P
26	A	824	LHG	C4-O6-P-O5
26	A	824	LHG	O7-C5-C6-O8
26	B	843	LHG	C4-O6-P-O5
26	B	843	LHG	C8-C7-O7-C5
26	F	301	LHG	O9-C7-O7-C5
26	F	301	LHG	C8-C7-O7-C5
26	G	203	LHG	O10-C23-O8-C6
26	G	203	LHG	C24-C23-O8-C6
26	X	314	LHG	C3-O3-P-O5
27	1	315	MGE	C2D-C1D-O3G-C3G
27	1	315	MGE	O6D-C1D-O3G-C3G
27	3	305	MGE	O1B-C1B-O2G-C2G
27	F	303	MGE	C2D-C1D-O3G-C3G
30	A	825	CL0	C1A-C2A-CAA-CBA
31	B	841	DGD	C2B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
31	B	841	DGD	O2G-C2G-C3G-O3G
31	J	104	DGD	C2B-C1B-O2G-C2G
21	3	307	CHL	O1D-CGD-O2D-CED
21	4	309	CHL	O1D-CGD-O2D-CED
22	A	834	CLA	O1D-CGD-O2D-CED
22	A	858	CLA	O1D-CGD-O2D-CED
22	B	801	CLA	O1D-CGD-O2D-CED
22	B	845	CLA	O1D-CGD-O2D-CED
22	B	803	CLA	C4C-C3C-CAC-CBC
22	B	830	CLA	C2C-C3C-CAC-CBC
21	2	302	CHL	O1D-CGD-O2D-CED
22	A	805	CLA	O1D-CGD-O2D-CED
30	A	825	CL0	O1D-CGD-O2D-CED
21	4	309	CHL	CBD-CGD-O2D-CED
22	1	303	CLA	CBD-CGD-O2D-CED
22	1	307	CLA	CBD-CGD-O2D-CED
22	2	307	CLA	CBD-CGD-O2D-CED
22	A	802	CLA	CBD-CGD-O2D-CED
22	A	807	CLA	CBD-CGD-O2D-CED
22	A	808	CLA	CBD-CGD-O2D-CED
22	A	812	CLA	CBD-CGD-O2D-CED
22	A	826	CLA	CBD-CGD-O2D-CED
22	A	827	CLA	CBD-CGD-O2D-CED
22	A	834	CLA	CBD-CGD-O2D-CED
22	A	846	CLA	CBD-CGD-O2D-CED
22	A	849	CLA	CBD-CGD-O2D-CED
22	A	854	CLA	CBD-CGD-O2D-CED
22	A	859	CLA	CBD-CGD-O2D-CED
22	B	821	CLA	CBD-CGD-O2D-CED
22	B	825	CLA	CBD-CGD-O2D-CED
22	B	827	CLA	CBD-CGD-O2D-CED
22	B	830	CLA	CBD-CGD-O2D-CED
22	F	306	CLA	CBD-CGD-O2D-CED
30	A	825	CL0	CBD-CGD-O2D-CED
22	B	814	CLA	O1A-CGA-O2A-C1
22	O	208	CLA	O1A-CGA-O2A-C1
22	B	830	CLA	C4C-C3C-CAC-CBC
22	A	801	CLA	O1D-CGD-O2D-CED
22	A	846	CLA	O1D-CGD-O2D-CED
22	B	809	CLA	O1D-CGD-O2D-CED
22	B	821	CLA	O1D-CGD-O2D-CED
22	F	306	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	1	301	CHL	O1D-CGD-O2D-CED
22	1	307	CLA	O1D-CGD-O2D-CED
22	3	315	CLA	O1D-CGD-O2D-CED
22	A	812	CLA	O1D-CGD-O2D-CED
22	A	826	CLA	O1D-CGD-O2D-CED
22	A	853	CLA	O1D-CGD-O2D-CED
22	A	859	CLA	O1D-CGD-O2D-CED
22	B	831	CLA	O1D-CGD-O2D-CED
22	B	814	CLA	CBA-CGA-O2A-C1
22	O	208	CLA	CBA-CGA-O2A-C1
21	2	309	CHL	CBD-CGD-O2D-CED
21	X	308	CHL	CBD-CGD-O2D-CED
21	Z	303	CHL	CBD-CGD-O2D-CED
22	2	304	CLA	CBD-CGD-O2D-CED
22	2	317	CLA	CBD-CGD-O2D-CED
22	4	311	CLA	CBD-CGD-O2D-CED
22	B	848	CLA	CBD-CGD-O2D-CED
22	B	803	CLA	C2C-C3C-CAC-CBC
22	3	310	CLA	O1A-CGA-O2A-C1
22	B	845	CLA	O1A-CGA-O2A-C1
22	B	852	CLA	O1A-CGA-O2A-C1
27	F	303	MGE	O1A-C1A-O1G-C1G
27	F	304	MGE	O1A-C1A-O1G-C1G
22	B	822	CLA	O1D-CGD-O2D-CED
22	B	824	CLA	O1D-CGD-O2D-CED
22	B	828	CLA	O1D-CGD-O2D-CED
22	A	838	CLA	C4C-C3C-CAC-CBC
22	3	310	CLA	O1D-CGD-O2D-CED
21	Y	305	CHL	CBD-CGD-O2D-CED
22	4	316	CLA	CBD-CGD-O2D-CED
22	G	205	CLA	CBD-CGD-O2D-CED
22	Z	313	CLA	CBD-CGD-O2D-CED
22	1	304	CLA	O1D-CGD-O2D-CED
26	B	843	LHG	O9-C7-O7-C5
31	B	841	DGD	O1B-C1B-O2G-C2G
31	J	104	DGD	O1B-C1B-O2G-C2G
22	B	847	CLA	O1A-CGA-O2A-C1
22	1	307	CLA	C3-C5-C6-C7
22	A	803	CLA	C3-C5-C6-C7
22	A	808	CLA	C3-C5-C6-C7
22	A	809	CLA	C3-C5-C6-C7
22	A	810	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	A	812	CLA	C3-C5-C6-C7
22	A	833	CLA	C3-C5-C6-C7
22	A	838	CLA	C3-C5-C6-C7
22	A	843	CLA	C3-C5-C6-C7
22	A	850	CLA	C3-C5-C6-C7
22	A	855	CLA	C3-C5-C6-C7
22	B	803	CLA	C3-C5-C6-C7
22	B	804	CLA	C3-C5-C6-C7
22	B	806	CLA	C3-C5-C6-C7
22	B	809	CLA	C3-C5-C6-C7
22	B	811	CLA	C3-C5-C6-C7
22	B	812	CLA	C3-C5-C6-C7
22	B	813	CLA	C3-C5-C6-C7
22	B	816	CLA	C3-C5-C6-C7
22	B	819	CLA	C3-C5-C6-C7
22	B	823	CLA	C3-C5-C6-C7
22	B	824	CLA	C3-C5-C6-C7
22	B	833	CLA	C3-C5-C6-C7
22	G	206	CLA	C3-C5-C6-C7
22	O	207	CLA	C3-C5-C6-C7
22	Y	311	CLA	C3-C5-C6-C7
22	A	829	CLA	CBA-CGA-O2A-C1
22	B	823	CLA	CBA-CGA-O2A-C1
22	B	845	CLA	CBA-CGA-O2A-C1
22	B	852	CLA	CBA-CGA-O2A-C1
27	F	303	MGE	C2A-C1A-O1G-C1G
27	F	304	MGE	C2A-C1A-O1G-C1G
27	3	305	MGE	C2B-C1B-O2G-C2G
22	B	806	CLA	O1D-CGD-O2D-CED
21	Z	305	CHL	CBD-CGD-O2D-CED
22	3	316	CLA	CBD-CGD-O2D-CED
22	A	838	CLA	C2C-C3C-CAC-CBC
22	X	313	CLA	CBA-CGA-O2A-C1
22	B	853	CLA	C3-C5-C6-C7
22	A	833	CLA	C4-C3-C5-C6
22	A	836	CLA	C4-C3-C5-C6
22	B	806	CLA	C4-C3-C5-C6
22	B	813	CLA	C4-C3-C5-C6
22	B	818	CLA	C4-C3-C5-C6
22	3	309	CLA	C2-C3-C5-C6
22	A	836	CLA	C2-C3-C5-C6
22	A	852	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	B	815	CLA	C2-C3-C5-C6
21	Y	306	CHL	CBD-CGD-O2D-CED
22	1	308	CLA	CBD-CGD-O2D-CED
22	B	819	CLA	CBD-CGD-O2D-CED
21	X	302	CHL	C2A-CAA-CBA-CGA
21	X	307	CHL	C2A-CAA-CBA-CGA
21	Y	304	CHL	C2A-CAA-CBA-CGA
21	Y	306	CHL	C2A-CAA-CBA-CGA
21	Y	313	CHL	C2A-CAA-CBA-CGA
21	Z	303	CHL	C2A-CAA-CBA-CGA
21	Z	304	CHL	C2A-CAA-CBA-CGA
21	Z	312	CHL	C2A-CAA-CBA-CGA
22	2	308	CLA	C2A-CAA-CBA-CGA
22	A	803	CLA	C2A-CAA-CBA-CGA
22	A	810	CLA	C2A-CAA-CBA-CGA
22	A	833	CLA	C2A-CAA-CBA-CGA
22	B	825	CLA	C2A-CAA-CBA-CGA
22	L	306	CLA	C2A-CAA-CBA-CGA
22	A	826	CLA	C3-C5-C6-C7
22	B	801	CLA	C3-C5-C6-C7
22	B	831	CLA	C3-C5-C6-C7
22	B	845	CLA	C3-C5-C6-C7
22	B	851	CLA	C3-C5-C6-C7
22	L	306	CLA	C3-C5-C6-C7
22	O	208	CLA	C3-C5-C6-C7
22	3	310	CLA	CBA-CGA-O2A-C1
22	B	833	CLA	CBA-CGA-O2A-C1
26	B	843	LHG	C10-C11-C12-C13
22	A	835	CLA	O1D-CGD-O2D-CED
22	B	827	CLA	O1D-CGD-O2D-CED
22	1	303	CLA	O1D-CGD-O2D-CED
22	2	307	CLA	O1D-CGD-O2D-CED
22	A	808	CLA	O1D-CGD-O2D-CED
22	A	829	CLA	O1A-CGA-O2A-C1
22	A	852	CLA	O1A-CGA-O2A-C1
22	B	803	CLA	O1A-CGA-O2A-C1
22	B	807	CLA	O1A-CGA-O2A-C1
22	B	823	CLA	O1A-CGA-O2A-C1
22	B	833	CLA	O1A-CGA-O2A-C1
22	B	825	CLA	O1D-CGD-O2D-CED
25	1	312	BCR	C15-C16-C17-C18
25	1	312	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
25	2	312	BCR	C9-C10-C11-C12
25	B	840	BCR	C15-C16-C17-C18
25	G	202	BCR	C19-C20-C21-C22
21	X	302	CHL	CBD-CGD-O2D-CED
21	Y	313	CHL	CBD-CGD-O2D-CED
21	Z	312	CHL	CBD-CGD-O2D-CED
22	2	318	CLA	CBD-CGD-O2D-CED
22	A	833	CLA	CBD-CGD-O2D-CED
22	A	852	CLA	CBD-CGD-O2D-CED
22	B	823	CLA	CBD-CGD-O2D-CED
22	B	850	CLA	CBD-CGD-O2D-CED
22	1	317	CLA	C3-C5-C6-C7
22	2	318	CLA	C3-C5-C6-C7
22	A	801	CLA	C3-C5-C6-C7
22	A	849	CLA	C3-C5-C6-C7
22	B	847	CLA	C3-C5-C6-C7
22	A	852	CLA	CBA-CGA-O2A-C1
22	B	803	CLA	CBA-CGA-O2A-C1
22	B	807	CLA	CBA-CGA-O2A-C1
22	B	817	CLA	CBA-CGA-O2A-C1
22	G	206	CLA	CBA-CGA-O2A-C1
22	2	318	CLA	O1A-CGA-O2A-C1
27	3	305	MGE	O6D-C5D-C6D-O5D
22	A	827	CLA	O1D-CGD-O2D-CED
22	A	802	CLA	O1D-CGD-O2D-CED
21	X	307	CHL	CBD-CGD-O2D-CED
21	X	309	CHL	CBD-CGD-O2D-CED
22	A	809	CLA	CBD-CGD-O2D-CED
22	O	208	CLA	CBD-CGD-O2D-CED
22	X	313	CLA	O1A-CGA-O2A-C1
22	X	303	CLA	CBD-CGD-O2D-CED
22	B	808	CLA	C3-C5-C6-C7
22	2	318	CLA	CBA-CGA-O2A-C1
22	B	847	CLA	CBA-CGA-O2A-C1
26	B	843	LHG	C5-C4-O6-P
22	G	206	CLA	O1A-CGA-O2A-C1
22	A	859	CLA	C4-C3-C5-C6
22	B	808	CLA	C4-C3-C5-C6
22	B	811	CLA	C4-C3-C5-C6
22	B	831	CLA	C4-C3-C5-C6
22	A	859	CLA	C2-C3-C5-C6
22	B	808	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	B	811	CLA	C2-C3-C5-C6
22	B	831	CLA	C2-C3-C5-C6
31	O	201	DGD	O6D-C5D-C6D-O5D
26	4	302	LHG	C23-C24-C25-C26
21	3	314	CHL	C2A-CAA-CBA-CGA
21	Y	305	CHL	C2A-CAA-CBA-CGA
22	B	851	CLA	C2A-CAA-CBA-CGA
22	A	807	CLA	O1D-CGD-O2D-CED
27	F	303	MGE	O6D-C1D-O3G-C3G
31	J	104	DGD	O6E-C1E-O5D-C6D
22	4	304	CLA	CBA-CGA-O2A-C1
31	O	201	DGD	C2A-C1A-O1G-C1G
22	B	826	CLA	CBD-CGD-O2D-CED
22	B	830	CLA	O1D-CGD-O2D-CED
22	A	854	CLA	O1D-CGD-O2D-CED
22	B	817	CLA	O1A-CGA-O2A-C1
22	A	849	CLA	O1D-CGD-O2D-CED
22	B	848	CLA	O1D-CGD-O2D-CED
21	X	305	CHL	CBD-CGD-O2D-CED
31	O	201	DGD	O1A-C1A-O1G-C1G
22	B	848	CLA	C3-C5-C6-C7
22	Z	309	CLA	CBA-CGA-O2A-C1
22	2	308	CLA	CBA-CGA-O2A-C1
22	A	801	CLA	CBA-CGA-O2A-C1
22	A	809	CLA	CBA-CGA-O2A-C1
22	B	812	CLA	CBA-CGA-O2A-C1
22	B	851	CLA	CBA-CGA-O2A-C1
27	1	315	MGE	C2A-C1A-O1G-C1G
27	3	304	MGE	C2A-C1A-O1G-C1G
31	O	201	DGD	C4D-C5D-C6D-O5D
27	1	315	MGE	C1B-C2B-C3B-C4B
26	B	843	LHG	C26-C27-C28-C29
26	B	843	LHG	C30-C31-C32-C33
22	A	831	CLA	C13-C15-C16-C17
22	B	808	CLA	C13-C15-C16-C17
22	B	818	CLA	C5-C6-C7-C8
22	B	822	CLA	C13-C15-C16-C17
22	B	831	CLA	C13-C15-C16-C17
22	B	847	CLA	C10-C11-C12-C13
22	L	306	CLA	C5-C6-C7-C8
26	4	302	LHG	O2-C2-C3-O3
22	A	809	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	851	CLA	O1A-CGA-O2A-C1
27	F	304	MGE	O6D-C5D-C6D-O5D
22	A	833	CLA	C2-C3-C5-C6
22	B	813	CLA	C2-C3-C5-C6
22	B	818	CLA	C2-C3-C5-C6
22	A	859	CLA	C6-C7-C8-C9
22	B	816	CLA	C6-C7-C8-C9
22	B	822	CLA	C11-C10-C8-C9
22	B	831	CLA	C14-C13-C15-C16
22	B	847	CLA	C14-C13-C15-C16
22	B	851	CLA	C14-C13-C15-C16
22	L	306	CLA	C11-C12-C13-C14
22	L	306	CLA	C14-C13-C15-C16
22	O	207	CLA	C11-C12-C13-C14
21	Z	304	CHL	CBD-CGD-O2D-CED
22	B	803	CLA	C8-C10-C11-C12
21	2	309	CHL	C2A-CAA-CBA-CGA
22	1	302	CLA	C2A-CAA-CBA-CGA
22	3	309	CLA	C2A-CAA-CBA-CGA
23	4	322	LUT	C7-C8-C9-C19
25	1	312	BCR	C37-C22-C23-C24
25	B	834	BCR	C7-C8-C9-C34
25	B	837	BCR	C7-C8-C9-C34
25	B	839	BCR	C37-C22-C23-C24
25	B	840	BCR	C36-C18-C19-C20
25	G	202	BCR	C7-C8-C9-C34
25	I	101	BCR	C37-C22-C23-C24
25	J	103	BCR	C7-C8-C9-C34
23	4	322	LUT	C7-C8-C9-C10
24	1	311	XAT	C31-C32-C33-C34
25	1	312	BCR	C17-C18-C19-C20
25	1	312	BCR	C21-C22-C23-C24
25	B	837	BCR	C7-C8-C9-C10
25	B	839	BCR	C21-C22-C23-C24
25	B	840	BCR	C17-C18-C19-C20
25	G	202	BCR	C7-C8-C9-C10
25	I	101	BCR	C21-C22-C23-C24
31	B	841	DGD	C1B-C2B-C3B-C4B
22	A	802	CLA	C5-C6-C7-C8
22	A	831	CLA	C15-C16-C17-C18
22	A	838	CLA	C8-C10-C11-C12
22	B	847	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	B	850	CLA	C5-C6-C7-C8
21	Z	303	CHL	O1D-CGD-O2D-CED
21	Z	305	CHL	CBA-CGA-O2A-C1
21	Y	304	CHL	CBD-CGD-O2D-CED
27	3	305	MGE	C4D-C5D-C6D-O5D
22	1	317	CLA	C8-C10-C11-C12
22	A	803	CLA	CBA-CGA-O2A-C1
22	A	842	CLA	CBA-CGA-O2A-C1
22	B	808	CLA	CBA-CGA-O2A-C1
22	B	815	CLA	CBA-CGA-O2A-C1
22	3	309	CLA	C8-C10-C11-C12
22	A	807	CLA	C5-C6-C7-C8
22	A	831	CLA	C10-C11-C12-C13
22	A	846	CLA	C10-C11-C12-C13
22	B	816	CLA	C13-C15-C16-C17
22	B	830	CLA	C13-C15-C16-C17
22	L	306	CLA	C15-C16-C17-C18
22	O	208	CLA	C5-C6-C7-C8
31	O	201	DGD	C1A-C2A-C3A-C4A
21	2	309	CHL	O1D-CGD-O2D-CED
22	A	808	CLA	C13-C15-C16-C17
22	A	842	CLA	C8-C10-C11-C12
22	B	803	CLA	C5-C6-C7-C8
22	B	806	CLA	C5-C6-C7-C8
22	B	807	CLA	C15-C16-C17-C18
22	B	809	CLA	C8-C10-C11-C12
22	B	814	CLA	C5-C6-C7-C8
22	B	819	CLA	C5-C6-C7-C8
22	B	827	CLA	C8-C10-C11-C12
22	B	845	CLA	C10-C11-C12-C13
28	B	832	PQN	C15-C16-C17-C18
26	B	843	LHG	C23-C24-C25-C26
27	1	315	MGE	C1A-C2A-C3A-C4A
22	B	830	CLA	C5-C6-C7-C8
22	B	831	CLA	C10-C11-C12-C13
22	A	805	CLA	CBA-CGA-O2A-C1
22	A	810	CLA	C5-C6-C7-C8
22	A	833	CLA	C10-C11-C12-C13
22	A	850	CLA	C8-C10-C11-C12
31	J	104	DGD	C1B-C2B-C3B-C4B
22	A	806	CLA	CBD-CGD-O2D-CED
22	B	847	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	L	306	CLA	C11-C12-C13-C15
22	A	801	CLA	O1A-CGA-O2A-C1
27	1	315	MGE	O1A-C1A-O1G-C1G
24	1	311	XAT	C33-C34-C35-C15
24	3	302	XAT	C13-C14-C15-C35
22	B	829	CLA	CBD-CGD-O2D-CED
21	4	308	CHL	C2A-CAA-CBA-CGA
21	4	309	CHL	C2A-CAA-CBA-CGA
22	1	317	CLA	C2A-CAA-CBA-CGA
22	2	303	CLA	C2A-CAA-CBA-CGA
22	4	306	CLA	C2A-CAA-CBA-CGA
22	B	815	CLA	C2A-CAA-CBA-CGA
21	X	308	CHL	O1D-CGD-O2D-CED
21	Y	305	CHL	O1D-CGD-O2D-CED
22	G	205	CLA	O1D-CGD-O2D-CED
22	A	858	CLA	C15-C16-C17-C18
22	Y	312	CLA	CBA-CGA-O2A-C1
22	B	812	CLA	O1A-CGA-O2A-C1
27	3	304	MGE	O1A-C1A-O1G-C1G
31	J	104	DGD	O6D-C1D-O3G-C3G
22	A	802	CLA	C3-C5-C6-C7
22	B	815	CLA	C3-C5-C6-C7
22	B	804	CLA	C15-C16-C17-C18
22	4	311	CLA	O1D-CGD-O2D-CED
22	2	308	CLA	O1A-CGA-O2A-C1
22	4	304	CLA	O1A-CGA-O2A-C1
22	A	803	CLA	O1A-CGA-O2A-C1
21	X	302	CHL	CBA-CGA-O2A-C1
26	F	301	LHG	C7-C8-C9-C10
27	F	304	MGE	C4D-C5D-C6D-O5D
22	2	317	CLA	O1D-CGD-O2D-CED
22	A	842	CLA	O1A-CGA-O2A-C1
22	2	304	CLA	O1D-CGD-O2D-CED
22	2	307	CLA	C5-C6-C7-C8
22	3	312	CLA	C8-C10-C11-C12
22	A	807	CLA	C8-C10-C11-C12
22	A	810	CLA	C8-C10-C11-C12
22	A	852	CLA	C10-C11-C12-C13
22	A	853	CLA	C15-C16-C17-C18
22	B	803	CLA	C10-C11-C12-C13
22	B	807	CLA	C5-C6-C7-C8
26	2	315	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
26	A	822	LHG	C4-O6-P-O3
22	A	806	CLA	CBA-CGA-O2A-C1
22	B	806	CLA	CBA-CGA-O2A-C1
22	A	810	CLA	C13-C15-C16-C17
22	Z	313	CLA	O1D-CGD-O2D-CED
22	4	316	CLA	O1D-CGD-O2D-CED
21	Y	303	CHL	C2A-CAA-CBA-CGA
22	1	307	CLA	C2A-CAA-CBA-CGA
22	A	843	CLA	C2A-CAA-CBA-CGA
22	A	827	CLA	C16-C17-C18-C19
22	4	304	CLA	C3-C5-C6-C7
22	A	857	CLA	C3-C5-C6-C7
22	A	810	CLA	CBA-CGA-O2A-C1
22	B	831	CLA	CBA-CGA-O2A-C1
22	A	838	CLA	C10-C11-C12-C13
22	B	819	CLA	O1D-CGD-O2D-CED
23	2	310	LUT	C39-C29-C30-C31
25	2	312	BCR	C35-C13-C14-C15
22	3	310	CLA	C3-C5-C6-C7
26	A	820	LHG	C13-C14-C15-C16
21	Z	305	CHL	O1D-CGD-O2D-CED
22	B	830	CLA	C16-C17-C18-C19
26	B	843	LHG	C11-C12-C13-C14
21	Y	306	CHL	O1D-CGD-O2D-CED
22	3	316	CLA	O1D-CGD-O2D-CED
26	A	821	LHG	C5-C4-O6-P
26	3	306	LHG	C11-C12-C13-C14
27	3	304	MGE	C1A-C2A-C3A-C4A
22	3	309	CLA	CBA-CGA-O2A-C1
22	A	807	CLA	CBA-CGA-O2A-C1
22	Y	311	CLA	CBA-CGA-O2A-C1
26	B	843	LHG	C24-C23-O8-C6
22	A	805	CLA	O1A-CGA-O2A-C1
22	B	815	CLA	O1A-CGA-O2A-C1
22	B	850	CLA	O1D-CGD-O2D-CED
22	A	809	CLA	C4-C3-C5-C6
22	A	831	CLA	C4-C3-C5-C6
22	B	818	CLA	C6-C7-C8-C9
22	B	830	CLA	C11-C10-C8-C9
22	B	851	CLA	C11-C10-C8-C9
21	Z	312	CHL	O1D-CGD-O2D-CED
27	F	304	MGE	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
22	A	836	CLA	C10-C11-C12-C13
21	2	302	CHL	C2A-CAA-CBA-CGA
21	2	321	CHL	C2A-CAA-CBA-CGA
22	A	827	CLA	C2A-CAA-CBA-CGA
22	A	854	CLA	C2A-CAA-CBA-CGA
22	B	807	CLA	C2A-CAA-CBA-CGA
22	A	806	CLA	O1A-CGA-O2A-C1
24	1	311	XAT	C27-C28-C29-C39
24	1	311	XAT	C31-C32-C33-C40
25	3	303	BCR	C7-C8-C9-C34
26	1	314	LHG	C17-C18-C19-C20
24	1	311	XAT	C27-C28-C29-C30
22	3	309	CLA	C3-C5-C6-C7
22	A	807	CLA	C3-C5-C6-C7
22	A	844	CLA	C3-C5-C6-C7
22	A	859	CLA	C3-C5-C6-C7
26	A	822	LHG	C24-C25-C26-C27
26	B	843	LHG	C9-C10-C11-C12
21	3	314	CHL	C4B-C3B-CAB-CBB
22	1	304	CLA	C4B-C3B-CAB-CBB
22	1	317	CLA	C4B-C3B-CAB-CBB
22	1	319	CLA	C4B-C3B-CAB-CBB
22	2	320	CLA	C4B-C3B-CAB-CBB
22	A	808	CLA	C4B-C3B-CAB-CBB
22	A	850	CLA	C4B-C3B-CAB-CBB
22	A	856	CLA	C4B-C3B-CAB-CBB
22	B	804	CLA	C4B-C3B-CAB-CBB
22	B	805	CLA	C4B-C3B-CAB-CBB
22	B	815	CLA	C4B-C3B-CAB-CBB
22	B	820	CLA	C4B-C3B-CAB-CBB
22	A	812	CLA	C6-C7-C8-C10
22	A	838	CLA	C16-C17-C18-C20
22	B	830	CLA	C16-C17-C18-C20
22	B	845	CLA	C16-C17-C18-C20
22	A	831	CLA	C8-C10-C11-C12
31	B	841	DGD	C4A-C5A-C6A-C7A
21	Z	304	CHL	CBA-CGA-O2A-C1
22	X	303	CLA	CBA-CGA-O2A-C1
22	1	318	CLA	CBD-CGD-O2D-CED
22	Y	308	CLA	CBD-CGD-O2D-CED
22	A	810	CLA	C15-C16-C17-C18
22	B	806	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	808	CLA	O1A-CGA-O2A-C1
22	B	831	CLA	O1A-CGA-O2A-C1
31	J	104	DGD	C3B-C4B-C5B-C6B
22	B	829	CLA	CBA-CGA-O2A-C1
26	B	843	LHG	C12-C13-C14-C15
22	A	833	CLA	O1D-CGD-O2D-CED
21	2	321	CHL	C3A-C2A-CAA-CBA
21	4	307	CHL	C3A-C2A-CAA-CBA
21	X	306	CHL	C3A-C2A-CAA-CBA
22	1	306	CLA	C3A-C2A-CAA-CBA
22	3	310	CLA	C3A-C2A-CAA-CBA
22	3	312	CLA	C3A-C2A-CAA-CBA
22	3	320	CLA	C3A-C2A-CAA-CBA
22	4	313	CLA	C3A-C2A-CAA-CBA
22	4	318	CLA	C3A-C2A-CAA-CBA
22	A	802	CLA	C3A-C2A-CAA-CBA
22	A	809	CLA	C3A-C2A-CAA-CBA
22	A	827	CLA	C3A-C2A-CAA-CBA
22	A	834	CLA	C3A-C2A-CAA-CBA
22	A	849	CLA	C3A-C2A-CAA-CBA
22	A	852	CLA	C3A-C2A-CAA-CBA
22	B	805	CLA	C3A-C2A-CAA-CBA
22	B	811	CLA	C3A-C2A-CAA-CBA
22	B	816	CLA	C3A-C2A-CAA-CBA
22	B	823	CLA	C3A-C2A-CAA-CBA
22	B	831	CLA	C3A-C2A-CAA-CBA
22	B	850	CLA	C3A-C2A-CAA-CBA
22	B	851	CLA	C3A-C2A-CAA-CBA
22	B	852	CLA	C3A-C2A-CAA-CBA
22	K	202	CLA	C3A-C2A-CAA-CBA
22	L	306	CLA	C3A-C2A-CAA-CBA
22	O	209	CLA	C3A-C2A-CAA-CBA
22	X	304	CLA	C3A-C2A-CAA-CBA
22	X	310	CLA	C3A-C2A-CAA-CBA
22	Y	302	CLA	C3A-C2A-CAA-CBA
22	Y	308	CLA	C3A-C2A-CAA-CBA
22	Y	309	CLA	C3A-C2A-CAA-CBA
22	Z	306	CLA	C3A-C2A-CAA-CBA
22	Z	309	CLA	C3A-C2A-CAA-CBA
22	A	838	CLA	C15-C16-C17-C18
22	B	847	CLA	C5-C6-C7-C8
22	A	812	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	A	827	CLA	C16-C17-C18-C20
21	X	302	CHL	O1D-CGD-O2D-CED
21	Y	313	CHL	O1D-CGD-O2D-CED
22	A	852	CLA	O1D-CGD-O2D-CED
21	2	301	CHL	CBD-CGD-O2D-CED
21	X	306	CHL	CBD-CGD-O2D-CED
22	A	827	CLA	C3-C5-C6-C7
22	A	808	CLA	C4-C3-C5-C6
22	A	850	CLA	C4-C3-C5-C6
21	2	301	CHL	CBA-CGA-O2A-C1
22	2	319	CLA	CBA-CGA-O2A-C1
22	A	808	CLA	C2-C3-C5-C6
22	A	809	CLA	C2-C3-C5-C6
22	B	806	CLA	C2-C3-C5-C6
27	1	315	MGE	C2B-C3B-C4B-C5B
22	Y	302	CLA	CBA-CGA-O2A-C1
22	B	801	CLA	C2A-CAA-CBA-CGA
26	1	322	LHG	C27-C28-C29-C30
22	A	810	CLA	O1A-CGA-O2A-C1
27	1	315	MGE	C5B-C6B-C7B-C8B
22	Z	309	CLA	O1A-CGA-O2A-C1
21	3	314	CHL	C2B-C3B-CAB-CBB
21	X	307	CHL	C2B-C3B-CAB-CBB
22	1	304	CLA	C2B-C3B-CAB-CBB
22	1	317	CLA	C2B-C3B-CAB-CBB
22	1	319	CLA	C2B-C3B-CAB-CBB
22	2	320	CLA	C2B-C3B-CAB-CBB
22	3	311	CLA	C2B-C3B-CAB-CBB
22	4	306	CLA	C2B-C3B-CAB-CBB
22	4	311	CLA	C2B-C3B-CAB-CBB
22	A	808	CLA	C2B-C3B-CAB-CBB
22	A	827	CLA	C2B-C3B-CAB-CBB
22	A	842	CLA	C2B-C3B-CAB-CBB
22	A	853	CLA	C2B-C3B-CAB-CBB
22	A	856	CLA	C2B-C3B-CAB-CBB
22	A	858	CLA	C2B-C3B-CAB-CBB
22	B	801	CLA	C2B-C3B-CAB-CBB
22	B	804	CLA	C2B-C3B-CAB-CBB
22	B	805	CLA	C2B-C3B-CAB-CBB
22	B	809	CLA	C2B-C3B-CAB-CBB
22	B	815	CLA	C2B-C3B-CAB-CBB
22	B	819	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	B	820	CLA	C2B-C3B-CAB-CBB
22	B	831	CLA	C2B-C3B-CAB-CBB
22	B	846	CLA	C2B-C3B-CAB-CBB
22	B	853	CLA	C2B-C3B-CAB-CBB
22	G	205	CLA	C2B-C3B-CAB-CBB
22	H	201	CLA	C2B-C3B-CAB-CBB
22	Z	314	CLA	C2B-C3B-CAB-CBB
31	O	201	DGD	C8A-C9A-CAA-CBA
22	A	853	CLA	C13-C15-C16-C17
26	B	843	LHG	O10-C23-O8-C6
22	B	845	CLA	C16-C17-C18-C19
22	A	853	CLA	C3-C5-C6-C7
23	1	310	LUT	C5-C6-C7-C8
25	3	303	BCR	C23-C24-C25-C26
25	3	303	BCR	C23-C24-C25-C30
25	4	321	BCR	C1-C6-C7-C8
25	4	321	BCR	C5-C6-C7-C8
25	A	814	BCR	C5-C6-C7-C8
25	A	815	BCR	C23-C24-C25-C26
25	A	818	BCR	C1-C6-C7-C8
25	A	818	BCR	C23-C24-C25-C26
25	A	818	BCR	C23-C24-C25-C30
25	B	834	BCR	C23-C24-C25-C26
25	B	837	BCR	C23-C24-C25-C26
25	B	837	BCR	C23-C24-C25-C30
25	B	840	BCR	C23-C24-C25-C26
25	B	844	BCR	C23-C24-C25-C26
25	F	302	BCR	C23-C24-C25-C26
25	J	103	BCR	C23-C24-C25-C26
25	K	201	BCR	C23-C24-C25-C26
25	K	201	BCR	C23-C24-C25-C30
25	L	301	BCR	C5-C6-C7-C8
25	L	301	BCR	C23-C24-C25-C26
25	L	302	BCR	C23-C24-C25-C26
25	L	303	BCR	C1-C6-C7-C8
25	L	303	BCR	C5-C6-C7-C8
25	O	202	BCR	C1-C6-C7-C8
25	O	202	BCR	C23-C24-C25-C26
25	O	202	BCR	C23-C24-C25-C30
25	O	203	BCR	C23-C24-C25-C26
31	O	201	DGD	O6E-C5E-C6E-O5E
27	F	303	MGE	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
22	1	318	CLA	CBA-CGA-O2A-C1
22	A	859	CLA	CBA-CGA-O2A-C1
22	B	850	CLA	CBA-CGA-O2A-C1
22	A	801	CLA	C8-C10-C11-C12
22	Y	311	CLA	C10-C11-C12-C13
27	F	304	MGE	C2B-C1B-O2G-C2G
27	1	315	MGE	C6B-C7B-C8B-C9B
27	3	304	MGE	C3A-C4A-C5A-C6A
22	B	829	CLA	O1A-CGA-O2A-C1
22	Y	311	CLA	O1A-CGA-O2A-C1
22	L	306	CLA	C13-C15-C16-C17
22	1	318	CLA	C4-C3-C5-C6
22	A	846	CLA	C4-C3-C5-C6
22	B	807	CLA	C4-C3-C5-C6
22	B	809	CLA	C4-C3-C5-C6
22	B	823	CLA	O1D-CGD-O2D-CED
22	1	318	CLA	C2-C3-C5-C6
22	A	801	CLA	C6-C7-C8-C10
22	A	831	CLA	C2-C3-C5-C6
22	A	846	CLA	C2-C3-C5-C6
22	A	850	CLA	C2-C3-C5-C6
22	B	809	CLA	C2-C3-C5-C6
22	B	816	CLA	C6-C7-C8-C10
22	B	851	CLA	C6-C7-C8-C10
22	B	851	CLA	C11-C10-C8-C7
22	O	207	CLA	C11-C10-C8-C7
22	A	831	CLA	C3-C5-C6-C7
21	2	301	CHL	O1A-CGA-O2A-C1
22	2	319	CLA	O1A-CGA-O2A-C1
22	3	309	CLA	O1A-CGA-O2A-C1
22	A	807	CLA	O1A-CGA-O2A-C1
22	A	859	CLA	O1A-CGA-O2A-C1
22	K	203	CLA	C10-C11-C12-C13
22	A	853	CLA	C16-C17-C18-C20
27	F	303	MGE	O1B-C1B-O2G-C2G
21	Z	305	CHL	O1A-CGA-O2A-C1
22	1	317	CLA	CBA-CGA-O2A-C1
31	J	104	DGD	C2A-C1A-O1G-C1G
22	A	845	CLA	C2A-CAA-CBA-CGA
22	B	817	CLA	C2A-CAA-CBA-CGA
22	B	821	CLA	C2A-CAA-CBA-CGA
21	X	309	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	A	827	CLA	C13-C15-C16-C17
22	B	807	CLA	C3-C5-C6-C7
21	X	307	CHL	O1D-CGD-O2D-CED
27	F	303	MGE	C2B-C1B-O2G-C2G
24	1	311	XAT	C30-C31-C32-C33
21	Y	307	CHL	CBD-CGD-O2D-CED
22	B	815	CLA	CBD-CGD-O2D-CED
26	2	314	LHG	C23-C24-C25-C26
22	B	849	CLA	C3-C5-C6-C7
22	B	812	CLA	C10-C11-C12-C13
22	A	846	CLA	C15-C16-C17-C18
22	L	306	CLA	C4-C3-C5-C6
27	3	304	MGE	C1B-C2B-C3B-C4B
27	3	305	MGE	C1B-C2B-C3B-C4B
22	L	306	CLA	C2-C3-C5-C6
22	1	317	CLA	C11-C10-C8-C9
22	A	802	CLA	C14-C13-C15-C16
22	B	851	CLA	C6-C7-C8-C9
21	X	305	CHL	C2A-CAA-CBA-CGA
22	3	317	CLA	C2A-CAA-CBA-CGA
22	A	840	CLA	C2A-CAA-CBA-CGA
22	Y	312	CLA	O1A-CGA-O2A-C1
24	2	311	XAT	C27-C28-C29-C39
24	2	311	XAT	C27-C28-C29-C30
22	1	318	CLA	O1A-CGA-O2A-C1
22	B	850	CLA	O1A-CGA-O2A-C1
31	J	104	DGD	O1A-C1A-O1G-C1G
21	X	305	CHL	O1D-CGD-O2D-CED
21	2	321	CHL	C1A-C2A-CAA-CBA
21	4	307	CHL	C1A-C2A-CAA-CBA
21	X	306	CHL	C1A-C2A-CAA-CBA
21	X	309	CHL	C1A-C2A-CAA-CBA
22	1	304	CLA	C1A-C2A-CAA-CBA
22	1	306	CLA	C1A-C2A-CAA-CBA
22	2	303	CLA	C1A-C2A-CAA-CBA
22	2	304	CLA	C1A-C2A-CAA-CBA
22	3	310	CLA	C1A-C2A-CAA-CBA
22	3	312	CLA	C1A-C2A-CAA-CBA
22	3	320	CLA	C1A-C2A-CAA-CBA
22	4	313	CLA	C1A-C2A-CAA-CBA
22	4	318	CLA	C1A-C2A-CAA-CBA
22	A	802	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	A	805	CLA	C1A-C2A-CAA-CBA
22	A	834	CLA	C1A-C2A-CAA-CBA
22	A	836	CLA	C1A-C2A-CAA-CBA
22	A	840	CLA	C1A-C2A-CAA-CBA
22	A	848	CLA	C1A-C2A-CAA-CBA
22	B	804	CLA	C1A-C2A-CAA-CBA
22	B	811	CLA	C1A-C2A-CAA-CBA
22	B	812	CLA	C1A-C2A-CAA-CBA
22	B	816	CLA	C1A-C2A-CAA-CBA
22	B	817	CLA	C1A-C2A-CAA-CBA
22	B	819	CLA	C1A-C2A-CAA-CBA
22	B	822	CLA	C1A-C2A-CAA-CBA
22	B	823	CLA	C1A-C2A-CAA-CBA
22	B	825	CLA	C1A-C2A-CAA-CBA
22	B	833	CLA	C1A-C2A-CAA-CBA
22	B	852	CLA	C1A-C2A-CAA-CBA
22	K	202	CLA	C1A-C2A-CAA-CBA
22	L	306	CLA	C1A-C2A-CAA-CBA
22	X	310	CLA	C1A-C2A-CAA-CBA
22	Y	302	CLA	C1A-C2A-CAA-CBA
22	Y	308	CLA	C1A-C2A-CAA-CBA
22	Y	309	CLA	C1A-C2A-CAA-CBA
22	Z	306	CLA	C1A-C2A-CAA-CBA
22	Z	313	CLA	C1A-C2A-CAA-CBA
22	A	826	CLA	C16-C17-C18-C19
22	A	838	CLA	C16-C17-C18-C19
22	B	827	CLA	C3-C5-C6-C7
22	3	312	CLA	CBA-CGA-O2A-C1
22	A	809	CLA	O1D-CGD-O2D-CED
22	A	834	CLA	CBA-CGA-O2A-C1
21	Z	304	CHL	O1D-CGD-O2D-CED
26	3	306	LHG	C9-C10-C11-C12
22	A	850	CLA	C16-C17-C18-C20
26	B	843	LHG	C28-C29-C30-C31
27	1	315	MGE	C7B-C8B-C9B-CAB
26	4	302	LHG	C1-C2-C3-O3
26	A	820	LHG	C1-C2-C3-O3
27	F	304	MGE	O1B-C1B-O2G-C2G
27	1	315	MGE	C2B-C1B-O2G-C2G
22	1	317	CLA	O1A-CGA-O2A-C1
21	X	309	CHL	C2A-CAA-CBA-CGA
22	4	318	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	A	801	CLA	C2A-CAA-CBA-CGA
26	A	824	LHG	C4-C5-C6-O8
31	J	104	DGD	C5D-C6D-O5D-C1E
31	O	201	DGD	C5D-C6D-O5D-C1E
21	Y	304	CHL	O1D-CGD-O2D-CED
22	A	850	CLA	C15-C16-C17-C18
22	B	808	CLA	C8-C10-C11-C12
22	B	812	CLA	C5-C6-C7-C8
22	2	318	CLA	O1D-CGD-O2D-CED
22	O	207	CLA	C16-C17-C18-C20
22	1	308	CLA	O1D-CGD-O2D-CED
22	O	208	CLA	O1D-CGD-O2D-CED
22	A	843	CLA	CBA-CGA-O2A-C1
22	A	854	CLA	CBA-CGA-O2A-C1
22	B	803	CLA	C13-C15-C16-C17
26	B	843	LHG	C6-C5-O7-C7
22	3	319	CLA	C2A-CAA-CBA-CGA
22	L	306	CLA	C10-C11-C12-C13
22	A	829	CLA	C2-C1-O2A-CGA
27	N	201	MGE	C8B-C9B-CAB-CBB
22	B	814	CLA	C3-C5-C6-C7
26	A	824	LHG	C31-C32-C33-C34
21	X	302	CHL	O1A-CGA-O2A-C1
26	G	203	LHG	C2-C3-O3-P
22	B	805	CLA	CAA-CBA-CGA-O2A
22	B	811	CLA	CAA-CBA-CGA-O2A
22	A	806	CLA	O1D-CGD-O2D-CED
22	X	303	CLA	O1D-CGD-O2D-CED
22	3	312	CLA	O1A-CGA-O2A-C1
30	A	825	CL0	CAA-CBA-CGA-O2A
22	A	853	CLA	C16-C17-C18-C19
22	A	802	CLA	C4-C3-C5-C6
22	B	822	CLA	C4-C3-C5-C6
28	B	832	PQN	C14-C13-C15-C16
22	1	317	CLA	C11-C10-C8-C7
22	2	318	CLA	C11-C12-C13-C15
22	3	312	CLA	C6-C7-C8-C10
22	A	802	CLA	C12-C13-C15-C16
22	A	810	CLA	C11-C12-C13-C15
22	A	858	CLA	C11-C10-C8-C7
22	B	807	CLA	C11-C12-C13-C15
22	B	822	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	B	851	CLA	C12-C13-C15-C16
22	Y	311	CLA	C12-C13-C15-C16
22	2	318	CLA	C11-C12-C13-C14
22	3	310	CLA	C11-C10-C8-C9
22	A	844	CLA	C6-C7-C8-C9
22	A	858	CLA	C11-C10-C8-C9
22	A	859	CLA	C11-C10-C8-C9
22	B	804	CLA	C6-C7-C8-C9
22	B	807	CLA	C11-C12-C13-C14
22	B	845	CLA	C6-C7-C8-C9
22	B	847	CLA	C11-C10-C8-C9
22	B	848	CLA	C11-C10-C8-C9
22	O	207	CLA	C11-C10-C8-C9
26	2	313	LHG	C23-C24-C25-C26
22	B	826	CLA	CBA-CGA-O2A-C1
26	3	306	LHG	C28-C29-C30-C31
22	A	837	CLA	C2C-C3C-CAC-CBC
22	B	829	CLA	O1D-CGD-O2D-CED
22	B	804	CLA	CBA-CGA-O2A-C1
27	F	303	MGE	C1A-C2A-C3A-C4A
31	G	201	DGD	C1A-C2A-C3A-C4A
22	2	307	CLA	C10-C11-C12-C13
22	1	304	CLA	C5-C6-C7-C8
21	2	302	CHL	C2C-C3C-CAC-CBC
21	X	307	CHL	C4B-C3B-CAB-CBB
22	2	304	CLA	C4B-C3B-CAB-CBB
22	3	311	CLA	C4B-C3B-CAB-CBB
22	4	311	CLA	C4B-C3B-CAB-CBB
22	A	827	CLA	C4B-C3B-CAB-CBB
22	A	829	CLA	C4B-C3B-CAB-CBB
22	A	831	CLA	C4B-C3B-CAB-CBB
22	A	846	CLA	C4B-C3B-CAB-CBB
22	A	853	CLA	C4B-C3B-CAB-CBB
22	B	801	CLA	C4B-C3B-CAB-CBB
22	H	201	CLA	C4B-C3B-CAB-CBB
22	Z	314	CLA	C4B-C3B-CAB-CBB
22	3	310	CLA	C5-C6-C7-C8
26	A	822	LHG	O6-C4-C5-C6
22	A	810	CLA	C10-C11-C12-C13
22	B	830	CLA	C10-C11-C12-C13
22	2	307	CLA	C4-C3-C5-C6
22	B	804	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	B	816	CLA	C4-C3-C5-C6
22	2	307	CLA	C2-C3-C5-C6
22	A	802	CLA	C2-C3-C5-C6
30	A	825	CL0	CBA-CGA-O2A-C1
26	2	313	LHG	C5-C4-O6-P
22	B	826	CLA	O1D-CGD-O2D-CED
22	1	303	CLA	C3A-C2A-CAA-CBA
22	A	829	CLA	C3A-C2A-CAA-CBA
22	A	858	CLA	C3A-C2A-CAA-CBA
22	B	801	CLA	C3A-C2A-CAA-CBA
22	B	810	CLA	C3A-C2A-CAA-CBA
22	B	813	CLA	C3A-C2A-CAA-CBA
22	B	815	CLA	C3A-C2A-CAA-CBA
22	B	833	CLA	C3A-C2A-CAA-CBA
22	K	203	CLA	C3A-C2A-CAA-CBA
22	Z	314	CLA	C3A-C2A-CAA-CBA
30	A	825	CL0	C3A-C2A-CAA-CBA
21	X	306	CHL	O1D-CGD-O2D-CED
22	3	312	CLA	C15-C16-C17-C18
22	2	319	CLA	O2A-C1-C2-C3
27	F	304	MGE	O1G-C1G-C2G-C3G
27	F	304	MGE	C1G-C2G-C3G-O3G
31	J	104	DGD	O1G-C1G-C2G-C3G
26	B	842	LHG	C9-C10-C11-C12
22	A	801	CLA	C10-C11-C12-C13
22	B	803	CLA	C4-C3-C5-C6
22	B	804	CLA	C2-C3-C5-C6
31	G	201	DGD	C3B-C4B-C5B-C6B
22	B	846	CLA	CBA-CGA-O2A-C1
21	1	316	CHL	C3C-C2C-CMC-OMC
21	4	317	CHL	C3C-C2C-CMC-OMC
21	Z	303	CHL	C3C-C2C-CMC-OMC
26	4	302	LHG	C3-O3-P-O6
22	A	854	CLA	O1A-CGA-O2A-C1
22	2	307	CLA	C3-C5-C6-C7
22	A	826	CLA	C15-C16-C17-C18
22	B	827	CLA	CBA-CGA-O2A-C1
22	B	830	CLA	CBA-CGA-O2A-C1
22	B	826	CLA	O1A-CGA-O2A-C1
22	B	818	CLA	CAA-CBA-CGA-O2A
21	2	301	CHL	O1D-CGD-O2D-CED
21	1	316	CHL	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	3	315	CLA	C2B-C3B-CAB-CBB
22	A	831	CLA	C2B-C3B-CAB-CBB
22	A	846	CLA	C2B-C3B-CAB-CBB
22	A	850	CLA	C2B-C3B-CAB-CBB
22	A	843	CLA	O1A-CGA-O2A-C1
26	1	322	LHG	O7-C5-C6-O8
26	4	301	LHG	O7-C5-C6-O8
27	1	315	MGE	O2G-C2G-C3G-O3G
27	F	304	MGE	O2G-C2G-C3G-O3G
31	J	104	DGD	O1G-C1G-C2G-O2G
21	Y	307	CHL	O1D-CGD-O2D-CED
21	X	308	CHL	CBA-CGA-O2A-C1
31	B	841	DGD	C6A-C7A-C8A-C9A
22	A	810	CLA	C16-C17-C18-C19
22	A	826	CLA	C16-C17-C18-C20
22	B	851	CLA	C13-C15-C16-C17
28	A	811	PQN	C15-C16-C17-C18
31	G	201	DGD	C6A-C7A-C8A-C9A
22	A	809	CLA	C2-C1-O2A-CGA
22	B	803	CLA	C2-C3-C5-C6
22	B	814	CLA	C11-C10-C8-C9
22	B	817	CLA	C11-C10-C8-C9
22	Y	311	CLA	C14-C13-C15-C16
21	Z	304	CHL	O1A-CGA-O2A-C1
22	A	826	CLA	C5-C6-C7-C8
22	A	842	CLA	C5-C6-C7-C8
22	A	854	CLA	C13-C15-C16-C17
26	4	302	LHG	C2-C3-O3-P
26	O	204	LHG	C5-C4-O6-P
30	A	825	CL0	O1A-CGA-O2A-C1
22	A	849	CLA	C2A-CAA-CBA-CGA
22	A	850	CLA	C16-C17-C18-C19
25	A	815	BCR	C1-C6-C7-C8
25	A	815	BCR	C23-C24-C25-C30
25	A	819	BCR	C1-C6-C7-C8
25	B	834	BCR	C23-C24-C25-C30
25	B	844	BCR	C23-C24-C25-C30
25	L	301	BCR	C1-C6-C7-C8
25	L	302	BCR	C23-C24-C25-C30
22	3	309	CLA	CAA-CBA-CGA-O2A
22	Y	310	CLA	CAA-CBA-CGA-O2A
22	A	804	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	A	835	CLA	C1A-C2A-CAA-CBA
22	J	102	CLA	C1A-C2A-CAA-CBA
25	4	321	BCR	C21-C22-C23-C24
25	L	301	BCR	C7-C8-C9-C10
27	1	315	MGE	O1B-C1B-O2G-C2G
22	B	823	CLA	C10-C11-C12-C13
22	1	318	CLA	O1D-CGD-O2D-CED
26	2	315	LHG	O6-C4-C5-C6
22	3	310	CLA	C6-C7-C8-C10
22	3	310	CLA	C11-C10-C8-C7
22	A	808	CLA	C12-C13-C15-C16
22	A	838	CLA	C6-C7-C8-C10
22	B	804	CLA	C6-C7-C8-C10
22	B	814	CLA	C11-C10-C8-C7
22	B	817	CLA	C11-C10-C8-C7
22	B	831	CLA	C12-C13-C15-C16
22	B	845	CLA	C6-C7-C8-C10
22	B	848	CLA	C11-C10-C8-C7
28	B	832	PQN	C12-C13-C15-C16
26	F	301	LHG	C25-C26-C27-C28
22	B	827	CLA	C5-C6-C7-C8
22	A	846	CLA	C2A-CAA-CBA-CGA
22	L	305	CLA	C2A-CAA-CBA-CGA
25	2	312	BCR	C16-C17-C18-C36
22	2	320	CLA	CBA-CGA-O2A-C1
22	B	810	CLA	CBA-CGA-O2A-C1
22	Y	311	CLA	CAA-CBA-CGA-O2A
22	B	804	CLA	O1A-CGA-O2A-C1
27	F	303	MGE	C4B-C5B-C6B-C7B
21	3	314	CHL	CAD-CBD-CGD-O2D
21	Z	302	CHL	CAD-CBD-CGD-O2D
22	1	319	CLA	CAD-CBD-CGD-O2D
22	2	317	CLA	CAD-CBD-CGD-O2D
22	3	316	CLA	CAD-CBD-CGD-O2D
22	3	319	CLA	CAD-CBD-CGD-O2D
22	4	310	CLA	CAD-CBD-CGD-O2D
22	4	311	CLA	CAD-CBD-CGD-O2D
22	A	802	CLA	CAD-CBD-CGD-O2D
22	A	809	CLA	CAD-CBD-CGD-O2D
22	A	810	CLA	CAD-CBD-CGD-O2D
22	A	837	CLA	CAD-CBD-CGD-O2D
22	A	845	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	A	846	CLA	CAD-CBD-CGD-O2D
22	B	804	CLA	CAD-CBD-CGD-O2D
22	B	811	CLA	CAD-CBD-CGD-O2D
22	B	815	CLA	CAD-CBD-CGD-O2D
22	B	817	CLA	CAD-CBD-CGD-O2D
22	B	819	CLA	CAD-CBD-CGD-O2D
22	B	828	CLA	CAD-CBD-CGD-O2D
22	F	306	CLA	CAD-CBD-CGD-O2D
22	G	206	CLA	CAD-CBD-CGD-O2D
22	X	312	CLA	CAD-CBD-CGD-O2D
22	Y	312	CLA	CAD-CBD-CGD-O2D
30	A	825	CL0	CAD-CBD-CGD-O2D
22	A	859	CLA	C5-C6-C7-C8
26	2	315	LHG	C4-C5-C6-O8
26	O	204	LHG	C4-C5-C6-O8
27	3	305	MGE	C1G-C2G-C3G-O3G
27	F	303	MGE	O1G-C1G-C2G-C3G
31	B	841	DGD	C1G-C2G-C3G-O3G
22	2	308	CLA	CBD-CGD-O2D-CED
22	B	852	CLA	C3-C5-C6-C7
22	F	306	CLA	CAA-CBA-CGA-O2A
26	2	316	LHG	C25-C26-C27-C28
22	A	833	CLA	C16-C17-C18-C20
21	1	301	CHL	CHA-CBD-CGD-O1D
22	1	305	CLA	CHA-CBD-CGD-O1D
22	1	305	CLA	CHA-CBD-CGD-O2D
22	1	309	CLA	CHA-CBD-CGD-O1D
22	1	309	CLA	CHA-CBD-CGD-O2D
22	3	310	CLA	CHA-CBD-CGD-O1D
22	3	310	CLA	CHA-CBD-CGD-O2D
22	A	802	CLA	CHA-CBD-CGD-O1D
22	A	804	CLA	CHA-CBD-CGD-O1D
22	A	804	CLA	CHA-CBD-CGD-O2D
22	A	807	CLA	CHA-CBD-CGD-O1D
22	A	807	CLA	CHA-CBD-CGD-O2D
22	A	829	CLA	CHA-CBD-CGD-O1D
22	A	829	CLA	CHA-CBD-CGD-O2D
22	A	830	CLA	CHA-CBD-CGD-O1D
22	A	830	CLA	CHA-CBD-CGD-O2D
22	A	838	CLA	CHA-CBD-CGD-O1D
22	B	803	CLA	CHA-CBD-CGD-O1D
22	B	833	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	B	833	CLA	CHA-CBD-CGD-O2D
22	B	847	CLA	CHA-CBD-CGD-O1D
22	B	847	CLA	CHA-CBD-CGD-O2D
22	B	850	CLA	CHA-CBD-CGD-O1D
22	B	850	CLA	CHA-CBD-CGD-O2D
22	L	306	CLA	CHA-CBD-CGD-O1D
22	L	306	CLA	CHA-CBD-CGD-O2D
22	X	313	CLA	CHA-CBD-CGD-O1D
22	X	313	CLA	CHA-CBD-CGD-O2D
22	Z	311	CLA	CHA-CBD-CGD-O1D
22	B	831	CLA	CAA-CBA-CGA-O2A
22	3	312	CLA	C3-C5-C6-C7
22	B	827	CLA	O1A-CGA-O2A-C1
26	2	315	LHG	O7-C5-C6-O8
26	3	306	LHG	O7-C5-C6-O8
27	F	303	MGE	O1G-C1G-C2G-O2G
22	A	801	CLA	C12-C13-C15-C16
22	B	815	CLA	O1D-CGD-O2D-CED
22	B	830	CLA	O1A-CGA-O2A-C1
22	3	312	CLA	CAA-CBA-CGA-O2A
22	A	810	CLA	C16-C17-C18-C20
26	A	820	LHG	C24-C25-C26-C27
31	B	841	DGD	C5B-C6B-C7B-C8B
22	A	806	CLA	C3-C5-C6-C7
22	A	812	CLA	C4-C3-C5-C6
22	B	824	CLA	C4-C3-C5-C6
22	Y	311	CLA	C4-C3-C5-C6
21	Y	304	CHL	C2C-C3C-CAC-CBC
27	1	315	MGE	C4B-C5B-C6B-C7B
22	2	320	CLA	O1A-CGA-O2A-C1
22	A	812	CLA	C2-C3-C5-C6
22	3	308	CLA	C2A-CAA-CBA-CGA
22	B	806	CLA	C2A-CAA-CBA-CGA
22	K	202	CLA	C2A-CAA-CBA-CGA
21	X	305	CHL	CAA-CBA-CGA-O2A
26	O	204	LHG	O7-C7-C8-C9
25	3	303	BCR	C37-C22-C23-C24
31	G	201	DGD	C8B-C9B-CAB-CBB
26	2	314	LHG	C11-C10-C9-C8
23	2	310	LUT	C7-C8-C9-C10
25	J	101	BCR	C7-C8-C9-C10
21	4	308	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	Y	307	CHL	C1A-C2A-CAA-CBA
22	4	315	CLA	CHA-CBD-CGD-O2D
22	B	801	CLA	C1A-C2A-CAA-CBA
22	B	813	CLA	C1A-C2A-CAA-CBA
22	B	815	CLA	C1A-C2A-CAA-CBA
26	4	301	LHG	C4-O6-P-O3
26	X	314	LHG	C4-O6-P-O3
22	2	308	CLA	O1D-CGD-O2D-CED
26	1	313	LHG	C5-C4-O6-P
26	A	824	LHG	C5-C4-O6-P
22	B	807	CLA	C2-C3-C5-C6
22	B	816	CLA	C2-C3-C5-C6
22	Y	311	CLA	C2-C3-C5-C6
22	B	810	CLA	O1A-CGA-O2A-C1
21	1	301	CHL	C4B-C3B-CAB-CBB
21	1	316	CHL	C4B-C3B-CAB-CBB
21	2	309	CHL	C4B-C3B-CAB-CBB
21	2	321	CHL	C4B-C3B-CAB-CBB
21	4	317	CHL	C4B-C3B-CAB-CBB
21	X	302	CHL	C4B-C3B-CAB-CBB
21	X	305	CHL	C4B-C3B-CAB-CBB
21	X	306	CHL	C4B-C3B-CAB-CBB
21	X	308	CHL	C4B-C3B-CAB-CBB
21	X	309	CHL	C4B-C3B-CAB-CBB
21	Y	303	CHL	C4B-C3B-CAB-CBB
21	Y	304	CHL	C4B-C3B-CAB-CBB
21	Y	305	CHL	C4B-C3B-CAB-CBB
21	Y	306	CHL	C4B-C3B-CAB-CBB
21	Y	307	CHL	C4B-C3B-CAB-CBB
21	Z	301	CHL	C4B-C3B-CAB-CBB
21	Z	303	CHL	C4B-C3B-CAB-CBB
21	Z	304	CHL	C4B-C3B-CAB-CBB
21	Z	305	CHL	C4B-C3B-CAB-CBB
22	2	319	CLA	C4B-C3B-CAB-CBB
22	3	312	CLA	C4B-C3B-CAB-CBB
22	3	315	CLA	C4B-C3B-CAB-CBB
22	4	310	CLA	C4B-C3B-CAB-CBB
22	A	802	CLA	C4B-C3B-CAB-CBB
22	A	806	CLA	C4B-C3B-CAB-CBB
22	A	843	CLA	C4B-C3B-CAB-CBB
22	A	845	CLA	C4B-C3B-CAB-CBB
22	A	849	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	B	806	CLA	C4B-C3B-CAB-CBB
22	B	812	CLA	C4B-C3B-CAB-CBB
22	B	826	CLA	C4B-C3B-CAB-CBB
22	B	827	CLA	C4B-C3B-CAB-CBB
22	B	831	CLA	C4B-C3B-CAB-CBB
22	B	850	CLA	C4B-C3B-CAB-CBB
22	B	851	CLA	C4B-C3B-CAB-CBB
22	B	852	CLA	C4B-C3B-CAB-CBB
22	F	306	CLA	C4B-C3B-CAB-CBB
26	2	315	LHG	C4-O6-P-O5
26	A	822	LHG	C4-O6-P-O4
26	A	822	LHG	C4-O6-P-O5
22	B	818	CLA	C8-C10-C11-C12
22	X	303	CLA	O1A-CGA-O2A-C1
22	Y	302	CLA	O1A-CGA-O2A-C1
21	2	302	CHL	C4C-C3C-CAC-CBC
21	1	301	CHL	CAD-CBD-CGD-O1D
21	1	316	CHL	CAD-CBD-CGD-O1D
22	3	310	CLA	CAD-CBD-CGD-O1D
22	4	316	CLA	CAD-CBD-CGD-O1D
22	A	829	CLA	CAD-CBD-CGD-O1D
22	A	830	CLA	CAD-CBD-CGD-O1D
22	A	838	CLA	CAD-CBD-CGD-O1D
22	B	803	CLA	CAD-CBD-CGD-O1D
22	B	826	CLA	CAD-CBD-CGD-O1D
22	B	847	CLA	CAD-CBD-CGD-O1D
22	K	204	CLA	CAD-CBD-CGD-O1D
22	L	306	CLA	CAD-CBD-CGD-O1D
22	Z	311	CLA	CAD-CBD-CGD-O1D
26	F	301	LHG	C23-C24-C25-C26
22	A	802	CLA	C13-C15-C16-C17
22	3	309	CLA	C10-C11-C12-C13
22	A	808	CLA	O1A-CGA-O2A-C1
21	4	308	CHL	CAD-CBD-CGD-O2D
22	2	322	CLA	CAD-CBD-CGD-O2D
22	A	859	CLA	C6-C7-C8-C10
22	B	803	CLA	C12-C13-C15-C16
22	B	824	CLA	C2-C3-C5-C6
22	B	830	CLA	C12-C13-C15-C16
22	B	853	CLA	C3A-C2A-CAA-CBA
22	O	207	CLA	C11-C12-C13-C15
26	2	315	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
22	A	802	CLA	CAA-CBA-CGA-O2A
21	4	307	CHL	C2A-CAA-CBA-CGA
21	1	316	CHL	C1C-C2C-CMC-OMC
21	4	307	CHL	C1C-C2C-CMC-OMC
21	4	307	CHL	CAD-CBD-CGD-O1D
21	4	308	CHL	C1C-C2C-CMC-OMC
21	4	317	CHL	C1C-C2C-CMC-OMC
21	X	305	CHL	C1C-C2C-CMC-OMC
21	X	308	CHL	C1C-C2C-CMC-OMC
21	Y	303	CHL	C1C-C2C-CMC-OMC
21	Y	307	CHL	C1C-C2C-CMC-OMC
21	Y	313	CHL	C1C-C2C-CMC-OMC
21	Z	301	CHL	C1C-C2C-CMC-OMC
21	Z	303	CHL	C1C-C2C-CMC-OMC
21	Z	312	CHL	C1C-C2C-CMC-OMC
22	2	322	CLA	CAD-CBD-CGD-O1D
26	3	306	LHG	C4-C5-C6-O8
27	3	305	MGE	O1A-C1A-O1G-C1G
26	A	820	LHG	O7-C5-C6-O8
26	O	205	LHG	O7-C5-C6-O8
27	3	305	MGE	O2G-C2G-C3G-O3G
27	F	304	MGE	O1G-C1G-C2G-O2G
26	A	820	LHG	C25-C26-C27-C28
22	B	851	CLA	C10-C11-C12-C13
22	Y	311	CLA	C15-C16-C17-C18
27	N	201	MGE	C6B-C7B-C8B-C9B
26	F	301	LHG	C24-C23-O8-C6
26	1	322	LHG	O7-C7-C8-C9
22	A	844	CLA	C15-C16-C17-C18
22	A	838	CLA	C6-C7-C8-C9
22	1	317	CLA	CAA-CBA-CGA-O2A
22	2	308	CLA	C3-C5-C6-C7
22	A	834	CLA	O1A-CGA-O2A-C1
25	2	312	BCR	C18-C19-C20-C21
25	A	816	BCR	C10-C11-C12-C13
25	B	840	BCR	C18-C19-C20-C21
22	L	306	CLA	C16-C17-C18-C19
21	2	309	CHL	C2B-C3B-CAB-CBB
21	X	302	CHL	C2B-C3B-CAB-CBB
21	X	305	CHL	C2B-C3B-CAB-CBB
21	X	309	CHL	C2B-C3B-CAB-CBB
21	Y	304	CHL	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
21	Y	306	CHL	C2B-C3B-CAB-CBB
21	Z	303	CHL	C2B-C3B-CAB-CBB
21	Z	305	CHL	C2B-C3B-CAB-CBB
22	2	304	CLA	C2B-C3B-CAB-CBB
22	4	310	CLA	C2B-C3B-CAB-CBB
22	A	829	CLA	C2B-C3B-CAB-CBB
22	A	843	CLA	C2B-C3B-CAB-CBB
22	A	845	CLA	C2B-C3B-CAB-CBB
22	B	812	CLA	C2B-C3B-CAB-CBB
22	B	850	CLA	C2B-C3B-CAB-CBB
22	O	208	CLA	C4-C3-C5-C6
21	2	301	CHL	C1-C2-C3-C4
22	3	308	CLA	C1-C2-C3-C4
21	Z	301	CHL	CAA-CBA-CGA-O2A
26	A	822	LHG	C4-C5-O7-C7
27	3	305	MGE	C3G-C2G-O2G-C1B
22	3	318	CLA	C2A-CAA-CBA-CGA
22	A	838	CLA	C2A-CAA-CBA-CGA
22	A	853	CLA	C2A-CAA-CBA-CGA
22	X	313	CLA	C2A-CAA-CBA-CGA
22	Y	310	CLA	C2A-CAA-CBA-CGA
22	3	310	CLA	C2-C1-O2A-CGA
22	A	807	CLA	C2-C1-O2A-CGA
22	B	826	CLA	C2-C1-O2A-CGA
22	B	833	CLA	C2-C1-O2A-CGA
22	B	849	CLA	C2-C1-O2A-CGA
22	Y	311	CLA	C2-C1-O2A-CGA
22	Y	308	CLA	O1D-CGD-O2D-CED
26	2	314	LHG	C4-O6-P-O5
26	A	821	LHG	C4-O6-P-O5
26	B	842	LHG	C10-C11-C12-C13
22	2	307	CLA	O1A-CGA-O2A-C1
26	A	822	LHG	O6-C4-C5-O7
26	1	322	LHG	C9-C10-C11-C12
25	3	303	BCR	C5-C6-C7-C8
25	A	818	BCR	C5-C6-C7-C8
25	G	202	BCR	C5-C6-C7-C8
26	B	843	LHG	C27-C28-C29-C30
22	B	824	CLA	C5-C6-C7-C8
22	A	837	CLA	C4C-C3C-CAC-CBC
26	1	313	LHG	C4-O6-P-O3
26	3	306	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
26	4	302	LHG	C4-O6-P-O3
26	A	820	LHG	C4-O6-P-O3
26	A	823	LHG	C3-O3-P-O6
26	B	842	LHG	C4-O6-P-O3
26	B	843	LHG	C3-O3-P-O6
26	G	203	LHG	C3-O3-P-O6
26	X	314	LHG	C3-O3-P-O6
21	3	307	CHL	C2-C3-C5-C6
22	3	312	CLA	C5-C6-C7-C8
22	A	807	CLA	C11-C12-C13-C15
22	B	818	CLA	C6-C7-C8-C10
22	1	318	CLA	C3-C5-C6-C7
22	B	829	CLA	C3-C5-C6-C7
22	3	310	CLA	C6-C7-C8-C9
22	3	312	CLA	C6-C7-C8-C9
22	A	810	CLA	C11-C12-C13-C14
22	B	830	CLA	C14-C13-C15-C16
22	B	848	CLA	C8-C10-C11-C12
21	X	306	CHL	CBA-CGA-O2A-C1
22	B	822	CLA	CAA-CBA-CGA-O2A
22	L	306	CLA	C16-C17-C18-C20
22	A	838	CLA	CBA-CGA-O2A-C1
22	Y	311	CLA	C13-C15-C16-C17
22	B	801	CLA	C4-C3-C5-C6
22	2	307	CLA	CBA-CGA-O2A-C1
30	A	825	CL0	CAA-CBA-CGA-O1A
22	B	816	CLA	C5-C6-C7-C8
22	A	808	CLA	CBA-CGA-O2A-C1
22	4	304	CLA	C4B-C3B-CAB-CBB
22	B	813	CLA	C4B-C3B-CAB-CBB
24	3	302	XAT	C9-C10-C11-C12
22	4	304	CLA	CBD-CGD-O2D-CED
22	B	846	CLA	CBD-CGD-O2D-CED
22	2	304	CLA	C3-C5-C6-C7
22	A	836	CLA	C2-C1-O2A-CGA
22	B	818	CLA	C2-C1-O2A-CGA
22	B	853	CLA	C2-C1-O2A-CGA
22	A	841	CLA	CBD-CGD-O2D-CED
22	2	307	CLA	C2A-CAA-CBA-CGA
22	4	304	CLA	C2A-CAA-CBA-CGA
22	A	826	CLA	C2A-CAA-CBA-CGA
22	B	849	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
26	G	203	LHG	O7-C5-C6-O8
22	B	846	CLA	O1A-CGA-O2A-C1
22	3	308	CLA	CAA-CBA-CGA-O2A
27	F	303	MGE	C5A-C6A-C7A-C8A
22	4	306	CLA	C3A-C2A-CAA-CBA
22	A	805	CLA	C3A-C2A-CAA-CBA
22	A	810	CLA	C3A-C2A-CAA-CBA
22	A	854	CLA	C3A-C2A-CAA-CBA
22	B	824	CLA	C3A-C2A-CAA-CBA
21	Y	304	CHL	C4C-C3C-CAC-CBC
21	3	307	CHL	O2A-C1-C2-C3
22	Y	309	CLA	CAA-CBA-CGA-O2A
22	A	802	CLA	C11-C10-C8-C9
22	A	846	CLA	C11-C10-C8-C9
22	A	858	CLA	C6-C7-C8-C9
22	B	808	CLA	C11-C10-C8-C9
22	B	831	CLA	C11-C10-C8-C9
22	1	320	CLA	CAA-CBA-CGA-O2A
22	3	309	CLA	C11-C12-C13-C15
24	2	311	XAT	C40-C33-C34-C35
24	3	302	XAT	C40-C33-C34-C35
25	A	816	BCR	C16-C17-C18-C36
25	A	818	BCR	C11-C10-C9-C34
25	B	836	BCR	C11-C10-C9-C34
25	B	836	BCR	C20-C21-C22-C37
25	F	302	BCR	C35-C13-C14-C15
25	L	301	BCR	C11-C10-C9-C34
25	L	302	BCR	C20-C21-C22-C37
26	B	842	LHG	C4-C5-C6-O8
27	1	315	MGE	C1G-C2G-C3G-O3G
22	2	303	CLA	CAA-CBA-CGA-O1A
22	B	818	CLA	C2A-CAA-CBA-CGA
31	J	104	DGD	C2A-C3A-C4A-C5A
22	B	829	CLA	C10-C11-C12-C13
22	1	320	CLA	CAA-CBA-CGA-O1A
22	4	305	CLA	CAA-CBA-CGA-O1A
22	A	845	CLA	CAA-CBA-CGA-O1A
27	3	305	MGE	C1G-C2G-O2G-C1B
22	B	805	CLA	CAA-CBA-CGA-O1A
21	2	301	CHL	C1A-C2A-CAA-CBA
22	A	858	CLA	C1A-C2A-CAA-CBA
22	B	810	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	818	CLA	C1A-C2A-CAA-CBA
22	B	845	CLA	C1A-C2A-CAA-CBA
22	G	206	CLA	C1A-C2A-CAA-CBA
22	B	807	CLA	C6-C7-C8-C10
22	B	822	CLA	C11-C10-C8-C7
22	A	844	CLA	O1A-CGA-O2A-C1
22	B	849	CLA	O1A-CGA-O2A-C1
21	2	321	CHL	CAA-CBA-CGA-O2A
22	4	305	CLA	CAA-CBA-CGA-O2A
26	B	843	LHG	C4-O6-P-O3
21	4	308	CHL	CAA-CBA-CGA-O2A
22	A	845	CLA	CAA-CBA-CGA-O2A
26	B	842	LHG	C11-C10-C9-C8
21	Z	301	CHL	C2A-CAA-CBA-CGA
22	3	310	CLA	C2A-CAA-CBA-CGA
22	X	304	CLA	C2A-CAA-CBA-CGA
22	Y	312	CLA	C2A-CAA-CBA-CGA
22	A	838	CLA	O1A-CGA-O2A-C1
21	Z	312	CHL	CAA-CBA-CGA-O1A
22	2	303	CLA	CAA-CBA-CGA-O2A
22	A	807	CLA	C4-C3-C5-C6
22	O	207	CLA	C4-C3-C5-C6
22	O	208	CLA	C2-C3-C5-C6
21	1	301	CHL	C2B-C3B-CAB-CBB
21	2	321	CHL	C2B-C3B-CAB-CBB
21	4	317	CHL	C2B-C3B-CAB-CBB
21	X	306	CHL	C2B-C3B-CAB-CBB
21	X	308	CHL	C2B-C3B-CAB-CBB
21	Y	303	CHL	C2B-C3B-CAB-CBB
21	Y	305	CHL	C2B-C3B-CAB-CBB
21	Y	307	CHL	C2B-C3B-CAB-CBB
21	Z	301	CHL	C2B-C3B-CAB-CBB
21	Z	304	CHL	C2B-C3B-CAB-CBB
22	2	307	CLA	C2B-C3B-CAB-CBB
22	2	319	CLA	C2B-C3B-CAB-CBB
22	3	312	CLA	C2B-C3B-CAB-CBB
22	4	304	CLA	C2B-C3B-CAB-CBB
22	A	802	CLA	C2B-C3B-CAB-CBB
22	A	806	CLA	C2B-C3B-CAB-CBB
22	A	849	CLA	C2B-C3B-CAB-CBB
22	B	806	CLA	C2B-C3B-CAB-CBB
22	B	813	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	B	826	CLA	C2B-C3B-CAB-CBB
22	B	827	CLA	C2B-C3B-CAB-CBB
22	B	833	CLA	C2B-C3B-CAB-CBB
22	B	851	CLA	C2B-C3B-CAB-CBB
22	F	306	CLA	C2B-C3B-CAB-CBB
22	K	202	CLA	C2B-C3B-CAB-CBB
22	X	310	CLA	C2B-C3B-CAB-CBB
22	Y	308	CLA	C2B-C3B-CAB-CBB
22	Y	311	CLA	C2B-C3B-CAB-CBB
26	G	203	LHG	C26-C27-C28-C29
24	2	311	XAT	C32-C33-C34-C35
24	3	302	XAT	C32-C33-C34-C35
25	A	816	BCR	C16-C17-C18-C19
25	A	818	BCR	C11-C10-C9-C8
25	B	836	BCR	C11-C10-C9-C8
25	B	836	BCR	C20-C21-C22-C23
25	F	302	BCR	C12-C13-C14-C15
25	L	301	BCR	C11-C10-C9-C8
25	L	302	BCR	C20-C21-C22-C23
27	N	201	MGE	C3B-C4B-C5B-C6B
26	O	204	LHG	O7-C5-C6-O8
26	A	822	LHG	C3-O3-P-O5
26	2	314	LHG	C7-C8-C9-C10
27	F	304	MGE	C2B-C3B-C4B-C5B
22	B	849	CLA	C4-C3-C5-C6
22	B	852	CLA	C4-C3-C5-C6
22	1	318	CLA	C2-C1-O2A-CGA
22	2	307	CLA	C2-C1-O2A-CGA
22	A	806	CLA	C2-C1-O2A-CGA
22	B	808	CLA	C2-C1-O2A-CGA
22	B	813	CLA	C2-C1-O2A-CGA
22	O	208	CLA	C2-C1-O2A-CGA
21	2	321	CHL	CAA-CBA-CGA-O1A
21	Y	303	CHL	CAA-CBA-CGA-O2A
22	B	816	CLA	C11-C10-C8-C9
22	O	207	CLA	C6-C7-C8-C9
28	A	811	PQN	C16-C17-C18-C19
22	B	811	CLA	CAA-CBA-CGA-O1A
21	X	308	CHL	O1A-CGA-O2A-C1
22	A	858	CLA	C2C-C3C-CAC-CBC
21	X	307	CHL	CAA-CBA-CGA-O2A
22	Z	314	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	A	806	CLA	C2A-CAA-CBA-CGA
21	4	308	CHL	CAA-CBA-CGA-O1A
23	1	310	LUT	C1-C6-C7-C8
25	4	321	BCR	C23-C24-C25-C30
25	A	819	BCR	C5-C6-C7-C8
25	B	834	BCR	C1-C6-C7-C8
25	B	844	BCR	C1-C6-C7-C8
25	F	302	BCR	C1-C6-C7-C8
25	F	302	BCR	C23-C24-C25-C30
25	I	101	BCR	C1-C6-C7-C8
25	J	103	BCR	C23-C24-C25-C30
25	O	203	BCR	C23-C24-C25-C30
22	B	817	CLA	C8-C10-C11-C12
22	A	852	CLA	CAA-CBA-CGA-O2A
22	G	206	CLA	C5-C6-C7-C8
26	4	301	LHG	C24-C25-C26-C27
22	A	827	CLA	C4-C3-C5-C6
22	B	829	CLA	C4-C3-C5-C6
21	Y	306	CHL	CAA-CBA-CGA-O2A
22	B	808	CLA	C10-C11-C12-C13
22	A	846	CLA	C5-C6-C7-C8
21	Z	312	CHL	CAA-CBA-CGA-O2A
22	3	318	CLA	CAA-CBA-CGA-O2A
31	B	841	DGD	C1A-C2A-C3A-C4A
22	1	321	CLA	CAA-CBA-CGA-O2A
22	2	306	CLA	CAA-CBA-CGA-O2A
22	B	830	CLA	C8-C10-C11-C12
31	B	841	DGD	O6D-C5D-C6D-O5D
21	X	307	CHL	CAA-CBA-CGA-O1A
21	Y	303	CHL	CAA-CBA-CGA-O1A
22	1	302	CLA	CAA-CBA-CGA-O2A
22	2	307	CLA	C4B-C3B-CAB-CBB
22	K	202	CLA	C4B-C3B-CAB-CBB
22	O	210	CLA	C4B-C3B-CAB-CBB
28	B	832	PQN	C20-C21-C22-C23
27	F	303	MGE	C4A-C5A-C6A-C7A
22	A	807	CLA	C2-C3-C5-C6
22	A	859	CLA	C11-C10-C8-C7
22	B	801	CLA	C2-C3-C5-C6
22	B	849	CLA	C2-C3-C5-C6
22	O	208	CLA	C6-C7-C8-C10
21	Z	303	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	1	302	CLA	CAA-CBA-CGA-O1A
26	1	313	LHG	C11-C10-C9-C8
26	4	302	LHG	O7-C7-C8-C9
26	4	302	LHG	O7-C5-C6-O8
26	3	306	LHG	C13-C14-C15-C16
26	G	203	LHG	C27-C28-C29-C30
22	3	317	CLA	CAA-CBA-CGA-O2A
21	2	301	CHL	O2A-C1-C2-C3
26	2	313	LHG	O7-C7-C8-C9
21	4	309	CHL	CAA-CBA-CGA-O2A
22	4	306	CLA	CAA-CBA-CGA-O2A
22	4	313	CLA	CAA-CBA-CGA-O2A
22	A	839	CLA	CAA-CBA-CGA-O2A
22	N	202	CLA	CAA-CBA-CGA-O2A
25	B	835	BCR	C11-C10-C9-C34
25	G	202	BCR	C20-C21-C22-C37
26	A	824	LHG	C4-O6-P-O3
22	1	307	CLA	C4-C3-C5-C6
28	A	811	PQN	C14-C13-C15-C16
21	Y	304	CHL	CAA-CBA-CGA-O2A
21	Y	313	CHL	CAA-CBA-CGA-O2A
22	B	815	CLA	CAA-CBA-CGA-O2A
22	A	807	CLA	C11-C12-C13-C14
22	B	803	CLA	C14-C13-C15-C16
22	B	812	CLA	C6-C7-C8-C9
22	B	812	CLA	C11-C10-C8-C9
21	Y	305	CHL	CAA-CBA-CGA-O2A
22	B	811	CLA	CBD-CGD-O2D-CED
26	4	301	LHG	C23-C24-C25-C26
22	3	311	CLA	C3A-C2A-CAA-CBA
22	B	818	CLA	C3A-C2A-CAA-CBA
22	G	206	CLA	C3A-C2A-CAA-CBA
22	A	852	CLA	C8-C10-C11-C12
26	O	205	LHG	O8-C23-C24-C25
21	3	314	CHL	CAA-CBA-CGA-O2A
22	2	306	CLA	CAA-CBA-CGA-O1A
22	B	821	CLA	CAA-CBA-CGA-O2A
21	Y	305	CHL	CAD-CBD-CGD-O2D
22	2	304	CLA	CAD-CBD-CGD-O2D
22	2	308	CLA	CAD-CBD-CGD-O2D
22	3	318	CLA	CAD-CBD-CGD-O2D
22	A	803	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	A	804	CLA	CAD-CBD-CGD-O2D
22	A	807	CLA	CAD-CBD-CGD-O2D
22	A	812	CLA	CAD-CBD-CGD-O2D
22	A	836	CLA	CAD-CBD-CGD-O2D
22	A	839	CLA	CAD-CBD-CGD-O2D
22	A	840	CLA	CAD-CBD-CGD-O2D
22	A	842	CLA	CAD-CBD-CGD-O2D
22	A	847	CLA	CAD-CBD-CGD-O2D
22	A	851	CLA	CAD-CBD-CGD-O2D
22	A	859	CLA	CAD-CBD-CGD-O2D
22	B	820	CLA	CAD-CBD-CGD-O2D
22	B	821	CLA	CAD-CBD-CGD-O2D
22	B	830	CLA	CAD-CBD-CGD-O2D
22	F	305	CLA	CAD-CBD-CGD-O2D
22	G	205	CLA	CAD-CBD-CGD-O2D
22	L	307	CLA	CAD-CBD-CGD-O2D
22	O	208	CLA	CAD-CBD-CGD-O2D
22	O	209	CLA	CAD-CBD-CGD-O2D
22	X	304	CLA	CAD-CBD-CGD-O2D
22	X	310	CLA	CAD-CBD-CGD-O2D
22	A	844	CLA	C2A-CAA-CBA-CGA
22	B	803	CLA	C2A-CAA-CBA-CGA
22	B	807	CLA	C8-C10-C11-C12
22	B	828	CLA	CAA-CBA-CGA-O2A
22	A	826	CLA	C10-C11-C12-C13
26	1	314	LHG	C9-C10-C11-C12
22	A	854	CLA	C4-C3-C5-C6
21	4	307	CHL	CAA-CBA-CGA-O2A
21	X	309	CHL	CAA-CBA-CGA-O2A
26	4	301	LHG	C11-C10-C9-C8
22	B	852	CLA	C2-C3-C5-C6
22	O	207	CLA	C2-C3-C5-C6
22	Y	308	CLA	CBA-CGA-O2A-C1
22	A	838	CLA	CAA-CBA-CGA-O2A
22	B	813	CLA	CAA-CBA-CGA-O2A
22	X	303	CLA	CAA-CBA-CGA-O2A
31	O	201	DGD	O1G-C1A-C2A-C3A
24	4	320	XAT	O4-C6-C7-C8
21	Y	305	CHL	CAA-CBA-CGA-O1A
22	3	318	CLA	CAA-CBA-CGA-O1A
22	K	202	CLA	CAA-CBA-CGA-O2A
31	G	201	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
26	4	302	LHG	O8-C23-C24-C25
22	B	818	CLA	CAA-CBA-CGA-O1A
21	Y	306	CHL	CAA-CBA-CGA-O1A
22	3	321	CLA	CAA-CBA-CGA-O2A
22	G	207	CLA	CAA-CBA-CGA-O2A
22	L	307	CLA	CAA-CBA-CGA-O2A
22	2	303	CLA	CBD-CGD-O2D-CED
22	A	844	CLA	O2A-C1-C2-C3
22	B	806	CLA	O2A-C1-C2-C3
22	1	319	CLA	C2A-CAA-CBA-CGA
22	B	850	CLA	C2A-CAA-CBA-CGA
21	3	307	CHL	CAA-CBA-CGA-O2A
21	Z	303	CHL	CAA-CBA-CGA-O1A
22	1	321	CLA	CAA-CBA-CGA-O1A
21	1	301	CHL	CHA-CBD-CGD-O2D
21	1	316	CHL	CHA-CBD-CGD-O1D
21	X	308	CHL	CHA-CBD-CGD-O1D
21	X	308	CHL	CHA-CBD-CGD-O2D
22	1	307	CLA	CHA-CBD-CGD-O1D
22	1	307	CLA	CHA-CBD-CGD-O2D
22	3	309	CLA	CHA-CBD-CGD-O2D
22	3	315	CLA	CHA-CBD-CGD-O1D
22	3	315	CLA	CHA-CBD-CGD-O2D
22	A	802	CLA	CHA-CBD-CGD-O2D
22	A	808	CLA	CHA-CBD-CGD-O2D
22	A	831	CLA	CHA-CBD-CGD-O2D
22	A	838	CLA	CHA-CBD-CGD-O2D
22	A	849	CLA	CHA-CBD-CGD-O1D
22	A	849	CLA	CHA-CBD-CGD-O2D
22	A	853	CLA	CHA-CBD-CGD-O1D
22	A	853	CLA	CHA-CBD-CGD-O2D
22	A	854	CLA	CHA-CBD-CGD-O1D
22	A	854	CLA	CHA-CBD-CGD-O2D
22	A	855	CLA	CHA-CBD-CGD-O1D
22	B	803	CLA	CHA-CBD-CGD-O2D
22	B	823	CLA	CHA-CBD-CGD-O2D
22	Z	306	CLA	CHA-CBD-CGD-O1D
22	Z	311	CLA	CHA-CBD-CGD-O2D
21	3	314	CHL	CAA-CBA-CGA-O1A
21	4	307	CHL	CAA-CBA-CGA-O1A
22	3	321	CLA	CAA-CBA-CGA-O1A
22	4	306	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	4	313	CLA	CAA-CBA-CGA-O1A
22	K	202	CLA	CAA-CBA-CGA-O1A
22	B	847	CLA	C4-C3-C5-C6
22	X	304	CLA	CAA-CBA-CGA-O2A
27	N	201	MGE	O2G-C1B-C2B-C3B
22	1	307	CLA	C2-C3-C5-C6
22	A	827	CLA	C2-C3-C5-C6
22	B	829	CLA	C2-C3-C5-C6
26	A	821	LHG	O6-C4-C5-C6
25	2	312	BCR	C12-C13-C14-C15
25	B	835	BCR	C11-C10-C9-C8
21	Y	313	CHL	CAA-CBA-CGA-O1A
22	1	306	CLA	CAA-CBA-CGA-O2A
22	3	317	CLA	CAA-CBA-CGA-O1A
22	B	821	CLA	CAA-CBA-CGA-O1A
22	G	207	CLA	CAA-CBA-CGA-O1A
22	L	307	CLA	CAA-CBA-CGA-O1A
26	3	306	LHG	C24-C25-C26-C27
22	B	814	CLA	C13-C15-C16-C17
22	2	307	CLA	CAA-CBA-CGA-O2A
26	1	313	LHG	O7-C7-C8-C9
26	4	302	LHG	O9-C7-C8-C9
26	4	303	LHG	O7-C5-C6-O8
22	B	830	CLA	C15-C16-C17-C18
27	F	303	MGE	C7B-C8B-C9B-CAB
22	B	845	CLA	CAA-CBA-CGA-O2A
22	B	847	CLA	CAA-CBA-CGA-O2A
22	X	310	CLA	CAA-CBA-CGA-O2A
22	X	313	CLA	CAA-CBA-CGA-O2A
22	B	804	CLA	C2A-CAA-CBA-CGA
22	F	305	CLA	C2A-CAA-CBA-CGA
21	1	316	CHL	CAA-CBA-CGA-O2A
22	3	319	CLA	CAA-CBA-CGA-O2A
22	B	808	CLA	C4C-C3C-CAC-CBC
22	A	858	CLA	CAA-CBA-CGA-O2A
26	3	306	LHG	O8-C23-C24-C25
22	A	852	CLA	C11-C12-C13-C15
27	N	201	MGE	O1B-C1B-O2G-C2G
22	B	853	CLA	CAA-CBA-CGA-O2A
22	A	852	CLA	C11-C12-C13-C14
22	O	208	CLA	C6-C7-C8-C9
26	B	843	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
27	3	305	MGE	C3B-C4B-C5B-C6B
22	A	835	CLA	C2B-C3B-CAB-CBB
21	4	309	CHL	CAA-CBA-CGA-O1A
22	3	311	CLA	CAA-CBA-CGA-O2A
22	N	202	CLA	CAA-CBA-CGA-O1A
22	B	849	CLA	CBA-CGA-O2A-C1
22	B	850	CLA	C15-C16-C17-C18
22	Y	310	CLA	CAA-CBA-CGA-O1A
26	4	302	LHG	O10-C23-C24-C25
22	A	807	CLA	C2A-CAA-CBA-CGA
22	B	812	CLA	C2A-CAA-CBA-CGA
26	2	313	LHG	O9-C7-C8-C9
31	O	201	DGD	O1A-C1A-C2A-C3A
22	A	809	CLA	C14-C13-C15-C16
22	A	803	CLA	CAA-CBA-CGA-O2A
21	X	309	CHL	CAA-CBA-CGA-O1A
21	Y	304	CHL	CAA-CBA-CGA-O1A
31	B	841	DGD	C3B-C4B-C5B-C6B
22	A	839	CLA	CAA-CBA-CGA-O1A
22	A	838	CLA	CAA-CBA-CGA-O1A
22	B	815	CLA	CAA-CBA-CGA-O1A
26	4	301	LHG	O6-C4-C5-O7
21	4	317	CHL	CHA-CBD-CGD-O2D
21	Z	301	CHL	C1A-C2A-CAA-CBA
22	3	308	CLA	C1A-C2A-CAA-CBA
22	3	311	CLA	C1A-C2A-CAA-CBA
22	4	305	CLA	C1A-C2A-CAA-CBA
22	A	826	CLA	C1A-C2A-CAA-CBA
22	A	838	CLA	C1A-C2A-CAA-CBA
22	A	855	CLA	C1A-C2A-CAA-CBA
22	X	313	CLA	C1A-C2A-CAA-CBA
22	Y	310	CLA	C1A-C2A-CAA-CBA
22	B	828	CLA	CAA-CBA-CGA-O1A
22	1	307	CLA	C2-C1-O2A-CGA
22	A	812	CLA	C2-C1-O2A-CGA
22	B	809	CLA	C2-C1-O2A-CGA
22	A	807	CLA	C10-C11-C12-C13
22	A	844	CLA	CBA-CGA-O2A-C1
22	A	858	CLA	CAA-CBA-CGA-O1A
27	N	201	MGE	O1B-C1B-C2B-C3B
27	N	201	MGE	C7B-C8B-C9B-CAB
22	B	853	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	X	303	CLA	CAA-CBA-CGA-O1A
22	X	313	CLA	CAA-CBA-CGA-O1A
22	1	306	CLA	CAA-CBA-CGA-O1A
21	3	307	CHL	CAA-CBA-CGA-O1A
21	3	307	CHL	C4B-C3B-CAB-CBB
22	1	305	CLA	C4B-C3B-CAB-CBB
22	1	308	CLA	C4B-C3B-CAB-CBB
22	1	309	CLA	C4B-C3B-CAB-CBB
22	3	310	CLA	C4B-C3B-CAB-CBB
22	4	315	CLA	C4B-C3B-CAB-CBB
22	4	318	CLA	C4B-C3B-CAB-CBB
22	A	835	CLA	C4B-C3B-CAB-CBB
22	A	840	CLA	C4B-C3B-CAB-CBB
22	B	823	CLA	C4B-C3B-CAB-CBB
22	B	833	CLA	C4B-C3B-CAB-CBB
22	B	847	CLA	C4B-C3B-CAB-CBB
22	B	849	CLA	C4B-C3B-CAB-CBB
22	K	204	CLA	C4B-C3B-CAB-CBB
22	X	310	CLA	C4B-C3B-CAB-CBB
22	X	311	CLA	C4B-C3B-CAB-CBB
22	X	312	CLA	C4B-C3B-CAB-CBB
22	X	313	CLA	C4B-C3B-CAB-CBB
22	Y	302	CLA	C4B-C3B-CAB-CBB
22	Y	309	CLA	C4B-C3B-CAB-CBB
22	Y	311	CLA	C4B-C3B-CAB-CBB
22	Z	306	CLA	C4B-C3B-CAB-CBB
26	B	843	LHG	C3-O3-P-O5
26	B	843	LHG	C4-O6-P-O4
22	2	307	CLA	CAA-CBA-CGA-O1A
22	B	845	CLA	CAA-CBA-CGA-O1A
22	X	304	CLA	CAA-CBA-CGA-O1A
26	3	306	LHG	O10-C23-C24-C25
22	A	855	CLA	CAA-CBA-CGA-O2A
22	B	850	CLA	C3-C5-C6-C7
23	4	322	LUT	C5-C6-C7-C8
25	4	321	BCR	C23-C24-C25-C26
25	A	814	BCR	C1-C6-C7-C8
25	B	837	BCR	C5-C6-C7-C8
25	B	838	BCR	C23-C24-C25-C30
25	J	101	BCR	C1-C6-C7-C8
25	J	101	BCR	C5-C6-C7-C8
26	O	205	LHG	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
22	Y	302	CLA	CAA-CBA-CGA-O2A
22	B	814	CLA	C8-C10-C11-C12
26	1	322	LHG	C26-C27-C28-C29
22	G	206	CLA	C2A-CAA-CBA-CGA
22	A	803	CLA	CAA-CBA-CGA-O1A
22	X	310	CLA	CAA-CBA-CGA-O1A
22	B	850	CLA	CAA-CBA-CGA-O2A
26	2	315	LHG	C23-C24-C25-C26
22	3	319	CLA	CAA-CBA-CGA-O1A
22	3	308	CLA	CAD-CBD-CGD-O1D
22	A	839	CLA	CAD-CBD-CGD-O1D
22	A	853	CLA	CAD-CBD-CGD-O1D
22	B	810	CLA	CAD-CBD-CGD-O1D
22	O	210	CLA	CAD-CBD-CGD-O1D
26	G	203	LHG	C4-C5-O7-C7
22	F	306	CLA	CAA-CBA-CGA-O1A
22	Y	311	CLA	CAA-CBA-CGA-O1A
22	O	207	CLA	C8-C10-C11-C12
22	A	831	CLA	C14-C13-C15-C16
22	A	855	CLA	C14-C13-C15-C16
22	B	819	CLA	C6-C7-C8-C9
22	B	850	CLA	C14-C13-C15-C16
21	1	316	CHL	CAA-CBA-CGA-O1A
22	A	857	CLA	O1A-CGA-O2A-C1
22	3	309	CLA	CAA-CBA-CGA-O1A
26	F	301	LHG	C11-C10-C9-C8
22	4	318	CLA	CAA-CBA-CGA-O2A
22	B	849	CLA	CAA-CBA-CGA-O2A
22	K	204	CLA	CAA-CBA-CGA-O2A
22	Y	312	CLA	CAA-CBA-CGA-O2A
22	1	318	CLA	CAA-CBA-CGA-O2A
22	B	823	CLA	CAA-CBA-CGA-O2A
22	B	827	CLA	CAA-CBA-CGA-O2A
22	B	833	CLA	CAA-CBA-CGA-O2A
22	Y	301	CLA	CAA-CBA-CGA-O2A
26	A	824	LHG	O8-C23-C24-C25
26	G	204	LHG	O7-C7-C8-C9
22	3	311	CLA	CAA-CBA-CGA-O1A
31	O	201	DGD	C7A-C8A-C9A-CAA
26	4	301	LHG	C5-C4-O6-P
21	4	307	CHL	CAD-CBD-CGD-O2D
21	4	308	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	4	317	CHL	CAD-CBD-CGD-O2D
22	4	305	CLA	C3A-C2A-CAA-CBA
22	A	826	CLA	C3A-C2A-CAA-CBA
22	A	831	CLA	C12-C13-C15-C16
22	A	832	CLA	C3A-C2A-CAA-CBA
22	A	855	CLA	C3A-C2A-CAA-CBA
22	B	819	CLA	C3A-C2A-CAA-CBA
22	B	819	CLA	C6-C7-C8-C10
22	B	845	CLA	C3A-C2A-CAA-CBA
22	B	850	CLA	C12-C13-C15-C16
22	L	306	CLA	C12-C13-C15-C16
22	Y	310	CLA	C3A-C2A-CAA-CBA
28	A	811	PQN	C12-C13-C15-C16
22	B	851	CLA	CAA-CBA-CGA-O1A
22	2	305	CLA	CAA-CBA-CGA-O2A
22	A	806	CLA	CAA-CBA-CGA-O2A
22	A	853	CLA	CAA-CBA-CGA-O2A
22	B	819	CLA	CAA-CBA-CGA-O2A
22	B	851	CLA	CAA-CBA-CGA-O2A
22	Y	308	CLA	CAA-CBA-CGA-O2A
22	Z	311	CLA	CAA-CBA-CGA-O2A
24	3	302	XAT	C7-C8-C9-C10
25	G	202	BCR	C21-C22-C23-C24
22	B	827	CLA	CAA-CBA-CGA-O1A
22	B	847	CLA	CAA-CBA-CGA-O1A
22	B	850	CLA	CAA-CBA-CGA-O1A
26	1	313	LHG	O9-C7-C8-C9
26	2	316	LHG	C31-C32-C33-C34
26	B	842	LHG	O8-C23-C24-C25
26	F	301	LHG	O7-C7-C8-C9
22	A	855	CLA	O1D-CGD-O2D-CED
22	A	812	CLA	C5-C6-C7-C8
22	B	833	CLA	CAA-CBA-CGA-O1A
22	B	849	CLA	CAA-CBA-CGA-O1A
22	Y	308	CLA	CAA-CBA-CGA-O1A
26	A	824	LHG	O10-C23-C24-C25
22	L	305	CLA	CAA-CBA-CGA-O2A
31	J	104	DGD	CFA-CGA-CHA-CIA
22	B	812	CLA	C8-C10-C11-C12
22	A	843	CLA	CAA-CBA-CGA-O2A
26	A	820	LHG	O7-C7-C8-C9
22	A	856	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
30	A	825	CL0	C2A-CAA-CBA-CGA
22	A	809	CLA	C5-C6-C7-C8
22	4	318	CLA	CAA-CBA-CGA-O1A
22	B	819	CLA	CAA-CBA-CGA-O1A
22	B	823	CLA	CAA-CBA-CGA-O1A
22	Y	312	CLA	CAA-CBA-CGA-O1A
22	3	310	CLA	CAA-CBA-CGA-O2A
22	O	209	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

227 monomers are involved in 664 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	4	310	CLA	3	0
28	A	811	PQN	4	0
21	Z	302	CHL	2	0
22	A	830	CLA	6	0
22	B	820	CLA	2	0
22	B	807	CLA	8	0
22	2	318	CLA	7	0
26	2	316	LHG	2	0
26	2	315	LHG	1	0
22	A	834	CLA	4	0
22	B	816	CLA	10	0
22	K	203	CLA	2	0
25	G	202	BCR	4	0
22	B	827	CLA	7	0
26	3	306	LHG	3	0
22	B	846	CLA	2	0
22	B	847	CLA	5	0
25	I	101	BCR	5	0
26	2	313	LHG	2	0
22	A	833	CLA	3	0
26	A	820	LHG	5	0
25	K	201	BCR	5	0
26	B	843	LHG	9	0
22	A	809	CLA	5	0
22	1	320	CLA	2	0
22	G	206	CLA	4	0
24	2	311	XAT	9	0
22	B	818	CLA	6	0
29	C	102	SF4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	837	CLA	3	0
22	B	829	CLA	5	0
25	L	302	BCR	3	0
22	3	308	CLA	1	0
28	B	832	PQN	7	0
22	1	319	CLA	1	0
22	A	802	CLA	1	0
25	B	840	BCR	6	0
25	A	818	BCR	6	0
27	3	304	MGE	1	0
25	O	203	BCR	4	0
21	Y	313	CHL	1	0
21	2	302	CHL	4	0
22	4	312	CLA	1	0
22	A	803	CLA	3	0
25	A	816	BCR	6	0
21	4	317	CHL	1	0
22	A	859	CLA	3	0
27	3	305	MGE	2	0
31	B	841	DGD	4	0
25	B	844	BCR	6	0
22	A	831	CLA	5	0
25	2	312	BCR	12	0
22	2	308	CLA	3	0
22	3	313	CLA	1	0
22	A	845	CLA	2	0
22	X	303	CLA	2	0
22	Y	314	CLA	1	0
25	B	835	BCR	6	0
31	G	201	DGD	9	0
22	B	803	CLA	11	0
22	4	311	CLA	5	0
22	B	809	CLA	6	0
21	2	309	CHL	3	0
25	B	837	BCR	5	0
22	B	806	CLA	3	0
22	B	849	CLA	7	0
24	3	302	XAT	7	0
21	Z	305	CHL	1	0
22	A	847	CLA	2	0
22	A	838	CLA	10	0
21	2	301	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	3	311	CLA	1	0
22	3	317	CLA	2	0
22	L	307	CLA	4	0
22	1	304	CLA	5	0
22	B	845	CLA	4	0
22	3	312	CLA	6	0
26	G	203	LHG	1	0
21	Y	307	CHL	2	0
22	A	839	CLA	3	0
22	1	306	CLA	1	0
22	A	844	CLA	10	0
25	B	838	BCR	4	0
22	3	316	CLA	4	0
25	F	302	BCR	6	0
22	A	808	CLA	2	0
21	Y	304	CHL	1	0
21	3	307	CHL	2	0
22	F	306	CLA	2	0
22	K	204	CLA	6	0
21	Z	303	CHL	2	0
22	B	828	CLA	5	0
22	B	848	CLA	3	0
22	B	851	CLA	5	0
23	1	310	LUT	4	0
29	C	101	SF4	1	0
22	O	207	CLA	1	0
25	O	202	BCR	5	0
22	3	320	CLA	2	0
22	A	841	CLA	1	0
22	A	827	CLA	8	0
22	G	207	CLA	1	0
26	1	322	LHG	2	0
22	2	303	CLA	3	0
22	A	854	CLA	8	0
22	B	831	CLA	5	0
22	A	801	CLA	1	0
22	1	317	CLA	9	0
22	Y	311	CLA	2	0
26	1	314	LHG	2	0
22	1	318	CLA	3	0
22	B	802	CLA	4	0
22	2	322	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	2	317	CLA	1	0
22	O	208	CLA	4	0
25	1	312	BCR	6	0
24	4	320	XAT	5	0
26	F	301	LHG	3	0
22	A	812	CLA	3	0
22	B	817	CLA	4	0
22	A	856	CLA	2	0
22	A	853	CLA	13	0
26	A	821	LHG	1	0
22	B	819	CLA	6	0
22	A	857	CLA	7	0
22	A	840	CLA	3	0
22	A	846	CLA	9	0
22	B	804	CLA	6	0
22	B	824	CLA	2	0
22	G	205	CLA	7	0
25	L	303	BCR	3	0
22	A	832	CLA	3	0
26	4	301	LHG	3	0
25	B	836	BCR	4	0
25	J	101	BCR	6	0
22	A	855	CLA	8	0
22	A	858	CLA	8	0
26	G	204	LHG	1	0
31	O	201	DGD	4	0
22	A	805	CLA	1	0
22	B	825	CLA	4	0
25	A	817	BCR	10	0
27	N	201	MGE	2	0
21	1	316	CHL	2	0
22	B	850	CLA	5	0
24	1	311	XAT	4	0
26	A	823	LHG	3	0
25	A	814	BCR	4	0
22	B	808	CLA	7	0
22	4	316	CLA	3	0
22	3	309	CLA	4	0
25	J	103	BCR	5	0
21	4	309	CHL	4	0
22	3	318	CLA	1	0
22	A	810	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	829	CLA	2	0
22	X	304	CLA	1	0
22	A	836	CLA	3	0
22	A	806	CLA	2	0
22	A	850	CLA	2	0
22	B	815	CLA	5	0
22	B	833	CLA	3	0
22	3	310	CLA	2	0
22	1	308	CLA	1	0
22	L	306	CLA	12	0
25	L	301	BCR	6	0
22	X	301	CLA	1	0
22	B	814	CLA	7	0
22	O	209	CLA	1	0
23	4	322	LUT	6	0
25	A	819	BCR	5	0
23	4	319	LUT	3	0
25	A	815	BCR	3	0
27	F	303	MGE	2	0
21	3	314	CHL	1	0
25	L	304	BCR	1	0
26	A	824	LHG	2	0
22	4	304	CLA	2	0
22	1	321	CLA	2	0
22	4	313	CLA	2	0
22	A	804	CLA	2	0
22	B	811	CLA	5	0
22	2	307	CLA	1	0
22	B	852	CLA	6	0
22	B	812	CLA	5	0
21	4	308	CHL	1	0
21	Z	312	CHL	1	0
22	B	813	CLA	2	0
23	2	310	LUT	4	0
27	1	315	MGE	3	0
22	1	307	CLA	1	0
22	A	807	CLA	2	0
22	B	801	CLA	4	0
22	A	842	CLA	3	0
25	4	321	BCR	1	0
30	A	825	CL0	4	0
23	3	301	LUT	5	0

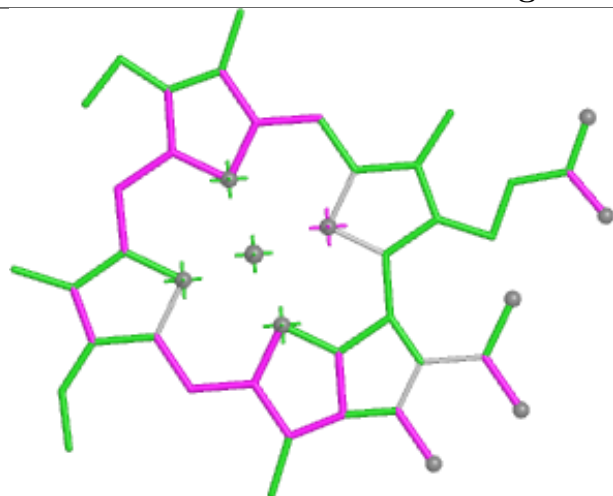
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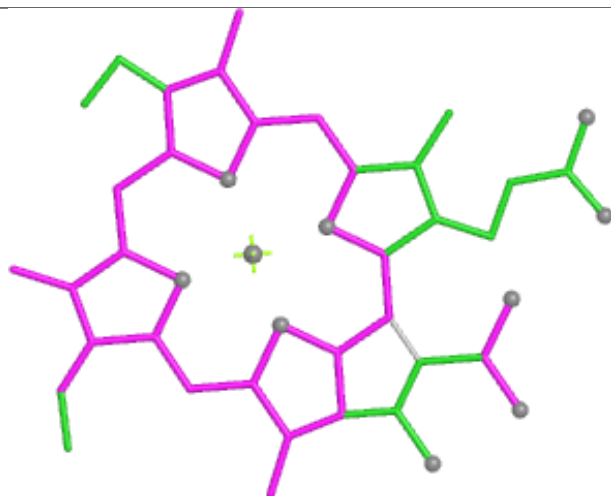
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	2	321	CHL	3	0
22	A	826	CLA	4	0
22	B	805	CLA	1	0
25	3	303	BCR	2	0
22	A	835	CLA	4	0
25	B	839	BCR	6	0
22	J	102	CLA	1	0
26	1	313	LHG	2	0
22	A	843	CLA	2	0
22	B	810	CLA	1	0
22	A	849	CLA	9	0
22	2	320	CLA	2	0
27	F	304	MGE	1	0
22	A	828	CLA	4	0
22	A	848	CLA	2	0
26	2	314	LHG	5	0
22	F	305	CLA	2	0
26	A	822	LHG	18	0
26	4	302	LHG	2	0
26	B	842	LHG	1	0
22	4	318	CLA	1	0
22	A	852	CLA	5	0
22	B	823	CLA	6	0
22	B	822	CLA	7	0
26	O	205	LHG	2	0
22	2	319	CLA	1	0
22	B	830	CLA	4	0
22	K	205	CLA	1	0
25	B	834	BCR	8	0
22	1	303	CLA	6	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.

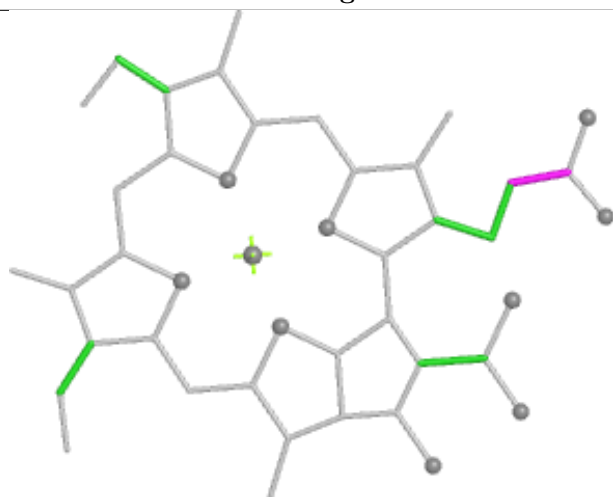
Ligand CLA 2 306



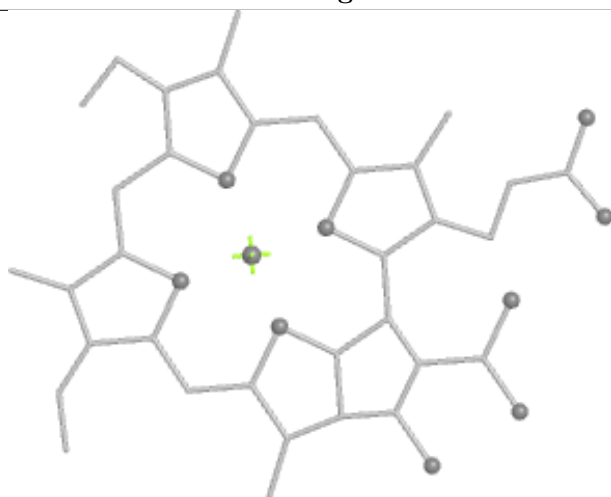
Bond lengths



Bond angles

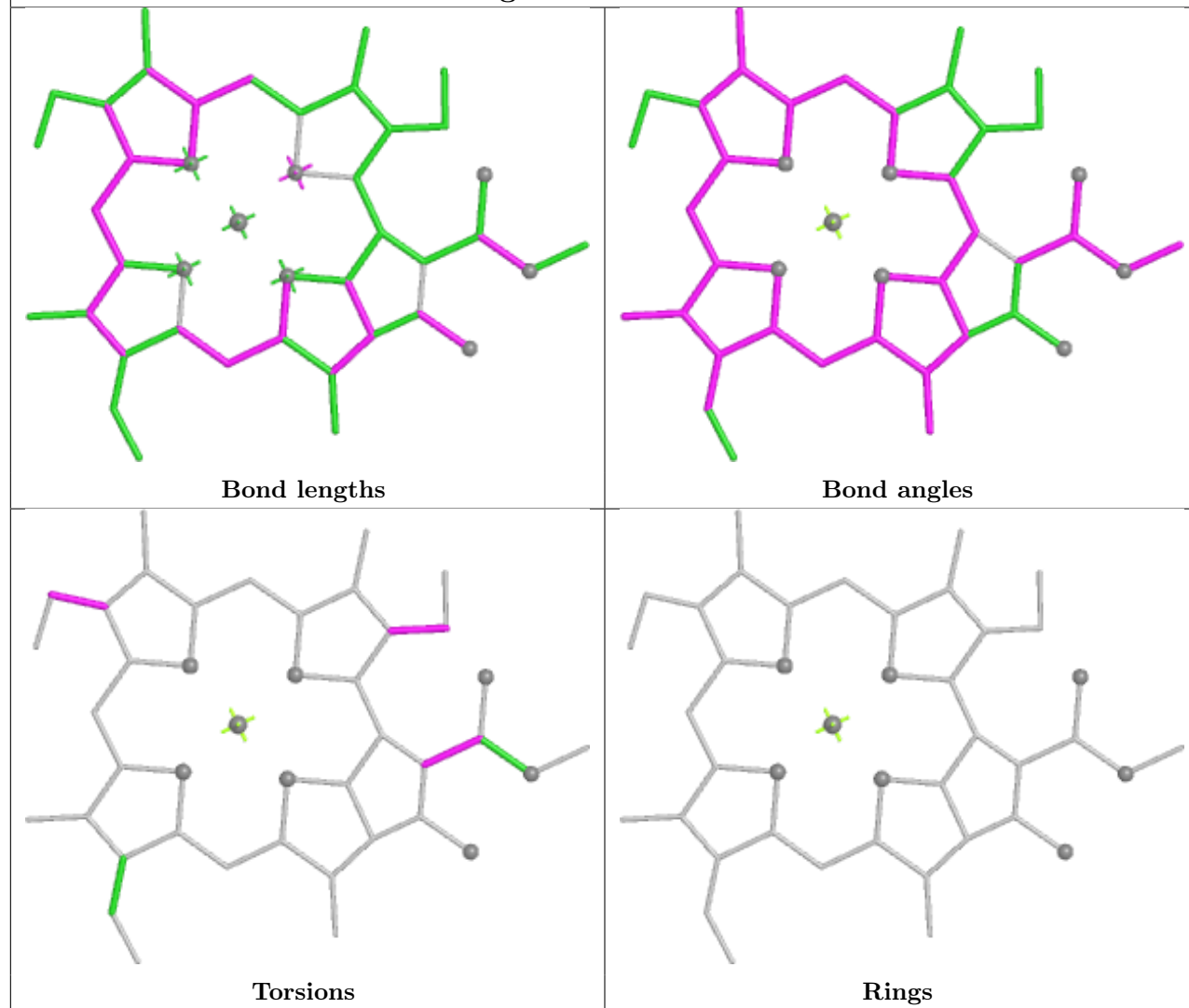


Torsions

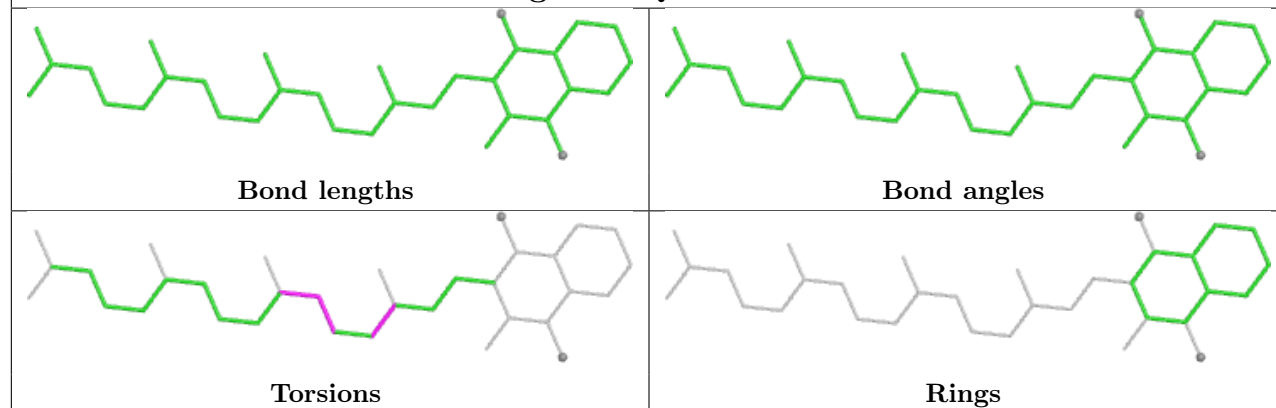


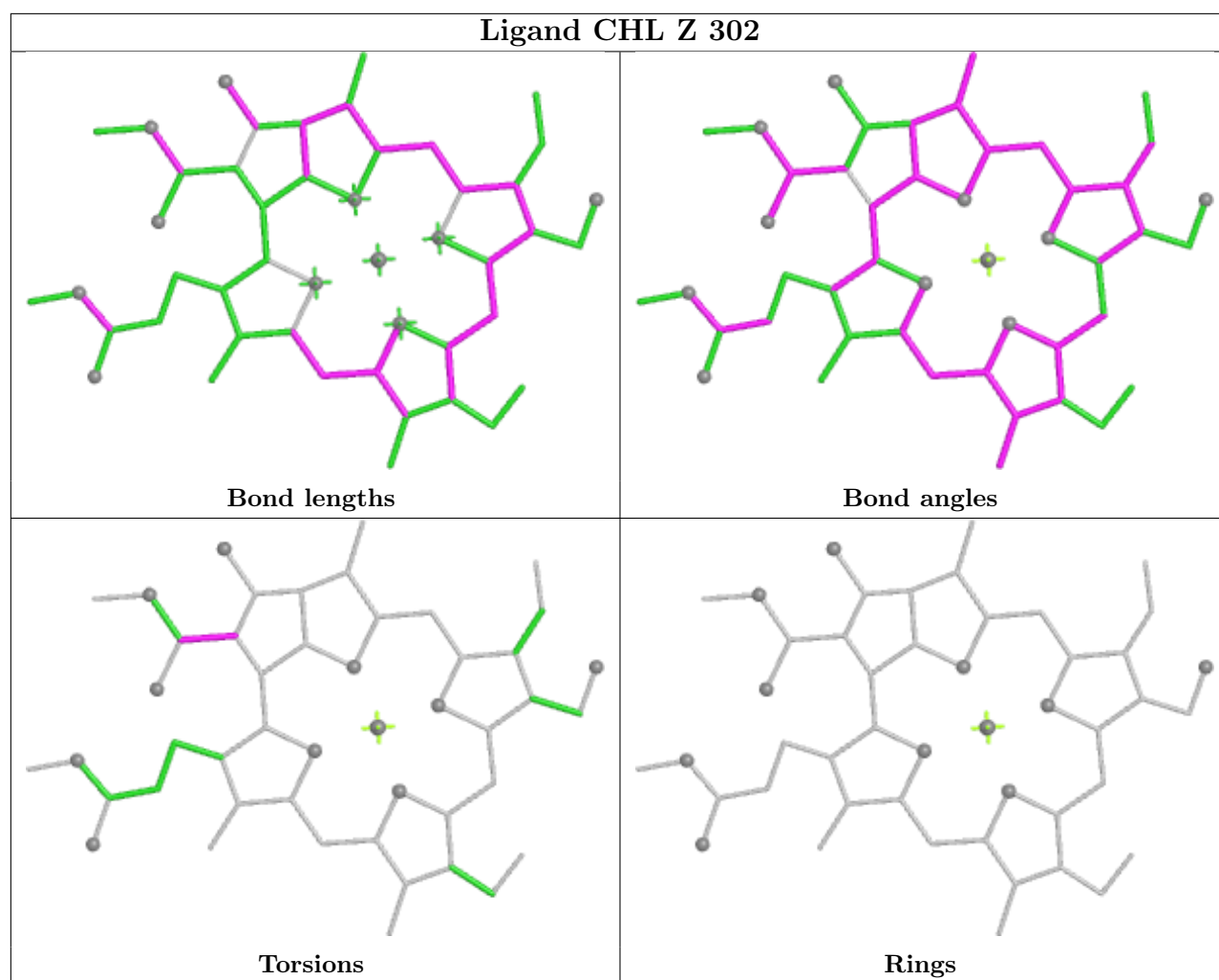
Rings

Ligand CLA 4 310

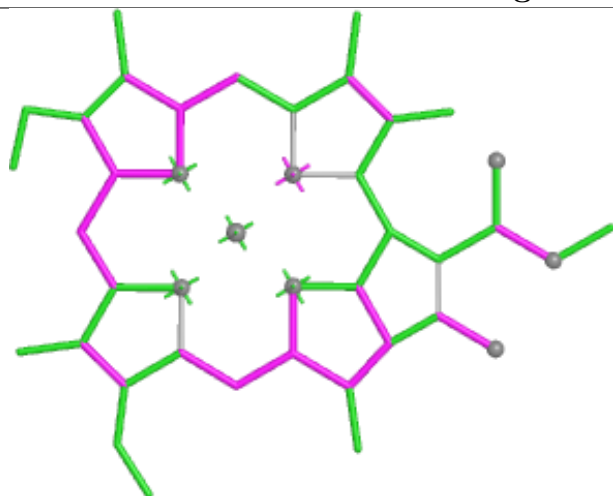


Ligand PQN A 811





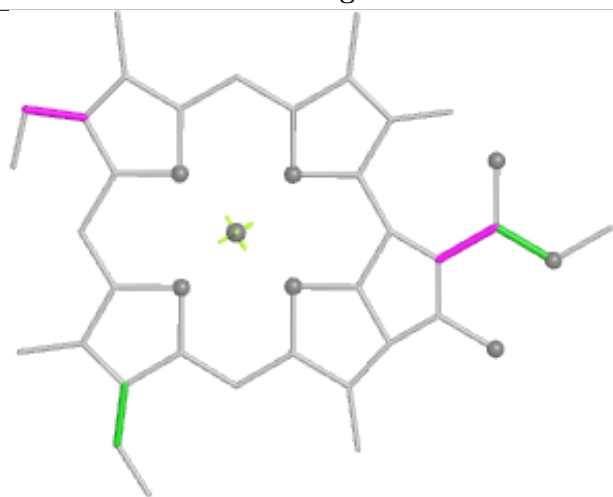
Ligand CLA O 210



Bond lengths



Bond angles

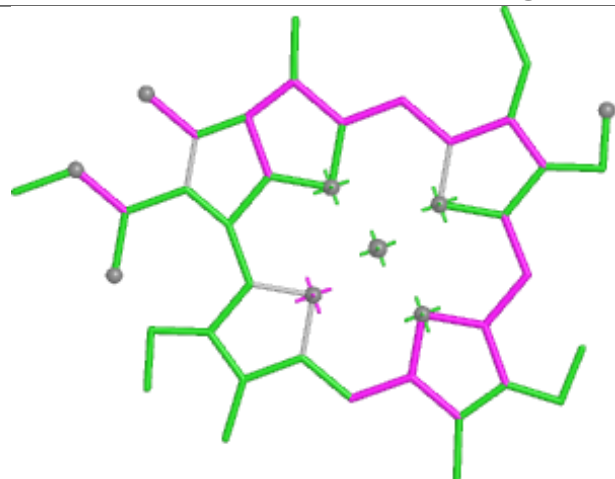


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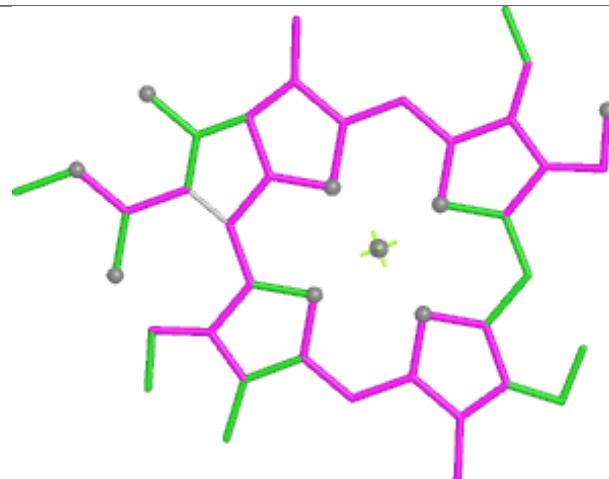


Rings

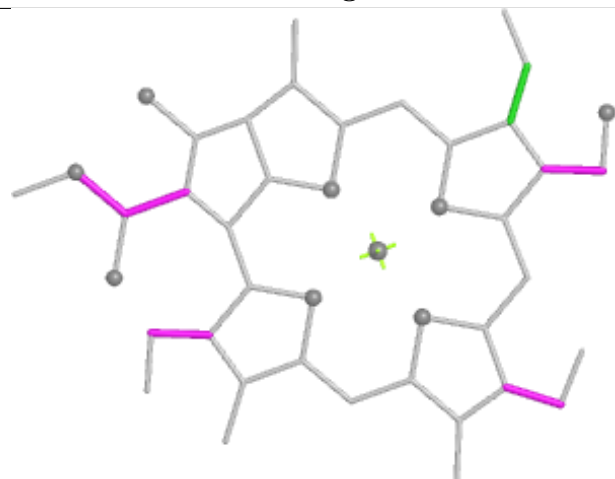
Ligand CHL 1 301



Bond lengths



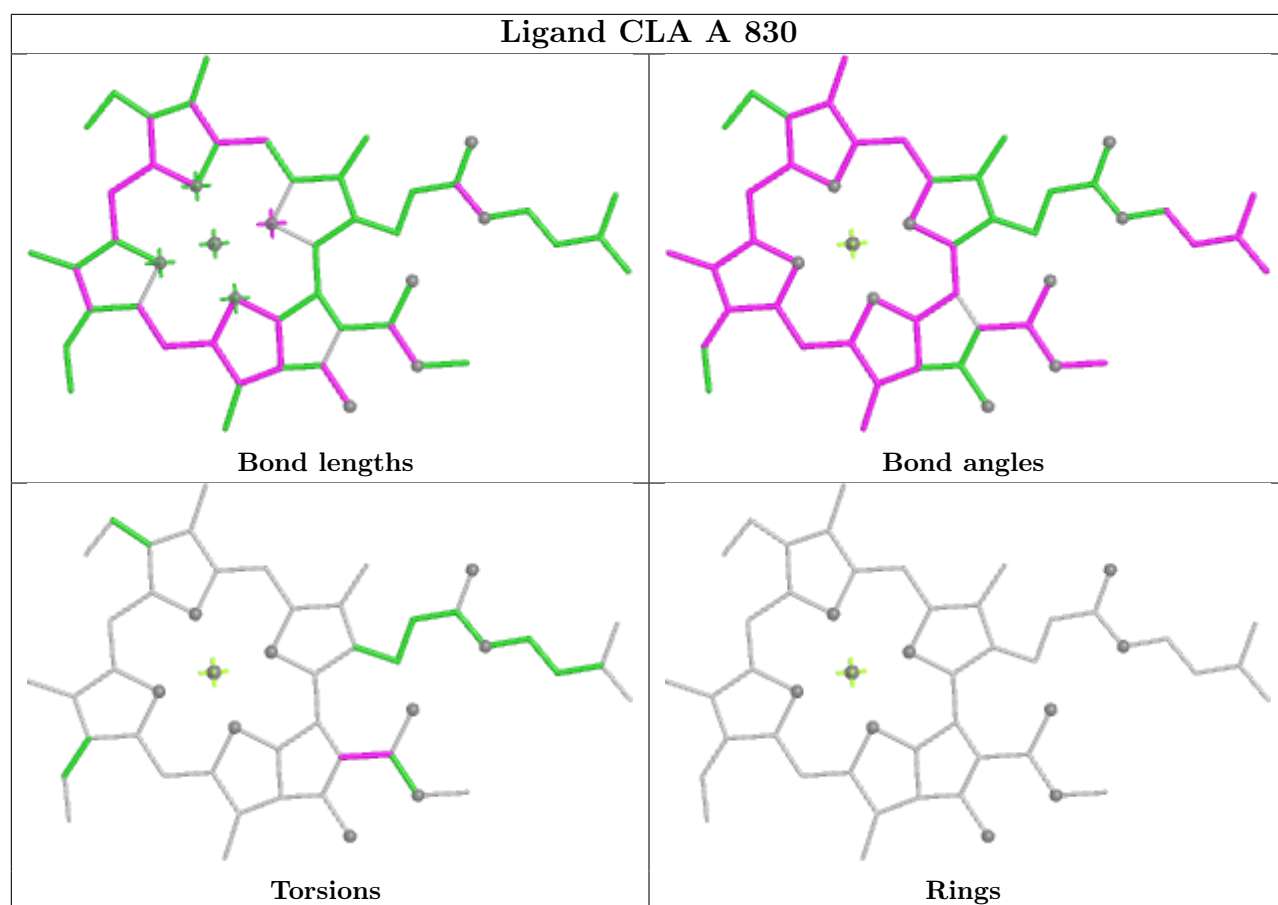
Bond angles

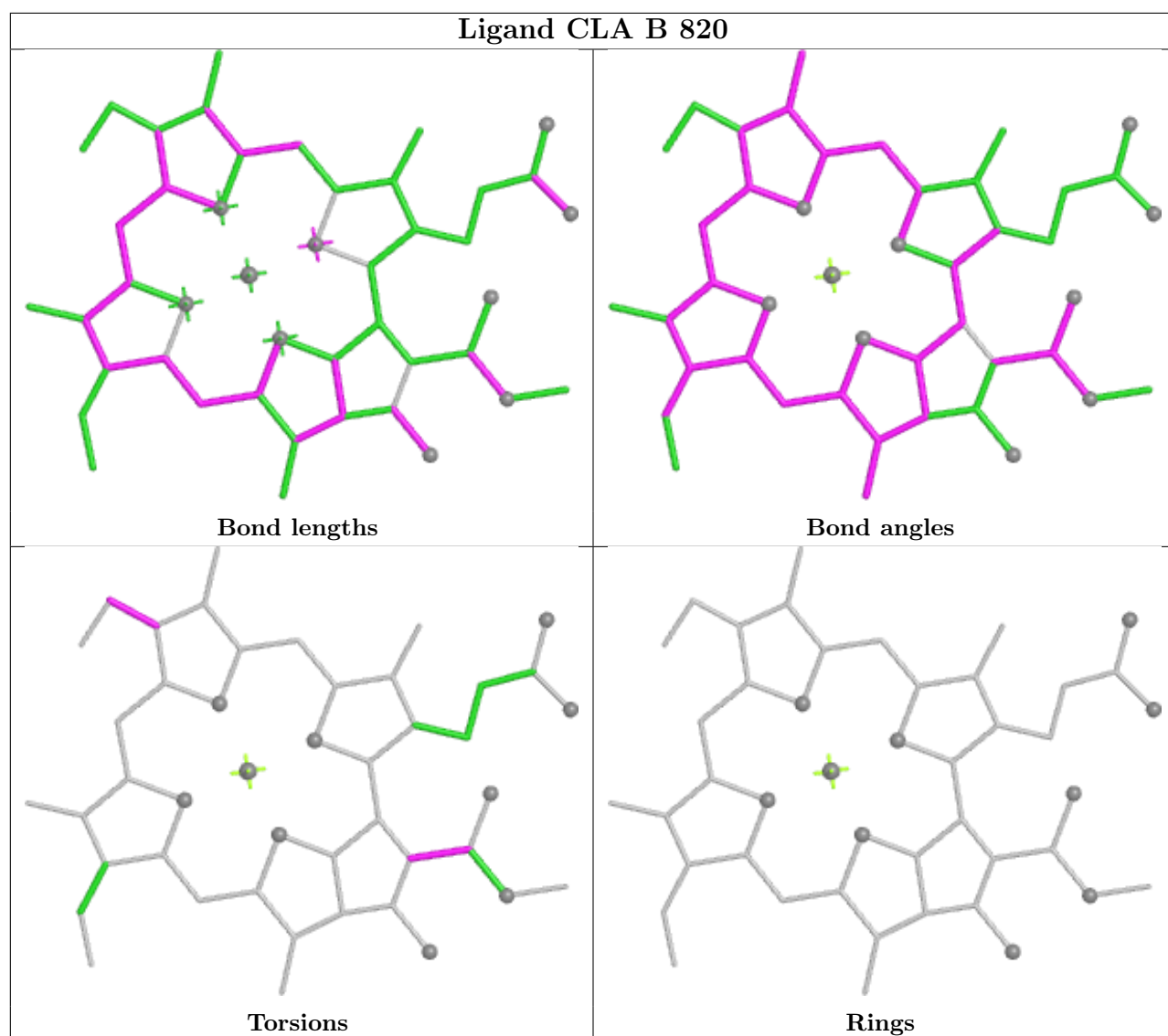


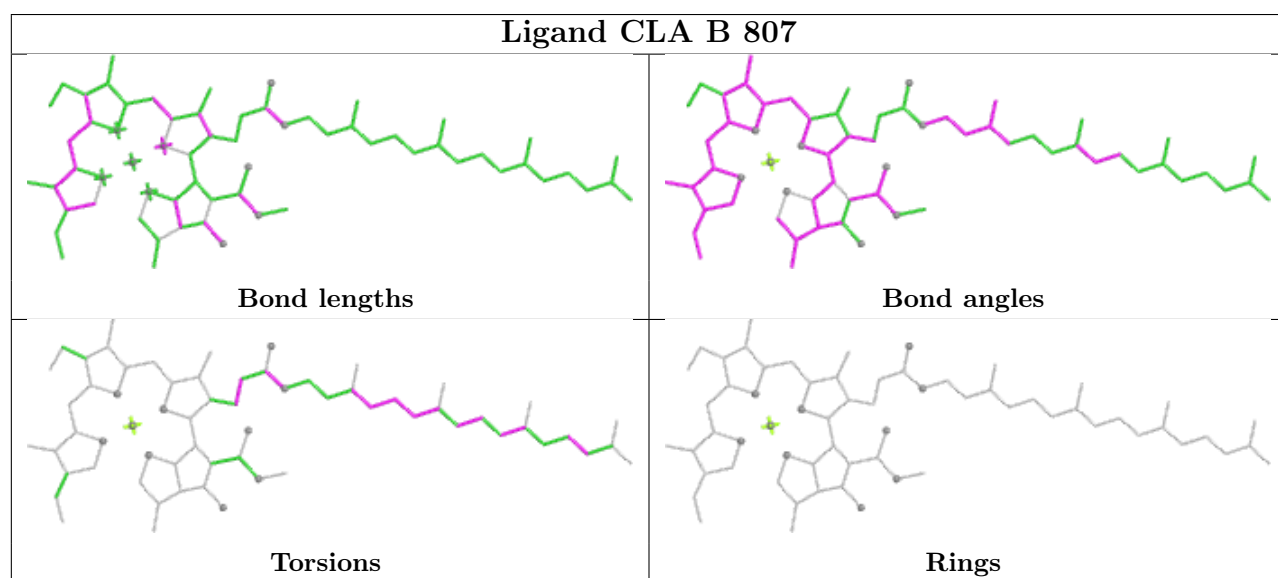
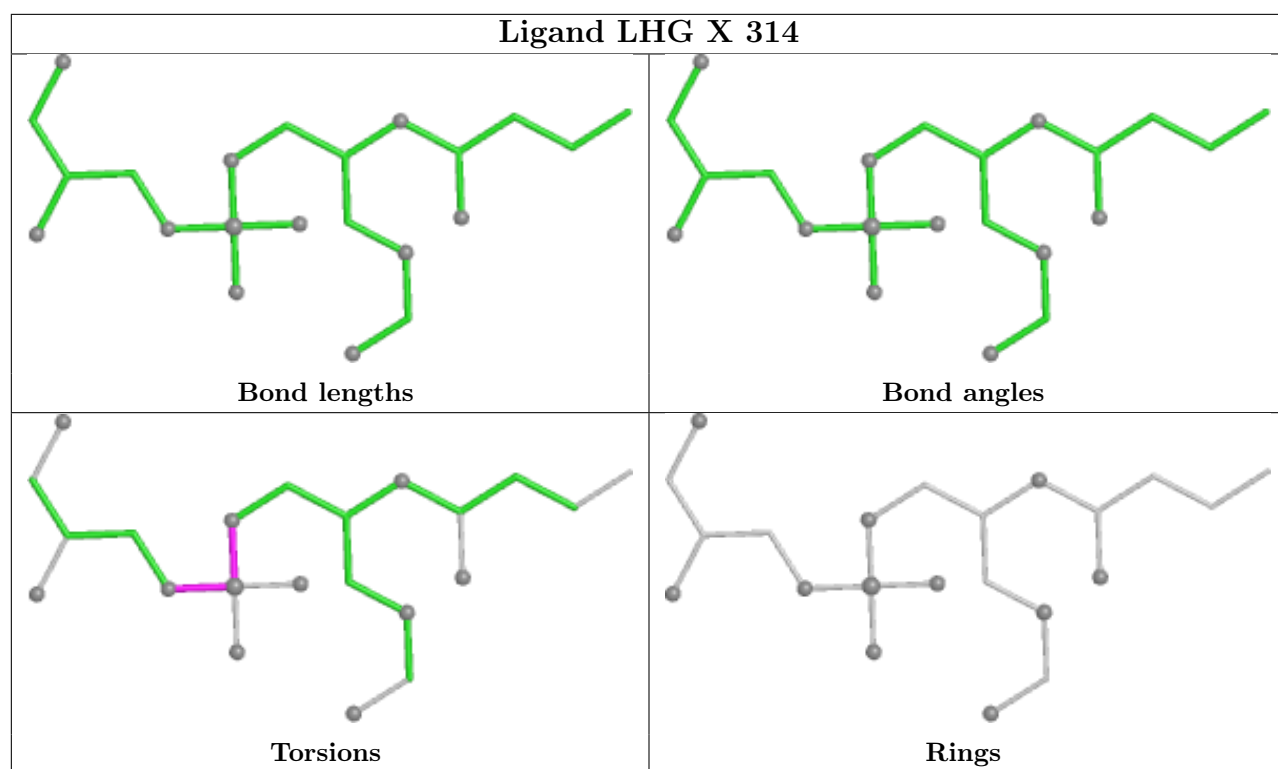
Torsions

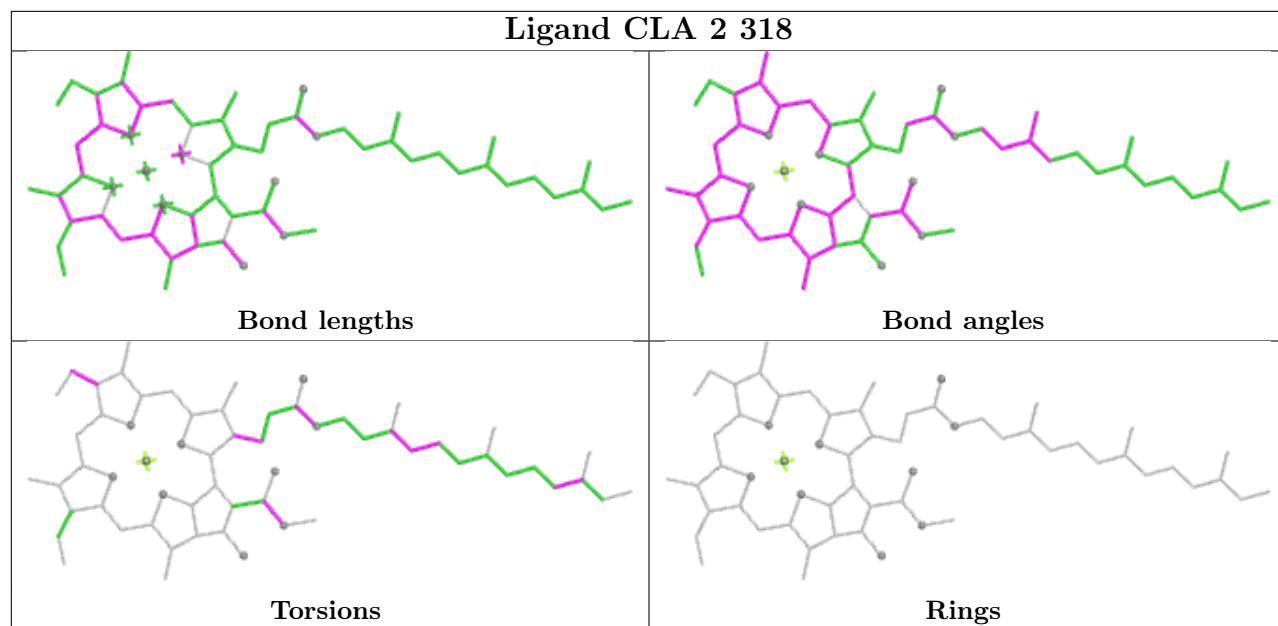


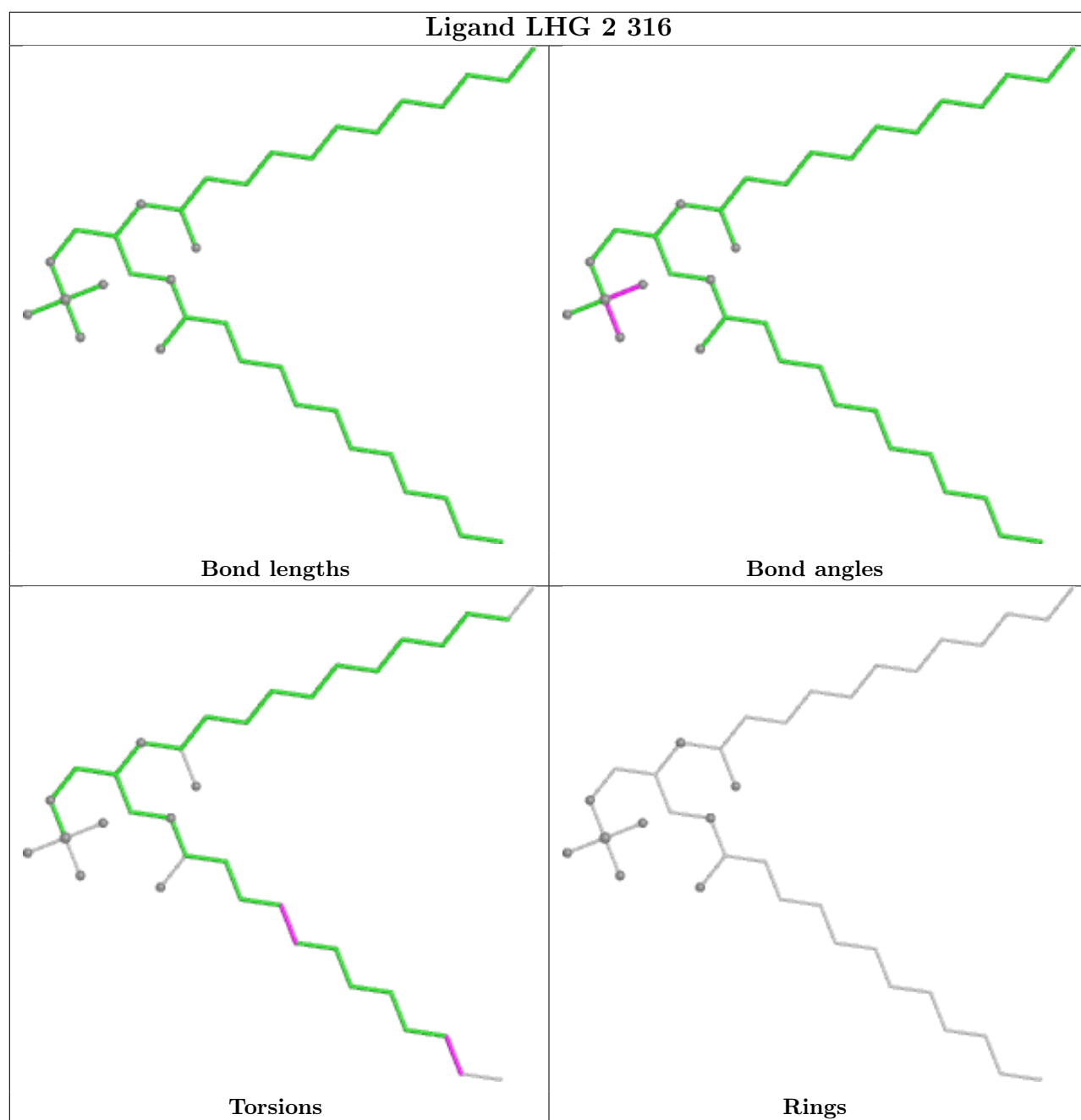
Rings

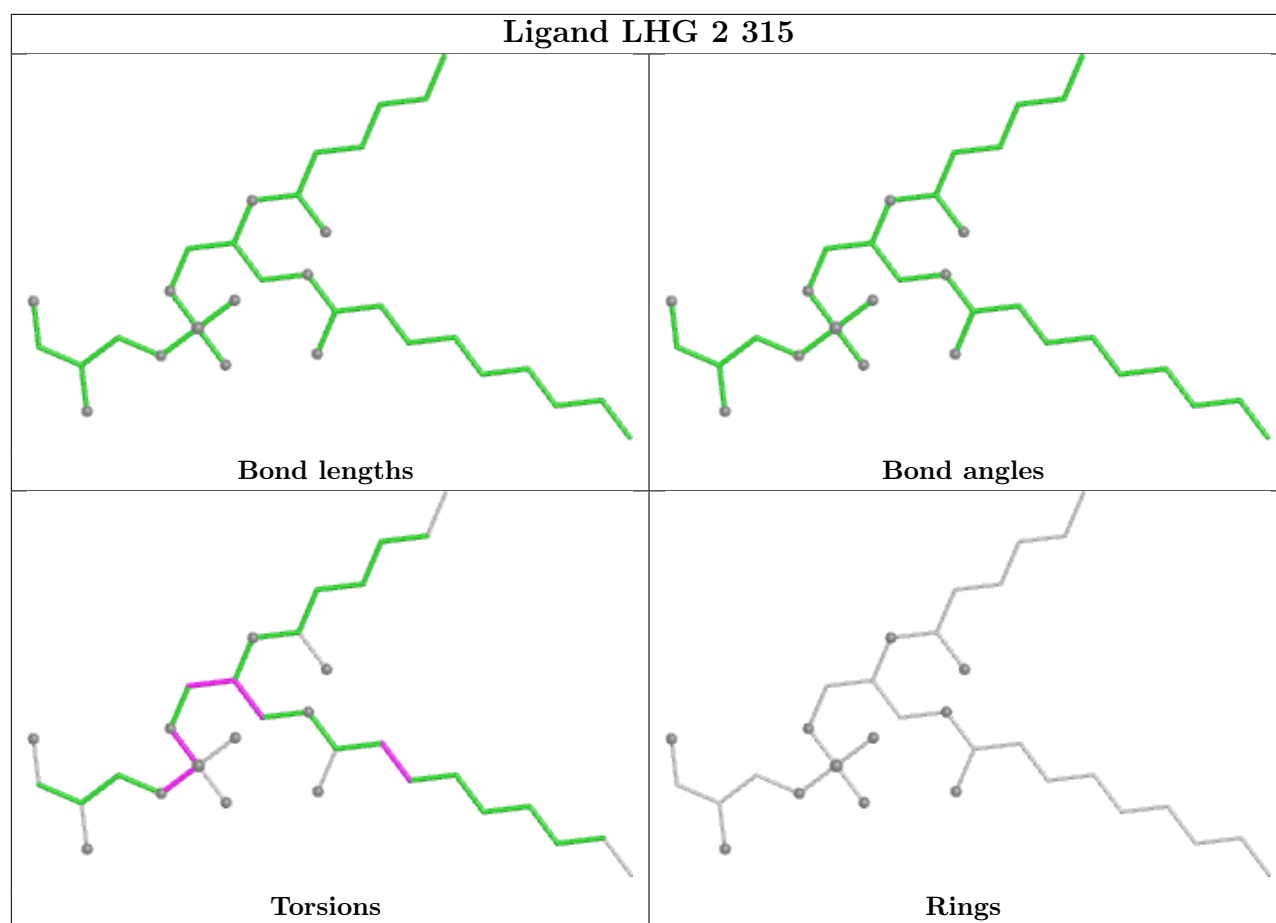




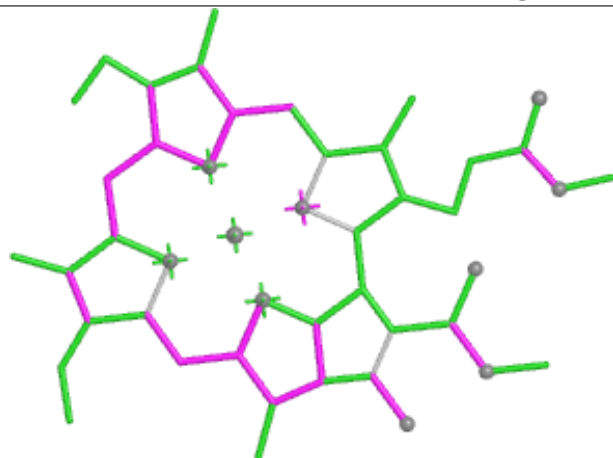




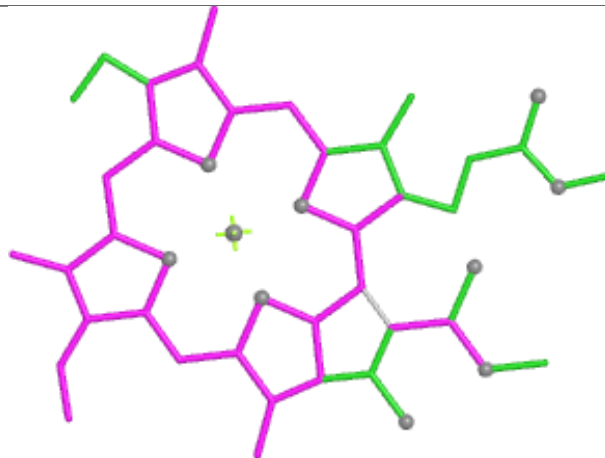




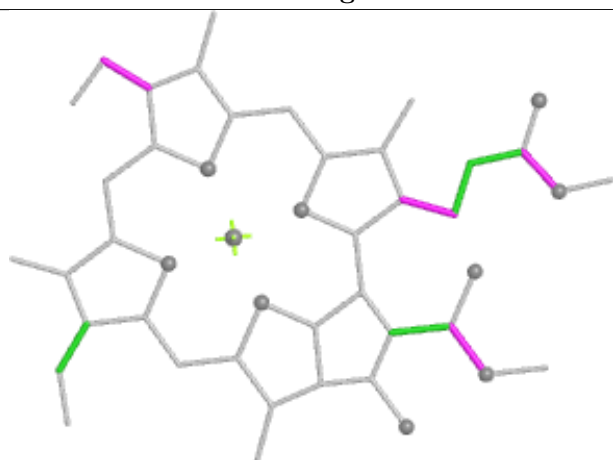
Ligand CLA A 834



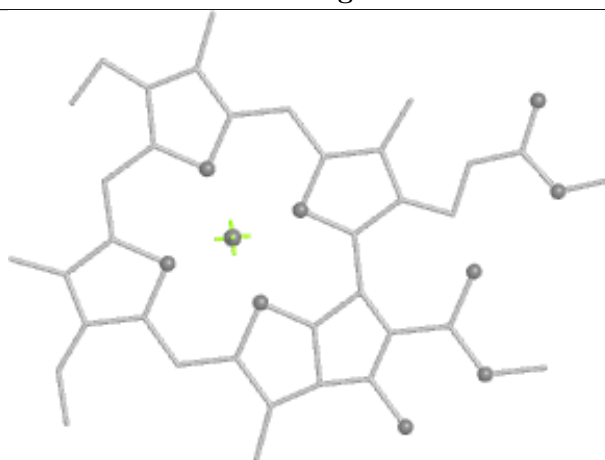
Bond lengths



Bond angles

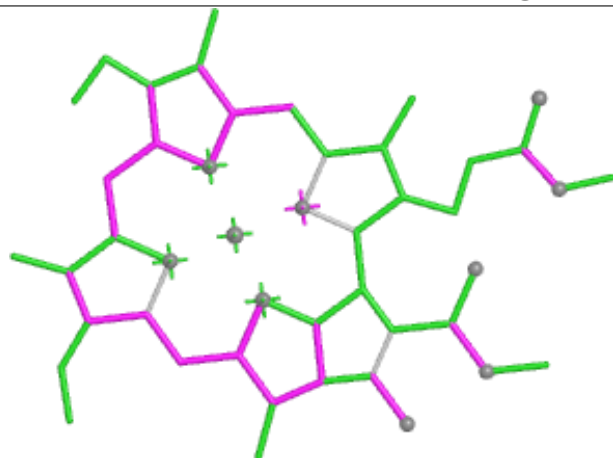


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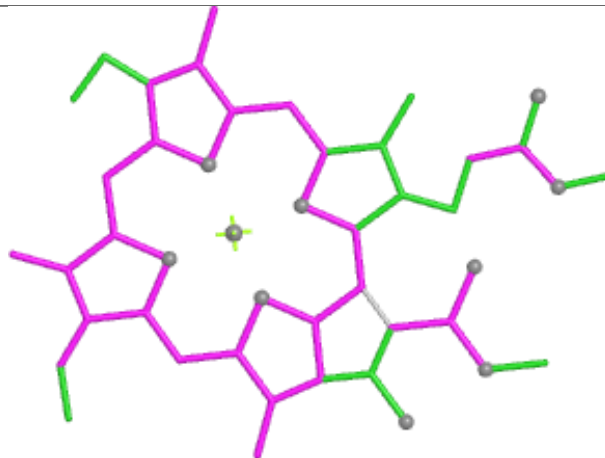


Rings

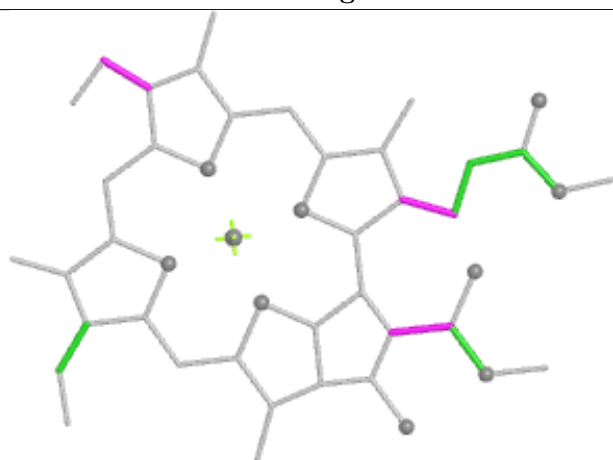
Ligand CLA Z 306



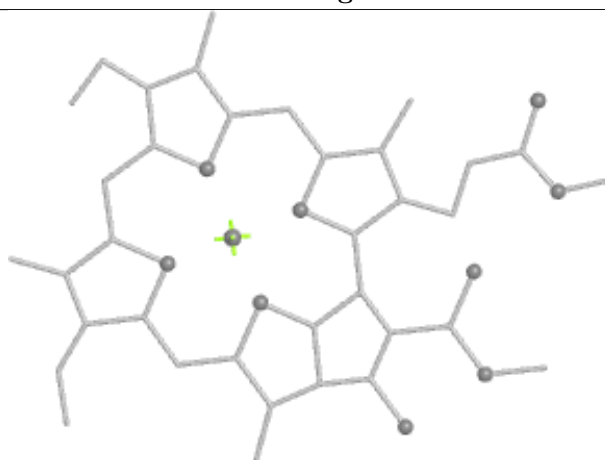
Bond lengths



Bond angles

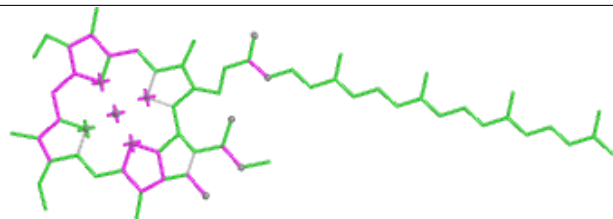


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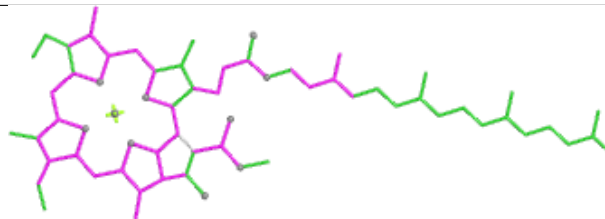


Rings

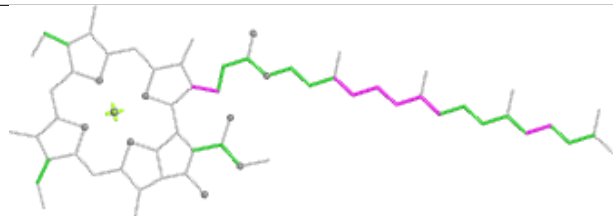
Ligand CLA B 816



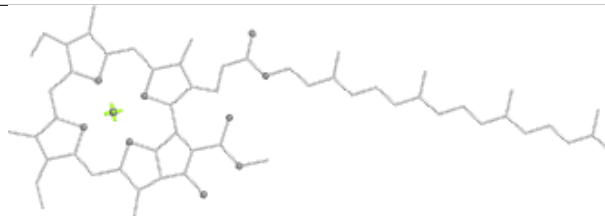
Bond lengths



Bond angles

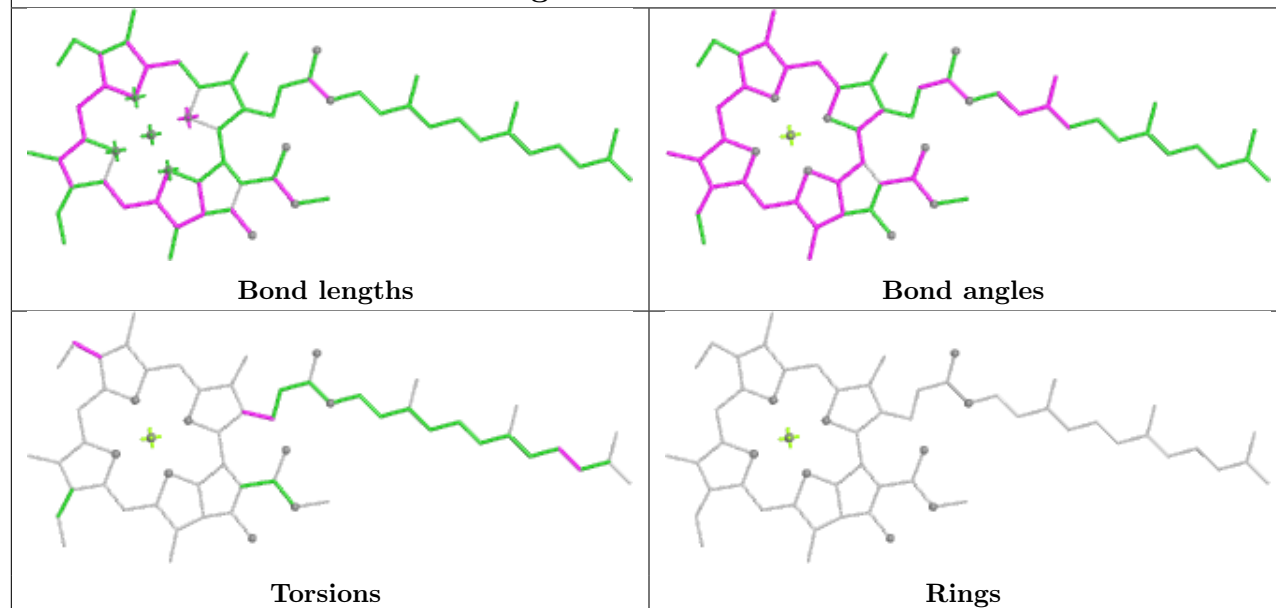


Torsions

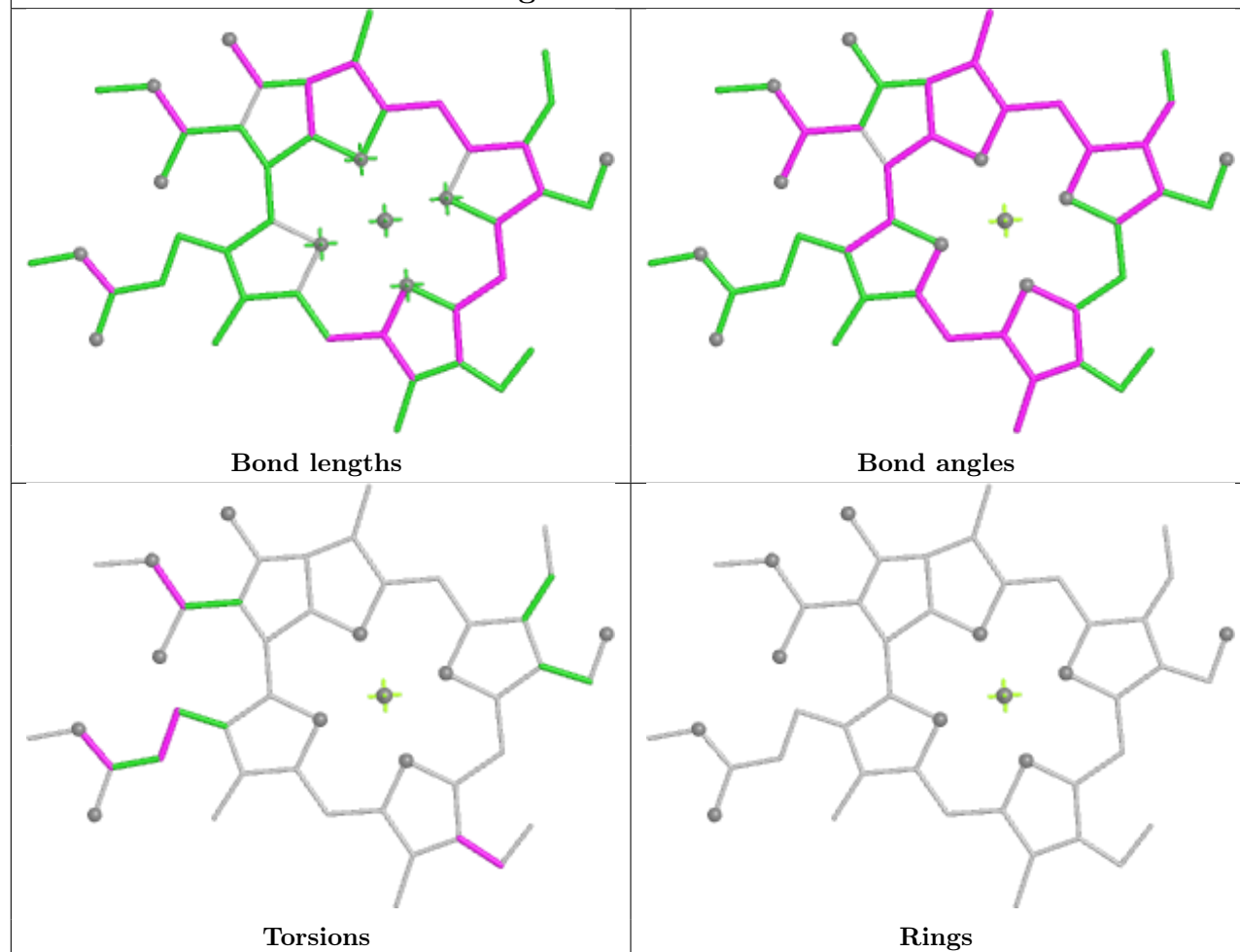


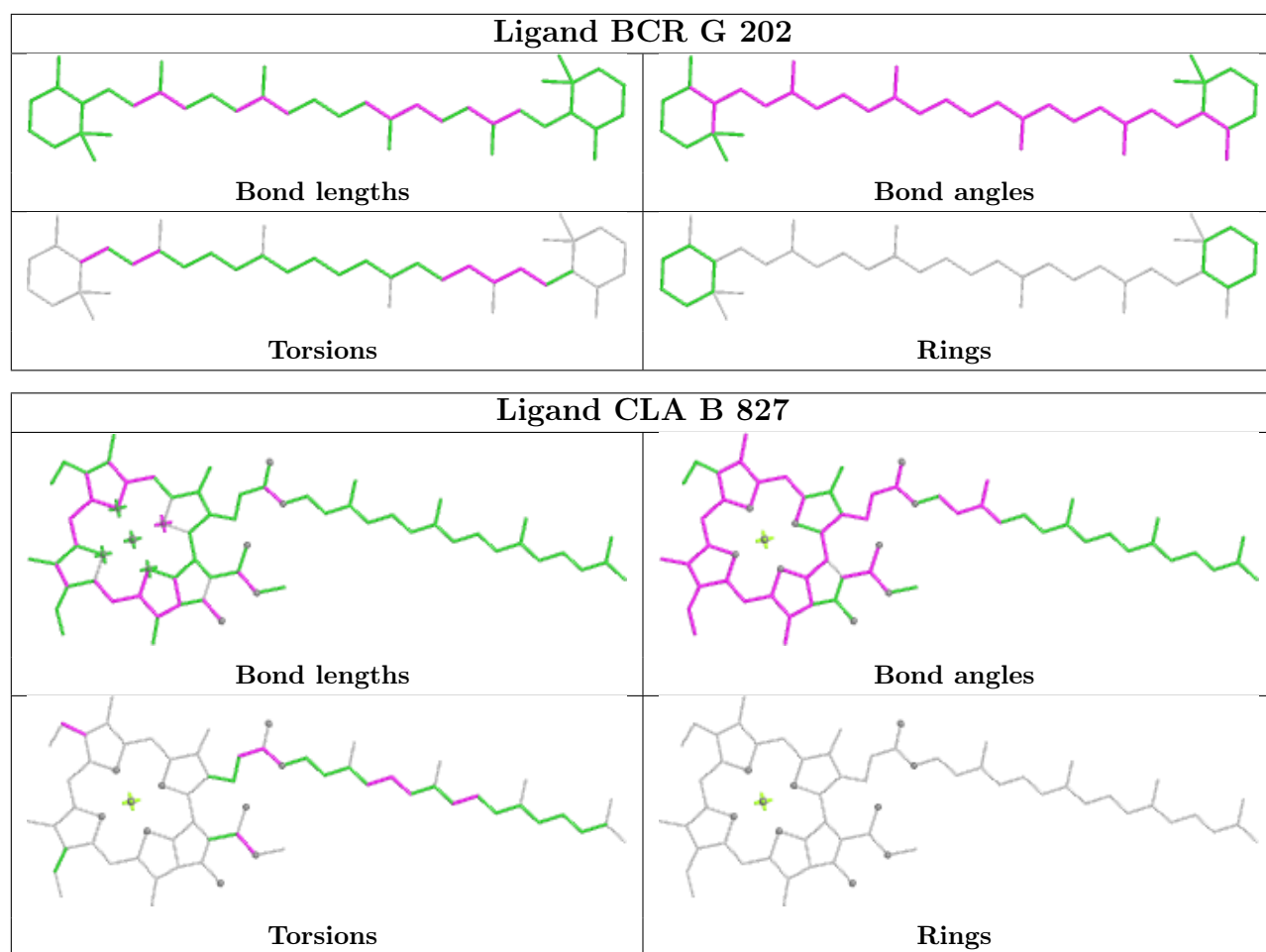
Rings

Ligand CLA K 203

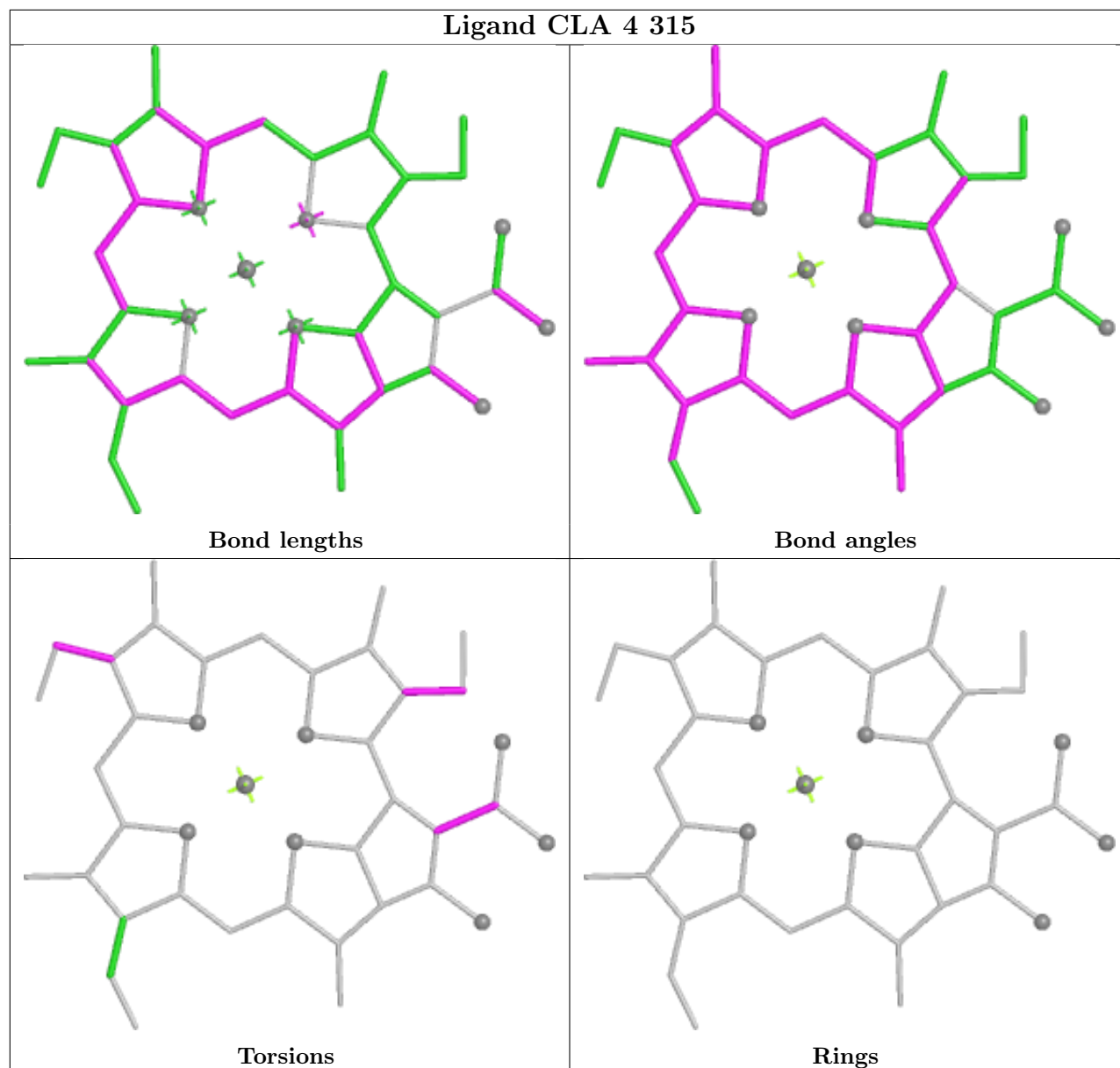


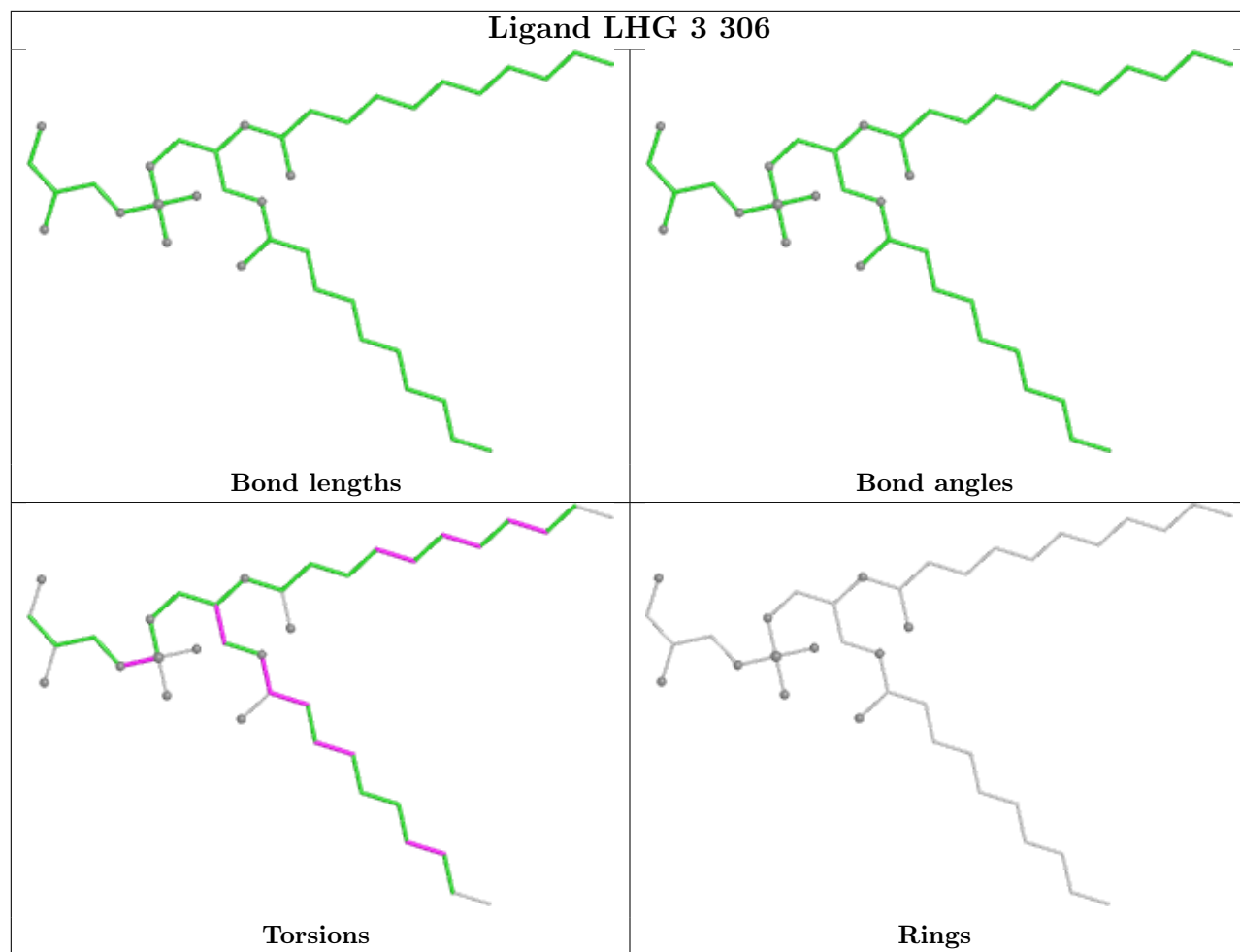
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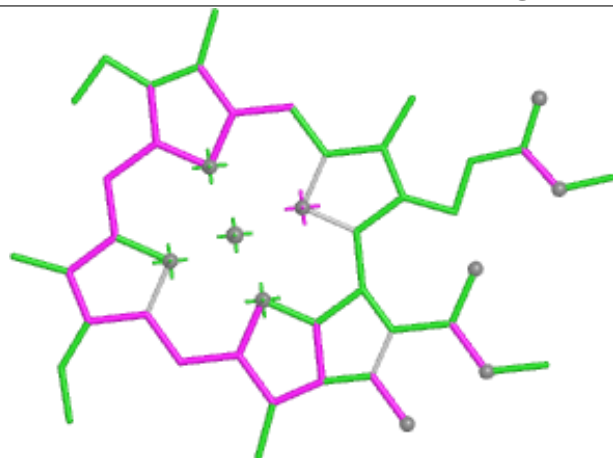


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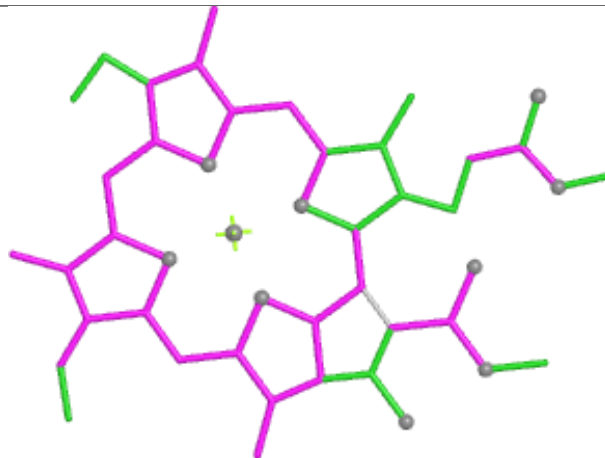




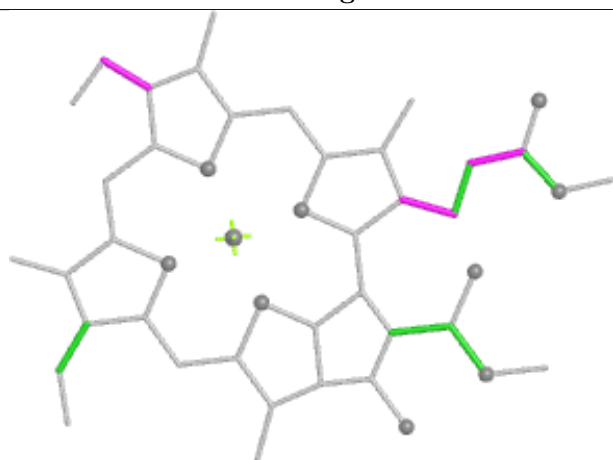
Ligand CLA Y 309



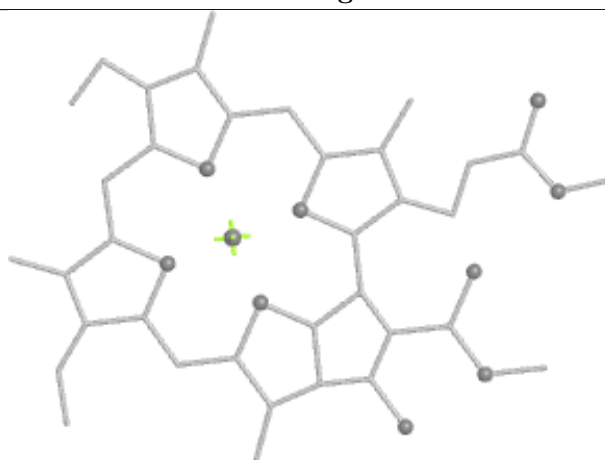
Bond lengths



Bond angles

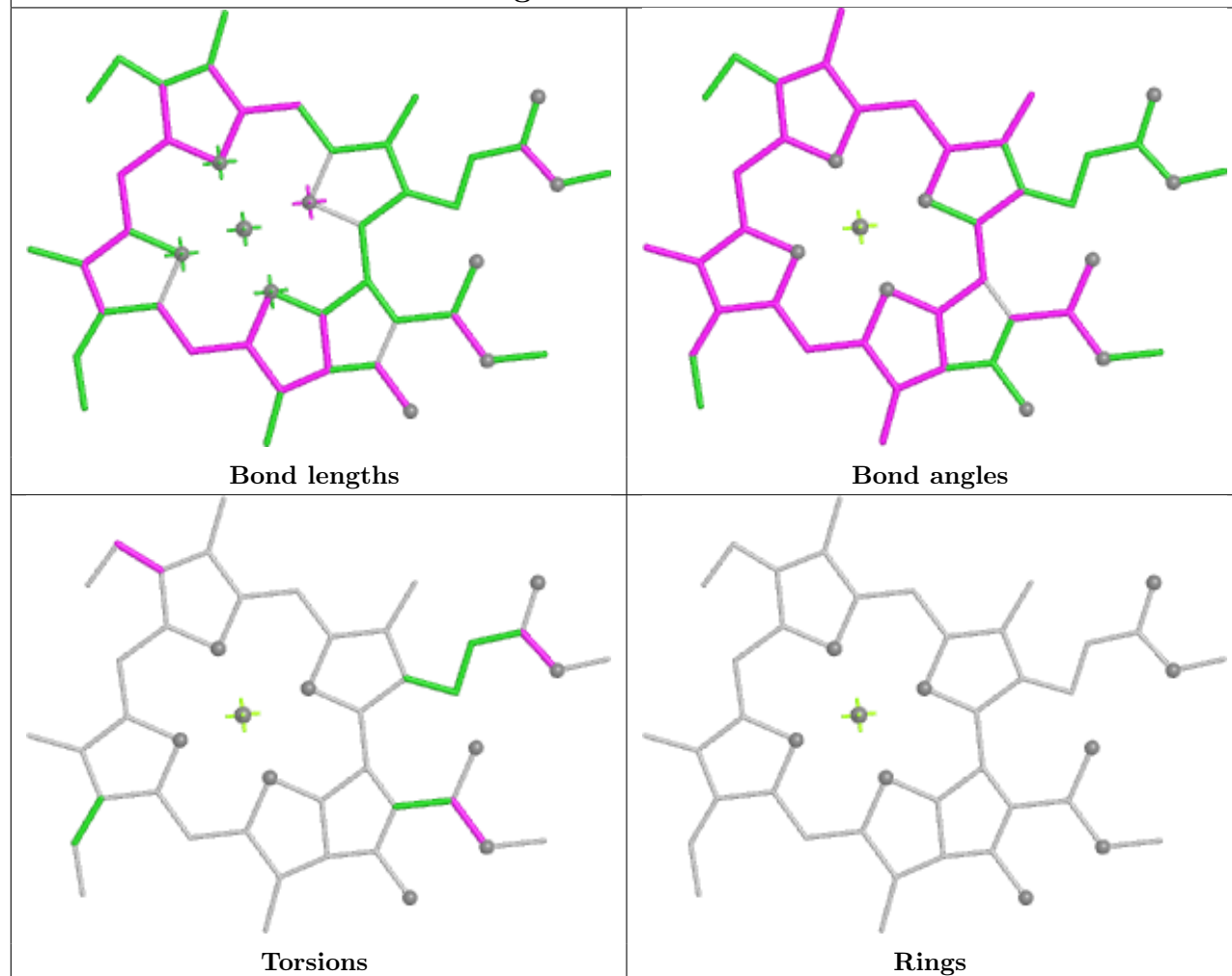


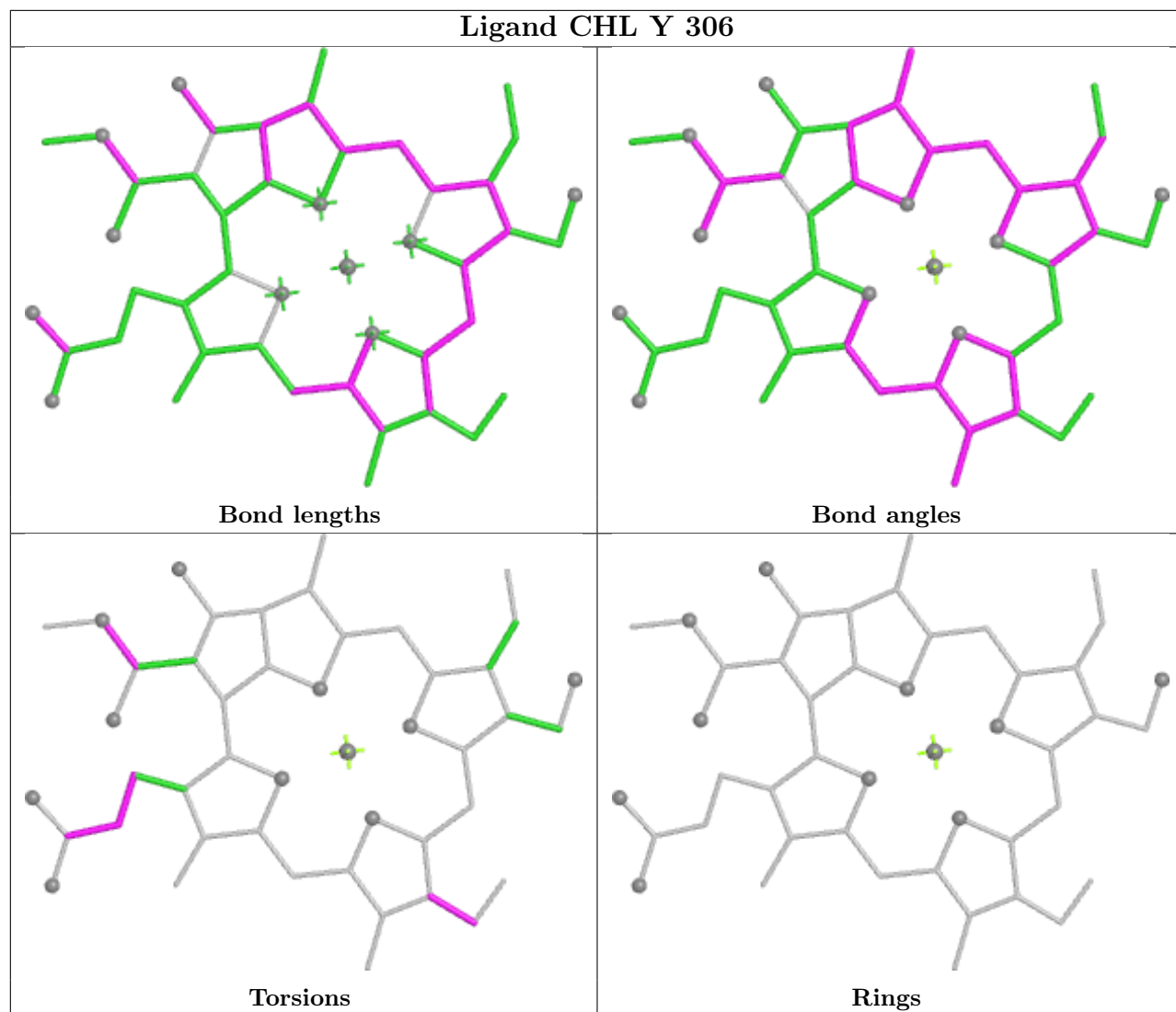
Torsions



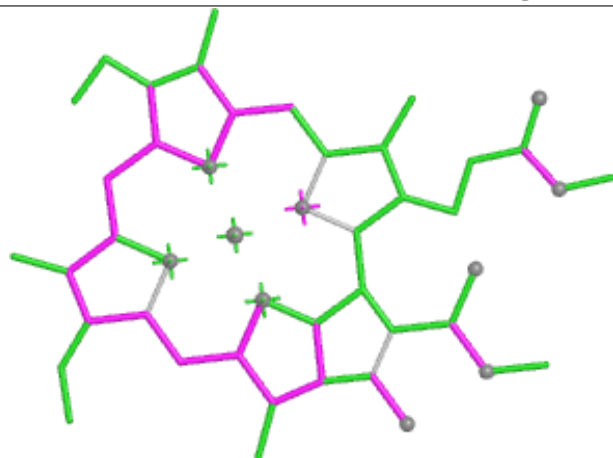
Rings

Ligand CLA B 846

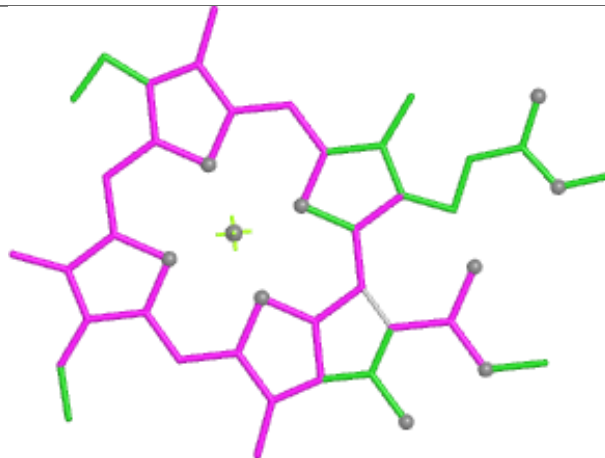




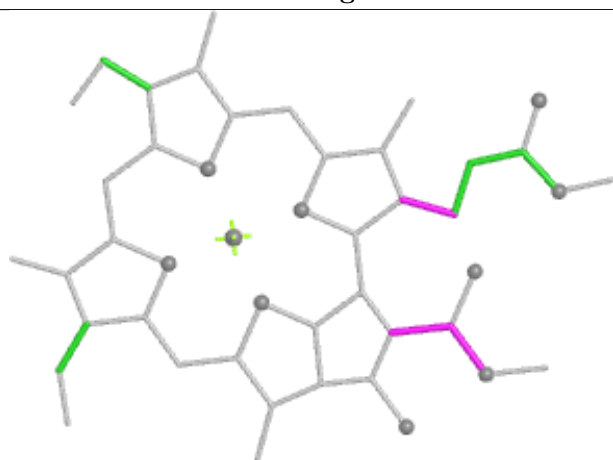
Ligand CLA Z 313



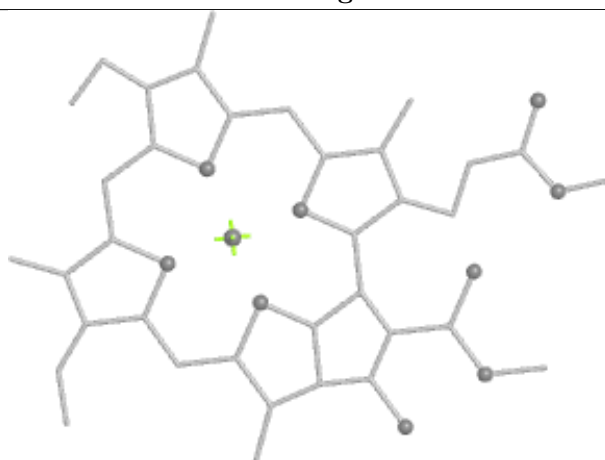
Bond lengths



Bond angles

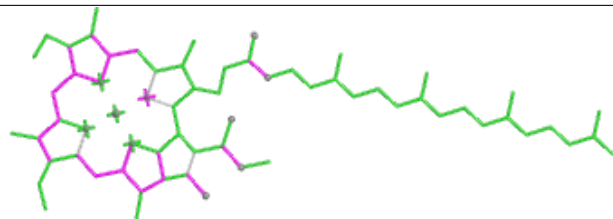


Torsions

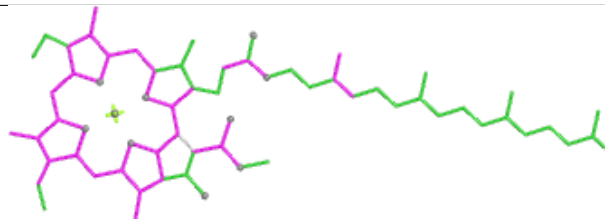


Rings

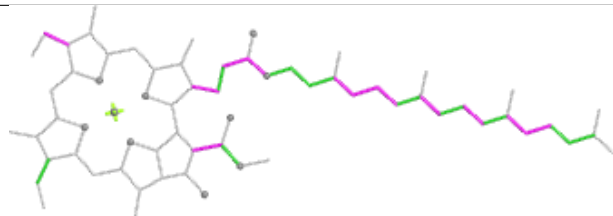
Ligand CLA B 847



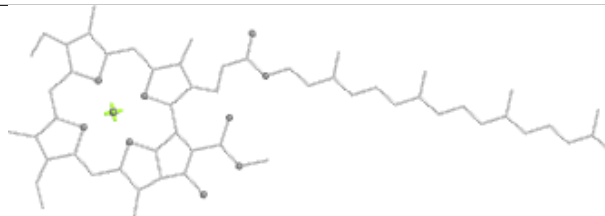
Bond lengths



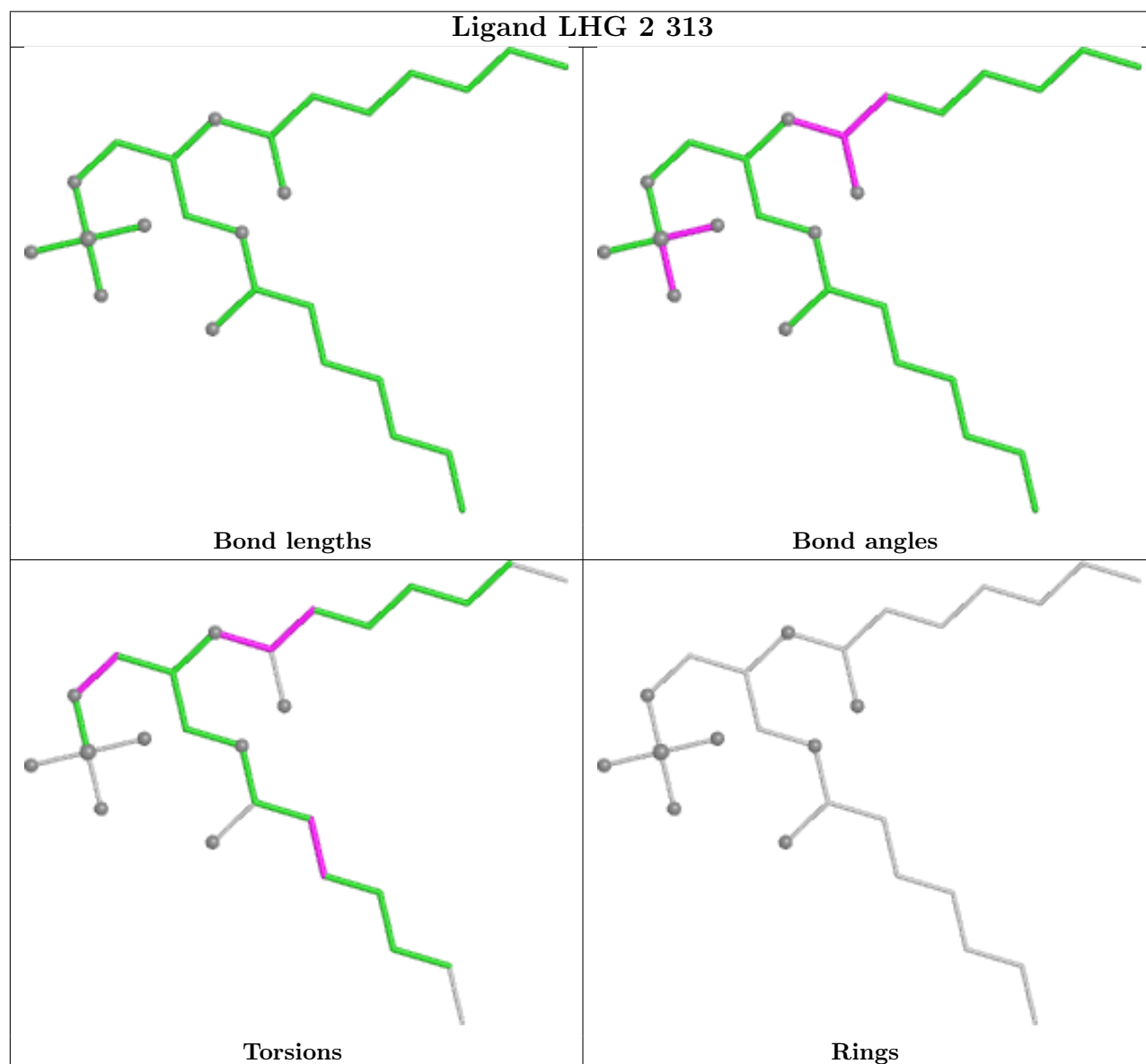
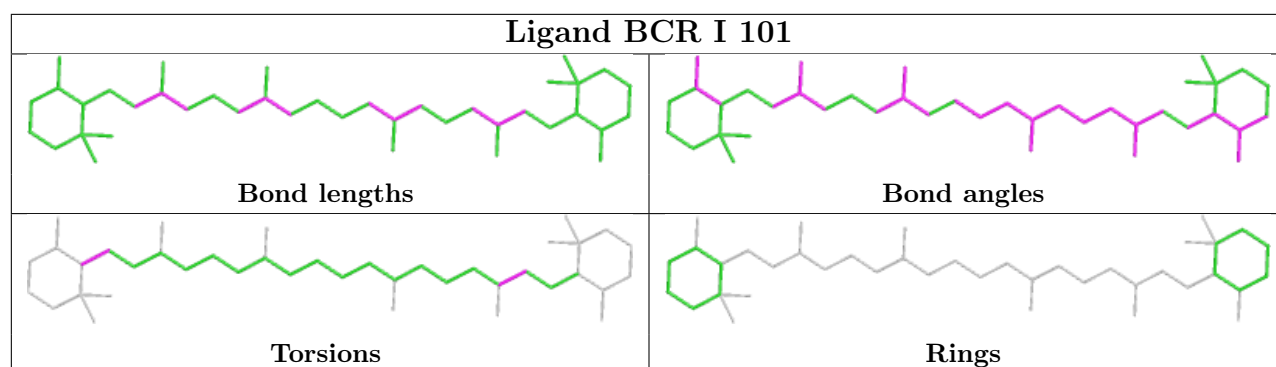
Bond angles

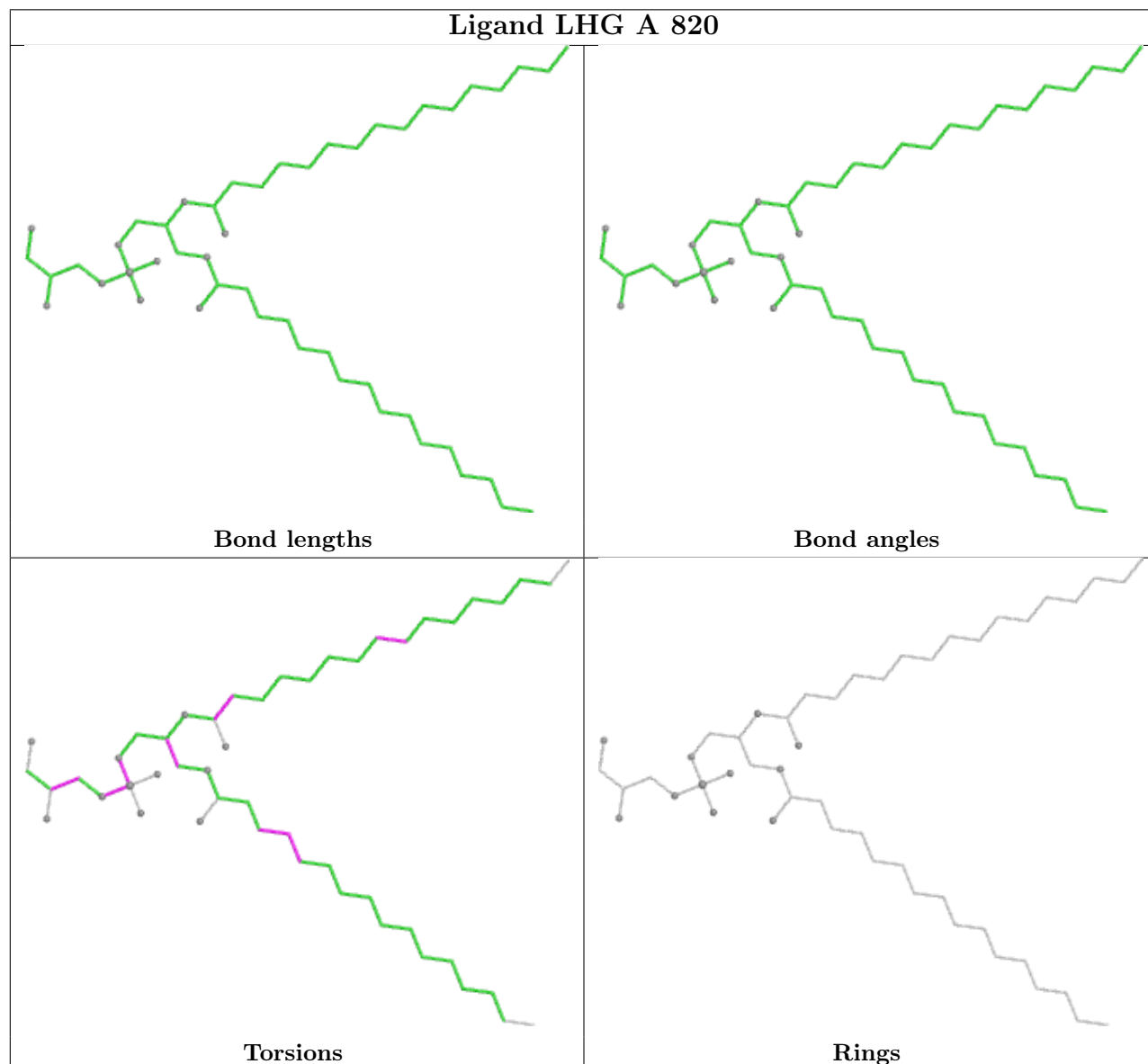
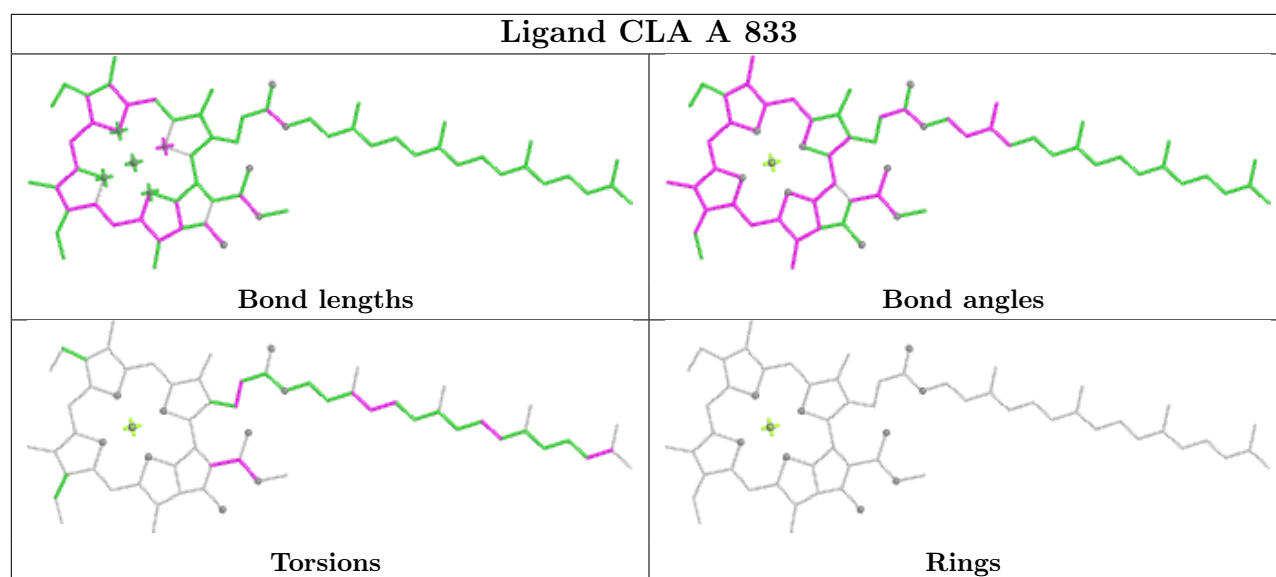


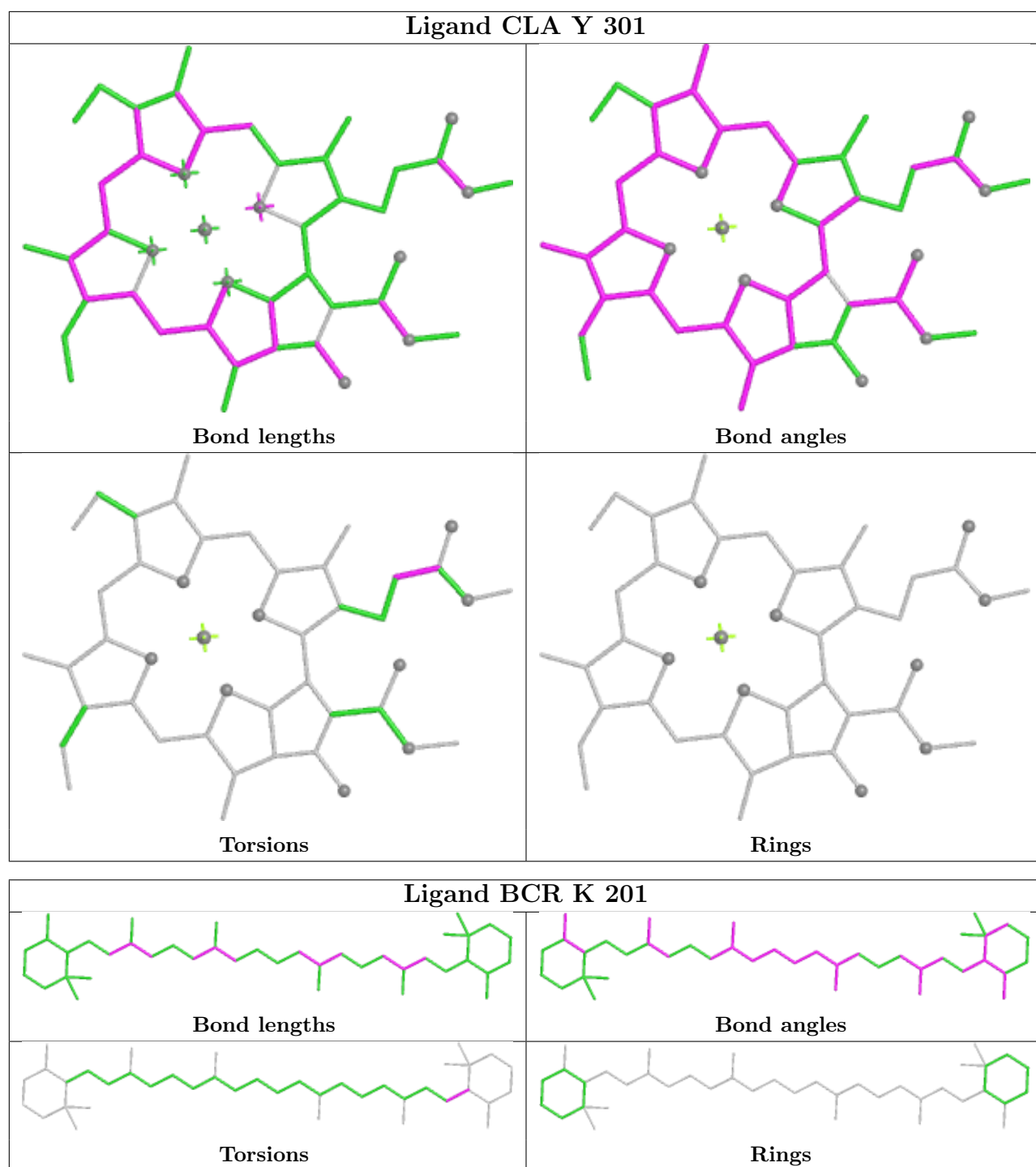
Torsions

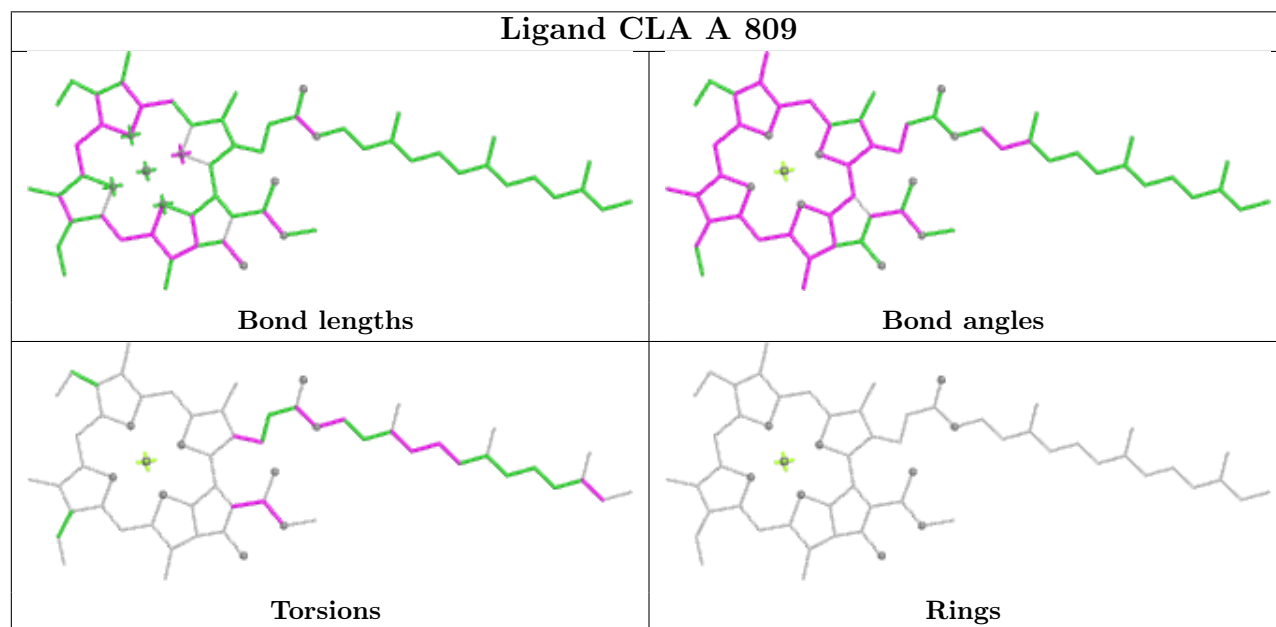
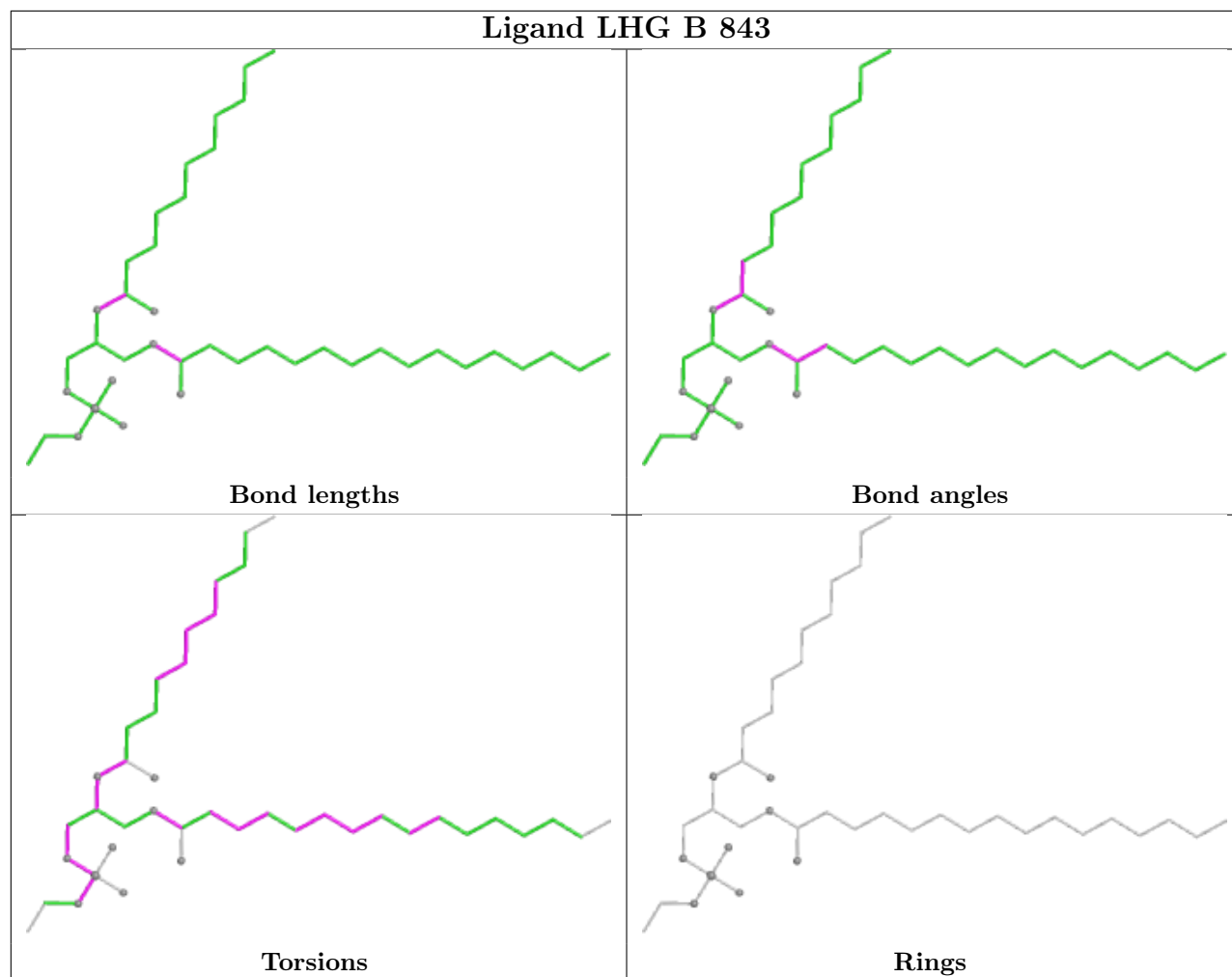


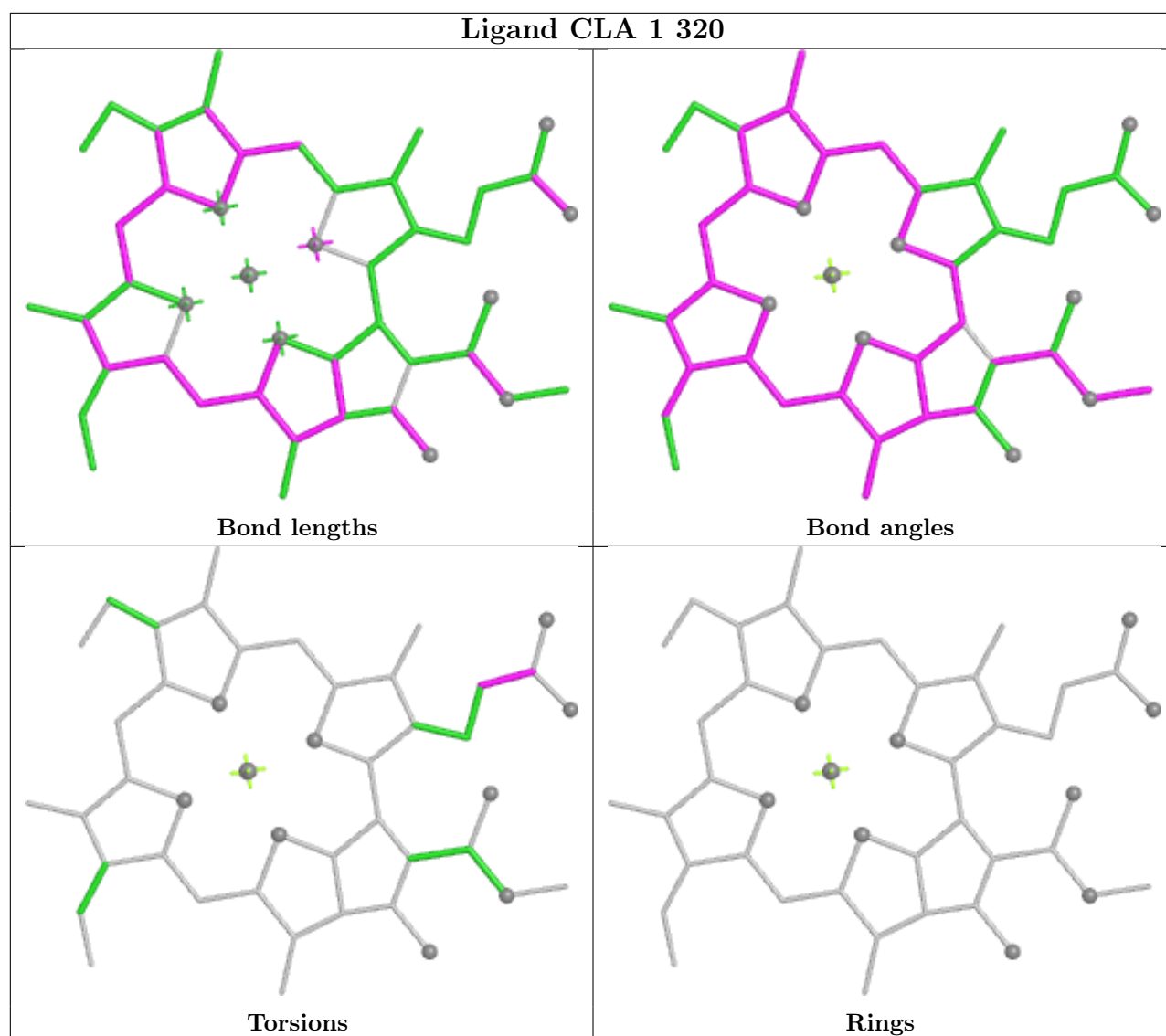
Rings

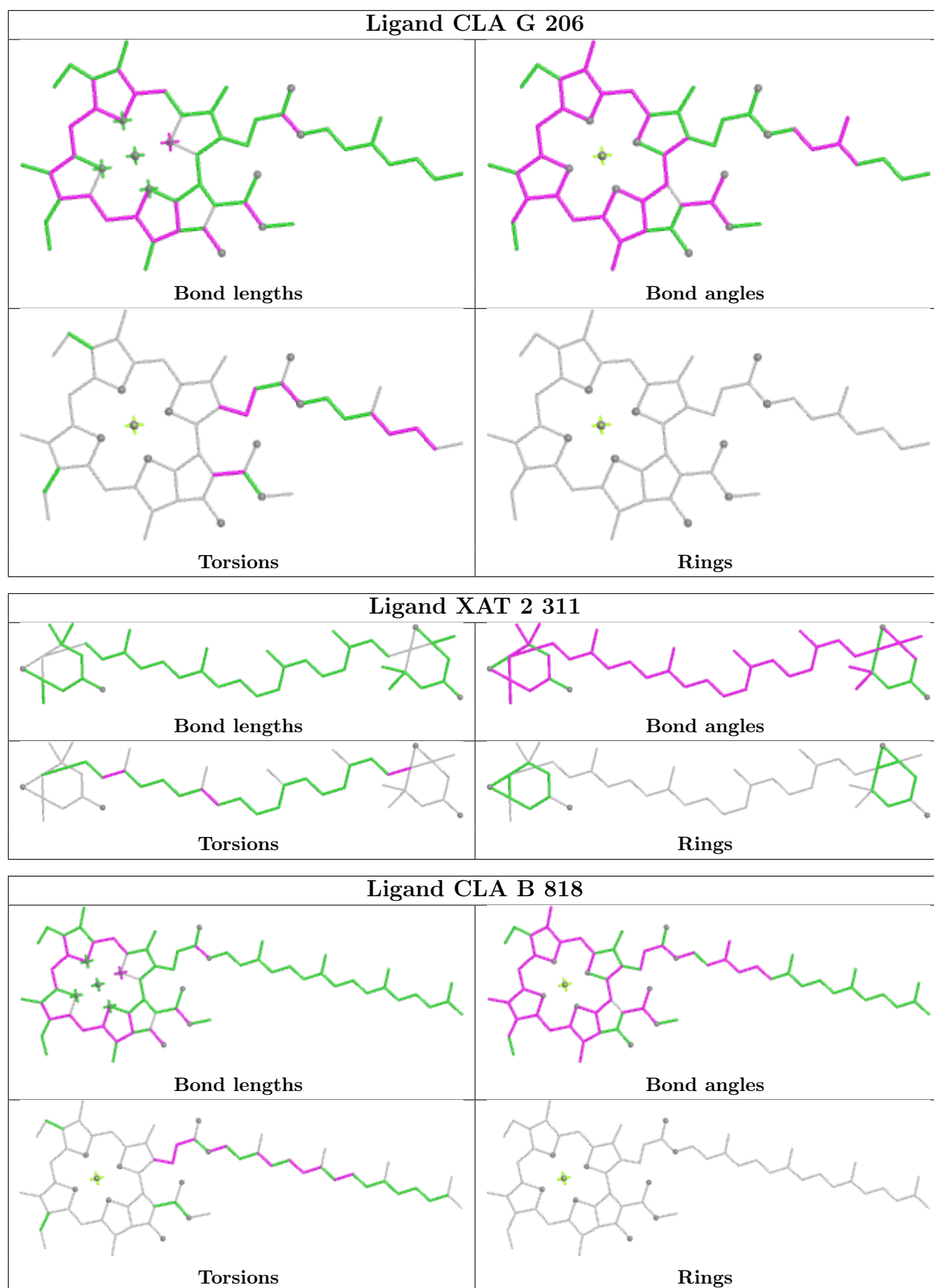


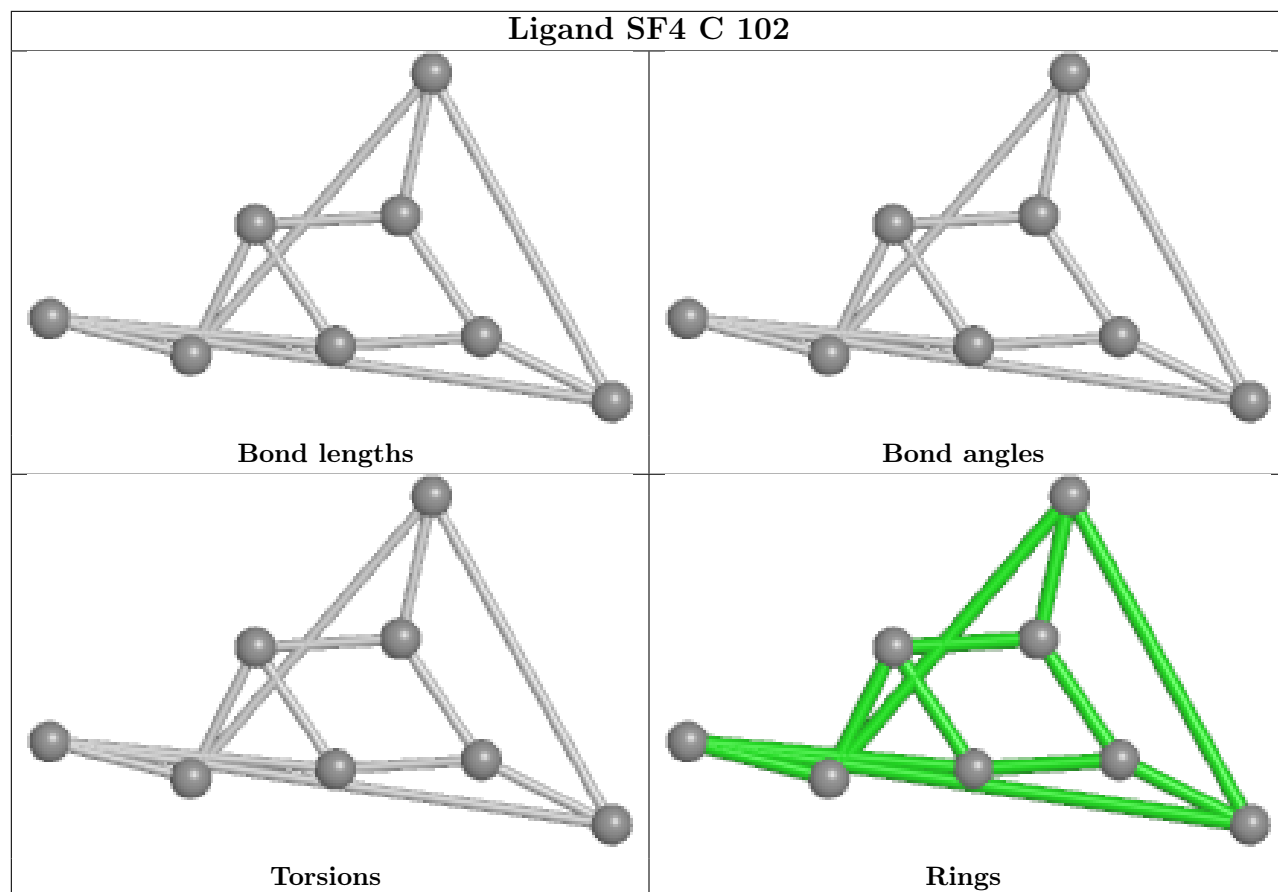




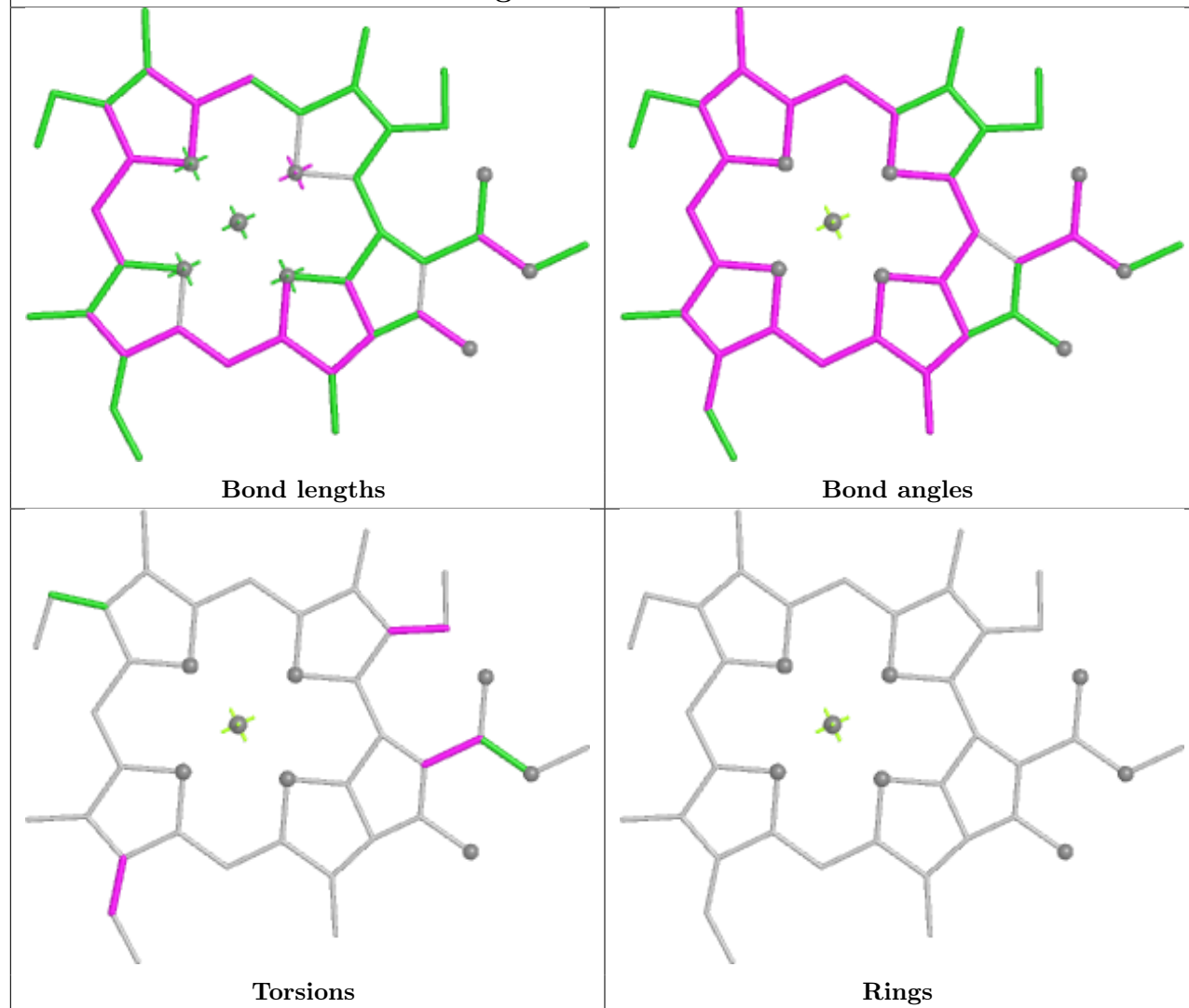




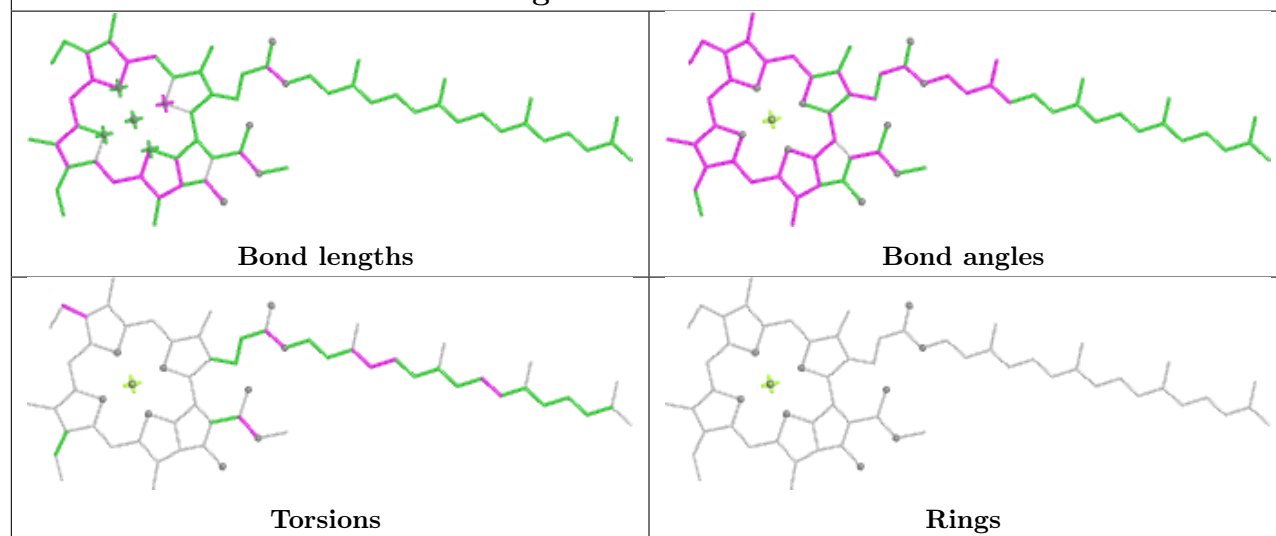


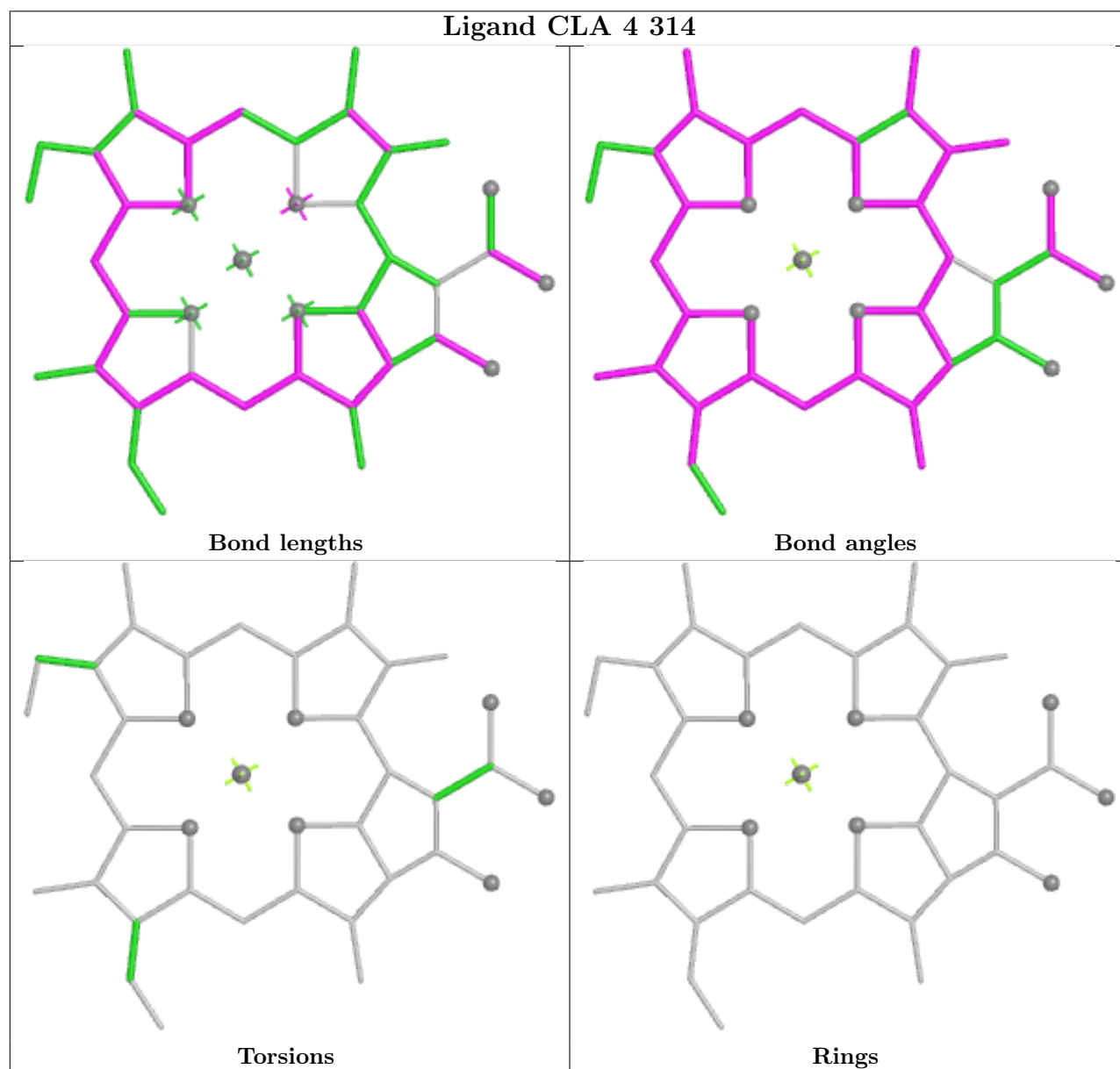
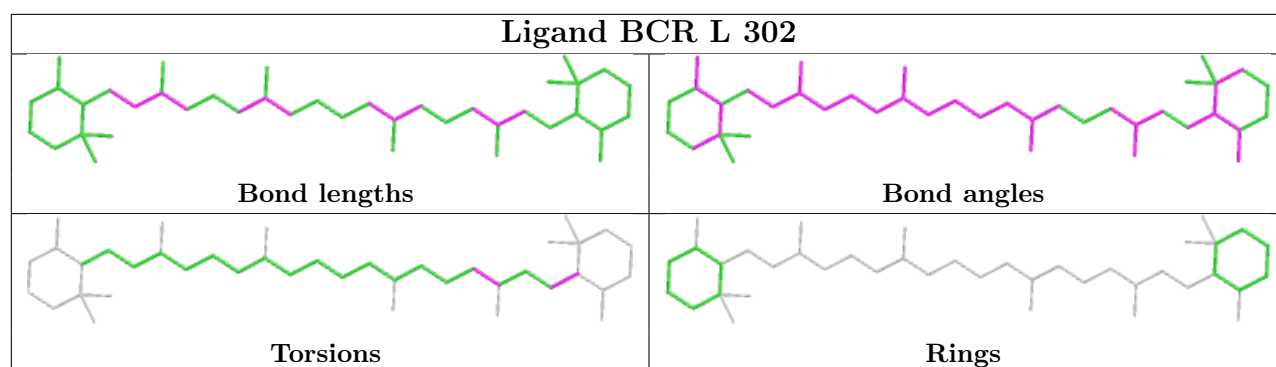


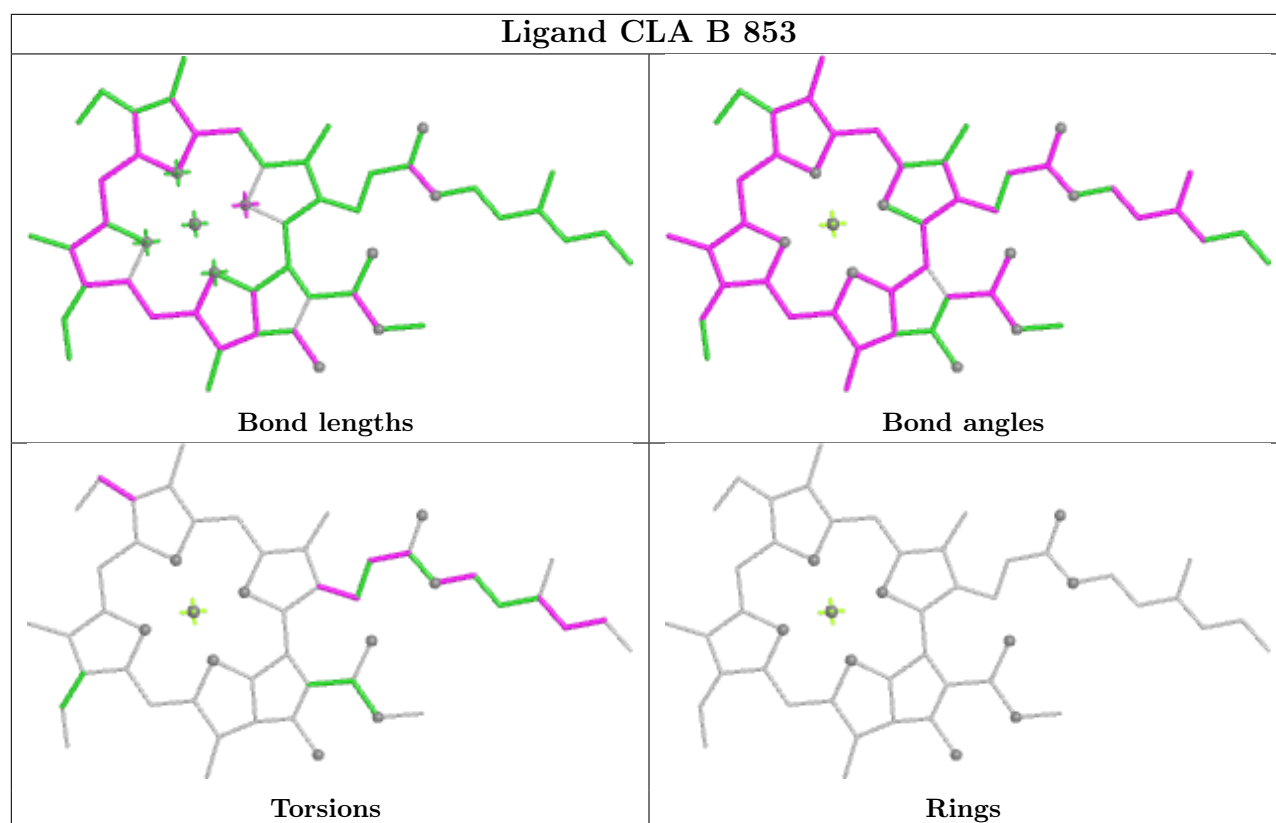
Ligand CLA A 837



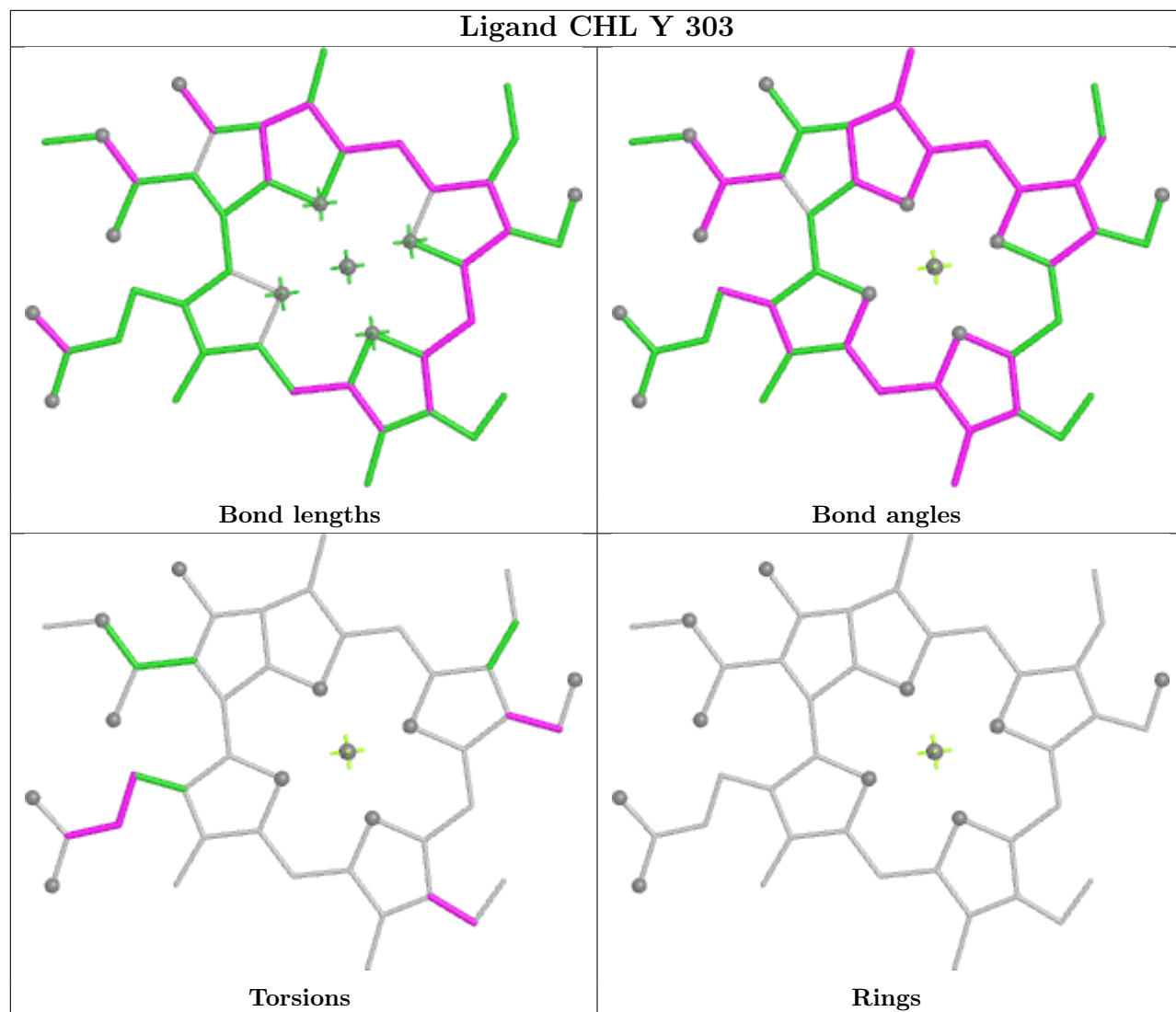
Ligand CLA B 829



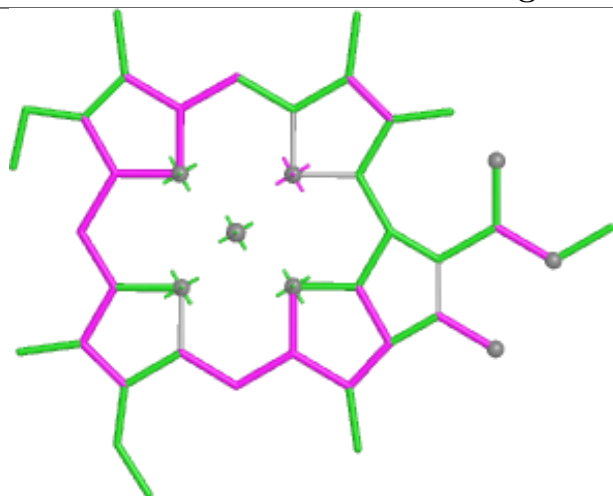




Ligand CHL Y 303



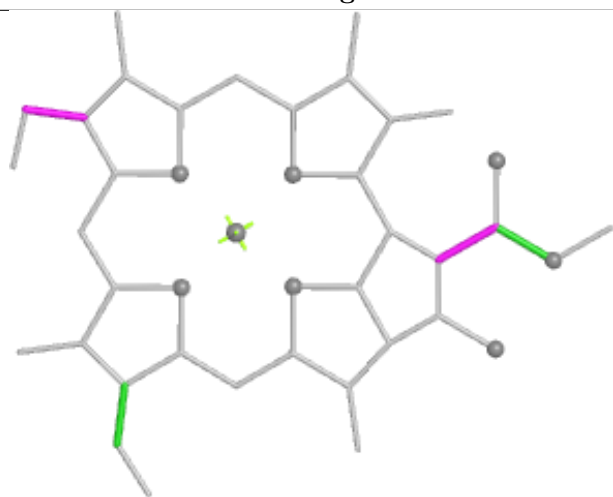
Ligand CLA 1 305



Bond lengths



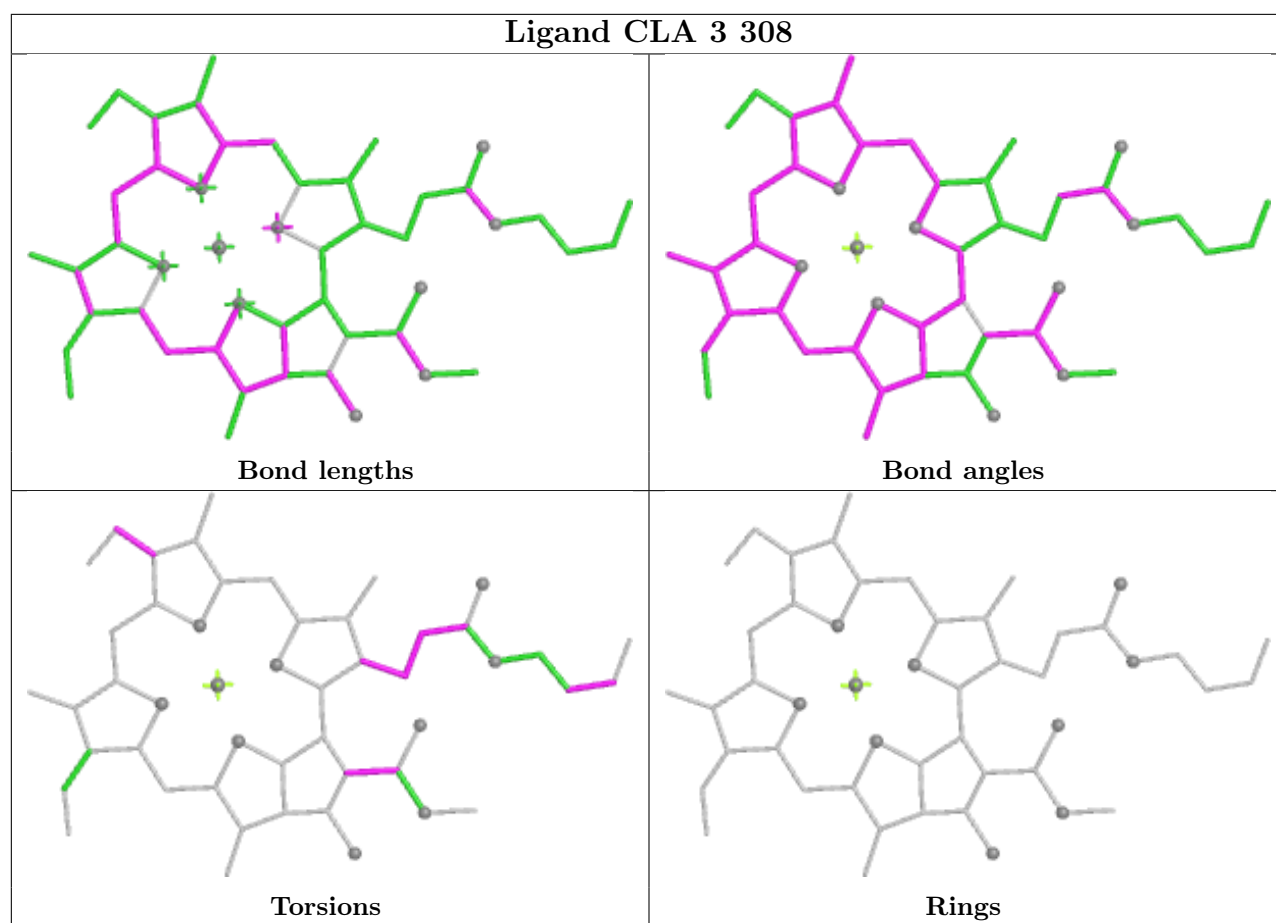
Bond angles



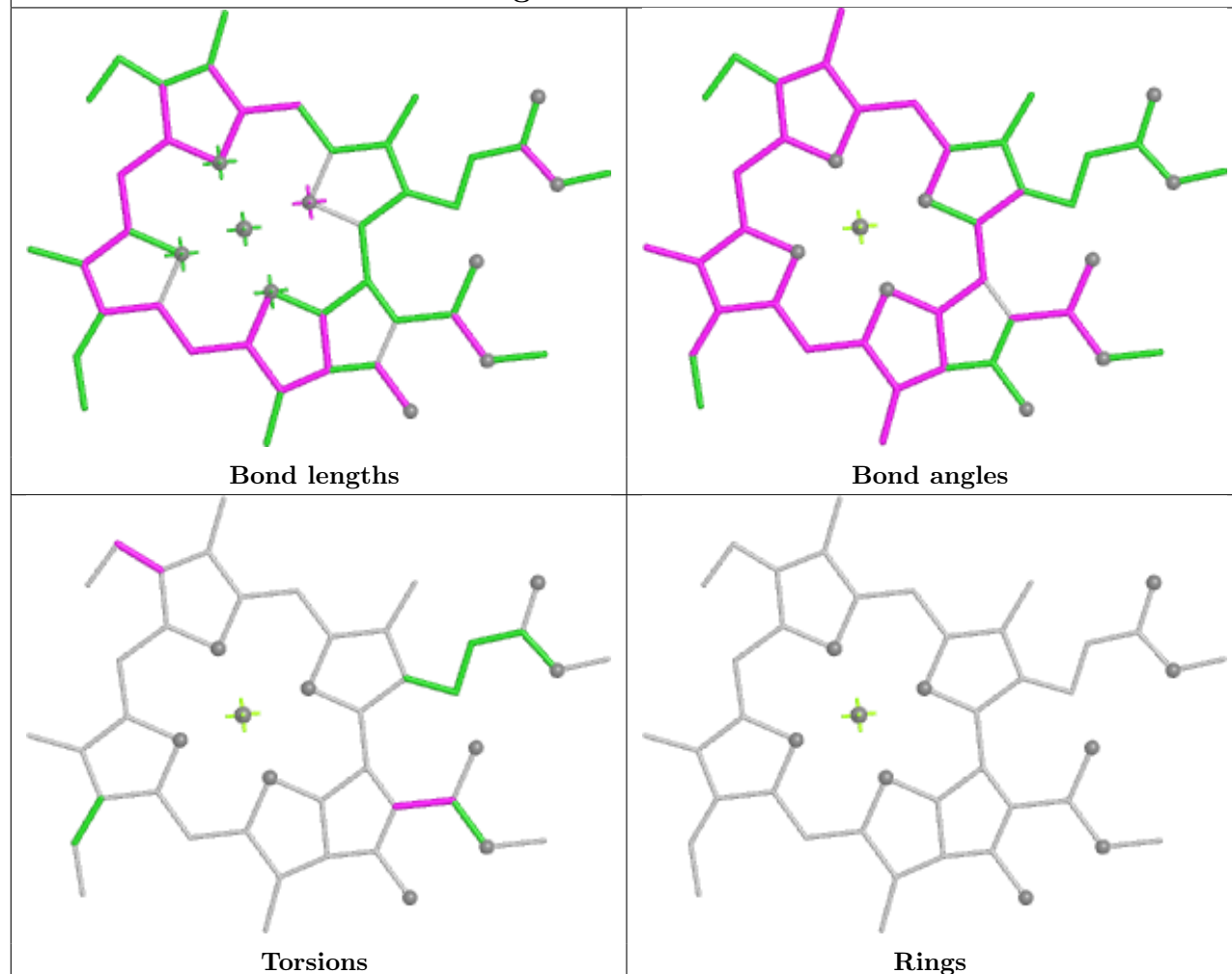
Torsions



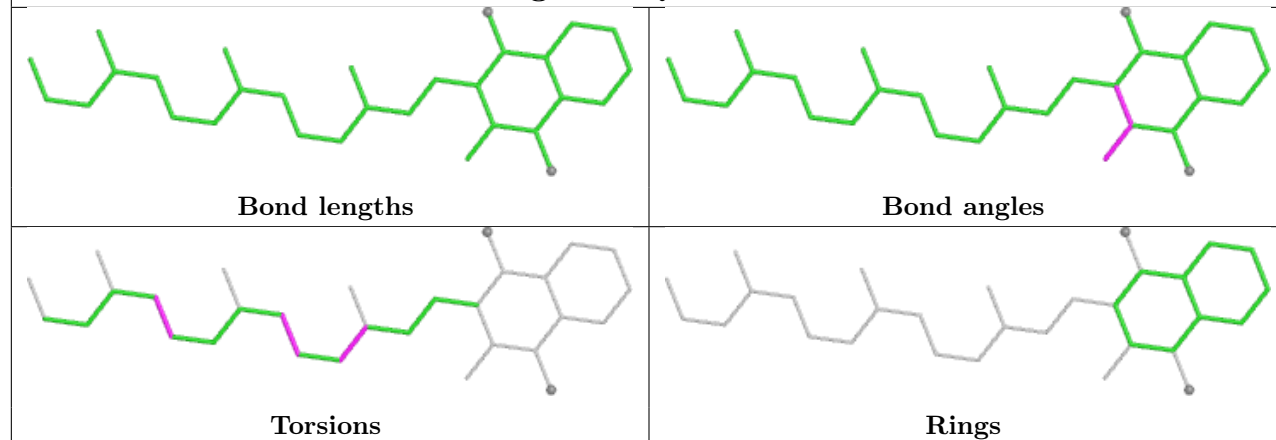
Rings



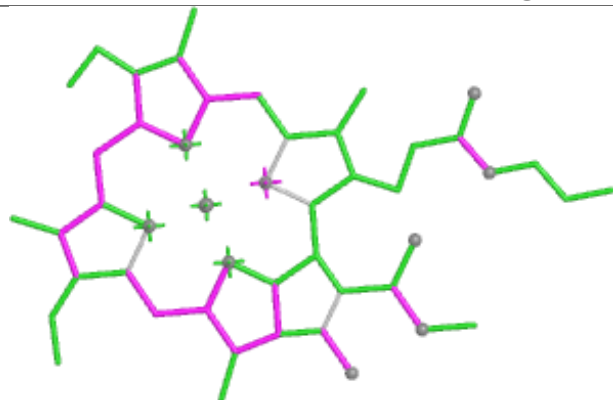
Ligand CLA X 312



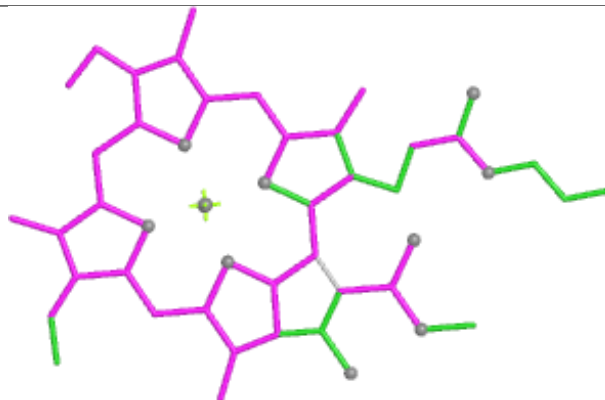
Ligand PQN B 832



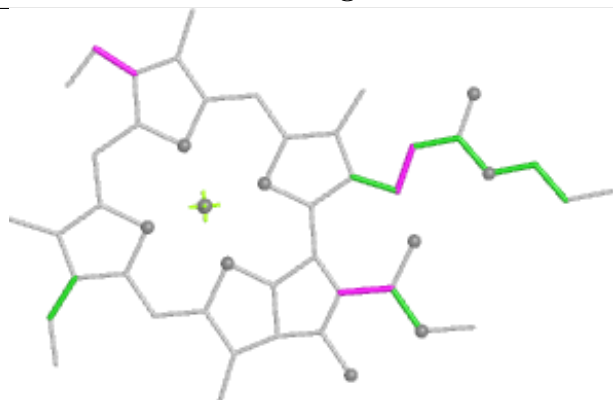
Ligand CLA 1 319



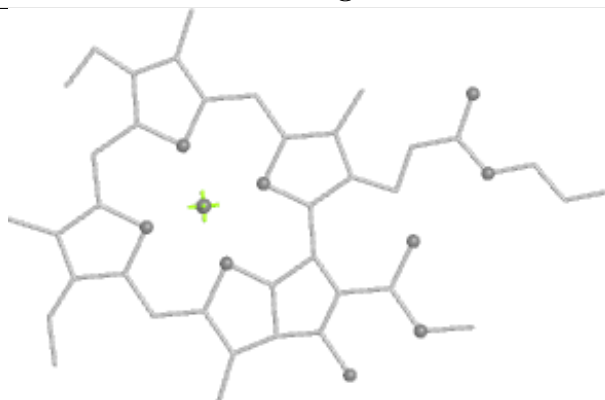
Bond lengths



Bond angles

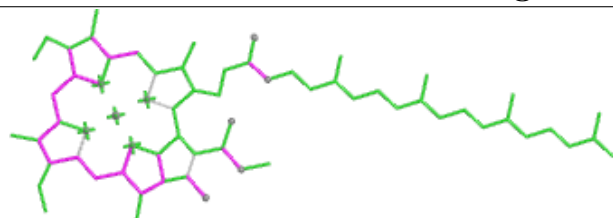


Torsions

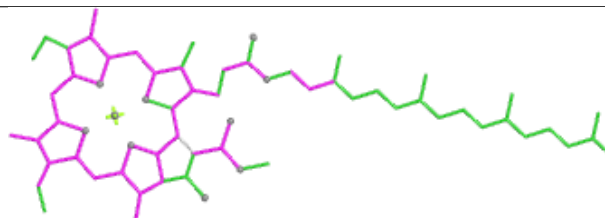


Rings

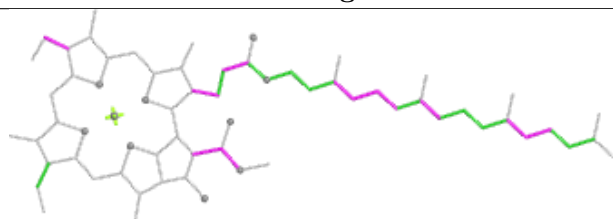
Ligand CLA A 802



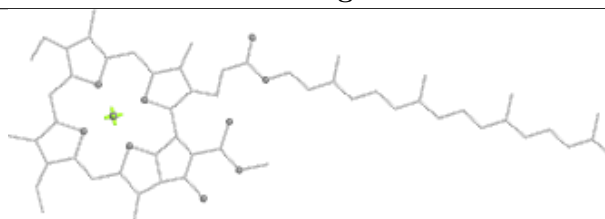
Bond lengths



Bond angles

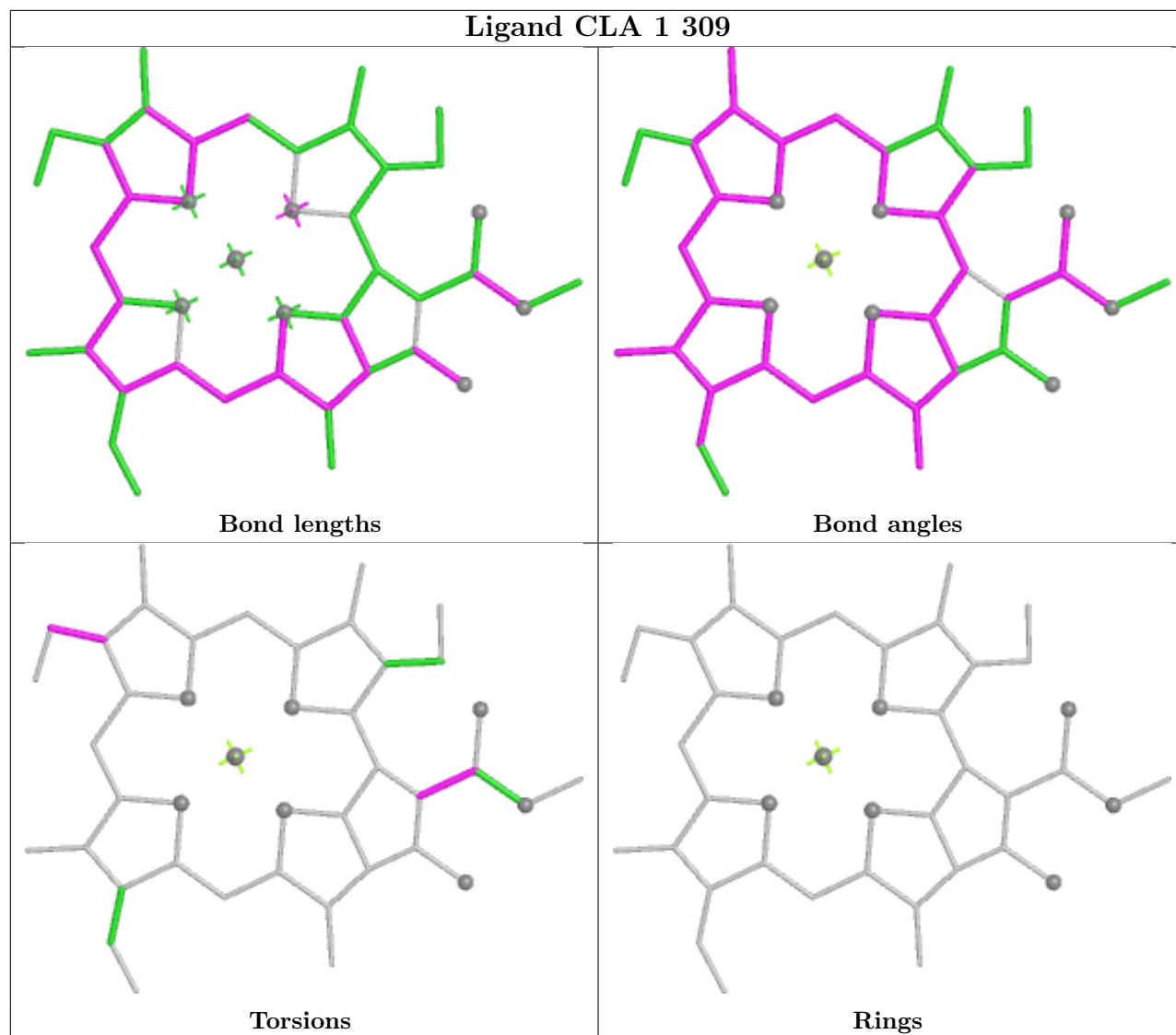


Torsions

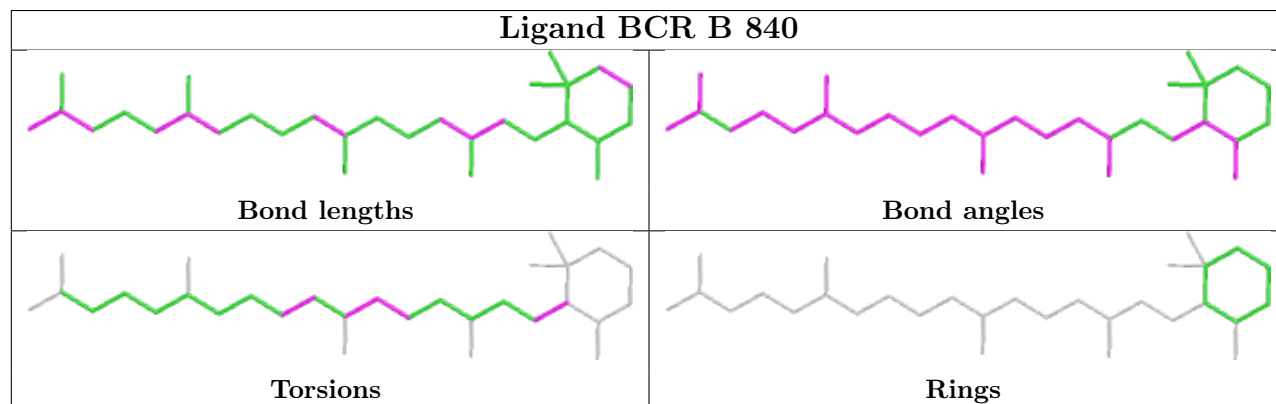


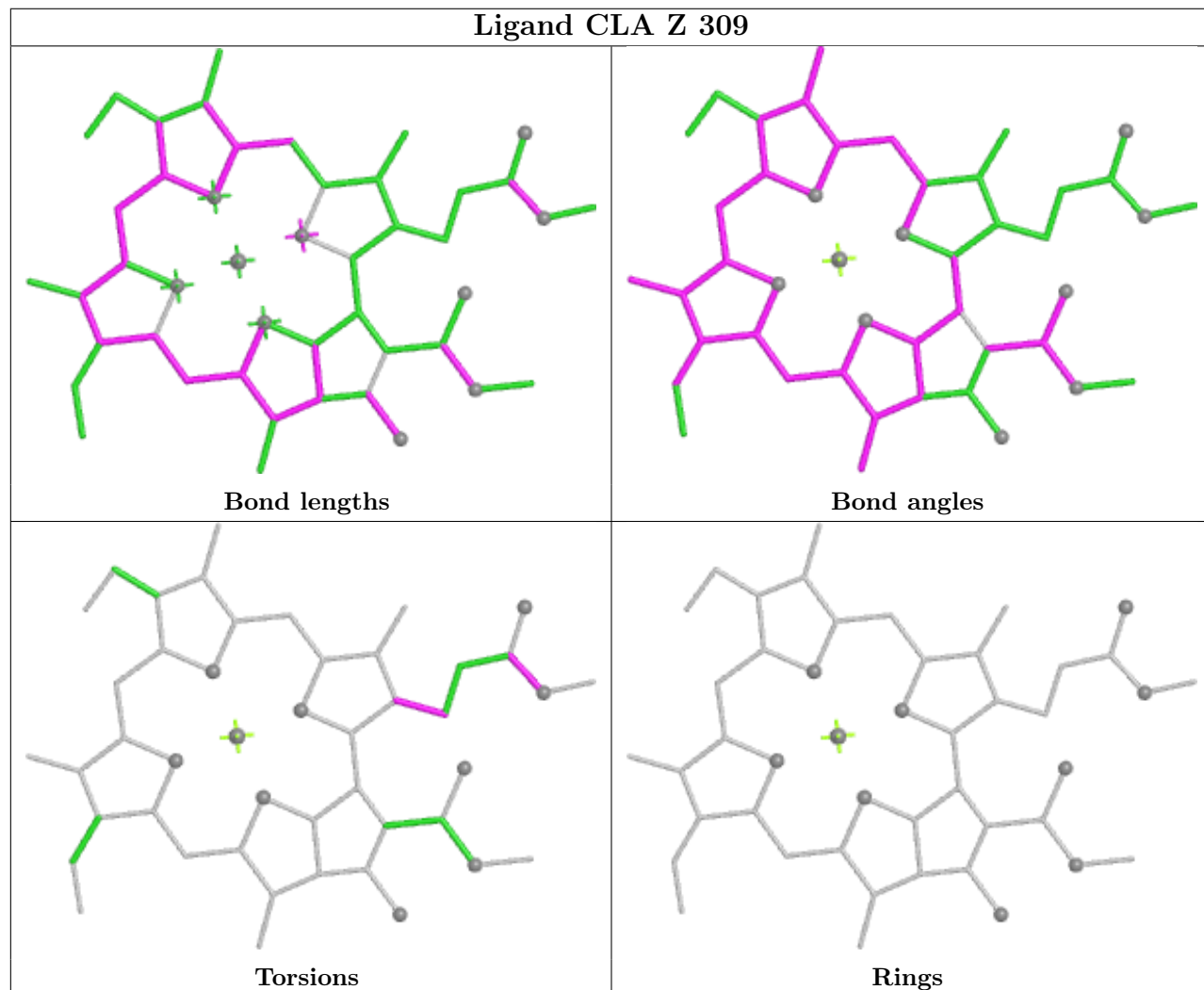
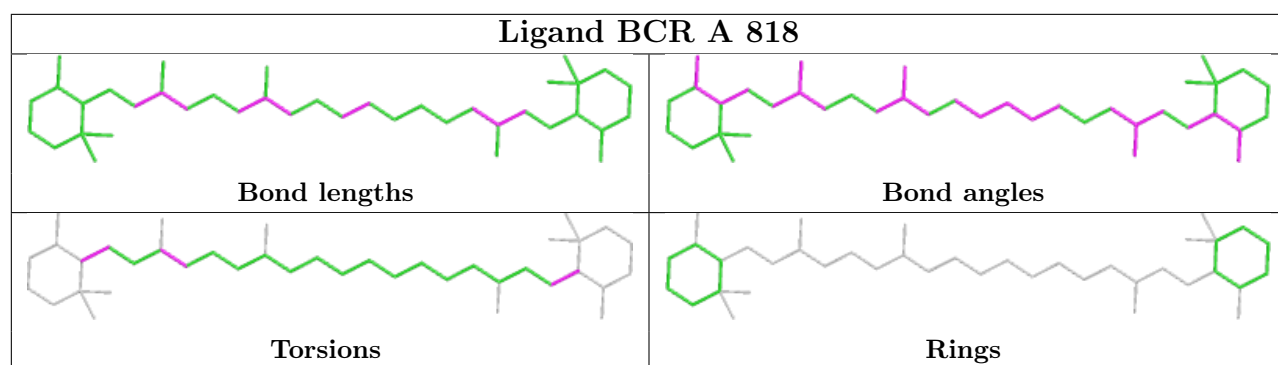
Rings

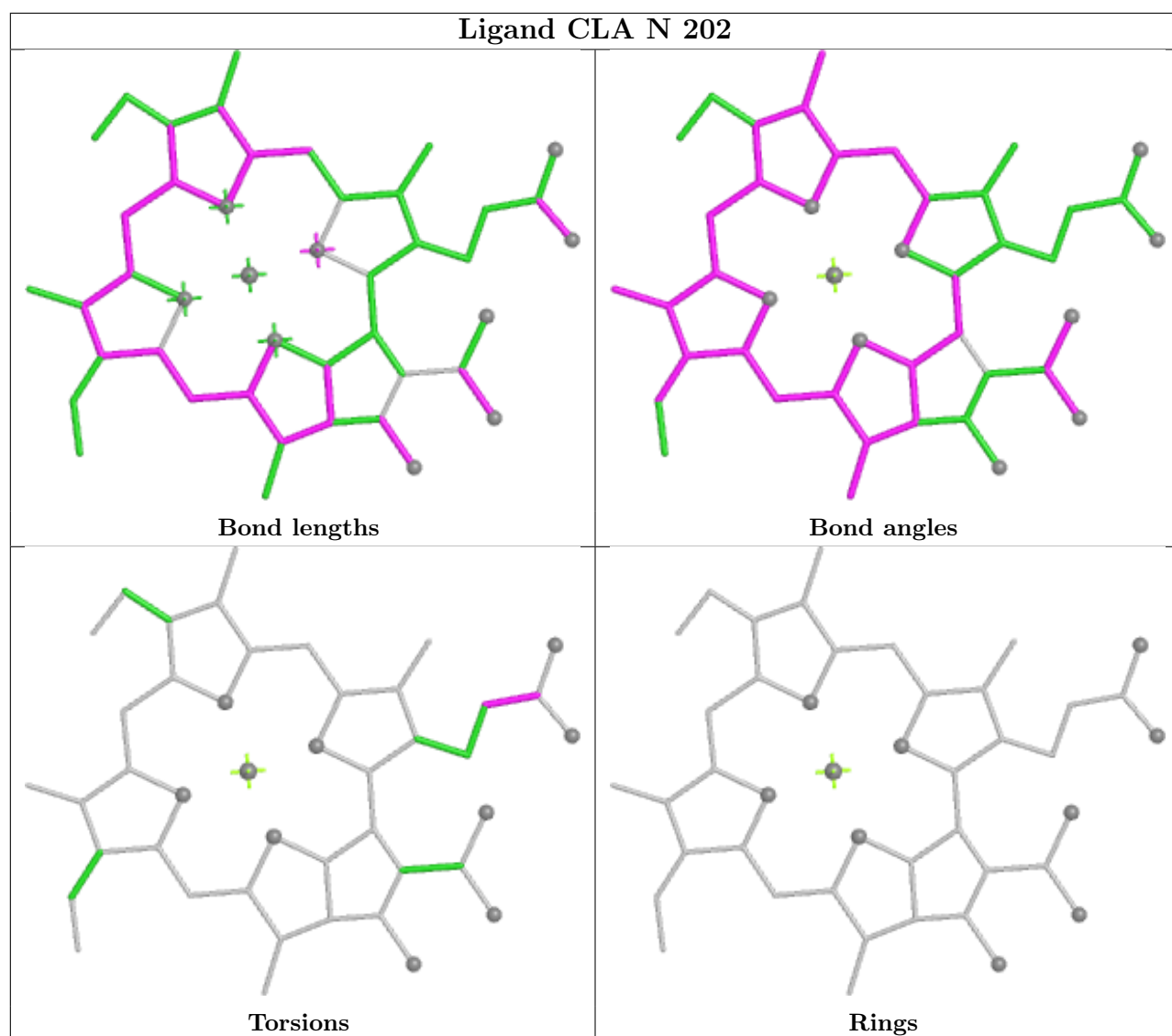
Ligand CLA 1 309

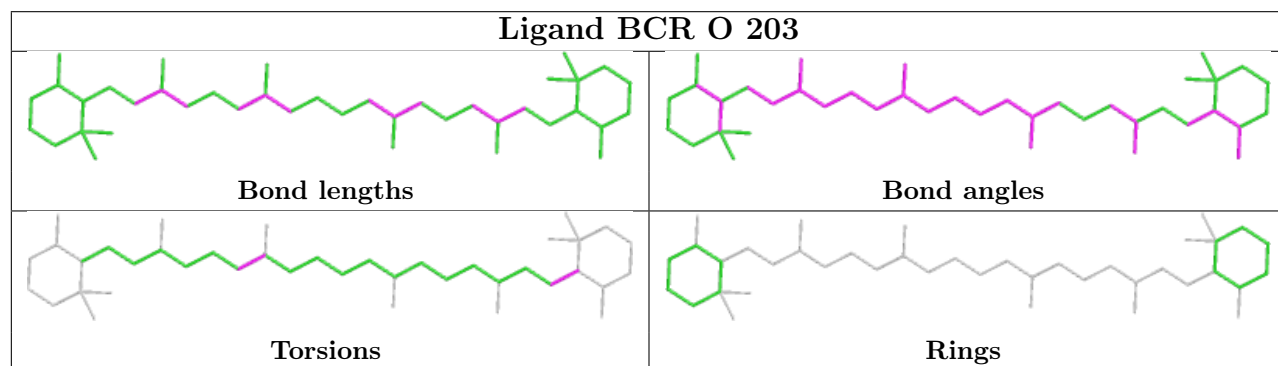
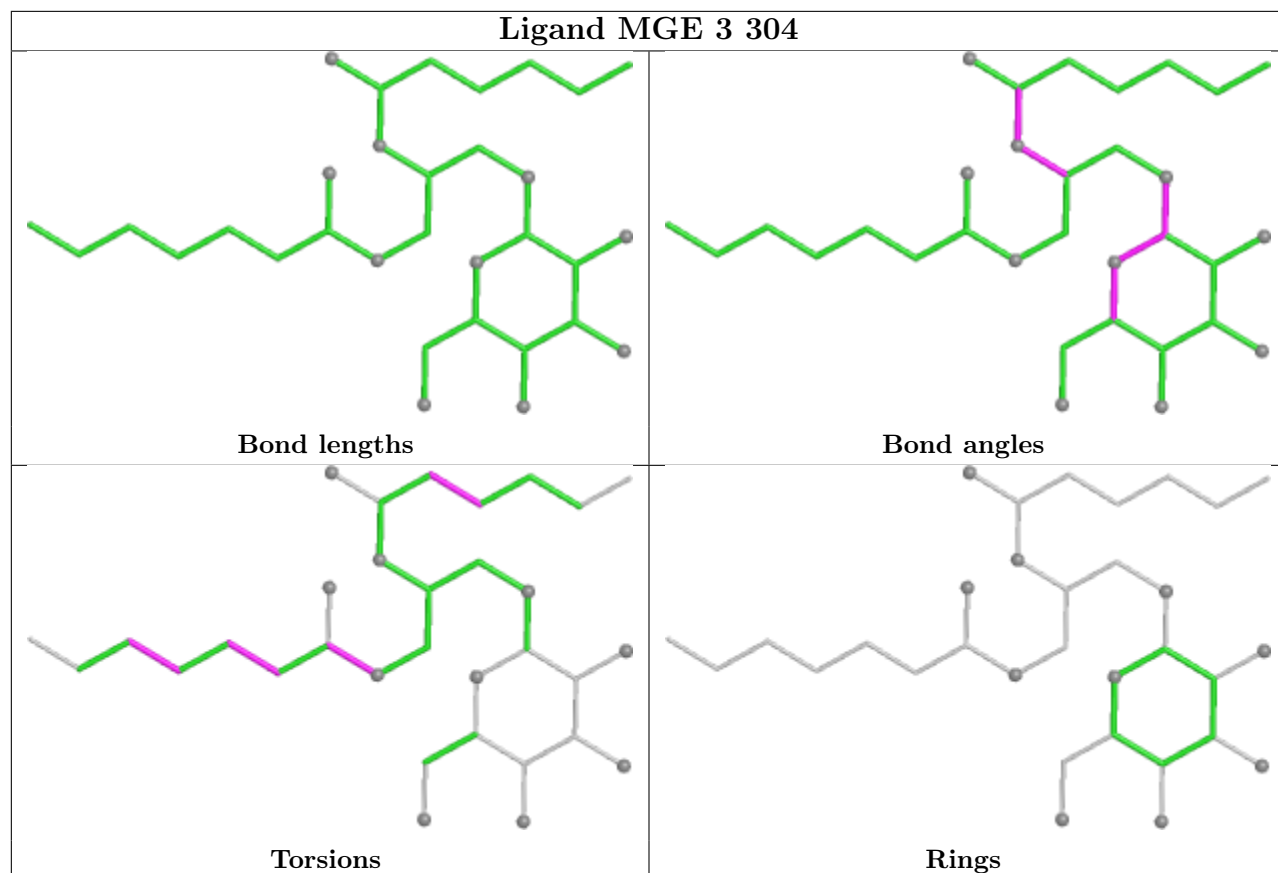


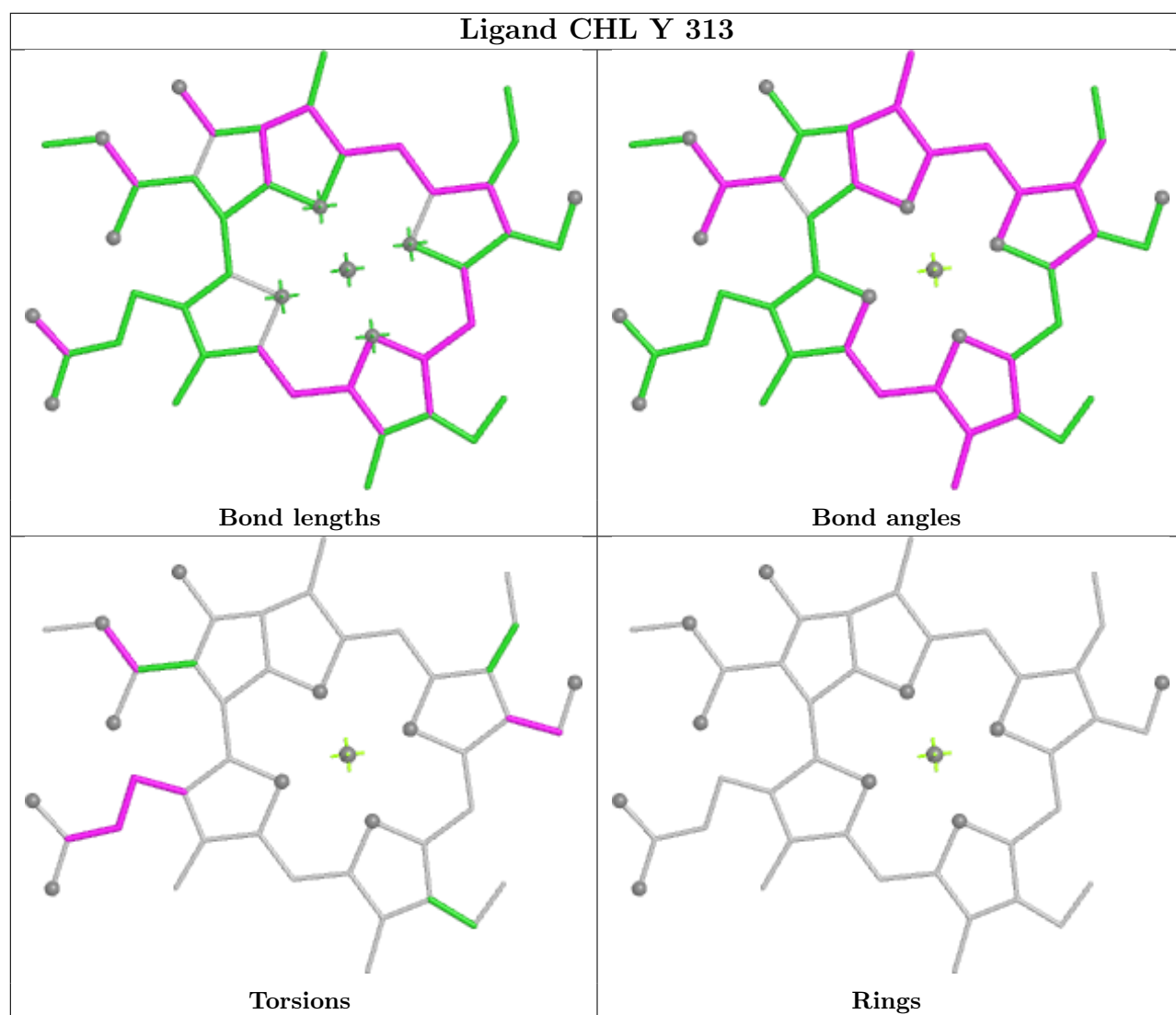
Ligand BCR B 840

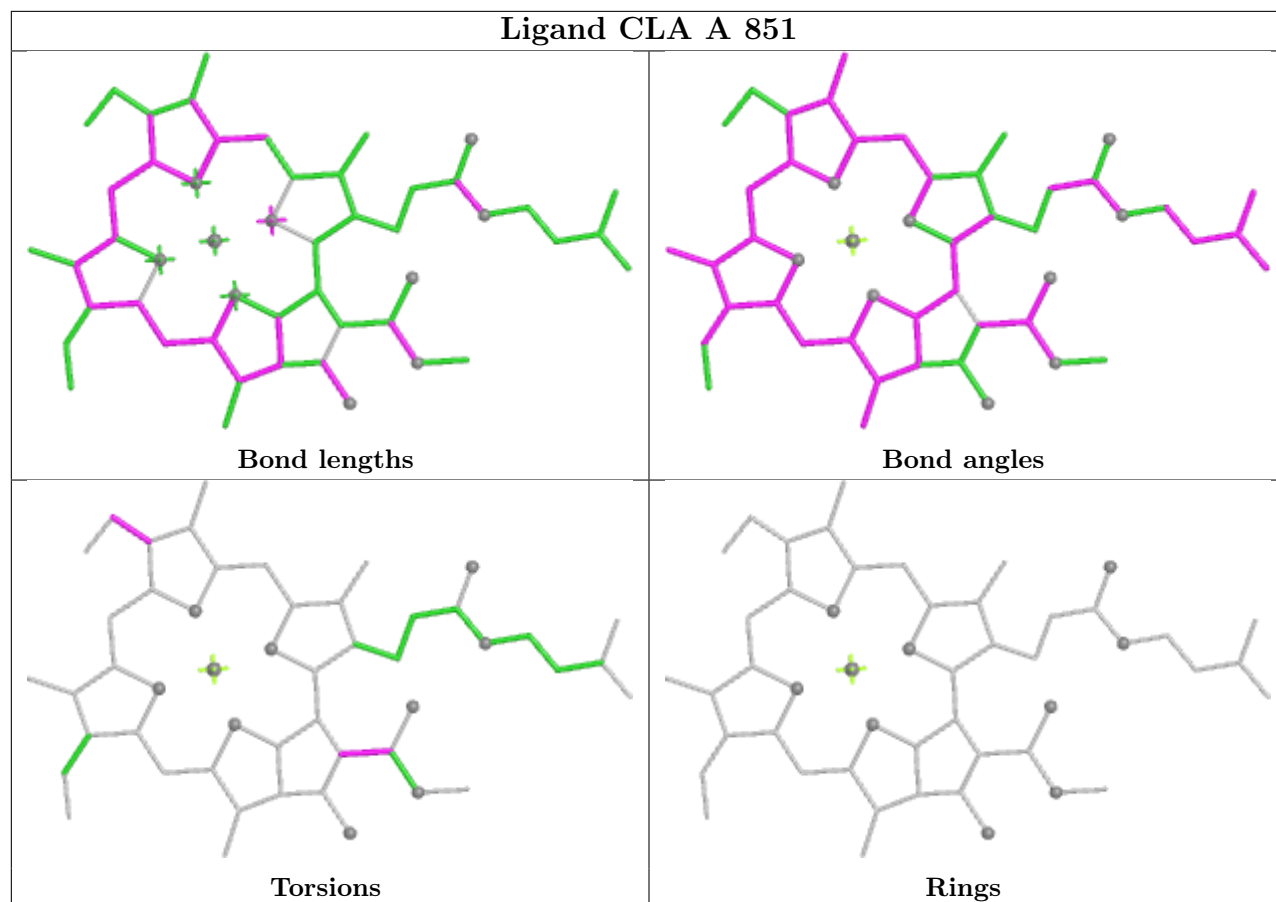


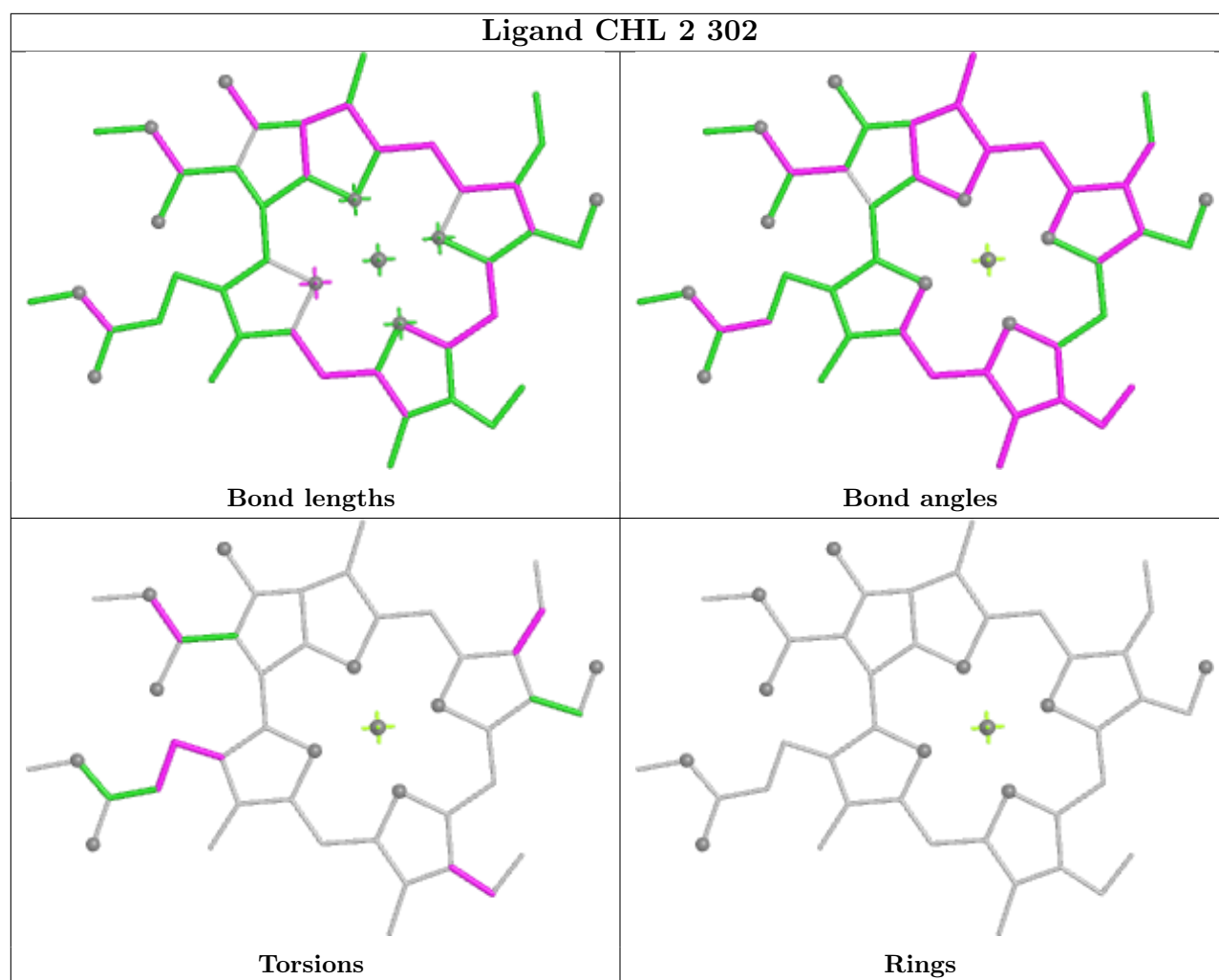




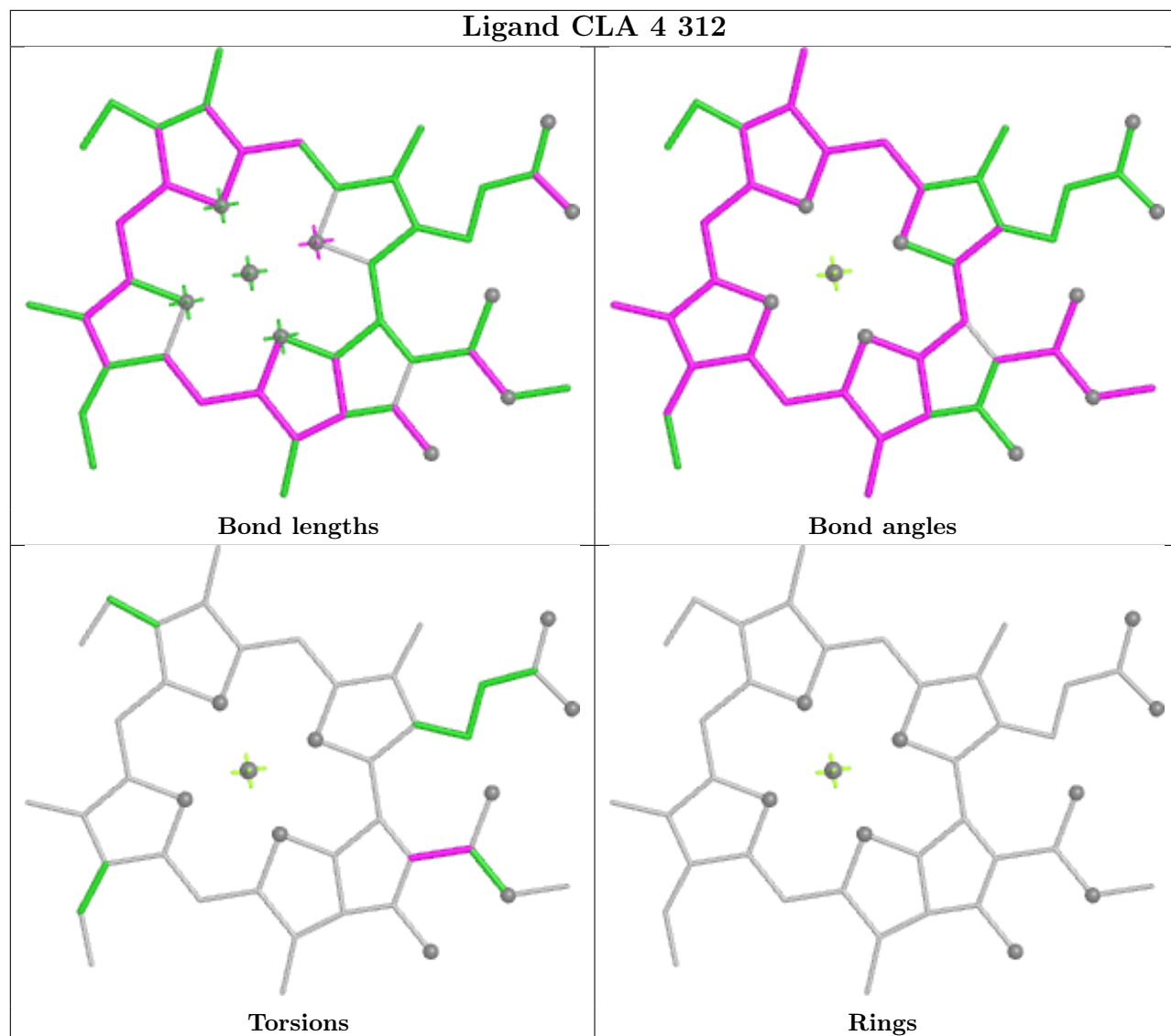


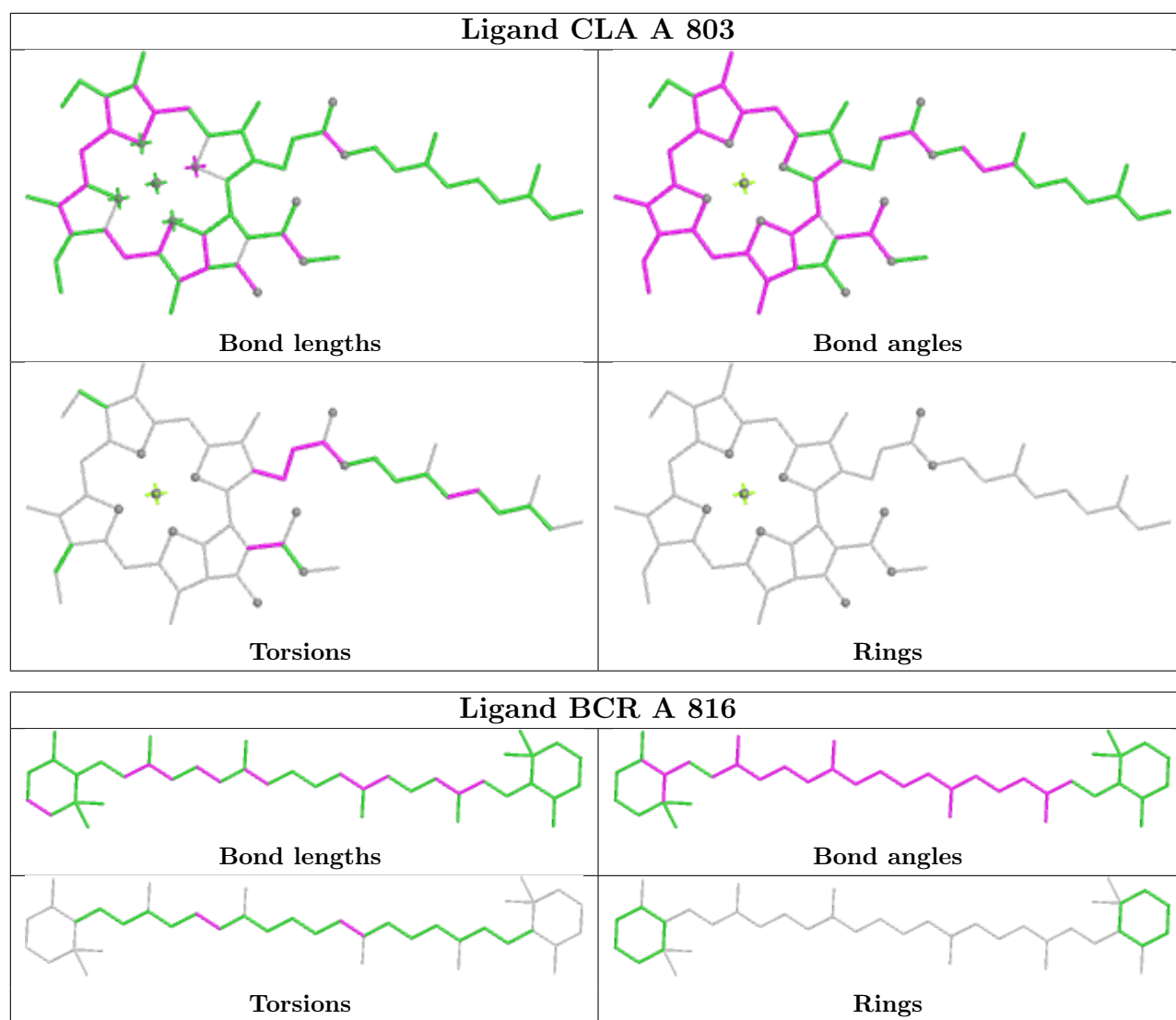




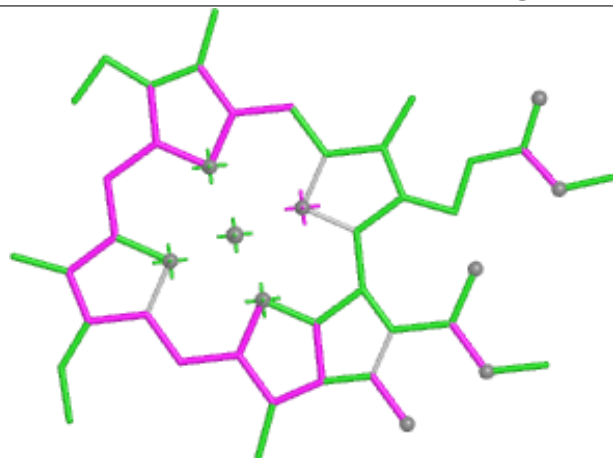


Ligand CLA 4 312

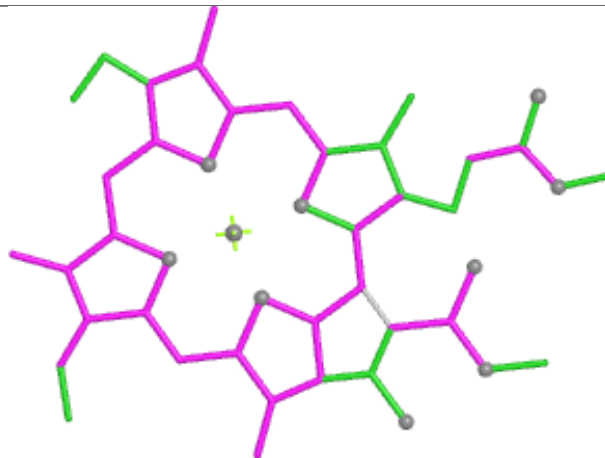




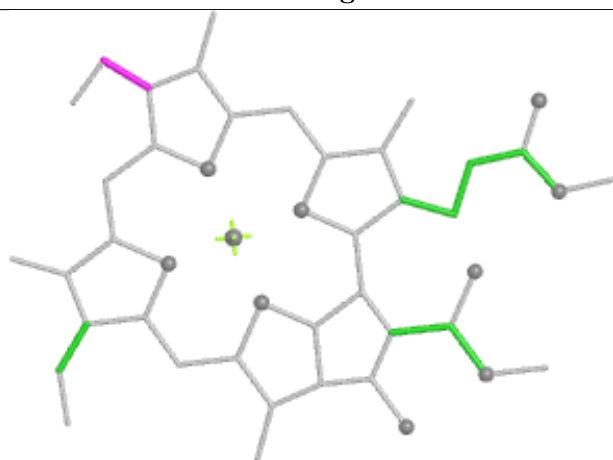
Ligand CLA X 311



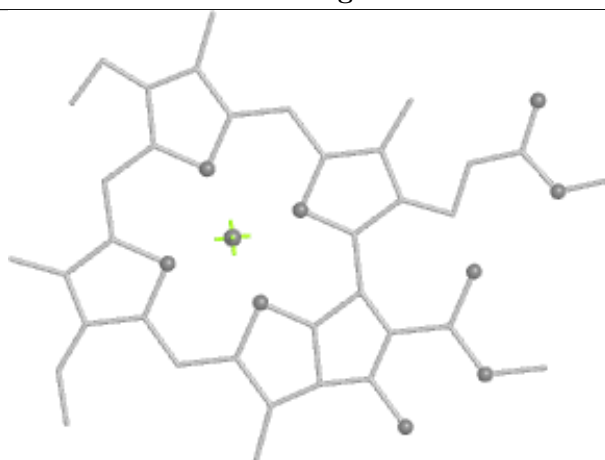
Bond lengths



Bond angles

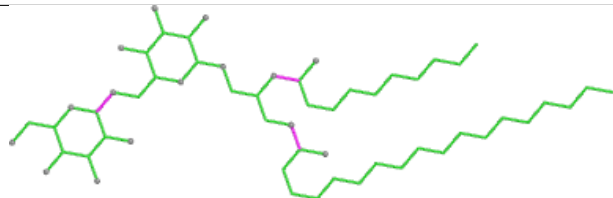


Torsions

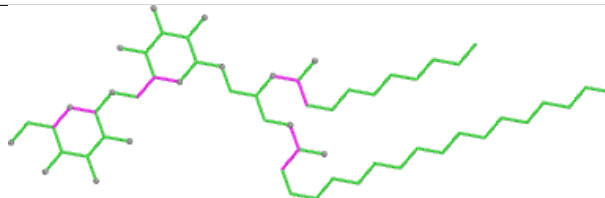


Rings

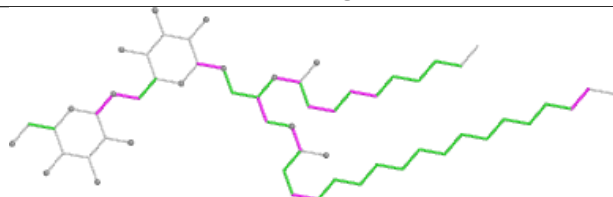
Ligand DGD J 104



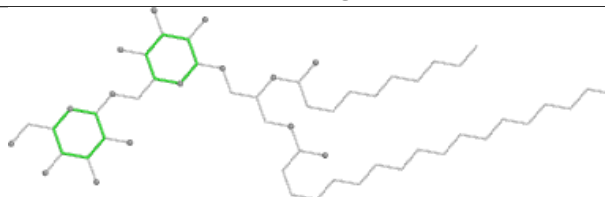
Bond lengths



Bond angles

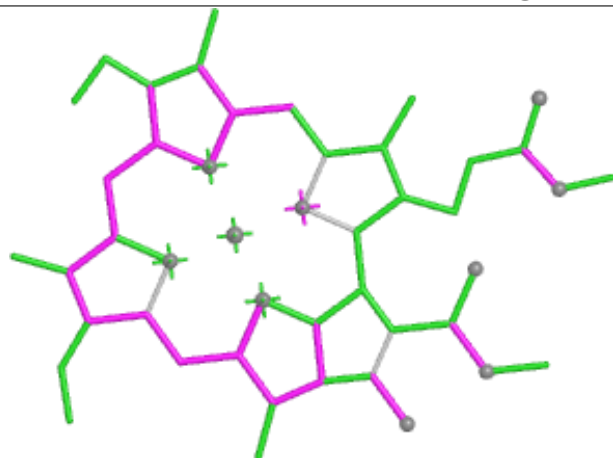


Torsions

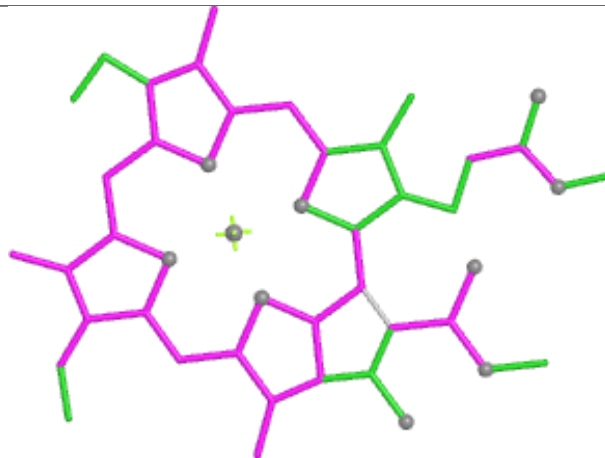


Rings

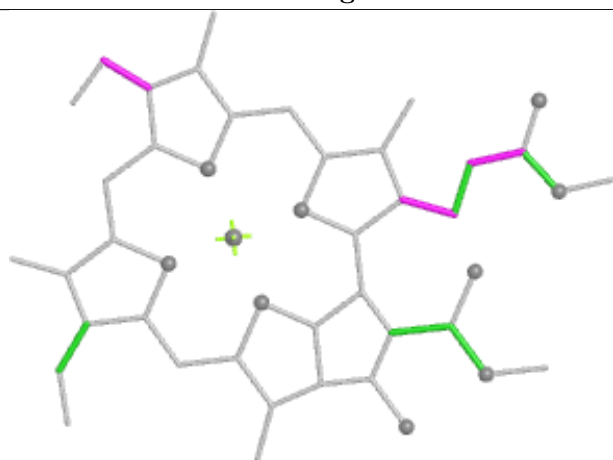
Ligand CLA Z 314



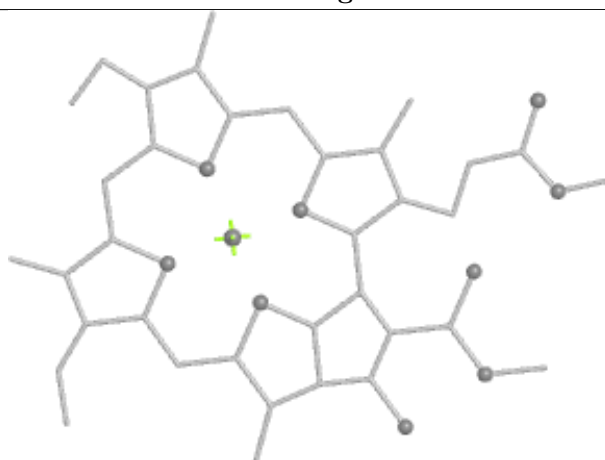
Bond lengths



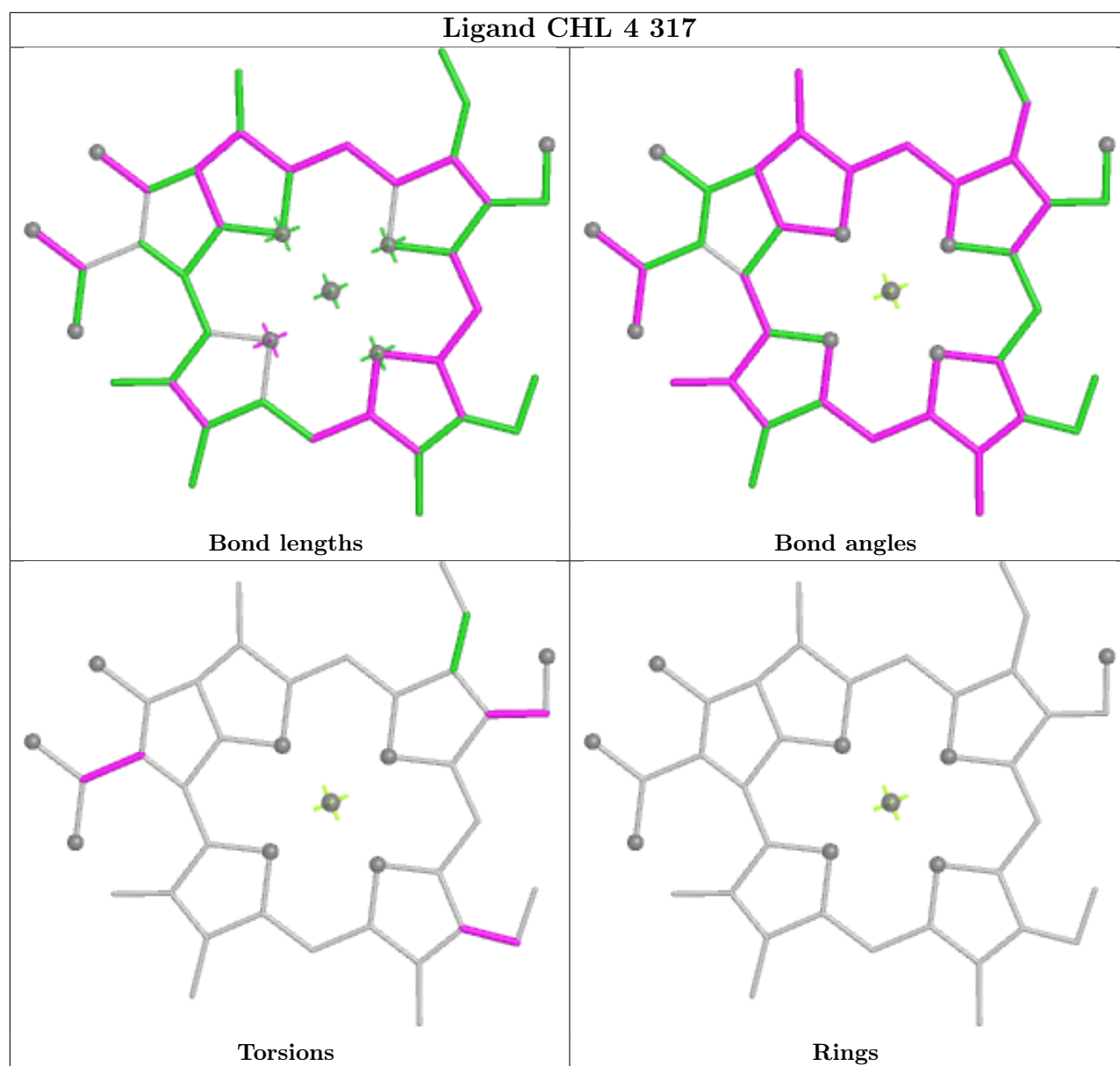
Bond angles

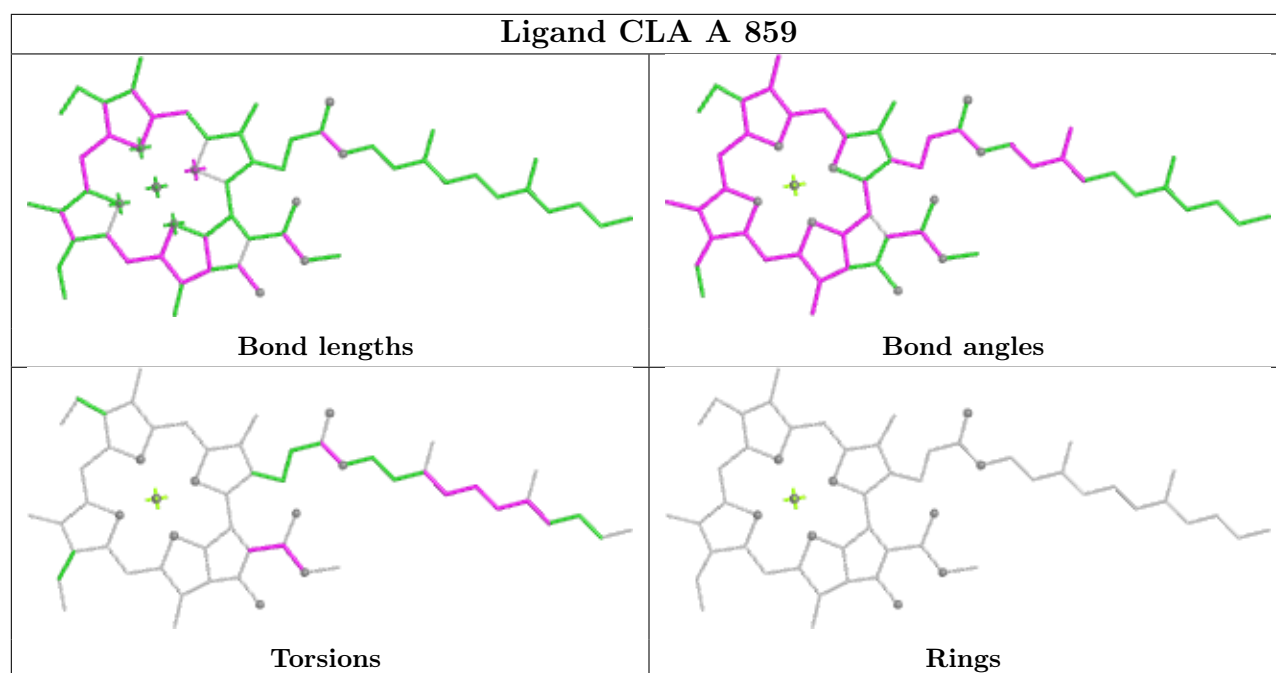


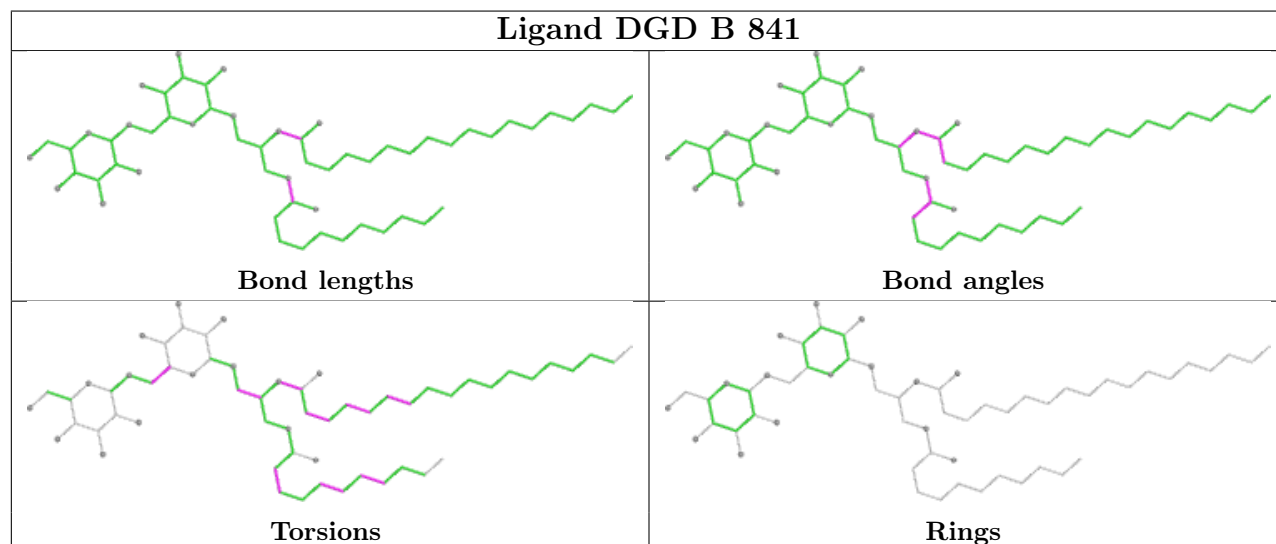
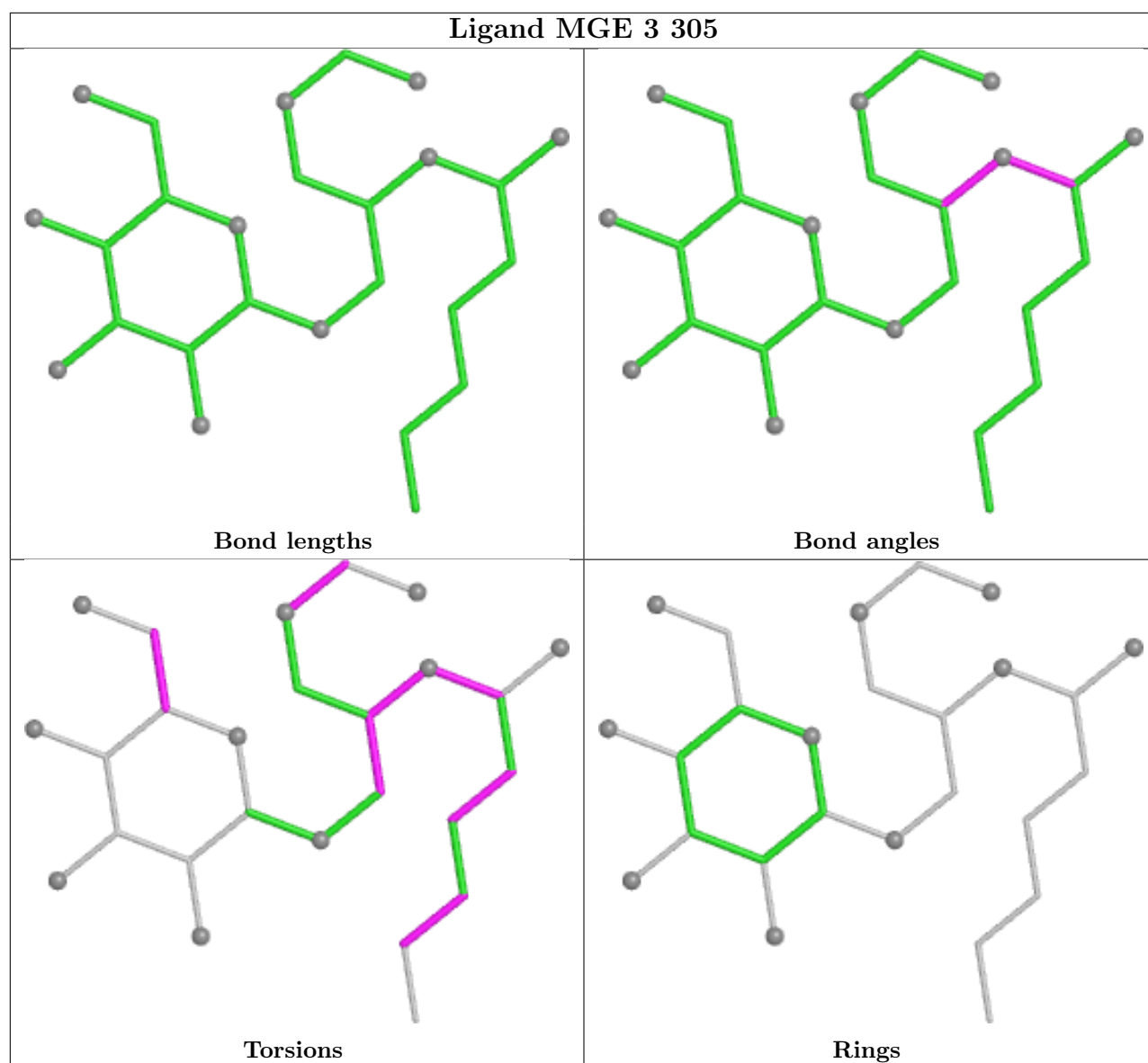
Torsions

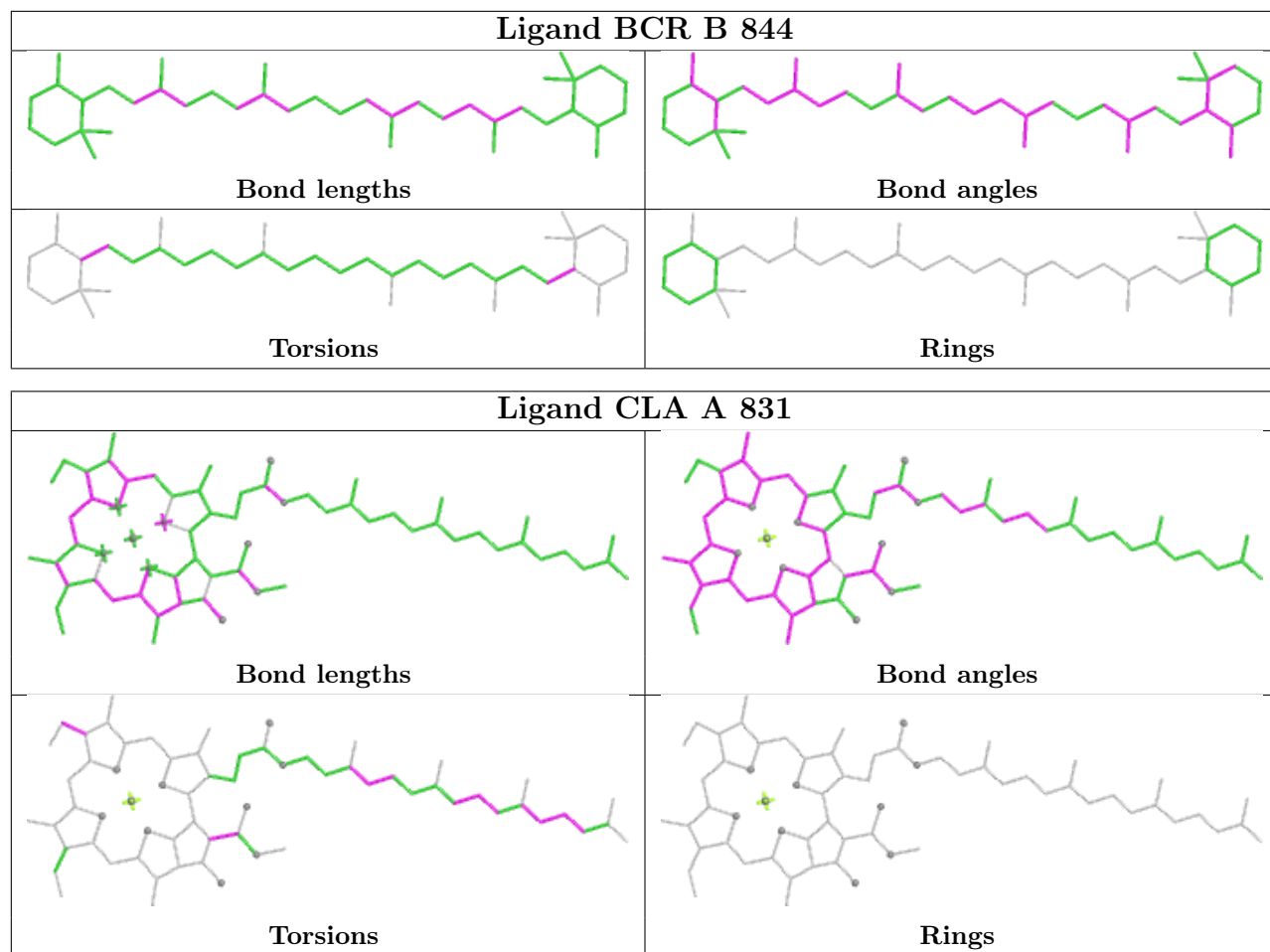


Rings

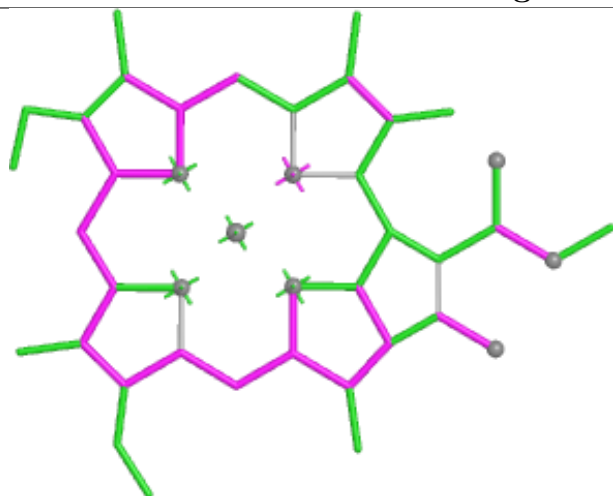




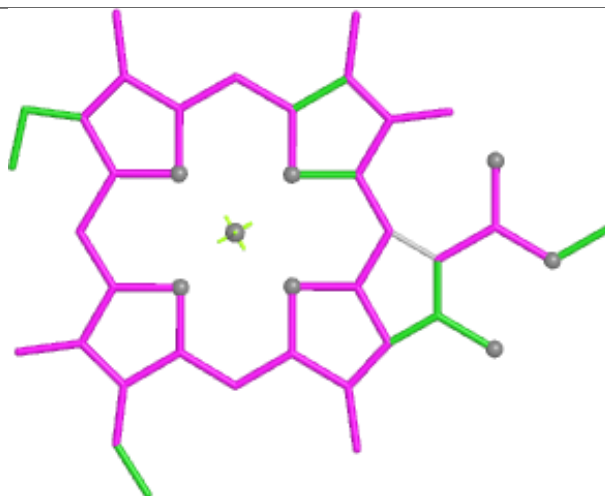




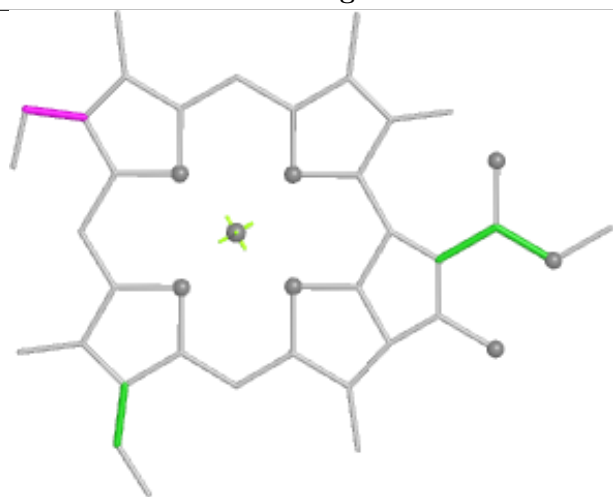
Ligand CLA H 201



Bond lengths



Bond angles

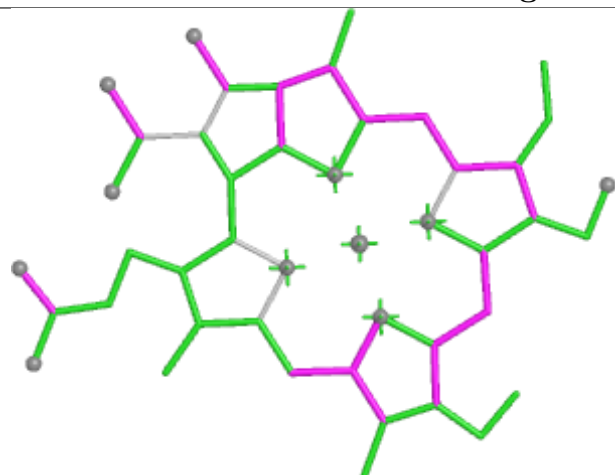


Torsions

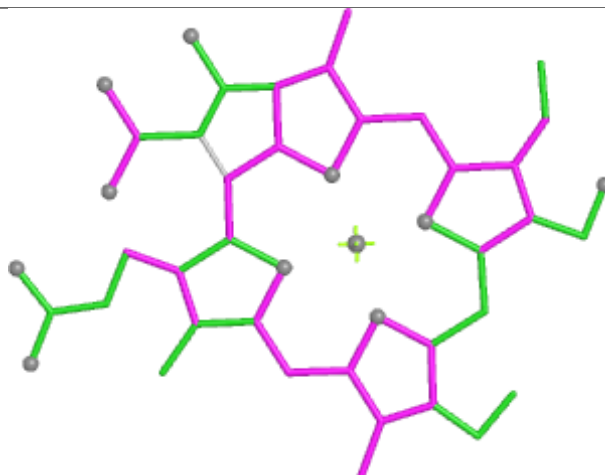


Rings

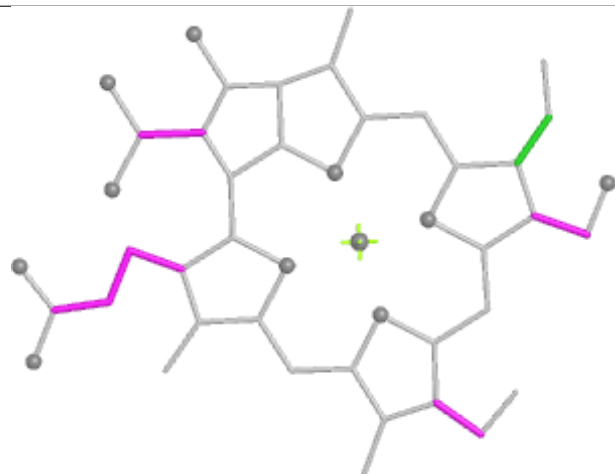
Ligand CHL 4 307



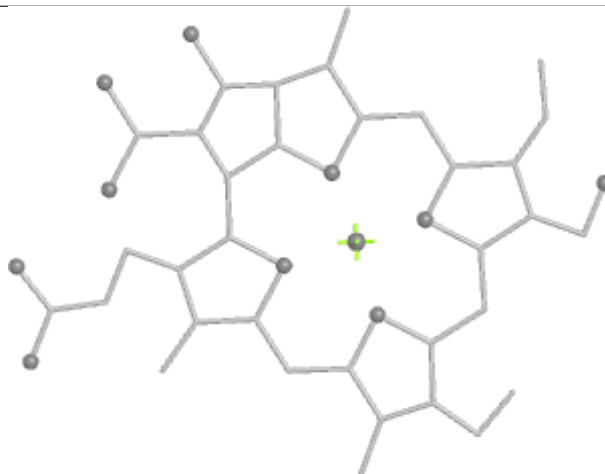
Bond lengths



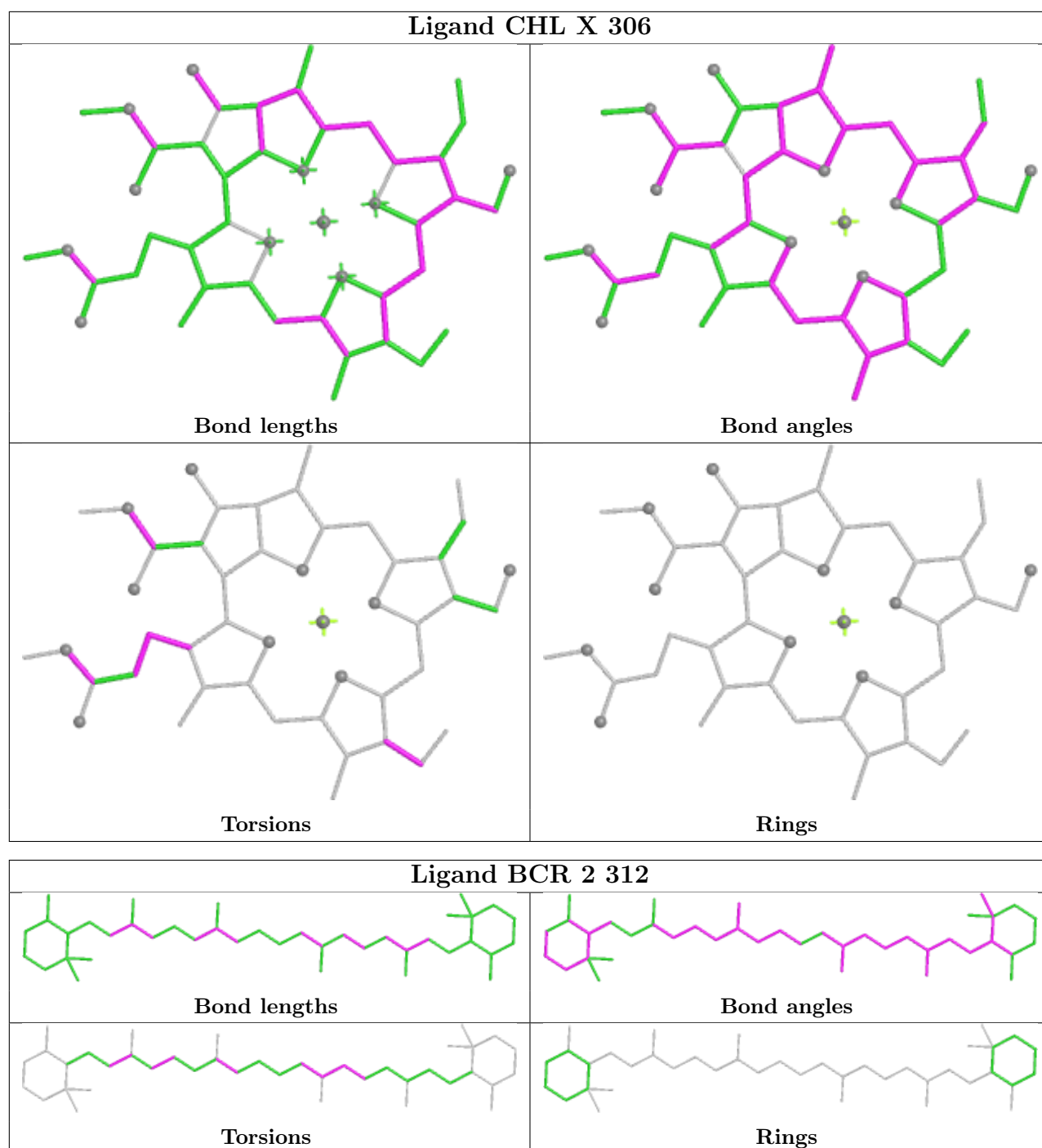
Bond angles

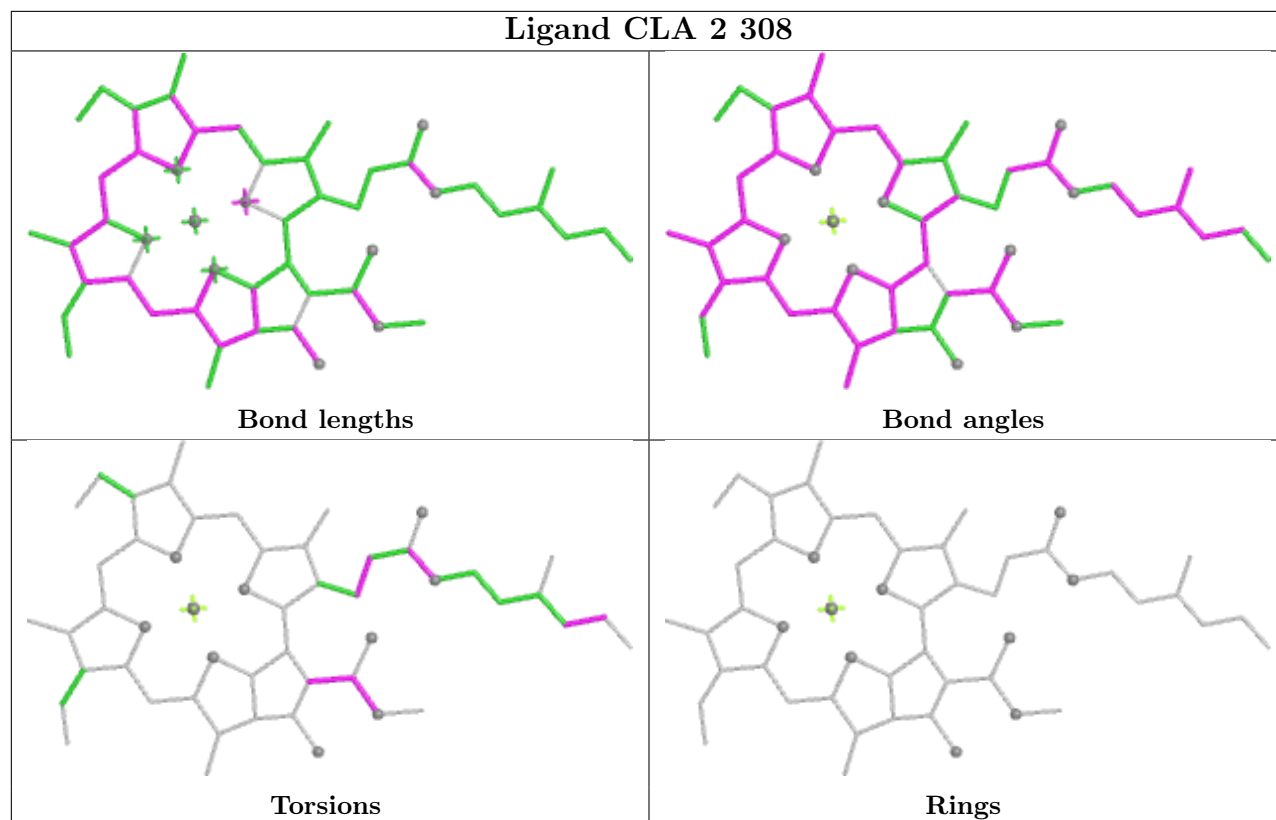


Torsions

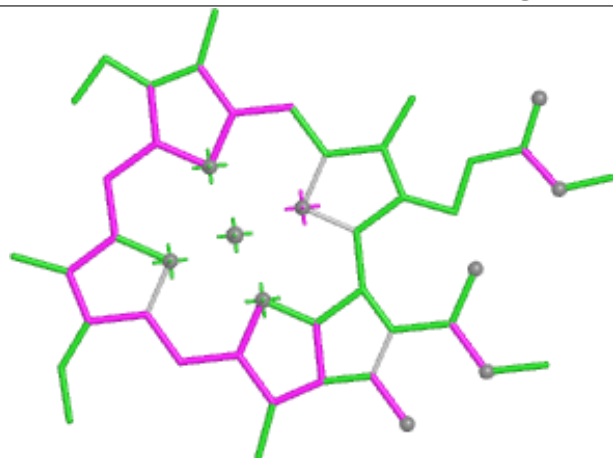


Rings

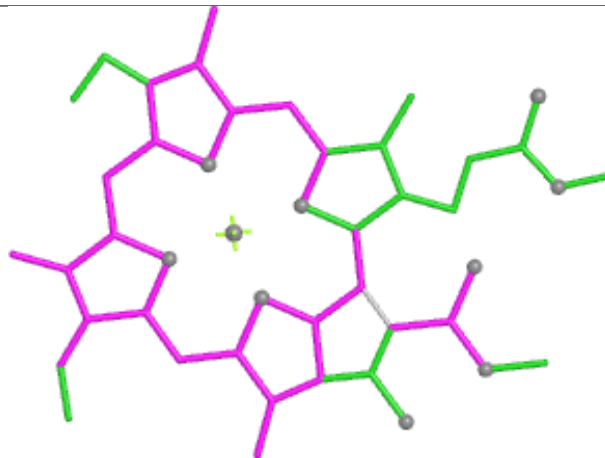




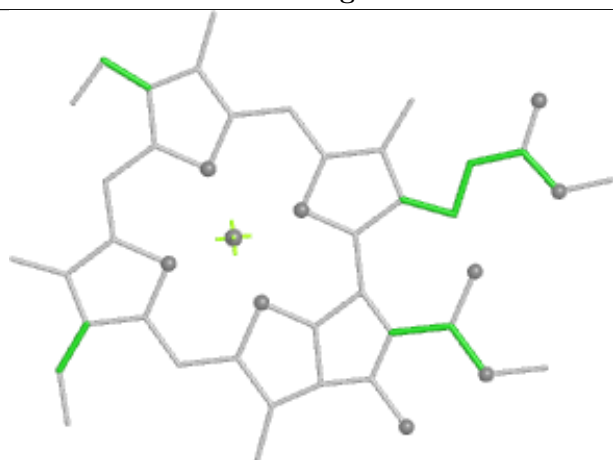
Ligand CLA Z 307



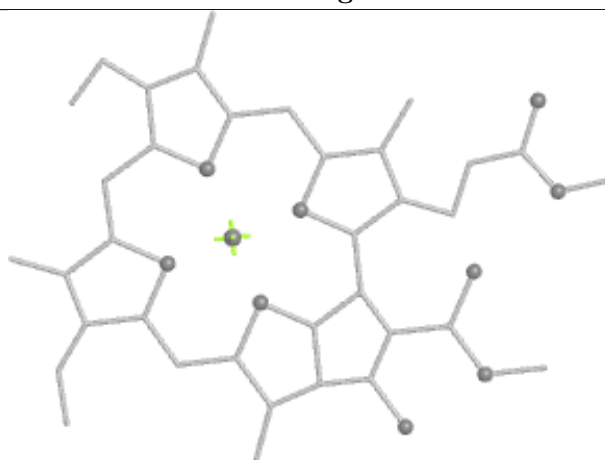
Bond lengths



Bond angles

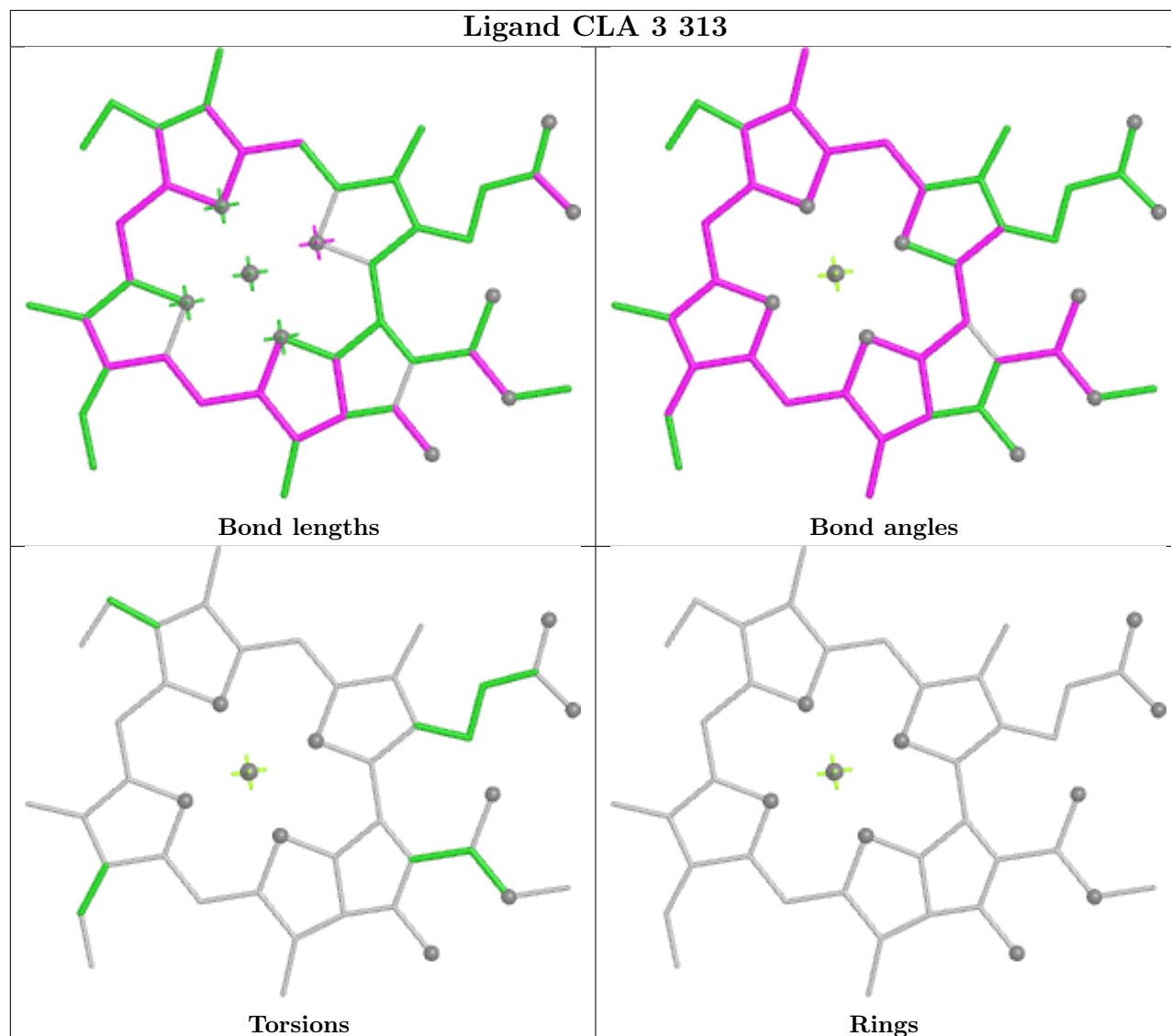


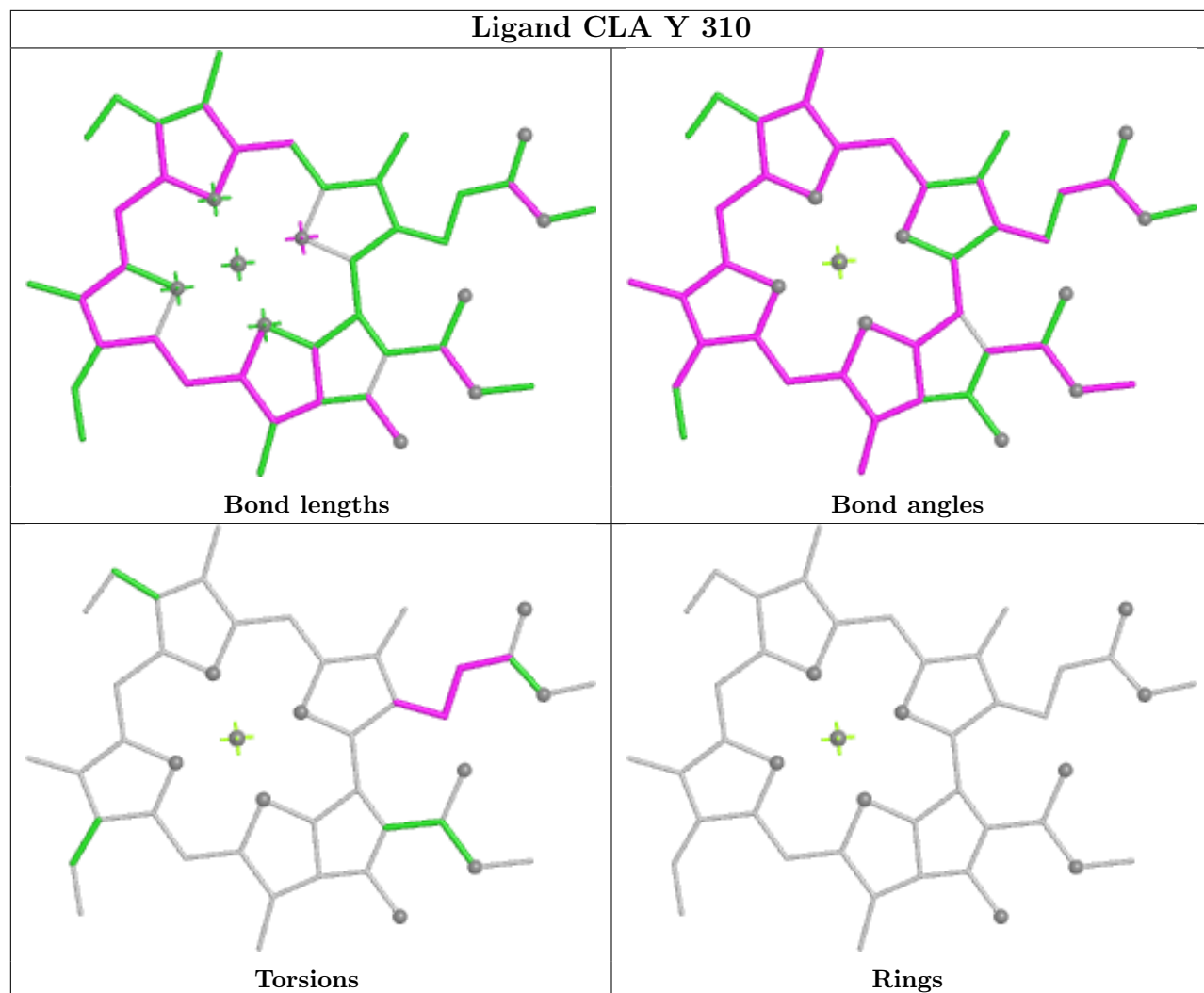
Torsions

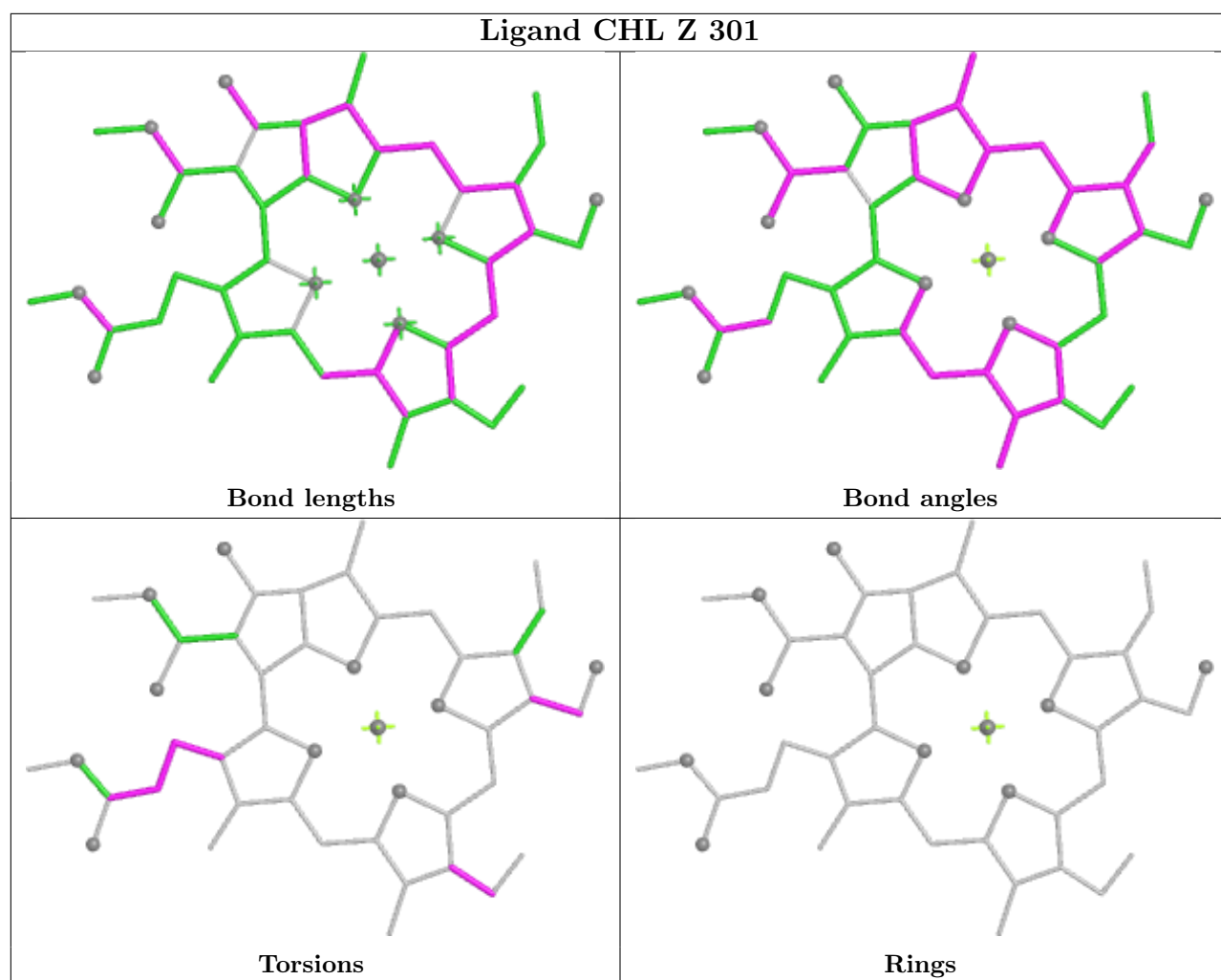


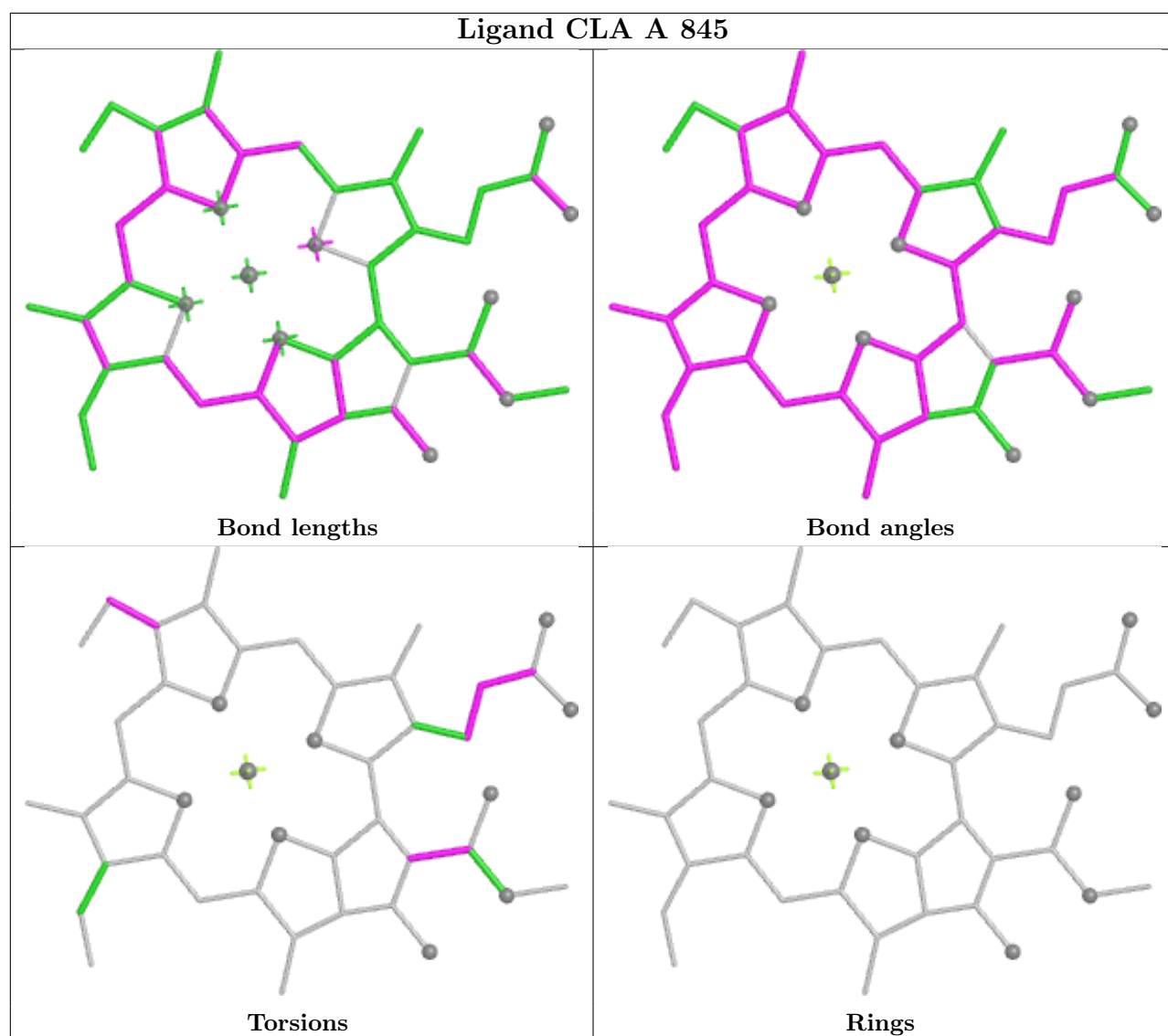
Rings

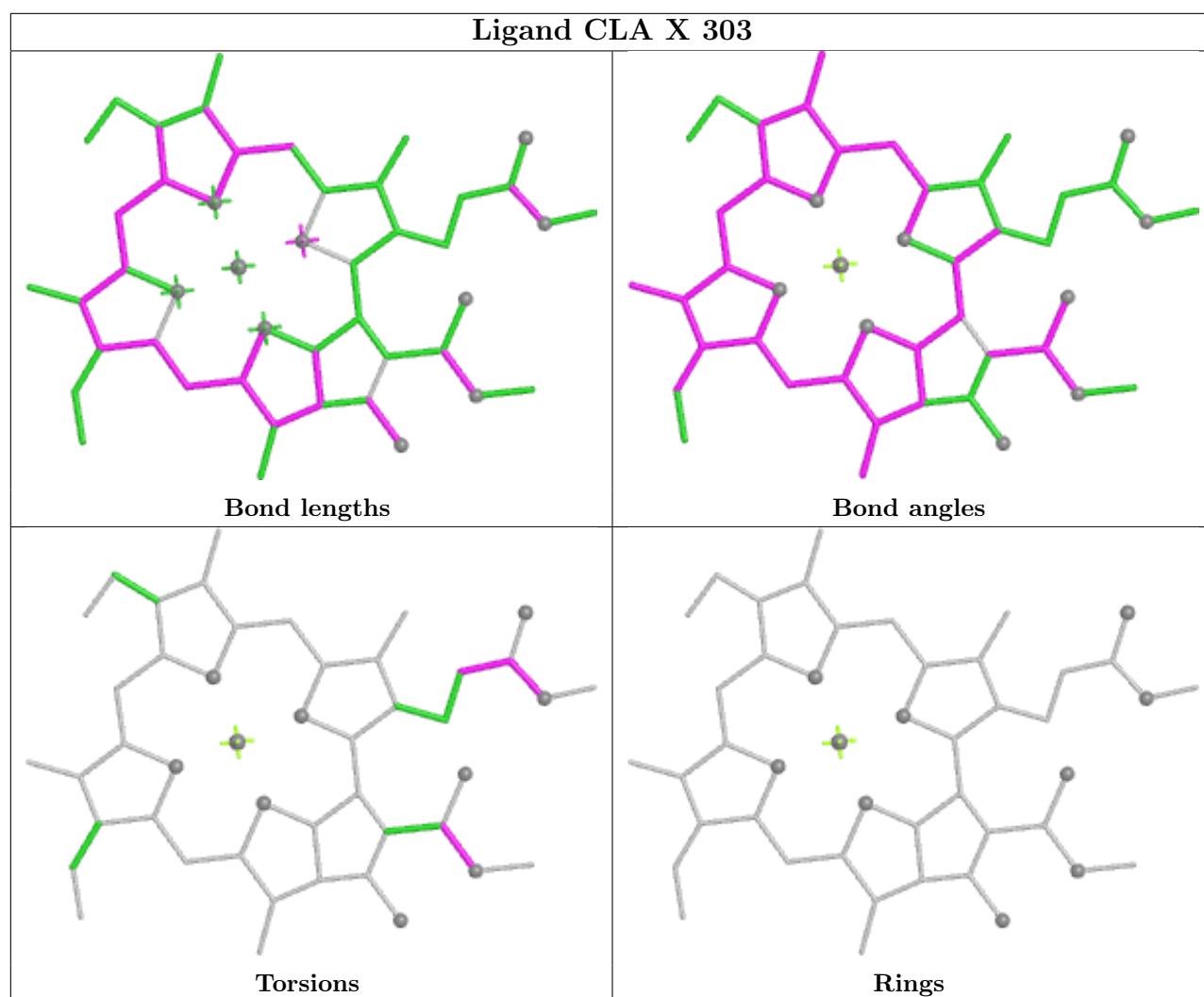
Ligand CLA 3 313

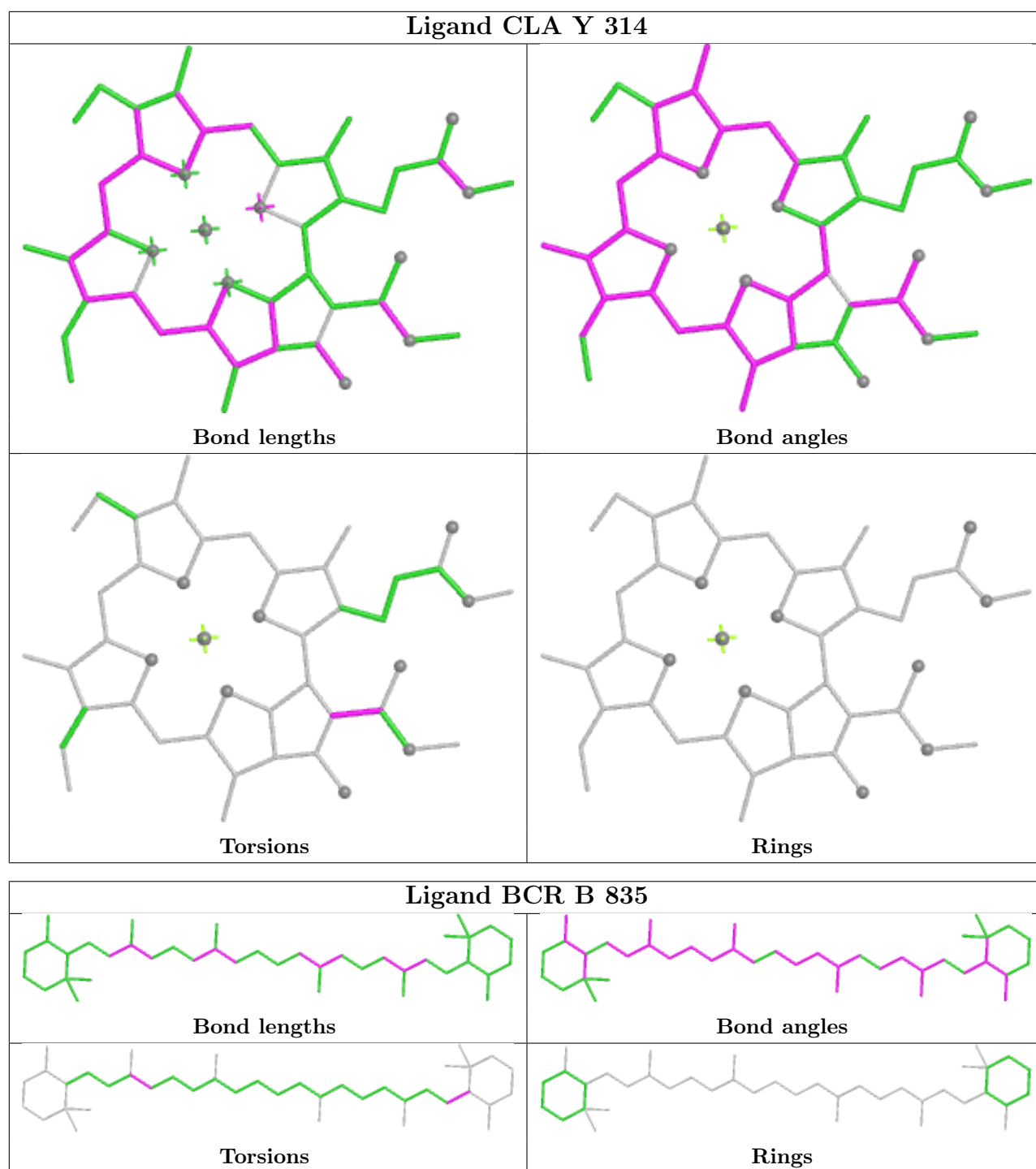


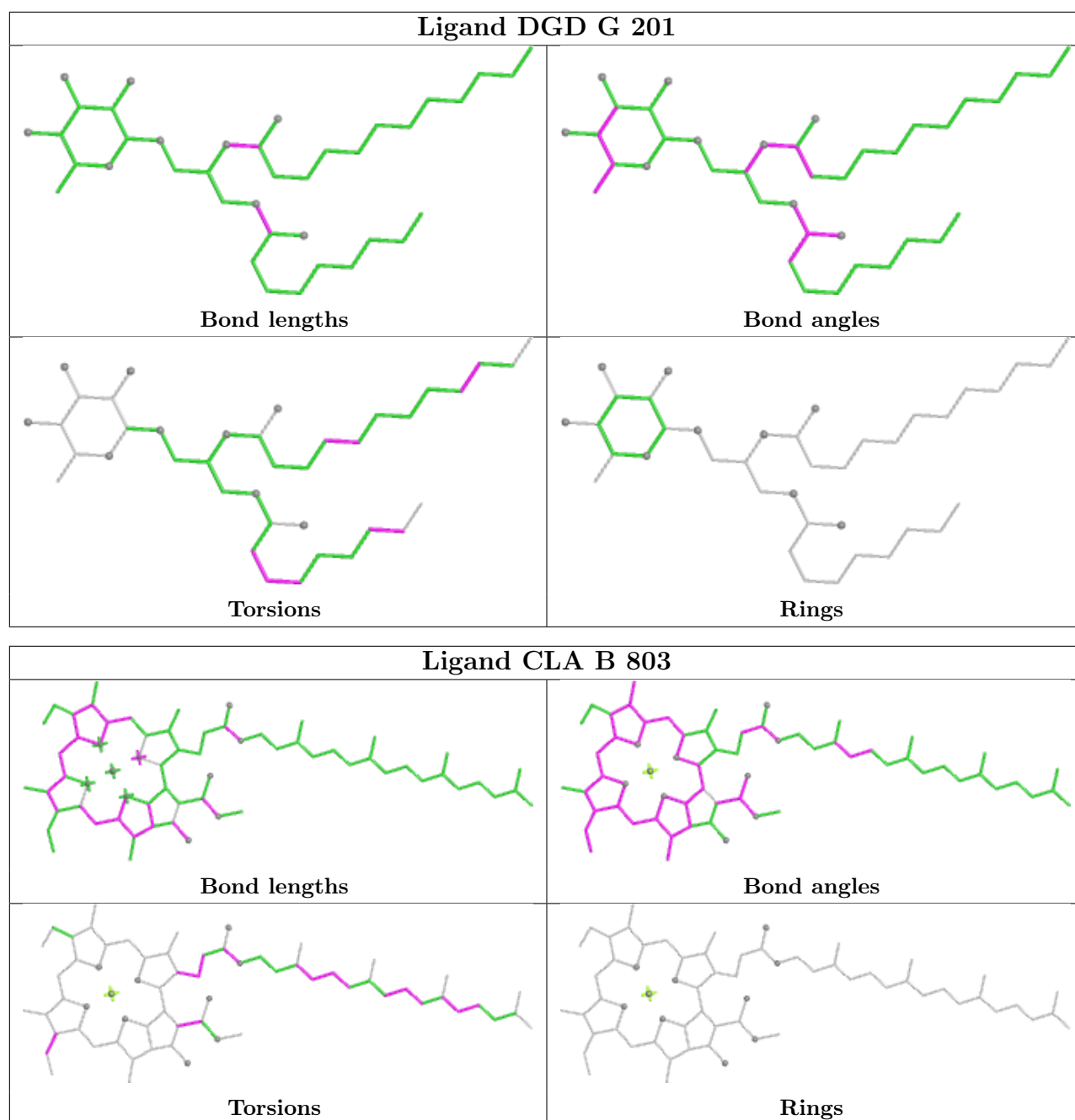




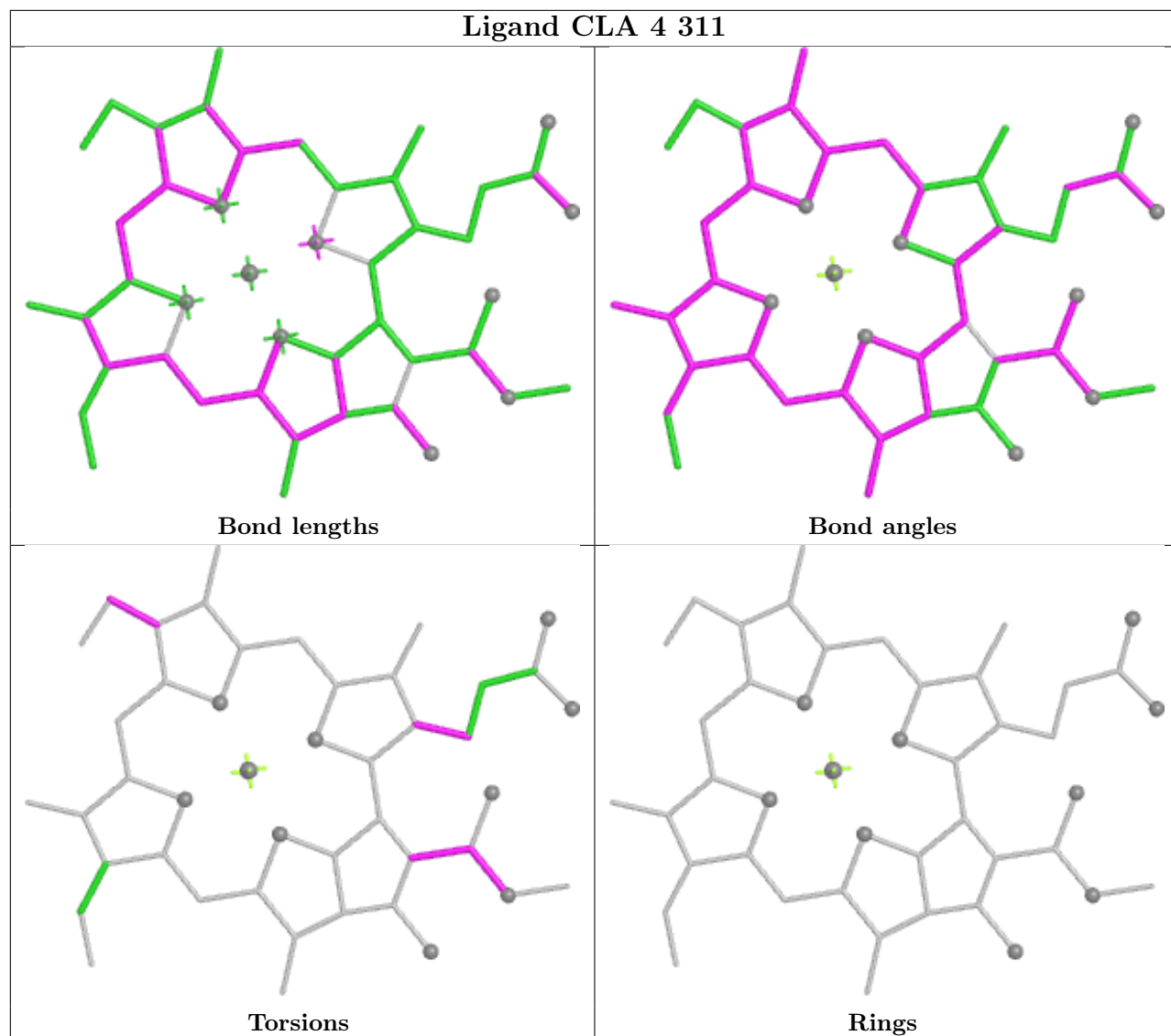




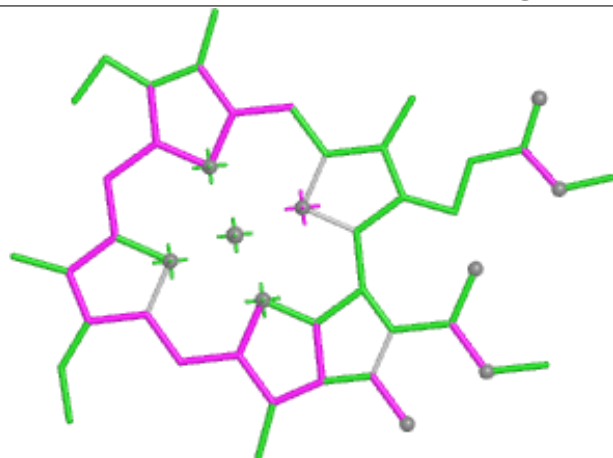




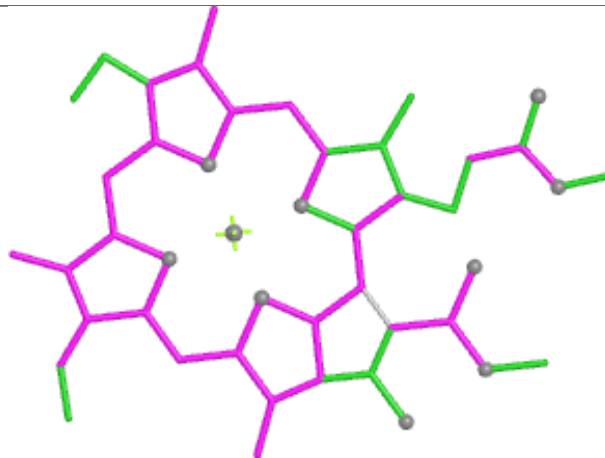
Ligand CLA 4 311



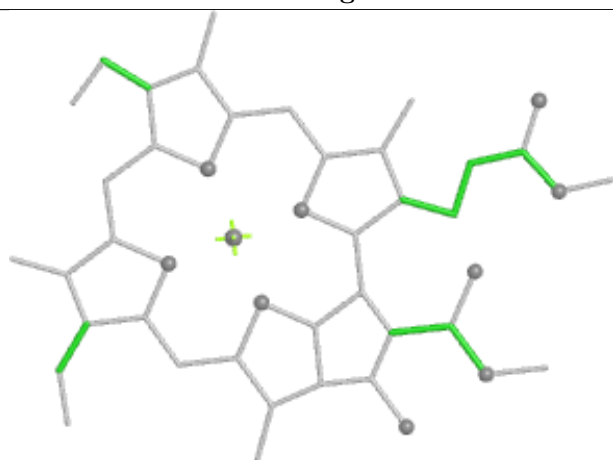
Ligand CLA Z 308



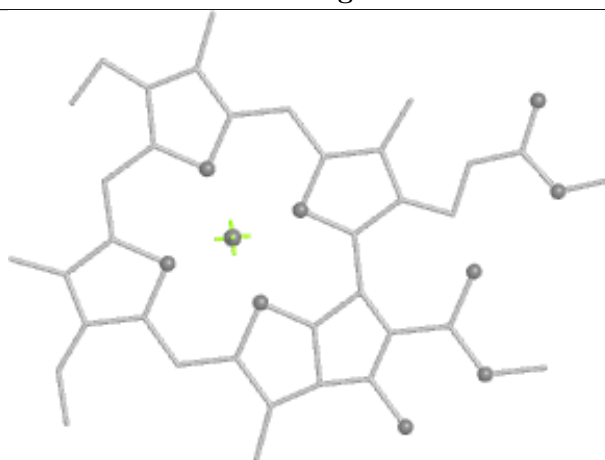
Bond lengths



Bond angles

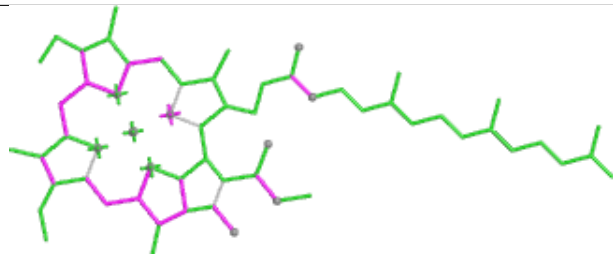


Torsions

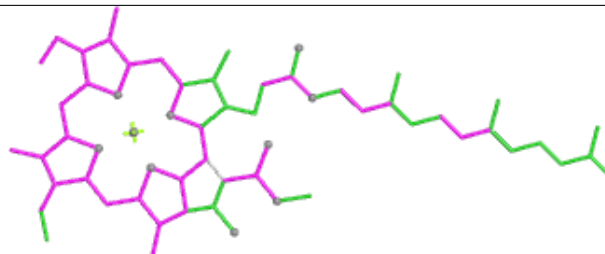


Rings

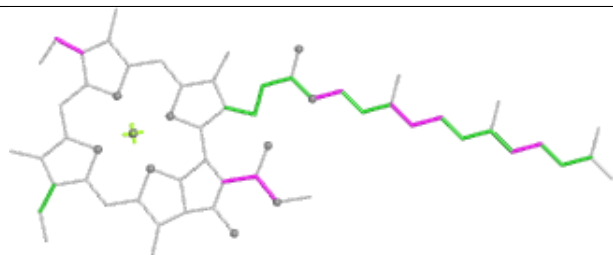
Ligand CLA B 809



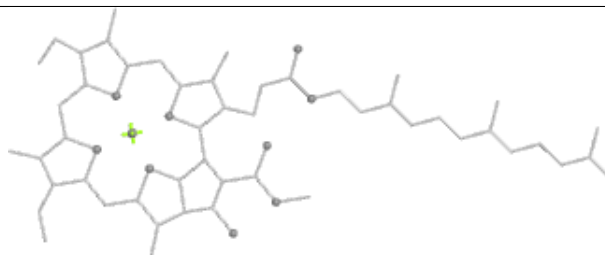
Bond lengths



Bond angles

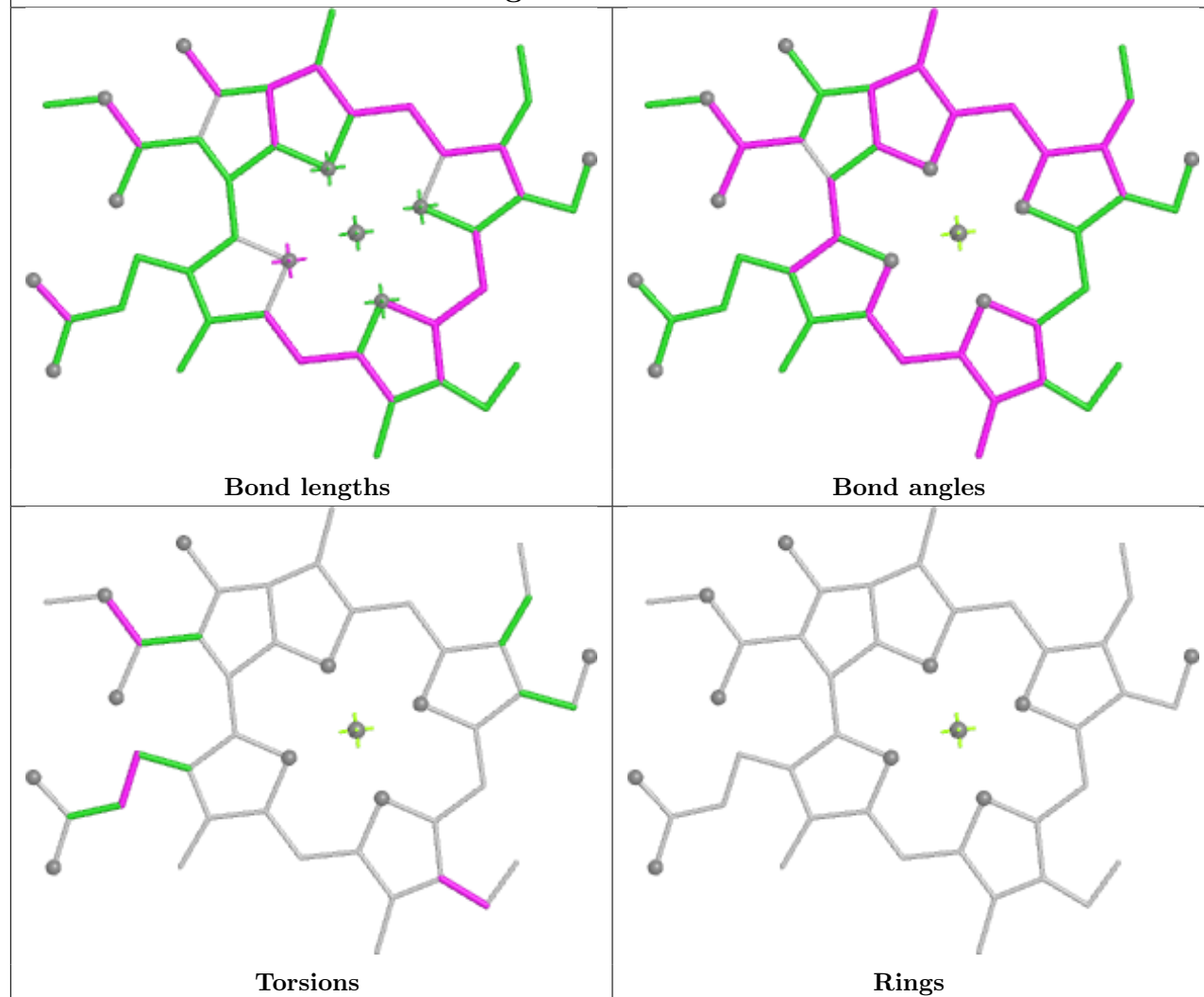


Torsions

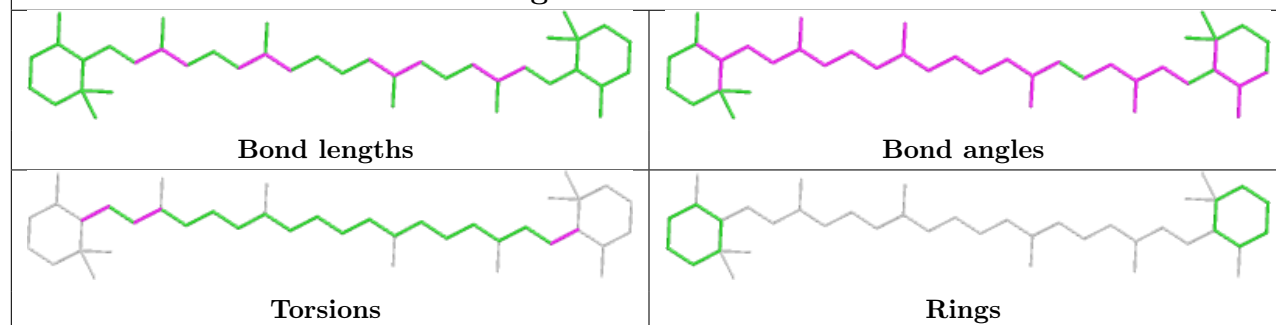


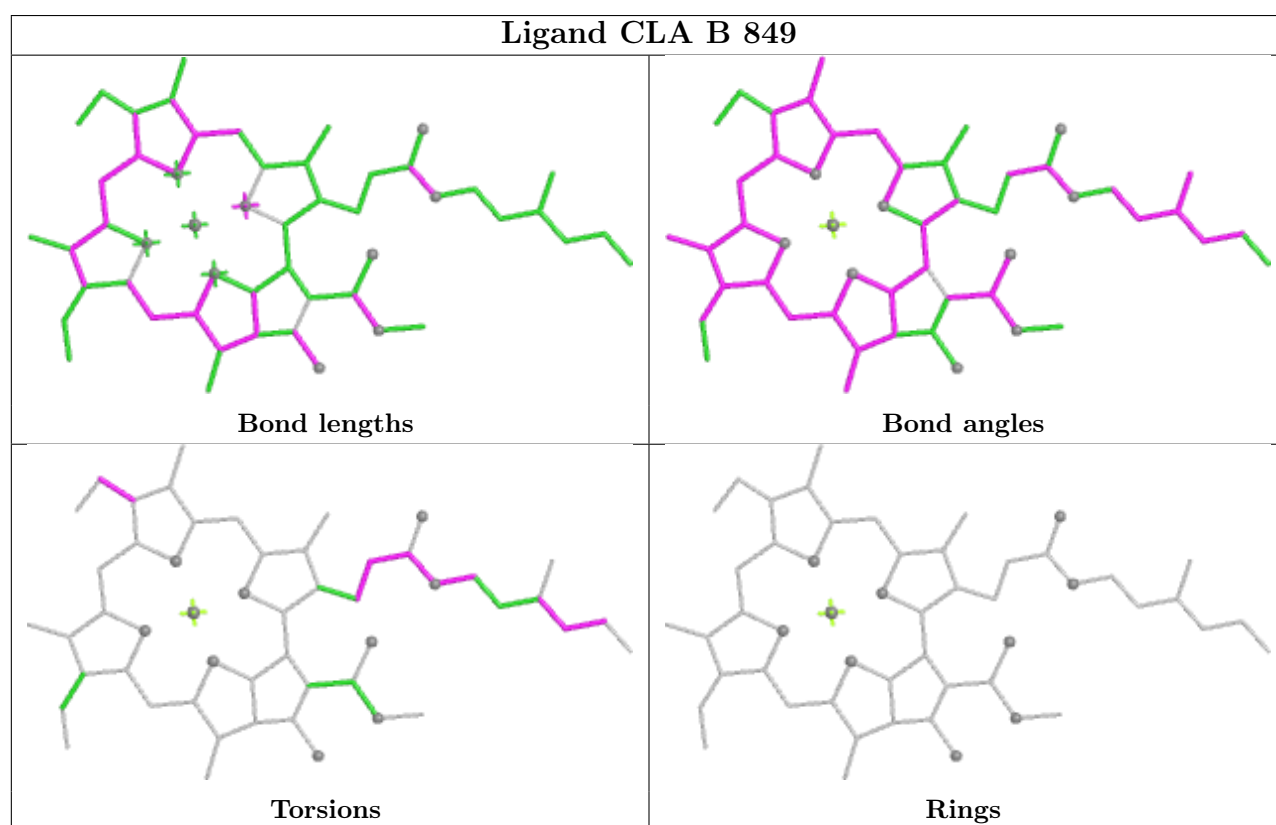
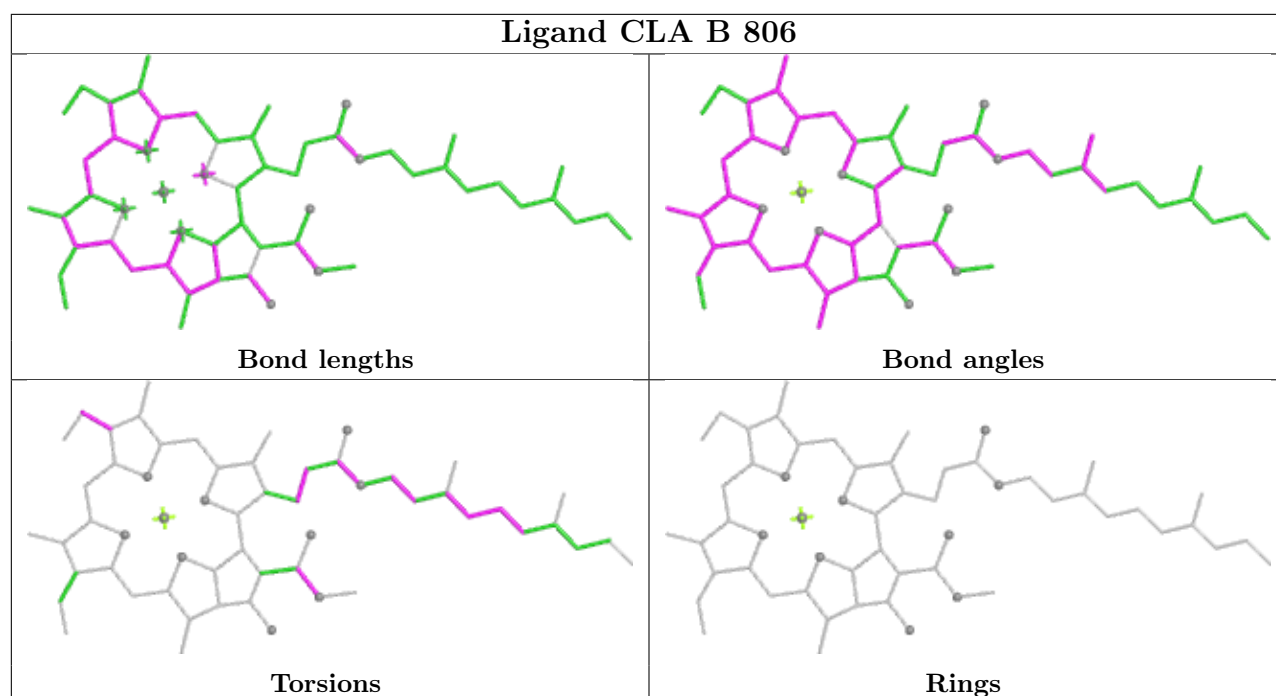
Rings

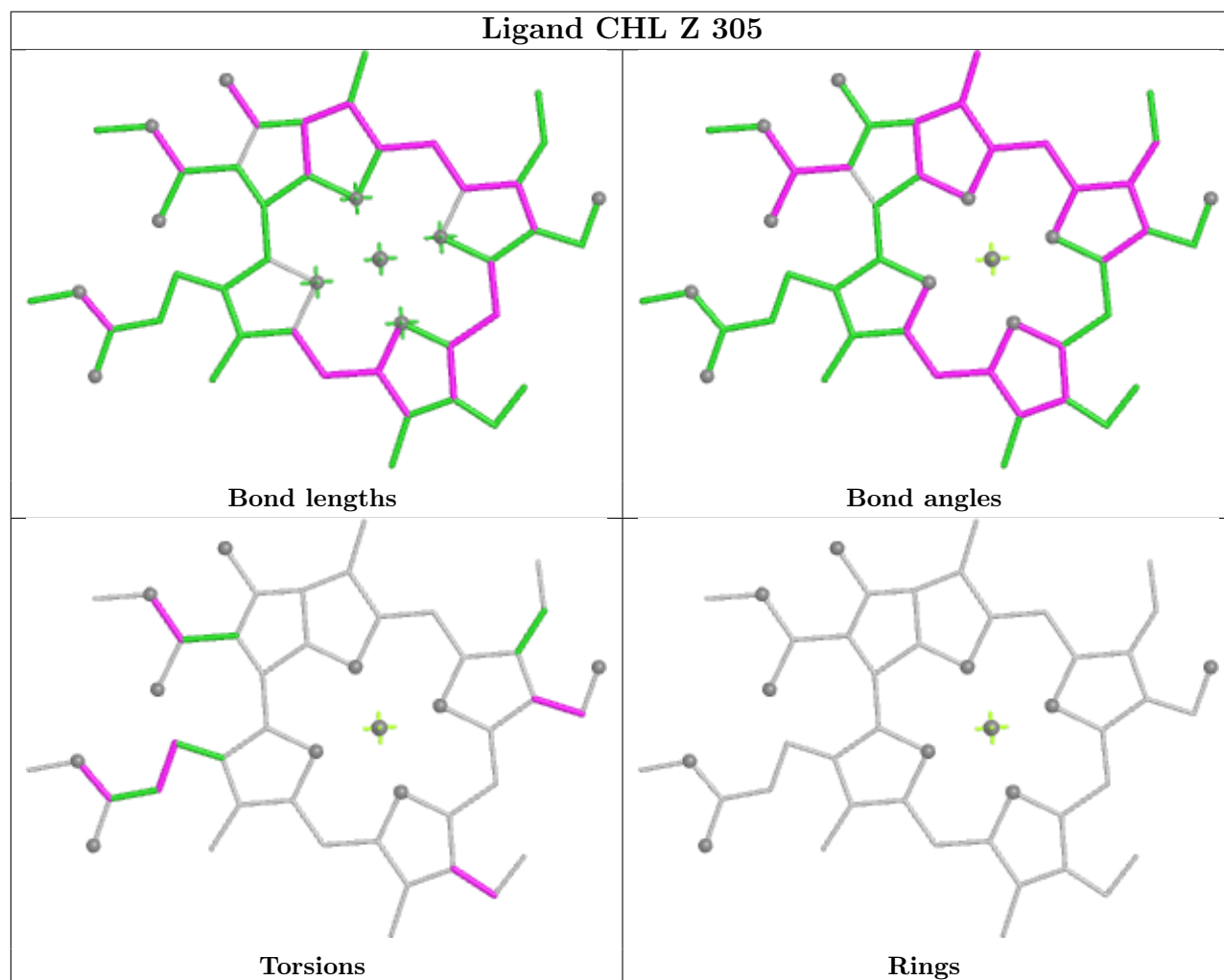
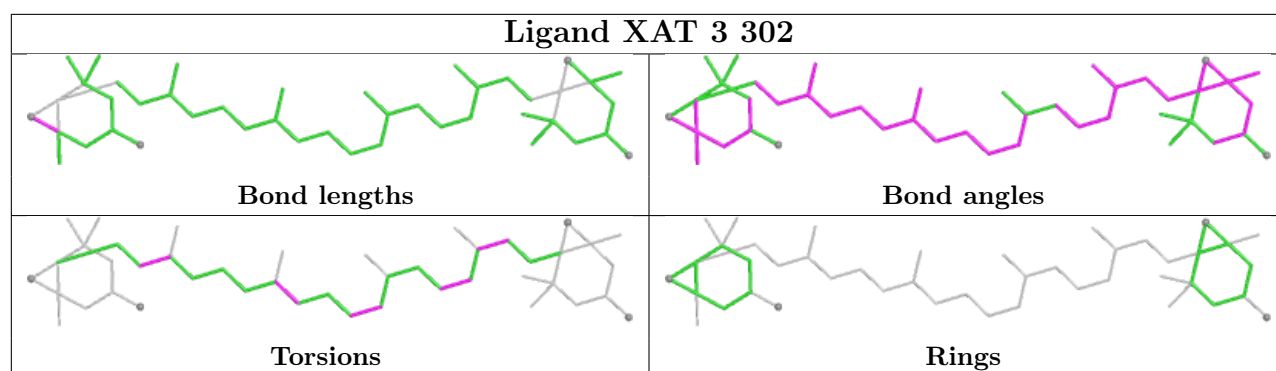
Ligand CHL 2 309



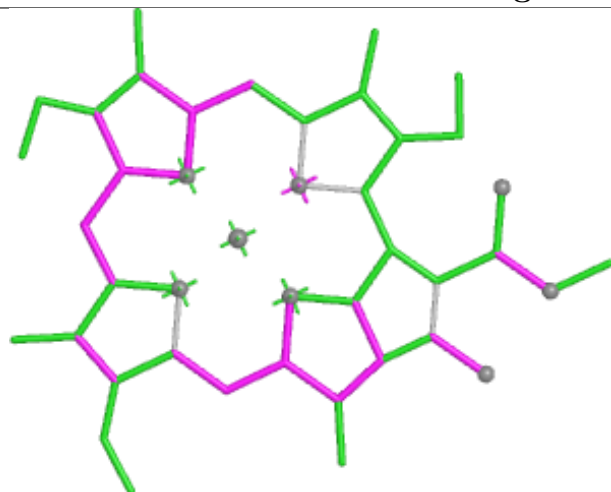
Ligand BCR B 837



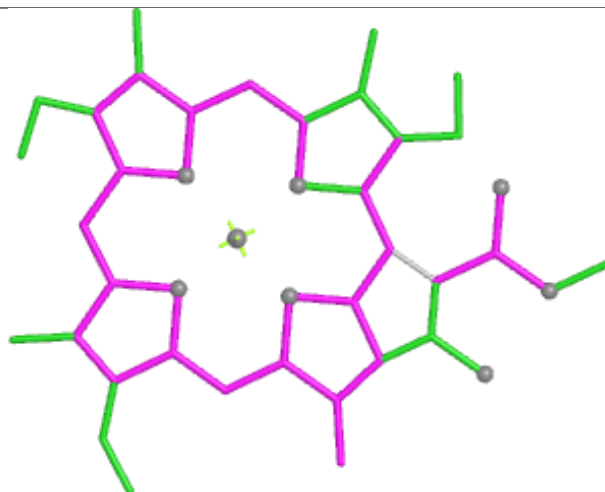




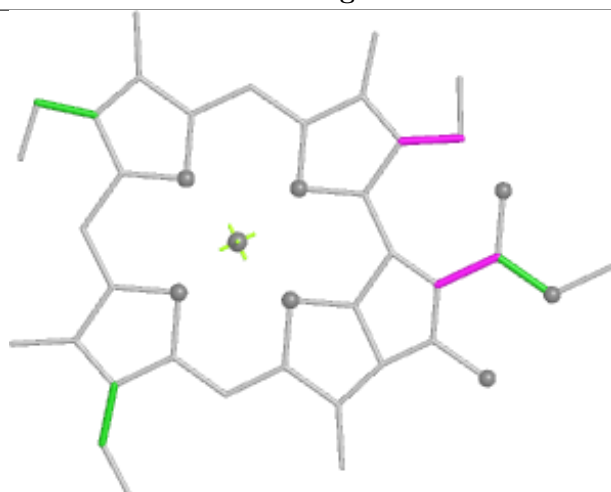
Ligand CLA A 847



Bond lengths



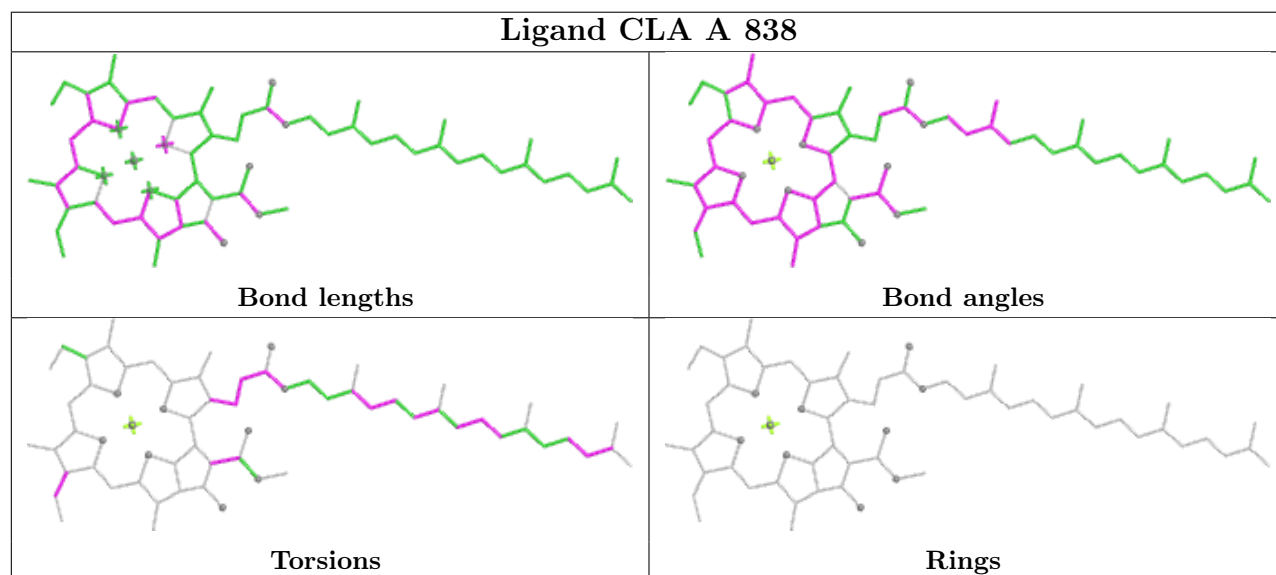
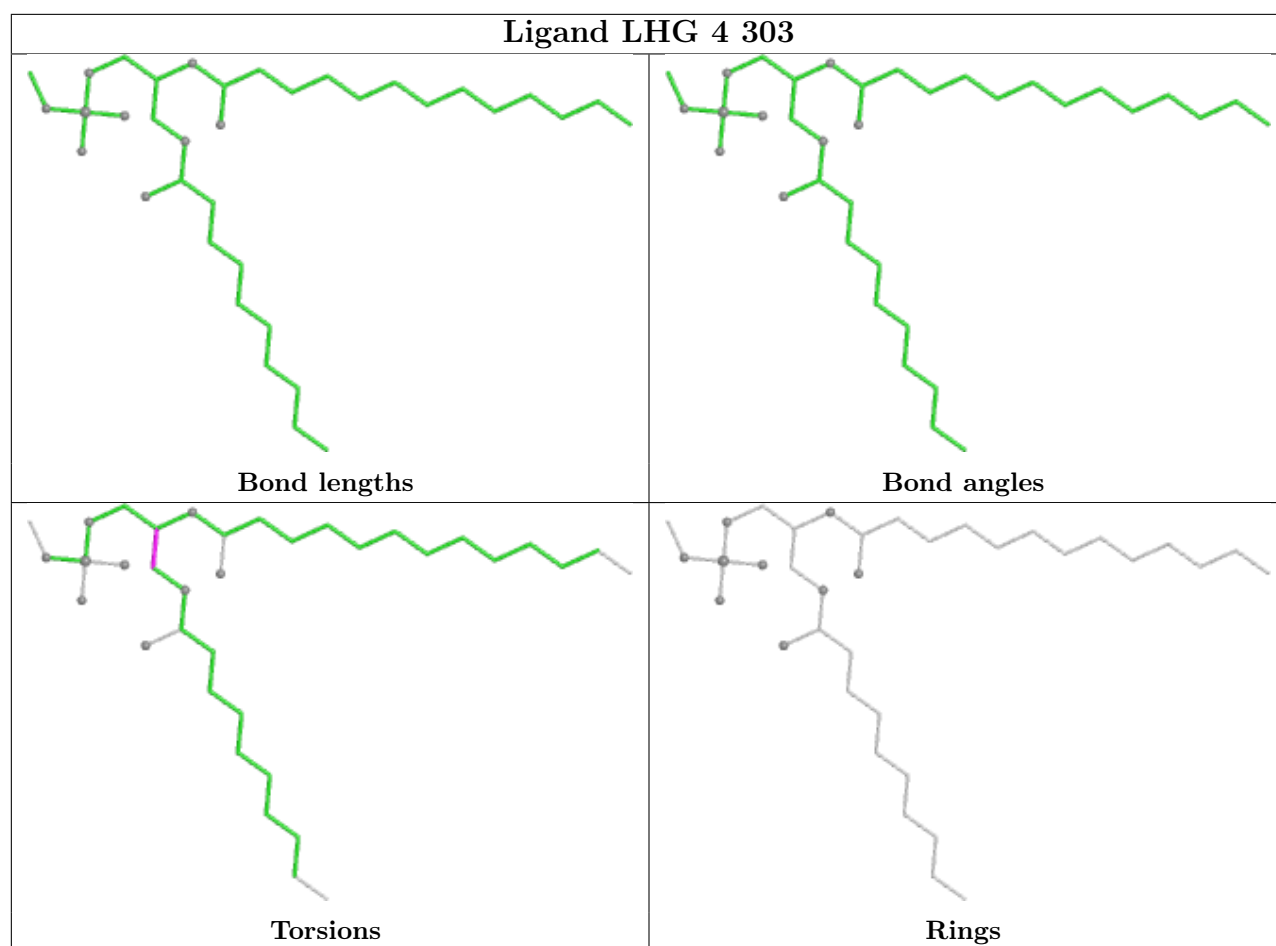
Bond angles

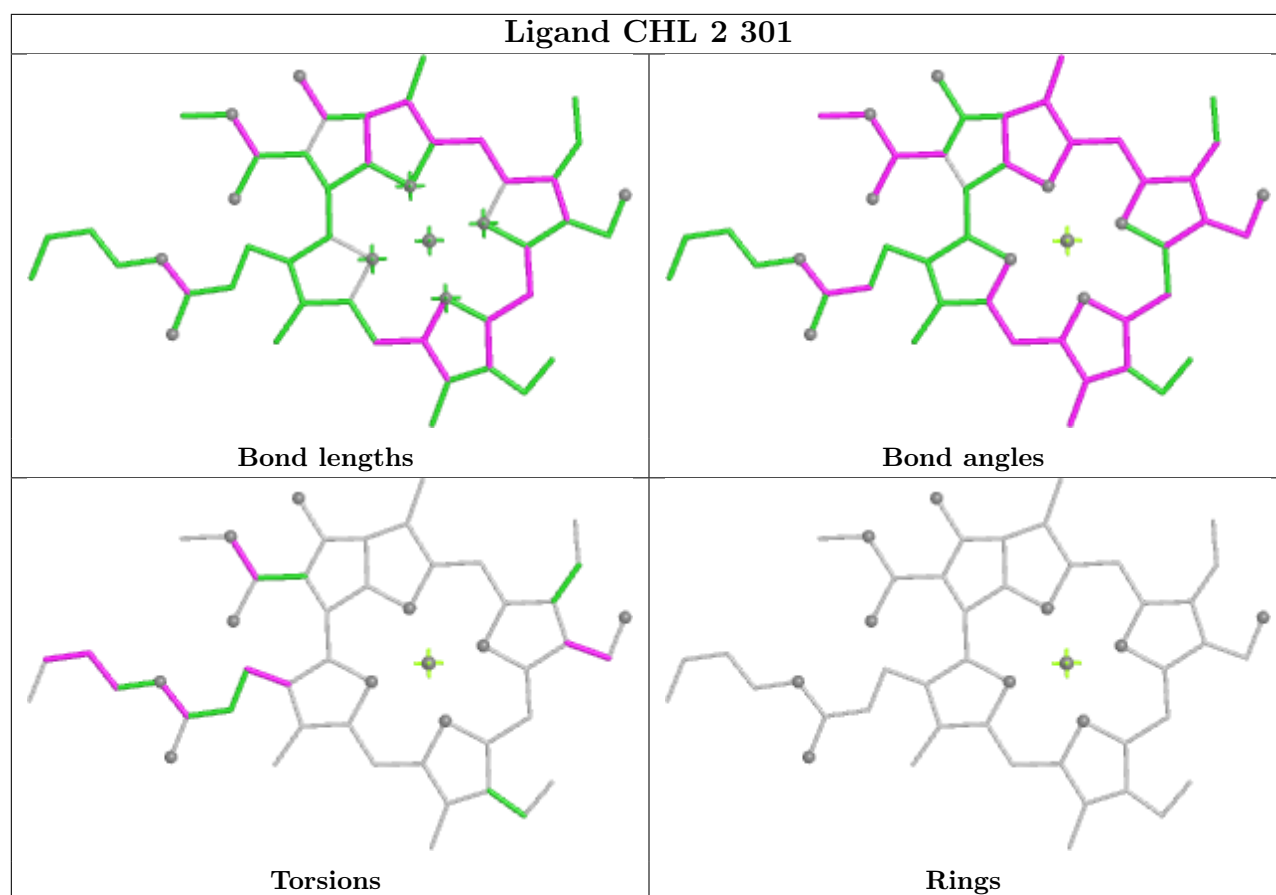


Torsions

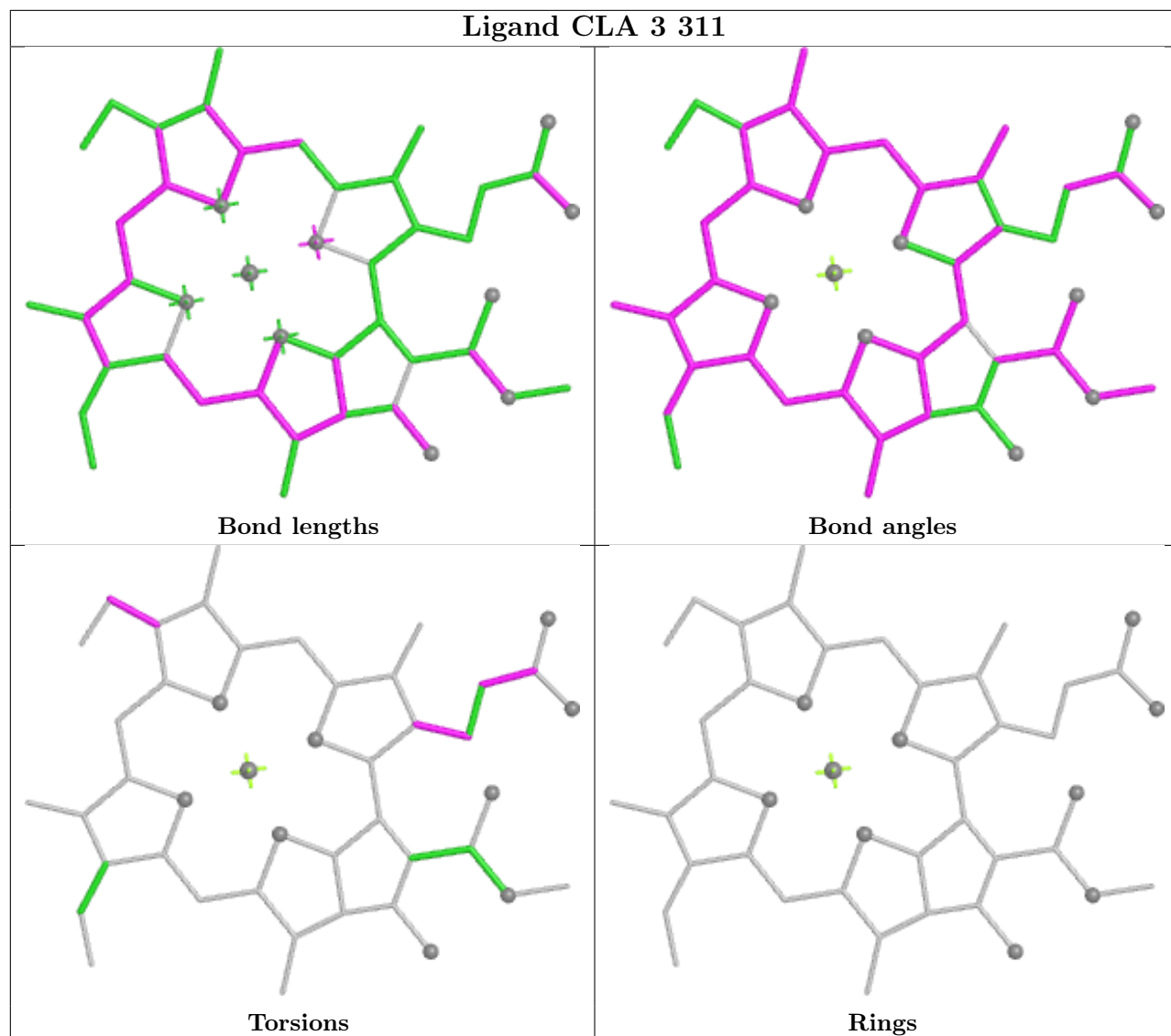


Rings

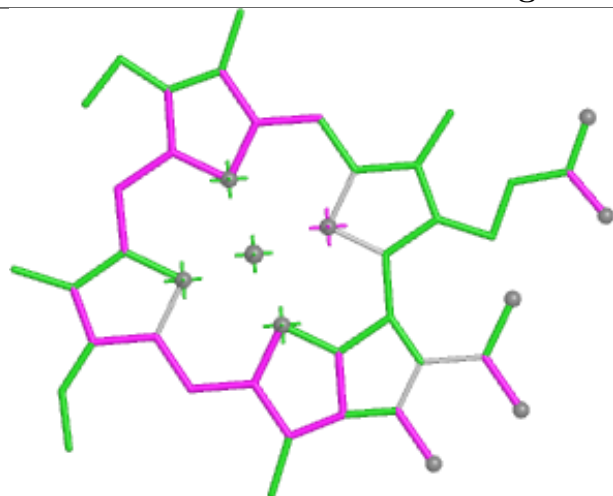




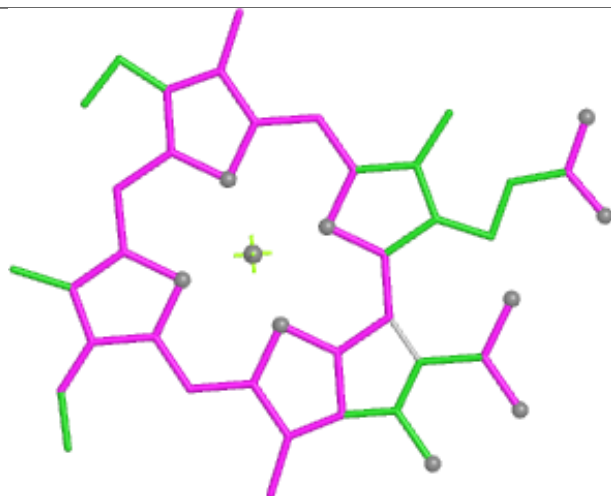
Ligand CLA 3 311



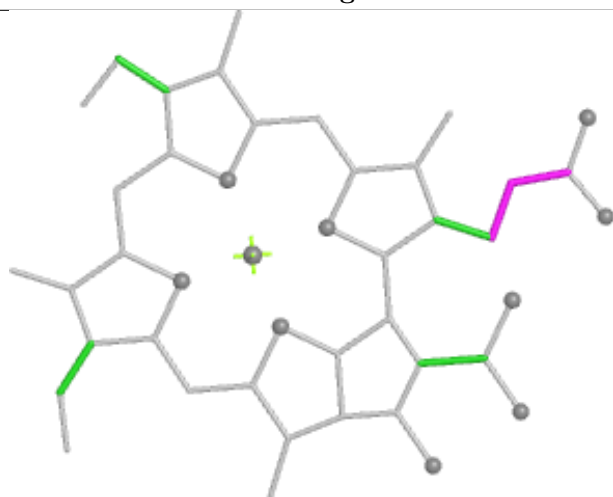
Ligand CLA 3 317



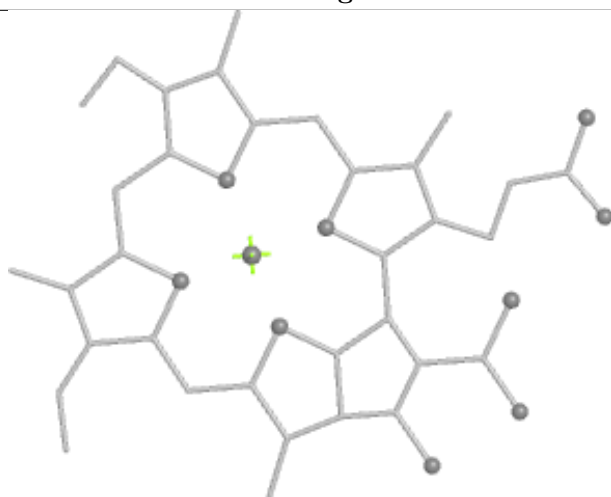
Bond lengths



Bond angles

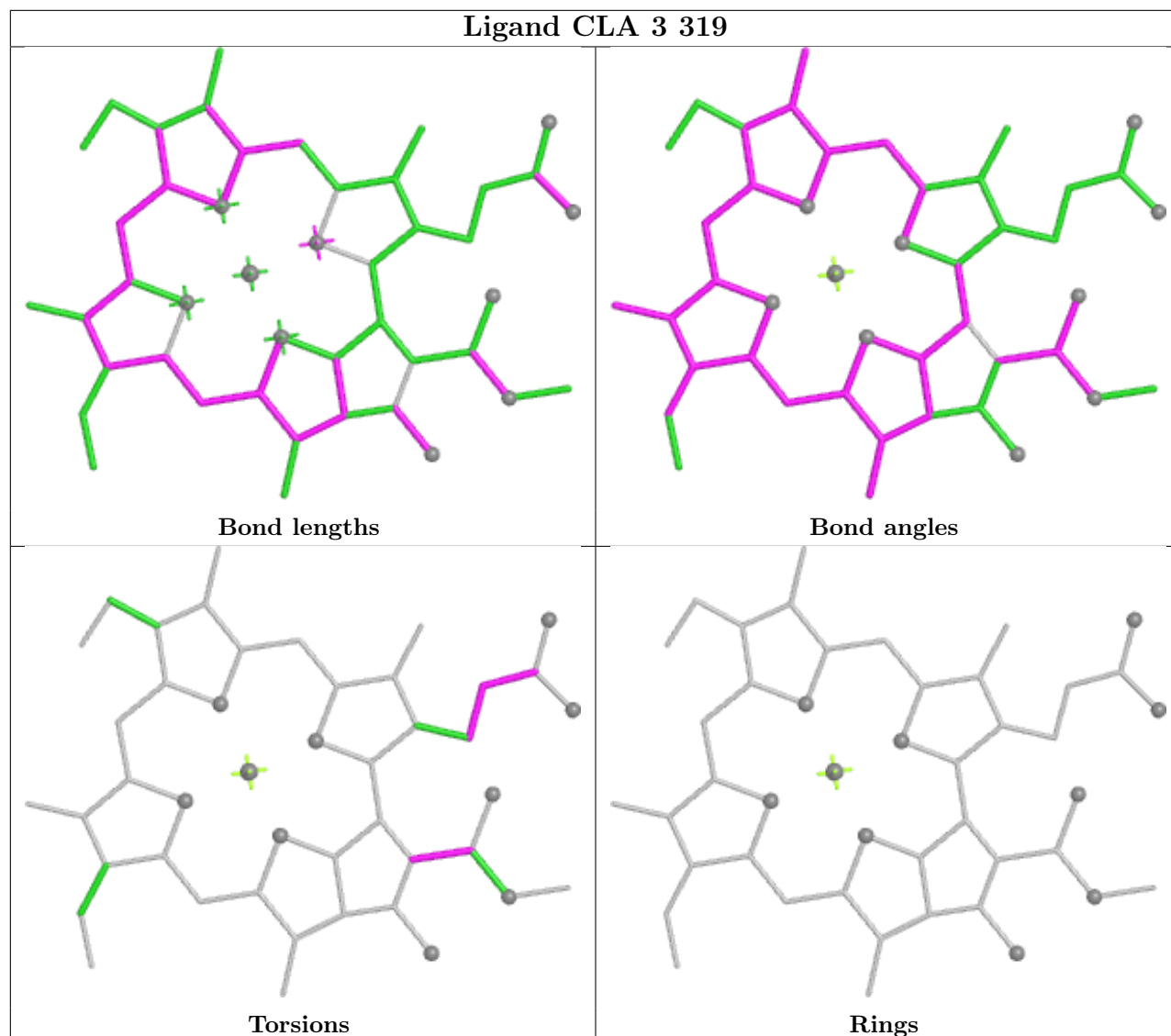


Torsions

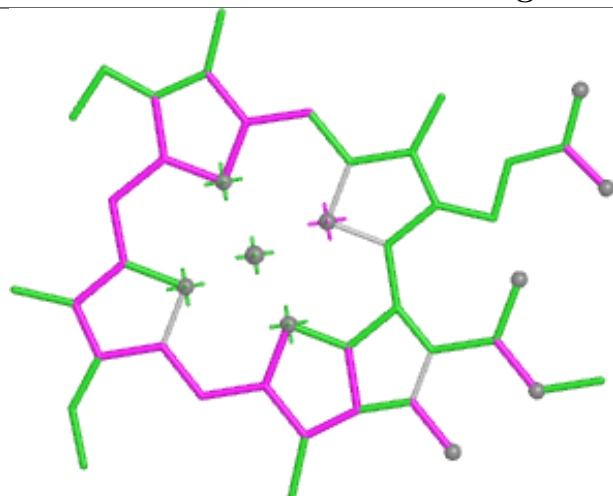


Rings

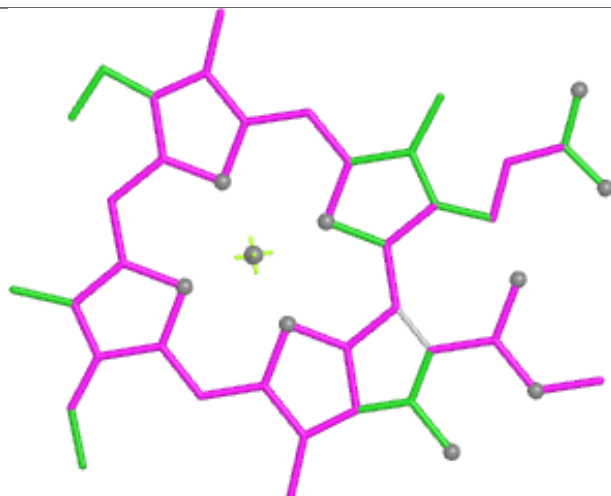
Ligand CLA 3 319



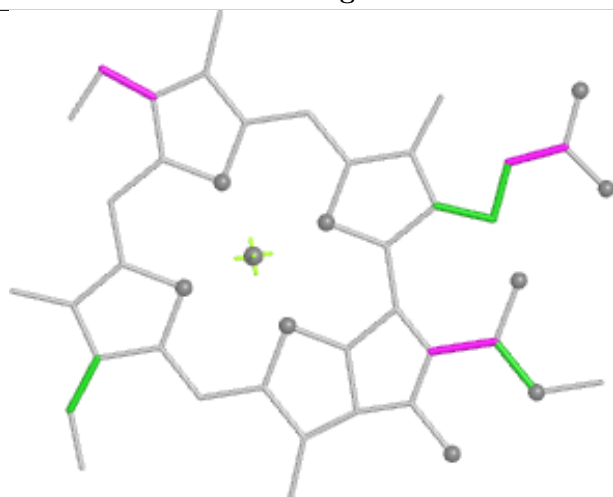
Ligand CLA L 307



Bond lengths



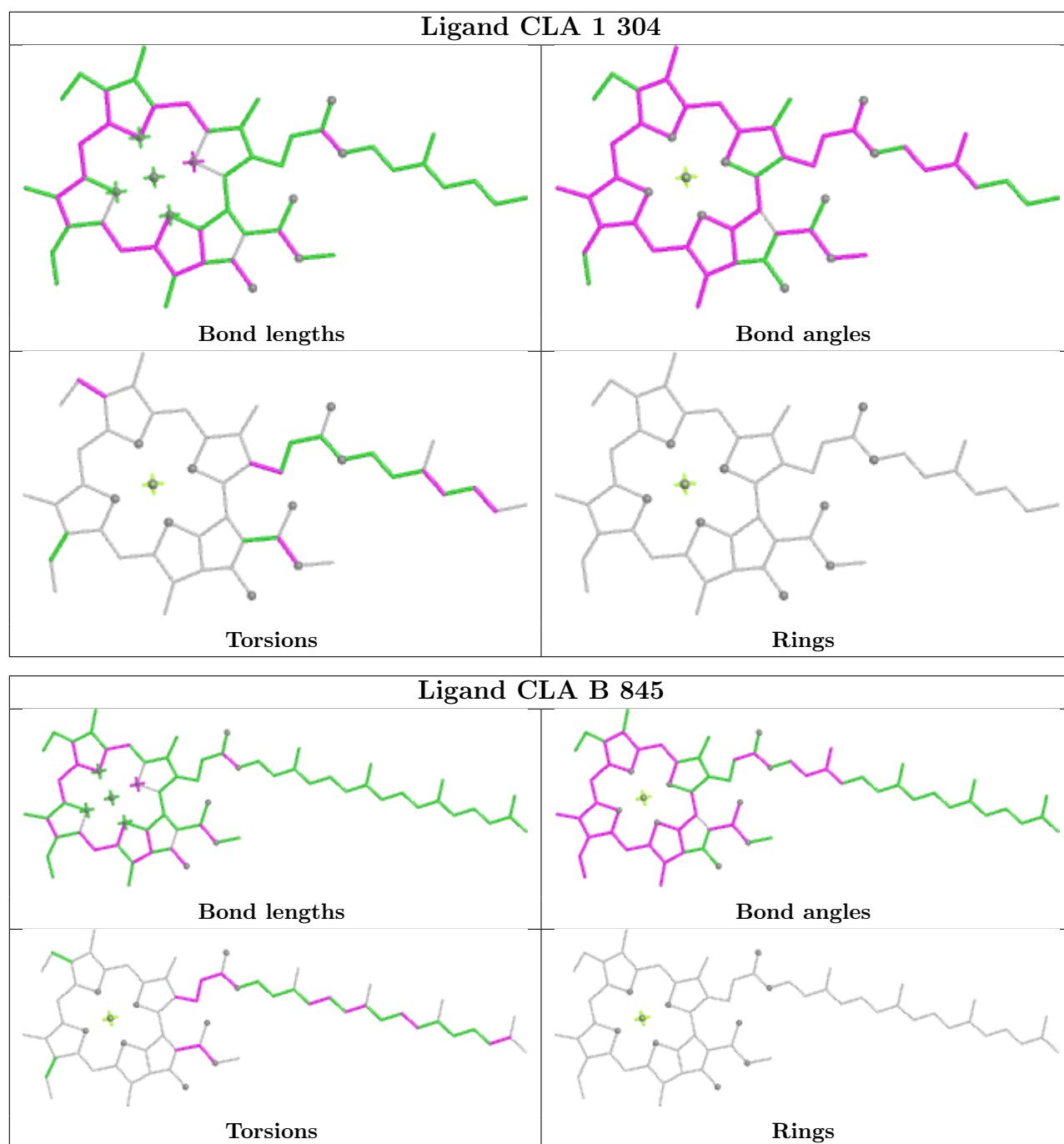
Bond angles



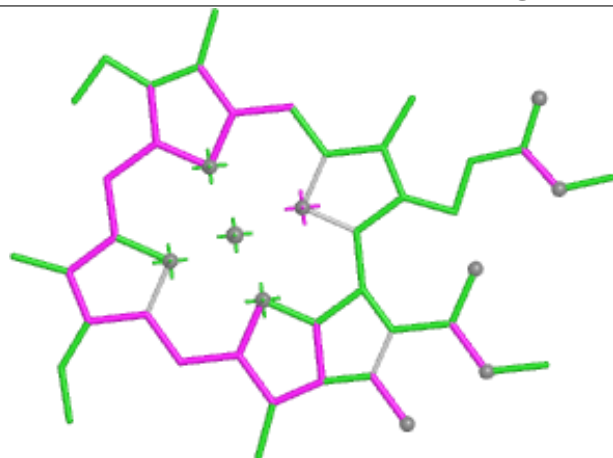
Torsions



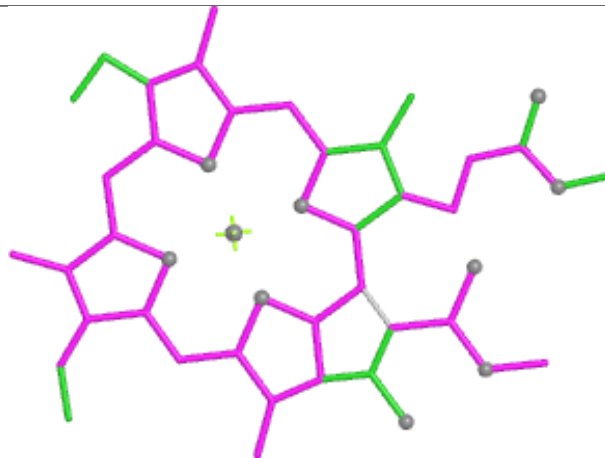
Rings



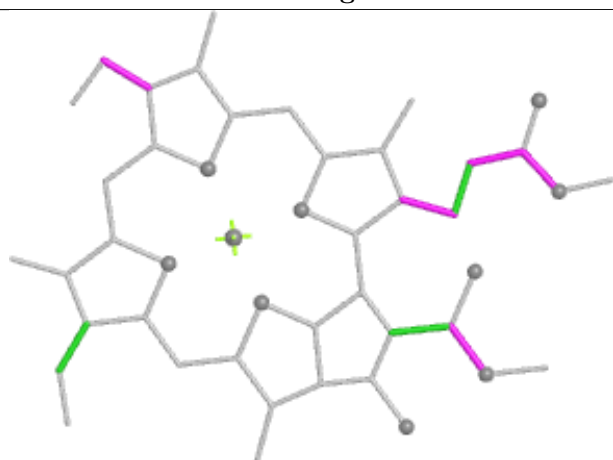
Ligand CLA Y 308



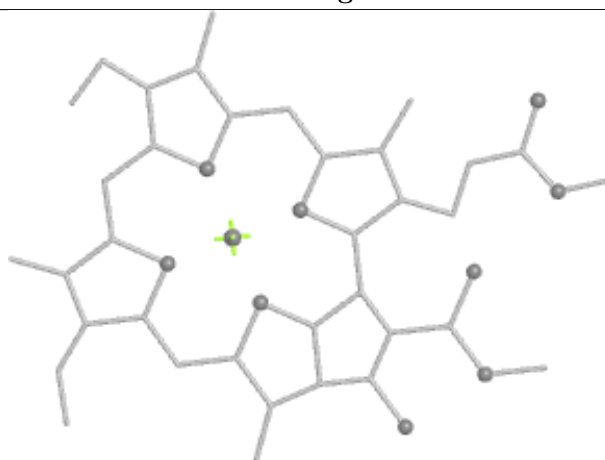
Bond lengths



Bond angles

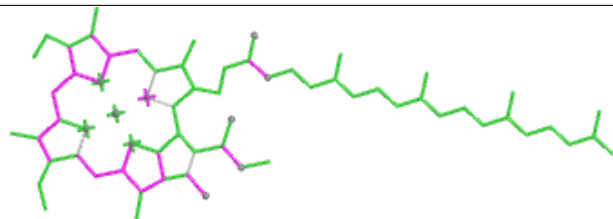


Torsions

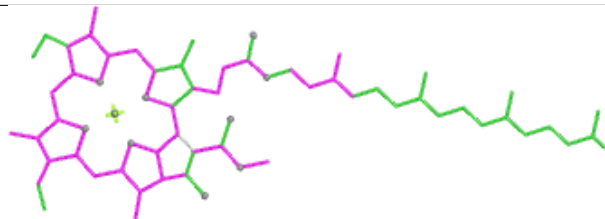


Rings

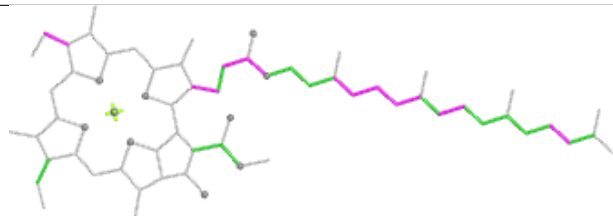
Ligand CLA 3 312



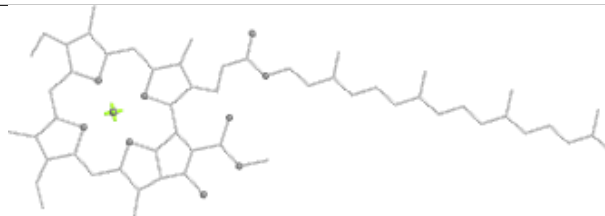
Bond lengths



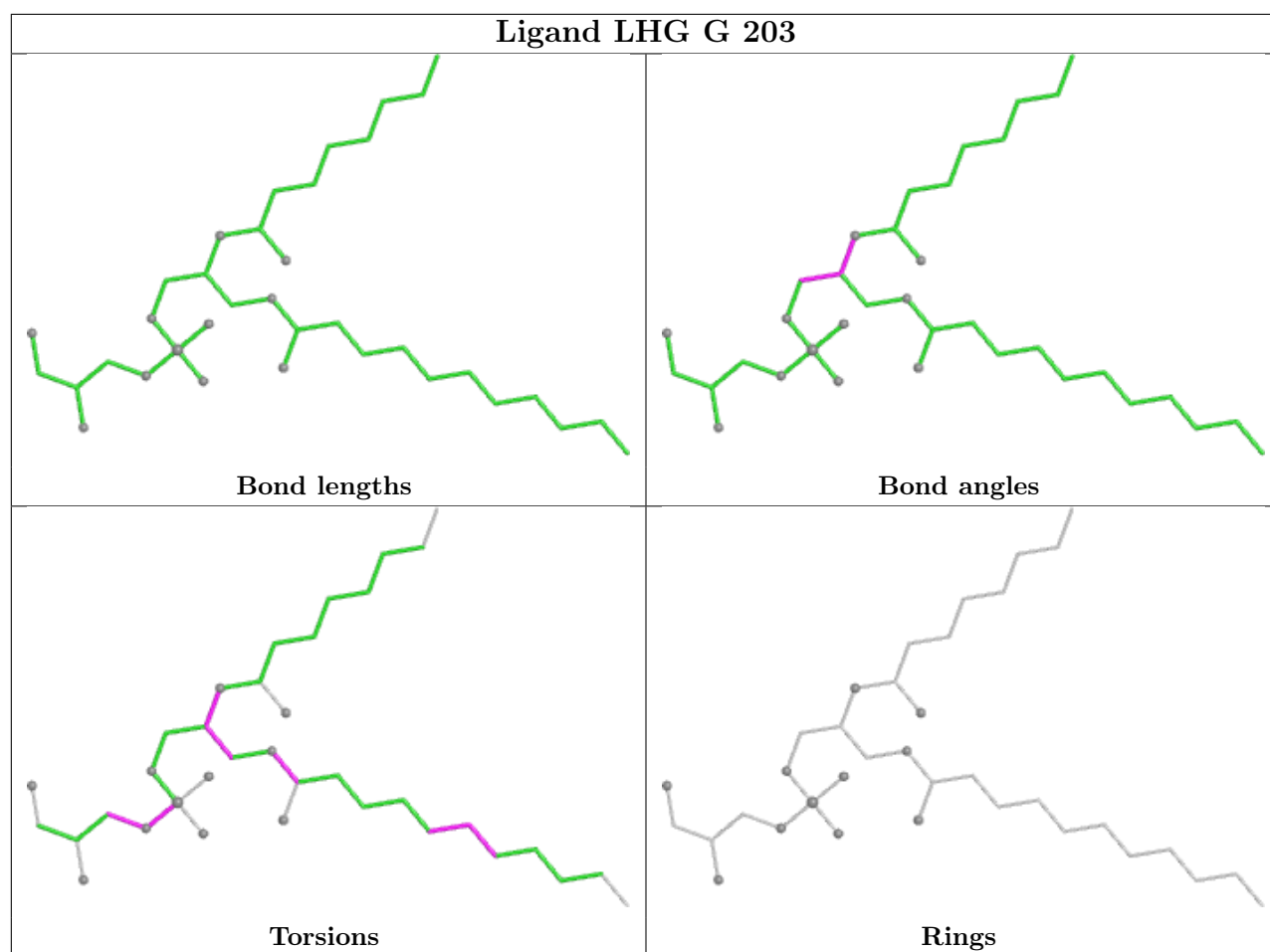
Bond angles

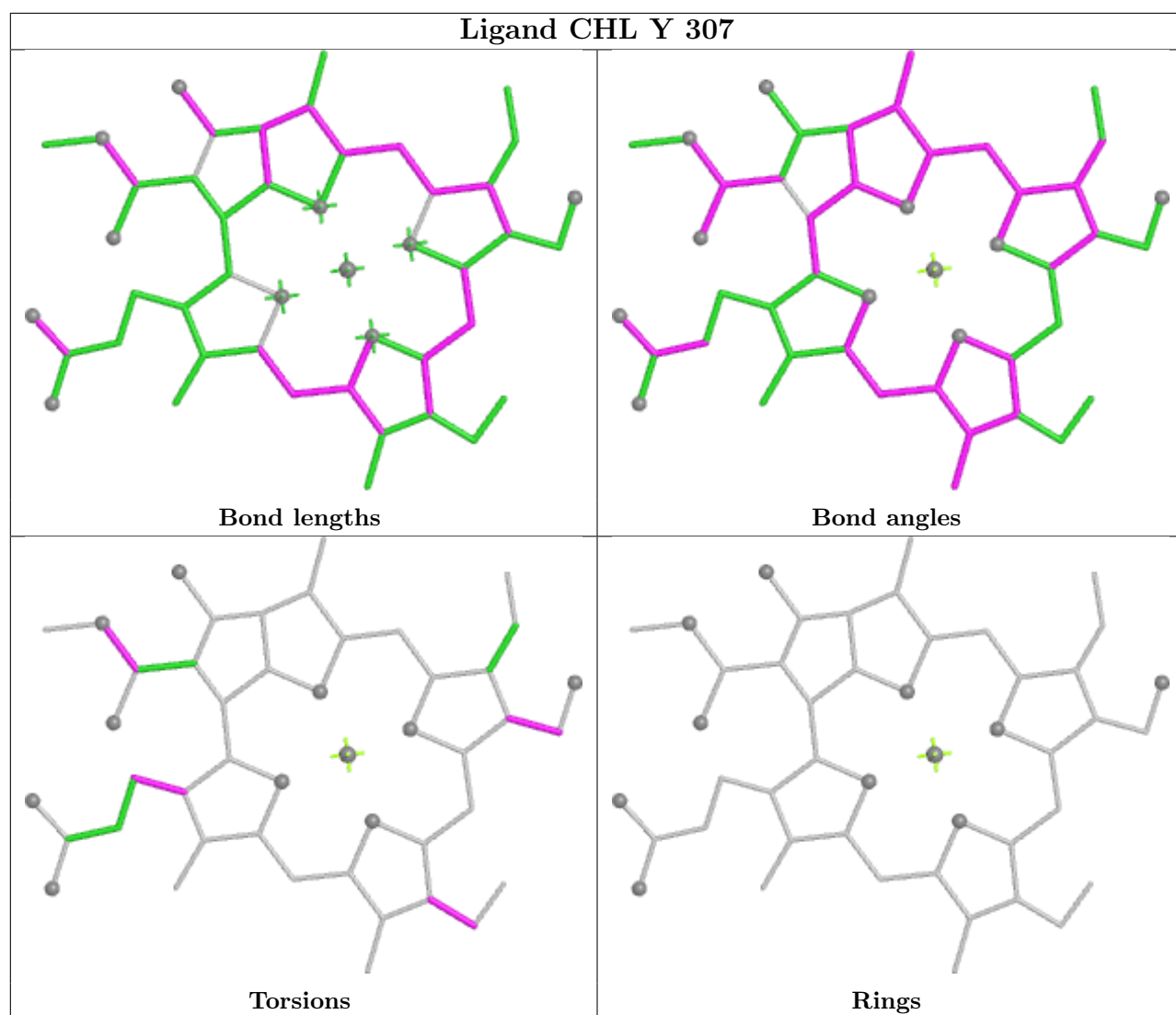


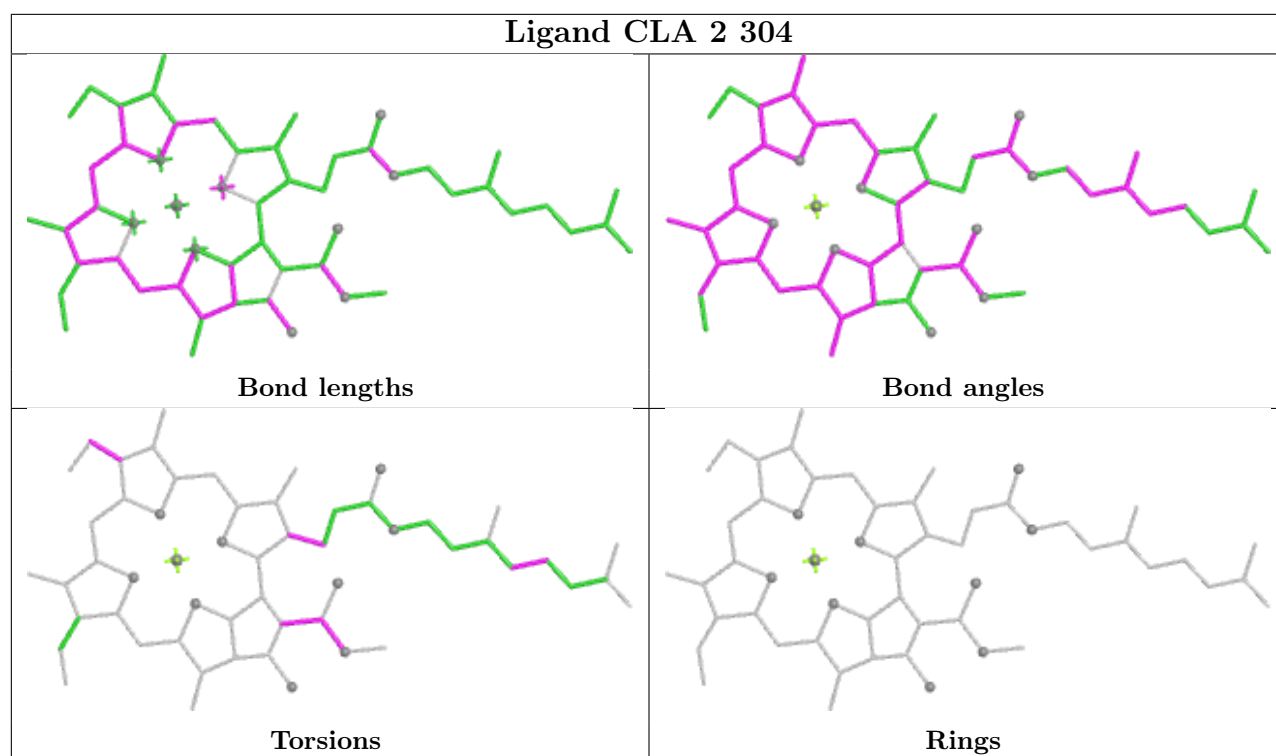
Torsions



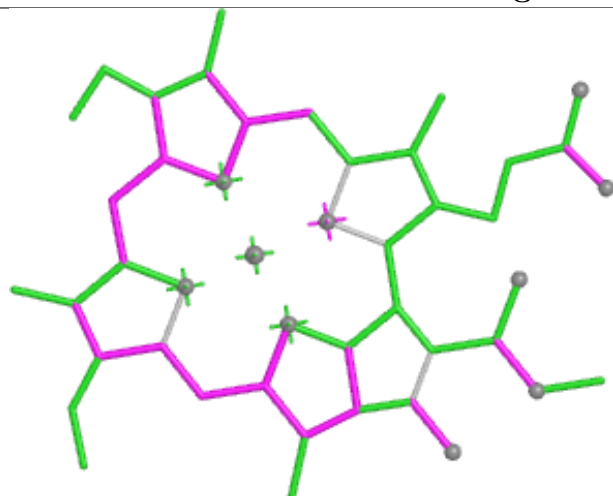
Rings



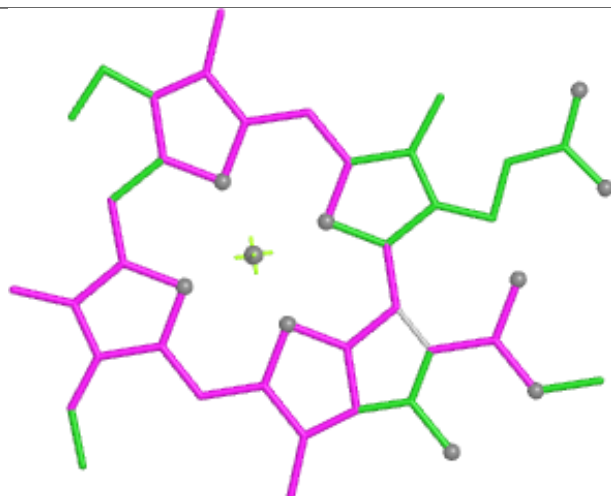




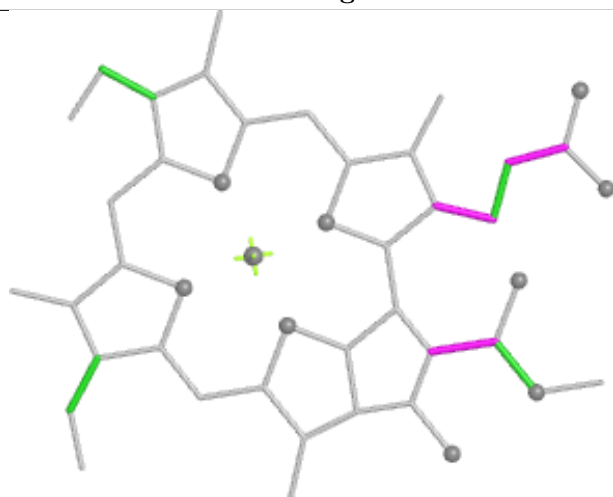
Ligand CLA A 839



Bond lengths



Bond angles

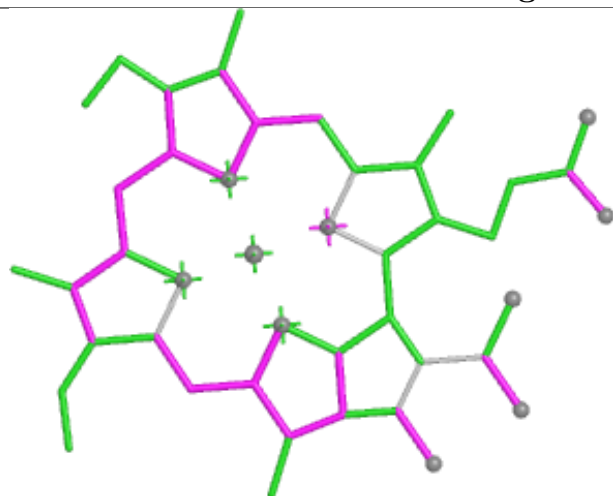


Torsions

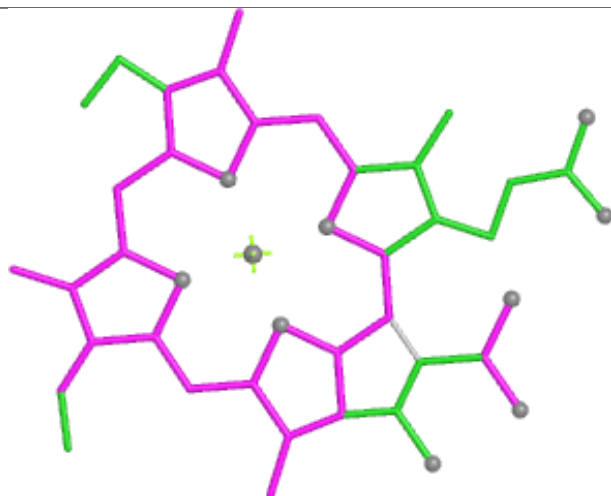


Rings

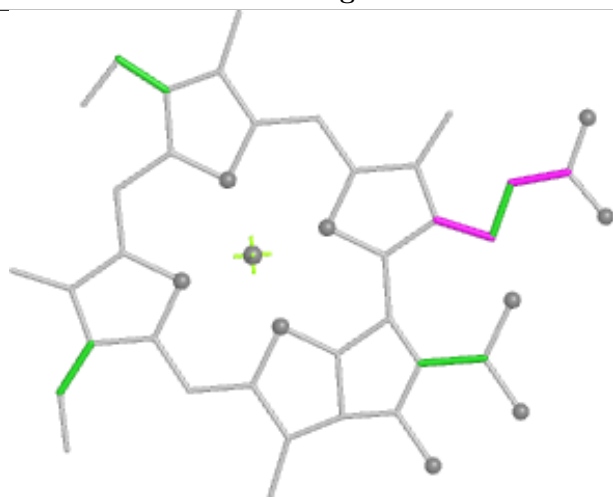
Ligand CLA 1 306



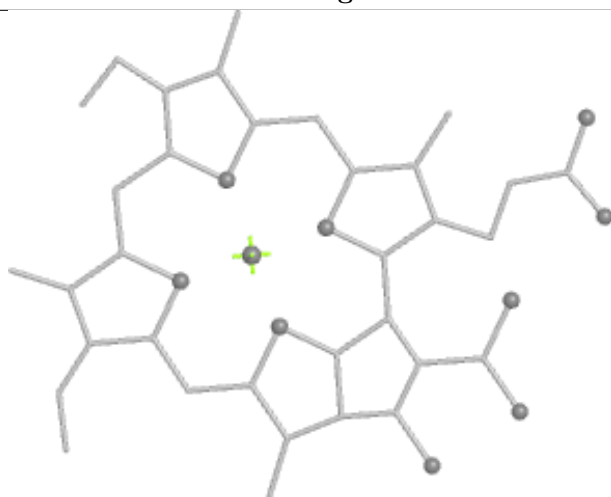
Bond lengths



Bond angles

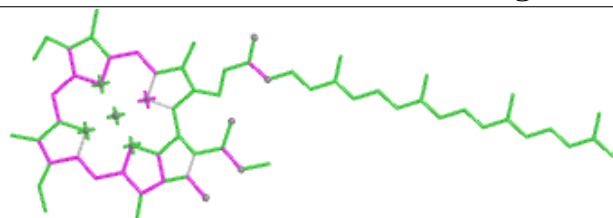


Torsions

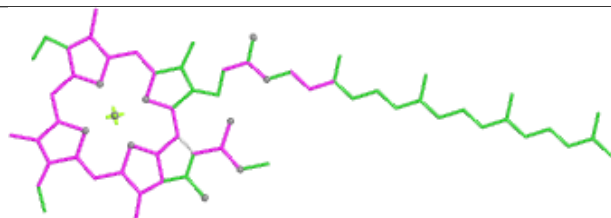


Rings

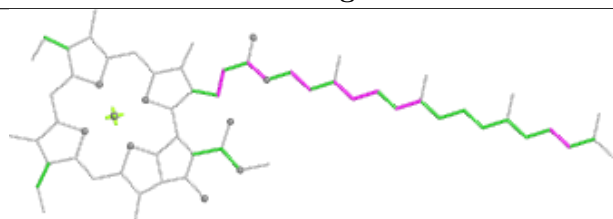
Ligand CLA A 844



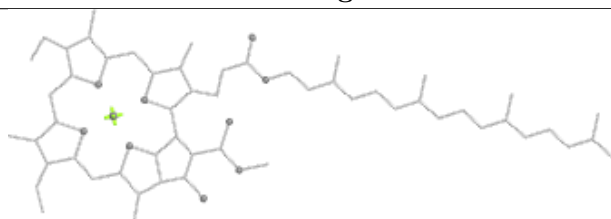
Bond lengths



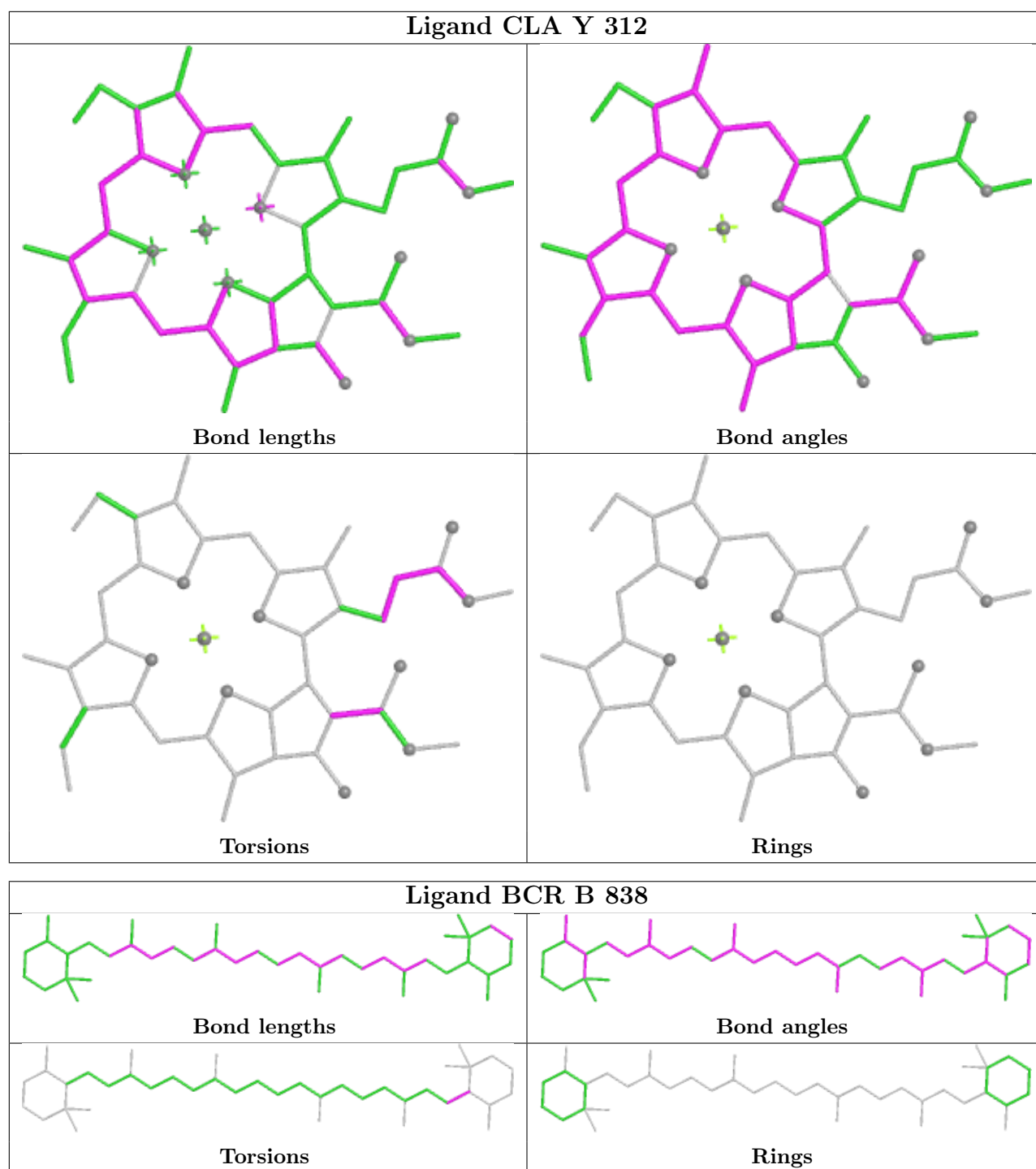
Bond angles



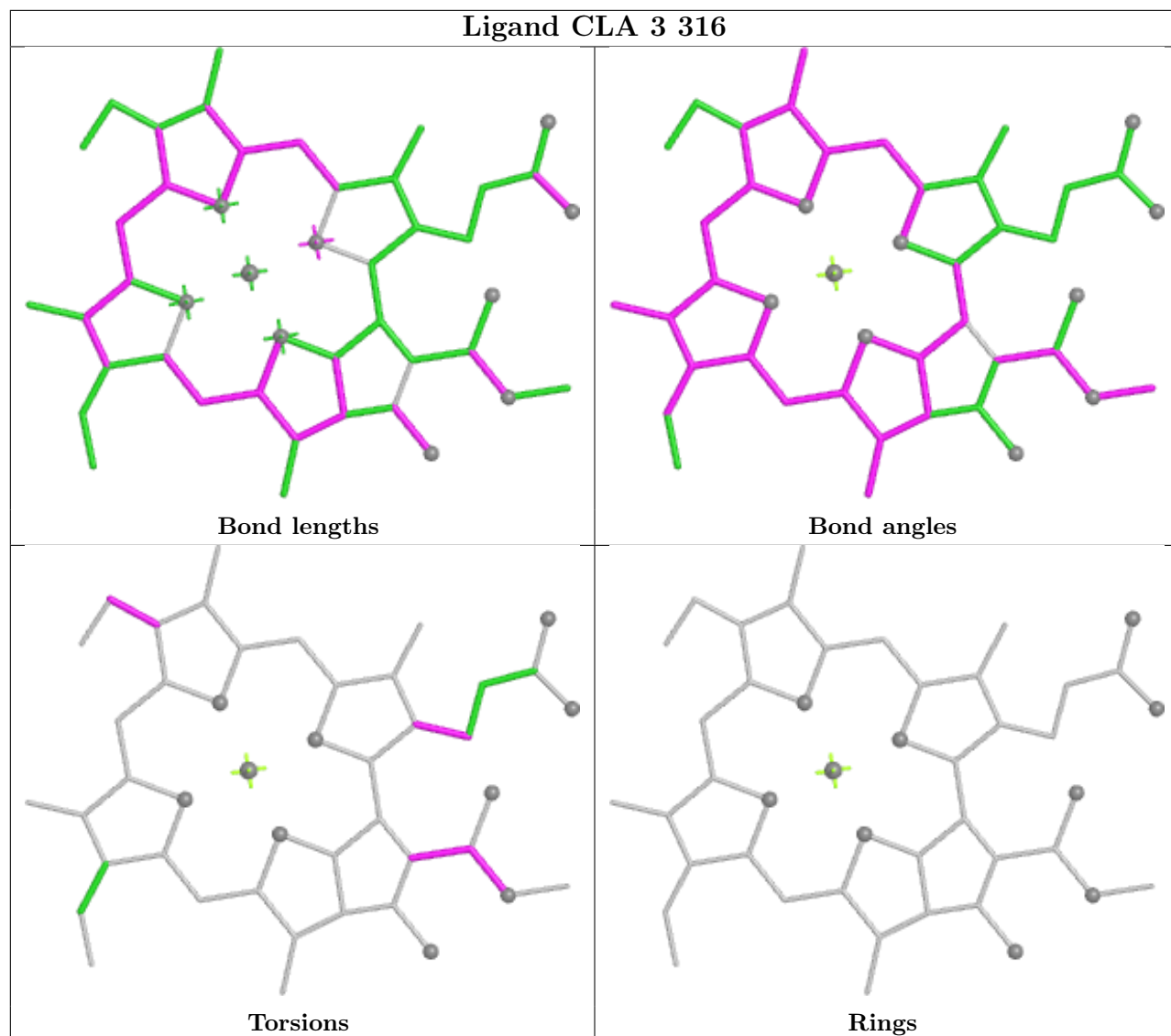
Torsions

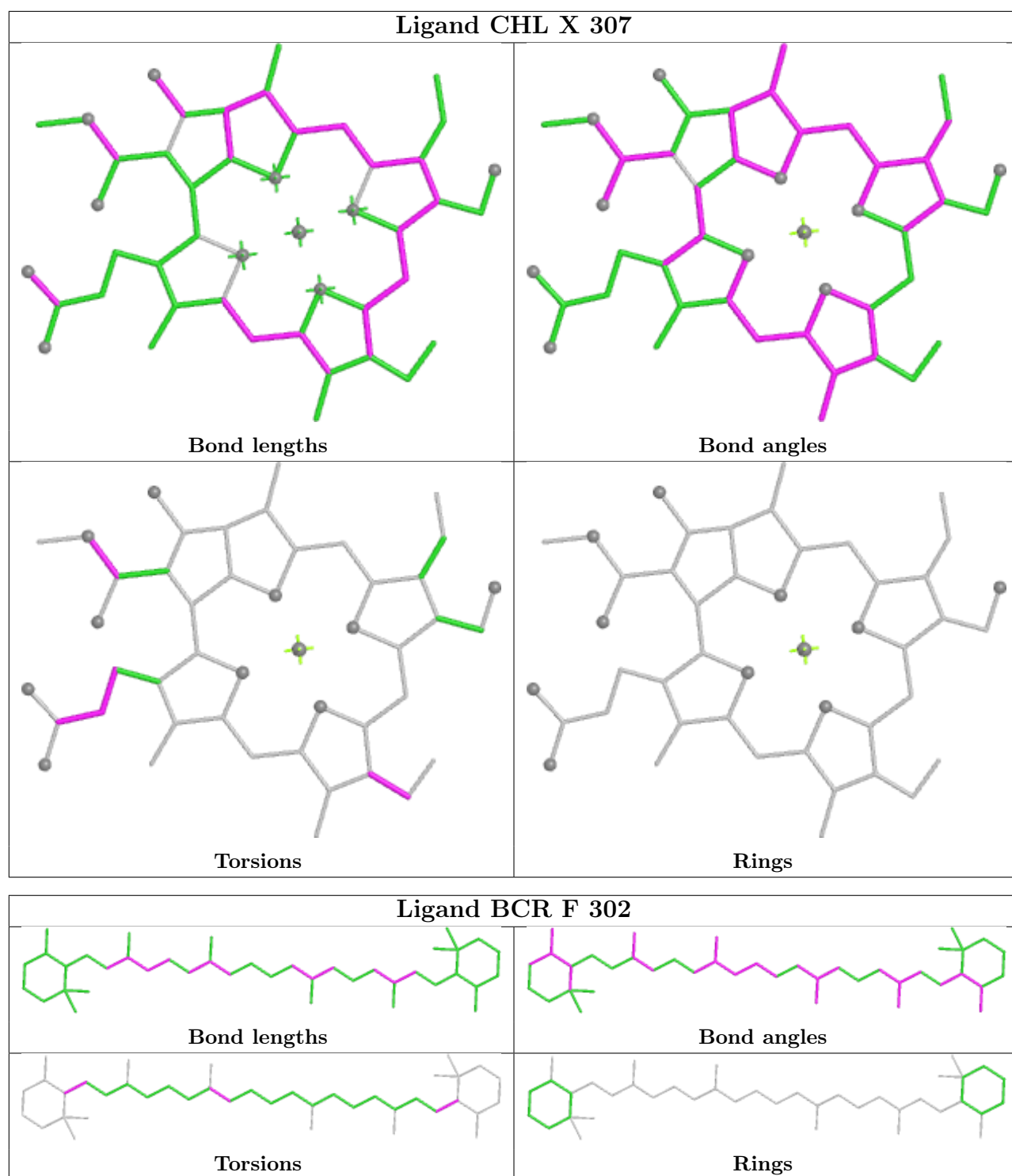


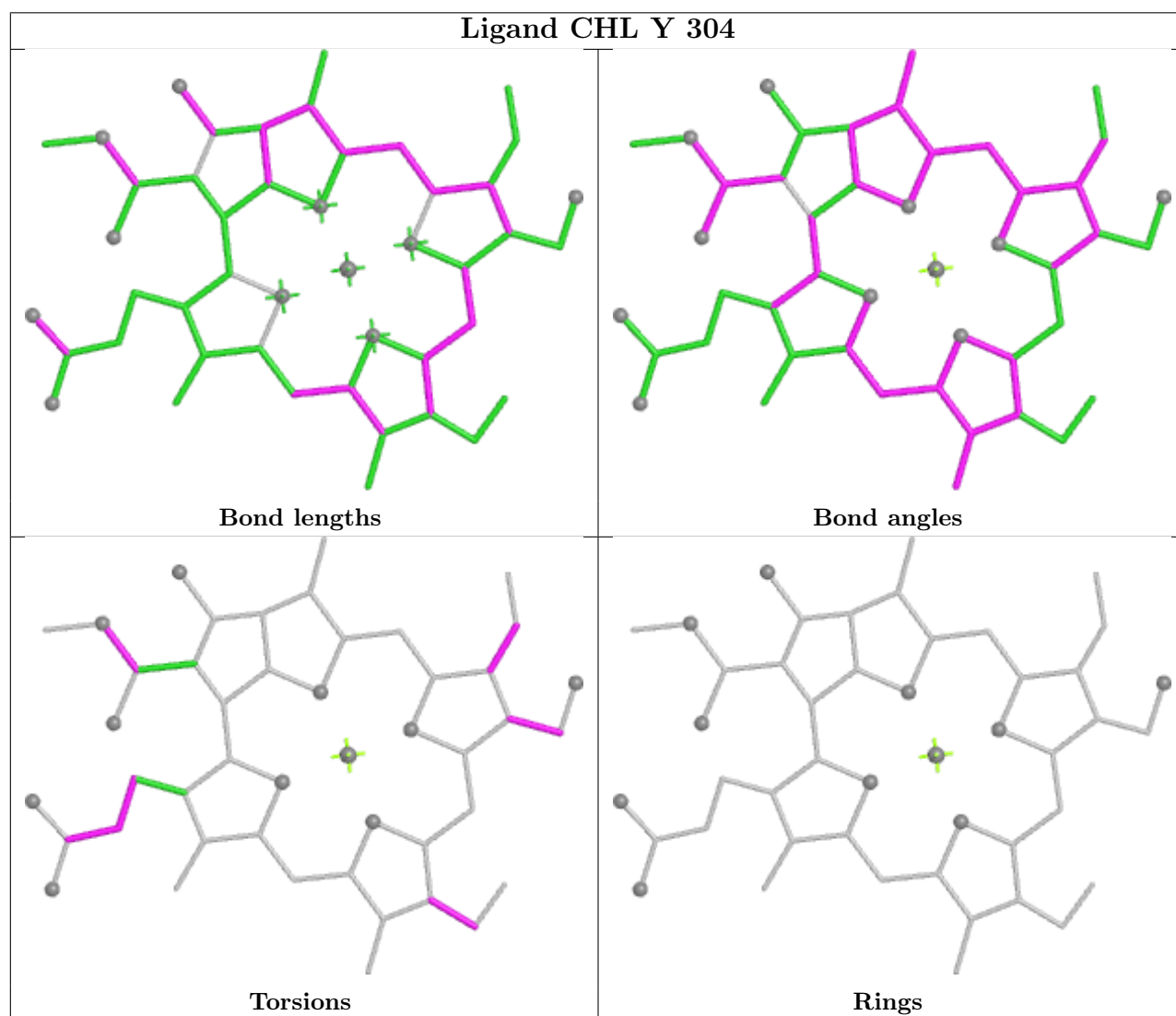
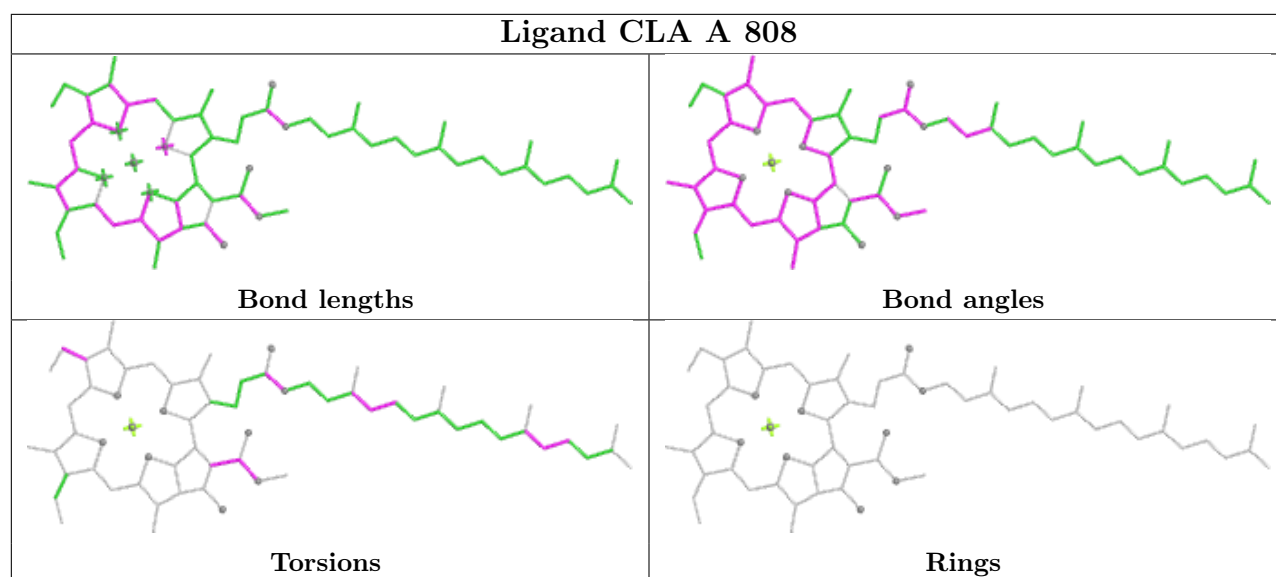
Rings

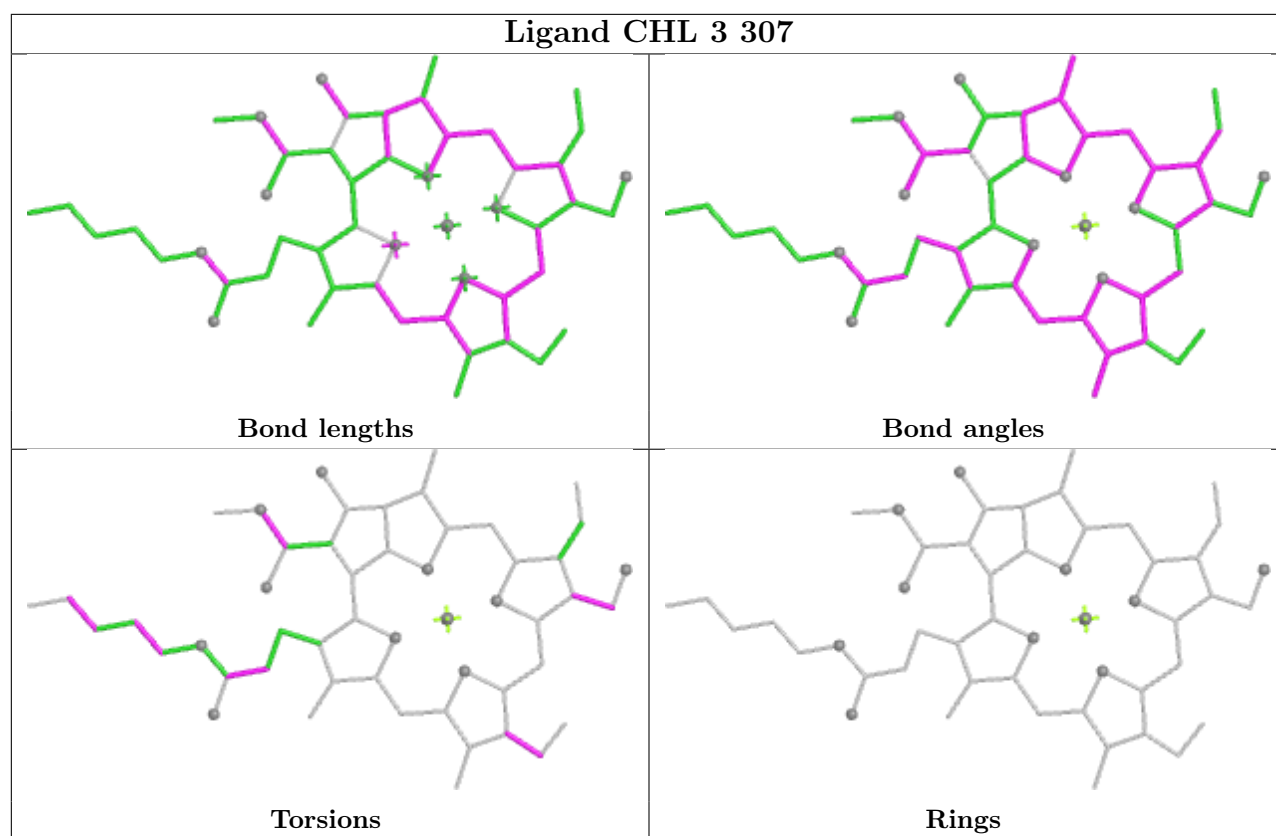


Ligand CLA 3 316

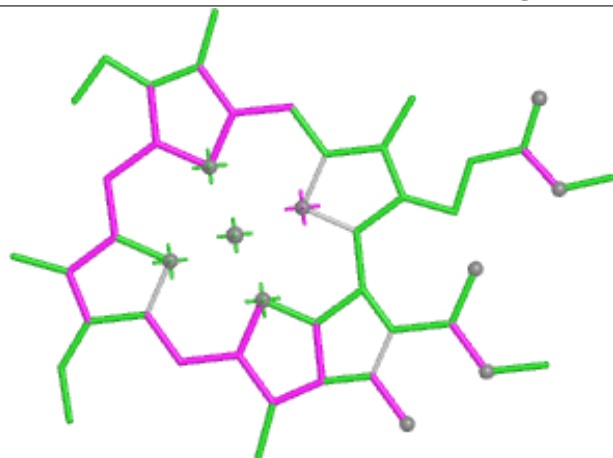




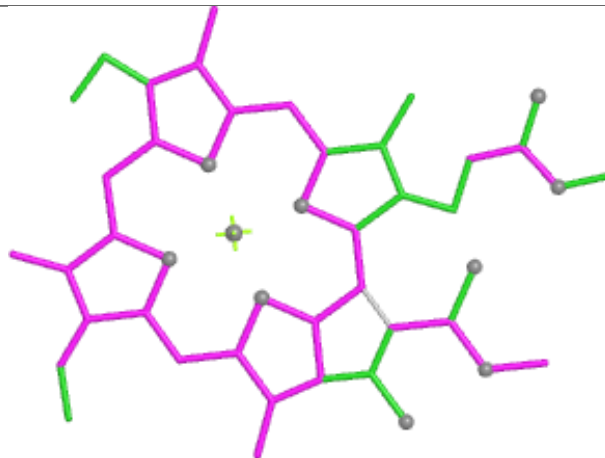




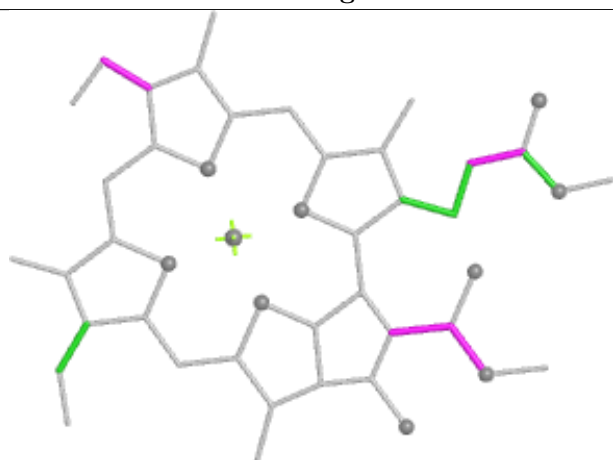
Ligand CLA F 306



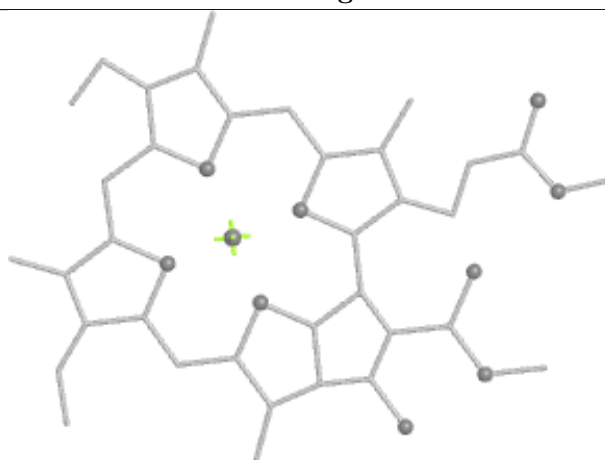
Bond lengths



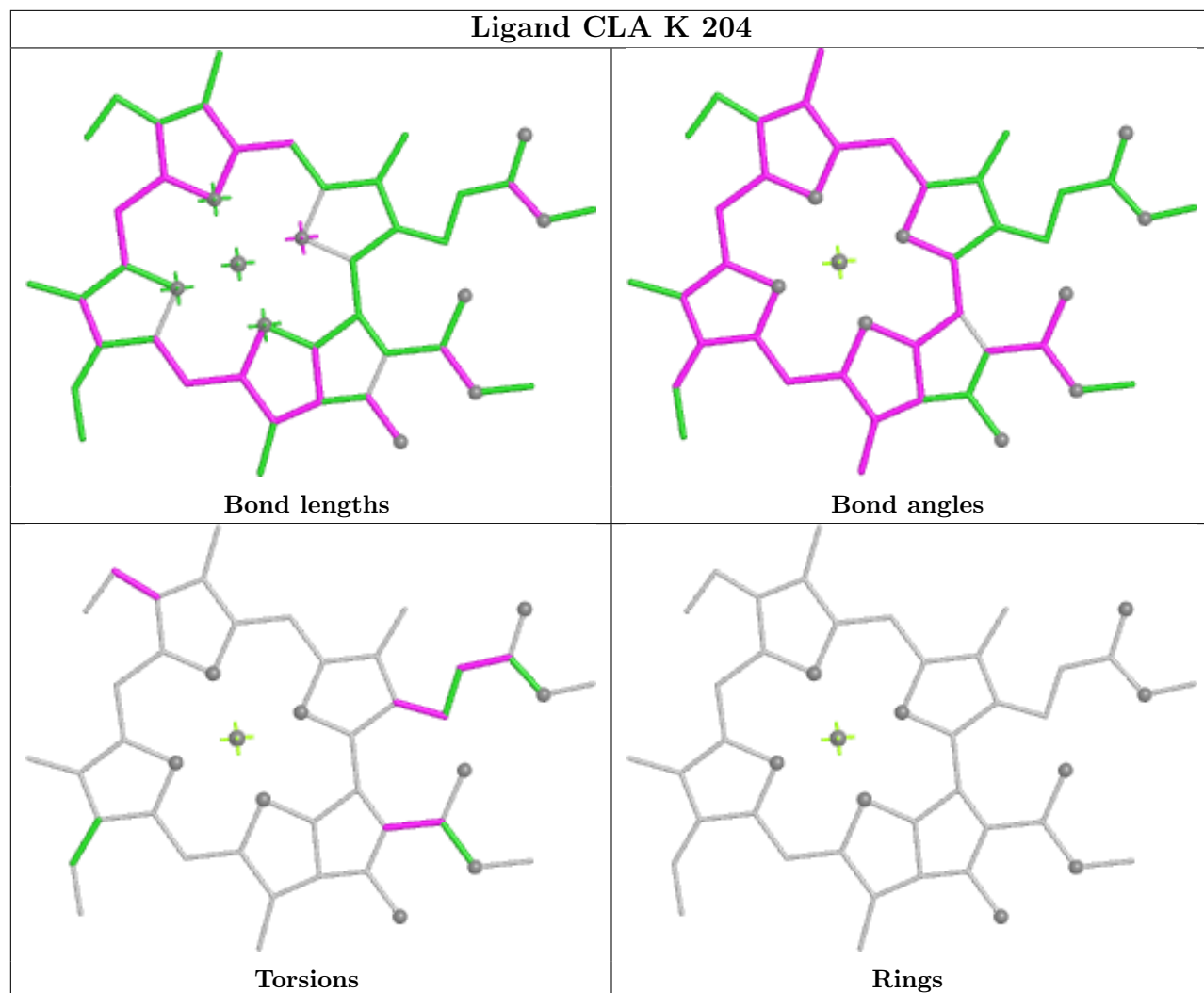
Bond angles



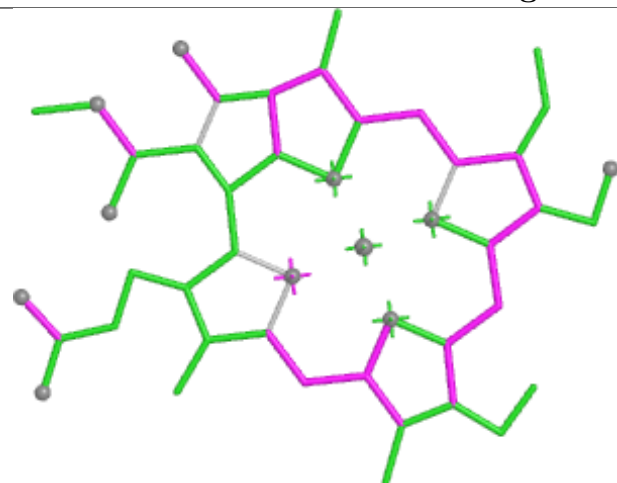
Torsions



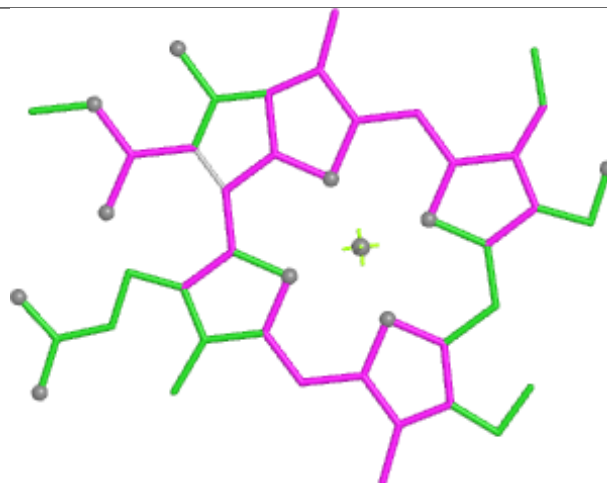
Rings



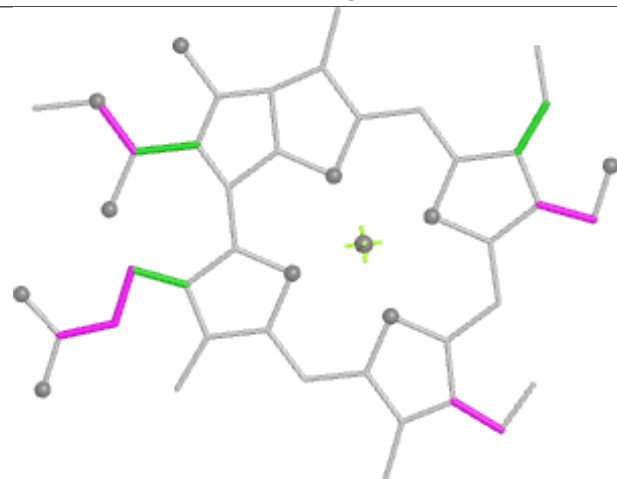
Ligand CHL Z 303



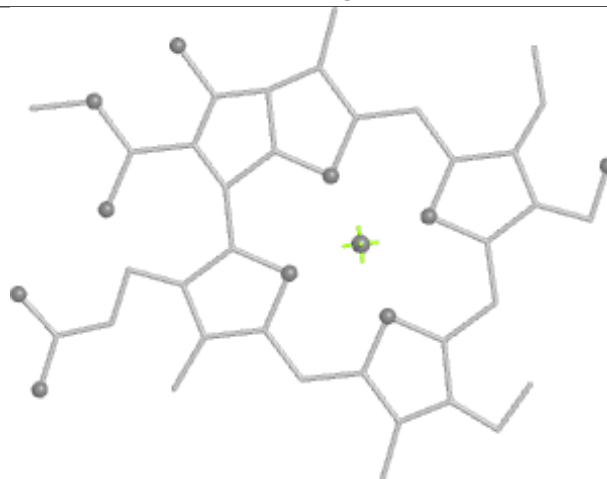
Bond lengths



Bond angles

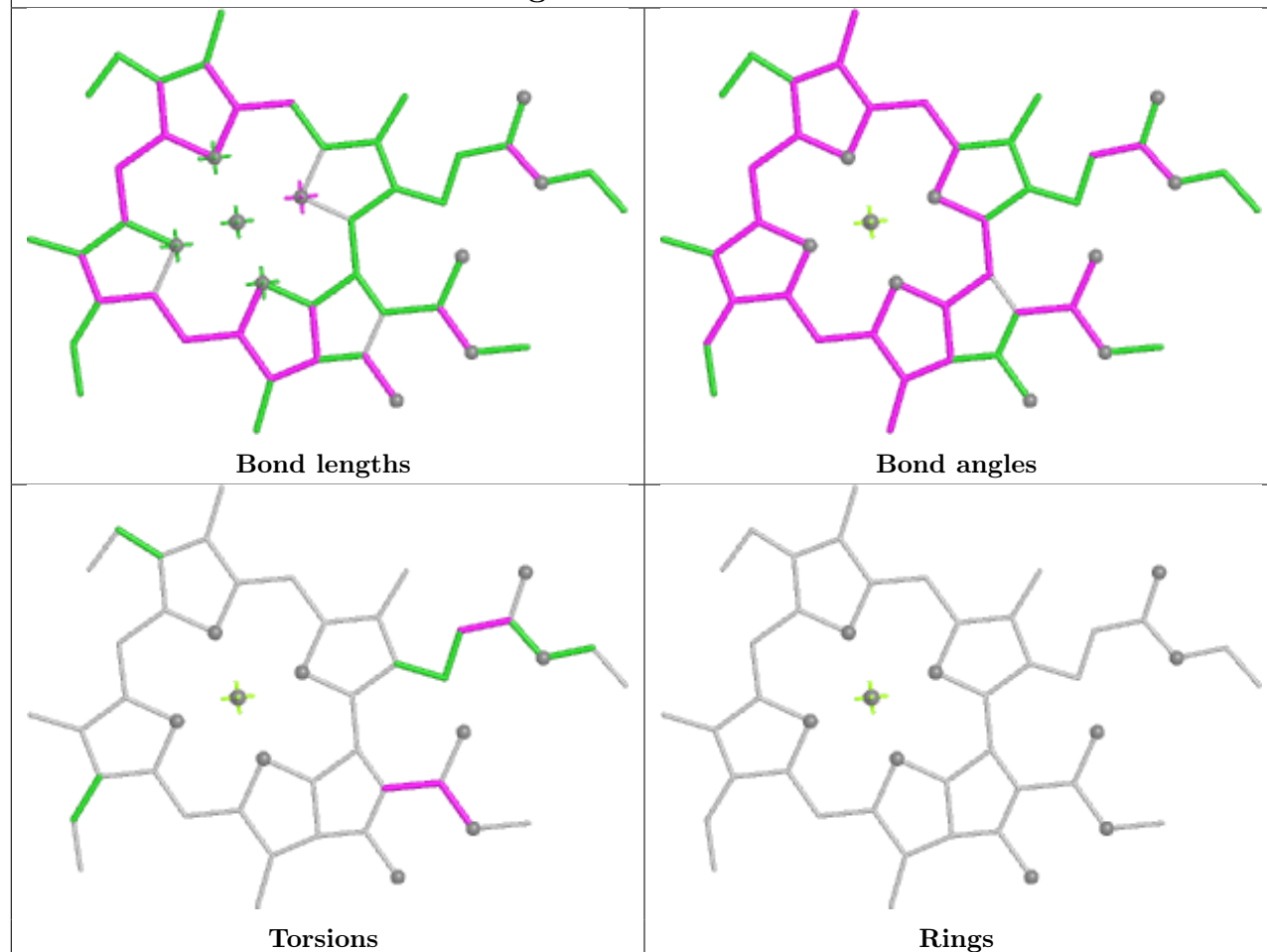


Torsions

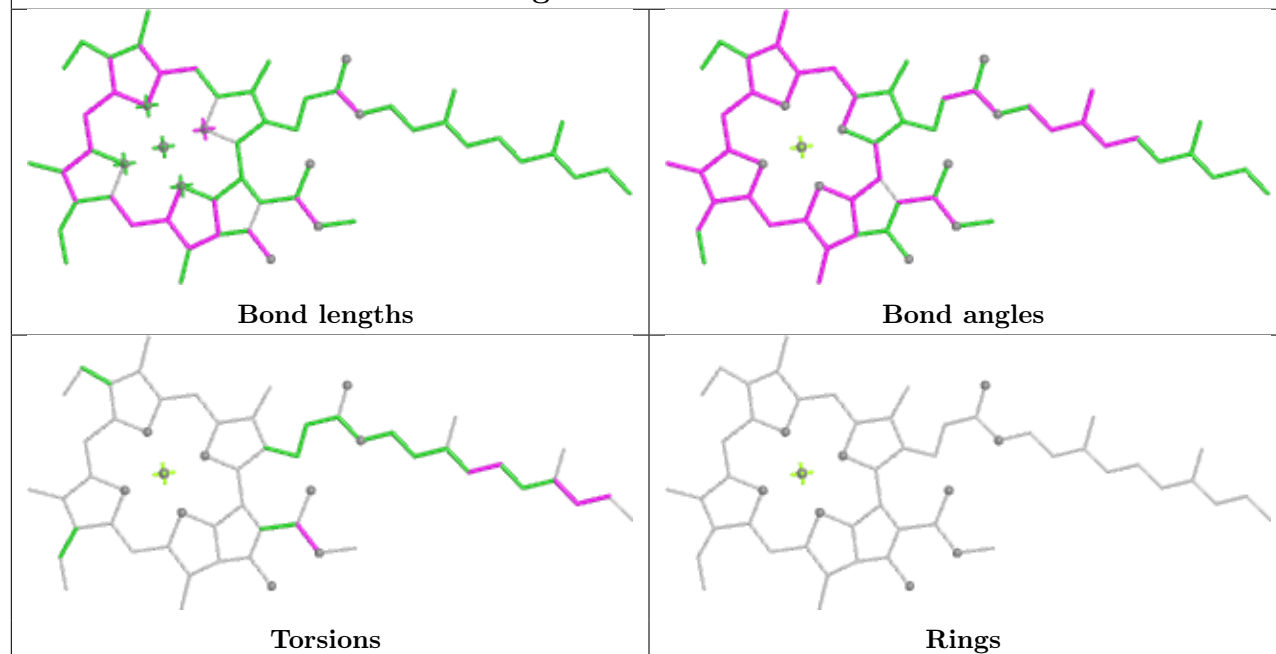


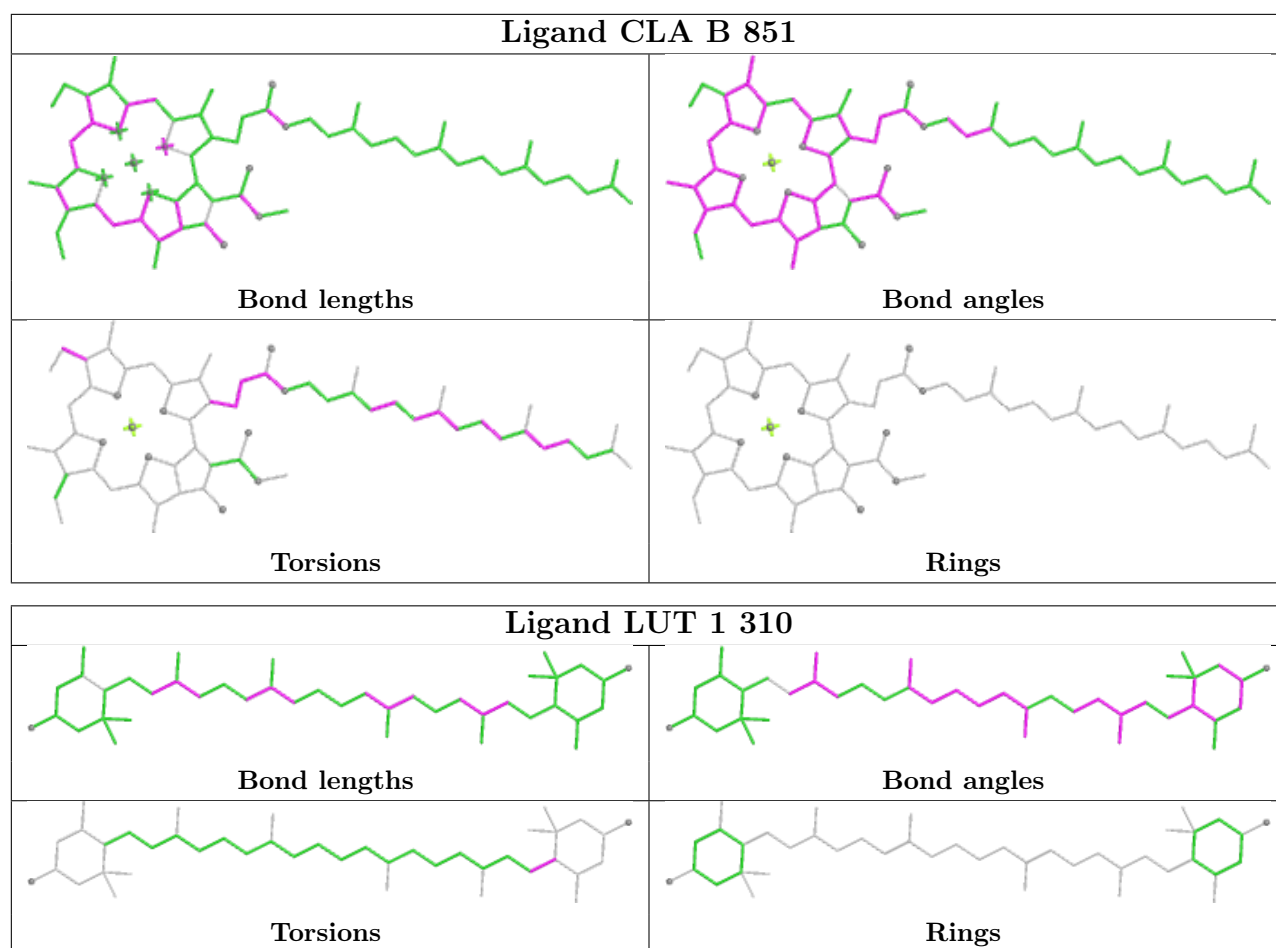
Rings

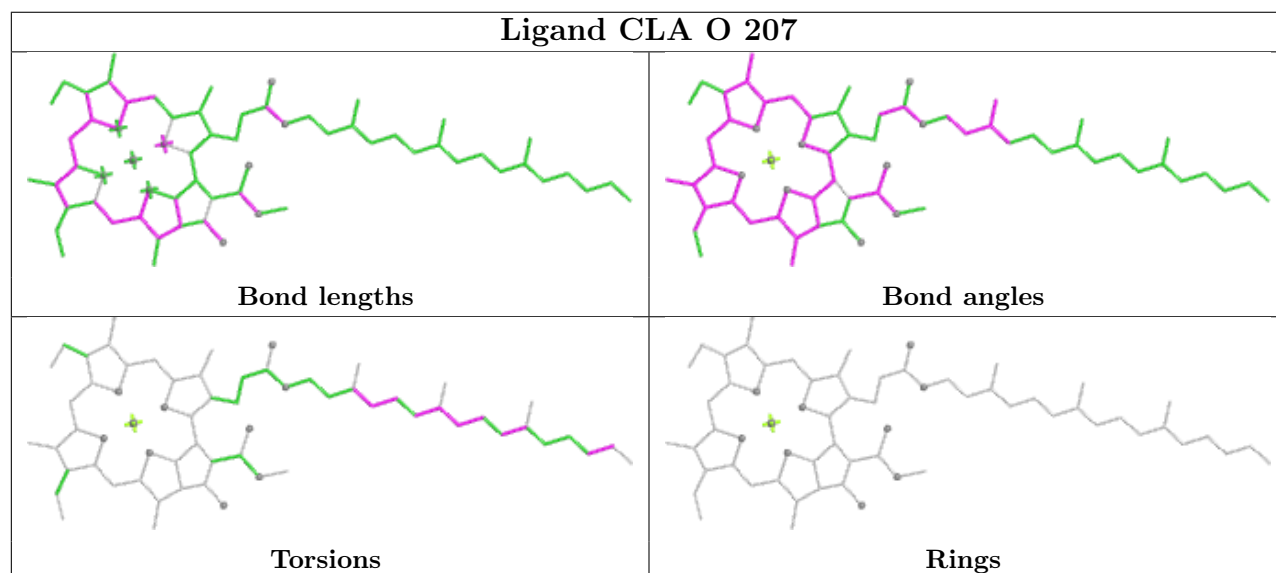
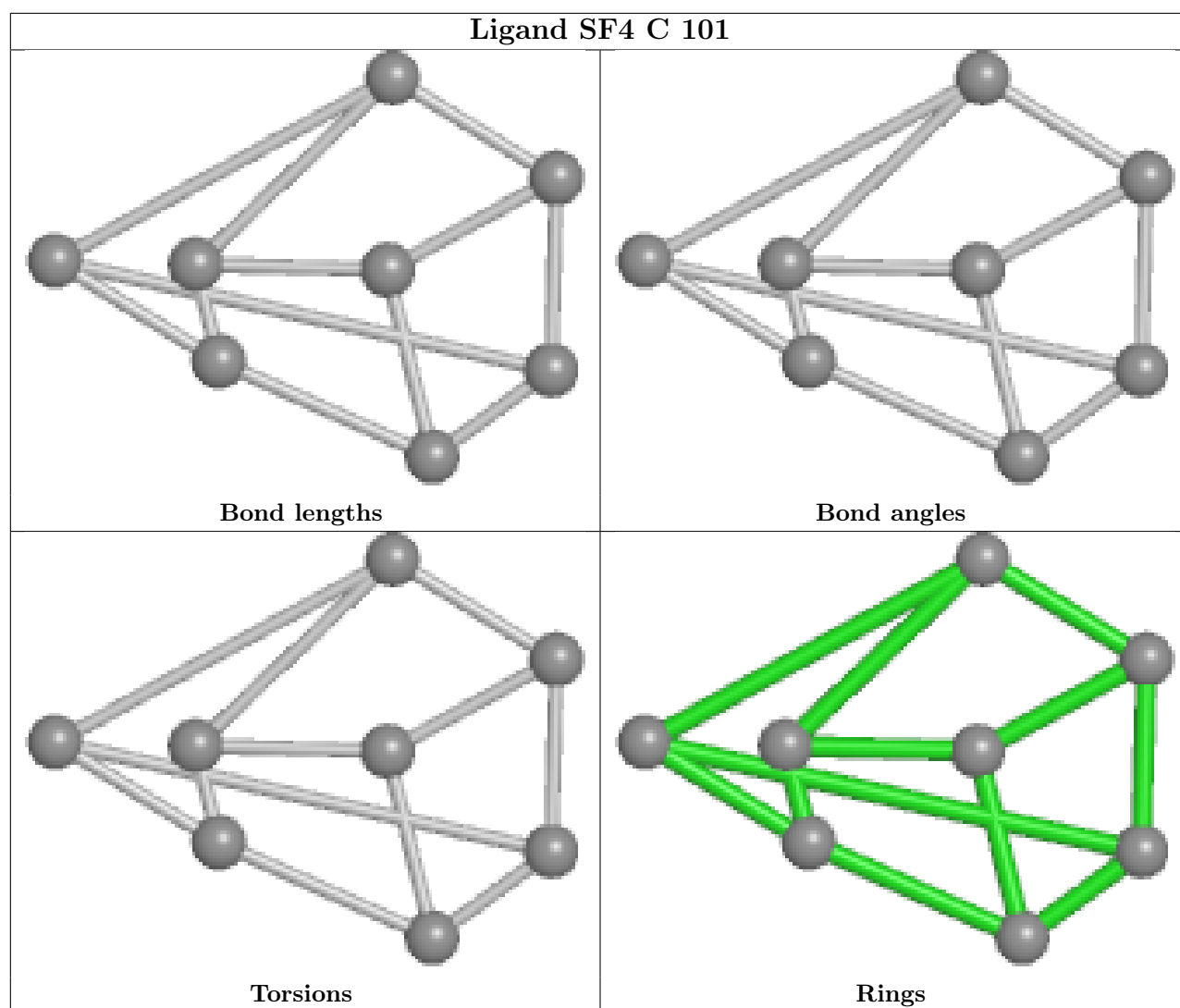
Ligand CLA B 828

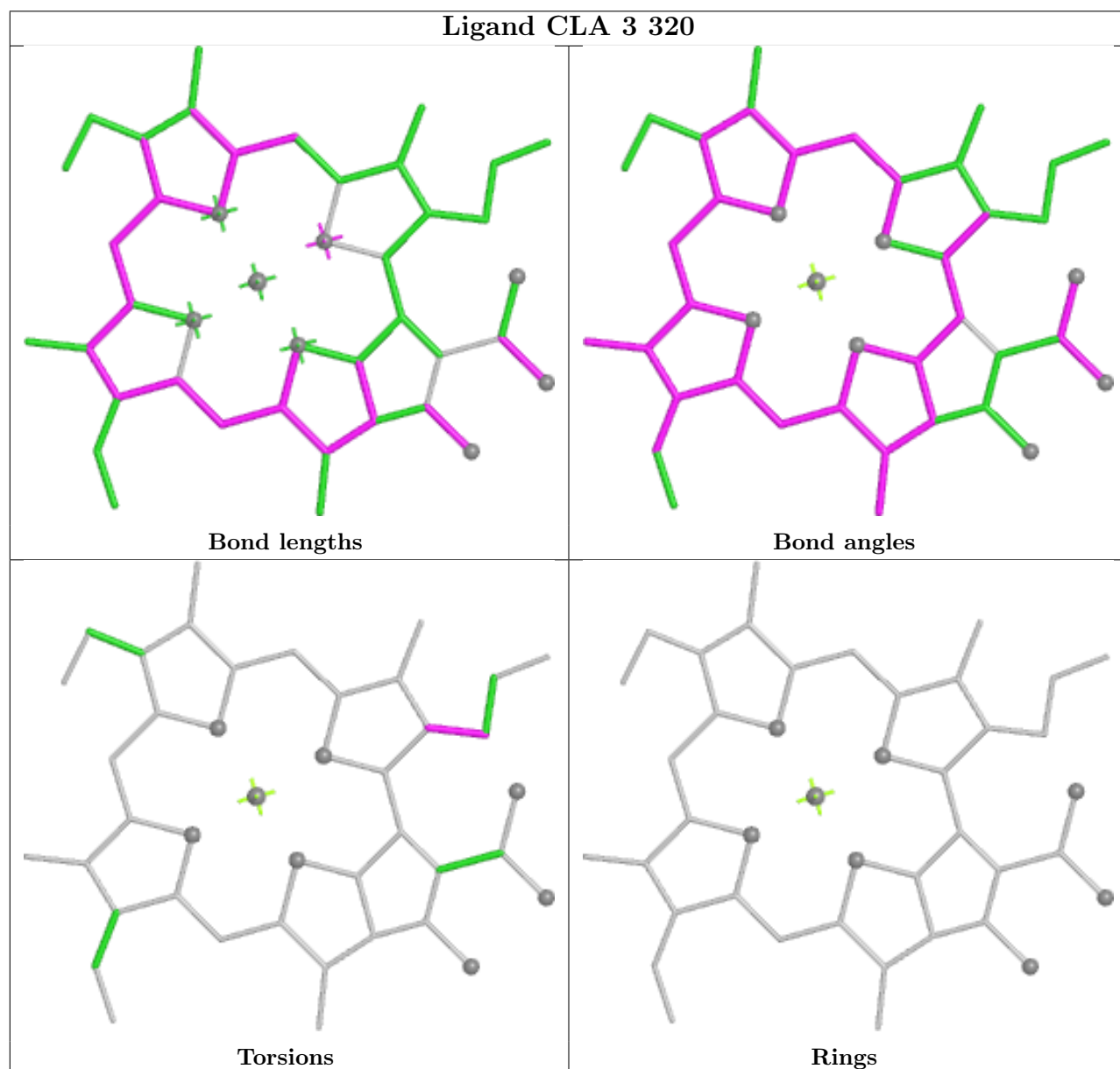
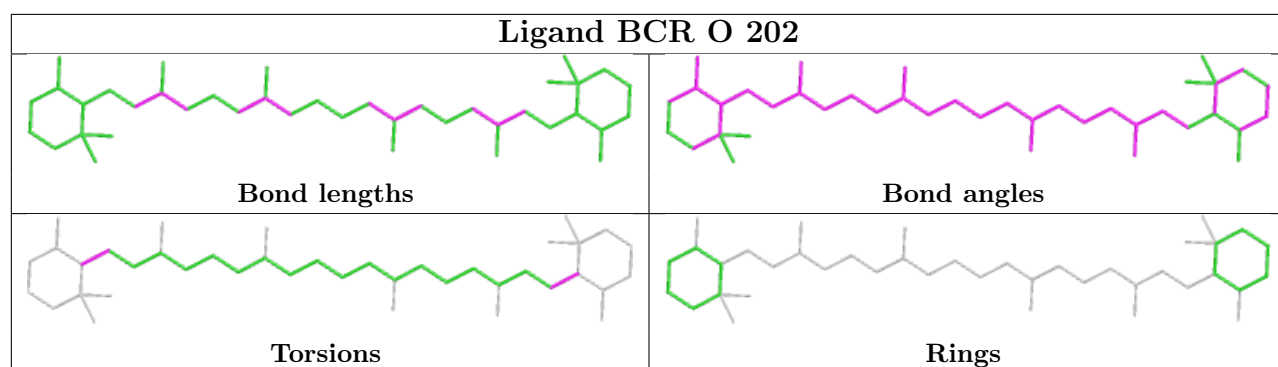


Ligand CLA B 848

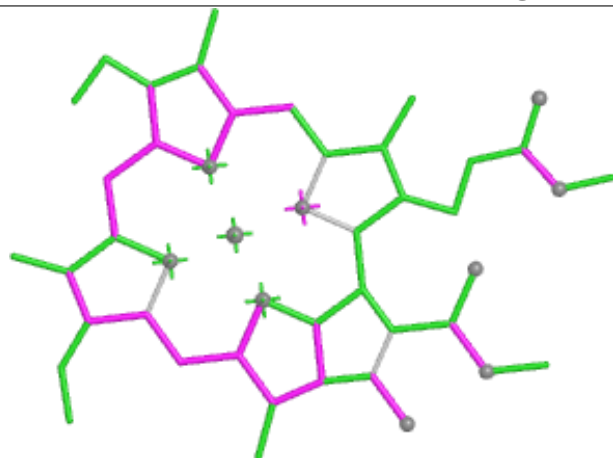




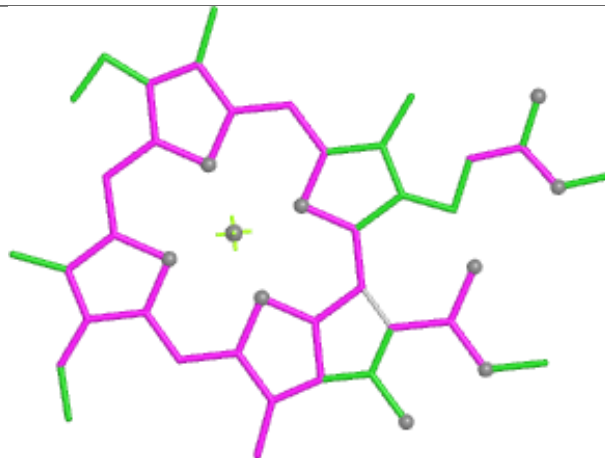




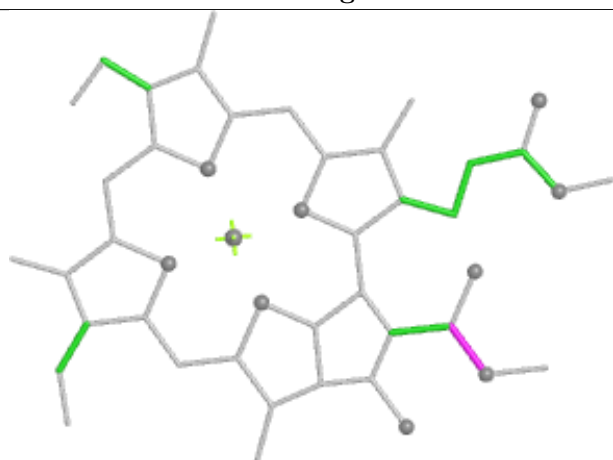
Ligand CLA A 841



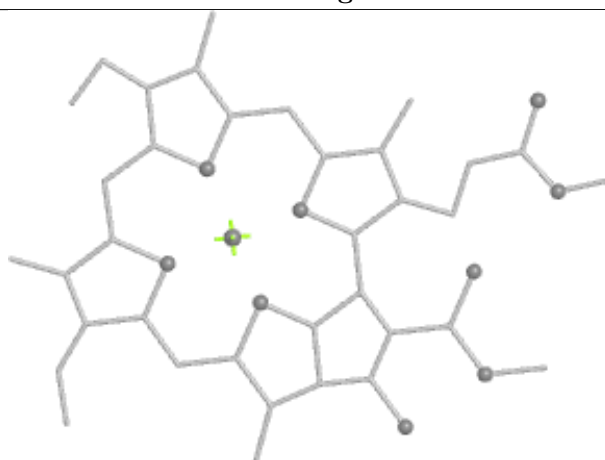
Bond lengths



Bond angles

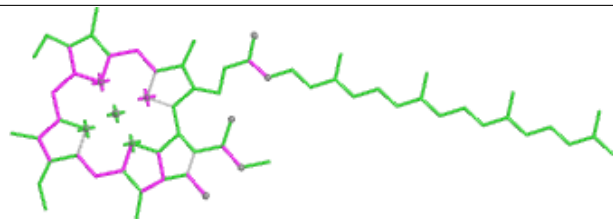


Torsions

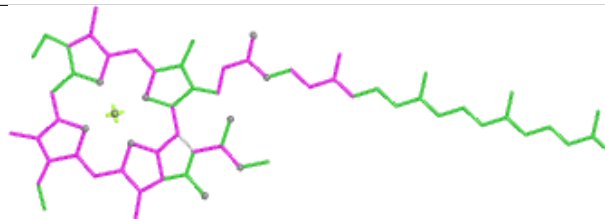


Rings

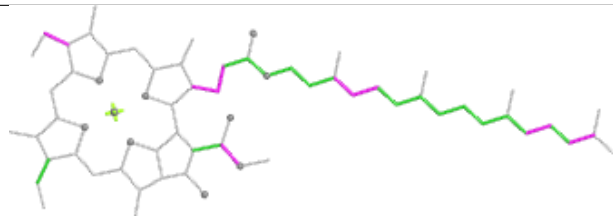
Ligand CLA A 827



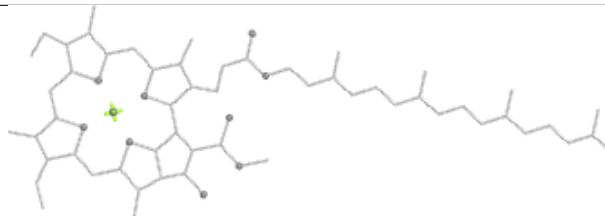
Bond lengths



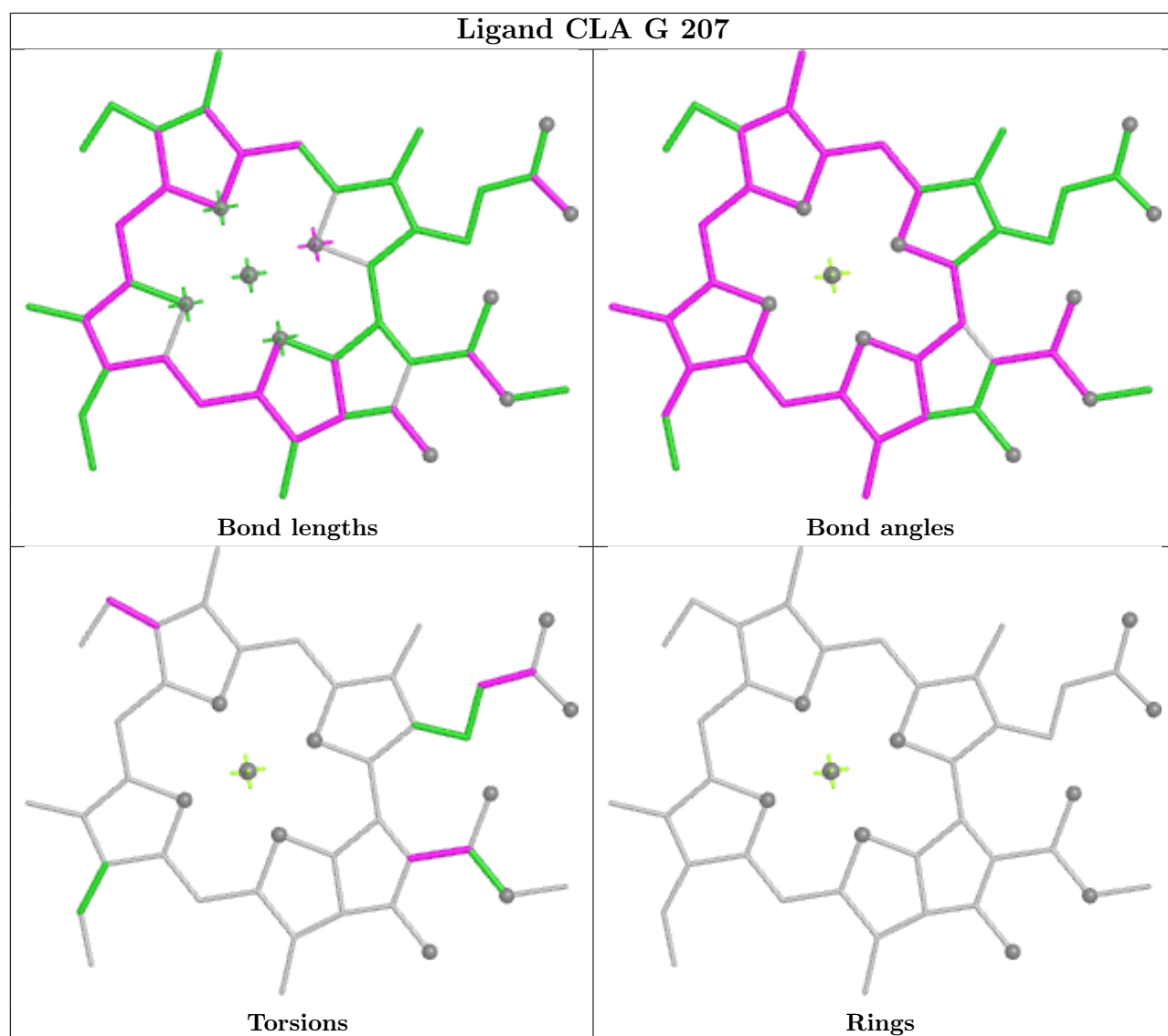
Bond angles

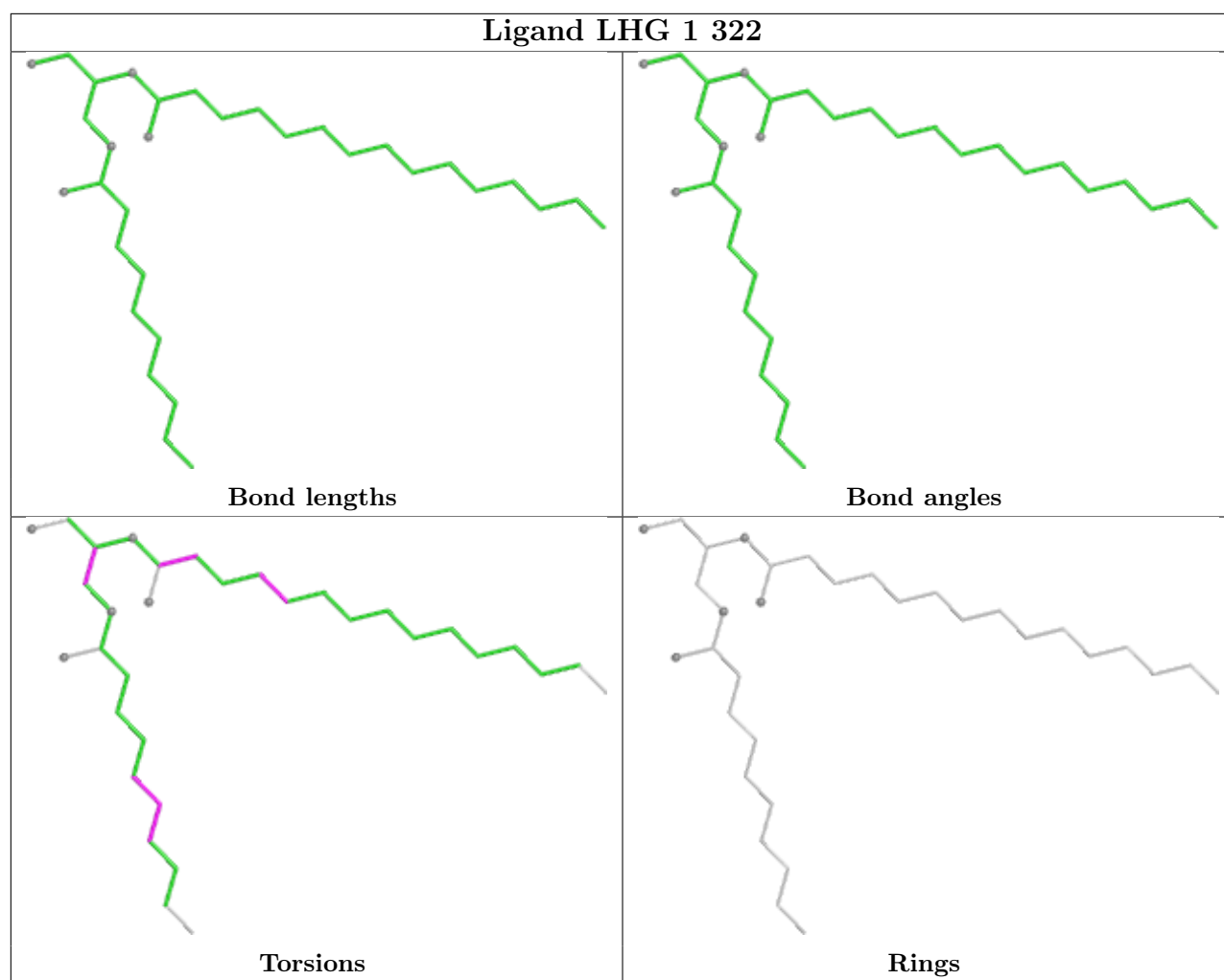


Torsions

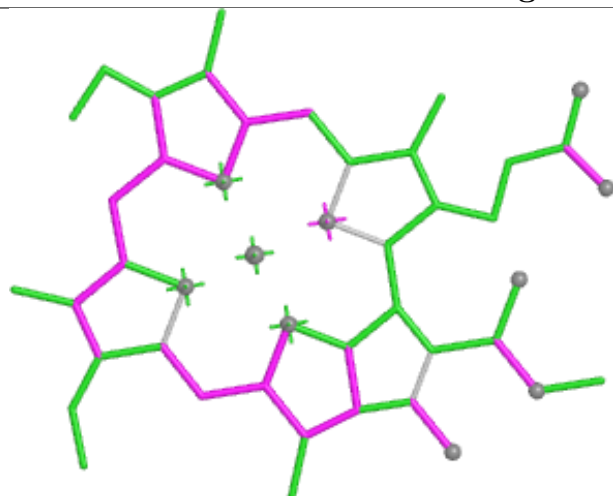


Rings

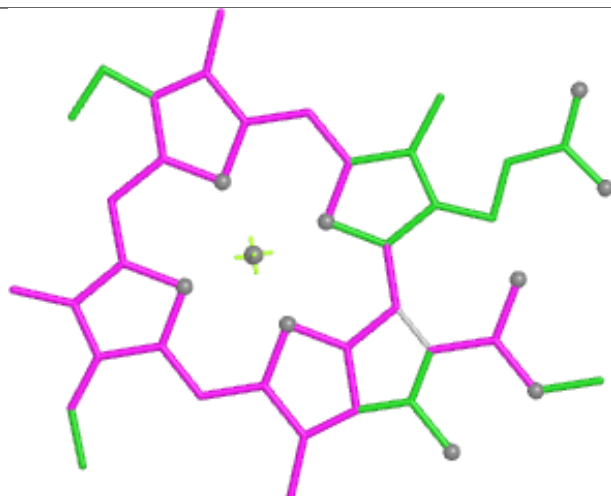




Ligand CLA 2 303



Bond lengths



Bond angles

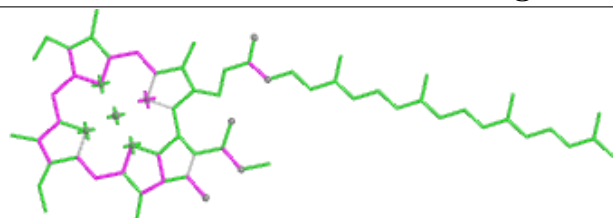


Torsions

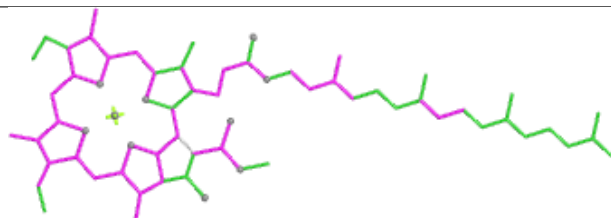


Rings

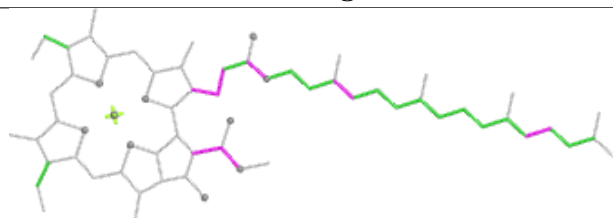
Ligand CLA A 854



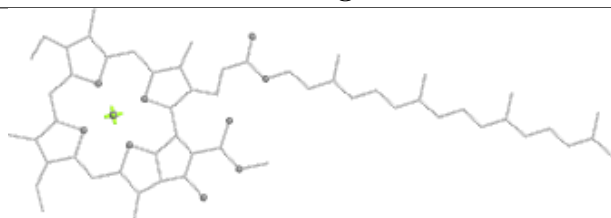
Bond lengths



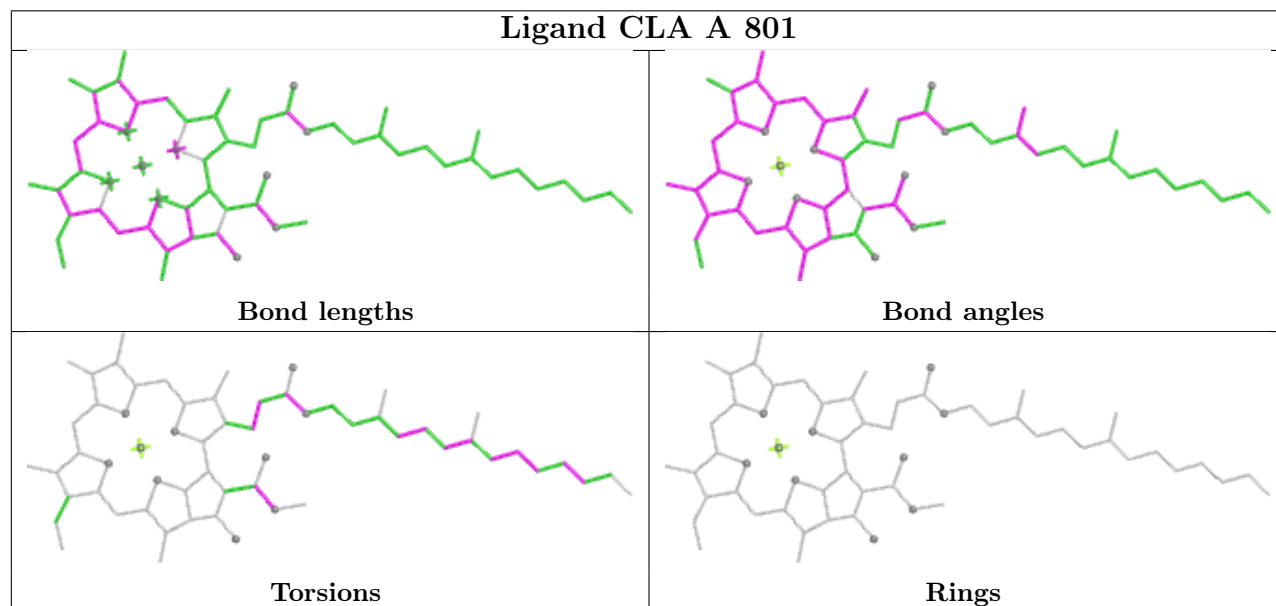
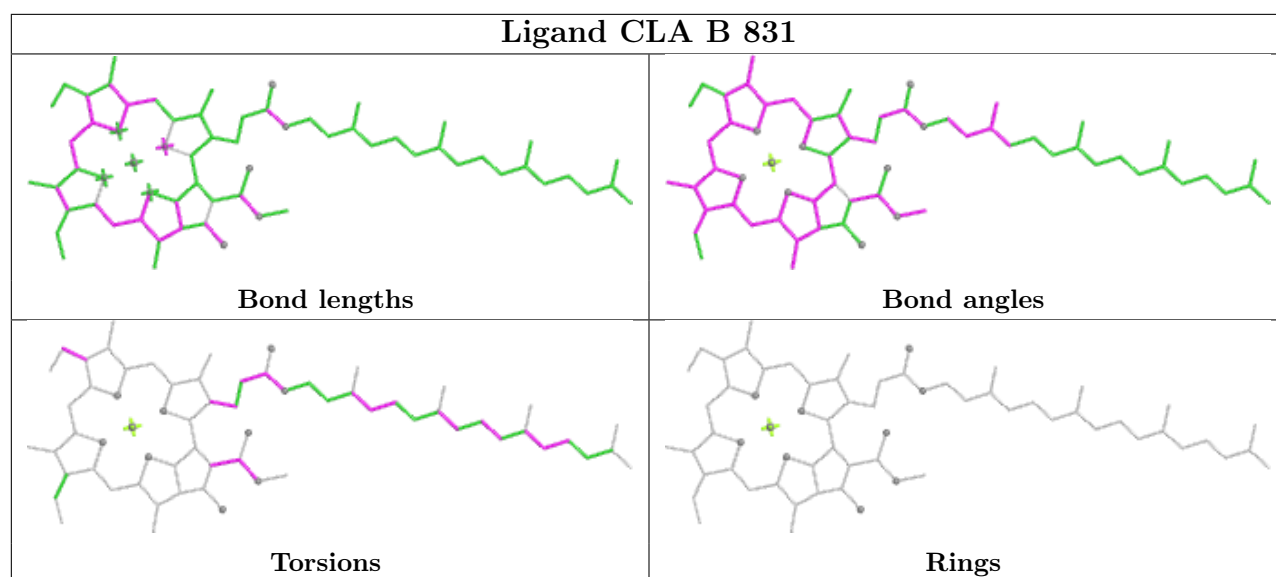
Bond angles



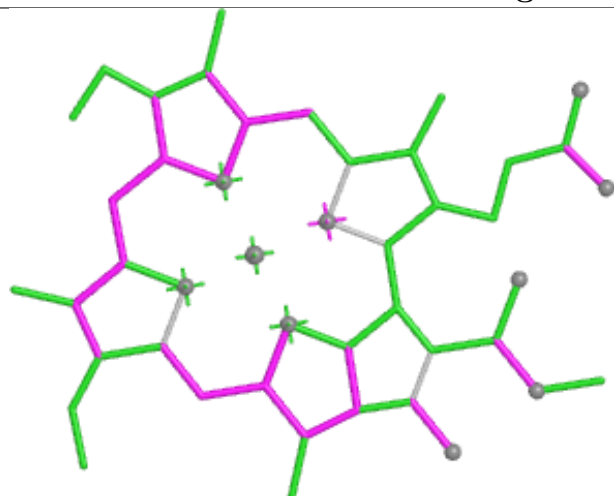
Torsions



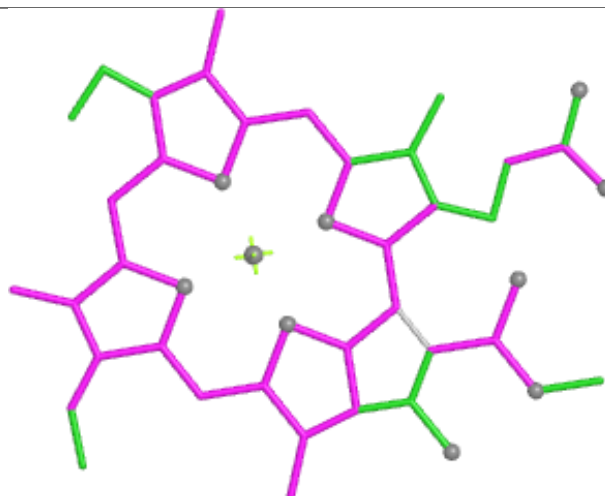
Rings



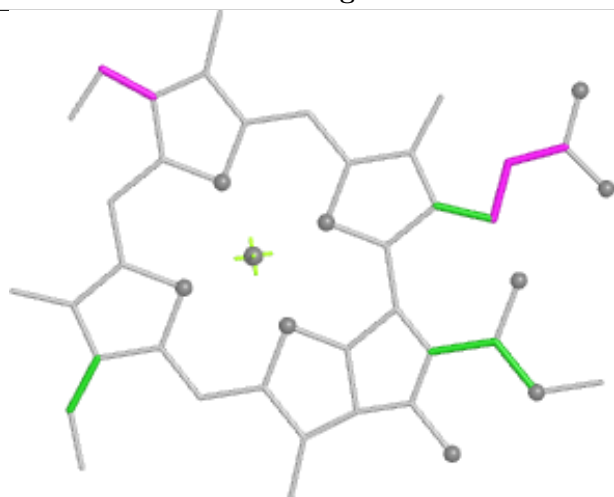
Ligand CLA L 305



Bond lengths



Bond angles

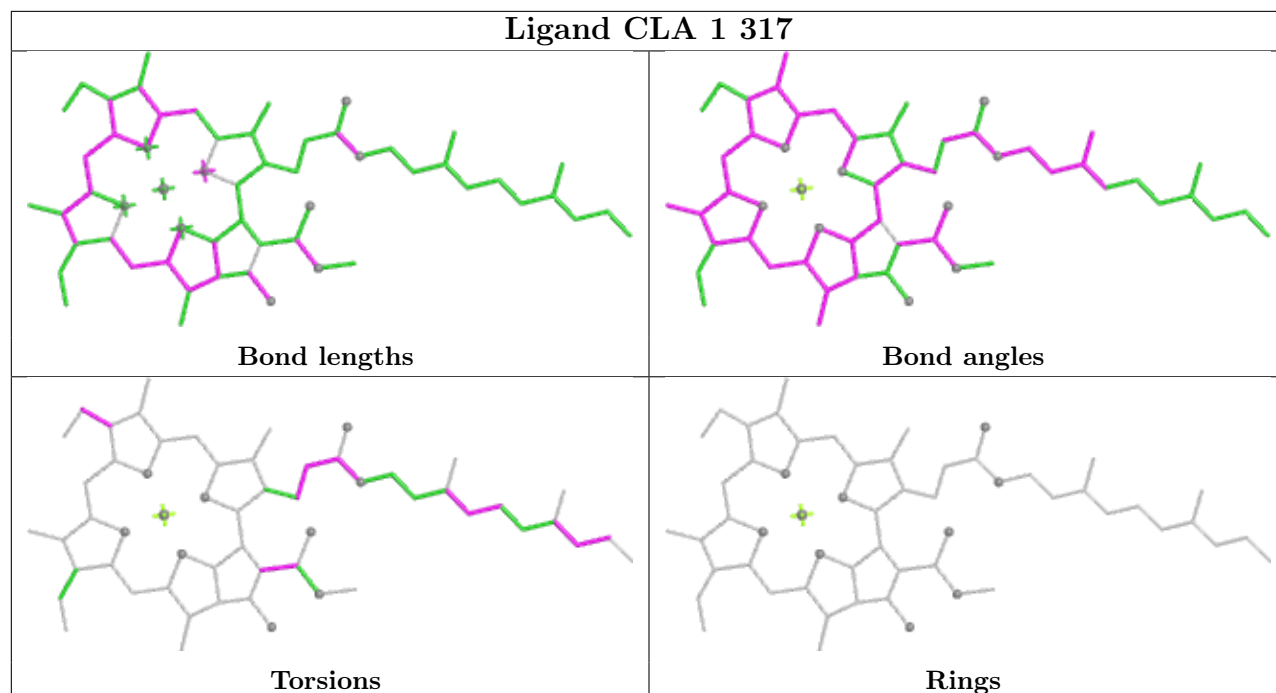


Torsions

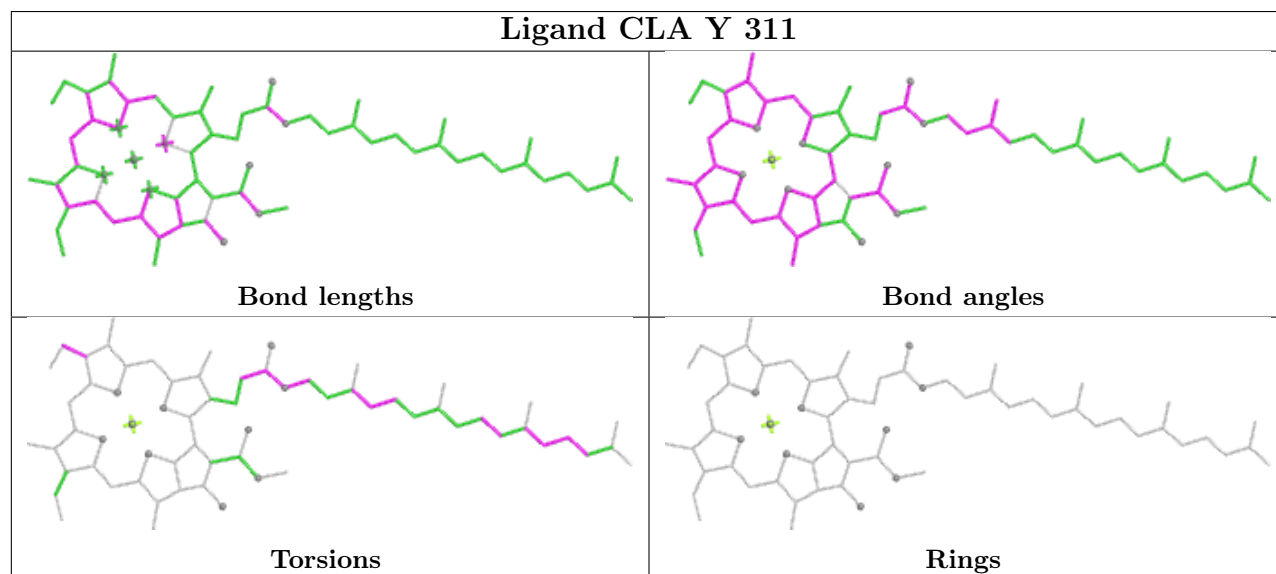


Rings

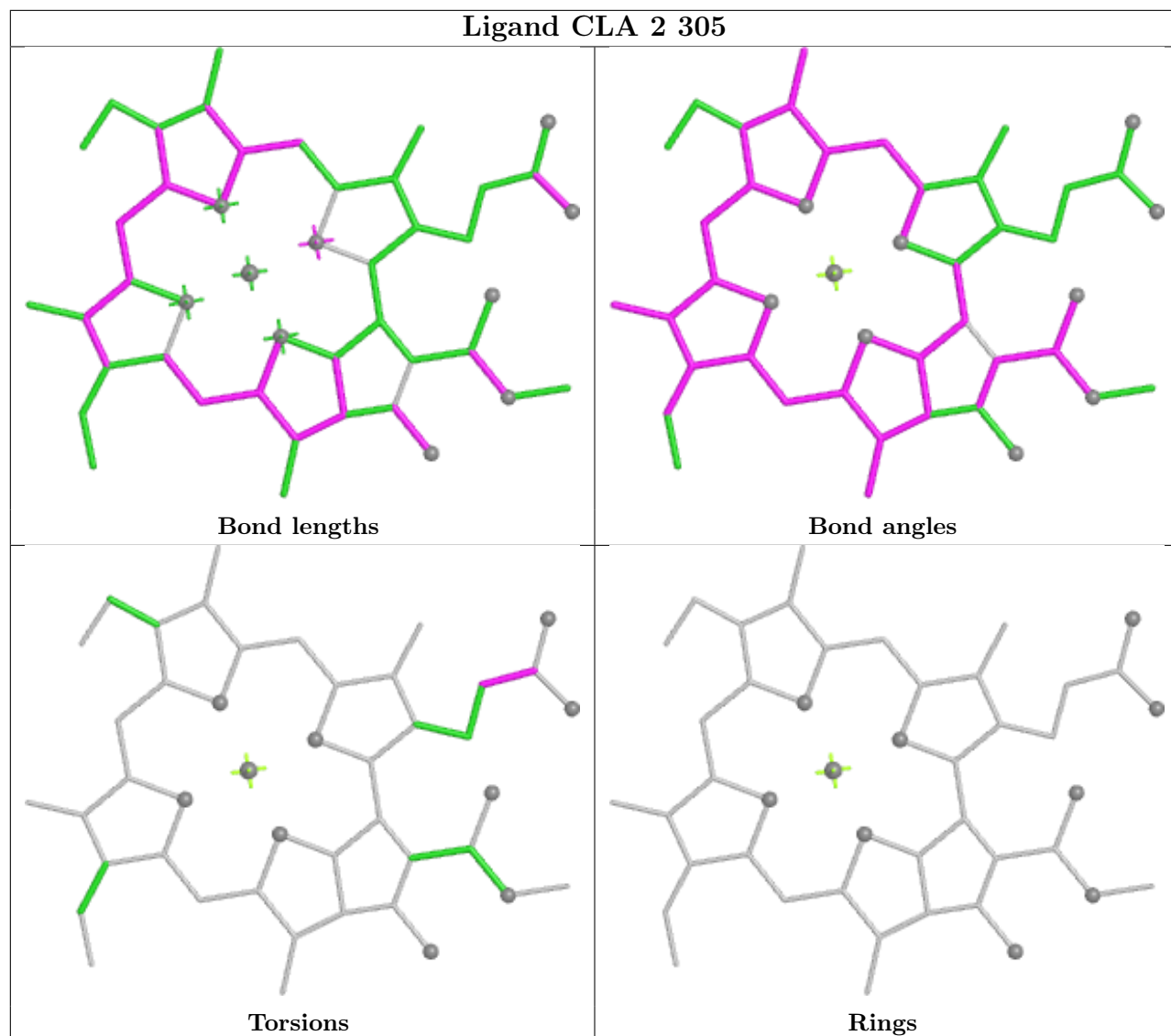
Ligand CLA 1 317

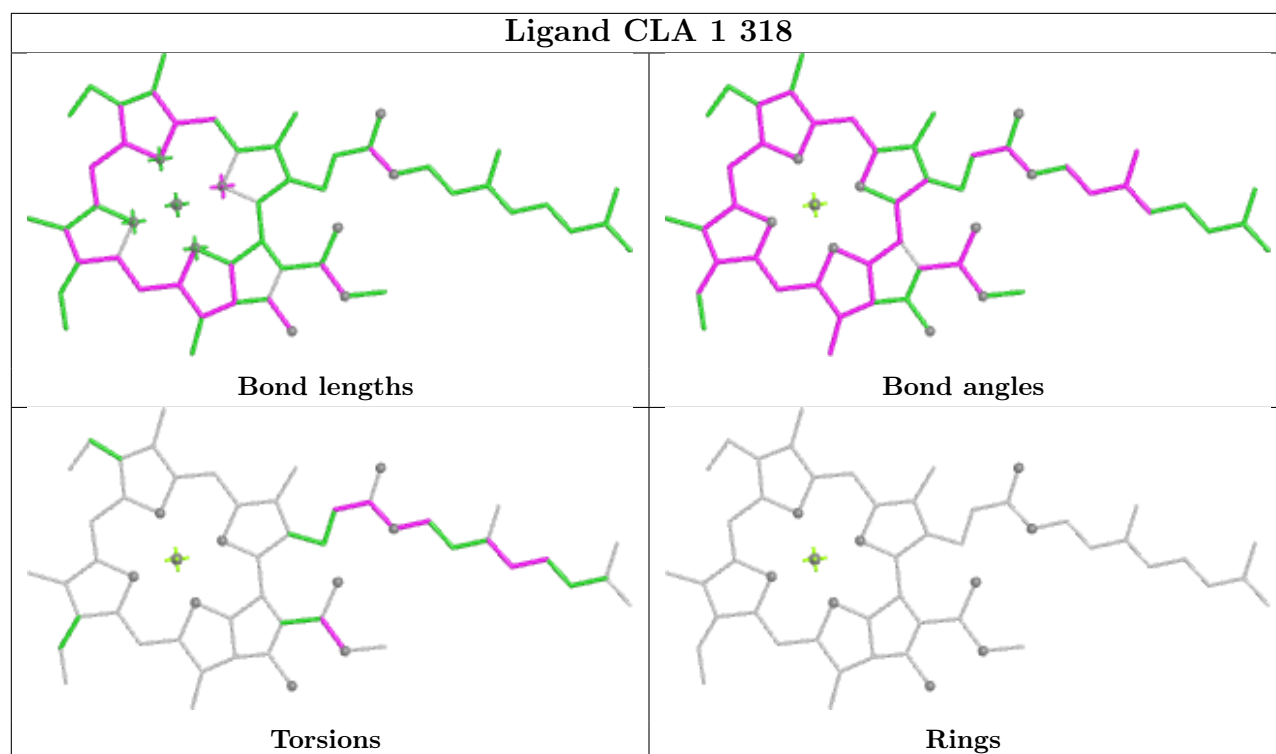
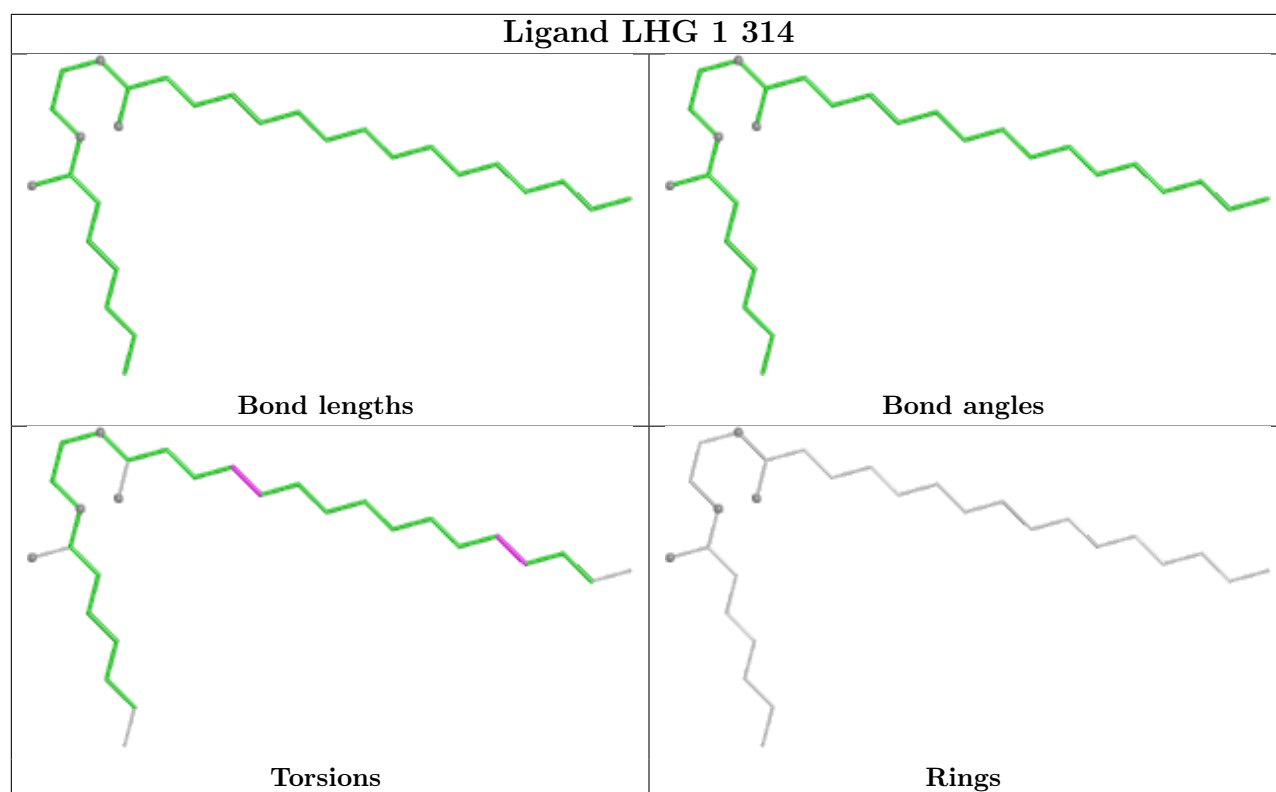


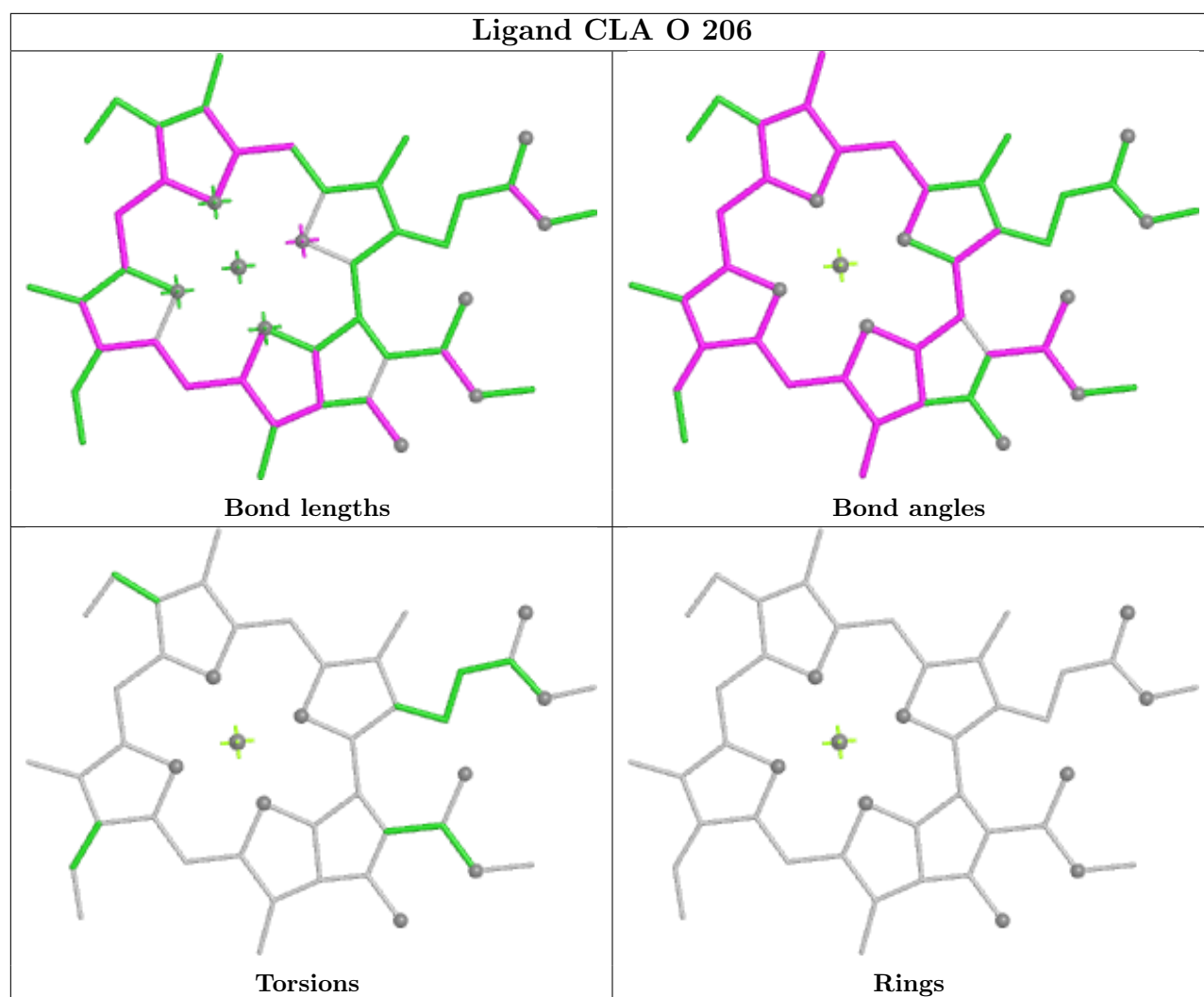
Ligand CLA Y 311

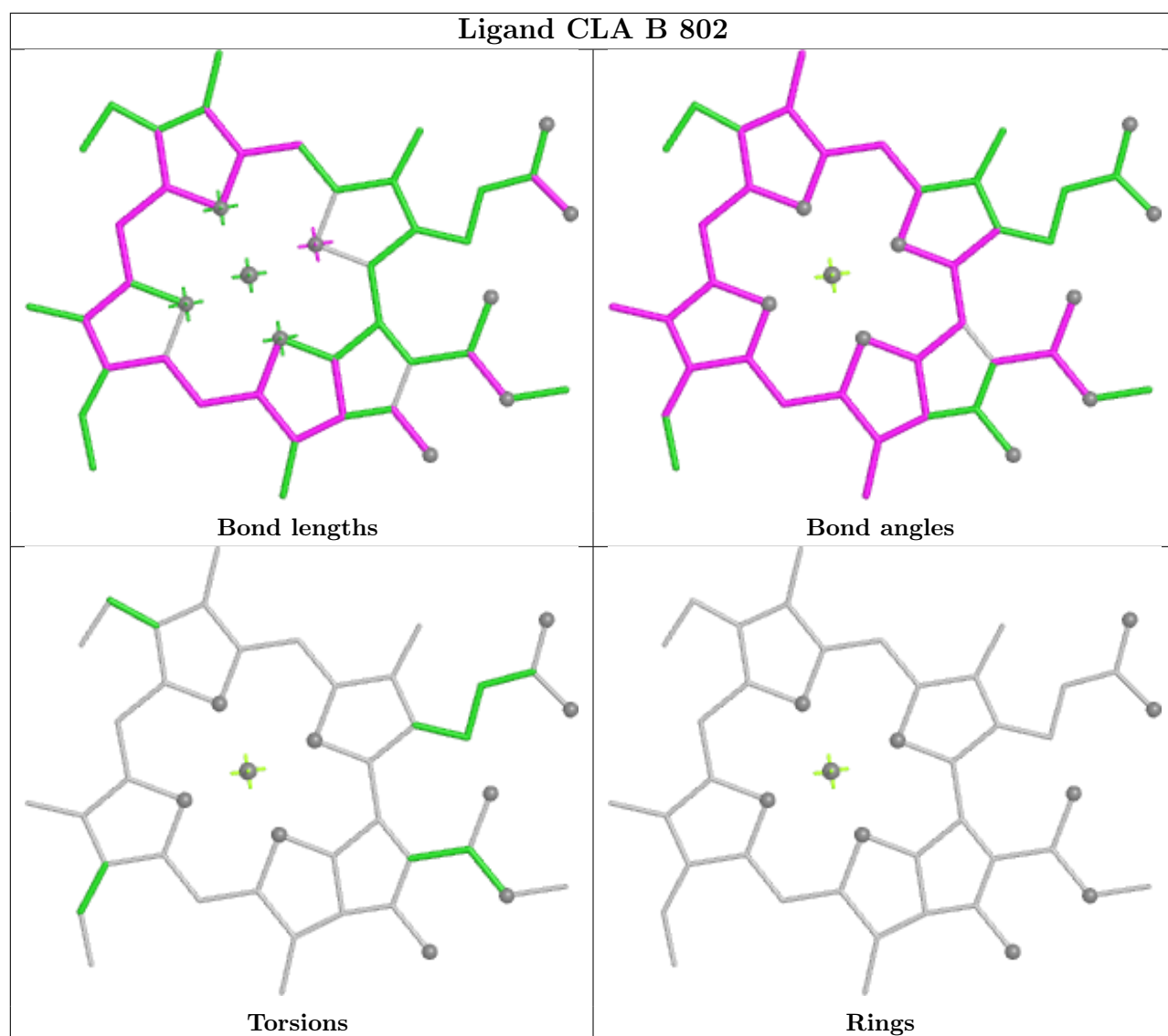


Ligand CLA 2 305

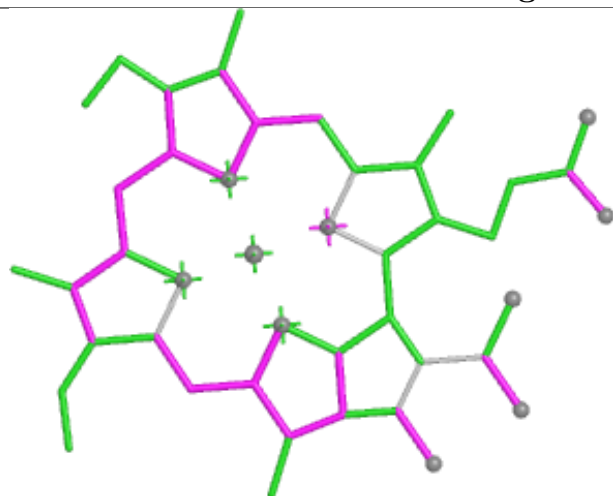




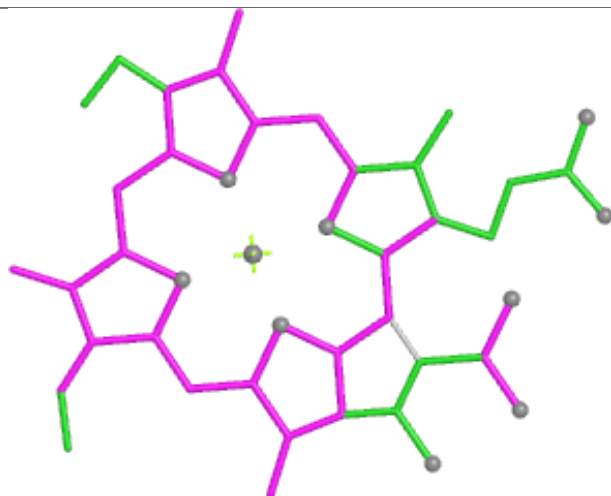




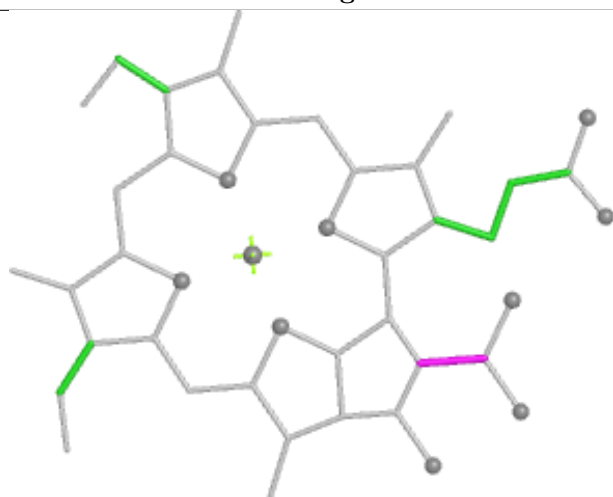
Ligand CLA 2 322



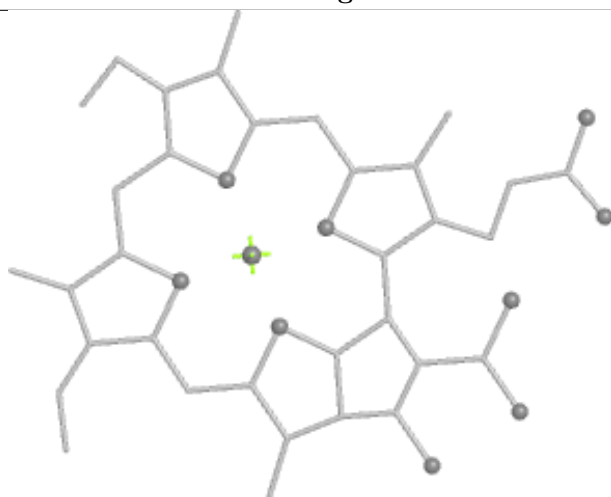
Bond lengths



Bond angles

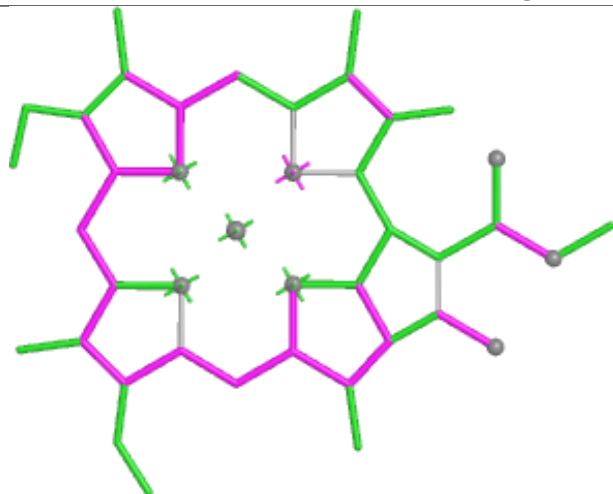


Torsions

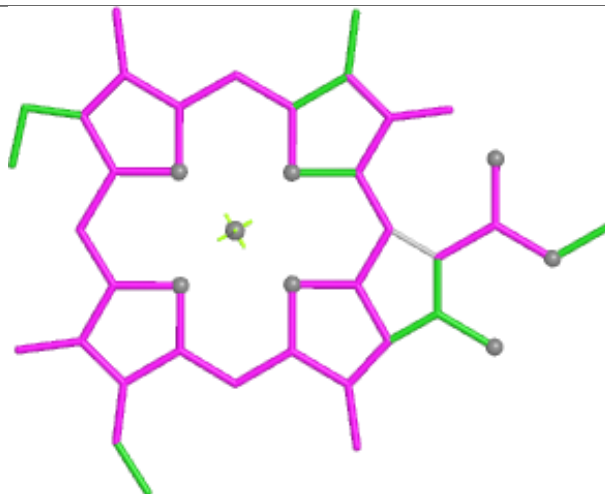


Rings

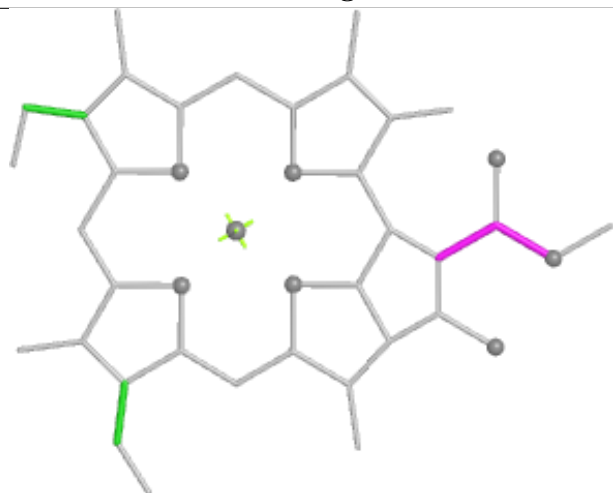
Ligand CLA 2 317



Bond lengths



Bond angles

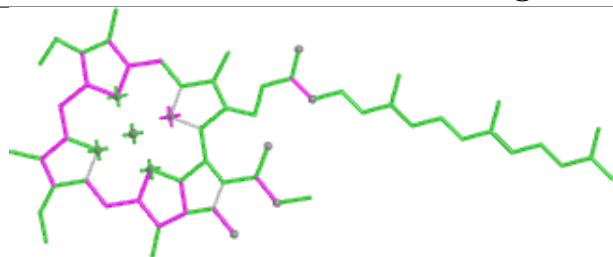


Torsions

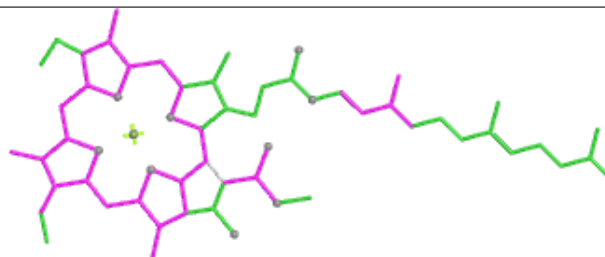


Rings

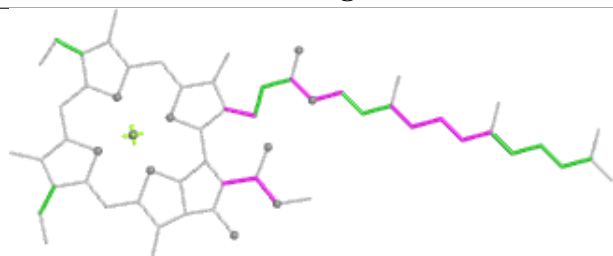
Ligand CLA O 208



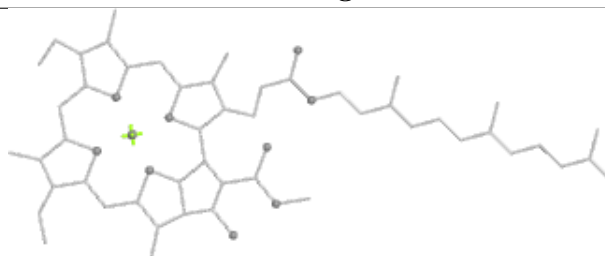
Bond lengths



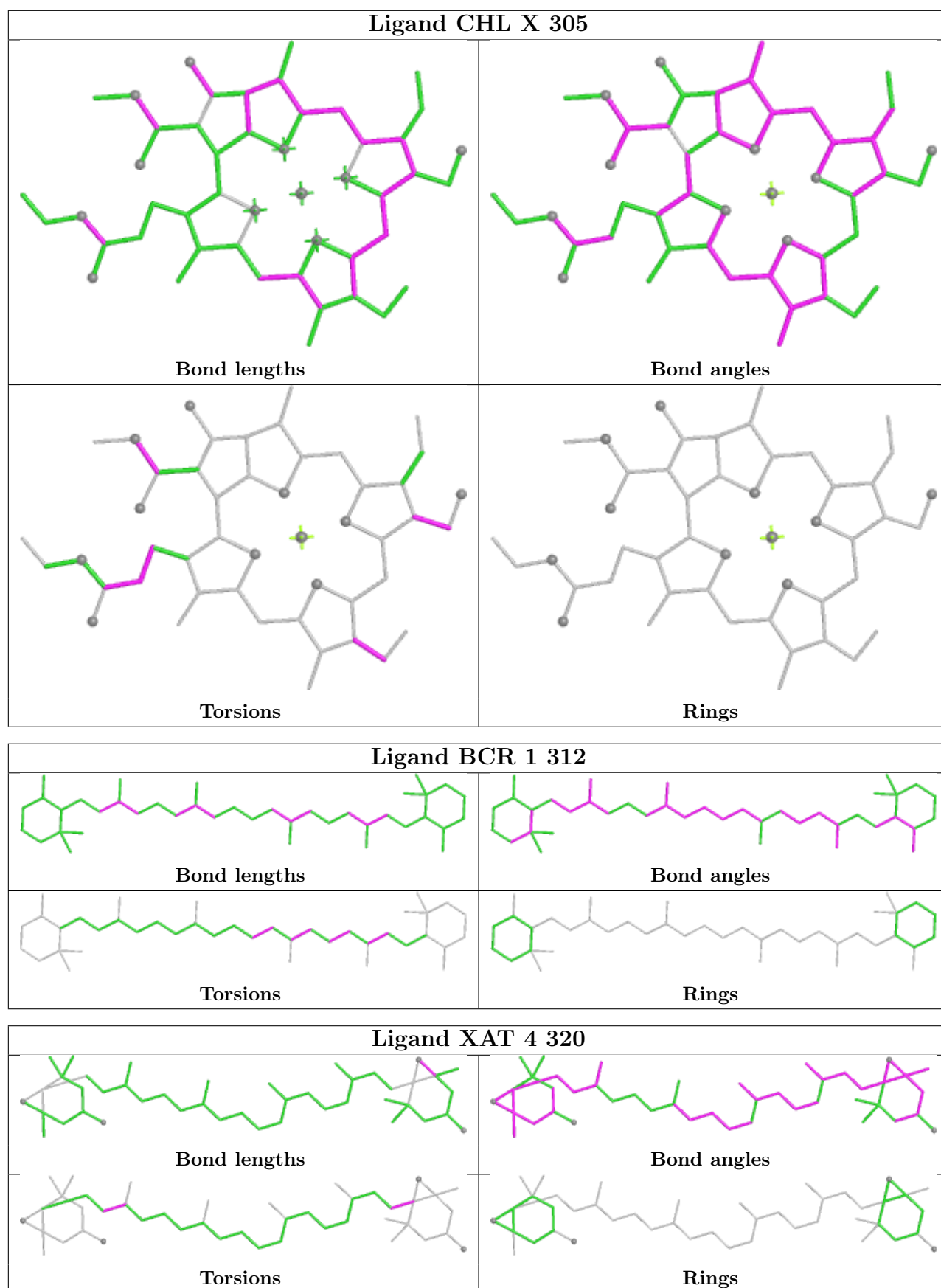
Bond angles

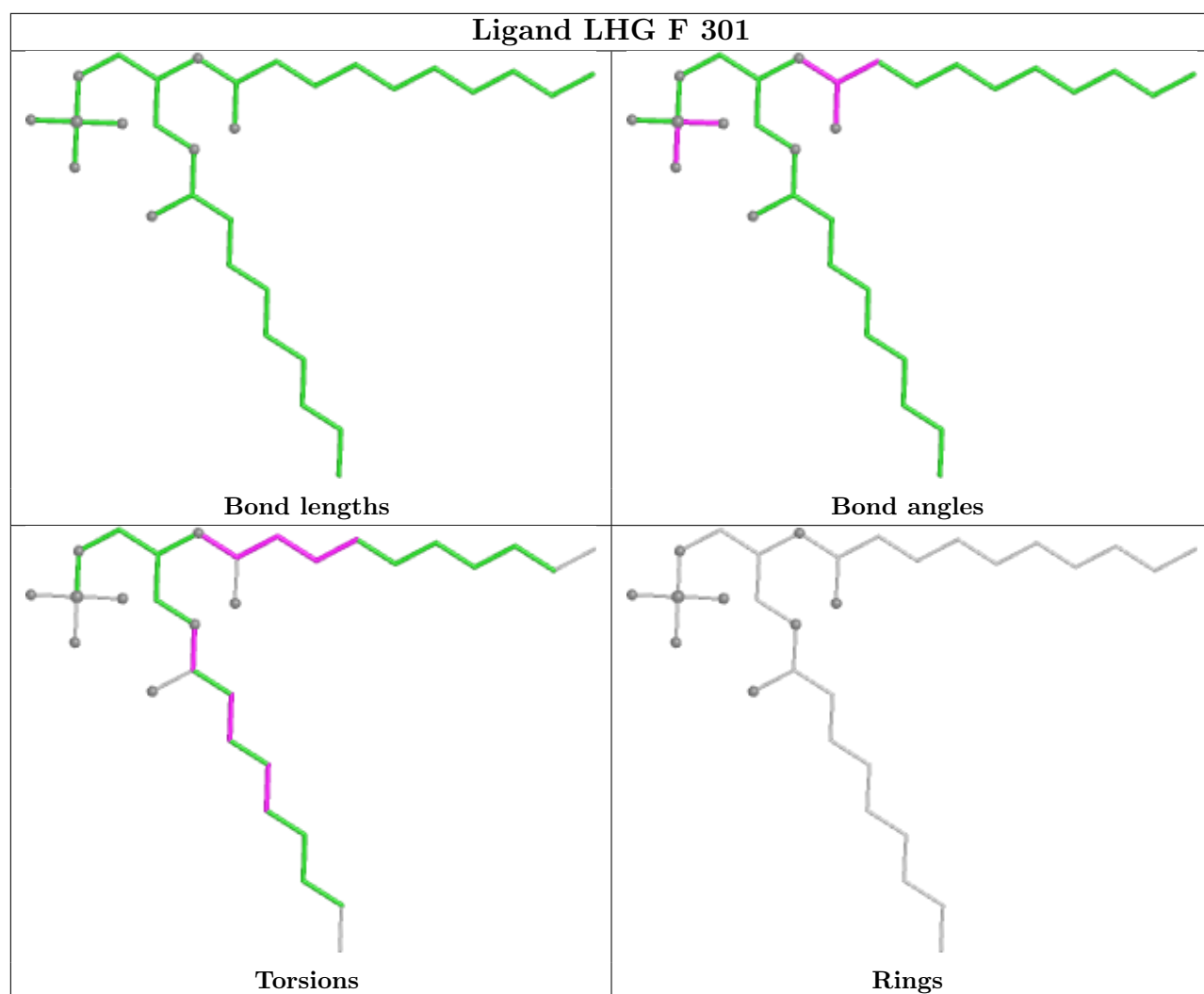


Torsions

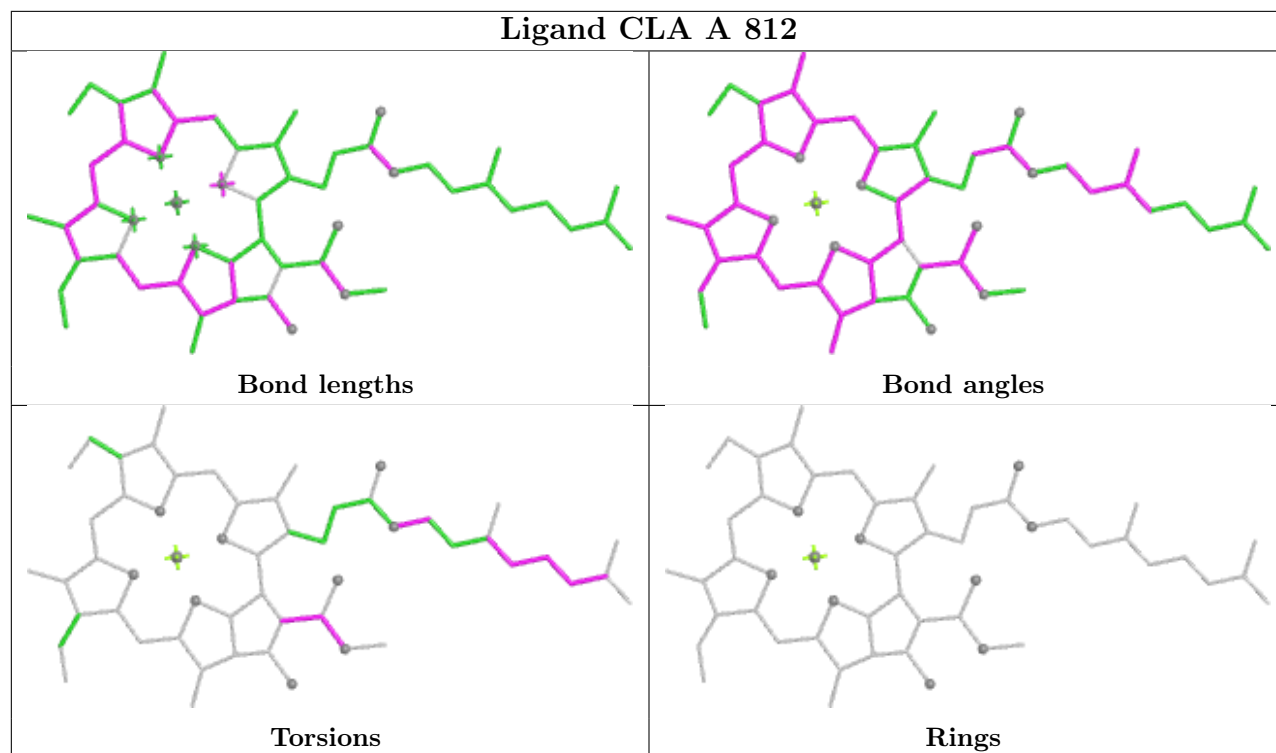


Rings

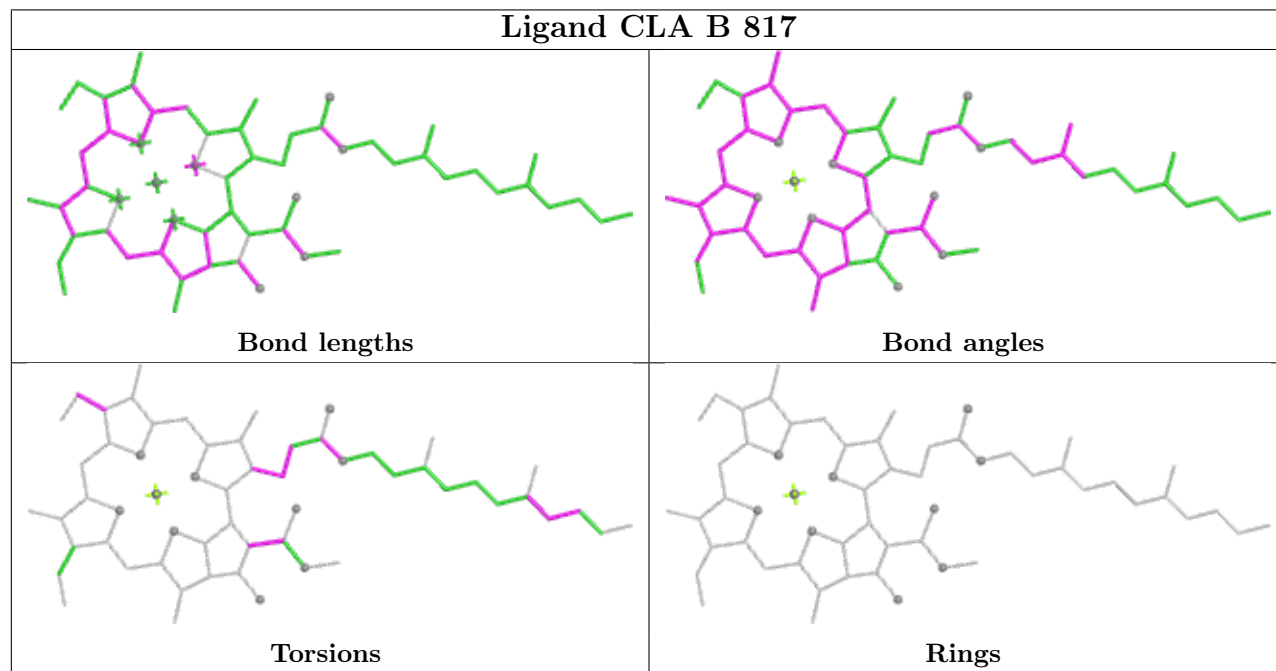


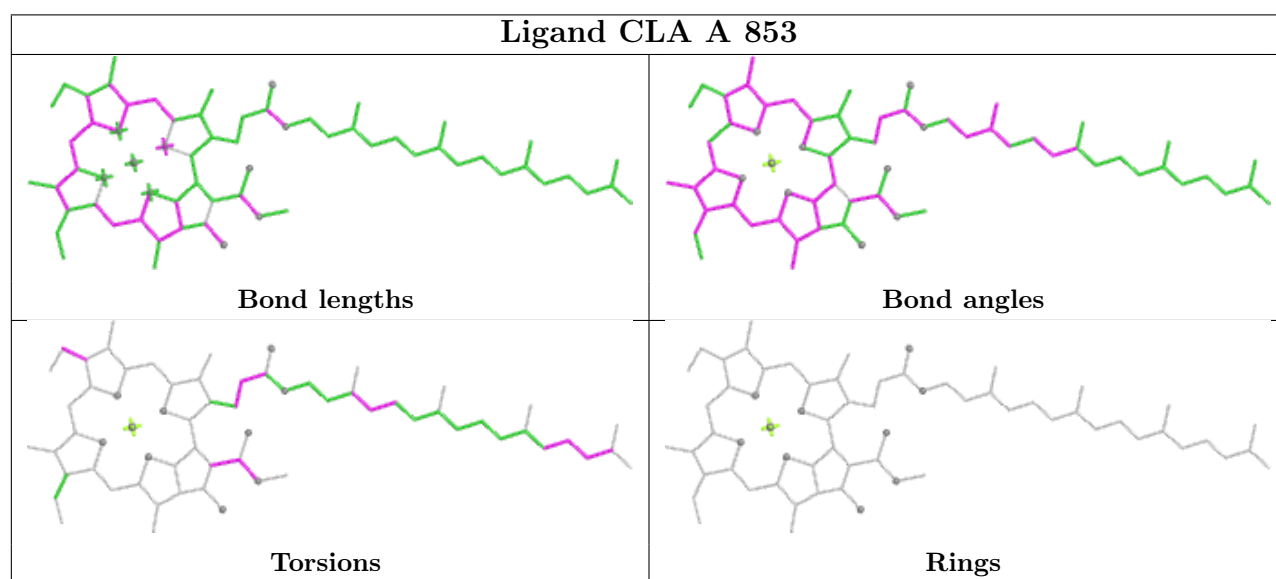
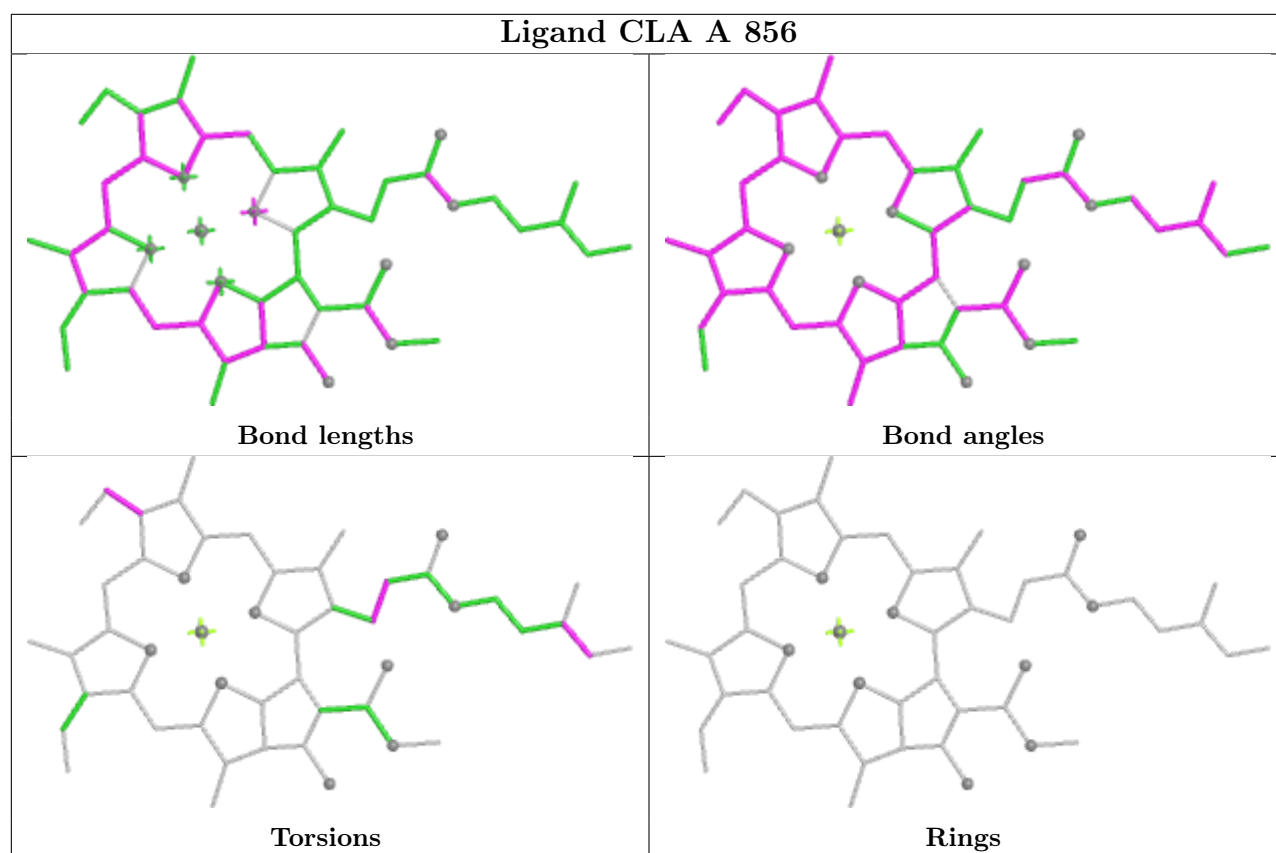


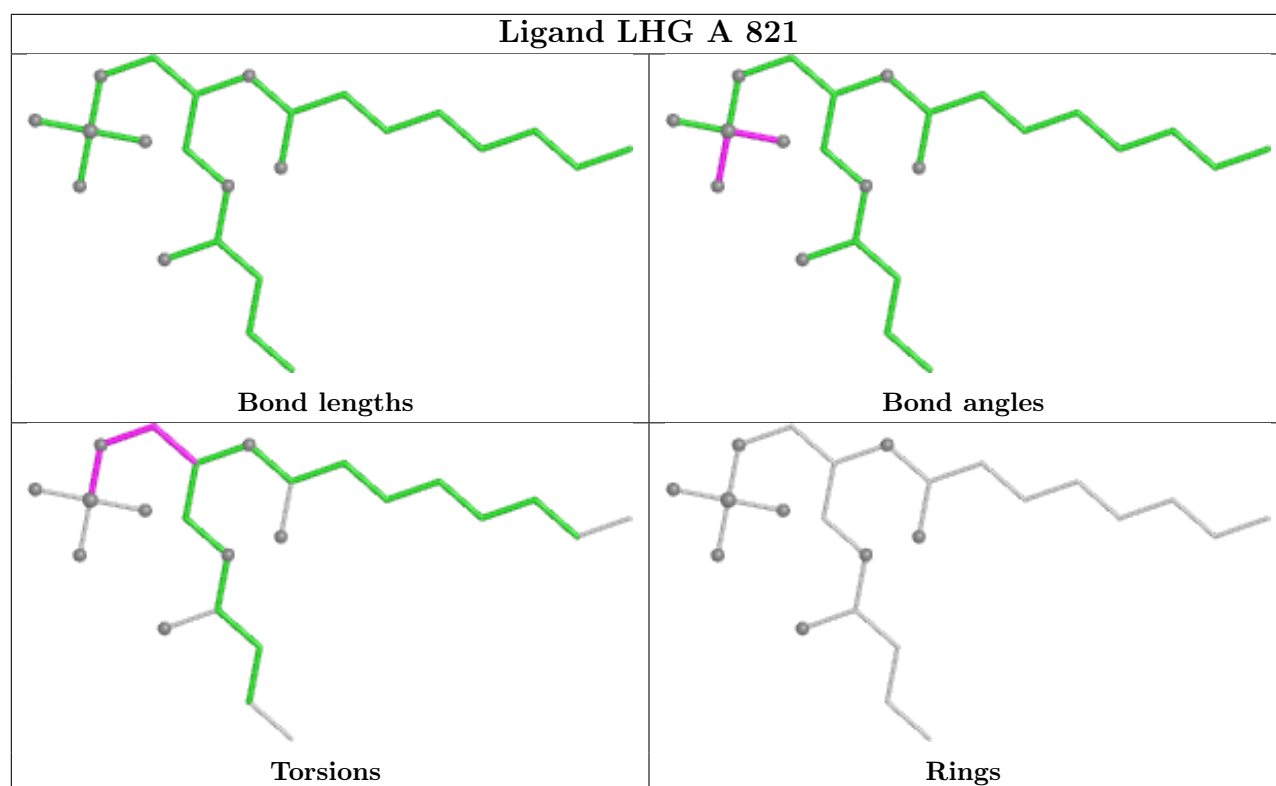
Ligand CLA A 812

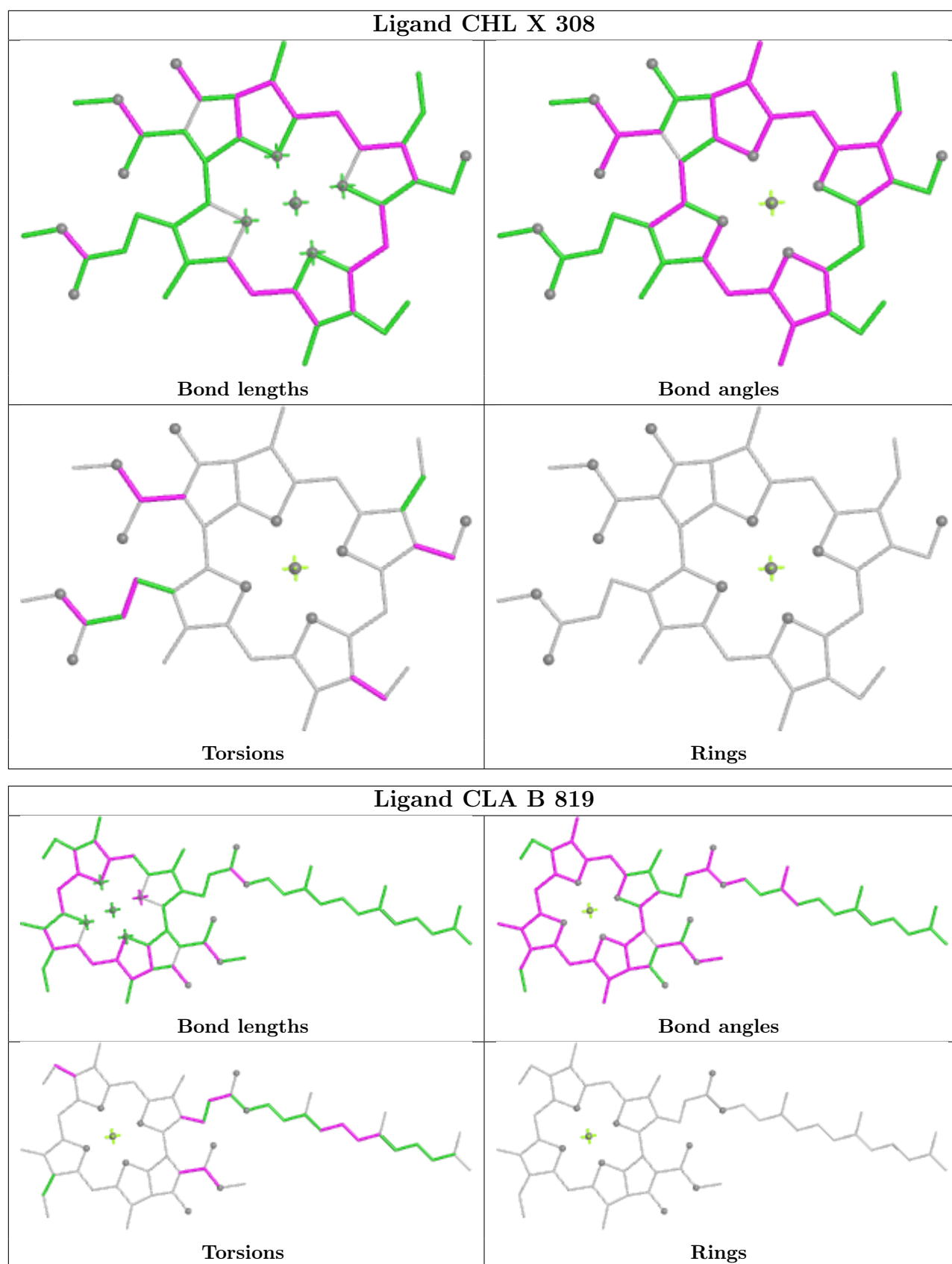


Ligand CLA B 817

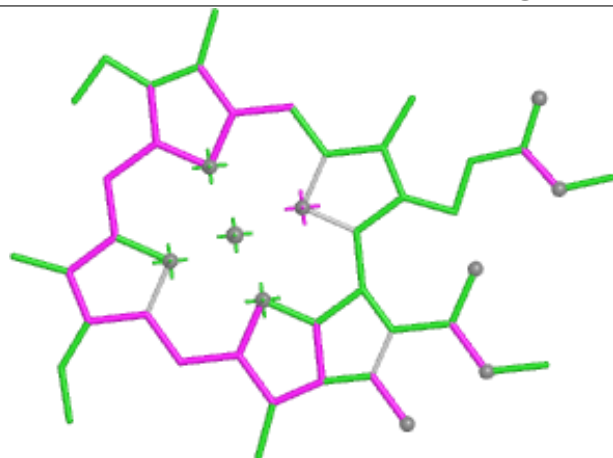




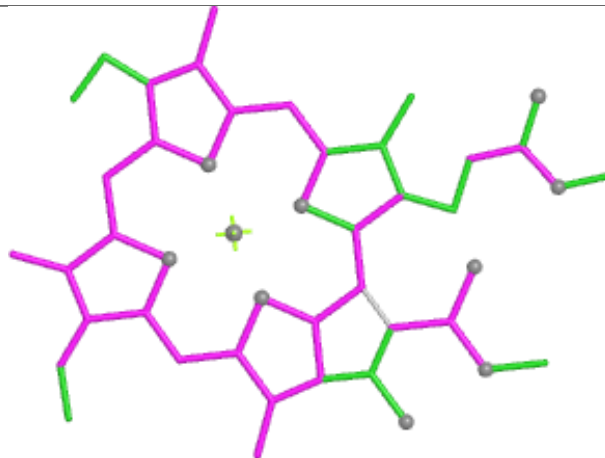




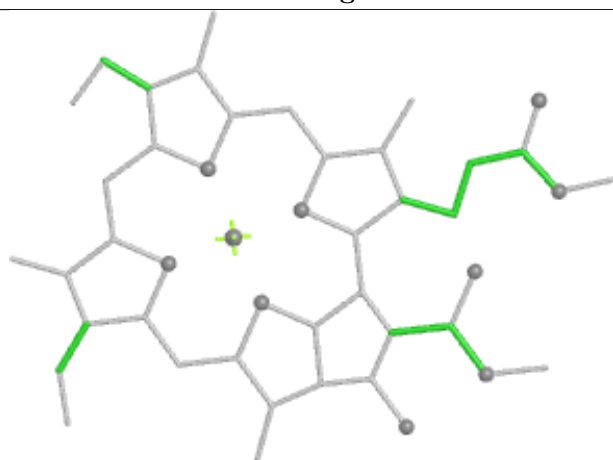
Ligand CLA Z 310



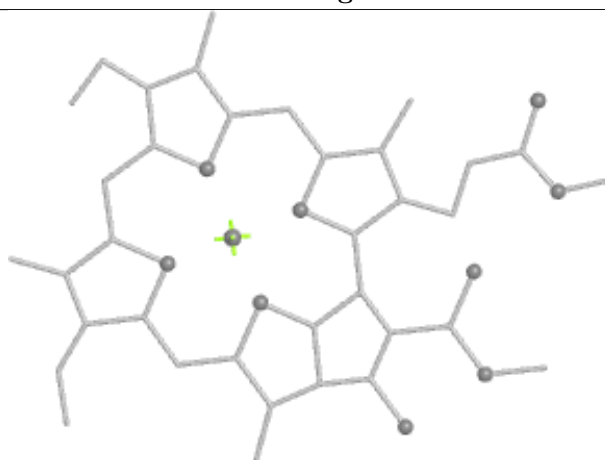
Bond lengths



Bond angles

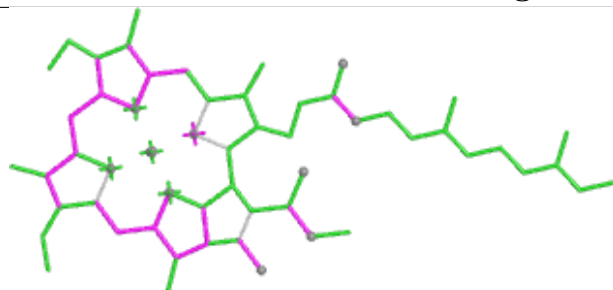


Torsions

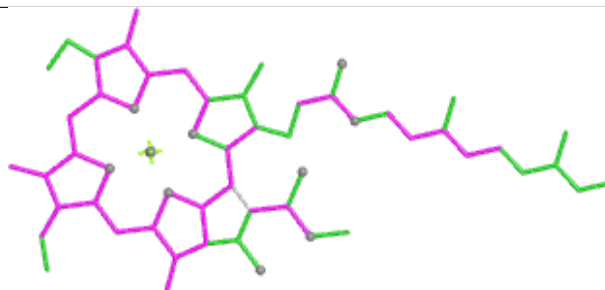


Rings

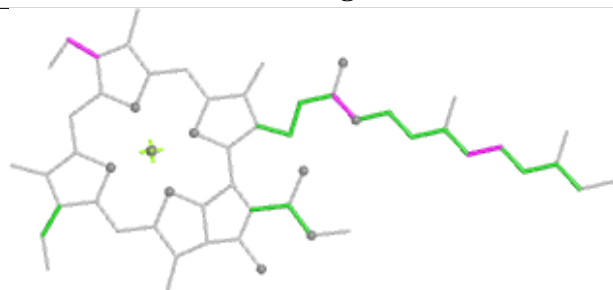
Ligand CLA A 857



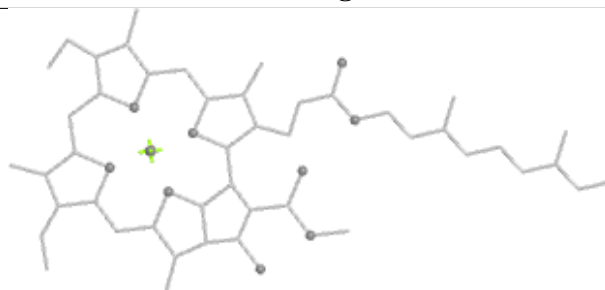
Bond lengths



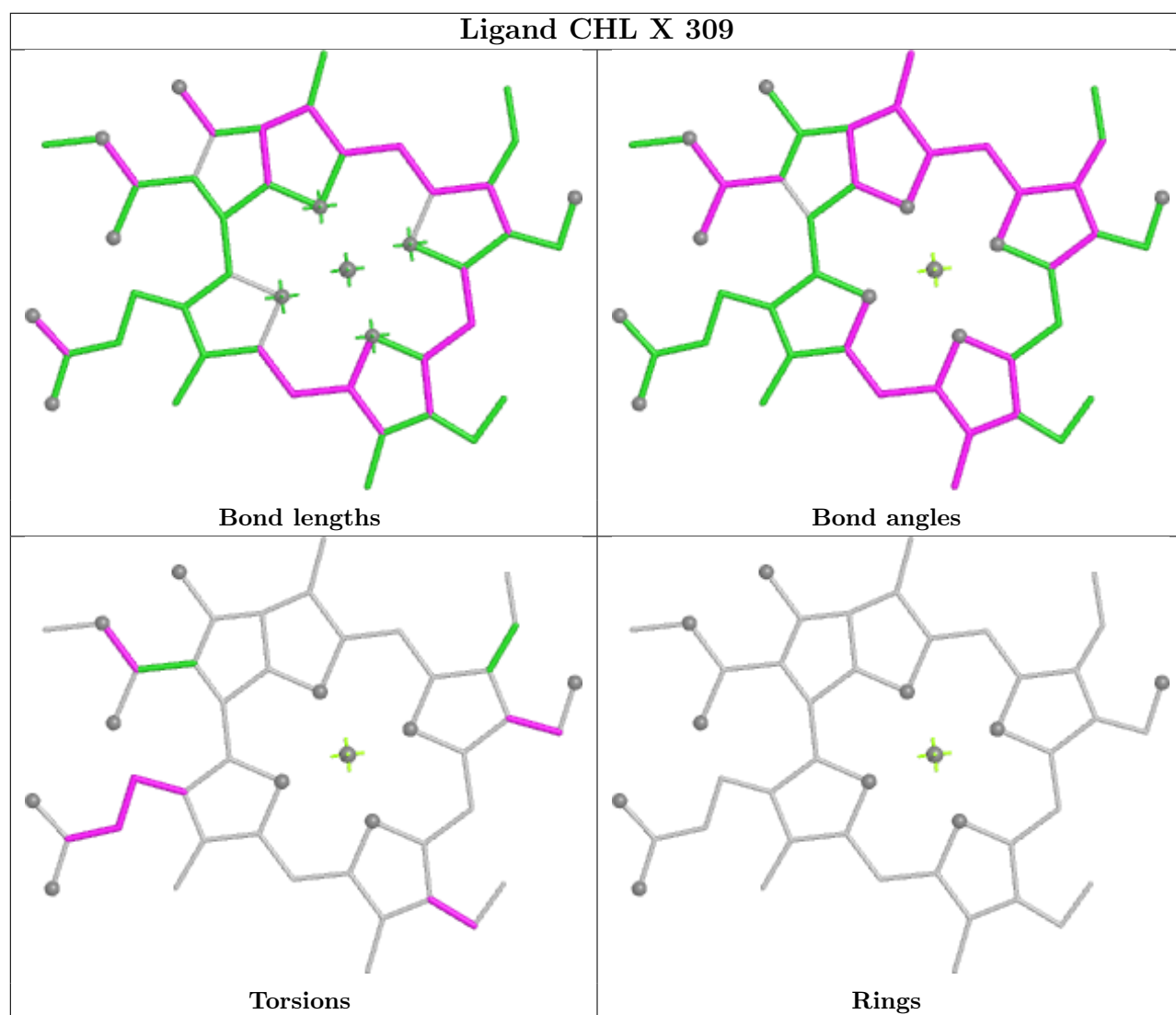
Bond angles

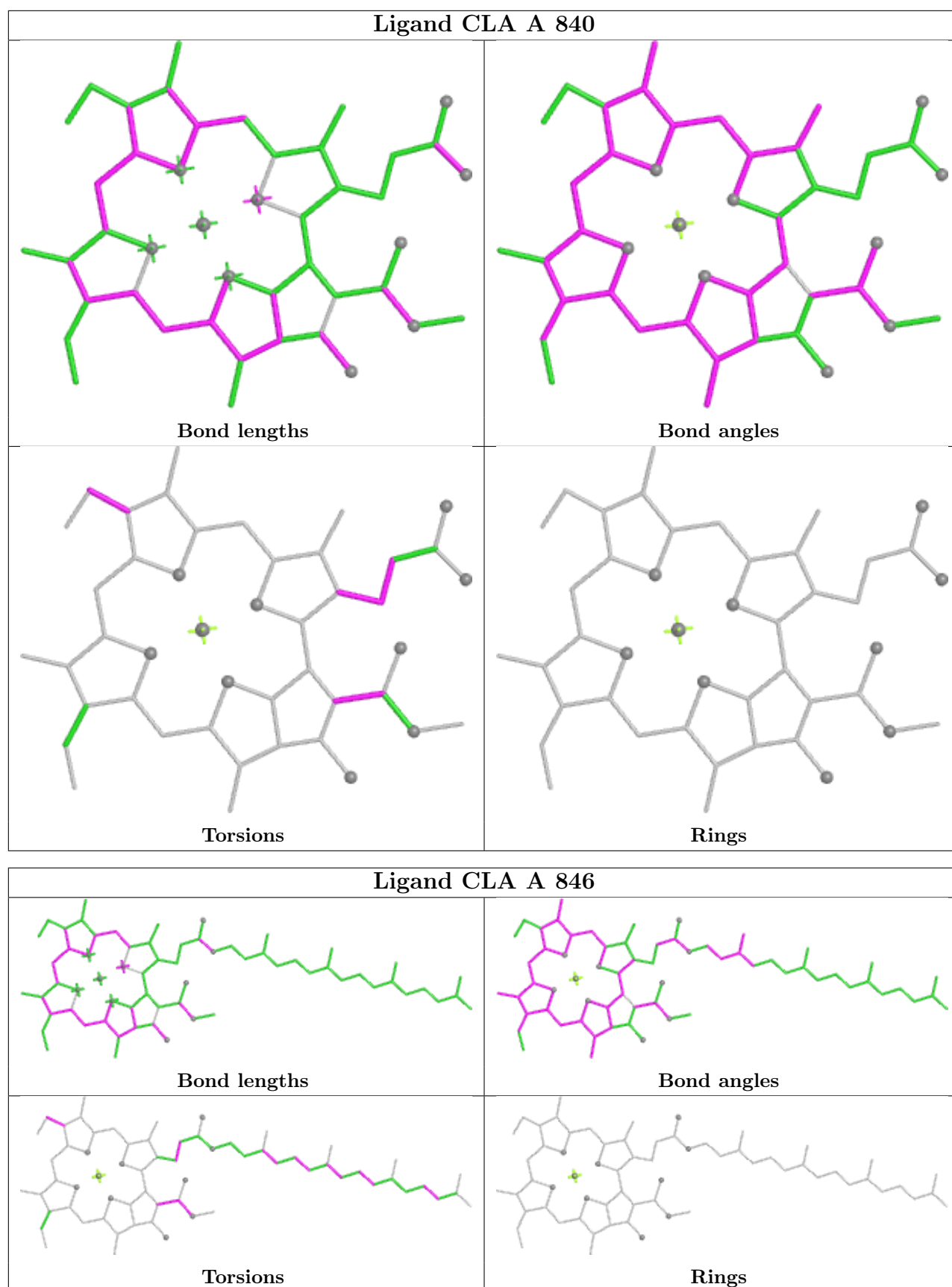


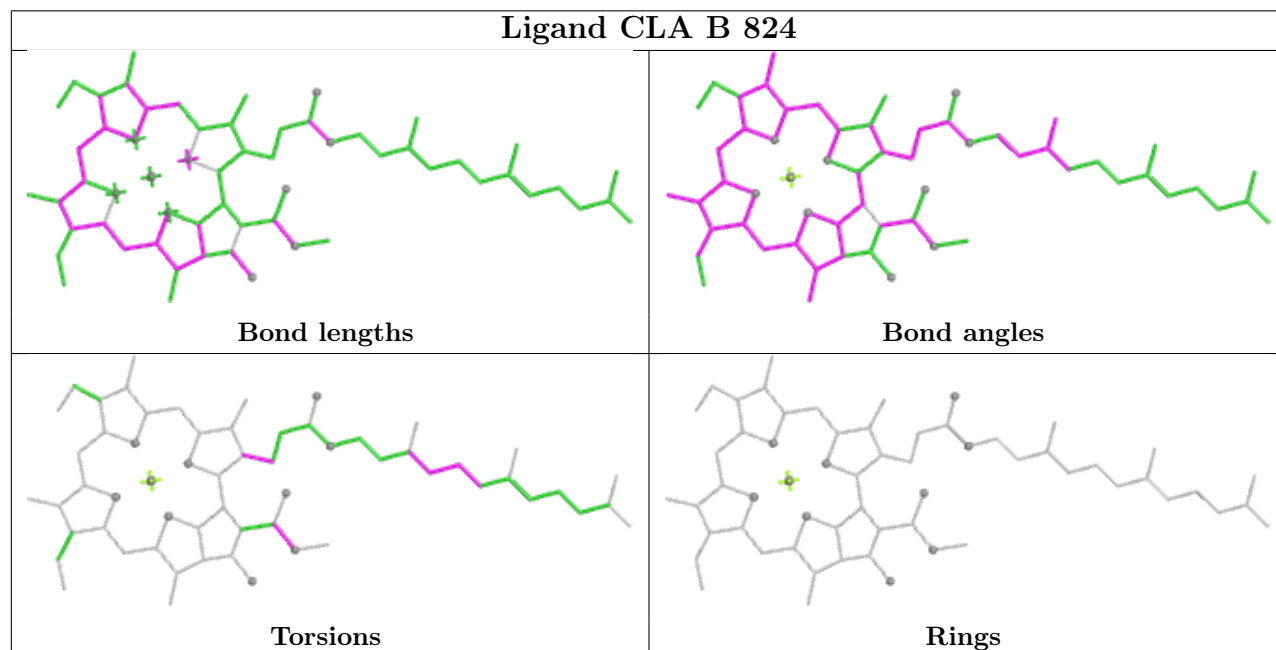
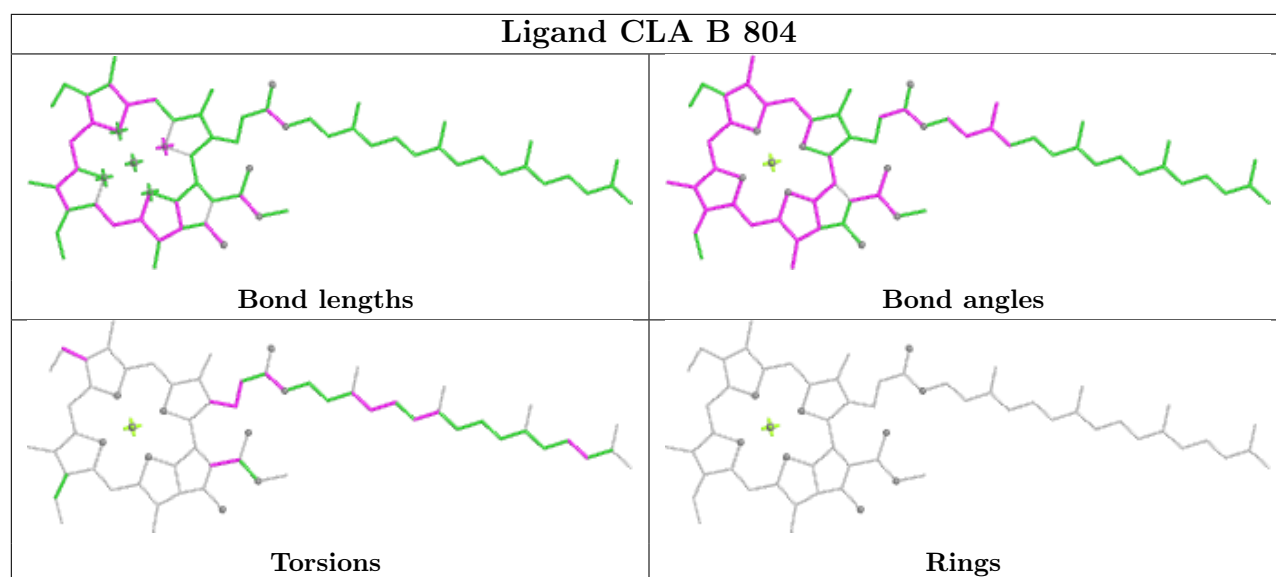
Torsions

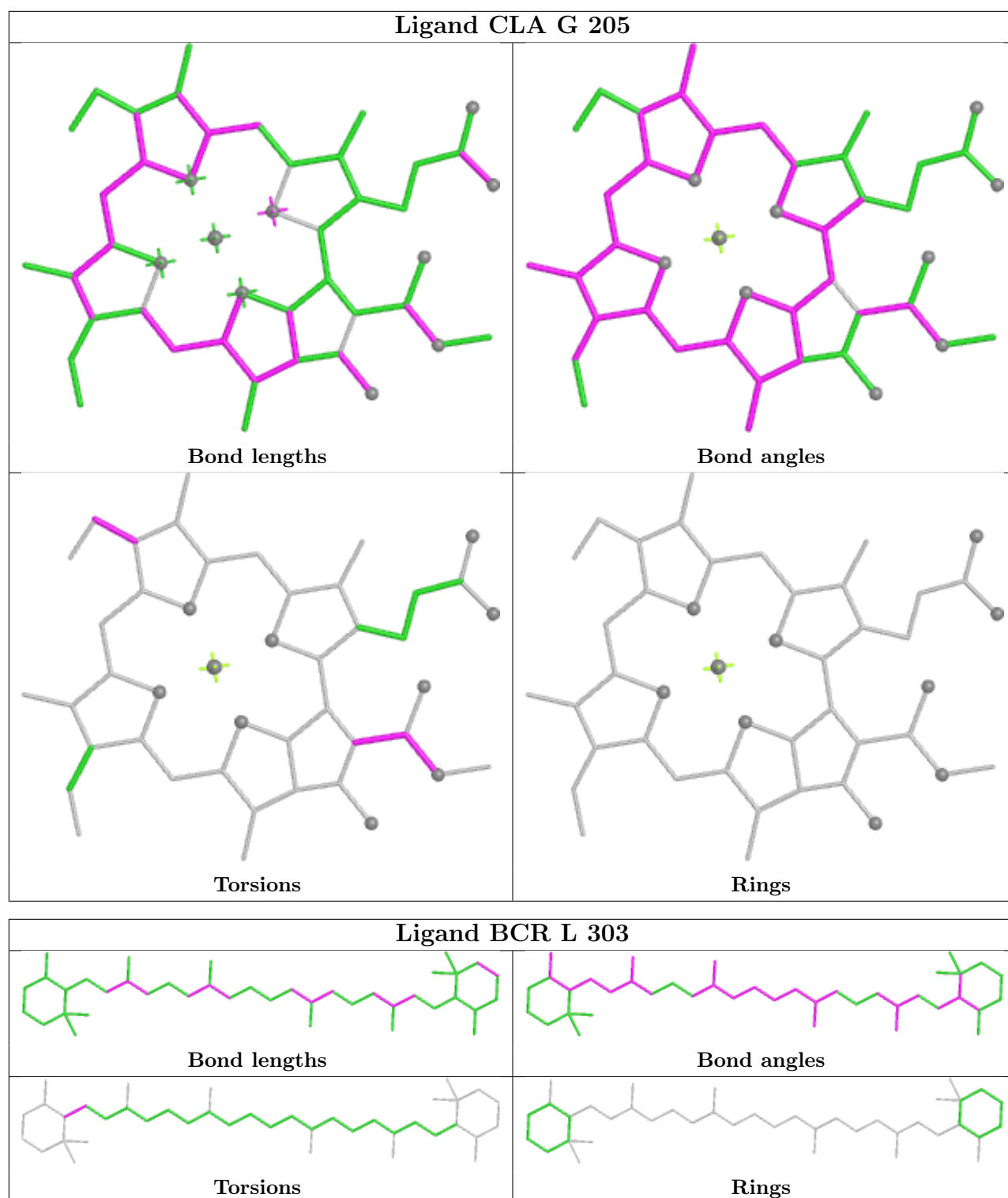


Rings

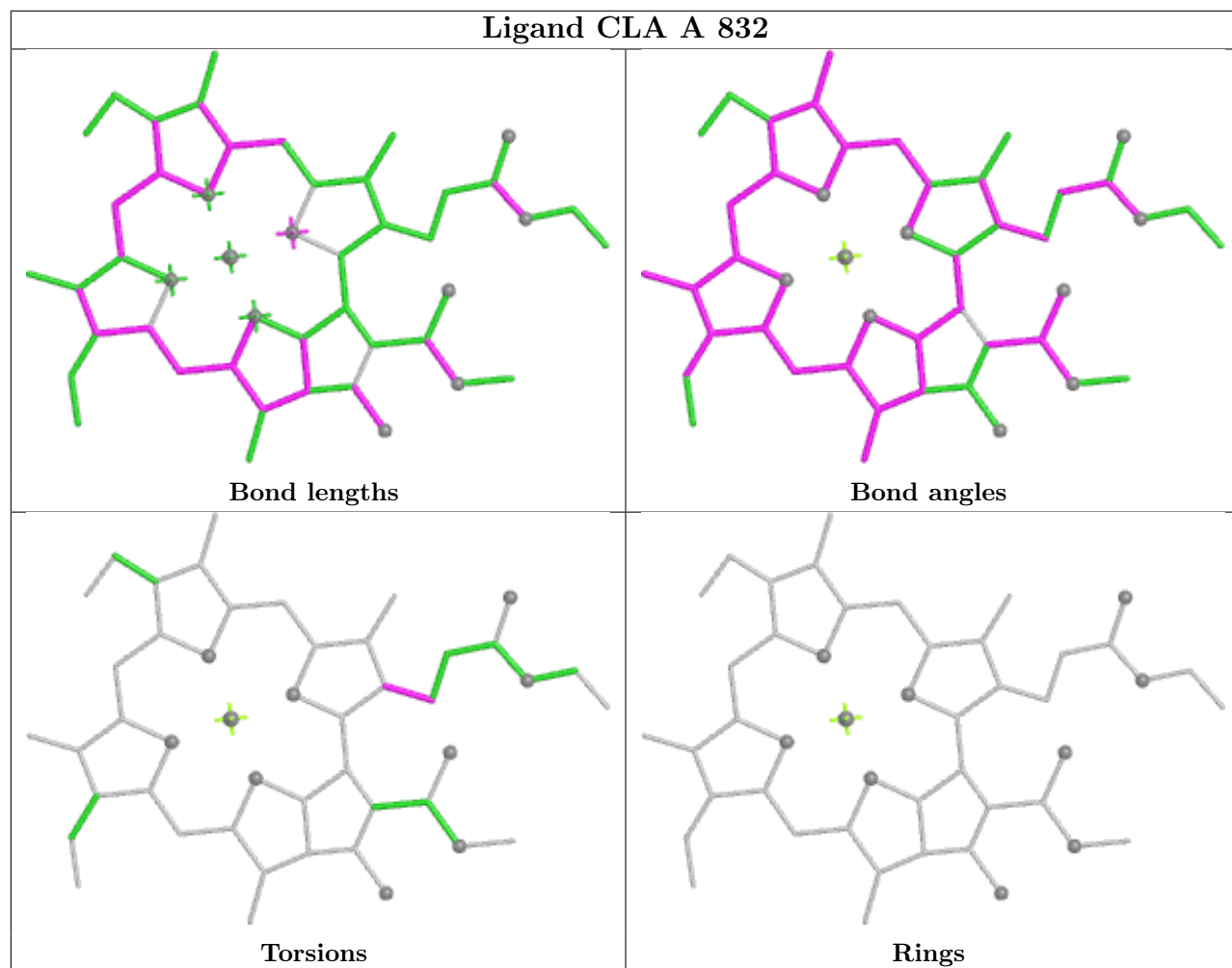


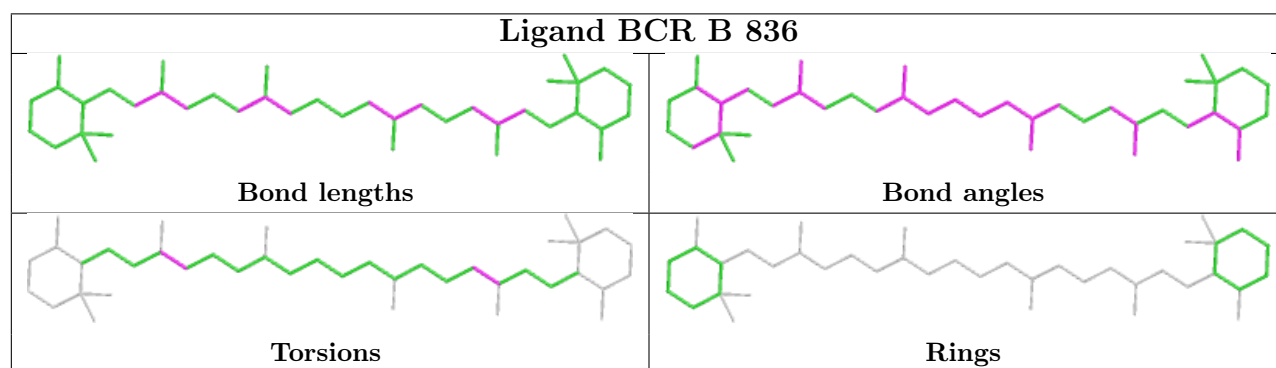
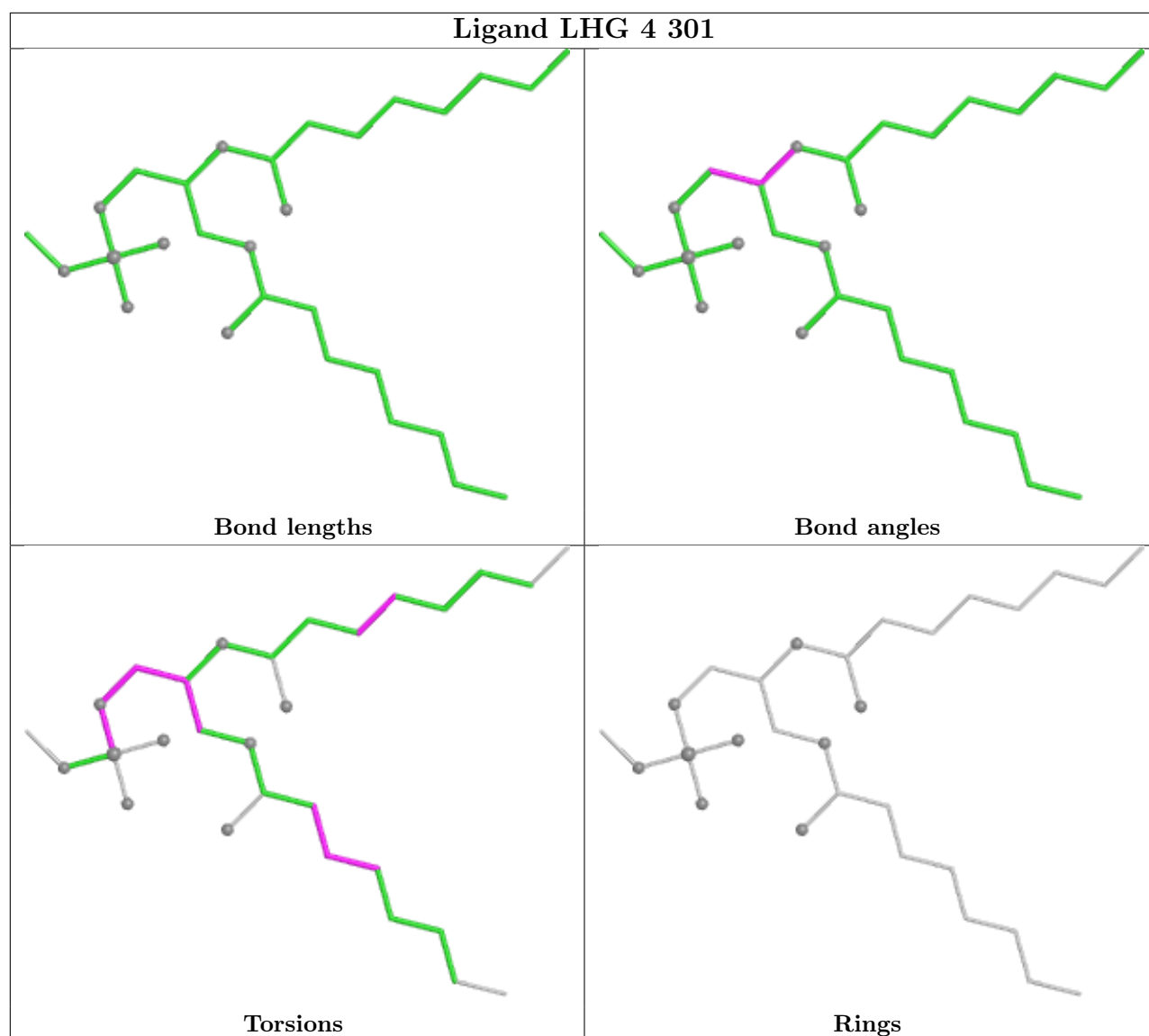


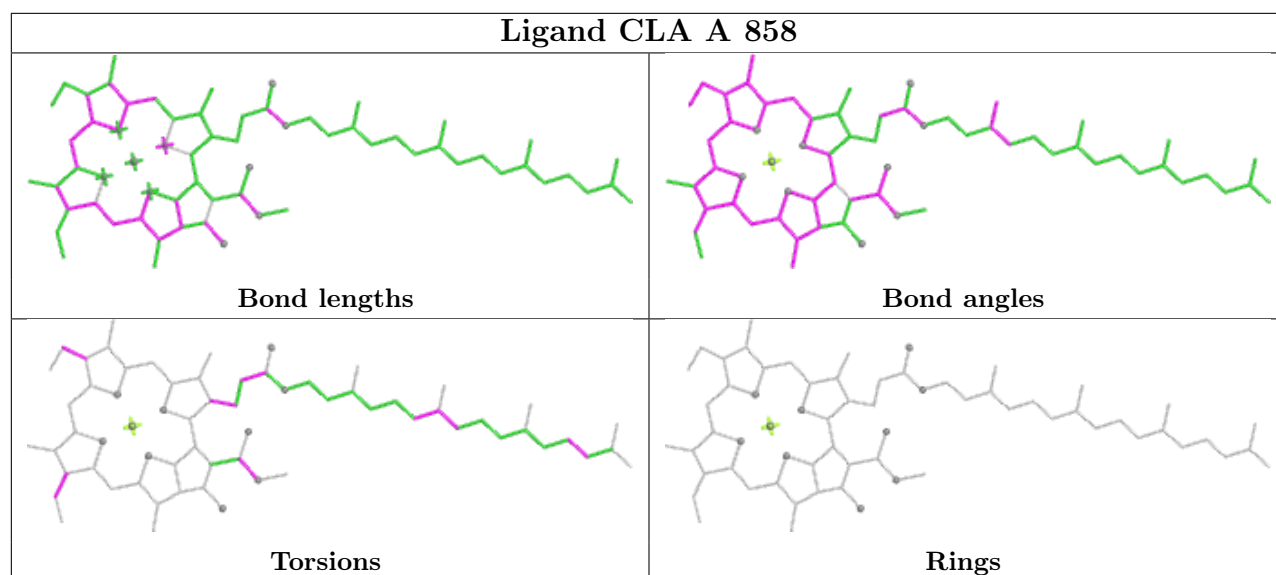
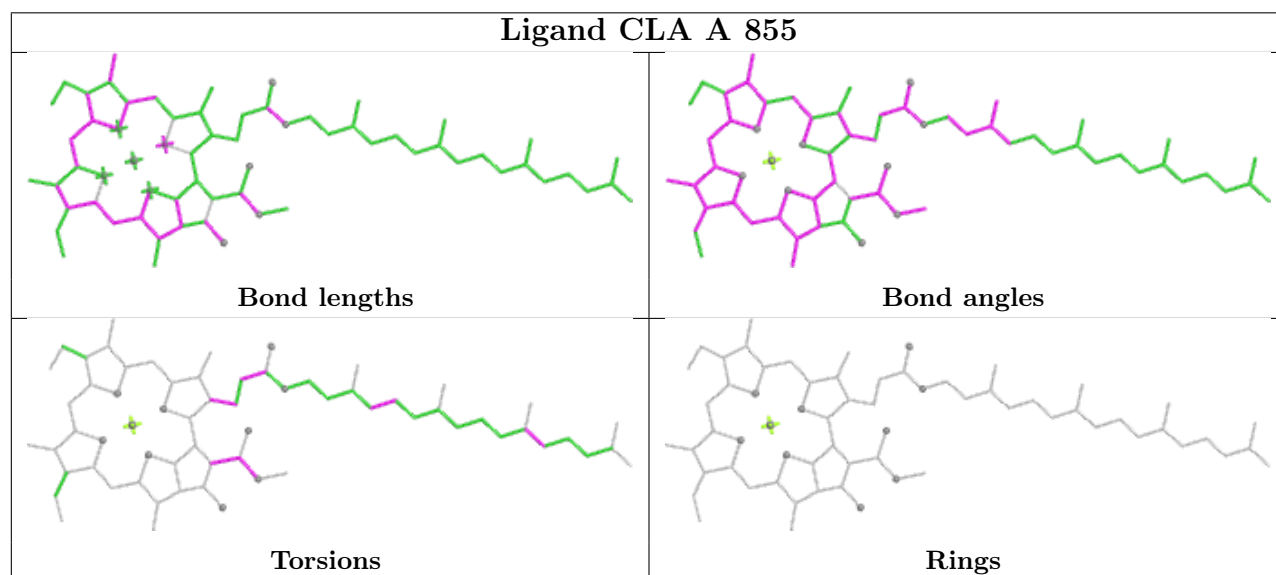
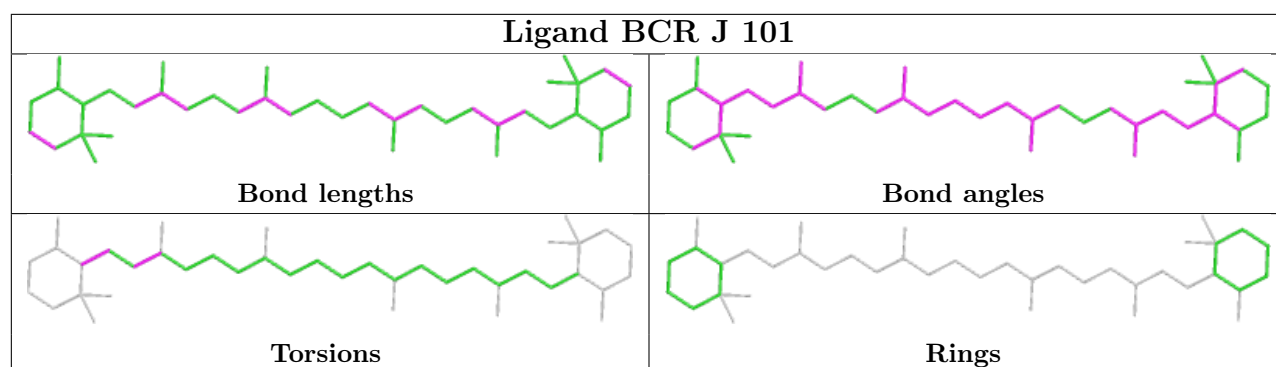


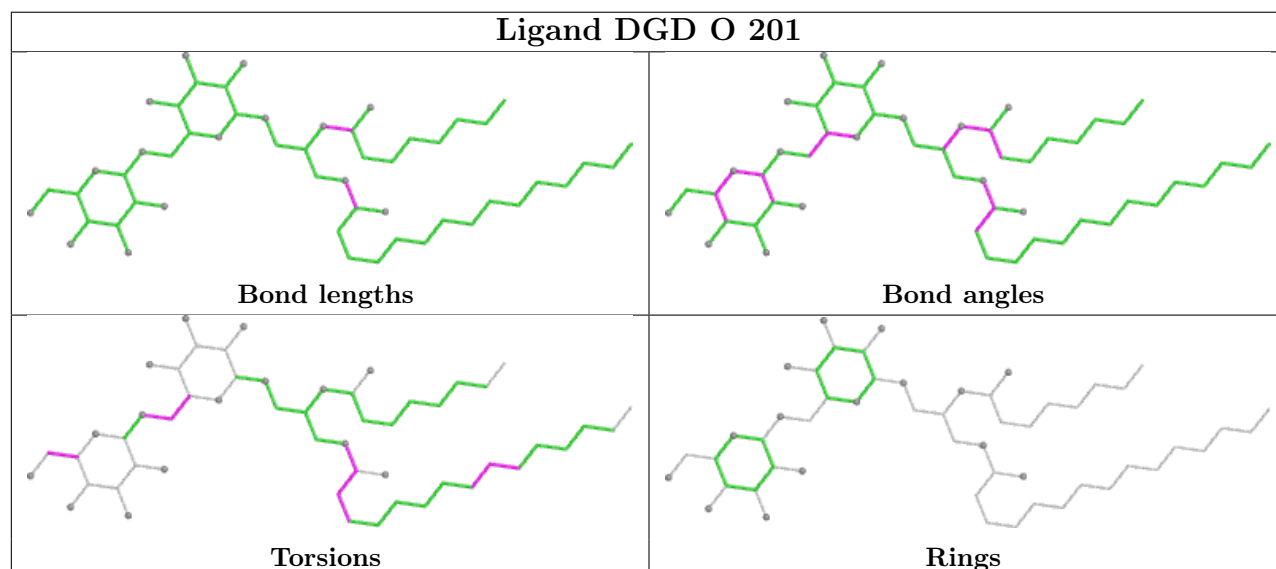
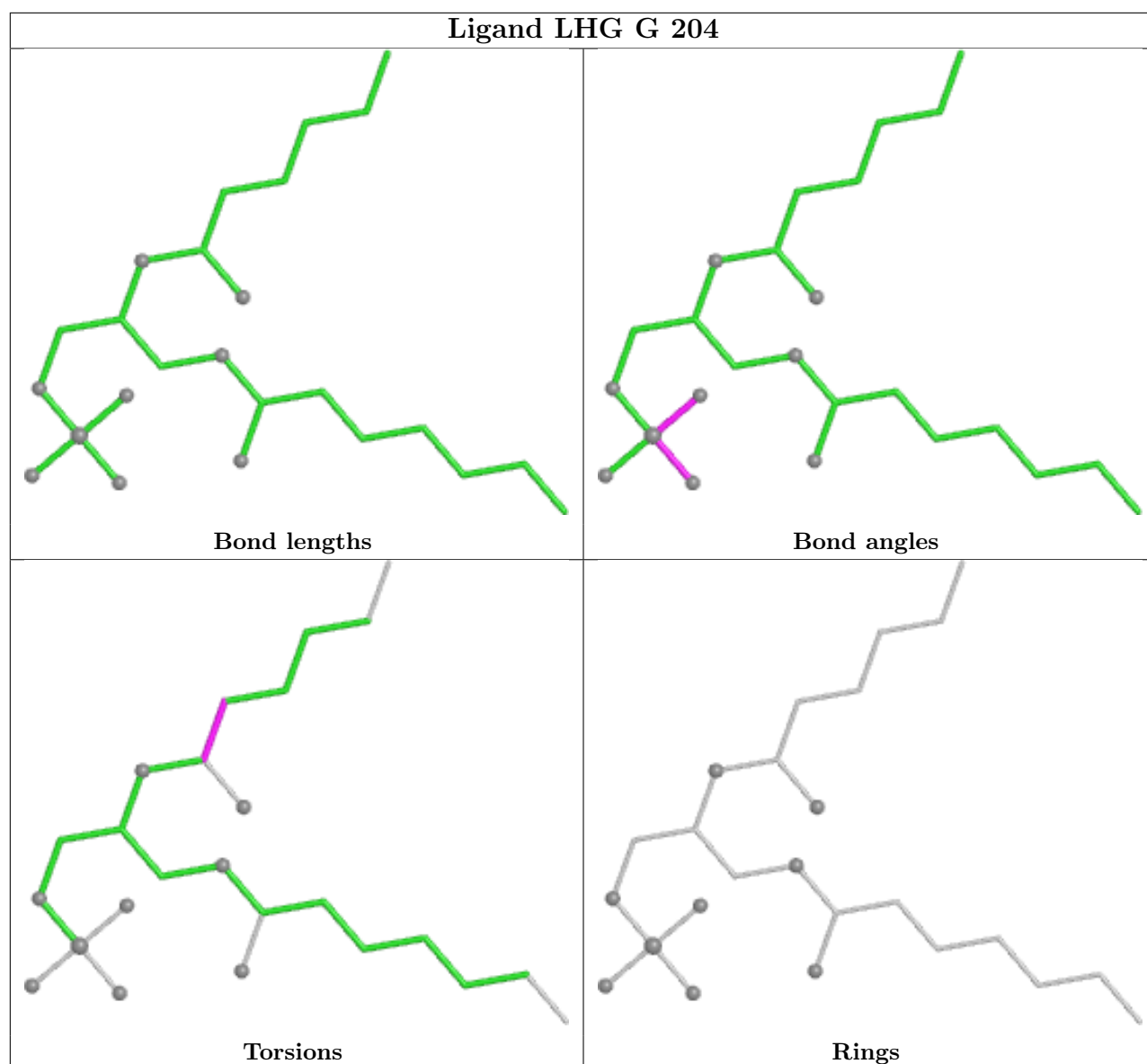


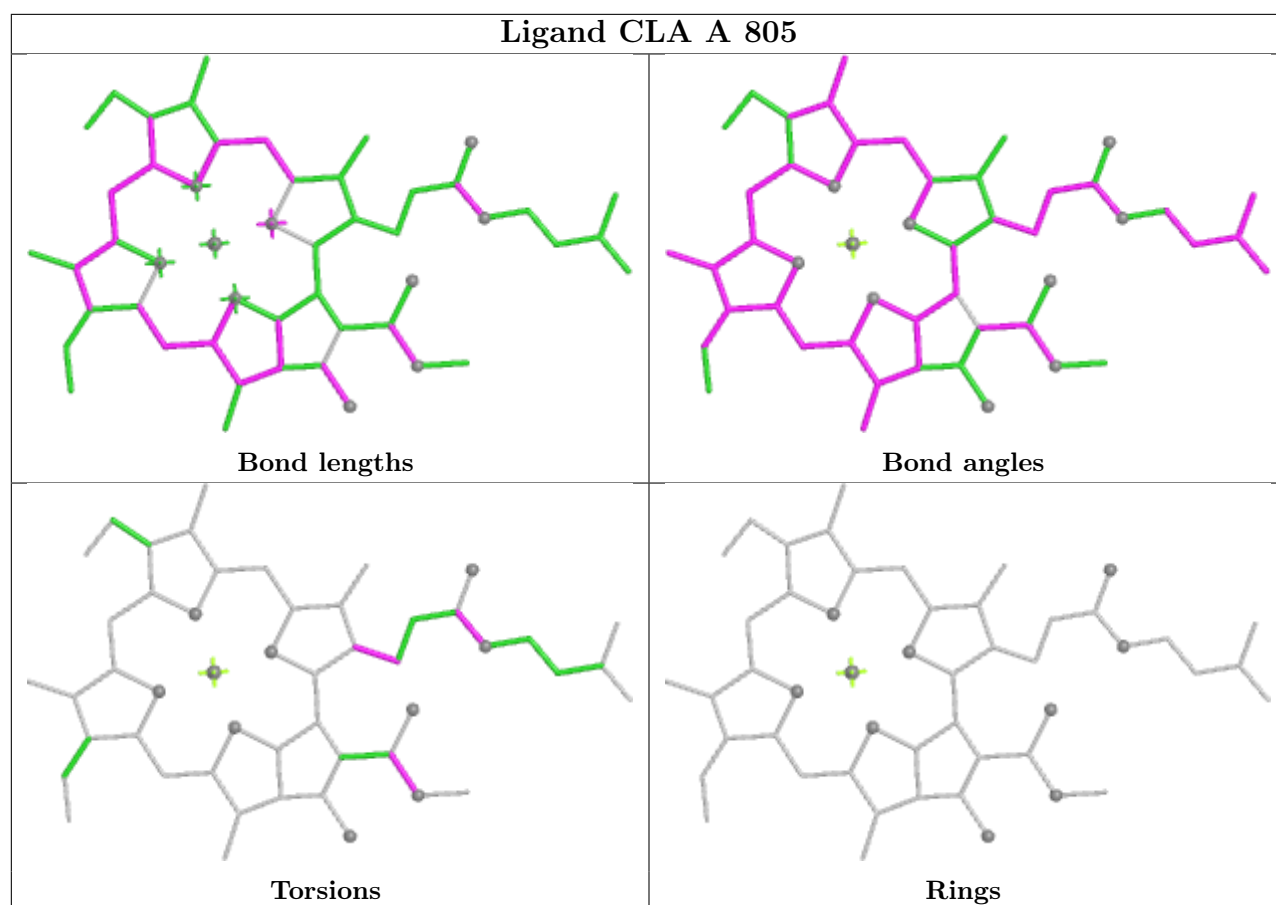
Ligand CLA A 832

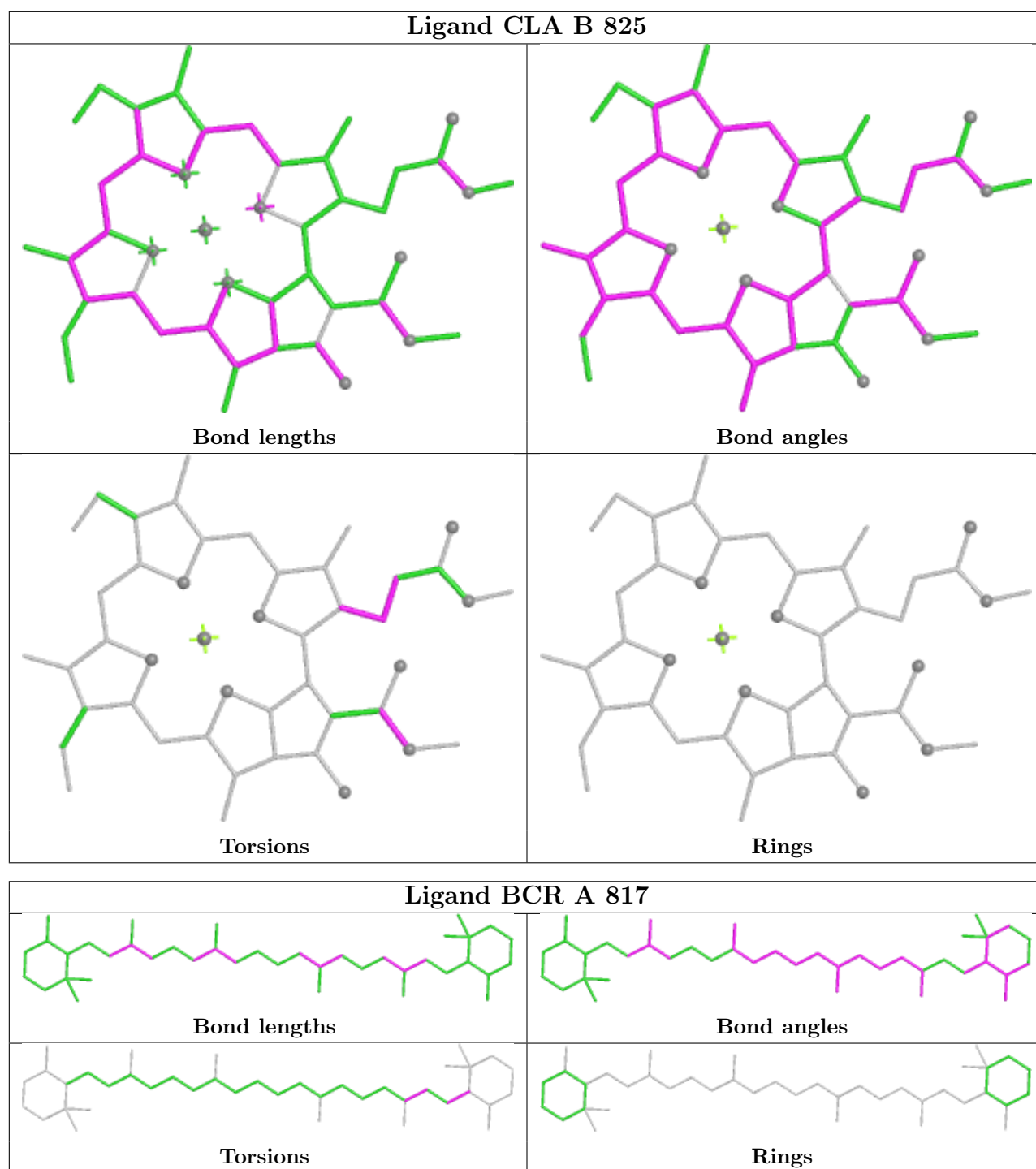


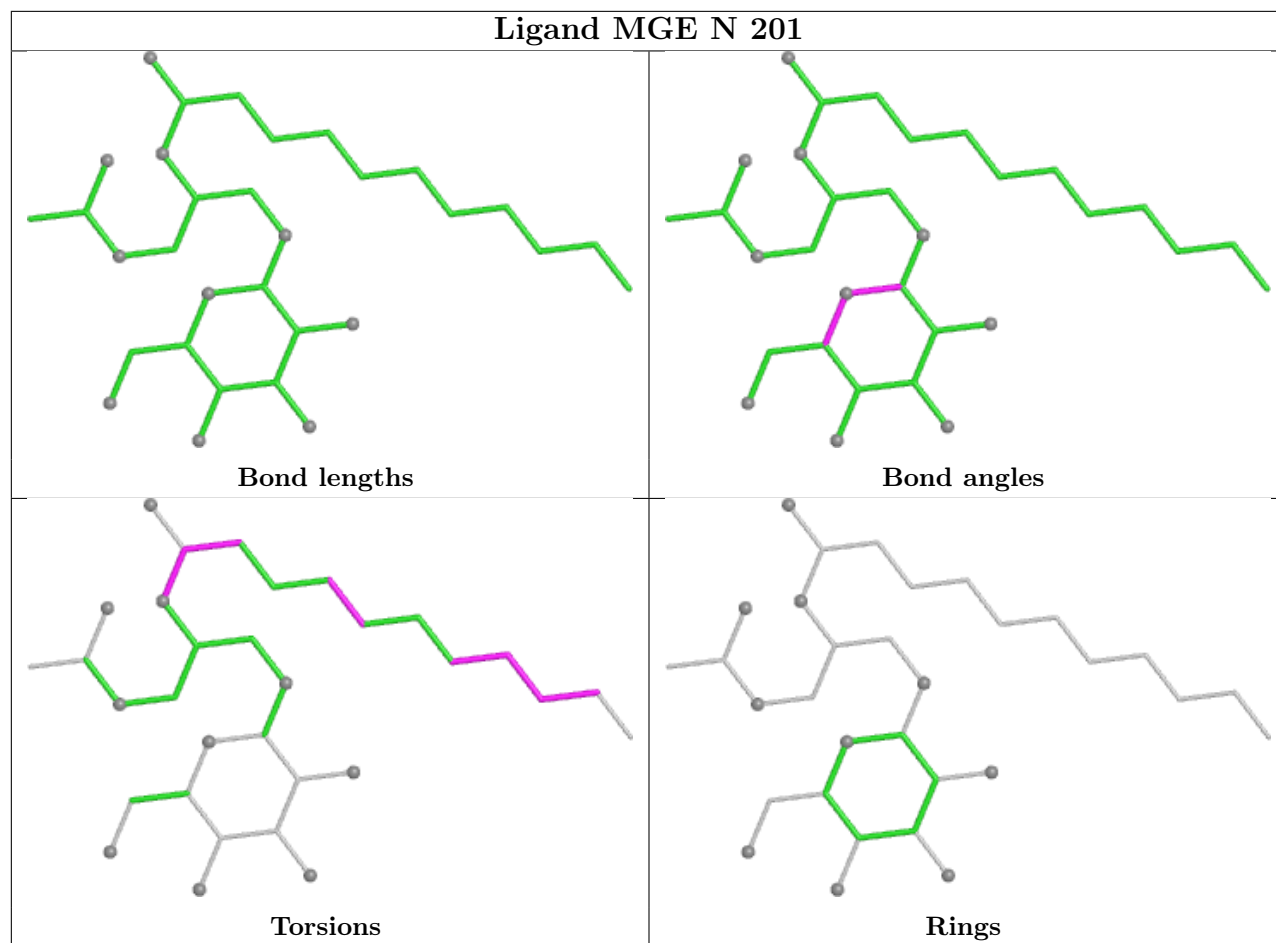




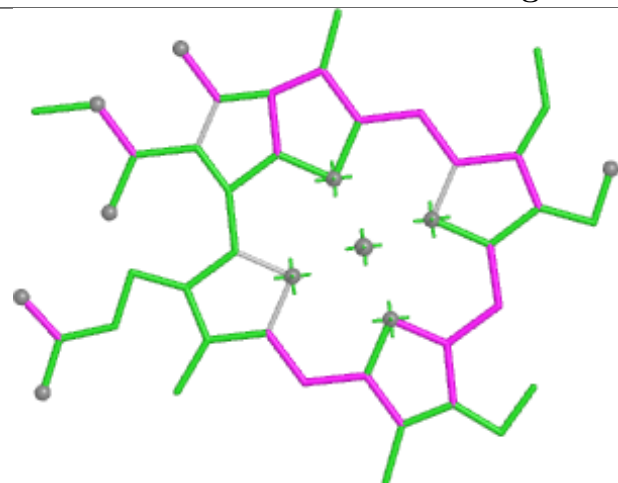




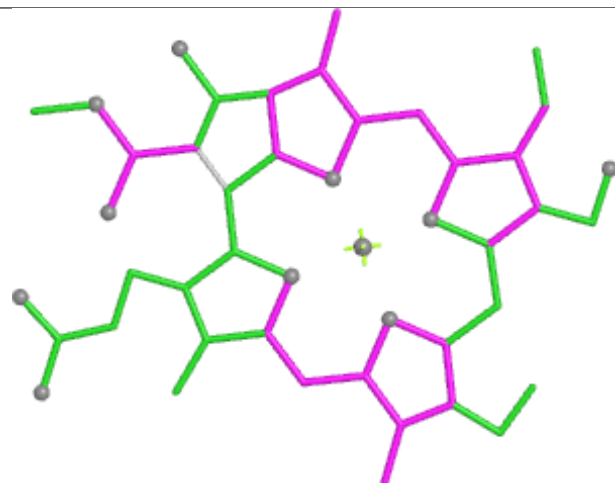




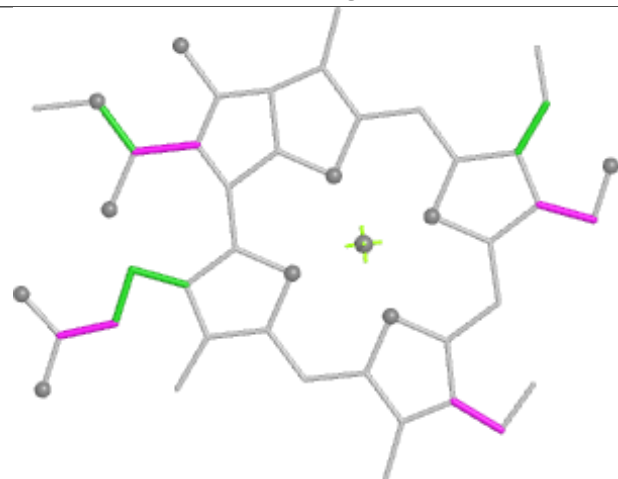
Ligand CHL 1 316



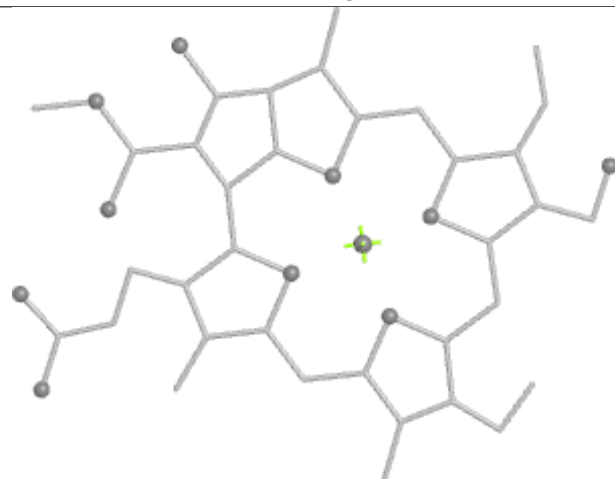
Bond lengths



Bond angles

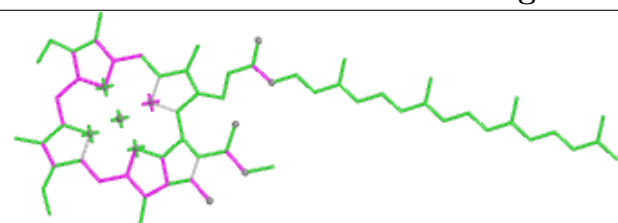


Torsions

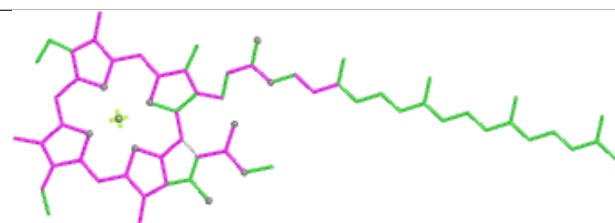


Rings

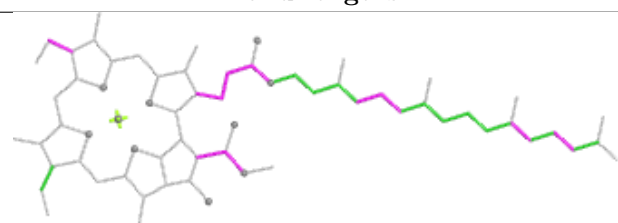
Ligand CLA B 850



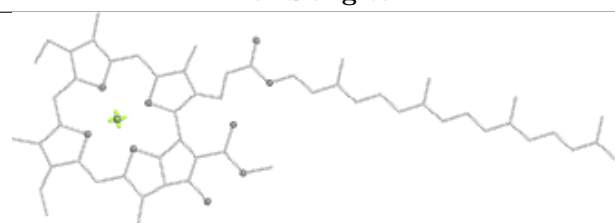
Bond lengths



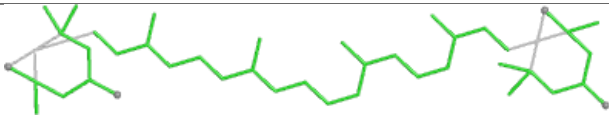
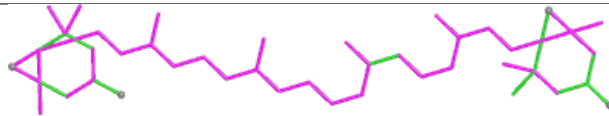
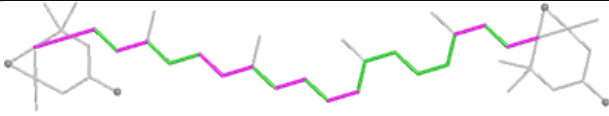
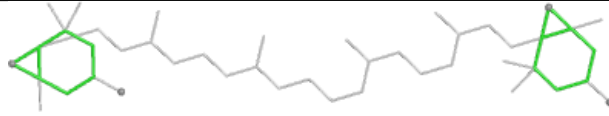
Bond angles

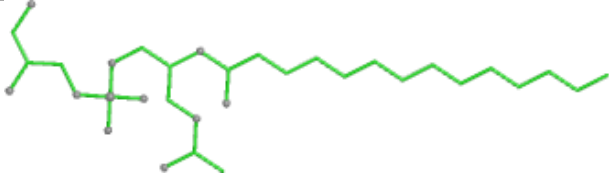
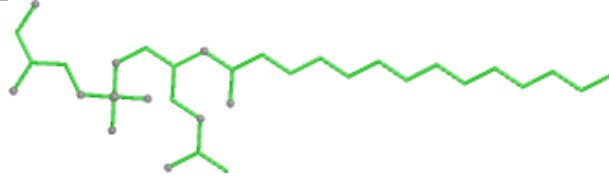
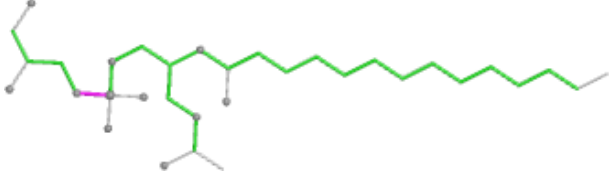
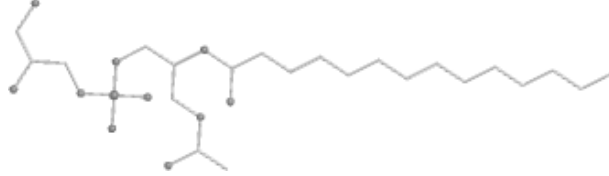


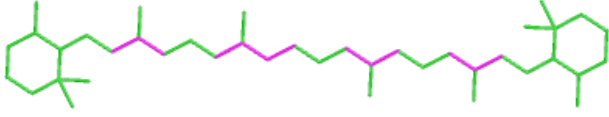
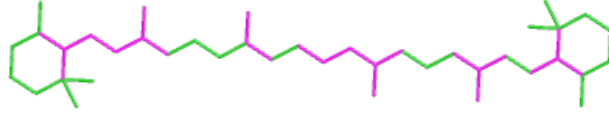
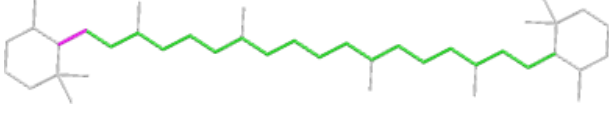
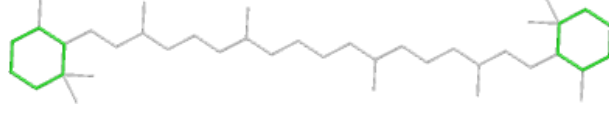
Torsions

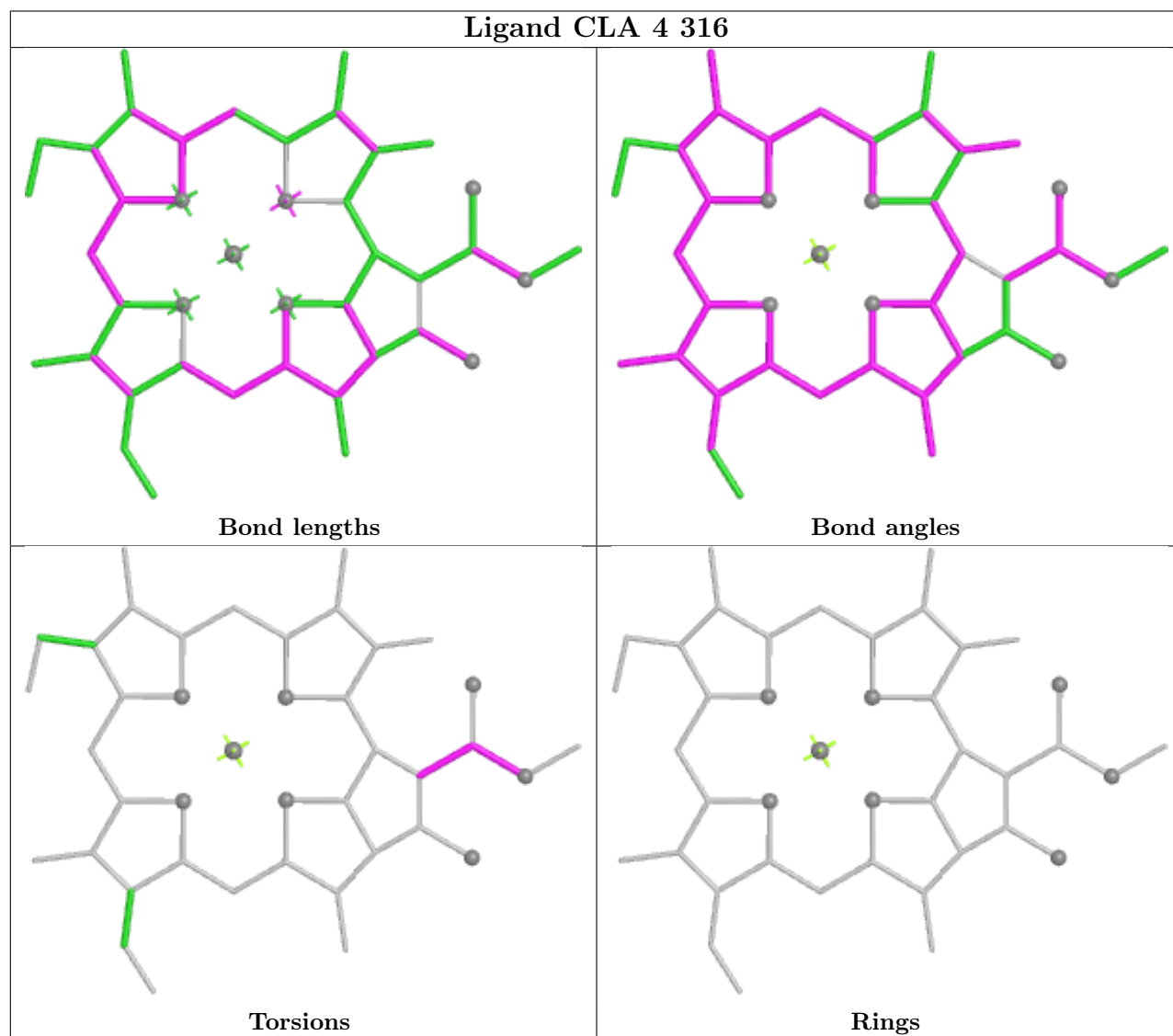
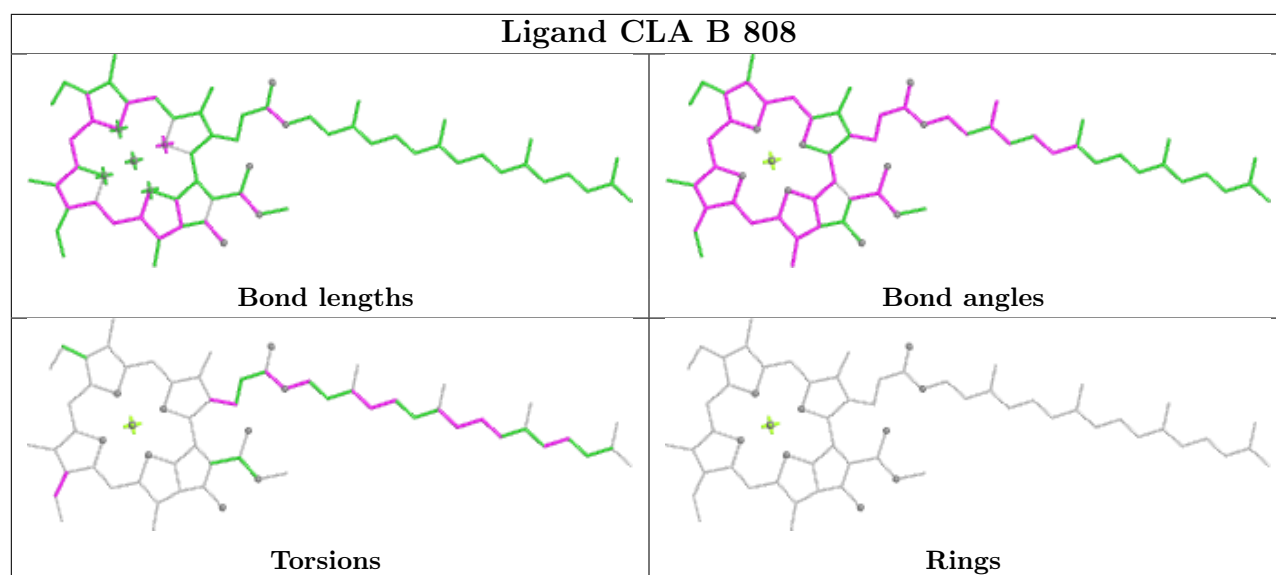


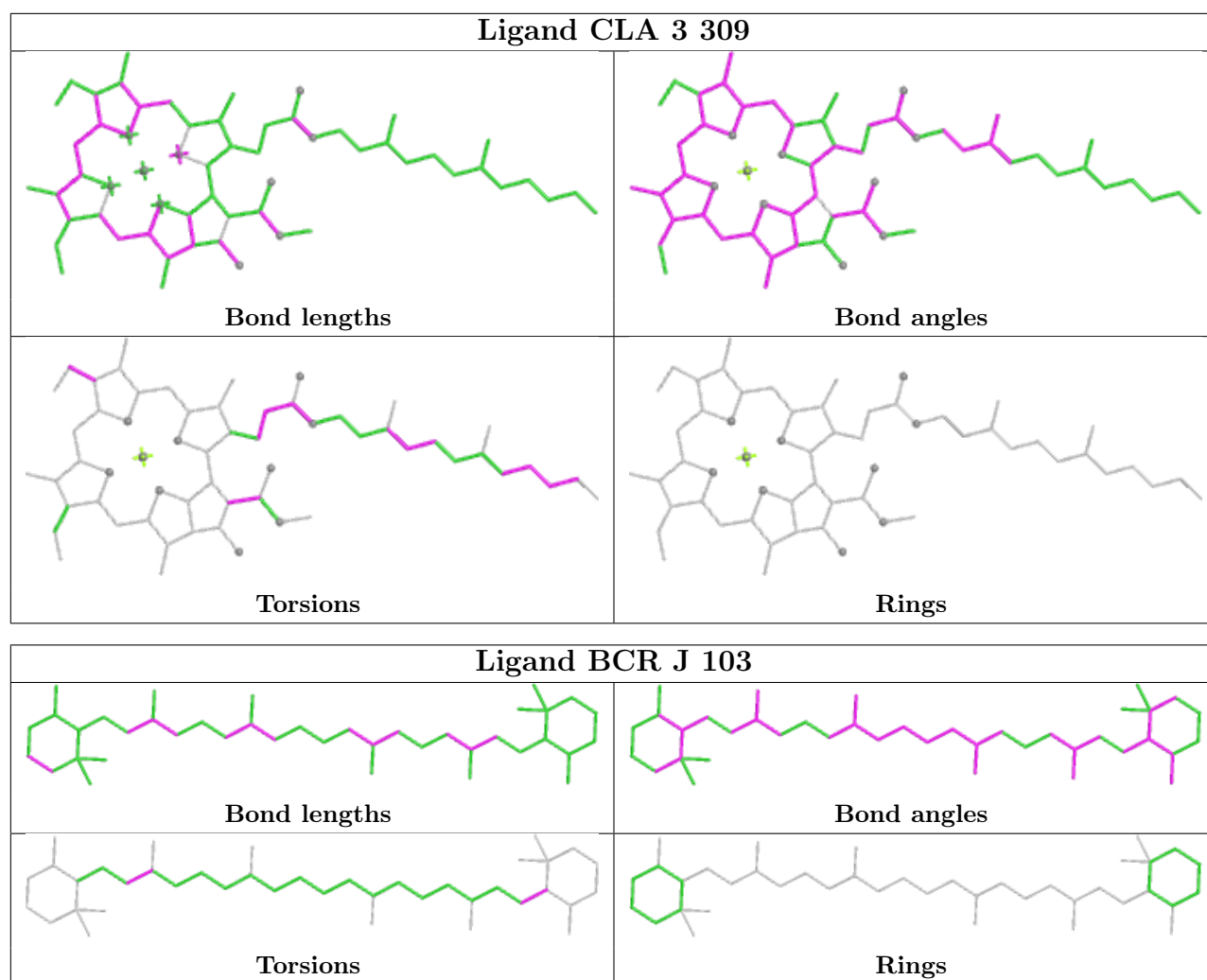
Rings

Ligand XAT 1 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

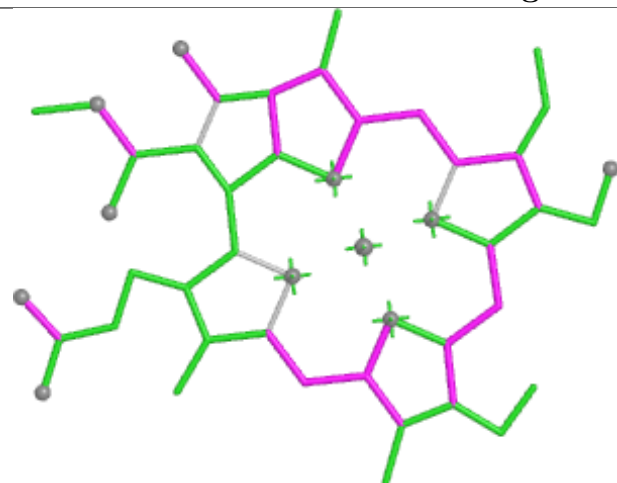
Ligand LHG A 823	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

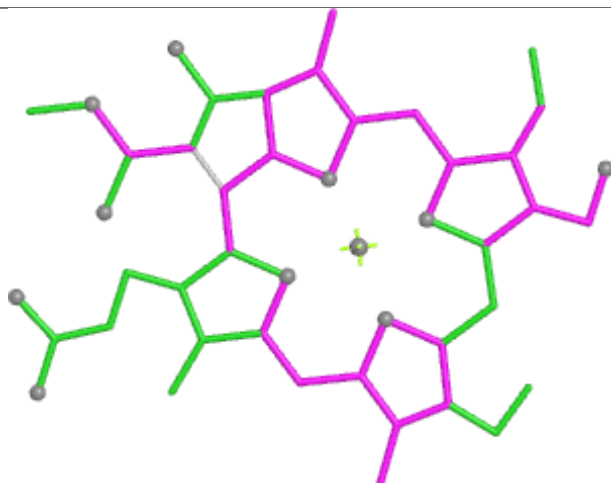




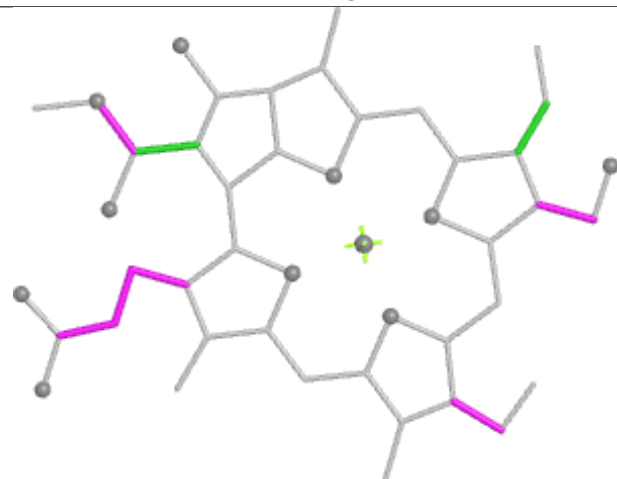
Ligand CHL 4 309



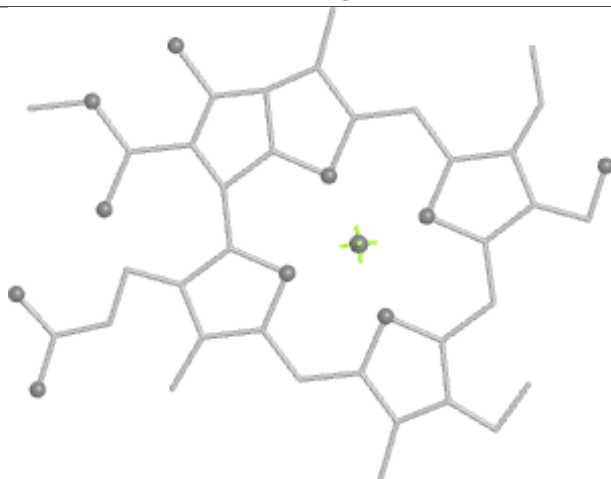
Bond lengths



Bond angles

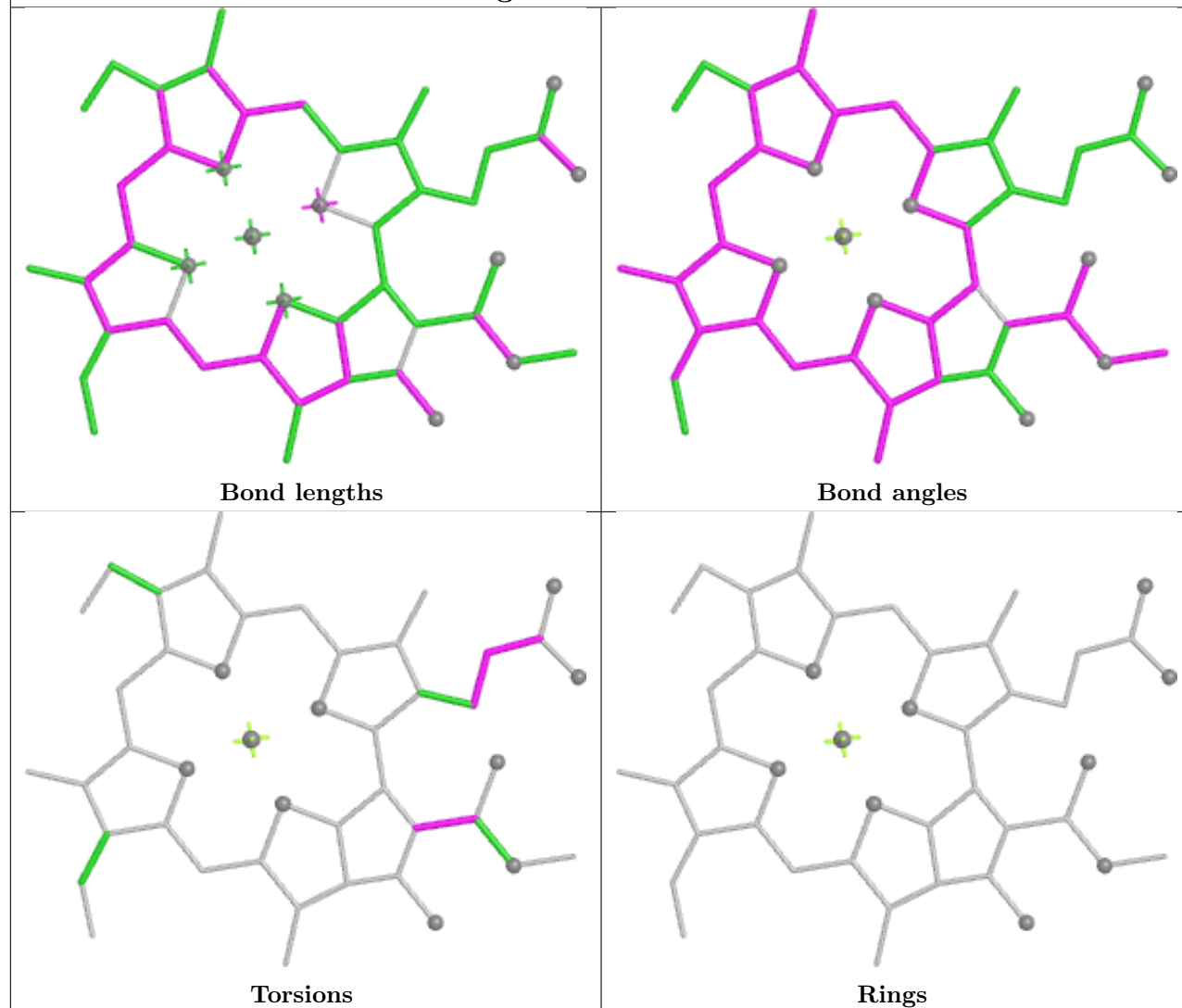


Torsions

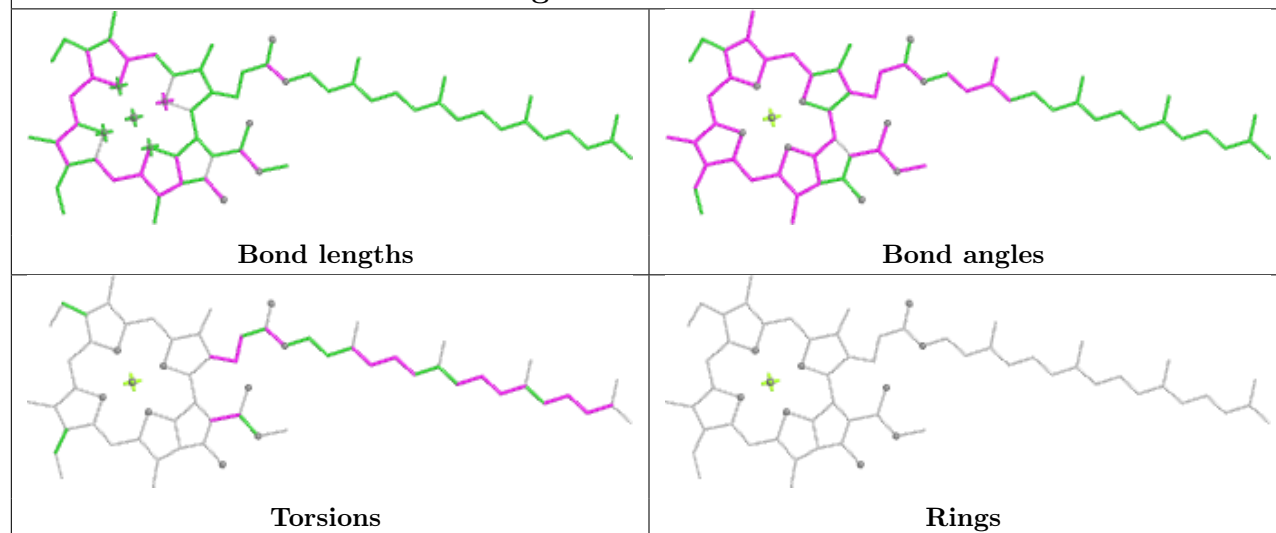


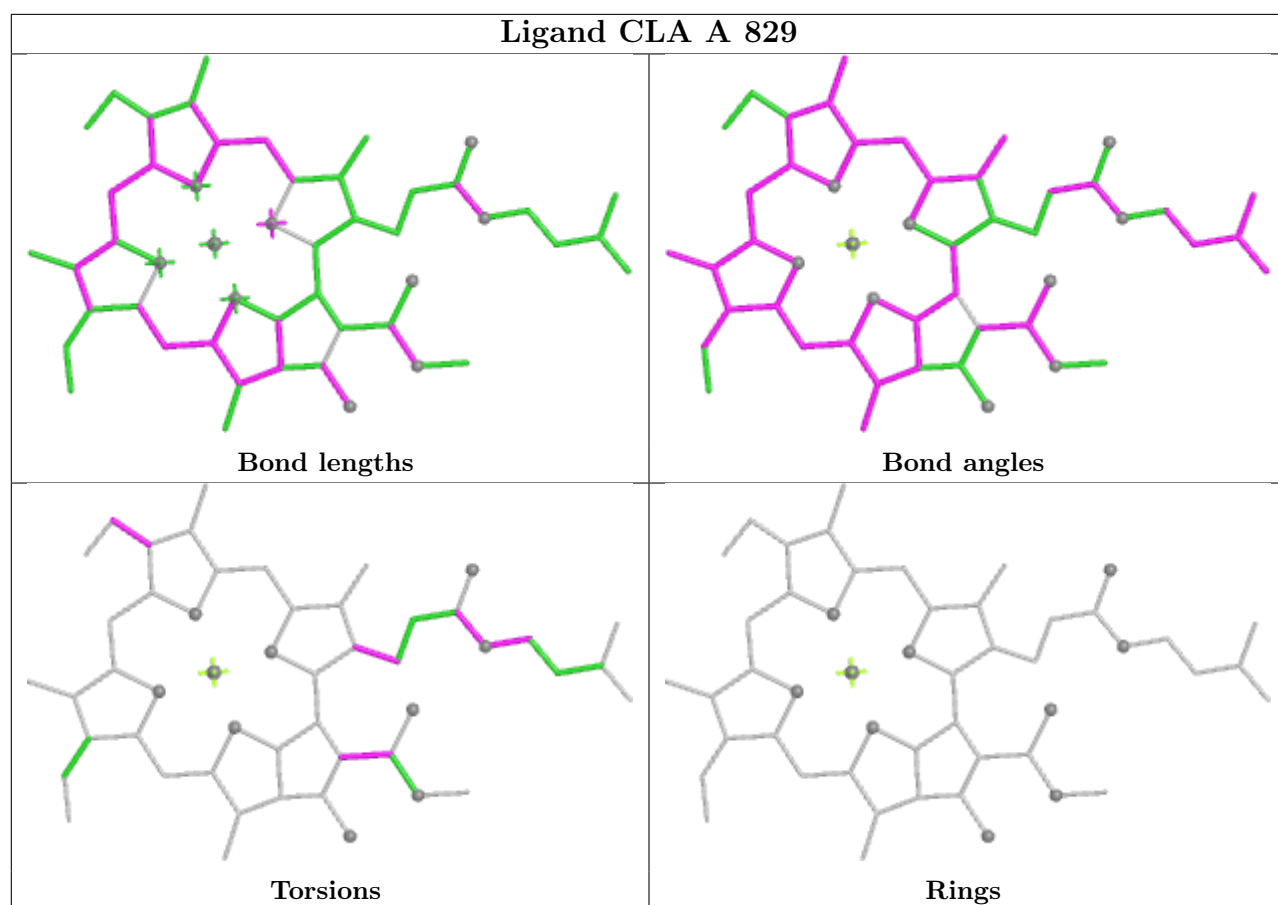
Rings

Ligand CLA 3 318

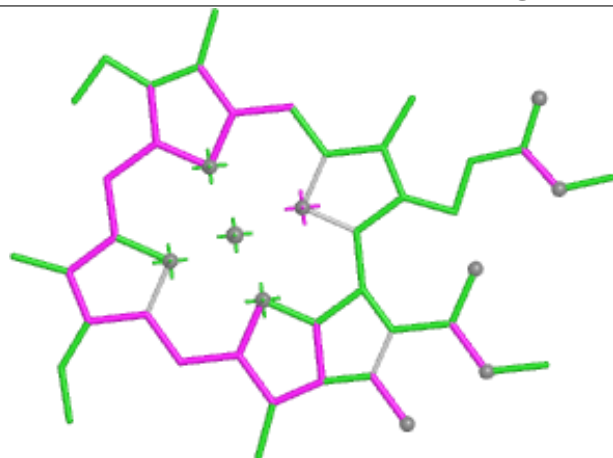


Ligand CLA A 810

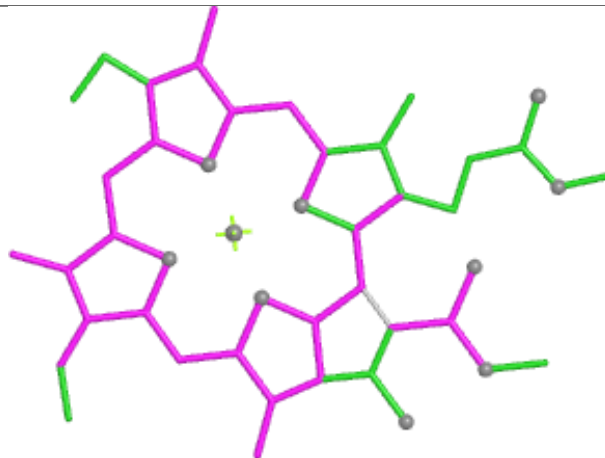




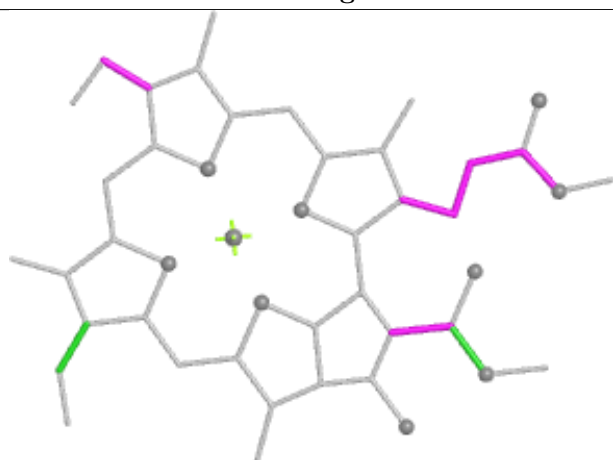
Ligand CLA X 313



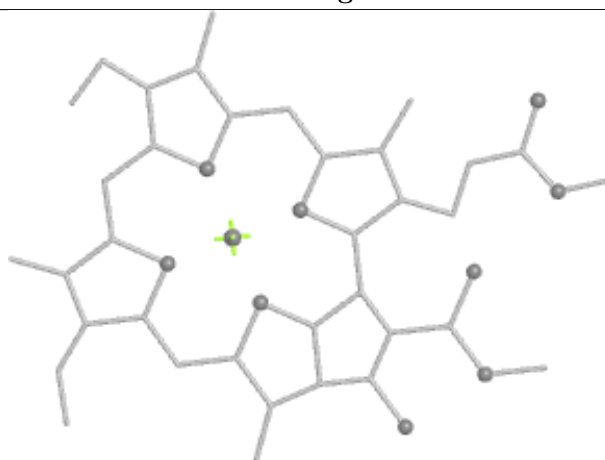
Bond lengths



Bond angles

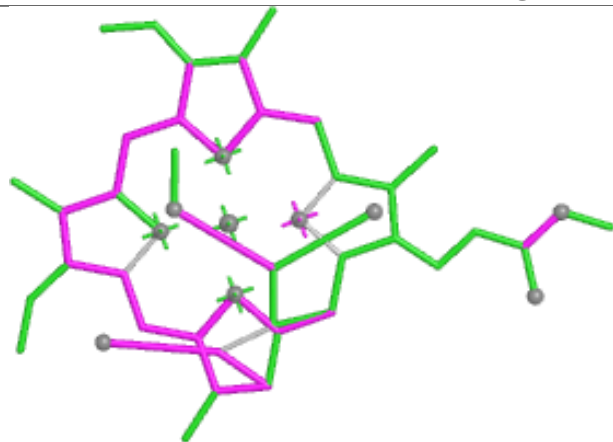


Torsions

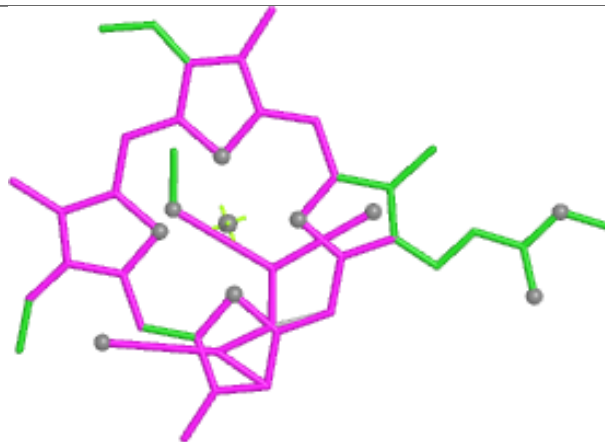


Rings

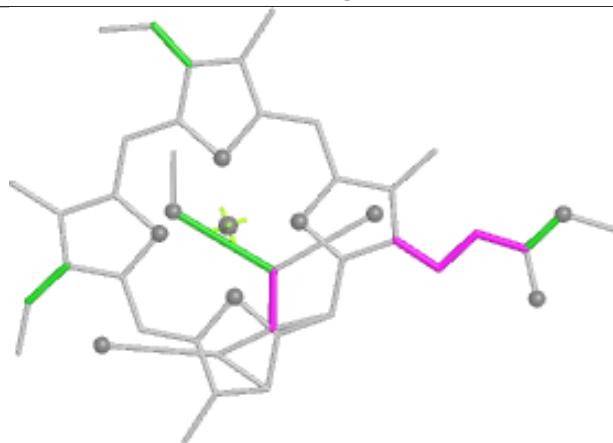
Ligand CLA X 304



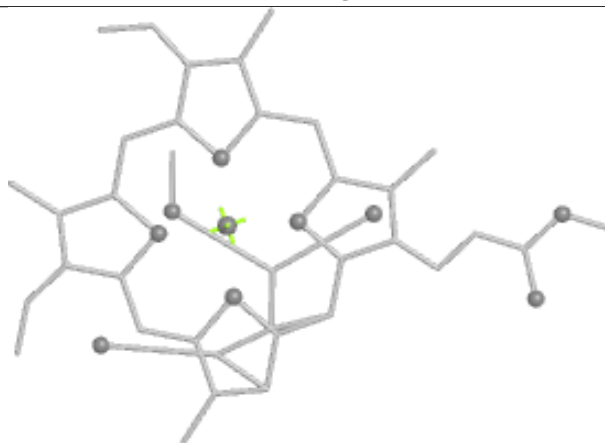
Bond lengths



Bond angles

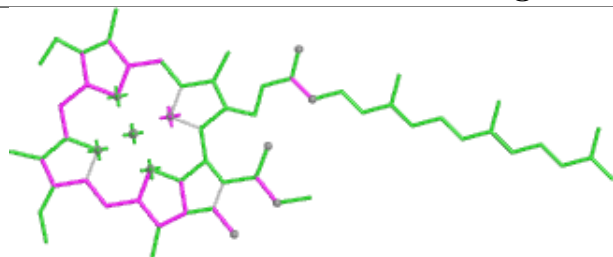


Torsions

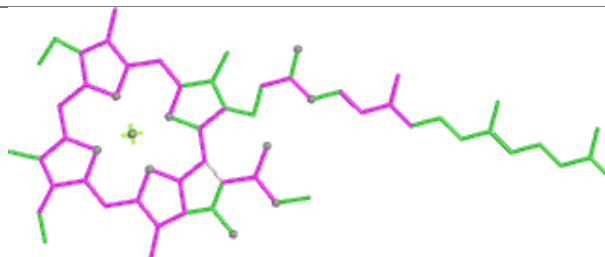


Rings

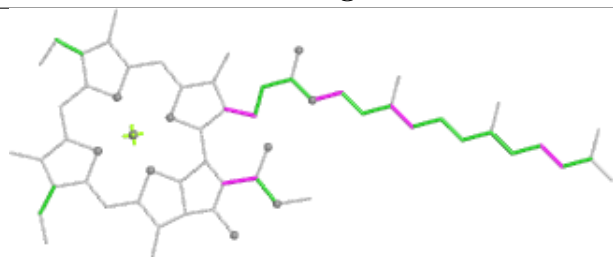
Ligand CLA A 836



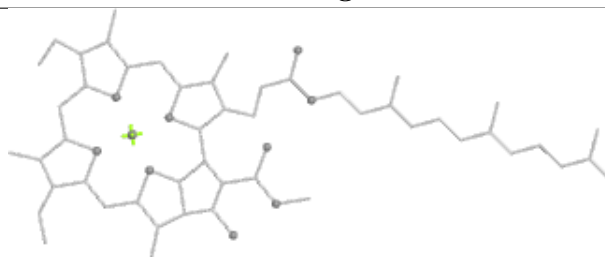
Bond lengths



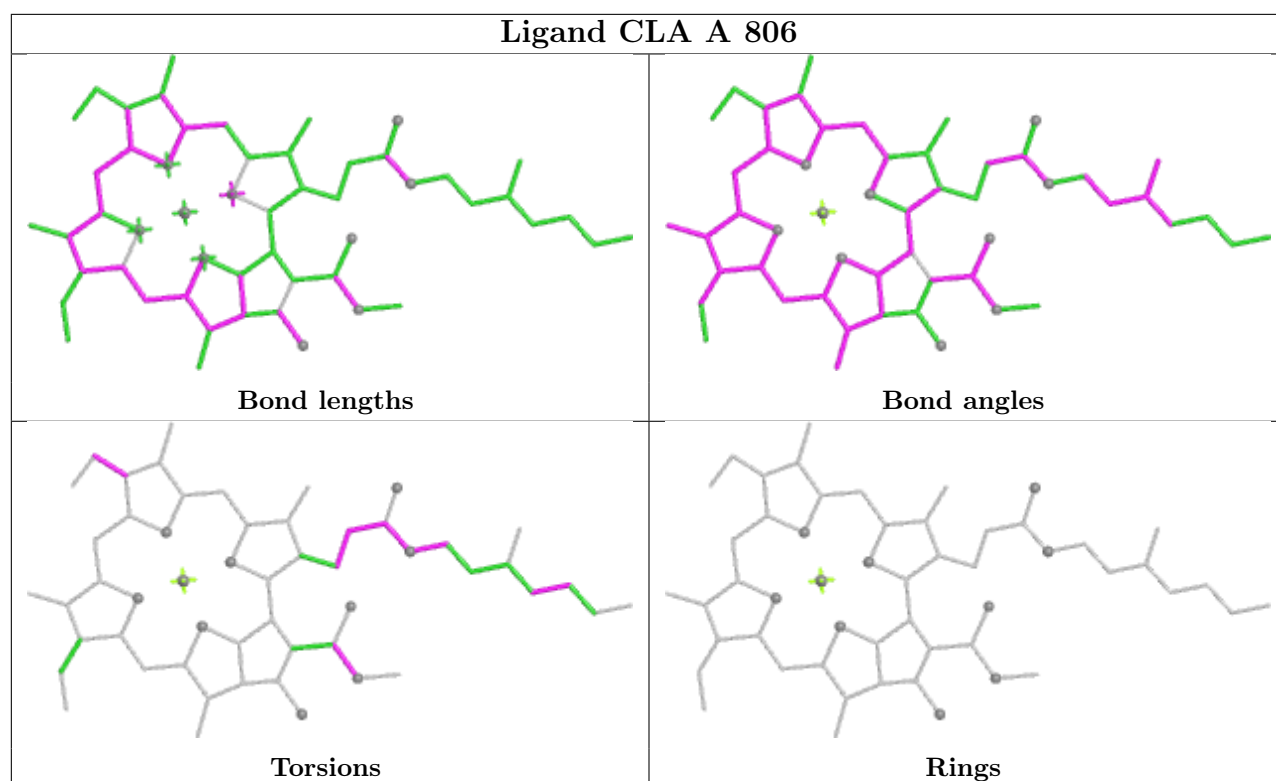
Bond angles



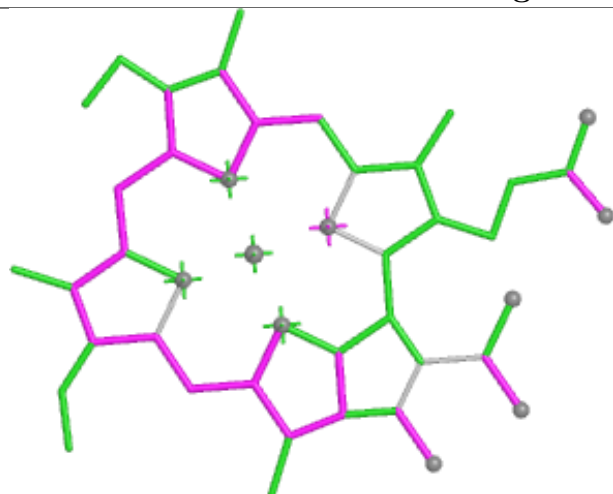
Torsions



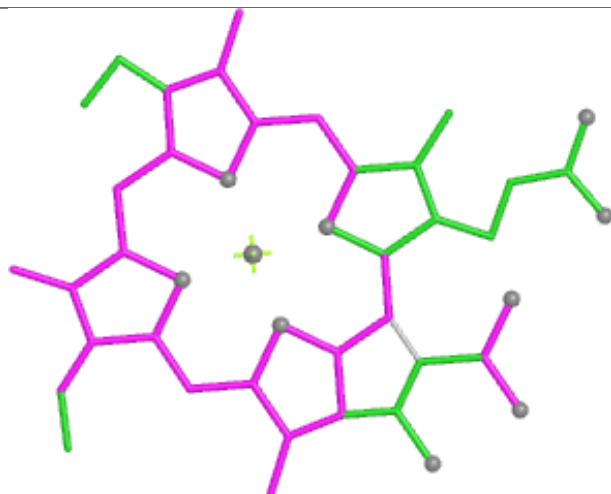
Rings



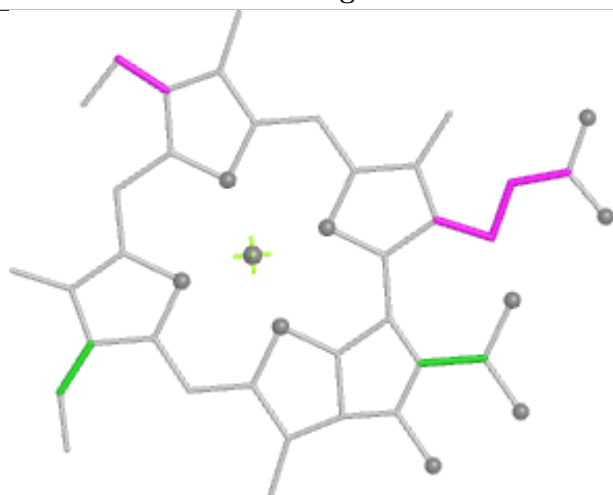
Ligand CLA K 202



Bond lengths



Bond angles

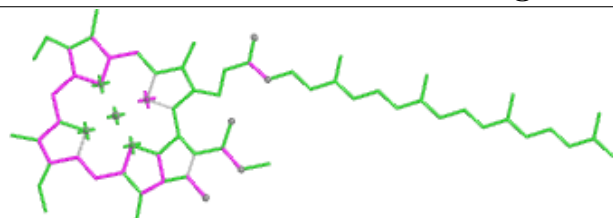


Torsions

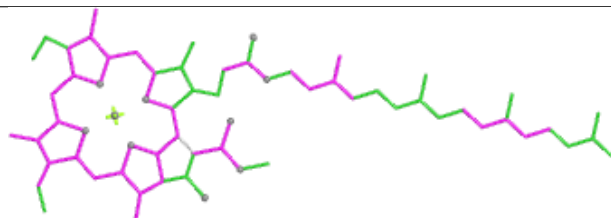


Rings

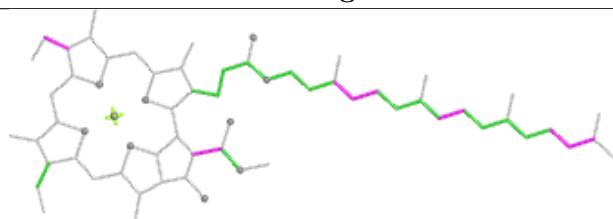
Ligand CLA A 850



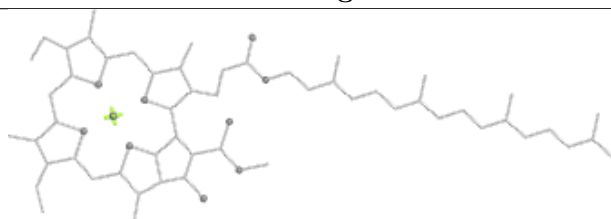
Bond lengths



Bond angles

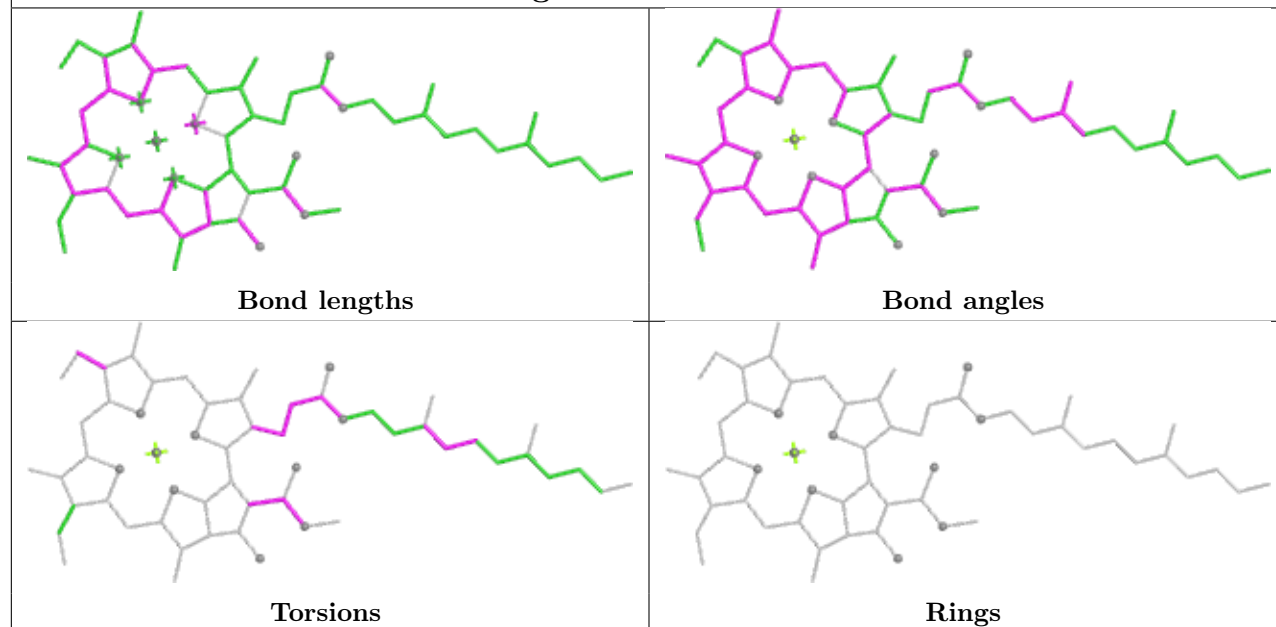


Torsions

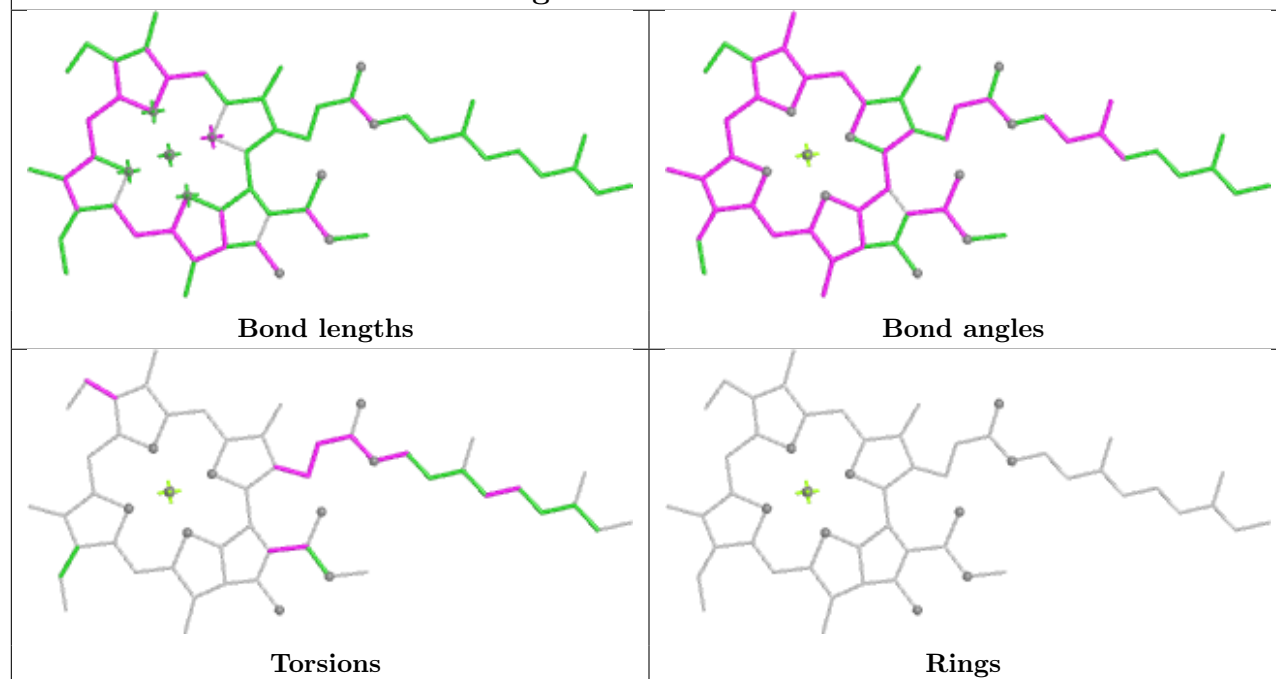


Rings

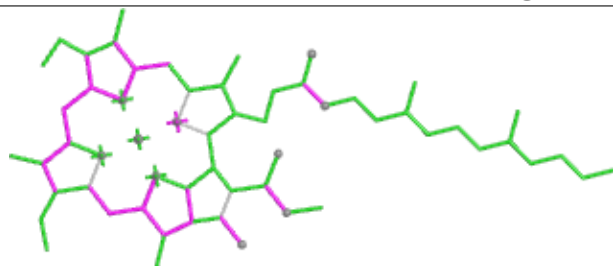
Ligand CLA B 815



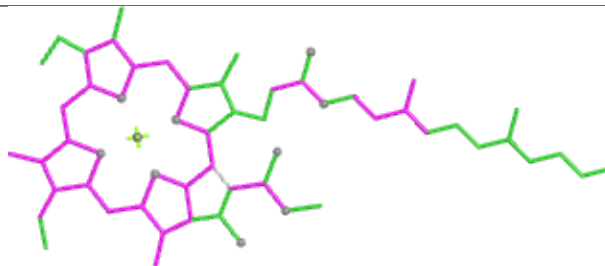
Ligand CLA B 833



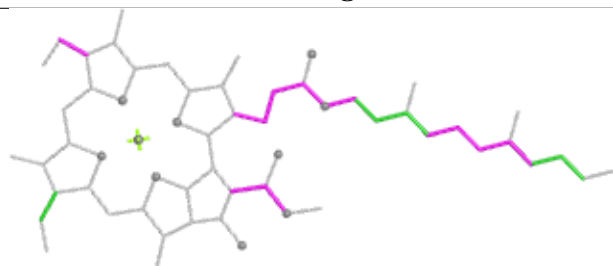
Ligand CLA 3 310



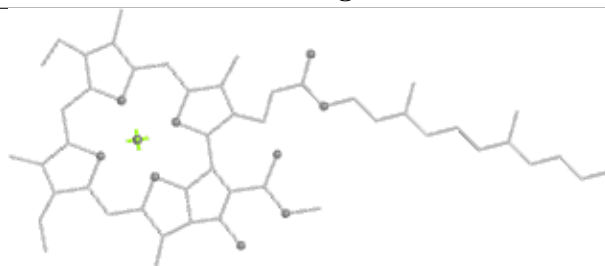
Bond lengths



Bond angles

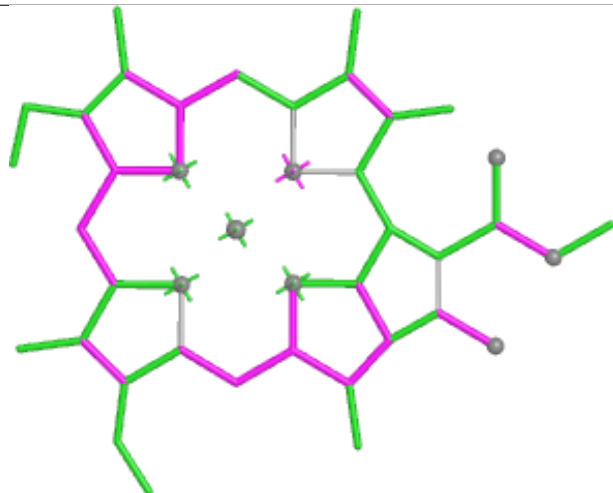


Torsions



Rings

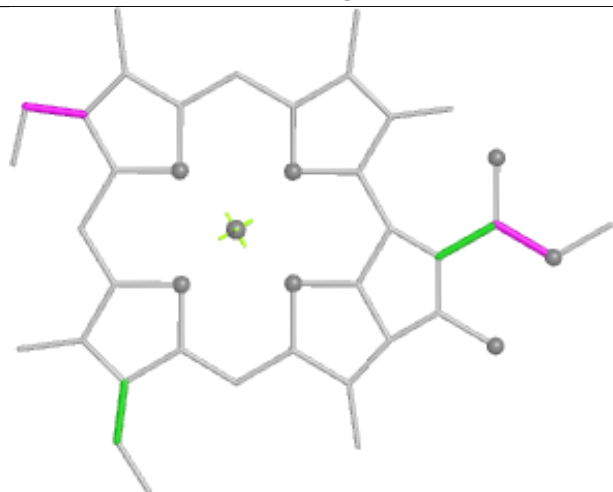
Ligand CLA 1 308



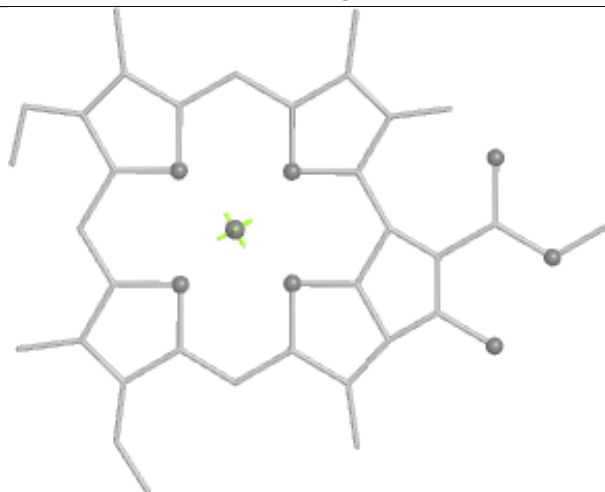
Bond lengths



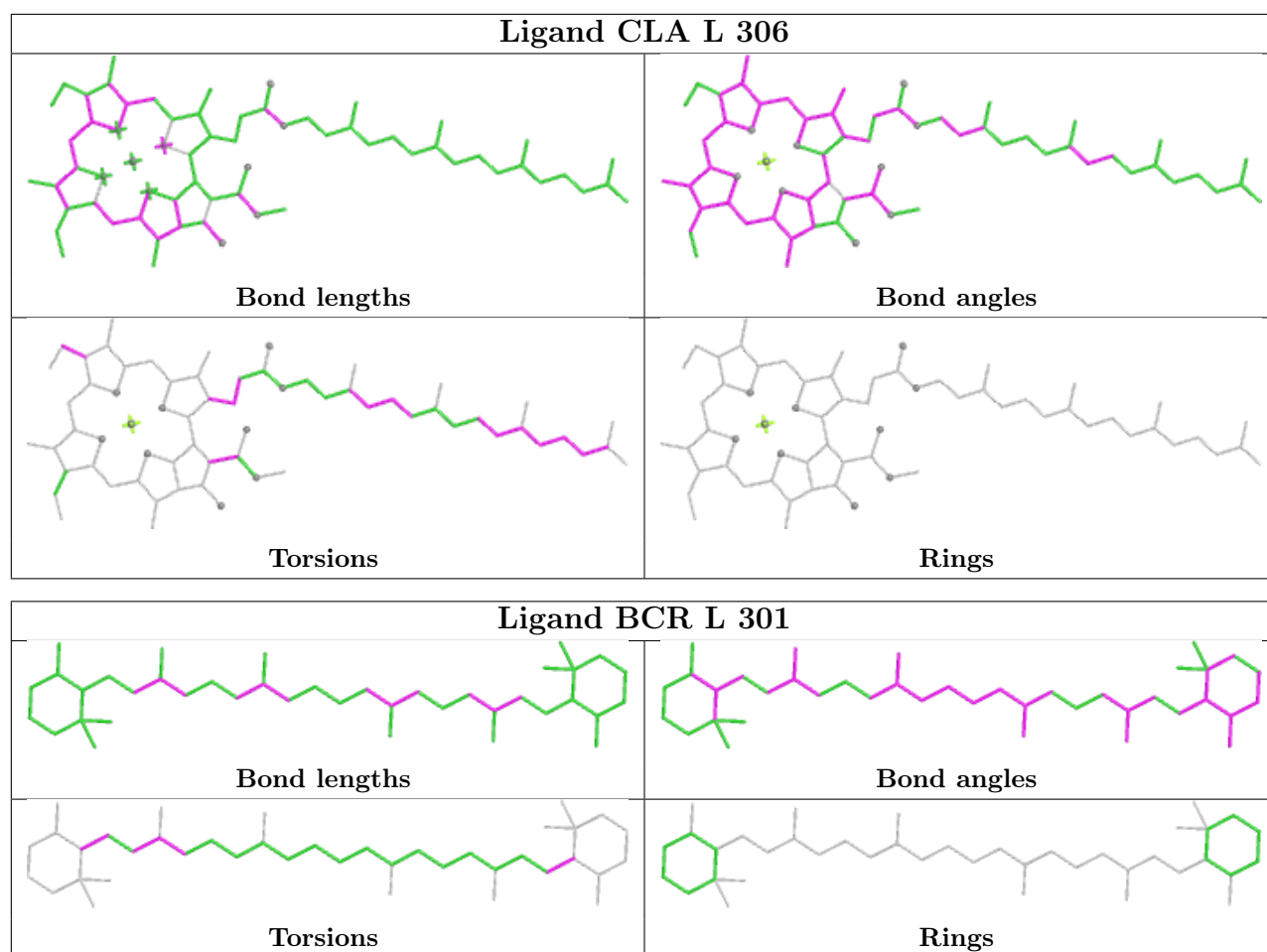
Bond angles



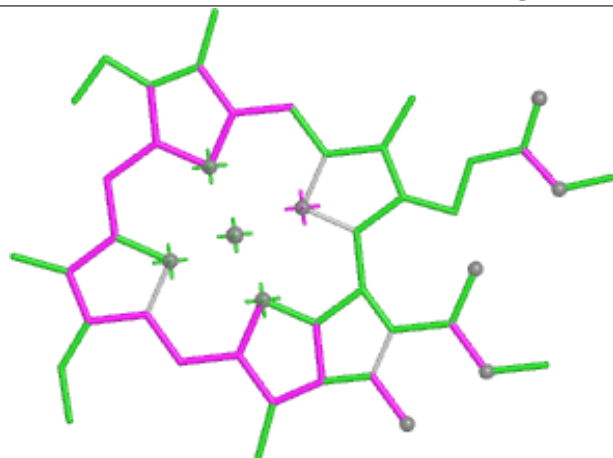
Torsions



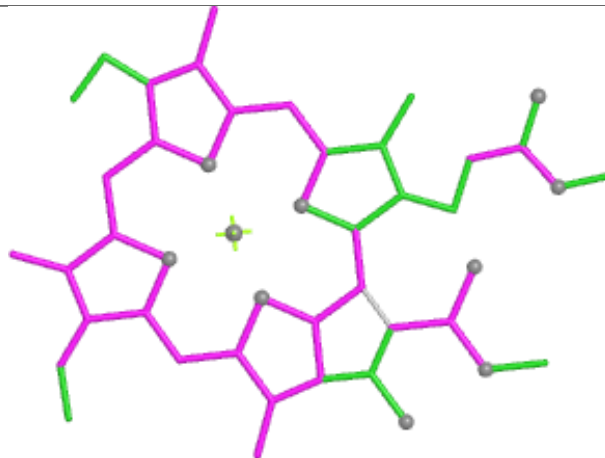
Rings



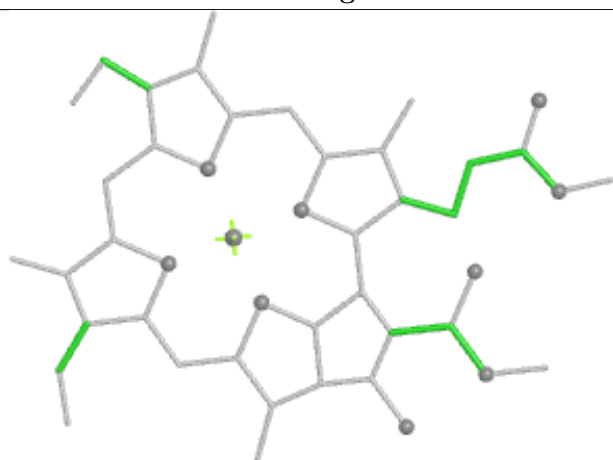
Ligand CLA X 301



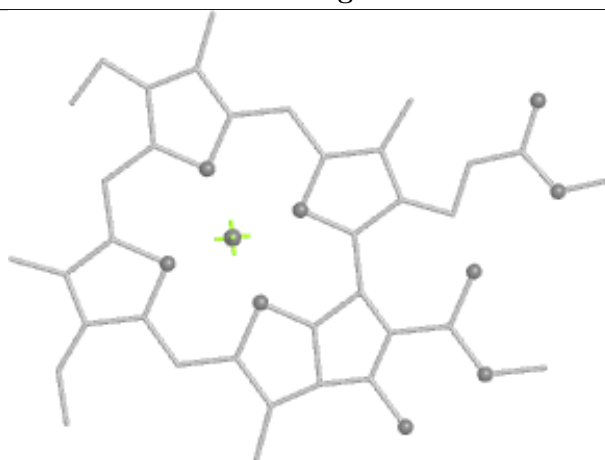
Bond lengths



Bond angles

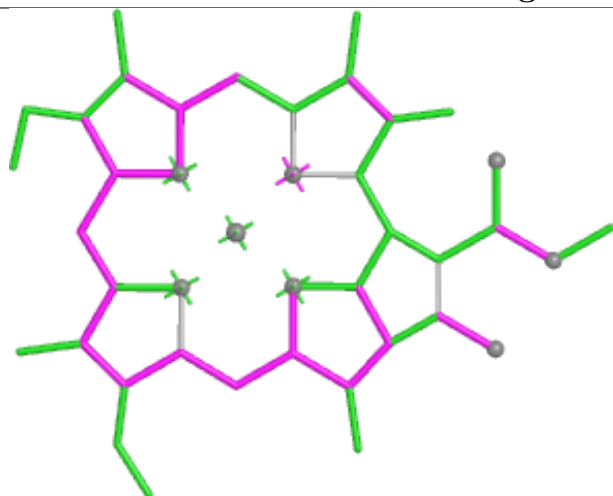


Torsions

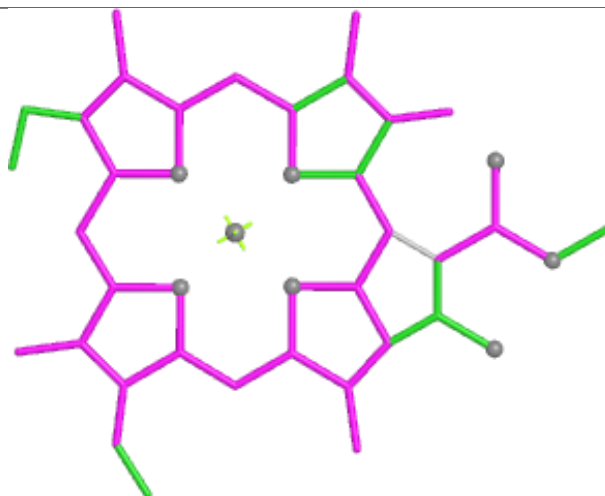


Rings

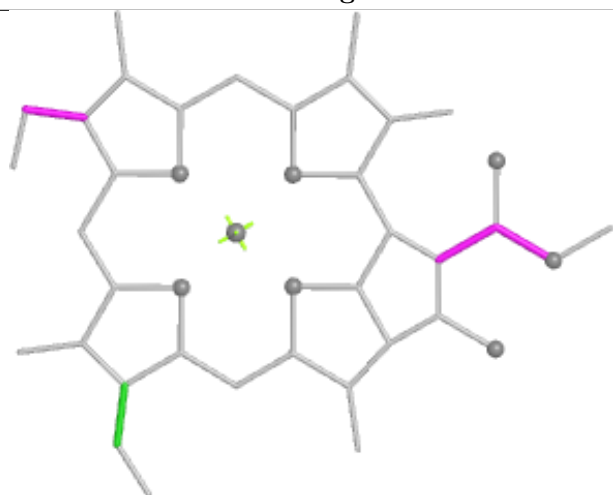
Ligand CLA 3 315



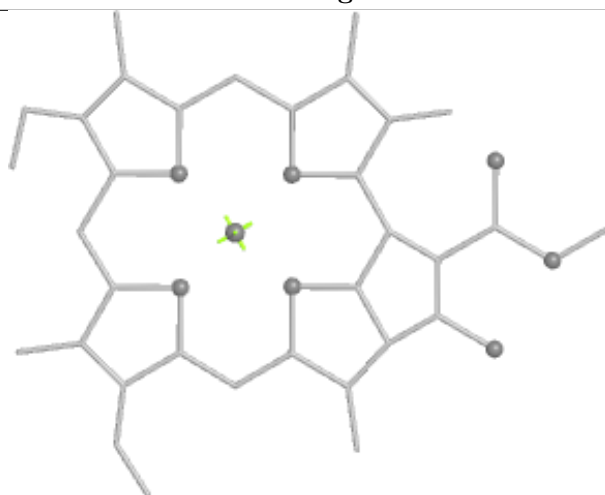
Bond lengths



Bond angles

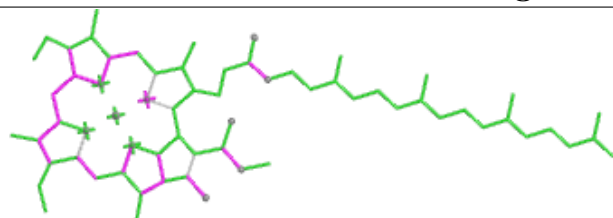


Torsions

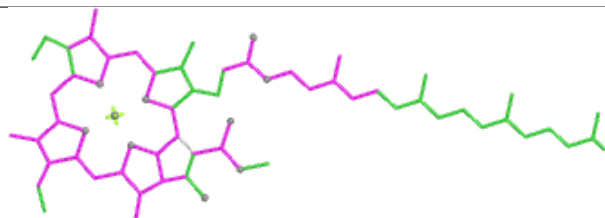


Rings

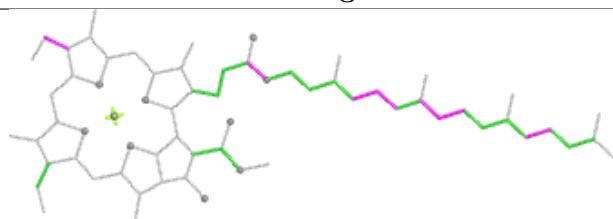
Ligand CLA B 814



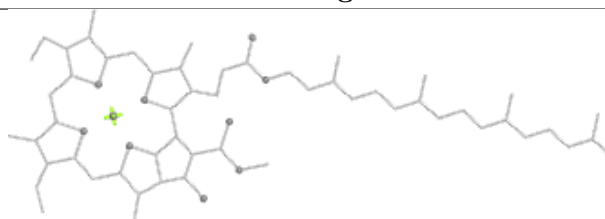
Bond lengths



Bond angles

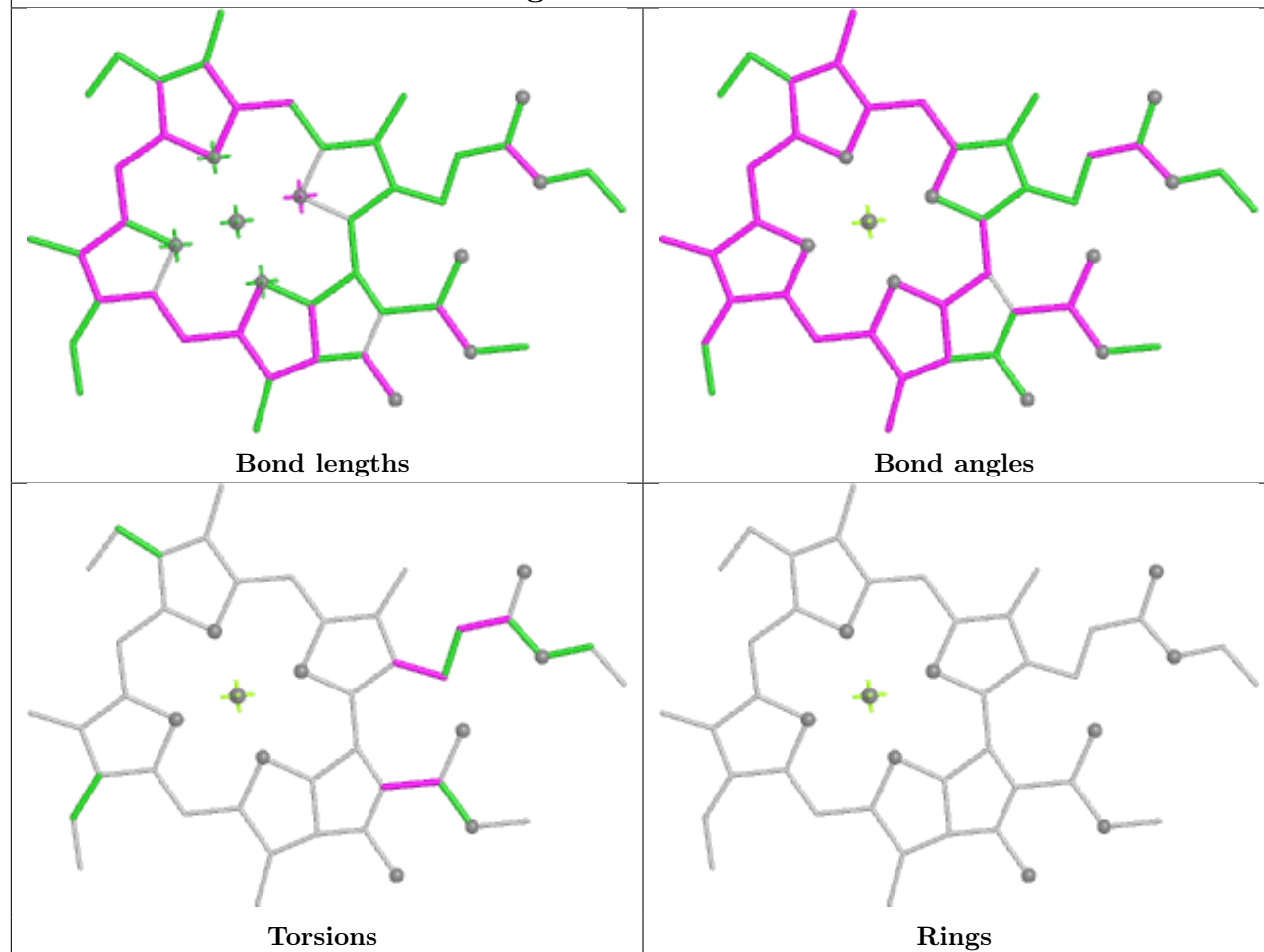


Torsions

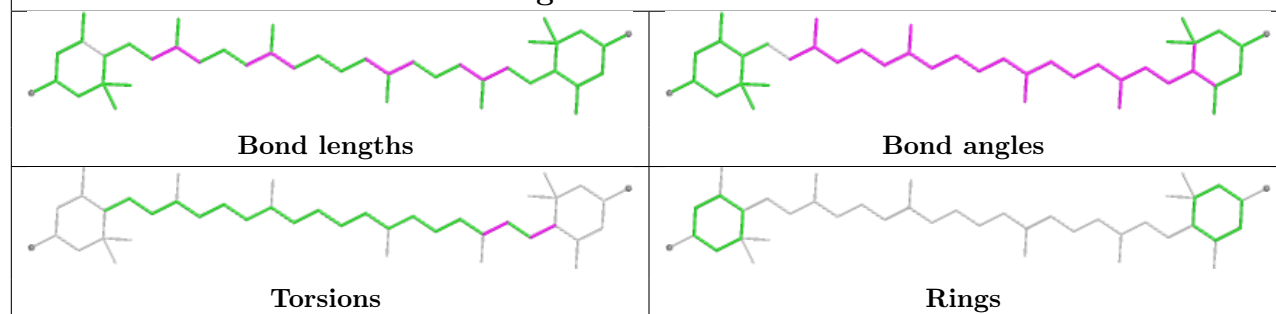


Rings

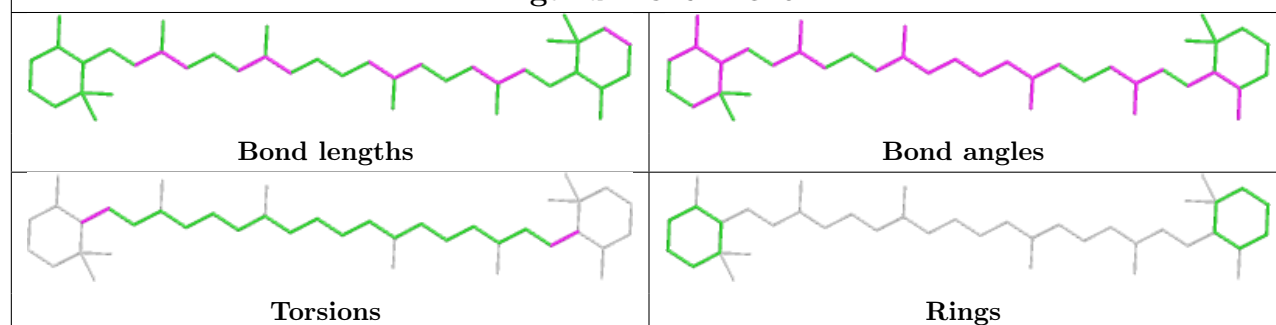
Ligand CLA O 209

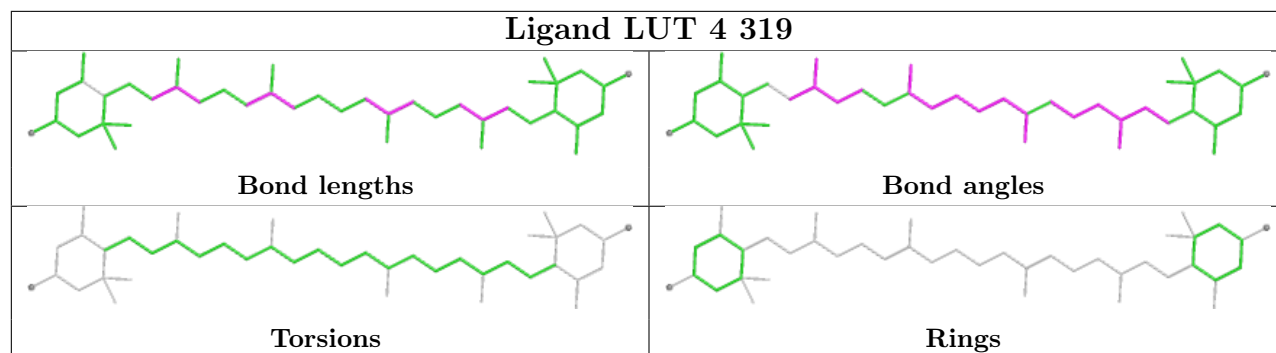
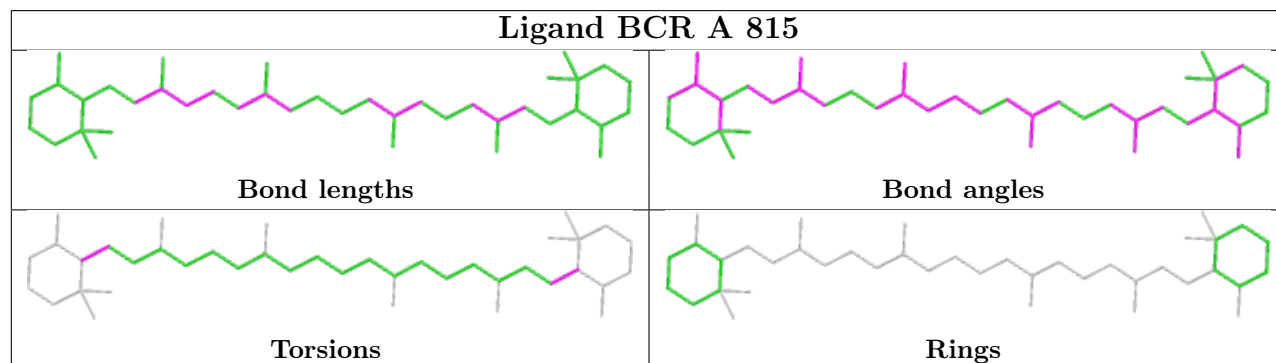
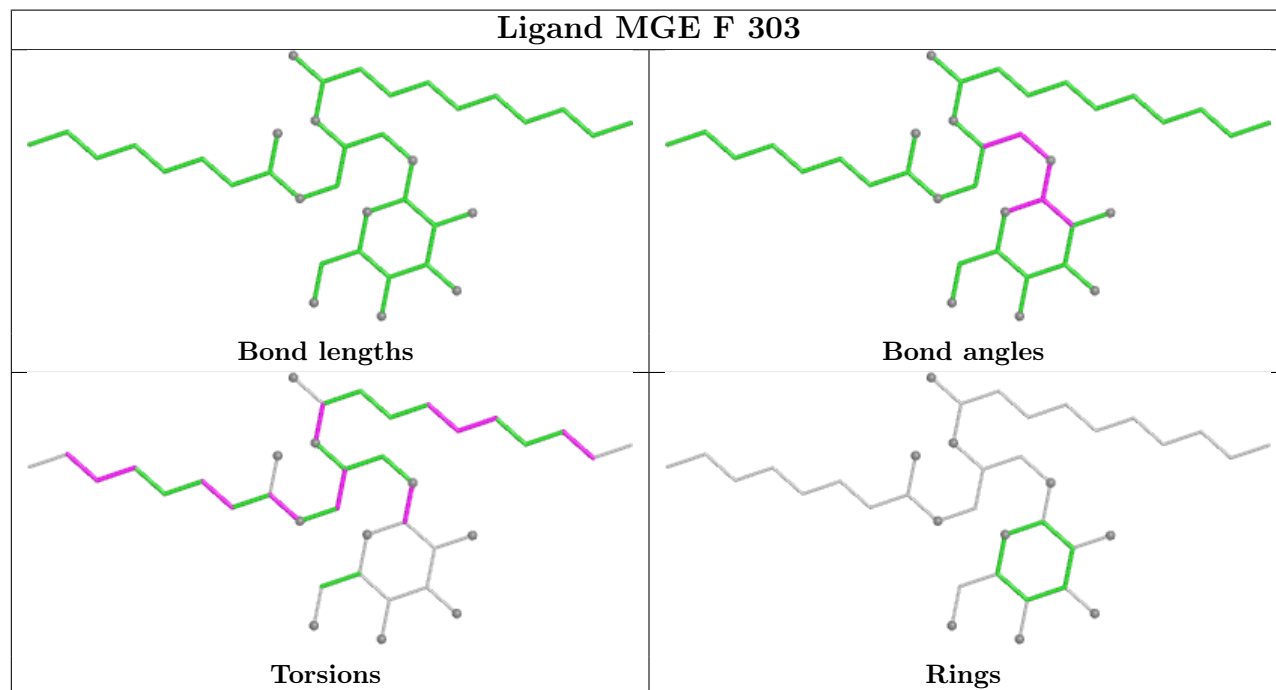


Ligand LUT 4 322

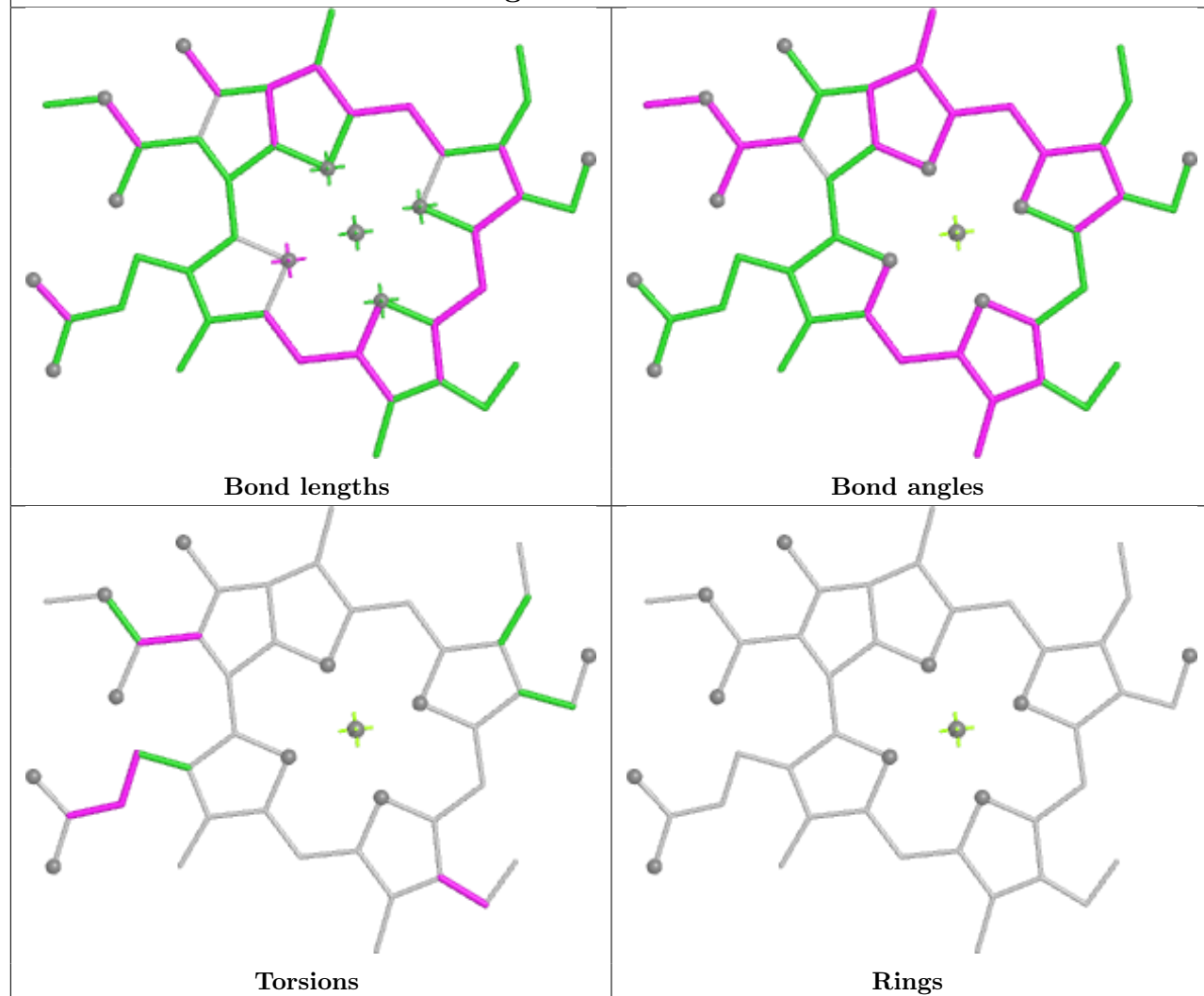


Ligand BCR A 819

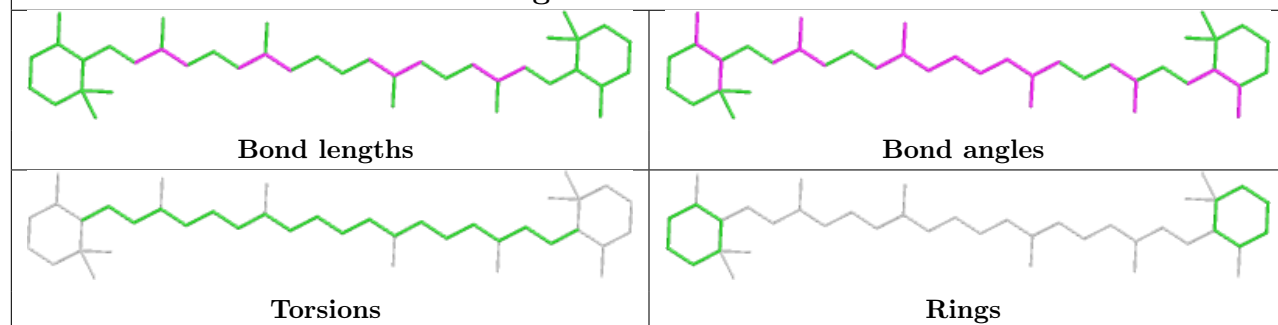


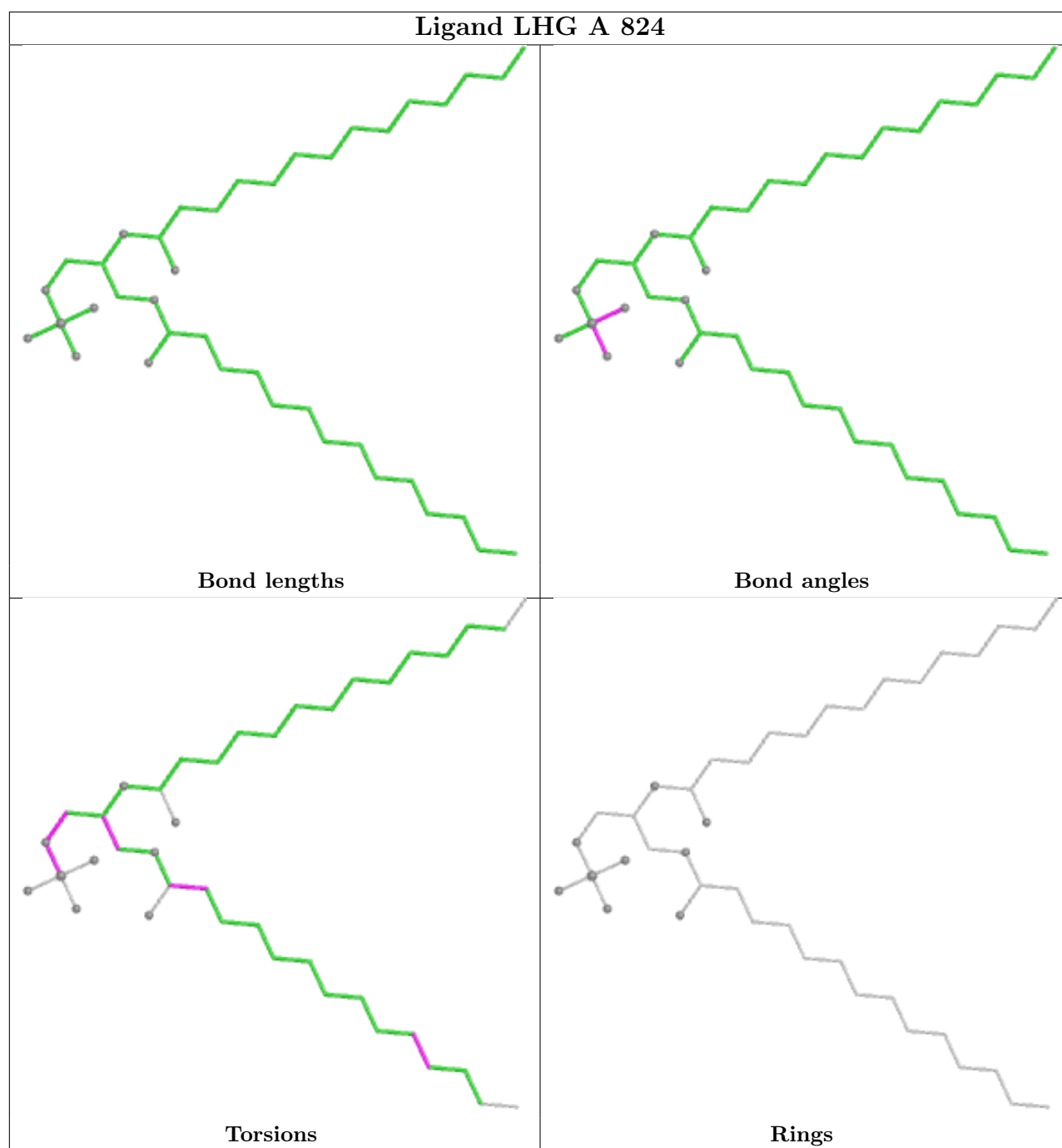
Ligand LUT 4 319**Ligand BCR A 815****Ligand MGE F 303**

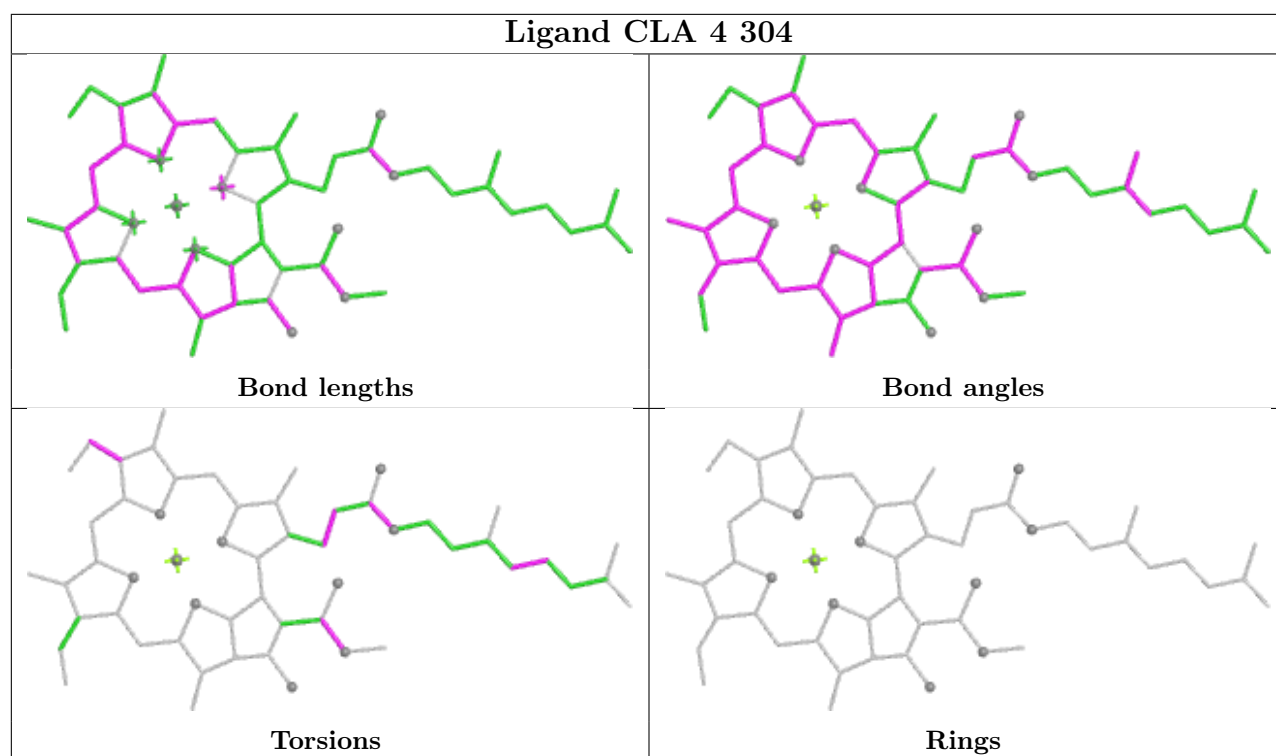
Ligand CHL 3 314



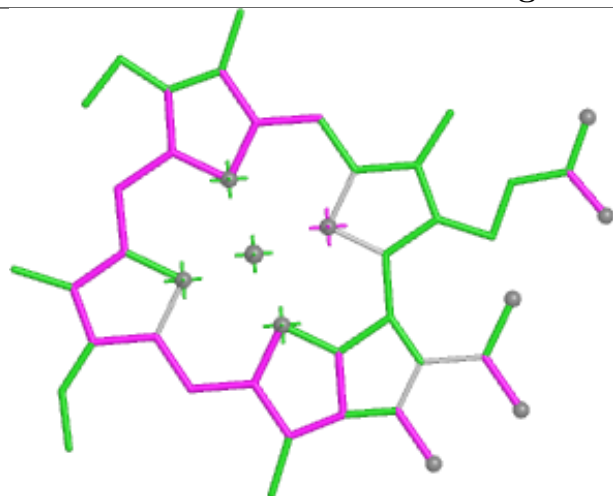
Ligand BCR L 304



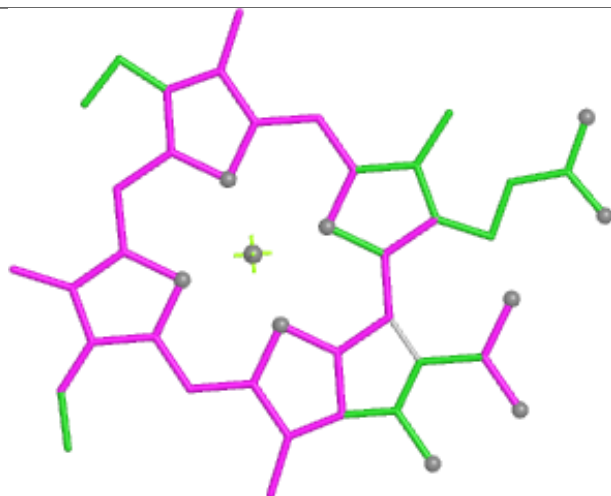




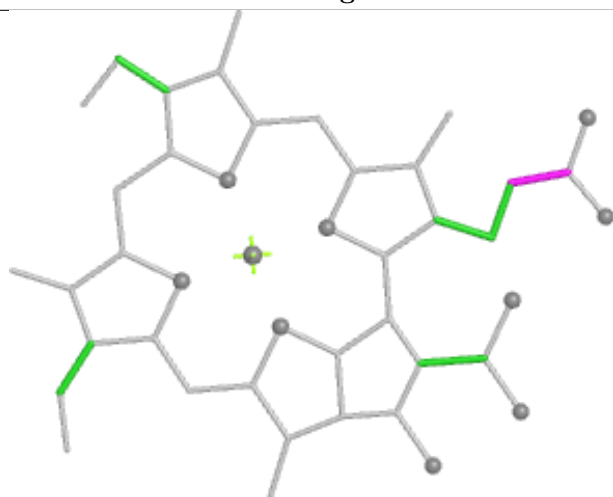
Ligand CLA 1 321



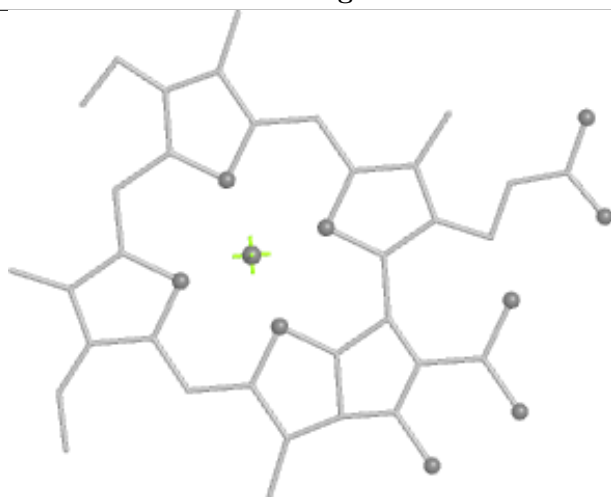
Bond lengths



Bond angles

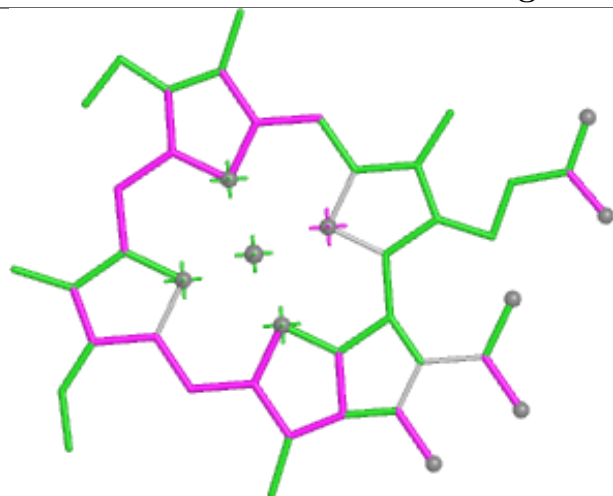


Torsions

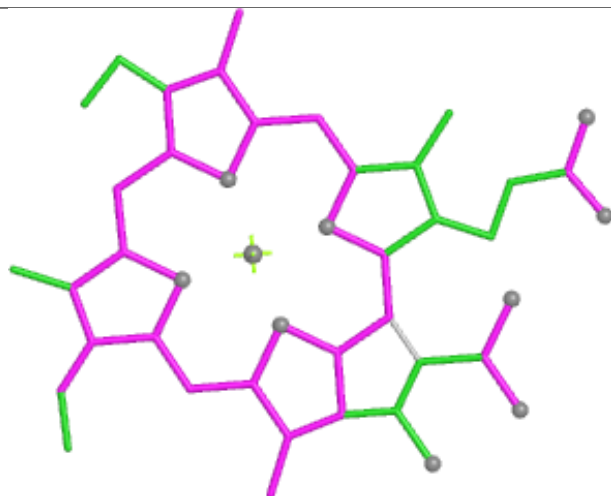


Rings

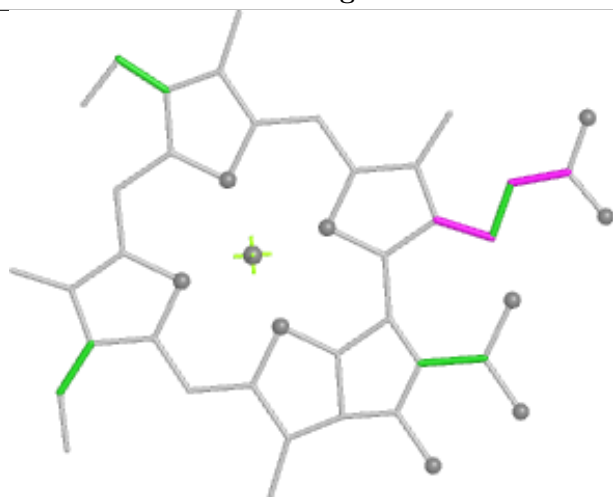
Ligand CLA 4 313



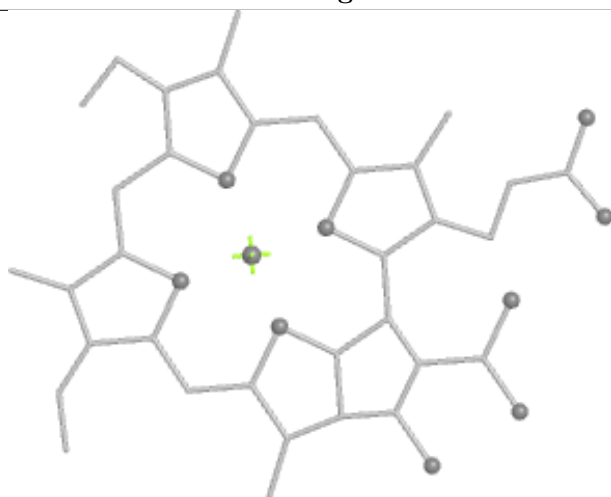
Bond lengths



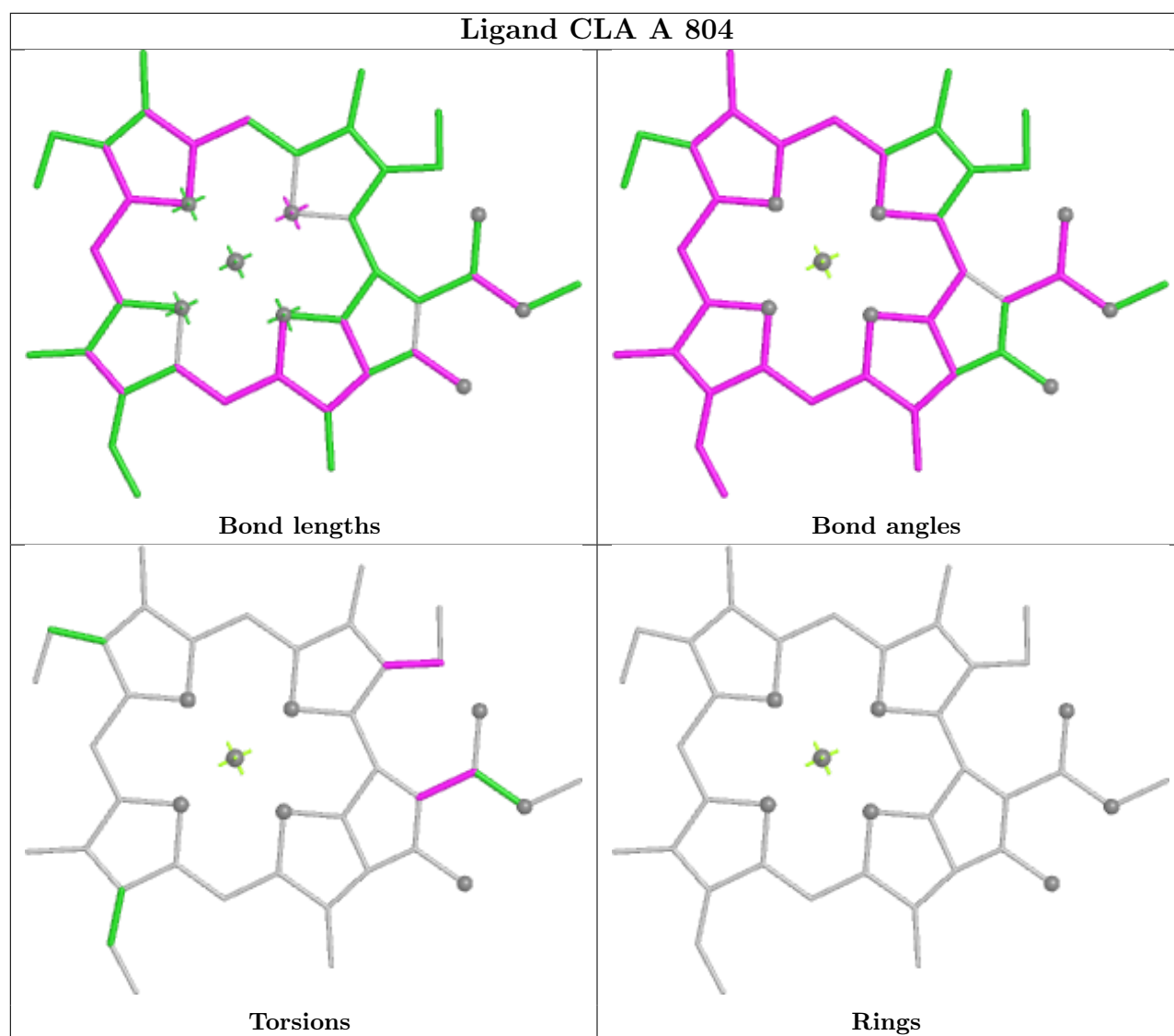
Bond angles



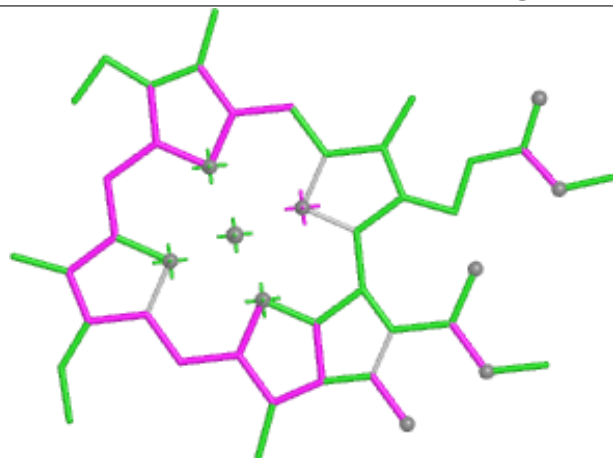
Torsions



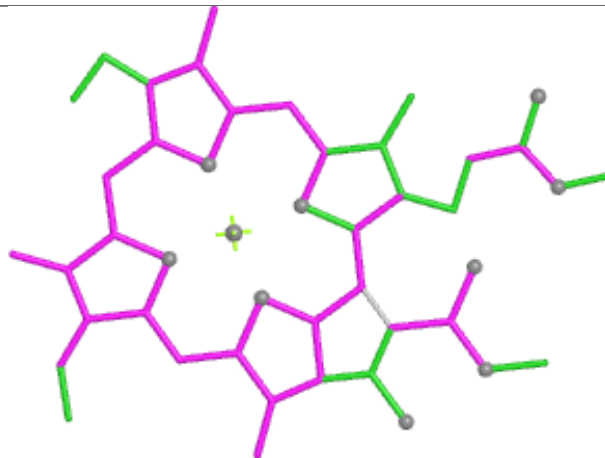
Rings



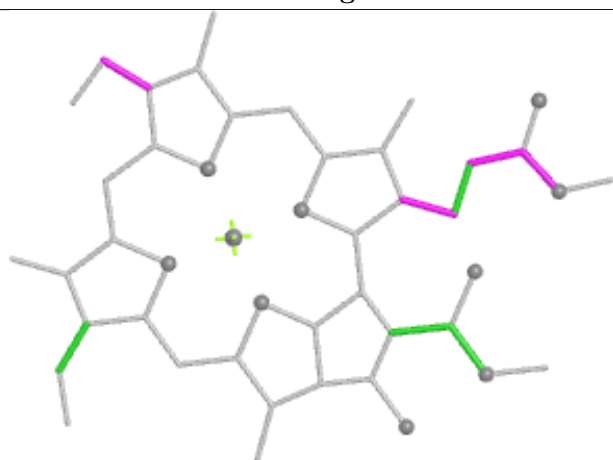
Ligand CLA Y 302



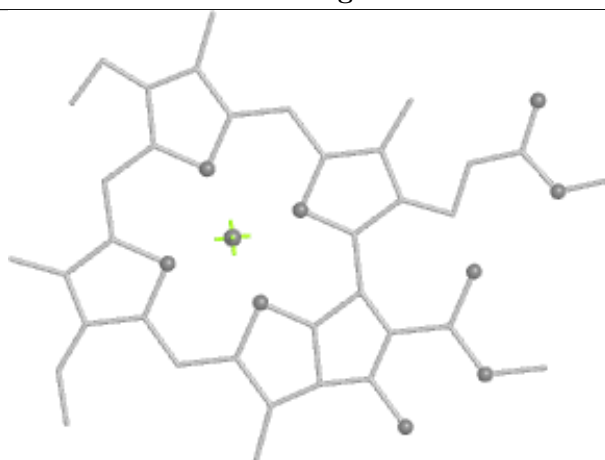
Bond lengths



Bond angles

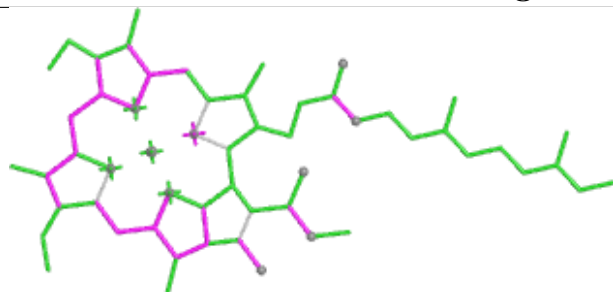


Torsions

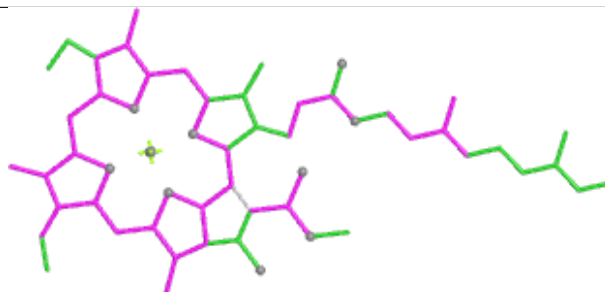


Rings

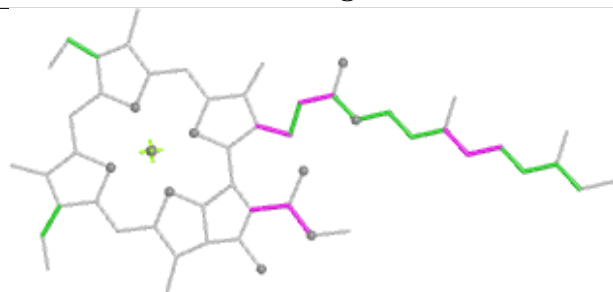
Ligand CLA B 811



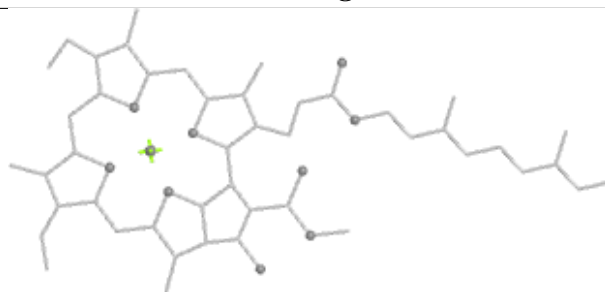
Bond lengths



Bond angles

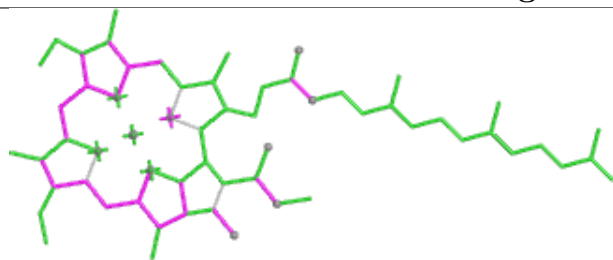


Torsions

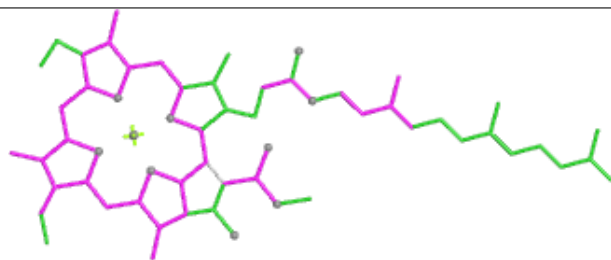


Rings

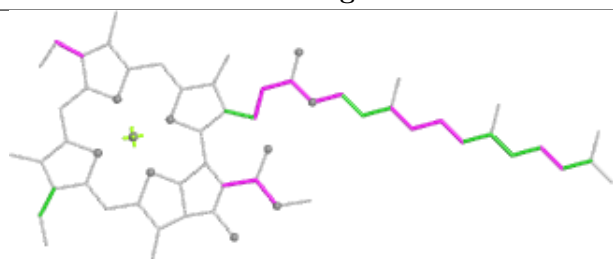
Ligand CLA 2 307



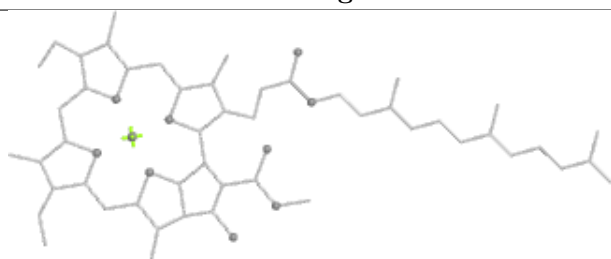
Bond lengths



Bond angles

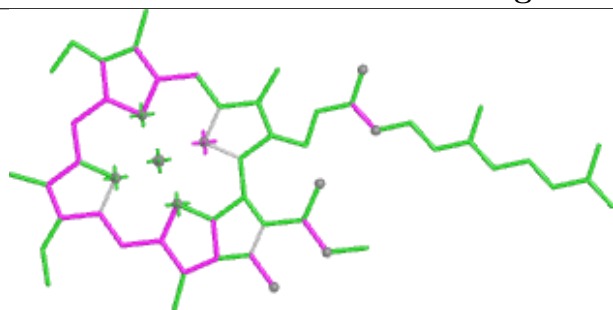


Torsions

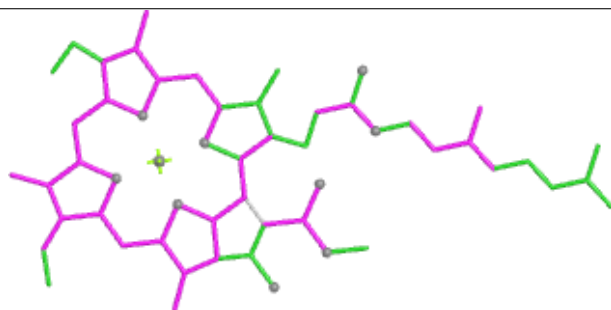


Rings

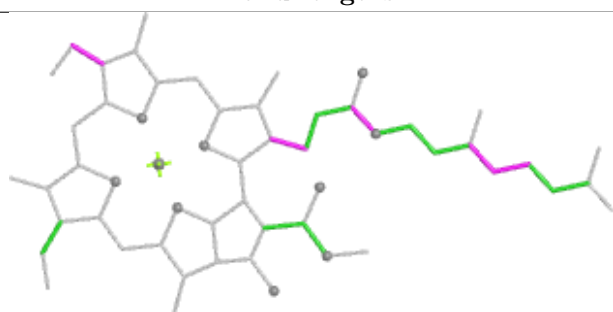
Ligand CLA B 852



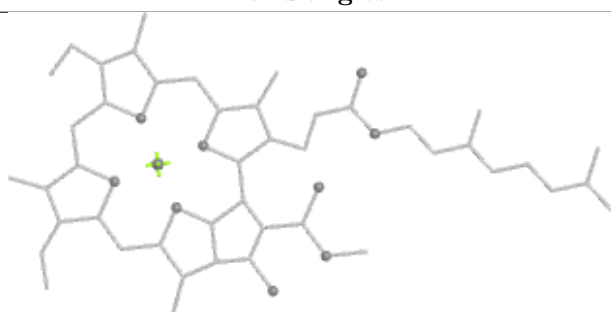
Bond lengths



Bond angles

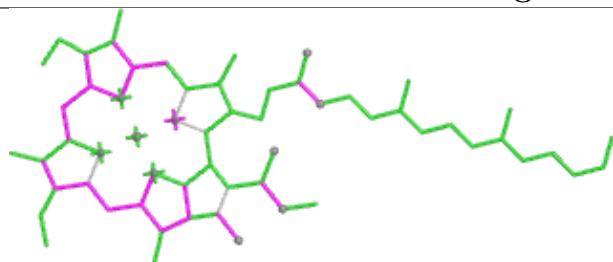


Torsions

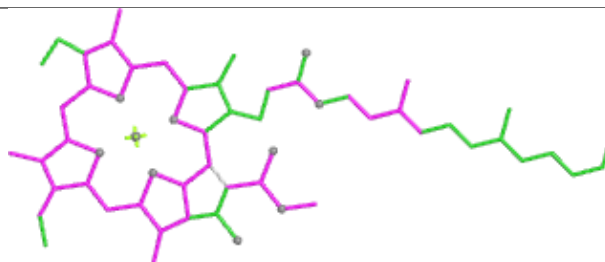


Rings

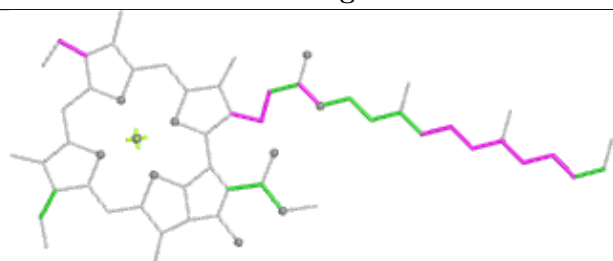
Ligand CLA B 812



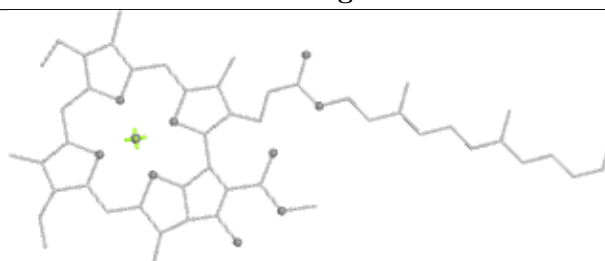
Bond lengths



Bond angles

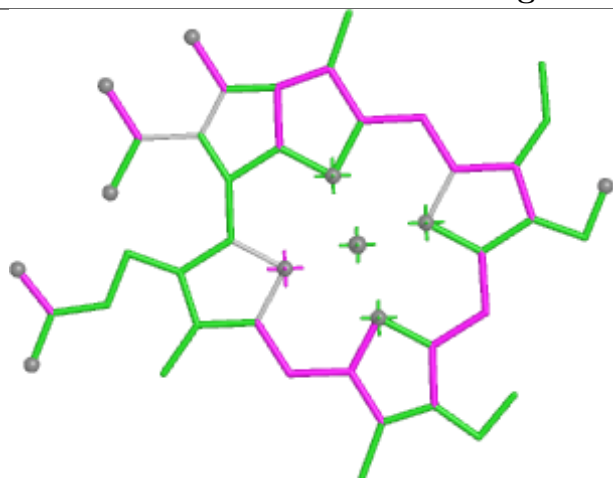


Torsions

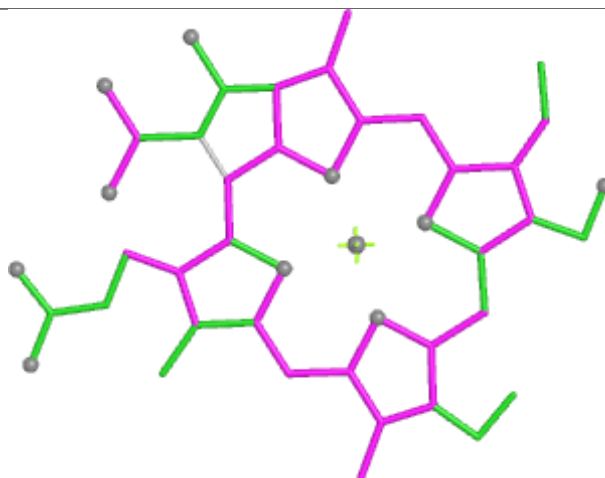


Rings

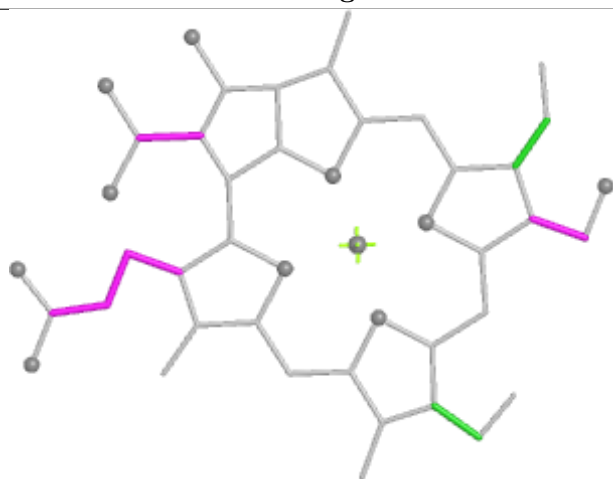
Ligand CHL 4 308



Bond lengths



Bond angles

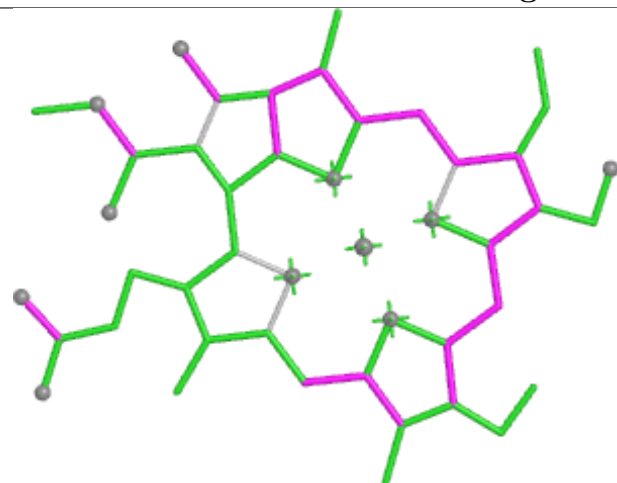


Torsions

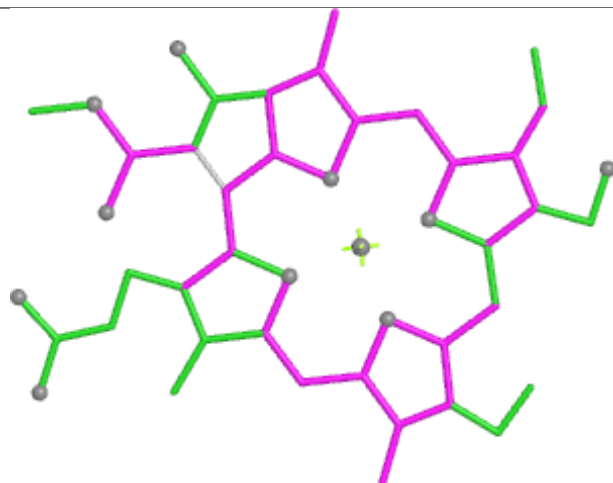


Rings

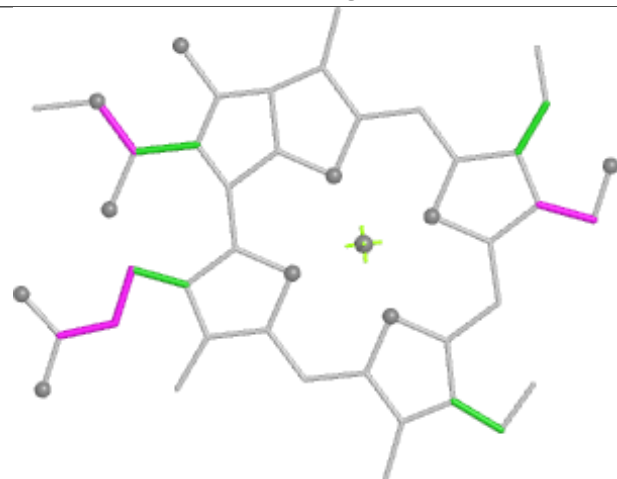
Ligand CHL Z 312



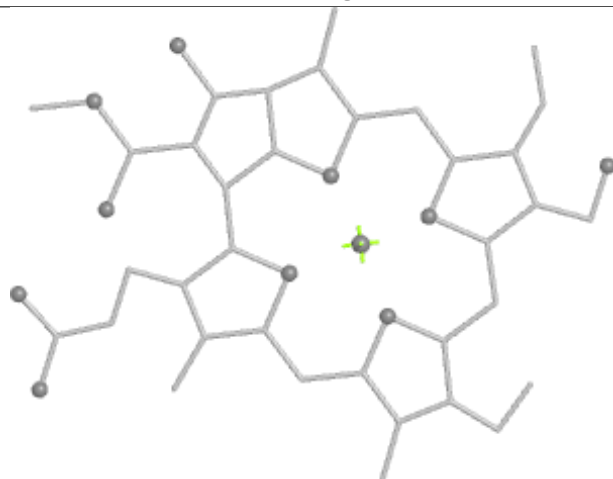
Bond lengths



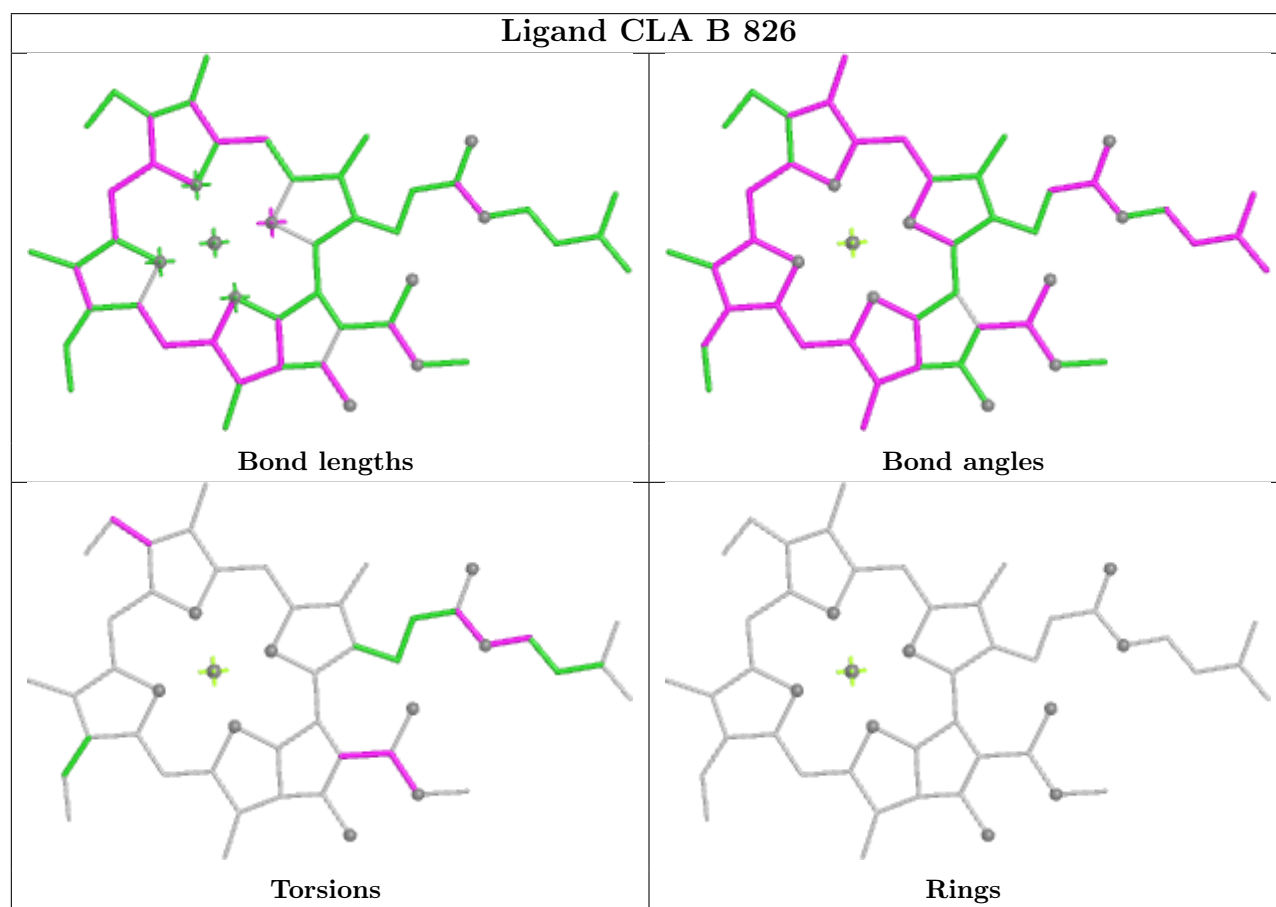
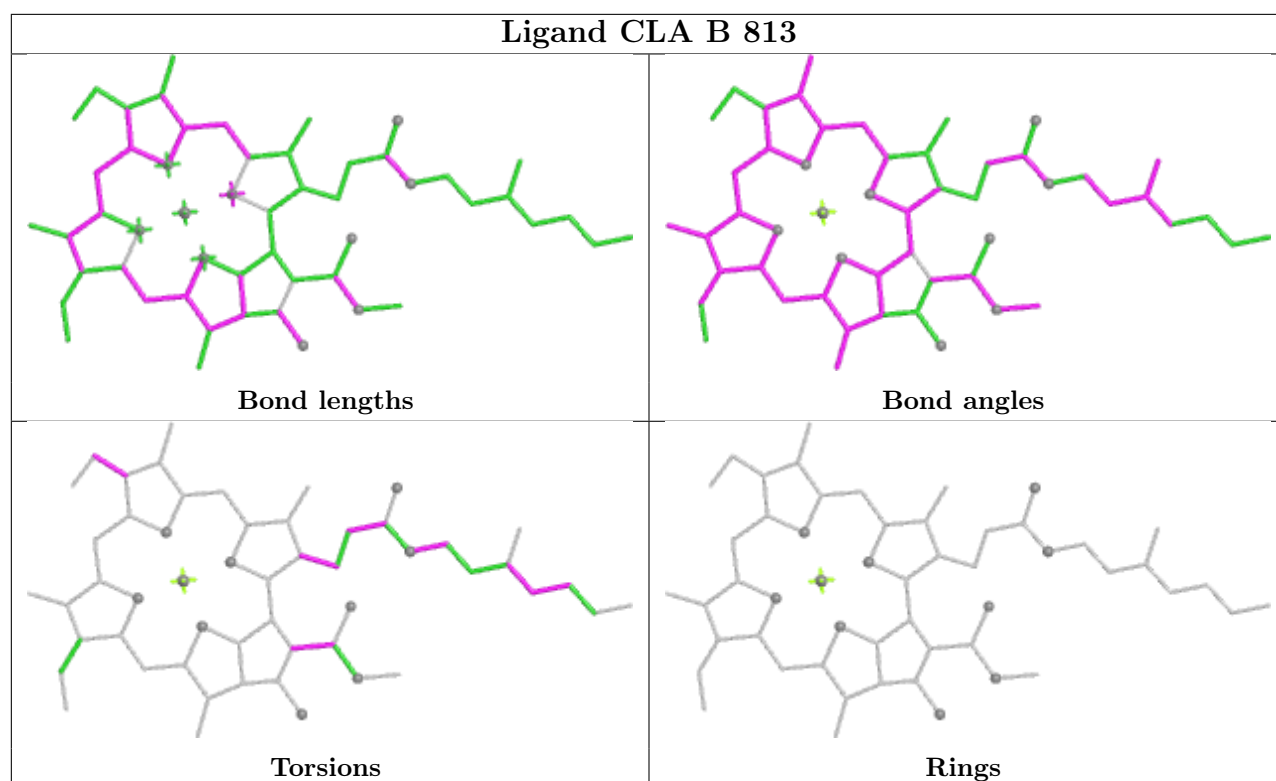
Bond angles

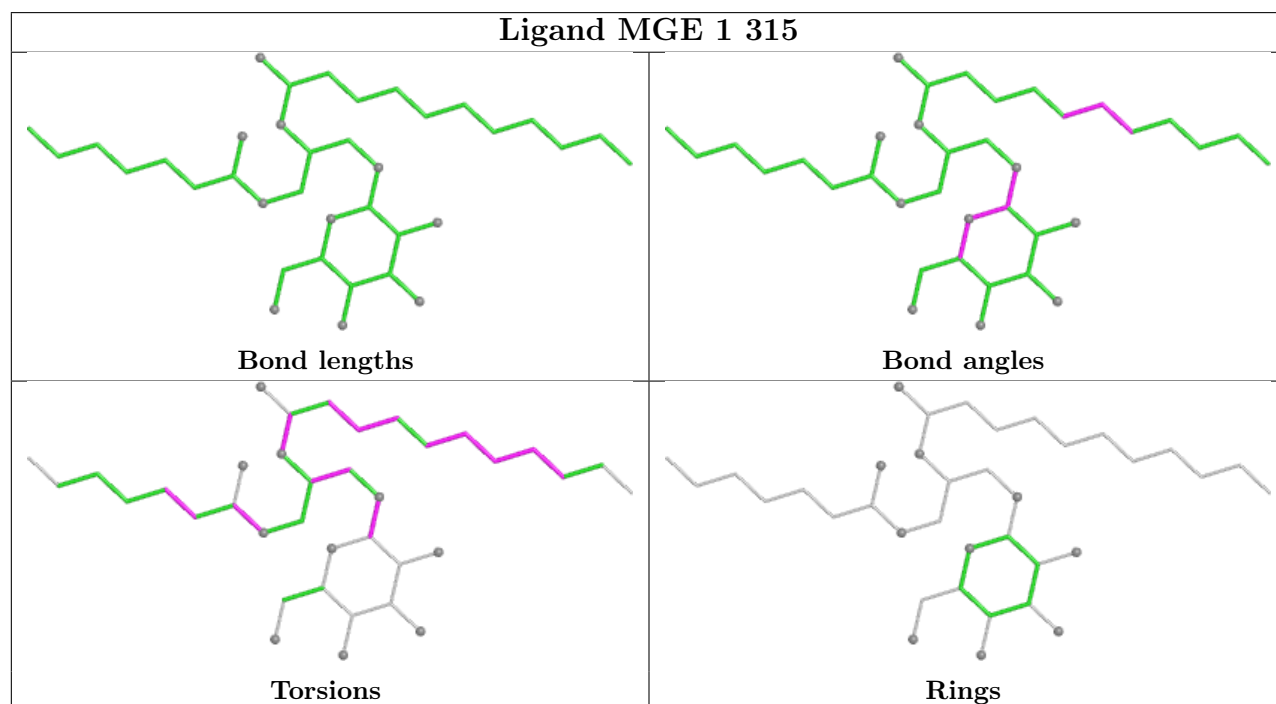
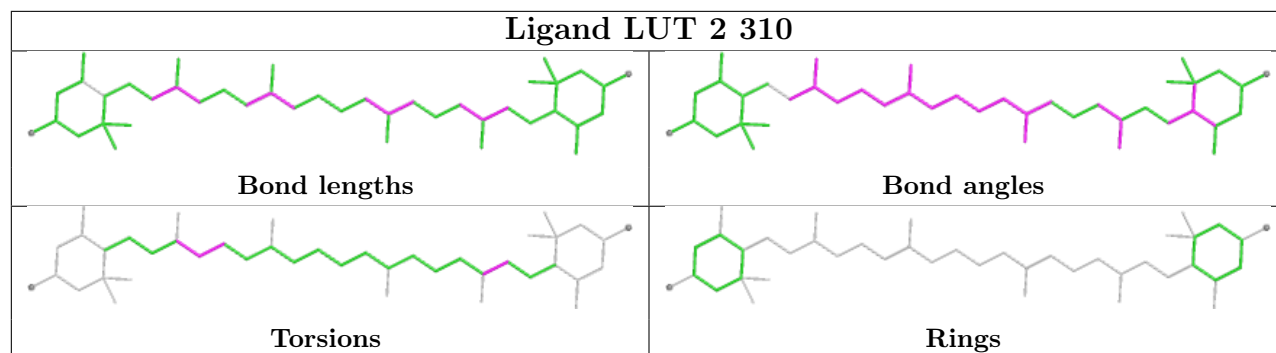


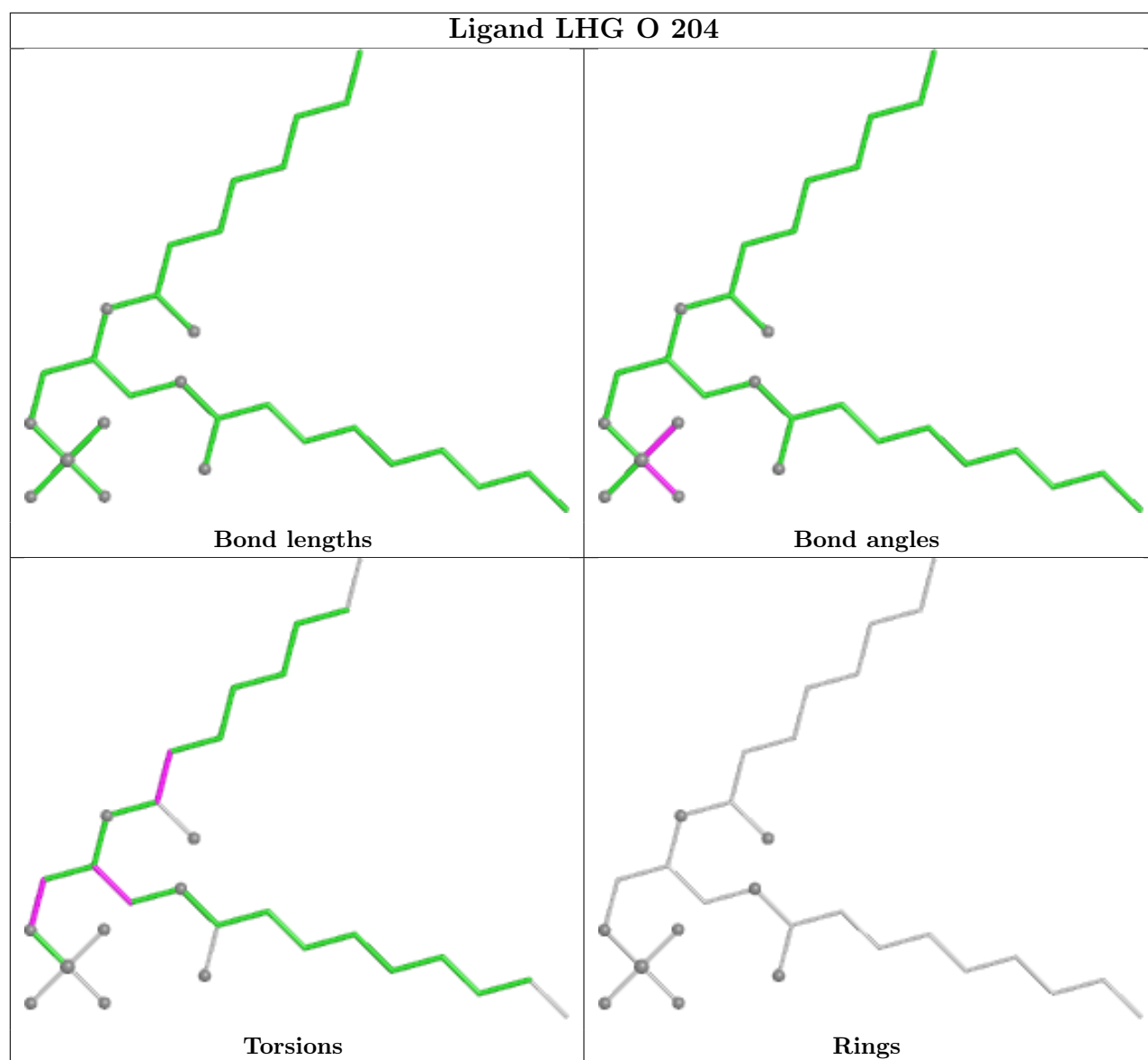
Torsions



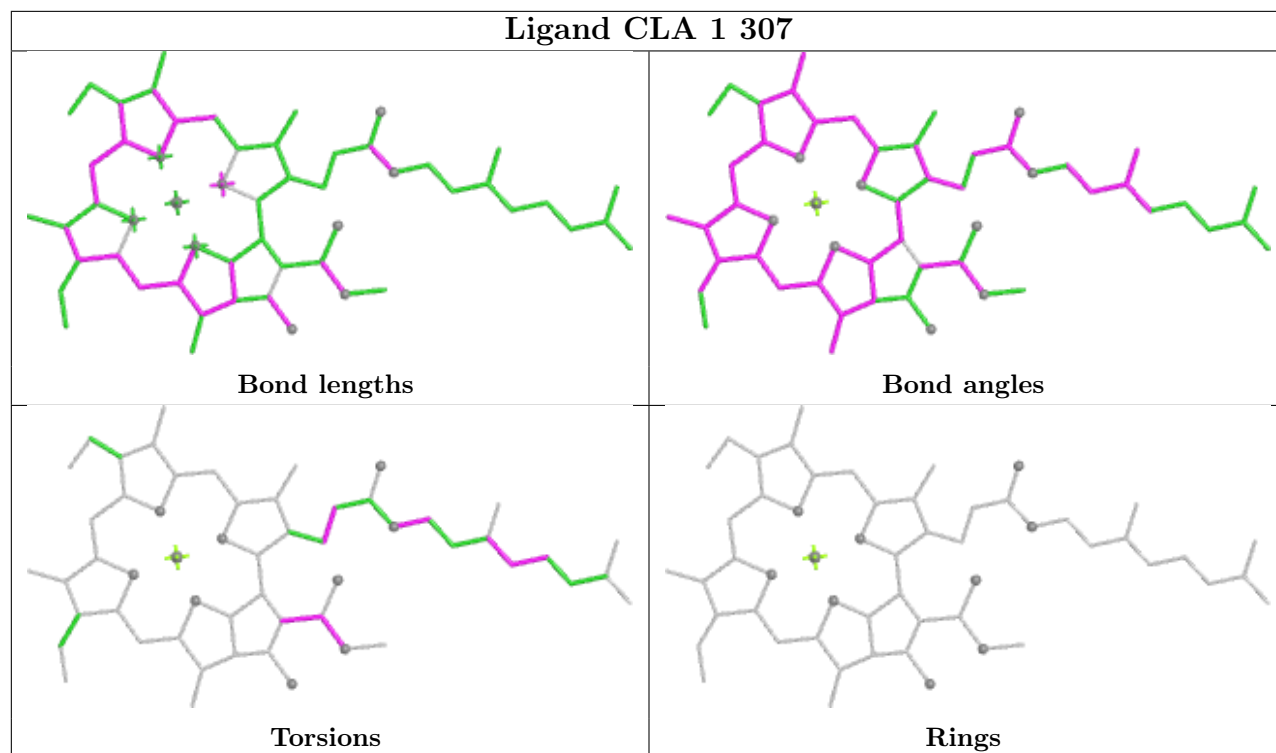
Rings



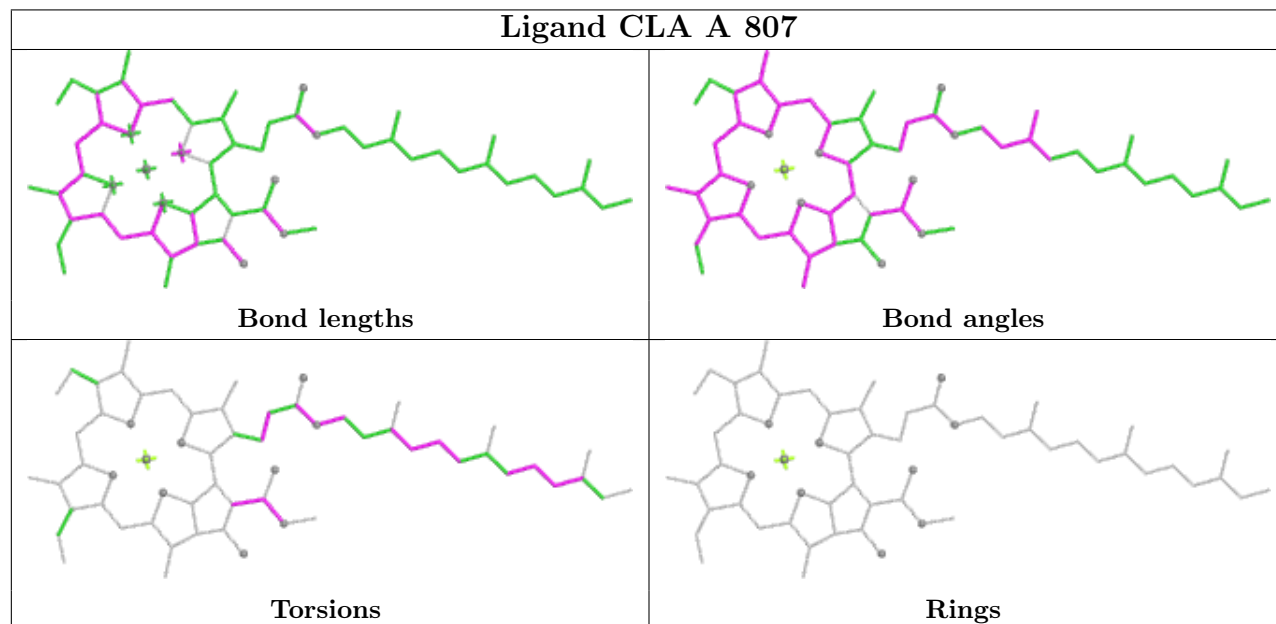


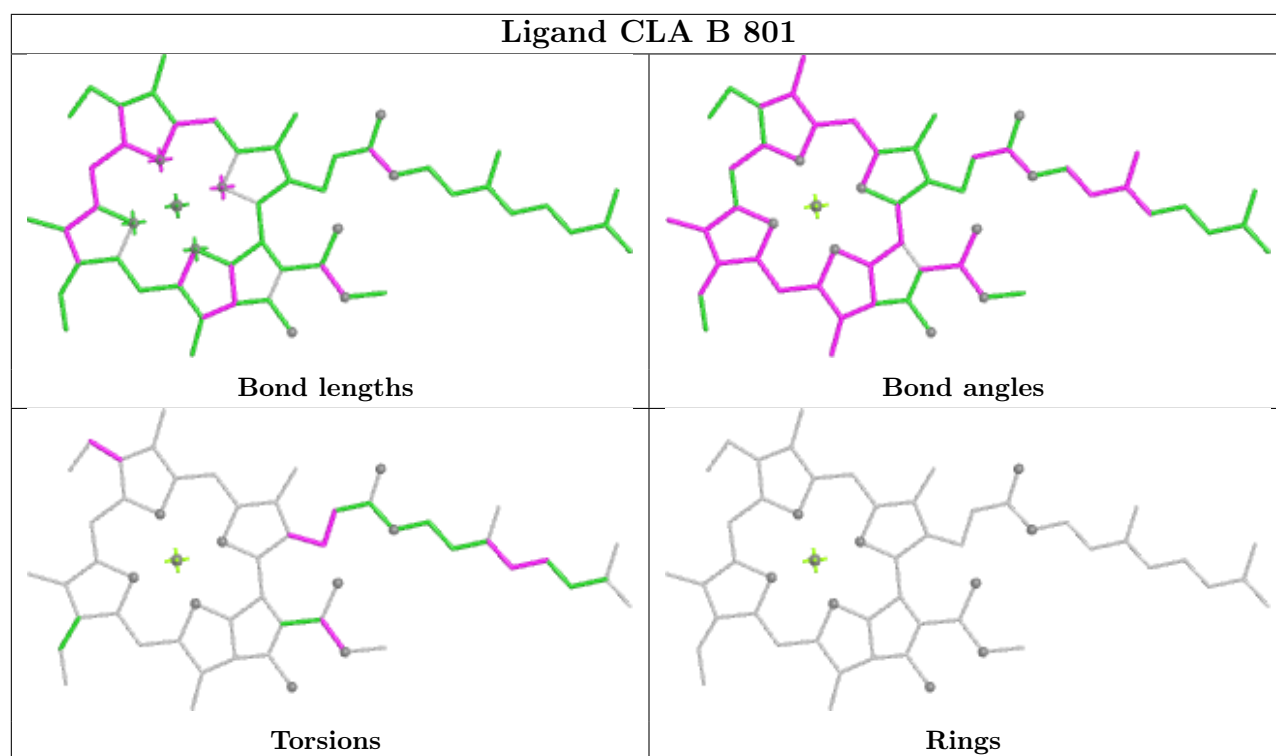


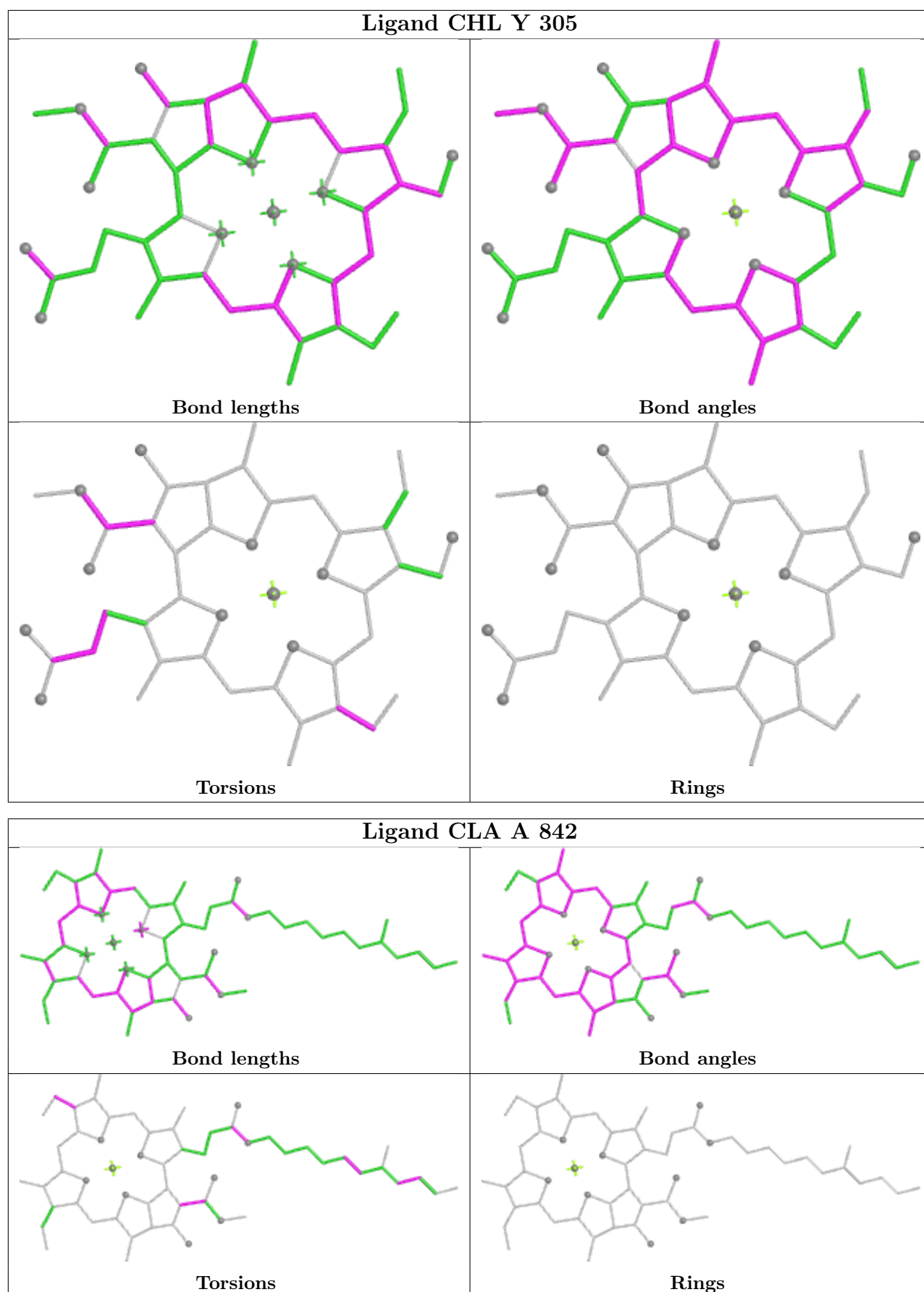
Ligand CLA 1 307

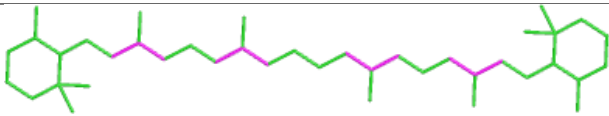
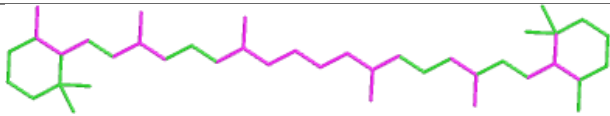
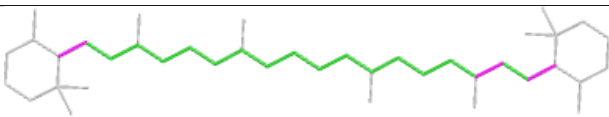
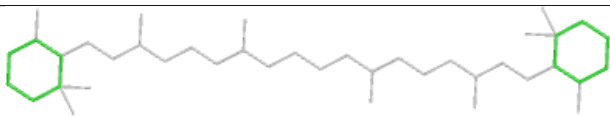


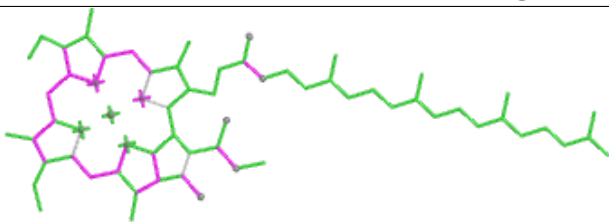
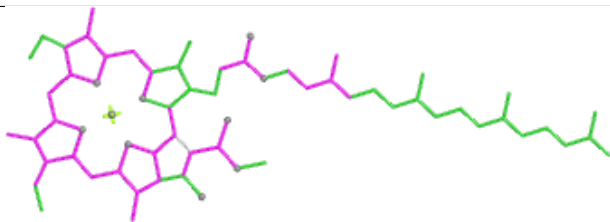
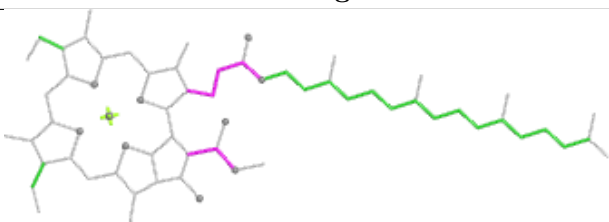
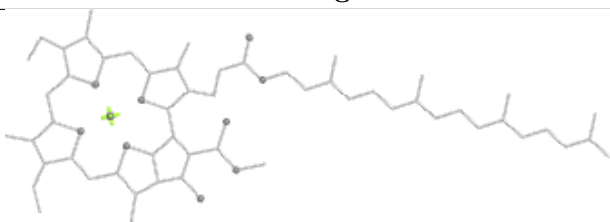
Ligand CLA A 807

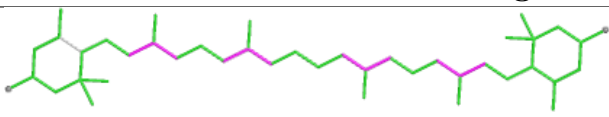
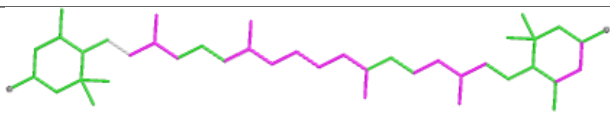
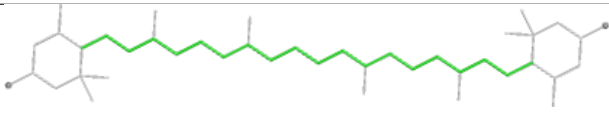
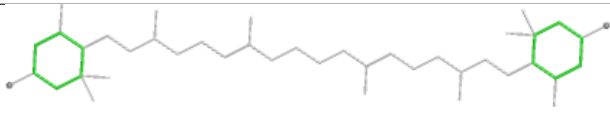




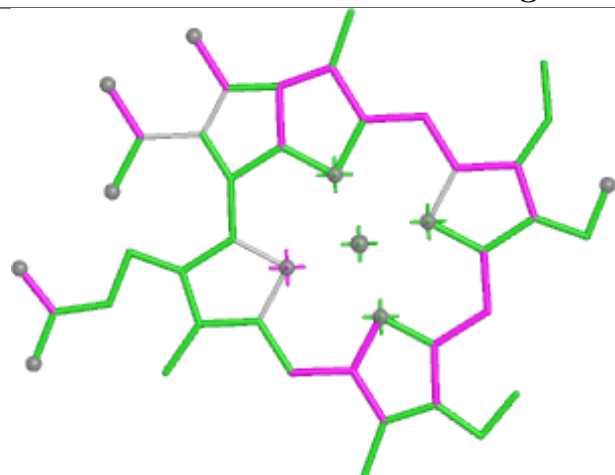


Ligand BCR 4 321	
	
Bond lengths	Bond angles
	
Torsions	Rings

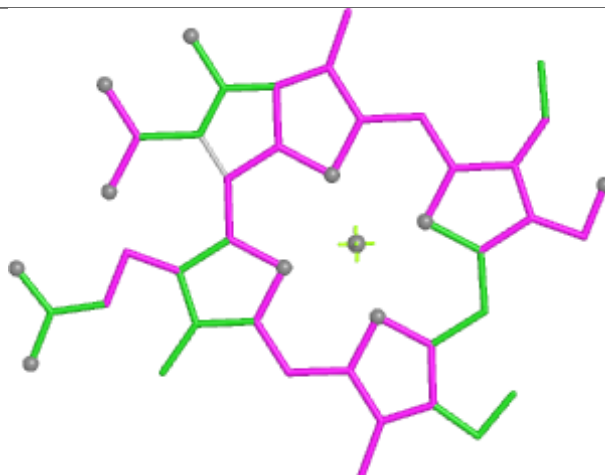
Ligand CL0 A 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 3 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

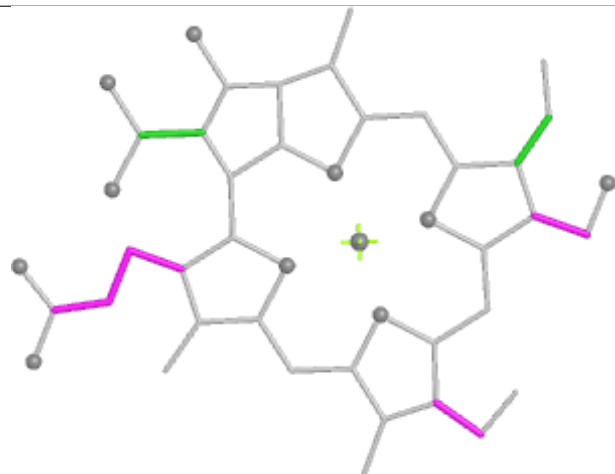
Ligand CHL 2 321



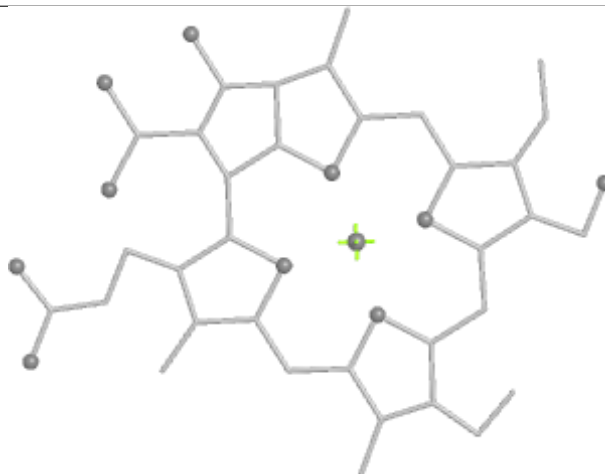
Bond lengths



Bond angles

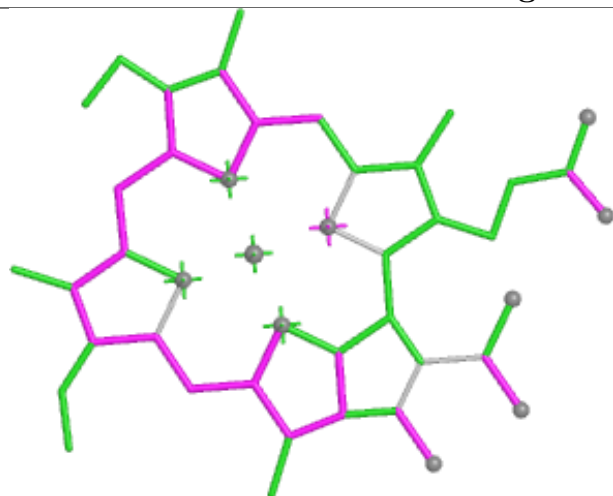


Torsions

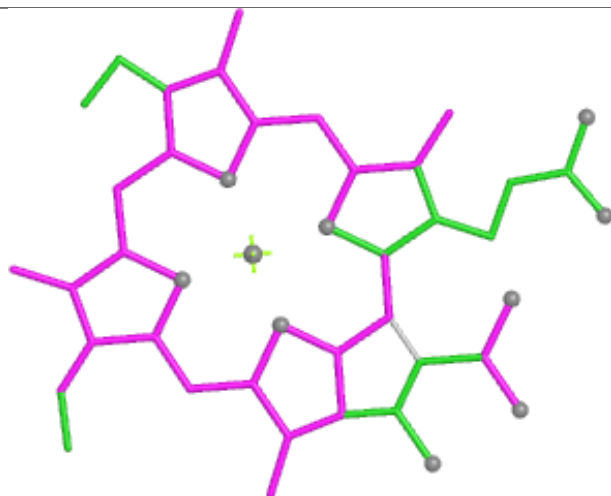


Rings

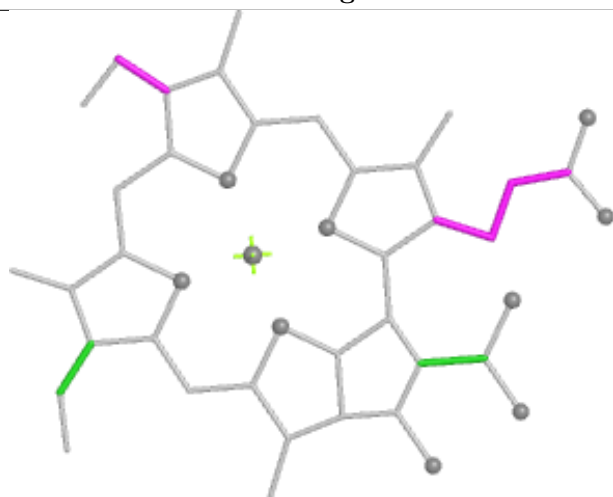
Ligand CLA 4 306



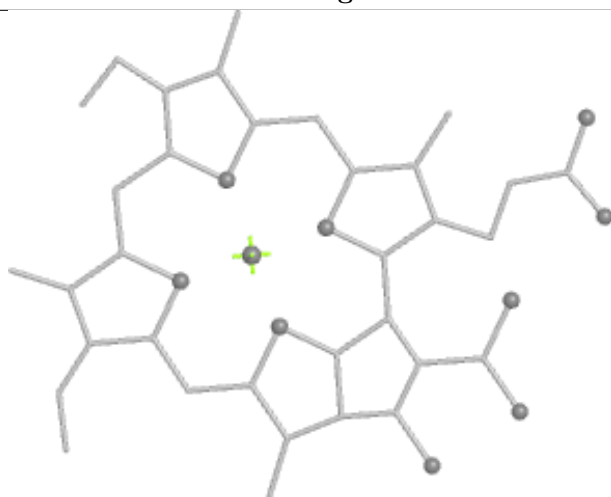
Bond lengths



Bond angles

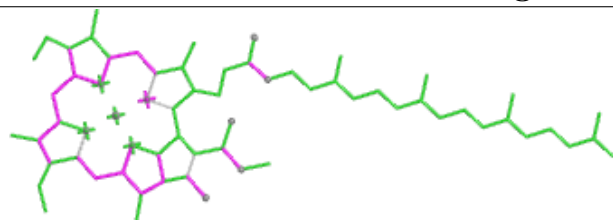


Torsions

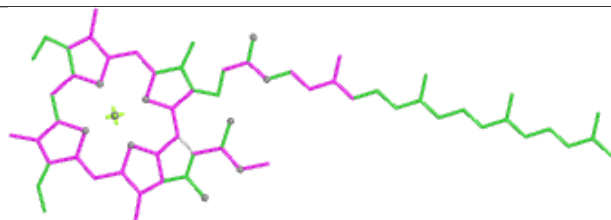


Rings

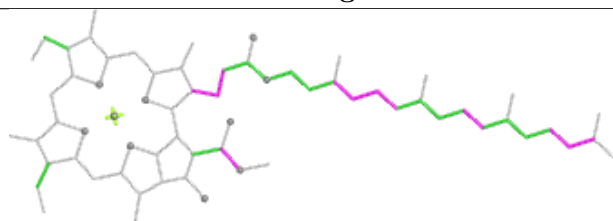
Ligand CLA A 826



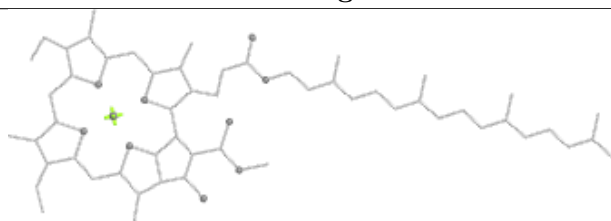
Bond lengths



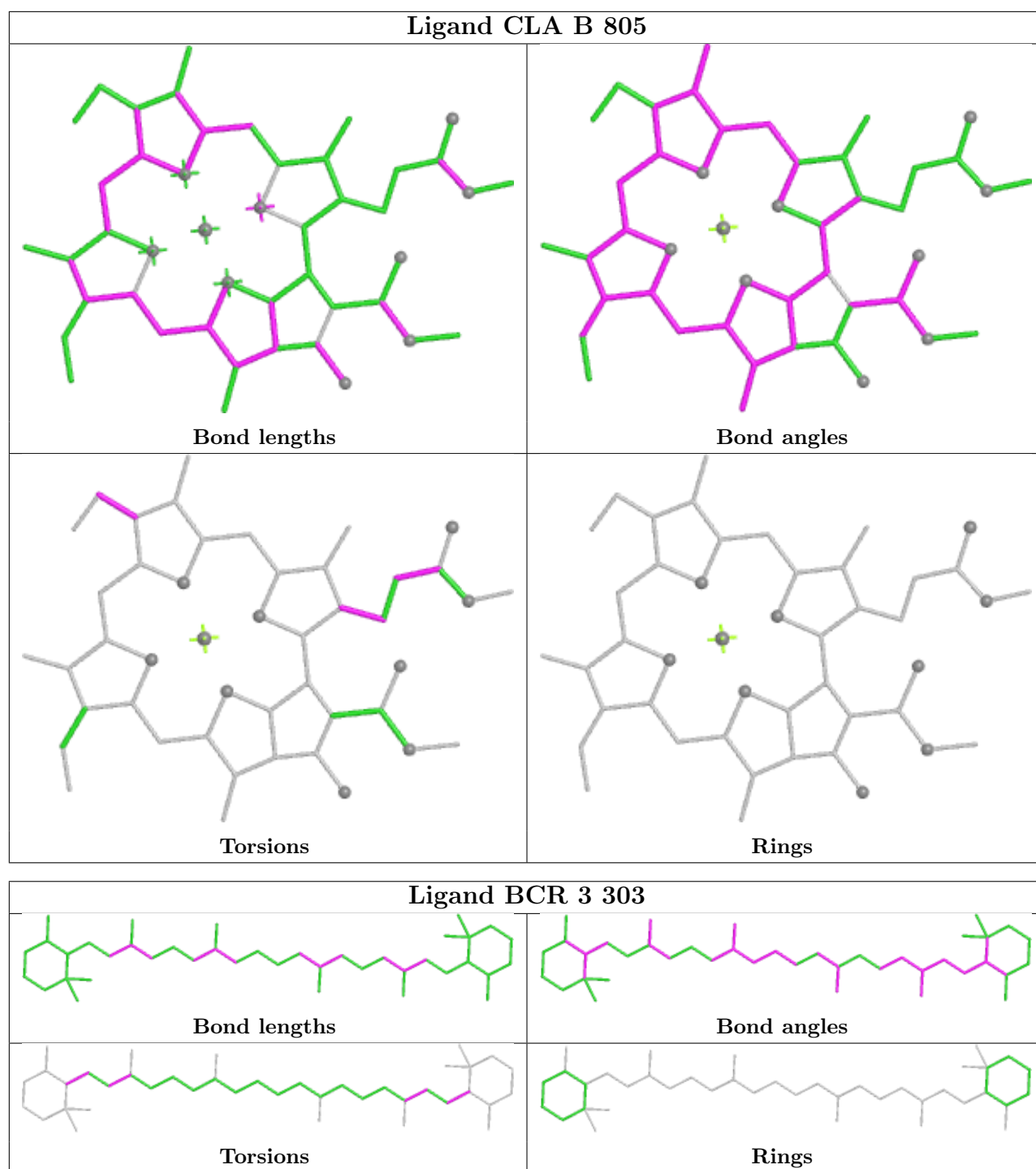
Bond angles

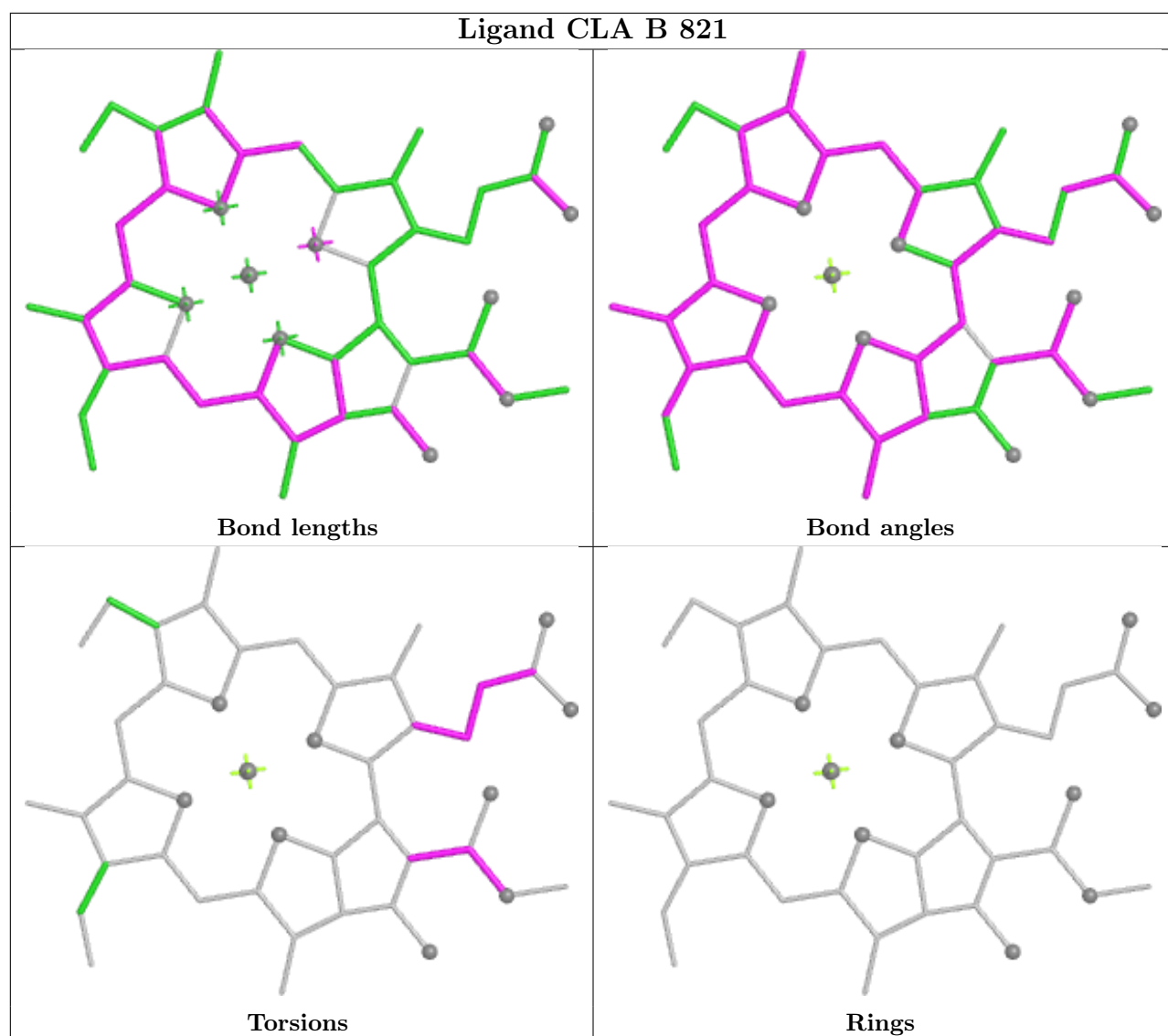


Torsions

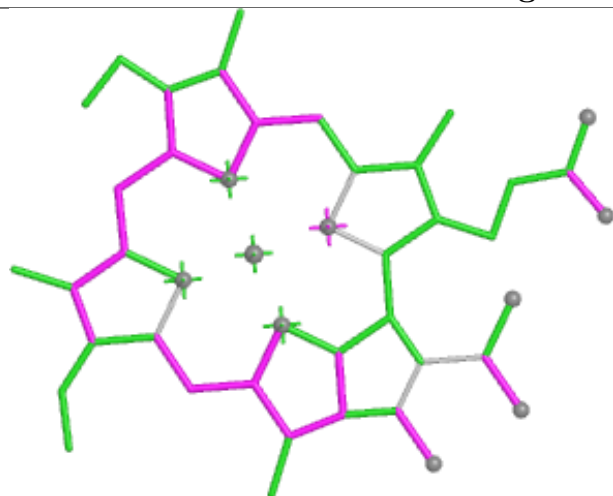


Rings

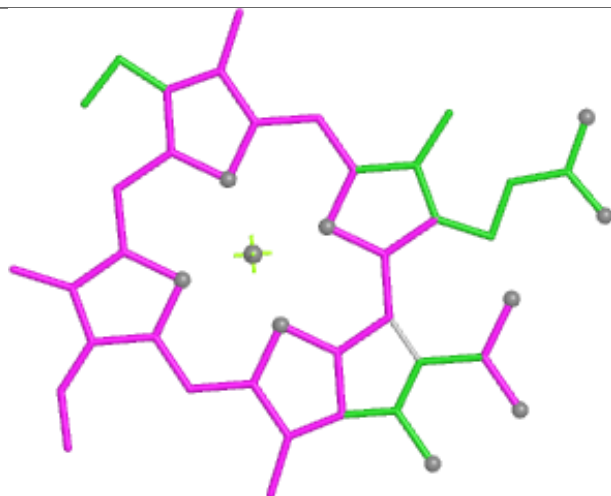




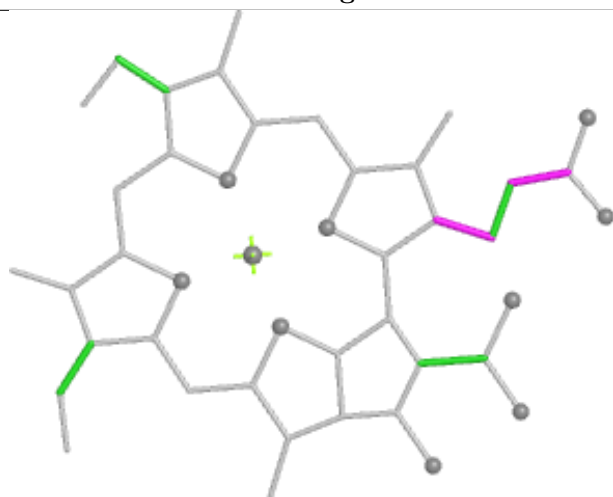
Ligand CLA 4 305



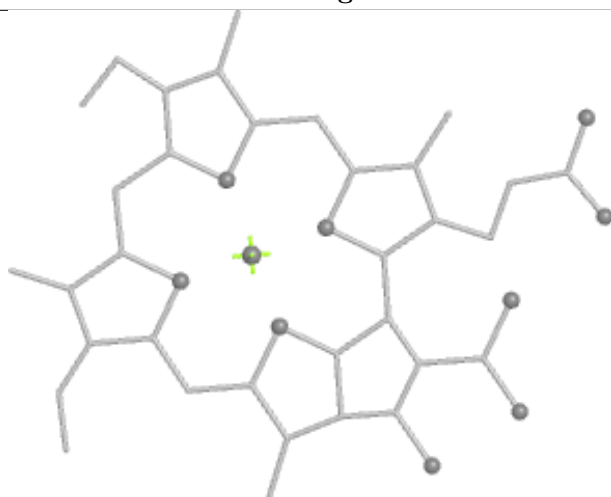
Bond lengths



Bond angles

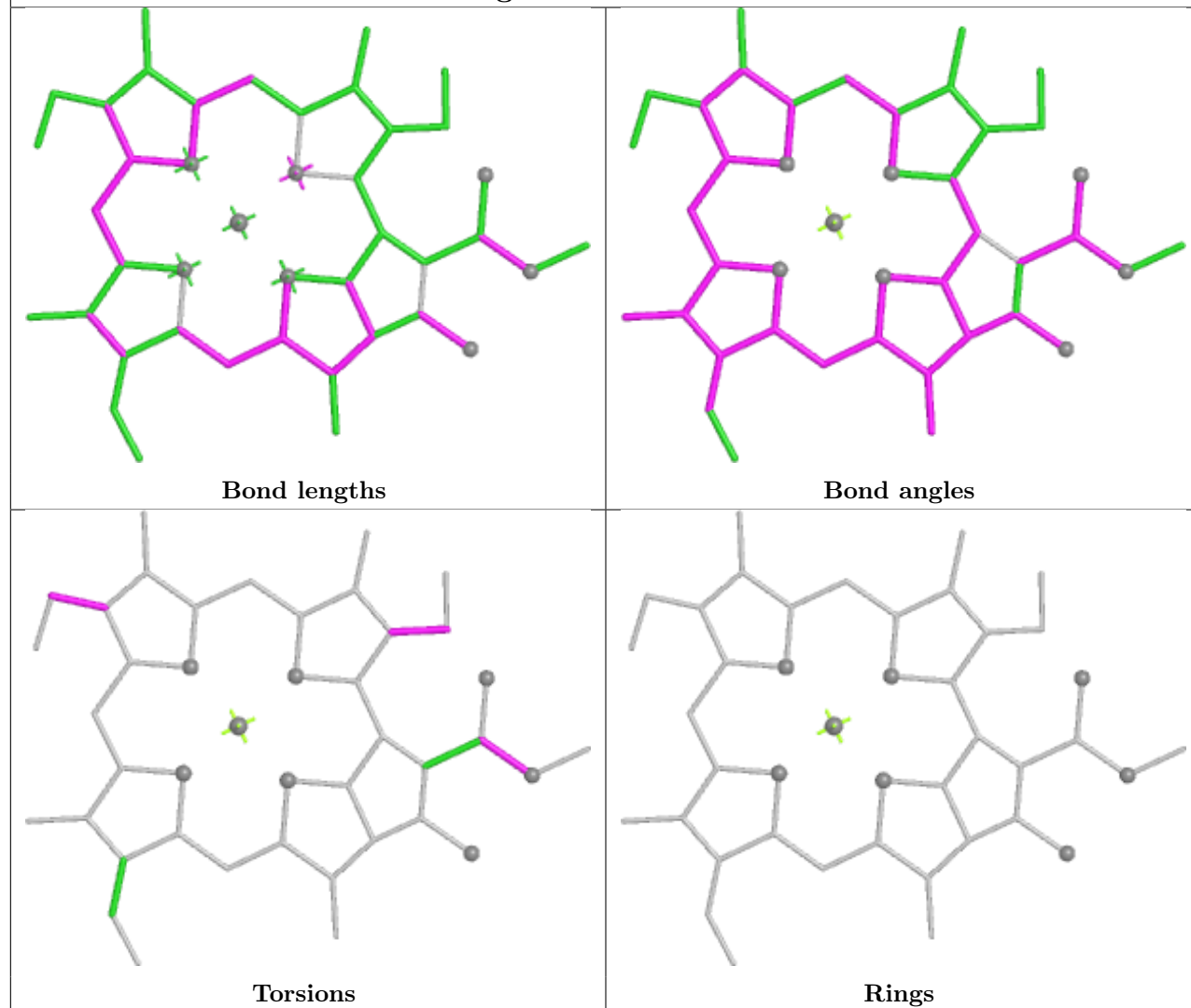


Torsions

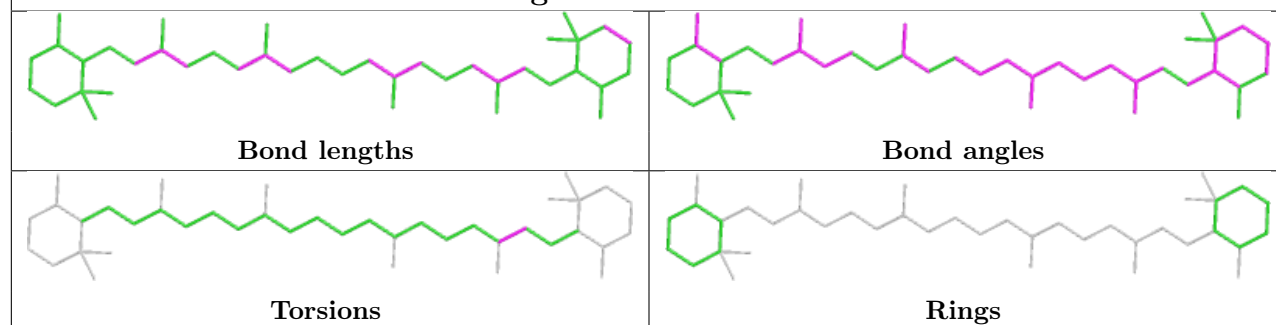


Rings

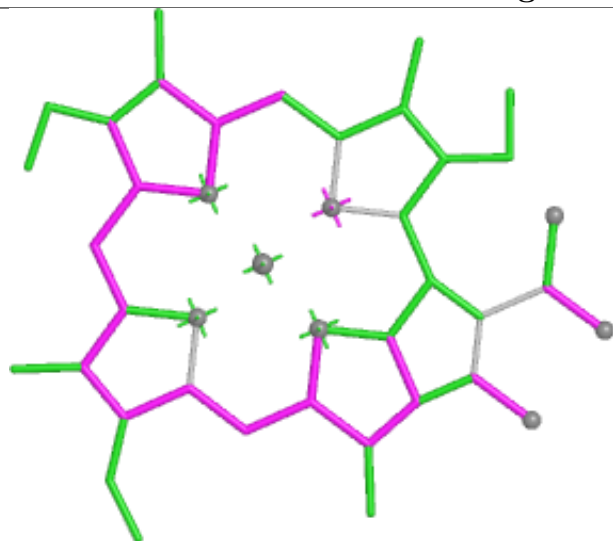
Ligand CLA A 835



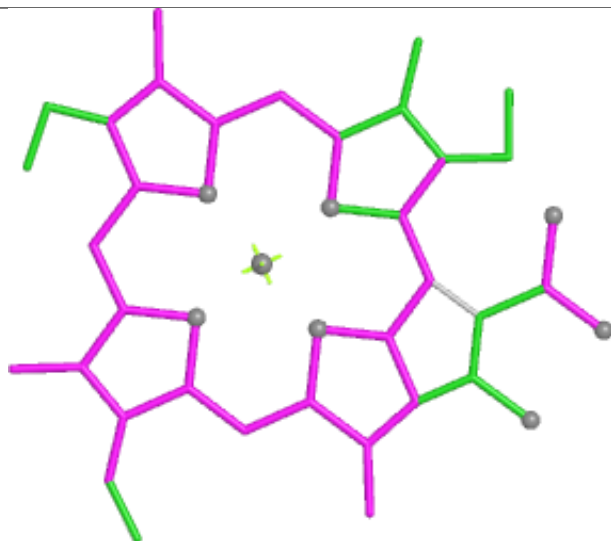
Ligand BCR B 839



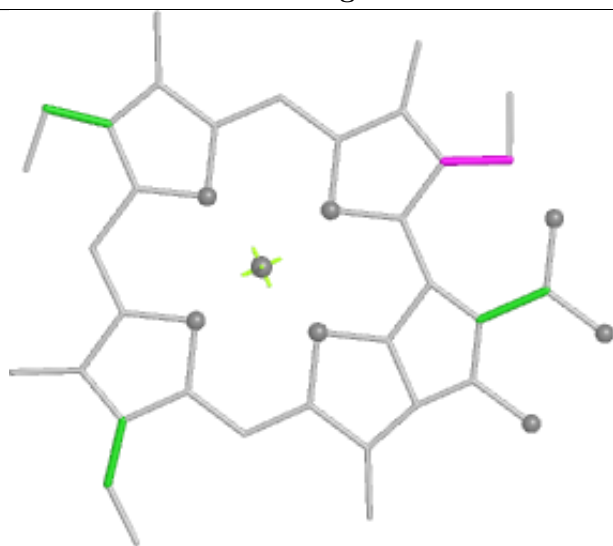
Ligand CLA J 102



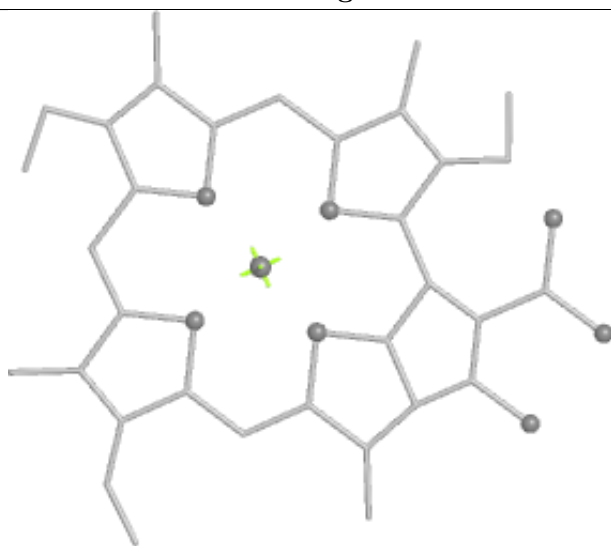
Bond lengths



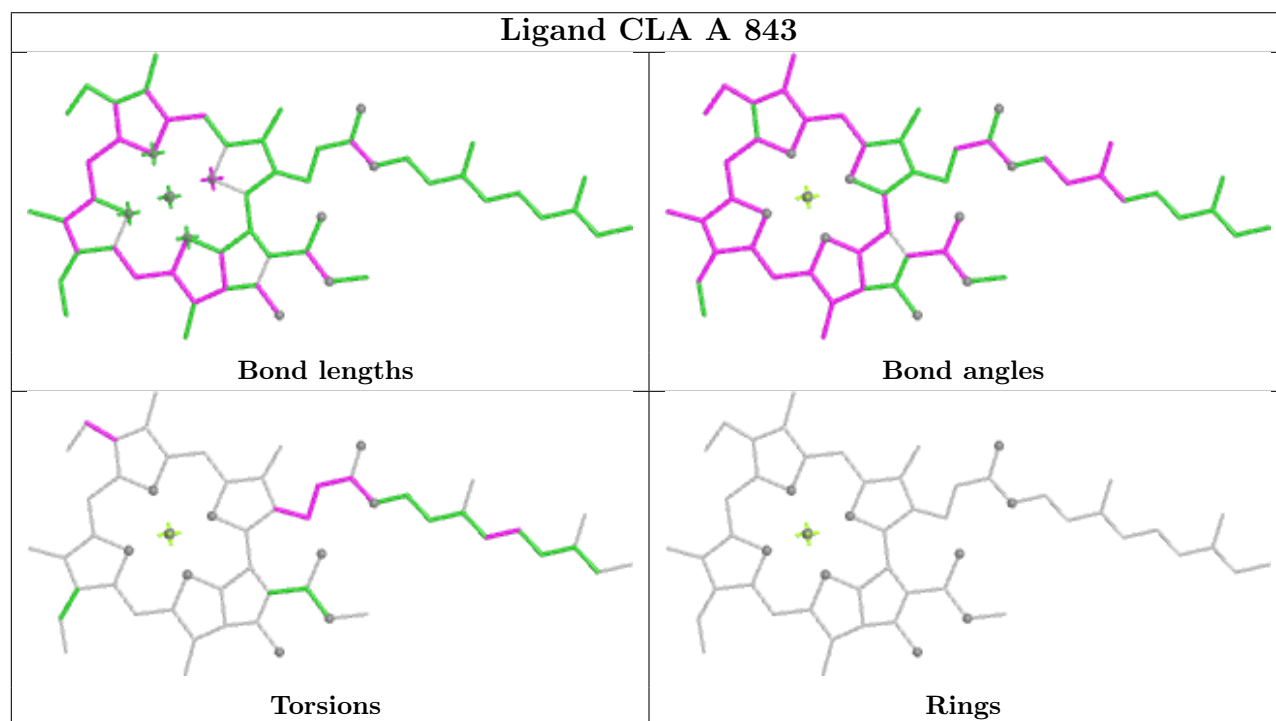
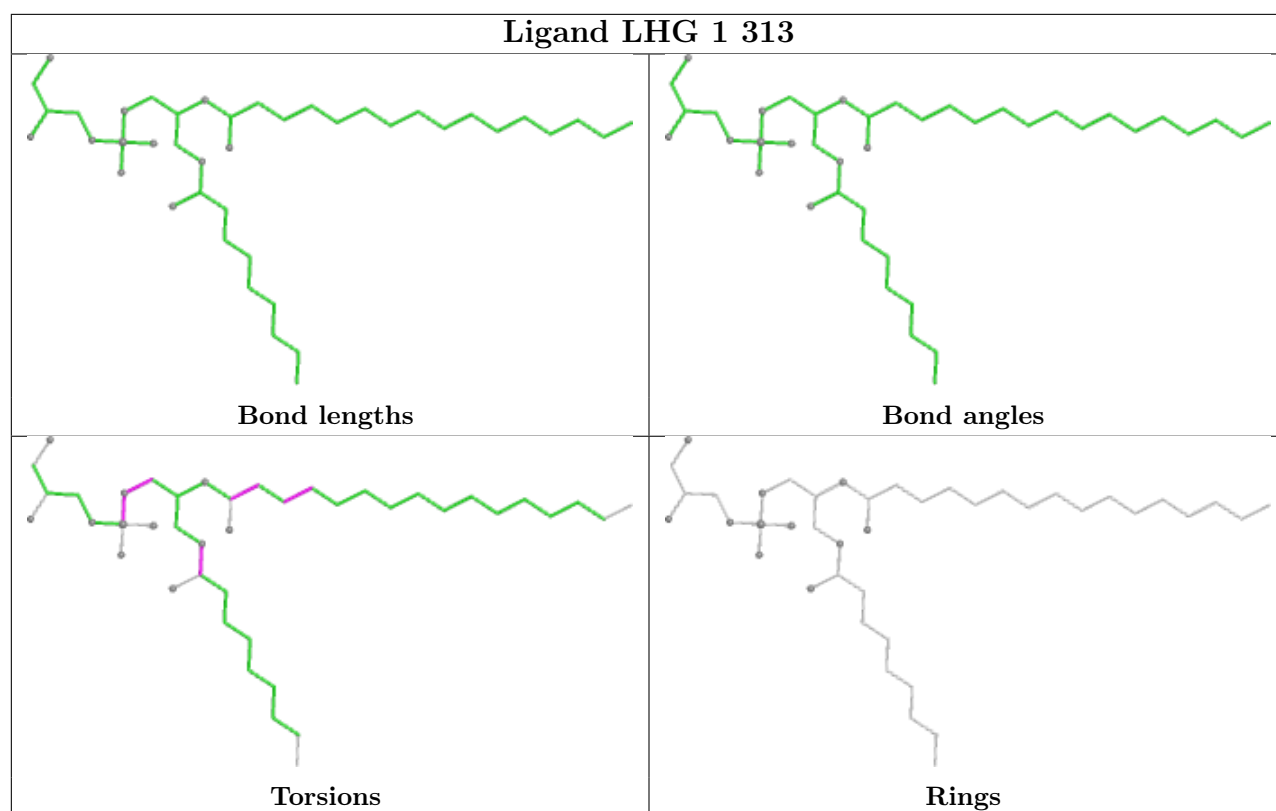
Bond angles



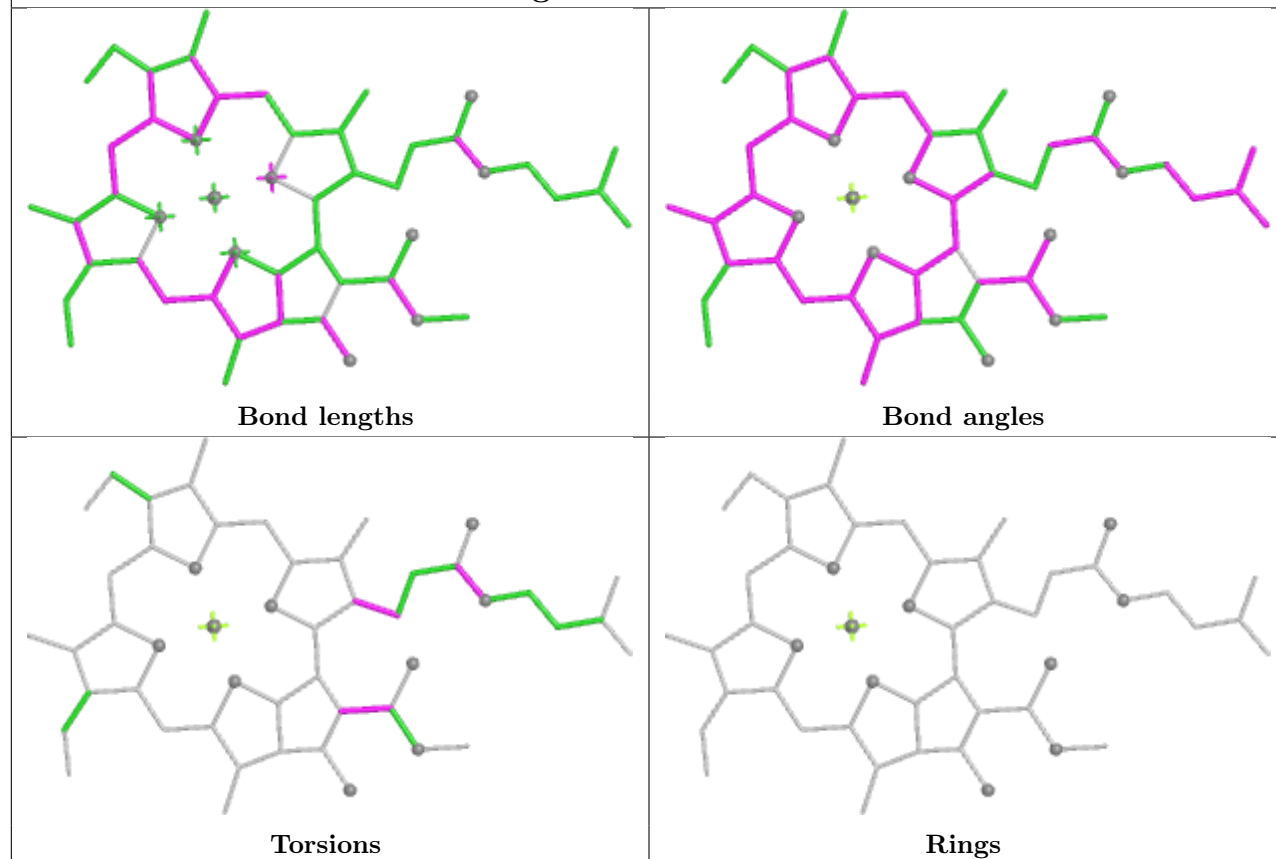
Torsions



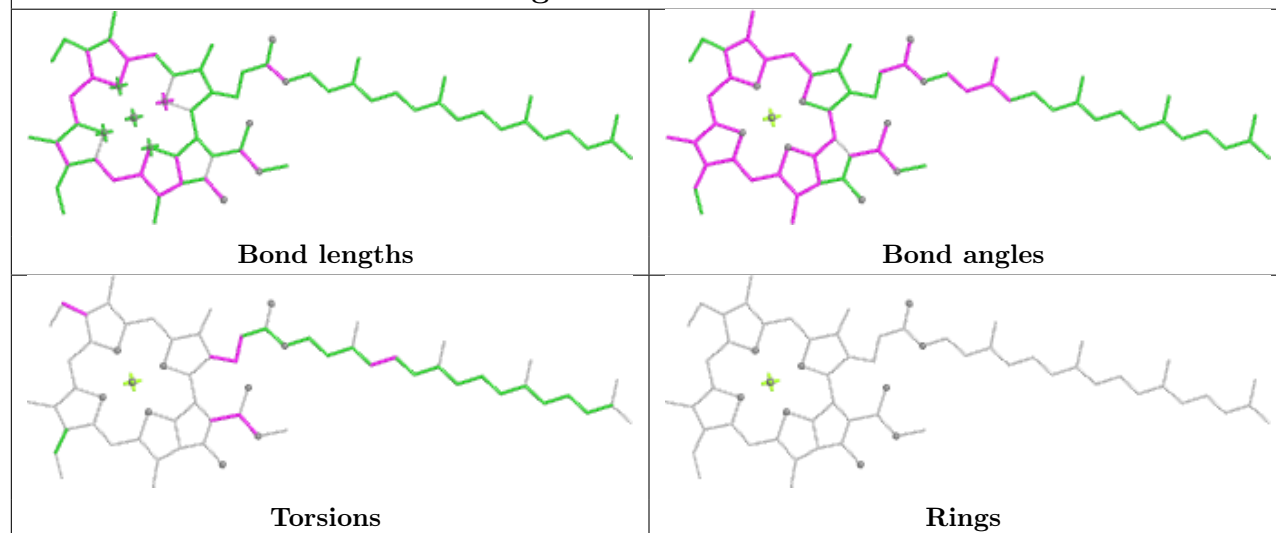
Rings



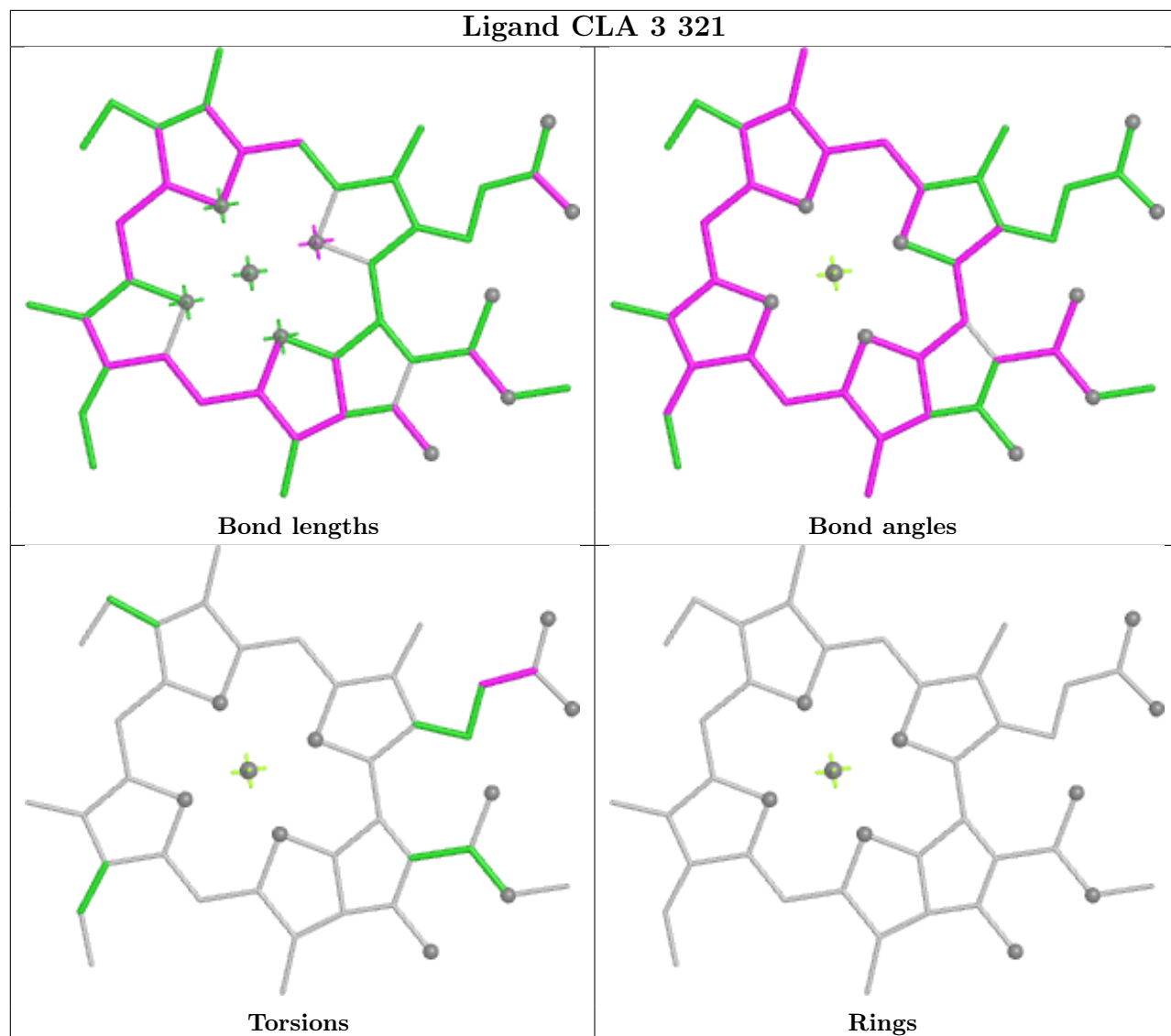
Ligand CLA B 810

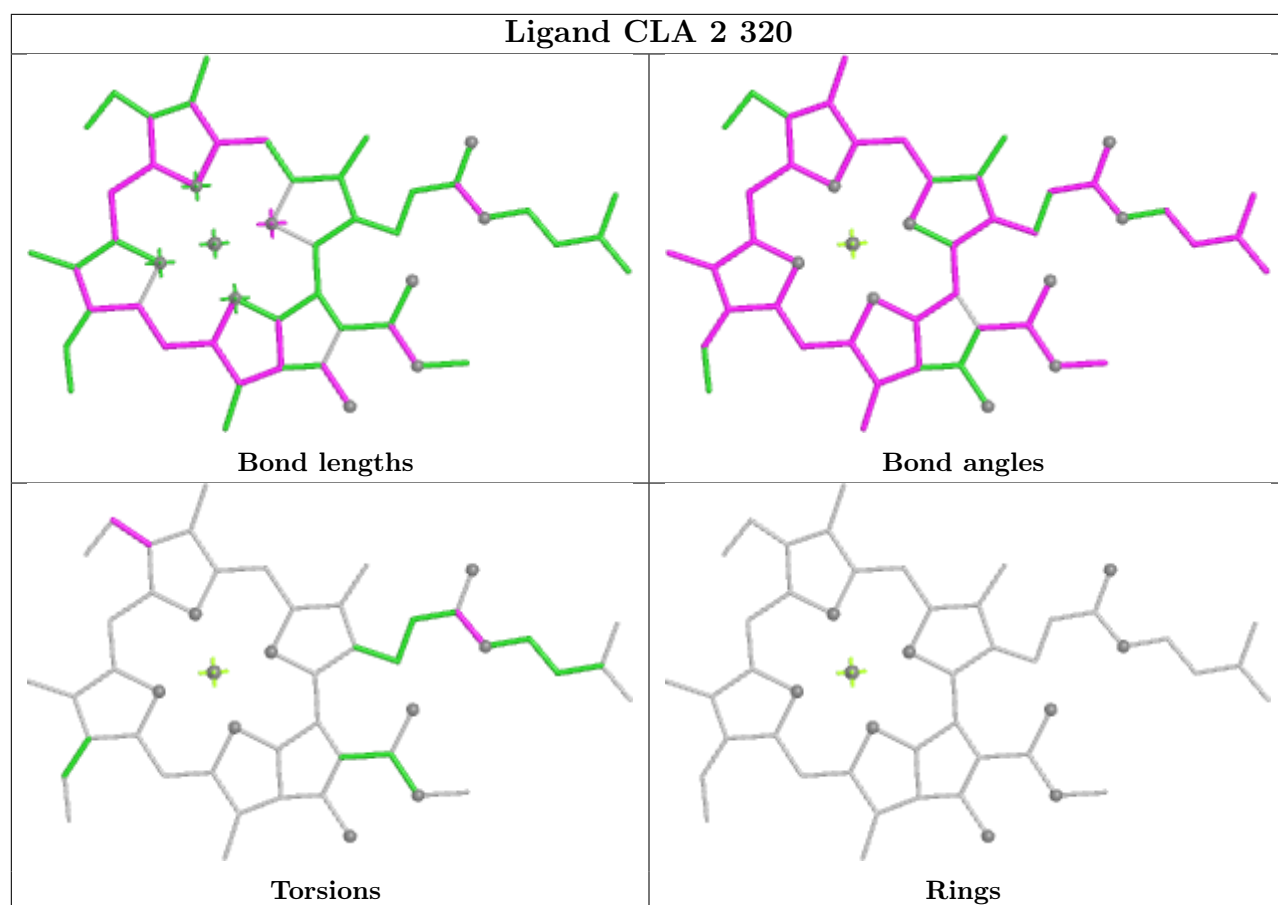


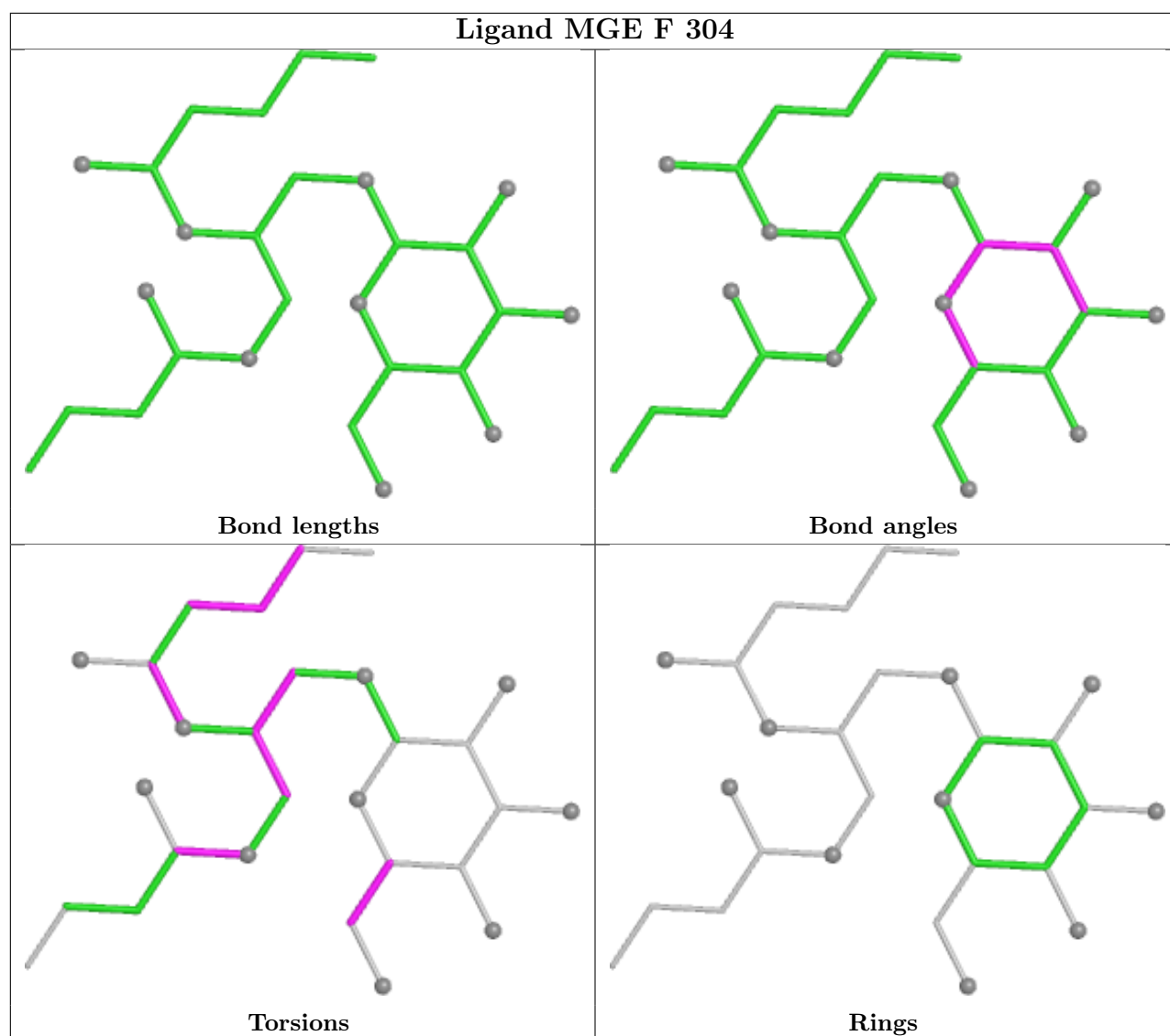
Ligand CLA A 849

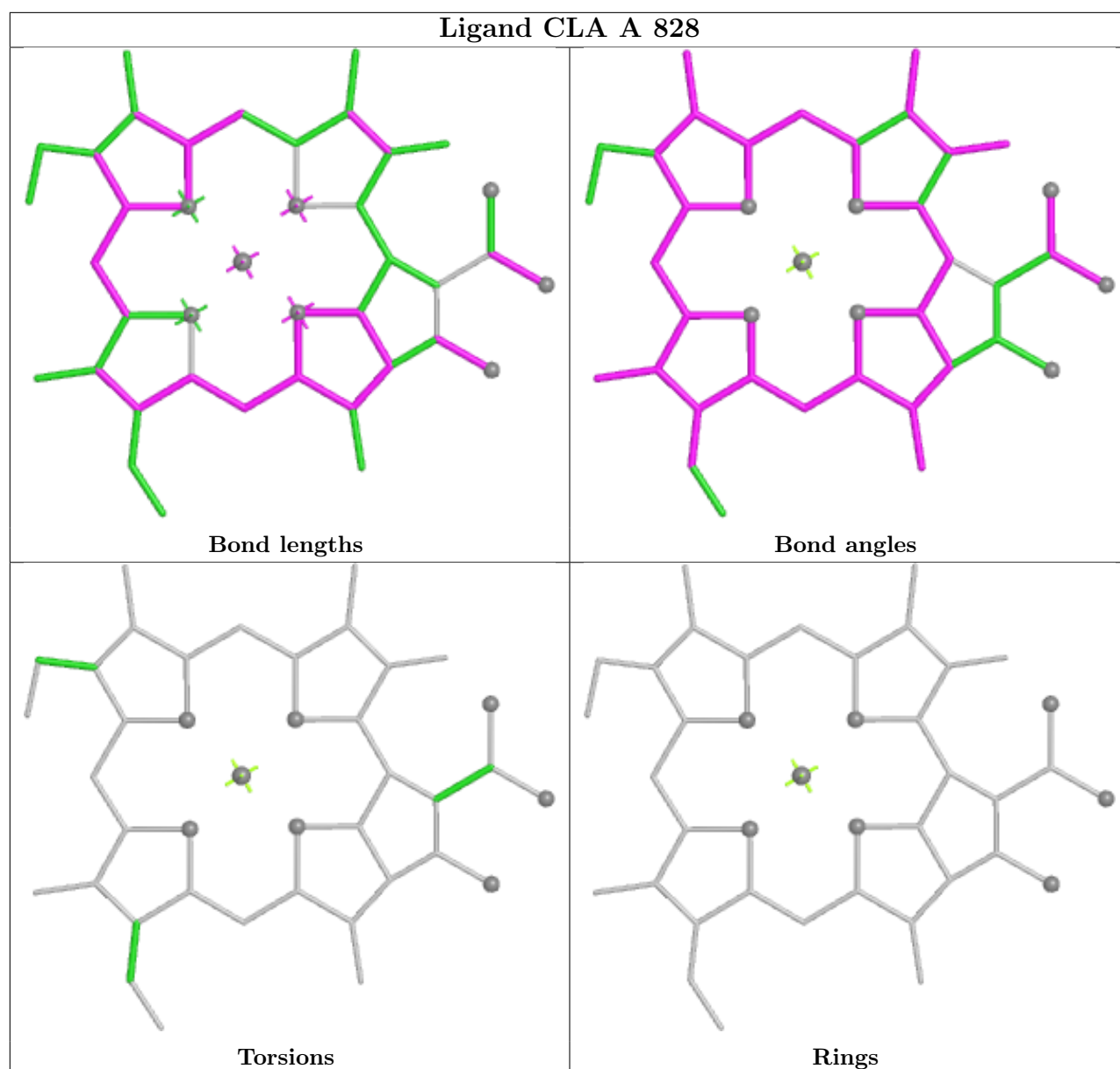


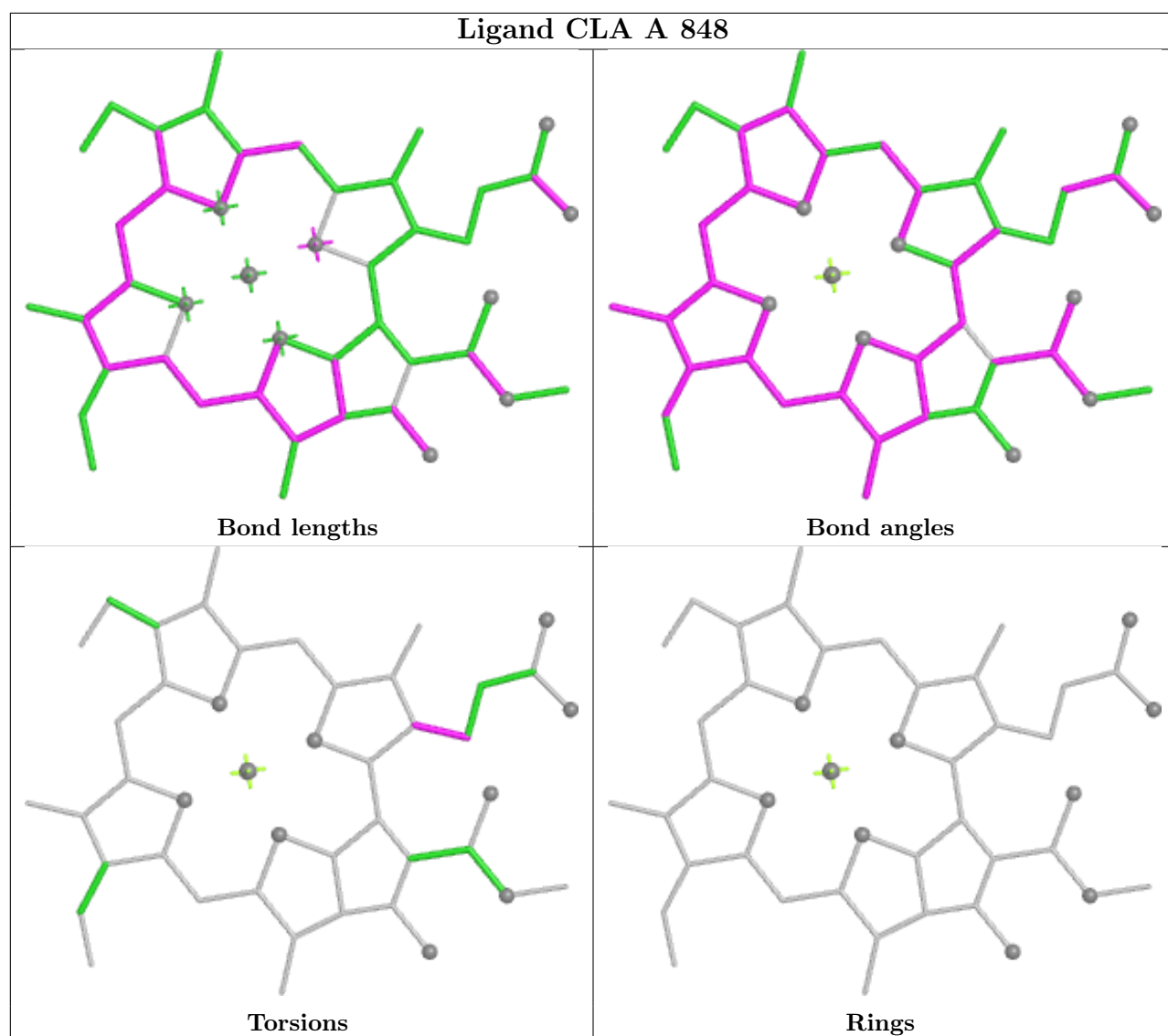
Ligand CLA 3 321

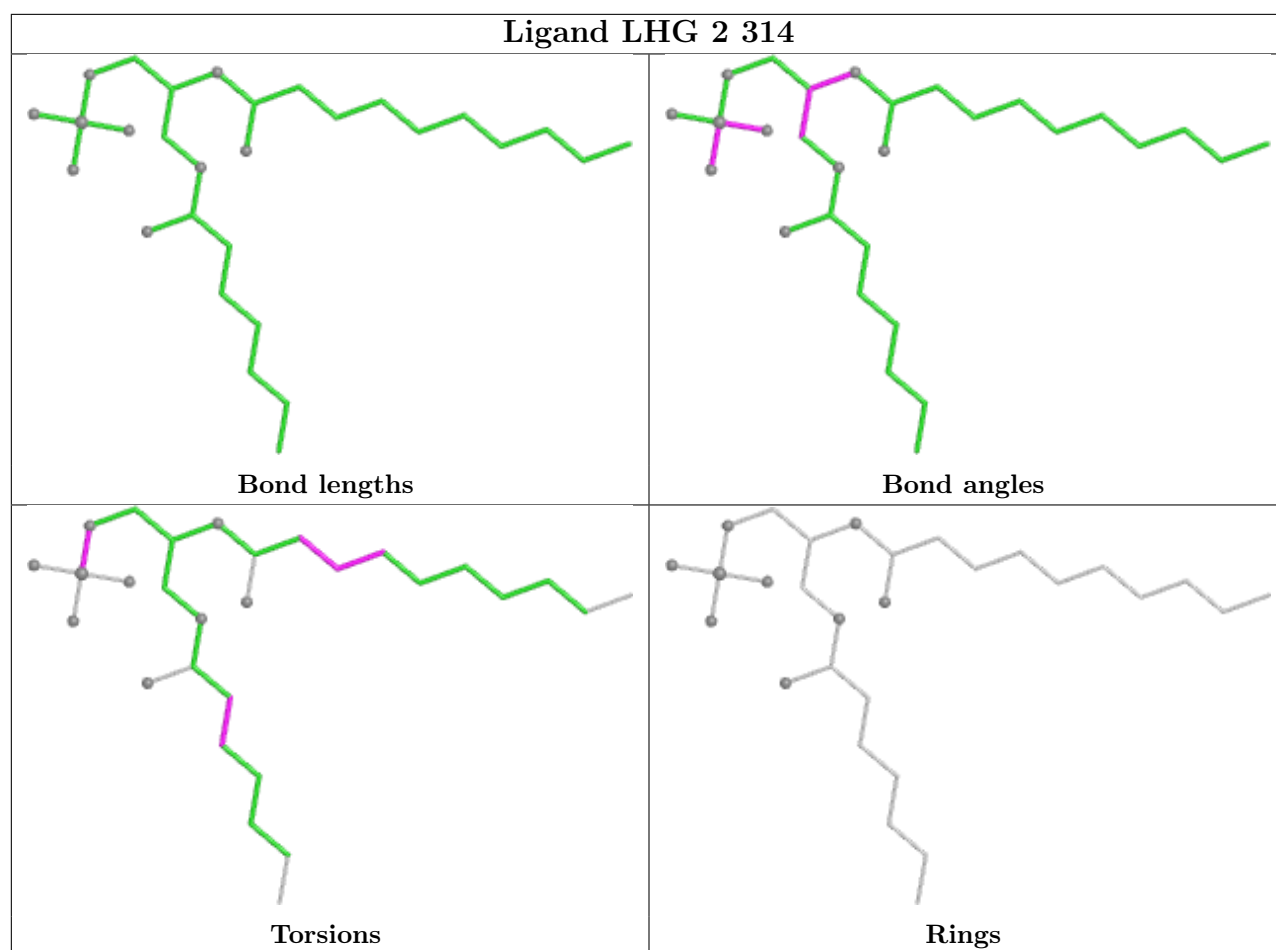




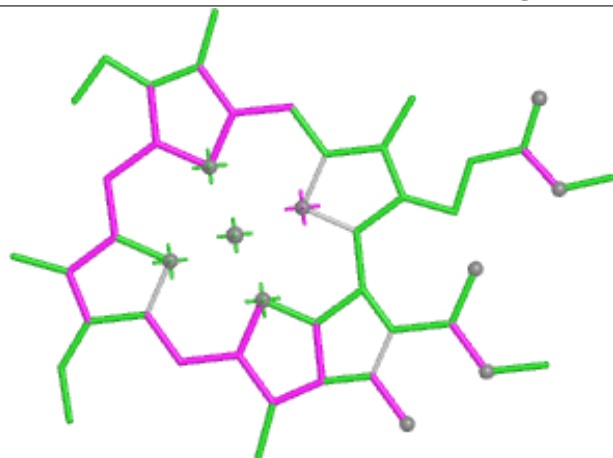




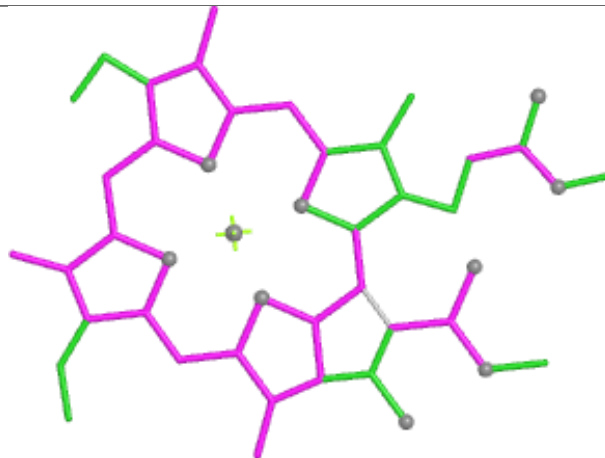




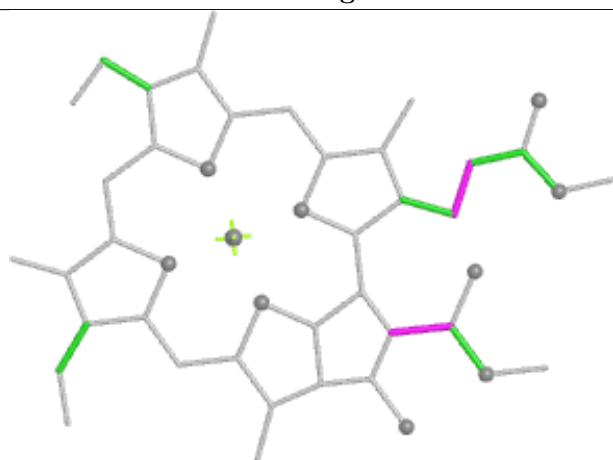
Ligand CLA F 305



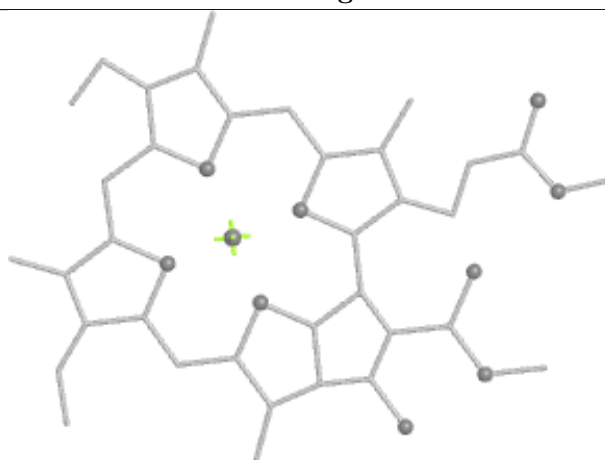
Bond lengths



Bond angles

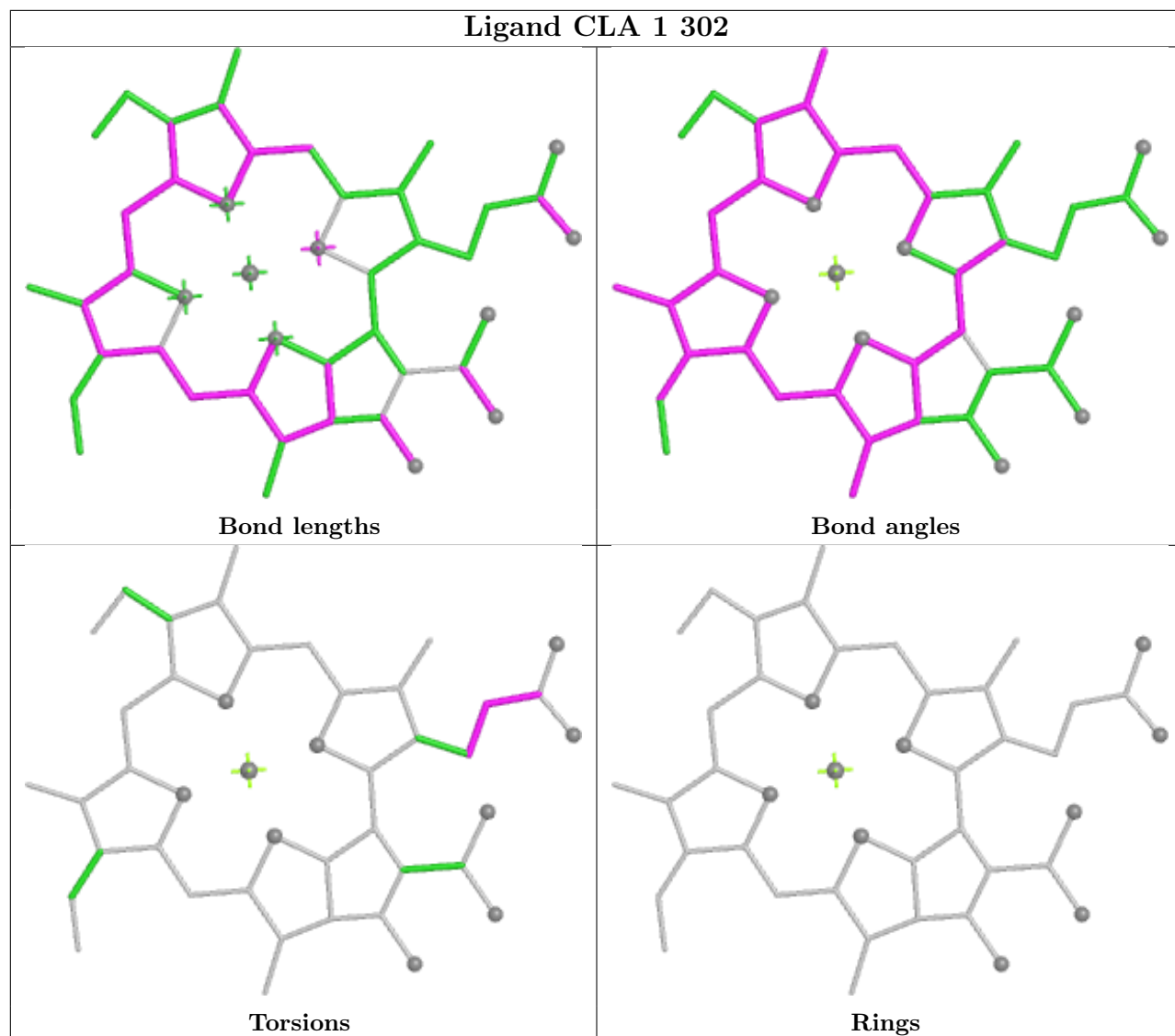


Torsions

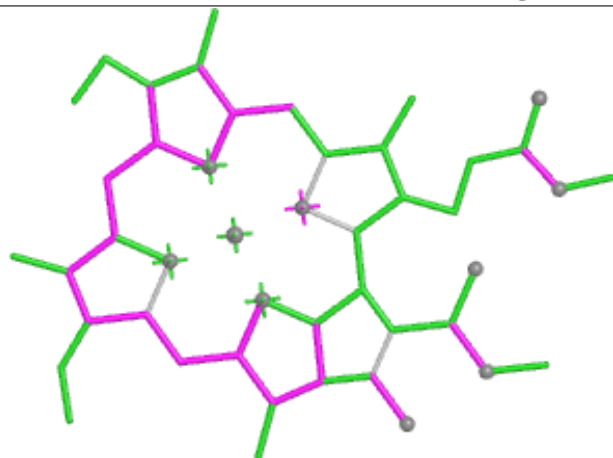


Rings

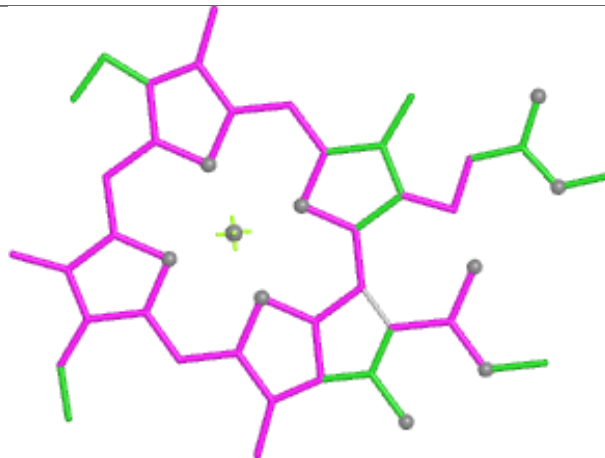
Ligand CLA 1 302



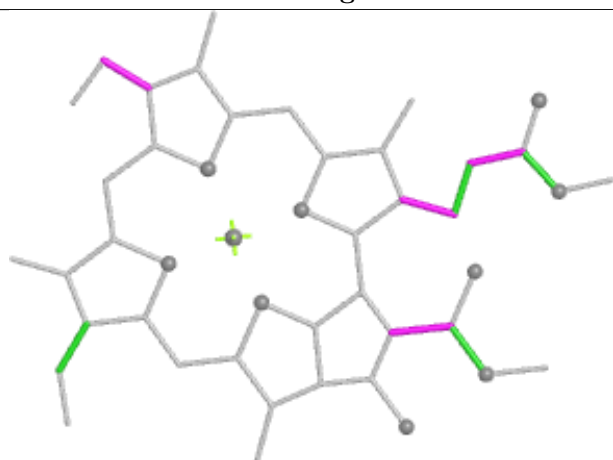
Ligand CLA X 310



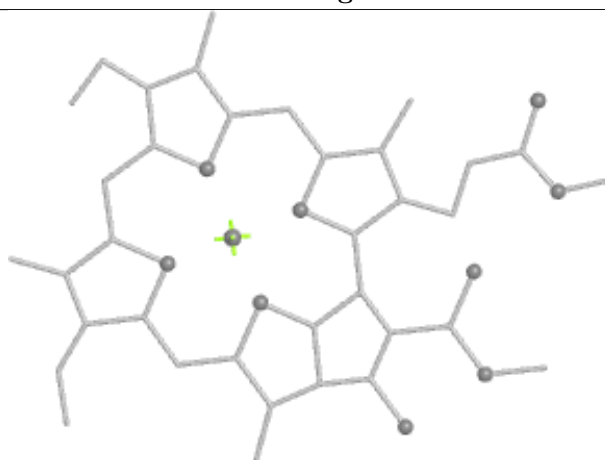
Bond lengths



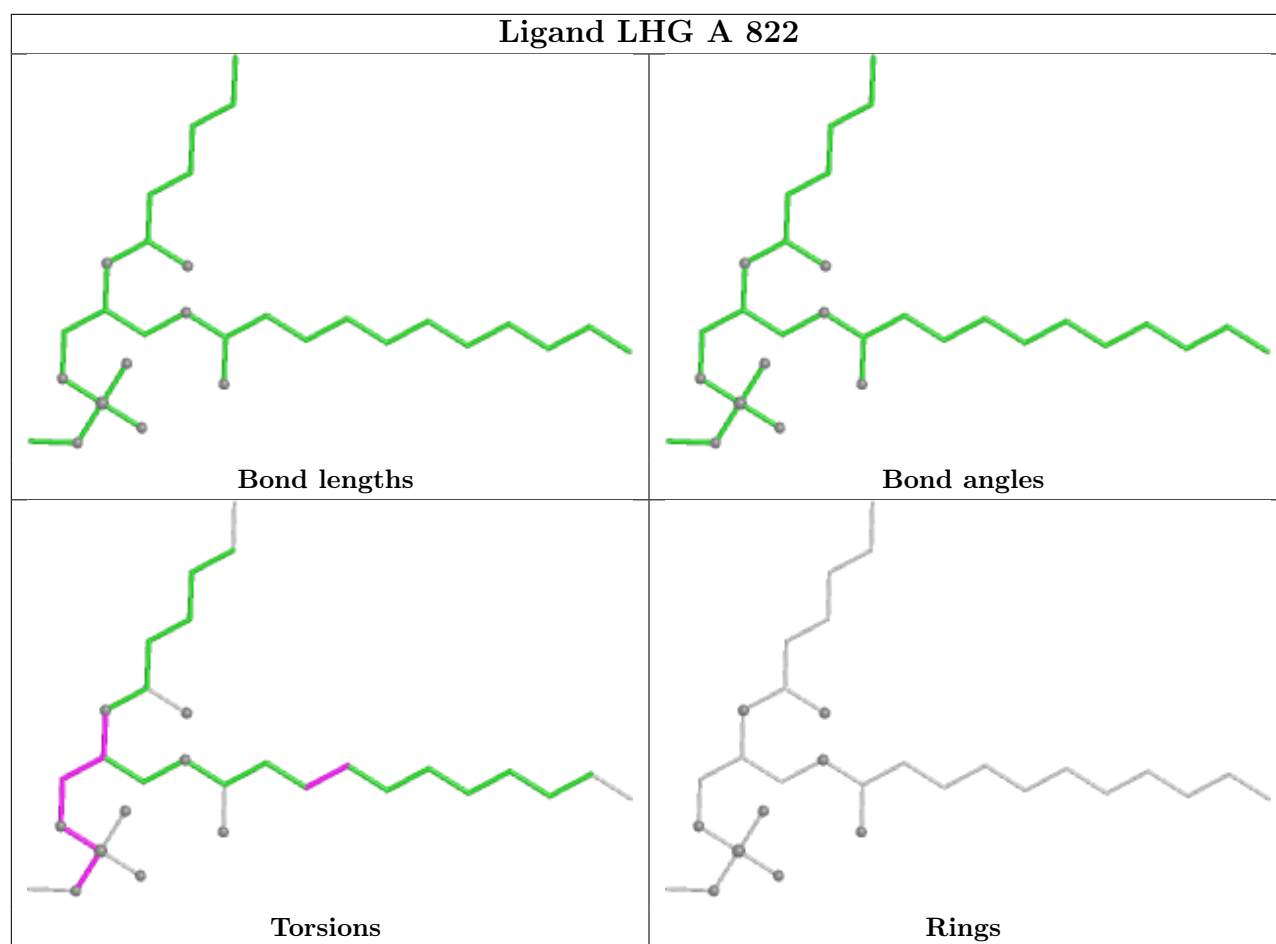
Bond angles



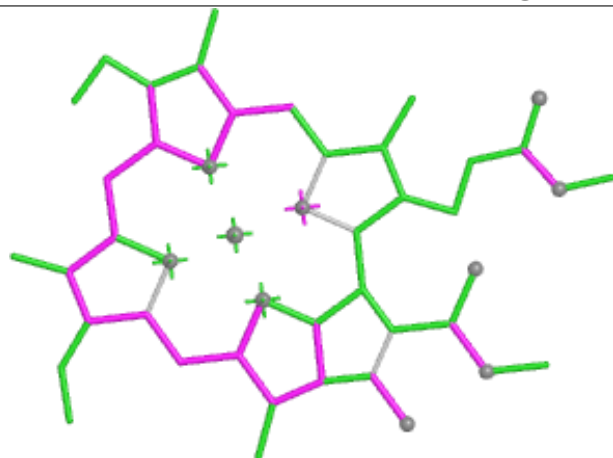
Torsions



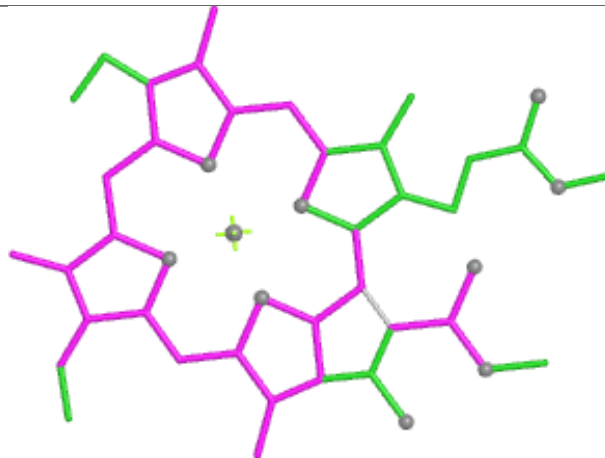
Rings



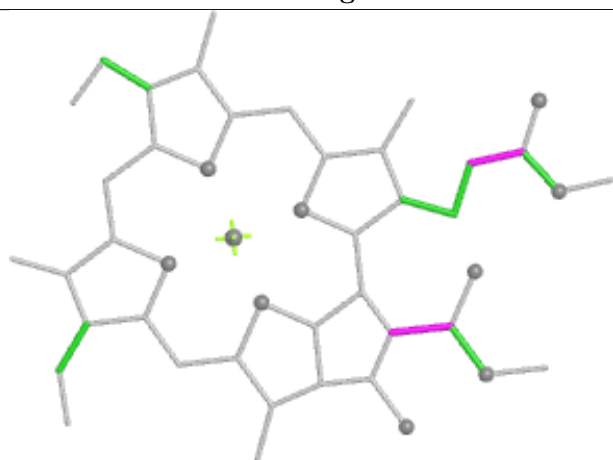
Ligand CLA Z 311



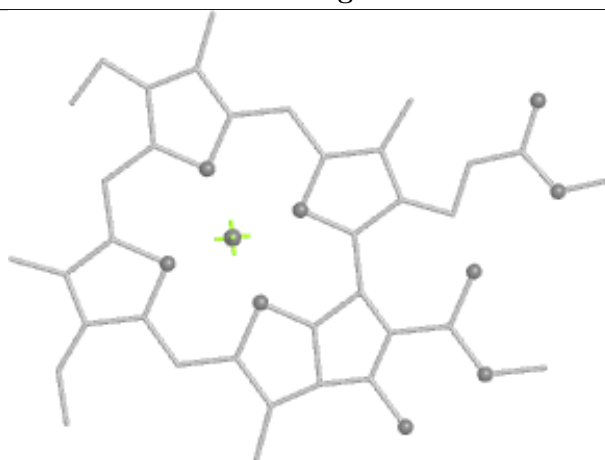
Bond lengths



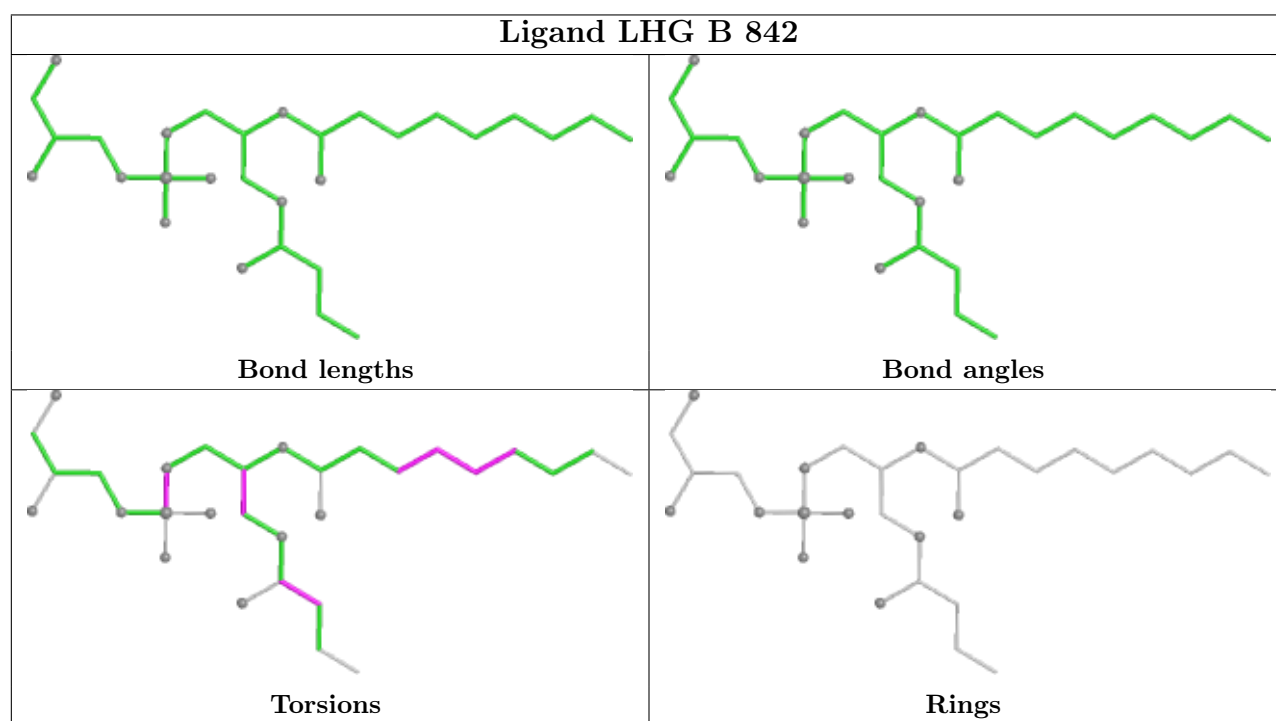
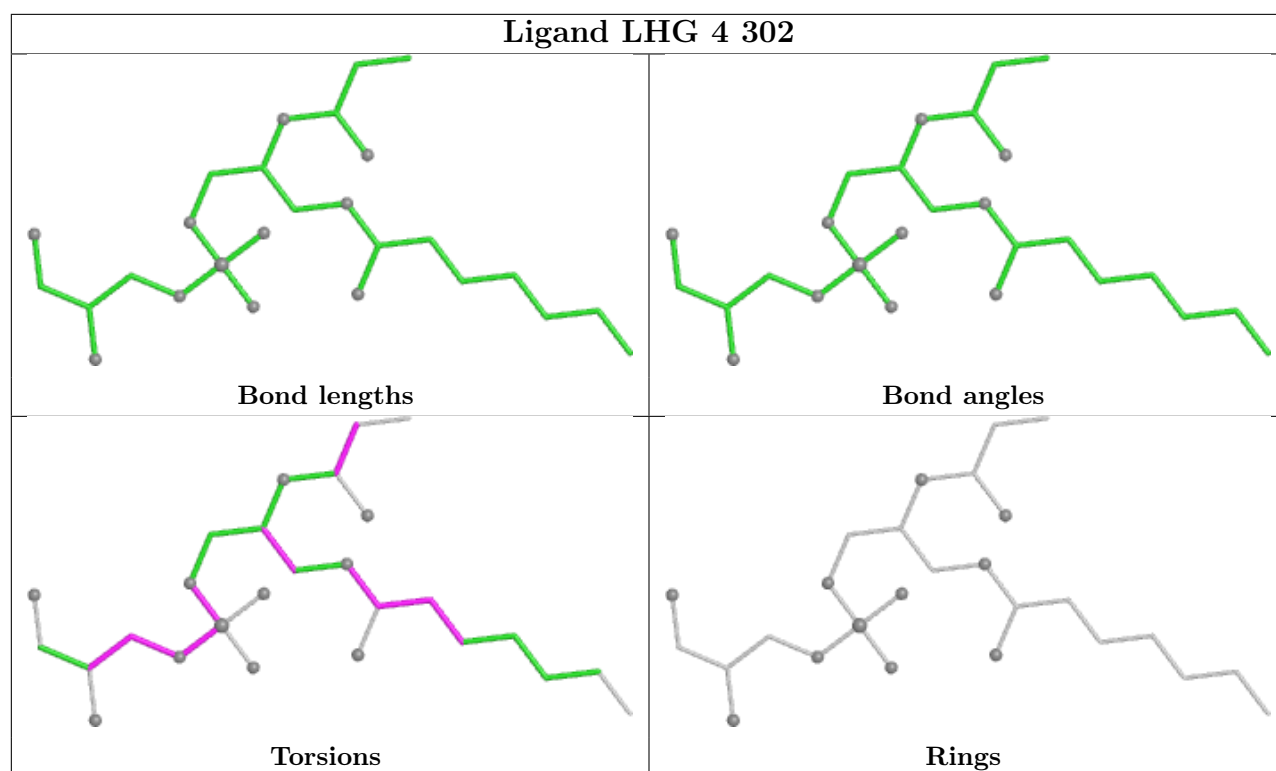
Bond angles



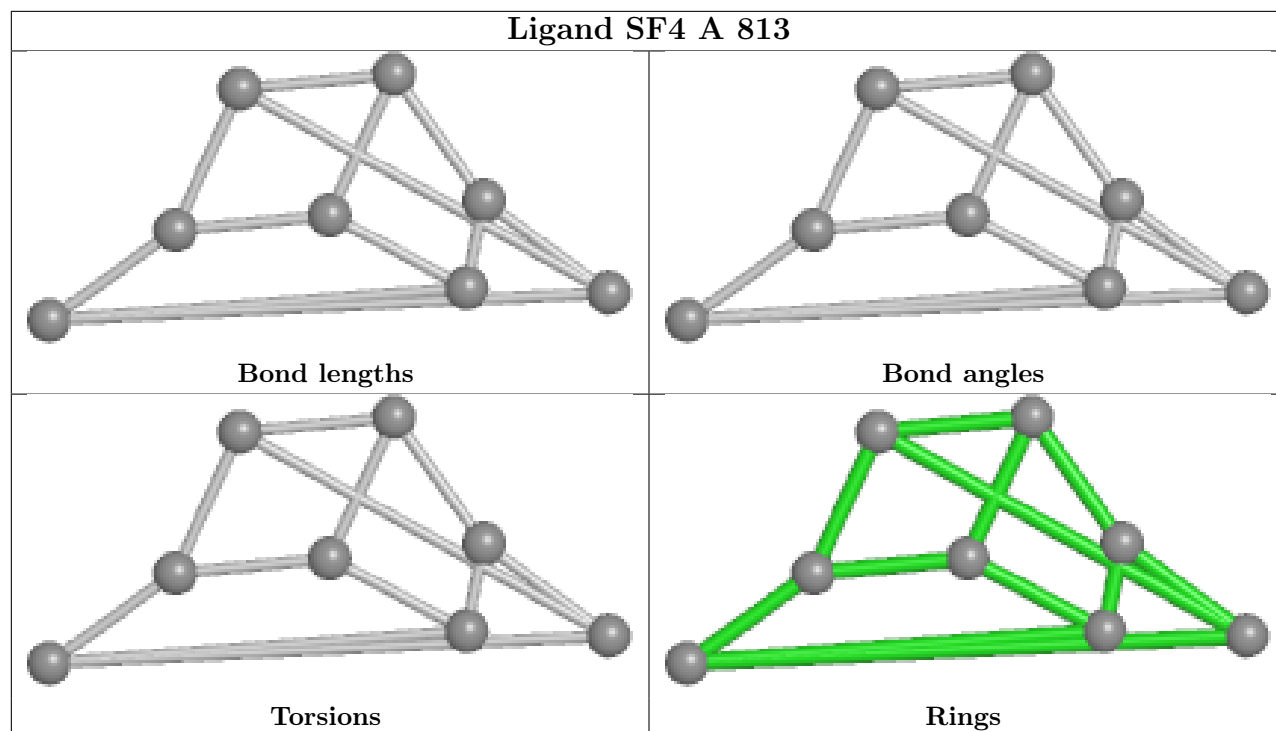
Torsions



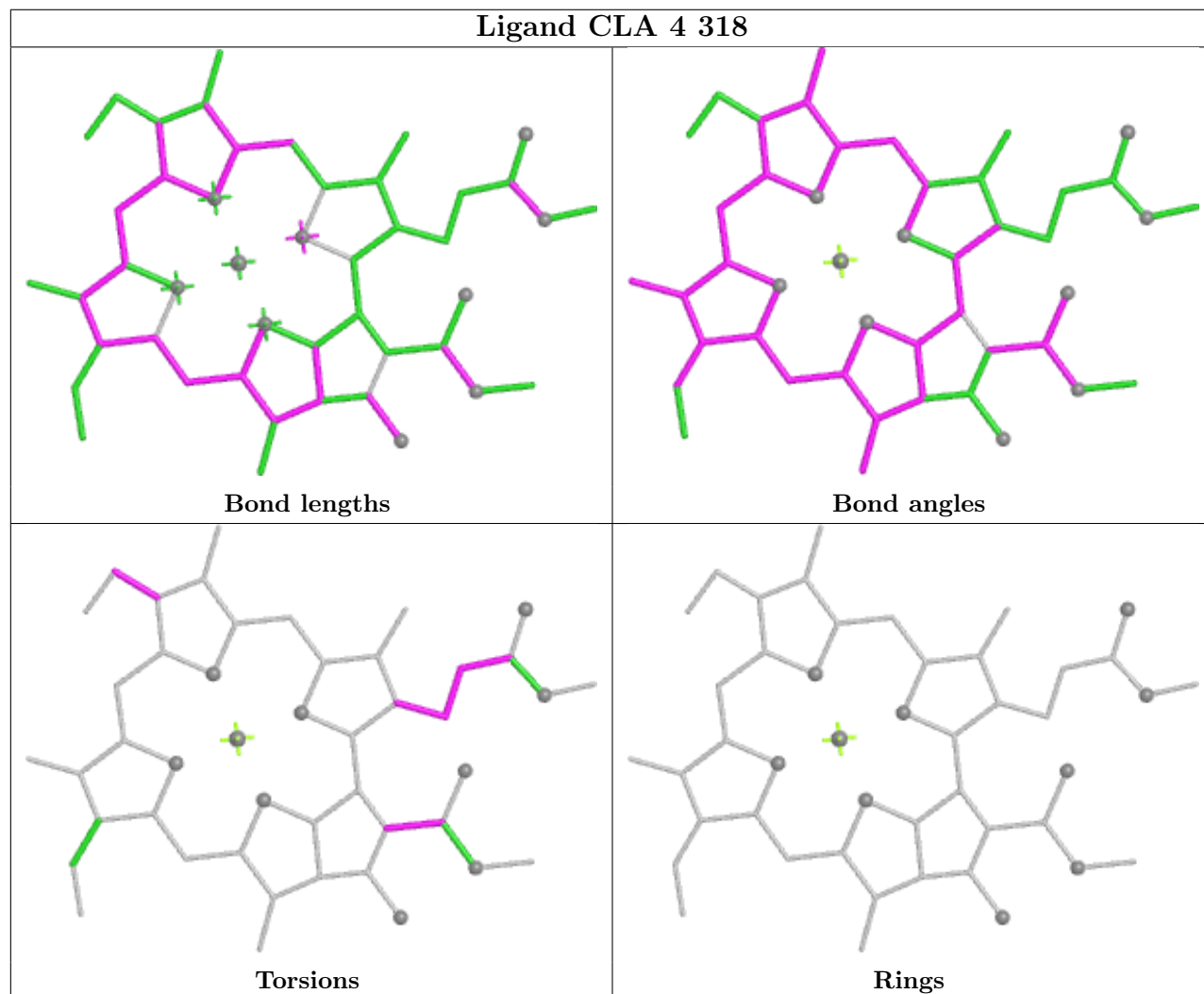
Rings



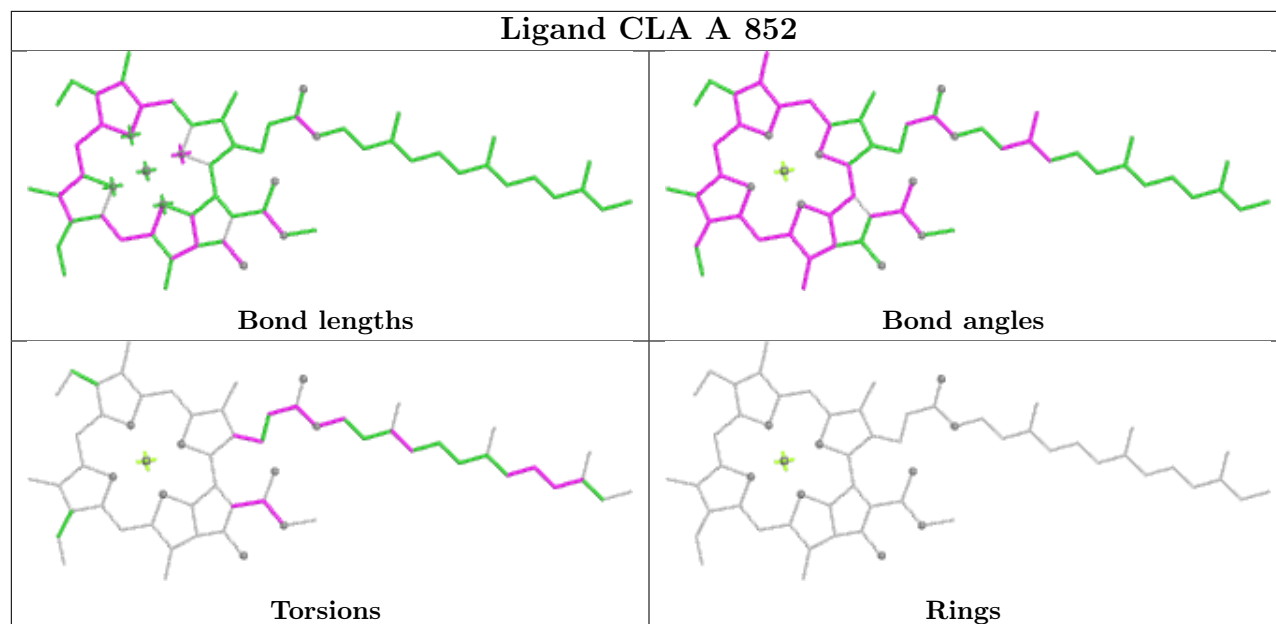
Ligand SF4 A 813



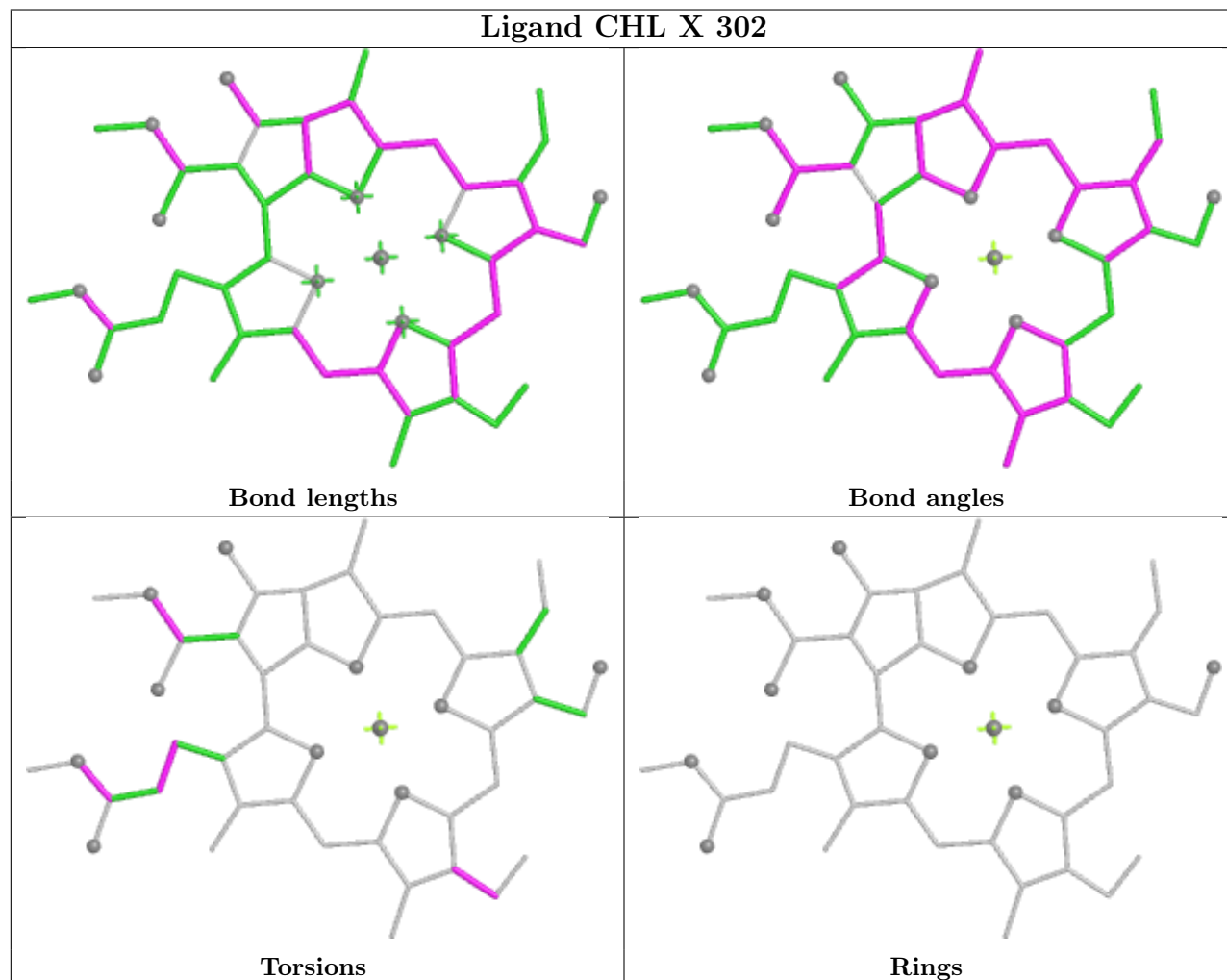
Ligand CLA 4 318

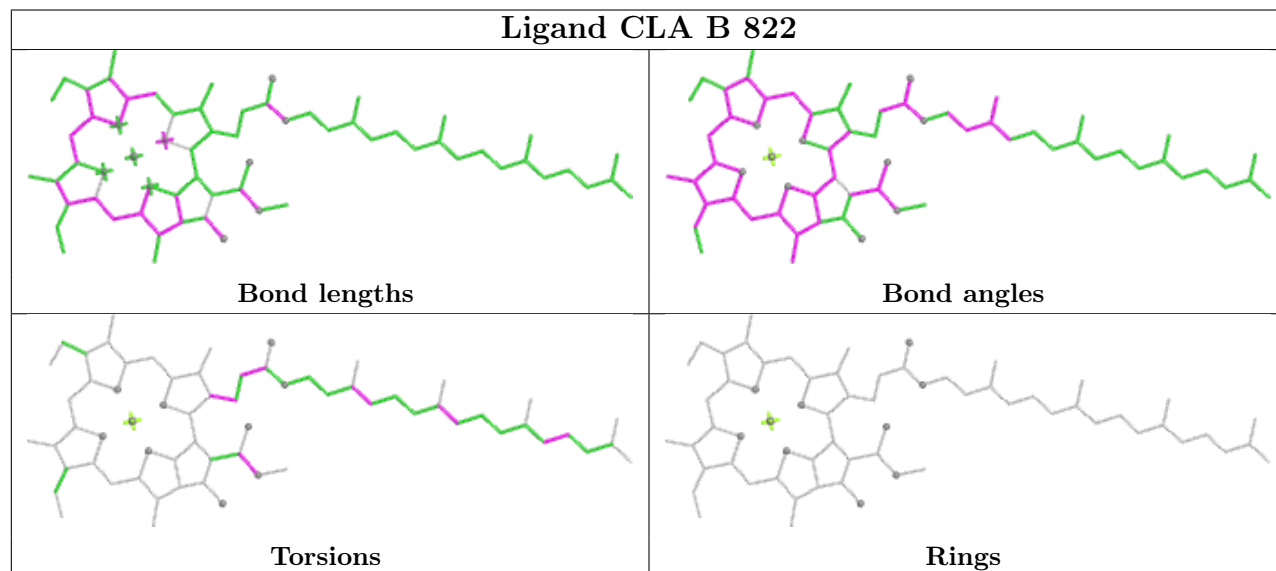
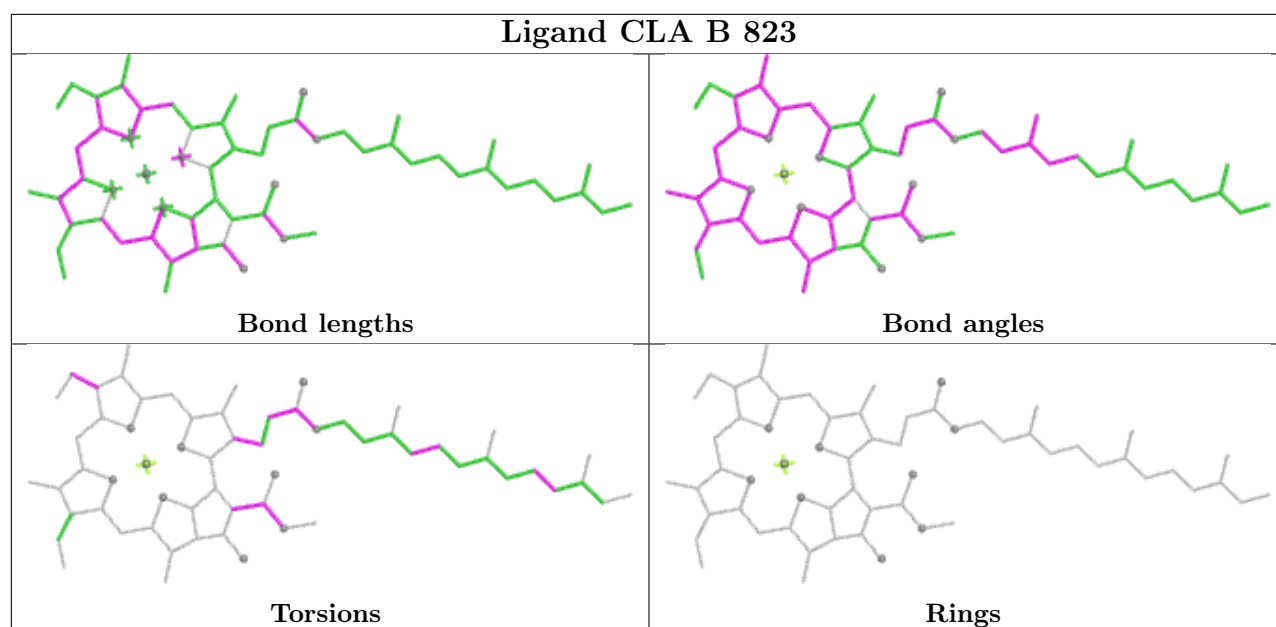


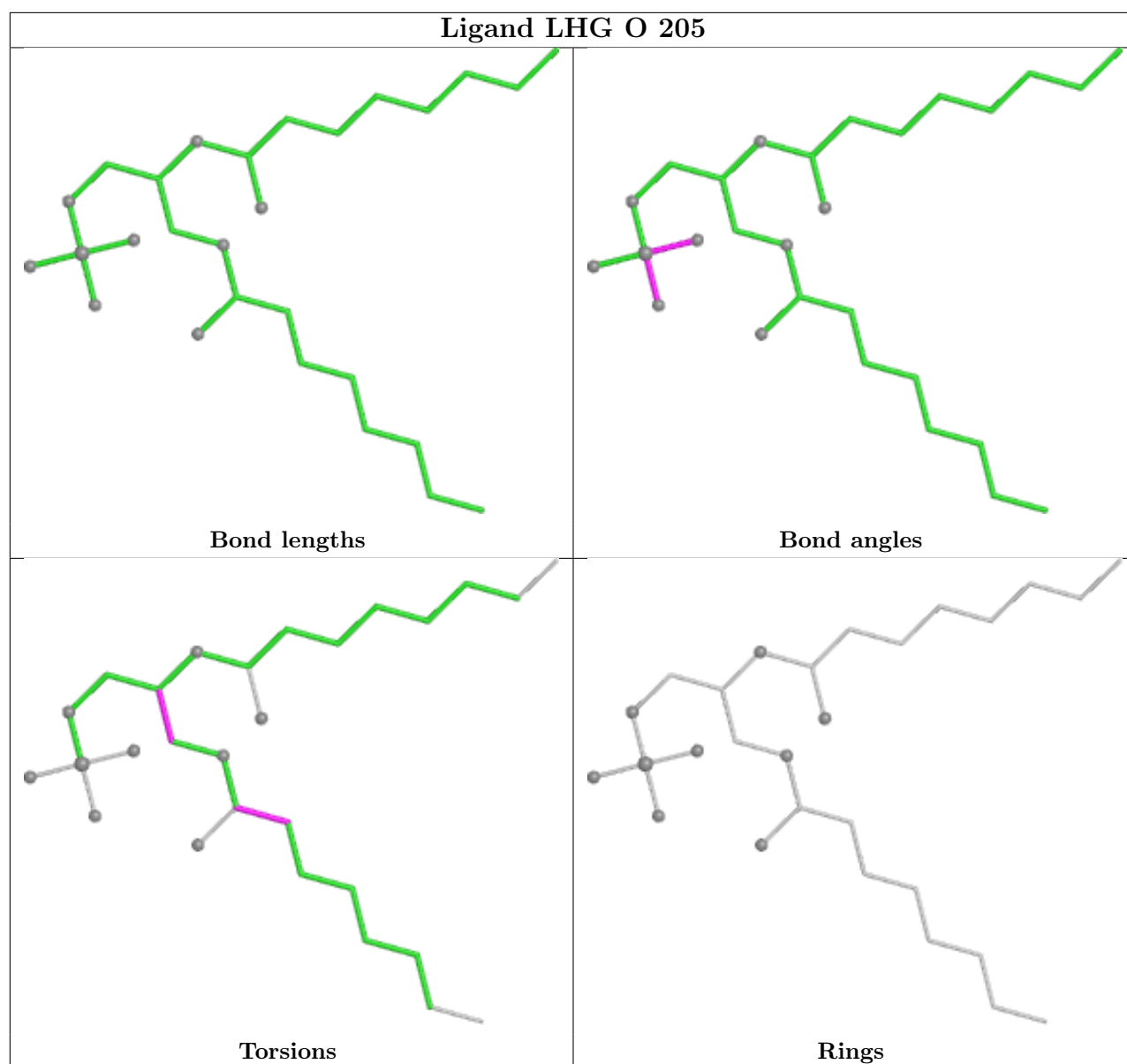
Ligand CLA A 852



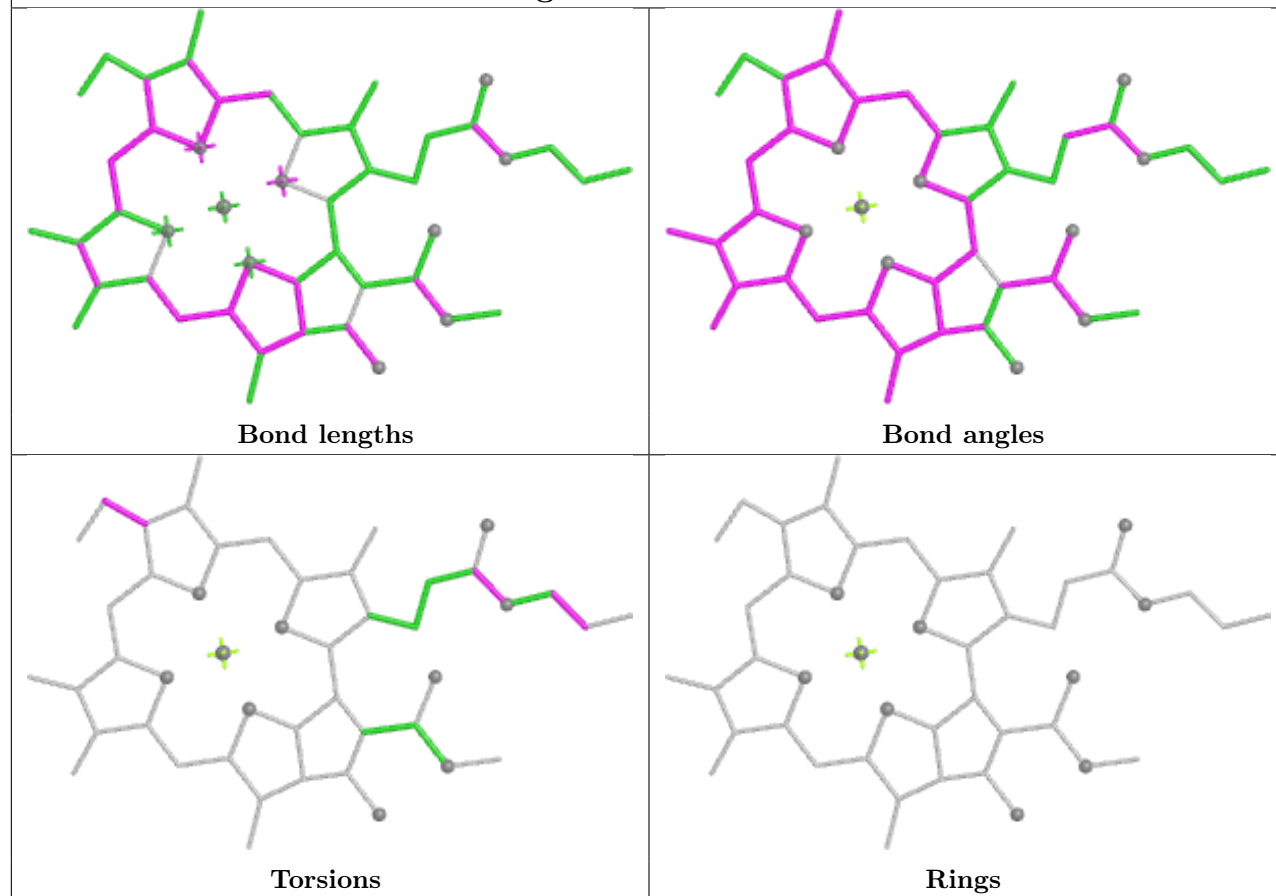
Ligand CHL X 302



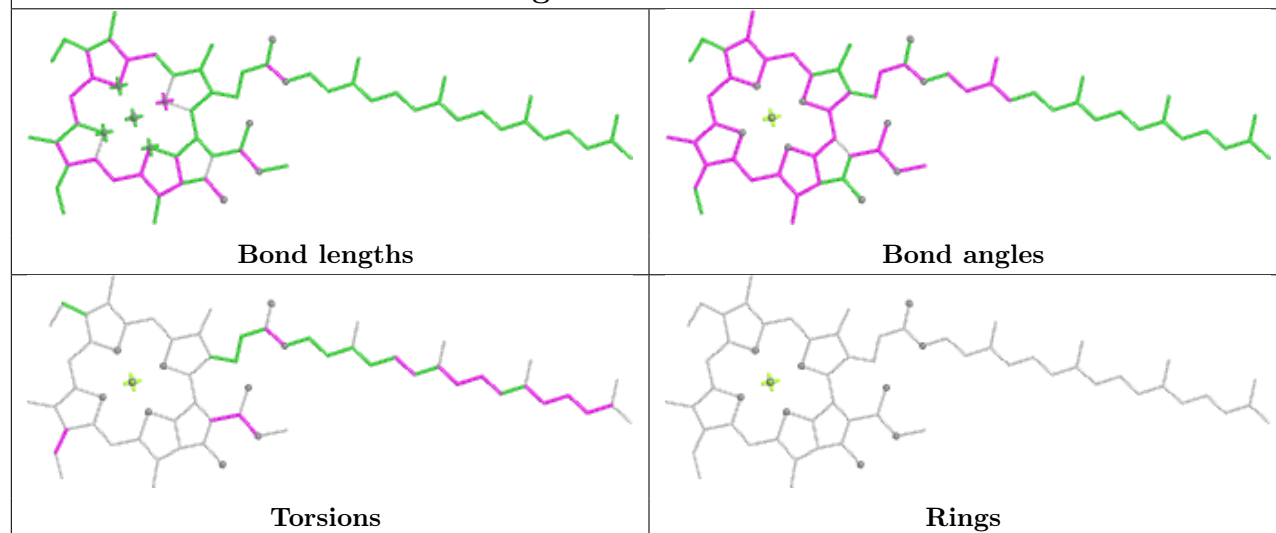




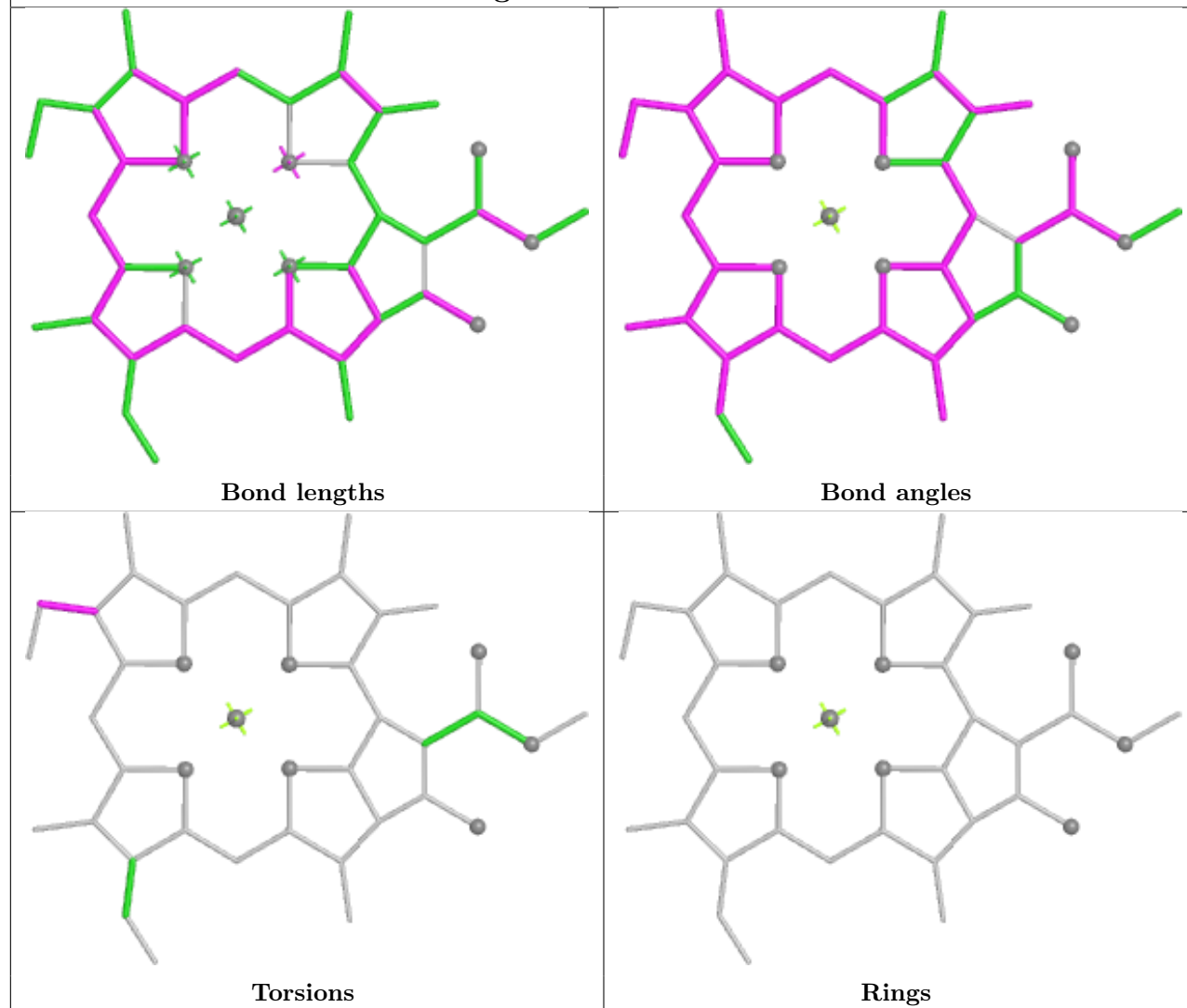
Ligand CLA 2 319



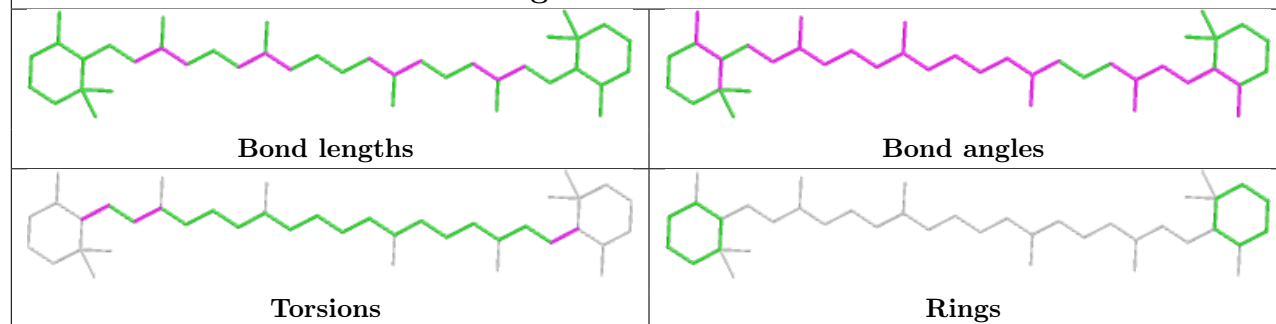
Ligand CLA B 830

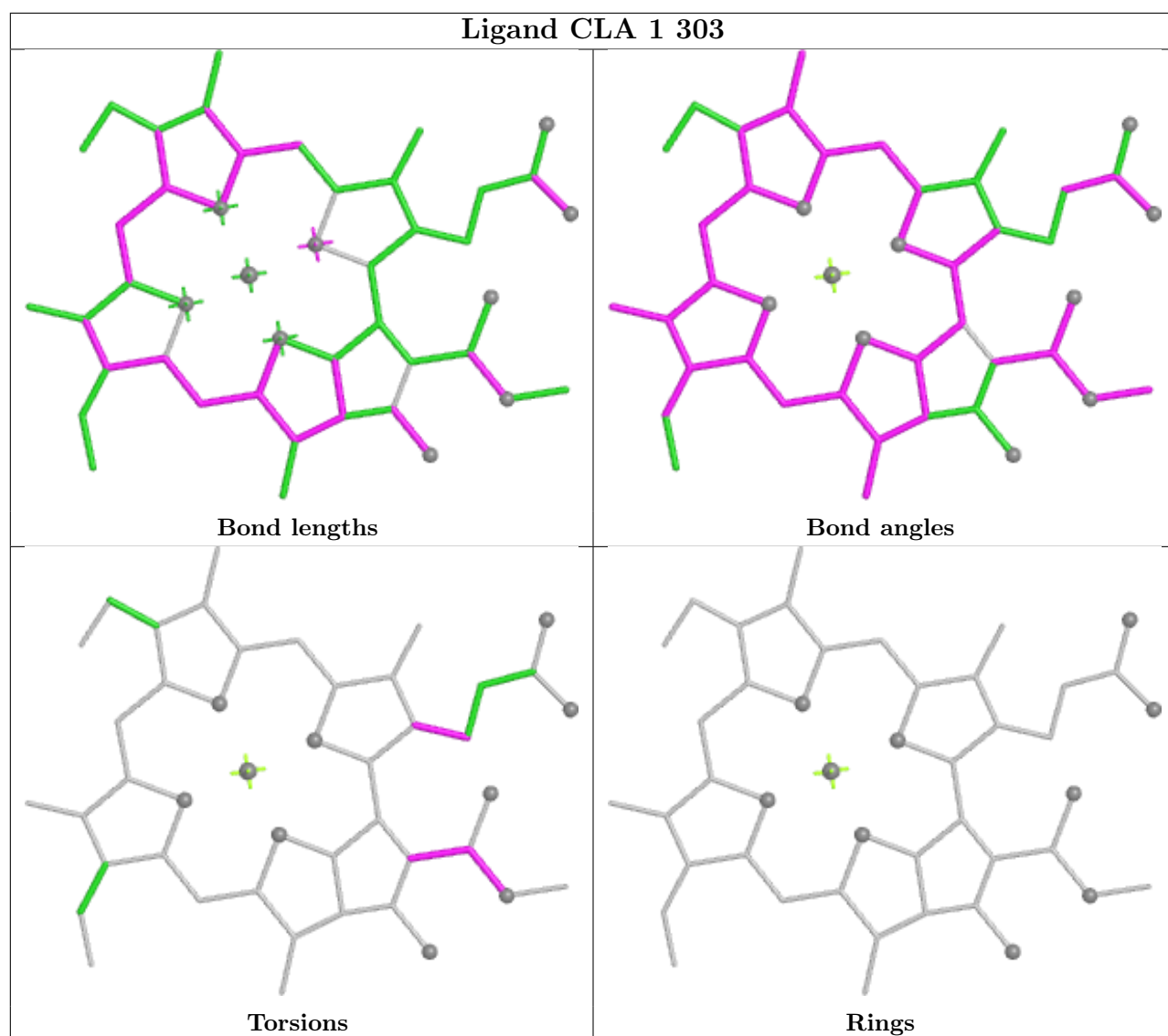


Ligand CLA K 205



Ligand BCR B 834





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

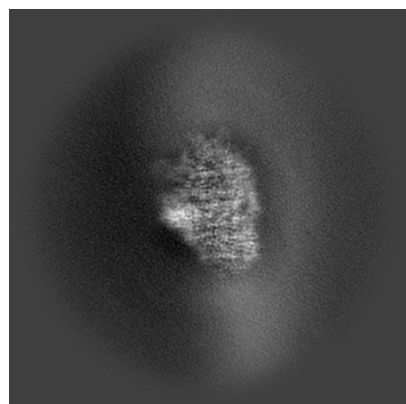
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66932. These allow visual inspection of the internal detail of the map and identification of artifacts.

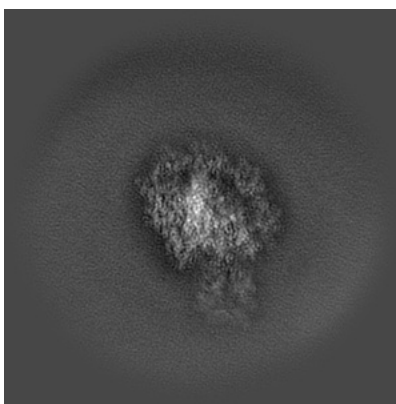
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

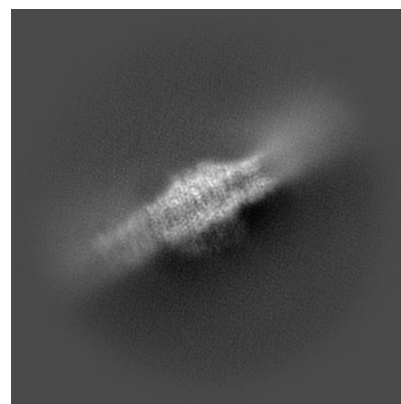
6.1.1 Primary map



X

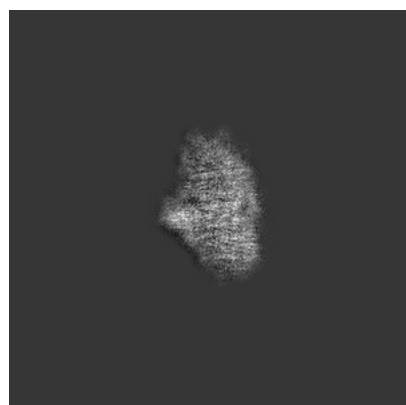


Y

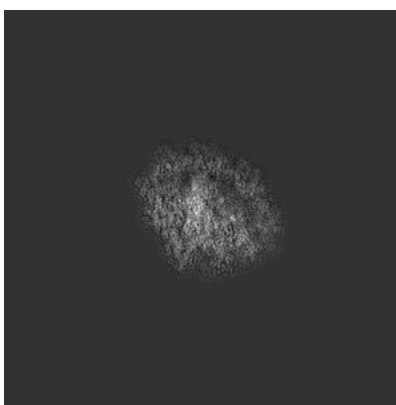


Z

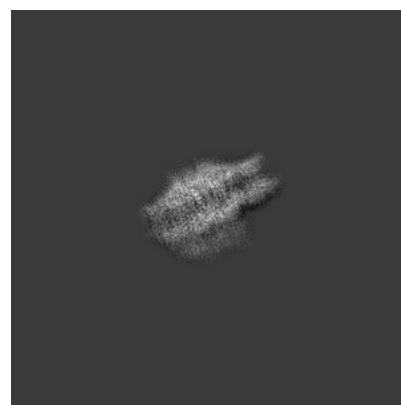
6.1.2 Raw map



X



Y

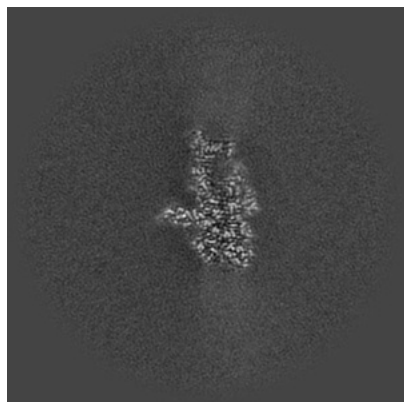


Z

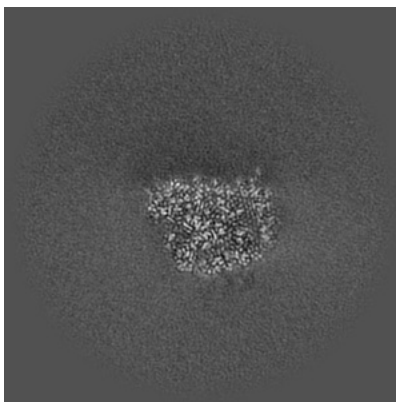
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

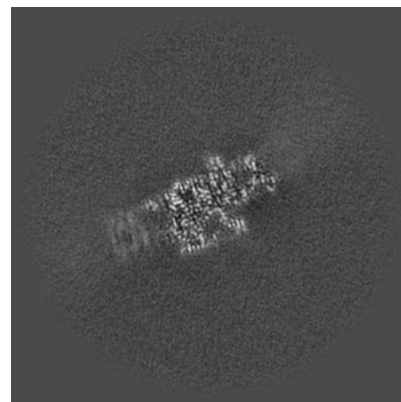
6.2.1 Primary map



X Index: 256

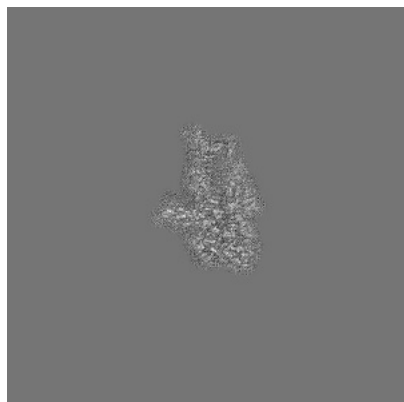


Y Index: 256

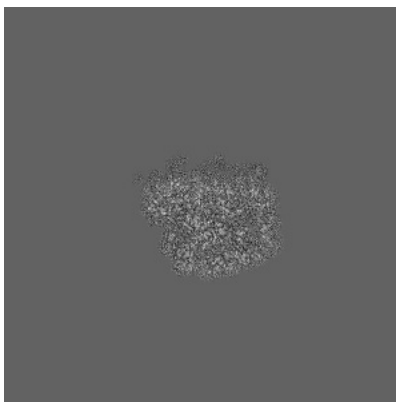


Z Index: 256

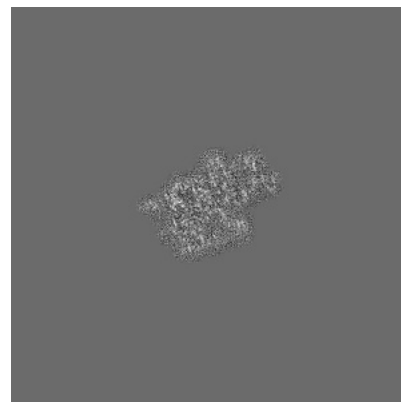
6.2.2 Raw map



X Index: 256



Y Index: 256

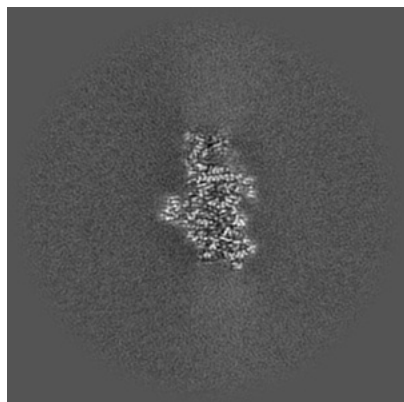


Z Index: 256

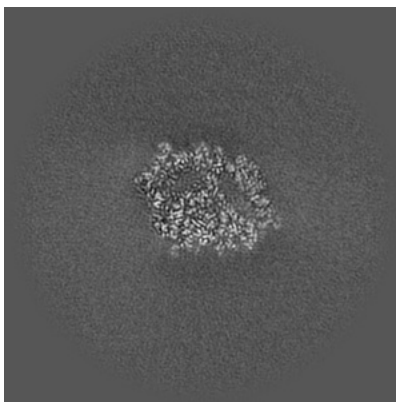
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

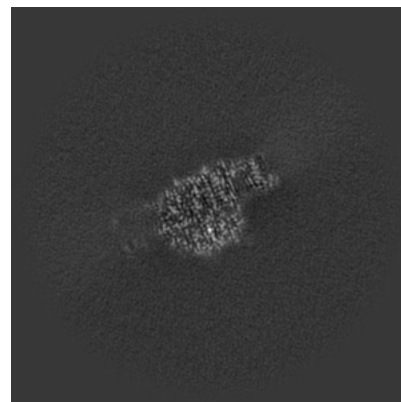
6.3.1 Primary map



X Index: 244

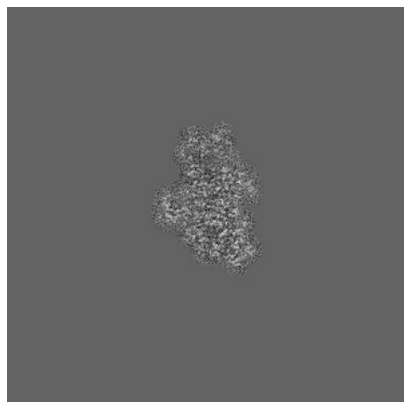


Y Index: 280

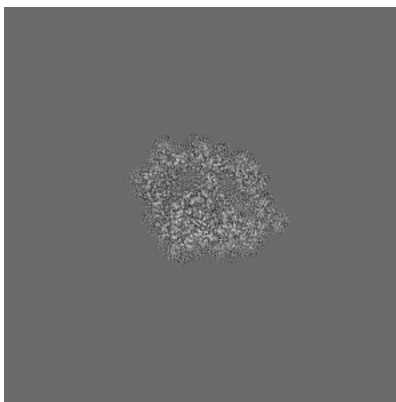


Z Index: 244

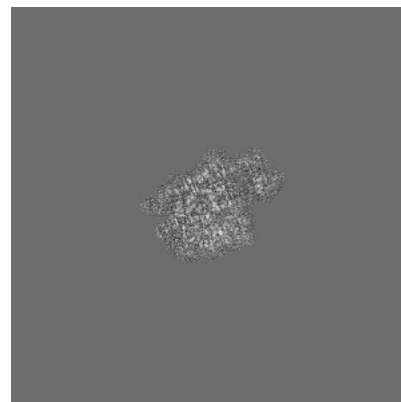
6.3.2 Raw map



X Index: 239



Y Index: 279

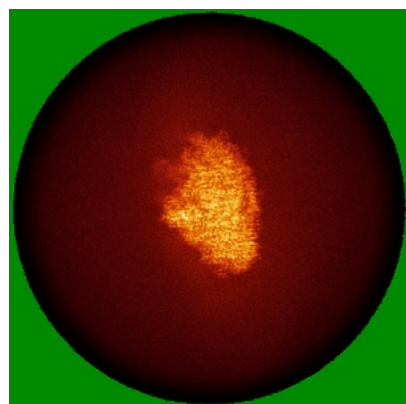


Z Index: 249

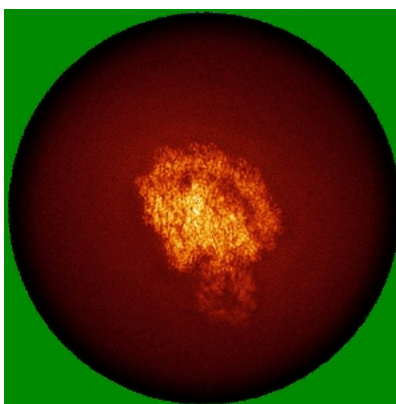
The images above show the largest variance slices of the map in three orthogonal directions.

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

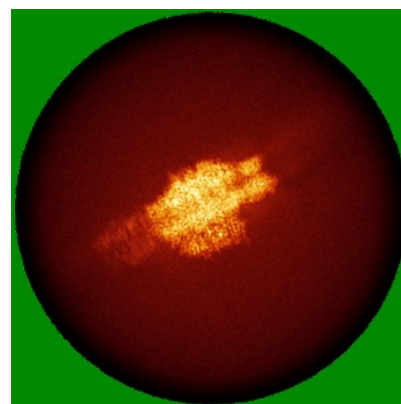
6.4.1 Primary map



X

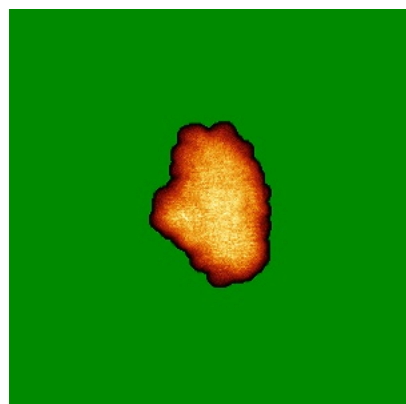


Y

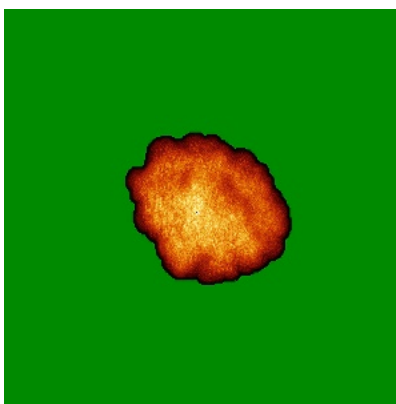


Z

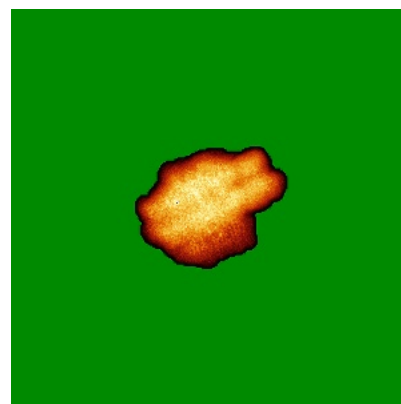
6.4.2 Raw map



X



Y

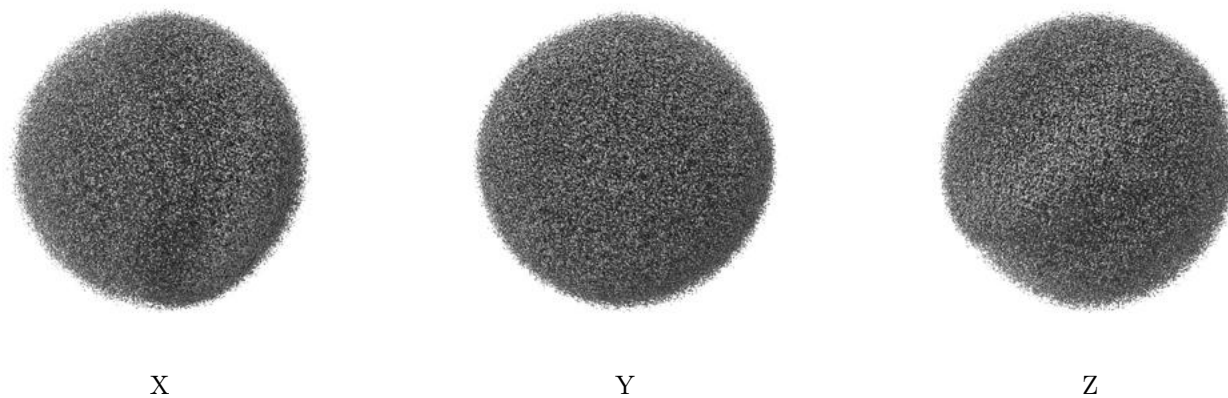


Z

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.

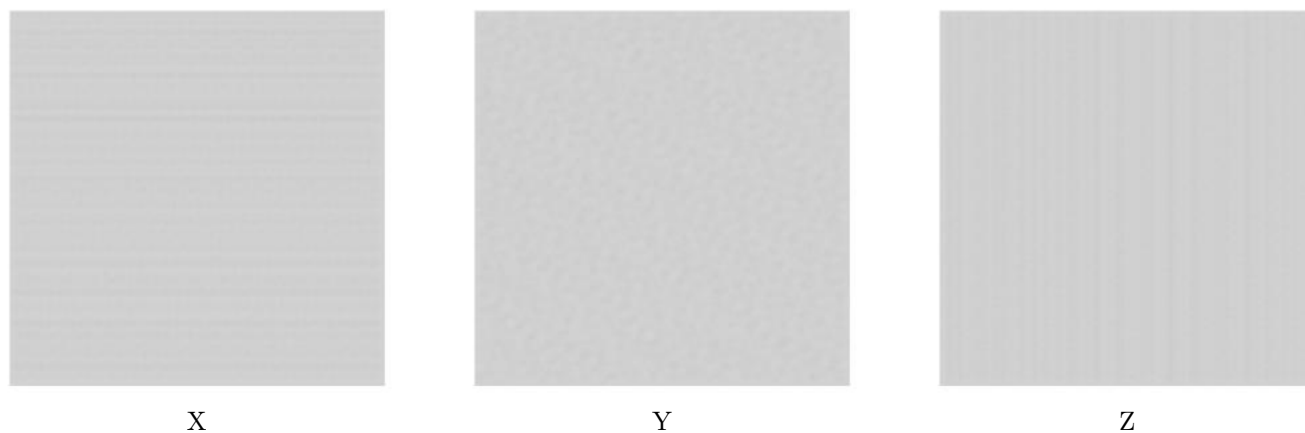
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. 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.

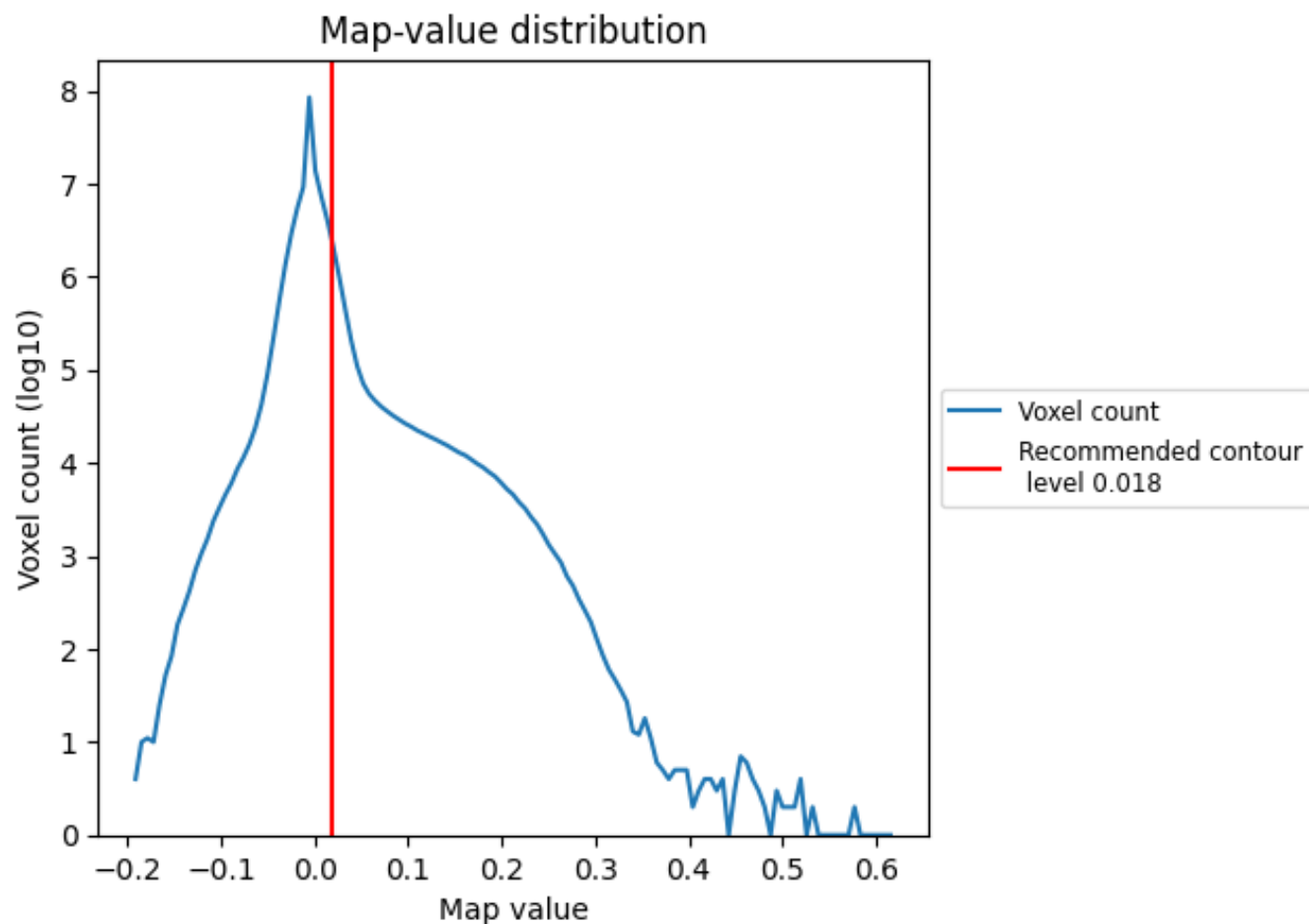
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

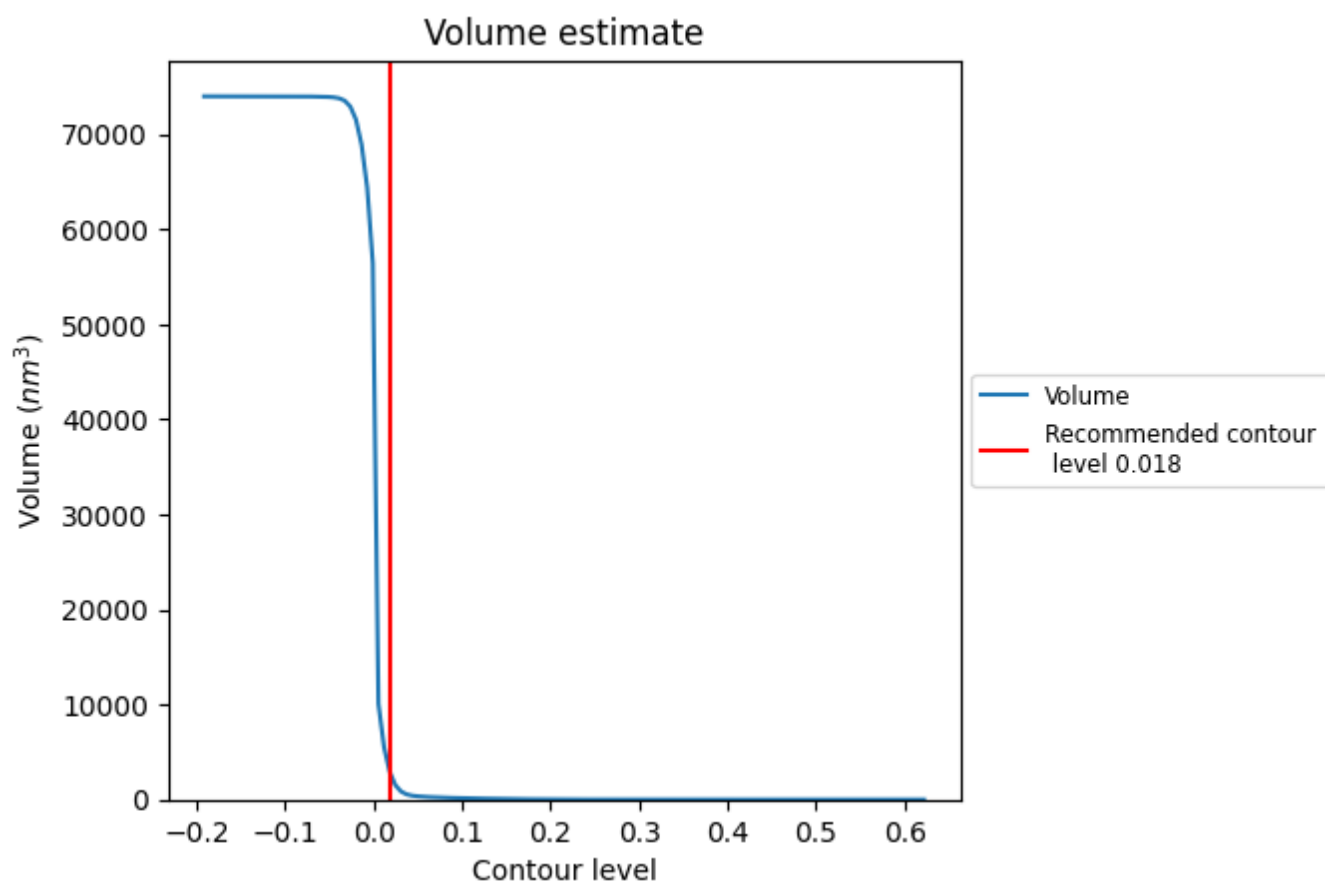
This section contains the results of statistical analysis of the map.

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.

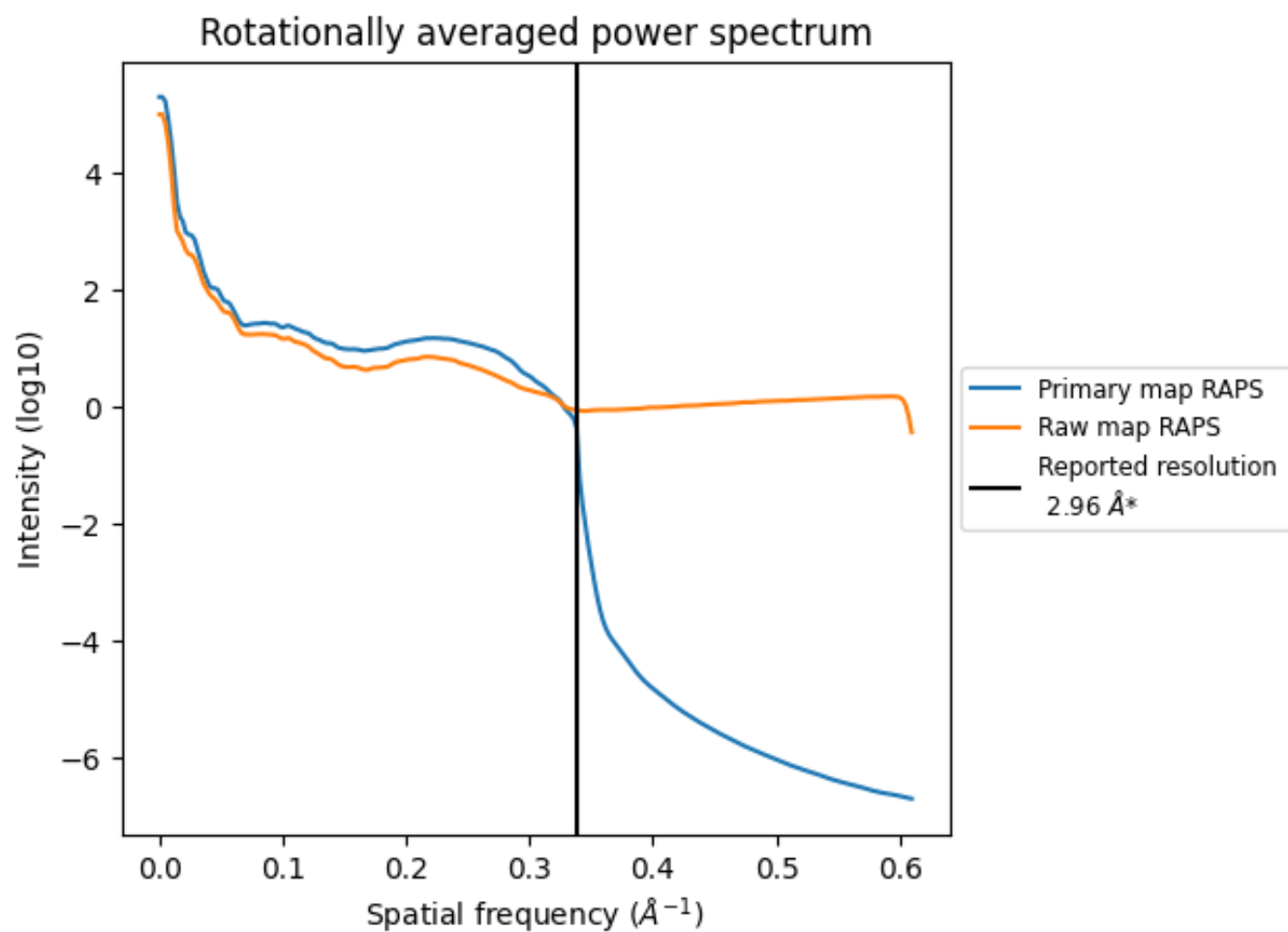
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3044 nm³; this corresponds to an approximate mass of 2750 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 ⓘ

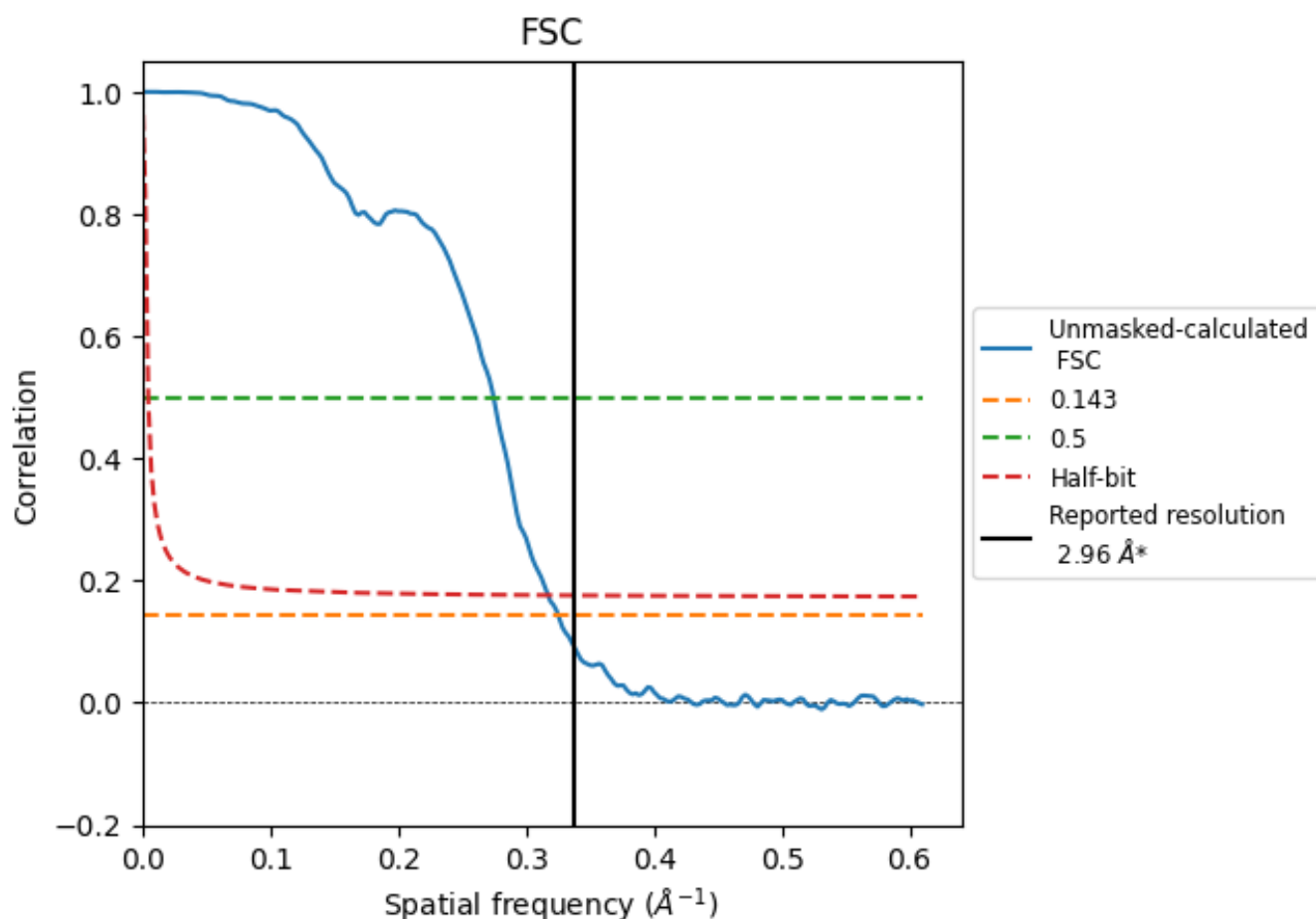


*Reported resolution corresponds to spatial frequency of 0.338 $\text{\AA}^{-1}$

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 0.338 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

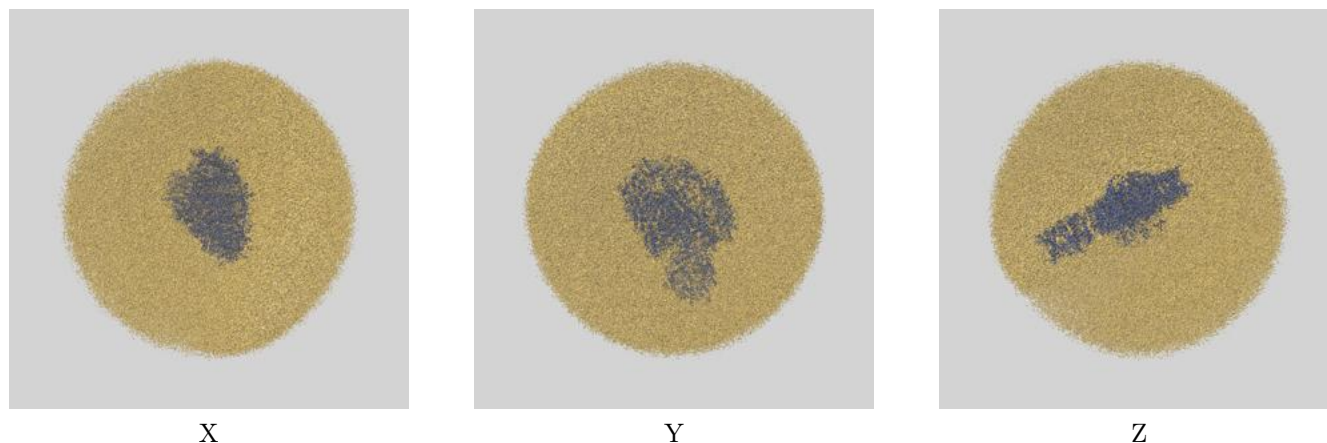
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.08	3.64	3.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

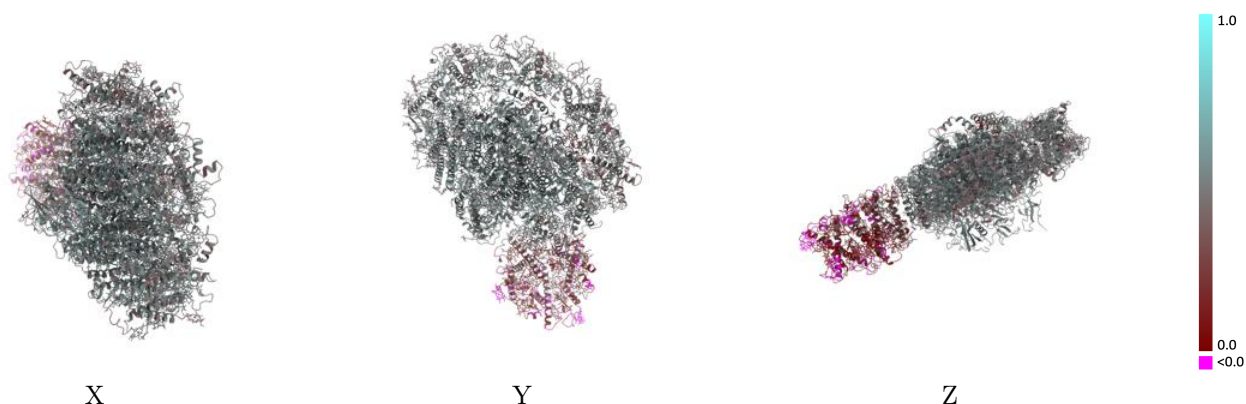
This section contains information regarding the fit between EMDB map EMD-66932 and PDB model 9XJ9. Per-residue inclusion information can be found in [section 3](#) on [page 29](#).

9.1 Map-model overlay [i](#)



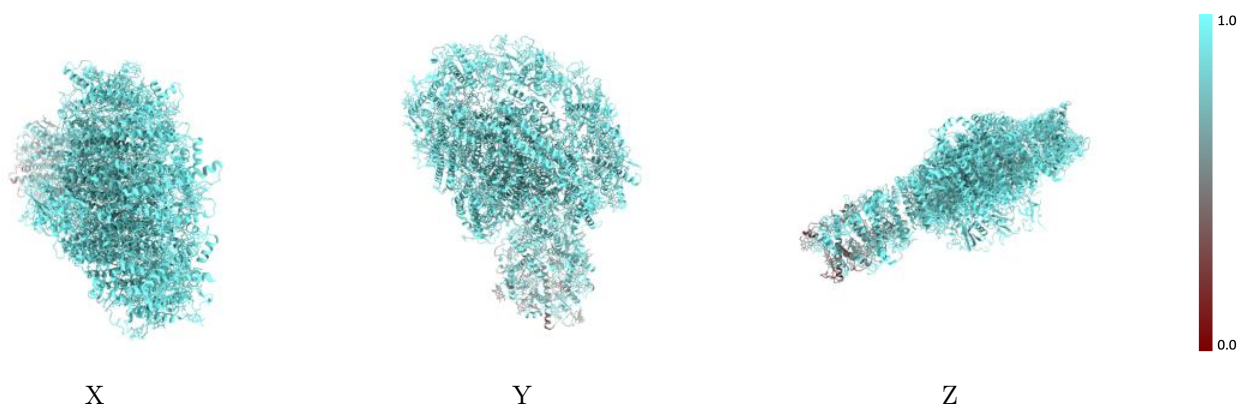
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



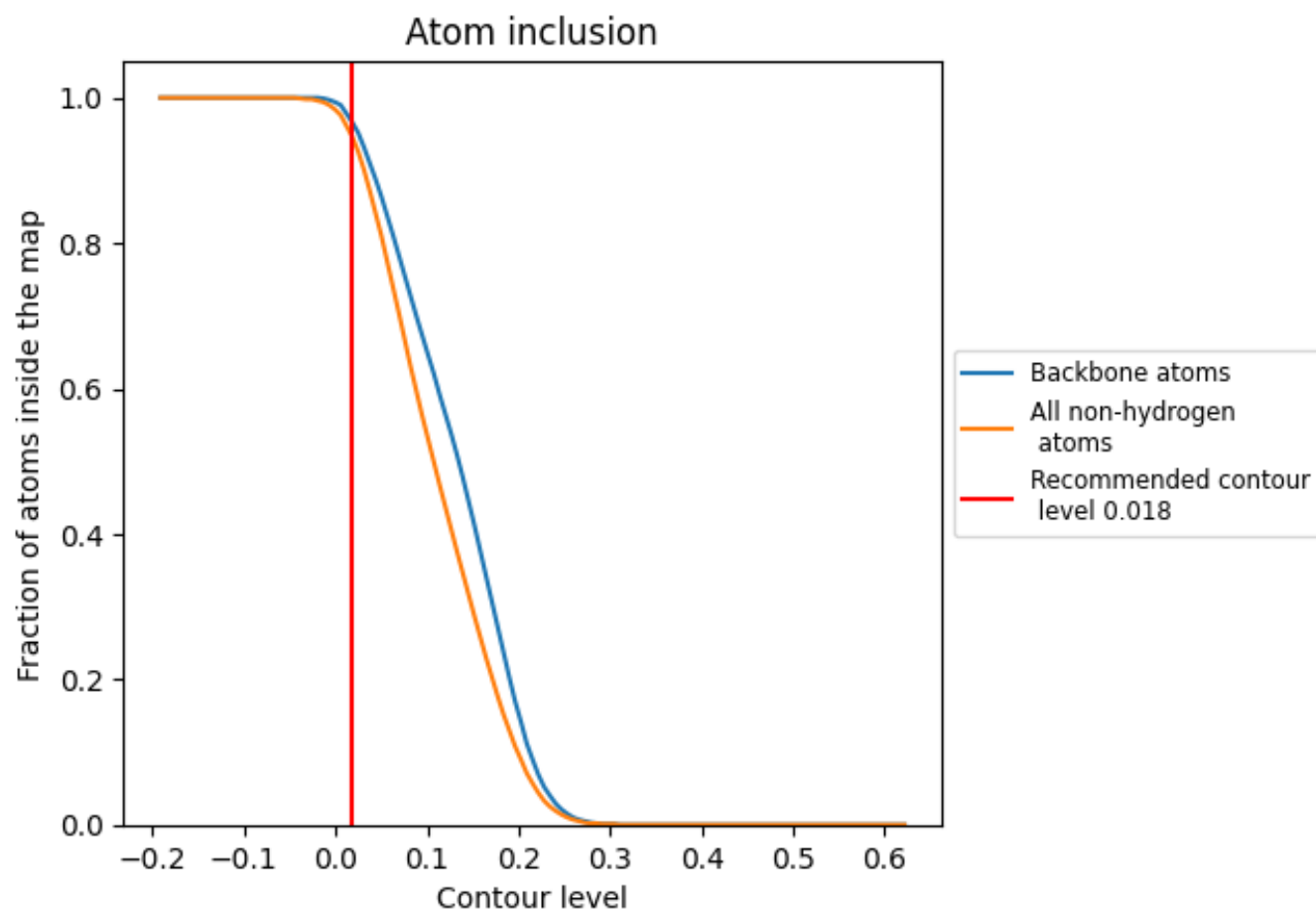
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9470	 0.4640
1	 0.9600	 0.4820
2	 0.9570	 0.4710
3	 0.9520	 0.4550
4	 0.9530	 0.4780
A	 0.9790	 0.5290
B	 0.9770	 0.5240
C	 0.9970	 0.5080
D	 0.9950	 0.5100
E	 1.0000	 0.5160
F	 0.9810	 0.5000
G	 0.9570	 0.4830
H	 0.9690	 0.4990
I	 0.9930	 0.5160
J	 0.9830	 0.4930
K	 0.9610	 0.4840
L	 0.9590	 0.5110
N	 0.9790	 0.4340
O	 0.9420	 0.4780
X	 0.6450	 0.1150
Y	 0.8280	 0.2120
Z	 0.8480	 0.2110

