Full wwPDB EM Validation Report (i)

Nov 14, 2022 – 07:02 PM JST

PDB ID	:	7D1T
EMDB ID	:	EMD-30547
Title	:	Cryo-EM Structure of PSII at 1.95 angstrom resolution
Authors	:	Kato, K.; Miyazaki, N.; Hamaguchi, T.; Nakajima, Y.; Akita, F.; Yonekura, K.; Shen, J.R.
Deposited on	:	2020-09-15
Resolution	:	1.95 Å(reported)
Based on initial model	:	3WU2

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 (i) 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 (1)) were used in the production of this report:

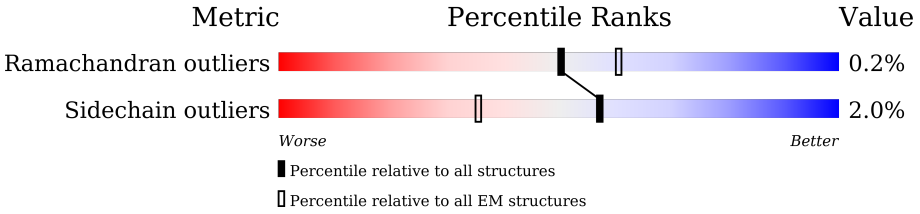
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.95 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	334	99%
1	a	334	99%
2	B	505	99%
2	b	505	99%
3	C	451	99%
3	c	451	99%
4	D	342	98%
4	d	342	98%
5	E	81	5% 96%

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Mol	Chain	Length	Quality of chain
5	e	81	5%, 96%
6	F	34	100%
6	f	34	100%
7	H	63	98%
7	h	63	98%
8	I	36	100%
8	i	36	100%
9	J	37	5%, 97%
9	j	37	5%, 97%
10	K	37	5%, 97%
10	k	37	5%, 97%
11	L	37	5%, 100%
11	l	37	5%, 100%
12	M	34	97%
12	m	34	97%
13	O	244	17%, 96%
13	o	244	17%, 96%
14	T	31	6%, 90%, 6%
14	t	31	6%, 90%, 6%
15	U	97	6%, 96%
15	u	97	6%, 96%
16	V	137	96%
16	v	137	96%
17	Y	30	17%, 87%, 10%
17	y	30	17%, 87%, 10%

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Mol	Chain	Length	Quality of chain
18	X	40	90% 5% 5%
18	x	40	90% 5% 5%
19	Z	62	29% 87% 13%
19	z	62	29% 87% 13%
20	R	34	88% 97%
20	r	34	88% 97%

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
24	CLA	A	405	X	-	-	-
24	CLA	B	601	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	514	X	-	-	-
24	CLA	D	401	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	a	405	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	c	514	X	-	-	-
24	CLA	d	401	X	-	-	-
24	CLA	d	404	X	-	-	-
33	BCT	D	403	-	X	-	-
33	BCT	d	403	-	X	-	-

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 52994 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	334	2634	1725	433	461	15	2	0
1	a	334	2634	1725	433	461	15	2	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	conflict	UNP P51765
a	279	PRO	ARG	conflict	UNP P51765

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	504	3969	2605	661	690	13	0	0
2	b	504	3969	2605	661	690	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	451	3486	2281	584	608	13	0	0
3	c	451	3486	2281	584	608	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	341	2718	1800	444	462	12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	341	2718	1800	444	462	12	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	81	661	432	107	122	0	0
5	e	81	661	432	107	122	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	34	275	187	45	42	1	0	0
6	f	34	275	187	45	42	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	63	498	333	80	83	2	0	0
7	h	63	498	333	80	83	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	36	296	200	46	49	1	0	0
8	i	36	296	200	46	49	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	36	257	174	40	42	1	0	0
9	j	36	257	174	40	42	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	K	37	293	204	43	46	0	0
10	k	37	293	204	43	46	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	conflict	UNP P19054
K	39	TRP	VAL	conflict	UNP P19054
k	33	LEU	PHE	conflict	UNP P19054
k	39	TRP	VAL	conflict	UNP P19054

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	37	304	202	48	53	1	0	0
11	l	37	304	202	48	53	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	33	260	173	38	48	1	0	0
12	m	33	260	173	38	48	1	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	conflict	UNP P12312
m	8	LEU	PHE	conflict	UNP P12312

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	O	244	1874	1170	317	383	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	o	244	1874	1170	317	383	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	T	30	258	181	36	39	2	0	0
14	t	30	258	181	36	39	2	0	0

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	U	97	774	491	129	154	0	0
15	u	97	774	491	129	154	0	0

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	V	137	1064	675	177	208	4	0	0
16	v	137	1064	675	177	208	4	0	0

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Y	27	200	131	35	31	3	0	0
17	y	27	200	131	35	31	3	0	0

- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	X	38	281	188	45	48	0	0
18	x	38	281	188	45	48	0	0

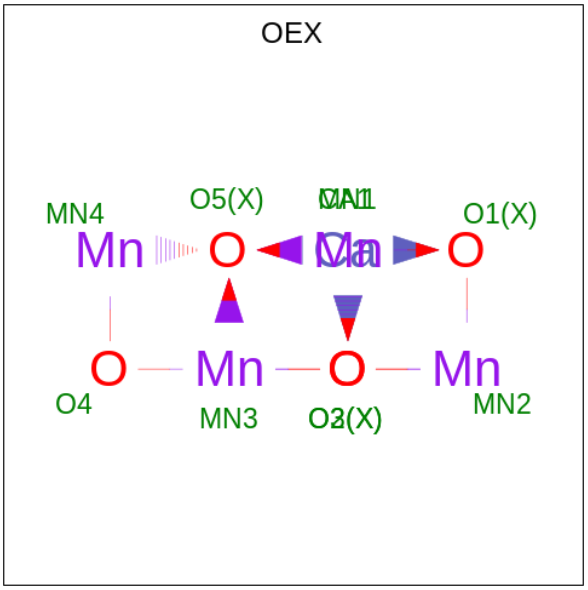
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Z	62	479	328	72	77	2	0	0
19	z	62	479	328	72	77	2	0	0

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	R	34	273	186	47	40	0	0
20	r	34	273	186	47	40	0	0

- Molecule 21 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
			Total	Ca	Mn	O	
21	A	1	10	1	4	5	0
21	a	1	10	1	4	5	0

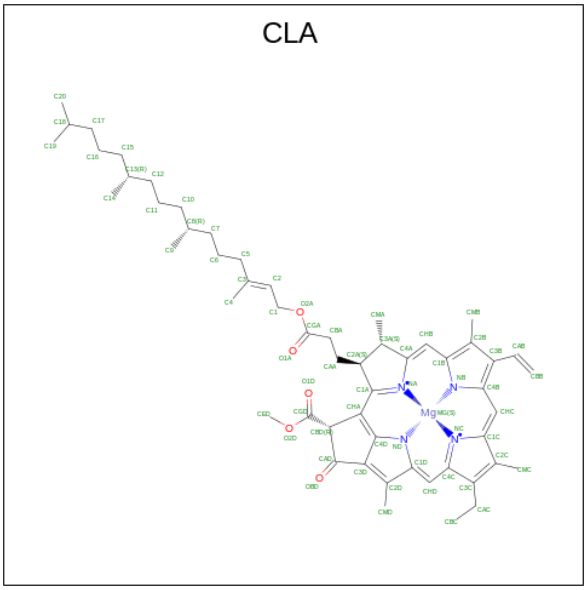
- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 23 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cl	
23	A	2	2	2	0
23	a	2	2	2	0

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	A	1	195	165	3	12	15	0
24	A	1	195	165	3	12	15	0
24	A	1	195	165	3	12	15	0
24	B	1	1040	880	16	64	80	0
24	B	1	1040	880	16	64	80	0
24	B	1	1040	880	16	64	80	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	C	1	845	715	13	52	65	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	D	1	195	165	3	12	15	0
			Total	C	Mg	N	O	
24	D	1	195	165	3	12	15	0
			Total	C	Mg	N	O	
24	D	1	195	165	3	12	15	0
			Total	C	Mg	N	O	
24	a	1	195	165	3	12	15	0
			Total	C	Mg	N	O	
24	a	1	195	165	3	12	15	0
			Total	C	Mg	N	O	
24	a	1	195	165	3	12	15	0
			Total	C	Mg	N	O	
24	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	b	1	1040	880	16	64	80	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
24	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
24	d	1	195	165	3	12	15	0
			Total	C	Mg	N	O	
24	d	1	195	165	3	12	15	0

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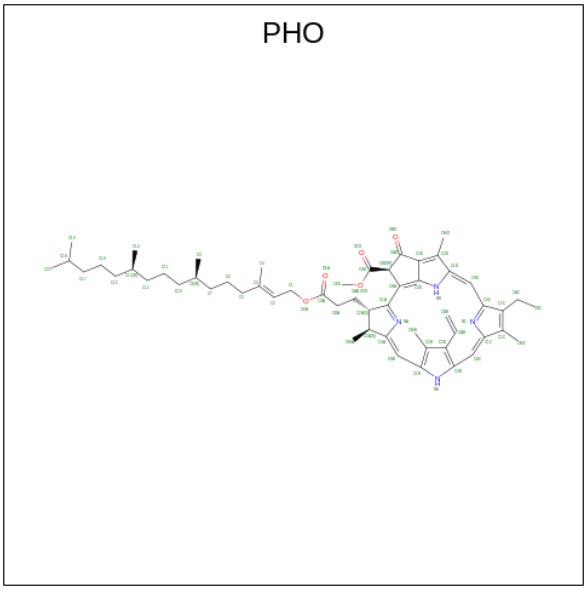
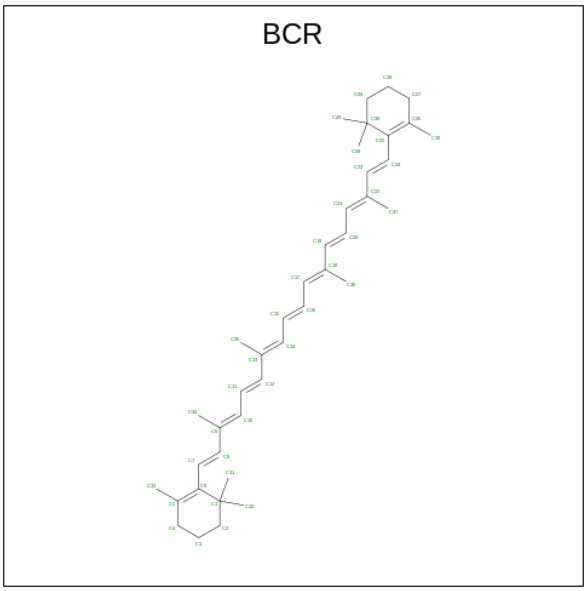
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	d	1	195	165	3	12	15	0

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
26	A	1	40	40	0
			Total	C	
26	B	1	120	120	0
			Total	C	
26	B	1	120	120	0
			Total	C	
26	B	1	120	120	0
			Total	C	
26	C	1	120	120	0
			Total	C	
26	C	1	120	120	0
			Total	C	
26	C	1	120	120	0
			Total	C	
26	D	1	40	40	0
			Total	C	
26	J	1	40	40	0
			Total	C	
26	T	1	40	40	0
			Total	C	
26	a	1	40	40	0
			Total	C	
26	b	1	120	120	0
			Total	C	
26	b	1	120	120	0
			Total	C	
26	b	1	120	120	0

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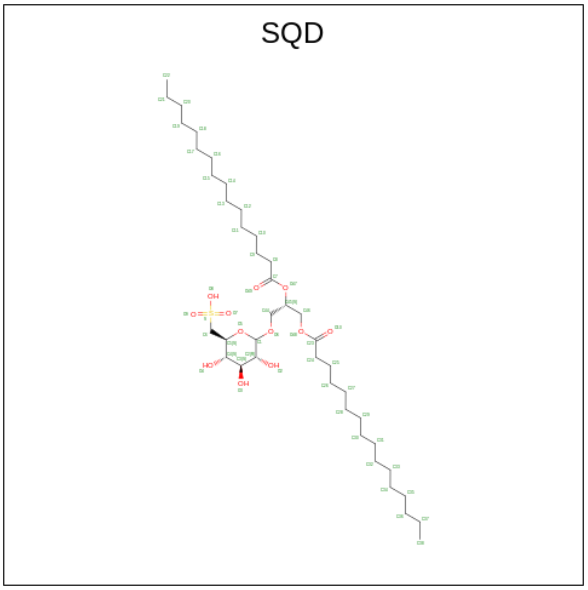
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
26	c	1	120	120	0
			Total	C	
26	c	1	120	120	0
			Total	C	
26	c	1	120	120	0
			Total	C	
26	d	1	40	40	0
			Total	C	
26	j	1	40	40	0
			Total	C	
26	t	1	40	40	0

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
27	A	1	108	82	24	2	0
			Total	C	O	S	
27	A	1	108	82	24	2	0
			Total	C	O	S	
27	B	1	54	41	12	1	0
			Total	C	O	S	
27	F	1	45	32	12	1	0
			Total	C	O	S	
27	L	1	54	41	12	1	0

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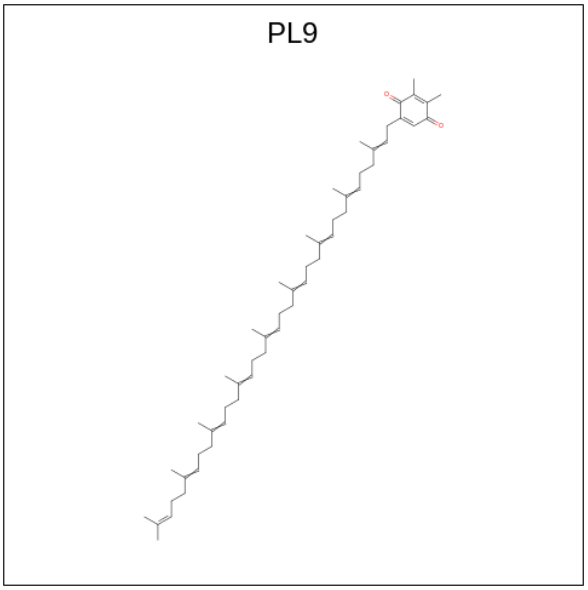
Mol	Chain	Residues	Atoms				AltConf
27	a	1	Total	C	O	S	0
			108	82	24	2	
27	a	1	Total	C	O	S	0
			108	82	24	2	
27	f	1	Total	C	O	S	0
			45	32	12	1	

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



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

- Molecule 29 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms			AltConf
29	A	2	Total	C	O	0
			59	49	10	

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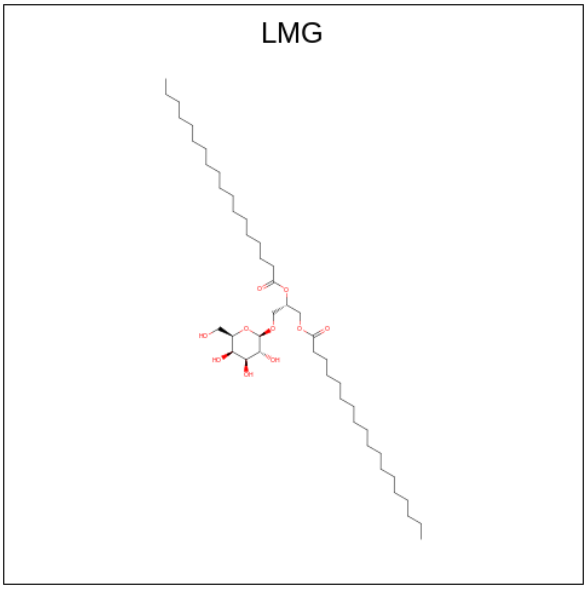
Mol	Chain	Residues	Atoms	AltConf
29	B	5	Total C 56 56	0
29	C	1	Total C 10 10	0
29	D	2	Total C O 56 51 5	0
29	E	1	Total C 10 10	0
29	I	2	Total C 17 17	0
29	J	1	Total C 10 10	0
29	K	1	Total C O 34 29 5	0
29	M	1	Total C 10 10	0
29	T	1	Total C 16 16	0
29	X	1	Total C 10 10	0
29	a	2	Total C O 59 49 10	0
29	b	5	Total C 56 56	0
29	c	1	Total C 10 10	0
29	d	2	Total C O 56 51 5	0
29	e	1	Total C 10 10	0
29	i	2	Total C 17 17	0
29	j	1	Total C 10 10	0
29	k	1	Total C O 34 29 5	0
29	m	1	Total C 10 10	0
29	t	1	Total C 16 16	0
29	x	1	Total C 10 10	0

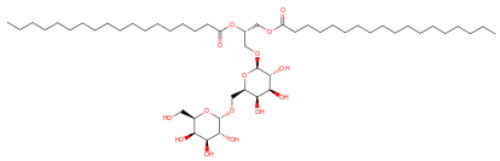
- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	B	1	51	41	10	0
			Total	C	O	
30	C	1	153	123	30	0
			Total	C	O	
30	C	1	153	123	30	0
			Total	C	O	
30	C	1	153	123	30	0
			Total	C	O	
30	D	1	51	41	10	0
			Total	C	O	
30	b	1	51	41	10	0
			Total	C	O	
30	c	1	153	123	30	0
			Total	C	O	
30	c	1	153	123	30	0
			Total	C	O	
30	c	1	153	123	30	0
			Total	C	O	
30	d	1	51	41	10	0

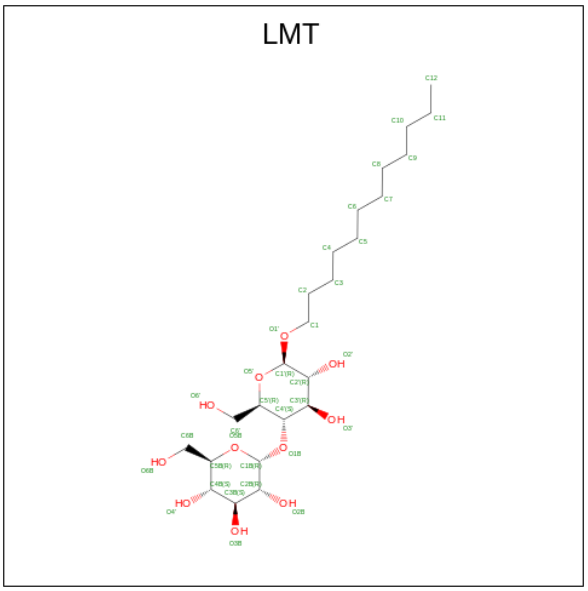
- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).

DGD



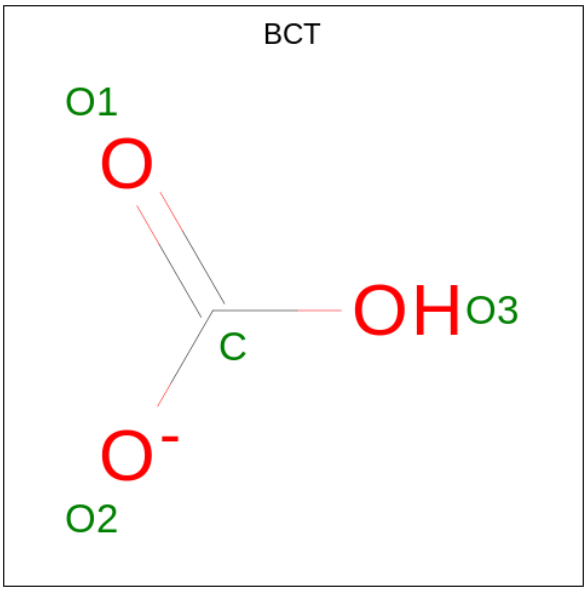
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	C	1	186	141	45	0
			Total	C	O	
31	C	1	186	141	45	0
			Total	C	O	
31	C	1	186	141	45	0
			Total	C	O	
31	H	1	62	47	15	0
			Total	C	O	
31	c	1	186	141	45	0
			Total	C	O	
31	c	1	186	141	45	0
			Total	C	O	
31	c	1	186	141	45	0
			Total	C	O	
31	h	1	62	47	15	0

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



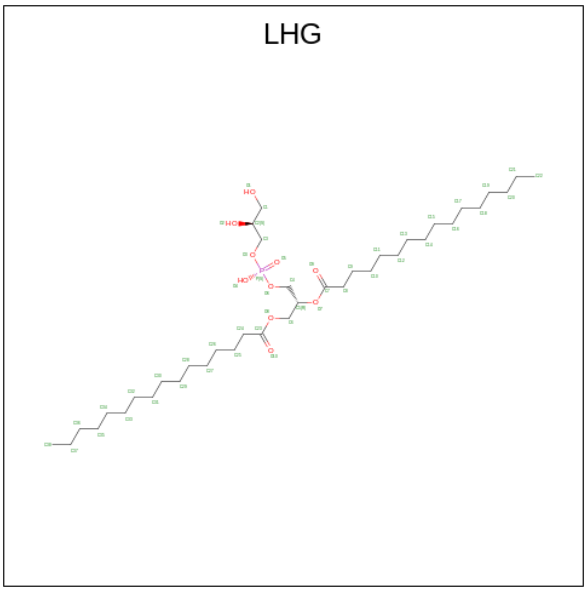
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
32	C	1	35	24	11	0
			Total	C	O	
32	J	1	24	18	6	0
			Total	C	O	
32	M	1	35	24	11	0
			Total	C	O	
32	Z	1	35	24	11	0
			Total	C	O	
32	c	1	35	24	11	0
			Total	C	O	
32	j	1	24	18	6	0
			Total	C	O	
32	m	1	35	24	11	0
			Total	C	O	
32	z	1	35	24	11	0

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
34	D	1	144	111	30	3	0

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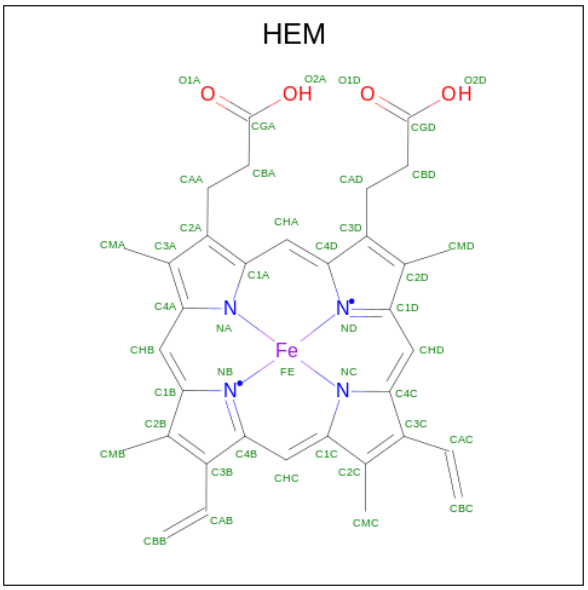
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
34	D	1	144	111	30	3	0
			Total	C	O	P	
34	D	1	144	111	30	3	0
			Total	C	O	P	
34	E	1	49	38	10	1	0
			Total	C	O	P	
34	L	1	49	38	10	1	0
			Total	C	O	P	
34	d	1	144	111	30	3	0
			Total	C	O	P	
34	d	1	144	111	30	3	0
			Total	C	O	P	
34	d	1	144	111	30	3	0
			Total	C	O	P	
34	e	1	49	38	10	1	0
			Total	C	O	P	
34	l	1	49	38	10	1	0

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

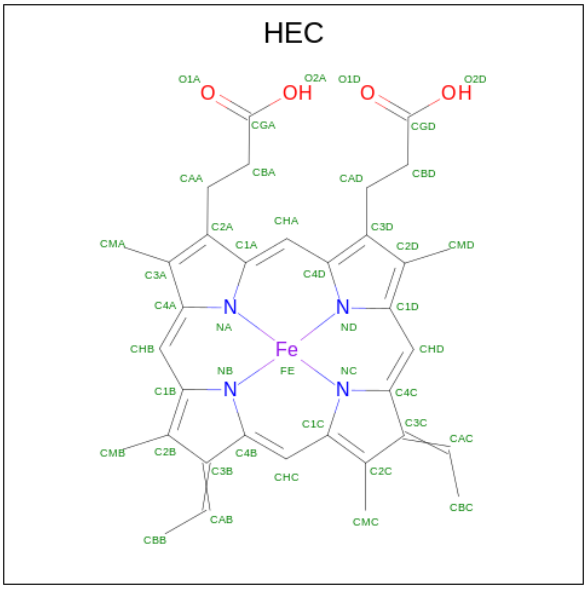


Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
35	E	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
35	e	1	43	34	1	4	4	0

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

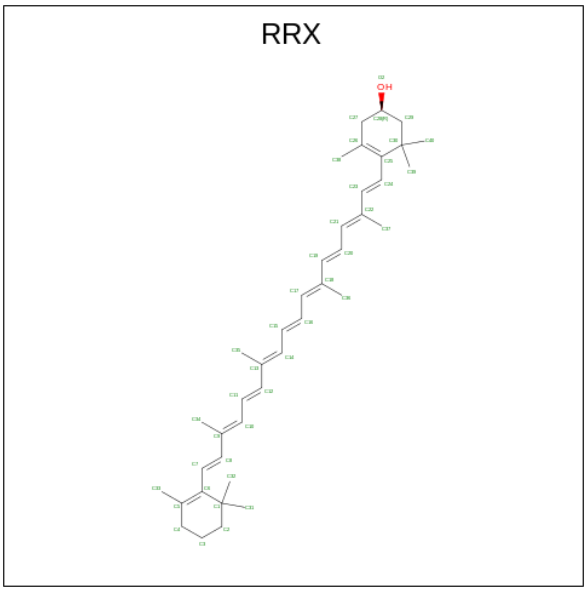
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
36	J	1	1	1	0
36	j	1	1	1	0

- Molecule 37 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: $C_{40}H_{56}O$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
38	X	1	41	40	1	0
38	x	1	41	40	1	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
39	A	152	152	152	0
39	B	298	298	298	0
39	C	220	220	220	0
39	D	154	154	154	0
39	E	26	26	26	0
39	F	5	5	5	0
39	H	38	38	38	0
39	I	13	13	13	0
39	J	11	11	11	0
39	K	3	3	3	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	O	
39	L	19	19	19	0
			Total	O	
39	M	8	8	8	0
			Total	O	
39	O	114	114	114	0
			Total	O	
39	T	9	9	9	0
			Total	O	
39	U	64	64	64	0
			Total	O	
39	V	78	78	78	0
			Total	O	
39	Y	2	2	2	0
			Total	O	
39	X	8	8	8	0
			Total	O	
39	a	152	152	152	0
			Total	O	
39	b	292	292	292	0
			Total	O	
39	c	220	220	220	0
			Total	O	
39	d	154	154	154	0
			Total	O	
39	e	26	26	26	0
			Total	O	
39	f	5	5	5	0
			Total	O	
39	h	38	38	38	0
			Total	O	
39	i	13	13	13	0
			Total	O	
39	j	11	11	11	0
			Total	O	
39	k	3	3	3	0
			Total	O	
39	l	13	13	13	0
			Total	O	
39	m	8	8	8	0
			Total	O	
39	o	114	114	114	0

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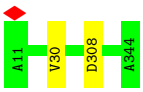
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
39	t	9	9	9	0
			Total	O	
39	u	64	64	64	0
			Total	O	
39	v	78	78	78	0
			Total	O	
39	y	2	2	2	0
			Total	O	
39	x	8	8	8	0

3 Residue-property plots (i)

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

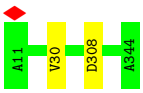
• Molecule 1: Photosystem II protein D1

Chain A: 99%



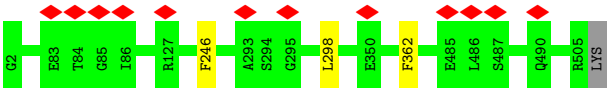
• Molecule 1: Photosystem II protein D1

Chain a: 99%



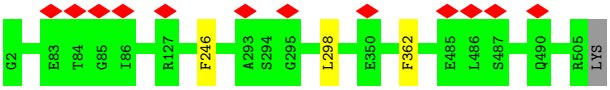
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 99%



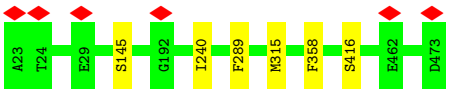
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b: 99%



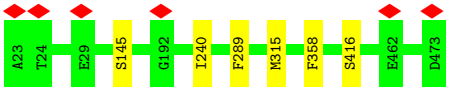
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 99%



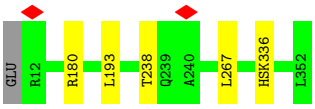
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 99%



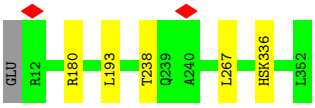
• Molecule 4: Photosystem II D2 protein

Chain D: 98%



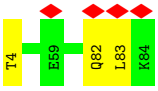
• Molecule 4: Photosystem II D2 protein

Chain d: 98%



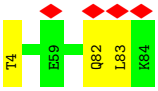
• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 5% 96%



• Molecule 5: Cytochrome b559 subunit alpha

Chain e: 5% 96%



• Molecule 6: Cytochrome b559 subunit beta

Chain F: 100%

There are no outlier residues recorded for this chain.

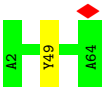
• Molecule 6: Cytochrome b559 subunit beta

Chain f: 100%

There are no outlier residues recorded for this chain.

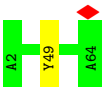
• Molecule 7: Photosystem II reaction center protein H

Chain H: 98%



• Molecule 7: Photosystem II reaction center protein H

Chain h: 98%



• Molecule 8: Photosystem II reaction center protein I

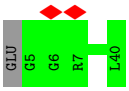
Chain I: 100%

• Molecule 8: Photosystem II reaction center protein I

Chain i: 100%

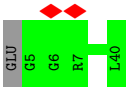
• Molecule 9: Photosystem II reaction center protein J

Chain J: 5% 97%



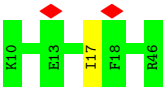
• Molecule 9: Photosystem II reaction center protein J

Chain j: 5% 97%



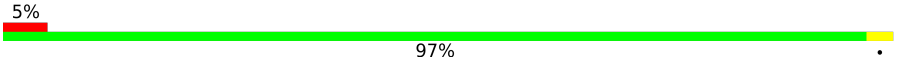
• Molecule 10: Photosystem II reaction center protein K

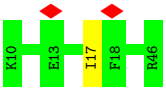
Chain K: 5% 97%



• Molecule 10: Photosystem II reaction center protein K

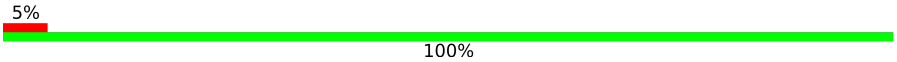
Chain k:





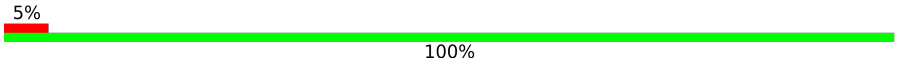
• Molecule 11: Photosystem II reaction center protein L

Chain L:



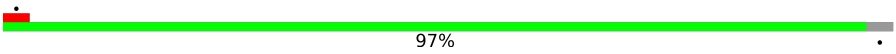
• Molecule 11: Photosystem II reaction center protein L

Chain l:



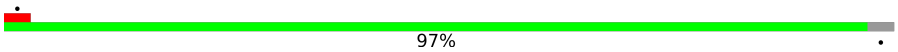
• Molecule 12: Photosystem II reaction center protein M

Chain M:



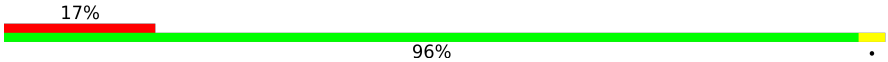
• Molecule 12: Photosystem II reaction center protein M

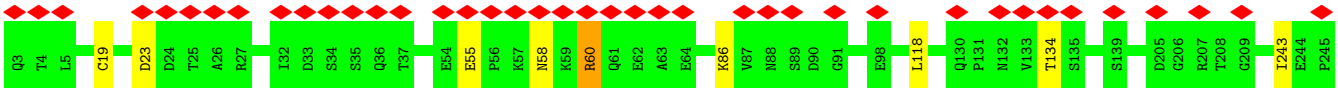
Chain m:



• Molecule 13: Photosystem II manganese-stabilizing polypeptide

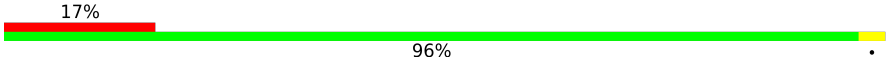
Chain O:

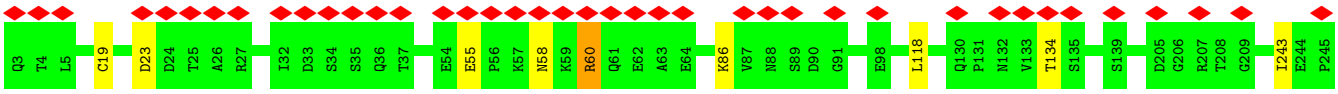




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

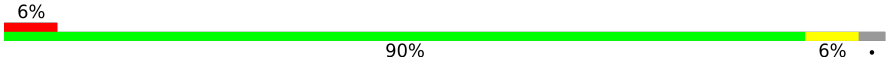
Chain o:

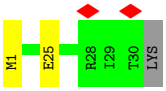




• Molecule 14: Photosystem II reaction center protein T

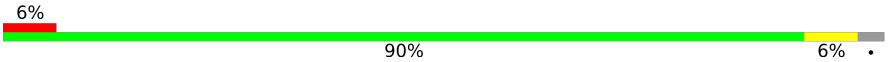
Chain T:

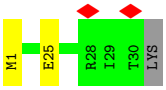




• Molecule 14: Photosystem II reaction center protein T

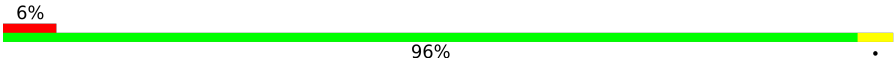
Chain t:

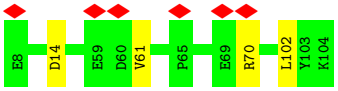




• Molecule 15: Photosystem II 12 kDa extrinsic protein

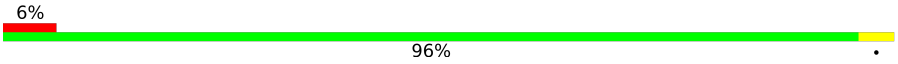
Chain U:

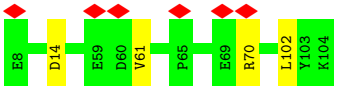




• Molecule 15: Photosystem II 12 kDa extrinsic protein

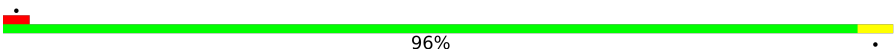
Chain u:

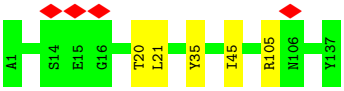




• Molecule 16: Cytochrome c-550

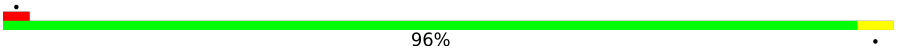
Chain V:

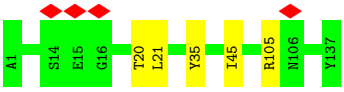




• Molecule 16: Cytochrome c-550

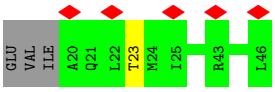
Chain v:





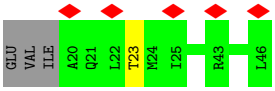
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



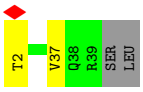
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



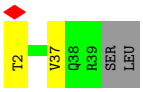
• Molecule 18: Photosystem II reaction center protein X

Chain X:



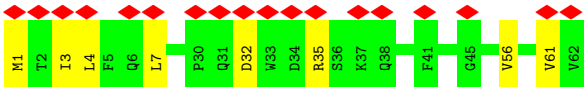
• Molecule 18: Photosystem II reaction center protein X

Chain x:



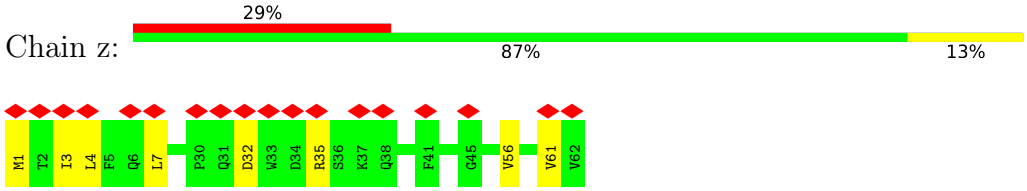
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



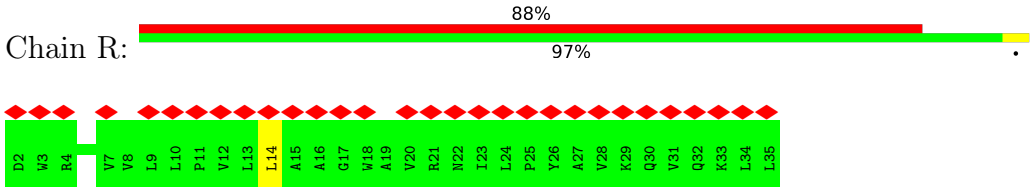
• Molecule 19: Photosystem II reaction center protein Z

Chain z:



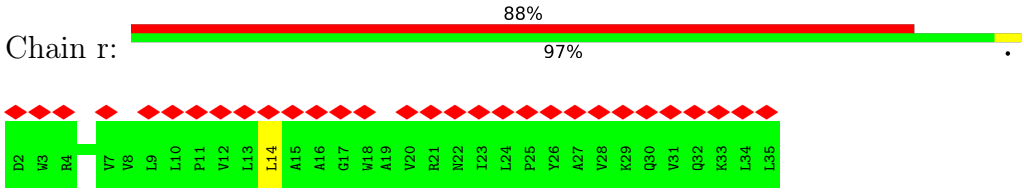
• Molecule 20: Photosystem II protein Y

Chain R:



• Molecule 20: Photosystem II protein Y

Chain r:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	174099	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	83	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.242	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	328.80002, 328.80002, 328.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	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: PL9, RRX, CLA, BCR, HSK, MG, LMT, PHO, SQD, BCT, LMG, OEX, FME, HEM, HEC, DGD, UNL, LHG, FE2, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.53	0/2718	0.66	1/3704 (0.0%)
1	a	0.53	0/2718	0.66	1/3704 (0.0%)
2	B	0.52	0/4109	0.62	0/5600
2	b	0.52	0/4109	0.62	0/5600
3	C	0.52	1/3599 (0.0%)	0.61	0/4900
3	c	0.52	1/3599 (0.0%)	0.61	0/4900
4	D	0.55	1/2800 (0.0%)	0.66	1/3814 (0.0%)
4	d	0.55	1/2800 (0.0%)	0.66	1/3814 (0.0%)
5	E	0.46	0/680	0.60	0/928
5	e	0.46	0/680	0.60	0/928
6	F	0.48	0/284	0.57	0/387
6	f	0.47	0/284	0.57	0/387
7	H	0.51	0/511	0.64	0/697
7	h	0.51	0/511	0.64	0/697
8	I	0.48	0/293	0.58	0/396
8	i	0.48	0/293	0.58	0/396
9	J	0.42	0/263	0.60	0/356
9	j	0.42	0/263	0.60	0/356
10	K	0.51	0/303	0.70	0/416
10	k	0.51	0/303	0.70	0/416
11	L	0.49	0/311	0.60	0/422
11	l	0.49	0/311	0.60	0/422
12	M	0.52	0/253	0.66	0/346
12	m	0.52	0/253	0.66	0/346
13	O	0.45	0/1905	0.68	0/2583
13	o	0.45	0/1905	0.68	0/2583
14	T	0.47	0/257	0.58	0/349
14	t	0.47	0/257	0.58	0/349
15	U	0.46	0/785	0.66	0/1064
15	u	0.46	0/785	0.66	0/1064
16	V	0.45	0/1085	0.60	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.45	0/1085	0.61	0/1473
17	Y	0.34	0/201	0.61	0/268
17	y	0.34	0/201	0.61	0/268
18	X	0.39	0/284	0.56	0/384
18	x	0.39	0/284	0.56	0/384
19	Z	0.43	0/490	0.58	0/669
19	z	0.42	0/490	0.58	0/669
20	R	0.38	0/279	0.71	0/383
20	r	0.38	0/279	0.71	0/383
All	All	0.50	4/42820 (0.0%)	0.63	4/58278 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	358	PHE	CD2-CE2	-5.64	1.27	1.39
4	D	193	LEU	C-N	-5.64	1.21	1.34
3	c	358	PHE	CD2-CE2	-5.64	1.27	1.39
4	d	193	LEU	C-N	-5.64	1.21	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	308	ASP	CB-CG-OD1	5.74	123.47	118.30
1	a	308	ASP	CB-CG-OD1	5.74	123.47	118.30
4	D	267	LEU	CB-CG-CD2	5.13	119.72	111.00
4	d	267	LEU	CB-CG-CD2	5.13	119.72	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/334 (100%)	326 (98%)	6 (2%)	1 (0%)	41	30
1	a	333/334 (100%)	326 (98%)	6 (2%)	1 (0%)	41	30
2	B	502/505 (99%)	495 (99%)	7 (1%)	0	100	100
2	b	502/505 (99%)	495 (99%)	7 (1%)	0	100	100
3	C	449/451 (100%)	443 (99%)	5 (1%)	1 (0%)	47	38
3	c	449/451 (100%)	443 (99%)	5 (1%)	1 (0%)	47	38
4	D	338/342 (99%)	332 (98%)	6 (2%)	0	100	100
4	d	338/342 (99%)	332 (98%)	6 (2%)	0	100	100
5	E	79/81 (98%)	79 (100%)	0	0	100	100
5	e	79/81 (98%)	79 (100%)	0	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	32/34 (94%)	32 (100%)	0	0	100	100
7	H	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
7	h	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
8	I	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
9	J	34/37 (92%)	31 (91%)	3 (9%)	0	100	100
9	j	34/37 (92%)	31 (91%)	3 (9%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	31/34 (91%)	31 (100%)	0	0	100	100
12	m	31/34 (91%)	31 (100%)	0	0	100	100
13	O	242/244 (99%)	231 (96%)	9 (4%)	2 (1%)	19	9
13	o	242/244 (99%)	231 (96%)	9 (4%)	2 (1%)	19	9
14	T	28/31 (90%)	28 (100%)	0	0	100	100
14	t	28/31 (90%)	28 (100%)	0	0	100	100
15	U	95/97 (98%)	90 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	u	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
16	V	135/137 (98%)	130 (96%)	4 (3%)	1 (1%)	22	11
16	v	135/137 (98%)	130 (96%)	4 (3%)	1 (1%)	22	11
17	Y	25/30 (83%)	25 (100%)	0	0	100	100
17	y	25/30 (83%)	25 (100%)	0	0	100	100
18	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
20	R	32/34 (94%)	32 (100%)	0	0	100	100
20	r	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5232/5332 (98%)	5120 (98%)	102 (2%)	10 (0%)	50	38

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
3	c	416	SER
13	O	58	ASN
13	o	58	ASN
13	O	60	ARG
13	o	60	ARG
1	A	30	VAL
16	V	45	ILE
1	a	30	VAL
16	v	45	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/269 (100%)	270 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	270/269 (100%)	270 (100%)	0	100	100
2	B	402/403 (100%)	399 (99%)	3 (1%)	84	82
2	b	402/403 (100%)	399 (99%)	3 (1%)	84	82
3	C	352/352 (100%)	348 (99%)	4 (1%)	73	71
3	c	352/352 (100%)	348 (99%)	4 (1%)	73	71
4	D	275/276 (100%)	273 (99%)	2 (1%)	84	82
4	d	275/276 (100%)	273 (99%)	2 (1%)	84	82
5	E	72/72 (100%)	69 (96%)	3 (4%)	30	17
5	e	72/72 (100%)	69 (96%)	3 (4%)	30	17
6	F	28/28 (100%)	28 (100%)	0	100	100
6	f	28/28 (100%)	28 (100%)	0	100	100
7	H	53/53 (100%)	52 (98%)	1 (2%)	57	50
7	h	53/53 (100%)	52 (98%)	1 (2%)	57	50
8	I	32/32 (100%)	32 (100%)	0	100	100
8	i	32/32 (100%)	32 (100%)	0	100	100
9	J	24/25 (96%)	24 (100%)	0	100	100
9	j	24/25 (96%)	24 (100%)	0	100	100
10	K	30/30 (100%)	29 (97%)	1 (3%)	38	26
10	k	30/30 (100%)	29 (97%)	1 (3%)	38	26
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	29/30 (97%)	29 (100%)	0	100	100
12	m	29/30 (97%)	29 (100%)	0	100	100
13	O	207/207 (100%)	199 (96%)	8 (4%)	32	19
13	o	207/207 (100%)	199 (96%)	8 (4%)	32	19
14	T	26/27 (96%)	25 (96%)	1 (4%)	33	21
14	t	26/27 (96%)	25 (96%)	1 (4%)	33	21
15	U	84/84 (100%)	80 (95%)	4 (5%)	25	12
15	u	84/84 (100%)	80 (95%)	4 (5%)	25	12
16	V	117/117 (100%)	113 (97%)	4 (3%)	37	25
16	v	117/117 (100%)	113 (97%)	4 (3%)	37	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Y	20/23 (87%)	19 (95%)	1 (5%)	24	11
17	y	20/23 (87%)	19 (95%)	1 (5%)	24	11
18	X	31/33 (94%)	29 (94%)	2 (6%)	17	6
18	x	31/33 (94%)	29 (94%)	2 (6%)	17	6
19	Z	52/52 (100%)	44 (85%)	8 (15%)	2	0
19	z	52/52 (100%)	44 (85%)	8 (15%)	2	0
20	R	29/29 (100%)	28 (97%)	1 (3%)	37	25
20	r	29/29 (100%)	28 (97%)	1 (3%)	37	25
All	All	4336/4354 (100%)	4250 (98%)	86 (2%)	57	48

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	246	PHE
2	B	298	LEU
2	B	362	PHE
3	C	145	SER
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
4	D	180	ARG
4	D	238	THR
5	E	4	THR
5	E	82	GLN
5	E	83	LEU
7	H	49	TYR
10	K	17	ILE
13	O	19	CYS
13	O	23	ASP
13	O	55	GLU
13	O	60	ARG
13	O	86	LYS
13	O	118	LEU
13	O	134	THR
13	O	243	ILE
14	T	25	GLU
15	U	14	ASP
15	U	61	VAL
15	U	70	ARG

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Mol	Chain	Res	Type
15	U	102	LEU
16	V	20	THR
16	V	21	LEU
16	V	35	TYR
16	V	105	ARG
17	Y	23	THR
18	X	2	THR
18	X	37	VAL
19	Z	1	MET
19	Z	3	ILE
19	Z	4	LEU
19	Z	7	LEU
19	Z	32	ASP
19	Z	35	ARG
19	Z	56	VAL
19	Z	61	VAL
20	R	14	LEU
2	b	246	PHE
2	b	298	LEU
2	b	362	PHE
3	c	145	SER
3	c	240	ILE
3	c	289	PHE
3	c	315	MET
4	d	180	ARG
4	d	238	THR
5	e	4	THR
5	e	82	GLN
5	e	83	LEU
7	h	49	TYR
10	k	17	ILE
13	o	19	CYS
13	o	23	ASP
13	o	55	GLU
13	o	60	ARG
13	o	86	LYS
13	o	118	LEU
13	o	134	THR
13	o	243	ILE
14	t	25	GLU
15	u	14	ASP
15	u	61	VAL

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Mol	Chain	Res	Type
15	u	70	ARG
15	u	102	LEU
16	v	20	THR
16	v	21	LEU
16	v	35	TYR
16	v	105	ARG
17	y	23	THR
18	x	2	THR
18	x	37	VAL
19	z	1	MET
19	z	3	ILE
19	z	4	LEU
19	z	7	LEU
19	z	32	ASP
19	z	35	ARG
19	z	56	VAL
19	z	61	VAL
20	r	14	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	331	ASN
3	C	229	ASN
3	C	313	GLN
3	C	415	ASN
5	E	74	GLN
7	H	50	ASN
12	M	5	GLN
13	O	36	GLN
13	O	88	ASN
13	O	104	GLN
13	O	196	GLN
15	U	31	ASN
16	V	34	GLN
20	R	22	ASN
2	b	331	ASN
3	c	229	ASN
3	c	313	GLN
3	c	415	ASN
7	h	50	ASN
12	m	5	GLN

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Mol	Chain	Res	Type
13	o	36	GLN
13	o	88	ASN
13	o	104	GLN
13	o	196	GLN
15	u	31	ASN
16	v	34	GLN
20	r	22	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
8	FME	i	1	8	8,9,10	1.02	0	7,9,11	0.86	0
12	FME	m	1	12	8,9,10	0.93	0	7,9,11	0.61	0
12	FME	M	1	12	8,9,10	0.93	0	7,9,11	0.61	0
14	FME	T	1	14	8,9,10	0.94	0	7,9,11	1.31	1 (14%)
4	HSK	d	336	4	7,11,12	1.34	1 (14%)	3,14,16	1.54	0
8	FME	I	1	8	8,9,10	1.02	0	7,9,11	0.86	0
14	FME	t	1	14	8,9,10	0.95	0	7,9,11	1.31	1 (14%)
4	HSK	D	336	4	7,11,12	1.31	1 (14%)	3,14,16	1.30	0

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
8	FME	i	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-
14	FME	T	1	14	-	0/7/9/11	-
4	HSK	d	336	4	-	0/5/6/8	0/1/1/1
8	FME	I	1	8	-	0/7/9/11	-
14	FME	t	1	14	-	0/7/9/11	-
4	HSK	D	336	4	-	0/5/6/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	336	HSK	CE1-ND1	2.70	1.40	1.36
4	D	336	HSK	CE1-ND1	2.54	1.39	1.36

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	C-CA-N	2.62	114.47	109.73
14	T	1	FME	C-CA-N	2.61	114.44	109.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	N-CA-CB-CG
12	m	1	FME	N-CA-CB-CG
12	M	1	FME	CB-CA-N-CN
12	m	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 196 ligands modelled in this entry, 8 are monoatomic and 36 are unknown - leaving 152 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CLA	B	607	39	65,73,73	1.87	16 (24%)	76,113,113	2.70	26 (34%)
24	CLA	c	514	-	65,73,73	2.02	18 (27%)	76,113,113	2.76	30 (39%)
27	SQD	A	410	-	53,54,54	1.05	6 (11%)	62,65,65	1.88	8 (12%)
30	LMG	c	520	-	51,51,55	0.95	4 (7%)	59,59,63	1.36	7 (11%)
24	CLA	c	513	-	65,73,73	1.84	15 (23%)	76,113,113	2.85	30 (39%)
24	CLA	B	608	-	65,73,73	1.88	17 (26%)	76,113,113	2.49	27 (35%)
34	LHG	E	101	-	48,48,48	0.71	1 (2%)	51,54,54	1.26	7 (13%)
24	CLA	c	503	-	65,73,73	1.93	17 (26%)	76,113,113	2.57	24 (31%)
26	BCR	j	104	-	41,41,41	1.16	3 (7%)	56,56,56	1.13	3 (5%)
24	CLA	C	508	39	65,73,73	1.91	17 (26%)	76,113,113	2.73	27 (35%)
26	BCR	B	618	-	41,41,41	1.10	3 (7%)	56,56,56	1.24	7 (12%)
32	LMT	J	102	-	24,24,36	1.01	1 (4%)	29,29,47	1.52	3 (10%)
28	PL9	a	411	-	55,55,55	1.53	8 (14%)	68,69,69	1.55	13 (19%)
24	CLA	c	505	39	65,73,73	1.89	15 (23%)	76,113,113	2.62	32 (42%)
31	DGD	c	519	-	63,63,67	1.20	7 (11%)	77,77,81	1.31	8 (10%)
24	CLA	c	506	-	65,73,73	1.84	19 (29%)	76,113,113	2.47	25 (32%)
24	CLA	B	605	-	65,73,73	1.86	17 (26%)	76,113,113	2.76	29 (38%)
33	BCT	D	403	22	2,3,3	1.85	1 (50%)	2,3,3	3.93	2 (100%)
24	CLA	a	406	39	65,73,73	1.87	17 (26%)	76,113,113	2.42	26 (34%)
26	BCR	c	522	-	41,41,41	1.02	1 (2%)	56,56,56	1.16	6 (10%)
32	LMT	m	102	-	36,36,36	1.38	6 (16%)	47,47,47	1.02	1 (2%)
24	CLA	c	511	-	65,73,73	1.95	17 (26%)	76,113,113	2.60	27 (35%)
24	CLA	b	609	39	65,73,73	1.87	16 (24%)	76,113,113	2.70	26 (34%)
21	OEX	A	401	39,3,1	0,15,15	-	-	-		
24	CLA	C	513	-	65,73,73	1.85	15 (23%)	76,113,113	2.85	30 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	OEX	a	401	39,3,1	0,15,15	-	-	-		
24	CLA	c	507	-	65,73,73	1.93	15 (23%)	76,113,113	2.69	30 (39%)
28	PL9	A	411	-	55,55,55	1.53	8 (14%)	68,69,69	1.56	13 (19%)
30	LMG	c	501	-	51,51,55	1.18	6 (11%)	59,59,63	1.38	8 (13%)
26	BCR	A	409	-	41,41,41	1.04	1 (2%)	56,56,56	1.27	7 (12%)
30	LMG	D	411	36	51,51,55	1.07	7 (13%)	59,59,63	1.32	7 (11%)
31	DGD	c	518	-	63,63,67	1.55	13 (20%)	77,77,81	1.44	11 (14%)
34	LHG	D	408	-	48,48,48	0.85	1 (2%)	51,54,54	1.23	8 (15%)
31	DGD	C	519	-	63,63,67	1.20	7 (11%)	77,77,81	1.31	8 (10%)
24	CLA	C	509	-	65,73,73	1.89	16 (24%)	76,113,113	2.80	30 (39%)
24	CLA	d	404	-	65,73,73	1.82	17 (26%)	76,113,113	2.67	24 (31%)
31	DGD	h	101	-	63,63,67	1.28	7 (11%)	77,77,81	1.28	9 (11%)
34	LHG	D	409	-	48,48,48	0.84	1 (2%)	51,54,54	1.11	3 (5%)
33	BCT	d	403	22	2,3,3	1.84	1 (50%)	2,3,3	3.92	2 (100%)
26	BCR	t	102	-	41,41,41	1.01	1 (2%)	56,56,56	1.27	7 (12%)
24	CLA	a	405	-	65,73,73	1.80	15 (23%)	76,113,113	2.45	23 (30%)
31	DGD	C	517	-	63,63,67	1.13	7 (11%)	77,77,81	1.44	11 (14%)
24	CLA	d	401	39	65,73,73	1.99	16 (24%)	76,113,113	2.86	29 (38%)
27	SQD	B	620	-	53,54,54	0.92	5 (9%)	62,65,65	2.23	11 (17%)
25	PHO	D	402	-	51,69,69	1.04	3 (5%)	47,99,99	1.51	8 (17%)
26	BCR	a	409	-	41,41,41	1.04	1 (2%)	56,56,56	1.27	7 (12%)
38	RRX	x	101	-	42,42,42	1.89	11 (26%)	57,58,58	2.01	16 (28%)
24	CLA	b	618	-	65,73,73	1.85	14 (21%)	76,113,113	2.65	31 (40%)
30	LMG	C	520	-	51,51,55	0.95	4 (7%)	59,59,63	1.36	7 (11%)
24	CLA	c	508	39	65,73,73	1.91	17 (26%)	76,113,113	2.73	27 (35%)
32	LMT	Z	101	-	36,36,36	1.30	6 (16%)	47,47,47	1.13	5 (10%)
24	CLA	B	614	-	65,73,73	1.85	15 (23%)	76,113,113	2.78	28 (36%)
31	DGD	H	101	-	63,63,67	1.27	7 (11%)	77,77,81	1.27	9 (11%)
30	LMG	C	523	-	51,51,55	0.86	2 (3%)	59,59,63	1.36	8 (13%)
24	CLA	b	612	39	65,73,73	1.86	17 (26%)	76,113,113	2.57	27 (35%)
24	CLA	A	405	-	65,73,73	1.80	15 (23%)	76,113,113	2.45	23 (30%)
27	SQD	A	412	-	53,54,54	0.97	5 (9%)	62,65,65	1.73	11 (17%)
25	PHO	A	407	-	51,69,69	1.15	6 (11%)	47,99,99	1.22	3 (6%)
26	BCR	C	522	-	41,41,41	1.02	1 (2%)	56,56,56	1.16	6 (10%)
27	SQD	f	101	-	44,45,54	1.10	5 (11%)	53,56,65	2.18	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CLA	B	609	-	65,73,73	1.82	15 (23%)	76,113,113	2.77	32 (42%)
26	BCR	b	620	-	41,41,41	1.10	3 (7%)	56,56,56	1.24	7 (12%)
27	SQD	F	101	-	44,45,54	1.10	5 (11%)	53,56,65	2.18	11 (20%)
24	CLA	c	510	-	65,73,73	1.98	16 (24%)	76,113,113	2.64	31 (40%)
26	BCR	c	516	-	41,41,41	1.02	1 (2%)	56,56,56	1.17	5 (8%)
26	BCR	B	619	-	41,41,41	1.11	2 (4%)	56,56,56	1.06	4 (7%)
24	CLA	B	615	-	65,73,73	1.84	15 (23%)	76,113,113	2.64	27 (35%)
24	CLA	C	512	3	65,73,73	1.92	15 (23%)	76,113,113	2.75	26 (34%)
26	BCR	C	516	-	41,41,41	1.02	1 (2%)	56,56,56	1.17	5 (8%)
27	SQD	a	410	-	53,54,54	1.05	6 (11%)	62,65,65	1.88	8 (12%)
24	CLA	D	401	39	65,73,73	1.99	16 (24%)	76,113,113	2.86	29 (38%)
24	CLA	d	405	-	65,73,73	1.94	18 (27%)	76,113,113	2.68	28 (36%)
24	CLA	C	505	39	65,73,73	1.89	15 (23%)	76,113,113	2.62	32 (42%)
24	CLA	C	510	-	65,73,73	1.97	16 (24%)	76,113,113	2.64	31 (40%)
24	CLA	B	612	-	65,73,73	1.88	15 (23%)	76,113,113	2.61	29 (38%)
24	CLA	C	511	-	65,73,73	1.95	17 (26%)	76,113,113	2.60	27 (35%)
28	PL9	D	407	-	55,55,55	1.90	11 (20%)	68,69,69	1.56	16 (23%)
37	HEC	v	201	16	32,50,50	2.14	5 (15%)	24,82,82	1.95	8 (33%)
27	SQD	a	412	-	53,54,54	0.97	5 (9%)	62,65,65	1.73	11 (17%)
26	BCR	J	104	-	41,41,41	1.16	3 (7%)	56,56,56	1.13	3 (5%)
31	DGD	C	518	-	63,63,67	1.55	13 (20%)	77,77,81	1.44	11 (14%)
31	DGD	c	517	-	63,63,67	1.13	7 (11%)	77,77,81	1.44	11 (14%)
24	CLA	B	613	-	65,73,73	1.87	18 (27%)	76,113,113	2.61	27 (35%)
24	CLA	D	404	-	65,73,73	1.82	17 (26%)	76,113,113	2.67	24 (31%)
32	LMT	c	521	-	36,36,36	1.32	5 (13%)	47,47,47	1.28	3 (6%)
24	CLA	c	504	-	65,73,73	1.84	18 (27%)	76,113,113	2.67	22 (28%)
24	CLA	A	406	39	65,73,73	1.87	17 (26%)	76,113,113	2.42	26 (34%)
24	CLA	B	606	-	65,73,73	2.00	18 (27%)	76,113,113	2.80	30 (39%)
30	LMG	C	501	-	51,51,55	1.18	6 (11%)	59,59,63	1.38	8 (13%)
32	LMT	C	521	-	36,36,36	1.31	5 (13%)	47,47,47	1.28	3 (6%)
24	CLA	b	610	-	65,73,73	1.89	17 (26%)	76,113,113	2.49	27 (35%)
24	CLA	b	603	39	65,73,73	1.95	19 (29%)	76,113,113	2.61	25 (32%)
24	CLA	C	502	-	65,73,73	1.91	17 (26%)	76,113,113	2.70	27 (35%)
24	CLA	C	504	-	65,73,73	1.84	18 (27%)	76,113,113	2.67	22 (28%)
26	BCR	c	515	-	41,41,41	1.16	3 (7%)	56,56,56	1.42	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CLA	B	611	-	65,73,73	1.80	14 (21%)	76,113,113	2.70	28 (36%)
24	CLA	b	613	-	65,73,73	1.80	14 (21%)	76,113,113	2.70	28 (36%)
32	LMT	z	101	-	36,36,36	1.30	6 (16%)	47,47,47	1.13	5 (10%)
34	LHG	d	408	-	48,48,48	0.85	1 (2%)	51,54,54	1.23	8 (15%)
26	BCR	C	515	-	41,41,41	1.16	3 (7%)	56,56,56	1.42	9 (16%)
34	LHG	e	101	-	48,48,48	0.72	1 (2%)	51,54,54	1.26	7 (13%)
24	CLA	C	503	-	65,73,73	1.92	17 (26%)	76,113,113	2.57	24 (31%)
30	LMG	B	621	-	51,51,55	1.05	3 (5%)	59,59,63	1.29	6 (10%)
24	CLA	C	514	-	65,73,73	2.01	18 (27%)	76,113,113	2.75	30 (39%)
35	HEM	E	103	5,6	41,50,50	1.45	4 (9%)	45,82,82	1.65	9 (20%)
30	LMG	c	523	-	51,51,55	0.85	2 (3%)	59,59,63	1.36	8 (13%)
24	CLA	B	602	-	65,73,73	1.85	17 (26%)	76,113,113	2.82	26 (34%)
24	CLA	A	408	-	65,73,73	1.88	14 (21%)	76,113,113	2.87	29 (38%)
24	CLA	b	616	-	65,73,73	1.85	15 (23%)	76,113,113	2.78	28 (36%)
26	BCR	T	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.27	7 (12%)
34	LHG	D	410	-	45,45,48	0.80	1 (2%)	48,51,54	1.17	4 (8%)
35	HEM	e	103	5,6	41,50,50	1.45	4 (9%)	45,82,82	1.65	9 (20%)
24	CLA	B	603	-	65,73,73	1.94	17 (26%)	76,113,113	2.66	31 (40%)
24	CLA	b	604	-	65,73,73	1.85	16 (24%)	76,113,113	2.82	27 (35%)
30	LMG	d	411	36	51,51,55	1.07	7 (13%)	59,59,63	1.32	7 (11%)
27	SQD	L	102	-	53,54,54	0.92	5 (9%)	62,65,65	2.23	11 (17%)
25	PHO	d	402	-	51,69,69	1.04	3 (5%)	47,99,99	1.51	8 (17%)
24	CLA	c	512	3	65,73,73	1.92	15 (23%)	76,113,113	2.75	26 (34%)
32	LMT	j	102	-	24,24,36	1.01	2 (8%)	29,29,47	1.51	3 (10%)
37	HEC	V	201	16	32,50,50	2.13	5 (15%)	24,82,82	1.95	8 (33%)
24	CLA	b	617	-	65,73,73	1.84	15 (23%)	76,113,113	2.64	27 (35%)
24	CLA	B	601	39	65,73,73	1.94	19 (29%)	76,113,113	2.60	25 (32%)
24	CLA	c	509	-	65,73,73	1.90	16 (24%)	76,113,113	2.81	30 (39%)
24	CLA	b	606	-	65,73,73	1.87	20 (30%)	76,113,113	2.66	31 (40%)
24	CLA	C	507	-	65,73,73	1.93	15 (23%)	76,113,113	2.69	30 (39%)
26	BCR	b	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.21	3 (5%)
26	BCR	b	621	-	41,41,41	1.11	2 (4%)	56,56,56	1.06	4 (7%)
26	BCR	d	406	-	41,41,41	1.17	3 (7%)	56,56,56	1.41	7 (12%)
34	LHG	L	101	-	48,48,48	0.70	0	51,54,54	1.12	4 (7%)
26	BCR	B	617	-	41,41,41	1.10	2 (4%)	56,56,56	1.21	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CLA	b	605	-	65,73,73	1.93	16 (24%)	76,113,113	2.66	31 (40%)
24	CLA	B	616	-	65,73,73	1.85	14 (21%)	76,113,113	2.65	32 (42%)
24	CLA	a	408	-	65,73,73	1.88	14 (21%)	76,113,113	2.87	29 (38%)
24	CLA	B	610	39	65,73,73	1.87	17 (26%)	76,113,113	2.55	27 (35%)
25	PHO	a	407	-	51,69,69	1.15	6 (11%)	47,99,99	1.22	3 (6%)
32	LMT	M	101	-	36,36,36	1.38	6 (16%)	47,47,47	1.02	1 (2%)
24	CLA	b	607	-	65,73,73	1.86	17 (26%)	76,113,113	2.76	29 (38%)
24	CLA	b	608	-	65,73,73	2.00	18 (27%)	76,113,113	2.81	30 (39%)
26	BCR	D	406	-	41,41,41	1.17	3 (7%)	56,56,56	1.41	7 (12%)
24	CLA	D	405	-	65,73,73	1.94	18 (27%)	76,113,113	2.68	29 (38%)
38	RRX	X	101	-	42,42,42	1.89	11 (26%)	57,58,58	2.00	16 (28%)
24	CLA	b	615	-	65,73,73	1.87	18 (27%)	76,113,113	2.61	27 (35%)
24	CLA	b	611	-	65,73,73	1.83	15 (23%)	76,113,113	2.77	32 (42%)
30	LMG	b	622	-	51,51,55	1.05	3 (5%)	59,59,63	1.29	6 (10%)
28	PL9	d	407	-	55,55,55	1.90	11 (20%)	68,69,69	1.56	16 (23%)
24	CLA	c	502	-	65,73,73	1.90	17 (26%)	76,113,113	2.70	28 (36%)
24	CLA	B	604	-	65,73,73	1.87	20 (30%)	76,113,113	2.66	31 (40%)
34	LHG	d	410	-	45,45,48	0.80	1 (2%)	48,51,54	1.17	4 (8%)
34	LHG	l	101	-	48,48,48	0.70	0	51,54,54	1.12	4 (7%)
34	LHG	d	409	-	48,48,48	0.84	1 (2%)	51,54,54	1.11	3 (5%)
24	CLA	C	506	-	65,73,73	1.84	19 (29%)	76,113,113	2.47	25 (32%)
24	CLA	b	614	-	65,73,73	1.88	16 (24%)	76,113,113	2.62	29 (38%)

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
24	CLA	B	607	39	1/1/15/20	9/37/115/115	-
24	CLA	c	514	-	1/1/15/20	10/37/115/115	-
27	SQD	A	410	-	-	12/49/69/69	0/1/1/1
30	LMG	c	520	-	-	21/46/66/70	0/1/1/1
24	CLA	c	513	-	1/1/15/20	12/37/115/115	-
24	CLA	B	608	-	-	2/37/115/115	-
34	LHG	E	101	-	-	25/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	503	-	-	10/37/115/115	-
26	BCR	j	104	-	-	11/29/63/63	0/2/2/2
24	CLA	C	508	39	1/1/15/20	10/37/115/115	-
26	BCR	B	618	-	-	5/29/63/63	0/2/2/2
32	LMT	J	102	-	-	4/15/35/61	0/1/1/2
28	PL9	a	411	-	-	18/53/73/73	0/1/1/1
24	CLA	c	505	39	1/1/15/20	6/37/115/115	-
31	DGD	c	519	-	-	14/51/91/95	0/2/2/2
24	CLA	c	506	-	1/1/15/20	7/37/115/115	-
24	CLA	B	605	-	1/1/15/20	7/37/115/115	-
24	CLA	a	406	39	-	9/37/115/115	-
26	BCR	c	522	-	-	12/29/63/63	0/2/2/2
32	LMT	m	102	-	-	4/21/61/61	0/2/2/2
24	CLA	c	511	-	1/1/15/20	6/37/115/115	-
24	CLA	b	609	39	1/1/15/20	9/37/115/115	-
24	CLA	C	513	-	1/1/15/20	12/37/115/115	-
24	CLA	c	507	-	1/1/15/20	9/37/115/115	-
28	PL9	A	411	-	-	18/53/73/73	0/1/1/1
30	LMG	c	501	-	-	29/46/66/70	0/1/1/1
26	BCR	A	409	-	-	9/29/63/63	0/2/2/2
30	LMG	D	411	36	-	16/46/66/70	0/1/1/1
31	DGD	c	518	-	-	26/51/91/95	0/2/2/2
34	LHG	D	408	-	-	16/53/53/53	-
31	DGD	C	519	-	-	14/51/91/95	0/2/2/2
24	CLA	C	509	-	1/1/15/20	6/37/115/115	-
24	CLA	d	404	-	1/1/15/20	2/37/115/115	-
31	DGD	h	101	-	-	10/51/91/95	0/2/2/2
34	LHG	D	409	-	-	19/53/53/53	-
26	BCR	t	102	-	-	10/29/63/63	0/2/2/2
24	CLA	a	405	-	1/1/15/20	4/37/115/115	-
31	DGD	C	517	-	-	12/51/91/95	0/2/2/2
24	CLA	d	401	39	1/1/15/20	7/37/115/115	-
27	SQD	B	620	-	-	26/49/69/69	0/1/1/1
25	PHO	D	402	-	-	3/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	a	409	-	-	9/29/63/63	0/2/2/2
38	RRX	x	101	-	-	3/29/65/65	0/2/2/2
24	CLA	b	618	-	1/1/15/20	6/37/115/115	-
30	LMG	C	520	-	-	21/46/66/70	0/1/1/1
24	CLA	c	508	39	1/1/15/20	10/37/115/115	-
32	LMT	Z	101	-	-	13/21/61/61	0/2/2/2
24	CLA	B	614	-	1/1/15/20	16/37/115/115	-
31	DGD	H	101	-	-	10/51/91/95	0/2/2/2
30	LMG	C	523	-	-	27/46/66/70	0/1/1/1
24	CLA	b	612	39	1/1/15/20	5/37/115/115	-
24	CLA	A	405	-	1/1/15/20	4/37/115/115	-
27	SQD	A	412	-	-	19/49/69/69	0/1/1/1
25	PHO	A	407	-	-	5/37/103/103	0/5/6/6
26	BCR	C	522	-	-	12/29/63/63	0/2/2/2
27	SQD	f	101	-	-	12/40/60/69	0/1/1/1
24	CLA	B	609	-	1/1/15/20	3/37/115/115	-
26	BCR	b	620	-	-	5/29/63/63	0/2/2/2
27	SQD	F	101	-	-	12/40/60/69	0/1/1/1
24	CLA	c	510	-	1/1/15/20	11/37/115/115	-
26	BCR	c	516	-	-	9/29/63/63	0/2/2/2
26	BCR	B	619	-	-	12/29/63/63	0/2/2/2
24	CLA	B	615	-	1/1/15/20	12/37/115/115	-
24	CLA	C	512	3	1/1/15/20	12/37/115/115	-
26	BCR	C	516	-	-	9/29/63/63	0/2/2/2
27	SQD	a	410	-	-	12/49/69/69	0/1/1/1
24	CLA	D	401	39	1/1/15/20	7/37/115/115	-
24	CLA	d	405	-	-	11/37/115/115	-
24	CLA	C	505	39	1/1/15/20	6/37/115/115	-
24	CLA	C	510	-	1/1/15/20	11/37/115/115	-
24	CLA	B	612	-	1/1/15/20	6/37/115/115	-
24	CLA	C	511	-	1/1/15/20	6/37/115/115	-
28	PL9	D	407	-	-	10/53/73/73	0/1/1/1
37	HEC	v	201	16	-	2/10/54/54	-
27	SQD	a	412	-	-	19/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	J	104	-	-	11/29/63/63	0/2/2/2
31	DGD	C	518	-	-	26/51/91/95	0/2/2/2
31	DGD	c	517	-	-	12/51/91/95	0/2/2/2
24	CLA	B	613	-	1/1/15/20	7/37/115/115	-
24	CLA	D	404	-	1/1/15/20	2/37/115/115	-
32	LMT	c	521	-	-	10/21/61/61	0/2/2/2
24	CLA	c	504	-	1/1/15/20	8/37/115/115	-
24	CLA	A	406	39	-	9/37/115/115	-
24	CLA	B	606	-	1/1/15/20	5/37/115/115	-
30	LMG	C	501	-	-	29/46/66/70	0/1/1/1
32	LMT	C	521	-	-	10/21/61/61	0/2/2/2
24	CLA	b	610	-	-	2/37/115/115	-
24	CLA	b	603	39	1/1/15/20	13/37/115/115	-
24	CLA	C	502	-	1/1/15/20	4/37/115/115	-
24	CLA	C	504	-	1/1/15/20	8/37/115/115	-
26	BCR	c	515	-	-	11/29/63/63	0/2/2/2
24	CLA	B	611	-	1/1/15/20	2/37/115/115	-
24	CLA	b	613	-	1/1/15/20	2/37/115/115	-
32	LMT	z	101	-	-	13/21/61/61	0/2/2/2
34	LHG	d	408	-	-	16/53/53/53	-
26	BCR	C	515	-	-	11/29/63/63	0/2/2/2
34	LHG	e	101	-	-	25/53/53/53	-
24	CLA	C	503	-	-	10/37/115/115	-
30	LMG	B	621	-	-	13/46/66/70	0/1/1/1
24	CLA	C	514	-	1/1/15/20	10/37/115/115	-
35	HEM	E	103	5,6	-	1/12/54/54	-
30	LMG	c	523	-	-	27/46/66/70	0/1/1/1
24	CLA	B	602	-	1/1/15/20	3/37/115/115	-
24	CLA	b	616	-	1/1/15/20	16/37/115/115	-
24	CLA	A	408	-	-	13/37/115/115	-
26	BCR	T	101	-	-	10/29/63/63	0/2/2/2
34	LHG	D	410	-	-	15/50/50/53	-
35	HEM	e	103	5,6	-	2/12/54/54	-
24	CLA	B	603	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	604	-	1/1/15/20	3/37/115/115	-
30	LMG	d	411	36	-	16/46/66/70	0/1/1/1
27	SQD	L	102	-	-	26/49/69/69	0/1/1/1
25	PHO	d	402	-	-	3/37/103/103	0/5/6/6
24	CLA	c	512	3	1/1/15/20	12/37/115/115	-
32	LMT	j	102	-	-	4/15/35/61	0/1/1/2
37	HEC	V	201	16	-	2/10/54/54	-
24	CLA	b	617	-	1/1/15/20	12/37/115/115	-
24	CLA	B	601	39	1/1/15/20	13/37/115/115	-
24	CLA	c	509	-	1/1/15/20	6/37/115/115	-
24	CLA	b	606	-	1/1/15/20	9/37/115/115	-
24	CLA	C	507	-	1/1/15/20	9/37/115/115	-
26	BCR	b	619	-	-	4/29/63/63	0/2/2/2
26	BCR	b	621	-	-	12/29/63/63	0/2/2/2
26	BCR	d	406	-	-	5/29/63/63	0/2/2/2
34	LHG	L	101	-	-	17/53/53/53	-
26	BCR	B	617	-	-	4/29/63/63	0/2/2/2
24	CLA	b	605	-	1/1/15/20	9/37/115/115	-
24	CLA	B	616	-	1/1/15/20	6/37/115/115	-
24	CLA	a	408	-	-	13/37/115/115	-
24	CLA	B	610	39	1/1/15/20	5/37/115/115	-
25	PHO	a	407	-	-	5/37/103/103	0/5/6/6
32	LMT	M	101	-	-	4/21/61/61	0/2/2/2
24	CLA	b	607	-	1/1/15/20	7/37/115/115	-
24	CLA	b	608	-	1/1/15/20	5/37/115/115	-
26	BCR	D	406	-	-	5/29/63/63	0/2/2/2
24	CLA	D	405	-	-	11/37/115/115	-
38	RRX	X	101	-	-	3/29/65/65	0/2/2/2
24	CLA	b	615	-	1/1/15/20	7/37/115/115	-
24	CLA	b	611	-	1/1/15/20	3/37/115/115	-
30	LMG	b	622	-	-	13/46/66/70	0/1/1/1
28	PL9	d	407	-	-	10/53/73/73	0/1/1/1
24	CLA	c	502	-	1/1/15/20	4/37/115/115	-
24	CLA	B	604	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LHG	d	410	-	-	15/50/50/53	-
34	LHG	l	101	-	-	17/53/53/53	-
34	LHG	d	409	-	-	19/53/53/53	-
24	CLA	C	506	-	1/1/15/20	7/37/115/115	-
24	CLA	b	614	-	1/1/15/20	6/37/115/115	-

All (1488) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	407	PL9	C3-C4	-7.64	1.36	1.49
28	d	407	PL9	C3-C4	-7.64	1.36	1.49
37	V	201	HEC	C2B-C3B	-6.92	1.33	1.40
37	v	201	HEC	C2B-C3B	-6.92	1.33	1.40
24	B	603	CLA	C3B-C2B	6.47	1.49	1.40
24	b	605	CLA	C3B-C2B	6.47	1.49	1.40
24	c	502	CLA	C3B-C2B	6.21	1.49	1.40
24	C	502	CLA	C3B-C2B	6.19	1.49	1.40
24	B	612	CLA	C3B-C2B	6.09	1.48	1.40
24	b	614	CLA	C3B-C2B	6.09	1.48	1.40
24	C	505	CLA	C3B-C2B	6.03	1.48	1.40
24	c	505	CLA	C3B-C2B	6.03	1.48	1.40
24	C	510	CLA	C3B-C2B	5.96	1.48	1.40
24	c	510	CLA	C3B-C2B	5.96	1.48	1.40
24	D	405	CLA	C3B-C2B	5.94	1.48	1.40
24	d	405	CLA	C3B-C2B	5.94	1.48	1.40
24	c	514	CLA	C3B-C2B	5.80	1.48	1.40
24	C	513	CLA	C3B-C2B	5.75	1.48	1.40
24	c	513	CLA	C3B-C2B	5.75	1.48	1.40
24	C	514	CLA	C3B-C2B	5.75	1.48	1.40
24	C	509	CLA	C3B-C2B	5.74	1.48	1.40
24	c	509	CLA	C3B-C2B	5.74	1.48	1.40
24	B	606	CLA	C3B-C2B	5.72	1.48	1.40
24	b	608	CLA	C3B-C2B	5.72	1.48	1.40
24	B	614	CLA	C3B-C2B	5.70	1.48	1.40
24	b	616	CLA	C3B-C2B	5.70	1.48	1.40
24	C	507	CLA	C3B-C2B	5.70	1.48	1.40
24	c	507	CLA	C3B-C2B	5.70	1.48	1.40
24	C	512	CLA	C3B-C2B	5.68	1.48	1.40
24	c	512	CLA	C3B-C2B	5.68	1.48	1.40
24	B	605	CLA	C3B-C2B	5.67	1.48	1.40
24	b	607	CLA	C3B-C2B	5.67	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	404	CLA	C3B-C2B	5.65	1.48	1.40
24	B	606	CLA	C1B-NB	-5.63	1.30	1.35
24	b	608	CLA	C1B-NB	-5.63	1.30	1.35
24	B	615	CLA	C3B-C2B	5.60	1.48	1.40
24	b	617	CLA	C3B-C2B	5.60	1.48	1.40
24	D	404	CLA	C3B-C2B	5.59	1.48	1.40
24	C	508	CLA	C3B-C2B	5.49	1.48	1.40
24	c	508	CLA	C3B-C2B	5.49	1.48	1.40
24	B	611	CLA	C3B-C2B	5.43	1.47	1.40
24	c	511	CLA	C3B-C2B	5.43	1.47	1.40
24	C	511	CLA	C3B-C2B	5.42	1.47	1.40
24	b	613	CLA	C3B-C2B	5.39	1.47	1.40
24	B	601	CLA	C3C-C2C	5.39	1.48	1.36
24	b	603	CLA	C3C-C2C	5.39	1.48	1.36
24	D	401	CLA	C1B-NB	-5.37	1.30	1.35
24	d	401	CLA	C1B-NB	-5.37	1.30	1.35
24	C	503	CLA	C3B-C2B	5.36	1.47	1.40
24	c	503	CLA	C3B-C2B	5.36	1.47	1.40
24	b	611	CLA	O2D-CGD	5.30	1.46	1.33
24	B	609	CLA	O2D-CGD	5.30	1.46	1.33
24	C	504	CLA	C3B-C2B	5.30	1.47	1.40
24	c	504	CLA	C3B-C2B	5.30	1.47	1.40
24	c	514	CLA	CHC-C1C	5.28	1.48	1.35
24	C	514	CLA	CHC-C1C	5.24	1.48	1.35
24	B	607	CLA	C3B-C2B	5.24	1.47	1.40
24	b	609	CLA	C3B-C2B	5.24	1.47	1.40
24	A	405	CLA	C3B-C2B	5.23	1.47	1.40
24	a	405	CLA	C3B-C2B	5.23	1.47	1.40
24	C	506	CLA	C3B-C2B	5.22	1.47	1.40
24	c	506	CLA	C3B-C2B	5.22	1.47	1.40
24	c	514	CLA	C3C-C2C	5.22	1.47	1.36
24	D	401	CLA	C3C-C2C	5.20	1.47	1.36
24	d	401	CLA	C3C-C2C	5.20	1.47	1.36
24	B	610	CLA	C3B-C2B	5.20	1.47	1.40
24	C	514	CLA	C3C-C2C	5.19	1.47	1.36
24	b	612	CLA	C3B-C2B	5.14	1.47	1.40
24	B	616	CLA	C3B-C2B	5.13	1.47	1.40
24	b	618	CLA	C3B-C2B	5.13	1.47	1.40
24	A	406	CLA	C3C-C2C	5.13	1.47	1.36
24	a	406	CLA	C3C-C2C	5.12	1.47	1.36
24	C	513	CLA	C3C-C2C	5.09	1.47	1.36
24	c	513	CLA	C3C-C2C	5.09	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	406	CLA	CHC-C1C	5.02	1.47	1.35
24	a	406	CLA	CHC-C1C	5.00	1.47	1.35
24	B	602	CLA	C3C-C2C	5.00	1.47	1.36
24	b	604	CLA	C3C-C2C	5.00	1.47	1.36
24	B	603	CLA	C3C-C2C	5.00	1.47	1.36
24	b	605	CLA	C3C-C2C	5.00	1.47	1.36
24	D	405	CLA	C3C-C2C	4.96	1.47	1.36
24	C	506	CLA	CHC-C1C	4.95	1.47	1.35
24	c	506	CLA	CHC-C1C	4.95	1.47	1.35
24	C	505	CLA	C3C-C2C	4.94	1.47	1.36
24	c	505	CLA	C3C-C2C	4.94	1.47	1.36
24	C	507	CLA	C3C-C2C	4.94	1.47	1.36
24	c	507	CLA	C3C-C2C	4.94	1.47	1.36
24	b	607	CLA	CHC-C1C	4.94	1.47	1.35
24	d	405	CLA	C3C-C2C	4.92	1.47	1.36
24	C	508	CLA	C3C-C2C	4.92	1.47	1.36
24	c	508	CLA	C3C-C2C	4.92	1.47	1.36
24	C	511	CLA	C3C-C2C	4.91	1.47	1.36
24	c	511	CLA	C3C-C2C	4.91	1.47	1.36
24	B	605	CLA	CHC-C1C	4.90	1.47	1.35
24	C	504	CLA	C3C-C2C	4.88	1.47	1.36
24	c	504	CLA	C3C-C2C	4.88	1.47	1.36
24	B	602	CLA	C3B-C2B	4.88	1.47	1.40
24	b	604	CLA	C3B-C2B	4.88	1.47	1.40
24	C	510	CLA	C3C-C2C	4.87	1.47	1.36
24	c	510	CLA	C3C-C2C	4.87	1.47	1.36
24	C	508	CLA	C4B-NB	-4.86	1.30	1.35
24	c	508	CLA	C4B-NB	-4.86	1.30	1.35
24	B	613	CLA	O2D-CGD	4.85	1.45	1.33
24	b	615	CLA	O2D-CGD	4.85	1.45	1.33
24	A	408	CLA	C3B-C2B	4.85	1.47	1.40
24	a	408	CLA	C3B-C2B	4.85	1.47	1.40
24	B	613	CLA	C3B-C2B	4.82	1.47	1.40
24	b	615	CLA	C3B-C2B	4.82	1.47	1.40
37	v	201	HEC	C3C-C2C	-4.81	1.35	1.40
24	C	510	CLA	O2D-CGD	4.75	1.44	1.33
24	c	510	CLA	O2D-CGD	4.75	1.44	1.33
24	A	408	CLA	C3C-C2C	4.75	1.46	1.36
24	a	408	CLA	C3C-C2C	4.75	1.46	1.36
24	C	502	CLA	O2D-CGD	4.74	1.44	1.33
24	c	502	CLA	O2D-CGD	4.74	1.44	1.33
24	B	602	CLA	CHC-C1C	4.74	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	604	CLA	CHC-C1C	4.74	1.47	1.35
24	b	608	CLA	C3C-C2C	4.73	1.46	1.36
37	V	201	HEC	C3C-C2C	-4.72	1.35	1.40
24	C	509	CLA	C3C-C2C	4.70	1.46	1.36
24	c	509	CLA	C3C-C2C	4.70	1.46	1.36
24	b	603	CLA	CHC-C1C	4.70	1.47	1.35
24	B	606	CLA	C3C-C2C	4.70	1.46	1.36
24	A	408	CLA	CHC-C1C	4.69	1.47	1.35
24	a	408	CLA	CHC-C1C	4.69	1.47	1.35
24	B	613	CLA	C3C-C2C	4.69	1.46	1.36
24	B	610	CLA	C3C-C2C	4.68	1.46	1.36
24	b	615	CLA	C3C-C2C	4.68	1.46	1.36
24	B	601	CLA	O2D-CGD	4.68	1.44	1.33
24	b	616	CLA	C3C-C2C	4.66	1.46	1.36
24	C	514	CLA	O2D-CGD	4.66	1.44	1.33
24	c	514	CLA	O2D-CGD	4.66	1.44	1.33
24	B	601	CLA	C3B-C2B	4.66	1.46	1.40
24	b	603	CLA	C3B-C2B	4.66	1.46	1.40
24	b	612	CLA	C3C-C2C	4.66	1.46	1.36
28	A	411	PL9	C3-C4	-4.66	1.41	1.49
28	a	411	PL9	C3-C4	-4.66	1.41	1.49
24	b	603	CLA	O2D-CGD	4.65	1.44	1.33
24	C	503	CLA	O2D-CGD	4.65	1.44	1.33
24	c	503	CLA	O2D-CGD	4.65	1.44	1.33
24	C	512	CLA	CHC-C1C	4.65	1.46	1.35
24	b	616	CLA	CHC-C1C	4.64	1.46	1.35
24	B	605	CLA	C3C-C2C	4.64	1.46	1.36
24	B	601	CLA	CHC-C1C	4.64	1.46	1.35
24	C	502	CLA	CHC-C1C	4.64	1.46	1.35
24	c	502	CLA	CHC-C1C	4.64	1.46	1.35
24	B	614	CLA	C3C-C2C	4.64	1.46	1.36
28	D	407	PL9	C7-C8	-4.63	1.44	1.50
28	d	407	PL9	C7-C8	-4.63	1.44	1.50
24	c	512	CLA	CHC-C1C	4.62	1.46	1.35
24	A	405	CLA	C3C-C2C	4.61	1.46	1.36
24	a	405	CLA	C3C-C2C	4.61	1.46	1.36
24	B	607	CLA	C1B-NB	-4.61	1.31	1.35
24	b	609	CLA	C1B-NB	-4.61	1.31	1.35
24	B	614	CLA	CHC-C1C	4.61	1.46	1.35
24	B	607	CLA	C3C-C2C	4.60	1.46	1.36
24	b	609	CLA	C3C-C2C	4.60	1.46	1.36
24	D	401	CLA	C3B-C2B	4.60	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	401	CLA	C3B-C2B	4.60	1.46	1.40
24	b	607	CLA	C3C-C2C	4.60	1.46	1.36
24	C	509	CLA	O2D-CGD	4.60	1.44	1.33
24	c	509	CLA	O2D-CGD	4.60	1.44	1.33
24	C	506	CLA	C3C-C2C	4.59	1.46	1.36
24	c	506	CLA	C3C-C2C	4.59	1.46	1.36
24	C	513	CLA	CHC-C1C	4.58	1.46	1.35
24	c	513	CLA	CHC-C1C	4.58	1.46	1.35
24	B	605	CLA	O2D-CGD	4.58	1.44	1.33
24	b	607	CLA	O2D-CGD	4.58	1.44	1.33
24	C	507	CLA	O2D-CGD	4.58	1.44	1.33
24	c	507	CLA	O2D-CGD	4.58	1.44	1.33
24	C	512	CLA	C3C-C2C	4.58	1.46	1.36
24	c	512	CLA	C3C-C2C	4.58	1.46	1.36
38	X	101	RRX	C8-C9	4.57	1.55	1.45
38	x	101	RRX	C8-C9	4.57	1.55	1.45
24	A	408	CLA	O2D-CGD	4.56	1.44	1.33
24	a	408	CLA	O2D-CGD	4.56	1.44	1.33
24	B	612	CLA	O2D-CGD	4.55	1.44	1.33
24	b	614	CLA	O2D-CGD	4.55	1.44	1.33
24	B	615	CLA	C3C-C2C	4.54	1.46	1.36
24	b	617	CLA	C3C-C2C	4.54	1.46	1.36
24	C	510	CLA	O2A-CGA	4.53	1.46	1.33
24	c	510	CLA	O2A-CGA	4.53	1.46	1.33
24	b	610	CLA	C3B-C2B	4.52	1.46	1.40
24	C	504	CLA	CHC-C1C	4.52	1.46	1.35
24	c	504	CLA	CHC-C1C	4.52	1.46	1.35
24	B	608	CLA	C3B-C2B	4.50	1.46	1.40
24	B	612	CLA	C3C-C2C	4.50	1.46	1.36
24	b	614	CLA	C3C-C2C	4.50	1.46	1.36
24	B	608	CLA	C1B-NB	-4.48	1.31	1.35
24	B	603	CLA	CHC-C1C	4.48	1.46	1.35
24	b	605	CLA	CHC-C1C	4.48	1.46	1.35
24	B	610	CLA	CHC-C1C	4.48	1.46	1.35
24	C	505	CLA	CHC-C1C	4.48	1.46	1.35
24	c	505	CLA	CHC-C1C	4.48	1.46	1.35
24	D	405	CLA	CHC-C1C	4.47	1.46	1.35
24	d	405	CLA	CHC-C1C	4.47	1.46	1.35
24	C	510	CLA	CHC-C1C	4.47	1.46	1.35
24	c	510	CLA	CHC-C1C	4.47	1.46	1.35
24	C	506	CLA	O2D-CGD	4.45	1.44	1.33
24	c	506	CLA	O2D-CGD	4.45	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	612	CLA	CHC-C1C	4.45	1.46	1.35
24	C	507	CLA	CHC-C1C	4.44	1.46	1.35
24	c	507	CLA	CHC-C1C	4.44	1.46	1.35
24	b	612	CLA	C1B-NB	-4.44	1.31	1.35
24	B	611	CLA	CHC-C1C	4.44	1.46	1.35
24	b	613	CLA	CHC-C1C	4.44	1.46	1.35
24	c	502	CLA	C3C-C2C	4.42	1.46	1.36
24	D	401	CLA	O2A-CGA	4.41	1.46	1.33
24	d	401	CLA	O2A-CGA	4.41	1.46	1.33
24	B	610	CLA	C1B-NB	-4.40	1.31	1.35
24	B	608	CLA	C3C-C2C	4.40	1.46	1.36
24	D	401	CLA	O2D-CGD	4.40	1.43	1.33
24	d	401	CLA	O2D-CGD	4.40	1.43	1.33
24	C	513	CLA	O2A-CGA	4.39	1.46	1.33
24	c	513	CLA	O2A-CGA	4.39	1.46	1.33
24	b	618	CLA	O2D-CGD	4.39	1.43	1.33
24	c	512	CLA	O2D-CGD	4.38	1.43	1.33
24	b	610	CLA	C3C-C2C	4.38	1.46	1.36
24	C	502	CLA	C3C-C2C	4.38	1.46	1.36
24	C	512	CLA	O2D-CGD	4.37	1.43	1.33
24	C	507	CLA	C1B-NB	-4.37	1.31	1.35
24	c	507	CLA	C1B-NB	-4.37	1.31	1.35
24	D	405	CLA	O2A-CGA	4.37	1.46	1.33
24	d	405	CLA	O2A-CGA	4.37	1.46	1.33
24	b	610	CLA	C1B-NB	-4.37	1.31	1.35
24	c	503	CLA	C3C-C2C	4.36	1.46	1.36
24	B	616	CLA	O2D-CGD	4.36	1.43	1.33
24	B	612	CLA	CHC-C1C	4.34	1.46	1.35
24	B	604	CLA	O2D-CGD	4.34	1.43	1.33
24	c	503	CLA	CHC-C1C	4.33	1.46	1.35
24	C	503	CLA	C3C-C2C	4.33	1.45	1.36
24	b	611	CLA	C3C-C2C	4.32	1.45	1.36
24	b	606	CLA	O2D-CGD	4.32	1.43	1.33
24	b	614	CLA	CHC-C1C	4.32	1.46	1.35
24	C	503	CLA	CHC-C1C	4.31	1.46	1.35
24	A	406	CLA	O2D-CGD	4.31	1.43	1.33
24	a	406	CLA	O2D-CGD	4.31	1.43	1.33
24	C	508	CLA	CHC-C1C	4.30	1.46	1.35
24	c	508	CLA	CHC-C1C	4.30	1.46	1.35
24	B	615	CLA	CHC-C1C	4.30	1.46	1.35
24	b	617	CLA	CHC-C1C	4.30	1.46	1.35
28	A	411	PL9	C7-C3	-4.29	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	513	CLA	O2D-CGD	4.29	1.43	1.33
24	B	606	CLA	CHC-C1C	4.29	1.46	1.35
24	B	611	CLA	O2D-CGD	4.28	1.43	1.33
24	b	613	CLA	O2D-CGD	4.28	1.43	1.33
24	C	514	CLA	C1D-ND	4.28	1.43	1.37
24	c	514	CLA	C1D-ND	4.28	1.43	1.37
37	V	201	HEC	CBB-CAB	-4.27	1.33	1.49
37	v	201	HEC	CBB-CAB	-4.27	1.33	1.49
24	b	608	CLA	CHC-C1C	4.27	1.45	1.35
24	d	404	CLA	C3C-C2C	4.27	1.45	1.36
24	B	609	CLA	C3C-C2C	4.26	1.45	1.36
28	a	411	PL9	C7-C3	-4.25	1.46	1.51
24	c	513	CLA	O2D-CGD	4.25	1.43	1.33
24	B	607	CLA	CHC-C1C	4.25	1.45	1.35
24	b	609	CLA	CHC-C1C	4.25	1.45	1.35
24	B	616	CLA	CHC-C1C	4.24	1.45	1.35
24	b	618	CLA	CHC-C1C	4.24	1.45	1.35
24	C	505	CLA	O2D-CGD	4.24	1.43	1.33
24	B	616	CLA	O2A-CGA	4.24	1.45	1.33
24	B	607	CLA	O2D-CGD	4.23	1.43	1.33
24	b	609	CLA	O2D-CGD	4.23	1.43	1.33
24	C	509	CLA	C1B-NB	-4.23	1.31	1.35
24	c	509	CLA	C1B-NB	-4.23	1.31	1.35
24	B	606	CLA	O2D-CGD	4.23	1.43	1.33
24	b	608	CLA	O2D-CGD	4.23	1.43	1.33
24	b	618	CLA	O2A-CGA	4.23	1.45	1.33
24	B	604	CLA	C3C-C2C	4.23	1.45	1.36
24	b	606	CLA	C3C-C2C	4.23	1.45	1.36
24	D	404	CLA	C3C-C2C	4.23	1.45	1.36
24	B	615	CLA	O2D-CGD	4.22	1.43	1.33
24	b	617	CLA	O2D-CGD	4.22	1.43	1.33
24	B	601	CLA	O2A-CGA	4.22	1.45	1.33
24	b	610	CLA	O2D-CGD	4.22	1.43	1.33
24	D	405	CLA	CHD-C1D	4.22	1.46	1.38
24	d	405	CLA	CHD-C1D	4.22	1.46	1.38
24	c	505	CLA	O2D-CGD	4.21	1.43	1.33
24	B	608	CLA	CHC-C1C	4.21	1.45	1.35
24	b	610	CLA	CHC-C1C	4.21	1.45	1.35
24	C	514	CLA	O2A-CGA	4.21	1.45	1.33
24	c	514	CLA	O2A-CGA	4.21	1.45	1.33
24	C	511	CLA	O2D-CGD	4.21	1.43	1.33
24	c	511	CLA	O2D-CGD	4.21	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	608	CLA	O2D-CGD	4.21	1.43	1.33
24	b	603	CLA	O2A-CGA	4.20	1.45	1.33
24	a	405	CLA	CHC-C1C	4.18	1.45	1.35
24	A	405	CLA	CHC-C1C	4.18	1.45	1.35
24	D	401	CLA	CHC-C1C	4.17	1.45	1.35
24	d	401	CLA	CHC-C1C	4.17	1.45	1.35
24	C	511	CLA	CHD-C1D	4.16	1.46	1.38
24	c	511	CLA	CHD-C1D	4.16	1.46	1.38
24	B	604	CLA	C1B-NB	-4.16	1.31	1.35
24	b	606	CLA	C1B-NB	-4.16	1.31	1.35
37	V	201	HEC	CBC-CAC	-4.15	1.33	1.49
37	v	201	HEC	CBC-CAC	-4.15	1.33	1.49
24	B	603	CLA	O2D-CGD	4.14	1.43	1.33
24	b	605	CLA	O2D-CGD	4.14	1.43	1.33
24	B	609	CLA	CHC-C1C	4.13	1.45	1.35
24	b	611	CLA	CHC-C1C	4.12	1.45	1.35
24	A	408	CLA	O2A-CGA	4.11	1.45	1.33
24	a	408	CLA	O2A-CGA	4.11	1.45	1.33
24	B	604	CLA	C3B-C2B	4.09	1.46	1.40
24	b	606	CLA	C3B-C2B	4.09	1.46	1.40
24	a	408	CLA	C1B-NB	-4.09	1.31	1.35
24	C	514	CLA	CHD-C1D	4.08	1.46	1.38
24	D	404	CLA	CHC-C1C	4.08	1.45	1.35
24	d	404	CLA	CHC-C1C	4.08	1.45	1.35
24	B	615	CLA	O2A-CGA	4.08	1.45	1.33
24	A	408	CLA	C1B-NB	-4.07	1.31	1.35
24	B	602	CLA	O2D-CGD	4.07	1.43	1.33
24	b	604	CLA	O2D-CGD	4.07	1.43	1.33
24	b	617	CLA	O2A-CGA	4.06	1.45	1.33
24	c	514	CLA	CHD-C1D	4.06	1.46	1.38
24	C	511	CLA	C1D-ND	4.06	1.42	1.37
24	c	511	CLA	C1D-ND	4.06	1.42	1.37
24	b	617	CLA	CHD-C1D	4.04	1.46	1.38
24	B	612	CLA	C1B-NB	-4.03	1.31	1.35
24	b	615	CLA	CHC-C1C	4.01	1.45	1.35
24	B	615	CLA	CHD-C1D	4.01	1.46	1.38
24	B	611	CLA	C3C-C2C	4.01	1.45	1.36
24	B	613	CLA	CHC-C1C	4.01	1.45	1.35
24	C	512	CLA	C1D-ND	4.01	1.42	1.37
24	c	512	CLA	C1D-ND	4.01	1.42	1.37
24	C	508	CLA	C1B-NB	-4.01	1.31	1.35
24	c	508	CLA	C1B-NB	-4.01	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	O2A-CGA	4.00	1.45	1.33
24	c	508	CLA	O2A-CGA	4.00	1.45	1.33
24	C	505	CLA	O2A-CGA	3.99	1.45	1.33
24	c	505	CLA	O2A-CGA	3.99	1.45	1.33
24	B	609	CLA	O2A-CGA	3.98	1.45	1.33
24	b	611	CLA	O2A-CGA	3.98	1.45	1.33
24	C	513	CLA	C3D-C2D	3.97	1.50	1.39
24	c	513	CLA	C3D-C2D	3.97	1.50	1.39
24	a	406	CLA	C3B-C2B	3.97	1.45	1.40
24	a	406	CLA	O2A-CGA	3.97	1.44	1.33
24	b	614	CLA	C1B-NB	-3.97	1.31	1.35
24	C	514	CLA	CHD-C4C	3.96	1.48	1.39
24	c	514	CLA	CHD-C4C	3.96	1.48	1.39
24	B	616	CLA	C3C-C2C	3.96	1.45	1.36
24	b	618	CLA	C3C-C2C	3.96	1.45	1.36
24	b	613	CLA	C3C-C2C	3.95	1.45	1.36
24	C	509	CLA	CHC-C1C	3.94	1.45	1.35
24	c	509	CLA	CHC-C1C	3.94	1.45	1.35
38	X	101	RRX	C12-C13	3.94	1.54	1.45
38	x	101	RRX	C12-C13	3.94	1.54	1.45
24	A	406	CLA	O2A-CGA	3.94	1.44	1.33
24	D	404	CLA	O2A-CGA	3.94	1.44	1.33
24	d	404	CLA	O2A-CGA	3.94	1.44	1.33
24	C	512	CLA	O2A-CGA	3.94	1.44	1.33
24	c	512	CLA	O2A-CGA	3.94	1.44	1.33
24	B	612	CLA	C1C-NC	-3.93	1.31	1.37
24	b	614	CLA	C1C-NC	-3.93	1.31	1.37
30	C	501	LMG	O1-C7	-3.93	1.36	1.43
30	c	501	LMG	O1-C7	-3.93	1.36	1.43
28	D	407	PL9	C7-C3	-3.93	1.47	1.51
28	d	407	PL9	C7-C3	-3.93	1.47	1.51
24	B	614	CLA	O2D-CGD	3.92	1.42	1.33
24	b	616	CLA	O2D-CGD	3.92	1.42	1.33
28	D	407	PL9	C31-C29	-3.92	1.43	1.51
38	X	101	RRX	C19-C18	3.91	1.54	1.45
38	x	101	RRX	C19-C18	3.91	1.54	1.45
24	b	616	CLA	O2A-CGA	3.91	1.44	1.33
24	A	406	CLA	C3B-C2B	3.91	1.45	1.40
24	A	405	CLA	O2D-CGD	3.91	1.42	1.33
24	a	405	CLA	O2D-CGD	3.91	1.42	1.33
24	D	405	CLA	O2D-CGD	3.91	1.42	1.33
24	d	405	CLA	O2D-CGD	3.91	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	O2A-CGA	3.90	1.44	1.33
30	C	501	LMG	C4-C5	3.90	1.61	1.53
30	c	501	LMG	C4-C5	3.90	1.61	1.53
24	C	503	CLA	O2A-CGA	3.89	1.44	1.33
24	c	503	CLA	O2A-CGA	3.89	1.44	1.33
28	d	407	PL9	C31-C29	-3.89	1.43	1.51
24	B	616	CLA	C1D-ND	3.89	1.42	1.37
24	b	618	CLA	C1D-ND	3.89	1.42	1.37
24	A	406	CLA	C1B-NB	-3.87	1.31	1.35
24	B	610	CLA	O2D-CGD	3.86	1.42	1.33
24	C	508	CLA	O2D-CGD	3.85	1.42	1.33
24	c	508	CLA	O2D-CGD	3.85	1.42	1.33
24	b	612	CLA	O2D-CGD	3.83	1.42	1.33
24	c	502	CLA	C1D-ND	3.82	1.42	1.37
24	a	406	CLA	C1B-NB	-3.81	1.31	1.35
24	B	616	CLA	C4B-NB	-3.80	1.31	1.35
24	b	618	CLA	C4B-NB	-3.80	1.31	1.35
24	D	401	CLA	CHD-C4C	3.80	1.47	1.39
24	d	401	CLA	CHD-C4C	3.80	1.47	1.39
24	C	511	CLA	C1B-NB	-3.79	1.31	1.35
24	c	511	CLA	C1B-NB	-3.79	1.31	1.35
24	A	406	CLA	C1D-ND	3.79	1.42	1.37
24	a	406	CLA	C1D-ND	3.79	1.42	1.37
24	b	604	CLA	O2A-CGA	3.78	1.44	1.33
24	b	613	CLA	C1B-NB	-3.77	1.31	1.35
24	B	615	CLA	C1B-NB	-3.76	1.31	1.35
24	b	617	CLA	C1B-NB	-3.76	1.31	1.35
24	B	602	CLA	O2A-CGA	3.76	1.44	1.33
24	D	404	CLA	O2D-CGD	3.76	1.42	1.33
24	d	404	CLA	O2D-CGD	3.76	1.42	1.33
24	a	408	CLA	CHD-C1D	3.76	1.45	1.38
24	B	602	CLA	CHD-C4C	3.76	1.47	1.39
24	b	604	CLA	CHD-C4C	3.76	1.47	1.39
24	B	611	CLA	C1B-NB	-3.75	1.31	1.35
26	D	406	BCR	C1-C6	-3.75	1.48	1.53
26	d	406	BCR	C1-C6	-3.75	1.48	1.53
24	C	502	CLA	C1D-ND	3.74	1.42	1.37
24	B	613	CLA	O2A-CGA	3.74	1.44	1.33
24	B	602	CLA	C1D-ND	3.74	1.42	1.37
24	b	604	CLA	C1D-ND	3.74	1.42	1.37
24	B	604	CLA	CHC-C1C	3.73	1.44	1.35
24	b	606	CLA	CHC-C1C	3.73	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	CHD-C1D	3.73	1.45	1.38
24	c	510	CLA	CHD-C1D	3.73	1.45	1.38
24	A	408	CLA	CHD-C1D	3.72	1.45	1.38
24	b	615	CLA	O2A-CGA	3.72	1.44	1.33
38	x	101	RRX	C23-C22	3.72	1.53	1.45
35	E	103	HEM	C3C-CAC	3.71	1.55	1.47
35	e	103	HEM	C3C-CAC	3.71	1.55	1.47
24	C	502	CLA	CHD-C1D	3.71	1.45	1.38
24	c	502	CLA	CHD-C1D	3.70	1.45	1.38
38	X	101	RRX	C23-C22	3.70	1.53	1.45
24	b	610	CLA	CHD-C1D	3.69	1.45	1.38
24	B	614	CLA	C4B-NB	-3.68	1.31	1.35
24	B	604	CLA	O2A-CGA	3.68	1.44	1.33
24	C	511	CLA	O2A-CGA	3.68	1.44	1.33
24	B	610	CLA	O2A-CGA	3.67	1.44	1.33
24	b	606	CLA	O2A-CGA	3.67	1.44	1.33
24	c	511	CLA	O2A-CGA	3.67	1.44	1.33
24	c	507	CLA	CHD-C1D	3.66	1.45	1.38
24	C	503	CLA	CHD-C1D	3.66	1.45	1.38
24	c	503	CLA	CHD-C1D	3.66	1.45	1.38
24	C	509	CLA	C1C-NC	-3.66	1.32	1.37
24	c	509	CLA	C1C-NC	-3.66	1.32	1.37
24	B	608	CLA	C4B-NB	-3.66	1.31	1.35
24	C	503	CLA	C4B-NB	-3.65	1.32	1.35
24	c	503	CLA	C4B-NB	-3.65	1.32	1.35
24	b	612	CLA	O2A-CGA	3.65	1.44	1.33
24	C	512	CLA	CHD-C4C	3.65	1.47	1.39
24	B	610	CLA	C3D-C2D	3.65	1.49	1.39
24	c	512	CLA	CHD-C4C	3.64	1.47	1.39
24	D	401	CLA	C1D-ND	3.64	1.42	1.37
24	d	401	CLA	C1D-ND	3.64	1.42	1.37
24	B	608	CLA	CHD-C1D	3.63	1.45	1.38
24	b	612	CLA	C3D-C2D	3.63	1.49	1.39
24	B	604	CLA	CHD-C1D	3.63	1.45	1.38
24	b	606	CLA	CHD-C1D	3.63	1.45	1.38
24	C	510	CLA	C3D-C2D	3.63	1.49	1.39
24	c	510	CLA	C3D-C2D	3.63	1.49	1.39
24	C	507	CLA	CHD-C1D	3.62	1.45	1.38
24	b	610	CLA	C4B-NB	-3.62	1.32	1.35
24	C	511	CLA	CHC-C1C	3.62	1.44	1.35
24	c	511	CLA	CHC-C1C	3.62	1.44	1.35
24	B	616	CLA	CHD-C4C	3.62	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	CLA	CHD-C4C	3.62	1.47	1.39
24	C	504	CLA	O2A-CGA	3.61	1.43	1.33
24	c	504	CLA	O2A-CGA	3.61	1.43	1.33
24	C	507	CLA	C1D-ND	3.61	1.42	1.37
24	c	507	CLA	C1D-ND	3.61	1.42	1.37
24	b	611	CLA	C1C-NC	-3.60	1.32	1.37
24	D	405	CLA	C1D-ND	3.60	1.42	1.37
24	d	405	CLA	C1D-ND	3.60	1.42	1.37
32	Z	101	LMT	O2B-C2B	-3.59	1.34	1.43
32	z	101	LMT	O2B-C2B	-3.59	1.34	1.43
24	b	604	CLA	C1B-NB	-3.59	1.32	1.35
24	b	610	CLA	O2A-CGA	3.58	1.43	1.33
24	B	609	CLA	C1C-NC	-3.58	1.32	1.37
24	C	505	CLA	CHD-C4C	3.58	1.47	1.39
24	c	505	CLA	CHD-C4C	3.58	1.47	1.39
24	D	401	CLA	CHD-C1D	3.58	1.45	1.38
24	d	401	CLA	CHD-C1D	3.58	1.45	1.38
31	C	518	DGD	O6D-C5D	-3.57	1.35	1.44
31	c	518	DGD	O6D-C5D	-3.57	1.35	1.44
24	b	611	CLA	C1B-NB	-3.56	1.32	1.35
30	B	621	LMG	C4-C5	3.56	1.60	1.53
30	b	622	LMG	C4-C5	3.56	1.60	1.53
24	C	511	CLA	CHD-C4C	3.56	1.47	1.39
24	c	511	CLA	CHD-C4C	3.56	1.47	1.39
24	A	405	CLA	O2A-CGA	3.56	1.43	1.33
24	a	405	CLA	O2A-CGA	3.56	1.43	1.33
24	C	506	CLA	O2A-CGA	3.56	1.43	1.33
24	c	506	CLA	O2A-CGA	3.56	1.43	1.33
24	C	510	CLA	C1B-NB	-3.55	1.32	1.35
24	c	510	CLA	C1B-NB	-3.55	1.32	1.35
24	B	608	CLA	O2A-CGA	3.55	1.43	1.33
31	C	518	DGD	O3D-C3D	-3.53	1.34	1.43
31	c	518	DGD	O3D-C3D	-3.53	1.34	1.43
24	B	603	CLA	C1B-NB	-3.53	1.32	1.35
24	b	605	CLA	C1B-NB	-3.53	1.32	1.35
24	B	609	CLA	C1D-ND	3.52	1.42	1.37
24	B	601	CLA	CHD-C1D	3.52	1.45	1.38
24	b	603	CLA	CHD-C1D	3.52	1.45	1.38
24	B	604	CLA	CHD-C4C	3.52	1.47	1.39
24	b	606	CLA	CHD-C4C	3.52	1.47	1.39
24	B	614	CLA	CHD-C4C	3.52	1.47	1.39
24	b	616	CLA	CHD-C4C	3.52	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	408	CLA	CHD-C4C	3.50	1.47	1.39
24	a	408	CLA	CHD-C4C	3.50	1.47	1.39
38	X	101	RRX	C15-C14	3.50	1.54	1.43
24	B	605	CLA	C1D-ND	3.50	1.42	1.37
24	b	607	CLA	C1D-ND	3.50	1.42	1.37
24	b	611	CLA	C3D-C2D	3.50	1.48	1.39
31	H	101	DGD	O4D-C4D	-3.50	1.34	1.43
31	h	101	DGD	O4D-C4D	-3.50	1.34	1.43
35	E	103	HEM	C3C-C2C	-3.49	1.35	1.40
35	e	103	HEM	C3C-C2C	-3.49	1.35	1.40
24	b	608	CLA	CHD-C1D	3.49	1.45	1.38
24	C	506	CLA	CHD-C4C	3.49	1.47	1.39
24	c	506	CLA	CHD-C4C	3.49	1.47	1.39
24	B	615	CLA	C3D-C2D	3.49	1.48	1.39
24	b	617	CLA	C3D-C2D	3.49	1.48	1.39
24	B	613	CLA	CHD-C1D	3.49	1.45	1.38
24	b	615	CLA	CHD-C1D	3.49	1.45	1.38
24	B	609	CLA	C3D-C2D	3.49	1.48	1.39
24	B	609	CLA	C3B-C2B	3.49	1.45	1.40
24	d	405	CLA	C3D-C2D	3.48	1.48	1.39
24	b	611	CLA	C1D-ND	3.48	1.42	1.37
24	B	607	CLA	CHD-C4C	3.48	1.47	1.39
24	b	609	CLA	CHD-C4C	3.48	1.47	1.39
24	B	606	CLA	O2A-CGA	3.48	1.43	1.33
24	b	608	CLA	O2A-CGA	3.48	1.43	1.33
24	C	504	CLA	CHD-C4C	3.47	1.47	1.39
24	c	504	CLA	CHD-C4C	3.47	1.47	1.39
38	x	101	RRX	C15-C14	3.47	1.54	1.43
24	B	602	CLA	C1B-NB	-3.47	1.32	1.35
24	B	601	CLA	C1D-ND	3.47	1.42	1.37
24	b	603	CLA	C1D-ND	3.47	1.42	1.37
24	b	616	CLA	C4B-NB	-3.47	1.32	1.35
24	D	405	CLA	C3D-C2D	3.47	1.48	1.39
24	B	616	CLA	CHD-C1D	3.47	1.45	1.38
24	b	618	CLA	CHD-C1D	3.47	1.45	1.38
24	C	505	CLA	CHD-C1D	3.46	1.45	1.38
24	c	505	CLA	CHD-C1D	3.46	1.45	1.38
24	C	510	CLA	C1D-ND	3.46	1.42	1.37
24	c	510	CLA	C1D-ND	3.46	1.42	1.37
24	C	504	CLA	O2D-CGD	3.46	1.41	1.33
24	c	504	CLA	O2D-CGD	3.46	1.41	1.33
24	B	606	CLA	CHD-C1D	3.46	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	509	CLA	C3D-C2D	3.46	1.48	1.39
24	c	509	CLA	C3D-C2D	3.46	1.48	1.39
31	C	519	DGD	O1G-C1G	-3.45	1.37	1.45
31	c	519	DGD	O1G-C1G	-3.45	1.37	1.45
31	C	518	DGD	O4D-C4D	-3.45	1.34	1.43
31	c	518	DGD	O4D-C4D	-3.45	1.34	1.43
24	B	601	CLA	CHD-C4C	3.45	1.47	1.39
24	b	603	CLA	CHD-C4C	3.45	1.47	1.39
24	C	504	CLA	C1D-ND	3.45	1.42	1.37
24	c	504	CLA	C1D-ND	3.45	1.42	1.37
31	C	518	DGD	C4D-C3D	3.44	1.61	1.52
31	c	518	DGD	C4D-C3D	3.44	1.61	1.52
24	b	610	CLA	CHD-C4C	3.44	1.47	1.39
24	B	608	CLA	CHD-C4C	3.44	1.47	1.39
24	D	405	CLA	CHD-C4C	3.43	1.47	1.39
24	d	405	CLA	CHD-C4C	3.43	1.47	1.39
24	B	609	CLA	CHD-C1D	3.42	1.45	1.38
24	b	613	CLA	C3D-C2D	3.42	1.48	1.39
24	b	611	CLA	C3B-C2B	3.42	1.45	1.40
34	D	408	LHG	O7-C5	-3.42	1.38	1.46
34	d	408	LHG	O7-C5	-3.42	1.38	1.46
24	b	611	CLA	CHD-C1D	3.42	1.45	1.38
24	A	408	CLA	C3D-C2D	3.41	1.48	1.39
24	B	611	CLA	C3D-C2D	3.41	1.48	1.39
24	a	408	CLA	C3D-C2D	3.41	1.48	1.39
24	B	601	CLA	C3D-C2D	3.41	1.48	1.39
24	b	603	CLA	C3D-C2D	3.41	1.48	1.39
24	B	607	CLA	O2A-CGA	3.41	1.43	1.33
24	b	609	CLA	O2A-CGA	3.41	1.43	1.33
24	D	401	CLA	C3D-C2D	3.41	1.48	1.39
24	d	401	CLA	C3D-C2D	3.41	1.48	1.39
24	D	404	CLA	C4B-NB	-3.41	1.32	1.35
24	d	404	CLA	C4B-NB	-3.41	1.32	1.35
24	C	514	CLA	C3D-C2D	3.40	1.48	1.39
24	c	514	CLA	C3D-C2D	3.40	1.48	1.39
24	B	609	CLA	C1B-NB	-3.40	1.32	1.35
28	a	411	PL9	C7-C8	-3.40	1.45	1.50
24	C	509	CLA	O2A-CGA	3.39	1.43	1.33
24	c	509	CLA	O2A-CGA	3.39	1.43	1.33
24	b	613	CLA	O2A-CGA	3.39	1.43	1.33
24	B	611	CLA	O2A-CGA	3.39	1.43	1.33
24	B	613	CLA	C1B-NB	-3.39	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	507	CLA	O2A-CGA	3.38	1.43	1.33
24	c	507	CLA	O2A-CGA	3.38	1.43	1.33
38	X	101	RRX	C16-C17	3.38	1.53	1.43
38	x	101	RRX	C16-C17	3.38	1.53	1.43
24	b	603	CLA	C1B-NB	-3.38	1.32	1.35
28	A	411	PL9	C7-C8	-3.38	1.45	1.50
24	C	503	CLA	C3D-C2D	3.37	1.48	1.39
24	c	503	CLA	C3D-C2D	3.37	1.48	1.39
24	C	502	CLA	O2A-CGA	3.37	1.43	1.33
24	C	509	CLA	C4B-NB	-3.37	1.32	1.35
24	c	509	CLA	C4B-NB	-3.37	1.32	1.35
24	C	502	CLA	C3D-C2D	3.36	1.48	1.39
24	b	607	CLA	C1B-NB	-3.36	1.32	1.35
24	B	605	CLA	C1B-NB	-3.35	1.32	1.35
24	C	506	CLA	CHD-C1D	3.35	1.44	1.38
24	c	506	CLA	CHD-C1D	3.35	1.44	1.38
24	B	606	CLA	CHD-C4C	3.35	1.46	1.39
24	b	608	CLA	CHD-C4C	3.34	1.46	1.39
24	c	502	CLA	C3D-C2D	3.34	1.48	1.39
24	B	613	CLA	C4B-NB	-3.34	1.32	1.35
24	b	615	CLA	C4B-NB	-3.34	1.32	1.35
24	C	512	CLA	C1B-NB	-3.34	1.32	1.35
24	c	512	CLA	C1B-NB	-3.34	1.32	1.35
24	c	502	CLA	O2A-CGA	3.34	1.43	1.33
24	c	512	CLA	C3D-C2D	3.34	1.48	1.39
32	M	101	LMT	O1'-C1'	-3.34	1.34	1.40
32	m	102	LMT	O1'-C1'	-3.34	1.34	1.40
38	X	101	RRX	C11-C10	3.32	1.53	1.43
38	x	101	RRX	C11-C10	3.32	1.53	1.43
24	B	606	CLA	C3D-C2D	3.32	1.48	1.39
24	b	608	CLA	C3D-C2D	3.32	1.48	1.39
24	b	615	CLA	C1B-NB	-3.32	1.32	1.35
24	A	408	CLA	OBD-CAD	3.31	1.28	1.22
24	a	408	CLA	OBD-CAD	3.31	1.28	1.22
24	B	605	CLA	CHD-C1D	3.31	1.44	1.38
24	b	607	CLA	CHD-C1D	3.31	1.44	1.38
24	B	612	CLA	O2A-CGA	3.31	1.43	1.33
24	C	512	CLA	C3D-C2D	3.31	1.48	1.39
24	C	505	CLA	C3D-C2D	3.30	1.48	1.39
24	c	505	CLA	C3D-C2D	3.30	1.48	1.39
24	C	513	CLA	CHD-C4C	3.30	1.46	1.39
24	c	513	CLA	CHD-C4C	3.30	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	601	CLA	C1B-NB	-3.30	1.32	1.35
24	b	603	CLA	C1C-NC	-3.30	1.32	1.37
24	B	608	CLA	C3D-C2D	3.30	1.48	1.39
24	b	610	CLA	C3D-C2D	3.29	1.48	1.39
24	B	610	CLA	C1C-NC	-3.29	1.32	1.37
24	C	503	CLA	C1D-ND	3.29	1.41	1.37
24	c	503	CLA	C1D-ND	3.29	1.41	1.37
24	b	614	CLA	O2A-CGA	3.29	1.42	1.33
24	D	404	CLA	C1B-NB	-3.28	1.32	1.35
24	d	404	CLA	C1B-NB	-3.28	1.32	1.35
32	z	101	LMT	O2'-C2'	-3.28	1.35	1.43
24	C	503	CLA	C1B-NB	-3.28	1.32	1.35
24	c	503	CLA	C1B-NB	-3.28	1.32	1.35
32	Z	101	LMT	O2'-C2'	-3.27	1.35	1.43
26	J	104	BCR	C1-C6	-3.27	1.49	1.53
27	f	101	SQD	O48-C23	3.27	1.42	1.33
24	A	406	CLA	C3D-C4D	-3.26	1.36	1.44
24	a	406	CLA	C3D-C4D	-3.26	1.36	1.44
24	B	606	CLA	C1D-ND	3.26	1.41	1.37
24	b	608	CLA	C1D-ND	3.26	1.41	1.37
26	j	104	BCR	C1-C6	-3.26	1.49	1.53
24	C	502	CLA	C1B-NB	-3.26	1.32	1.35
24	b	612	CLA	C1C-NC	-3.26	1.32	1.37
24	B	605	CLA	C3D-C2D	3.25	1.48	1.39
24	b	607	CLA	C3D-C2D	3.25	1.48	1.39
24	B	601	CLA	C1C-NC	-3.25	1.33	1.37
24	C	507	CLA	CHD-C4C	3.24	1.46	1.39
31	H	101	DGD	C4D-C5D	3.24	1.59	1.53
31	h	101	DGD	C4D-C5D	3.24	1.59	1.53
24	b	614	CLA	CHD-C1D	3.24	1.44	1.38
24	B	610	CLA	C1D-ND	3.23	1.41	1.37
27	F	101	SQD	O48-C23	3.23	1.42	1.33
24	B	612	CLA	CHD-C1D	3.23	1.44	1.38
24	c	507	CLA	CHD-C4C	3.23	1.46	1.39
24	b	612	CLA	CHD-C1D	3.23	1.44	1.38
24	B	611	CLA	C1D-ND	3.22	1.41	1.37
24	b	613	CLA	C1D-ND	3.22	1.41	1.37
24	C	510	CLA	C3D-C4D	-3.22	1.36	1.44
24	c	510	CLA	C3D-C4D	-3.22	1.36	1.44
24	D	401	CLA	C4B-NB	-3.22	1.32	1.35
24	d	401	CLA	C4B-NB	-3.22	1.32	1.35
24	C	510	CLA	CHD-C4C	3.21	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	518	DGD	O2G-C2G	-3.21	1.38	1.46
24	C	512	CLA	CHD-C1D	3.21	1.44	1.38
24	c	512	CLA	CHD-C1D	3.21	1.44	1.38
24	B	603	CLA	CHD-C1D	3.20	1.44	1.38
24	c	510	CLA	CHD-C4C	3.20	1.46	1.39
24	B	606	CLA	C4B-NB	-3.20	1.32	1.35
24	b	608	CLA	C4B-NB	-3.20	1.32	1.35
31	C	518	DGD	O2G-C2G	-3.20	1.38	1.46
24	B	615	CLA	CHD-C4C	3.19	1.46	1.39
24	B	610	CLA	CHD-C1D	3.19	1.44	1.38
38	X	101	RRX	C20-C21	3.19	1.53	1.43
38	x	101	RRX	C20-C21	3.19	1.53	1.43
24	c	502	CLA	C1B-NB	-3.19	1.32	1.35
24	C	511	CLA	C4B-NB	-3.19	1.32	1.35
24	c	511	CLA	C4B-NB	-3.19	1.32	1.35
24	B	603	CLA	C1C-NC	-3.18	1.33	1.37
24	b	605	CLA	C1C-NC	-3.18	1.33	1.37
24	B	603	CLA	O2A-CGA	3.18	1.42	1.33
31	C	518	DGD	O4E-C4E	-3.18	1.35	1.43
31	c	518	DGD	O4E-C4E	-3.18	1.35	1.43
24	C	508	CLA	CHD-C1D	3.18	1.44	1.38
24	b	605	CLA	CHD-C1D	3.18	1.44	1.38
24	c	508	CLA	CHD-C1D	3.18	1.44	1.38
31	c	519	DGD	O3E-C3E	-3.17	1.35	1.43
31	C	519	DGD	O3E-C3E	-3.17	1.35	1.43
24	D	401	CLA	C1C-NC	-3.17	1.33	1.37
24	d	401	CLA	C1C-NC	-3.17	1.33	1.37
24	C	508	CLA	C1D-ND	3.17	1.41	1.37
24	c	508	CLA	C1D-ND	3.17	1.41	1.37
24	c	503	CLA	C1C-NC	-3.17	1.33	1.37
24	B	607	CLA	C3D-C2D	3.17	1.47	1.39
24	b	609	CLA	C3D-C2D	3.17	1.47	1.39
24	B	614	CLA	C1C-NC	-3.16	1.33	1.37
24	b	616	CLA	C1C-NC	-3.16	1.33	1.37
32	C	521	LMT	O3'-C3'	-3.16	1.35	1.43
32	c	521	LMT	O3'-C3'	-3.16	1.35	1.43
24	B	603	CLA	C3D-C4D	-3.16	1.37	1.44
24	C	506	CLA	C1D-ND	3.16	1.41	1.37
24	c	506	CLA	C1D-ND	3.16	1.41	1.37
24	B	613	CLA	C3D-C2D	3.15	1.47	1.39
24	b	615	CLA	C3D-C2D	3.15	1.47	1.39
24	C	507	CLA	C3D-C2D	3.15	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	507	CLA	C3D-C2D	3.15	1.47	1.39
24	b	617	CLA	CHD-C4C	3.15	1.46	1.39
24	b	605	CLA	O2A-CGA	3.15	1.42	1.33
24	b	605	CLA	C3D-C4D	-3.15	1.37	1.44
24	B	611	CLA	CHD-C1D	3.14	1.44	1.38
24	b	613	CLA	CHD-C1D	3.14	1.44	1.38
24	C	503	CLA	C1C-NC	-3.12	1.33	1.37
24	C	504	CLA	CHD-C1D	3.12	1.44	1.38
24	c	504	CLA	CHD-C1D	3.12	1.44	1.38
31	C	518	DGD	C4E-C3E	3.12	1.60	1.52
31	c	518	DGD	C4E-C3E	3.12	1.60	1.52
24	C	511	CLA	C3D-C2D	3.11	1.47	1.39
24	c	511	CLA	C3D-C2D	3.11	1.47	1.39
24	b	616	CLA	C1B-NB	-3.11	1.32	1.35
24	B	602	CLA	CHD-C1D	3.11	1.44	1.38
24	b	604	CLA	CHD-C1D	3.11	1.44	1.38
26	B	617	BCR	C1-C6	-3.11	1.49	1.53
26	b	619	BCR	C1-C6	-3.11	1.49	1.53
24	B	605	CLA	CHD-C4C	3.10	1.46	1.39
24	b	607	CLA	CHD-C4C	3.10	1.46	1.39
24	C	502	CLA	CHD-C4C	3.09	1.46	1.39
24	c	502	CLA	CHD-C4C	3.09	1.46	1.39
24	D	404	CLA	CHD-C4C	3.09	1.46	1.39
24	c	503	CLA	CHD-C4C	3.09	1.46	1.39
24	d	404	CLA	CHD-C4C	3.09	1.46	1.39
24	B	616	CLA	C3D-C2D	3.08	1.47	1.39
24	b	618	CLA	C3D-C2D	3.08	1.47	1.39
24	B	613	CLA	C3D-C4D	-3.08	1.37	1.44
24	b	615	CLA	C3D-C4D	-3.08	1.37	1.44
24	b	612	CLA	C1D-ND	3.08	1.41	1.37
31	C	517	DGD	O5D-C6D	-3.08	1.38	1.43
24	C	503	CLA	C3D-C4D	-3.06	1.37	1.44
24	C	507	CLA	C3D-C4D	-3.06	1.37	1.44
24	c	503	CLA	C3D-C4D	-3.06	1.37	1.44
24	c	507	CLA	C3D-C4D	-3.06	1.37	1.44
24	C	512	CLA	OBD-CAD	3.06	1.27	1.22
24	c	512	CLA	OBD-CAD	3.06	1.27	1.22
24	a	408	CLA	C1D-ND	3.06	1.41	1.37
28	D	407	PL9	C6-C1	-3.05	1.43	1.48
24	C	509	CLA	CHD-C1D	3.05	1.44	1.38
24	c	509	CLA	CHD-C1D	3.05	1.44	1.38
24	B	616	CLA	C1B-NB	-3.05	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	CLA	C1B-NB	-3.05	1.32	1.35
24	b	610	CLA	C3D-C4D	-3.04	1.37	1.44
24	C	505	CLA	C3D-C4D	-3.04	1.37	1.44
24	c	505	CLA	C3D-C4D	-3.04	1.37	1.44
24	B	610	CLA	CHD-C4C	3.04	1.46	1.39
24	A	408	CLA	C1D-ND	3.04	1.41	1.37
24	B	607	CLA	C1C-NC	-3.04	1.33	1.37
24	b	609	CLA	C1C-NC	-3.04	1.33	1.37
24	C	513	CLA	CHD-C1D	3.03	1.44	1.38
24	c	513	CLA	CHD-C1D	3.03	1.44	1.38
24	C	503	CLA	CHD-C4C	3.03	1.46	1.39
24	B	604	CLA	C1C-NC	-3.03	1.33	1.37
24	b	606	CLA	C1C-NC	-3.03	1.33	1.37
24	C	505	CLA	C1D-ND	3.03	1.41	1.37
24	c	505	CLA	C1D-ND	3.03	1.41	1.37
24	A	405	CLA	C3D-C4D	-3.03	1.37	1.44
24	a	405	CLA	C3D-C4D	-3.03	1.37	1.44
31	c	517	DGD	O5D-C6D	-3.03	1.38	1.43
24	B	607	CLA	CHD-C1D	3.02	1.44	1.38
24	b	609	CLA	CHD-C1D	3.02	1.44	1.38
24	C	514	CLA	C1B-NB	-3.02	1.32	1.35
24	c	514	CLA	C1B-NB	-3.02	1.32	1.35
28	d	407	PL9	C6-C1	-3.02	1.43	1.48
25	A	407	PHO	CAC-C3C	-3.02	1.46	1.52
25	a	407	PHO	CAC-C3C	-3.02	1.46	1.52
31	C	518	DGD	O3G-C3G	-3.02	1.38	1.43
31	c	518	DGD	O3G-C3G	-3.02	1.38	1.43
24	C	511	CLA	C3D-C4D	-3.02	1.37	1.44
24	c	511	CLA	C3D-C4D	-3.02	1.37	1.44
24	b	612	CLA	CHD-C4C	3.01	1.46	1.39
24	B	609	CLA	CHD-C4C	3.01	1.46	1.39
24	D	404	CLA	C1C-NC	-3.00	1.33	1.37
24	d	404	CLA	C1C-NC	-3.00	1.33	1.37
24	A	406	CLA	CHD-C4C	2.99	1.46	1.39
24	a	406	CLA	CHD-C4C	2.99	1.46	1.39
24	B	608	CLA	C3D-C4D	-2.99	1.37	1.44
24	B	614	CLA	C3D-C4D	-2.99	1.37	1.44
24	b	611	CLA	CHD-C4C	2.98	1.46	1.39
27	A	410	SQD	O47-C45	-2.98	1.39	1.46
26	B	619	BCR	C30-C25	-2.98	1.49	1.53
26	b	621	BCR	C30-C25	-2.98	1.49	1.53
24	B	605	CLA	O2A-CGA	2.98	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	607	CLA	O2A-CGA	2.98	1.42	1.33
24	B	612	CLA	C4B-NB	-2.98	1.32	1.35
24	B	614	CLA	C1B-NB	-2.98	1.32	1.35
24	C	508	CLA	CHD-C4C	2.97	1.46	1.39
24	c	508	CLA	CHD-C4C	2.97	1.46	1.39
24	b	616	CLA	C3D-C4D	-2.97	1.37	1.44
34	D	409	LHG	O7-C5	-2.96	1.39	1.46
34	d	409	LHG	O7-C5	-2.96	1.39	1.46
24	B	613	CLA	CHD-C4C	2.96	1.46	1.39
24	b	615	CLA	CHD-C4C	2.96	1.46	1.39
31	C	517	DGD	O1G-C1G	-2.95	1.38	1.45
31	c	517	DGD	O1G-C1G	-2.95	1.38	1.45
27	a	410	SQD	O47-C45	-2.95	1.39	1.46
24	b	605	CLA	CHD-C4C	2.95	1.46	1.39
24	B	603	CLA	CHD-C4C	2.95	1.46	1.39
24	B	608	CLA	C1C-NC	-2.94	1.33	1.37
24	A	405	CLA	C1B-NB	-2.94	1.32	1.35
24	a	405	CLA	C1B-NB	-2.94	1.32	1.35
35	E	103	HEM	CAB-C3B	2.94	1.55	1.47
35	e	103	HEM	CAB-C3B	2.94	1.55	1.47
24	b	614	CLA	C4B-NB	-2.93	1.32	1.35
24	c	510	CLA	C4B-NB	-2.93	1.32	1.35
24	b	605	CLA	OBD-CAD	2.93	1.27	1.22
24	C	508	CLA	C3D-C2D	2.93	1.47	1.39
24	c	508	CLA	C3D-C2D	2.93	1.47	1.39
24	d	404	CLA	C3D-C4D	-2.92	1.37	1.44
24	B	604	CLA	C1D-ND	2.92	1.41	1.37
24	b	606	CLA	C1D-ND	2.92	1.41	1.37
24	D	405	CLA	C1B-NB	-2.92	1.32	1.35
24	d	405	CLA	C1B-NB	-2.92	1.32	1.35
25	A	407	PHO	CMC-C2C	-2.92	1.44	1.51
25	a	407	PHO	CMC-C2C	-2.92	1.44	1.51
24	B	615	CLA	C1C-NC	-2.92	1.33	1.37
24	b	617	CLA	C1C-NC	-2.92	1.33	1.37
24	A	406	CLA	CHD-C1D	2.92	1.44	1.38
24	a	406	CLA	CHD-C1D	2.92	1.44	1.38
24	D	404	CLA	C3D-C4D	-2.92	1.37	1.44
24	C	505	CLA	C1B-NB	-2.91	1.32	1.35
24	c	505	CLA	C1B-NB	-2.91	1.32	1.35
24	B	601	CLA	OBD-CAD	2.91	1.27	1.22
24	b	603	CLA	OBD-CAD	2.91	1.27	1.22
26	C	516	BCR	C1-C6	-2.91	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	516	BCR	C1-C6	-2.91	1.49	1.53
24	b	610	CLA	C1C-NC	-2.91	1.33	1.37
24	B	616	CLA	C3D-C4D	-2.91	1.37	1.44
24	b	618	CLA	C3D-C4D	-2.91	1.37	1.44
24	A	405	CLA	C1C-NC	-2.91	1.33	1.37
24	a	405	CLA	C1C-NC	-2.91	1.33	1.37
28	A	411	PL9	C53-C6	-2.91	1.44	1.50
24	B	606	CLA	OBD-CAD	2.90	1.27	1.22
28	d	407	PL9	C51-C49	-2.90	1.42	1.50
24	b	606	CLA	C3D-C2D	2.90	1.47	1.39
24	b	614	CLA	C3D-C2D	2.90	1.47	1.39
28	D	407	PL9	C51-C49	-2.89	1.42	1.50
24	B	604	CLA	C3D-C2D	2.88	1.47	1.39
31	C	517	DGD	O3E-C3E	-2.88	1.36	1.43
31	c	517	DGD	O3E-C3E	-2.88	1.36	1.43
31	C	518	DGD	C3E-C2E	2.88	1.59	1.52
31	c	518	DGD	C3E-C2E	2.88	1.59	1.52
27	B	620	SQD	O48-C23	2.88	1.41	1.33
27	L	102	SQD	O48-C23	2.88	1.41	1.33
24	C	506	CLA	C1B-NB	-2.87	1.32	1.35
24	c	506	CLA	C1B-NB	-2.87	1.32	1.35
24	C	510	CLA	C4B-NB	-2.87	1.32	1.35
31	C	517	DGD	O2D-C2D	-2.87	1.36	1.43
31	c	517	DGD	O2D-C2D	-2.87	1.36	1.43
24	A	405	CLA	CHD-C4C	2.87	1.45	1.39
24	a	405	CLA	CHD-C4C	2.87	1.45	1.39
24	C	513	CLA	C1D-ND	2.87	1.41	1.37
24	c	513	CLA	C1D-ND	2.87	1.41	1.37
24	B	603	CLA	OBD-CAD	2.87	1.27	1.22
28	a	411	PL9	C53-C6	-2.86	1.44	1.50
31	C	519	DGD	O3D-C3D	-2.86	1.36	1.43
31	c	519	DGD	O3D-C3D	-2.86	1.36	1.43
24	C	507	CLA	C1C-NC	-2.86	1.33	1.37
24	c	507	CLA	C1C-NC	-2.86	1.33	1.37
24	b	605	CLA	C3D-C2D	2.86	1.46	1.39
24	B	615	CLA	C1D-ND	2.86	1.41	1.37
24	b	617	CLA	C1D-ND	2.86	1.41	1.37
24	C	512	CLA	C1C-NC	-2.86	1.33	1.37
24	c	512	CLA	C1C-NC	-2.86	1.33	1.37
24	B	612	CLA	C3D-C2D	2.85	1.46	1.39
27	A	412	SQD	O48-C23	2.85	1.41	1.33
27	a	412	SQD	O48-C23	2.85	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	C1C-NC	-2.85	1.33	1.37
24	b	618	CLA	C1C-NC	-2.85	1.33	1.37
24	C	514	CLA	OBD-CAD	2.85	1.27	1.22
24	c	514	CLA	OBD-CAD	2.85	1.27	1.22
24	b	614	CLA	C3D-C4D	-2.85	1.37	1.44
24	B	606	CLA	C1C-NC	-2.84	1.33	1.37
24	A	405	CLA	O2D-CED	-2.84	1.38	1.45
24	a	405	CLA	O2D-CED	-2.84	1.38	1.45
24	B	612	CLA	C3D-C4D	-2.84	1.37	1.44
24	B	603	CLA	C3D-C2D	2.83	1.46	1.39
24	b	608	CLA	OBD-CAD	2.83	1.27	1.22
27	A	410	SQD	O2-C2	-2.83	1.36	1.43
27	a	410	SQD	O2-C2	-2.83	1.36	1.43
27	a	412	SQD	O47-C7	2.82	1.42	1.34
27	A	412	SQD	O47-C7	2.81	1.42	1.34
24	B	602	CLA	C3D-C2D	2.81	1.46	1.39
24	b	604	CLA	C3D-C2D	2.81	1.46	1.39
24	b	608	CLA	C1C-NC	-2.80	1.33	1.37
25	d	402	PHO	CAC-C3C	-2.80	1.47	1.52
24	B	604	CLA	C3D-C4D	-2.80	1.37	1.44
24	c	509	CLA	C1D-ND	2.80	1.41	1.37
24	b	611	CLA	OBD-CAD	2.80	1.27	1.22
24	B	612	CLA	CHD-C4C	2.80	1.45	1.39
24	b	614	CLA	CHD-C4C	2.80	1.45	1.39
31	C	519	DGD	O3G-C3G	-2.79	1.38	1.43
31	c	519	DGD	O3G-C3G	-2.79	1.38	1.43
25	D	402	PHO	CAC-C3C	-2.79	1.47	1.52
24	B	611	CLA	CHD-C4C	2.78	1.45	1.39
24	b	613	CLA	CHD-C4C	2.78	1.45	1.39
38	X	101	RRX	C10-C9	-2.78	1.32	1.35
38	x	101	RRX	C10-C9	-2.78	1.32	1.35
24	B	609	CLA	OBD-CAD	2.78	1.27	1.22
24	B	613	CLA	C1D-ND	2.77	1.41	1.37
24	b	615	CLA	C1D-ND	2.77	1.41	1.37
24	b	606	CLA	C3D-C4D	-2.77	1.37	1.44
24	B	607	CLA	C4B-NB	-2.77	1.32	1.35
24	b	609	CLA	C4B-NB	-2.77	1.32	1.35
26	D	406	BCR	C30-C25	-2.77	1.50	1.53
26	d	406	BCR	C30-C25	-2.77	1.50	1.53
26	B	619	BCR	C1-C6	-2.77	1.50	1.53
26	b	621	BCR	C1-C6	-2.77	1.50	1.53
27	F	101	SQD	O47-C7	2.76	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	f	101	SQD	O47-C7	2.76	1.42	1.34
28	a	411	PL9	C16-C14	-2.76	1.45	1.51
28	A	411	PL9	C16-C14	-2.76	1.45	1.51
24	C	508	CLA	C1C-NC	-2.76	1.33	1.37
24	c	508	CLA	C1C-NC	-2.76	1.33	1.37
24	b	613	CLA	C1C-NC	-2.76	1.33	1.37
24	B	611	CLA	C1C-NC	-2.75	1.33	1.37
24	C	509	CLA	C1D-ND	2.74	1.41	1.37
24	C	502	CLA	C3D-C4D	-2.73	1.38	1.44
32	M	101	LMT	O3'-C3'	-2.73	1.36	1.43
32	m	102	LMT	O3'-C3'	-2.73	1.36	1.43
25	D	402	PHO	CMD-C2D	-2.72	1.45	1.51
28	d	407	PL9	C41-C39	-2.72	1.45	1.51
25	d	402	PHO	CMD-C2D	-2.72	1.45	1.51
24	C	504	CLA	C3D-C2D	2.71	1.46	1.39
24	c	504	CLA	C3D-C2D	2.71	1.46	1.39
32	M	101	LMT	O3B-C3B	-2.71	1.36	1.43
32	m	102	LMT	O3B-C3B	-2.71	1.36	1.43
24	A	405	CLA	C4B-NB	-2.71	1.32	1.35
24	a	405	CLA	C4B-NB	-2.71	1.32	1.35
28	D	407	PL9	C41-C39	-2.70	1.45	1.51
24	C	504	CLA	C1B-NB	-2.70	1.32	1.35
24	c	504	CLA	C1B-NB	-2.70	1.32	1.35
24	C	509	CLA	CHD-C4C	2.70	1.45	1.39
24	c	509	CLA	CHD-C4C	2.70	1.45	1.39
24	C	502	CLA	OBD-CAD	2.69	1.27	1.22
24	B	607	CLA	C3D-C4D	-2.69	1.38	1.44
24	b	609	CLA	C3D-C4D	-2.69	1.38	1.44
31	h	101	DGD	O5D-C6D	-2.69	1.38	1.43
24	d	404	CLA	CHD-C1D	2.69	1.43	1.38
24	D	404	CLA	CHD-C1D	2.69	1.43	1.38
24	c	502	CLA	C3D-C4D	-2.68	1.38	1.44
31	C	519	DGD	O2D-C2D	-2.68	1.36	1.43
31	c	519	DGD	O2D-C2D	-2.68	1.36	1.43
24	C	503	CLA	OBD-CAD	2.68	1.27	1.22
24	c	503	CLA	OBD-CAD	2.68	1.27	1.22
24	C	513	CLA	OBD-CAD	2.67	1.27	1.22
24	c	513	CLA	OBD-CAD	2.67	1.27	1.22
24	B	614	CLA	C3D-C2D	2.65	1.46	1.39
31	H	101	DGD	O5D-C6D	-2.65	1.38	1.43
32	z	101	LMT	O3'-C3'	-2.65	1.36	1.43
32	Z	101	LMT	O3'-C3'	-2.64	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	CMD-C2D	-2.64	1.45	1.50
24	b	605	CLA	CMD-C2D	-2.64	1.45	1.50
26	B	618	BCR	C30-C25	-2.64	1.50	1.53
26	b	620	BCR	C30-C25	-2.64	1.50	1.53
24	c	502	CLA	OBD-CAD	2.64	1.27	1.22
24	b	616	CLA	C3D-C2D	2.64	1.46	1.39
31	C	518	DGD	O3E-C3E	-2.64	1.36	1.43
31	c	518	DGD	O3E-C3E	-2.64	1.36	1.43
24	B	602	CLA	C3D-C4D	-2.63	1.38	1.44
24	b	604	CLA	C3D-C4D	-2.63	1.38	1.44
26	C	522	BCR	C1-C6	-2.63	1.50	1.53
26	c	522	BCR	C1-C6	-2.63	1.50	1.53
24	A	405	CLA	CHD-C1D	2.63	1.43	1.38
24	a	405	CLA	CHD-C1D	2.63	1.43	1.38
26	D	406	BCR	C33-C5	-2.63	1.46	1.50
26	d	406	BCR	C33-C5	-2.63	1.46	1.50
24	B	609	CLA	C4D-CHA	2.63	1.47	1.38
24	b	611	CLA	C4D-CHA	2.63	1.47	1.38
24	C	508	CLA	OBD-CAD	2.61	1.27	1.22
24	c	508	CLA	OBD-CAD	2.61	1.27	1.22
30	d	411	LMG	O4-C4	-2.61	1.36	1.43
24	D	405	CLA	C3D-C4D	-2.61	1.38	1.44
24	d	405	CLA	C3D-C4D	-2.61	1.38	1.44
24	C	511	CLA	C1B-CHB	2.60	1.48	1.41
24	c	511	CLA	C1B-CHB	2.60	1.48	1.41
28	A	411	PL9	C36-C34	-2.60	1.45	1.51
28	a	411	PL9	C36-C34	-2.60	1.45	1.51
27	A	410	SQD	O3-C3	-2.60	1.36	1.43
27	a	410	SQD	O3-C3	-2.60	1.36	1.43
32	C	521	LMT	O4'-C4B	-2.60	1.36	1.43
32	c	521	LMT	O4'-C4B	-2.60	1.36	1.43
24	B	601	CLA	C3D-C4D	-2.60	1.38	1.44
24	b	603	CLA	C3D-C4D	-2.60	1.38	1.44
24	B	604	CLA	C1C-C2C	2.60	1.49	1.44
24	b	606	CLA	C1C-C2C	2.60	1.49	1.44
24	B	601	CLA	C4B-NB	-2.60	1.32	1.35
24	b	603	CLA	C4B-NB	-2.60	1.32	1.35
30	c	501	LMG	O7-C8	-2.59	1.40	1.46
30	D	411	LMG	O4-C4	-2.59	1.36	1.43
24	C	504	CLA	C1C-NC	-2.59	1.33	1.37
24	c	504	CLA	C1C-NC	-2.59	1.33	1.37
24	C	508	CLA	C3D-C4D	-2.59	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	508	CLA	C3D-C4D	-2.59	1.38	1.44
24	C	506	CLA	C3D-C2D	2.59	1.46	1.39
24	c	506	CLA	C3D-C2D	2.59	1.46	1.39
27	A	412	SQD	O2-C2	-2.59	1.36	1.43
27	a	412	SQD	O2-C2	-2.59	1.36	1.43
32	J	102	LMT	O3'-C3'	-2.58	1.36	1.43
27	F	101	SQD	O3-C3	-2.58	1.36	1.43
27	f	101	SQD	O3-C3	-2.58	1.36	1.43
32	j	102	LMT	O3'-C3'	-2.58	1.36	1.43
30	C	523	LMG	O2-C2	-2.58	1.36	1.43
30	c	523	LMG	O2-C2	-2.58	1.36	1.43
24	D	401	CLA	C4D-CHA	2.58	1.47	1.38
24	d	401	CLA	C4D-CHA	2.58	1.47	1.38
26	J	104	BCR	C33-C5	-2.58	1.46	1.50
24	C	511	CLA	OBD-CAD	2.58	1.26	1.22
30	C	501	LMG	O7-C8	-2.57	1.40	1.46
32	C	521	LMT	O2'-C2'	-2.57	1.36	1.43
32	c	521	LMT	O2'-C2'	-2.57	1.36	1.43
26	j	104	BCR	C33-C5	-2.57	1.46	1.50
24	B	604	CLA	C4B-NB	-2.57	1.32	1.35
24	b	606	CLA	C4B-NB	-2.57	1.32	1.35
30	C	523	LMG	O7-C8	-2.56	1.40	1.46
30	c	523	LMG	O7-C8	-2.56	1.40	1.46
24	D	404	CLA	C3D-C2D	2.56	1.46	1.39
24	d	404	CLA	C3D-C2D	2.56	1.46	1.39
26	C	515	BCR	C30-C25	-2.56	1.50	1.53
26	c	515	BCR	C30-C25	-2.56	1.50	1.53
24	a	406	CLA	C1C-C2C	2.56	1.49	1.44
24	D	404	CLA	O2D-CED	-2.55	1.39	1.45
24	d	404	CLA	O2D-CED	-2.55	1.39	1.45
24	B	605	CLA	C3D-C4D	-2.55	1.38	1.44
24	b	607	CLA	C3D-C4D	-2.55	1.38	1.44
27	F	101	SQD	O4-C4	-2.55	1.37	1.43
27	f	101	SQD	O4-C4	-2.55	1.37	1.43
24	C	506	CLA	CMD-C2D	-2.55	1.45	1.50
24	c	506	CLA	CMD-C2D	-2.55	1.45	1.50
24	B	604	CLA	CMB-C2B	-2.55	1.46	1.51
24	b	606	CLA	CMB-C2B	-2.55	1.46	1.51
27	A	410	SQD	O48-C23	2.55	1.40	1.33
27	a	410	SQD	O48-C23	2.55	1.40	1.33
24	A	406	CLA	C1C-C2C	2.54	1.49	1.44
24	B	606	CLA	C1C-C2C	2.54	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	511	CLA	OBD-CAD	2.54	1.26	1.22
26	B	618	BCR	C1-C6	-2.54	1.50	1.53
26	b	620	BCR	C1-C6	-2.54	1.50	1.53
24	C	505	CLA	C1C-NC	-2.53	1.34	1.37
24	c	505	CLA	C1C-NC	-2.53	1.34	1.37
26	T	101	BCR	C30-C25	-2.53	1.50	1.53
26	t	102	BCR	C30-C25	-2.53	1.50	1.53
24	b	607	CLA	C1C-NC	-2.53	1.34	1.37
24	C	506	CLA	C3D-C4D	-2.53	1.38	1.44
24	c	506	CLA	C3D-C4D	-2.53	1.38	1.44
31	C	518	DGD	O5D-C6D	-2.53	1.39	1.43
31	c	518	DGD	O5D-C6D	-2.53	1.39	1.43
24	C	513	CLA	C4D-CHA	2.53	1.47	1.38
24	c	513	CLA	C4D-CHA	2.53	1.47	1.38
24	B	602	CLA	OBD-CAD	2.52	1.26	1.22
24	b	604	CLA	OBD-CAD	2.52	1.26	1.22
24	C	511	CLA	C4D-CHA	2.51	1.47	1.38
24	c	511	CLA	C4D-CHA	2.51	1.47	1.38
24	B	607	CLA	C4D-CHA	2.51	1.47	1.38
24	B	606	CLA	C3D-C4D	-2.51	1.38	1.44
24	b	608	CLA	C3D-C4D	-2.51	1.38	1.44
24	B	611	CLA	C3D-C4D	-2.51	1.38	1.44
24	b	613	CLA	C3D-C4D	-2.51	1.38	1.44
24	C	502	CLA	C4B-NB	-2.51	1.33	1.35
24	b	606	CLA	OBD-CAD	2.50	1.26	1.22
24	B	608	CLA	C1D-ND	2.50	1.40	1.37
24	C	514	CLA	C3D-C4D	-2.50	1.38	1.44
24	c	514	CLA	C3D-C4D	-2.50	1.38	1.44
28	D	407	PL9	C52-C5	-2.50	1.45	1.50
24	B	615	CLA	C3D-C4D	-2.50	1.38	1.44
24	b	617	CLA	C3D-C4D	-2.50	1.38	1.44
24	b	609	CLA	C4D-CHA	2.49	1.47	1.38
24	B	605	CLA	C1C-NC	-2.49	1.34	1.37
26	C	515	BCR	C1-C6	-2.49	1.50	1.53
26	c	515	BCR	C1-C6	-2.49	1.50	1.53
24	A	406	CLA	C3D-C2D	2.49	1.45	1.39
24	a	406	CLA	C3D-C2D	2.49	1.45	1.39
24	b	608	CLA	C1C-C2C	2.49	1.49	1.44
24	B	615	CLA	C4D-CHA	2.48	1.47	1.38
24	b	617	CLA	C4D-CHA	2.48	1.47	1.38
28	d	407	PL9	C52-C5	-2.47	1.45	1.50
24	B	609	CLA	C3D-C4D	-2.47	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	M	101	LMT	O2B-C2B	-2.47	1.37	1.43
32	m	102	LMT	O2B-C2B	-2.47	1.37	1.43
24	b	611	CLA	C3D-C4D	-2.47	1.38	1.44
24	B	604	CLA	OBD-CAD	2.47	1.26	1.22
32	Z	101	LMT	O4'-C4B	-2.46	1.37	1.43
32	z	101	LMT	O4'-C4B	-2.46	1.37	1.43
27	B	620	SQD	O47-C7	2.46	1.41	1.34
27	L	102	SQD	O47-C7	2.46	1.41	1.34
24	b	610	CLA	C1D-ND	2.46	1.40	1.37
31	C	517	DGD	C1D-C2D	2.46	1.59	1.52
31	c	517	DGD	C1D-C2D	2.46	1.59	1.52
24	A	405	CLA	C3D-C2D	2.46	1.45	1.39
24	a	405	CLA	C3D-C2D	2.46	1.45	1.39
24	B	610	CLA	C4B-NB	-2.46	1.33	1.35
32	Z	101	LMT	O3B-C3B	-2.45	1.37	1.43
32	z	101	LMT	O3B-C3B	-2.45	1.37	1.43
33	D	403	BCT	O2-C	-2.45	1.12	1.33
33	d	403	BCT	O2-C	-2.45	1.12	1.33
24	C	503	CLA	C1B-CHB	2.45	1.47	1.41
24	c	503	CLA	C1B-CHB	2.45	1.47	1.41
27	B	620	SQD	O4-C4	-2.44	1.37	1.43
30	D	411	LMG	O7-C8	-2.44	1.40	1.46
27	L	102	SQD	O4-C4	-2.44	1.37	1.43
24	C	504	CLA	O2D-CED	-2.43	1.39	1.45
24	c	504	CLA	O2D-CED	-2.43	1.39	1.45
30	D	411	LMG	O3-C3	-2.43	1.37	1.43
30	d	411	LMG	O3-C3	-2.43	1.37	1.43
24	c	502	CLA	C4B-NB	-2.43	1.33	1.35
24	C	506	CLA	C1C-NC	-2.43	1.34	1.37
24	c	506	CLA	C1C-NC	-2.43	1.34	1.37
24	C	505	CLA	C4B-NB	-2.43	1.33	1.35
24	c	505	CLA	C4B-NB	-2.43	1.33	1.35
24	C	510	CLA	C4D-CHA	2.43	1.47	1.38
24	c	510	CLA	C4D-CHA	2.43	1.47	1.38
24	B	614	CLA	CHD-C1D	2.42	1.43	1.38
24	b	616	CLA	CHD-C1D	2.42	1.43	1.38
24	D	404	CLA	C1B-CHB	2.42	1.47	1.41
24	d	404	CLA	C1B-CHB	2.42	1.47	1.41
26	B	618	BCR	C38-C26	-2.42	1.47	1.50
26	b	620	BCR	C38-C26	-2.42	1.47	1.50
24	C	509	CLA	C1B-CHB	2.42	1.47	1.41
24	c	509	CLA	C1B-CHB	2.42	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	405	CLA	C4B-NB	-2.42	1.33	1.35
24	d	405	CLA	C4B-NB	-2.42	1.33	1.35
24	b	612	CLA	C3D-C4D	-2.41	1.38	1.44
24	B	610	CLA	OBD-CAD	2.41	1.26	1.22
30	c	520	LMG	C7-C8	2.41	1.58	1.50
24	C	514	CLA	C4B-NB	-2.40	1.33	1.35
30	d	411	LMG	O7-C8	-2.40	1.40	1.46
24	b	608	CLA	C4D-CHA	2.40	1.46	1.38
24	B	601	CLA	C4D-CHA	2.40	1.46	1.38
24	b	603	CLA	C4D-CHA	2.40	1.46	1.38
24	B	605	CLA	C4B-NB	-2.40	1.33	1.35
24	b	607	CLA	C4B-NB	-2.40	1.33	1.35
24	C	505	CLA	C4D-CHA	2.40	1.46	1.38
24	c	505	CLA	C4D-CHA	2.40	1.46	1.38
24	B	608	CLA	C4D-CHA	2.39	1.46	1.38
24	B	606	CLA	C4D-CHA	2.39	1.46	1.38
28	d	407	PL9	C53-C6	-2.39	1.45	1.50
25	A	407	PHO	C1C-NC	-2.39	1.31	1.38
25	a	407	PHO	C1C-NC	-2.39	1.31	1.38
34	e	101	LHG	O8-C6	-2.39	1.39	1.45
24	B	616	CLA	C4D-CHA	2.39	1.46	1.38
24	b	618	CLA	C4D-CHA	2.39	1.46	1.38
30	C	501	LMG	C4-C3	2.39	1.58	1.52
30	c	501	LMG	C4-C3	2.39	1.58	1.52
24	B	610	CLA	C3D-C4D	-2.38	1.38	1.44
24	B	607	CLA	C1D-ND	2.38	1.40	1.37
24	b	609	CLA	C1D-ND	2.38	1.40	1.37
35	E	103	HEM	C4D-ND	-2.38	1.36	1.40
35	e	103	HEM	C4D-ND	-2.38	1.36	1.40
24	b	612	CLA	OBD-CAD	2.38	1.26	1.22
30	C	520	LMG	C7-C8	2.38	1.58	1.50
24	a	408	CLA	C4B-NB	-2.38	1.33	1.35
24	b	610	CLA	C4D-CHA	2.38	1.46	1.38
25	A	407	PHO	CMD-C2D	-2.38	1.45	1.51
25	a	407	PHO	CMD-C2D	-2.38	1.45	1.51
24	D	405	CLA	C1C-NC	-2.38	1.34	1.37
24	d	405	CLA	C1C-NC	-2.38	1.34	1.37
24	C	504	CLA	C4B-NB	-2.37	1.33	1.35
24	c	504	CLA	C4B-NB	-2.37	1.33	1.35
27	a	410	SQD	O4-C4	-2.37	1.37	1.43
24	c	514	CLA	C4B-NB	-2.37	1.33	1.35
28	D	407	PL9	C53-C6	-2.37	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	408	CLA	C4B-NB	-2.37	1.33	1.35
30	b	622	LMG	C9-C8	2.36	1.58	1.50
24	A	406	CLA	C1C-NC	-2.36	1.34	1.37
24	C	509	CLA	C3D-C4D	-2.36	1.38	1.44
24	c	509	CLA	C3D-C4D	-2.36	1.38	1.44
30	B	621	LMG	C9-C8	2.36	1.57	1.50
24	B	613	CLA	C1C-NC	-2.36	1.34	1.37
24	b	615	CLA	C1C-NC	-2.36	1.34	1.37
24	a	406	CLA	C1C-NC	-2.36	1.34	1.37
24	C	511	CLA	C1C-NC	-2.35	1.34	1.37
24	c	511	CLA	C1C-NC	-2.35	1.34	1.37
24	B	605	CLA	C4D-CHA	2.35	1.46	1.38
24	b	607	CLA	C4D-CHA	2.35	1.46	1.38
34	E	101	LHG	O8-C6	-2.35	1.39	1.45
24	A	406	CLA	OBD-CAD	2.35	1.26	1.22
24	a	406	CLA	OBD-CAD	2.35	1.26	1.22
28	A	411	PL9	C12-C13	-2.35	1.42	1.50
28	a	411	PL9	C12-C13	-2.35	1.42	1.50
27	B	620	SQD	O3-C3	-2.34	1.37	1.43
27	L	102	SQD	O3-C3	-2.34	1.37	1.43
24	C	513	CLA	C1C-C2C	2.34	1.49	1.44
24	c	513	CLA	C1C-C2C	2.34	1.49	1.44
24	C	514	CLA	C4D-CHA	2.34	1.46	1.38
24	c	514	CLA	C4D-CHA	2.34	1.46	1.38
27	A	410	SQD	O4-C4	-2.34	1.37	1.43
26	A	409	BCR	C1-C6	-2.34	1.50	1.53
26	a	409	BCR	C1-C6	-2.34	1.50	1.53
24	B	607	CLA	C4C-C3C	2.34	1.49	1.45
24	b	609	CLA	C4C-C3C	2.34	1.49	1.45
24	D	401	CLA	C3D-C4D	-2.33	1.38	1.44
24	d	401	CLA	C3D-C4D	-2.33	1.38	1.44
24	b	612	CLA	C4B-NB	-2.33	1.33	1.35
24	C	514	CLA	C1C-NC	-2.33	1.34	1.37
24	c	514	CLA	C1C-NC	-2.33	1.34	1.37
24	C	503	CLA	C4D-CHA	2.33	1.46	1.38
24	c	503	CLA	C4D-CHA	2.33	1.46	1.38
24	D	404	CLA	C4C-C3C	2.32	1.49	1.45
24	C	513	CLA	C4B-CHC	2.32	1.47	1.41
24	c	513	CLA	C4B-CHC	2.32	1.47	1.41
24	D	405	CLA	C1C-C2C	2.32	1.49	1.44
24	d	405	CLA	C1C-C2C	2.32	1.49	1.44
24	B	605	CLA	C1C-C2C	2.32	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	607	CLA	C1C-C2C	2.32	1.49	1.44
24	D	405	CLA	C1B-CHB	2.31	1.47	1.41
24	d	405	CLA	C1B-CHB	2.31	1.47	1.41
24	C	504	CLA	OBD-CAD	2.31	1.26	1.22
24	c	504	CLA	OBD-CAD	2.31	1.26	1.22
31	C	518	DGD	O3G-C1D	-2.31	1.36	1.40
31	c	518	DGD	O3G-C1D	-2.31	1.36	1.40
30	C	520	LMG	O2-C2	-2.30	1.37	1.43
30	c	520	LMG	O2-C2	-2.30	1.37	1.43
24	C	510	CLA	C1C-NC	-2.30	1.34	1.37
24	c	510	CLA	C1C-NC	-2.30	1.34	1.37
24	C	506	CLA	C1C-C2C	2.29	1.49	1.44
24	c	506	CLA	C1C-C2C	2.29	1.49	1.44
24	C	502	CLA	C4D-CHA	2.29	1.46	1.38
24	c	502	CLA	C4D-CHA	2.29	1.46	1.38
24	C	506	CLA	C1B-CHB	2.29	1.47	1.41
24	c	506	CLA	C1B-CHB	2.29	1.47	1.41
32	Z	101	LMT	O1'-C1'	-2.29	1.36	1.40
32	z	101	LMT	O1'-C1'	-2.29	1.36	1.40
30	C	520	LMG	C4-C5	2.29	1.57	1.53
30	c	520	LMG	C4-C5	2.29	1.57	1.53
24	B	602	CLA	C4D-CHA	2.29	1.46	1.38
24	b	604	CLA	C4D-CHA	2.29	1.46	1.38
24	d	404	CLA	C4C-C3C	2.29	1.49	1.45
24	B	613	CLA	C4D-CHA	2.28	1.46	1.38
24	b	615	CLA	C4D-CHA	2.28	1.46	1.38
24	B	610	CLA	C1B-CHB	2.28	1.47	1.41
37	V	201	HEC	CAD-C3D	2.28	1.55	1.52
37	v	201	HEC	CAD-C3D	2.28	1.55	1.52
24	B	610	CLA	O2D-CED	-2.28	1.40	1.45
24	C	513	CLA	C1B-CHB	2.27	1.47	1.41
24	c	513	CLA	C1B-CHB	2.27	1.47	1.41
24	d	404	CLA	C1D-ND	2.27	1.40	1.37
24	B	614	CLA	C4D-CHA	2.27	1.46	1.38
24	b	616	CLA	C4D-CHA	2.27	1.46	1.38
30	C	501	LMG	O1-C1	-2.27	1.36	1.40
30	c	501	LMG	O1-C1	-2.27	1.36	1.40
24	b	611	CLA	CMB-C2B	-2.26	1.46	1.51
26	J	104	BCR	C30-C25	-2.26	1.50	1.53
26	j	104	BCR	C30-C25	-2.26	1.50	1.53
24	D	404	CLA	C1C-C2C	2.26	1.48	1.44
24	d	404	CLA	C1C-C2C	2.26	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	412	SQD	O3-C3	-2.26	1.37	1.43
27	a	412	SQD	O3-C3	-2.26	1.37	1.43
31	H	101	DGD	O2E-C2E	-2.26	1.37	1.43
31	h	101	DGD	O2E-C2E	-2.26	1.37	1.43
24	b	612	CLA	C1B-CHB	2.26	1.47	1.41
24	D	404	CLA	C1D-ND	2.26	1.40	1.37
24	D	401	CLA	C4C-C3C	2.25	1.48	1.45
24	d	401	CLA	C4C-C3C	2.25	1.48	1.45
30	D	411	LMG	C3-C2	2.25	1.58	1.52
30	d	411	LMG	C3-C2	2.25	1.58	1.52
24	C	509	CLA	OBD-CAD	2.25	1.26	1.22
24	c	509	CLA	OBD-CAD	2.25	1.26	1.22
24	D	405	CLA	C4D-CHA	2.25	1.46	1.38
24	d	405	CLA	C4D-CHA	2.25	1.46	1.38
24	C	513	CLA	C3D-C4D	-2.25	1.39	1.44
24	c	513	CLA	C3D-C4D	-2.25	1.39	1.44
24	b	612	CLA	O2D-CED	-2.25	1.40	1.45
28	A	411	PL9	C10-C9	-2.24	1.44	1.50
24	C	504	CLA	C1B-CHB	2.24	1.47	1.41
24	c	504	CLA	C1B-CHB	2.24	1.47	1.41
24	B	614	CLA	C1D-ND	2.24	1.40	1.37
24	b	616	CLA	C1D-ND	2.24	1.40	1.37
27	f	101	SQD	O2-C2	-2.24	1.37	1.43
30	B	621	LMG	O7-C8	-2.24	1.41	1.46
31	H	101	DGD	C4D-C3D	2.24	1.58	1.52
31	h	101	DGD	C4D-C3D	2.24	1.58	1.52
24	B	602	CLA	C4B-NB	-2.24	1.33	1.35
24	C	512	CLA	C3D-C4D	-2.24	1.39	1.44
24	c	512	CLA	C3D-C4D	-2.24	1.39	1.44
24	C	512	CLA	C4D-CHA	2.23	1.46	1.38
24	c	512	CLA	C4D-CHA	2.23	1.46	1.38
24	C	504	CLA	C3D-C4D	-2.23	1.39	1.44
24	c	504	CLA	C3D-C4D	-2.23	1.39	1.44
27	B	620	SQD	O2-C2	-2.23	1.37	1.43
27	L	102	SQD	O2-C2	-2.23	1.37	1.43
34	D	410	LHG	C4-C5	2.23	1.57	1.50
34	d	410	LHG	C4-C5	2.23	1.57	1.50
31	C	519	DGD	O4E-C4E	-2.23	1.37	1.43
24	B	604	CLA	MG-NA	2.22	2.11	2.06
24	b	606	CLA	MG-NA	2.22	2.11	2.06
24	B	604	CLA	C1B-CHB	2.22	1.47	1.41
24	b	606	CLA	C1B-CHB	2.22	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	518	DGD	O2E-C2E	-2.22	1.37	1.43
31	c	518	DGD	O2E-C2E	-2.22	1.37	1.43
24	B	604	CLA	C4C-C3C	2.22	1.48	1.45
24	b	606	CLA	C4C-C3C	2.22	1.48	1.45
24	B	608	CLA	OBD-CAD	2.22	1.26	1.22
28	a	411	PL9	C10-C9	-2.21	1.45	1.50
27	F	101	SQD	O2-C2	-2.21	1.37	1.43
31	c	519	DGD	O4E-C4E	-2.21	1.37	1.43
24	C	507	CLA	C4D-CHA	2.21	1.46	1.38
24	c	507	CLA	C4D-CHA	2.21	1.46	1.38
30	b	622	LMG	O7-C8	-2.21	1.41	1.46
31	H	101	DGD	O2G-C2G	-2.21	1.41	1.46
31	h	101	DGD	O2G-C2G	-2.21	1.41	1.46
24	B	601	CLA	C4B-CHC	2.21	1.47	1.41
24	b	603	CLA	C4B-CHC	2.21	1.47	1.41
25	A	407	PHO	CBD-CGD	-2.20	1.49	1.52
25	a	407	PHO	CBD-CGD	-2.20	1.49	1.52
24	B	602	CLA	C1C-C2C	2.20	1.48	1.44
24	b	604	CLA	C1C-C2C	2.20	1.48	1.44
24	b	610	CLA	OBD-CAD	2.20	1.26	1.22
24	A	406	CLA	C4D-CHA	2.20	1.46	1.38
24	a	406	CLA	C4D-CHA	2.20	1.46	1.38
24	B	603	CLA	C1B-CHB	2.20	1.47	1.41
24	b	605	CLA	C1B-CHB	2.20	1.47	1.41
24	B	613	CLA	C1B-CHB	2.18	1.47	1.41
24	B	601	CLA	C1C-C2C	2.18	1.48	1.44
24	b	604	CLA	C4B-NB	-2.17	1.33	1.35
24	C	510	CLA	C1C-C2C	2.17	1.48	1.44
24	c	510	CLA	C1C-C2C	2.17	1.48	1.44
26	B	617	BCR	C33-C5	-2.17	1.47	1.50
26	b	619	BCR	C33-C5	-2.17	1.47	1.50
24	c	514	CLA	C4C-C3C	2.17	1.48	1.45
30	C	501	LMG	O4-C4	-2.16	1.37	1.43
24	B	607	CLA	OBD-CAD	2.16	1.26	1.22
24	b	609	CLA	OBD-CAD	2.16	1.26	1.22
24	B	614	CLA	C1C-C2C	2.16	1.48	1.44
24	b	616	CLA	C1C-C2C	2.16	1.48	1.44
24	B	604	CLA	C4D-CHA	2.16	1.46	1.38
24	b	606	CLA	C4D-CHA	2.16	1.46	1.38
24	C	512	CLA	C1B-CHB	2.16	1.47	1.41
24	c	512	CLA	C1B-CHB	2.16	1.47	1.41
24	b	615	CLA	C1B-CHB	2.15	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	501	LMG	O4-C4	-2.15	1.37	1.43
24	C	506	CLA	C4B-CHC	2.15	1.47	1.41
24	c	506	CLA	C4B-CHC	2.15	1.47	1.41
30	D	411	LMG	C7-C8	2.15	1.57	1.50
24	B	601	CLA	C4C-C3C	2.15	1.48	1.45
24	b	603	CLA	C4C-C3C	2.15	1.48	1.45
30	d	411	LMG	C7-C8	2.15	1.57	1.50
24	b	603	CLA	C1C-C2C	2.14	1.48	1.44
24	B	613	CLA	C1C-C2C	2.13	1.48	1.44
24	c	509	CLA	C4D-CHA	2.13	1.46	1.38
38	X	101	RRX	C24-C25	2.13	1.52	1.45
38	x	101	RRX	C24-C25	2.13	1.52	1.45
24	C	514	CLA	C1C-C2C	2.13	1.48	1.44
24	a	408	CLA	C4D-CHA	2.13	1.46	1.38
24	A	408	CLA	C4D-CHA	2.12	1.46	1.38
24	B	610	CLA	C4D-CHA	2.12	1.46	1.38
24	C	502	CLA	C1C-NC	-2.12	1.34	1.37
24	c	502	CLA	C1C-NC	-2.12	1.34	1.37
24	C	507	CLA	C1B-CHB	2.12	1.46	1.41
24	c	507	CLA	C1B-CHB	2.12	1.46	1.41
24	B	612	CLA	C1C-C2C	2.12	1.48	1.44
24	b	614	CLA	C1C-C2C	2.12	1.48	1.44
24	C	506	CLA	OBD-CAD	2.12	1.26	1.22
24	D	405	CLA	OBD-CAD	2.12	1.26	1.22
24	c	506	CLA	OBD-CAD	2.12	1.26	1.22
24	d	405	CLA	OBD-CAD	2.12	1.26	1.22
24	b	612	CLA	C4D-CHA	2.12	1.45	1.38
32	C	521	LMT	O1'-C1'	-2.11	1.36	1.40
32	c	521	LMT	O1'-C1'	-2.11	1.36	1.40
24	b	608	CLA	C4C-C3C	2.11	1.48	1.45
24	a	408	CLA	C3D-C4D	-2.11	1.39	1.44
24	C	509	CLA	C4D-CHA	2.11	1.45	1.38
27	A	412	SQD	O4-C4	-2.11	1.38	1.43
24	b	604	CLA	C1B-CHB	2.11	1.46	1.41
30	C	520	LMG	O7-C8	-2.11	1.41	1.46
30	c	520	LMG	O7-C8	-2.11	1.41	1.46
27	a	410	SQD	O5-C5	-2.11	1.39	1.44
24	A	408	CLA	C3D-C4D	-2.11	1.39	1.44
24	D	401	CLA	OBD-CAD	2.10	1.26	1.22
24	d	401	CLA	OBD-CAD	2.10	1.26	1.22
24	C	510	CLA	C1B-CHB	2.10	1.46	1.41
24	c	510	CLA	C1B-CHB	2.10	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	406	CLA	MG-ND	-2.10	2.01	2.05
24	a	406	CLA	MG-ND	-2.10	2.01	2.05
24	B	603	CLA	C4C-C3C	2.10	1.48	1.45
24	b	605	CLA	C4C-C3C	2.10	1.48	1.45
24	C	514	CLA	C4B-CHC	2.10	1.46	1.41
24	c	514	CLA	C4B-CHC	2.10	1.46	1.41
24	C	508	CLA	C4D-CHA	2.10	1.45	1.38
24	c	508	CLA	C4D-CHA	2.10	1.45	1.38
24	B	603	CLA	C4B-NB	-2.10	1.33	1.35
24	b	605	CLA	C4B-NB	-2.10	1.33	1.35
32	M	101	LMT	O2'-C2'	-2.10	1.38	1.43
24	B	605	CLA	C4B-CHC	2.10	1.46	1.41
24	b	607	CLA	C4B-CHC	2.10	1.46	1.41
24	C	514	CLA	C4C-C3C	2.10	1.48	1.45
24	B	609	CLA	CMB-C2B	-2.10	1.47	1.51
24	C	506	CLA	C4C-C3C	2.09	1.48	1.45
24	c	506	CLA	C4C-C3C	2.09	1.48	1.45
31	C	519	DGD	O2G-C2G	-2.09	1.41	1.46
31	c	519	DGD	O2G-C2G	-2.09	1.41	1.46
24	d	405	CLA	C4C-C3C	2.09	1.48	1.45
24	b	615	CLA	C1C-C2C	2.09	1.48	1.44
24	C	508	CLA	C1C-C2C	2.09	1.48	1.44
24	c	508	CLA	C1C-C2C	2.09	1.48	1.44
24	a	405	CLA	C1C-C2C	2.09	1.48	1.44
24	A	405	CLA	C1C-C2C	2.09	1.48	1.44
24	B	602	CLA	C1B-CHB	2.09	1.46	1.41
24	C	506	CLA	C4D-CHA	2.09	1.45	1.38
24	c	506	CLA	C4D-CHA	2.09	1.45	1.38
24	c	514	CLA	C1C-C2C	2.08	1.48	1.44
24	B	606	CLA	C4C-C3C	2.08	1.48	1.45
24	C	504	CLA	C1C-C2C	2.08	1.48	1.44
24	c	504	CLA	C1C-C2C	2.08	1.48	1.44
30	D	411	LMG	C4-C5	2.08	1.57	1.53
30	d	411	LMG	C4-C5	2.08	1.57	1.53
28	d	407	PL9	C36-C34	-2.08	1.47	1.51
24	b	613	CLA	O2A-C1	-2.07	1.40	1.46
28	D	407	PL9	C50-C49	-2.07	1.44	1.50
28	d	407	PL9	C50-C49	-2.07	1.44	1.50
32	c	521	LMT	O2B-C2B	-2.07	1.38	1.43
27	a	412	SQD	O4-C4	-2.07	1.38	1.43
24	b	607	CLA	C1B-CHB	2.07	1.46	1.41
27	A	410	SQD	O5-C5	-2.07	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	613	CLA	MG-ND	-2.06	2.01	2.05
24	b	615	CLA	MG-ND	-2.06	2.01	2.05
24	C	502	CLA	C1B-CHB	2.06	1.46	1.41
32	m	102	LMT	O2'-C2'	-2.06	1.38	1.43
24	B	605	CLA	C1B-CHB	2.06	1.46	1.41
25	D	402	PHO	CMC-C2C	-2.06	1.46	1.51
25	d	402	PHO	CMC-C2C	-2.06	1.46	1.51
24	a	406	CLA	C1B-CHB	2.06	1.46	1.41
24	B	611	CLA	C4D-CHA	2.06	1.45	1.38
24	b	613	CLA	C4D-CHA	2.06	1.45	1.38
38	X	101	RRX	C21-C22	-2.06	1.33	1.35
38	x	101	RRX	C21-C22	-2.06	1.33	1.35
28	D	407	PL9	C36-C34	-2.06	1.47	1.51
24	b	610	CLA	O2A-C1	-2.05	1.40	1.46
24	b	614	CLA	C4B-CHC	2.05	1.46	1.41
24	B	608	CLA	O2A-C1	-2.05	1.40	1.46
24	D	405	CLA	C4C-C3C	2.05	1.48	1.45
30	D	411	LMG	O2-C2	-2.05	1.38	1.43
30	d	411	LMG	O2-C2	-2.05	1.38	1.43
24	B	611	CLA	O2A-C1	-2.04	1.40	1.46
26	C	515	BCR	C33-C5	-2.04	1.47	1.50
26	c	515	BCR	C33-C5	-2.04	1.47	1.50
32	C	521	LMT	O2B-C2B	-2.04	1.38	1.43
24	A	406	CLA	C1B-CHB	2.04	1.46	1.41
24	c	508	CLA	O2D-CED	-2.04	1.40	1.45
24	B	608	CLA	C4C-C3C	2.04	1.48	1.45
24	b	610	CLA	C4C-C3C	2.04	1.48	1.45
24	B	615	CLA	C1B-CHB	2.04	1.46	1.41
24	b	617	CLA	C1B-CHB	2.04	1.46	1.41
24	B	612	CLA	C4B-CHC	2.04	1.46	1.41
24	A	405	CLA	MG-ND	-2.04	2.01	2.05
24	a	405	CLA	MG-ND	-2.04	2.01	2.05
31	h	101	DGD	O2D-C2D	-2.04	1.38	1.43
24	B	615	CLA	OBD-CAD	2.03	1.26	1.22
24	b	617	CLA	OBD-CAD	2.03	1.26	1.22
24	C	504	CLA	C4D-CHA	2.03	1.45	1.38
24	c	504	CLA	C4D-CHA	2.03	1.45	1.38
31	c	517	DGD	O4D-C4D	-2.03	1.38	1.43
24	c	502	CLA	C1B-CHB	2.03	1.46	1.41
32	M	101	LMT	O4'-C4B	-2.03	1.38	1.43
32	m	102	LMT	O4'-C4B	-2.03	1.38	1.43
24	C	503	CLA	O2A-C1	-2.03	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	503	CLA	O2A-C1	-2.03	1.40	1.46
24	b	608	CLA	C1B-CHB	2.03	1.46	1.41
24	B	602	CLA	C4B-CHC	2.02	1.46	1.41
24	B	603	CLA	C1D-ND	2.02	1.40	1.37
24	C	511	CLA	C4C-C3C	2.02	1.48	1.45
24	c	511	CLA	C4C-C3C	2.02	1.48	1.45
24	b	603	CLA	C1B-CHB	2.02	1.46	1.41
31	C	517	DGD	O4E-C4E	-2.02	1.38	1.43
31	c	517	DGD	O4E-C4E	-2.02	1.38	1.43
32	j	102	LMT	C3'-C2'	2.02	1.57	1.52
24	C	508	CLA	O2D-CED	-2.02	1.40	1.45
24	B	601	CLA	C1B-CHB	2.01	1.46	1.41
24	B	613	CLA	CMB-C2B	-2.01	1.47	1.51
24	b	615	CLA	CMB-C2B	-2.01	1.47	1.51
31	H	101	DGD	O2D-C2D	-2.01	1.38	1.43
24	C	507	CLA	C4B-NB	-2.01	1.33	1.35
24	c	507	CLA	C4B-NB	-2.01	1.33	1.35
31	C	517	DGD	O4D-C4D	-2.01	1.38	1.43
24	b	614	CLA	C1D-ND	2.01	1.40	1.37
24	C	502	CLA	C1C-C2C	2.01	1.48	1.44
24	c	502	CLA	C1C-C2C	2.01	1.48	1.44
24	B	606	CLA	C1B-CHB	2.01	1.46	1.41
25	A	407	PHO	OBD-CAD	-2.00	1.19	1.22
25	a	407	PHO	OBD-CAD	-2.00	1.19	1.22
24	C	505	CLA	C1B-CHB	2.00	1.46	1.41
24	c	505	CLA	C1B-CHB	2.00	1.46	1.41
24	B	612	CLA	C4D-CHA	2.00	1.45	1.38
24	b	614	CLA	C4D-CHA	2.00	1.45	1.38

All (2526) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	L	102	SQD	O6-C1-C2	10.58	124.81	108.30
27	B	620	SQD	O6-C1-C2	10.57	124.81	108.30
24	C	513	CLA	C2D-C1D-ND	10.29	117.69	110.10
24	c	513	CLA	C2D-C1D-ND	10.29	117.69	110.10
24	B	614	CLA	C1D-ND-C4D	-10.01	99.23	106.33
24	b	616	CLA	C1D-ND-C4D	-10.01	99.23	106.33
24	D	401	CLA	C1D-ND-C4D	-9.90	99.30	106.33
24	d	401	CLA	C1D-ND-C4D	-9.90	99.30	106.33
24	c	509	CLA	C2D-C1D-ND	9.88	117.38	110.10
24	C	509	CLA	C2D-C1D-ND	9.85	117.36	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	408	CLA	C2D-C1D-ND	9.80	117.33	110.10
24	a	408	CLA	C1D-ND-C4D	-9.75	99.41	106.33
24	A	408	CLA	C2D-C1D-ND	9.74	117.28	110.10
24	A	408	CLA	C1D-ND-C4D	-9.70	99.44	106.33
24	D	401	CLA	C2D-C1D-ND	9.56	117.15	110.10
24	d	401	CLA	C2D-C1D-ND	9.56	117.15	110.10
24	B	602	CLA	C1D-ND-C4D	-9.52	99.57	106.33
24	b	604	CLA	C1D-ND-C4D	-9.52	99.57	106.33
27	a	410	SQD	O6-C1-C2	9.50	123.13	108.30
27	A	410	SQD	O6-C1-C2	9.47	123.08	108.30
24	C	512	CLA	C1D-ND-C4D	-9.42	99.64	106.33
24	c	512	CLA	C1D-ND-C4D	-9.42	99.64	106.33
24	c	509	CLA	C1D-ND-C4D	-9.31	99.72	106.33
24	C	504	CLA	C1D-ND-C4D	-9.31	99.72	106.33
24	c	504	CLA	C1D-ND-C4D	-9.31	99.72	106.33
24	d	404	CLA	C1D-ND-C4D	-9.25	99.76	106.33
24	C	509	CLA	C1D-ND-C4D	-9.24	99.77	106.33
24	D	404	CLA	C1D-ND-C4D	-9.23	99.78	106.33
24	C	513	CLA	C1D-ND-C4D	-9.16	99.83	106.33
24	c	513	CLA	C1D-ND-C4D	-9.16	99.83	106.33
24	B	611	CLA	C1D-ND-C4D	-9.08	99.89	106.33
24	b	613	CLA	C1D-ND-C4D	-9.08	99.89	106.33
24	C	508	CLA	C1D-ND-C4D	-9.04	99.91	106.33
24	c	508	CLA	C1D-ND-C4D	-9.04	99.91	106.33
24	b	613	CLA	C2D-C1D-ND	8.79	116.58	110.10
24	B	611	CLA	C2D-C1D-ND	8.78	116.57	110.10
24	D	405	CLA	C1D-ND-C4D	-8.68	100.17	106.33
24	d	405	CLA	C1D-ND-C4D	-8.68	100.17	106.33
24	B	605	CLA	C1D-ND-C4D	-8.67	100.17	106.33
24	b	607	CLA	C1D-ND-C4D	-8.67	100.17	106.33
24	B	614	CLA	C2D-C1D-ND	8.61	116.45	110.10
24	b	616	CLA	C2D-C1D-ND	8.56	116.42	110.10
24	c	512	CLA	C2D-C1D-ND	8.56	116.42	110.10
24	B	602	CLA	C2D-C1D-ND	8.53	116.39	110.10
24	b	604	CLA	C2D-C1D-ND	8.53	116.39	110.10
24	C	504	CLA	C2D-C1D-ND	8.52	116.38	110.10
24	C	512	CLA	C2D-C1D-ND	8.52	116.38	110.10
24	c	504	CLA	C2D-C1D-ND	8.52	116.38	110.10
24	C	514	CLA	C1D-ND-C4D	-8.39	100.37	106.33
24	c	514	CLA	C1D-ND-C4D	-8.39	100.37	106.33
24	C	503	CLA	C1D-ND-C4D	-8.39	100.37	106.33
24	c	503	CLA	C1D-ND-C4D	-8.39	100.37	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	605	CLA	C2D-C1D-ND	8.39	116.29	110.10
24	b	607	CLA	C2D-C1D-ND	8.39	116.29	110.10
24	C	508	CLA	C2D-C1D-ND	8.35	116.26	110.10
24	c	508	CLA	C2D-C1D-ND	8.35	116.26	110.10
24	B	609	CLA	C1D-ND-C4D	-8.28	100.45	106.33
24	c	502	CLA	C1D-ND-C4D	-8.26	100.46	106.33
24	b	612	CLA	C2D-C1D-ND	8.25	116.19	110.10
24	C	502	CLA	C1D-ND-C4D	-8.24	100.48	106.33
24	d	404	CLA	C2D-C1D-ND	8.21	116.15	110.10
24	D	404	CLA	C2D-C1D-ND	8.21	116.15	110.10
24	C	511	CLA	C2C-C1C-NC	8.19	117.65	109.97
24	c	511	CLA	C2C-C1C-NC	8.19	117.65	109.97
24	B	606	CLA	C1D-ND-C4D	-8.19	100.52	106.33
24	B	610	CLA	C2D-C1D-ND	8.18	116.14	110.10
24	b	608	CLA	C1D-ND-C4D	-8.17	100.53	106.33
24	B	607	CLA	C1D-ND-C4D	-8.15	100.54	106.33
24	b	609	CLA	C1D-ND-C4D	-8.15	100.54	106.33
24	b	611	CLA	C1D-ND-C4D	-8.14	100.55	106.33
27	f	101	SQD	O6-C1-C2	8.11	120.96	108.30
27	F	101	SQD	O6-C1-C2	8.11	120.96	108.30
24	B	601	CLA	C1D-ND-C4D	-8.00	100.65	106.33
24	b	603	CLA	C1D-ND-C4D	-8.00	100.65	106.33
24	B	609	CLA	C2D-C1D-ND	7.97	115.98	110.10
24	B	615	CLA	C1D-ND-C4D	-7.93	100.70	106.33
24	b	617	CLA	C1D-ND-C4D	-7.93	100.70	106.33
24	B	615	CLA	C2D-C1D-ND	7.92	115.94	110.10
24	b	617	CLA	C2D-C1D-ND	7.92	115.94	110.10
24	b	611	CLA	C2D-C1D-ND	7.88	115.91	110.10
24	C	506	CLA	C1D-ND-C4D	-7.85	100.76	106.33
24	c	506	CLA	C1D-ND-C4D	-7.85	100.76	106.33
24	b	612	CLA	C1D-ND-C4D	-7.81	100.79	106.33
24	C	505	CLA	C1D-ND-C4D	-7.80	100.79	106.33
24	c	505	CLA	C1D-ND-C4D	-7.80	100.79	106.33
24	B	610	CLA	C1D-ND-C4D	-7.80	100.80	106.33
24	C	502	CLA	C2D-C1D-ND	7.75	115.81	110.10
24	c	502	CLA	C2D-C1D-ND	7.74	115.81	110.10
24	D	401	CLA	CHD-C1D-ND	-7.69	117.38	124.45
24	d	401	CLA	CHD-C1D-ND	-7.69	117.38	124.45
24	C	514	CLA	C2D-C1D-ND	7.67	115.75	110.10
24	c	514	CLA	C2D-C1D-ND	7.67	115.75	110.10
24	B	607	CLA	C2D-C1D-ND	7.63	115.73	110.10
24	b	609	CLA	C2D-C1D-ND	7.63	115.73	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	614	CLA	C1D-ND-C4D	-7.61	100.93	106.33
24	B	601	CLA	C2D-C1D-ND	7.60	115.71	110.10
24	b	603	CLA	C2D-C1D-ND	7.60	115.71	110.10
24	B	612	CLA	C1D-ND-C4D	-7.58	100.95	106.33
24	b	608	CLA	C2D-C1D-ND	7.58	115.69	110.10
24	B	613	CLA	C2D-C1D-ND	7.57	115.69	110.10
24	b	615	CLA	C2D-C1D-ND	7.57	115.69	110.10
24	B	606	CLA	C2D-C1D-ND	7.56	115.68	110.10
24	C	507	CLA	C2D-C1D-ND	7.56	115.67	110.10
24	c	507	CLA	C2D-C1D-ND	7.56	115.67	110.10
24	C	507	CLA	C1D-ND-C4D	-7.54	100.98	106.33
24	c	507	CLA	C1D-ND-C4D	-7.54	100.98	106.33
24	B	616	CLA	C1D-ND-C4D	-7.48	101.02	106.33
24	b	618	CLA	C1D-ND-C4D	-7.48	101.02	106.33
24	C	510	CLA	C1D-ND-C4D	-7.47	101.03	106.33
24	c	510	CLA	C1D-ND-C4D	-7.47	101.03	106.33
24	B	613	CLA	C1D-ND-C4D	-7.45	101.04	106.33
24	b	615	CLA	C1D-ND-C4D	-7.45	101.04	106.33
24	C	505	CLA	C2D-C1D-ND	7.34	115.51	110.10
24	c	505	CLA	C2D-C1D-ND	7.34	115.51	110.10
24	C	503	CLA	C2D-C1D-ND	7.29	115.47	110.10
24	c	503	CLA	C2D-C1D-ND	7.29	115.47	110.10
24	C	511	CLA	CMD-C2D-C1D	7.29	137.56	124.71
24	c	511	CLA	CMD-C2D-C1D	7.29	137.56	124.71
24	b	614	CLA	C2D-C1D-ND	7.28	115.47	110.10
24	B	612	CLA	C2D-C1D-ND	7.25	115.45	110.10
24	B	605	CLA	O2D-CGD-CBD	7.24	124.12	111.27
24	b	607	CLA	O2D-CGD-CBD	7.24	124.12	111.27
24	B	602	CLA	CMD-C2D-C1D	7.19	137.38	124.71
24	b	604	CLA	CMD-C2D-C1D	7.19	137.38	124.71
24	B	612	CLA	O2D-CGD-CBD	7.13	123.94	111.27
24	b	614	CLA	O2D-CGD-CBD	7.12	123.93	111.27
24	C	510	CLA	C2D-C1D-ND	7.07	115.31	110.10
24	c	510	CLA	C2D-C1D-ND	7.07	115.31	110.10
24	B	603	CLA	C1D-ND-C4D	-7.06	101.32	106.33
24	B	604	CLA	C2C-C1C-NC	7.06	116.59	109.97
24	b	606	CLA	C2C-C1C-NC	7.06	116.59	109.97
24	d	405	CLA	C2D-C1D-ND	7.02	115.28	110.10
24	D	405	CLA	C2D-C1D-ND	7.01	115.27	110.10
24	b	605	CLA	C1D-ND-C4D	-6.98	101.37	106.33
24	a	408	CLA	CHD-C1D-ND	-6.95	118.07	124.45
24	A	408	CLA	CHD-C1D-ND	-6.87	118.14	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	405	CLA	CMD-C2D-C1D	6.86	136.80	124.71
24	a	405	CLA	CMD-C2D-C1D	6.86	136.80	124.71
24	B	613	CLA	CMD-C2D-C1D	6.84	136.76	124.71
24	b	615	CLA	CMD-C2D-C1D	6.84	136.76	124.71
24	B	606	CLA	CMD-C2D-C1D	6.83	136.75	124.71
24	b	608	CLA	CMD-C2D-C1D	6.83	136.74	124.71
24	C	508	CLA	CMD-C2D-C1D	6.82	136.73	124.71
24	c	508	CLA	CMD-C2D-C1D	6.82	136.73	124.71
24	D	404	CLA	CMD-C2D-C1D	6.81	136.71	124.71
24	b	610	CLA	C1D-ND-C4D	-6.80	101.50	106.33
24	d	404	CLA	CMD-C2D-C1D	6.80	136.70	124.71
24	B	602	CLA	CHD-C1D-ND	-6.80	118.21	124.45
24	b	604	CLA	CHD-C1D-ND	-6.80	118.21	124.45
24	D	401	CLA	C2C-C1C-NC	6.75	116.30	109.97
24	d	401	CLA	C2C-C1C-NC	6.75	116.30	109.97
24	B	608	CLA	C1D-ND-C4D	-6.75	101.54	106.33
24	C	504	CLA	CMD-C2D-C1D	6.69	136.51	124.71
24	c	504	CLA	CMD-C2D-C1D	6.69	136.51	124.71
24	B	614	CLA	CHD-C1D-ND	-6.64	118.35	124.45
24	b	616	CLA	CHD-C1D-ND	-6.64	118.35	124.45
24	b	611	CLA	CHD-C4C-C3C	-6.63	115.10	124.84
24	B	609	CLA	CHD-C4C-C3C	-6.62	115.10	124.84
24	B	616	CLA	C2D-C1D-ND	6.62	114.98	110.10
24	b	618	CLA	C2D-C1D-ND	6.62	114.98	110.10
24	B	604	CLA	O2D-CGD-CBD	6.58	122.96	111.27
24	b	617	CLA	CHD-C1D-ND	-6.55	118.44	124.45
24	b	606	CLA	O2D-CGD-CBD	6.55	122.90	111.27
24	A	406	CLA	CMD-C2D-C1D	6.54	136.25	124.71
24	C	514	CLA	CMD-C2D-C1D	6.54	136.25	124.71
24	a	406	CLA	CMD-C2D-C1D	6.54	136.25	124.71
24	c	514	CLA	CMD-C2D-C1D	6.54	136.25	124.71
24	c	512	CLA	CMD-C2D-C1D	6.54	136.24	124.71
24	B	608	CLA	C2C-C1C-NC	6.53	116.09	109.97
24	A	406	CLA	C1D-ND-C4D	-6.52	101.70	106.33
24	a	406	CLA	C1D-ND-C4D	-6.52	101.70	106.33
24	B	607	CLA	CMD-C2D-C1D	6.52	136.20	124.71
24	b	609	CLA	CMD-C2D-C1D	6.52	136.20	124.71
24	C	512	CLA	CMD-C2D-C1D	6.51	136.19	124.71
24	B	615	CLA	CHD-C1D-ND	-6.51	118.47	124.45
24	B	607	CLA	C2C-C1C-NC	6.50	116.07	109.97
24	b	609	CLA	C2C-C1C-NC	6.50	116.07	109.97
24	b	610	CLA	C2C-C1C-NC	6.48	116.04	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	514	CLA	O2D-CGD-CBD	6.47	122.77	111.27
24	c	514	CLA	O2D-CGD-CBD	6.47	122.77	111.27
24	c	503	CLA	C2C-C1C-NC	6.45	116.02	109.97
24	d	405	CLA	CMD-C2D-C1D	6.43	136.05	124.71
24	D	405	CLA	CMD-C2D-C1D	6.41	136.01	124.71
24	C	503	CLA	C2C-C1C-NC	6.41	115.97	109.97
24	C	507	CLA	CMD-C2D-C1D	6.41	136.00	124.71
24	c	507	CLA	CMD-C2D-C1D	6.41	136.00	124.71
24	b	603	CLA	O2D-CGD-CBD	6.41	122.65	111.27
24	A	405	CLA	C1D-ND-C4D	-6.40	101.79	106.33
24	a	405	CLA	C1D-ND-C4D	-6.40	101.79	106.33
24	B	601	CLA	O2D-CGD-CBD	6.37	122.59	111.27
24	C	511	CLA	C1D-ND-C4D	-6.37	101.81	106.33
24	c	511	CLA	C1D-ND-C4D	-6.37	101.81	106.33
24	B	603	CLA	C2C-C1C-NC	6.36	115.93	109.97
24	b	605	CLA	C2C-C1C-NC	6.36	115.93	109.97
24	A	406	CLA	CHD-C4C-C3C	-6.36	115.50	124.84
24	a	406	CLA	CHD-C4C-C3C	-6.35	115.51	124.84
24	B	612	CLA	CHD-C4C-C3C	-6.33	115.53	124.84
24	b	614	CLA	CHD-C4C-C3C	-6.33	115.53	124.84
24	B	604	CLA	C1D-ND-C4D	-6.31	101.85	106.33
24	b	606	CLA	C1D-ND-C4D	-6.31	101.85	106.33
24	c	502	CLA	CHD-C1D-ND	-6.31	118.66	124.45
24	B	616	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
24	b	618	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
24	C	505	CLA	CMD-C2D-C1D	6.26	135.74	124.71
24	c	505	CLA	CMD-C2D-C1D	6.26	135.74	124.71
24	C	502	CLA	CHD-C1D-ND	-6.24	118.72	124.45
24	b	611	CLA	C2C-C1C-NC	6.23	115.81	109.97
24	C	502	CLA	C2C-C1C-NC	6.22	115.80	109.97
24	c	502	CLA	C2C-C1C-NC	6.22	115.80	109.97
24	C	513	CLA	CHD-C4C-C3C	-6.19	115.74	124.84
24	c	513	CLA	CHD-C4C-C3C	-6.19	115.74	124.84
24	C	509	CLA	C2C-C1C-NC	6.18	115.76	109.97
24	c	509	CLA	C2C-C1C-NC	6.18	115.76	109.97
24	B	609	CLA	C2C-C1C-NC	6.14	115.72	109.97
24	B	603	CLA	C2D-C1D-ND	6.14	114.63	110.10
24	a	405	CLA	C2C-C1C-NC	6.12	115.70	109.97
24	A	405	CLA	C2C-C1C-NC	6.12	115.70	109.97
24	b	605	CLA	C2D-C1D-ND	6.12	114.61	110.10
24	C	506	CLA	O2D-CGD-CBD	6.11	122.13	111.27
24	c	506	CLA	O2D-CGD-CBD	6.11	122.13	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	504	CLA	CHD-C4C-C3C	-6.10	115.87	124.84
24	c	504	CLA	CHD-C4C-C3C	-6.10	115.87	124.84
24	C	502	CLA	CMD-C2D-C1D	6.08	135.43	124.71
24	c	502	CLA	CMD-C2D-C1D	6.07	135.41	124.71
24	B	613	CLA	C2C-C1C-NC	6.04	115.63	109.97
24	b	615	CLA	C2C-C1C-NC	6.02	115.61	109.97
24	b	612	CLA	C2C-C1C-NC	6.01	115.60	109.97
24	b	603	CLA	C2C-C1C-NC	6.00	115.59	109.97
24	B	609	CLA	CMD-C2D-C1D	6.00	135.29	124.71
24	C	508	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
24	c	508	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
24	b	608	CLA	CHD-C4C-C3C	-5.98	116.06	124.84
24	B	604	CLA	CMD-C2D-C1D	5.97	135.24	124.71
24	b	606	CLA	CMD-C2D-C1D	5.97	135.24	124.71
24	C	506	CLA	CMD-C2D-C1D	5.97	135.23	124.71
24	c	506	CLA	CMD-C2D-C1D	5.97	135.23	124.71
24	c	514	CLA	CHD-C1D-ND	-5.96	118.98	124.45
24	b	611	CLA	CMD-C2D-C1D	5.95	135.21	124.71
24	C	514	CLA	CHD-C1D-ND	-5.94	118.99	124.45
24	D	405	CLA	CHD-C1D-ND	-5.94	119.00	124.45
24	d	405	CLA	CHD-C1D-ND	-5.94	119.00	124.45
24	C	506	CLA	C2D-C1D-ND	5.94	114.48	110.10
24	c	506	CLA	C2D-C1D-ND	5.94	114.48	110.10
24	B	613	CLA	CHD-C1D-ND	-5.93	119.00	124.45
24	b	615	CLA	CHD-C1D-ND	-5.93	119.00	124.45
24	B	606	CLA	CHD-C4C-C3C	-5.93	116.13	124.84
24	b	611	CLA	O2D-CGD-CBD	5.93	121.80	111.27
24	c	513	CLA	O2D-CGD-CBD	5.91	121.77	111.27
24	B	609	CLA	O2D-CGD-CBD	5.91	121.77	111.27
24	C	513	CLA	O2D-CGD-CBD	5.91	121.77	111.27
24	C	510	CLA	CMD-C2D-C1D	5.90	135.11	124.71
24	c	510	CLA	CMD-C2D-C1D	5.90	135.11	124.71
24	B	601	CLA	C2C-C1C-NC	5.90	115.50	109.97
24	B	610	CLA	C2C-C1C-NC	5.88	115.48	109.97
24	B	608	CLA	C2D-C1D-ND	5.85	114.42	110.10
24	b	610	CLA	C2D-C1D-ND	5.85	114.41	110.10
24	B	607	CLA	CHD-C1D-ND	-5.84	119.09	124.45
24	b	609	CLA	CHD-C1D-ND	-5.84	119.09	124.45
24	B	601	CLA	CMD-C2D-C1D	5.83	134.99	124.71
24	b	603	CLA	CMD-C2D-C1D	5.83	134.98	124.71
24	b	609	CLA	O2D-CGD-CBD	5.82	121.61	111.27
24	B	607	CLA	O2D-CGD-CBD	5.81	121.59	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	620	SQD	O7-S-C6	5.79	113.82	106.94
27	L	102	SQD	O7-S-C6	5.77	113.80	106.94
24	C	510	CLA	CHD-C1D-ND	-5.74	119.17	124.45
24	c	510	CLA	CHD-C1D-ND	-5.74	119.17	124.45
24	B	602	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
24	b	604	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
24	C	508	CLA	C2C-C1C-NC	5.73	115.34	109.97
24	c	508	CLA	C2C-C1C-NC	5.73	115.34	109.97
24	C	512	CLA	CHD-C4C-C3C	-5.73	116.42	124.84
24	C	509	CLA	O2D-CGD-CBD	5.72	121.44	111.27
24	c	509	CLA	O2D-CGD-CBD	5.72	121.44	111.27
24	C	509	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
24	c	509	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
24	B	611	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
24	b	613	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
24	c	512	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
24	c	505	CLA	O2D-CGD-CBD	5.69	121.38	111.27
24	C	505	CLA	O2D-CGD-CBD	5.68	121.36	111.27
24	d	404	CLA	CHD-C1D-ND	-5.66	119.25	124.45
24	A	405	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
24	a	405	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
24	D	404	CLA	CHD-C1D-ND	-5.64	119.27	124.45
24	C	513	CLA	CHD-C1D-ND	-5.64	119.27	124.45
24	c	513	CLA	CHD-C1D-ND	-5.64	119.27	124.45
24	C	511	CLA	C1C-C2C-C3C	-5.63	101.04	106.96
24	c	511	CLA	C1C-C2C-C3C	-5.63	101.04	106.96
24	B	614	CLA	CMD-C2D-C1D	5.62	134.62	124.71
24	b	608	CLA	CHD-C1D-ND	-5.62	119.29	124.45
24	B	615	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
24	b	617	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
24	B	612	CLA	C3C-C4C-NC	5.60	116.85	110.57
24	b	614	CLA	C3C-C4C-NC	5.60	116.85	110.57
24	B	608	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
24	B	606	CLA	CHD-C1D-ND	-5.60	119.31	124.45
24	b	613	CLA	CMD-C2D-C1D	5.58	134.54	124.71
24	B	611	CLA	CMD-C2D-C1D	5.58	134.54	124.71
24	c	502	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
24	b	610	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
24	b	616	CLA	CMD-C2D-C1D	5.57	134.53	124.71
24	c	507	CLA	CHD-C4C-C3C	-5.57	116.66	124.84
24	a	408	CLA	CMD-C2D-C1D	5.56	134.51	124.71
24	B	616	CLA	CMD-C2D-C1D	5.56	134.51	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	618	CLA	CMD-C2D-C1D	5.56	134.51	124.71
24	A	408	CLA	CMD-C2D-C1D	5.55	134.50	124.71
24	C	502	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
24	C	507	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
24	b	608	CLA	O2D-CGD-CBD	5.54	121.12	111.27
24	B	606	CLA	O2D-CGD-CBD	5.53	121.09	111.27
24	B	602	CLA	O2D-CGD-CBD	5.52	121.08	111.27
24	b	604	CLA	O2D-CGD-CBD	5.52	121.08	111.27
24	B	613	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
24	b	615	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
24	C	508	CLA	CHD-C1D-ND	-5.51	119.39	124.45
24	c	508	CLA	CHD-C1D-ND	-5.51	119.39	124.45
24	B	605	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
24	b	607	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
24	C	511	CLA	CHD-C4C-C3C	-5.48	116.79	124.84
24	c	511	CLA	CHD-C4C-C3C	-5.48	116.79	124.84
24	b	612	CLA	CHD-C4C-C3C	-5.48	116.79	124.84
24	B	610	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
24	C	510	CLA	C2C-C1C-NC	5.43	115.06	109.97
24	c	510	CLA	C2C-C1C-NC	5.43	115.06	109.97
24	B	606	CLA	C2C-C1C-NC	5.41	115.04	109.97
24	b	608	CLA	C2C-C1C-NC	5.41	115.04	109.97
24	D	401	CLA	C3D-C2D-C1D	-5.39	98.48	105.83
24	d	401	CLA	C3D-C2D-C1D	-5.39	98.48	105.83
24	b	613	CLA	C3D-C2D-C1D	-5.38	98.48	105.83
24	A	408	CLA	C2C-C1C-NC	5.38	115.01	109.97
24	a	408	CLA	C2C-C1C-NC	5.38	115.01	109.97
27	L	102	SQD	O8-S-C6	5.37	114.30	105.74
24	B	604	CLA	C2D-C1D-ND	5.37	114.06	110.10
24	b	606	CLA	C2D-C1D-ND	5.37	114.06	110.10
24	B	603	CLA	O2D-CGD-CBD	5.37	120.81	111.27
24	b	605	CLA	O2D-CGD-CBD	5.37	120.81	111.27
24	D	405	CLA	O2D-CGD-CBD	5.37	120.80	111.27
24	d	405	CLA	O2D-CGD-CBD	5.37	120.80	111.27
27	B	620	SQD	O8-S-C6	5.36	114.28	105.74
24	C	505	CLA	C2C-C1C-NC	5.35	114.99	109.97
24	c	505	CLA	C2C-C1C-NC	5.35	114.99	109.97
24	B	611	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
24	A	408	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
24	a	408	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
24	B	616	CLA	C2C-C1C-NC	5.34	114.97	109.97
24	b	618	CLA	C2C-C1C-NC	5.34	114.97	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	604	CLA	CHD-C4C-C3C	-5.33	117.00	124.84
24	b	606	CLA	CHD-C4C-C3C	-5.33	117.00	124.84
24	a	408	CLA	C3D-C2D-C1D	-5.33	98.56	105.83
24	A	406	CLA	C2D-C1D-ND	5.32	114.03	110.10
24	a	406	CLA	C2D-C1D-ND	5.32	114.03	110.10
24	A	408	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
24	C	513	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
24	c	513	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
24	B	603	CLA	CMD-C2D-C1D	5.31	134.07	124.71
24	b	605	CLA	CMD-C2D-C1D	5.31	134.07	124.71
24	D	404	CLA	C2C-C1C-NC	5.31	114.95	109.97
24	d	404	CLA	C2C-C1C-NC	5.31	114.95	109.97
24	D	401	CLA	C1C-C2C-C3C	-5.31	101.38	106.96
24	d	401	CLA	C1C-C2C-C3C	-5.31	101.38	106.96
24	D	405	CLA	CHD-C4C-C3C	-5.31	117.04	124.84
24	C	509	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
24	c	509	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
24	d	405	CLA	CHD-C4C-C3C	-5.29	117.06	124.84
24	C	502	CLA	C1C-C2C-C3C	-5.29	101.40	106.96
24	C	511	CLA	O2D-CGD-CBD	5.28	120.66	111.27
24	c	511	CLA	O2D-CGD-CBD	5.28	120.66	111.27
24	C	505	CLA	CHD-C1D-ND	-5.28	119.60	124.45
24	c	505	CLA	CHD-C1D-ND	-5.28	119.60	124.45
24	C	504	CLA	C2C-C1C-NC	5.28	114.92	109.97
24	c	504	CLA	C2C-C1C-NC	5.28	114.92	109.97
24	c	502	CLA	C1C-C2C-C3C	-5.27	101.41	106.96
24	C	506	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
24	c	506	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
24	B	604	CLA	C1C-C2C-C3C	-5.27	101.42	106.96
24	b	606	CLA	C1C-C2C-C3C	-5.27	101.42	106.96
24	B	601	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
24	b	603	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
27	A	412	SQD	C4-C3-C2	5.27	120.02	110.82
24	C	506	CLA	C2C-C1C-NC	5.26	114.90	109.97
24	c	506	CLA	C2C-C1C-NC	5.26	114.90	109.97
24	C	503	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
24	c	503	CLA	CHD-C4C-C3C	-5.25	117.12	124.84
27	a	412	SQD	C4-C3-C2	5.25	119.99	110.82
24	C	507	CLA	C2C-C1C-NC	5.24	114.88	109.97
24	c	507	CLA	C2C-C1C-NC	5.24	114.88	109.97
24	B	610	CLA	CMD-C2D-C1D	5.22	133.91	124.71
27	a	412	SQD	O7-S-C6	5.21	113.14	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	612	CLA	CMD-C2D-C1D	5.21	133.90	124.71
24	A	405	CLA	C2D-C1D-ND	5.21	113.94	110.10
24	a	405	CLA	C2D-C1D-ND	5.21	113.94	110.10
24	c	510	CLA	CHD-C4C-C3C	-5.19	117.22	124.84
24	C	514	CLA	C4A-NA-C1A	-5.18	104.38	106.71
24	c	514	CLA	C4A-NA-C1A	-5.18	104.38	106.71
24	b	607	CLA	C2C-C1C-NC	5.18	114.83	109.97
27	F	101	SQD	O9-S-C6	5.18	113.10	106.94
24	b	616	CLA	CHD-C4C-C3C	-5.17	117.25	124.84
27	f	101	SQD	O9-S-C6	5.17	113.08	106.94
24	B	613	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
24	b	615	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
27	A	412	SQD	O7-S-C6	5.16	113.07	106.94
24	C	510	CLA	CHD-C4C-C3C	-5.16	117.26	124.84
24	B	614	CLA	CHD-C4C-C3C	-5.16	117.26	124.84
24	B	615	CLA	C2C-C1C-NC	5.16	114.80	109.97
24	b	617	CLA	C2C-C1C-NC	5.16	114.80	109.97
24	a	405	CLA	C3C-C4C-NC	5.15	116.35	110.57
24	A	405	CLA	C3C-C4C-NC	5.15	116.35	110.57
24	B	613	CLA	C1C-C2C-C3C	-5.15	101.54	106.96
24	B	605	CLA	C2C-C1C-NC	5.15	114.79	109.97
24	B	609	CLA	CHD-C1D-ND	-5.14	119.73	124.45
24	A	406	CLA	C3C-C4C-NC	5.14	116.33	110.57
24	C	511	CLA	CHD-C1D-ND	-5.14	119.73	124.45
24	c	511	CLA	CHD-C1D-ND	-5.14	119.73	124.45
24	C	507	CLA	CHD-C1D-ND	-5.14	119.73	124.45
24	c	507	CLA	CHD-C1D-ND	-5.13	119.74	124.45
24	B	607	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
24	b	609	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
24	B	616	CLA	CHD-C1D-ND	-5.13	119.74	124.45
24	b	618	CLA	CHD-C1D-ND	-5.13	119.74	124.45
24	a	406	CLA	C3C-C4C-NC	5.12	116.32	110.57
24	C	510	CLA	O2D-CGD-CBD	5.12	120.36	111.27
24	c	510	CLA	O2D-CGD-CBD	5.12	120.36	111.27
24	C	512	CLA	C2C-C1C-NC	5.12	114.77	109.97
24	c	512	CLA	C2C-C1C-NC	5.12	114.77	109.97
24	B	601	CLA	CHD-C1D-ND	-5.11	119.75	124.45
24	b	603	CLA	CHD-C1D-ND	-5.11	119.75	124.45
24	C	512	CLA	CHD-C1D-ND	-5.11	119.76	124.45
24	c	512	CLA	CHD-C1D-ND	-5.11	119.76	124.45
24	C	507	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
24	c	507	CLA	C3D-C2D-C1D	-5.11	98.86	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	615	CLA	C1C-C2C-C3C	-5.11	101.59	106.96
24	b	611	CLA	CHD-C1D-ND	-5.10	119.77	124.45
24	C	513	CLA	C3C-C4C-NC	5.10	116.29	110.57
24	c	513	CLA	C3C-C4C-NC	5.10	116.29	110.57
24	B	611	CLA	C2C-C1C-NC	5.09	114.74	109.97
24	b	613	CLA	C2C-C1C-NC	5.07	114.72	109.97
24	B	605	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
24	b	607	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
24	B	614	CLA	C2C-C1C-NC	5.05	114.70	109.97
24	b	616	CLA	C2C-C1C-NC	5.05	114.70	109.97
33	D	403	BCT	O2-C-O1	5.03	132.58	119.55
24	B	611	CLA	CHD-C1D-ND	-5.02	119.84	124.45
24	b	613	CLA	CHD-C1D-ND	-5.02	119.84	124.45
33	d	403	BCT	O2-C-O1	5.02	132.56	119.55
24	B	602	CLA	C3D-C2D-C1D	-5.02	98.99	105.83
24	b	604	CLA	C3D-C2D-C1D	-5.02	98.99	105.83
24	b	608	CLA	C3C-C4C-NC	5.01	116.19	110.57
24	B	615	CLA	CMD-C2D-C1D	5.00	133.53	124.71
24	b	617	CLA	CMD-C2D-C1D	5.00	133.53	124.71
24	A	405	CLA	CAA-C2A-C3A	-5.00	99.08	112.78
24	a	405	CLA	CAA-C2A-C3A	-5.00	99.08	112.78
24	B	614	CLA	O2D-CGD-CBD	4.99	120.14	111.27
24	C	503	CLA	O2D-CGD-CBD	4.99	120.14	111.27
24	b	616	CLA	O2D-CGD-CBD	4.99	120.14	111.27
24	C	509	CLA	C3C-C4C-NC	4.99	116.17	110.57
24	c	509	CLA	C3C-C4C-NC	4.99	116.17	110.57
24	A	406	CLA	C2C-C1C-NC	4.99	114.65	109.97
24	B	606	CLA	C3C-C4C-NC	4.99	116.17	110.57
24	c	503	CLA	O2D-CGD-CBD	4.99	120.13	111.27
24	B	612	CLA	C2C-C1C-NC	4.98	114.64	109.97
24	b	614	CLA	C2C-C1C-NC	4.98	114.64	109.97
24	B	604	CLA	C4A-NA-C1A	-4.98	104.47	106.71
24	c	512	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
24	a	406	CLA	C2C-C1C-NC	4.95	114.61	109.97
24	B	605	CLA	CHD-C1D-ND	-4.94	119.92	124.45
24	b	607	CLA	CHD-C1D-ND	-4.94	119.92	124.45
24	b	616	CLA	C3D-C4D-ND	4.94	118.22	110.24
24	C	504	CLA	C3C-C4C-NC	4.93	116.10	110.57
24	c	504	CLA	C3C-C4C-NC	4.93	116.10	110.57
24	C	512	CLA	C3D-C2D-C1D	-4.92	99.11	105.83
24	d	404	CLA	C3C-C4C-NC	4.92	116.09	110.57
24	B	614	CLA	C3D-C4D-ND	4.91	118.19	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	605	CLA	CMD-C2D-C1D	4.91	133.37	124.71
24	b	607	CLA	CMD-C2D-C1D	4.91	133.37	124.71
24	C	514	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
24	c	514	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
24	C	512	CLA	C3B-C4B-NB	4.91	115.55	109.21
24	c	512	CLA	C3B-C4B-NB	4.91	115.55	109.21
24	b	606	CLA	C4A-NA-C1A	-4.90	104.50	106.71
24	D	404	CLA	C3C-C4C-NC	4.90	116.06	110.57
24	D	401	CLA	O2D-CGD-CBD	4.90	119.97	111.27
24	d	401	CLA	O2D-CGD-CBD	4.89	119.96	111.27
24	C	504	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
24	c	504	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
24	b	611	CLA	C3C-C4C-NC	4.87	116.04	110.57
24	C	514	CLA	CHD-C4C-C3C	-4.87	117.68	124.84
24	c	514	CLA	CHD-C4C-C3C	-4.87	117.68	124.84
24	C	509	CLA	CMB-C2B-C3B	4.86	133.77	124.68
24	c	509	CLA	CMB-C2B-C3B	4.86	133.77	124.68
24	C	502	CLA	O2D-CGD-CBD	4.84	119.87	111.27
24	c	502	CLA	O2D-CGD-CBD	4.84	119.87	111.27
24	D	401	CLA	CMD-C2D-C1D	4.84	133.24	124.71
24	d	401	CLA	CMD-C2D-C1D	4.84	133.24	124.71
24	C	508	CLA	O2D-CGD-CBD	4.84	119.87	111.27
24	c	508	CLA	O2D-CGD-CBD	4.84	119.87	111.27
24	B	609	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
24	B	609	CLA	C3C-C4C-NC	4.84	116.00	110.57
24	B	603	CLA	CHD-C4C-C3C	-4.83	117.74	124.84
24	b	611	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
24	b	605	CLA	CHD-C4C-C3C	-4.83	117.75	124.84
24	C	513	CLA	C2C-C1C-NC	4.82	114.48	109.97
24	c	513	CLA	C2C-C1C-NC	4.82	114.48	109.97
24	D	405	CLA	C3D-C4D-ND	4.80	118.01	110.24
24	d	405	CLA	C3D-C4D-ND	4.80	118.01	110.24
38	X	101	RRX	C7-C8-C9	-4.80	118.98	126.23
38	x	101	RRX	C7-C8-C9	-4.80	118.98	126.23
24	B	607	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
24	b	609	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
25	D	402	PHO	CMB-C2B-C3B	4.78	133.63	124.68
25	d	402	PHO	CMB-C2B-C3B	4.78	133.63	124.68
24	B	607	CLA	C3C-C4C-NC	4.78	115.94	110.57
24	b	609	CLA	C3C-C4C-NC	4.78	115.94	110.57
24	C	508	CLA	C3C-C4C-NC	4.78	115.93	110.57
24	c	508	CLA	C3C-C4C-NC	4.78	115.93	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	405	CLA	C2C-C1C-NC	4.77	114.44	109.97
24	d	405	CLA	C2C-C1C-NC	4.77	114.44	109.97
24	A	408	CLA	O2D-CGD-CBD	4.77	119.74	111.27
24	a	408	CLA	O2D-CGD-CBD	4.77	119.74	111.27
24	B	616	CLA	O2D-CGD-CBD	4.77	119.74	111.27
24	b	618	CLA	O2D-CGD-CBD	4.76	119.73	111.27
24	B	606	CLA	CMB-C2B-C3B	4.76	133.59	124.68
24	b	608	CLA	CMB-C2B-C3B	4.76	133.59	124.68
24	b	612	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
24	B	610	CLA	C3D-C2D-C1D	-4.75	99.36	105.83
38	X	101	RRX	C16-C17-C18	-4.74	120.55	127.31
38	x	101	RRX	C16-C17-C18	-4.74	120.55	127.31
24	C	511	CLA	C2D-C1D-ND	4.73	113.59	110.10
24	c	511	CLA	C2D-C1D-ND	4.73	113.59	110.10
24	B	606	CLA	C3B-C4B-NB	4.72	115.32	109.21
24	b	608	CLA	C3B-C4B-NB	4.72	115.32	109.21
24	D	405	CLA	C3B-C4B-NB	4.70	115.29	109.21
24	d	405	CLA	C3B-C4B-NB	4.70	115.29	109.21
24	C	503	CLA	CMD-C2D-C1D	4.70	132.99	124.71
24	c	503	CLA	CMD-C2D-C1D	4.70	132.99	124.71
24	C	508	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
24	c	508	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
24	d	404	CLA	CHD-C4C-C3C	-4.68	117.96	124.84
24	B	614	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
24	C	504	CLA	CHD-C1D-ND	-4.67	120.17	124.45
24	c	504	CLA	CHD-C1D-ND	-4.67	120.17	124.45
27	A	410	SQD	O8-S-C6	4.66	113.17	105.74
24	D	404	CLA	CHD-C4C-C3C	-4.66	117.99	124.84
24	C	511	CLA	C3C-C4C-NC	4.66	115.80	110.57
24	c	511	CLA	C3C-C4C-NC	4.66	115.80	110.57
24	b	616	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
24	C	505	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
24	c	505	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
24	A	408	CLA	C1C-C2C-C3C	-4.65	102.07	106.96
24	a	408	CLA	C1C-C2C-C3C	-4.65	102.07	106.96
24	B	615	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
24	b	617	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
24	C	502	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
27	a	410	SQD	O8-S-C6	4.64	113.13	105.74
24	D	404	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
24	b	608	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
24	B	616	CLA	C3D-C2D-C1D	-4.63	99.51	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	618	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
24	B	616	CLA	C1D-CHD-C4C	-4.63	116.06	126.06
24	b	618	CLA	C1D-CHD-C4C	-4.63	116.06	126.06
24	d	404	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
35	e	103	HEM	CBD-CAD-C3D	-4.63	99.76	112.63
24	B	606	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
24	B	615	CLA	C3C-C4C-NC	4.62	115.76	110.57
24	b	617	CLA	C3C-C4C-NC	4.62	115.76	110.57
35	E	103	HEM	CBD-CAD-C3D	-4.62	99.80	112.63
32	J	102	LMT	C3'-C4'-C5'	-4.61	102.01	110.24
24	C	507	CLA	C4A-NA-C1A	-4.60	104.64	106.71
24	c	502	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
24	B	607	CLA	CAC-C3C-C4C	4.60	130.77	124.81
24	b	609	CLA	CAC-C3C-C4C	4.60	130.77	124.81
24	B	602	CLA	C4A-NA-C1A	-4.60	104.64	106.71
24	b	604	CLA	C4A-NA-C1A	-4.60	104.64	106.71
24	B	611	CLA	C3D-C4D-ND	4.59	117.67	110.24
24	b	613	CLA	C3D-C4D-ND	4.59	117.67	110.24
24	C	505	CLA	CHD-C4C-C3C	-4.59	118.09	124.84
24	c	505	CLA	CHD-C4C-C3C	-4.59	118.09	124.84
32	j	102	LMT	C3'-C4'-C5'	-4.59	102.06	110.24
24	B	601	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
24	b	603	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
24	C	512	CLA	C3C-C4C-NC	4.58	115.70	110.57
24	c	512	CLA	C3C-C4C-NC	4.57	115.70	110.57
24	b	612	CLA	CHD-C1D-ND	-4.55	120.27	124.45
27	F	101	SQD	O9-S-O7	-4.52	98.30	113.95
24	C	510	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
24	c	510	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
27	f	101	SQD	O9-S-O7	-4.52	98.30	113.95
38	X	101	RRX	C20-C21-C22	-4.52	120.87	127.31
38	x	101	RRX	C20-C21-C22	-4.52	120.87	127.31
24	C	508	CLA	C1C-C2C-C3C	-4.51	102.22	106.96
24	c	508	CLA	C1C-C2C-C3C	-4.51	102.22	106.96
24	d	404	CLA	C3D-C4D-ND	4.50	117.51	110.24
24	D	404	CLA	C3D-C4D-ND	4.49	117.50	110.24
24	b	614	CLA	CHD-C1D-ND	-4.49	120.33	124.45
24	c	507	CLA	C4A-NA-C1A	-4.48	104.69	106.71
24	C	512	CLA	C3D-C4D-ND	4.48	117.48	110.24
24	c	512	CLA	C3D-C4D-ND	4.48	117.48	110.24
24	D	404	CLA	CAA-C2A-C3A	-4.47	100.54	112.78
24	d	404	CLA	CAA-C2A-C3A	-4.47	100.54	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	614	CLA	CMD-C2D-C1D	4.47	132.59	124.71
24	b	605	CLA	CAC-C3C-C4C	4.45	130.59	124.81
24	D	405	CLA	C3C-C4C-NC	4.45	115.56	110.57
24	B	603	CLA	C4-C3-C5	4.44	122.74	115.27
24	B	603	CLA	CAC-C3C-C4C	4.44	130.57	124.81
24	B	612	CLA	CHD-C1D-ND	-4.43	120.38	124.45
24	b	605	CLA	C4-C3-C5	4.43	122.72	115.27
24	d	405	CLA	C3C-C4C-NC	4.43	115.54	110.57
24	B	612	CLA	CMD-C2D-C1D	4.42	132.50	124.71
24	D	401	CLA	C3D-C4D-ND	4.42	117.39	110.24
24	d	401	CLA	C3D-C4D-ND	4.42	117.39	110.24
28	A	411	PL9	C7-C3-C4	4.40	120.46	116.88
24	C	513	CLA	C4A-NA-C1A	-4.40	104.73	106.71
24	c	513	CLA	C4A-NA-C1A	-4.40	104.73	106.71
24	B	607	CLA	C3B-C4B-NB	4.40	114.90	109.21
24	b	609	CLA	C3B-C4B-NB	4.40	114.89	109.21
24	C	507	CLA	O2D-CGD-CBD	4.38	119.06	111.27
24	c	507	CLA	O2D-CGD-CBD	4.38	119.06	111.27
24	B	608	CLA	C1C-C2C-C3C	-4.38	102.35	106.96
27	f	101	SQD	O7-S-C6	4.38	112.14	106.94
24	b	606	CLA	C1-C2-C3	-4.37	118.48	126.04
24	b	610	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
24	a	408	CLA	C3D-C4D-ND	4.36	117.30	110.24
24	A	408	CLA	C3D-C4D-ND	4.36	117.30	110.24
24	B	610	CLA	CHD-C1D-ND	-4.36	120.44	124.45
24	C	506	CLA	C3C-C4C-NC	4.36	115.46	110.57
24	c	506	CLA	C3C-C4C-NC	4.36	115.46	110.57
24	b	612	CLA	C3C-C4C-NC	4.36	115.46	110.57
24	B	604	CLA	C1-C2-C3	-4.36	118.51	126.04
28	a	411	PL9	C7-C3-C4	4.34	120.41	116.88
24	b	603	CLA	C1C-C2C-C3C	-4.34	102.39	106.96
27	F	101	SQD	O7-S-C6	4.34	112.09	106.94
24	C	504	CLA	C3D-C4D-ND	4.33	117.25	110.24
24	c	504	CLA	C3D-C4D-ND	4.33	117.25	110.24
24	B	611	CLA	O2D-CGD-CBD	4.33	118.96	111.27
24	b	613	CLA	O2D-CGD-CBD	4.33	118.96	111.27
24	c	503	CLA	C3C-C4C-NC	4.32	115.42	110.57
24	C	507	CLA	C3B-C4B-NB	4.32	114.79	109.21
24	c	507	CLA	C3B-C4B-NB	4.32	114.79	109.21
24	b	610	CLA	C1D-CHD-C4C	-4.31	116.76	126.06
24	d	404	CLA	CAC-C3C-C4C	4.31	130.40	124.81
24	c	514	CLA	CAC-C3C-C4C	4.31	130.40	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	606	CLA	C4A-NA-C1A	-4.31	104.77	106.71
24	b	608	CLA	C4A-NA-C1A	-4.31	104.77	106.71
24	C	510	CLA	CMB-C2B-C3B	4.30	132.73	124.68
24	c	510	CLA	CMB-C2B-C3B	4.30	132.73	124.68
24	B	603	CLA	C3C-C4C-NC	4.30	115.39	110.57
24	b	605	CLA	C3C-C4C-NC	4.30	115.39	110.57
24	B	601	CLA	C1C-C2C-C3C	-4.29	102.44	106.96
24	B	608	CLA	C1D-CHD-C4C	-4.29	116.79	126.06
24	C	514	CLA	CAC-C3C-C4C	4.29	130.38	124.81
24	D	401	CLA	CHD-C4C-C3C	-4.29	118.53	124.84
24	d	401	CLA	CHD-C4C-C3C	-4.29	118.53	124.84
24	D	404	CLA	CAC-C3C-C4C	4.29	130.37	124.81
24	b	616	CLA	C1C-C2C-C3C	-4.28	102.45	106.96
27	F	101	SQD	O47-C7-C8	4.28	120.72	111.50
27	f	101	SQD	O47-C7-C8	4.28	120.72	111.50
24	D	405	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
24	B	607	CLA	C3D-C4D-ND	4.28	117.15	110.24
24	b	609	CLA	C3D-C4D-ND	4.28	117.15	110.24
24	C	503	CLA	C3C-C4C-NC	4.27	115.36	110.57
27	A	410	SQD	O9-S-C6	4.26	112.00	106.94
27	a	410	SQD	O9-S-C6	4.26	112.00	106.94
24	c	502	CLA	CMB-C2B-C3B	4.26	132.65	124.68
24	d	405	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
24	B	614	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
24	A	406	CLA	O2D-CGD-CBD	4.25	118.82	111.27
24	a	406	CLA	O2D-CGD-CBD	4.25	118.82	111.27
24	B	615	CLA	C4A-NA-C1A	-4.25	104.80	106.71
24	b	617	CLA	C4A-NA-C1A	-4.25	104.80	106.71
24	c	509	CLA	C3D-C4D-ND	4.24	117.10	110.24
24	C	503	CLA	CHD-C1D-ND	-4.24	120.56	124.45
24	c	503	CLA	CHD-C1D-ND	-4.24	120.56	124.45
24	B	612	CLA	C4C-C3C-C2C	-4.23	100.73	106.90
24	b	614	CLA	C4C-C3C-C2C	-4.23	100.73	106.90
24	C	502	CLA	CMB-C2B-C3B	4.22	132.58	124.68
24	C	509	CLA	C3D-C4D-ND	4.22	117.07	110.24
24	C	510	CLA	C3C-C4C-NC	4.22	115.30	110.57
34	D	410	LHG	O4-P-O5	4.22	133.09	112.24
34	d	410	LHG	O4-P-O5	4.22	133.09	112.24
24	b	610	CLA	O2D-CGD-CBD	4.21	118.75	111.27
24	B	604	CLA	C3C-C4C-NC	4.21	115.29	110.57
24	b	606	CLA	C3C-C4C-NC	4.21	115.29	110.57
24	B	610	CLA	C3C-C4C-NC	4.20	115.28	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	510	CLA	C3C-C4C-NC	4.20	115.28	110.57
24	C	514	CLA	CMB-C2B-C3B	4.20	132.53	124.68
24	B	608	CLA	O2D-CGD-CBD	4.19	118.72	111.27
24	B	603	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
24	b	605	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
34	l	101	LHG	O4-P-O5	4.17	132.88	112.24
34	L	101	LHG	O4-P-O5	4.17	132.88	112.24
24	A	406	CLA	C1D-CHD-C4C	-4.17	117.06	126.06
24	a	406	CLA	C1D-CHD-C4C	-4.17	117.06	126.06
24	c	514	CLA	CMB-C2B-C3B	4.17	132.48	124.68
24	A	405	CLA	CHD-C1D-ND	-4.16	120.63	124.45
24	a	405	CLA	CHD-C1D-ND	-4.16	120.63	124.45
24	C	504	CLA	C1D-CHD-C4C	-4.16	117.09	126.06
24	c	504	CLA	C1D-CHD-C4C	-4.16	117.09	126.06
24	C	509	CLA	O2D-CGD-O1D	-4.15	115.72	123.84
24	c	509	CLA	O2D-CGD-O1D	-4.15	115.72	123.84
24	B	602	CLA	C3D-C4D-ND	4.15	116.95	110.24
24	b	604	CLA	C3D-C4D-ND	4.15	116.95	110.24
24	c	514	CLA	O2D-CGD-O1D	-4.15	115.73	123.84
24	C	514	CLA	O2D-CGD-O1D	-4.14	115.73	123.84
24	B	601	CLA	C3C-C4C-NC	4.14	115.21	110.57
24	b	603	CLA	C3C-C4C-NC	4.14	115.21	110.57
24	B	609	CLA	C3D-C4D-ND	4.13	116.93	110.24
24	A	406	CLA	C3D-C2D-C1D	-4.13	100.20	105.83
24	a	406	CLA	C3D-C2D-C1D	-4.13	100.20	105.83
24	B	605	CLA	C3C-C4C-NC	4.12	115.19	110.57
24	b	607	CLA	C3C-C4C-NC	4.12	115.19	110.57
24	B	603	CLA	CMB-C2B-C3B	4.12	132.38	124.68
27	A	410	SQD	O9-S-O7	-4.12	99.71	113.95
27	a	410	SQD	O9-S-O7	-4.12	99.71	113.95
24	b	605	CLA	CMB-C2B-C3B	4.11	132.37	124.68
24	b	611	CLA	C3D-C4D-ND	4.10	116.87	110.24
24	C	504	CLA	CAC-C3C-C4C	4.10	130.13	124.81
24	c	504	CLA	CAC-C3C-C4C	4.10	130.13	124.81
24	C	505	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
24	c	505	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
28	d	407	PL9	O1-C4-C3	-4.09	116.21	120.72
32	C	521	LMT	O1B-C4'-C3'	4.09	118.15	107.28
32	c	521	LMT	O1B-C4'-C3'	4.09	118.15	107.28
28	D	407	PL9	O1-C4-C3	-4.08	116.22	120.72
24	B	603	CLA	C3D-C4D-ND	4.08	116.84	110.24
24	C	503	CLA	C3D-C2D-C1D	-4.08	100.26	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	503	CLA	C3D-C2D-C1D	-4.08	100.26	105.83
24	B	606	CLA	C3D-C4D-ND	4.08	116.84	110.24
24	b	605	CLA	C3D-C4D-ND	4.08	116.84	110.24
27	B	620	SQD	O47-C7-C8	4.08	120.29	111.50
27	L	102	SQD	O47-C7-C8	4.08	120.29	111.50
24	b	608	CLA	C3D-C4D-ND	4.08	116.83	110.24
24	c	507	CLA	CBC-CAC-C3C	-4.07	101.20	112.43
24	C	507	CLA	CBC-CAC-C3C	-4.07	101.20	112.43
24	C	503	CLA	C3D-C4D-ND	4.06	116.81	110.24
24	c	503	CLA	C3D-C4D-ND	4.06	116.81	110.24
34	E	101	LHG	O4-P-O5	4.05	132.28	112.24
34	e	101	LHG	O4-P-O5	4.05	132.28	112.24
24	C	505	CLA	C3B-C4B-NB	4.05	114.45	109.21
24	c	505	CLA	C3B-C4B-NB	4.05	114.45	109.21
24	C	509	CLA	CMD-C2D-C1D	4.05	131.84	124.71
24	c	509	CLA	CMD-C2D-C1D	4.05	131.84	124.71
24	C	512	CLA	O2D-CGD-CBD	4.03	118.44	111.27
24	c	512	CLA	O2D-CGD-CBD	4.03	118.43	111.27
24	C	510	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
24	c	510	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
24	B	614	CLA	C3B-C4B-NB	4.02	114.40	109.21
24	C	508	CLA	C3D-C4D-ND	4.01	116.72	110.24
24	c	508	CLA	C3D-C4D-ND	4.01	116.72	110.24
24	b	607	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
31	C	517	DGD	C6D-O5D-C1E	4.00	121.56	113.74
24	c	503	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
24	B	608	CLA	CAC-C3C-C4C	4.00	130.00	124.81
24	B	605	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
31	c	517	DGD	C6D-O5D-C1E	4.00	121.55	113.74
24	C	512	CLA	C1-C2-C3	-4.00	119.13	126.04
24	c	512	CLA	C1-C2-C3	-4.00	119.13	126.04
24	b	610	CLA	CAC-C3C-C4C	4.00	130.00	124.81
24	b	616	CLA	C3B-C4B-NB	3.98	114.36	109.21
24	B	605	CLA	C4-C3-C5	3.98	121.96	115.27
24	B	605	CLA	C3D-C4D-ND	3.97	116.66	110.24
24	b	607	CLA	C3D-C4D-ND	3.97	116.66	110.24
24	b	605	CLA	O2A-CGA-CBA	3.97	124.37	111.91
24	b	614	CLA	C3D-C2D-C1D	-3.97	100.41	105.83
24	C	510	CLA	C3B-C4B-NB	3.97	114.34	109.21
24	C	503	CLA	C1C-C2C-C3C	-3.96	102.79	106.96
24	b	607	CLA	C4-C3-C5	3.96	121.94	115.27
24	B	616	CLA	C4A-NA-C1A	-3.96	104.92	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	618	CLA	C4A-NA-C1A	-3.96	104.92	106.71
24	c	510	CLA	C3B-C4B-NB	3.96	114.33	109.21
24	B	603	CLA	O2A-CGA-CBA	3.95	124.32	111.91
35	e	103	HEM	CBA-CAA-C2A	-3.95	105.87	112.62
24	c	509	CLA	CHD-C1D-ND	-3.95	120.82	124.45
35	E	103	HEM	CBA-CAA-C2A	-3.95	105.88	112.62
37	v	201	HEC	CMB-C2B-C1B	-3.95	122.39	128.46
24	B	612	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
37	V	201	HEC	CMB-C2B-C1B	-3.94	122.41	128.46
24	B	602	CLA	C1-O2A-CGA	3.94	126.78	116.44
24	c	511	CLA	C3B-C4B-NB	3.93	114.29	109.21
24	B	611	CLA	CAC-C3C-C4C	3.93	129.91	124.81
24	b	613	CLA	CAC-C3C-C4C	3.93	129.91	124.81
27	f	101	SQD	C4-C3-C2	3.93	117.68	110.82
24	d	404	CLA	CMC-C2C-C1C	3.93	131.02	125.04
24	C	509	CLA	CHD-C1D-ND	-3.93	120.84	124.45
24	b	611	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
24	a	405	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
24	C	511	CLA	C3B-C4B-NB	3.92	114.28	109.21
24	A	405	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
24	b	604	CLA	C1-O2A-CGA	3.92	126.73	116.44
24	B	615	CLA	C3D-C4D-ND	3.92	116.58	110.24
24	b	617	CLA	C3D-C4D-ND	3.92	116.58	110.24
24	D	404	CLA	CMC-C2C-C1C	3.92	131.01	125.04
24	c	514	CLA	C2C-C1C-NC	3.92	113.64	109.97
27	F	101	SQD	C4-C3-C2	3.92	117.66	110.82
24	A	408	CLA	C4-C3-C5	3.91	121.85	115.27
24	a	408	CLA	C4-C3-C5	3.91	121.85	115.27
24	C	509	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
24	c	509	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
24	b	612	CLA	C3D-C4D-ND	3.91	116.56	110.24
24	B	602	CLA	C2C-C1C-NC	3.90	113.63	109.97
24	b	604	CLA	C2C-C1C-NC	3.90	113.63	109.97
24	C	513	CLA	C3D-C4D-ND	3.90	116.55	110.24
24	c	513	CLA	C3D-C4D-ND	3.90	116.55	110.24
24	B	610	CLA	C3D-C4D-ND	3.89	116.53	110.24
24	C	514	CLA	C2C-C1C-NC	3.88	113.61	109.97
24	C	506	CLA	C3D-C4D-ND	3.88	116.52	110.24
24	c	506	CLA	C3D-C4D-ND	3.88	116.52	110.24
24	b	610	CLA	C3D-C4D-ND	3.88	116.52	110.24
24	B	615	CLA	C3B-C4B-NB	3.87	114.21	109.21
24	b	617	CLA	C3B-C4B-NB	3.87	114.21	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	613	CLA	C3C-C4C-NC	3.87	114.91	110.57
24	b	615	CLA	C3C-C4C-NC	3.87	114.91	110.57
24	B	604	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
24	b	606	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
24	C	507	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
24	c	507	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
24	B	608	CLA	C3D-C4D-ND	3.85	116.47	110.24
24	A	405	CLA	C3D-C4D-ND	3.85	116.47	110.24
24	a	405	CLA	C3D-C4D-ND	3.85	116.47	110.24
24	B	609	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
24	C	503	CLA	O2D-CGD-O1D	-3.84	116.33	123.84
24	c	503	CLA	O2D-CGD-O1D	-3.84	116.33	123.84
31	C	517	DGD	O3G-C3G-C2G	-3.84	101.64	110.90
24	B	602	CLA	C3C-C4C-NC	3.84	114.87	110.57
24	b	604	CLA	C3C-C4C-NC	3.84	114.87	110.57
24	C	502	CLA	C3D-C4D-ND	3.84	116.44	110.24
31	c	517	DGD	O3G-C3G-C2G	-3.83	101.65	110.90
24	B	603	CLA	CHD-C1D-ND	-3.83	120.93	124.45
24	c	502	CLA	C3D-C4D-ND	3.83	116.43	110.24
35	E	103	HEM	CMC-C2C-C3C	3.83	131.84	124.68
35	e	103	HEM	CMC-C2C-C3C	3.83	131.84	124.68
24	C	505	CLA	C3C-C4C-NC	3.82	114.86	110.57
24	c	505	CLA	C3C-C4C-NC	3.82	114.86	110.57
24	b	610	CLA	CMC-C2C-C1C	3.82	130.86	125.04
24	C	502	CLA	CMC-C2C-C1C	3.82	130.86	125.04
24	c	502	CLA	CMC-C2C-C1C	3.82	130.86	125.04
24	b	605	CLA	CHD-C1D-ND	-3.81	120.95	124.45
24	b	610	CLA	C4A-NA-C1A	-3.81	104.99	106.71
24	B	608	CLA	CMC-C2C-C1C	3.81	130.84	125.04
24	B	611	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
24	B	615	CLA	C4C-C3C-C2C	-3.81	101.34	106.90
24	b	617	CLA	C4C-C3C-C2C	-3.81	101.34	106.90
24	B	605	CLA	CMB-C2B-C3B	3.81	131.81	124.68
24	b	607	CLA	CMB-C2B-C3B	3.81	131.81	124.68
24	B	603	CLA	CBA-CAA-C2A	3.81	125.11	113.86
24	b	605	CLA	CBA-CAA-C2A	3.81	125.11	113.86
24	B	601	CLA	C3D-C4D-ND	3.81	116.39	110.24
24	b	603	CLA	C3D-C4D-ND	3.81	116.39	110.24
24	C	514	CLA	C3D-C4D-ND	3.80	116.39	110.24
24	c	514	CLA	C3D-C4D-ND	3.80	116.39	110.24
24	B	608	CLA	C4A-NA-C1A	-3.80	105.00	106.71
24	b	611	CLA	C1D-CHD-C4C	-3.80	117.86	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	504	CLA	O2D-CGD-CBD	3.80	118.02	111.27
24	c	504	CLA	O2D-CGD-CBD	3.80	118.02	111.27
24	b	611	CLA	C3B-C4B-NB	3.80	114.12	109.21
24	B	609	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
24	b	613	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
26	D	406	BCR	C24-C23-C22	-3.79	120.51	126.23
24	d	404	CLA	C4C-C3C-C2C	-3.79	101.38	106.90
24	C	505	CLA	C3D-C4D-ND	3.79	116.36	110.24
24	c	505	CLA	C3D-C4D-ND	3.79	116.36	110.24
26	d	406	BCR	C24-C23-C22	-3.78	120.52	126.23
24	D	404	CLA	C4C-C3C-C2C	-3.78	101.39	106.90
24	c	507	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
24	C	509	CLA	C4C-C3C-C2C	-3.76	101.42	106.90
24	c	509	CLA	C4C-C3C-C2C	-3.76	101.42	106.90
24	C	507	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
24	B	613	CLA	CMB-C2B-C3B	3.75	131.70	124.68
24	b	615	CLA	CMB-C2B-C3B	3.75	131.70	124.68
24	B	607	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
24	b	609	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
24	C	508	CLA	C3B-C4B-NB	3.74	114.05	109.21
24	c	508	CLA	C3B-C4B-NB	3.74	114.05	109.21
24	B	609	CLA	C3B-C4B-NB	3.74	114.04	109.21
38	X	101	RRX	C11-C10-C9	-3.74	121.98	127.31
38	x	101	RRX	C11-C10-C9	-3.74	121.98	127.31
24	b	614	CLA	C3D-C4D-ND	3.74	116.28	110.24
38	x	101	RRX	C38-C26-C25	-3.73	120.34	124.53
27	a	412	SQD	O9-S-O7	-3.72	101.06	113.95
24	A	406	CLA	C4C-C3C-C2C	-3.72	101.47	106.90
24	b	616	CLA	C3C-C4C-NC	3.72	114.74	110.57
38	X	101	RRX	C38-C26-C25	-3.72	120.36	124.53
27	A	412	SQD	O9-S-O7	-3.71	101.09	113.95
24	B	612	CLA	C3D-C4D-ND	3.71	116.24	110.24
24	B	614	CLA	CMC-C2C-C1C	3.71	130.69	125.04
24	b	616	CLA	CMC-C2C-C1C	3.71	130.69	125.04
27	a	412	SQD	O47-C7-C8	3.71	119.49	111.50
24	B	614	CLA	C3C-C4C-NC	3.71	114.73	110.57
24	C	503	CLA	C3B-C4B-NB	3.71	114.00	109.21
24	b	614	CLA	C3B-C4B-NB	3.71	114.00	109.21
24	c	503	CLA	C3B-C4B-NB	3.71	114.00	109.21
24	b	616	CLA	CAC-C3C-C4C	3.70	129.61	124.81
24	B	603	CLA	C4A-NA-C1A	-3.70	105.04	106.71
24	b	605	CLA	C4A-NA-C1A	-3.70	105.04	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	412	SQD	O47-C7-C8	3.70	119.47	111.50
24	C	504	CLA	C4C-C3C-C2C	-3.70	101.51	106.90
24	c	504	CLA	C4C-C3C-C2C	-3.70	101.51	106.90
24	b	608	CLA	C4C-C3C-C2C	-3.70	101.51	106.90
38	X	101	RRX	C33-C5-C6	-3.69	120.38	124.53
38	x	101	RRX	C33-C5-C6	-3.69	120.38	124.53
24	a	406	CLA	C4C-C3C-C2C	-3.69	101.52	106.90
24	B	612	CLA	C3B-C4B-NB	3.68	113.97	109.21
24	c	502	CLA	C3B-C4B-NB	3.68	113.97	109.21
24	C	510	CLA	C3D-C4D-ND	3.67	116.18	110.24
24	c	510	CLA	C3D-C4D-ND	3.67	116.18	110.24
24	B	616	CLA	C3C-C4C-NC	3.67	114.69	110.57
24	b	618	CLA	C3C-C4C-NC	3.67	114.69	110.57
24	B	603	CLA	C3D-C2D-C1D	-3.67	100.82	105.83
24	B	614	CLA	CAC-C3C-C4C	3.66	129.56	124.81
24	B	610	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
24	B	613	CLA	C3B-C4B-NB	3.66	113.94	109.21
24	b	615	CLA	C3B-C4B-NB	3.66	113.94	109.21
24	b	605	CLA	C3D-C2D-C1D	-3.66	100.84	105.83
24	B	606	CLA	C4C-C3C-C2C	-3.66	101.57	106.90
24	b	612	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
24	B	610	CLA	CAA-C2A-C3A	-3.66	102.77	112.78
27	B	620	SQD	C4-C3-C2	3.65	117.20	110.82
24	A	408	CLA	CAA-C2A-C3A	-3.65	102.78	112.78
34	D	409	LHG	O4-P-O5	3.65	130.30	112.24
34	d	409	LHG	O4-P-O5	3.65	130.30	112.24
24	C	502	CLA	C3B-C4B-NB	3.65	113.93	109.21
24	B	608	CLA	CMD-C2D-C1D	3.65	131.15	124.71
27	L	102	SQD	C4-C3-C2	3.65	117.19	110.82
24	B	604	CLA	CMC-C2C-C1C	3.64	130.59	125.04
24	b	606	CLA	CMC-C2C-C1C	3.64	130.59	125.04
24	B	604	CLA	O2D-CGD-O1D	-3.64	116.72	123.84
24	C	509	CLA	CAC-C3C-C4C	3.64	129.53	124.81
24	c	509	CLA	CAC-C3C-C4C	3.64	129.53	124.81
24	a	408	CLA	CAA-C2A-C3A	-3.64	102.81	112.78
24	c	502	CLA	C3C-C4C-NC	3.64	114.65	110.57
24	b	605	CLA	O2A-CGA-O1A	-3.63	114.42	123.59
24	B	605	CLA	O2D-CGD-O1D	-3.63	116.74	123.84
24	b	607	CLA	O2D-CGD-O1D	-3.63	116.74	123.84
24	A	405	CLA	C3B-C4B-NB	3.63	113.90	109.21
24	a	405	CLA	C3B-C4B-NB	3.63	113.90	109.21
24	B	616	CLA	C3B-C4B-NB	3.63	113.90	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	618	CLA	C3B-C4B-NB	3.63	113.90	109.21
24	B	603	CLA	O2A-CGA-O1A	-3.63	114.44	123.59
24	b	606	CLA	O2D-CGD-O1D	-3.62	116.75	123.84
24	C	514	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
24	b	610	CLA	CMD-C2D-C1D	3.62	131.09	124.71
24	b	612	CLA	CAA-C2A-C3A	-3.62	102.88	112.78
34	D	408	LHG	O4-P-O5	3.61	130.11	112.24
34	d	408	LHG	O4-P-O5	3.61	130.11	112.24
24	c	514	CLA	C1D-CHD-C4C	-3.61	118.26	126.06
37	v	201	HEC	CMC-C2C-C1C	-3.61	122.91	128.46
24	b	610	CLA	C3C-C4C-NC	3.61	114.62	110.57
24	B	610	CLA	O2D-CGD-CBD	3.61	117.68	111.27
24	C	503	CLA	C1-C2-C3	-3.61	119.81	126.04
24	c	503	CLA	C1-C2-C3	-3.61	119.81	126.04
26	C	522	BCR	C24-C23-C22	-3.60	120.79	126.23
26	c	522	BCR	C24-C23-C22	-3.60	120.79	126.23
24	C	502	CLA	C3C-C4C-NC	3.60	114.61	110.57
24	B	608	CLA	C3C-C4C-NC	3.60	114.61	110.57
24	d	401	CLA	CMA-C3A-C2A	-3.60	99.31	113.83
24	D	401	CLA	CMA-C3A-C2A	-3.60	99.31	113.83
24	C	507	CLA	CHC-C1C-C2C	-3.59	116.78	126.72
24	c	507	CLA	CHC-C1C-C2C	-3.59	116.78	126.72
24	B	616	CLA	C3D-C4D-ND	3.59	116.05	110.24
24	b	618	CLA	C3D-C4D-ND	3.59	116.05	110.24
26	c	515	BCR	C24-C23-C22	-3.59	120.81	126.23
24	C	512	CLA	C4C-C3C-C2C	-3.59	101.66	106.90
24	A	405	CLA	CMB-C2B-C3B	3.59	131.39	124.68
24	a	405	CLA	CMB-C2B-C3B	3.59	131.39	124.68
24	C	511	CLA	C3D-C4D-ND	3.59	116.04	110.24
24	c	511	CLA	C3D-C4D-ND	3.59	116.04	110.24
24	c	512	CLA	C4C-C3C-C2C	-3.58	101.67	106.90
24	b	613	CLA	CMB-C2B-C3B	3.58	131.38	124.68
37	V	201	HEC	CMC-C2C-C1C	-3.58	122.96	128.46
24	C	513	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
24	c	513	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
24	B	613	CLA	C3D-C4D-ND	3.58	116.03	110.24
24	b	615	CLA	C3D-C4D-ND	3.58	116.03	110.24
26	D	406	BCR	C7-C8-C9	-3.58	120.83	126.23
26	d	406	BCR	C7-C8-C9	-3.58	120.83	126.23
24	C	506	CLA	C4A-NA-C1A	-3.58	105.10	106.71
24	c	506	CLA	C4A-NA-C1A	-3.58	105.10	106.71
24	B	611	CLA	CMB-C2B-C3B	3.58	131.37	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	506	CLA	CHD-C1D-ND	-3.56	121.18	124.45
24	c	506	CLA	CHD-C1D-ND	-3.56	121.18	124.45
24	B	603	CLA	CAA-C2A-C3A	-3.56	103.03	112.78
24	b	605	CLA	CAA-C2A-C3A	-3.56	103.03	112.78
27	f	101	SQD	O8-S-C6	3.56	111.41	105.74
24	B	607	CLA	C4C-C3C-C2C	-3.56	101.71	106.90
24	b	609	CLA	C4C-C3C-C2C	-3.56	101.71	106.90
24	b	611	CLA	CBC-CAC-C3C	-3.56	102.63	112.43
26	C	515	BCR	C24-C23-C22	-3.56	120.86	126.23
24	A	408	CLA	C3C-C4C-NC	3.55	114.56	110.57
24	a	408	CLA	C3C-C4C-NC	3.55	114.56	110.57
24	B	608	CLA	CHD-C1D-ND	-3.55	121.19	124.45
24	C	503	CLA	C1D-CHD-C4C	-3.55	118.40	126.06
24	b	614	CLA	C2A-C1A-CHA	-3.55	117.65	123.86
24	A	405	CLA	C3D-C2D-C1D	-3.55	100.99	105.83
24	a	405	CLA	C3D-C2D-C1D	-3.55	100.99	105.83
24	B	609	CLA	CBC-CAC-C3C	-3.54	102.67	112.43
24	c	503	CLA	C1D-CHD-C4C	-3.54	118.43	126.06
24	C	506	CLA	C1D-CHD-C4C	-3.54	118.43	126.06
24	c	506	CLA	C1D-CHD-C4C	-3.54	118.43	126.06
27	F	101	SQD	O8-S-C6	3.53	111.37	105.74
24	C	513	CLA	CMD-C2D-C1D	3.53	130.94	124.71
24	c	513	CLA	CMD-C2D-C1D	3.53	130.94	124.71
24	B	610	CLA	O2A-CGA-CBA	3.53	122.99	111.91
24	C	506	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
24	c	506	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
24	b	612	CLA	O2A-CGA-CBA	3.53	122.98	111.91
24	A	408	CLA	CBC-CAC-C3C	-3.52	102.72	112.43
24	a	408	CLA	CBC-CAC-C3C	-3.52	102.72	112.43
24	A	408	CLA	C3B-C4B-NB	3.52	113.77	109.21
24	B	612	CLA	C2A-C1A-CHA	-3.52	117.70	123.86
24	A	405	CLA	C4C-C3C-C2C	-3.52	101.77	106.90
24	a	405	CLA	C4C-C3C-C2C	-3.52	101.77	106.90
24	a	408	CLA	C3B-C4B-NB	3.52	113.76	109.21
24	C	511	CLA	C3D-C2D-C1D	-3.52	101.03	105.83
24	c	511	CLA	C3D-C2D-C1D	-3.52	101.03	105.83
24	b	610	CLA	CHD-C1D-ND	-3.51	121.22	124.45
32	c	521	LMT	C3'-C4'-C5'	-3.51	102.87	110.93
24	B	615	CLA	O2D-CGD-CBD	3.51	117.50	111.27
24	b	617	CLA	O2D-CGD-CBD	3.51	117.50	111.27
24	b	612	CLA	CHC-C1C-C2C	-3.51	117.02	126.72
24	B	604	CLA	C3B-C4B-NB	3.51	113.74	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	606	CLA	C3B-C4B-NB	3.51	113.74	109.21
24	c	503	CLA	CHC-C1C-C2C	-3.50	117.03	126.72
32	C	521	LMT	C3'-C4'-C5'	-3.50	102.90	110.93
24	b	604	CLA	CAA-C2A-C3A	-3.50	103.20	112.78
24	B	602	CLA	CAA-C2A-C3A	-3.50	103.20	112.78
24	C	503	CLA	CHC-C1C-C2C	-3.49	117.08	126.72
24	c	510	CLA	CAC-C3C-C4C	3.48	129.32	124.81
24	B	616	CLA	CAC-C3C-C4C	3.48	129.32	124.81
24	b	618	CLA	CAC-C3C-C4C	3.48	129.32	124.81
24	b	608	CLA	C1D-CHD-C4C	-3.48	118.56	126.06
24	C	510	CLA	CAC-C3C-C4C	3.47	129.32	124.81
24	B	610	CLA	CHC-C1C-C2C	-3.47	117.12	126.72
24	b	612	CLA	O2D-CGD-CBD	3.47	117.44	111.27
24	B	616	CLA	CHD-C4C-NC	3.47	129.66	124.20
24	b	618	CLA	CHD-C4C-NC	3.47	129.66	124.20
24	D	401	CLA	CED-O2D-CGD	3.47	123.78	115.94
24	d	401	CLA	CED-O2D-CGD	3.47	123.78	115.94
24	B	604	CLA	CHD-C1D-ND	-3.46	121.27	124.45
24	b	606	CLA	CHD-C1D-ND	-3.46	121.27	124.45
24	b	612	CLA	C4C-C3C-C2C	-3.46	101.85	106.90
24	b	615	CLA	CMC-C2C-C1C	3.46	130.31	125.04
24	B	606	CLA	C1D-CHD-C4C	-3.46	118.60	126.06
24	B	613	CLA	CMC-C2C-C1C	3.46	130.30	125.04
27	B	620	SQD	O9-S-O7	-3.45	101.99	113.95
27	L	102	SQD	O9-S-O7	-3.45	101.99	113.95
24	B	602	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
24	b	604	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
24	D	405	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
24	b	608	CLA	CAC-C3C-C4C	3.44	129.27	124.81
24	b	613	CLA	C3B-C4B-NB	3.43	113.64	109.21
31	C	518	DGD	O6D-C1D-O3G	-3.43	101.85	109.97
24	B	604	CLA	C3D-C2D-C1D	-3.43	101.15	105.83
24	C	510	CLA	CMC-C2C-C1C	3.43	130.26	125.04
24	c	510	CLA	CMC-C2C-C1C	3.43	130.26	125.04
24	d	405	CLA	C1C-C2C-C3C	-3.43	103.36	106.96
24	D	401	CLA	C3B-C4B-NB	3.43	113.64	109.21
24	d	401	CLA	C3B-C4B-NB	3.43	113.64	109.21
31	c	518	DGD	O6D-C1D-O3G	-3.42	101.87	109.97
24	C	504	CLA	C4A-NA-C1A	-3.42	105.17	106.71
24	c	504	CLA	C4A-NA-C1A	-3.42	105.17	106.71
24	B	608	CLA	C11-C12-C13	-3.42	104.87	115.92
24	b	610	CLA	C11-C12-C13	-3.42	104.87	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	606	CLA	C3D-C4D-ND	3.41	115.76	110.24
24	B	606	CLA	CAC-C3C-C4C	3.41	129.24	124.81
24	B	605	CLA	CMC-C2C-C1C	3.41	130.24	125.04
24	b	606	CLA	C1-O2A-CGA	3.41	125.39	116.44
24	B	610	CLA	C4C-C3C-C2C	-3.41	101.93	106.90
24	B	611	CLA	C3B-C4B-NB	3.41	113.62	109.21
24	B	604	CLA	C1-O2A-CGA	3.41	125.39	116.44
24	b	606	CLA	C3D-C2D-C1D	-3.41	101.18	105.83
24	A	406	CLA	C3D-C4D-ND	3.40	115.74	110.24
24	a	406	CLA	C3D-C4D-ND	3.40	115.74	110.24
24	C	513	CLA	CMC-C2C-C1C	3.40	130.22	125.04
24	C	508	CLA	CAC-C3C-C2C	3.40	133.34	127.53
24	B	604	CLA	C3D-C4D-ND	3.40	115.73	110.24
24	C	511	CLA	CHC-C1C-C2C	-3.40	117.32	126.72
24	c	511	CLA	CHC-C1C-C2C	-3.40	117.32	126.72
24	b	613	CLA	C3C-C4C-NC	3.40	114.38	110.57
24	c	513	CLA	CMC-C2C-C1C	3.40	130.21	125.04
24	b	603	CLA	O2D-CGD-O1D	-3.40	117.20	123.84
24	B	611	CLA	C3C-C4C-NC	3.39	114.38	110.57
24	B	602	CLA	C3B-C4B-NB	3.39	113.60	109.21
24	c	508	CLA	CAC-C3C-C2C	3.39	133.33	127.53
28	A	411	PL9	C7-C3-C2	-3.39	118.84	123.30
24	b	607	CLA	CMC-C2C-C1C	3.39	130.20	125.04
24	B	615	CLA	CED-O2D-CGD	3.39	123.59	115.94
24	b	617	CLA	CED-O2D-CGD	3.39	123.59	115.94
24	B	601	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
24	d	404	CLA	C3B-C4B-NB	3.38	113.58	109.21
24	B	603	CLA	C3B-C4B-NB	3.38	113.58	109.21
24	b	605	CLA	C3B-C4B-NB	3.38	113.58	109.21
31	C	518	DGD	O3G-C3G-C2G	-3.38	102.75	110.90
31	c	518	DGD	O3G-C3G-C2G	-3.38	102.75	110.90
24	b	610	CLA	CMB-C2B-C3B	3.38	130.99	124.68
24	C	505	CLA	CHC-C1C-C2C	-3.37	117.40	126.72
24	c	505	CLA	CHC-C1C-C2C	-3.37	117.40	126.72
24	D	404	CLA	C3B-C4B-NB	3.36	113.56	109.21
24	C	507	CLA	CAA-C2A-C3A	-3.36	103.58	112.78
24	B	611	CLA	CHC-C1C-C2C	-3.35	117.44	126.72
24	B	608	CLA	CMB-C2B-C3B	3.35	130.95	124.68
24	c	507	CLA	CAA-C2A-C3A	-3.35	103.60	112.78
24	b	608	CLA	CAA-C2A-C3A	-3.35	103.60	112.78
28	a	411	PL9	C7-C3-C2	-3.35	118.89	123.30
24	D	405	CLA	C4C-C3C-C2C	-3.35	102.02	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	608	CLA	C1-C2-C3	-3.35	120.25	126.04
24	b	610	CLA	C1-C2-C3	-3.35	120.25	126.04
24	d	405	CLA	C4C-C3C-C2C	-3.35	102.02	106.90
24	B	606	CLA	CAA-C2A-C3A	-3.34	103.63	112.78
24	C	509	CLA	CHC-C1C-C2C	-3.34	117.48	126.72
24	c	509	CLA	CHC-C1C-C2C	-3.34	117.48	126.72
24	b	611	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
24	b	613	CLA	CHC-C1C-C2C	-3.34	117.49	126.72
24	b	604	CLA	C3B-C4B-NB	3.34	113.53	109.21
24	B	609	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
24	C	513	CLA	C4C-C3C-C2C	-3.33	102.04	106.90
24	c	513	CLA	C4C-C3C-C2C	-3.33	102.04	106.90
24	B	611	CLA	C1D-CHD-C4C	-3.33	118.87	126.06
24	b	613	CLA	C1D-CHD-C4C	-3.33	118.87	126.06
24	B	608	CLA	C3D-C2D-C1D	-3.33	101.29	105.83
24	B	615	CLA	CHC-C1C-C2C	-3.32	117.52	126.72
24	b	617	CLA	CHC-C1C-C2C	-3.32	117.52	126.72
24	b	610	CLA	CMA-C3A-C2A	-3.32	100.43	113.83
24	B	608	CLA	CMA-C3A-C2A	-3.32	100.43	113.83
24	B	616	CLA	C4-C3-C5	3.32	120.86	115.27
24	b	618	CLA	C4-C3-C5	3.32	120.86	115.27
24	c	512	CLA	CED-O2D-CGD	3.32	123.44	115.94
24	B	616	CLA	CHC-C1C-C2C	-3.31	117.56	126.72
24	b	618	CLA	CHC-C1C-C2C	-3.31	117.56	126.72
24	C	512	CLA	CAC-C3C-C4C	3.30	129.10	124.81
24	B	613	CLA	C1-C2-C3	-3.30	120.33	126.04
37	v	201	HEC	CMC-C2C-C3C	3.30	129.70	125.82
24	C	507	CLA	C3C-C4C-NC	3.30	114.27	110.57
24	c	507	CLA	C3C-C4C-NC	3.30	114.27	110.57
24	A	408	CLA	CHB-C4A-NA	3.30	129.08	124.51
24	C	512	CLA	CED-O2D-CGD	3.30	123.40	115.94
24	a	408	CLA	CHB-C4A-NA	3.30	129.07	124.51
25	A	407	PHO	CMB-C2B-C3B	3.30	130.85	124.68
25	a	407	PHO	CMB-C2B-C3B	3.30	130.85	124.68
24	c	512	CLA	CAC-C3C-C4C	3.30	129.09	124.81
24	b	615	CLA	C1-C2-C3	-3.29	120.35	126.04
24	C	512	CLA	C1D-CHD-C4C	-3.29	118.95	126.06
24	B	603	CLA	C4C-C3C-C2C	-3.29	102.10	106.90
24	b	605	CLA	C4C-C3C-C2C	-3.29	102.10	106.90
24	A	406	CLA	C3B-C4B-NB	3.29	113.46	109.21
24	a	406	CLA	C3B-C4B-NB	3.29	113.46	109.21
24	C	514	CLA	C3C-C4C-NC	3.29	114.26	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	x	101	RRX	C24-C23-C22	-3.29	121.27	126.23
24	b	610	CLA	C3D-C2D-C1D	-3.29	101.35	105.83
24	c	514	CLA	C3C-C4C-NC	3.28	114.25	110.57
26	A	409	BCR	C15-C14-C13	-3.28	122.62	127.31
38	x	101	RRX	C23-C24-C25	-3.28	117.98	127.20
24	c	512	CLA	C1D-CHD-C4C	-3.28	118.97	126.06
37	V	201	HEC	CMC-C2C-C3C	3.28	129.68	125.82
24	C	506	CLA	CAC-C3C-C4C	3.28	129.07	124.81
24	c	506	CLA	CAC-C3C-C4C	3.28	129.07	124.81
24	A	405	CLA	C1D-CHD-C4C	-3.28	118.98	126.06
24	a	405	CLA	C1D-CHD-C4C	-3.28	118.98	126.06
31	C	519	DGD	O3G-C3G-C2G	-3.27	103.00	110.90
31	c	519	DGD	O3G-C3G-C2G	-3.27	103.00	110.90
26	a	409	BCR	C15-C14-C13	-3.27	122.64	127.31
24	B	610	CLA	C1D-CHD-C4C	-3.27	119.00	126.06
24	b	612	CLA	C3B-C4B-NB	3.27	113.43	109.21
24	C	507	CLA	C3D-C4D-ND	3.27	115.52	110.24
24	c	507	CLA	C3D-C4D-ND	3.27	115.52	110.24
24	B	616	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
24	b	618	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
24	C	504	CLA	CMC-C2C-C1C	3.26	130.01	125.04
24	c	504	CLA	CMC-C2C-C1C	3.26	130.01	125.04
38	X	101	RRX	C23-C24-C25	-3.26	118.04	127.20
24	C	506	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
24	c	506	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
24	b	612	CLA	C1D-CHD-C4C	-3.26	119.02	126.06
38	X	101	RRX	C24-C23-C22	-3.26	121.31	126.23
24	B	615	CLA	CAC-C3C-C4C	3.25	129.03	124.81
24	b	617	CLA	CAC-C3C-C4C	3.25	129.03	124.81
27	A	412	SQD	O5-C5-C4	3.25	115.60	109.69
24	a	406	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
24	b	616	CLA	CAA-C2A-C3A	-3.25	103.88	112.78
24	B	612	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
24	b	614	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
24	B	601	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
24	b	603	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
24	B	614	CLA	CAA-C2A-C3A	-3.24	103.90	112.78
38	X	101	RRX	C10-C11-C12	-3.24	113.11	123.22
38	x	101	RRX	C10-C11-C12	-3.24	113.11	123.22
25	D	402	PHO	O2D-CGD-O1D	-3.24	117.51	123.84
25	d	402	PHO	O2D-CGD-O1D	-3.24	117.51	123.84
24	B	603	CLA	C1D-CHD-C4C	-3.23	119.08	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	412	SQD	O5-C5-C4	3.23	115.56	109.69
24	C	502	CLA	C1D-CHD-C4C	-3.23	119.08	126.06
24	A	406	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
24	B	613	CLA	O2D-CGD-CBD	3.23	117.00	111.27
24	b	615	CLA	O2D-CGD-CBD	3.23	117.00	111.27
24	A	408	CLA	CMC-C2C-C1C	3.23	129.95	125.04
24	a	408	CLA	CMC-C2C-C1C	3.23	129.95	125.04
24	b	614	CLA	C4-C3-C5	3.22	120.69	115.27
24	b	605	CLA	C5-C3-C2	-3.22	114.60	121.12
24	b	617	CLA	C1-O2A-CGA	3.22	124.89	116.44
24	b	605	CLA	C1D-CHD-C4C	-3.22	119.11	126.06
24	C	505	CLA	CAC-C3C-C4C	3.22	128.99	124.81
24	c	505	CLA	CAC-C3C-C4C	3.22	128.99	124.81
24	B	603	CLA	C5-C3-C2	-3.22	114.60	121.12
24	B	606	CLA	C1C-C2C-C3C	-3.21	103.58	106.96
24	c	502	CLA	C1D-CHD-C4C	-3.21	119.12	126.06
24	B	616	CLA	C1-O2A-CGA	3.21	124.87	116.44
24	B	612	CLA	C4-C3-C5	3.21	120.67	115.27
24	C	502	CLA	CHC-C1C-C2C	-3.21	117.85	126.72
24	c	502	CLA	CHC-C1C-C2C	-3.21	117.85	126.72
24	D	405	CLA	CMC-C2C-C1C	3.21	129.92	125.04
24	d	405	CLA	CMC-C2C-C1C	3.21	129.92	125.04
24	C	508	CLA	C1D-CHD-C4C	-3.20	119.14	126.06
24	c	508	CLA	C1D-CHD-C4C	-3.20	119.14	126.06
24	A	406	CLA	CAC-C3C-C4C	3.20	128.97	124.81
24	C	506	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
24	c	506	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
24	B	615	CLA	C1-O2A-CGA	3.20	124.84	116.44
24	a	406	CLA	CAC-C3C-C4C	3.20	128.96	124.81
24	b	618	CLA	C1-O2A-CGA	3.20	124.83	116.44
24	D	401	CLA	CBC-CAC-C3C	-3.19	103.62	112.43
24	c	503	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
24	d	401	CLA	CBC-CAC-C3C	-3.19	103.64	112.43
24	C	513	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
24	b	608	CLA	C1C-C2C-C3C	-3.19	103.61	106.96
24	C	514	CLA	CAA-C2A-C3A	-3.19	104.05	112.78
24	c	514	CLA	CAA-C2A-C3A	-3.19	104.05	112.78
24	C	511	CLA	CAA-C2A-C3A	-3.18	104.07	112.78
24	B	602	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
24	b	604	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
24	C	503	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
24	B	615	CLA	C1D-CHD-C4C	-3.17	119.21	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	511	CLA	CAA-C2A-C3A	-3.17	104.10	112.78
24	B	606	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
24	b	608	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
24	C	505	CLA	CMB-C2B-C3B	3.16	130.59	124.68
24	c	505	CLA	CMB-C2B-C3B	3.16	130.59	124.68
24	b	617	CLA	C1D-CHD-C4C	-3.16	119.24	126.06
24	B	611	CLA	CHD-C4C-NC	3.16	129.18	124.20
24	c	513	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
24	b	613	CLA	CHD-C4C-NC	3.15	129.17	124.20
24	C	504	CLA	C1C-C2C-C3C	-3.15	103.64	106.96
24	c	504	CLA	C1C-C2C-C3C	-3.15	103.64	106.96
24	C	510	CLA	C1-O2A-CGA	3.15	124.71	116.44
30	C	501	LMG	O6-C1-O1	-3.15	102.51	109.97
30	c	501	LMG	O6-C1-O1	-3.15	102.51	109.97
24	B	616	CLA	CBC-CAC-C3C	-3.14	103.76	112.43
24	b	618	CLA	CBC-CAC-C3C	-3.14	103.76	112.43
24	c	510	CLA	C1-O2A-CGA	3.14	124.68	116.44
24	C	512	CLA	C1C-C2C-C3C	-3.14	103.66	106.96
24	c	512	CLA	C1C-C2C-C3C	-3.14	103.66	106.96
24	C	507	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
24	c	507	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
24	C	504	CLA	C3B-C4B-NB	3.12	113.25	109.21
24	c	504	CLA	C3B-C4B-NB	3.12	113.25	109.21
30	B	621	LMG	O7-C10-O9	-3.11	116.18	123.70
30	b	622	LMG	O7-C10-O9	-3.11	116.18	123.70
24	B	610	CLA	C3B-C4B-NB	3.11	113.22	109.21
27	B	620	SQD	O47-C7-O49	-3.10	116.21	123.70
27	L	102	SQD	O47-C7-O49	-3.10	116.21	123.70
24	C	505	CLA	CAA-CBA-CGA	3.10	122.31	113.25
24	c	505	CLA	CAA-CBA-CGA	3.10	122.31	113.25
24	c	514	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
24	c	514	CLA	C3B-C4B-NB	3.09	113.20	109.21
26	C	515	BCR	C7-C8-C9	-3.08	121.57	126.23
24	b	603	CLA	CHC-C1C-C2C	-3.08	118.19	126.72
24	c	507	CLA	CHD-C4C-NC	3.08	129.06	124.20
24	C	513	CLA	C3B-C4B-NB	3.08	113.19	109.21
24	c	513	CLA	C3B-C4B-NB	3.08	113.19	109.21
24	B	614	CLA	CMB-C2B-C3B	3.08	130.43	124.68
24	b	616	CLA	CMB-C2B-C3B	3.08	130.43	124.68
24	c	503	CLA	CAC-C3C-C4C	3.08	128.80	124.81
24	C	514	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
24	b	611	CLA	CHC-C1C-C2C	-3.07	118.22	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	519	DGD	O6D-C1D-O3G	-3.07	102.71	109.97
24	B	601	CLA	CHC-C1C-C2C	-3.07	118.24	126.72
24	B	604	CLA	O2A-CGA-CBA	3.07	121.53	111.91
37	V	201	HEC	CMB-C2B-C3B	3.06	129.42	125.82
37	v	201	HEC	CMB-C2B-C3B	3.06	129.42	125.82
24	C	507	CLA	CHD-C4C-NC	3.06	129.03	124.20
27	a	412	SQD	O9-S-C6	3.06	110.58	106.94
24	b	611	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
24	b	606	CLA	O2A-CGA-CBA	3.06	121.51	111.91
31	c	519	DGD	O6D-C1D-O3G	-3.06	102.73	109.97
24	b	609	CLA	C1-C2-C3	-3.06	120.76	126.04
24	C	514	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
24	C	514	CLA	C3B-C4B-NB	3.06	113.16	109.21
24	C	503	CLA	CAC-C3C-C4C	3.05	128.77	124.81
24	c	514	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
24	B	605	CLA	C3B-C4B-NB	3.05	113.15	109.21
24	b	607	CLA	C3B-C4B-NB	3.05	113.15	109.21
24	B	604	CLA	CHC-C1C-C2C	-3.05	118.28	126.72
24	b	606	CLA	CHC-C1C-C2C	-3.05	118.28	126.72
26	c	515	BCR	C7-C8-C9	-3.05	121.63	126.23
24	C	507	CLA	CMB-C2B-C3B	3.05	130.38	124.68
24	c	507	CLA	CMB-C2B-C3B	3.05	130.38	124.68
24	B	613	CLA	C4A-NA-C1A	-3.05	105.34	106.71
24	b	615	CLA	C4A-NA-C1A	-3.05	105.34	106.71
24	B	609	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
27	A	412	SQD	O9-S-C6	3.04	110.56	106.94
24	a	405	CLA	CHC-C1C-C2C	-3.04	118.31	126.72
24	A	405	CLA	CHC-C1C-C2C	-3.04	118.31	126.72
31	c	519	DGD	CDB-CCB-CBB	-3.04	99.00	114.42
24	A	408	CLA	CED-O2D-CGD	3.04	122.81	115.94
24	a	408	CLA	CED-O2D-CGD	3.04	122.81	115.94
31	C	519	DGD	CDB-CCB-CBB	-3.03	99.03	114.42
32	Z	101	LMT	C3'-C4'-C5'	-3.03	103.97	110.93
32	z	101	LMT	C3'-C4'-C5'	-3.03	103.98	110.93
24	B	606	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
24	B	607	CLA	C1-C2-C3	-3.02	120.81	126.04
24	B	601	CLA	C1D-CHD-C4C	-3.02	119.54	126.06
24	b	603	CLA	C1D-CHD-C4C	-3.02	119.54	126.06
24	B	604	CLA	C6-C7-C8	-3.02	106.16	115.92
24	b	606	CLA	C6-C7-C8	-3.02	106.16	115.92
24	B	612	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
24	b	614	CLA	C1C-C2C-C3C	-3.02	103.78	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	508	CLA	CBC-CAC-C3C	-3.02	104.11	112.43
24	B	609	CLA	CHC-C1C-C2C	-3.01	118.39	126.72
24	b	608	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
26	B	618	BCR	C29-C30-C25	3.01	115.11	110.48
26	b	620	BCR	C29-C30-C25	3.01	115.11	110.48
24	c	508	CLA	CMB-C2B-C3B	3.01	130.30	124.68
31	c	518	DGD	CBB-CAB-C9B	-3.00	99.17	114.42
28	d	407	PL9	O2-C1-C6	3.00	125.79	120.59
24	C	508	CLA	CMB-C2B-C3B	3.00	130.29	124.68
24	b	610	CLA	C3B-C4B-NB	3.00	113.09	109.21
24	B	616	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
24	b	618	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
27	B	620	SQD	C1-O5-C5	-3.00	107.80	113.69
24	C	508	CLA	CBC-CAC-C3C	-3.00	104.17	112.43
31	C	518	DGD	CBB-CAB-C9B	-3.00	99.21	114.42
24	C	509	CLA	C1D-CHD-C4C	-2.99	119.61	126.06
24	c	509	CLA	C1D-CHD-C4C	-2.99	119.61	126.06
24	B	607	CLA	CHC-C1C-C2C	-2.99	118.46	126.72
24	b	609	CLA	CHC-C1C-C2C	-2.99	118.46	126.72
27	L	102	SQD	C1-O5-C5	-2.99	107.83	113.69
24	d	404	CLA	CMB-C2B-C3B	2.98	130.26	124.68
24	D	401	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
24	d	401	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
24	B	608	CLA	C3B-C4B-NB	2.98	113.06	109.21
26	B	617	BCR	C29-C30-C25	2.98	115.06	110.48
26	b	619	BCR	C29-C30-C25	2.98	115.06	110.48
24	D	404	CLA	CMB-C2B-C3B	2.97	130.24	124.68
24	D	401	CLA	C1-O2A-CGA	2.97	124.25	116.44
24	d	401	CLA	C1-O2A-CGA	2.97	124.25	116.44
24	D	405	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
24	d	405	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
25	D	402	PHO	O1D-CGD-CBD	2.97	129.68	124.74
25	d	402	PHO	O1D-CGD-CBD	2.97	129.68	124.74
24	B	601	CLA	C4A-NA-C1A	-2.96	105.38	106.71
24	b	603	CLA	C4A-NA-C1A	-2.96	105.38	106.71
28	D	407	PL9	O2-C1-C6	2.96	125.71	120.59
24	B	602	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
24	b	604	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
24	B	609	CLA	CHD-C4C-NC	2.95	128.86	124.20
24	d	404	CLA	C1C-C2C-C3C	-2.95	103.85	106.96
27	F	101	SQD	O48-C23-C24	2.94	121.14	111.91
24	c	508	CLA	C4-C3-C5	2.94	120.22	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	506	CLA	CMC-C2C-C1C	2.94	129.52	125.04
24	c	506	CLA	CMC-C2C-C1C	2.94	129.52	125.04
27	f	101	SQD	O48-C23-C24	2.94	121.14	111.91
24	B	615	CLA	C6-C7-C8	-2.93	106.43	115.92
24	b	611	CLA	CHD-C4C-NC	2.93	128.83	124.20
24	b	617	CLA	C6-C7-C8	-2.93	106.44	115.92
24	D	404	CLA	C1C-C2C-C3C	-2.93	103.87	106.96
24	B	605	CLA	C1D-CHD-C4C	-2.93	119.73	126.06
24	b	607	CLA	C1D-CHD-C4C	-2.93	119.73	126.06
24	c	510	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
24	A	408	CLA	CMB-C2B-C3B	2.93	130.16	124.68
24	a	408	CLA	CMB-C2B-C3B	2.93	130.16	124.68
24	C	505	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
24	c	505	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
24	D	405	CLA	C4A-NA-C1A	-2.93	105.39	106.71
24	d	405	CLA	C4A-NA-C1A	-2.93	105.39	106.71
28	d	407	PL9	C40-C39-C41	2.93	120.19	115.27
24	C	510	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
24	C	513	CLA	C1D-CHD-C4C	-2.92	119.75	126.06
24	c	513	CLA	C1D-CHD-C4C	-2.92	119.75	126.06
35	E	103	HEM	C3B-C2B-C1B	2.92	108.65	106.49
35	e	103	HEM	C3B-C2B-C1B	2.92	108.65	106.49
30	C	523	LMG	O8-C28-O10	-2.92	116.22	123.59
30	c	523	LMG	O8-C28-O10	-2.92	116.22	123.59
26	B	618	BCR	C30-C25-C26	-2.92	118.50	122.61
26	b	620	BCR	C30-C25-C26	-2.92	118.50	122.61
28	D	407	PL9	C40-C39-C41	2.92	120.18	115.27
24	C	508	CLA	C4-C3-C5	2.92	120.17	115.27
24	C	508	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
24	c	508	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
24	b	613	CLA	C1-C2-C3	-2.91	121.00	126.04
24	B	606	CLA	C4-C3-C5	2.91	120.17	115.27
24	b	608	CLA	C4-C3-C5	2.91	120.17	115.27
26	C	515	BCR	C27-C26-C25	2.91	126.95	122.73
26	c	515	BCR	C27-C26-C25	2.91	126.95	122.73
27	F	101	SQD	O5-C1-C2	-2.90	104.21	110.35
24	B	608	CLA	CHD-C4C-NC	2.90	128.78	124.20
37	v	201	HEC	CBD-CAD-C3D	-2.90	107.67	112.62
24	B	602	CLA	CED-O2D-CGD	2.90	122.50	115.94
24	b	604	CLA	CED-O2D-CGD	2.90	122.50	115.94
24	C	513	CLA	CHB-C4A-NA	2.90	128.52	124.51
24	c	513	CLA	CHB-C4A-NA	2.90	128.52	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	410	SQD	C1-C2-C3	-2.90	103.96	110.00
27	a	410	SQD	C1-C2-C3	-2.90	103.96	110.00
24	D	401	CLA	CMB-C2B-C3B	2.90	130.10	124.68
24	d	401	CLA	CMB-C2B-C3B	2.90	130.10	124.68
24	B	603	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
24	b	605	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
27	f	101	SQD	O5-C1-C2	-2.89	104.22	110.35
24	B	611	CLA	C1-C2-C3	-2.89	121.04	126.04
24	b	611	CLA	CAC-C3C-C4C	2.89	128.56	124.81
24	B	612	CLA	O1D-CGD-CBD	-2.89	118.57	124.48
24	D	401	CLA	C3C-C4C-NC	2.88	113.81	110.57
24	d	401	CLA	C3C-C4C-NC	2.88	113.81	110.57
24	b	614	CLA	O1D-CGD-CBD	-2.88	118.58	124.48
24	D	401	CLA	C1-C2-C3	-2.88	121.06	126.04
24	d	401	CLA	C1-C2-C3	-2.88	121.06	126.04
37	V	201	HEC	CBD-CAD-C3D	-2.88	107.71	112.62
24	B	612	CLA	CAC-C3C-C4C	2.88	128.54	124.81
24	b	614	CLA	CAC-C3C-C4C	2.88	128.54	124.81
24	D	404	CLA	O2A-CGA-CBA	2.88	120.94	111.91
24	d	404	CLA	O2A-CGA-CBA	2.88	120.94	111.91
24	b	610	CLA	CHD-C4C-NC	2.87	128.73	124.20
24	B	602	CLA	CHD-C4C-NC	2.87	128.72	124.20
24	b	604	CLA	CHD-C4C-NC	2.87	128.72	124.20
28	D	407	PL9	C7-C8-C9	-2.87	122.02	126.79
28	d	407	PL9	C7-C8-C9	-2.87	122.02	126.79
24	A	406	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
24	a	406	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
24	B	604	CLA	C11-C12-C13	-2.87	106.65	115.92
24	b	606	CLA	C11-C12-C13	-2.87	106.65	115.92
24	C	514	CLA	C4-C3-C5	2.86	120.09	115.27
24	c	514	CLA	C4-C3-C5	2.86	120.09	115.27
24	C	513	CLA	CMA-C3A-C4A	-2.86	104.08	111.77
24	c	513	CLA	CMA-C3A-C4A	-2.86	104.08	111.77
27	A	410	SQD	C4-C3-C2	2.86	115.82	110.82
27	a	410	SQD	C4-C3-C2	2.86	115.82	110.82
30	B	621	LMG	C40-C39-C38	-2.86	99.90	114.42
30	b	622	LMG	C40-C39-C38	-2.86	99.90	114.42
30	B	621	LMG	O6-C1-O1	-2.86	103.21	109.97
30	b	622	LMG	O6-C1-O1	-2.86	103.21	109.97
24	c	505	CLA	CED-O2D-CGD	2.85	122.39	115.94
24	B	614	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
24	C	507	CLA	C4C-C3C-C2C	-2.85	102.74	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	507	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
24	c	510	CLA	C1-C2-C3	-2.85	121.11	126.04
31	H	101	DGD	C3D-C4D-C5D	-2.85	105.16	110.24
31	h	101	DGD	C3D-C4D-C5D	-2.85	105.16	110.24
24	B	607	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
24	b	609	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
24	b	616	CLA	CHC-C1C-C2C	-2.85	118.85	126.72
26	C	515	BCR	C38-C26-C27	-2.85	108.15	113.62
26	c	515	BCR	C38-C26-C27	-2.85	108.15	113.62
31	H	101	DGD	C6D-C5D-C4D	2.85	118.03	112.09
31	h	101	DGD	C6D-C5D-C4D	2.85	118.03	112.09
24	B	611	CLA	CBC-CAC-C3C	-2.84	104.59	112.43
24	b	613	CLA	CBC-CAC-C3C	-2.84	104.59	112.43
24	C	502	CLA	CHD-C4C-NC	2.84	128.68	124.20
24	c	502	CLA	CHD-C4C-NC	2.84	128.68	124.20
32	z	101	LMT	C3B-C4B-C5B	-2.84	105.17	110.24
24	B	609	CLA	CAC-C3C-C4C	2.84	128.50	124.81
24	A	408	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
24	a	408	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
34	d	408	LHG	O8-C23-C24	2.84	120.82	111.91
24	C	505	CLA	CED-O2D-CGD	2.84	122.36	115.94
24	C	510	CLA	C1-C2-C3	-2.84	121.13	126.04
24	b	607	CLA	C1-C2-C3	-2.84	121.13	126.04
24	B	601	CLA	CAA-C2A-C3A	-2.84	105.01	112.78
24	b	603	CLA	CAA-C2A-C3A	-2.84	105.01	112.78
24	B	608	CLA	CHC-C1C-C2C	-2.83	118.88	126.72
24	c	510	CLA	C1D-CHD-C4C	-2.83	119.95	126.06
24	B	606	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
34	D	408	LHG	O8-C23-C24	2.83	120.79	111.91
24	b	610	CLA	CHC-C1C-C2C	-2.83	118.90	126.72
24	b	608	CLA	CHC-C1C-C2C	-2.83	118.90	126.72
32	Z	101	LMT	C3B-C4B-C5B	-2.83	105.20	110.24
24	C	512	CLA	CHC-C1C-C2C	-2.82	118.91	126.72
27	A	412	SQD	O6-C1-C2	2.82	112.71	108.30
27	a	412	SQD	O6-C1-C2	2.82	112.71	108.30
24	B	605	CLA	C1-C2-C3	-2.82	121.17	126.04
24	C	506	CLA	C3D-C2D-C1D	-2.82	101.98	105.83
24	c	506	CLA	C3D-C2D-C1D	-2.82	101.98	105.83
30	d	411	LMG	O6-C1-O1	-2.82	103.30	109.97
28	a	411	PL9	O1-C4-C3	-2.82	117.62	120.72
24	C	510	CLA	C1D-CHD-C4C	-2.82	119.98	126.06
24	c	512	CLA	CHC-C1C-C2C	-2.81	118.94	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	611	CLA	C4A-NA-C1A	-2.81	105.44	106.71
24	b	614	CLA	C4D-CHA-C1A	-2.81	117.83	121.25
30	D	411	LMG	O6-C1-O1	-2.81	103.32	109.97
31	C	518	DGD	CDB-CCB-CBB	-2.81	100.18	114.42
31	c	518	DGD	CDB-CCB-CBB	-2.81	100.18	114.42
24	B	605	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
24	B	615	CLA	CHA-C1A-NA	-2.80	119.98	126.40
24	b	617	CLA	CHA-C1A-NA	-2.80	119.98	126.40
24	C	508	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
24	c	508	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
28	A	411	PL9	O1-C4-C3	-2.80	117.64	120.72
24	C	505	CLA	CMA-C3A-C4A	-2.80	104.25	111.77
24	c	505	CLA	CMA-C3A-C4A	-2.80	104.25	111.77
24	C	511	CLA	C4-C3-C5	2.80	119.98	115.27
24	B	612	CLA	C1D-CHD-C4C	-2.80	120.02	126.06
24	b	607	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
24	C	513	CLA	O2A-CGA-CBA	2.80	120.69	111.91
24	c	513	CLA	O2A-CGA-CBA	2.80	120.69	111.91
24	D	405	CLA	C4-C3-C5	2.80	119.98	115.27
24	d	405	CLA	C4-C3-C5	2.80	119.98	115.27
24	B	612	CLA	C4D-CHA-C1A	-2.80	117.85	121.25
24	C	510	CLA	C4A-NA-C1A	-2.79	105.45	106.71
38	X	101	RRX	C16-C15-C14	-2.79	117.75	123.47
30	D	411	LMG	C6-C5-C4	-2.79	106.46	113.00
30	d	411	LMG	C6-C5-C4	-2.79	106.46	113.00
25	D	402	PHO	C4A-C3A-C2A	-2.79	100.19	102.84
25	d	402	PHO	C4A-C3A-C2A	-2.79	100.19	102.84
24	b	614	CLA	C1D-CHD-C4C	-2.79	120.05	126.06
24	B	601	CLA	C3B-C4B-NB	2.78	112.81	109.21
24	b	603	CLA	C3B-C4B-NB	2.78	112.81	109.21
34	D	408	LHG	C11-C10-C9	-2.78	100.29	114.42
34	d	408	LHG	C11-C10-C9	-2.78	100.29	114.42
24	C	503	CLA	CMB-C2B-C3B	2.78	129.88	124.68
24	c	503	CLA	CMB-C2B-C3B	2.78	129.88	124.68
24	C	511	CLA	C1D-CHD-C4C	-2.78	120.06	126.06
24	c	511	CLA	C1D-CHD-C4C	-2.78	120.06	126.06
24	B	612	CLA	CMB-C2B-C3B	2.78	129.88	124.68
24	b	614	CLA	CMB-C2B-C3B	2.78	129.88	124.68
24	c	510	CLA	C4A-NA-C1A	-2.78	105.46	106.71
38	x	101	RRX	C16-C15-C14	-2.78	117.79	123.47
24	B	602	CLA	C1D-CHD-C4C	-2.77	120.07	126.06
24	b	604	CLA	C1D-CHD-C4C	-2.77	120.07	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	513	CLA	C1-C2-C3	-2.77	121.25	126.04
24	c	513	CLA	C1-C2-C3	-2.77	121.25	126.04
24	B	605	CLA	CAC-C3C-C4C	2.77	128.41	124.81
24	b	607	CLA	CAC-C3C-C4C	2.77	128.41	124.81
24	B	609	CLA	C4A-NA-C1A	-2.77	105.46	106.71
31	H	101	DGD	C3E-C4E-C5E	-2.77	105.30	110.24
31	h	101	DGD	C3E-C4E-C5E	-2.77	105.30	110.24
24	A	405	CLA	CHB-C4A-NA	2.76	128.34	124.51
24	a	405	CLA	CHB-C4A-NA	2.76	128.34	124.51
24	C	506	CLA	C3B-C4B-NB	2.76	112.78	109.21
24	c	506	CLA	C3B-C4B-NB	2.76	112.78	109.21
28	D	407	PL9	C8-C7-C3	2.76	119.79	111.98
28	d	407	PL9	C8-C7-C3	2.76	119.79	111.98
35	e	103	HEM	C4B-CHC-C1C	2.76	126.20	122.56
34	e	101	LHG	C11-C10-C9	-2.76	100.42	114.42
24	c	511	CLA	C4-C3-C5	2.76	119.91	115.27
35	E	103	HEM	C4B-CHC-C1C	2.76	126.19	122.56
24	A	406	CLA	C4A-NA-C1A	-2.75	105.47	106.71
24	a	406	CLA	C4A-NA-C1A	-2.75	105.47	106.71
24	a	405	CLA	C7-C6-C5	-2.75	105.88	113.36
26	B	618	BCR	C15-C16-C17	-2.75	117.83	123.47
26	b	620	BCR	C15-C16-C17	-2.75	117.83	123.47
34	E	101	LHG	C11-C10-C9	-2.75	100.46	114.42
24	B	612	CLA	O2A-CGA-CBA	2.75	120.54	111.91
24	D	405	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
24	d	405	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
24	b	614	CLA	O2A-CGA-CBA	2.75	120.53	111.91
24	A	406	CLA	C1-C2-C3	-2.74	121.30	126.04
24	a	406	CLA	C1-C2-C3	-2.74	121.30	126.04
24	D	405	CLA	CHC-C1C-C2C	-2.74	119.13	126.72
24	d	405	CLA	CHC-C1C-C2C	-2.74	119.13	126.72
26	B	619	BCR	C24-C23-C22	-2.74	122.09	126.23
24	A	405	CLA	C7-C6-C5	-2.74	105.92	113.36
28	d	407	PL9	C36-C34-C33	-2.74	115.58	121.12
28	D	407	PL9	C36-C34-C33	-2.73	115.59	121.12
24	B	614	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
24	B	607	CLA	C1D-CHD-C4C	-2.73	120.17	126.06
24	b	609	CLA	C1D-CHD-C4C	-2.73	120.17	126.06
24	B	609	CLA	CMC-C2C-C1C	2.73	129.19	125.04
24	C	507	CLA	CHC-C1C-NC	2.72	128.34	124.20
24	c	507	CLA	CHC-C1C-NC	2.72	128.34	124.20
26	t	102	BCR	C33-C5-C6	-2.72	121.47	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	505	CLA	C1D-CHD-C4C	-2.72	120.19	126.06
24	c	505	CLA	C1D-CHD-C4C	-2.72	120.19	126.06
26	b	621	BCR	C24-C23-C22	-2.72	122.12	126.23
24	b	616	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
24	B	616	CLA	C7-C6-C5	-2.72	105.97	113.36
24	b	618	CLA	C7-C6-C5	-2.72	105.97	113.36
24	C	509	CLA	CMB-C2B-C1B	-2.71	124.29	128.46
24	c	509	CLA	CMB-C2B-C1B	-2.71	124.29	128.46
24	d	401	CLA	CAA-C2A-C3A	-2.71	105.35	112.78
24	D	405	CLA	CMB-C2B-C3B	2.71	129.75	124.68
24	d	405	CLA	CMB-C2B-C3B	2.71	129.75	124.68
24	B	613	CLA	CHC-C1C-C2C	-2.71	119.23	126.72
24	C	510	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
24	c	510	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
26	T	101	BCR	C33-C5-C6	-2.70	121.49	124.53
34	e	101	LHG	C20-C19-C18	-2.70	100.70	114.42
24	C	506	CLA	CHC-C1C-C2C	-2.70	119.24	126.72
24	c	506	CLA	CHC-C1C-C2C	-2.70	119.24	126.72
24	D	401	CLA	CAA-C2A-C3A	-2.70	105.38	112.78
34	E	101	LHG	C20-C19-C18	-2.70	100.71	114.42
26	C	515	BCR	C15-C16-C17	-2.70	117.94	123.47
24	C	511	CLA	CMD-C2D-C3D	-2.70	121.41	127.61
24	c	511	CLA	CMD-C2D-C3D	-2.70	121.41	127.61
24	A	408	CLA	CHD-C4C-NC	2.70	128.45	124.20
24	a	408	CLA	CHD-C4C-NC	2.70	128.45	124.20
24	B	616	CLA	CMA-C3A-C4A	-2.70	104.53	111.77
24	b	618	CLA	CMA-C3A-C4A	-2.70	104.53	111.77
31	C	518	DGD	C6D-O5D-C1E	2.69	119.00	113.74
31	c	518	DGD	C6D-O5D-C1E	2.69	119.00	113.74
24	b	615	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
26	C	516	BCR	C7-C8-C9	-2.68	122.18	126.23
26	c	516	BCR	C7-C8-C9	-2.68	122.18	126.23
24	B	613	CLA	C1-O2A-CGA	2.68	123.49	116.44
26	c	515	BCR	C15-C16-C17	-2.68	117.98	123.47
24	C	509	CLA	C3B-C4B-NB	2.68	112.68	109.21
24	c	509	CLA	C3B-C4B-NB	2.68	112.68	109.21
24	c	507	CLA	C1-C2-C3	-2.68	121.41	126.04
24	b	615	CLA	C1-O2A-CGA	2.68	123.47	116.44
24	b	611	CLA	CMC-C2C-C1C	2.68	129.12	125.04
26	B	617	BCR	C38-C26-C27	-2.68	108.47	113.62
26	b	619	BCR	C38-C26-C27	-2.68	108.47	113.62
38	X	101	RRX	C15-C14-C13	-2.68	123.49	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	517	DGD	CDB-CCB-CBB	-2.67	100.85	114.42
38	x	101	RRX	C15-C14-C13	-2.67	123.50	127.31
31	c	517	DGD	CDB-CCB-CBB	-2.67	100.87	114.42
34	D	409	LHG	O8-C23-C24	2.67	120.28	111.91
30	B	621	LMG	O8-C28-O10	-2.67	116.86	123.59
24	b	607	CLA	CHC-C1C-C2C	-2.67	119.35	126.72
24	B	605	CLA	CHC-C1C-C2C	-2.67	119.35	126.72
24	C	504	CLA	CHC-C1C-C2C	-2.66	119.35	126.72
24	c	504	CLA	CHC-C1C-C2C	-2.66	119.35	126.72
24	B	601	CLA	CAC-C3C-C4C	2.66	128.26	124.81
24	b	603	CLA	CAC-C3C-C4C	2.66	128.26	124.81
24	C	510	CLA	C11-C12-C13	-2.66	107.33	115.92
24	c	510	CLA	C11-C12-C13	-2.66	107.33	115.92
30	b	622	LMG	O8-C28-O10	-2.66	116.89	123.59
24	b	609	CLA	CAA-C2A-C3A	-2.66	105.51	112.78
24	C	507	CLA	C1-C2-C3	-2.65	121.45	126.04
31	c	518	DGD	O3G-C1D-C2D	-2.65	104.16	108.30
24	C	514	CLA	CHB-C4A-NA	2.65	128.18	124.51
24	c	514	CLA	CHB-C4A-NA	2.65	128.18	124.51
34	d	409	LHG	O8-C23-C24	2.65	120.23	111.91
31	C	518	DGD	O3G-C1D-C2D	-2.65	104.16	108.30
24	B	605	CLA	O1D-CGD-CBD	-2.65	119.06	124.48
24	b	607	CLA	O1D-CGD-CBD	-2.65	119.06	124.48
24	C	510	CLA	CAA-C2A-C3A	-2.65	105.53	112.78
24	c	510	CLA	CAA-C2A-C3A	-2.65	105.53	112.78
31	C	518	DGD	O6D-C5D-C6D	-2.65	101.32	106.67
27	a	412	SQD	C3-C4-C5	2.65	114.96	110.24
28	A	411	PL9	C21-C19-C18	-2.65	115.76	121.12
28	a	411	PL9	C21-C19-C18	-2.65	115.76	121.12
24	B	615	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
24	b	617	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
31	C	517	DGD	O2G-C1B-O1B	-2.64	117.31	123.70
31	c	517	DGD	O2G-C1B-O1B	-2.64	117.31	123.70
30	C	523	LMG	C1-C2-C3	-2.64	104.49	110.00
30	c	523	LMG	C1-C2-C3	-2.64	104.49	110.00
24	B	607	CLA	CAA-C2A-C3A	-2.64	105.54	112.78
30	C	501	LMG	C40-C39-C38	-2.64	101.01	114.42
30	c	501	LMG	C40-C39-C38	-2.64	101.01	114.42
24	B	602	CLA	CBC-CAC-C3C	-2.64	105.15	112.43
24	b	604	CLA	CBC-CAC-C3C	-2.64	105.15	112.43
24	b	611	CLA	CHA-C1A-NA	-2.64	120.35	126.40
31	H	101	DGD	CDB-CCB-CBB	-2.64	101.02	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	h	101	DGD	CDB-CCB-CBB	-2.64	101.02	114.42
24	B	611	CLA	CMC-C2C-C1C	2.64	129.05	125.04
24	B	609	CLA	CHA-C1A-NA	-2.63	120.38	126.40
24	D	401	CLA	O2A-CGA-CBA	2.63	120.16	111.91
24	d	401	CLA	O2A-CGA-CBA	2.63	120.16	111.91
24	C	505	CLA	CHB-C4A-NA	2.63	128.15	124.51
24	c	505	CLA	CHB-C4A-NA	2.63	128.15	124.51
24	C	511	CLA	C4C-C3C-C2C	-2.63	103.07	106.90
24	c	511	CLA	C4C-C3C-C2C	-2.63	103.07	106.90
31	c	518	DGD	O6D-C5D-C6D	-2.63	101.36	106.67
24	D	401	CLA	CMC-C2C-C3C	2.63	133.25	126.12
24	d	401	CLA	CMC-C2C-C3C	2.63	133.25	126.12
24	b	612	CLA	CMB-C2B-C3B	2.63	129.59	124.68
24	A	408	CLA	CAC-C3C-C4C	2.63	128.22	124.81
24	a	408	CLA	CAC-C3C-C4C	2.63	128.22	124.81
28	d	407	PL9	O2-C1-C2	-2.62	115.77	121.78
24	b	607	CLA	CHB-C4A-NA	2.62	128.14	124.51
27	A	412	SQD	C3-C4-C5	2.62	114.91	110.24
24	c	514	CLA	CHC-C1C-C2C	-2.62	119.48	126.72
28	D	407	PL9	O2-C1-C2	-2.62	115.78	121.78
24	D	405	CLA	CHB-C4A-NA	2.62	128.13	124.51
24	d	405	CLA	CHB-C4A-NA	2.62	128.13	124.51
30	c	523	LMG	O1-C1-C2	-2.61	104.23	108.30
24	B	613	CLA	CHD-C4C-NC	2.61	128.32	124.20
24	b	615	CLA	CHD-C4C-NC	2.61	128.32	124.20
24	B	605	CLA	CHB-C4A-NA	2.61	128.12	124.51
31	C	518	DGD	O3D-C3D-C4D	-2.61	104.32	110.35
31	c	518	DGD	O3D-C3D-C4D	-2.61	104.32	110.35
24	C	514	CLA	CHC-C1C-C2C	-2.61	119.51	126.72
24	A	405	CLA	CAA-C2A-C1A	-2.61	103.43	111.97
24	a	405	CLA	CAA-C2A-C1A	-2.61	103.43	111.97
25	D	402	PHO	C1B-NB-C4B	2.60	112.44	107.09
25	d	402	PHO	C1B-NB-C4B	2.60	112.44	107.09
24	b	616	CLA	C4-C3-C5	2.60	119.65	115.27
24	B	614	CLA	C4-C3-C5	2.60	119.64	115.27
28	D	407	PL9	C20-C19-C21	2.60	119.64	115.27
30	C	523	LMG	O1-C1-C2	-2.60	104.25	108.30
24	B	615	CLA	CMA-C3A-C4A	-2.59	104.81	111.77
24	b	617	CLA	CMA-C3A-C4A	-2.59	104.81	111.77
24	C	510	CLA	O2A-CGA-CBA	2.59	120.04	111.91
24	c	510	CLA	O2A-CGA-CBA	2.59	120.04	111.91
28	d	407	PL9	C31-C32-C33	-2.59	103.36	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	d	407	PL9	C20-C19-C21	2.59	119.63	115.27
24	B	602	CLA	C4-C3-C5	2.59	119.63	115.27
24	b	604	CLA	C4-C3-C5	2.59	119.63	115.27
24	C	510	CLA	CED-O2D-CGD	2.59	121.79	115.94
24	c	510	CLA	CED-O2D-CGD	2.59	121.79	115.94
38	X	101	RRX	C30-C29-C28	-2.59	107.80	113.64
38	x	101	RRX	C30-C29-C28	-2.59	107.80	113.64
24	C	510	CLA	CHC-C1C-C2C	-2.58	119.58	126.72
24	c	510	CLA	CHC-C1C-C2C	-2.58	119.58	126.72
28	D	407	PL9	C22-C23-C24	-2.58	121.44	127.66
28	d	407	PL9	C22-C23-C24	-2.58	121.44	127.66
32	J	102	LMT	C1-O1'-C1'	2.58	118.11	113.84
32	j	102	LMT	C1-O1'-C1'	2.58	118.11	113.84
24	C	502	CLA	O2A-CGA-O1A	-2.58	117.09	123.59
28	d	407	PL9	C41-C39-C38	-2.58	115.90	121.12
24	b	613	CLA	CMC-C2C-C1C	2.57	128.96	125.04
28	D	407	PL9	C31-C32-C33	-2.57	103.42	111.88
28	a	411	PL9	O2-C1-C6	2.57	125.04	120.59
26	D	406	BCR	C1-C6-C5	-2.57	118.99	122.61
26	d	406	BCR	C1-C6-C5	-2.57	118.99	122.61
24	c	502	CLA	CBC-CAC-C3C	-2.57	105.34	112.43
24	b	610	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
24	C	502	CLA	CBC-CAC-C3C	-2.57	105.35	112.43
24	B	608	CLA	C4C-C3C-C2C	-2.57	103.16	106.90
31	c	517	DGD	O3E-C3E-C2E	-2.56	104.42	110.35
24	c	502	CLA	O2A-CGA-O1A	-2.56	117.12	123.59
28	A	411	PL9	O2-C1-C6	2.56	125.03	120.59
38	X	101	RRX	C8-C7-C6	-2.56	120.00	127.20
38	x	101	RRX	C8-C7-C6	-2.56	120.00	127.20
24	b	616	CLA	O2A-CGA-O1A	-2.56	117.12	123.59
31	C	517	DGD	O3E-C3E-C2E	-2.56	104.42	110.35
24	b	609	CLA	CAA-CBA-CGA	2.56	120.73	113.25
24	B	610	CLA	CMB-C2B-C3B	2.56	129.47	124.68
30	C	520	LMG	C40-C39-C38	-2.56	101.44	114.42
24	A	408	CLA	O2A-CGA-CBA	2.56	119.93	111.91
24	a	408	CLA	O2A-CGA-CBA	2.56	119.93	111.91
24	B	601	CLA	CBC-CAC-C3C	-2.56	105.39	112.43
24	b	603	CLA	CBC-CAC-C3C	-2.56	105.39	112.43
24	B	607	CLA	CAA-CBA-CGA	2.55	120.72	113.25
24	C	511	CLA	CMB-C2B-C3B	2.55	129.46	124.68
30	c	520	LMG	C40-C39-C38	-2.55	101.46	114.42
24	c	502	CLA	CAC-C3C-C4C	2.55	128.12	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	C	501	LMG	O3-C3-C2	-2.55	104.46	110.35
30	c	501	LMG	O3-C3-C2	-2.55	104.46	110.35
24	B	616	CLA	C4-C3-C2	-2.55	117.14	123.68
24	b	618	CLA	C4-C3-C2	-2.55	117.14	123.68
24	A	406	CLA	CHD-C1D-ND	-2.55	122.11	124.45
24	a	406	CLA	CHD-C1D-ND	-2.55	122.11	124.45
24	B	614	CLA	O2A-CGA-O1A	-2.55	117.16	123.59
31	C	517	DGD	O2D-C2D-C3D	-2.55	104.46	110.35
31	c	517	DGD	O2D-C2D-C3D	-2.55	104.46	110.35
24	C	512	CLA	CMB-C2B-C3B	2.55	129.44	124.68
24	c	512	CLA	CMB-C2B-C3B	2.55	129.44	124.68
24	b	612	CLA	C1-C2-C3	-2.54	121.64	126.04
32	C	521	LMT	O5B-C5B-C4B	2.54	114.31	109.69
32	c	521	LMT	O5B-C5B-C4B	2.54	114.31	109.69
28	D	407	PL9	C7-C3-C4	2.54	118.94	116.88
28	d	407	PL9	C7-C3-C4	2.54	118.94	116.88
24	B	610	CLA	C1-C2-C3	-2.54	121.65	126.04
24	B	606	CLA	C11-C10-C8	-2.54	107.71	115.92
24	b	608	CLA	C11-C10-C8	-2.54	107.71	115.92
24	B	607	CLA	CMB-C2B-C3B	2.54	129.43	124.68
24	B	603	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
24	b	605	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
24	c	511	CLA	CMB-C2B-C3B	2.54	129.43	124.68
28	D	407	PL9	C41-C39-C38	-2.54	115.98	121.12
24	b	609	CLA	CMB-C2B-C3B	2.54	129.43	124.68
24	D	404	CLA	CHC-C1C-C2C	-2.53	119.71	126.72
24	d	404	CLA	CHC-C1C-C2C	-2.53	119.71	126.72
24	A	408	CLA	C1D-CHD-C4C	-2.53	120.59	126.06
30	C	520	LMG	O1-C1-C2	-2.53	104.35	108.30
30	c	520	LMG	O1-C1-C2	-2.53	104.35	108.30
24	B	602	CLA	CHC-C1C-C2C	-2.53	119.72	126.72
24	b	604	CLA	CHC-C1C-C2C	-2.53	119.72	126.72
24	D	404	CLA	CMA-C3A-C2A	-2.53	103.62	113.83
24	d	404	CLA	CMA-C3A-C2A	-2.53	103.62	113.83
24	C	502	CLA	CAA-C2A-C3A	-2.53	105.85	112.78
24	c	502	CLA	CAA-C2A-C3A	-2.53	105.85	112.78
24	c	511	CLA	C1-O2A-CGA	2.53	123.08	116.44
32	z	101	LMT	O5B-C5B-C4B	2.53	114.28	109.69
24	B	609	CLA	CHB-C4A-NA	2.53	128.01	124.51
24	b	607	CLA	CED-O2D-CGD	2.52	121.65	115.94
24	C	511	CLA	C1-O2A-CGA	2.52	123.06	116.44
24	B	606	CLA	C11-C12-C13	-2.52	107.77	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	D	407	PL9	C12-C13-C14	-2.52	121.59	127.66
28	d	407	PL9	C12-C13-C14	-2.52	121.59	127.66
24	a	408	CLA	C1D-CHD-C4C	-2.52	120.62	126.06
32	m	102	LMT	O1'-C1-C2	-2.52	100.74	109.56
24	A	406	CLA	CHD-C4C-NC	2.52	128.17	124.20
24	a	406	CLA	CHD-C4C-NC	2.52	128.17	124.20
24	C	503	CLA	CAA-C2A-C3A	-2.51	105.89	112.78
24	c	503	CLA	CAA-C2A-C3A	-2.51	105.89	112.78
24	B	605	CLA	CED-O2D-CGD	2.51	121.62	115.94
24	b	608	CLA	C11-C12-C13	-2.51	107.80	115.92
24	B	616	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
24	b	618	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
24	C	514	CLA	O2A-CGA-CBA	2.51	119.79	111.91
24	c	514	CLA	O2A-CGA-CBA	2.51	119.79	111.91
24	d	404	CLA	C1-C2-C3	-2.51	121.70	126.04
32	M	101	LMT	O1'-C1-C2	-2.51	100.77	109.56
35	E	103	HEM	C1B-NB-C4B	2.51	107.67	105.07
35	e	103	HEM	C1B-NB-C4B	2.51	107.67	105.07
24	C	505	CLA	C4-C3-C5	2.51	119.49	115.27
24	c	505	CLA	C4-C3-C5	2.51	119.49	115.27
24	C	510	CLA	CBC-CAC-C3C	-2.51	105.52	112.43
24	c	510	CLA	CBC-CAC-C3C	-2.51	105.52	112.43
24	b	611	CLA	CHB-C4A-NA	2.50	127.97	124.51
24	C	511	CLA	C4A-NA-C1A	-2.50	105.58	106.71
24	c	511	CLA	C4A-NA-C1A	-2.50	105.58	106.71
24	D	405	CLA	C1-C2-C3	-2.50	121.72	126.04
24	d	405	CLA	C1-C2-C3	-2.50	121.72	126.04
24	D	404	CLA	C1-C2-C3	-2.50	121.72	126.04
24	C	502	CLA	C7-C6-C5	-2.50	106.58	113.36
24	c	502	CLA	C7-C6-C5	-2.50	106.58	113.36
24	B	602	CLA	CMC-C2C-C1C	2.50	128.84	125.04
24	b	604	CLA	CMC-C2C-C1C	2.50	128.84	125.04
32	Z	101	LMT	O5B-C5B-C4B	2.49	114.22	109.69
24	B	602	CLA	C1-C2-C3	-2.49	121.73	126.04
24	b	604	CLA	C1-C2-C3	-2.49	121.73	126.04
24	C	513	CLA	C1-O2A-CGA	2.49	122.97	116.44
24	c	513	CLA	C1-O2A-CGA	2.49	122.97	116.44
24	c	506	CLA	C1-C2-C3	-2.49	121.74	126.04
26	C	515	BCR	C16-C15-C14	-2.49	118.38	123.47
30	C	520	LMG	C38-C37-C36	-2.48	101.81	114.42
24	b	608	CLA	CMC-C2C-C1C	2.48	128.82	125.04
24	C	502	CLA	CAC-C3C-C4C	2.48	128.03	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	T	101	BCR	C31-C1-C6	2.48	114.32	110.30
26	t	102	BCR	C31-C1-C6	2.48	114.32	110.30
24	B	610	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
24	c	505	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
30	d	411	LMG	C40-C39-C38	-2.48	101.84	114.42
30	c	520	LMG	C38-C37-C36	-2.48	101.84	114.42
24	C	505	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
24	B	611	CLA	C4C-C3C-C2C	-2.48	103.29	106.90
30	c	501	LMG	O7-C10-O9	-2.48	117.72	123.70
24	b	612	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
31	C	518	DGD	O2E-C2E-C1E	-2.48	104.03	110.05
31	c	518	DGD	O2E-C2E-C1E	-2.48	104.03	110.05
30	D	411	LMG	C40-C39-C38	-2.47	101.87	114.42
24	D	401	CLA	C4A-NA-C1A	-2.47	105.59	106.71
24	d	401	CLA	C4A-NA-C1A	-2.47	105.59	106.71
30	C	501	LMG	O7-C10-O9	-2.47	117.73	123.70
24	c	503	CLA	C16-C17-C18	-2.47	104.35	115.98
24	D	405	CLA	O2A-CGA-CBA	2.47	119.65	111.91
24	d	405	CLA	O2A-CGA-CBA	2.47	119.65	111.91
24	C	503	CLA	C16-C17-C18	-2.47	104.35	115.98
26	T	101	BCR	C15-C14-C13	-2.47	123.79	127.31
26	t	102	BCR	C15-C14-C13	-2.47	123.79	127.31
26	B	619	BCR	C27-C26-C25	2.47	126.31	122.73
26	b	621	BCR	C27-C26-C25	2.47	126.31	122.73
24	C	511	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
24	C	504	CLA	C1-O2A-CGA	2.46	122.91	116.44
24	c	504	CLA	C1-O2A-CGA	2.46	122.91	116.44
24	b	613	CLA	C4C-C3C-C2C	-2.46	103.31	106.90
24	C	506	CLA	C1-C2-C3	-2.46	121.79	126.04
24	B	606	CLA	CMC-C2C-C1C	2.46	128.78	125.04
24	b	607	CLA	CBC-CAC-C3C	-2.46	105.66	112.43
24	C	505	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
24	c	505	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
31	c	517	DGD	O5D-C6D-C5D	-2.46	104.50	109.05
24	C	505	CLA	CBC-CAC-C3C	-2.46	105.66	112.43
24	c	505	CLA	CBC-CAC-C3C	-2.46	105.66	112.43
24	c	502	CLA	C1-C2-C3	-2.46	121.80	126.04
24	C	502	CLA	C1-C2-C3	-2.45	121.80	126.04
26	T	101	BCR	C35-C13-C14	-2.45	119.49	122.92
26	t	102	BCR	C35-C13-C14	-2.45	119.49	122.92
31	C	517	DGD	O5D-C6D-C5D	-2.45	104.51	109.05
24	c	514	CLA	CHD-C4C-NC	2.45	128.07	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	c	515	BCR	C16-C15-C14	-2.45	118.45	123.47
24	A	406	CLA	CMA-C3A-C4A	-2.45	105.19	111.77
24	a	406	CLA	CMA-C3A-C4A	-2.45	105.19	111.77
24	a	405	CLA	O2A-CGA-CBA	2.45	119.59	111.91
24	C	514	CLA	CHD-C4C-NC	2.45	128.06	124.20
24	c	511	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
24	B	605	CLA	CBC-CAC-C3C	-2.45	105.69	112.43
24	A	405	CLA	O2A-CGA-CBA	2.44	119.58	111.91
24	C	508	CLA	CHB-C4A-NA	2.44	127.89	124.51
24	c	508	CLA	CHB-C4A-NA	2.44	127.89	124.51
24	b	610	CLA	O2A-CGA-CBA	2.44	119.58	111.91
24	B	614	CLA	CED-O2D-CGD	2.44	121.45	115.94
24	b	616	CLA	CED-O2D-CGD	2.44	121.45	115.94
24	B	608	CLA	O2A-CGA-CBA	2.44	119.56	111.91
24	c	514	CLA	CMC-C2C-C1C	2.44	128.75	125.04
24	B	601	CLA	CHB-C4A-NA	2.44	127.88	124.51
24	b	603	CLA	CHB-C4A-NA	2.44	127.88	124.51
26	D	406	BCR	C38-C26-C27	-2.44	108.94	113.62
26	d	406	BCR	C38-C26-C27	-2.44	108.94	113.62
24	C	506	CLA	C1-O2A-CGA	2.43	122.83	116.44
24	B	612	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
24	b	616	CLA	O2A-CGA-CBA	2.43	119.54	111.91
24	C	505	CLA	C1-C2-C3	-2.43	121.83	126.04
24	c	505	CLA	C1-C2-C3	-2.43	121.83	126.04
24	B	610	CLA	CAC-C3C-C4C	2.43	127.97	124.81
24	b	614	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
24	C	504	CLA	CHD-C4C-NC	2.43	128.03	124.20
24	c	504	CLA	CHD-C4C-NC	2.43	128.03	124.20
30	C	520	LMG	O1-C7-C8	-2.43	105.04	110.90
30	c	520	LMG	O1-C7-C8	-2.43	105.04	110.90
24	C	508	CLA	CHD-C4C-NC	2.43	128.03	124.20
24	c	508	CLA	CHD-C4C-NC	2.43	128.03	124.20
24	D	405	CLA	C1D-CHD-C4C	-2.43	120.82	126.06
24	d	405	CLA	C1D-CHD-C4C	-2.43	120.82	126.06
24	C	507	CLA	OBD-CAD-C3D	-2.43	122.68	128.52
24	c	507	CLA	OBD-CAD-C3D	-2.43	122.68	128.52
24	c	506	CLA	C1-O2A-CGA	2.42	122.80	116.44
24	c	508	CLA	C11-C12-C13	-2.42	108.09	115.92
24	B	614	CLA	O2A-CGA-CBA	2.42	119.50	111.91
31	h	101	DGD	C1D-C2D-C3D	-2.42	104.95	110.00
24	C	514	CLA	C2A-C1A-CHA	-2.42	119.63	123.86
24	c	514	CLA	C2A-C1A-CHA	-2.42	119.63	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	614	CLA	CAA-C2A-C3A	-2.42	106.16	112.78
26	B	619	BCR	C1-C6-C5	-2.42	119.21	122.61
24	C	507	CLA	C2A-C1A-CHA	-2.42	119.64	123.86
24	c	507	CLA	C2A-C1A-CHA	-2.42	119.64	123.86
24	C	513	CLA	CHA-C1A-NA	-2.42	120.87	126.40
24	c	513	CLA	CHA-C1A-NA	-2.42	120.87	126.40
24	B	604	CLA	C4C-C3C-C2C	-2.41	103.38	106.90
24	b	606	CLA	C4C-C3C-C2C	-2.41	103.38	106.90
24	B	605	CLA	CHD-C4C-NC	2.41	128.01	124.20
24	b	607	CLA	CHD-C4C-NC	2.41	128.01	124.20
24	B	613	CLA	CHB-C4A-NA	2.41	127.85	124.51
24	b	615	CLA	CHB-C4A-NA	2.41	127.85	124.51
24	B	614	CLA	CMA-C3A-C2A	-2.41	104.09	113.83
26	C	522	BCR	C11-C10-C9	-2.41	123.87	127.31
26	c	522	BCR	C11-C10-C9	-2.41	123.87	127.31
24	C	508	CLA	C11-C12-C13	-2.41	108.13	115.92
30	C	523	LMG	O7-C10-O9	-2.41	117.88	123.70
30	c	523	LMG	O7-C10-O9	-2.41	117.88	123.70
24	b	616	CLA	CMA-C3A-C2A	-2.41	104.11	113.83
24	C	514	CLA	CMC-C2C-C1C	2.41	128.71	125.04
26	A	409	BCR	C20-C21-C22	-2.41	123.87	127.31
26	a	409	BCR	C20-C21-C22	-2.41	123.87	127.31
28	A	411	PL9	C37-C38-C39	-2.41	121.87	127.66
28	a	411	PL9	C37-C38-C39	-2.41	121.87	127.66
24	B	612	CLA	CAA-C2A-C3A	-2.40	106.19	112.78
24	B	614	CLA	CHD-C4C-NC	2.40	127.99	124.20
24	b	616	CLA	CHD-C4C-NC	2.40	127.99	124.20
24	B	615	CLA	CMB-C2B-C3B	2.40	129.17	124.68
24	b	617	CLA	CMB-C2B-C3B	2.40	129.17	124.68
24	C	514	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
24	c	514	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
31	C	519	DGD	C1E-O6E-C5E	2.40	118.39	113.69
31	c	519	DGD	C1E-O6E-C5E	2.40	118.39	113.69
24	A	408	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
24	a	408	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
31	H	101	DGD	C1D-C2D-C3D	-2.39	105.01	110.00
24	c	509	CLA	C11-C10-C8	-2.39	108.18	115.92
34	d	410	LHG	O8-C23-C24	2.39	119.42	111.91
24	D	401	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
24	d	401	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
28	D	407	PL9	C7-C3-C2	-2.39	120.16	123.30
28	d	407	PL9	C7-C3-C2	-2.39	120.16	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	D	406	BCR	C4-C5-C6	2.39	126.20	122.73
26	d	406	BCR	C4-C5-C6	2.39	126.20	122.73
24	B	604	CLA	CAC-C3C-C4C	2.39	127.91	124.81
24	b	606	CLA	CAC-C3C-C4C	2.39	127.91	124.81
26	b	621	BCR	C1-C6-C5	-2.39	119.25	122.61
24	A	406	CLA	CED-O2D-CGD	2.39	121.34	115.94
24	a	406	CLA	CED-O2D-CGD	2.39	121.34	115.94
24	C	509	CLA	C11-C10-C8	-2.39	108.20	115.92
24	B	613	CLA	C1D-CHD-C4C	-2.39	120.91	126.06
24	b	615	CLA	C1D-CHD-C4C	-2.39	120.91	126.06
31	H	101	DGD	O6D-C1D-O3G	-2.38	104.33	109.97
31	h	101	DGD	O6D-C1D-O3G	-2.38	104.33	109.97
24	B	616	CLA	CMB-C2B-C3B	2.38	129.13	124.68
24	b	618	CLA	CMB-C2B-C3B	2.38	129.13	124.68
24	C	509	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
24	c	509	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
34	D	410	LHG	O8-C23-C24	2.38	119.37	111.91
26	B	617	BCR	C30-C25-C26	-2.38	119.26	122.61
26	b	619	BCR	C30-C25-C26	-2.38	119.26	122.61
24	C	513	CLA	CHD-C4C-NC	2.38	127.95	124.20
24	c	513	CLA	CHD-C4C-NC	2.38	127.95	124.20
33	D	403	BCT	O3-C-O1	-2.37	113.39	119.55
24	c	505	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
28	A	411	PL9	C22-C23-C24	-2.37	121.94	127.66
28	a	411	PL9	C22-C23-C24	-2.37	121.94	127.66
24	C	510	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
24	c	510	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
24	C	508	CLA	C1-C2-C3	-2.37	121.94	126.04
30	C	520	LMG	O2-C2-C1	-2.37	104.29	110.05
30	c	520	LMG	O2-C2-C1	-2.37	104.29	110.05
24	B	609	CLA	CAA-C2A-C3A	-2.37	106.29	112.78
26	A	409	BCR	C27-C26-C25	2.37	126.17	122.73
26	a	409	BCR	C27-C26-C25	2.37	126.17	122.73
24	C	514	CLA	CBC-CAC-C3C	-2.37	105.91	112.43
24	B	605	CLA	CAA-C2A-C3A	-2.37	106.30	112.78
24	b	607	CLA	CAA-C2A-C3A	-2.37	106.30	112.78
24	B	615	CLA	CHB-C4A-NA	2.37	127.78	124.51
24	b	617	CLA	CHB-C4A-NA	2.37	127.78	124.51
24	b	612	CLA	C4-C3-C5	2.37	119.25	115.27
24	a	406	CLA	CBC-CAC-C3C	-2.36	105.91	112.43
24	C	505	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
24	B	612	CLA	CMA-C3A-C2A	-2.36	104.30	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	614	CLA	CMA-C3A-C2A	-2.36	104.30	113.83
26	B	619	BCR	C2-C1-C6	2.36	114.11	110.48
24	A	406	CLA	CBC-CAC-C3C	-2.36	105.92	112.43
24	c	514	CLA	CBC-CAC-C3C	-2.36	105.92	112.43
24	B	610	CLA	C4-C3-C5	2.36	119.24	115.27
24	B	614	CLA	CHB-C4A-NA	2.36	127.77	124.51
24	b	616	CLA	CHB-C4A-NA	2.36	127.77	124.51
24	c	508	CLA	C1-C2-C3	-2.36	121.97	126.04
25	D	402	PHO	CMC-C2C-C3C	2.36	129.39	124.94
30	D	411	LMG	C38-C37-C36	-2.36	102.46	114.42
30	d	411	LMG	C38-C37-C36	-2.35	102.48	114.42
33	d	403	BCT	O3-C-O1	-2.35	113.44	119.55
24	B	604	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
24	B	611	CLA	C7-C6-C5	-2.35	106.97	113.36
24	C	513	CLA	CAC-C3C-C4C	2.35	127.86	124.81
24	c	513	CLA	CAC-C3C-C4C	2.35	127.86	124.81
24	B	610	CLA	CHD-C4C-NC	2.35	127.91	124.20
24	B	607	CLA	CED-O2D-CGD	2.35	121.25	115.94
24	b	609	CLA	CED-O2D-CGD	2.35	121.25	115.94
24	D	401	CLA	C4C-C3C-C2C	-2.35	103.47	106.90
24	d	401	CLA	C4C-C3C-C2C	-2.35	103.47	106.90
24	A	405	CLA	CMD-C2D-C3D	-2.35	122.21	127.61
24	a	405	CLA	CMD-C2D-C3D	-2.35	122.21	127.61
26	b	621	BCR	C2-C1-C6	2.35	114.09	110.48
25	d	402	PHO	CMC-C2C-C3C	2.34	129.36	124.94
24	b	612	CLA	CAC-C3C-C4C	2.34	127.85	124.81
28	a	411	PL9	C15-C14-C16	-2.34	111.33	115.27
24	B	611	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
24	b	611	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
24	A	408	CLA	C5-C3-C2	-2.34	116.38	121.12
24	a	408	CLA	C5-C3-C2	-2.34	116.38	121.12
26	C	515	BCR	C11-C10-C9	-2.34	123.97	127.31
26	c	515	BCR	C11-C10-C9	-2.34	123.97	127.31
24	D	401	CLA	CHB-C4A-NA	2.34	127.75	124.51
24	d	401	CLA	CHB-C4A-NA	2.34	127.75	124.51
24	b	606	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
24	C	510	CLA	CMA-C3A-C2A	-2.34	104.39	113.83
24	D	405	CLA	CAA-C2A-C3A	-2.34	106.37	112.78
24	d	405	CLA	CAA-C2A-C3A	-2.34	106.37	112.78
24	B	609	CLA	CMB-C2B-C1B	2.34	132.06	128.46
24	b	613	CLA	CAA-C2A-C3A	-2.34	106.38	112.78
24	c	510	CLA	CMA-C3A-C2A	-2.34	104.40	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	411	PL9	C15-C14-C16	-2.34	111.34	115.27
24	B	611	CLA	CHC-C1C-NC	2.34	127.75	124.20
30	C	523	LMG	C38-C37-C36	-2.33	102.58	114.42
30	c	523	LMG	C38-C37-C36	-2.33	102.58	114.42
24	C	508	CLA	O2A-CGA-CBA	2.33	119.23	111.91
24	c	508	CLA	O2A-CGA-CBA	2.33	119.23	111.91
24	C	513	CLA	CHC-C1C-C2C	-2.33	120.28	126.72
24	c	513	CLA	CHC-C1C-C2C	-2.33	120.28	126.72
24	c	509	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
24	A	406	CLA	CMA-C3A-C2A	-2.33	104.44	113.83
24	a	406	CLA	CMA-C3A-C2A	-2.33	104.44	113.83
25	A	407	PHO	CMC-C2C-C3C	2.33	129.33	124.94
25	a	407	PHO	CMC-C2C-C3C	2.33	129.33	124.94
24	b	613	CLA	C7-C6-C5	-2.33	107.04	113.36
24	C	512	CLA	CHD-C4C-NC	2.33	127.87	124.20
24	B	607	CLA	C4-C3-C5	2.32	119.17	115.27
24	b	609	CLA	C4-C3-C5	2.32	119.17	115.27
24	b	613	CLA	CHC-C1C-NC	2.32	127.72	124.20
37	v	201	HEC	CBA-CAA-C2A	-2.32	108.70	112.60
26	C	516	BCR	C27-C26-C25	2.32	126.10	122.73
24	C	504	CLA	CMB-C2B-C3B	2.32	129.01	124.68
24	c	504	CLA	CMB-C2B-C3B	2.32	129.01	124.68
24	B	613	CLA	C7-C6-C5	-2.32	107.07	113.36
24	D	405	CLA	CMA-C3A-C4A	-2.31	105.55	111.77
24	d	405	CLA	CMA-C3A-C4A	-2.31	105.55	111.77
24	b	615	CLA	C7-C6-C5	-2.31	107.07	113.36
24	c	512	CLA	CHD-C4C-NC	2.31	127.85	124.20
26	J	104	BCR	C38-C26-C27	-2.31	109.17	113.62
26	j	104	BCR	C38-C26-C27	-2.31	109.17	113.62
24	C	512	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
24	c	512	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
24	b	616	CLA	CBA-CAA-C2A	2.31	120.69	113.86
24	C	512	CLA	C1-O2A-CGA	2.31	122.51	116.44
24	c	512	CLA	C1-O2A-CGA	2.31	122.51	116.44
24	B	614	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
24	b	616	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
24	C	509	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
24	C	505	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
24	c	505	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
24	C	512	CLA	O2A-CGA-CBA	2.31	119.15	111.91
24	b	611	CLA	CMB-C2B-C1B	2.31	132.01	128.46
37	V	201	HEC	CBA-CAA-C2A	-2.31	108.72	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	508	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
24	c	508	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
24	B	616	CLA	CMC-C2C-C1C	2.30	128.55	125.04
24	b	618	CLA	CMC-C2C-C1C	2.30	128.55	125.04
30	B	621	LMG	O3-C3-C2	-2.30	105.02	110.35
30	b	622	LMG	O3-C3-C2	-2.30	105.02	110.35
24	B	613	CLA	CAA-C2A-C3A	-2.30	106.47	112.78
24	b	615	CLA	CAA-C2A-C3A	-2.30	106.47	112.78
30	C	523	LMG	O6-C1-O1	-2.30	104.52	109.97
24	C	513	CLA	CBC-CAC-C3C	-2.30	106.08	112.43
24	c	513	CLA	CBC-CAC-C3C	-2.30	106.08	112.43
24	b	610	CLA	C4-C3-C5	2.30	119.14	115.27
24	B	614	CLA	CBA-CAA-C2A	2.30	120.65	113.86
24	B	611	CLA	CED-O2D-CGD	2.30	121.13	115.94
24	b	613	CLA	CED-O2D-CGD	2.30	121.13	115.94
26	a	409	BCR	C38-C26-C27	-2.30	109.20	113.62
26	C	516	BCR	C30-C25-C26	-2.30	119.38	122.61
26	c	516	BCR	C30-C25-C26	-2.30	119.38	122.61
27	F	101	SQD	O5-C5-C4	2.30	113.86	109.69
24	c	502	CLA	O2A-CGA-CBA	2.30	119.11	111.91
24	c	512	CLA	O2A-CGA-CBA	2.30	119.11	111.91
26	c	516	BCR	C27-C26-C25	2.29	126.06	122.73
24	A	406	CLA	CAA-CBA-CGA	2.29	119.96	113.25
30	c	523	LMG	O6-C1-O1	-2.29	104.54	109.97
27	f	101	SQD	O5-C5-C4	2.29	113.86	109.69
24	C	508	CLA	CMC-C2C-C1C	2.29	128.53	125.04
24	c	508	CLA	CMC-C2C-C1C	2.29	128.53	125.04
24	B	603	CLA	CMC-C2C-C1C	2.29	128.53	125.04
24	b	605	CLA	CMC-C2C-C1C	2.29	128.53	125.04
28	a	411	PL9	O2-C1-C2	-2.29	116.53	121.78
26	A	409	BCR	C38-C26-C27	-2.29	109.22	113.62
24	B	610	CLA	CMC-C2C-C1C	2.29	128.53	125.04
28	A	411	PL9	O2-C1-C2	-2.29	116.54	121.78
24	B	608	CLA	C4-C3-C5	2.29	119.12	115.27
24	C	502	CLA	O2A-CGA-CBA	2.28	119.08	111.91
26	C	522	BCR	C38-C26-C27	-2.28	109.23	113.62
26	c	522	BCR	C38-C26-C27	-2.28	109.23	113.62
24	C	507	CLA	CGD-CBD-CAD	-2.28	103.34	110.73
24	c	507	CLA	CGD-CBD-CAD	-2.28	103.34	110.73
24	B	614	CLA	C1D-CHD-C4C	-2.28	121.14	126.06
24	b	616	CLA	C1D-CHD-C4C	-2.28	121.14	126.06
27	B	620	SQD	O48-C23-C24	2.28	119.06	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	L	102	SQD	O48-C23-C24	2.28	119.06	111.91
24	a	406	CLA	CAA-CBA-CGA	2.28	119.91	113.25
24	B	615	CLA	CHC-C1C-NC	2.28	127.66	124.20
24	b	617	CLA	CHC-C1C-NC	2.28	127.66	124.20
24	C	503	CLA	CHB-C4A-NA	2.28	127.66	124.51
24	c	503	CLA	CHB-C4A-NA	2.28	127.66	124.51
34	L	101	LHG	C11-C10-C9	-2.28	102.86	114.42
34	l	101	LHG	C11-C10-C9	-2.28	102.86	114.42
24	B	610	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
24	b	615	CLA	C4C-C3C-C2C	-2.28	103.58	106.90
26	a	409	BCR	C16-C17-C18	-2.28	124.06	127.31
24	C	509	CLA	CBC-CAC-C3C	-2.27	106.16	112.43
24	c	509	CLA	CBC-CAC-C3C	-2.27	106.16	112.43
34	d	408	LHG	C27-C26-C25	-2.27	102.88	114.42
34	D	408	LHG	C27-C26-C25	-2.27	102.89	114.42
24	C	511	CLA	CMC-C2C-C1C	2.27	128.50	125.04
24	c	511	CLA	CMC-C2C-C1C	2.27	128.50	125.04
24	B	603	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
24	b	605	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
24	C	508	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
24	c	508	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
31	c	518	DGD	O2D-C2D-C1D	-2.27	104.53	110.05
32	Z	101	LMT	O5B-C5B-C6B	2.27	112.07	106.44
24	C	503	CLA	C6-C5-C3	-2.27	107.51	113.45
24	c	503	CLA	C6-C5-C3	-2.27	107.51	113.45
34	e	101	LHG	C18-C17-C16	-2.26	102.93	114.42
26	B	618	BCR	C28-C27-C26	-2.26	110.04	114.08
24	C	506	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
24	c	506	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
24	B	607	CLA	CBC-CAC-C3C	-2.26	106.19	112.43
24	b	609	CLA	CBC-CAC-C3C	-2.26	106.19	112.43
30	C	501	LMG	C7-O1-C1	-2.26	109.32	113.74
30	c	501	LMG	C7-O1-C1	-2.26	109.32	113.74
34	E	101	LHG	C18-C17-C16	-2.26	102.96	114.42
24	D	404	CLA	CED-O2D-CGD	2.26	121.05	115.94
24	d	404	CLA	CED-O2D-CGD	2.26	121.05	115.94
31	C	518	DGD	O2D-C2D-C1D	-2.26	104.56	110.05
24	D	405	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
24	d	405	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
28	A	411	PL9	C31-C32-C33	-2.26	104.47	111.88
28	a	411	PL9	C31-C32-C33	-2.26	104.47	111.88
32	z	101	LMT	O5B-C5B-C6B	2.26	112.04	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b	620	BCR	C28-C27-C26	-2.25	110.05	114.08
24	b	612	CLA	CMC-C2C-C1C	2.25	128.47	125.04
24	B	613	CLA	C4C-C3C-C2C	-2.25	103.61	106.90
24	b	612	CLA	CHD-C4C-NC	2.25	127.75	124.20
24	b	613	CLA	CMA-C3A-C4A	-2.25	105.72	111.77
24	b	608	CLA	CHD-C4C-NC	2.25	127.75	124.20
31	H	101	DGD	CAB-C9B-C8B	-2.25	103.02	114.42
31	h	101	DGD	CAB-C9B-C8B	-2.25	103.02	114.42
24	C	505	CLA	CHC-C1C-NC	2.25	127.61	124.20
24	c	505	CLA	CHC-C1C-NC	2.25	127.61	124.20
24	c	509	CLA	C1-C2-C3	-2.24	122.16	126.04
26	A	409	BCR	C16-C17-C18	-2.24	124.11	127.31
24	C	505	CLA	C1-O2A-CGA	2.24	122.33	116.44
24	c	505	CLA	C1-O2A-CGA	2.24	122.33	116.44
35	E	103	HEM	C4C-CHD-C1D	2.24	125.52	122.56
35	e	103	HEM	C4C-CHD-C1D	2.24	125.52	122.56
24	B	611	CLA	CMA-C3A-C4A	-2.24	105.75	111.77
26	c	516	BCR	C35-C13-C14	-2.24	119.79	122.92
24	C	502	CLA	CHB-C4A-NA	2.24	127.61	124.51
24	c	502	CLA	CHB-C4A-NA	2.24	127.60	124.51
31	C	519	DGD	C3G-C2G-C1G	-2.23	106.50	111.79
31	c	519	DGD	C3G-C2G-C1G	-2.23	106.50	111.79
26	B	618	BCR	C27-C26-C25	2.23	125.97	122.73
26	b	620	BCR	C27-C26-C25	2.23	125.97	122.73
24	b	606	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
24	C	507	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
24	c	507	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
24	b	603	CLA	O2A-CGA-CBA	2.23	118.90	111.91
31	H	101	DGD	C4E-C3E-C2E	-2.23	106.93	110.82
31	h	101	DGD	C4E-C3E-C2E	-2.23	106.93	110.82
24	B	601	CLA	O2A-CGA-CBA	2.23	118.90	111.91
24	b	611	CLA	C4-C3-C5	2.23	119.02	115.27
24	B	604	CLA	CAA-C2A-C3A	-2.23	106.68	112.78
24	B	604	CLA	CHD-C4C-NC	2.22	127.71	124.20
24	b	606	CLA	CHD-C4C-NC	2.22	127.71	124.20
24	B	606	CLA	CHD-C4C-NC	2.22	127.71	124.20
24	c	511	CLA	O2A-CGA-CBA	2.22	118.88	111.91
24	b	610	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
30	D	411	LMG	C1-C2-C3	-2.22	105.37	110.00
30	d	411	LMG	C1-C2-C3	-2.22	105.37	110.00
26	B	618	BCR	C24-C23-C22	-2.22	122.88	126.23
26	b	620	BCR	C24-C23-C22	-2.22	122.88	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	408	CLA	C4C-C3C-C2C	-2.22	103.66	106.90
24	a	408	CLA	C4C-C3C-C2C	-2.22	103.66	106.90
25	D	402	PHO	CED-O2D-CGD	2.22	120.95	115.94
25	d	402	PHO	CED-O2D-CGD	2.22	120.95	115.94
24	C	502	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
24	c	502	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
26	T	101	BCR	C39-C30-C25	2.22	113.89	110.30
26	t	102	BCR	C39-C30-C25	2.22	113.89	110.30
26	C	516	BCR	C35-C13-C14	-2.22	119.82	122.92
24	B	601	CLA	CHD-C4C-NC	2.21	127.69	124.20
24	b	603	CLA	CHD-C4C-NC	2.21	127.69	124.20
34	D	410	LHG	O8-C23-O10	-2.21	118.01	123.59
24	C	509	CLA	C1-C2-C3	-2.21	122.22	126.04
28	A	411	PL9	C20-C19-C18	-2.21	118.00	123.68
28	a	411	PL9	C20-C19-C18	-2.21	118.00	123.68
38	X	101	RRX	C4-C5-C6	-2.21	119.52	122.73
38	x	101	RRX	C4-C5-C6	-2.21	119.52	122.73
24	B	612	CLA	CHC-C1C-C2C	-2.21	120.61	126.72
24	b	614	CLA	CHC-C1C-C2C	-2.21	120.61	126.72
24	b	613	CLA	C6-C5-C3	2.21	119.25	113.45
27	f	101	SQD	C1-C2-C3	-2.21	105.39	110.00
26	D	406	BCR	C35-C13-C12	2.21	121.56	118.08
24	C	511	CLA	O2A-CGA-CBA	2.21	118.84	111.91
24	B	609	CLA	C4-C3-C5	2.21	118.98	115.27
24	C	512	CLA	C7-C6-C5	-2.21	107.36	113.36
24	c	512	CLA	C7-C6-C5	-2.21	107.36	113.36
26	J	104	BCR	C1-C6-C5	-2.21	119.51	122.61
24	B	608	CLA	CAA-C2A-C3A	-2.21	106.74	112.78
26	T	101	BCR	C38-C26-C27	-2.21	109.38	113.62
24	b	603	CLA	C4-C3-C5	2.20	118.98	115.27
24	C	505	CLA	CMC-C2C-C1C	2.20	128.39	125.04
24	c	505	CLA	CMC-C2C-C1C	2.20	128.39	125.04
26	t	102	BCR	C38-C26-C27	-2.20	109.39	113.62
34	d	410	LHG	O8-C23-O10	-2.20	118.04	123.59
24	B	609	CLA	O2A-CGA-CBA	2.20	118.82	111.91
24	b	611	CLA	C1-C2-C3	-2.20	122.24	126.04
24	B	611	CLA	C6-C5-C3	2.20	119.21	113.45
24	C	507	CLA	CMC-C2C-C3C	2.20	132.08	126.12
24	c	507	CLA	CMC-C2C-C3C	2.20	132.08	126.12
24	c	510	CLA	O2A-C1-C2	2.19	114.40	108.64
24	B	609	CLA	C1-C2-C3	-2.19	122.25	126.04
31	H	101	DGD	O3G-C3G-C2G	-2.19	105.61	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	h	101	DGD	O3G-C3G-C2G	-2.19	105.61	110.90
30	D	411	LMG	C22-C21-C20	-2.19	103.30	114.42
30	d	411	LMG	C22-C21-C20	-2.19	103.30	114.42
24	B	609	CLA	CED-O2D-CGD	2.19	120.89	115.94
24	C	510	CLA	O2A-C1-C2	2.19	114.39	108.64
24	C	512	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
24	c	512	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
24	B	607	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
24	b	609	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
24	b	611	CLA	CED-O2D-CGD	2.19	120.89	115.94
24	b	611	CLA	O2A-CGA-CBA	2.19	118.78	111.91
26	D	406	BCR	C27-C26-C25	2.19	125.91	122.73
26	d	406	BCR	C27-C26-C25	2.19	125.91	122.73
24	B	615	CLA	CHD-C4C-NC	2.19	127.65	124.20
24	b	617	CLA	CHD-C4C-NC	2.19	127.65	124.20
26	d	406	BCR	C35-C13-C12	2.19	121.52	118.08
24	B	604	CLA	C11-C10-C8	-2.19	108.85	115.92
24	b	606	CLA	C11-C10-C8	-2.19	108.85	115.92
24	b	612	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
34	L	101	LHG	C27-C26-C25	-2.18	103.33	114.42
26	C	515	BCR	C31-C1-C6	2.18	113.84	110.30
27	F	101	SQD	C1-C2-C3	-2.18	105.45	110.00
24	B	616	CLA	CHA-C1A-NA	-2.18	121.41	126.40
24	b	618	CLA	CHA-C1A-NA	-2.18	121.41	126.40
24	B	601	CLA	C4-C3-C5	2.18	118.94	115.27
24	B	605	CLA	C4A-NA-C1A	-2.18	105.73	106.71
34	l	101	LHG	C27-C26-C25	-2.18	103.37	114.42
24	B	606	CLA	CHA-C1A-NA	-2.17	121.42	126.40
24	b	608	CLA	CHA-C1A-NA	-2.17	121.42	126.40
24	B	604	CLA	CHA-C1A-NA	-2.17	121.42	126.40
24	b	606	CLA	CHA-C1A-NA	-2.17	121.42	126.40
26	j	104	BCR	C1-C6-C5	-2.17	119.55	122.61
24	b	612	CLA	CAA-CBA-CGA	-2.17	106.91	113.25
24	b	611	CLA	CMA-C3A-C2A	-2.17	105.07	113.83
30	c	501	LMG	C38-C37-C36	-2.17	103.42	114.42
24	B	609	CLA	CMA-C3A-C2A	-2.17	105.09	113.83
24	D	401	CLA	CHD-C4C-NC	2.17	127.62	124.20
24	d	401	CLA	CHD-C4C-NC	2.17	127.62	124.20
28	d	407	PL9	C32-C33-C34	-2.17	122.45	127.66
30	C	501	LMG	C38-C37-C36	-2.17	103.43	114.42
25	d	402	PHO	CMD-C2D-C3D	2.16	128.73	124.68
24	B	612	CLA	CHD-C4C-NC	2.16	127.61	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	614	CLA	CHD-C4C-NC	2.16	127.61	124.20
31	C	519	DGD	CBB-CAB-C9B	-2.16	103.45	114.42
31	c	519	DGD	CBB-CAB-C9B	-2.16	103.45	114.42
24	B	610	CLA	CAA-CBA-CGA	-2.16	106.94	113.25
24	C	512	CLA	CAA-C2A-C1A	2.16	119.06	111.97
24	c	512	CLA	CAA-C2A-C1A	2.16	119.06	111.97
34	d	410	LHG	C18-C17-C16	-2.16	103.46	114.42
26	c	515	BCR	C31-C1-C6	2.16	113.80	110.30
24	C	507	CLA	CMA-C3A-C4A	-2.16	105.97	111.77
34	e	101	LHG	C5-O7-C7	-2.16	112.48	117.79
24	C	513	CLA	C16-C15-C13	-2.16	108.95	115.92
24	c	513	CLA	C16-C15-C13	-2.16	108.95	115.92
28	D	407	PL9	C32-C33-C34	-2.16	122.47	127.66
34	D	410	LHG	C18-C17-C16	-2.16	103.48	114.42
26	t	102	BCR	C7-C8-C9	-2.15	122.98	126.23
26	T	101	BCR	C7-C8-C9	-2.15	122.98	126.23
25	D	402	PHO	CMD-C2D-C3D	2.15	128.70	124.68
24	b	607	CLA	C4A-NA-C1A	-2.15	105.74	106.71
24	a	406	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
24	C	509	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
24	d	401	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
24	B	616	CLA	CHC-C1C-NC	2.15	127.46	124.20
24	b	618	CLA	CHC-C1C-NC	2.15	127.46	124.20
24	A	406	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
34	D	408	LHG	O8-C6-C5	-2.15	102.19	108.43
24	c	507	CLA	CMA-C3A-C4A	-2.14	106.01	111.77
34	E	101	LHG	C5-O7-C7	-2.14	112.52	117.79
26	a	409	BCR	C24-C23-C22	-2.14	123.00	126.23
24	c	509	CLA	CAA-C2A-C3A	-2.14	106.92	112.78
24	B	615	CLA	CBC-CAC-C3C	-2.14	106.53	112.43
24	b	617	CLA	CBC-CAC-C3C	-2.14	106.53	112.43
31	C	517	DGD	O5E-C6E-C5E	-2.14	103.95	111.29
34	d	408	LHG	O8-C6-C5	-2.14	102.21	108.43
26	C	522	BCR	C27-C26-C25	2.14	125.83	122.73
26	c	522	BCR	C27-C26-C25	2.14	125.83	122.73
24	A	408	CLA	OBD-CAD-C3D	-2.14	123.38	128.52
24	a	408	CLA	OBD-CAD-C3D	-2.14	123.38	128.52
24	b	609	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
31	C	517	DGD	O6E-C1E-O5D	-2.13	104.92	109.97
24	D	401	CLA	CAA-CBA-CGA	2.13	119.48	113.25
24	d	401	CLA	CAA-CBA-CGA	2.13	119.48	113.25
27	A	412	SQD	C45-O47-C7	2.13	123.04	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	412	SQD	C45-O47-C7	2.13	123.04	117.79
31	c	517	DGD	O5E-C6E-C5E	-2.13	103.98	111.29
24	B	603	CLA	CBC-CAC-C3C	-2.13	106.57	112.43
24	D	401	CLA	C2A-C1A-CHA	-2.13	120.14	123.86
24	c	509	CLA	CED-O2D-CGD	2.12	120.74	115.94
31	c	517	DGD	O6E-C1E-O5D	-2.12	104.94	109.97
24	B	607	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
31	c	517	DGD	C3G-C2G-C1G	-2.12	106.77	111.79
24	D	404	CLA	O2D-CGD-CBD	2.12	115.04	111.27
24	d	404	CLA	O2D-CGD-CBD	2.12	115.04	111.27
24	A	405	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
24	a	405	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
30	B	621	LMG	C38-C37-C36	-2.12	103.66	114.42
30	b	622	LMG	C38-C37-C36	-2.12	103.66	114.42
32	Z	101	LMT	C1B-O5B-C5B	2.12	117.85	113.69
24	b	603	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
24	b	605	CLA	CBC-CAC-C3C	-2.12	106.59	112.43
24	a	408	CLA	C7-C6-C5	-2.12	107.61	113.36
27	B	620	SQD	O5-C1-C2	-2.12	105.87	110.35
27	L	102	SQD	O5-C1-C2	-2.12	105.87	110.35
24	B	613	CLA	CHA-C1A-NA	-2.12	121.55	126.40
24	b	615	CLA	CHA-C1A-NA	-2.12	121.55	126.40
34	D	409	LHG	C20-C19-C18	-2.12	103.69	114.42
34	d	409	LHG	C20-C19-C18	-2.12	103.69	114.42
24	B	603	CLA	CHB-C4A-NA	2.12	127.44	124.51
24	b	605	CLA	CHB-C4A-NA	2.12	127.44	124.51
24	C	509	CLA	CED-O2D-CGD	2.11	120.72	115.94
28	A	411	PL9	C12-C13-C14	-2.11	122.58	127.66
28	a	411	PL9	C12-C13-C14	-2.11	122.58	127.66
32	z	101	LMT	C1B-O5B-C5B	2.11	117.83	113.69
31	C	517	DGD	C3G-C2G-C1G	-2.11	106.80	111.79
24	C	509	CLA	O2A-CGA-CBA	2.11	118.52	111.91
24	c	509	CLA	O2A-CGA-CBA	2.11	118.52	111.91
25	A	407	PHO	CBA-CAA-C2A	-2.11	107.65	113.81
24	C	506	CLA	CMD-C2D-C3D	-2.11	122.77	127.61
24	c	506	CLA	CMD-C2D-C3D	-2.11	122.77	127.61
24	A	408	CLA	C7-C6-C5	-2.11	107.64	113.36
24	C	503	CLA	CHD-C4C-NC	2.10	127.52	124.20
26	A	409	BCR	C24-C23-C22	-2.10	123.06	126.23
24	C	507	CLA	CAC-C3C-C4C	2.10	127.54	124.81
24	c	507	CLA	CAC-C3C-C4C	2.10	127.54	124.81
24	B	601	CLA	O1D-CGD-CBD	-2.10	120.19	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	C	523	LMG	O2-C2-C1	-2.10	104.95	110.05
30	c	523	LMG	O2-C2-C1	-2.10	104.95	110.05
24	c	511	CLA	OBD-CAD-C3D	-2.10	123.47	128.52
30	C	523	LMG	C40-C39-C38	-2.10	103.78	114.42
30	c	523	LMG	C40-C39-C38	-2.10	103.78	114.42
24	C	511	CLA	OBD-CAD-C3D	-2.10	123.48	128.52
27	B	620	SQD	C1-C2-C3	-2.09	105.63	110.00
27	L	102	SQD	C1-C2-C3	-2.09	105.63	110.00
24	C	513	CLA	CAA-C2A-C1A	2.09	118.83	111.97
24	c	513	CLA	CAA-C2A-C1A	2.09	118.83	111.97
24	c	502	CLA	C4A-NA-C1A	-2.09	105.77	106.71
24	c	510	CLA	CHD-C4C-NC	2.09	127.50	124.20
28	d	407	PL9	C36-C37-C38	-2.09	105.01	111.88
25	a	407	PHO	CBA-CAA-C2A	-2.09	107.70	113.81
24	C	509	CLA	C4A-NA-C1A	-2.09	105.77	106.71
24	c	509	CLA	C4A-NA-C1A	-2.09	105.77	106.71
26	J	104	BCR	C27-C26-C25	2.09	125.76	122.73
26	j	104	BCR	C27-C26-C25	2.09	125.76	122.73
24	B	605	CLA	C6-C7-C8	-2.09	109.18	115.92
24	B	612	CLA	CHB-C4A-NA	2.08	127.39	124.51
24	b	614	CLA	CHB-C4A-NA	2.08	127.39	124.51
24	B	603	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
24	b	605	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
24	B	610	CLA	CHC-C1C-NC	2.08	127.36	124.20
28	D	407	PL9	C36-C37-C38	-2.08	105.04	111.88
24	b	612	CLA	CHC-C1C-NC	2.08	127.36	124.20
32	J	102	LMT	C1'-C2'-C3'	2.08	114.33	110.00
31	C	517	DGD	C1E-O6E-C5E	2.08	117.77	113.69
24	B	606	CLA	CED-O2D-CGD	2.08	120.64	115.94
24	C	509	CLA	CMA-C3A-C2A	-2.08	105.44	113.83
27	A	412	SQD	O48-C23-C24	2.08	118.42	111.91
27	a	412	SQD	O48-C23-C24	2.08	118.42	111.91
26	C	516	BCR	C2-C1-C6	2.08	113.68	110.48
26	c	516	BCR	C2-C1-C6	2.08	113.68	110.48
24	B	613	CLA	CBC-CAC-C3C	-2.08	106.71	112.43
24	b	615	CLA	CBC-CAC-C3C	-2.08	106.71	112.43
24	C	506	CLA	CMB-C2B-C3B	2.07	128.56	124.68
24	c	506	CLA	CMB-C2B-C3B	2.07	128.56	124.68
24	c	509	CLA	CMA-C3A-C2A	-2.07	105.46	113.83
24	b	607	CLA	C6-C7-C8	-2.07	109.22	115.92
32	j	102	LMT	C1'-C2'-C3'	2.07	114.31	110.00
38	x	101	RRX	C37-C22-C23	2.07	121.34	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	517	DGD	C1E-O6E-C5E	2.07	117.75	113.69
24	c	503	CLA	CHD-C4C-NC	2.07	127.46	124.20
34	L	101	LHG	C20-C19-C18	-2.06	103.95	114.42
24	D	404	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
24	d	404	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
24	b	608	CLA	CED-O2D-CGD	2.06	120.60	115.94
34	l	101	LHG	C20-C19-C18	-2.06	103.95	114.42
26	C	515	BCR	C15-C14-C13	-2.06	124.37	127.31
24	D	404	CLA	C1D-CHD-C4C	-2.06	121.61	126.06
38	X	101	RRX	C37-C22-C23	2.06	121.32	118.08
38	x	101	RRX	C34-C9-C8	2.06	121.32	118.08
24	C	506	CLA	CHD-C4C-NC	2.06	127.45	124.20
24	c	506	CLA	CHD-C4C-NC	2.06	127.45	124.20
30	C	520	LMG	O8-C28-O10	-2.06	118.40	123.59
30	c	520	LMG	O8-C28-O10	-2.06	118.40	123.59
26	a	409	BCR	C20-C19-C18	-2.06	120.64	126.42
27	A	410	SQD	O48-C23-C24	2.06	118.36	111.91
27	a	410	SQD	O48-C23-C24	2.06	118.36	111.91
26	C	522	BCR	C40-C30-C25	2.06	113.64	110.30
26	c	522	BCR	C40-C30-C25	2.06	113.64	110.30
24	d	404	CLA	C1D-CHD-C4C	-2.06	121.62	126.06
24	b	611	CLA	CMA-C3A-C4A	-2.06	106.25	111.77
24	B	603	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
24	b	605	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
26	B	618	BCR	C15-C14-C13	-2.05	124.38	127.31
26	b	620	BCR	C15-C14-C13	-2.05	124.38	127.31
24	c	511	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
26	A	409	BCR	C20-C19-C18	-2.05	120.66	126.42
34	d	408	LHG	O8-C23-O10	-2.05	118.42	123.59
24	C	510	CLA	CHD-C4C-NC	2.05	127.43	124.20
24	B	606	CLA	CMA-C3A-C2A	-2.05	105.56	113.83
24	B	602	CLA	OBD-CAD-C3D	-2.04	123.60	128.52
24	b	604	CLA	OBD-CAD-C3D	-2.04	123.60	128.52
24	B	604	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
38	X	101	RRX	C34-C9-C8	2.04	121.30	118.08
26	C	522	BCR	C2-C1-C6	2.04	113.63	110.48
26	c	522	BCR	C2-C1-C6	2.04	113.63	110.48
24	b	608	CLA	CMA-C3A-C2A	-2.04	105.59	113.83
24	C	511	CLA	CHD-C4C-NC	2.04	127.42	124.20
24	c	511	CLA	CHD-C4C-NC	2.04	127.42	124.20
26	c	515	BCR	C15-C14-C13	-2.04	124.40	127.31
34	E	101	LHG	C27-C26-C25	-2.04	104.07	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	V	201	HEC	CMA-C3A-C2A	2.04	128.79	124.94
31	C	519	DGD	O2G-C1B-C2B	2.04	115.89	111.50
31	c	519	DGD	O2G-C1B-C2B	2.04	115.89	111.50
34	e	101	LHG	C27-C26-C25	-2.04	104.08	114.42
24	B	616	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
24	b	618	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
30	c	501	LMG	O2-C2-C1	-2.04	105.10	110.05
34	D	408	LHG	O8-C23-O10	-2.04	118.45	123.59
24	B	604	CLA	CMB-C2B-C3B	2.04	128.49	124.68
24	b	606	CLA	CMB-C2B-C3B	2.04	128.49	124.68
24	C	511	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
24	C	504	CLA	CHA-C1A-NA	-2.03	121.74	126.40
24	c	504	CLA	CHA-C1A-NA	-2.03	121.74	126.40
24	b	606	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
34	D	408	LHG	C18-C17-C16	-2.03	104.12	114.42
34	d	408	LHG	C18-C17-C16	-2.03	104.12	114.42
24	B	609	CLA	CMA-C3A-C4A	-2.03	106.32	111.77
37	v	201	HEC	CMA-C3A-C2A	2.03	128.77	124.94
27	a	412	SQD	O8-S-C6	2.03	108.97	105.74
30	C	520	LMG	O6-C1-O1	-2.03	105.17	109.97
30	c	520	LMG	O6-C1-O1	-2.03	105.17	109.97
30	d	411	LMG	C17-C16-C15	-2.03	104.13	114.42
30	C	501	LMG	O2-C2-C1	-2.03	105.12	110.05
31	C	519	DGD	CAB-C9B-C8B	-2.03	104.14	114.42
31	c	519	DGD	CAB-C9B-C8B	-2.03	104.14	114.42
24	D	405	CLA	CHD-C4C-NC	2.03	127.40	124.20
24	d	405	CLA	CHD-C4C-NC	2.03	127.40	124.20
24	B	609	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
24	b	611	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
24	D	405	CLA	CAC-C3C-C4C	2.02	127.44	124.81
24	B	612	CLA	C11-C12-C13	-2.02	109.38	115.92
24	b	614	CLA	C11-C12-C13	-2.02	109.38	115.92
34	D	408	LHG	C20-C19-C18	-2.02	104.15	114.42
34	d	408	LHG	C20-C19-C18	-2.02	104.15	114.42
24	c	502	CLA	C4C-C3C-C2C	-2.02	103.95	106.90
27	A	410	SQD	O48-C23-O10	-2.02	118.48	123.59
27	a	410	SQD	O48-C23-O10	-2.02	118.48	123.59
24	A	405	CLA	CAC-C3C-C4C	2.02	127.44	124.81
24	a	405	CLA	CAC-C3C-C4C	2.02	127.44	124.81
28	A	411	PL9	C50-C49-C48	-2.02	116.80	122.65
37	V	201	HEC	CAA-CBA-CGA	-2.02	108.09	113.76
24	B	606	CLA	O2A-CGA-CBA	2.02	118.25	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	608	CLA	O2A-CGA-CBA	2.02	118.25	111.91
24	C	514	CLA	CMA-C3A-C2A	-2.02	105.67	113.83
24	c	514	CLA	CMA-C3A-C2A	-2.02	105.67	113.83
34	E	101	LHG	O8-C6-C5	-2.02	102.55	108.43
24	A	406	CLA	CHA-C1A-NA	-2.02	121.77	126.40
24	a	406	CLA	CHA-C1A-NA	-2.02	121.77	126.40
24	b	610	CLA	CBC-CAC-C3C	-2.02	106.86	112.43
24	B	611	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
24	b	613	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
24	C	509	CLA	CHD-C4C-NC	2.02	127.39	124.20
24	c	509	CLA	CHD-C4C-NC	2.02	127.39	124.20
27	A	412	SQD	O8-S-C6	2.02	108.96	105.74
24	C	505	CLA	C4A-NA-C1A	-2.02	105.80	106.71
24	c	505	CLA	C4A-NA-C1A	-2.02	105.80	106.71
24	B	616	CLA	C6-C5-C3	2.02	118.74	113.45
24	b	618	CLA	C6-C5-C3	2.02	118.74	113.45
34	e	101	LHG	O8-C6-C5	-2.02	102.56	108.43
30	D	411	LMG	C17-C16-C15	-2.02	104.19	114.42
35	e	103	HEM	O2A-CGA-CBA	2.02	120.50	114.03
37	v	201	HEC	CAA-CBA-CGA	-2.01	108.11	113.76
28	a	411	PL9	C50-C49-C48	-2.01	116.83	122.65
31	C	518	DGD	O3E-C3E-C2E	-2.01	105.70	110.35
31	c	518	DGD	O3E-C3E-C2E	-2.01	105.70	110.35
35	E	103	HEM	C4D-ND-C1D	2.01	107.15	105.07
35	e	103	HEM	C4D-ND-C1D	2.01	107.15	105.07
24	C	514	CLA	OBD-CAD-C3D	-2.01	123.68	128.52
24	c	514	CLA	OBD-CAD-C3D	-2.01	123.68	128.52
24	C	502	CLA	C4A-NA-C1A	-2.01	105.80	106.71
24	C	513	CLA	CMA-C3A-C2A	-2.01	105.73	113.83
24	c	513	CLA	CMA-C3A-C2A	-2.01	105.73	113.83
24	B	616	CLA	C11-C12-C13	-2.01	109.43	115.92
24	B	608	CLA	CBC-CAC-C3C	-2.01	106.90	112.43
35	E	103	HEM	O2A-CGA-CBA	2.01	120.47	114.03
24	B	613	CLA	CED-O2D-CGD	2.01	120.47	115.94
24	b	615	CLA	CED-O2D-CGD	2.01	120.47	115.94
24	b	604	CLA	CMA-C3A-C4A	-2.00	106.39	111.77
30	C	501	LMG	C1-C2-C3	-2.00	105.83	110.00
30	c	501	LMG	C1-C2-C3	-2.00	105.83	110.00

All (60) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	B	601	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND
24	B	604	CLA	ND
24	B	605	CLA	ND
24	B	606	CLA	ND
24	B	607	CLA	ND
24	B	609	CLA	ND
24	B	610	CLA	ND
24	B	611	CLA	ND
24	B	612	CLA	ND
24	B	613	CLA	ND
24	B	614	CLA	ND
24	B	615	CLA	ND
24	B	616	CLA	ND
24	C	502	CLA	ND
24	C	504	CLA	ND
24	C	505	CLA	ND
24	C	506	CLA	ND
24	C	507	CLA	ND
24	C	508	CLA	ND
24	C	509	CLA	ND
24	C	510	CLA	ND
24	C	511	CLA	ND
24	C	512	CLA	ND
24	C	513	CLA	ND
24	C	514	CLA	ND
24	D	401	CLA	ND
24	D	404	CLA	ND
24	a	405	CLA	ND
24	b	603	CLA	ND
24	b	604	CLA	ND
24	b	605	CLA	ND
24	b	606	CLA	ND
24	b	607	CLA	ND
24	b	608	CLA	ND
24	b	609	CLA	ND
24	b	611	CLA	ND
24	b	612	CLA	ND
24	b	613	CLA	ND

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Mol	Chain	Res	Type	Atom
24	b	614	CLA	ND
24	b	615	CLA	ND
24	b	616	CLA	ND
24	b	617	CLA	ND
24	b	618	CLA	ND
24	c	502	CLA	ND
24	c	504	CLA	ND
24	c	505	CLA	ND
24	c	506	CLA	ND
24	c	507	CLA	ND
24	c	508	CLA	ND
24	c	509	CLA	ND
24	c	510	CLA	ND
24	c	511	CLA	ND
24	c	512	CLA	ND
24	c	513	CLA	ND
24	c	514	CLA	ND
24	d	401	CLA	ND
24	d	404	CLA	ND

All (1523) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	406	CLA	CHA-CBD-CGD-O1D
24	A	406	CLA	CHA-CBD-CGD-O2D
24	B	601	CLA	C14-C13-C15-C16
24	B	603	CLA	C2-C3-C5-C6
24	B	603	CLA	C4-C3-C5-C6
24	B	605	CLA	C2-C3-C5-C6
24	B	605	CLA	C4-C3-C5-C6
24	B	606	CLA	CHA-CBD-CGD-O1D
24	B	606	CLA	CHA-CBD-CGD-O2D
24	B	614	CLA	CHA-CBD-CGD-O1D
24	B	614	CLA	CHA-CBD-CGD-O2D
24	B	614	CLA	CAD-CBD-CGD-O1D
24	C	503	CLA	CHA-CBD-CGD-O1D
24	C	503	CLA	CHA-CBD-CGD-O2D
24	C	503	CLA	CAD-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	C	510	CLA	C2-C1-O2A-CGA
24	a	406	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	a	406	CLA	CHA-CBD-CGD-O2D
24	b	603	CLA	C14-C13-C15-C16
24	b	605	CLA	C2-C3-C5-C6
24	b	605	CLA	C4-C3-C5-C6
24	b	607	CLA	C2-C3-C5-C6
24	b	607	CLA	C4-C3-C5-C6
24	b	608	CLA	CHA-CBD-CGD-O1D
24	b	608	CLA	CHA-CBD-CGD-O2D
24	b	616	CLA	CHA-CBD-CGD-O1D
24	b	616	CLA	CHA-CBD-CGD-O2D
24	b	616	CLA	CAD-CBD-CGD-O1D
24	c	503	CLA	CHA-CBD-CGD-O1D
24	c	503	CLA	CHA-CBD-CGD-O2D
24	c	503	CLA	CAD-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O2D
24	c	510	CLA	C2-C1-O2A-CGA
26	A	409	BCR	C36-C18-C19-C20
26	B	617	BCR	C1-C6-C7-C8
26	B	618	BCR	C7-C8-C9-C34
26	B	619	BCR	C7-C8-C9-C10
26	B	619	BCR	C7-C8-C9-C34
26	B	619	BCR	C21-C22-C23-C24
26	B	619	BCR	C37-C22-C23-C24
26	C	515	BCR	C7-C8-C9-C34
26	C	515	BCR	C11-C12-C13-C35
26	C	515	BCR	C37-C22-C23-C24
26	C	516	BCR	C7-C8-C9-C34
26	C	516	BCR	C11-C12-C13-C14
26	C	516	BCR	C11-C12-C13-C35
26	C	516	BCR	C23-C24-C25-C30
26	C	522	BCR	C1-C6-C7-C8
26	C	522	BCR	C11-C10-C9-C8
26	C	522	BCR	C11-C10-C9-C34
26	C	522	BCR	C11-C12-C13-C35
26	D	406	BCR	C7-C8-C9-C10
26	D	406	BCR	C21-C22-C23-C24
26	D	406	BCR	C37-C22-C23-C24
26	D	406	BCR	C22-C23-C24-C25
26	J	104	BCR	C5-C6-C7-C8
26	J	104	BCR	C7-C8-C9-C34
26	J	104	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
26	J	104	BCR	C37-C22-C23-C24
26	T	101	BCR	C1-C6-C7-C8
26	T	101	BCR	C7-C8-C9-C10
26	T	101	BCR	C21-C22-C23-C24
26	T	101	BCR	C37-C22-C23-C24
26	a	409	BCR	C36-C18-C19-C20
26	b	619	BCR	C1-C6-C7-C8
26	b	620	BCR	C7-C8-C9-C34
26	b	621	BCR	C7-C8-C9-C10
26	b	621	BCR	C7-C8-C9-C34
26	b	621	BCR	C21-C22-C23-C24
26	b	621	BCR	C37-C22-C23-C24
26	c	515	BCR	C7-C8-C9-C34
26	c	515	BCR	C11-C12-C13-C35
26	c	515	BCR	C37-C22-C23-C24
26	c	516	BCR	C7-C8-C9-C34
26	c	516	BCR	C11-C12-C13-C14
26	c	516	BCR	C11-C12-C13-C35
26	c	516	BCR	C23-C24-C25-C30
26	c	522	BCR	C1-C6-C7-C8
26	c	522	BCR	C11-C10-C9-C8
26	c	522	BCR	C11-C10-C9-C34
26	c	522	BCR	C11-C12-C13-C35
26	d	406	BCR	C7-C8-C9-C10
26	d	406	BCR	C21-C22-C23-C24
26	d	406	BCR	C37-C22-C23-C24
26	d	406	BCR	C22-C23-C24-C25
26	j	104	BCR	C5-C6-C7-C8
26	j	104	BCR	C7-C8-C9-C34
26	j	104	BCR	C21-C22-C23-C24
26	j	104	BCR	C37-C22-C23-C24
26	t	102	BCR	C1-C6-C7-C8
26	t	102	BCR	C7-C8-C9-C10
26	t	102	BCR	C21-C22-C23-C24
26	t	102	BCR	C37-C22-C23-C24
27	A	412	SQD	C5-C6-S-O7
27	A	412	SQD	C5-C6-S-O8
27	A	412	SQD	C5-C6-S-O9
27	B	620	SQD	O10-C23-O48-C46
27	B	620	SQD	C24-C23-O48-C46
27	L	102	SQD	O10-C23-O48-C46
27	L	102	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
27	a	412	SQD	C5-C6-S-O7
27	a	412	SQD	C5-C6-S-O8
27	a	412	SQD	C5-C6-S-O9
28	A	411	PL9	C12-C13-C14-C16
28	A	411	PL9	C18-C19-C21-C22
28	A	411	PL9	C27-C28-C29-C30
28	A	411	PL9	C27-C28-C29-C31
28	A	411	PL9	C28-C29-C31-C32
28	A	411	PL9	C37-C38-C39-C40
28	D	407	PL9	C42-C43-C44-C45
28	D	407	PL9	C44-C46-C47-C48
28	D	407	PL9	C47-C48-C49-C51
28	a	411	PL9	C12-C13-C14-C16
28	a	411	PL9	C18-C19-C21-C22
28	a	411	PL9	C27-C28-C29-C30
28	a	411	PL9	C27-C28-C29-C31
28	a	411	PL9	C28-C29-C31-C32
28	a	411	PL9	C37-C38-C39-C40
28	d	407	PL9	C42-C43-C44-C45
28	d	407	PL9	C44-C46-C47-C48
28	d	407	PL9	C47-C48-C49-C51
32	Z	101	LMT	C2-C1-O1'-C1'
32	z	101	LMT	C2-C1-O1'-C1'
34	D	408	LHG	C3-O3-P-O4
34	D	409	LHG	O1-C1-C2-C3
34	D	409	LHG	O2-C2-C3-O3
34	D	409	LHG	C3-O3-P-O5
34	D	409	LHG	C4-O6-P-O3
34	D	409	LHG	C4-O6-P-O4
34	D	409	LHG	C4-O6-P-O5
34	E	101	LHG	C3-O3-P-O5
34	E	101	LHG	C3-O3-P-O6
34	d	408	LHG	C3-O3-P-O4
34	d	409	LHG	O1-C1-C2-C3
34	d	409	LHG	O2-C2-C3-O3
34	d	409	LHG	C3-O3-P-O5
34	d	409	LHG	C4-O6-P-O3
34	d	409	LHG	C4-O6-P-O4
34	d	409	LHG	C4-O6-P-O5
34	e	101	LHG	C3-O3-P-O5
34	e	101	LHG	C3-O3-P-O6
27	F	101	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
27	f	101	SQD	O10-C23-O48-C46
32	C	521	LMT	C3'-C4'-O1B-C1B
32	c	521	LMT	C3'-C4'-O1B-C1B
24	B	614	CLA	C3-C5-C6-C7
24	B	615	CLA	C3-C5-C6-C7
24	b	616	CLA	C3-C5-C6-C7
24	b	617	CLA	C3-C5-C6-C7
27	F	101	SQD	C24-C23-O48-C46
27	f	101	SQD	C24-C23-O48-C46
32	Z	101	LMT	O5'-C5'-C6'-O6'
32	z	101	LMT	O5'-C5'-C6'-O6'
28	D	407	PL9	C47-C48-C49-C50
28	d	407	PL9	C47-C48-C49-C50
24	B	601	CLA	C4-C3-C5-C6
24	D	405	CLA	C4-C3-C5-C6
24	b	603	CLA	C4-C3-C5-C6
24	d	405	CLA	C4-C3-C5-C6
24	D	405	CLA	C2-C3-C5-C6
24	d	405	CLA	C2-C3-C5-C6
24	B	606	CLA	C2A-CAA-CBA-CGA
24	b	608	CLA	C2A-CAA-CBA-CGA
24	B	601	CLA	C3-C5-C6-C7
24	b	603	CLA	C3-C5-C6-C7
24	C	510	CLA	CBA-CGA-O2A-C1
24	c	510	CLA	CBA-CGA-O2A-C1
28	A	411	PL9	C22-C23-C24-C25
28	a	411	PL9	C22-C23-C24-C25
28	A	411	PL9	C17-C18-C19-C21
28	A	411	PL9	C22-C23-C24-C26
28	a	411	PL9	C17-C18-C19-C21
28	a	411	PL9	C22-C23-C24-C26
30	C	523	LMG	C4-C5-C6-O5
30	c	523	LMG	C4-C5-C6-O5
32	J	102	LMT	O5'-C5'-C6'-O6'
32	j	102	LMT	O5'-C5'-C6'-O6'
24	B	604	CLA	CBD-CGD-O2D-CED
24	C	514	CLA	CBD-CGD-O2D-CED
24	b	606	CLA	CBD-CGD-O2D-CED
24	c	514	CLA	CBD-CGD-O2D-CED
30	C	523	LMG	C29-C28-O8-C9
30	c	523	LMG	C29-C28-O8-C9
32	Z	101	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
32	z	101	LMT	C4'-C5'-C6'-O6'
28	A	411	PL9	C47-C48-C49-C50
28	a	411	PL9	C47-C48-C49-C50
25	D	402	PHO	CBD-CGD-O2D-CED
25	d	402	PHO	CBD-CGD-O2D-CED
27	A	410	SQD	C12-C13-C14-C15
27	a	410	SQD	C12-C13-C14-C15
24	C	510	CLA	O1A-CGA-O2A-C1
24	c	510	CLA	O1A-CGA-O2A-C1
24	A	408	CLA	C4-C3-C5-C6
24	B	614	CLA	C4-C3-C5-C6
24	C	508	CLA	C4-C3-C5-C6
24	a	408	CLA	C4-C3-C5-C6
24	b	616	CLA	C4-C3-C5-C6
24	c	508	CLA	C4-C3-C5-C6
28	A	411	PL9	C20-C19-C21-C22
28	a	411	PL9	C20-C19-C21-C22
24	A	408	CLA	C2-C3-C5-C6
24	B	614	CLA	C2-C3-C5-C6
24	C	508	CLA	C2-C3-C5-C6
24	a	408	CLA	C2-C3-C5-C6
24	b	616	CLA	C2-C3-C5-C6
24	c	508	CLA	C2-C3-C5-C6
30	C	523	LMG	O6-C5-C6-O5
30	c	523	LMG	O6-C5-C6-O5
28	A	411	PL9	C24-C26-C27-C28
28	A	411	PL9	C44-C46-C47-C48
28	D	407	PL9	C39-C41-C42-C43
28	a	411	PL9	C24-C26-C27-C28
28	a	411	PL9	C44-C46-C47-C48
28	d	407	PL9	C39-C41-C42-C43
24	B	601	CLA	C2-C3-C5-C6
24	b	603	CLA	C2-C3-C5-C6
24	B	607	CLA	C6-C7-C8-C9
24	C	503	CLA	C14-C13-C15-C16
24	C	505	CLA	C11-C12-C13-C14
24	b	609	CLA	C6-C7-C8-C9
24	c	503	CLA	C14-C13-C15-C16
24	c	505	CLA	C11-C12-C13-C14
25	A	407	PHO	C14-C13-C15-C16
25	a	407	PHO	C14-C13-C15-C16
26	A	409	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
26	B	618	BCR	C11-C12-C13-C35
26	B	618	BCR	C37-C22-C23-C24
26	C	515	BCR	C36-C18-C19-C20
26	J	104	BCR	C36-C18-C19-C20
26	T	101	BCR	C7-C8-C9-C34
26	a	409	BCR	C7-C8-C9-C34
26	b	620	BCR	C11-C12-C13-C35
26	b	620	BCR	C37-C22-C23-C24
26	c	515	BCR	C36-C18-C19-C20
26	j	104	BCR	C36-C18-C19-C20
26	t	102	BCR	C7-C8-C9-C34
34	D	408	LHG	C23-C24-C25-C26
34	d	408	LHG	C23-C24-C25-C26
32	M	101	LMT	O5'-C5'-C6'-O6'
32	m	102	LMT	O5'-C5'-C6'-O6'
24	A	406	CLA	C15-C16-C17-C18
24	A	408	CLA	C8-C10-C11-C12
24	a	406	CLA	C15-C16-C17-C18
24	a	408	CLA	C8-C10-C11-C12
24	c	509	CLA	C8-C10-C11-C12
27	F	101	SQD	C7-C8-C9-C10
27	f	101	SQD	C7-C8-C9-C10
30	B	621	LMG	C28-C29-C30-C31
30	b	622	LMG	C28-C29-C30-C31
32	Z	101	LMT	C2B-C1B-O1B-C4'
32	z	101	LMT	C2B-C1B-O1B-C4'
24	B	614	CLA	C10-C11-C12-C13
24	C	504	CLA	C15-C16-C17-C18
24	C	509	CLA	C8-C10-C11-C12
24	C	509	CLA	C10-C11-C12-C13
24	C	513	CLA	C15-C16-C17-C18
24	C	514	CLA	C5-C6-C7-C8
24	D	405	CLA	C5-C6-C7-C8
24	b	616	CLA	C10-C11-C12-C13
24	c	504	CLA	C15-C16-C17-C18
24	c	509	CLA	C10-C11-C12-C13
24	c	513	CLA	C15-C16-C17-C18
24	c	514	CLA	C5-C6-C7-C8
24	d	405	CLA	C5-C6-C7-C8
34	D	409	LHG	O1-C1-C2-O2
34	d	409	LHG	O1-C1-C2-O2
27	B	620	SQD	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
27	L	102	SQD	C23-C24-C25-C26
30	C	501	LMG	C28-C29-C30-C31
30	C	520	LMG	C28-C29-C30-C31
30	c	501	LMG	C28-C29-C30-C31
30	c	520	LMG	C28-C29-C30-C31
34	E	101	LHG	C23-C24-C25-C26
34	e	101	LHG	C23-C24-C25-C26
24	B	613	CLA	C8-C10-C11-C12
24	b	615	CLA	C8-C10-C11-C12
31	C	518	DGD	C1A-C2A-C3A-C4A
31	c	518	DGD	C1A-C2A-C3A-C4A
24	A	406	CLA	C6-C7-C8-C10
24	B	613	CLA	C11-C10-C8-C7
24	a	406	CLA	C6-C7-C8-C10
24	b	615	CLA	C11-C10-C8-C7
24	B	604	CLA	C3-C5-C6-C7
24	C	514	CLA	C3-C5-C6-C7
24	b	606	CLA	C3-C5-C6-C7
24	c	514	CLA	C3-C5-C6-C7
32	Z	101	LMT	O5B-C1B-O1B-C4'
32	z	101	LMT	O5B-C1B-O1B-C4'
24	B	601	CLA	C15-C16-C17-C18
24	b	603	CLA	C15-C16-C17-C18
32	Z	101	LMT	O5'-C1'-O1'-C1
32	z	101	LMT	O5'-C1'-O1'-C1
28	A	411	PL9	C9-C11-C12-C13
28	a	411	PL9	C9-C11-C12-C13
32	C	521	LMT	O5B-C5B-C6B-O6B
32	c	521	LMT	O5B-C5B-C6B-O6B
30	C	523	LMG	O9-C10-O7-C8
30	c	523	LMG	O9-C10-O7-C8
24	C	512	CLA	C3-C5-C6-C7
24	c	512	CLA	C3-C5-C6-C7
24	B	610	CLA	C15-C16-C17-C18
24	b	612	CLA	C15-C16-C17-C18
32	J	102	LMT	C4'-C5'-C6'-O6'
32	j	102	LMT	C4'-C5'-C6'-O6'
24	B	608	CLA	C13-C15-C16-C17
24	b	610	CLA	C13-C15-C16-C17
34	D	409	LHG	C3-O3-P-O6
34	L	101	LHG	C4-O6-P-O3
34	d	409	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
34	l	101	LHG	C4-O6-P-O3
24	C	513	CLA	CBA-CGA-O2A-C1
24	c	513	CLA	CBA-CGA-O2A-C1
27	A	410	SQD	C7-C8-C9-C10
27	a	410	SQD	C7-C8-C9-C10
34	D	409	LHG	C1-C2-C3-O3
34	d	409	LHG	C1-C2-C3-O3
32	Z	101	LMT	O1'-C1-C2-C3
32	z	101	LMT	O1'-C1-C2-C3
24	C	512	CLA	C8-C10-C11-C12
24	c	512	CLA	C8-C10-C11-C12
32	Z	101	LMT	O5B-C5B-C6B-O6B
32	z	101	LMT	O5B-C5B-C6B-O6B
27	L	102	SQD	C11-C10-C9-C8
31	C	517	DGD	C2A-C3A-C4A-C5A
31	c	517	DGD	C2A-C3A-C4A-C5A
24	B	603	CLA	CBD-CGD-O2D-CED
24	C	503	CLA	CBD-CGD-O2D-CED
24	b	605	CLA	CBD-CGD-O2D-CED
24	c	503	CLA	CBD-CGD-O2D-CED
27	F	101	SQD	C8-C7-O47-C45
27	f	101	SQD	C8-C7-O47-C45
30	C	501	LMG	C11-C10-O7-C8
30	c	501	LMG	C11-C10-O7-C8
24	D	404	CLA	C15-C16-C17-C18
24	d	404	CLA	C15-C16-C17-C18
26	A	409	BCR	C11-C10-C9-C34
26	A	409	BCR	C20-C21-C22-C37
26	B	617	BCR	C11-C10-C9-C34
26	B	619	BCR	C16-C17-C18-C36
26	C	515	BCR	C20-C21-C22-C37
26	T	101	BCR	C20-C21-C22-C37
26	a	409	BCR	C11-C10-C9-C34
26	a	409	BCR	C20-C21-C22-C37
26	b	619	BCR	C11-C10-C9-C34
26	b	621	BCR	C16-C17-C18-C36
26	c	515	BCR	C20-C21-C22-C37
26	t	102	BCR	C20-C21-C22-C37
27	B	620	SQD	C11-C10-C9-C8
27	F	101	SQD	C34-C35-C36-C37
27	f	101	SQD	C34-C35-C36-C37
30	B	621	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
30	B	621	LMG	C33-C34-C35-C36
30	B	621	LMG	C35-C36-C37-C38
30	B	621	LMG	C36-C37-C38-C39
30	C	501	LMG	C35-C36-C37-C38
30	b	622	LMG	C15-C16-C17-C18
30	b	622	LMG	C33-C34-C35-C36
30	b	622	LMG	C35-C36-C37-C38
30	b	622	LMG	C36-C37-C38-C39
30	c	501	LMG	C35-C36-C37-C38
31	C	518	DGD	C6B-C7B-C8B-C9B
31	H	101	DGD	CAA-CBA-CCA-CDA
31	c	518	DGD	C6B-C7B-C8B-C9B
31	h	101	DGD	CAA-CBA-CCA-CDA
34	E	101	LHG	C27-C28-C29-C30
34	e	101	LHG	C27-C28-C29-C30
24	C	502	CLA	C16-C17-C18-C19
24	C	511	CLA	C16-C17-C18-C19
24	c	502	CLA	C16-C17-C18-C19
24	c	511	CLA	C16-C17-C18-C19
24	C	512	CLA	CBA-CGA-O2A-C1
24	c	512	CLA	CBA-CGA-O2A-C1
34	D	410	LHG	C12-C13-C14-C15
34	d	408	LHG	C27-C28-C29-C30
34	d	410	LHG	C12-C13-C14-C15
34	d	410	LHG	C13-C14-C15-C16
34	D	408	LHG	C27-C28-C29-C30
34	D	410	LHG	C13-C14-C15-C16
27	A	410	SQD	C10-C11-C12-C13
27	a	410	SQD	C10-C11-C12-C13
30	B	621	LMG	C18-C19-C20-C21
30	C	520	LMG	C12-C13-C14-C15
30	D	411	LMG	C30-C31-C32-C33
30	b	622	LMG	C18-C19-C20-C21
30	c	520	LMG	C12-C13-C14-C15
30	d	411	LMG	C30-C31-C32-C33
31	C	517	DGD	C3A-C4A-C5A-C6A
31	c	517	DGD	C3A-C4A-C5A-C6A
31	C	518	DGD	C6A-C7A-C8A-C9A
31	c	518	DGD	C6A-C7A-C8A-C9A
30	C	520	LMG	C10-C11-C12-C13
30	c	520	LMG	C10-C11-C12-C13
34	E	101	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
34	e	101	LHG	C7-C8-C9-C10
26	A	409	BCR	C20-C21-C22-C23
26	B	619	BCR	C11-C10-C9-C8
26	C	515	BCR	C20-C21-C22-C23
26	T	101	BCR	C11-C10-C9-C8
26	T	101	BCR	C20-C21-C22-C23
26	a	409	BCR	C20-C21-C22-C23
26	b	621	BCR	C11-C10-C9-C8
26	c	515	BCR	C20-C21-C22-C23
26	t	102	BCR	C11-C10-C9-C8
26	t	102	BCR	C20-C21-C22-C23
31	C	518	DGD	C2E-C1E-O5D-C6D
31	c	518	DGD	C2E-C1E-O5D-C6D
32	Z	101	LMT	C2'-C1'-O1'-C1
32	z	101	LMT	C2'-C1'-O1'-C1
27	F	101	SQD	C9-C10-C11-C12
27	f	101	SQD	C9-C10-C11-C12
30	C	501	LMG	C39-C40-C41-C42
30	c	501	LMG	C39-C40-C41-C42
34	D	408	LHG	C29-C30-C31-C32
34	d	408	LHG	C29-C30-C31-C32
24	C	513	CLA	O1A-CGA-O2A-C1
24	c	513	CLA	O1A-CGA-O2A-C1
24	C	507	CLA	C16-C17-C18-C19
24	C	513	CLA	C16-C17-C18-C19
24	c	507	CLA	C16-C17-C18-C19
24	c	513	CLA	C16-C17-C18-C19
25	A	407	PHO	C4-C3-C5-C6
25	a	407	PHO	C4-C3-C5-C6
28	D	407	PL9	C32-C33-C34-C35
28	D	407	PL9	C45-C44-C46-C47
28	d	407	PL9	C32-C33-C34-C35
28	d	407	PL9	C45-C44-C46-C47
30	B	621	LMG	C38-C39-C40-C41
30	C	501	LMG	C37-C38-C39-C40
30	b	622	LMG	C38-C39-C40-C41
30	c	501	LMG	C37-C38-C39-C40
31	C	518	DGD	C4B-C5B-C6B-C7B
31	c	518	DGD	C4B-C5B-C6B-C7B
24	A	408	CLA	C11-C10-C8-C9
24	C	506	CLA	C11-C12-C13-C14
24	a	408	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	c	506	CLA	C11-C12-C13-C14
24	C	508	CLA	C2A-CAA-CBA-CGA
24	c	508	CLA	C2A-CAA-CBA-CGA
34	D	410	LHG	O1-C1-C2-C3
34	E	101	LHG	O1-C1-C2-C3
34	d	410	LHG	O1-C1-C2-C3
34	e	101	LHG	O1-C1-C2-C3
27	A	412	SQD	C27-C28-C29-C30
27	B	620	SQD	C24-C25-C26-C27
27	L	102	SQD	C24-C25-C26-C27
27	a	412	SQD	C25-C26-C27-C28
27	a	412	SQD	C27-C28-C29-C30
30	B	621	LMG	C34-C35-C36-C37
30	C	523	LMG	C12-C13-C14-C15
30	C	523	LMG	C31-C32-C33-C34
30	b	622	LMG	C34-C35-C36-C37
30	c	523	LMG	C12-C13-C14-C15
30	c	523	LMG	C31-C32-C33-C34
31	H	101	DGD	C5B-C6B-C7B-C8B
31	h	101	DGD	C5B-C6B-C7B-C8B
34	D	408	LHG	C7-C8-C9-C10
34	d	408	LHG	C7-C8-C9-C10
27	A	412	SQD	C25-C26-C27-C28
30	B	621	LMG	C30-C31-C32-C33
30	C	520	LMG	C31-C32-C33-C34
30	C	523	LMG	C17-C18-C19-C20
30	C	523	LMG	C18-C19-C20-C21
30	D	411	LMG	C37-C38-C39-C40
30	b	622	LMG	C30-C31-C32-C33
30	c	501	LMG	C30-C31-C32-C33
30	c	520	LMG	C31-C32-C33-C34
30	c	523	LMG	C18-C19-C20-C21
30	d	411	LMG	C37-C38-C39-C40
31	C	518	DGD	C3B-C4B-C5B-C6B
31	c	518	DGD	C3B-C4B-C5B-C6B
34	D	408	LHG	C30-C31-C32-C33
34	d	408	LHG	C30-C31-C32-C33
34	d	410	LHG	C28-C29-C30-C31
24	C	511	CLA	C16-C17-C18-C20
24	c	511	CLA	C16-C17-C18-C20
31	C	518	DGD	O6D-C1D-O3G-C3G
31	C	518	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
31	c	518	DGD	O6D-C1D-O3G-C3G
31	c	518	DGD	O6E-C1E-O5D-C6D
27	B	620	SQD	C28-C29-C30-C31
27	B	620	SQD	C30-C31-C32-C33
27	L	102	SQD	C28-C29-C30-C31
27	L	102	SQD	C30-C31-C32-C33
30	C	501	LMG	C18-C19-C20-C21
30	C	501	LMG	C30-C31-C32-C33
30	D	411	LMG	C35-C36-C37-C38
30	c	501	LMG	C18-C19-C20-C21
30	c	523	LMG	C17-C18-C19-C20
30	d	411	LMG	C35-C36-C37-C38
31	C	519	DGD	CAB-CBB-CCB-CDB
31	c	519	DGD	CAB-CBB-CCB-CDB
34	D	410	LHG	C28-C29-C30-C31
30	C	520	LMG	C11-C12-C13-C14
30	c	520	LMG	C11-C12-C13-C14
31	C	518	DGD	C4A-C5A-C6A-C7A
31	C	518	DGD	C8A-C9A-CAA-CBA
31	c	518	DGD	C4A-C5A-C6A-C7A
31	c	518	DGD	C8A-C9A-CAA-CBA
32	C	521	LMT	C6-C7-C8-C9
32	c	521	LMT	C6-C7-C8-C9
34	e	101	LHG	C16-C17-C18-C19
27	A	412	SQD	C11-C12-C13-C14
27	B	620	SQD	C13-C14-C15-C16
27	L	102	SQD	C13-C14-C15-C16
27	a	412	SQD	C11-C12-C13-C14
30	B	621	LMG	C17-C18-C19-C20
30	b	622	LMG	C17-C18-C19-C20
31	C	518	DGD	C3A-C4A-C5A-C6A
31	C	518	DGD	C5B-C6B-C7B-C8B
31	c	518	DGD	C3A-C4A-C5A-C6A
31	c	518	DGD	C5B-C6B-C7B-C8B
34	E	101	LHG	C16-C17-C18-C19
27	B	620	SQD	C16-C17-C18-C19
27	L	102	SQD	C16-C17-C18-C19
30	C	501	LMG	C12-C13-C14-C15
31	C	518	DGD	C9A-CAA-CBA-CCA
31	c	518	DGD	C9A-CAA-CBA-CCA
30	D	411	LMG	C14-C15-C16-C17
30	c	501	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
30	d	411	LMG	C14-C15-C16-C17
31	C	517	DGD	CBA-CCA-CDA-CEA
31	C	519	DGD	CBA-CCA-CDA-CEA
31	H	101	DGD	CBA-CCA-CDA-CEA
31	c	517	DGD	CBA-CCA-CDA-CEA
31	c	519	DGD	CBA-CCA-CDA-CEA
31	h	101	DGD	CBA-CCA-CDA-CEA
34	E	101	LHG	C15-C16-C17-C18
34	E	101	LHG	C17-C18-C19-C20
34	e	101	LHG	C15-C16-C17-C18
34	e	101	LHG	C17-C18-C19-C20
24	C	512	CLA	O1A-CGA-O2A-C1
24	c	512	CLA	O1A-CGA-O2A-C1
24	B	615	CLA	C16-C17-C18-C19
24	C	502	CLA	C16-C17-C18-C20
24	b	617	CLA	C16-C17-C18-C19
24	c	502	CLA	C16-C17-C18-C20
31	C	519	DGD	C7B-C8B-C9B-CAB
31	c	519	DGD	C7B-C8B-C9B-CAB
34	E	101	LHG	C18-C19-C20-C21
25	D	402	PHO	O1D-CGD-O2D-CED
25	d	402	PHO	O1D-CGD-O2D-CED
30	C	523	LMG	O1-C7-C8-C9
30	c	523	LMG	O1-C7-C8-C9
24	C	504	CLA	CBD-CGD-O2D-CED
24	c	504	CLA	CBD-CGD-O2D-CED
30	D	411	LMG	C17-C18-C19-C20
30	d	411	LMG	C17-C18-C19-C20
34	e	101	LHG	C18-C19-C20-C21
24	B	609	CLA	C4-C3-C5-C6
25	A	407	PHO	C2-C3-C5-C6
25	a	407	PHO	C2-C3-C5-C6
28	A	411	PL9	C13-C14-C16-C17
28	a	411	PL9	C13-C14-C16-C17
24	D	401	CLA	C2C-C3C-CAC-CBC
24	d	401	CLA	C2C-C3C-CAC-CBC
27	B	620	SQD	C11-C12-C13-C14
27	L	102	SQD	C11-C12-C13-C14
24	b	606	CLA	O1A-CGA-O2A-C1
24	A	408	CLA	C16-C17-C18-C19
24	a	408	CLA	C16-C17-C18-C19
24	B	606	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	b	608	CLA	C15-C16-C17-C18
32	C	521	LMT	C1-C2-C3-C4
32	c	521	LMT	C1-C2-C3-C4
32	z	101	LMT	C6-C7-C8-C9
24	B	604	CLA	O1A-CGA-O2A-C1
32	Z	101	LMT	C6-C7-C8-C9
27	A	410	SQD	C34-C35-C36-C37
27	A	412	SQD	C10-C11-C12-C13
27	a	410	SQD	C34-C35-C36-C37
27	a	412	SQD	C10-C11-C12-C13
24	D	401	CLA	C15-C16-C17-C18
24	d	401	CLA	C15-C16-C17-C18
26	B	617	BCR	C5-C6-C7-C8
26	C	515	BCR	C1-C6-C7-C8
26	C	515	BCR	C5-C6-C7-C8
26	C	516	BCR	C23-C24-C25-C26
26	C	522	BCR	C5-C6-C7-C8
26	J	104	BCR	C1-C6-C7-C8
26	T	101	BCR	C5-C6-C7-C8
26	b	619	BCR	C5-C6-C7-C8
26	c	515	BCR	C1-C6-C7-C8
26	c	515	BCR	C5-C6-C7-C8
26	c	516	BCR	C23-C24-C25-C26
26	c	522	BCR	C5-C6-C7-C8
26	j	104	BCR	C1-C6-C7-C8
26	t	102	BCR	C5-C6-C7-C8
38	X	101	RRX	C23-C24-C25-C30
38	x	101	RRX	C23-C24-C25-C30
27	B	620	SQD	C14-C15-C16-C17
24	B	604	CLA	CBA-CGA-O2A-C1
24	b	606	CLA	CBA-CGA-O2A-C1
24	A	408	CLA	C5-C6-C7-C8
24	B	612	CLA	C10-C11-C12-C13
24	D	405	CLA	C13-C15-C16-C17
24	a	408	CLA	C5-C6-C7-C8
24	b	614	CLA	C10-C11-C12-C13
24	d	405	CLA	C13-C15-C16-C17
27	L	102	SQD	C14-C15-C16-C17
30	C	501	LMG	C16-C17-C18-C19
30	C	520	LMG	C34-C35-C36-C37
30	c	501	LMG	C16-C17-C18-C19
30	c	520	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
30	C	523	LMG	C16-C17-C18-C19
30	c	523	LMG	C16-C17-C18-C19
31	C	519	DGD	C6B-C7B-C8B-C9B
31	c	519	DGD	C6B-C7B-C8B-C9B
27	A	410	SQD	C11-C12-C13-C14
27	a	410	SQD	C11-C12-C13-C14
24	b	611	CLA	C4-C3-C5-C6
24	A	408	CLA	C11-C10-C8-C7
24	A	408	CLA	C11-C12-C13-C15
24	B	609	CLA	C2-C3-C5-C6
24	B	614	CLA	C11-C12-C13-C15
24	B	615	CLA	C6-C7-C8-C10
24	C	506	CLA	C11-C12-C13-C15
24	a	408	CLA	C11-C10-C8-C7
24	a	408	CLA	C11-C12-C13-C15
24	b	611	CLA	C2-C3-C5-C6
24	b	616	CLA	C11-C12-C13-C15
24	b	617	CLA	C6-C7-C8-C10
24	c	506	CLA	C11-C12-C13-C15
34	E	101	LHG	C34-C35-C36-C37
34	e	101	LHG	C34-C35-C36-C37
38	X	101	RRX	C9-C10-C11-C12
38	x	101	RRX	C9-C10-C11-C12
24	C	510	CLA	C16-C17-C18-C20
24	c	510	CLA	C16-C17-C18-C20
31	C	518	DGD	CBA-CCA-CDA-CEA
31	c	518	DGD	CBA-CCA-CDA-CEA
24	C	502	CLA	C2A-CAA-CBA-CGA
24	c	502	CLA	C2A-CAA-CBA-CGA
24	B	604	CLA	C5-C6-C7-C8
24	B	606	CLA	C13-C15-C16-C17
24	b	606	CLA	C5-C6-C7-C8
24	b	608	CLA	C13-C15-C16-C17
27	A	412	SQD	C24-C25-C26-C27
27	a	412	SQD	C24-C25-C26-C27
24	B	604	CLA	O1D-CGD-O2D-CED
24	b	606	CLA	O1D-CGD-O2D-CED
31	C	518	DGD	C7A-C8A-C9A-CAA
31	c	518	DGD	C7A-C8A-C9A-CAA
30	C	520	LMG	C15-C16-C17-C18
30	c	520	LMG	C15-C16-C17-C18
30	d	411	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
31	C	518	DGD	CCB-CDB-CEB-CFB
31	c	518	DGD	CCB-CDB-CEB-CFB
28	A	411	PL9	C39-C41-C42-C43
28	a	411	PL9	C39-C41-C42-C43
30	D	411	LMG	C32-C33-C34-C35
31	C	518	DGD	CCA-CDA-CEA-CFA
31	c	518	DGD	CCA-CDA-CEA-CFA
30	C	523	LMG	C11-C10-O7-C8
30	c	523	LMG	C11-C10-O7-C8
30	C	523	LMG	C38-C39-C40-C41
30	D	411	LMG	C36-C37-C38-C39
30	c	523	LMG	C38-C39-C40-C41
30	d	411	LMG	C36-C37-C38-C39
32	C	521	LMT	C4'-C5'-C6'-O6'
32	c	521	LMT	C4'-C5'-C6'-O6'
24	B	615	CLA	C8-C10-C11-C12
24	b	617	CLA	C8-C10-C11-C12
27	A	412	SQD	C23-C24-C25-C26
27	a	412	SQD	C23-C24-C25-C26
27	A	412	SQD	O6-C44-C45-O47
27	a	412	SQD	O6-C44-C45-O47
30	C	520	LMG	C16-C17-C18-C19
31	C	519	DGD	C9B-CAB-CBB-CCB
31	c	519	DGD	C9B-CAB-CBB-CCB
30	c	520	LMG	C16-C17-C18-C19
30	C	523	LMG	C32-C33-C34-C35
24	A	406	CLA	C6-C7-C8-C9
24	B	614	CLA	C11-C12-C13-C14
24	B	615	CLA	C6-C7-C8-C9
24	C	507	CLA	C11-C12-C13-C14
24	a	406	CLA	C6-C7-C8-C9
24	b	616	CLA	C11-C12-C13-C14
24	b	617	CLA	C6-C7-C8-C9
24	c	507	CLA	C11-C12-C13-C14
30	c	523	LMG	C32-C33-C34-C35
30	C	501	LMG	C13-C14-C15-C16
30	c	501	LMG	C13-C14-C15-C16
31	C	518	DGD	C2B-C3B-C4B-C5B
32	Z	101	LMT	C7-C8-C9-C10
30	D	411	LMG	O6-C5-C6-O5
30	d	411	LMG	O6-C5-C6-O5
31	c	518	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
32	z	101	LMT	C7-C8-C9-C10
34	d	409	LHG	C26-C27-C28-C29
34	l	101	LHG	C29-C30-C31-C32
30	C	523	LMG	O10-C28-O8-C9
30	c	523	LMG	O10-C28-O8-C9
24	A	406	CLA	C1A-C2A-CAA-CBA
24	C	502	CLA	C1A-C2A-CAA-CBA
24	C	503	CLA	C1A-C2A-CAA-CBA
24	C	507	CLA	C1A-C2A-CAA-CBA
24	C	512	CLA	C1A-C2A-CAA-CBA
24	D	401	CLA	C1A-C2A-CAA-CBA
24	a	406	CLA	C1A-C2A-CAA-CBA
24	c	502	CLA	C1A-C2A-CAA-CBA
24	c	503	CLA	C1A-C2A-CAA-CBA
24	c	507	CLA	C1A-C2A-CAA-CBA
24	c	512	CLA	C1A-C2A-CAA-CBA
24	d	401	CLA	C1A-C2A-CAA-CBA
24	A	408	CLA	C16-C17-C18-C20
24	C	507	CLA	C16-C17-C18-C20
24	C	513	CLA	C16-C17-C18-C20
24	a	408	CLA	C16-C17-C18-C20
24	c	507	CLA	C16-C17-C18-C20
24	c	513	CLA	C16-C17-C18-C20
27	F	101	SQD	O49-C7-O47-C45
27	f	101	SQD	O49-C7-O47-C45
34	D	409	LHG	C26-C27-C28-C29
34	L	101	LHG	C29-C30-C31-C32
24	C	504	CLA	C8-C10-C11-C12
24	c	504	CLA	C8-C10-C11-C12
30	C	520	LMG	C32-C33-C34-C35
30	c	520	LMG	C32-C33-C34-C35
32	C	521	LMT	C4-C5-C6-C7
32	c	521	LMT	C4-C5-C6-C7
27	A	410	SQD	C30-C31-C32-C33
27	A	412	SQD	C17-C18-C19-C20
27	a	410	SQD	C30-C31-C32-C33
27	a	412	SQD	C17-C18-C19-C20
34	D	409	LHG	C23-C24-C25-C26
34	d	409	LHG	C23-C24-C25-C26
27	A	412	SQD	C26-C27-C28-C29
27	B	620	SQD	C27-C28-C29-C30
27	L	102	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
27	a	412	SQD	C26-C27-C28-C29
30	C	501	LMG	C31-C32-C33-C34
30	c	501	LMG	C31-C32-C33-C34
24	B	615	CLA	C16-C17-C18-C20
24	b	617	CLA	C16-C17-C18-C20
31	C	517	DGD	C5B-C6B-C7B-C8B
31	c	517	DGD	C5B-C6B-C7B-C8B
30	C	520	LMG	C38-C39-C40-C41
30	c	520	LMG	C38-C39-C40-C41
34	D	408	LHG	C33-C34-C35-C36
34	d	408	LHG	C33-C34-C35-C36
30	c	501	LMG	C29-C30-C31-C32
34	L	101	LHG	C14-C15-C16-C17
34	l	101	LHG	C14-C15-C16-C17
30	C	501	LMG	C29-C30-C31-C32
30	C	523	LMG	C20-C21-C22-C23
30	c	501	LMG	C33-C34-C35-C36
30	c	523	LMG	C20-C21-C22-C23
24	C	510	CLA	C10-C11-C12-C13
24	c	510	CLA	C10-C11-C12-C13
31	C	517	DGD	O6E-C5E-C6E-O5E
31	c	517	DGD	O6E-C5E-C6E-O5E
24	C	514	CLA	O1D-CGD-O2D-CED
30	C	501	LMG	C33-C34-C35-C36
30	C	523	LMG	C7-C8-C9-O8
30	c	523	LMG	C7-C8-C9-O8
32	j	102	LMT	C4-C5-C6-C7
30	C	523	LMG	C33-C34-C35-C36
30	c	523	LMG	C33-C34-C35-C36
31	H	101	DGD	CDB-CEB-CFB-CGB
31	h	101	DGD	CDB-CEB-CFB-CGB
32	J	102	LMT	C4-C5-C6-C7
30	C	523	LMG	C8-C7-O1-C1
30	c	523	LMG	C8-C7-O1-C1
31	C	518	DGD	C5D-C6D-O5D-C1E
31	c	518	DGD	C5D-C6D-O5D-C1E
24	c	514	CLA	O1D-CGD-O2D-CED
27	B	620	SQD	C29-C30-C31-C32
27	L	102	SQD	C29-C30-C31-C32
30	C	523	LMG	C34-C35-C36-C37
30	c	523	LMG	C34-C35-C36-C37
30	D	411	LMG	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
30	d	411	LMG	C22-C23-C24-C25
34	E	101	LHG	O1-C1-C2-O2
34	e	101	LHG	O1-C1-C2-O2
26	C	516	BCR	C35-C13-C14-C15
26	C	522	BCR	C20-C21-C22-C37
26	c	516	BCR	C35-C13-C14-C15
26	c	522	BCR	C20-C21-C22-C37
30	D	411	LMG	C13-C14-C15-C16
30	d	411	LMG	C13-C14-C15-C16
31	c	517	DGD	CDA-CEA-CFA-CGA
34	D	410	LHG	C32-C33-C34-C35
31	C	517	DGD	CDA-CEA-CFA-CGA
34	d	410	LHG	C32-C33-C34-C35
30	D	411	LMG	C19-C20-C21-C22
30	d	411	LMG	C19-C20-C21-C22
30	C	501	LMG	C32-C33-C34-C35
30	c	501	LMG	C32-C33-C34-C35
32	Z	101	LMT	C2-C3-C4-C5
32	z	101	LMT	C2-C3-C4-C5
24	A	408	CLA	C15-C16-C17-C18
24	a	408	CLA	C15-C16-C17-C18
24	B	601	CLA	C5-C6-C7-C8
24	b	603	CLA	C5-C6-C7-C8
26	B	617	BCR	C11-C10-C9-C8
26	C	515	BCR	C16-C17-C18-C19
26	J	104	BCR	C11-C10-C9-C8
26	b	619	BCR	C11-C10-C9-C8
26	c	515	BCR	C16-C17-C18-C19
26	j	104	BCR	C11-C10-C9-C8
31	C	518	DGD	C2D-C1D-O3G-C3G
31	c	518	DGD	C2D-C1D-O3G-C3G
27	B	620	SQD	C31-C32-C33-C34
27	L	102	SQD	C31-C32-C33-C34
24	C	512	CLA	C15-C16-C17-C18
32	C	521	LMT	C5-C6-C7-C8
32	c	521	LMT	C5-C6-C7-C8
30	C	520	LMG	C14-C15-C16-C17
30	c	520	LMG	C14-C15-C16-C17
24	c	512	CLA	C15-C16-C17-C18
24	B	614	CLA	C6-C7-C8-C10
24	C	505	CLA	C11-C12-C13-C15
24	C	507	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	C	509	CLA	C12-C13-C15-C16
24	C	512	CLA	C6-C7-C8-C10
24	b	616	CLA	C6-C7-C8-C10
24	c	505	CLA	C11-C12-C13-C15
24	c	507	CLA	C11-C12-C13-C15
24	c	509	CLA	C12-C13-C15-C16
24	c	512	CLA	C6-C7-C8-C10
24	B	614	CLA	C6-C7-C8-C9
24	C	509	CLA	C14-C13-C15-C16
24	b	616	CLA	C6-C7-C8-C9
24	c	509	CLA	C14-C13-C15-C16
34	L	101	LHG	C16-C17-C18-C19
34	l	101	LHG	C16-C17-C18-C19
24	B	603	CLA	C5-C6-C7-C8
24	b	605	CLA	C5-C6-C7-C8
30	c	523	LMG	C19-C20-C21-C22
30	C	523	LMG	C19-C20-C21-C22
27	A	412	SQD	C19-C20-C21-C22
27	a	412	SQD	C19-C20-C21-C22
34	D	408	LHG	C1-C2-C3-O3
34	d	408	LHG	C1-C2-C3-O3
30	B	621	LMG	O9-C10-O7-C8
30	b	622	LMG	O9-C10-O7-C8
34	L	101	LHG	C30-C31-C32-C33
34	l	101	LHG	C30-C31-C32-C33
24	B	615	CLA	C13-C15-C16-C17
24	b	617	CLA	C13-C15-C16-C17
34	D	409	LHG	O6-C4-C5-C6
34	d	409	LHG	O6-C4-C5-C6
27	A	410	SQD	C32-C33-C34-C35
27	a	410	SQD	C32-C33-C34-C35
34	D	408	LHG	C12-C13-C14-C15
34	d	408	LHG	C12-C13-C14-C15
24	C	514	CLA	C4-C3-C5-C6
24	c	514	CLA	C4-C3-C5-C6
28	A	411	PL9	C30-C29-C31-C32
28	a	411	PL9	C30-C29-C31-C32
28	D	407	PL9	C43-C44-C46-C47
28	d	407	PL9	C43-C44-C46-C47
32	Z	101	LMT	C1-C2-C3-C4
32	z	101	LMT	C1-C2-C3-C4
31	C	517	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
31	C	519	DGD	CCA-CDA-CEA-CFA
31	c	517	DGD	C4B-C5B-C6B-C7B
31	c	519	DGD	CCA-CDA-CEA-CFA
30	C	501	LMG	C38-C39-C40-C41
30	c	501	LMG	C38-C39-C40-C41
24	C	514	CLA	CBA-CGA-O2A-C1
24	c	514	CLA	CBA-CGA-O2A-C1
24	C	503	CLA	O1D-CGD-O2D-CED
24	c	503	CLA	O1D-CGD-O2D-CED
34	D	409	LHG	C16-C17-C18-C19
34	d	409	LHG	C16-C17-C18-C19
32	C	521	LMT	O5'-C5'-C6'-O6'
32	c	521	LMT	O5'-C5'-C6'-O6'
24	D	405	CLA	CBA-CGA-O2A-C1
24	d	405	CLA	CBA-CGA-O2A-C1
31	C	519	DGD	CCB-CDB-CEB-CFB
31	c	519	DGD	CCB-CDB-CEB-CFB
24	B	615	CLA	C10-C11-C12-C13
24	b	617	CLA	C10-C11-C12-C13
27	A	412	SQD	O6-C44-C45-C46
27	a	412	SQD	O6-C44-C45-C46
30	C	520	LMG	O1-C7-C8-C9
30	c	520	LMG	O1-C7-C8-C9
27	B	620	SQD	C12-C13-C14-C15
27	L	102	SQD	C12-C13-C14-C15
27	B	620	SQD	C32-C33-C34-C35
27	L	102	SQD	C32-C33-C34-C35
24	C	510	CLA	C16-C17-C18-C19
24	c	510	CLA	C16-C17-C18-C19
24	C	514	CLA	C2-C3-C5-C6
24	c	514	CLA	C2-C3-C5-C6
24	A	405	CLA	C2C-C3C-CAC-CBC
24	a	405	CLA	C2C-C3C-CAC-CBC
27	B	620	SQD	C25-C26-C27-C28
27	L	102	SQD	C25-C26-C27-C28
24	B	607	CLA	C3-C5-C6-C7
24	b	609	CLA	C3-C5-C6-C7
24	B	603	CLA	C8-C10-C11-C12
24	b	605	CLA	C8-C10-C11-C12
30	C	520	LMG	C22-C23-C24-C25
30	c	520	LMG	C22-C23-C24-C25
34	L	101	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
34	l	101	LHG	O6-C4-C5-O7
30	C	520	LMG	C33-C34-C35-C36
30	c	520	LMG	C33-C34-C35-C36
31	c	519	DGD	CBB-CCB-CDB-CEB
31	C	519	DGD	CBB-CCB-CDB-CEB
34	D	410	LHG	C11-C12-C13-C14
34	d	410	LHG	C11-C12-C13-C14
30	C	520	LMG	O1-C7-C8-O7
30	c	520	LMG	O1-C7-C8-O7
30	C	520	LMG	C35-C36-C37-C38
30	c	520	LMG	C35-C36-C37-C38
27	B	620	SQD	O49-C7-O47-C45
27	L	102	SQD	O49-C7-O47-C45
24	B	615	CLA	C2-C3-C5-C6
24	B	613	CLA	C11-C10-C8-C9
24	B	614	CLA	C14-C13-C15-C16
24	B	615	CLA	C14-C13-C15-C16
24	C	510	CLA	C6-C7-C8-C9
24	b	615	CLA	C11-C10-C8-C9
24	b	616	CLA	C14-C13-C15-C16
24	b	617	CLA	C14-C13-C15-C16
24	c	510	CLA	C6-C7-C8-C9
30	B	621	LMG	C21-C22-C23-C24
34	D	410	LHG	C15-C16-C17-C18
34	d	410	LHG	C15-C16-C17-C18
34	D	410	LHG	C2-C3-O3-P
34	d	410	LHG	C2-C3-O3-P
30	b	622	LMG	C21-C22-C23-C24
24	C	504	CLA	C16-C17-C18-C20
24	c	504	CLA	C16-C17-C18-C20
24	A	408	CLA	C3-C5-C6-C7
24	a	408	CLA	C3-C5-C6-C7
26	A	409	BCR	C1-C6-C7-C8
26	A	409	BCR	C5-C6-C7-C8
26	B	619	BCR	C23-C24-C25-C26
26	B	619	BCR	C23-C24-C25-C30
26	C	522	BCR	C23-C24-C25-C26
26	a	409	BCR	C1-C6-C7-C8
26	a	409	BCR	C5-C6-C7-C8
26	b	621	BCR	C23-C24-C25-C26
26	b	621	BCR	C23-C24-C25-C30
26	c	522	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
31	H	101	DGD	O2G-C1B-C2B-C3B
31	h	101	DGD	O2G-C1B-C2B-C3B
32	M	101	LMT	C4'-C5'-C6'-O6'
32	m	102	LMT	C4'-C5'-C6'-O6'
31	H	101	DGD	CCA-CDA-CEA-CFA
31	h	101	DGD	CCA-CDA-CEA-CFA
26	J	104	BCR	C7-C8-C9-C10
26	j	104	BCR	C7-C8-C9-C10
30	B	621	LMG	C13-C14-C15-C16
30	b	622	LMG	C13-C14-C15-C16
24	B	607	CLA	C5-C6-C7-C8
24	C	513	CLA	C10-C11-C12-C13
24	b	609	CLA	C5-C6-C7-C8
24	c	513	CLA	C10-C11-C12-C13
24	B	616	CLA	C13-C15-C16-C17
24	b	618	CLA	C13-C15-C16-C17
34	L	101	LHG	O6-C4-C5-C6
34	l	101	LHG	O6-C4-C5-C6
34	E	101	LHG	C9-C10-C11-C12
34	e	101	LHG	C9-C10-C11-C12
24	B	601	CLA	C12-C13-C15-C16
24	B	605	CLA	C11-C12-C13-C15
24	B	614	CLA	C12-C13-C15-C16
24	B	615	CLA	C12-C13-C15-C16
24	D	405	CLA	C11-C10-C8-C7
24	b	603	CLA	C12-C13-C15-C16
24	b	607	CLA	C11-C12-C13-C15
24	b	616	CLA	C12-C13-C15-C16
24	b	617	CLA	C2-C3-C5-C6
24	b	617	CLA	C12-C13-C15-C16
24	d	405	CLA	C11-C10-C8-C7
26	C	522	BCR	C19-C20-C21-C22
26	c	522	BCR	C19-C20-C21-C22
24	C	508	CLA	C16-C17-C18-C19
24	c	508	CLA	C16-C17-C18-C19
34	d	410	LHG	C31-C32-C33-C34
24	B	601	CLA	C2A-CAA-CBA-CGA
24	b	603	CLA	C2A-CAA-CBA-CGA
34	D	410	LHG	C31-C32-C33-C34
26	B	619	BCR	C20-C21-C22-C37
26	J	104	BCR	C35-C13-C14-C15
26	J	104	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
26	J	104	BCR	C20-C21-C22-C37
26	b	621	BCR	C20-C21-C22-C37
26	j	104	BCR	C35-C13-C14-C15
26	j	104	BCR	C16-C17-C18-C36
26	j	104	BCR	C20-C21-C22-C37
34	d	409	LHG	C30-C31-C32-C33
34	D	409	LHG	C30-C31-C32-C33
30	C	501	LMG	C17-C18-C19-C20
30	c	501	LMG	C17-C18-C19-C20
34	E	101	LHG	C10-C11-C12-C13
34	e	101	LHG	C10-C11-C12-C13
24	B	603	CLA	CAD-CBD-CGD-O2D
24	B	604	CLA	CAD-CBD-CGD-O2D
24	B	613	CLA	CAD-CBD-CGD-O2D
24	B	614	CLA	CAD-CBD-CGD-O2D
24	C	503	CLA	CAD-CBD-CGD-O2D
24	C	510	CLA	CAD-CBD-CGD-O2D
24	b	605	CLA	CAD-CBD-CGD-O2D
24	b	606	CLA	CAD-CBD-CGD-O2D
24	b	615	CLA	CAD-CBD-CGD-O2D
24	b	616	CLA	CAD-CBD-CGD-O2D
24	c	503	CLA	CAD-CBD-CGD-O2D
24	c	510	CLA	CAD-CBD-CGD-O2D
27	F	101	SQD	C25-C26-C27-C28
27	f	101	SQD	C25-C26-C27-C28
24	B	615	CLA	C4-C3-C5-C6
27	F	101	SQD	O5-C1-O6-C44
27	f	101	SQD	O5-C1-O6-C44
24	C	510	CLA	C8-C10-C11-C12
24	c	510	CLA	C8-C10-C11-C12
24	C	514	CLA	O1A-CGA-O2A-C1
24	c	514	CLA	O1A-CGA-O2A-C1
34	D	409	LHG	O6-C4-C5-O7
34	d	409	LHG	O6-C4-C5-O7
31	c	517	DGD	C6A-C7A-C8A-C9A
30	C	520	LMG	C40-C41-C42-C43
30	C	523	LMG	C14-C15-C16-C17
30	c	520	LMG	C40-C41-C42-C43
30	c	523	LMG	C14-C15-C16-C17
31	C	517	DGD	C6A-C7A-C8A-C9A
24	B	601	CLA	CHA-CBD-CGD-O1D
24	B	601	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	B	605	CLA	CHA-CBD-CGD-O1D
24	C	505	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	D	401	CLA	CHA-CBD-CGD-O2D
24	b	603	CLA	CHA-CBD-CGD-O1D
24	b	603	CLA	CHA-CBD-CGD-O2D
24	b	607	CLA	CHA-CBD-CGD-O1D
24	c	505	CLA	CHA-CBD-CGD-O1D
24	c	508	CLA	CHA-CBD-CGD-O1D
24	c	508	CLA	CHA-CBD-CGD-O2D
24	d	401	CLA	CHA-CBD-CGD-O2D
27	A	410	SQD	O6-C44-C45-O47
27	a	410	SQD	O6-C44-C45-O47
30	C	523	LMG	O7-C8-C9-O8
30	c	523	LMG	O7-C8-C9-O8
24	b	617	CLA	C4-C3-C5-C6
30	C	520	LMG	C36-C37-C38-C39
24	D	405	CLA	O1A-CGA-O2A-C1
24	d	405	CLA	O1A-CGA-O2A-C1
30	c	520	LMG	C36-C37-C38-C39
32	c	521	LMT	C3-C4-C5-C6
34	l	101	LHG	C31-C32-C33-C34
34	D	409	LHG	O9-C7-O7-C5
34	d	409	LHG	O9-C7-O7-C5
24	B	605	CLA	C11-C12-C13-C14
24	b	607	CLA	C11-C12-C13-C14
32	C	521	LMT	C3-C4-C5-C6
34	L	101	LHG	C31-C32-C33-C34
24	C	508	CLA	C5-C6-C7-C8
24	c	508	CLA	C5-C6-C7-C8
24	C	503	CLA	C16-C17-C18-C20
24	D	405	CLA	C16-C17-C18-C19
24	c	503	CLA	C16-C17-C18-C20
24	d	405	CLA	C16-C17-C18-C19
26	C	522	BCR	C7-C8-C9-C34
26	c	522	BCR	C7-C8-C9-C34
26	C	515	BCR	C21-C22-C23-C24
26	c	515	BCR	C21-C22-C23-C24
31	C	519	DGD	CDA-CEA-CFA-CGA
31	c	519	DGD	CDA-CEA-CFA-CGA
24	C	514	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	c	514	CLA	C1A-C2A-CAA-CBA
30	D	411	LMG	C21-C22-C23-C24
30	d	411	LMG	C21-C22-C23-C24
34	l	101	LHG	C12-C13-C14-C15
34	L	101	LHG	C12-C13-C14-C15
32	M	101	LMT	C4B-C5B-C6B-O6B
32	m	102	LMT	C4B-C5B-C6B-O6B
30	C	520	LMG	C30-C31-C32-C33
30	c	520	LMG	C30-C31-C32-C33
34	L	101	LHG	C34-C35-C36-C37
34	D	409	LHG	C3-O3-P-O4
34	L	101	LHG	C4-O6-P-O5
34	d	409	LHG	C3-O3-P-O4
34	l	101	LHG	C4-O6-P-O5
30	c	501	LMG	C15-C16-C17-C18
34	e	101	LHG	C13-C14-C15-C16
34	l	101	LHG	C34-C35-C36-C37
24	B	612	CLA	CBA-CGA-O2A-C1
24	b	614	CLA	CBA-CGA-O2A-C1
28	d	407	PL9	C37-C38-C39-C40
30	C	501	LMG	C15-C16-C17-C18
34	E	101	LHG	C13-C14-C15-C16
34	E	101	LHG	C28-C29-C30-C31
34	e	101	LHG	C28-C29-C30-C31
24	B	601	CLA	CAD-CBD-CGD-O1D
24	B	605	CLA	CAD-CBD-CGD-O1D
24	B	609	CLA	CAD-CBD-CGD-O1D
24	C	505	CLA	CAD-CBD-CGD-O1D
24	b	603	CLA	CAD-CBD-CGD-O1D
24	b	607	CLA	CAD-CBD-CGD-O1D
24	b	611	CLA	CAD-CBD-CGD-O1D
24	c	505	CLA	CAD-CBD-CGD-O1D
24	A	405	CLA	C13-C15-C16-C17
24	a	405	CLA	C13-C15-C16-C17
24	B	612	CLA	O1A-CGA-O2A-C1
24	b	614	CLA	O1A-CGA-O2A-C1
30	C	523	LMG	C37-C38-C39-C40
30	c	523	LMG	C37-C38-C39-C40
30	C	501	LMG	C36-C37-C38-C39
30	c	501	LMG	C36-C37-C38-C39
24	A	406	CLA	C11-C10-C8-C7
24	C	503	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	C	508	CLA	C11-C10-C8-C7
24	C	512	CLA	C12-C13-C15-C16
24	a	406	CLA	C11-C10-C8-C7
24	c	503	CLA	C12-C13-C15-C16
24	c	508	CLA	C11-C10-C8-C7
24	c	512	CLA	C12-C13-C15-C16
31	C	517	DGD	O6D-C5D-C6D-O5D
31	c	517	DGD	O6D-C5D-C6D-O5D
27	A	412	SQD	C16-C17-C18-C19
27	a	412	SQD	C16-C17-C18-C19
30	c	501	LMG	C14-C15-C16-C17
28	D	407	PL9	C37-C38-C39-C40
30	C	501	LMG	O1-C7-C8-C9
30	C	501	LMG	C14-C15-C16-C17
30	c	501	LMG	O1-C7-C8-C9
30	C	501	LMG	O1-C7-C8-O7
30	C	523	LMG	O1-C7-C8-O7
30	c	501	LMG	O1-C7-C8-O7
30	c	523	LMG	O1-C7-C8-O7
31	C	518	DGD	C2G-C3G-O3G-C1D
31	c	518	DGD	C2G-C3G-O3G-C1D
24	D	405	CLA	C10-C11-C12-C13
24	d	405	CLA	C10-C11-C12-C13
30	D	411	LMG	C20-C21-C22-C23
30	d	411	LMG	C20-C21-C22-C23
34	D	408	LHG	C24-C25-C26-C27
24	B	616	CLA	C10-C11-C12-C13
24	b	618	CLA	C10-C11-C12-C13
34	d	408	LHG	C24-C25-C26-C27
24	B	604	CLA	C11-C12-C13-C14
24	C	512	CLA	C6-C7-C8-C9
24	C	512	CLA	C14-C13-C15-C16
24	D	405	CLA	C11-C10-C8-C9
24	b	606	CLA	C11-C12-C13-C14
24	c	512	CLA	C6-C7-C8-C9
24	c	512	CLA	C14-C13-C15-C16
24	d	405	CLA	C11-C10-C8-C9
26	T	101	BCR	C22-C23-C24-C25
26	t	102	BCR	C22-C23-C24-C25
31	C	519	DGD	O6D-C1D-O3G-C3G
34	D	409	LHG	C34-C35-C36-C37
34	d	409	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
30	C	501	LMG	O9-C10-O7-C8
30	c	501	LMG	O9-C10-O7-C8
30	C	501	LMG	C11-C12-C13-C14
34	l	101	LHG	C13-C14-C15-C16
30	c	501	LMG	C11-C12-C13-C14
34	E	101	LHG	O8-C23-C24-C25
34	L	101	LHG	C13-C14-C15-C16
34	e	101	LHG	O8-C23-C24-C25
34	l	101	LHG	C10-C11-C12-C13
31	C	517	DGD	O1B-C1B-O2G-C2G
31	c	517	DGD	O1B-C1B-O2G-C2G
34	L	101	LHG	O10-C23-O8-C6
34	l	101	LHG	O10-C23-O8-C6
24	B	614	CLA	C2-C1-O2A-CGA
24	b	616	CLA	C2-C1-O2A-CGA
34	L	101	LHG	C10-C11-C12-C13
26	B	618	BCR	C23-C24-C25-C26
26	C	522	BCR	C23-C24-C25-C30
26	b	620	BCR	C23-C24-C25-C26
26	c	522	BCR	C23-C24-C25-C30
24	A	405	CLA	C4C-C3C-CAC-CBC
24	a	405	CLA	C4C-C3C-CAC-CBC
31	c	519	DGD	O6D-C1D-O3G-C3G
34	D	410	LHG	C29-C30-C31-C32
34	d	410	LHG	C29-C30-C31-C32
27	B	620	SQD	C9-C10-C11-C12
27	L	102	SQD	C9-C10-C11-C12
24	C	513	CLA	C11-C10-C8-C7
24	c	513	CLA	C11-C10-C8-C7
24	C	508	CLA	C11-C10-C8-C9
24	c	508	CLA	C11-C10-C8-C9
24	C	504	CLA	C16-C17-C18-C19
24	C	508	CLA	C16-C17-C18-C20
24	c	504	CLA	C16-C17-C18-C19
24	c	508	CLA	C16-C17-C18-C20
34	E	101	LHG	O9-C7-O7-C5
34	e	101	LHG	O9-C7-O7-C5
27	B	620	SQD	C26-C27-C28-C29
27	L	102	SQD	C26-C27-C28-C29
30	C	523	LMG	C15-C16-C17-C18
30	c	523	LMG	C15-C16-C17-C18
32	C	521	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
32	c	521	LMT	C5'-C4'-O1B-C1B
31	C	519	DGD	C8A-C9A-CAA-CBA
31	C	517	DGD	C4D-C5D-C6D-O5D
31	c	517	DGD	C4D-C5D-C6D-O5D
31	c	519	DGD	C8A-C9A-CAA-CBA
34	E	101	LHG	O6-C4-C5-O7
34	e	101	LHG	O6-C4-C5-O7
32	J	102	LMT	C11-C10-C9-C8
32	j	102	LMT	C11-C10-C9-C8
31	H	101	DGD	C7B-C8B-C9B-CAB
31	h	101	DGD	C7B-C8B-C9B-CAB
24	B	607	CLA	C8-C10-C11-C12
24	b	609	CLA	C8-C10-C11-C12
27	a	412	SQD	O49-C7-O47-C45
30	C	523	LMG	C29-C30-C31-C32
30	c	523	LMG	C29-C30-C31-C32
34	D	410	LHG	C10-C11-C12-C13
34	d	410	LHG	C10-C11-C12-C13
24	A	408	CLA	C2-C1-O2A-CGA
24	B	608	CLA	C2-C1-O2A-CGA
24	B	613	CLA	C2-C1-O2A-CGA
24	a	408	CLA	C2-C1-O2A-CGA
24	b	610	CLA	C2-C1-O2A-CGA
24	b	615	CLA	C2-C1-O2A-CGA
24	C	510	CLA	C13-C15-C16-C17
24	c	510	CLA	C13-C15-C16-C17
24	B	611	CLA	O1D-CGD-O2D-CED
24	b	613	CLA	O1D-CGD-O2D-CED
24	B	610	CLA	C2A-CAA-CBA-CGA
24	b	612	CLA	C2A-CAA-CBA-CGA
27	B	620	SQD	C10-C11-C12-C13
27	L	102	SQD	C10-C11-C12-C13
27	A	412	SQD	O49-C7-O47-C45
30	c	520	LMG	C17-C18-C19-C20
30	C	520	LMG	C17-C18-C19-C20
28	A	411	PL9	C4-C3-C7-C8
28	a	411	PL9	C4-C3-C7-C8
24	B	601	CLA	CAA-CBA-CGA-O2A
24	b	603	CLA	CAA-CBA-CGA-O2A
24	A	406	CLA	C11-C10-C8-C9
24	A	408	CLA	C14-C13-C15-C16
24	C	507	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	a	406	CLA	C11-C10-C8-C9
24	c	507	CLA	C11-C10-C8-C9
24	D	405	CLA	C16-C17-C18-C20
24	d	405	CLA	C16-C17-C18-C20
26	B	619	BCR	C35-C13-C14-C15
26	C	516	BCR	C11-C10-C9-C34
26	b	621	BCR	C35-C13-C14-C15
26	c	516	BCR	C11-C10-C9-C34
27	A	410	SQD	O6-C44-C45-C46
27	a	410	SQD	O6-C44-C45-C46
31	H	101	DGD	C8A-C9A-CAA-CBA
31	h	101	DGD	C8A-C9A-CAA-CBA
27	A	410	SQD	C15-C16-C17-C18
27	a	410	SQD	C15-C16-C17-C18
27	A	412	SQD	C31-C32-C33-C34
27	a	412	SQD	C31-C32-C33-C34
24	A	405	CLA	C15-C16-C17-C18
24	a	405	CLA	C15-C16-C17-C18
24	B	601	CLA	C1A-C2A-CAA-CBA
24	C	504	CLA	C1A-C2A-CAA-CBA
24	b	603	CLA	C1A-C2A-CAA-CBA
24	c	504	CLA	C1A-C2A-CAA-CBA
24	B	604	CLA	C11-C12-C13-C15
24	B	610	CLA	C12-C13-C15-C16
24	B	616	CLA	C12-C13-C15-C16
24	b	606	CLA	C11-C12-C13-C15
24	b	612	CLA	C12-C13-C15-C16
24	b	618	CLA	C12-C13-C15-C16
34	D	408	LHG	C32-C33-C34-C35
34	d	408	LHG	C32-C33-C34-C35
34	D	408	LHG	C3-O3-P-O6
34	E	101	LHG	C4-O6-P-O3
34	d	408	LHG	C3-O3-P-O6
34	e	101	LHG	C4-O6-P-O3
31	H	101	DGD	C9B-CAB-CBB-CCB
31	h	101	DGD	C9B-CAB-CBB-CCB
30	d	411	LMG	C28-C29-C30-C31
31	C	519	DGD	O6E-C5E-C6E-O5E
31	c	519	DGD	O6E-C5E-C6E-O5E
24	B	614	CLA	C5-C6-C7-C8
24	b	616	CLA	C5-C6-C7-C8
31	c	518	DGD	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
31	C	518	DGD	CBB-CCB-CDB-CEB
30	D	411	LMG	C28-C29-C30-C31
24	C	506	CLA	C2-C3-C5-C6
24	c	506	CLA	C2-C3-C5-C6
37	V	201	HEC	CAD-CBD-CGD-O1D
37	v	201	HEC	CAD-CBD-CGD-O1D
26	D	406	BCR	C13-C14-C15-C16
26	d	406	BCR	C13-C14-C15-C16
34	D	409	LHG	C13-C14-C15-C16
34	d	409	LHG	C13-C14-C15-C16
34	E	101	LHG	C11-C10-C9-C8
34	e	101	LHG	C11-C10-C9-C8
24	C	512	CLA	C2-C1-O2A-CGA
24	C	514	CLA	C2-C1-O2A-CGA
24	c	512	CLA	C2-C1-O2A-CGA
24	c	514	CLA	C2-C1-O2A-CGA
24	d	404	CLA	C2-C1-O2A-CGA
24	B	602	CLA	C15-C16-C17-C18
24	b	604	CLA	C15-C16-C17-C18
24	a	408	CLA	C14-C13-C15-C16
30	d	411	LMG	C33-C34-C35-C36
30	D	411	LMG	C33-C34-C35-C36
34	l	101	LHG	C25-C26-C27-C28
34	L	101	LHG	C25-C26-C27-C28
24	B	607	CLA	C2A-CAA-CBA-CGA
24	b	609	CLA	C2A-CAA-CBA-CGA
37	V	201	HEC	CAD-CBD-CGD-O2D
37	v	201	HEC	CAD-CBD-CGD-O2D
26	A	409	BCR	C23-C24-C25-C30
26	B	618	BCR	C23-C24-C25-C30
26	B	619	BCR	C1-C6-C7-C8
26	C	516	BCR	C1-C6-C7-C8
26	C	516	BCR	C5-C6-C7-C8
26	a	409	BCR	C23-C24-C25-C30
26	b	620	BCR	C23-C24-C25-C30
26	b	621	BCR	C1-C6-C7-C8
26	c	516	BCR	C1-C6-C7-C8
26	c	516	BCR	C5-C6-C7-C8
34	e	101	LHG	C33-C34-C35-C36
27	F	101	SQD	O47-C7-C8-C9
27	f	101	SQD	O47-C7-C8-C9
34	E	101	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
24	B	602	CLA	O1A-CGA-O2A-C1
24	b	604	CLA	O1A-CGA-O2A-C1
38	X	101	RRX	C19-C20-C21-C22
38	x	101	RRX	C19-C20-C21-C22
34	D	410	LHG	O10-C23-O8-C6
34	d	410	LHG	O10-C23-O8-C6
27	A	412	SQD	C45-C44-O6-C1
27	B	620	SQD	C45-C44-O6-C1
27	F	101	SQD	C45-C44-O6-C1
27	L	102	SQD	C45-C44-O6-C1
27	a	412	SQD	C45-C44-O6-C1
27	f	101	SQD	C45-C44-O6-C1
24	B	610	CLA	O1D-CGD-O2D-CED
27	A	412	SQD	C28-C29-C30-C31
27	a	412	SQD	C28-C29-C30-C31
24	C	504	CLA	O1D-CGD-O2D-CED
24	c	504	CLA	O1D-CGD-O2D-CED
30	D	411	LMG	C10-C11-C12-C13
30	d	411	LMG	C10-C11-C12-C13
24	B	603	CLA	O1D-CGD-O2D-CED
24	b	605	CLA	O1D-CGD-O2D-CED
24	c	507	CLA	C10-C11-C12-C13
24	c	506	CLA	C4-C3-C5-C6
24	C	507	CLA	C10-C11-C12-C13
34	D	408	LHG	C11-C12-C13-C14
34	d	408	LHG	C11-C12-C13-C14
31	C	519	DGD	C2D-C1D-O3G-C3G
31	c	519	DGD	C2D-C1D-O3G-C3G
24	b	612	CLA	O1D-CGD-O2D-CED
24	C	505	CLA	C15-C16-C17-C18
24	c	505	CLA	C15-C16-C17-C18
24	D	401	CLA	C4C-C3C-CAC-CBC
24	d	401	CLA	C4C-C3C-CAC-CBC
24	B	616	CLA	C14-C13-C15-C16
24	C	513	CLA	C11-C10-C8-C9
24	b	618	CLA	C14-C13-C15-C16
24	c	513	CLA	C11-C10-C8-C9
24	B	607	CLA	C3A-C2A-CAA-CBA
24	b	609	CLA	C3A-C2A-CAA-CBA
31	C	519	DGD	O1A-C1A-O1G-C1G
31	c	519	DGD	O1A-C1A-O1G-C1G
24	B	610	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	B	612	CLA	CAD-CBD-CGD-O2D
24	C	504	CLA	CAD-CBD-CGD-O2D
24	C	507	CLA	CAD-CBD-CGD-O2D
24	C	513	CLA	CAD-CBD-CGD-O2D
24	b	612	CLA	CAD-CBD-CGD-O2D
24	b	614	CLA	CAD-CBD-CGD-O2D
24	c	504	CLA	CAD-CBD-CGD-O2D
24	c	507	CLA	CAD-CBD-CGD-O2D
24	c	513	CLA	CAD-CBD-CGD-O2D
24	D	404	CLA	C2-C1-O2A-CGA
24	C	511	CLA	CAA-CBA-CGA-O2A
24	c	511	CLA	CAA-CBA-CGA-O2A
27	A	410	SQD	O47-C7-C8-C9
27	a	410	SQD	O47-C7-C8-C9
30	C	501	LMG	O8-C28-C29-C30
24	C	506	CLA	C4-C3-C5-C6
30	c	501	LMG	O8-C28-C29-C30
34	d	410	LHG	C14-C15-C16-C17
26	C	515	BCR	C11-C12-C13-C14
26	c	515	BCR	C11-C12-C13-C14
34	D	410	LHG	C14-C15-C16-C17
30	C	501	LMG	C19-C20-C21-C22
30	c	501	LMG	C19-C20-C21-C22
24	C	506	CLA	CAA-CBA-CGA-O2A
24	c	506	CLA	CAA-CBA-CGA-O2A
34	D	408	LHG	O2-C2-C3-O3
34	d	408	LHG	O2-C2-C3-O3
24	C	505	CLA	CHA-CBD-CGD-O2D
24	C	510	CLA	CHA-CBD-CGD-O1D
24	D	401	CLA	CHA-CBD-CGD-O1D
24	c	505	CLA	CHA-CBD-CGD-O2D
24	c	510	CLA	CHA-CBD-CGD-O1D
24	d	401	CLA	CHA-CBD-CGD-O1D
30	C	523	LMG	O8-C28-C29-C30
30	c	523	LMG	O8-C28-C29-C30
31	H	101	DGD	CBB-CCB-CDB-CEB
31	h	101	DGD	CBB-CCB-CDB-CEB
24	B	613	CLA	CAA-CBA-CGA-O2A
24	B	616	CLA	CAA-CBA-CGA-O2A
24	C	513	CLA	CAA-CBA-CGA-O2A
24	b	615	CLA	CAA-CBA-CGA-O2A
24	c	513	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	c	517	DGD	O2G-C1B-C2B-C3B
34	D	410	LHG	O8-C23-C24-C25
34	d	410	LHG	O8-C23-C24-C25
31	C	518	DGD	C5A-C6A-C7A-C8A
31	c	518	DGD	C5A-C6A-C7A-C8A
24	b	605	CLA	C13-C15-C16-C17
31	C	517	DGD	O2G-C1B-C2B-C3B
25	A	407	PHO	CHA-CBD-CGD-O1D
25	A	407	PHO	CHA-CBD-CGD-O2D
25	D	402	PHO	CHA-CBD-CGD-O2D
25	a	407	PHO	CHA-CBD-CGD-O1D
25	a	407	PHO	CHA-CBD-CGD-O2D
25	d	402	PHO	CHA-CBD-CGD-O2D
27	F	101	SQD	C28-C29-C30-C31
27	f	101	SQD	C28-C29-C30-C31
24	b	618	CLA	CAA-CBA-CGA-O2A
27	B	620	SQD	O48-C23-C24-C25
27	L	102	SQD	O48-C23-C24-C25
34	D	410	LHG	C17-C18-C19-C20
34	d	410	LHG	C17-C18-C19-C20
34	D	408	LHG	C25-C26-C27-C28
24	C	507	CLA	C11-C10-C8-C7
24	c	507	CLA	C11-C10-C8-C7
28	D	407	PL9	C4-C3-C7-C8
28	d	407	PL9	C4-C3-C7-C8
24	B	603	CLA	C13-C15-C16-C17
31	C	518	DGD	CAA-CBA-CCA-CDA
31	c	518	DGD	CAA-CBA-CCA-CDA
24	B	612	CLA	C11-C10-C8-C9
24	b	614	CLA	C11-C10-C8-C9
30	C	501	LMG	O9-C10-C11-C12
30	c	501	LMG	O9-C10-C11-C12
34	d	408	LHG	C25-C26-C27-C28
24	B	607	CLA	O1A-CGA-O2A-C1
24	b	609	CLA	O1A-CGA-O2A-C1
27	A	410	SQD	C9-C10-C11-C12
27	a	410	SQD	C9-C10-C11-C12
24	c	511	CLA	CAA-CBA-CGA-O1A
32	M	101	LMT	O5B-C5B-C6B-O6B
24	C	511	CLA	CAA-CBA-CGA-O1A
27	B	620	SQD	O49-C7-C8-C9
27	L	102	SQD	O49-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
32	m	102	LMT	O5B-C5B-C6B-O6B
24	C	511	CLA	C2-C1-O2A-CGA
24	c	511	CLA	C2-C1-O2A-CGA
31	C	518	DGD	O1B-C1B-C2B-C3B
31	c	518	DGD	O1B-C1B-C2B-C3B
24	D	401	CLA	C16-C17-C18-C20
24	c	506	CLA	C16-C17-C18-C19
24	d	401	CLA	C16-C17-C18-C20
24	B	611	CLA	CBD-CGD-O2D-CED
24	b	613	CLA	CBD-CGD-O2D-CED
35	E	103	HEM	CAA-CBA-CGA-O2A
35	e	103	HEM	CAA-CBA-CGA-O2A
34	D	408	LHG	C3-O3-P-O5
34	E	101	LHG	C4-O6-P-O5
34	d	408	LHG	C3-O3-P-O5
34	e	101	LHG	C4-O6-P-O5
24	C	506	CLA	C16-C17-C18-C19
34	E	101	LHG	O6-C4-C5-C6
34	e	101	LHG	O6-C4-C5-C6
30	C	501	LMG	C20-C21-C22-C23
30	c	501	LMG	C20-C21-C22-C23
26	B	619	BCR	C5-C6-C7-C8
26	b	621	BCR	C5-C6-C7-C8
24	B	602	CLA	C13-C15-C16-C17
24	b	604	CLA	C13-C15-C16-C17
24	C	506	CLA	CAA-CBA-CGA-O1A
24	c	506	CLA	CAA-CBA-CGA-O1A
34	l	101	LHG	C17-C18-C19-C20
30	C	520	LMG	C4-C5-C6-O5
31	C	518	DGD	C8B-C9B-CAB-CBB
31	c	518	DGD	C8B-C9B-CAB-CBB
34	L	101	LHG	C17-C18-C19-C20
30	c	520	LMG	C4-C5-C6-O5
24	B	607	CLA	CAD-CBD-CGD-O1D
24	b	609	CLA	CAD-CBD-CGD-O1D
24	B	605	CLA	C10-C11-C12-C13
30	C	501	LMG	O7-C10-C11-C12
30	c	501	LMG	O7-C10-C11-C12
34	e	101	LHG	C30-C31-C32-C33
24	b	607	CLA	C10-C11-C12-C13
34	E	101	LHG	C30-C31-C32-C33
27	B	620	SQD	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
27	L	102	SQD	O10-C23-C24-C25
24	B	603	CLA	C6-C7-C8-C10
24	B	607	CLA	C6-C7-C8-C10
24	B	612	CLA	C11-C10-C8-C7
24	C	512	CLA	C11-C12-C13-C15
24	b	605	CLA	C6-C7-C8-C10
24	b	609	CLA	C6-C7-C8-C10
24	b	614	CLA	C11-C10-C8-C7
24	c	512	CLA	C11-C12-C13-C15
24	B	616	CLA	CAA-CBA-CGA-O1A
24	b	618	CLA	CAA-CBA-CGA-O1A
34	L	101	LHG	O7-C7-C8-C9
34	l	101	LHG	O7-C7-C8-C9
26	A	409	BCR	C17-C18-C19-C20
26	C	522	BCR	C11-C12-C13-C14
26	C	522	BCR	C21-C22-C23-C24
26	a	409	BCR	C17-C18-C19-C20
26	c	522	BCR	C11-C12-C13-C14
26	c	522	BCR	C21-C22-C23-C24
24	C	513	CLA	CAA-CBA-CGA-O1A
24	c	513	CLA	CAA-CBA-CGA-O1A
24	C	513	CLA	C8-C10-C11-C12
24	c	513	CLA	C8-C10-C11-C12
30	c	501	LMG	O10-C28-C29-C30
27	B	620	SQD	O47-C7-C8-C9
27	L	102	SQD	O47-C7-C8-C9
24	C	511	CLA	C8-C10-C11-C12
24	c	511	CLA	C8-C10-C11-C12
24	A	406	CLA	C2A-CAA-CBA-CGA
24	a	406	CLA	C2A-CAA-CBA-CGA
24	B	613	CLA	CAA-CBA-CGA-O1A
24	b	615	CLA	CAA-CBA-CGA-O1A
30	C	501	LMG	O10-C28-C29-C30
35	e	103	HEM	CAD-CBD-CGD-O1D

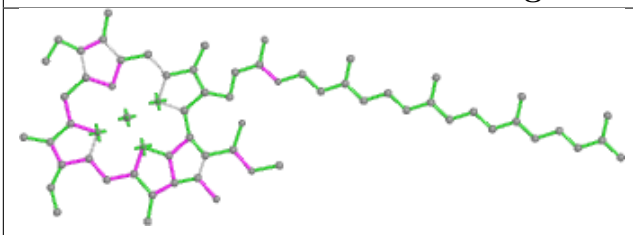
There are no ring outliers.

No monomer is involved in short contacts.

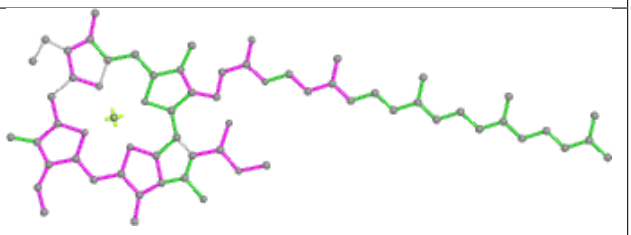
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

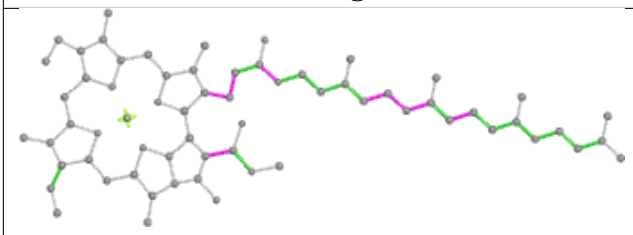
Ligand CLA B 607



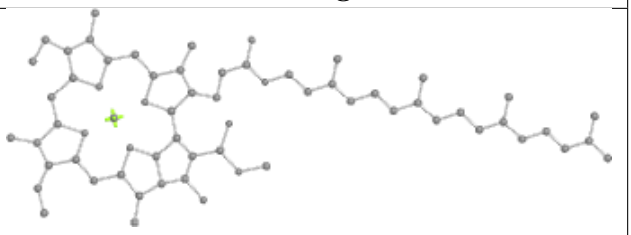
Bond lengths



Bond angles

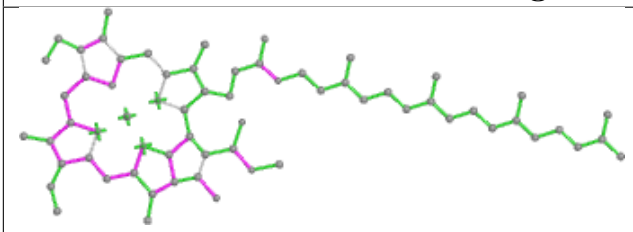


Torsions

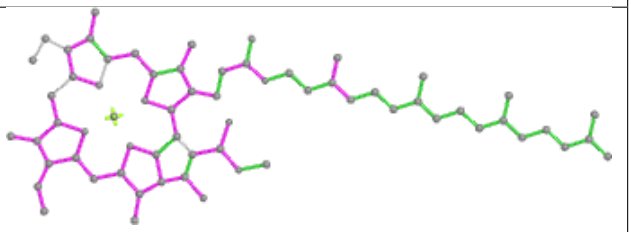


Rings

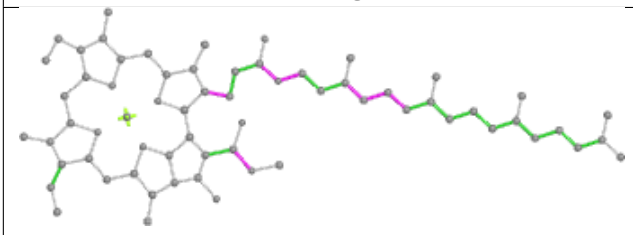
Ligand CLA c 514



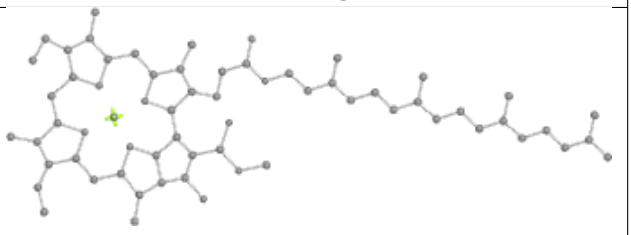
Bond lengths



Bond angles

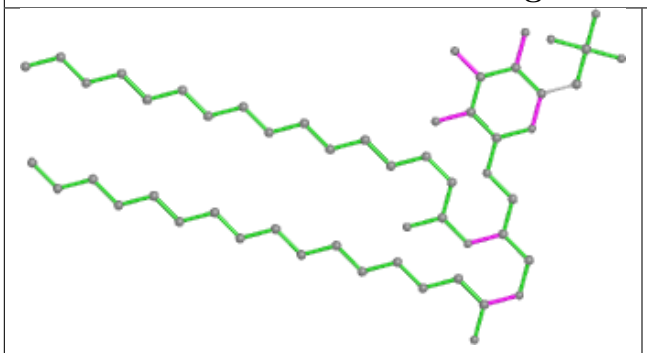


Torsions



Rings

Ligand SQD A 410



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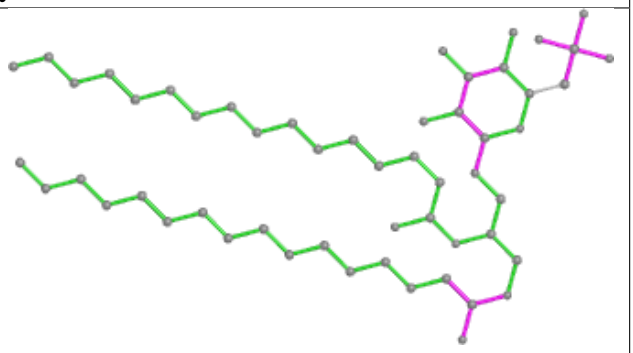
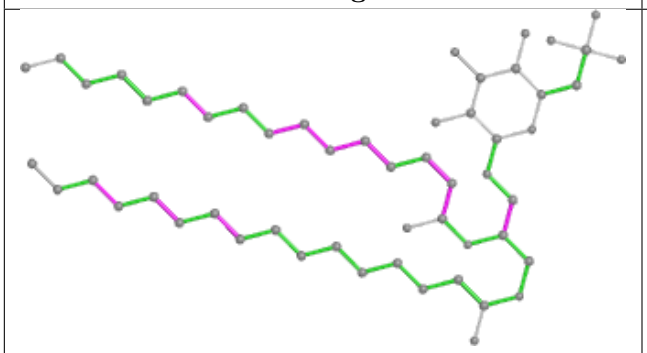
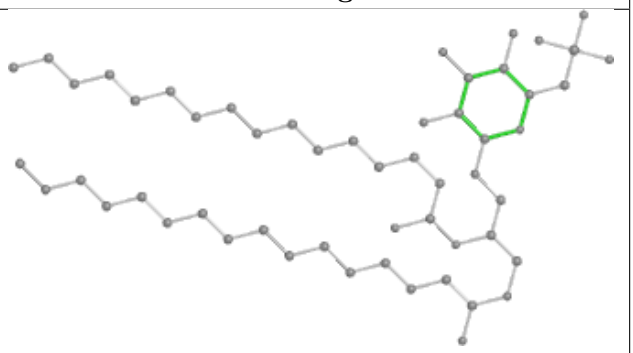


Bond angles

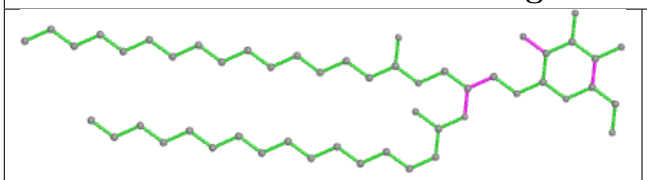


Torsions

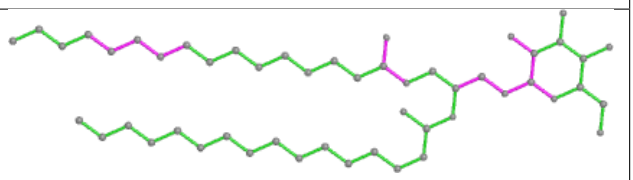


Rings

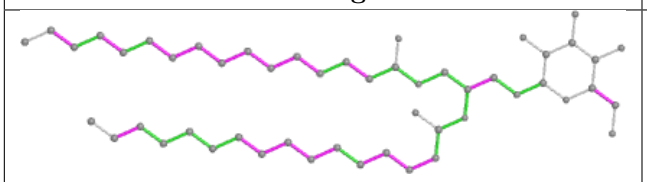
Ligand LMG c 520



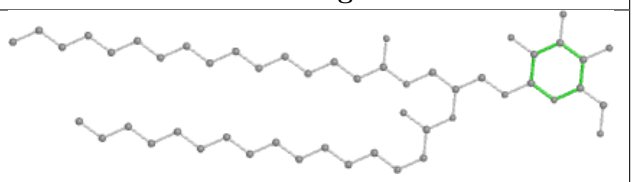
Bond lengths



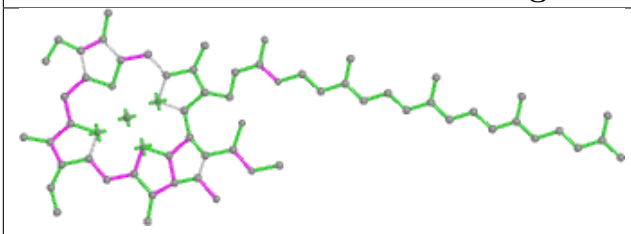
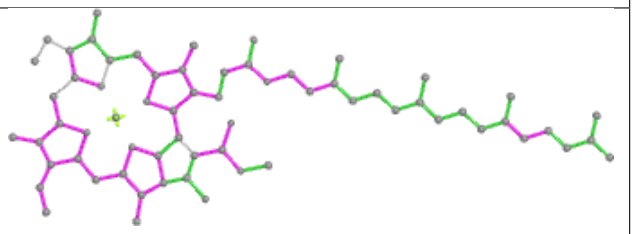
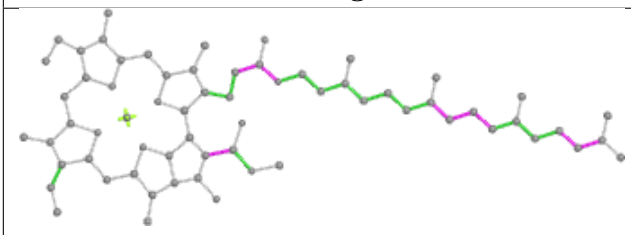
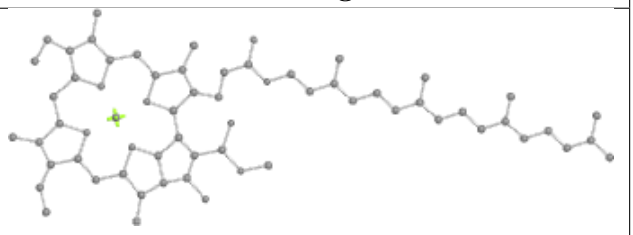
Bond angles

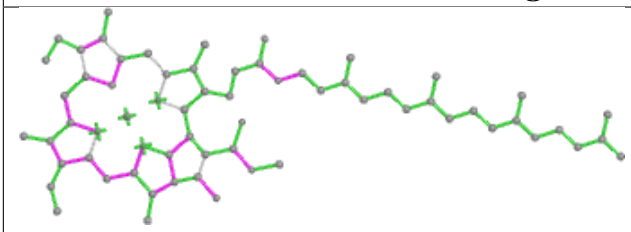
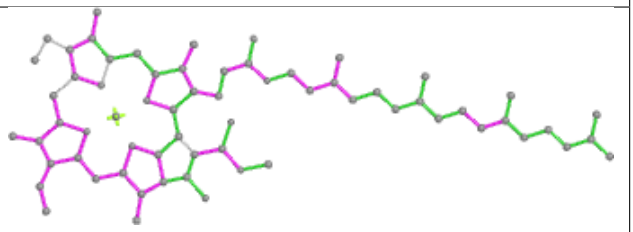
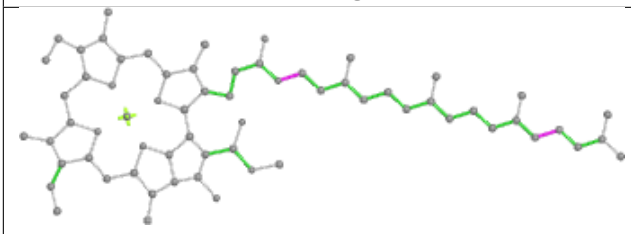
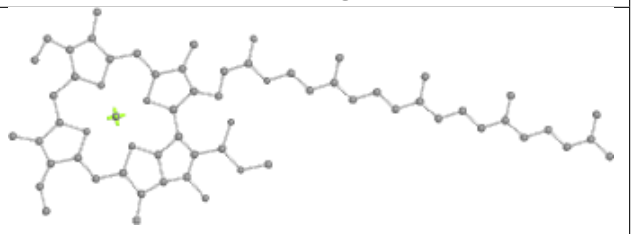


Torsions

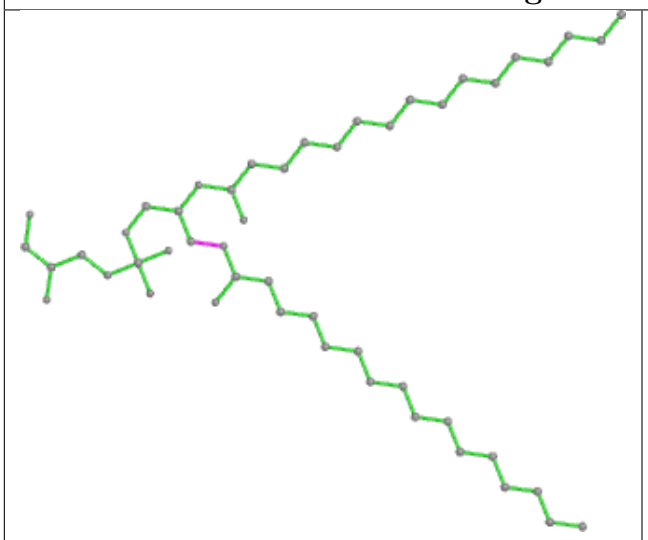


Rings

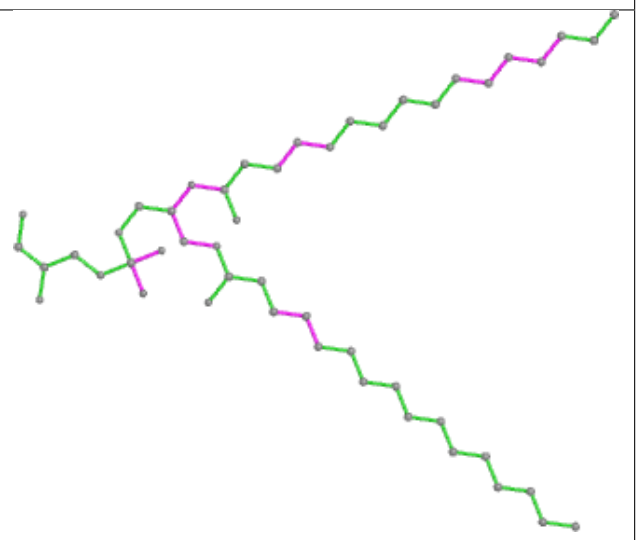
Ligand CLA c 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

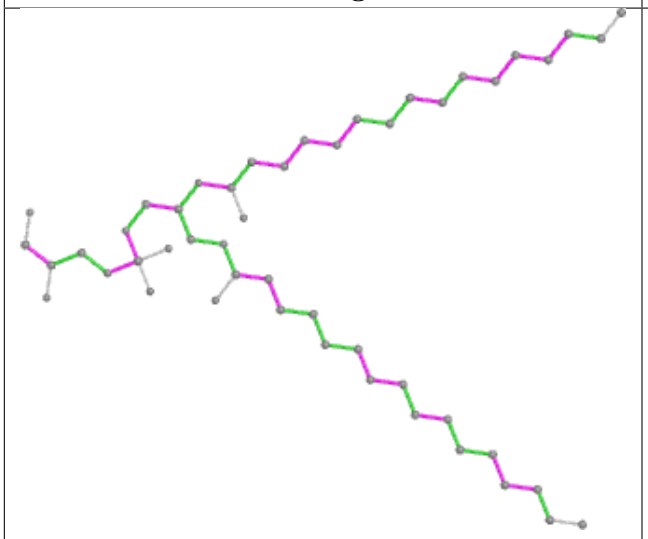
Ligand LHG E 101



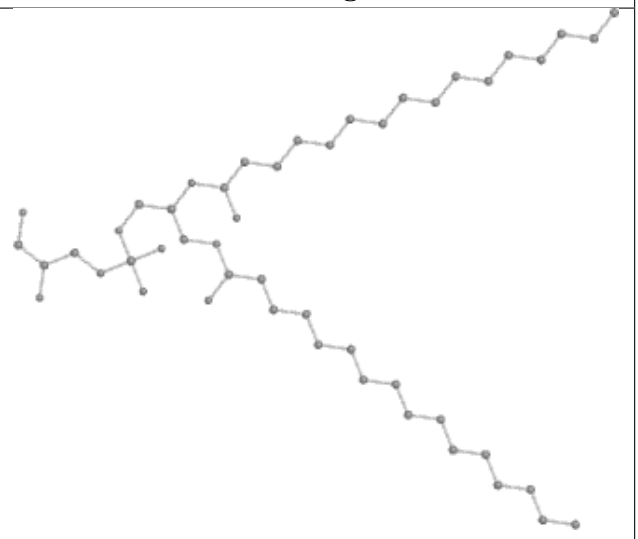
Bond lengths



Bond angles

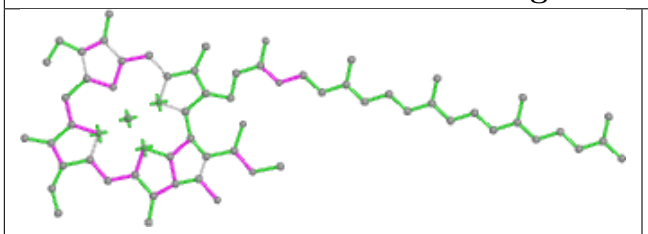


Torsions

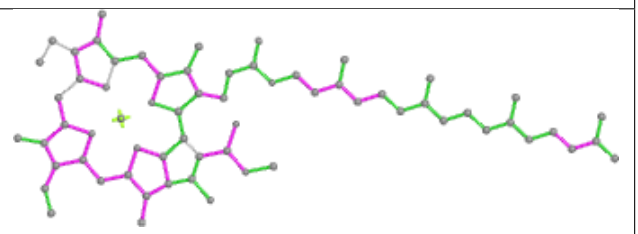


Rings

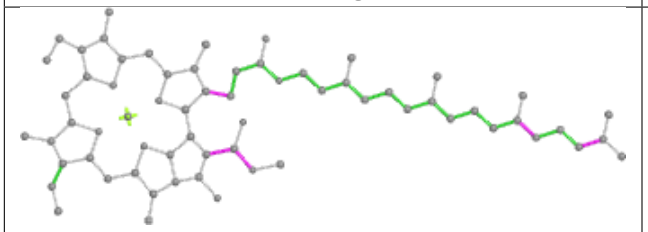
Ligand CLA c 503



Bond lengths



Bond angles



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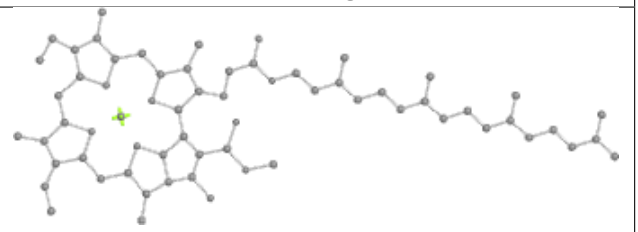
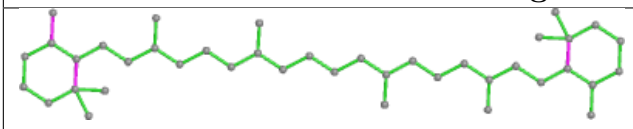
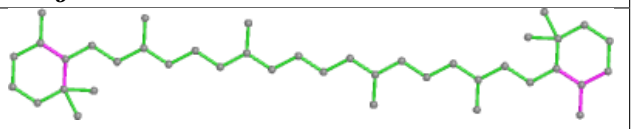


Rings

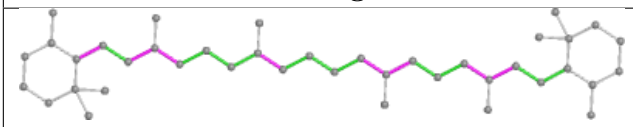
Ligand BCR j 104



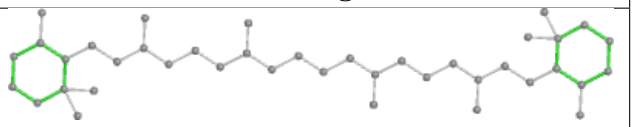
Bond lengths



Bond angles

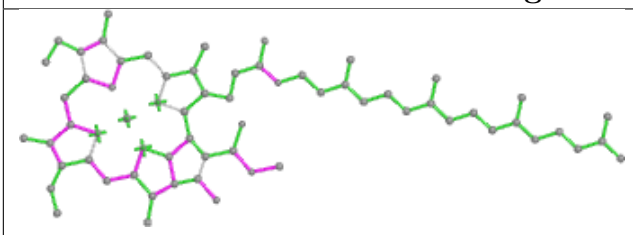


Torsions

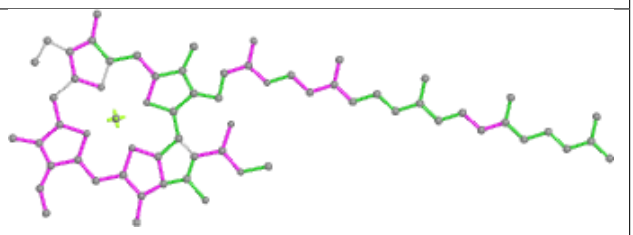


Rings

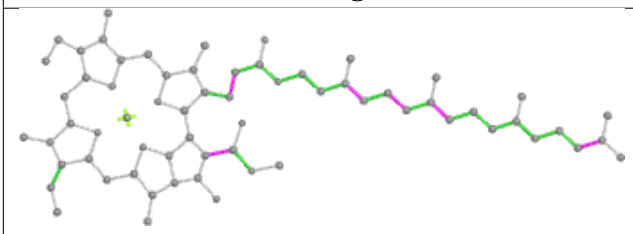
Ligand CLA C 508



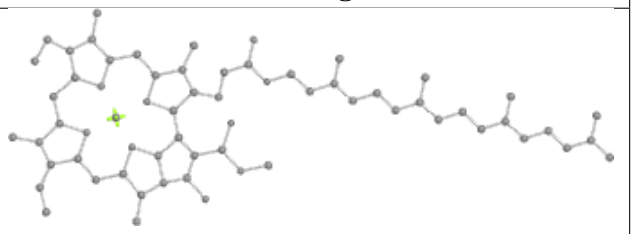
Bond lengths



Bond angles

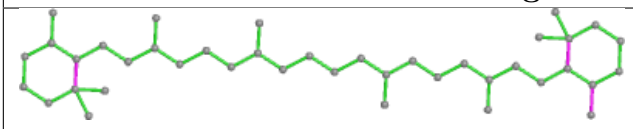


Torsions



Rings

Ligand BCR B 618



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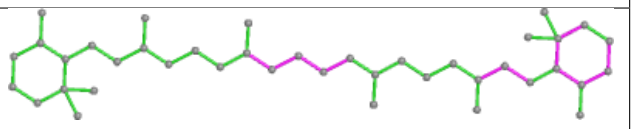
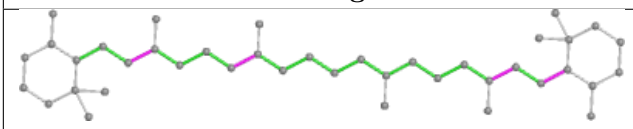


Bond angles



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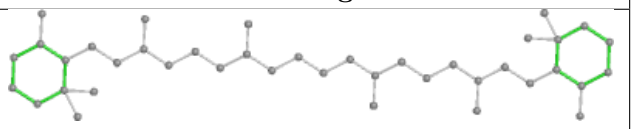
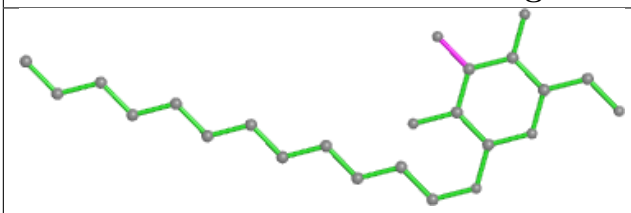
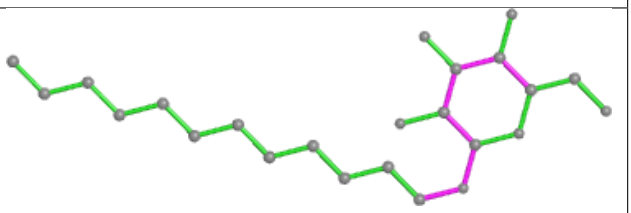


Rings

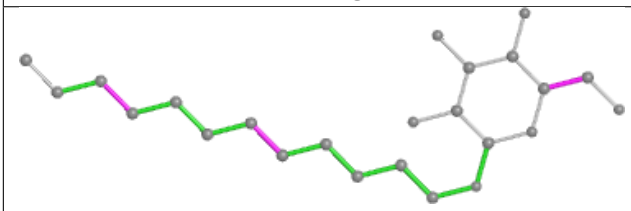
Ligand LMT J 102



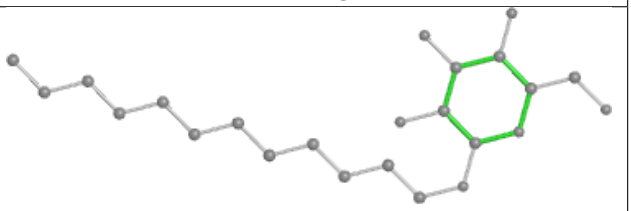
Bond lengths



Bond angles

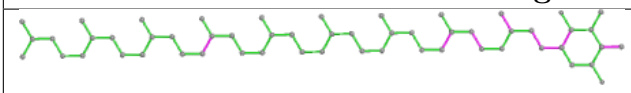


Torsions

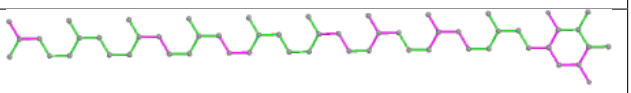


Rings

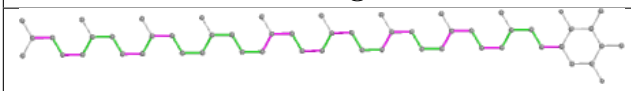
Ligand PL9 a 411



Bond lengths



Bond angles



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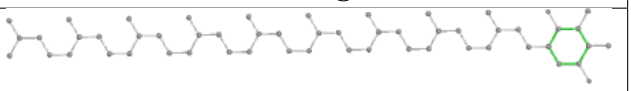
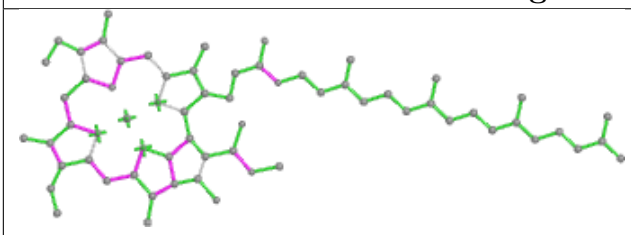
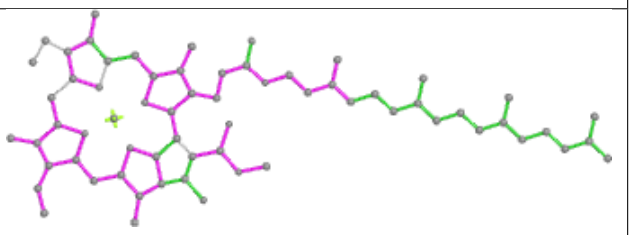


Rings

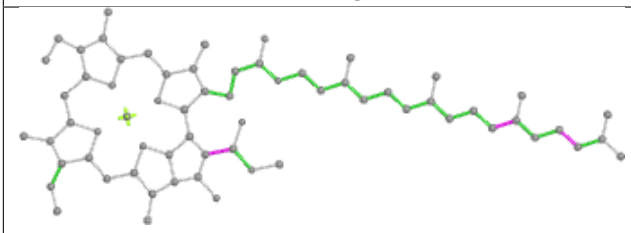
Ligand CLA c 505



Bond lengths



Bond angles



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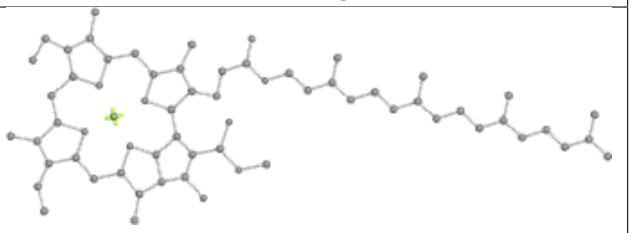
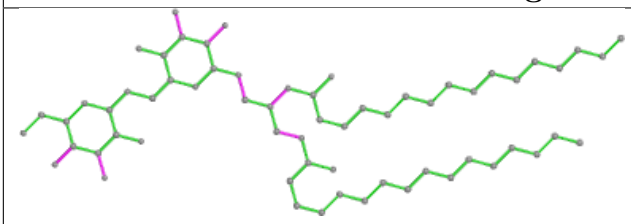
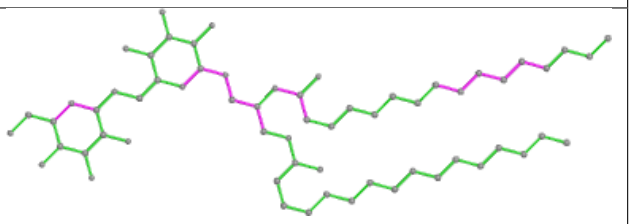


Rings

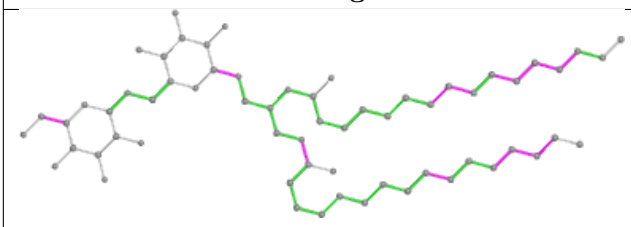
Ligand DGD c 519



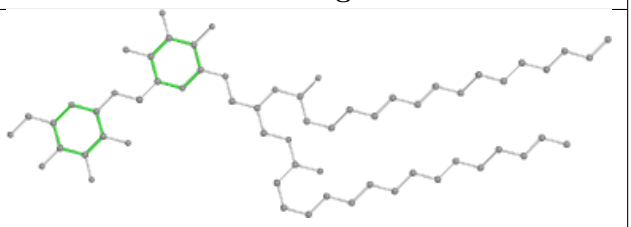
Bond lengths



Bond angles

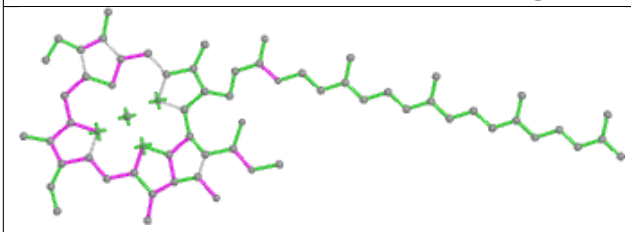


Torsions

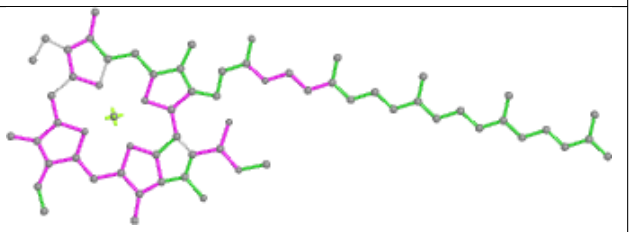


Rings

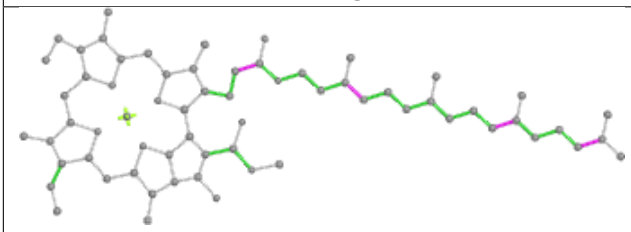
Ligand CLA c 506



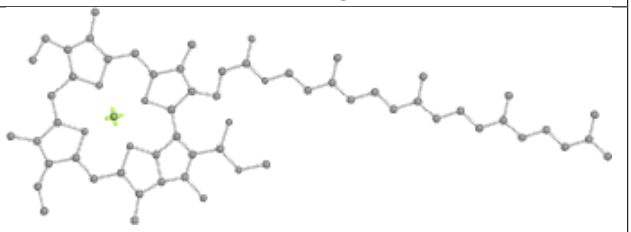
Bond lengths



Bond angles

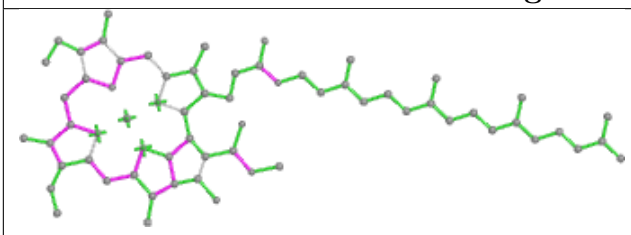


Torsions

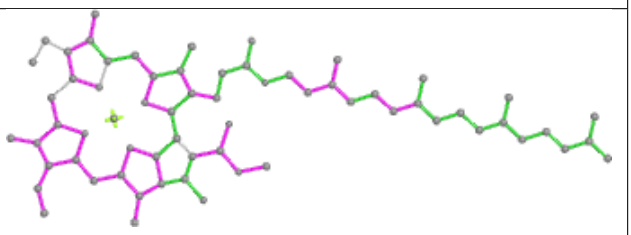


Rings

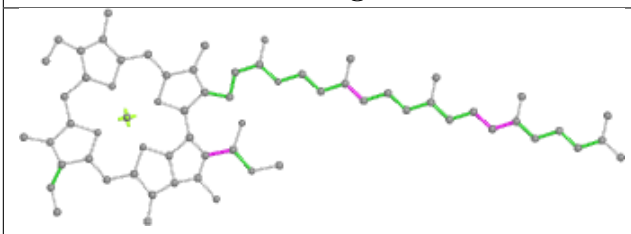
Ligand CLA B 605



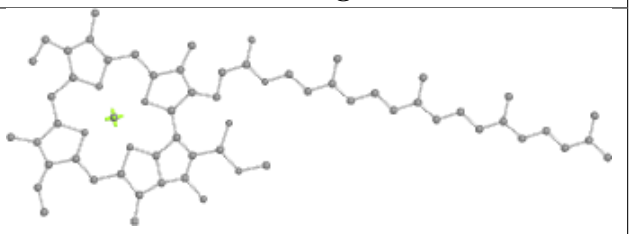
Bond lengths



Bond angles

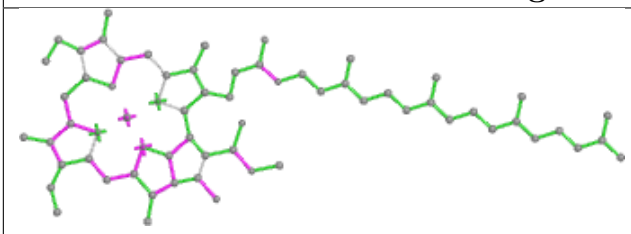


Torsions

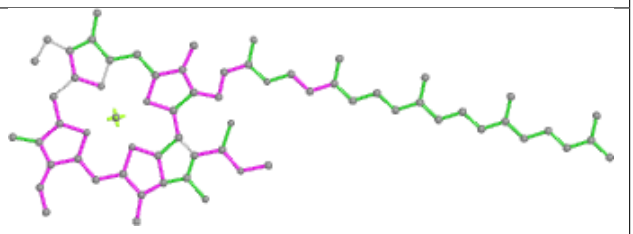


Rings

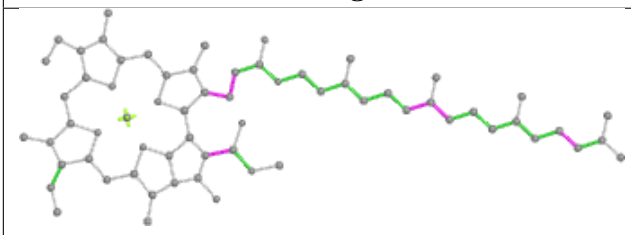
Ligand CLA a 406



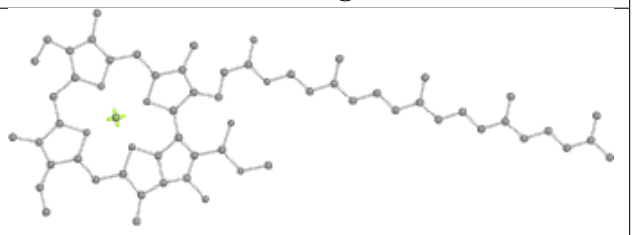
Bond lengths



Bond angles

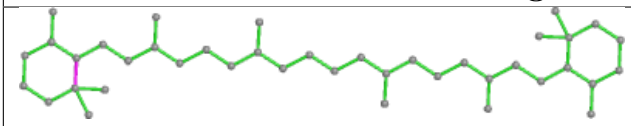


Torsions

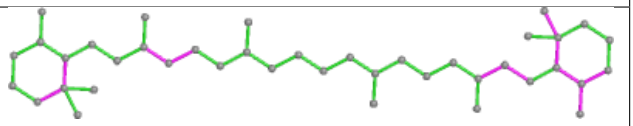


Rings

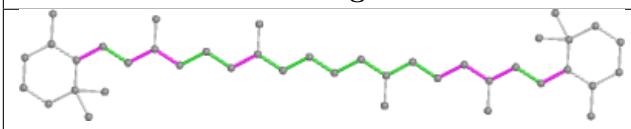
Ligand BCR c 522



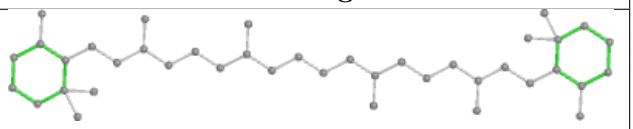
Bond lengths



Bond angles

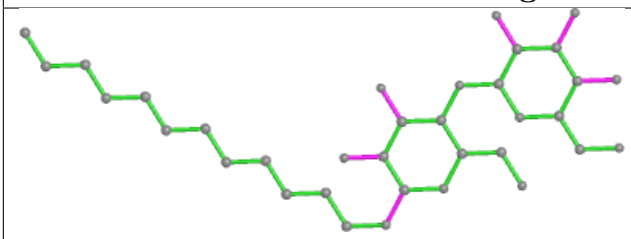


Torsions

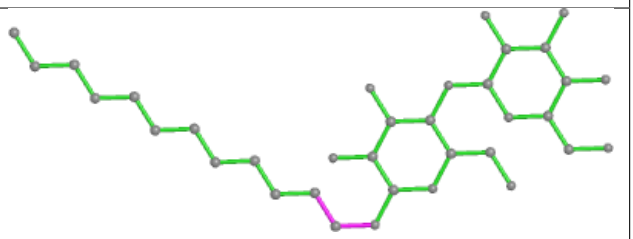


Rings

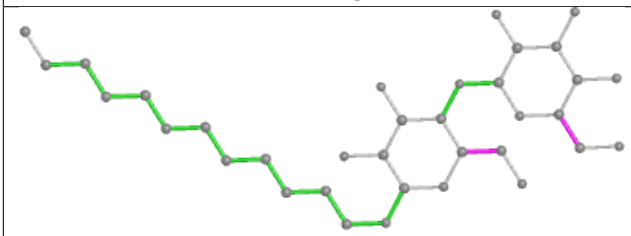
Ligand LMT m 102



Bond lengths



Bond angles



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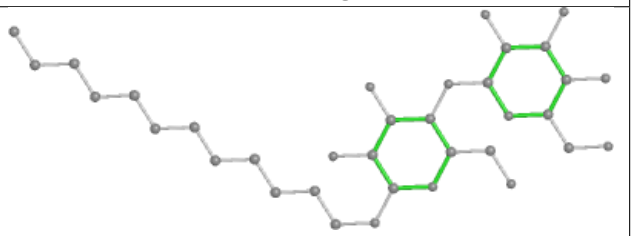
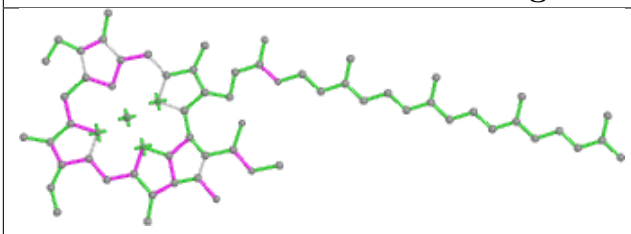
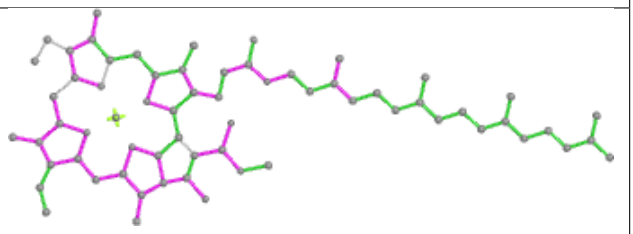
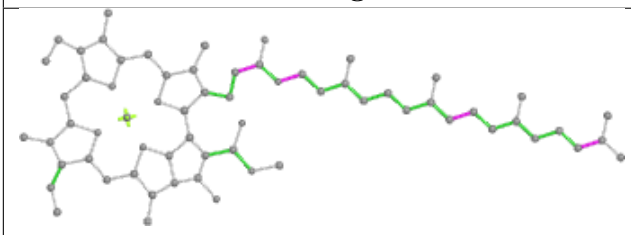
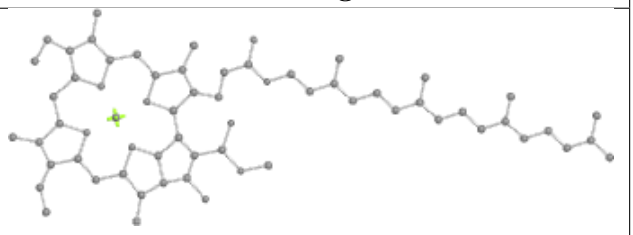
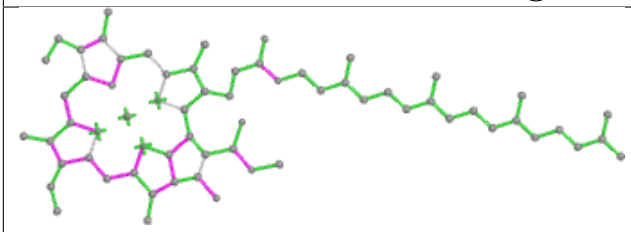
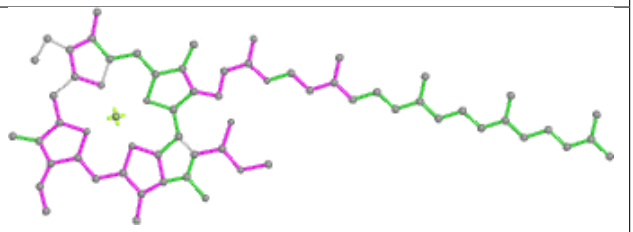
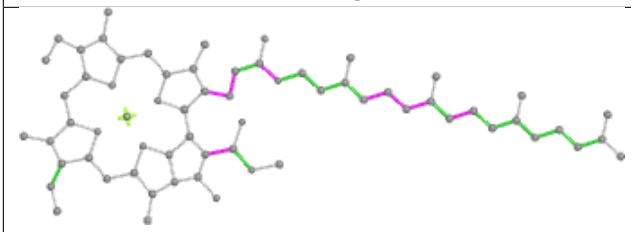
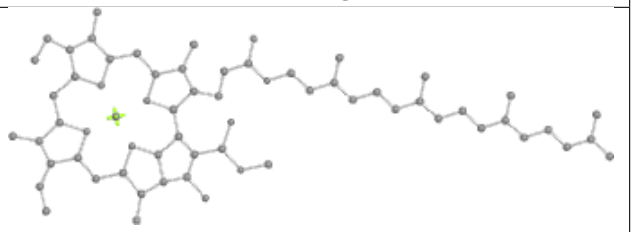
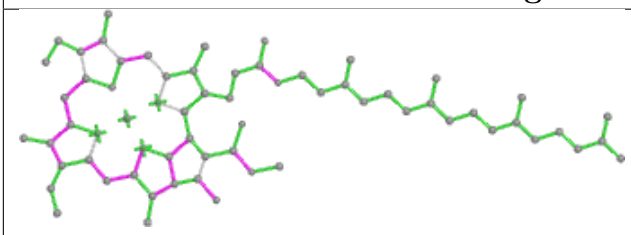
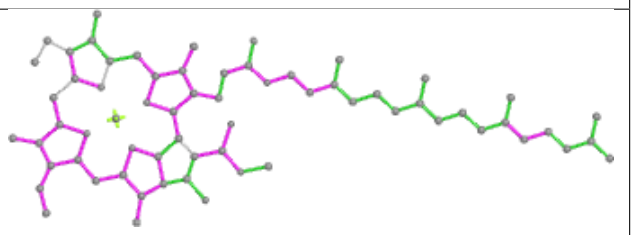
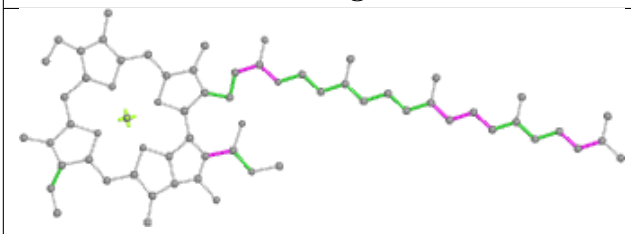
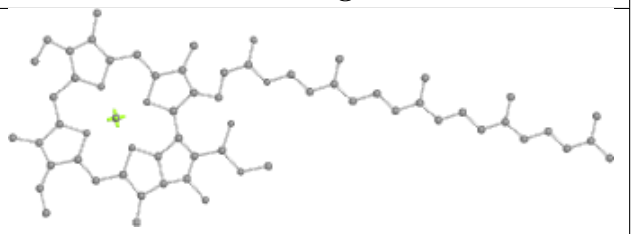


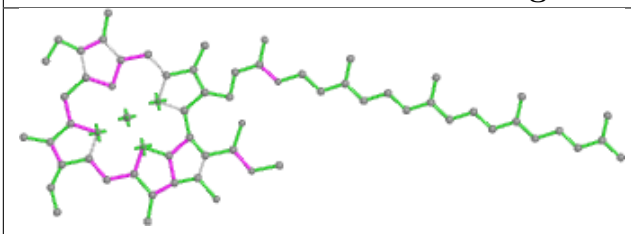
Rings

Ligand CLA c 511	
 Bond lengths	 Bond angles
 Torsions	 Rings

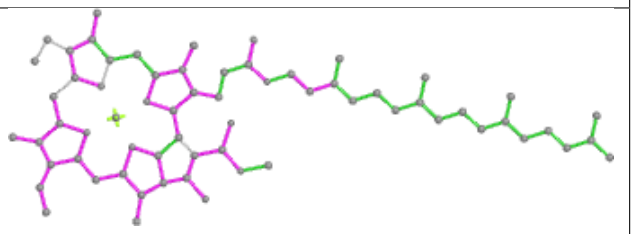
Ligand CLA b 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

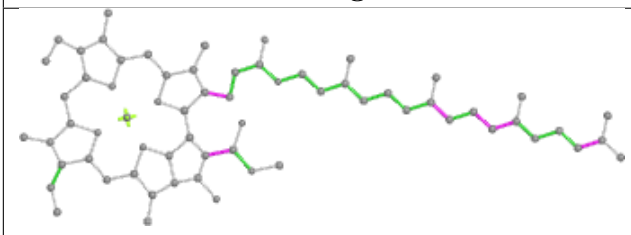
Ligand CLA c 507



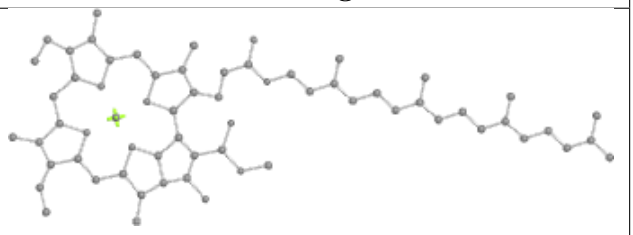
Bond lengths



Bond angles

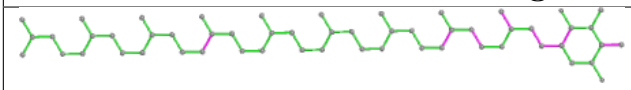


Torsions



Rings

Ligand PL9 A 411



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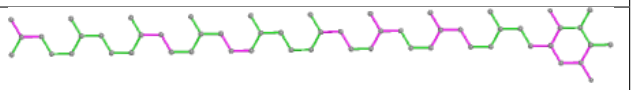
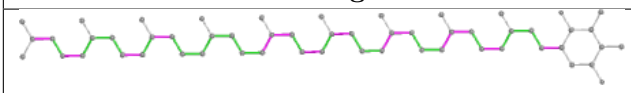
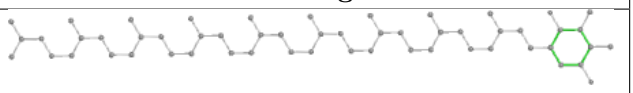


Bond angles

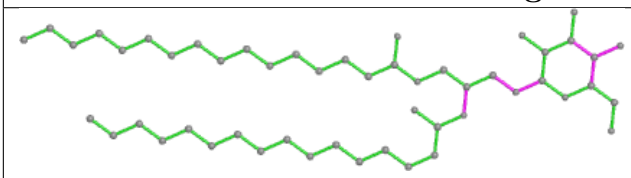


Torsions

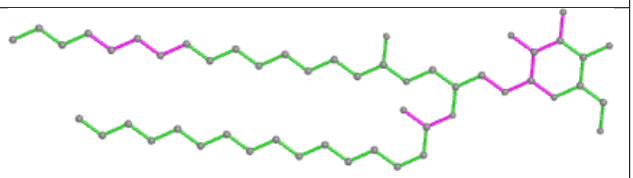


Rings

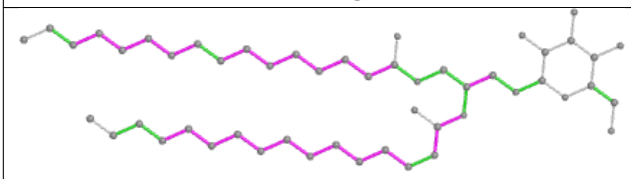
Ligand LMG c 501



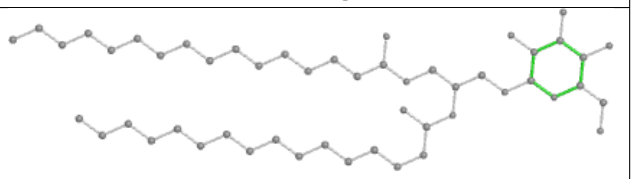
Bond lengths



Bond angles

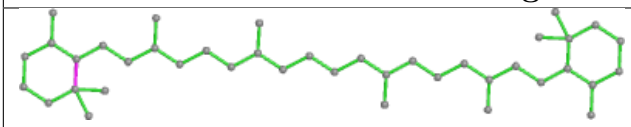


Torsions

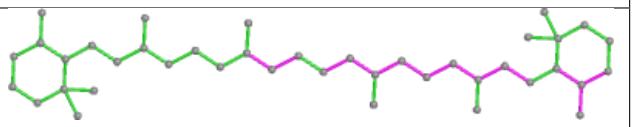


Rings

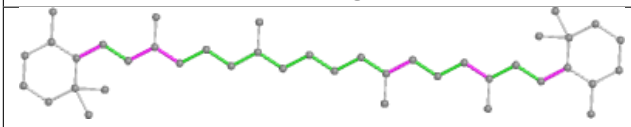
Ligand BCR A 409



Bond lengths

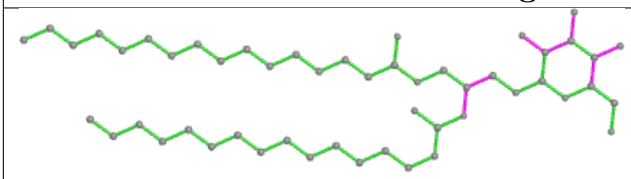
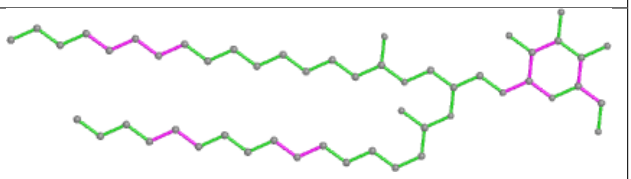
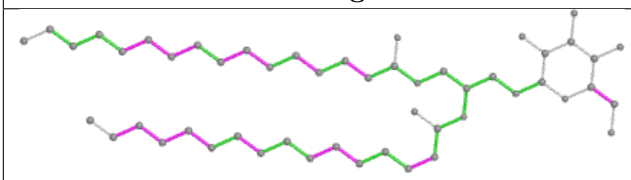
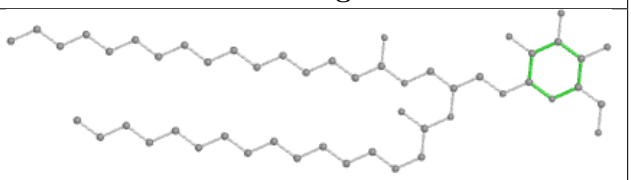


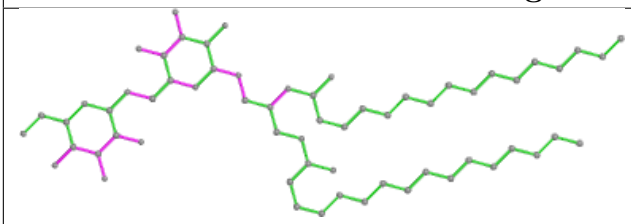
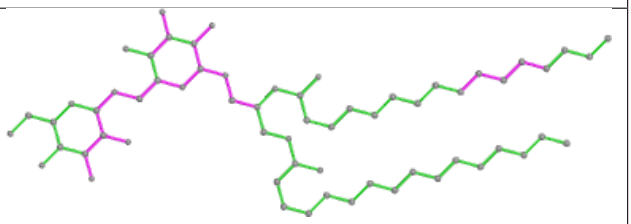
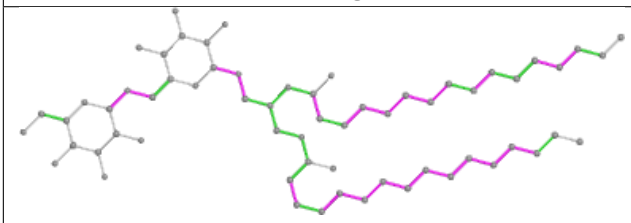
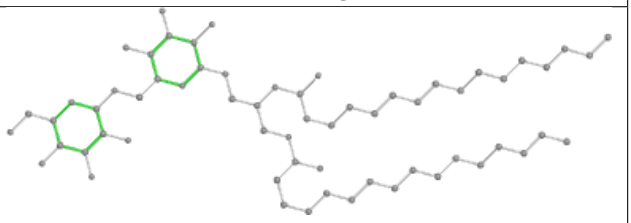
Bond angles



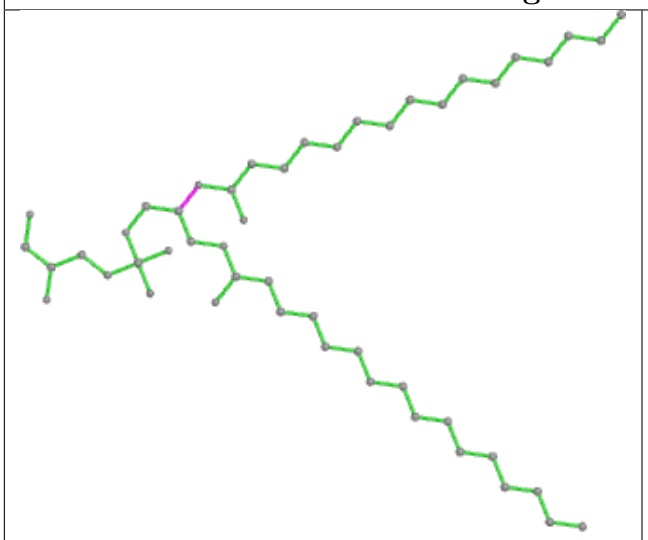
Torsions

Rings

Ligand LMG D 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DGD c 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG D 408



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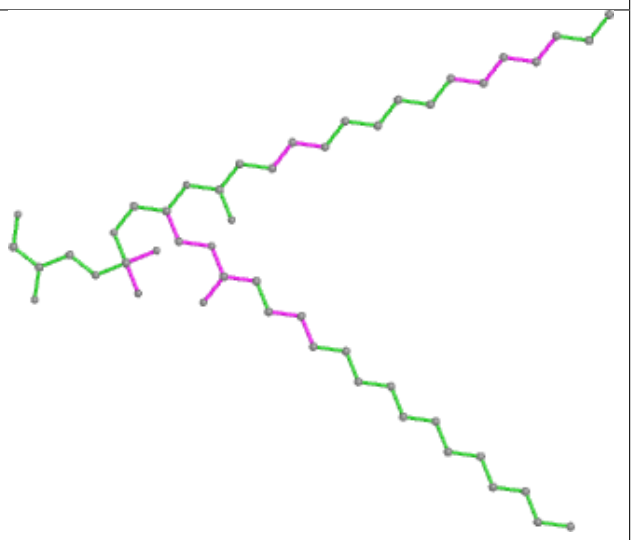

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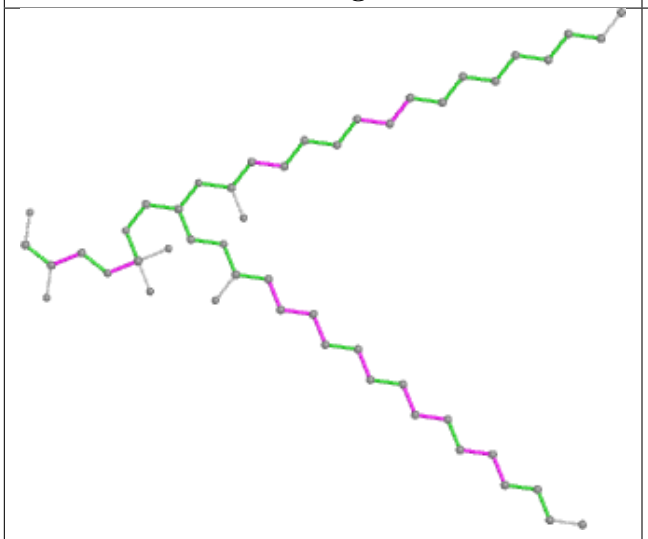

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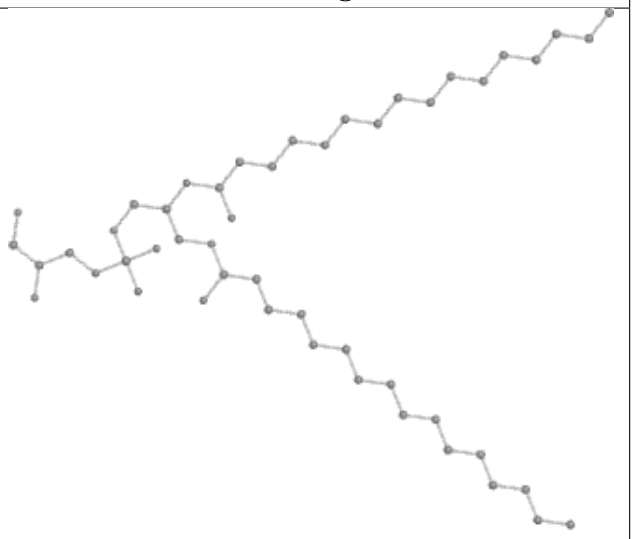
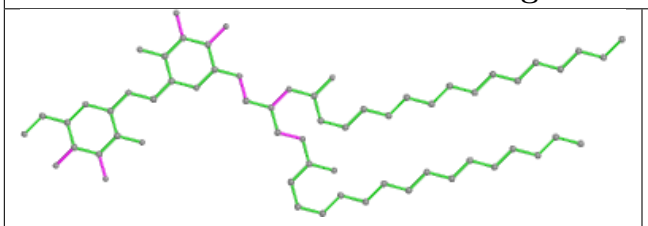


Rings

Ligand DGD C 519



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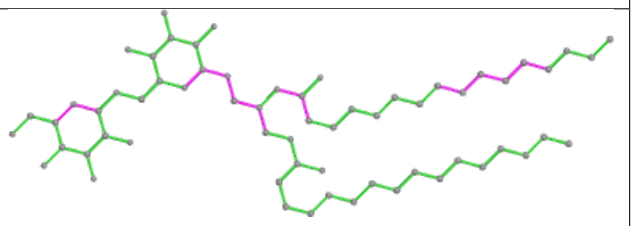

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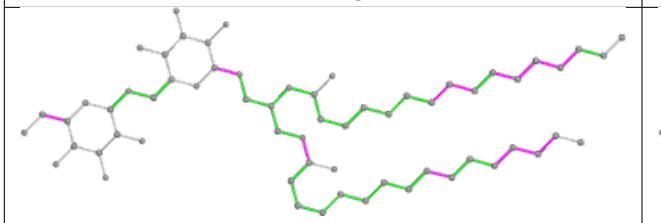

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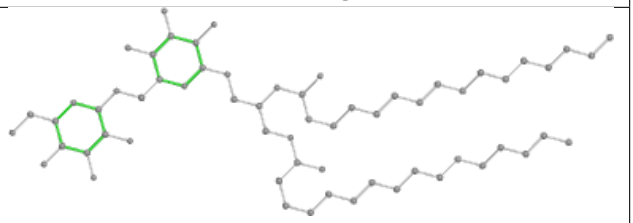
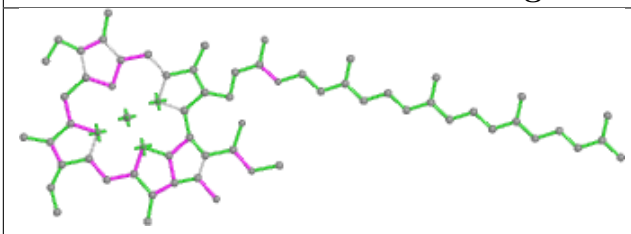


Rings

Ligand CLA C 509



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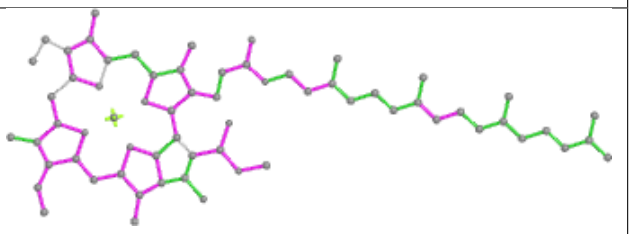

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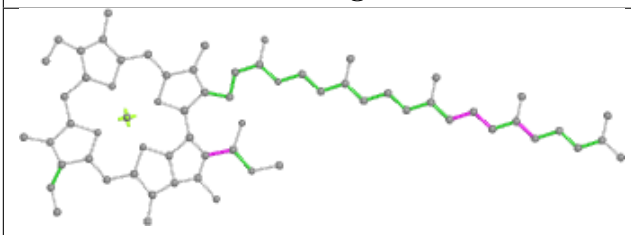

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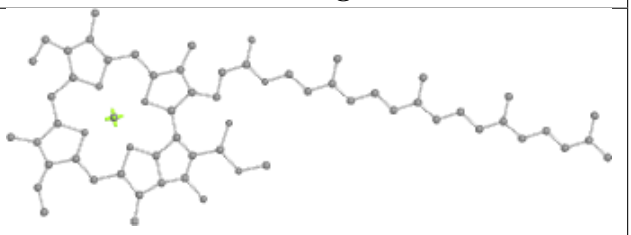
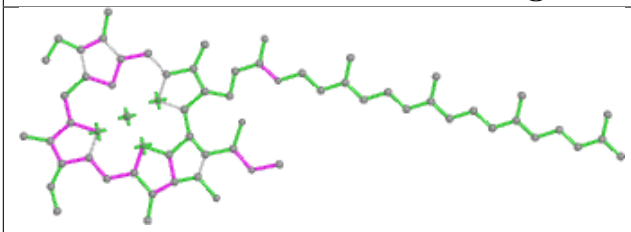


Rings

Ligand CLA d 404



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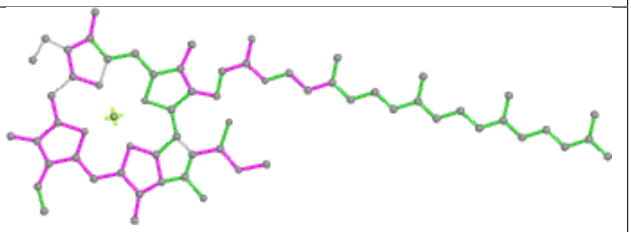

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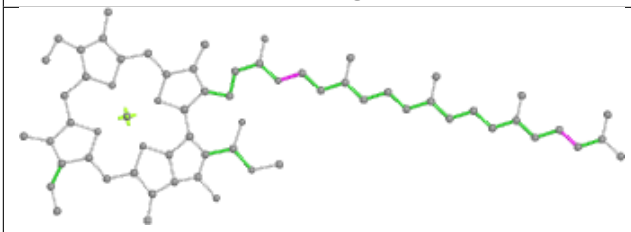

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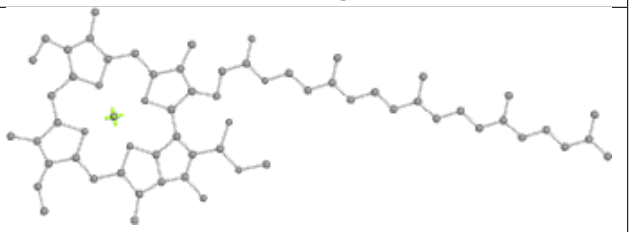
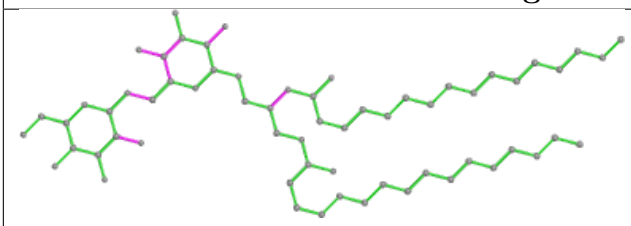


Rings

Ligand DGD h 101



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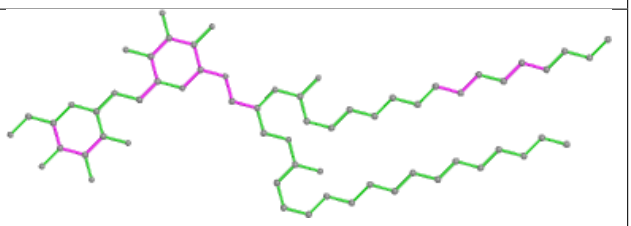

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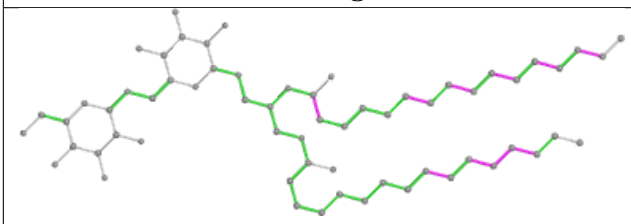

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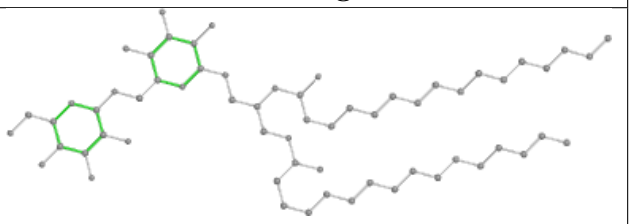
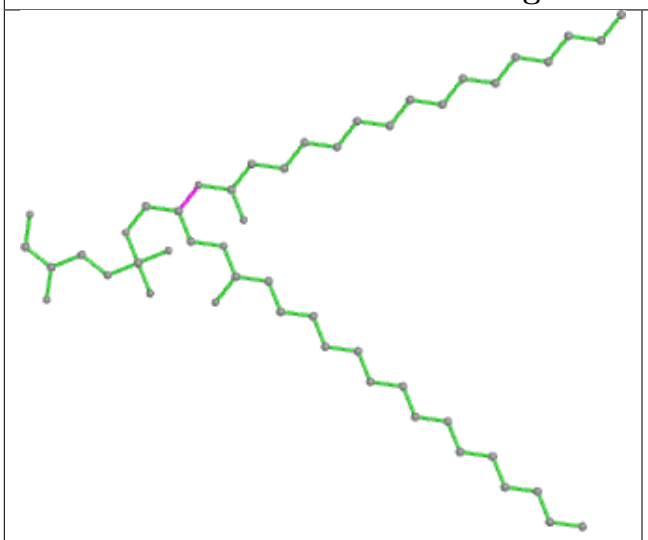


Rings

Ligand LHG D 409



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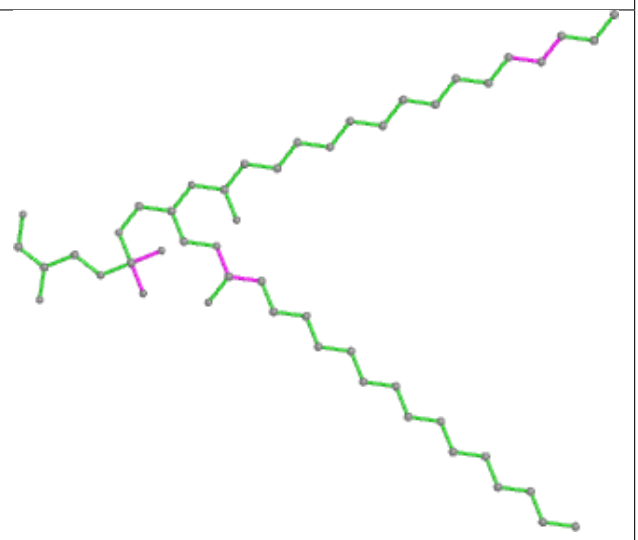

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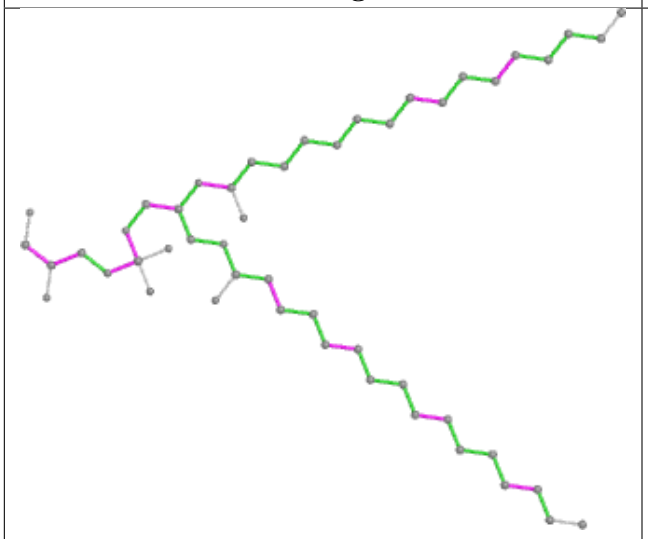

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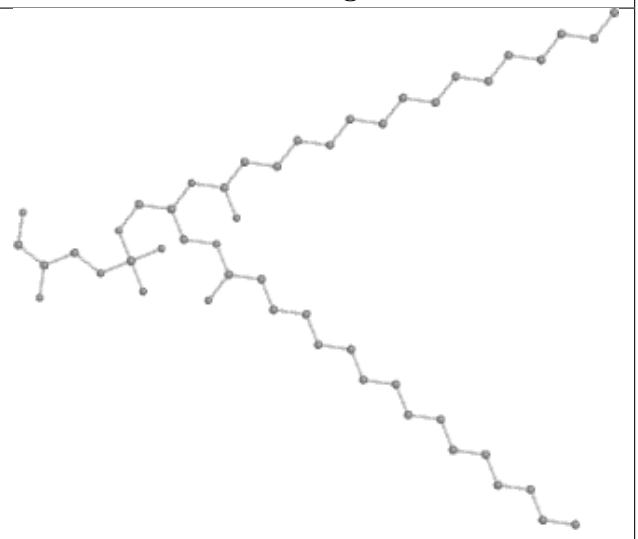
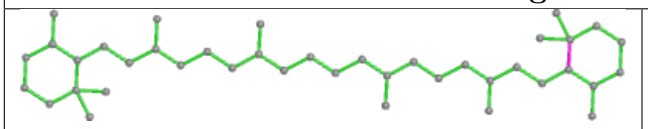


Rings

Ligand BCR t 102



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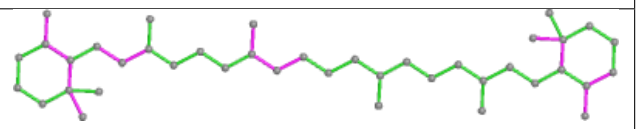

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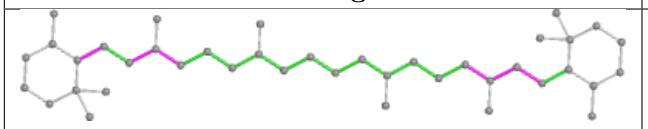

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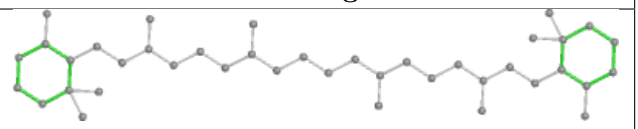

Rings

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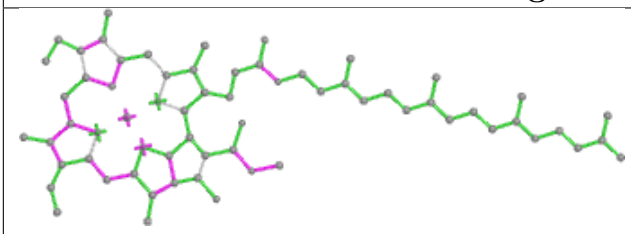

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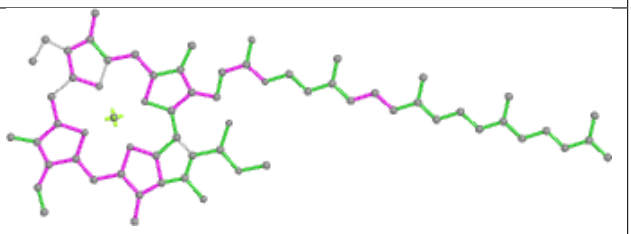

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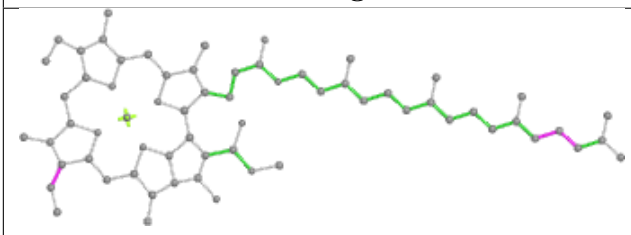

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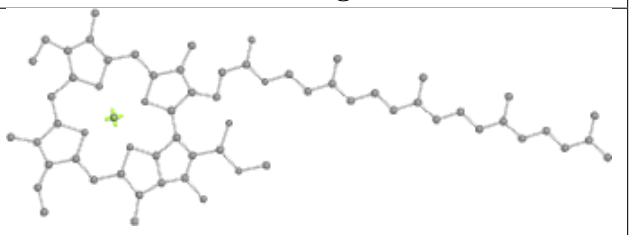

Rings

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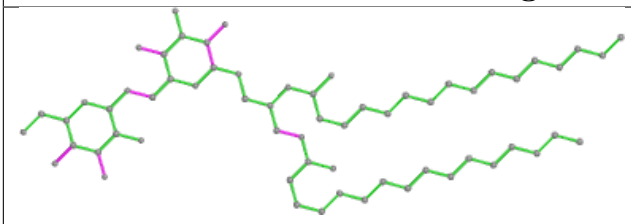

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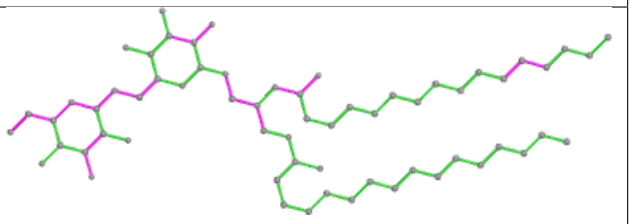

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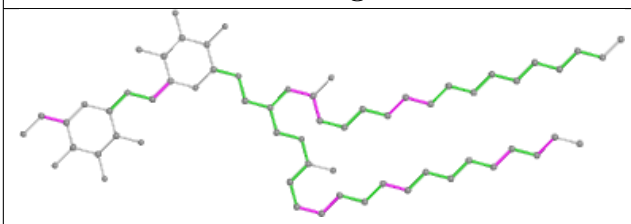

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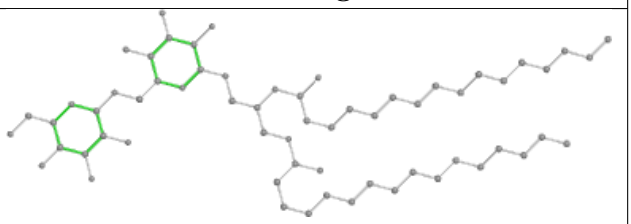
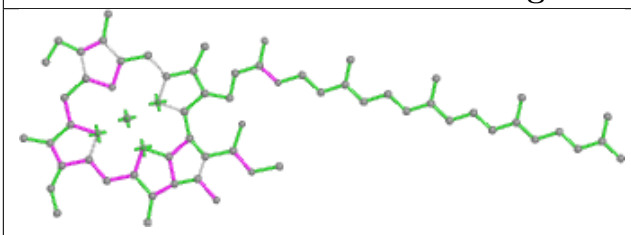


Rings

Ligand CLA d 401



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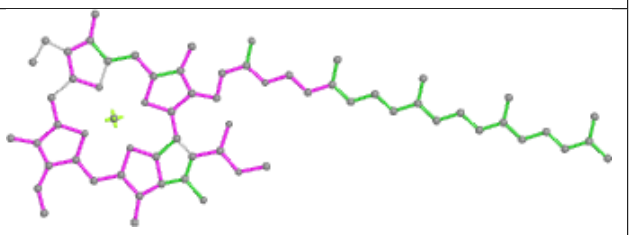

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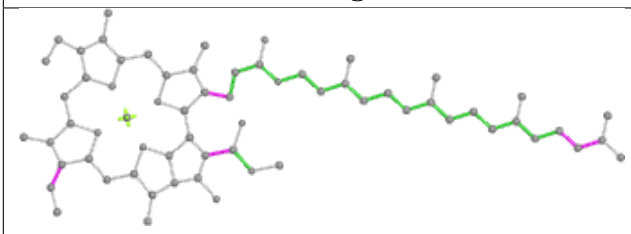

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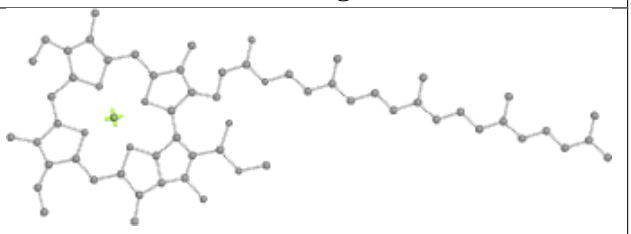

Rings

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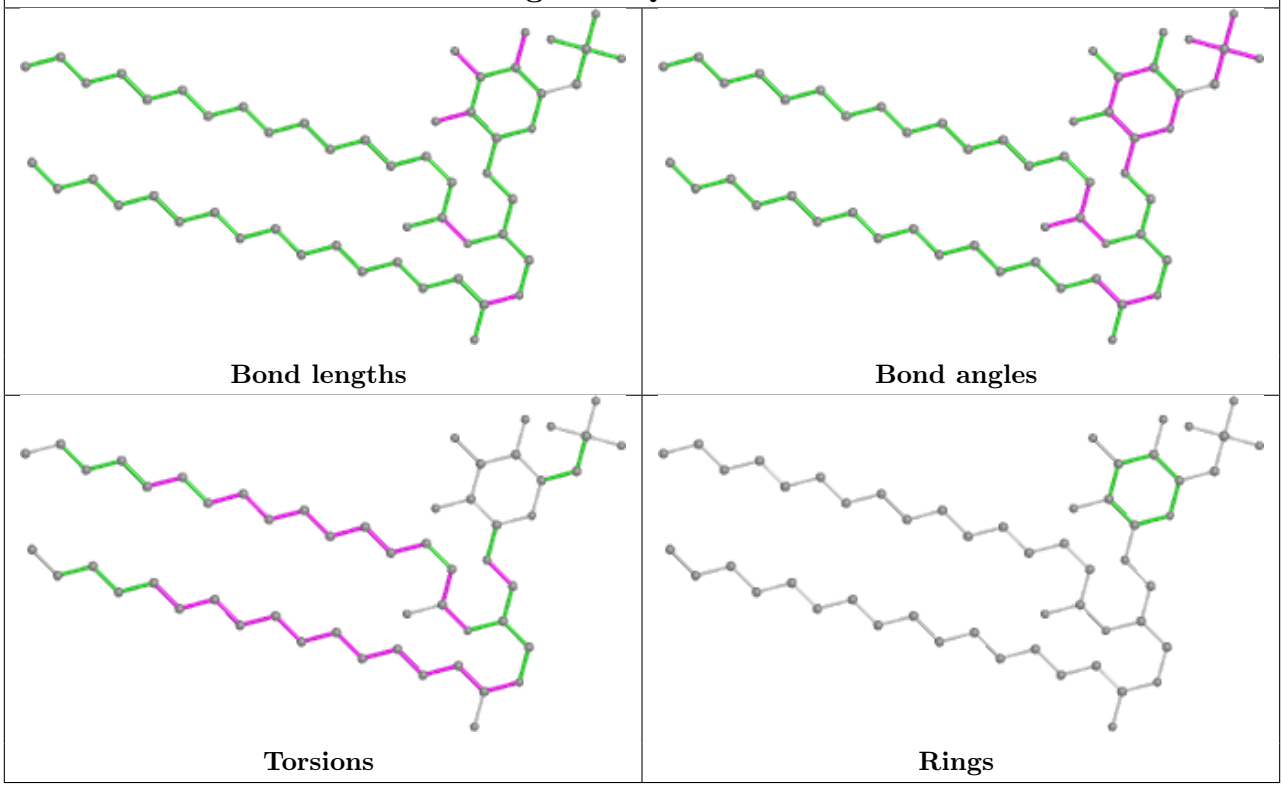

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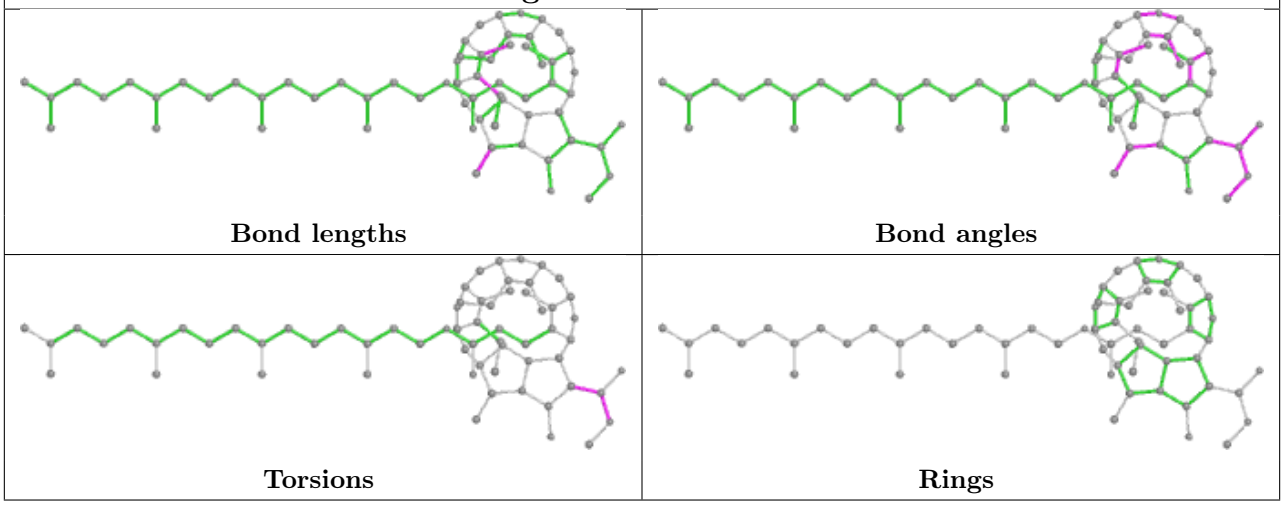

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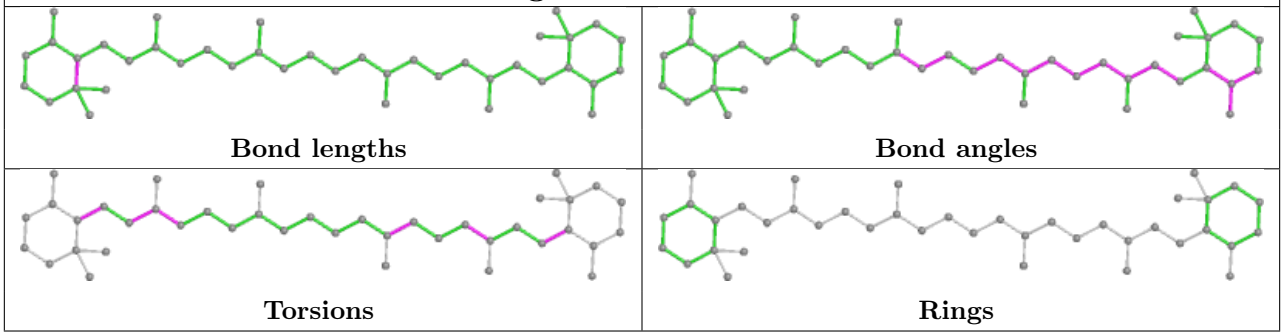
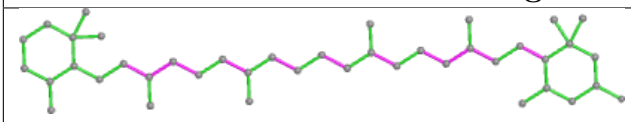
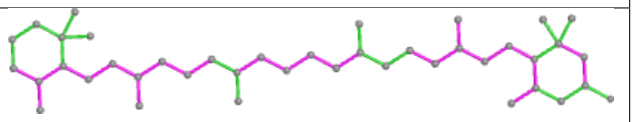


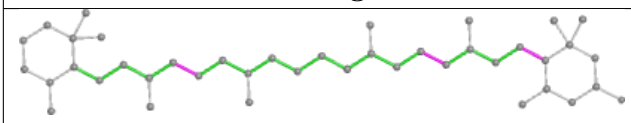
Ligand RRX x 101



Bond lengths



Bond angles



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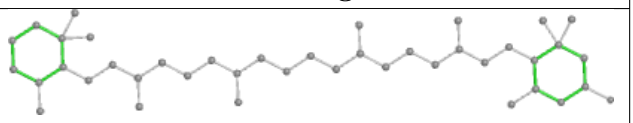
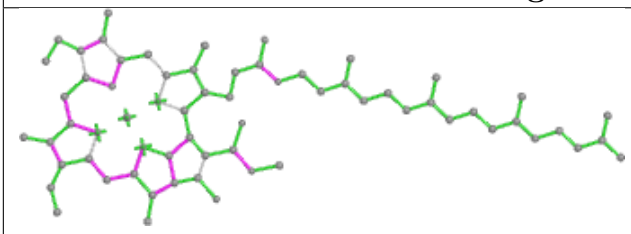
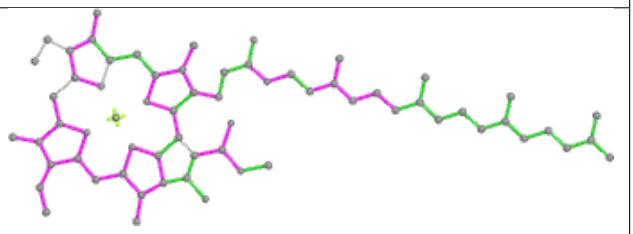


Rings

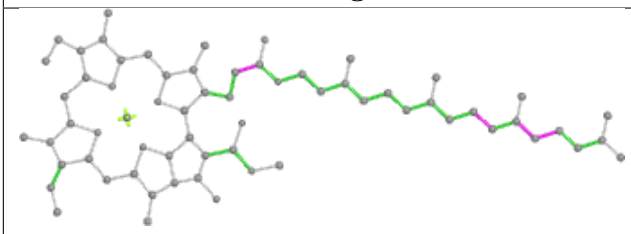
Ligand CLA b 618



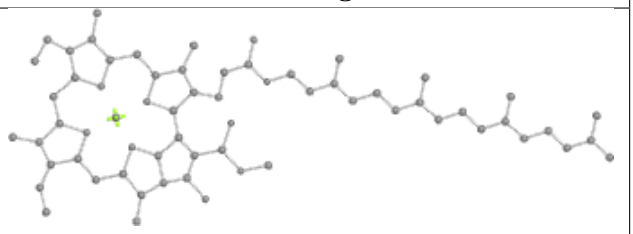
Bond lengths



Bond angles

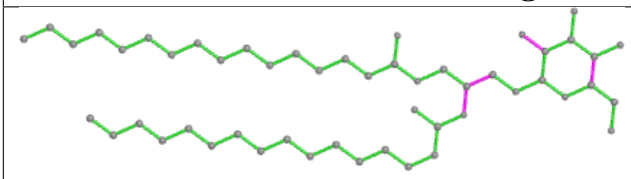


Torsions



Rings

Ligand LMG C 520



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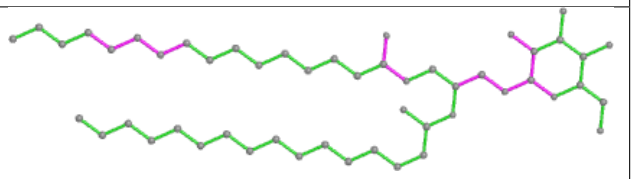
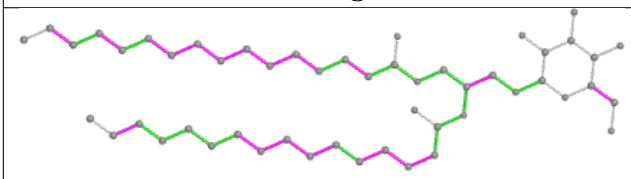


Bond angles



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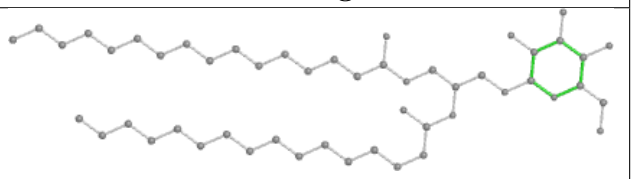
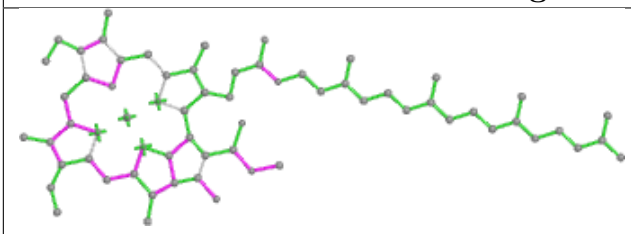


Rings

Ligand CLA c 508



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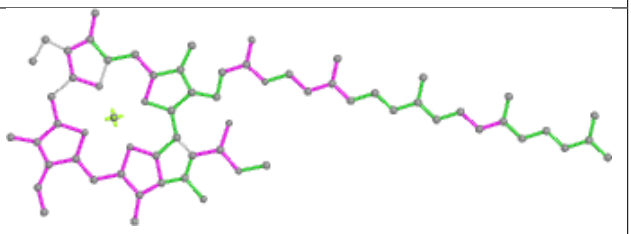
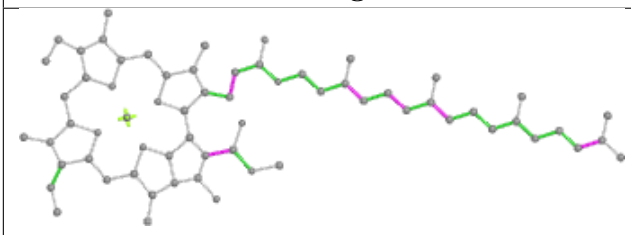
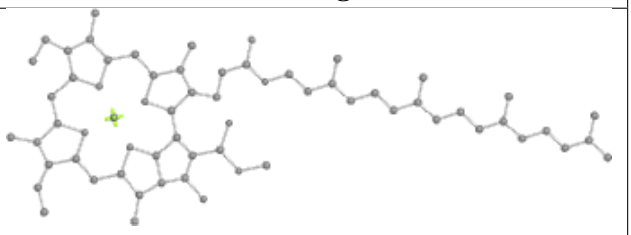


Bond angles

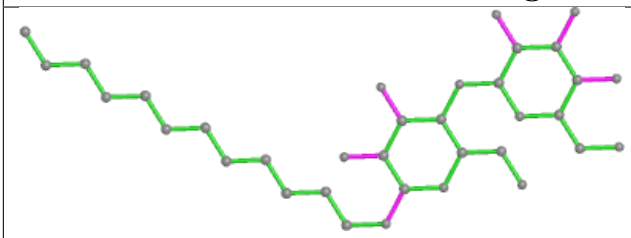


Torsions



Rings

Ligand LMT Z 101



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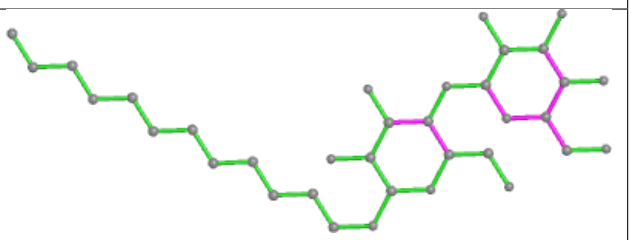
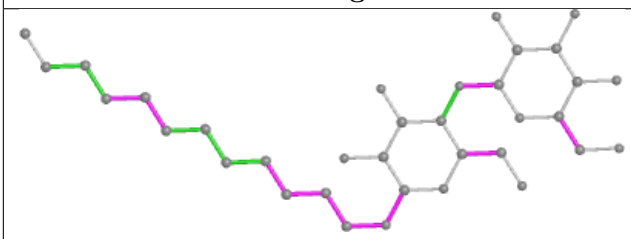


Bond angles



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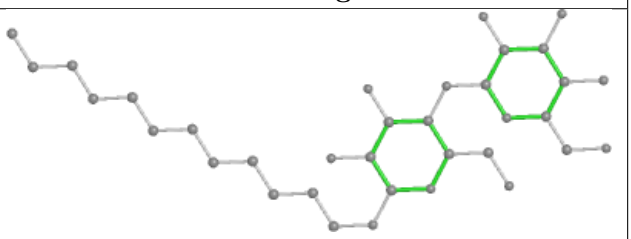
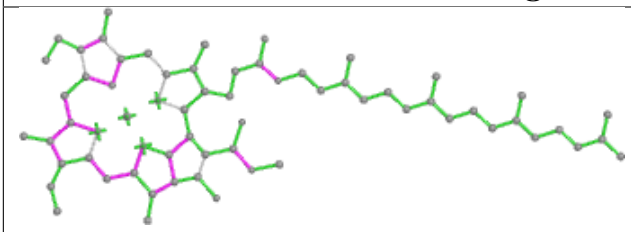


Rings

Ligand CLA B 614



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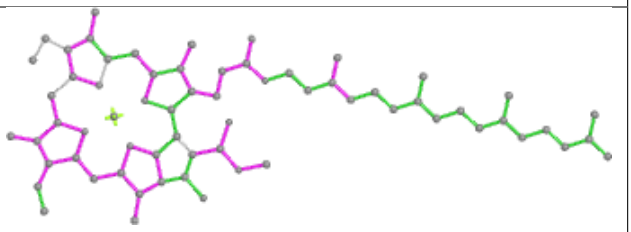
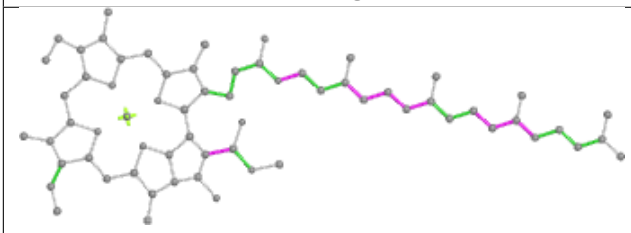


Bond angles



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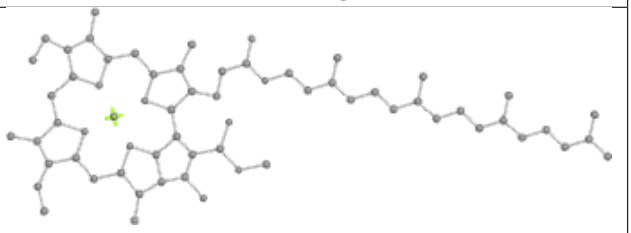
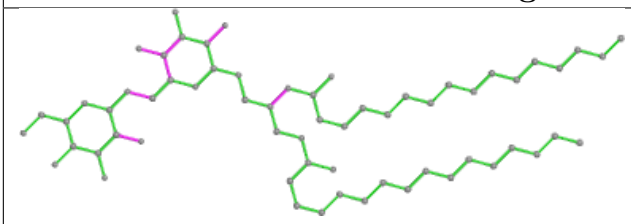


Rings

Ligand DGD H 101



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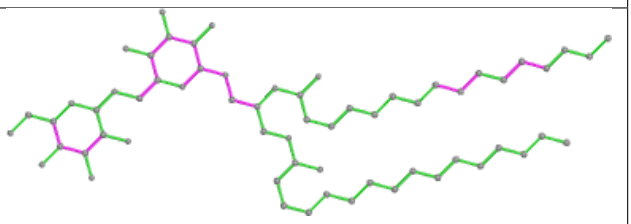
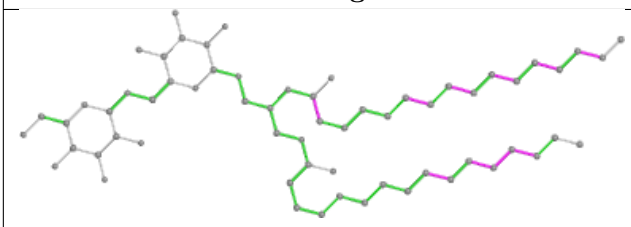


Bond angles



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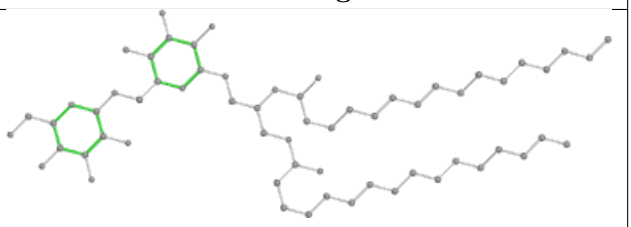
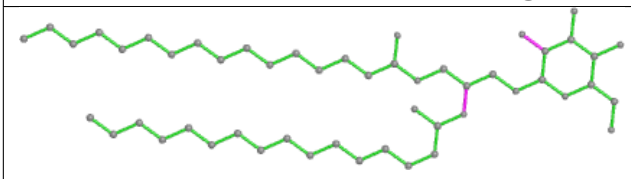


Rings

Ligand LMG C 523



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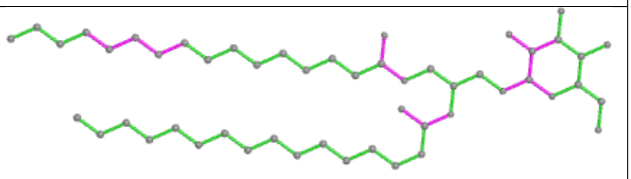
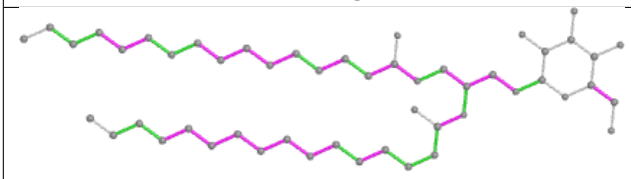


Bond angles



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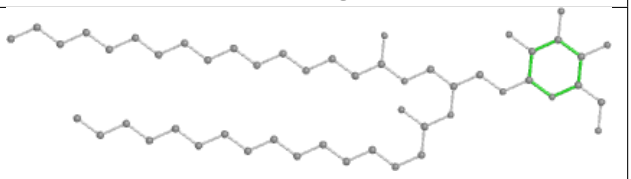
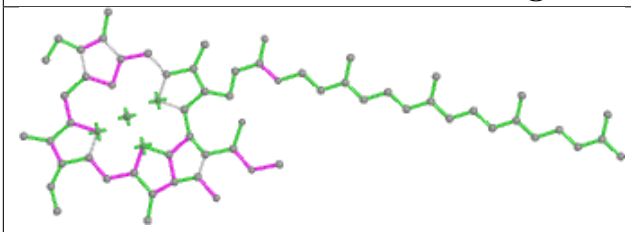


Rings

Ligand CLA b 612



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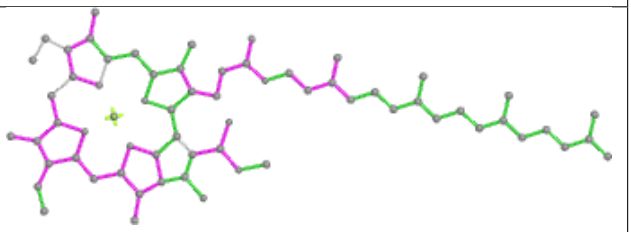
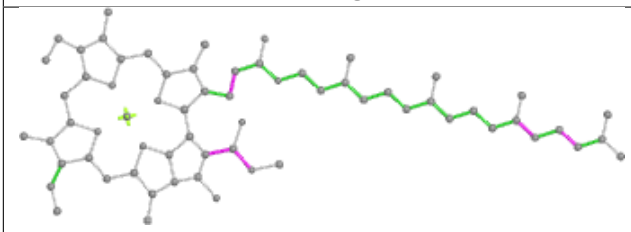


Bond angles



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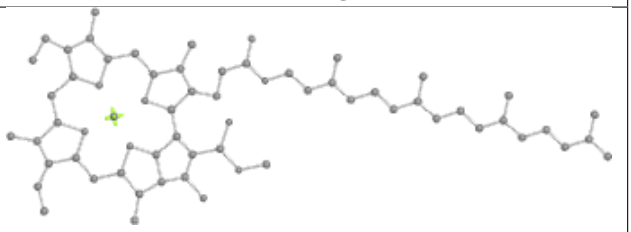
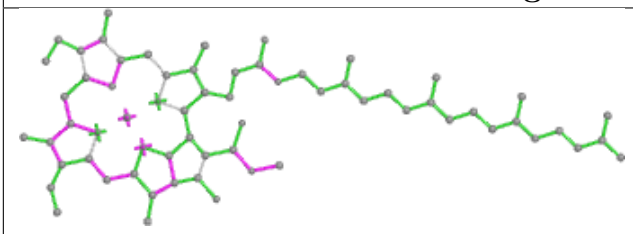
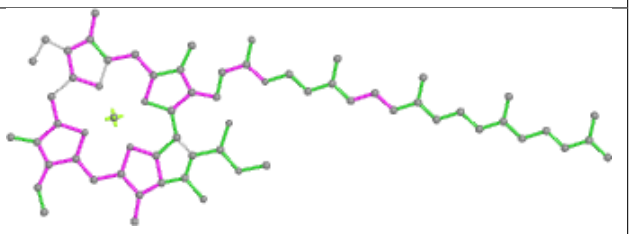


Rings

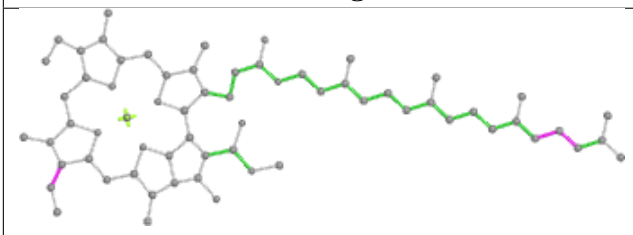
Ligand CLA A 405



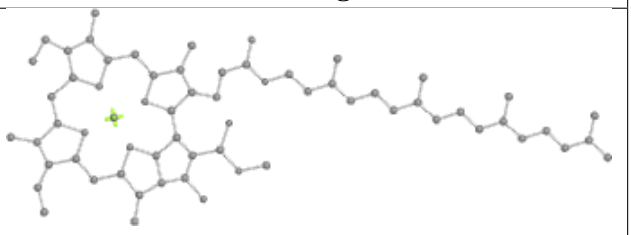
Bond lengths



Bond angles

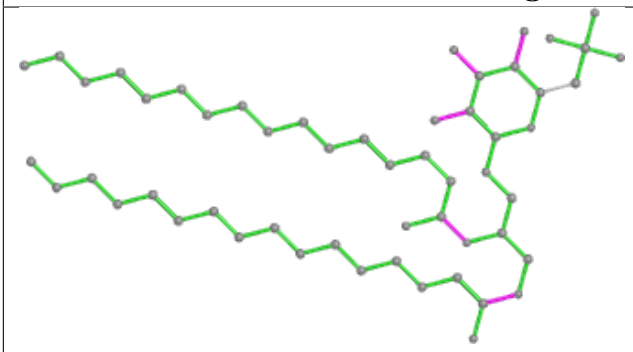


Torsions



Rings

Ligand SQD A 412



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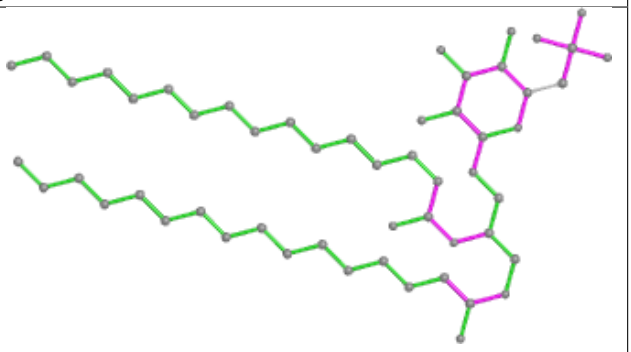
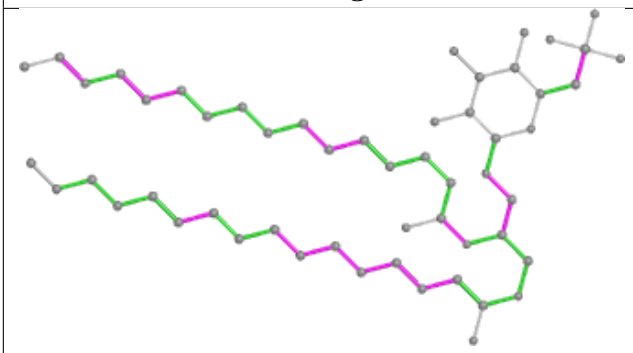


Bond angles



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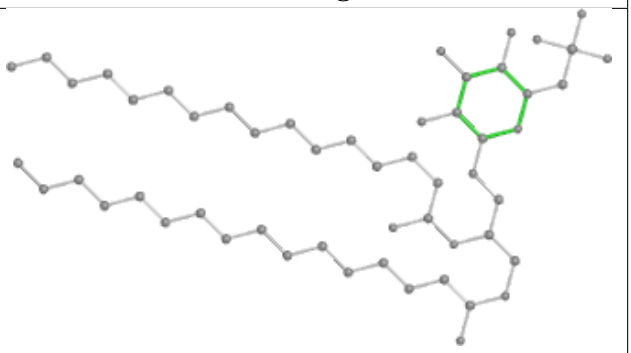
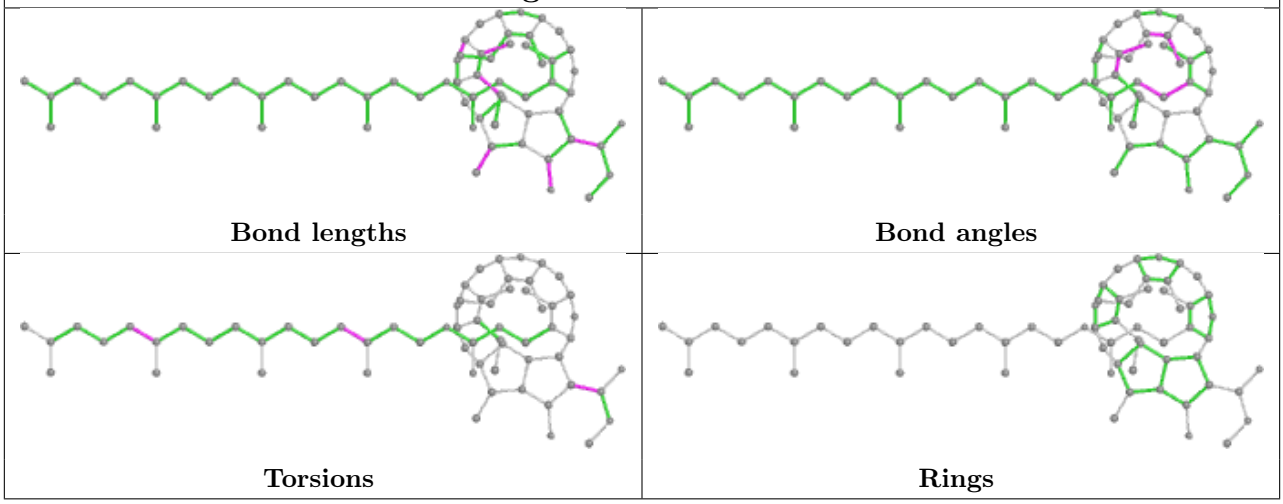
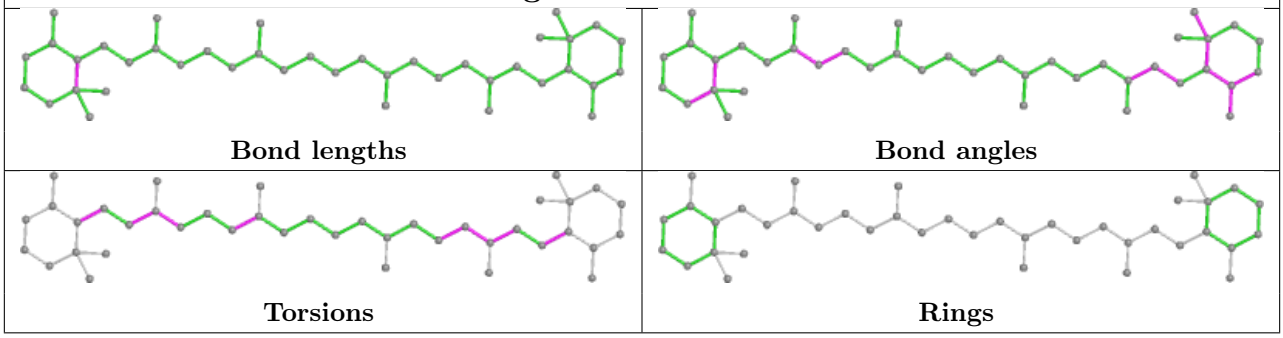


Rings

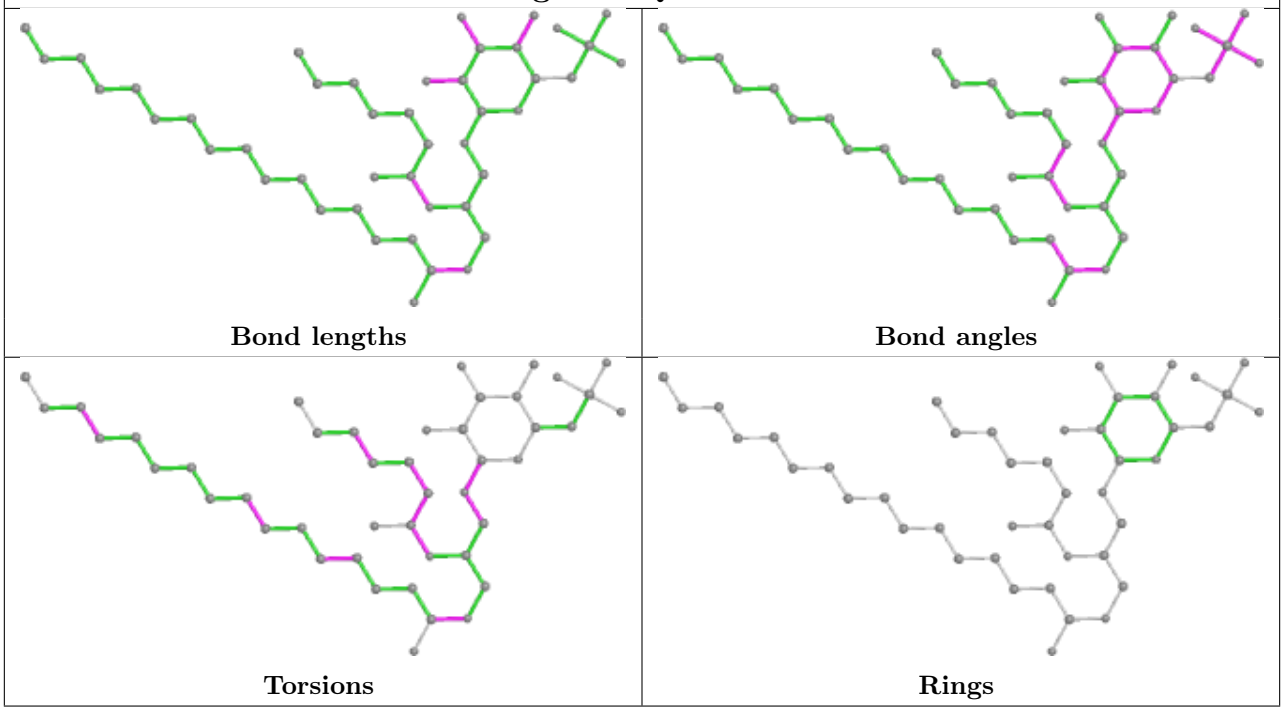
Ligand PHO A 407



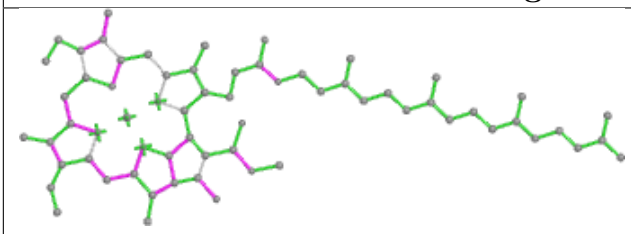
Ligand BCR C 522



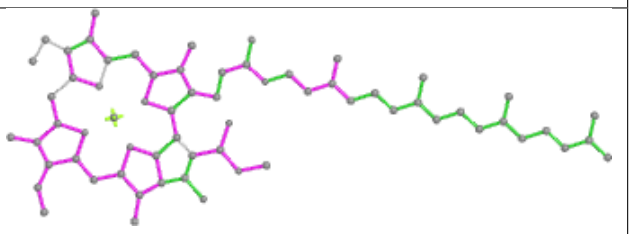
Ligand SQD f 101



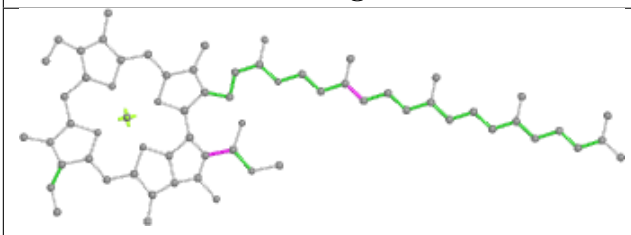
Ligand CLA B 609



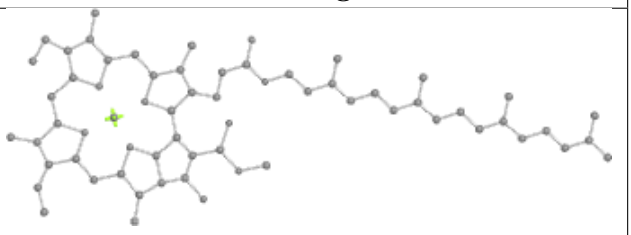
Bond lengths



Bond angles

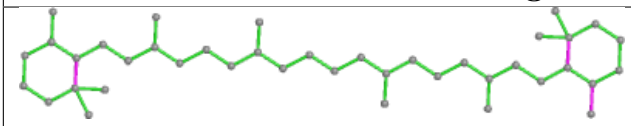


Torsions



Rings

Ligand BCR b 620



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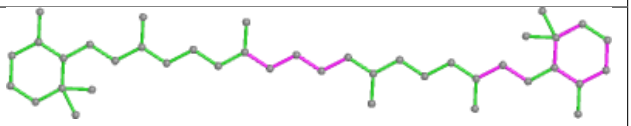
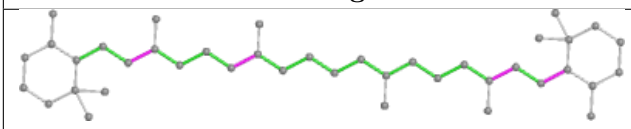


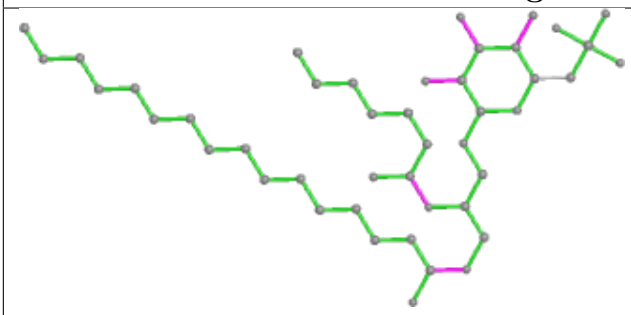
Bond angles



Torsions

Rings

Ligand SQD F 101



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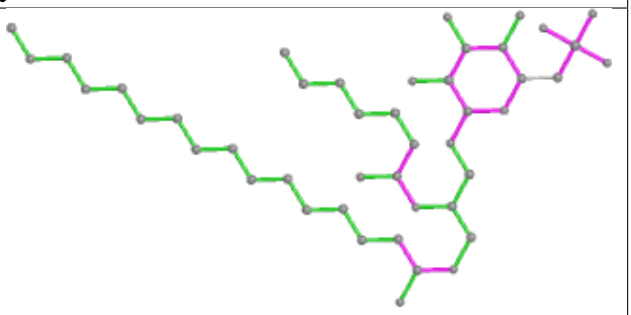
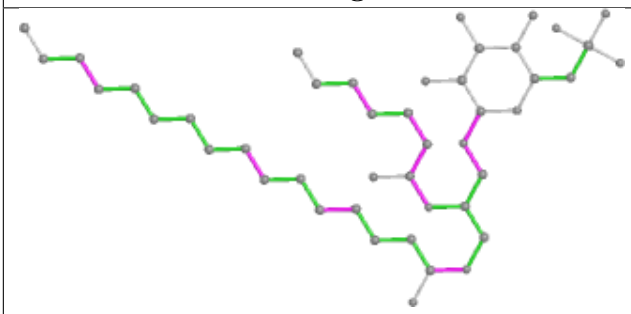
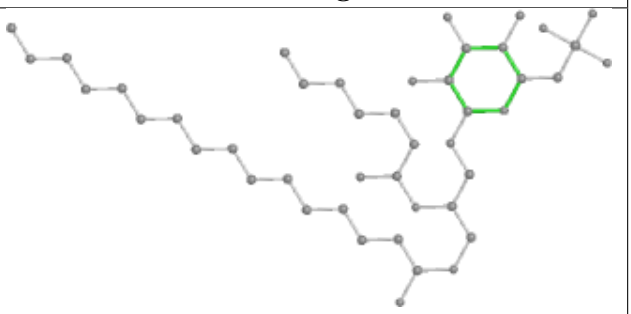


Bond angles

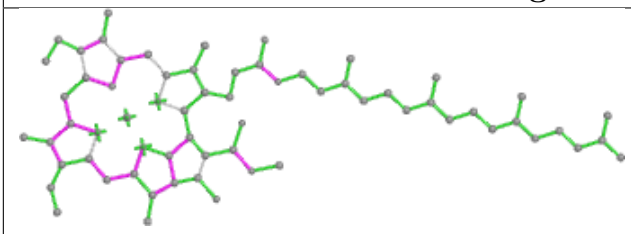


Torsions

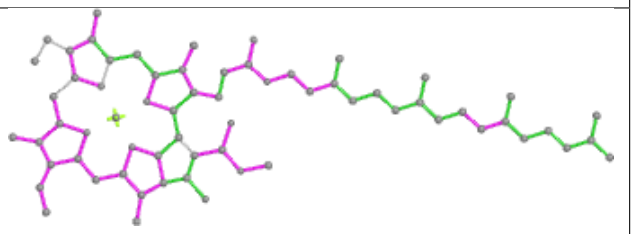


Rings

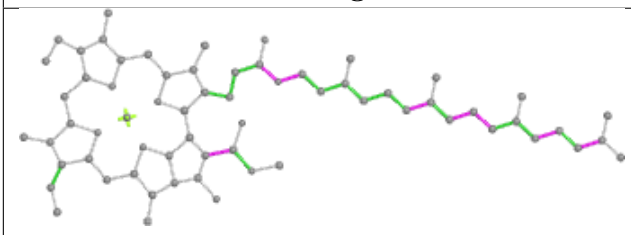
Ligand CLA c 510



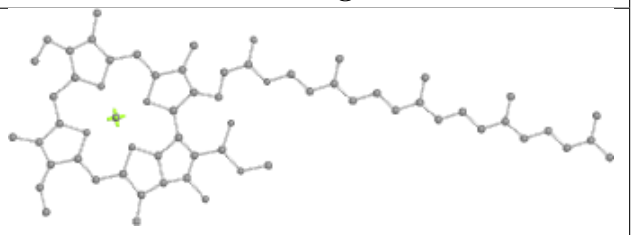
Bond lengths



Bond angles

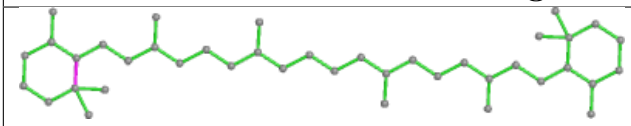


Torsions



Rings

Ligand BCR c 516



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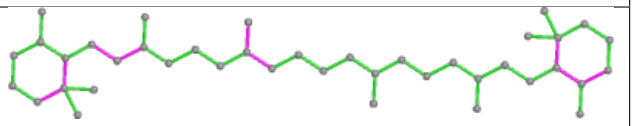

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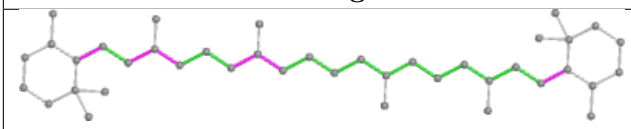
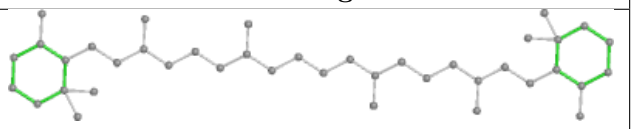
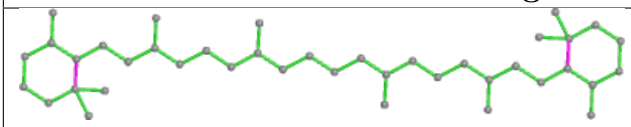


Torsions



Rings

Ligand BCR B 619



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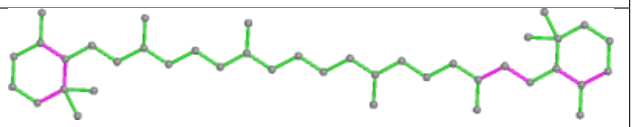
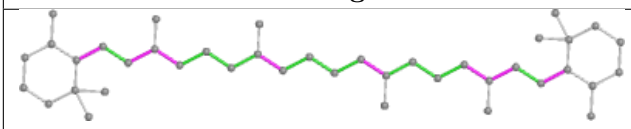


Bond angles



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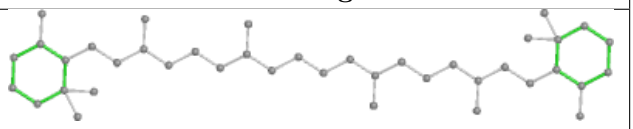
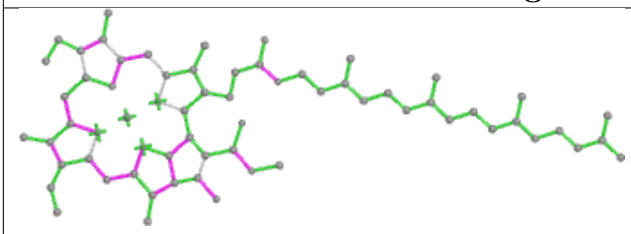


Rings

Ligand CLA B 615



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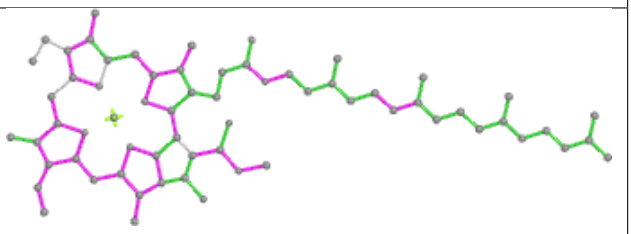

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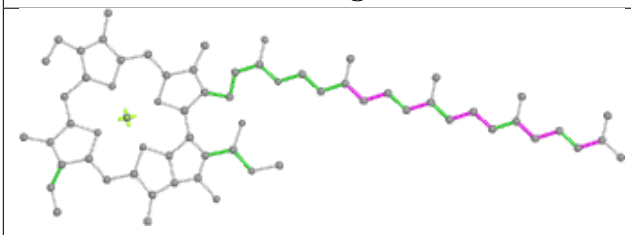

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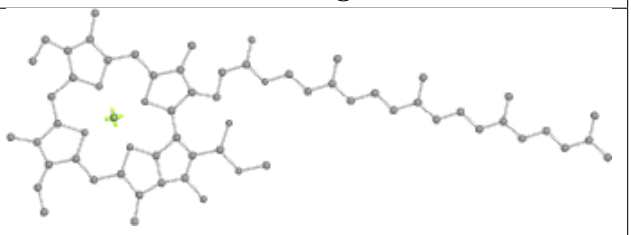
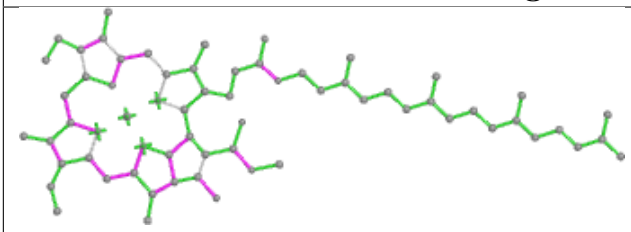


Rings

Ligand CLA C 512



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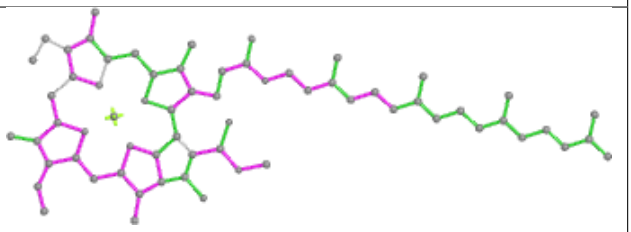

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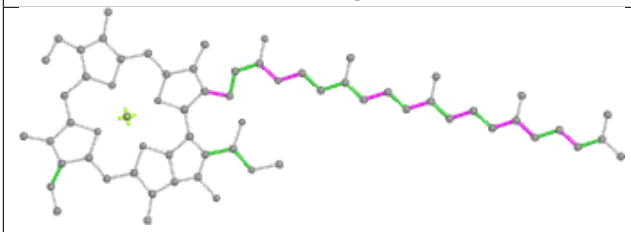

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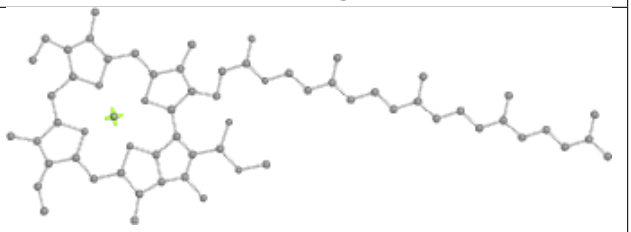
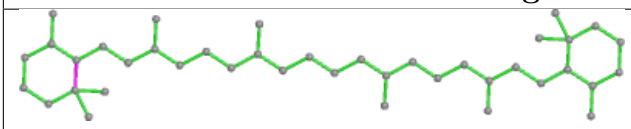


Rings

Ligand BCR C 516



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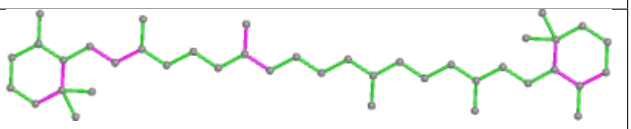
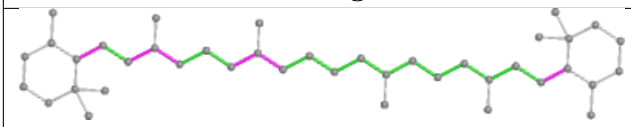


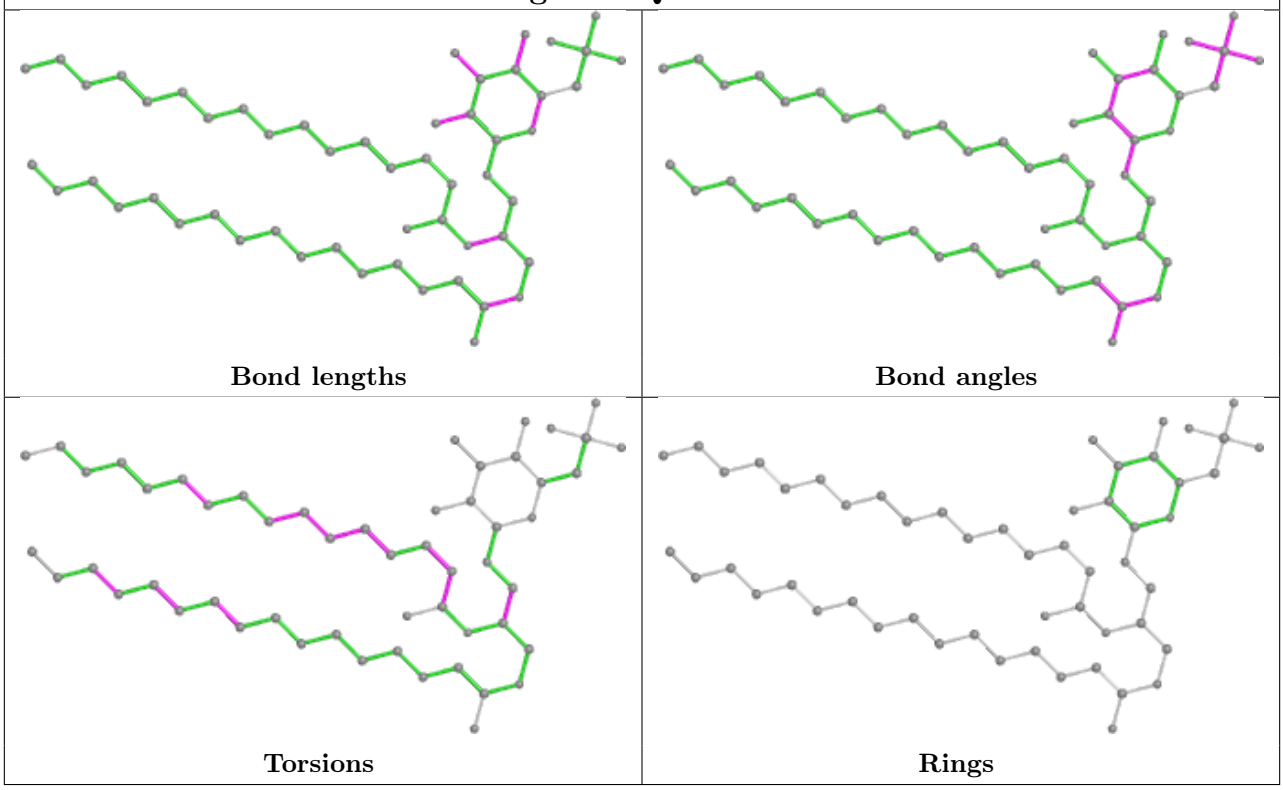
Bond angles



Torsions

Rings

Ligand SQD a 410



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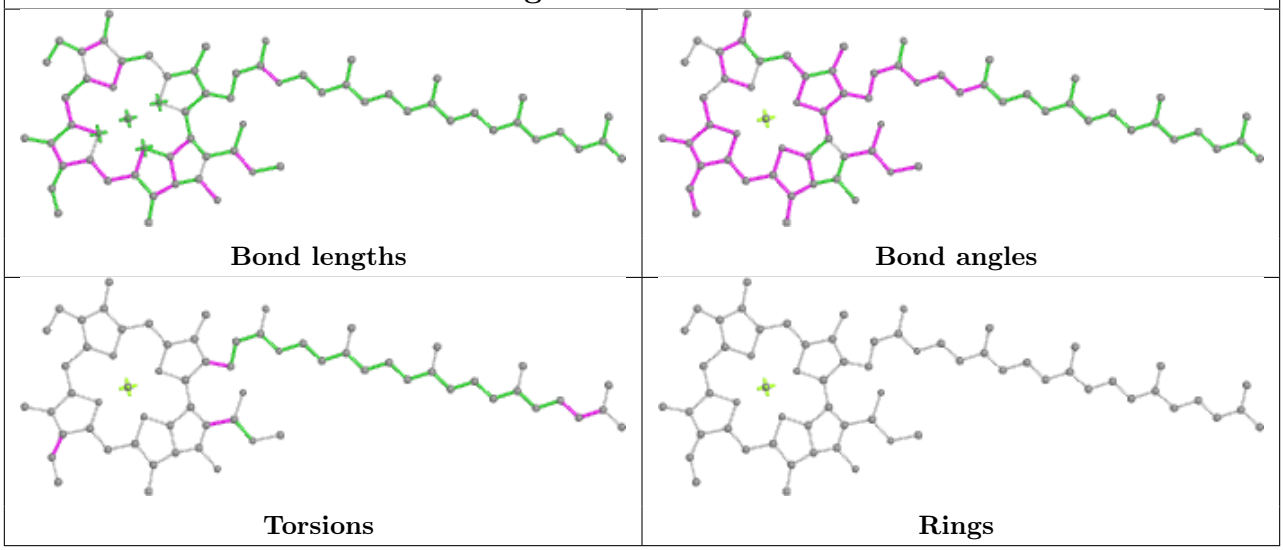

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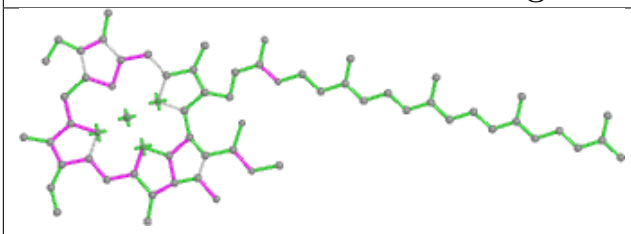

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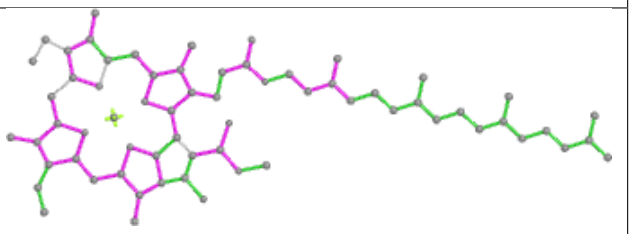
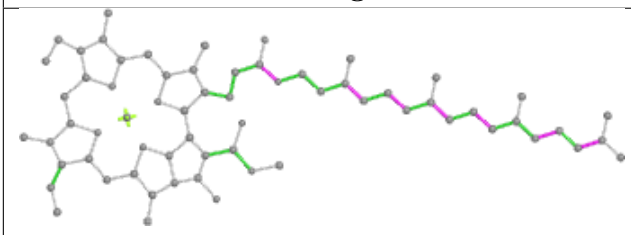


Bond angles



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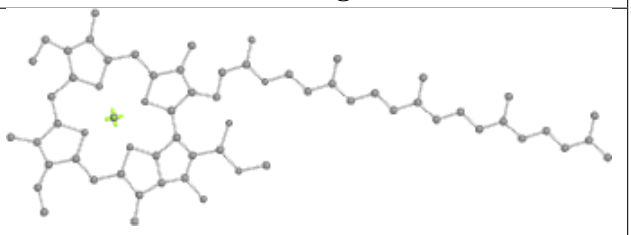
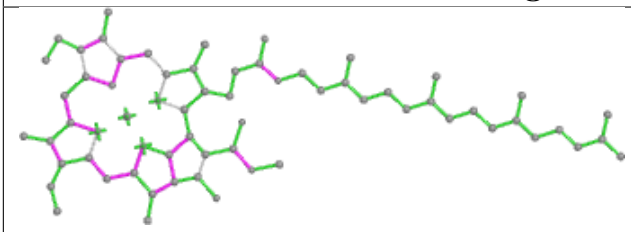


Rings

Ligand CLA C 505



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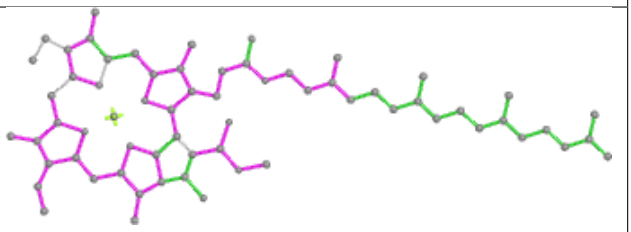
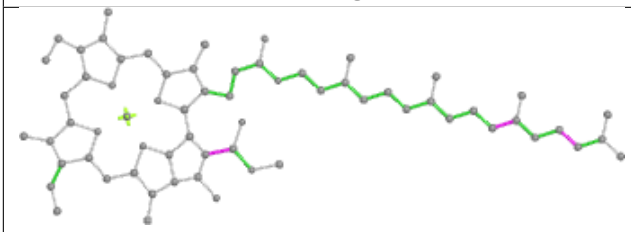


Bond angles



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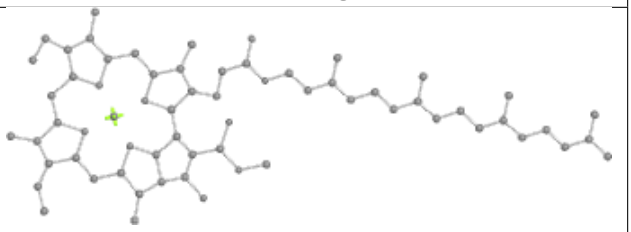

Rings

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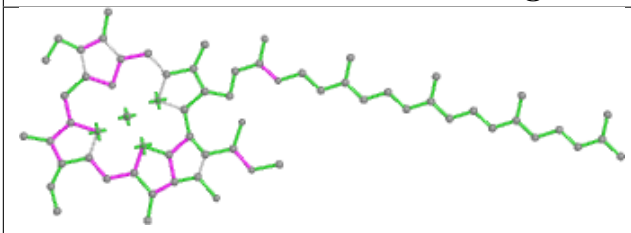

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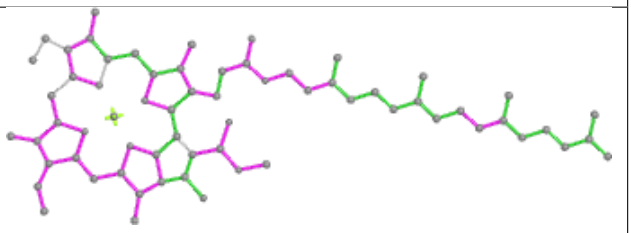

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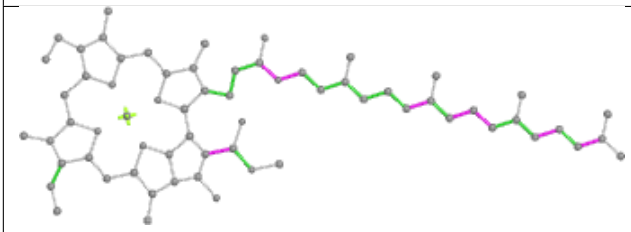

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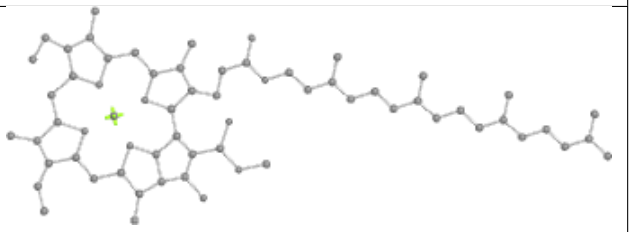

Rings

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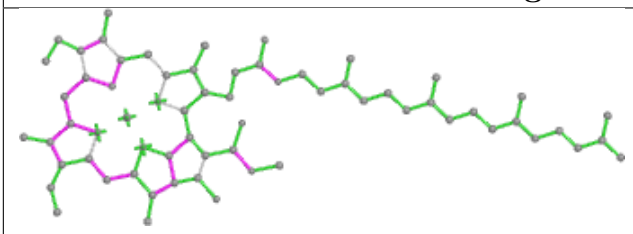

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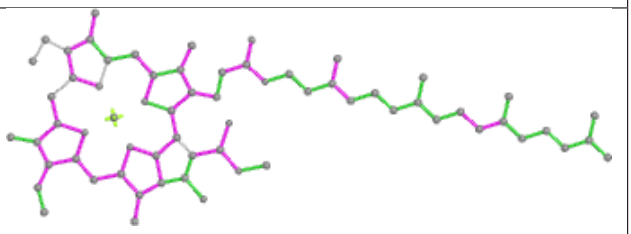

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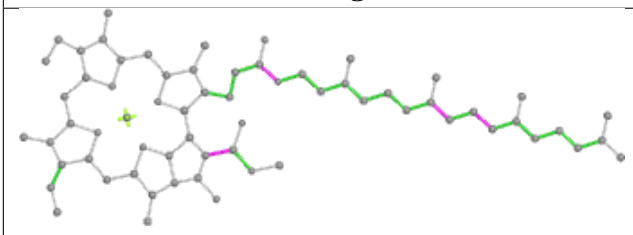

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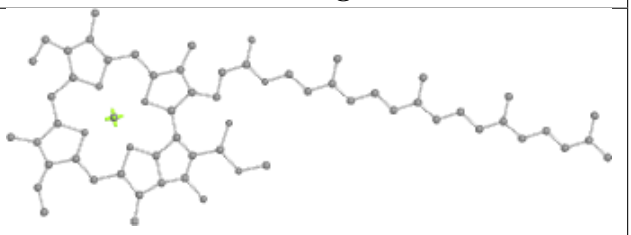
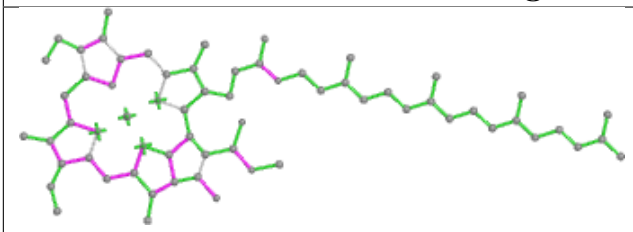


Rings

Ligand CLA C 511



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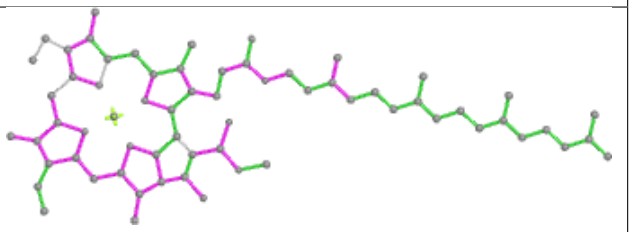
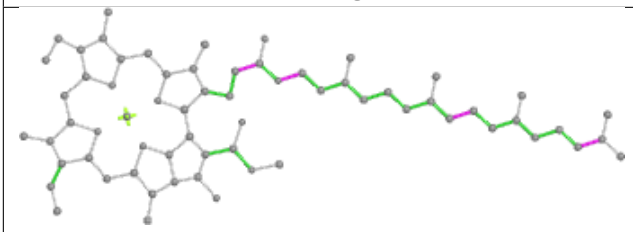


Bond angles



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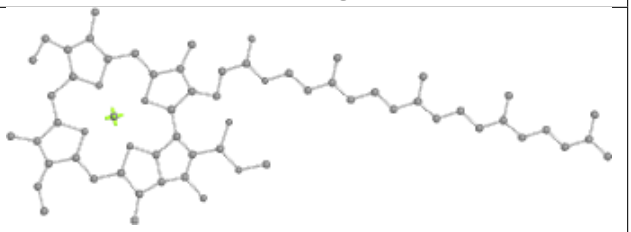
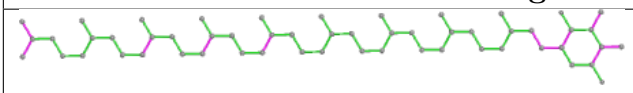


Rings

Ligand PL9 D 407



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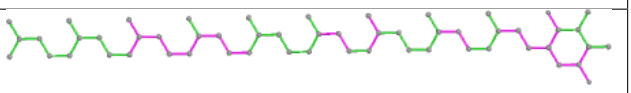
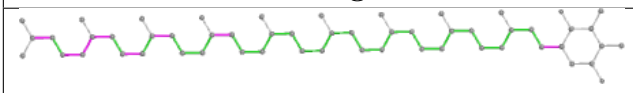


Bond angles



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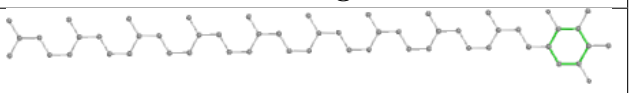
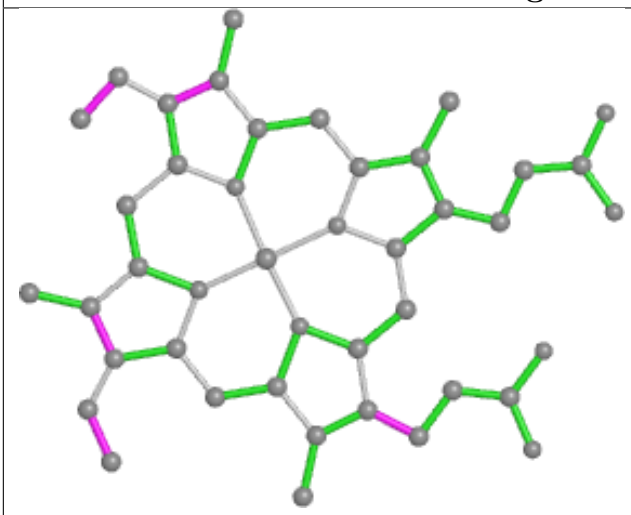


Rings

Ligand HEC v 201



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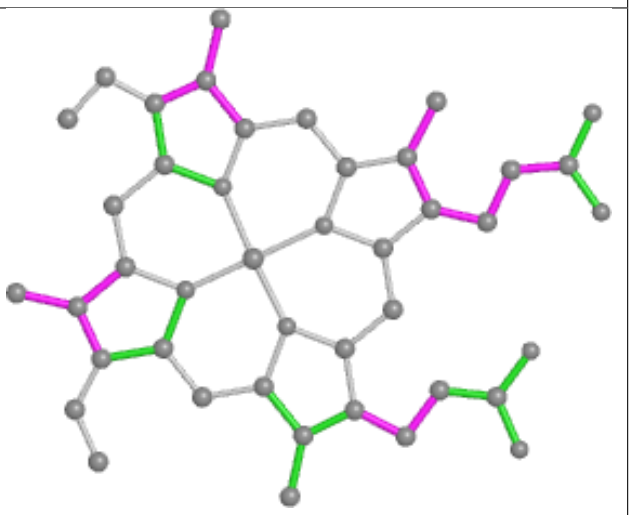
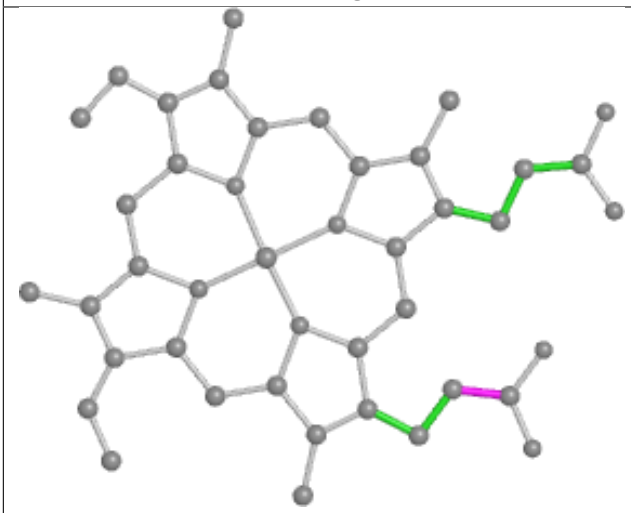
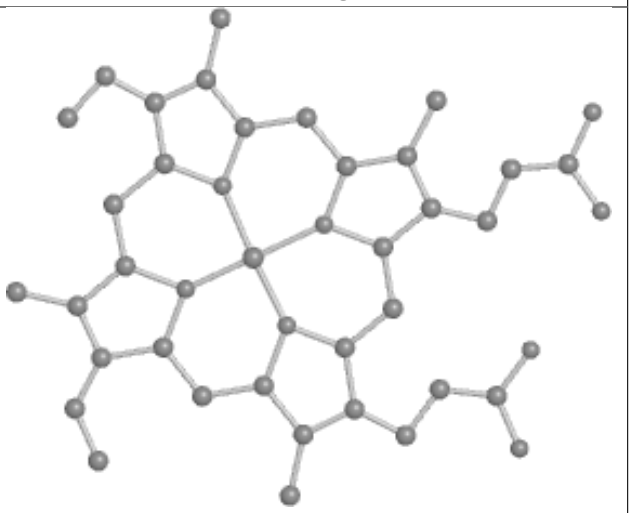


Bond angles

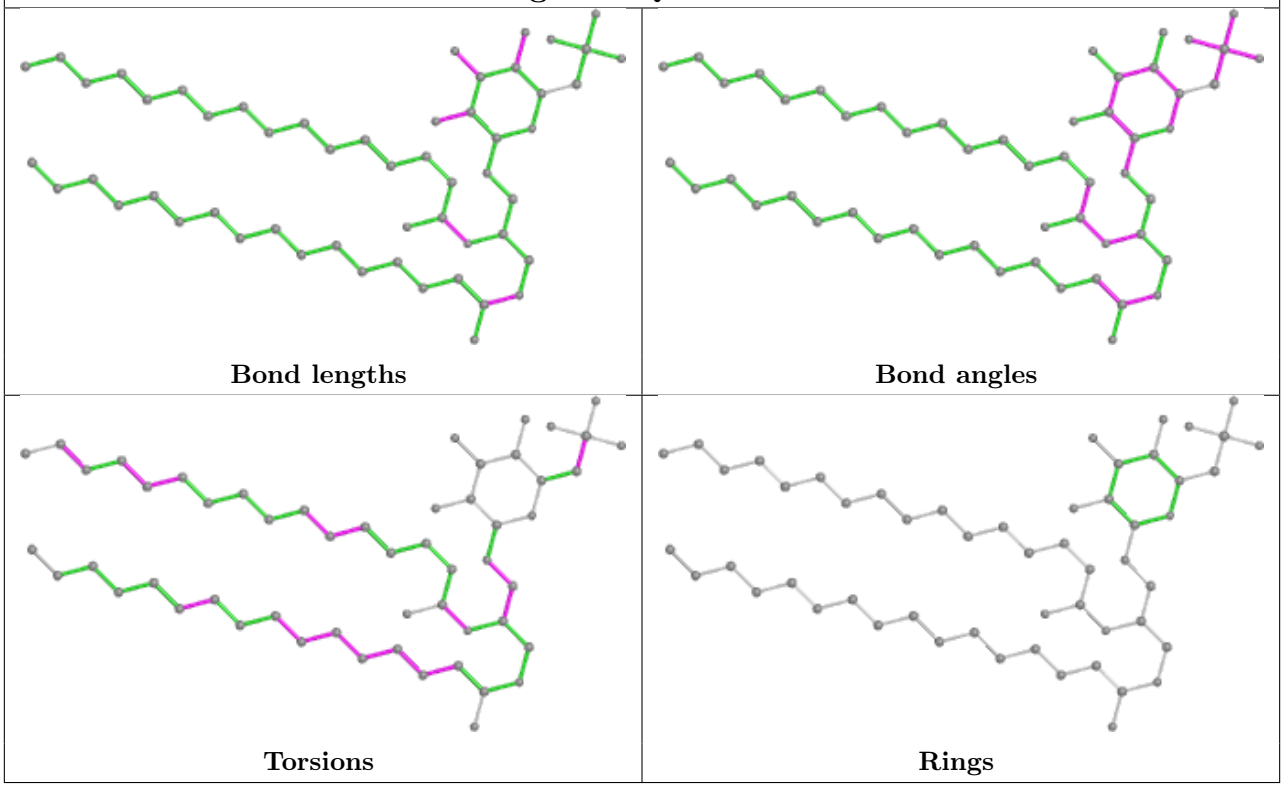


Torsions

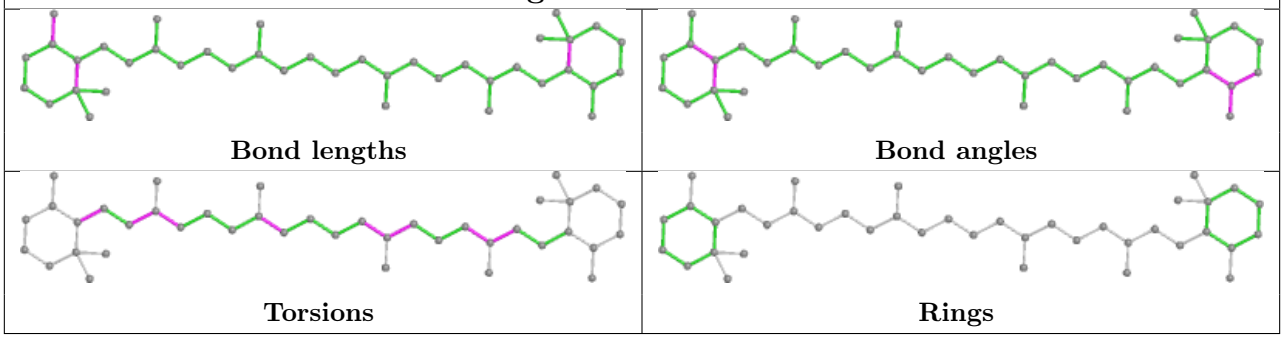


Rings

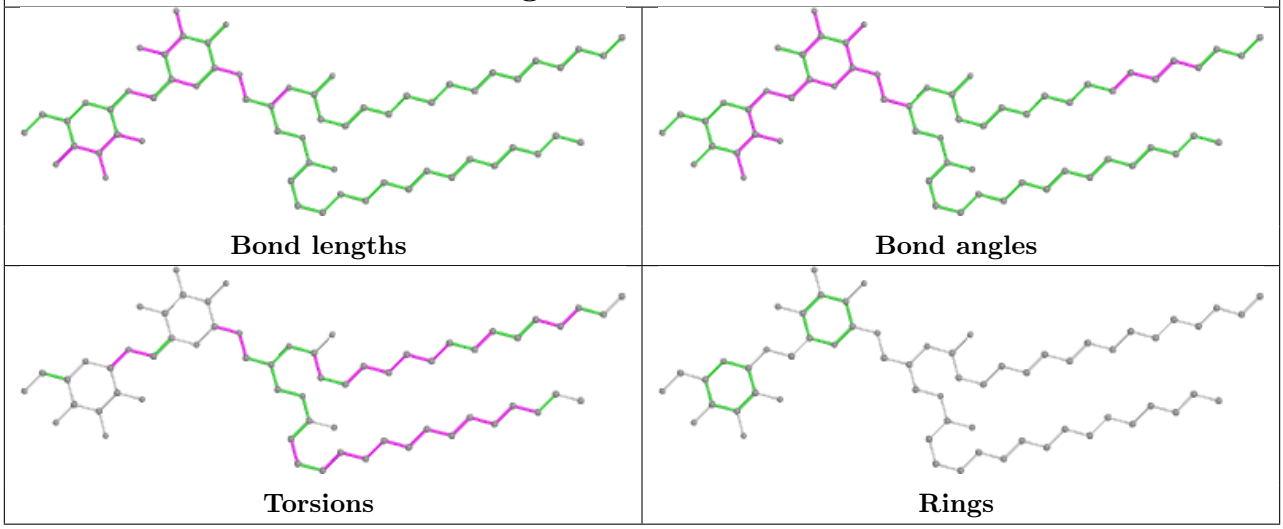
Ligand SQD a 412



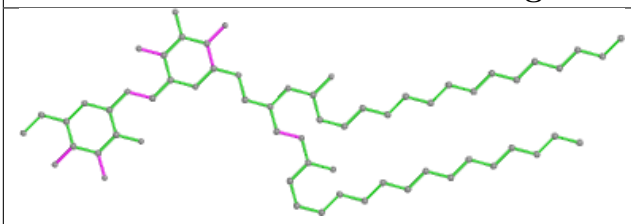
Ligand BCR J 104



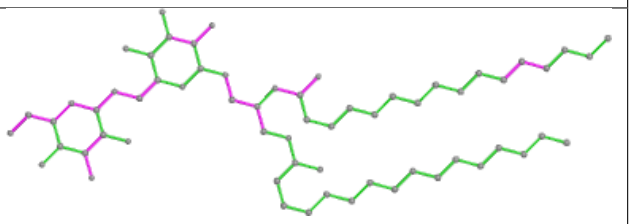
Ligand DGD C 518



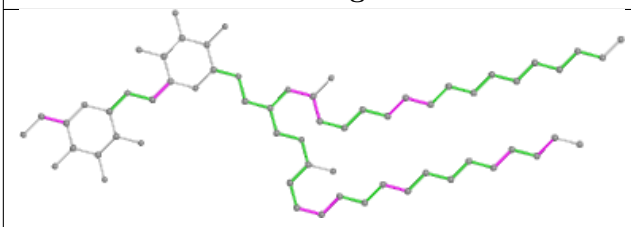
Ligand DGD c 517



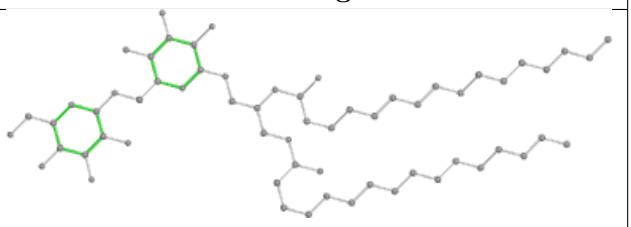
Bond lengths



Bond angles

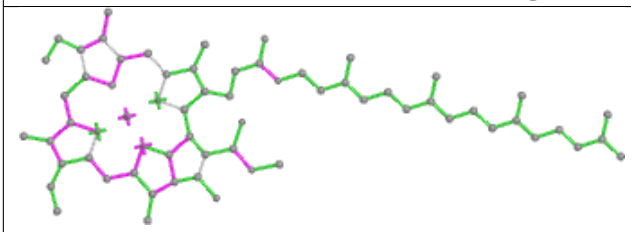


Torsions



Rings

Ligand CLA B 613



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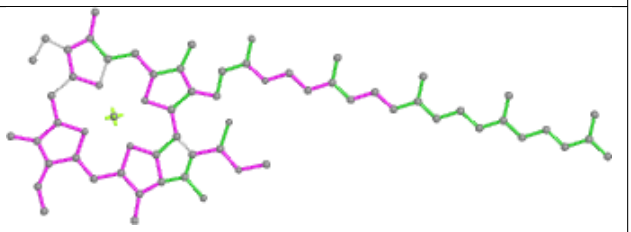
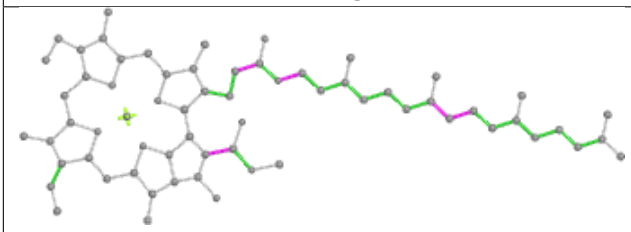
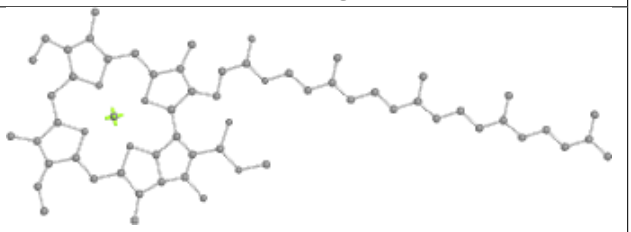


Bond angles

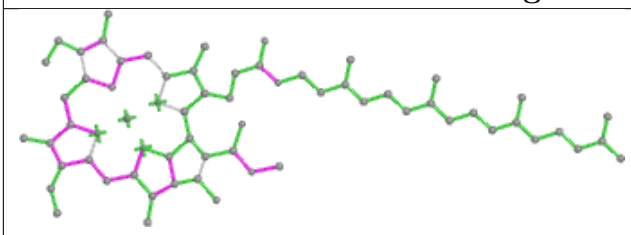


Torsions

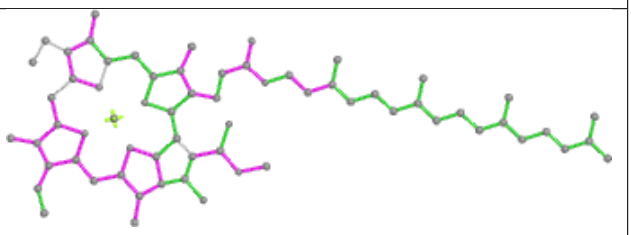


Rings

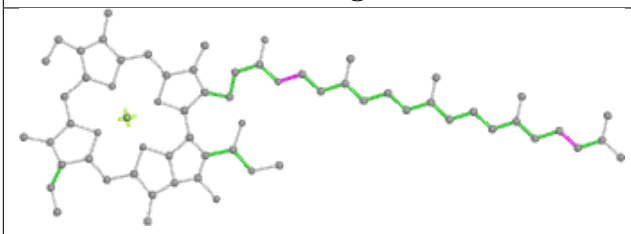
Ligand CLA D 404



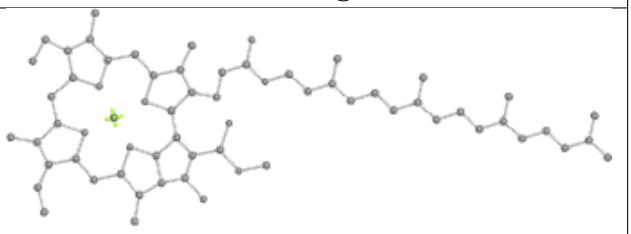
Bond lengths



Bond angles

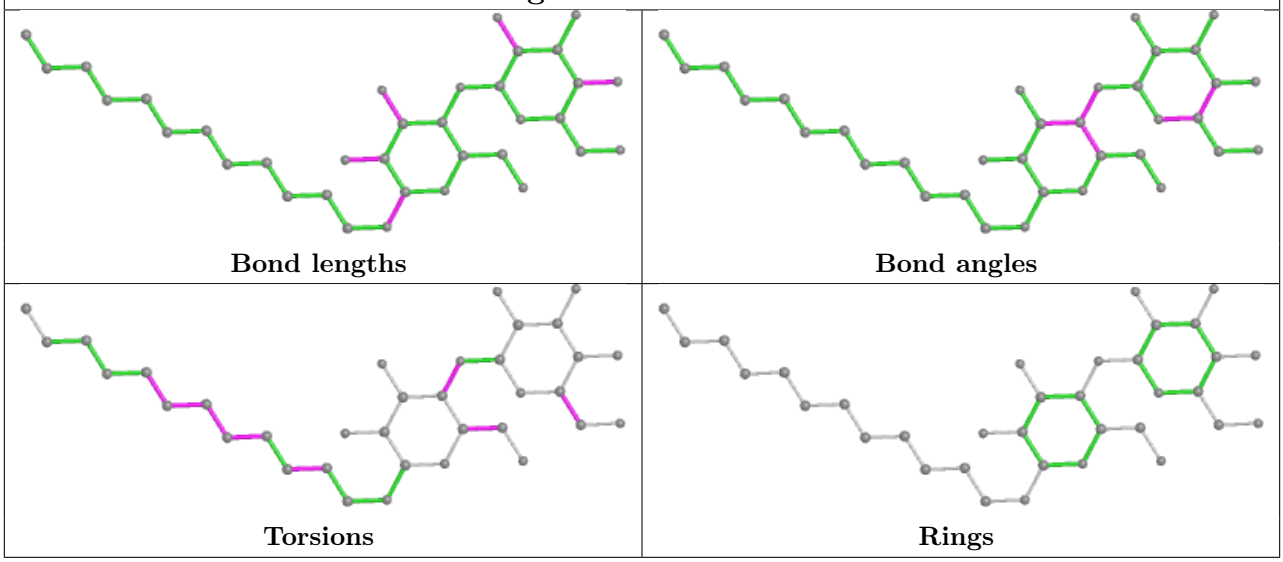


Torsions

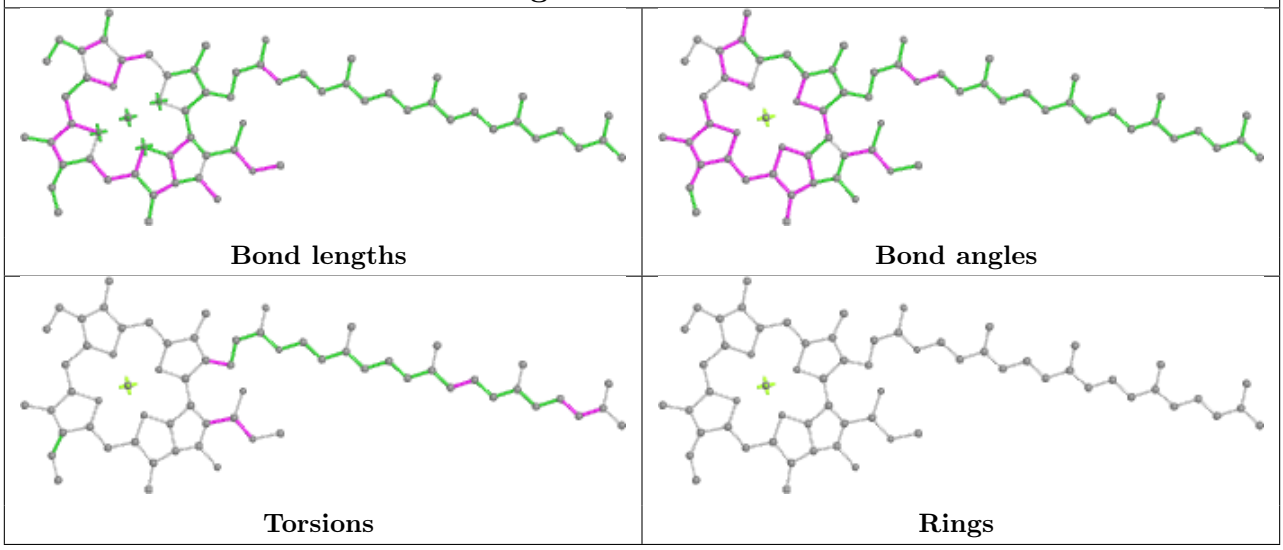


Rings

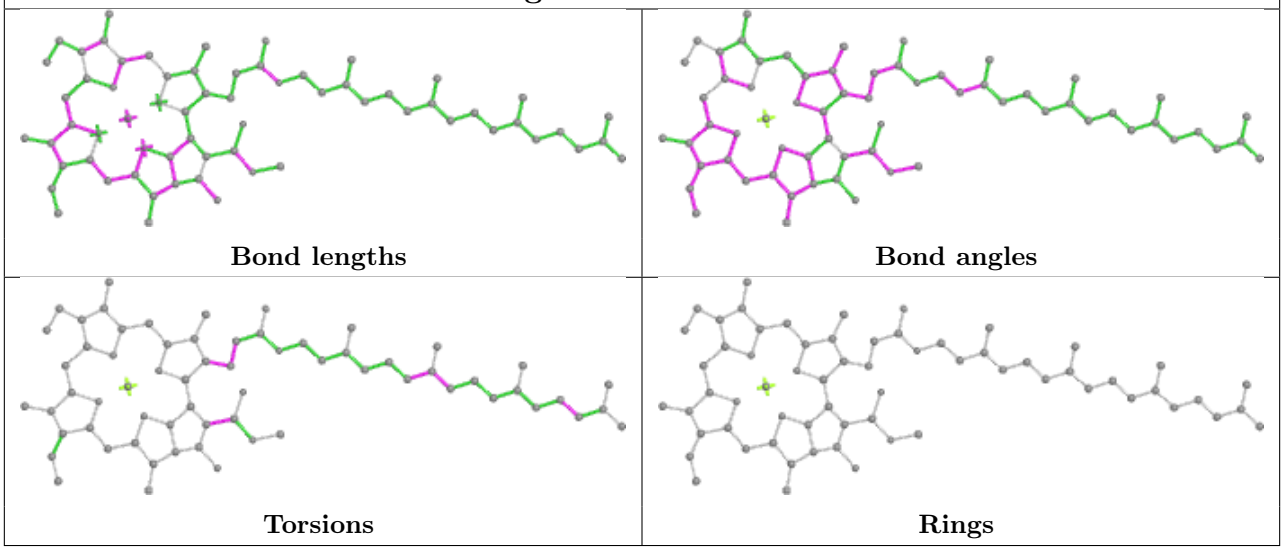
Ligand LMT c 521



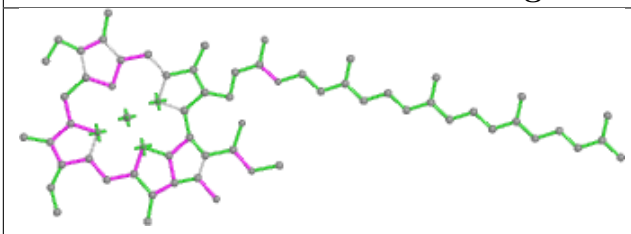
Ligand CLA c 504



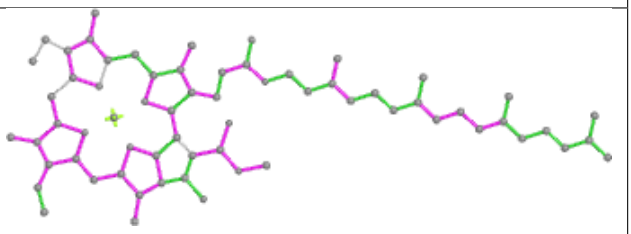
Ligand CLA A 406



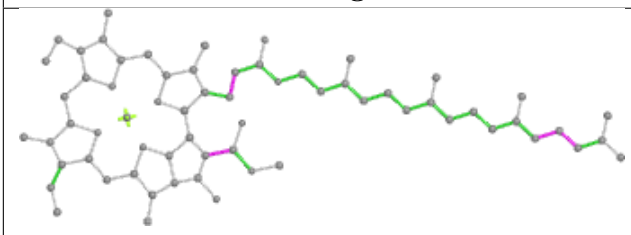
Ligand CLA B 606



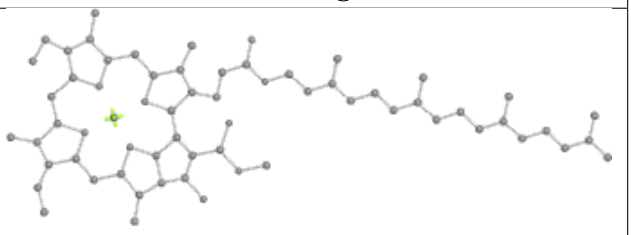
Bond lengths



Bond angles

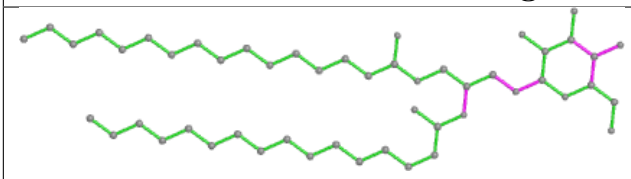


Torsions



Rings

Ligand LMG C 501



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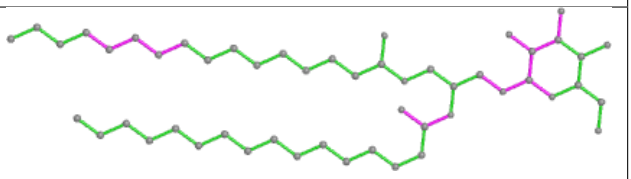
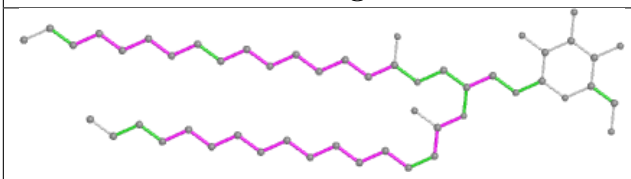
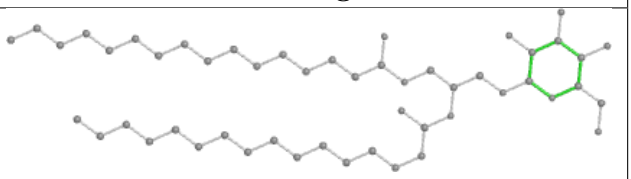


Bond angles

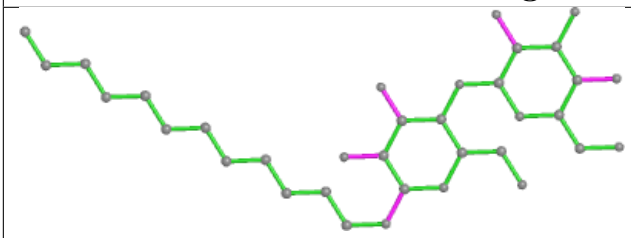


Torsions

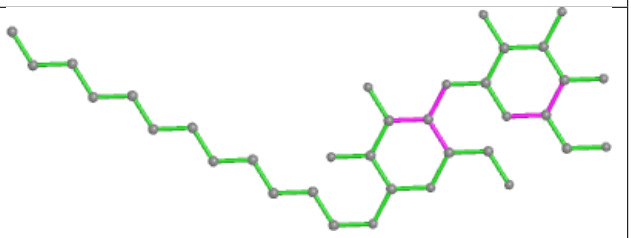


Rings

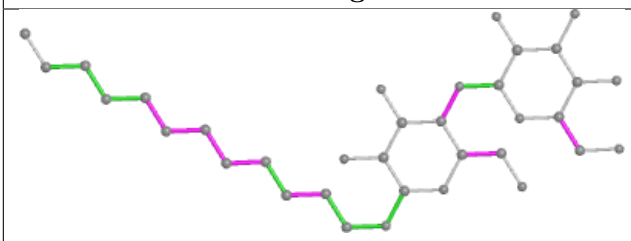
Ligand LMT C 521



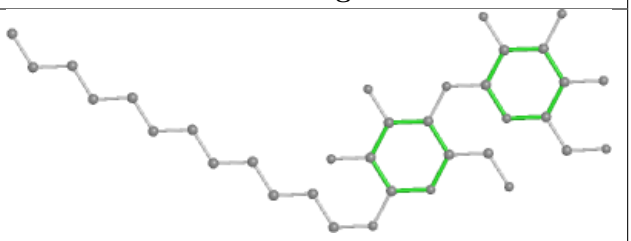
Bond lengths



Bond angles

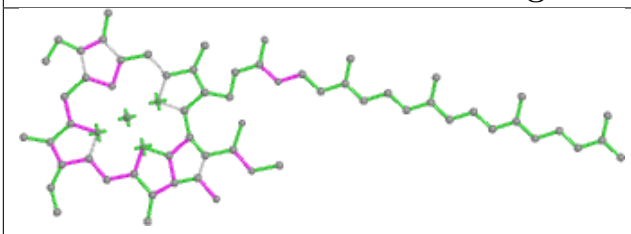


Torsions



Rings

Ligand CLA b 610



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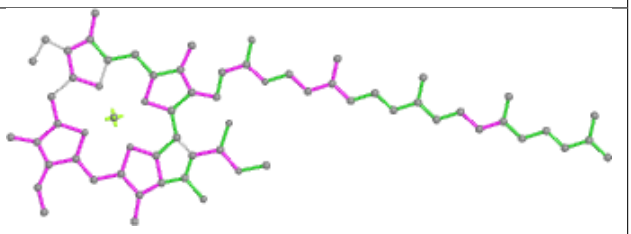
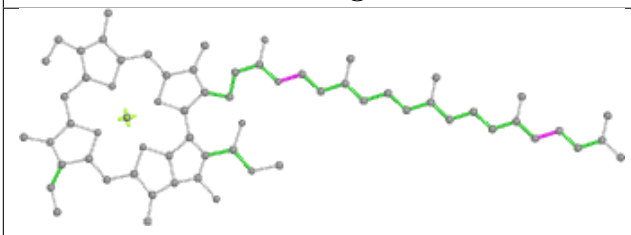
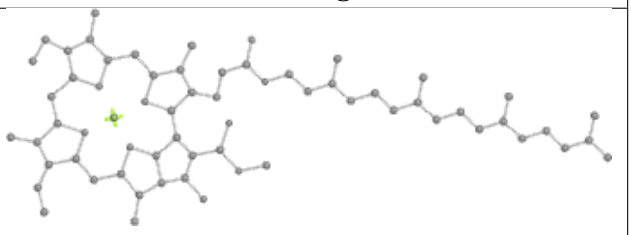


Bond angles

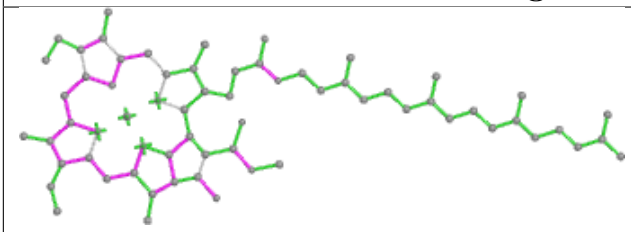


Torsions

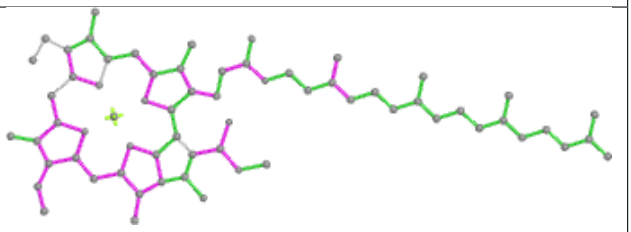


Rings

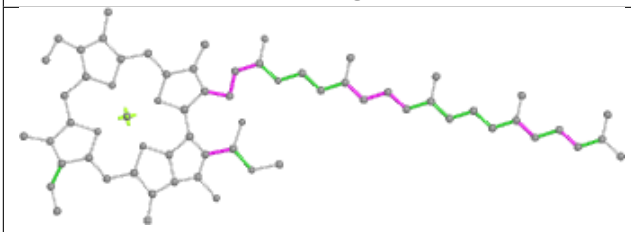
Ligand CLA b 603



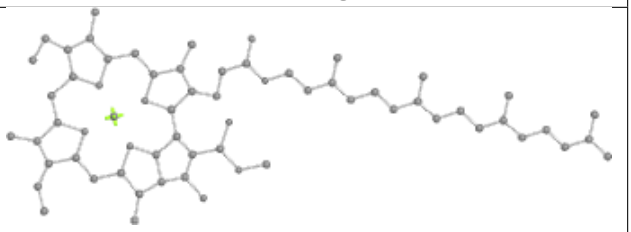
Bond lengths



Bond angles

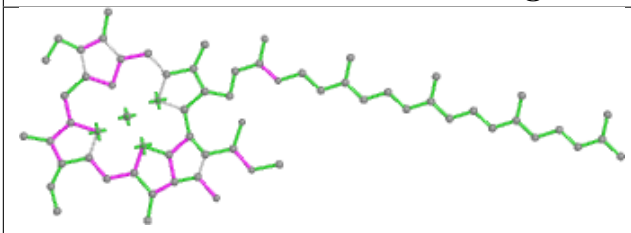


Torsions



Rings

Ligand CLA C 502



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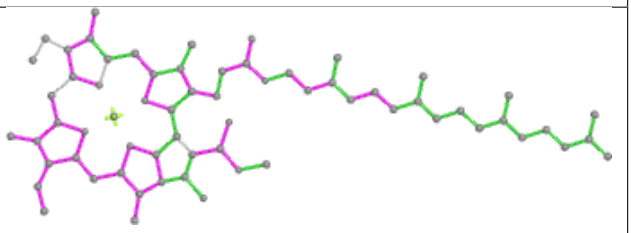
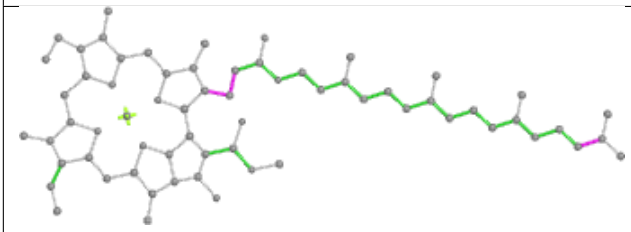


Bond angles



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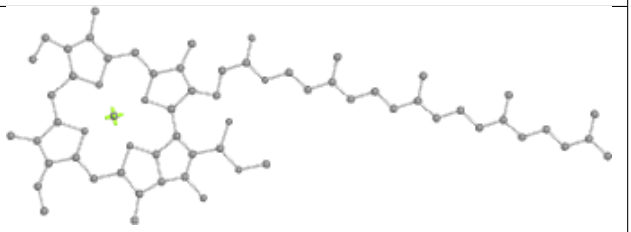
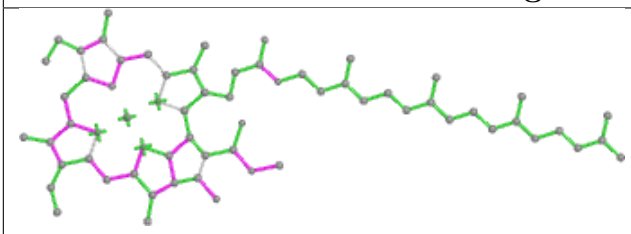


Rings

Ligand CLA C 504



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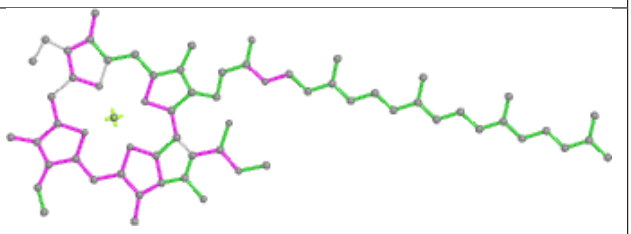
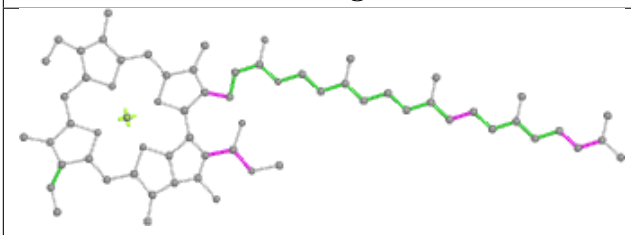
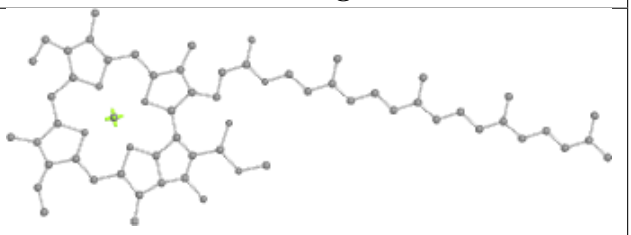


Bond angles

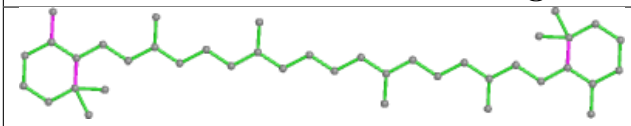


Torsions



Rings

Ligand BCR c 515



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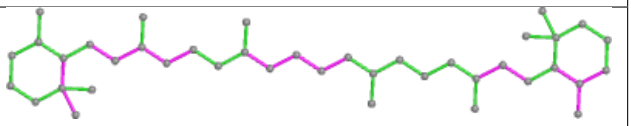
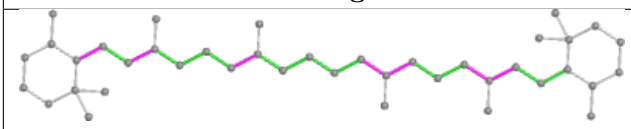


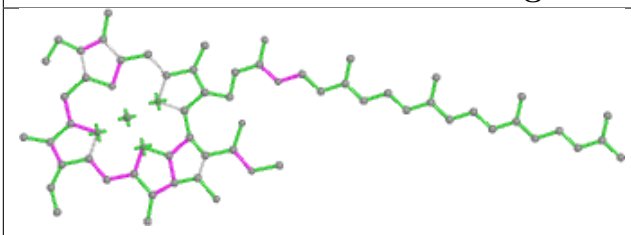
Bond angles



Torsions

Rings

Ligand CLA B 611



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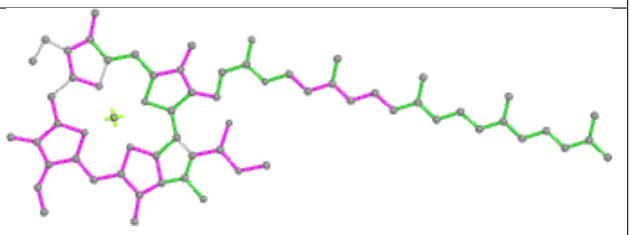
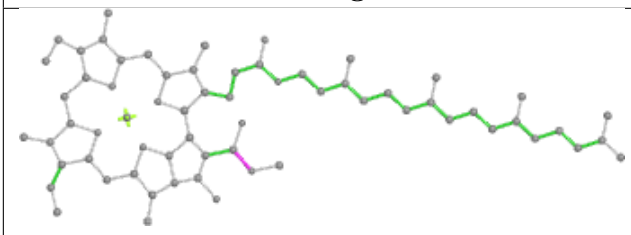
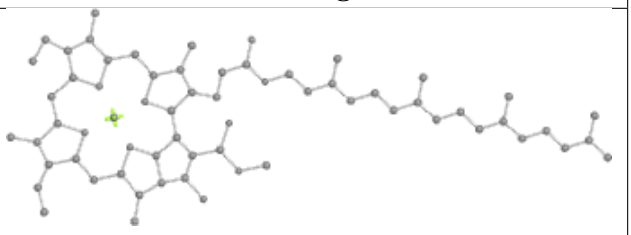


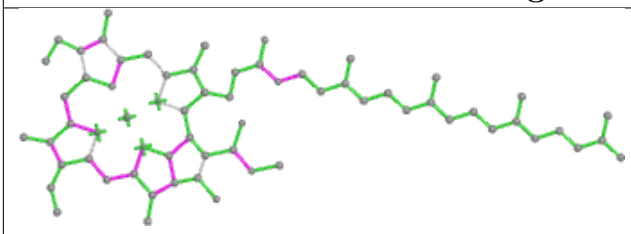
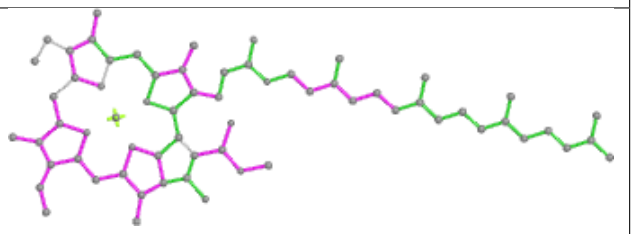
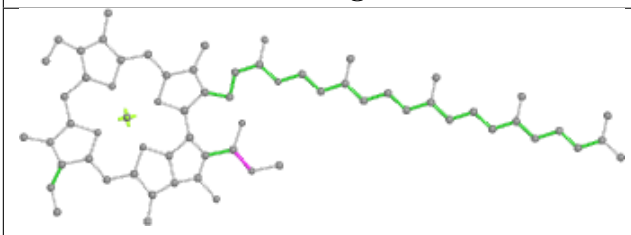
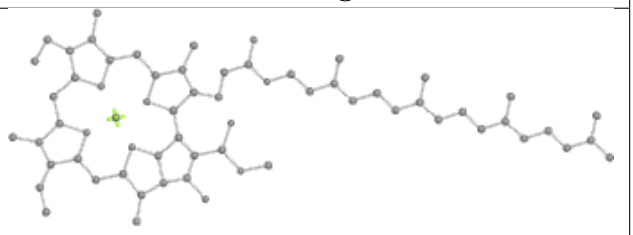
Bond angles

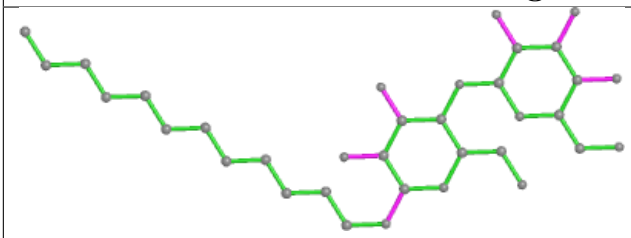
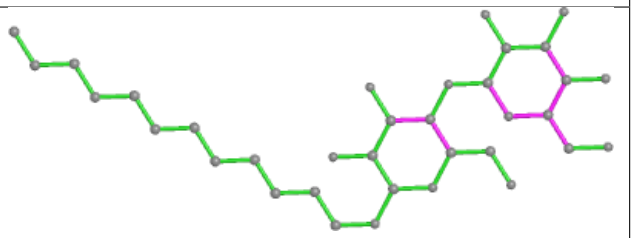
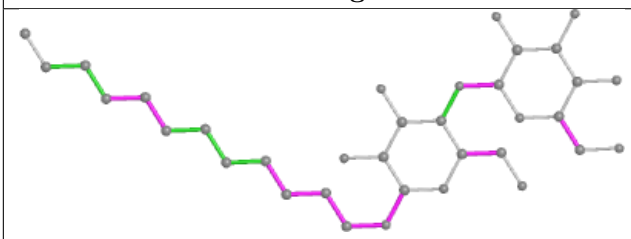
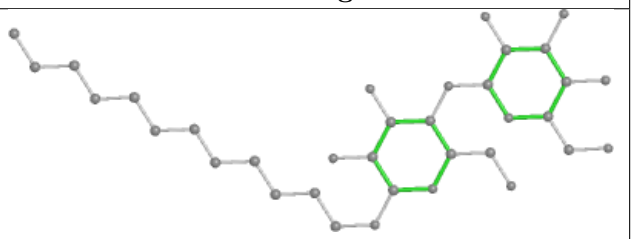


Torsions

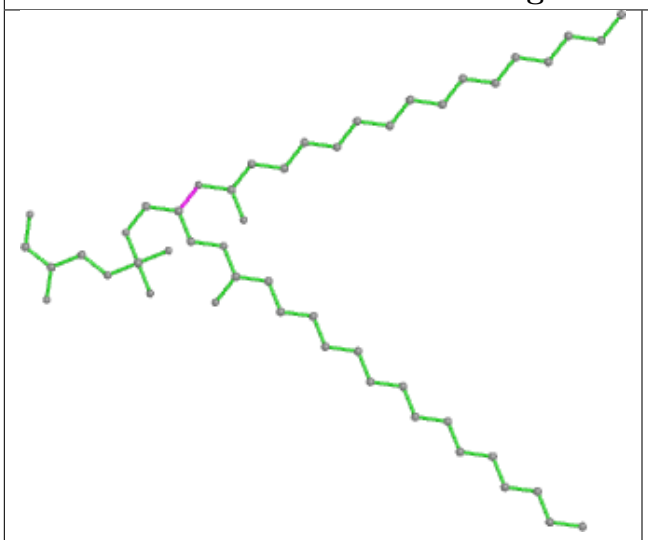


Rings

Ligand CLA b 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT z 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG d 408



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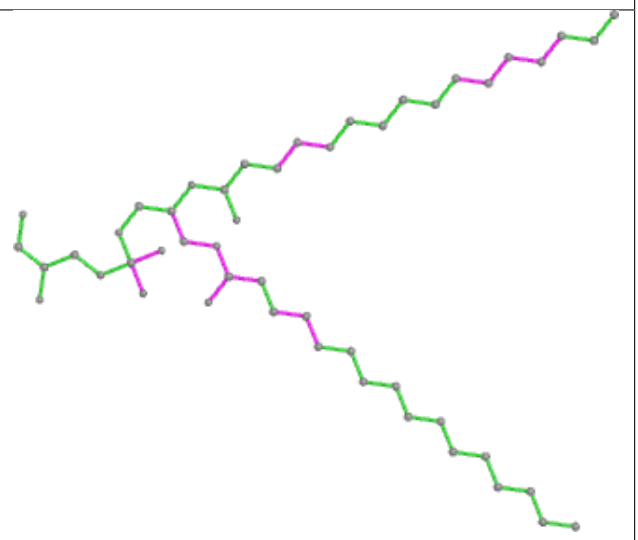
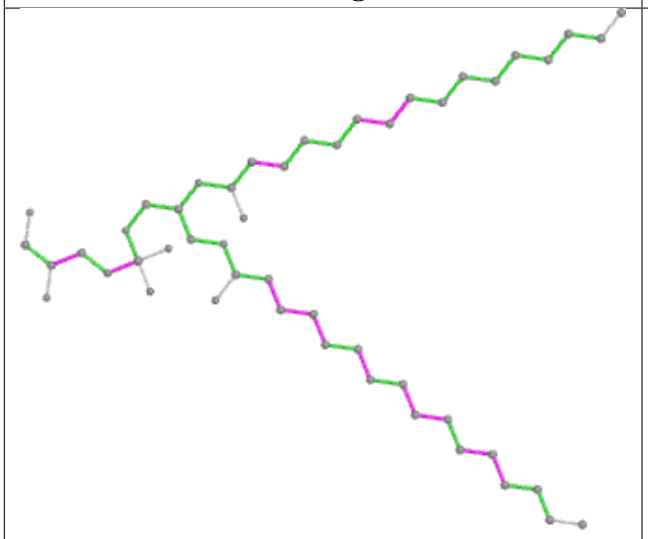
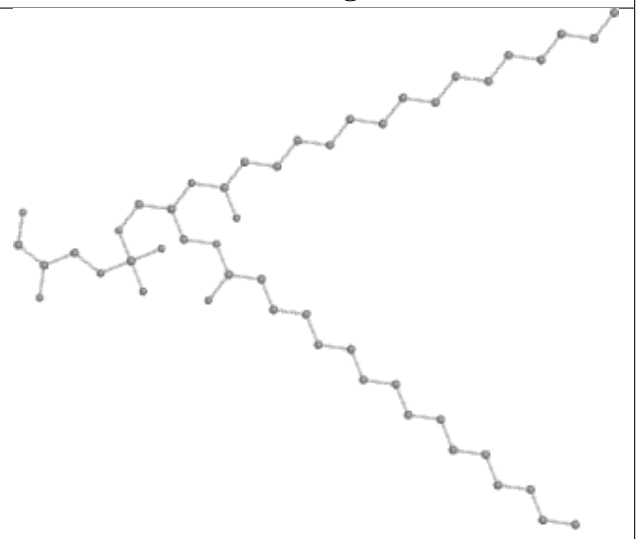


Bond angles

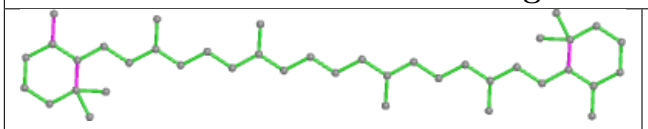


Torsions



Rings

Ligand BCR C 515



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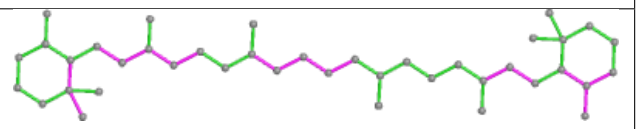

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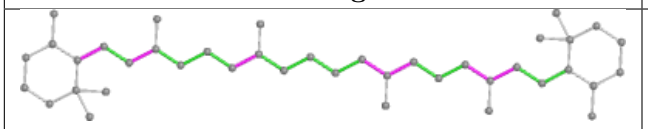

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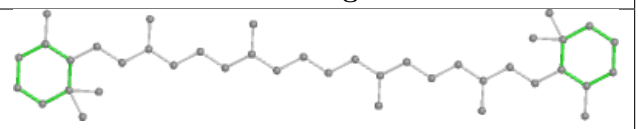
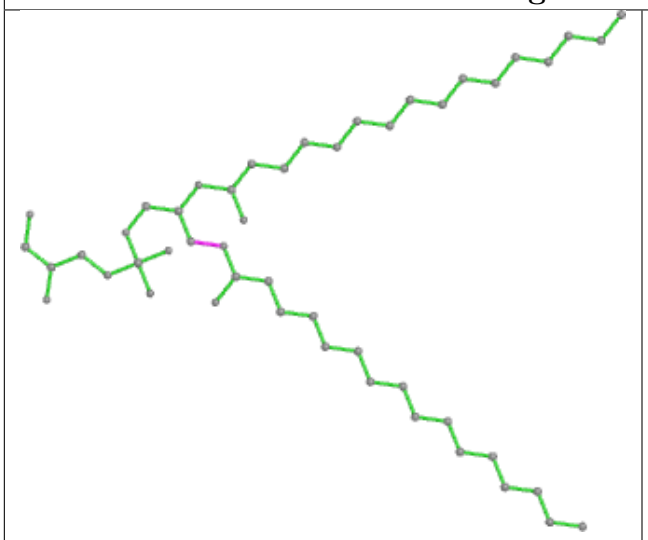


Rings

Ligand LHG e 101



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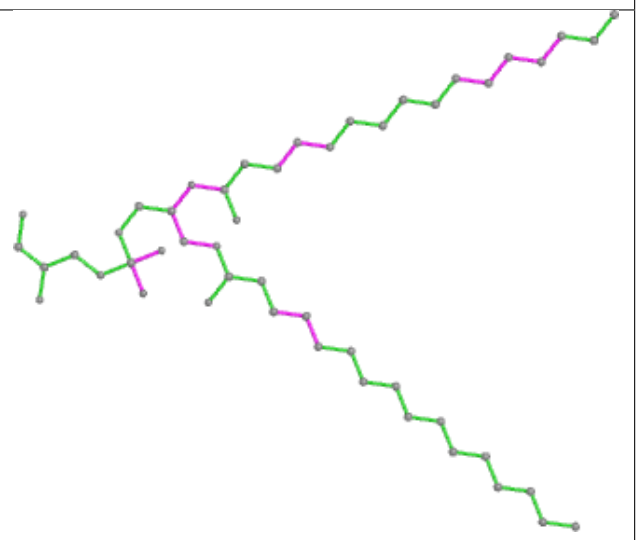

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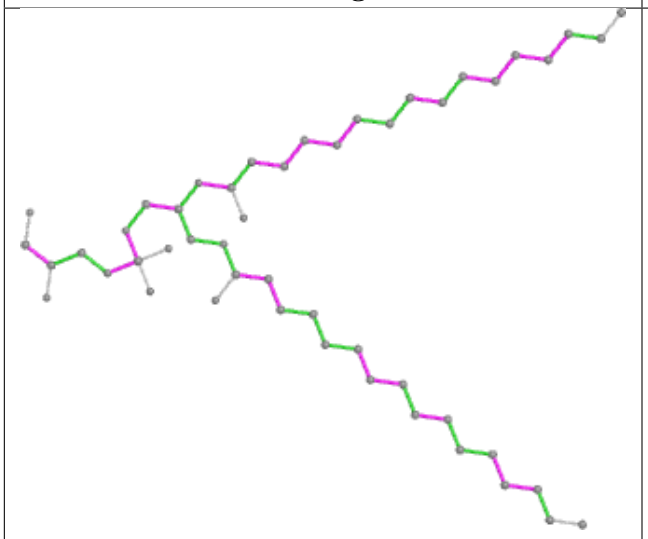

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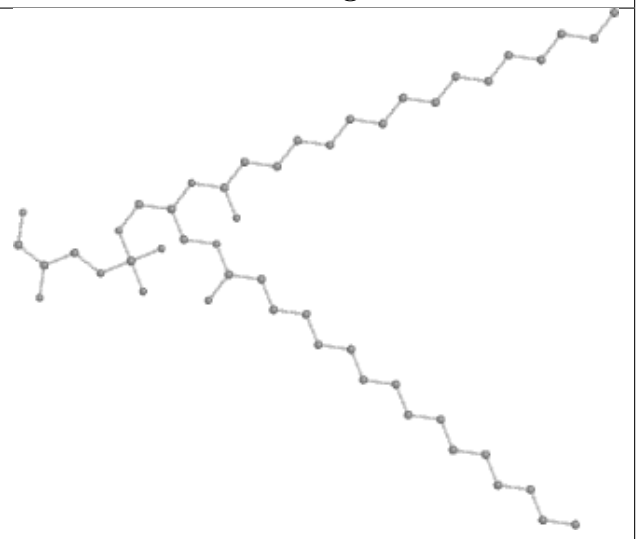
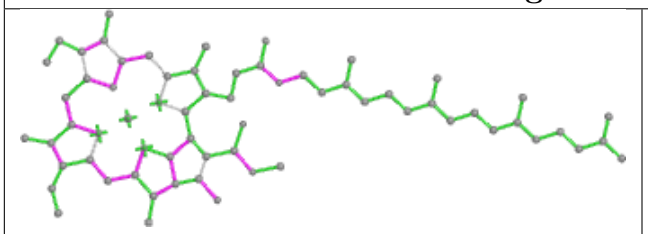


Rings

Ligand CLA C 503



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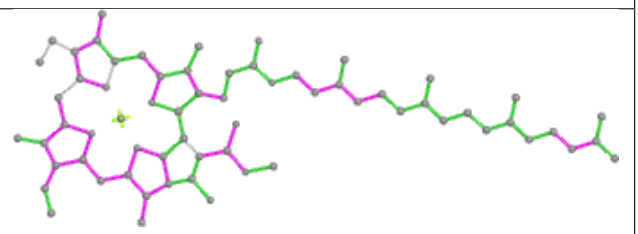
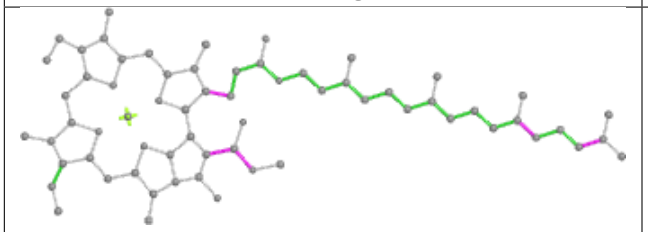


Bond angles



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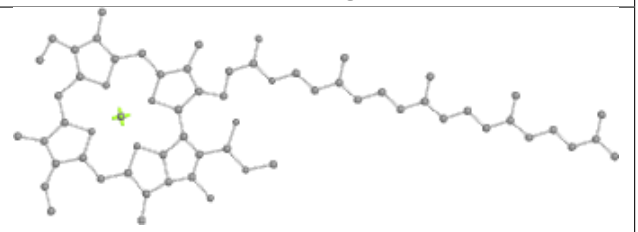
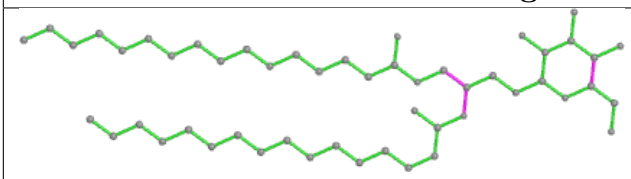
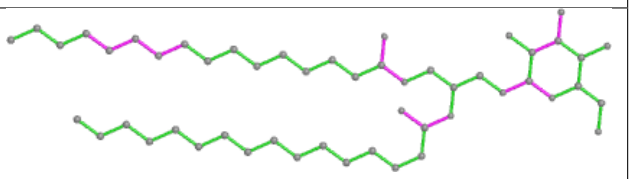
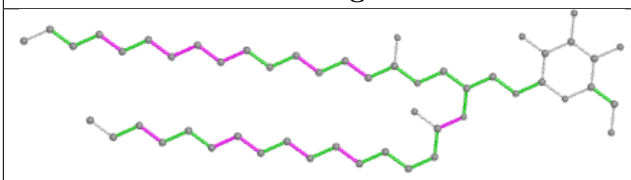
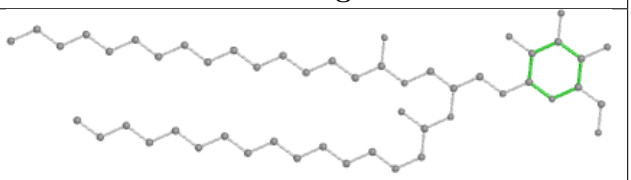
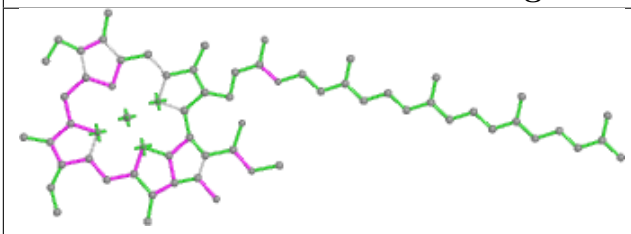
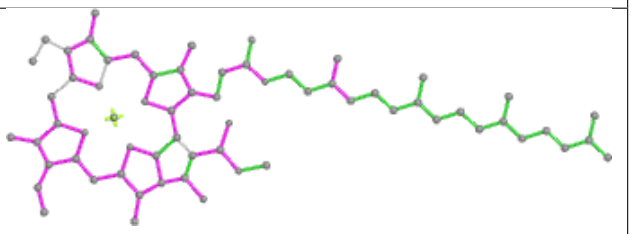
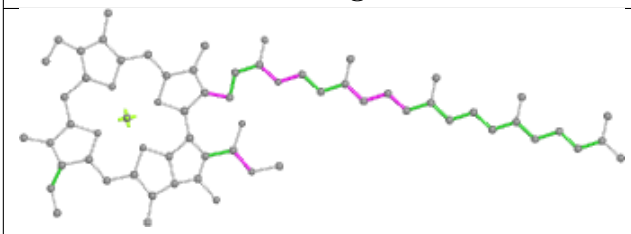
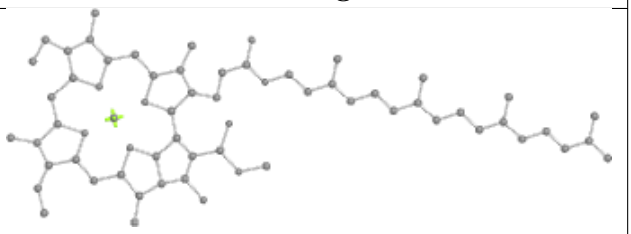
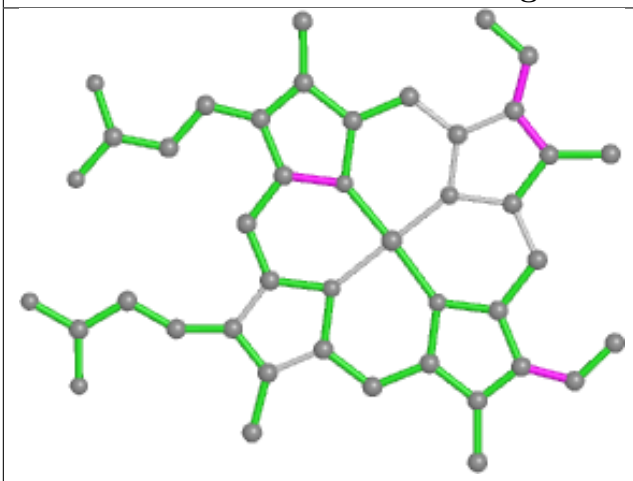


Rings

Ligand LMG B 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEM E 103



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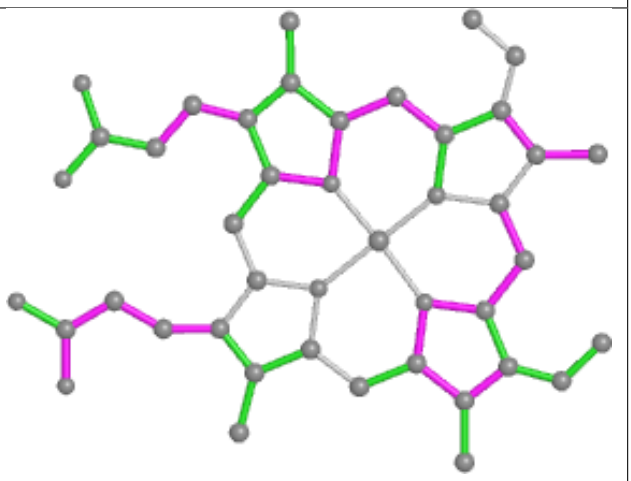
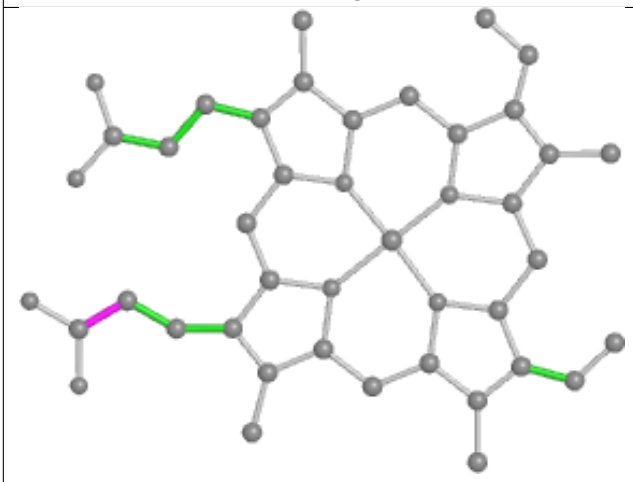
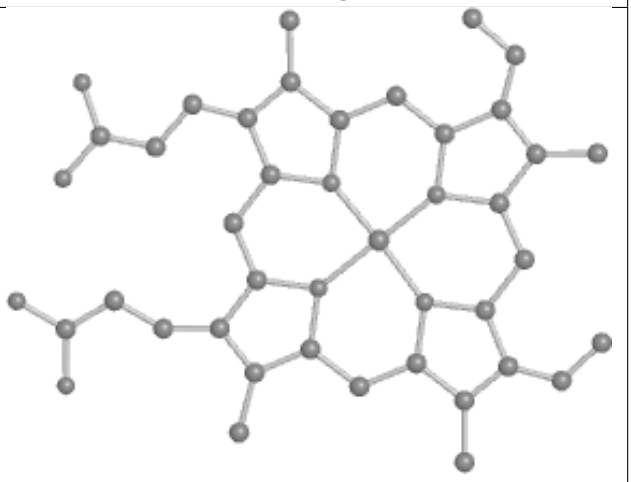


Bond angles

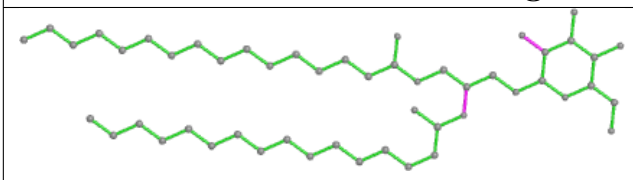


Torsions



Rings

Ligand LMG c 523



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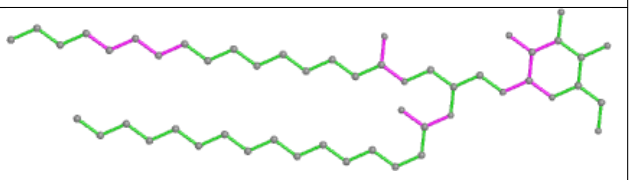

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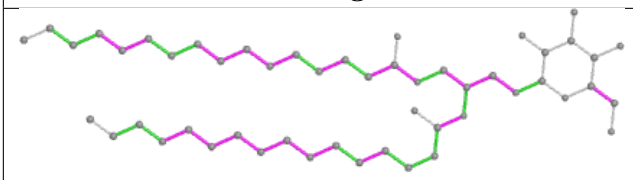

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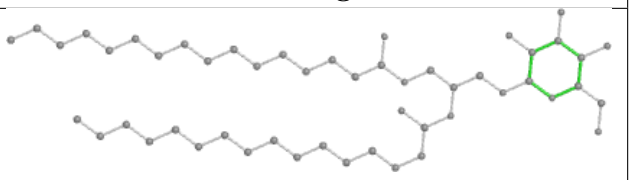
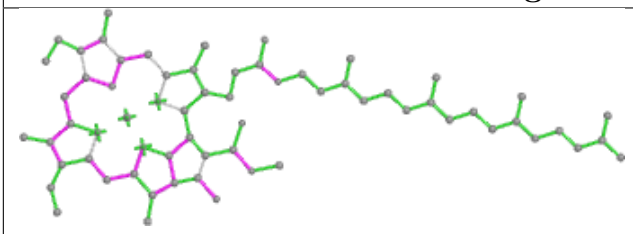


Rings

Ligand CLA B 602



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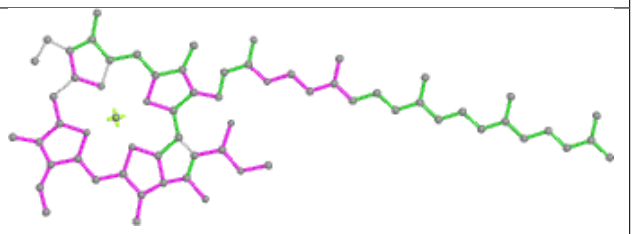
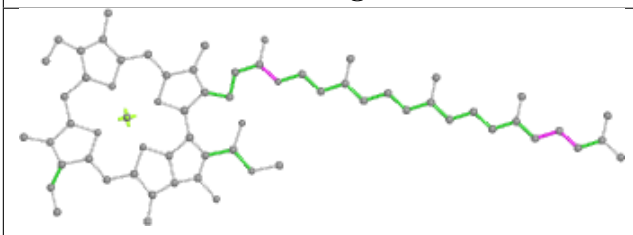


Bond angles



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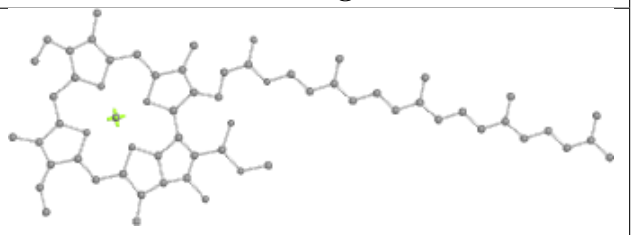
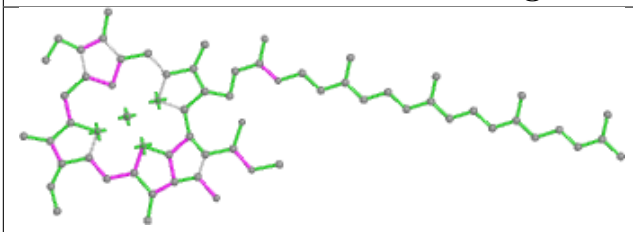


Rings

Ligand CLA A 408



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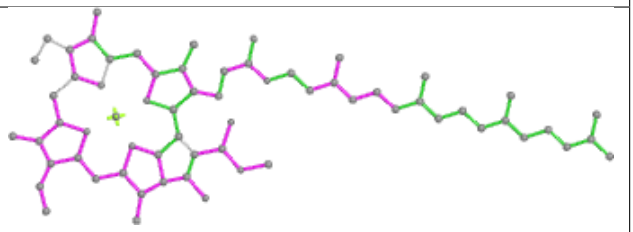

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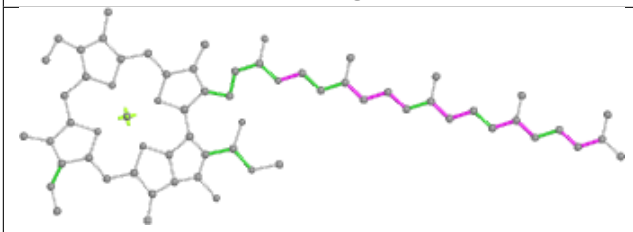

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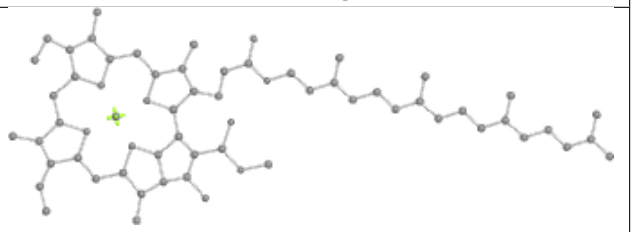
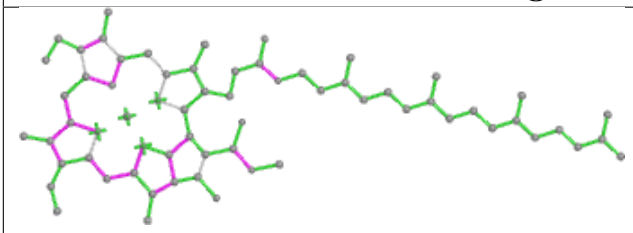


Rings

Ligand CLA b 616



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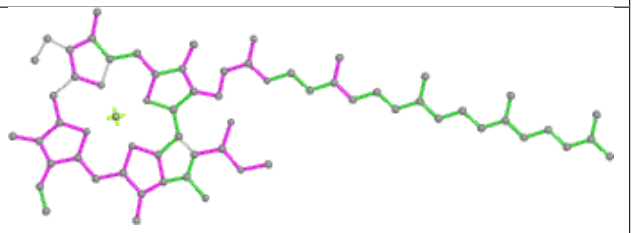
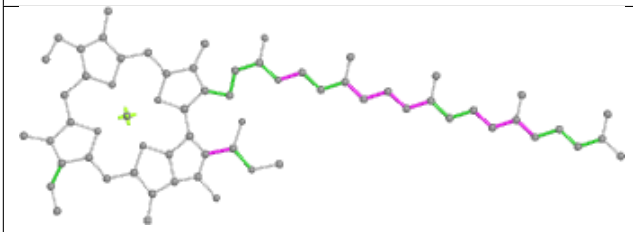


Bond angles



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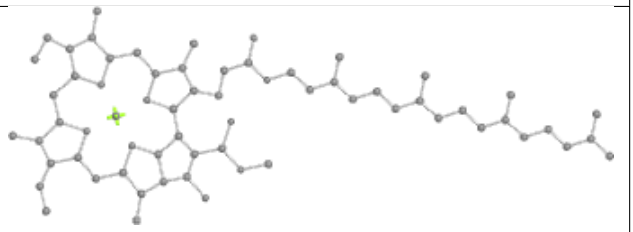
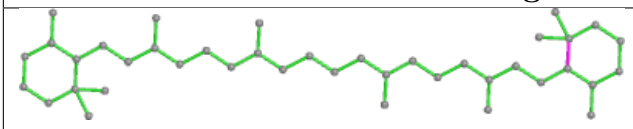
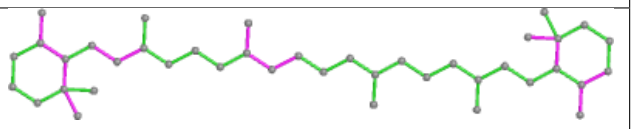


Rings

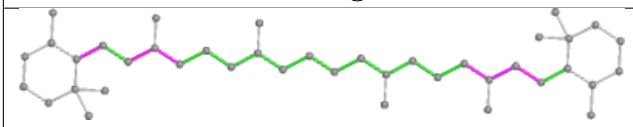
Ligand BCR T 101



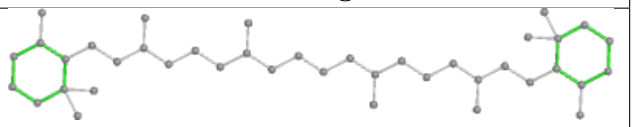
Bond lengths



Bond angles

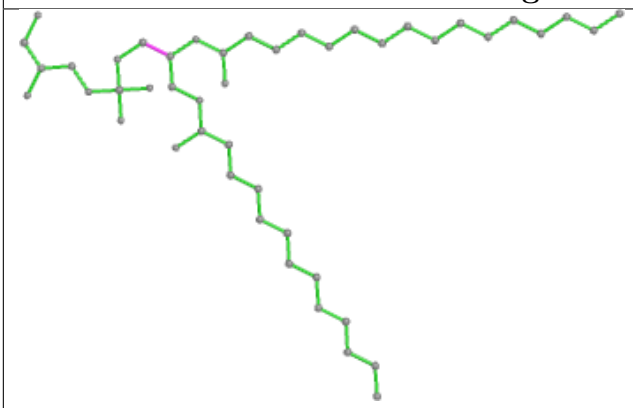


Torsions

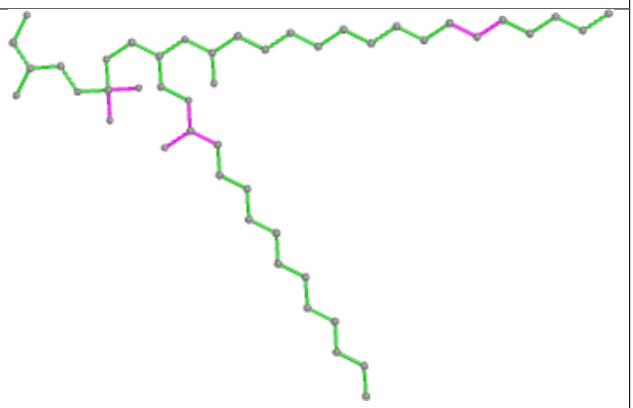


Rings

Ligand LHG D 410



Bond lengths



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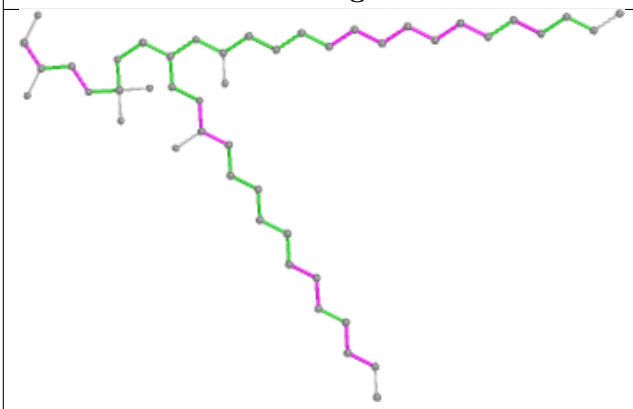

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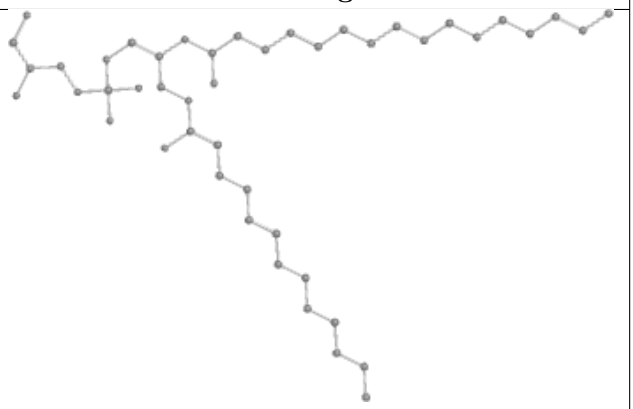
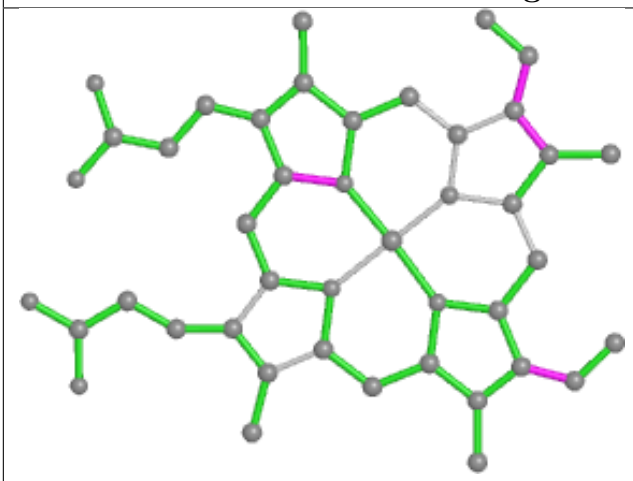
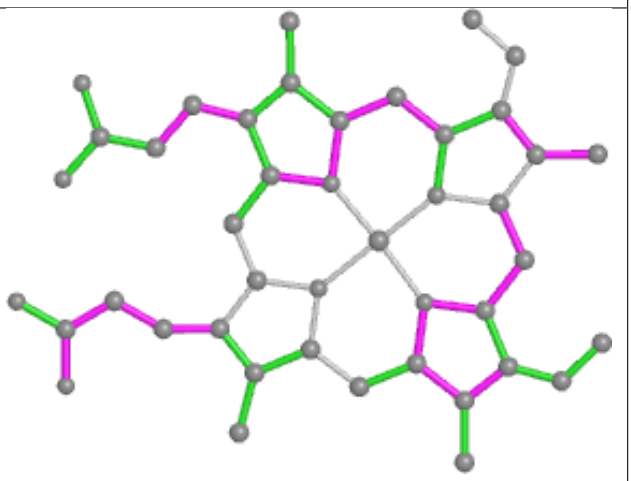


Rings

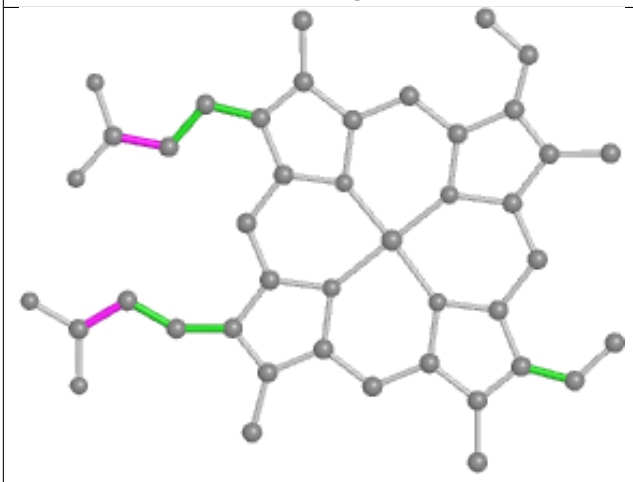
Ligand HEM e 103



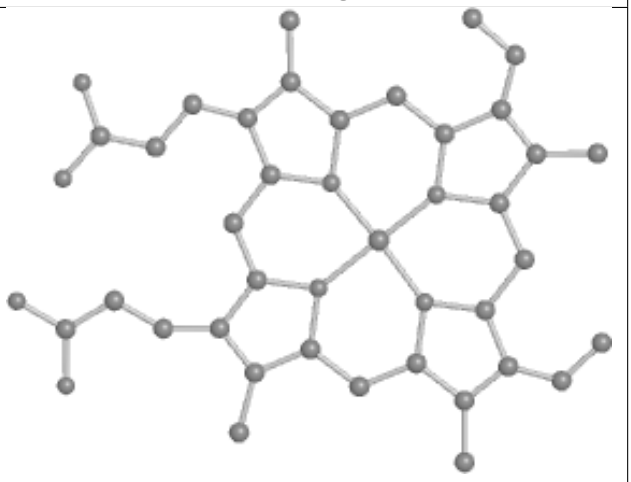
Bond lengths



Bond angles

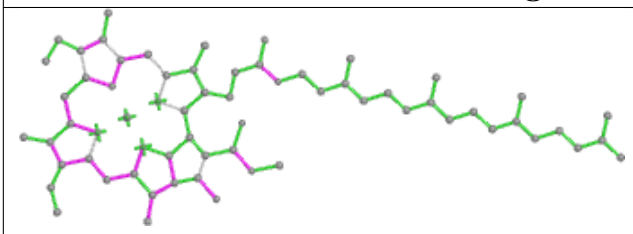


Torsions



Rings

Ligand CLA B 603



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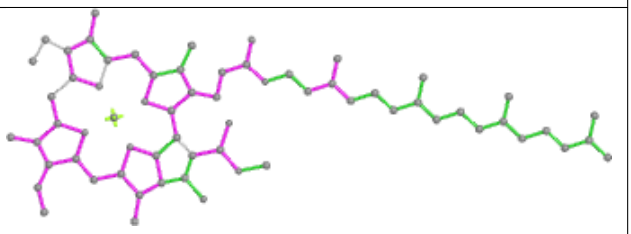
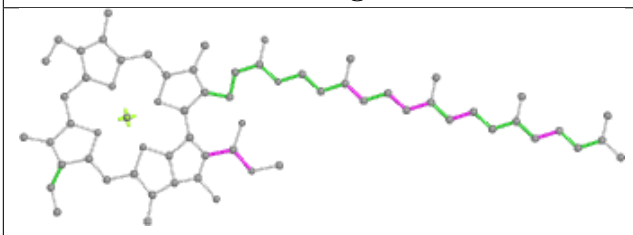


Bond angles



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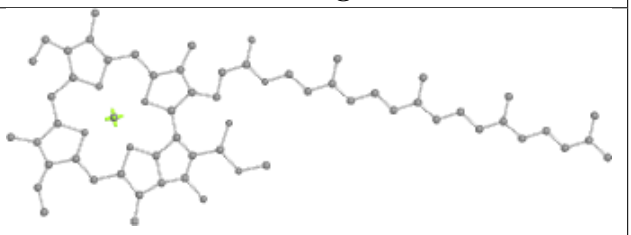
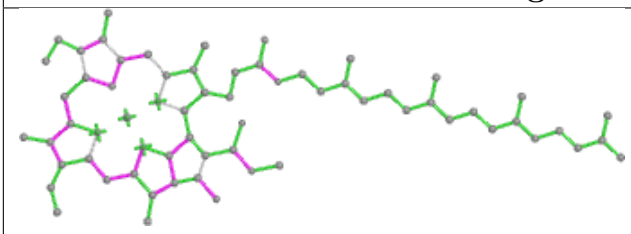
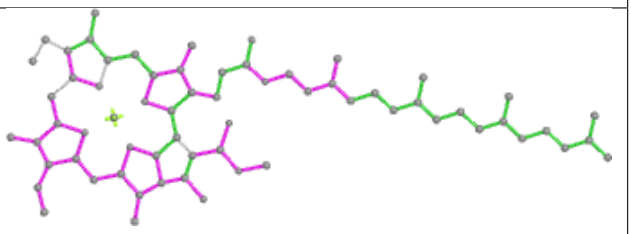
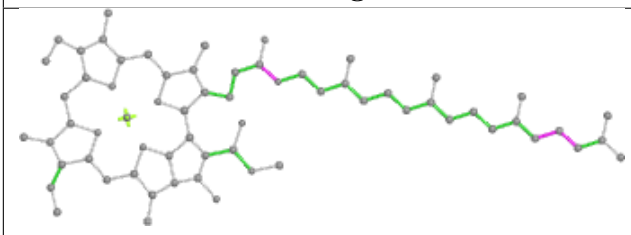
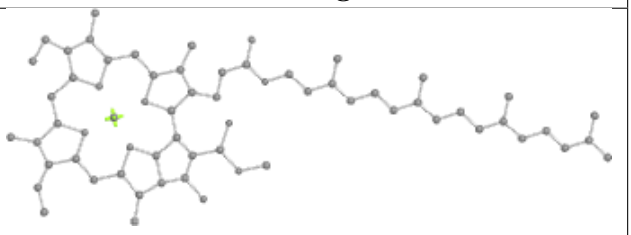
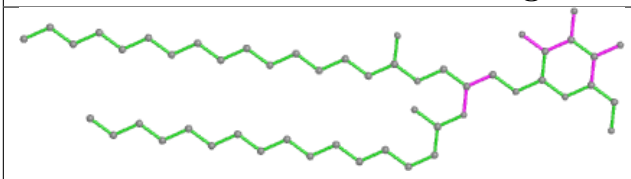
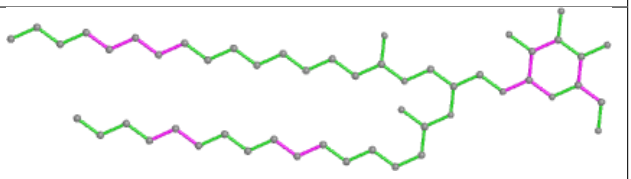
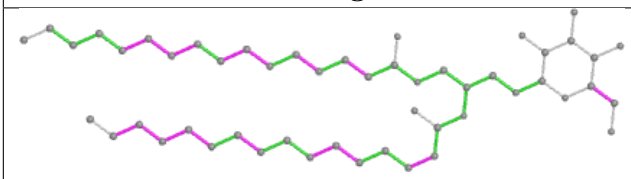
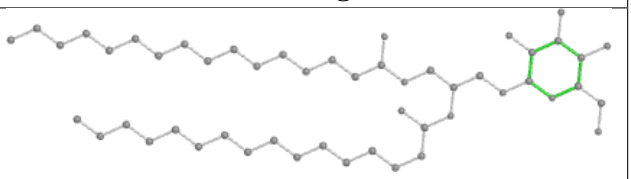
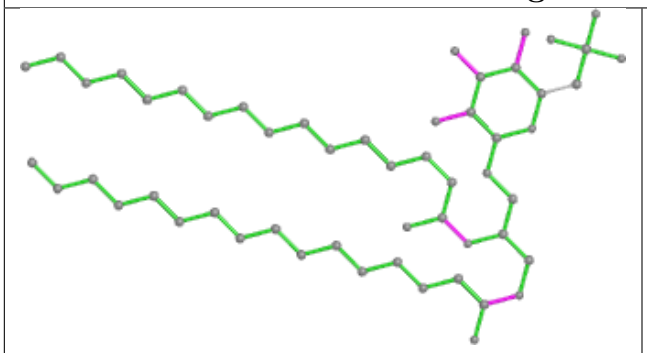


Rings

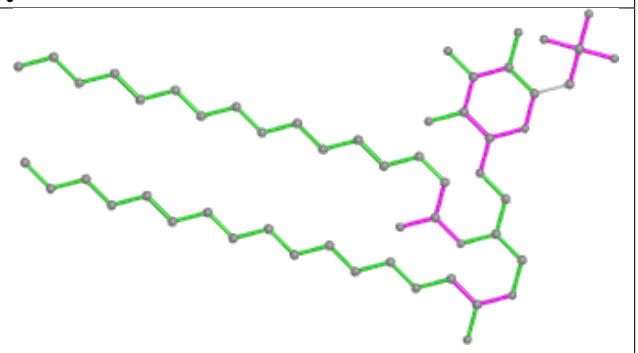
Ligand CLA b 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG d 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

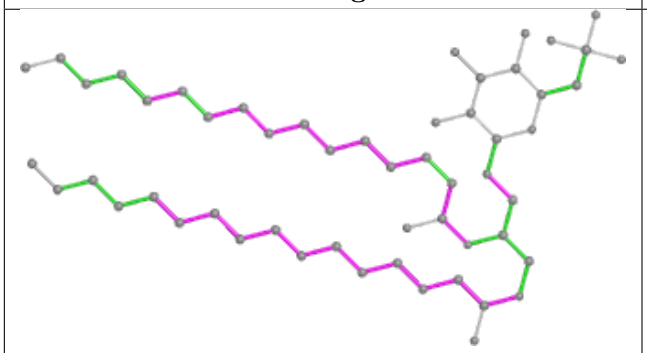
Ligand SQD L 102



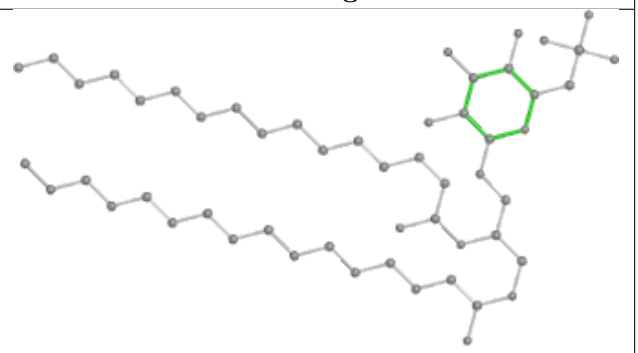
Bond lengths



Bond angles

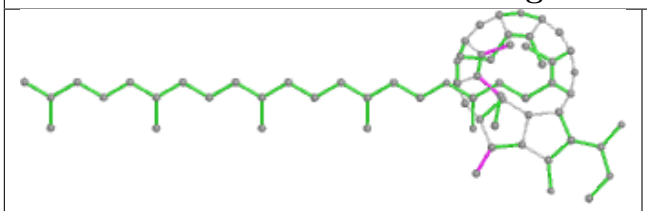


Torsions

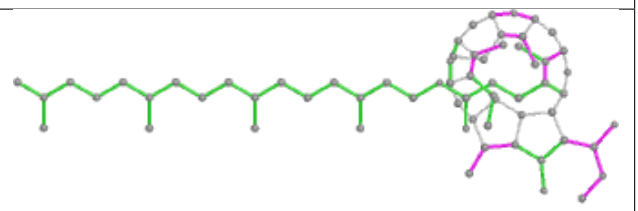


Rings

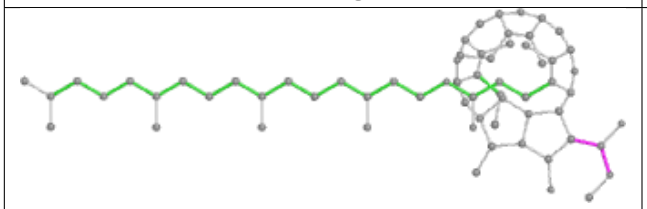
Ligand PHO d 402



Bond lengths



Bond angles



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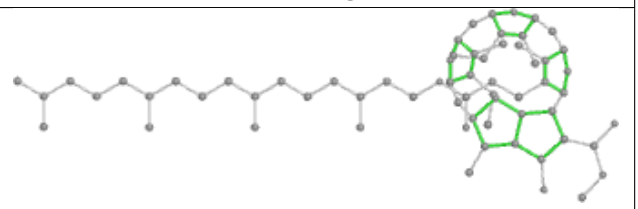
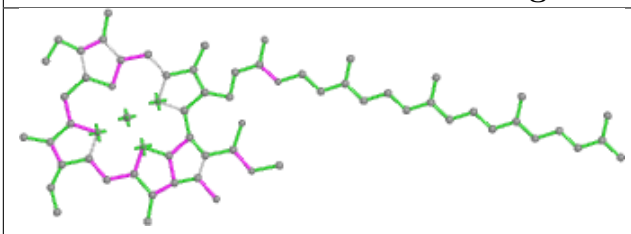
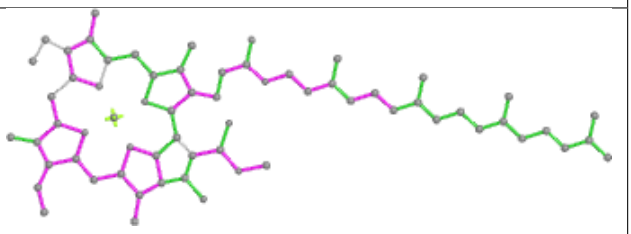
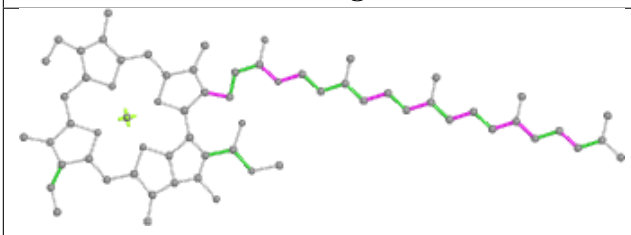
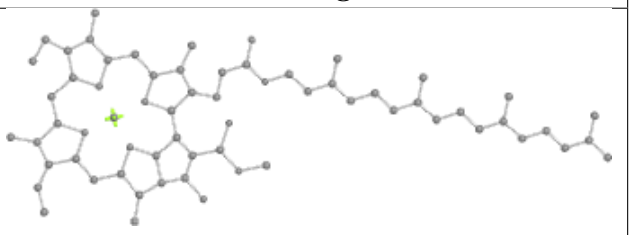
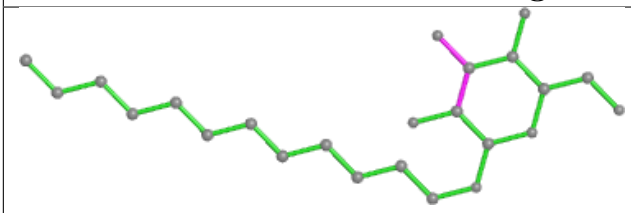
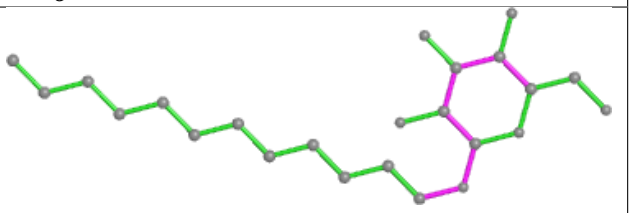
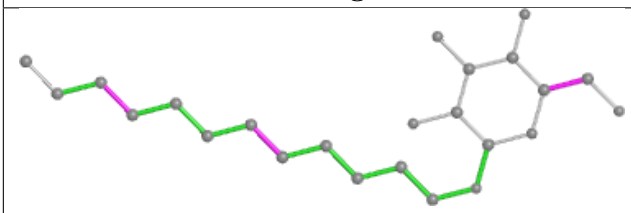
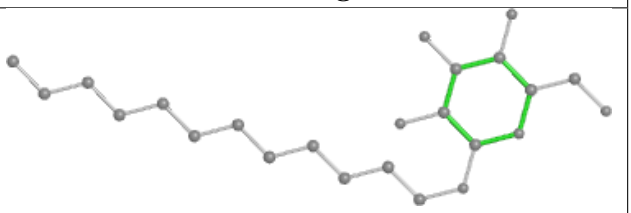
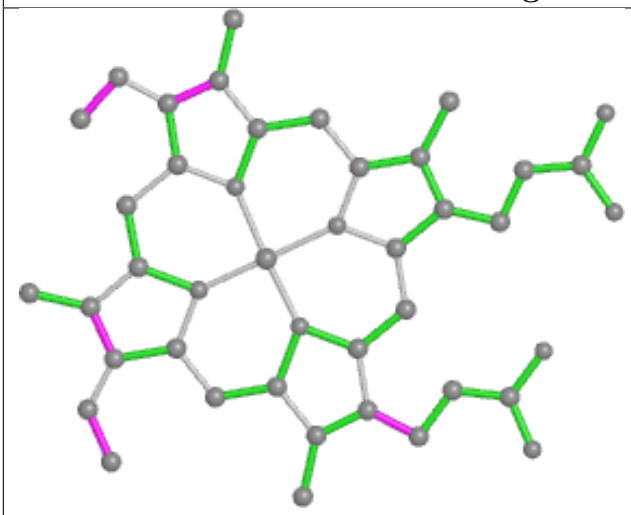


Rings

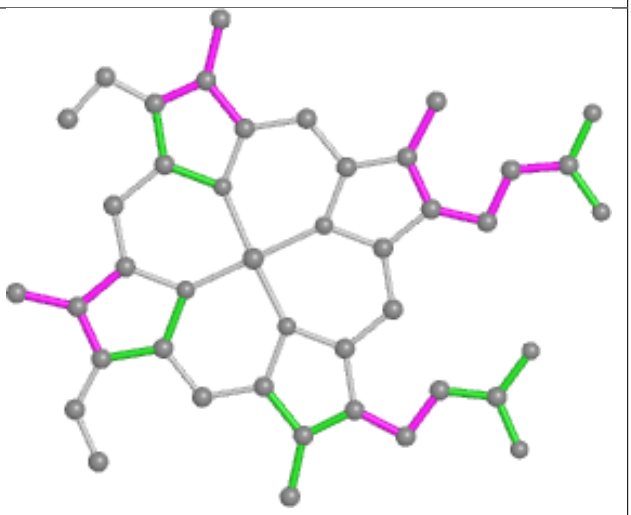
Ligand CLA c 512	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT j 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

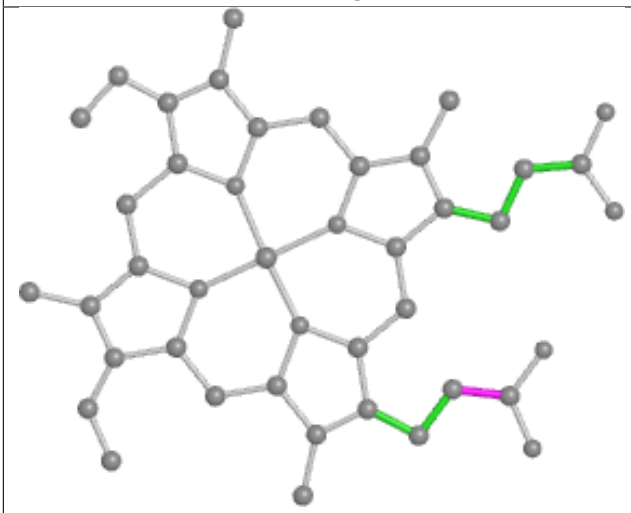
Ligand HEC V 201



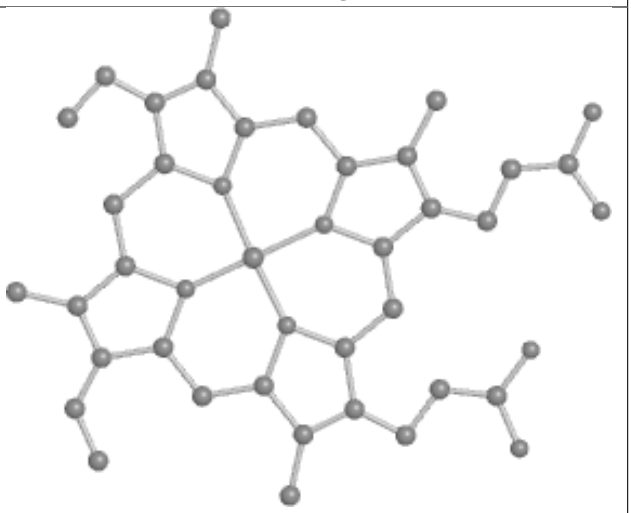
Bond lengths



Bond angles

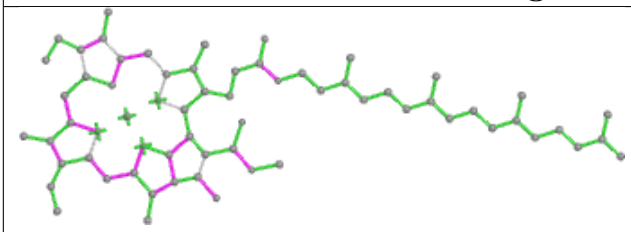


Torsions

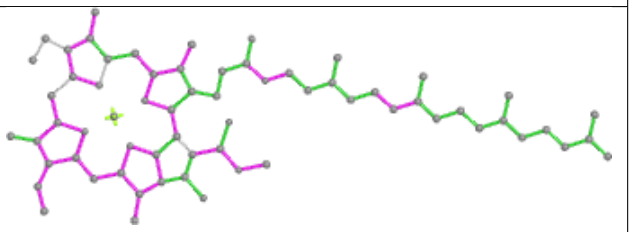


Rings

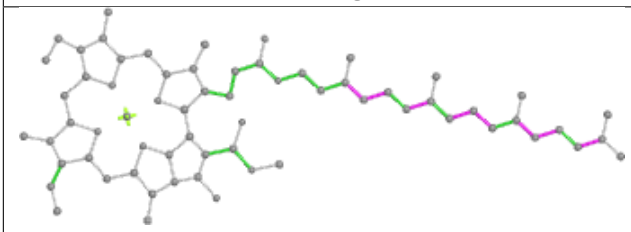
Ligand CLA b 617



Bond lengths



Bond angles



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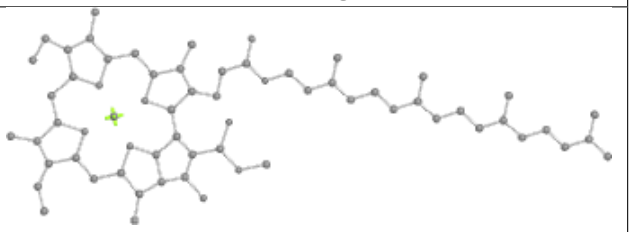
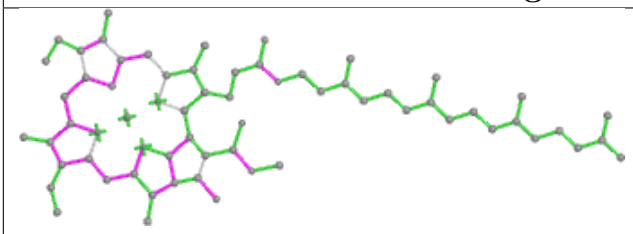
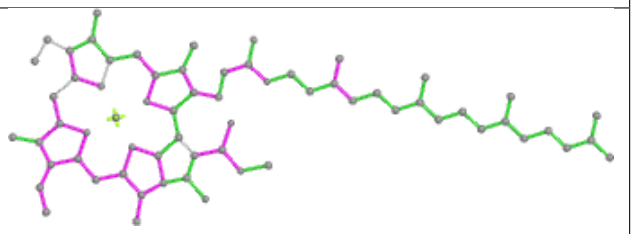


Rings

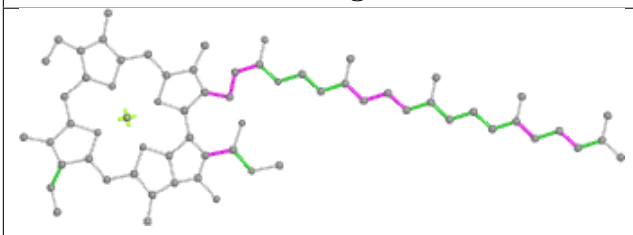
Ligand CLA B 601



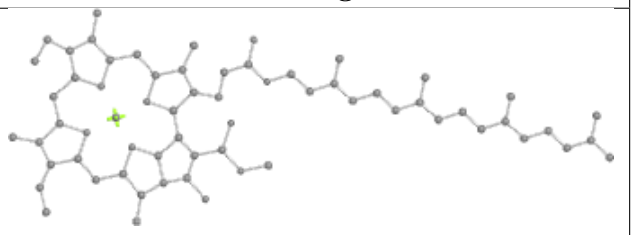
Bond lengths



Bond angles

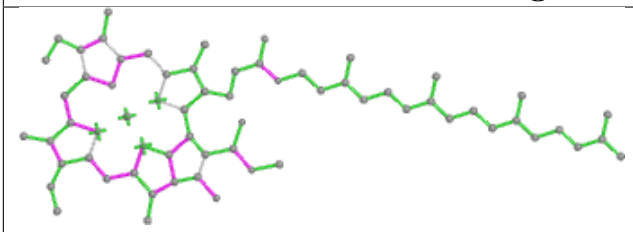


Torsions

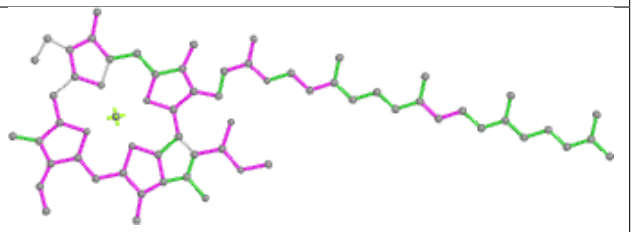


Rings

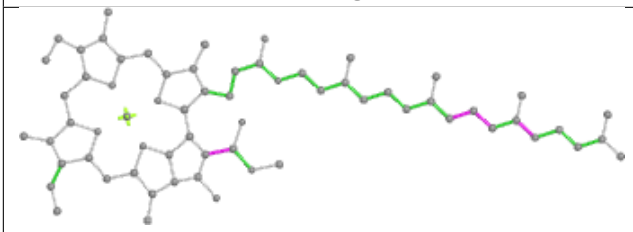
Ligand CLA c 509



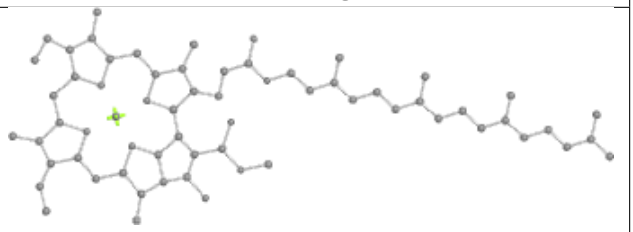
Bond lengths



Bond angles

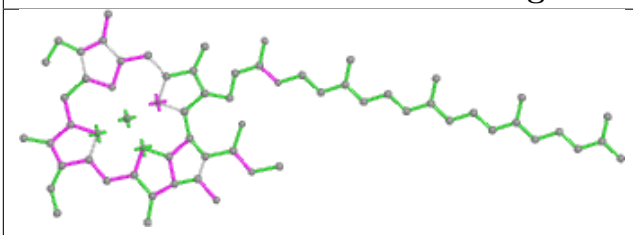


Torsions

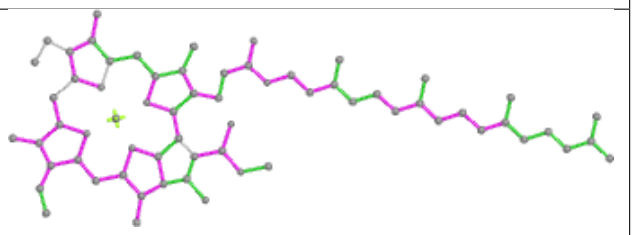


Rings

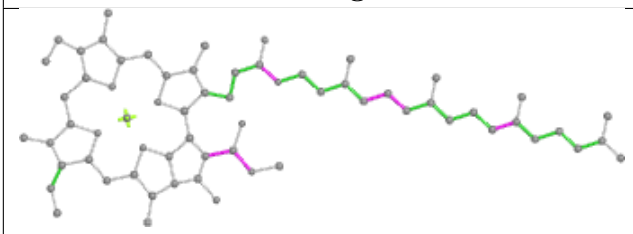
Ligand CLA b 606



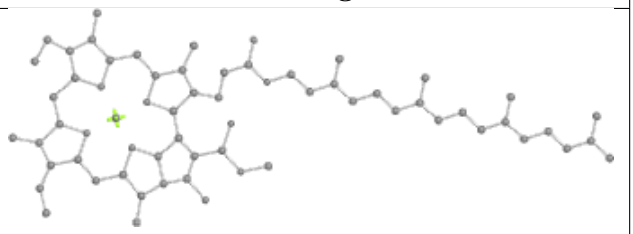
Bond lengths



Bond angles

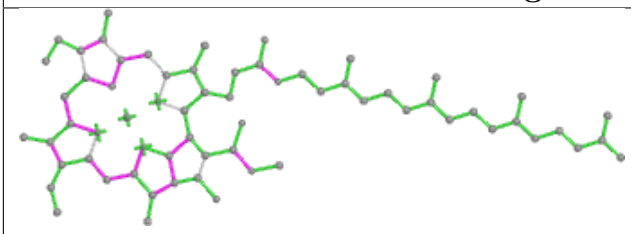


Torsions



Rings

Ligand CLA C 507



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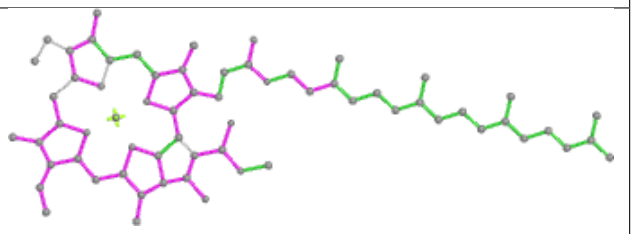
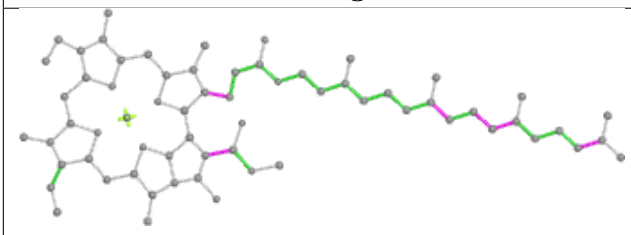
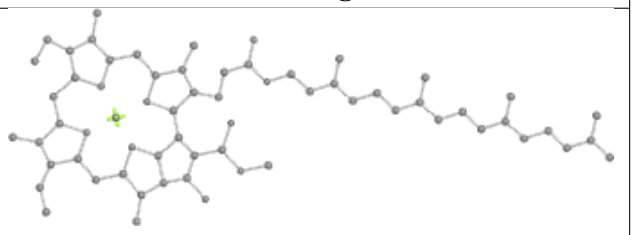


Bond angles

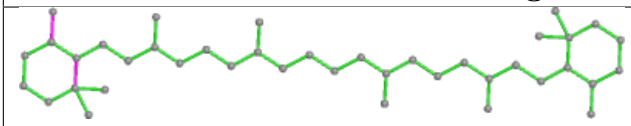


Torsions



Rings

Ligand BCR b 619



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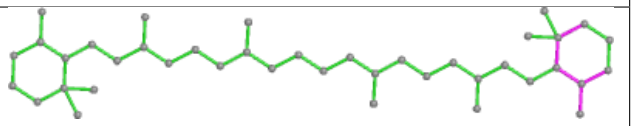
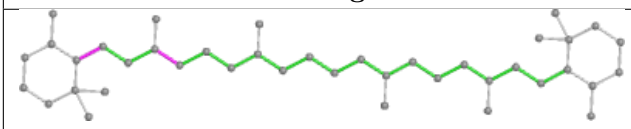
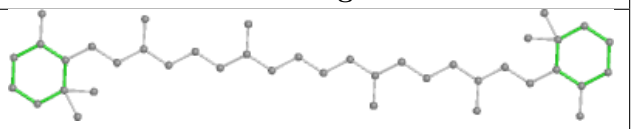


Bond angles

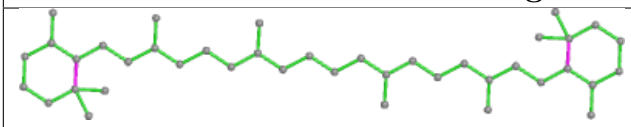


Torsions



Rings

Ligand BCR b 621



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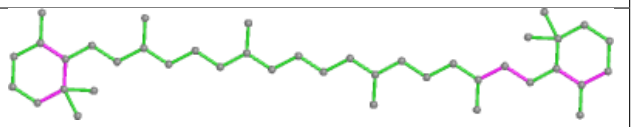
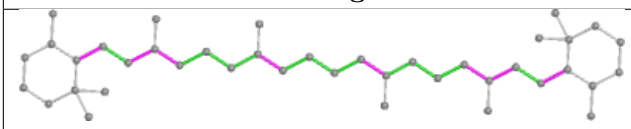
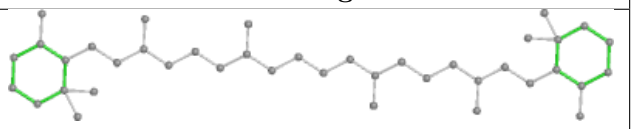


Bond angles

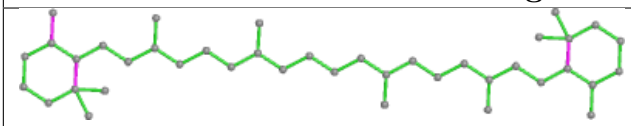


Torsions



Rings

Ligand BCR d 406



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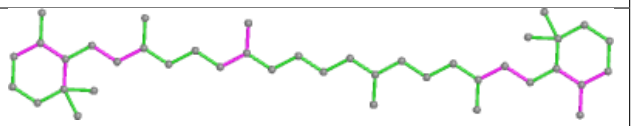
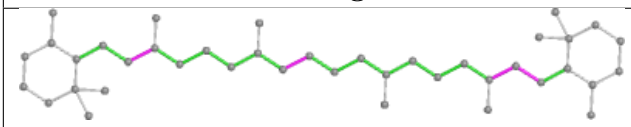


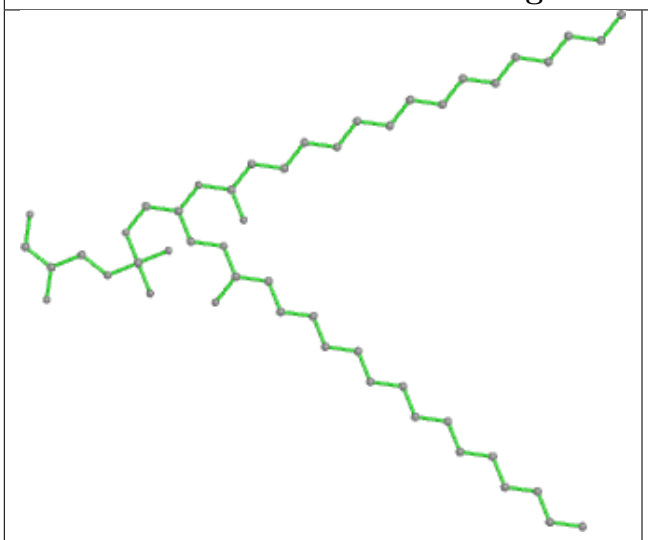
Bond angles



Torsions

Rings

Ligand LHG L 101



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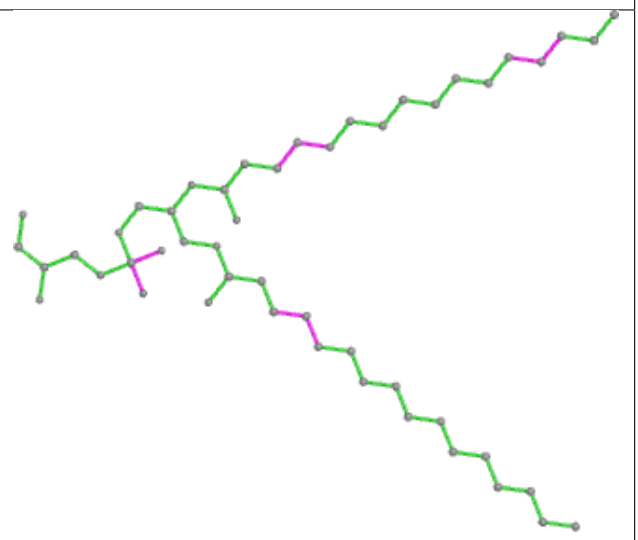
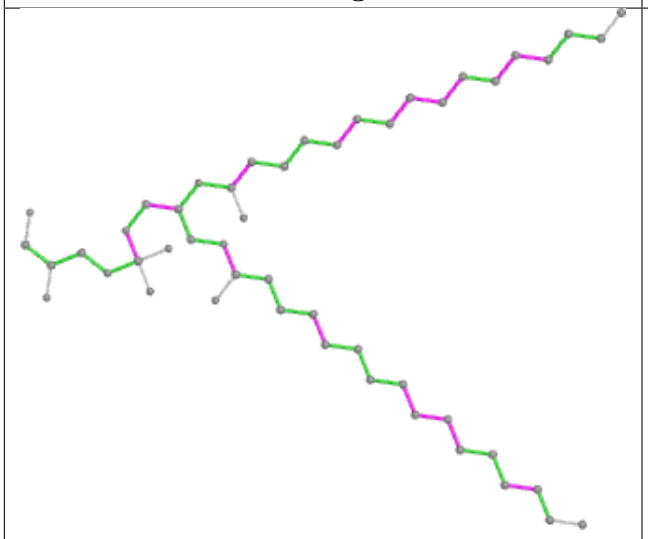
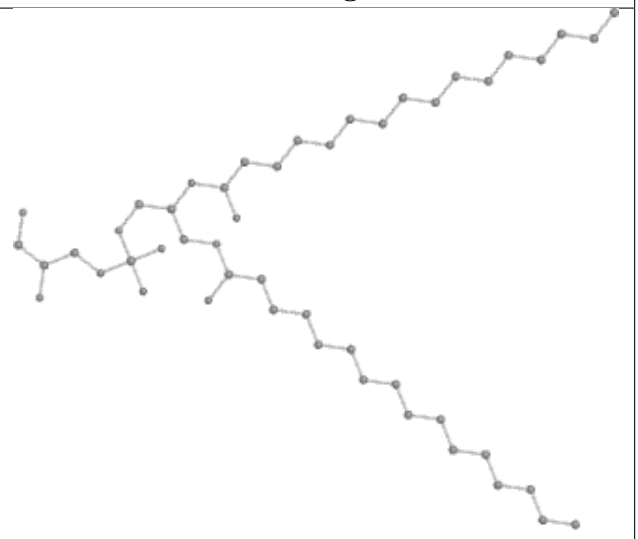


Bond angles

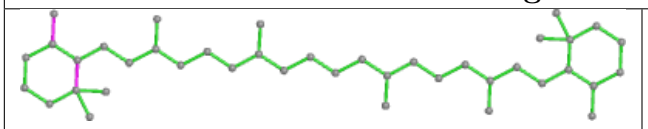


Torsions



Rings

Ligand BCR B 617



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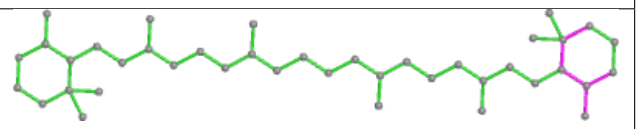
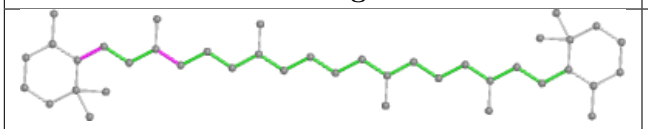


Bond angles



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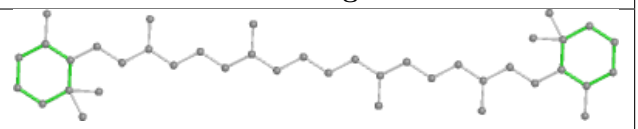
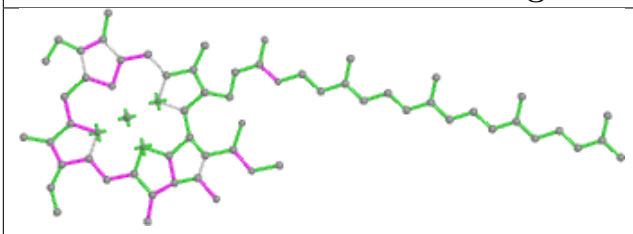


Rings

Ligand CLA b 605



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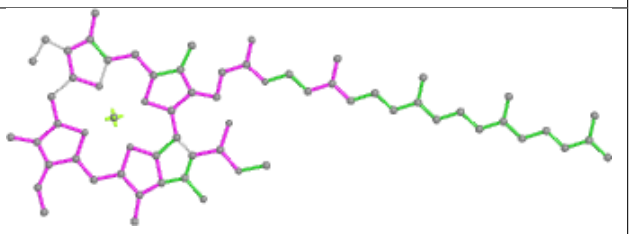
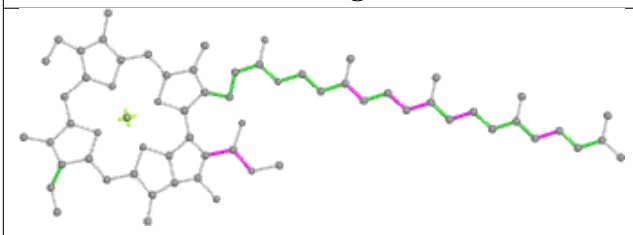
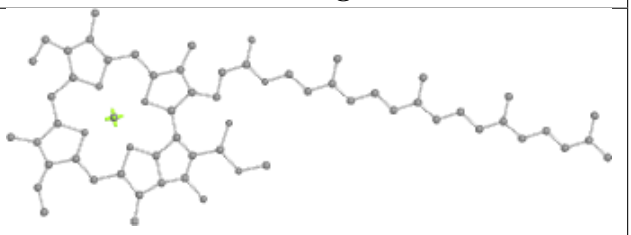


Bond angles

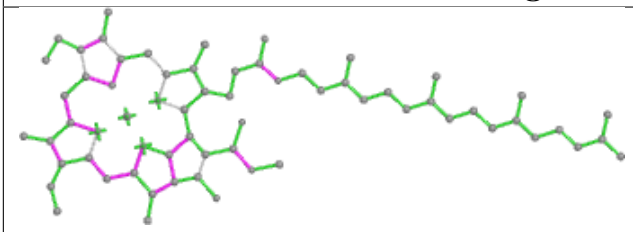


Torsions



Rings

Ligand CLA B 616



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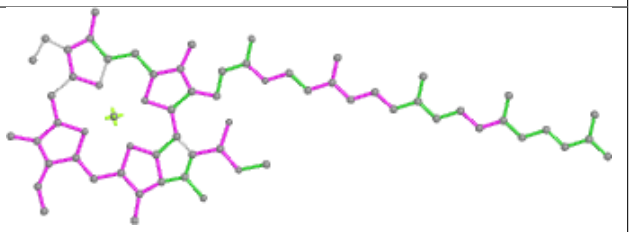

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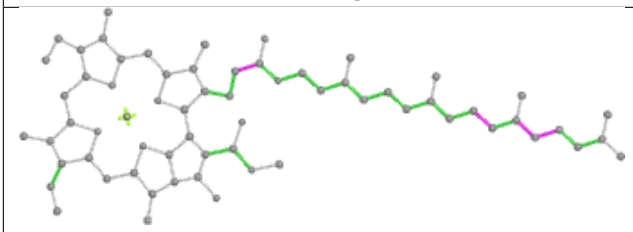

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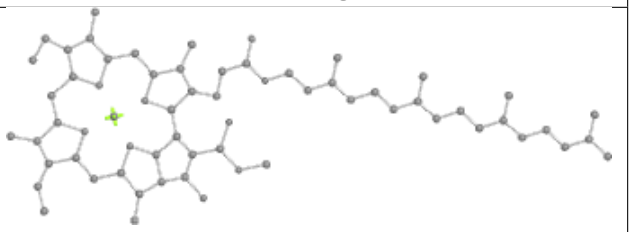
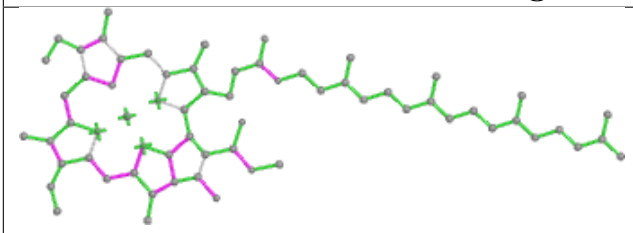


Rings

Ligand CLA a 408



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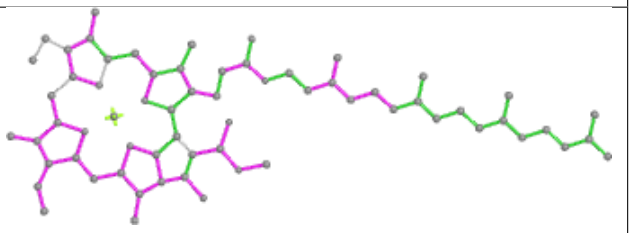
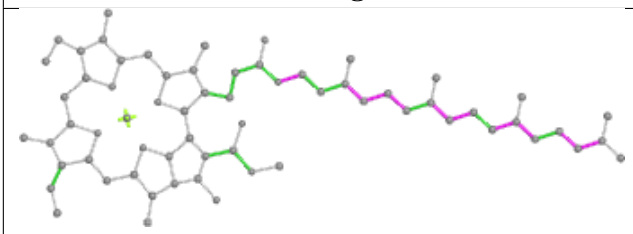


Bond angles



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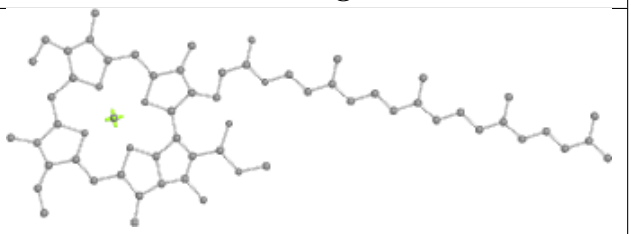
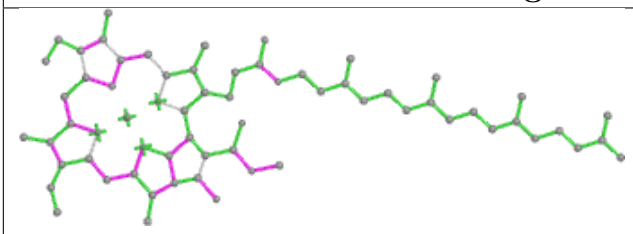


Rings

Ligand CLA B 610



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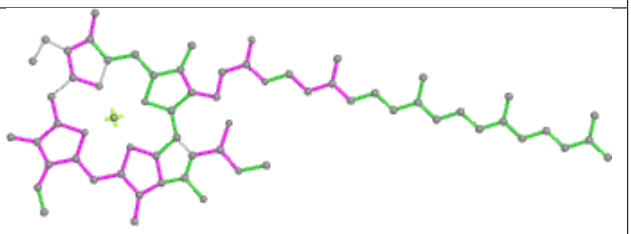
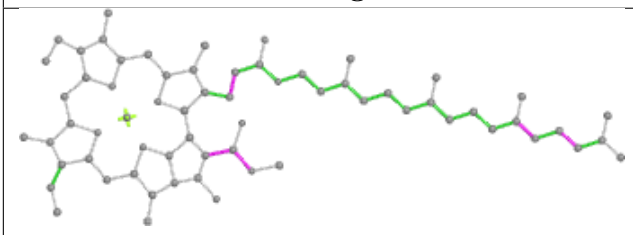


Bond angles



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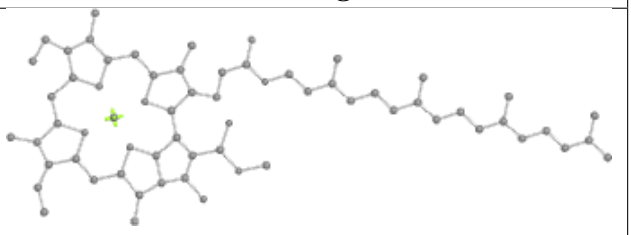
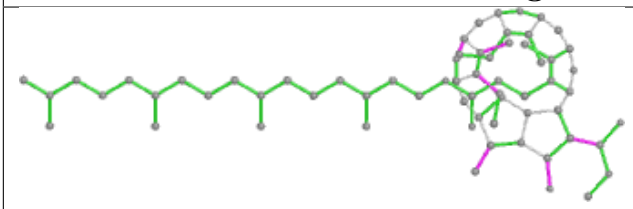


Rings

Ligand PHO a 407



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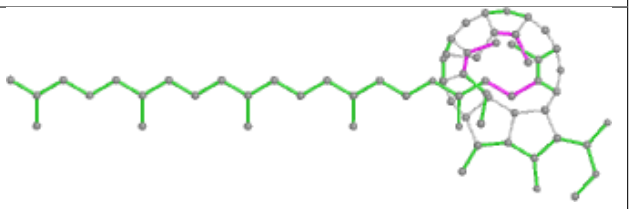
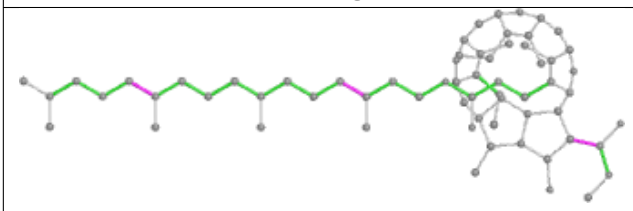


Bond angles



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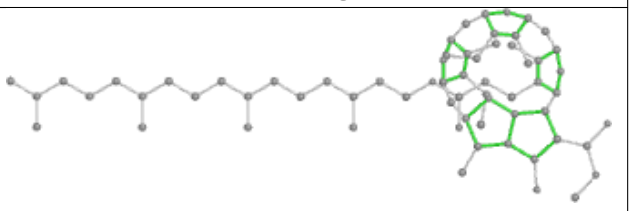
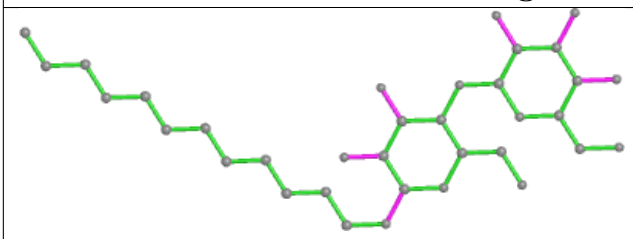
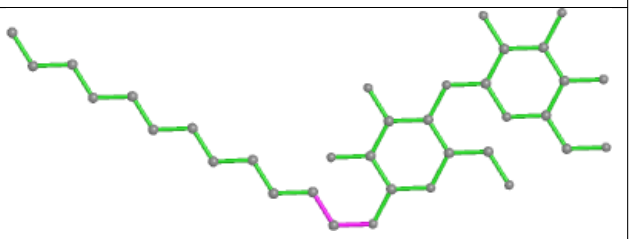


Rings

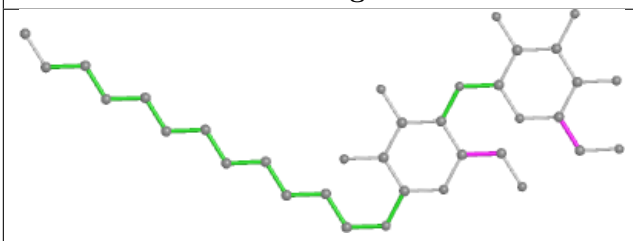
Ligand LMT M 101



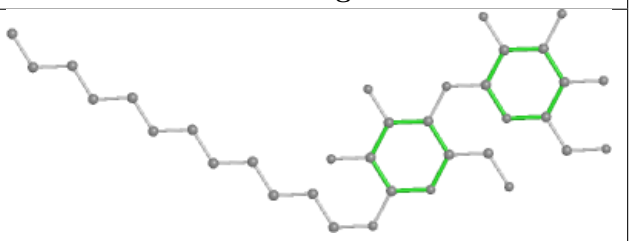
Bond lengths



Bond angles

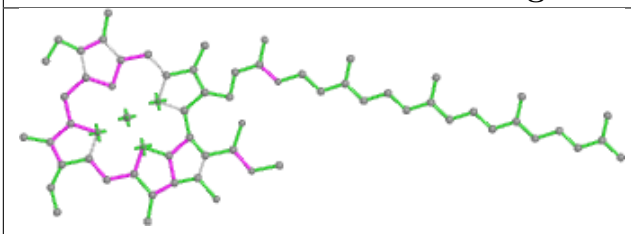


Torsions

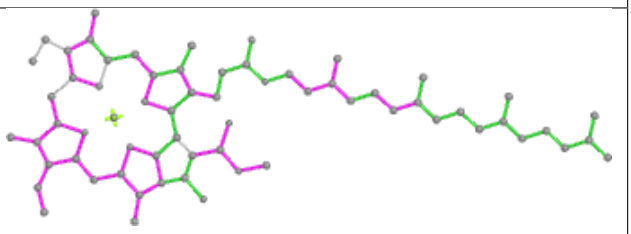


Rings

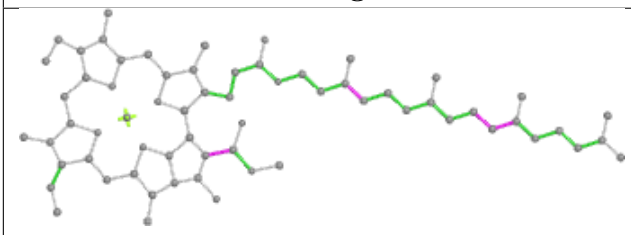
Ligand CLA b 607



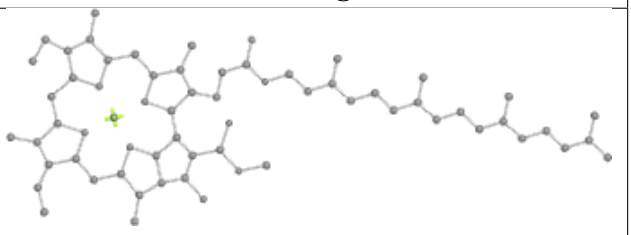
Bond lengths



Bond angles

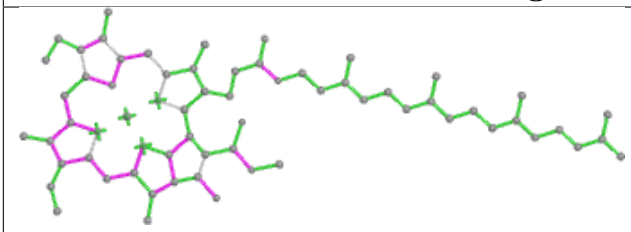


Torsions



Rings

Ligand CLA b 608



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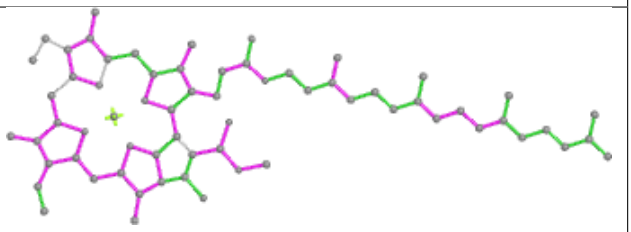
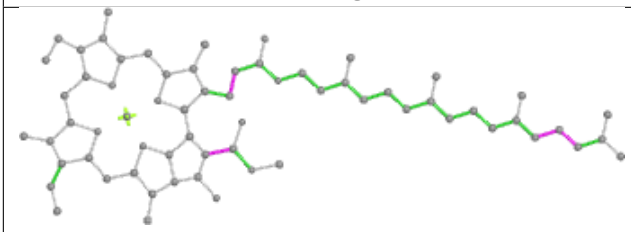
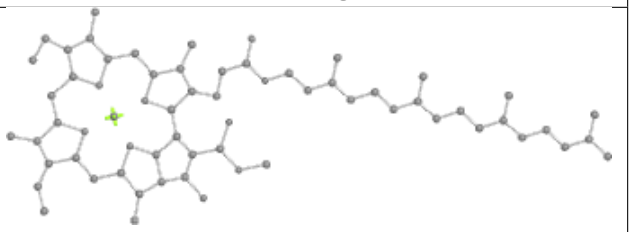


Bond angles

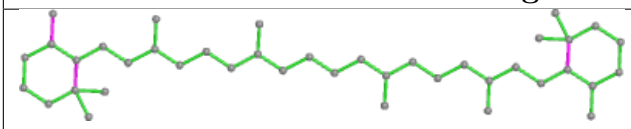


Torsions



Rings

Ligand BCR D 406



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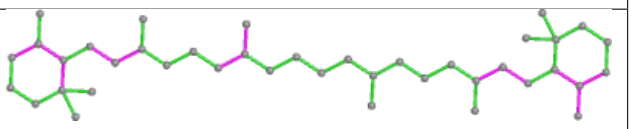
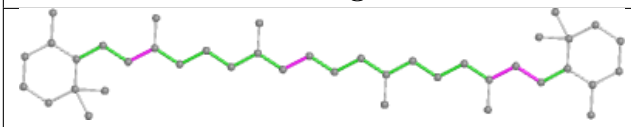


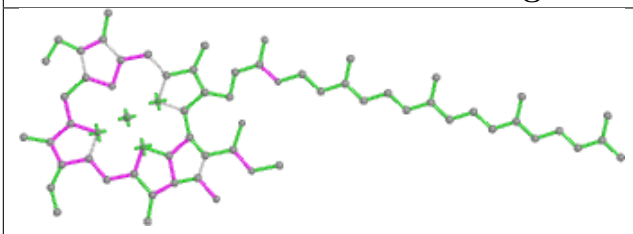
Bond angles



Torsions

Rings

Ligand CLA D 405



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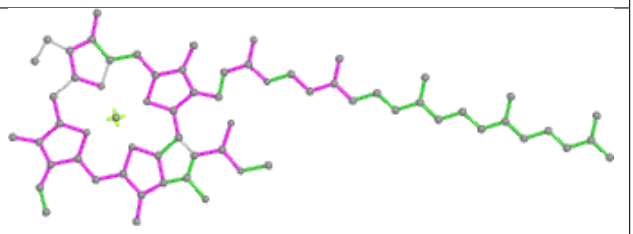
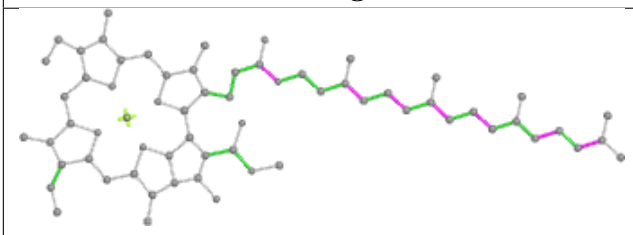
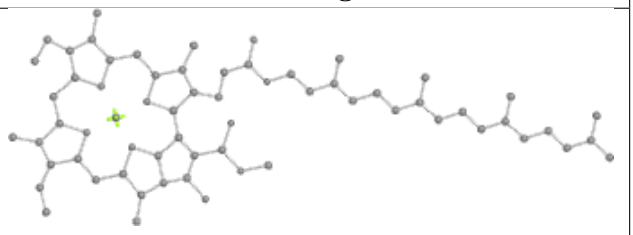


Bond angles

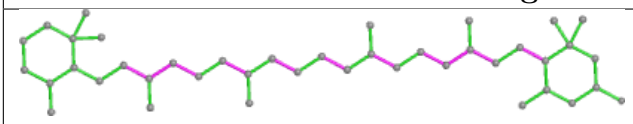


Torsions



Rings

Ligand RRX X 101



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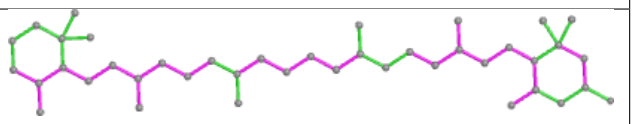
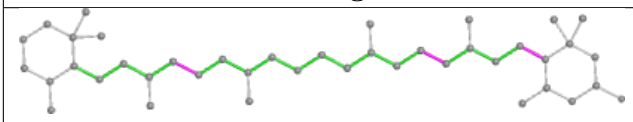


Bond angles



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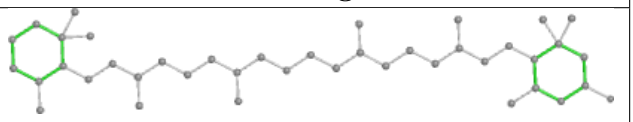
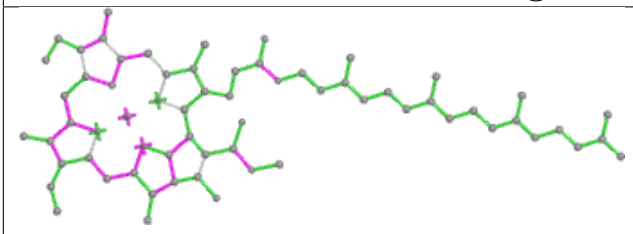


Rings

Ligand CLA b 615



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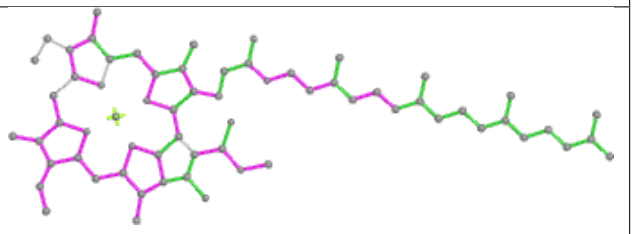
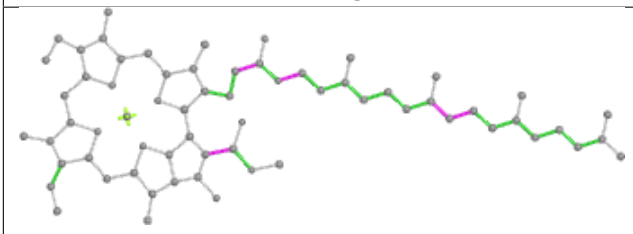


Bond angles



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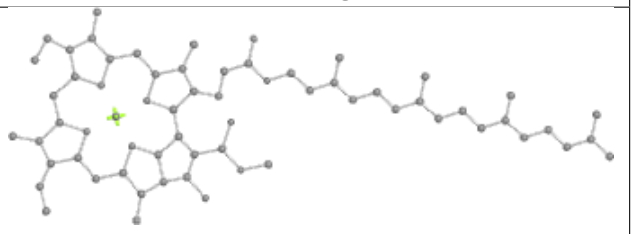
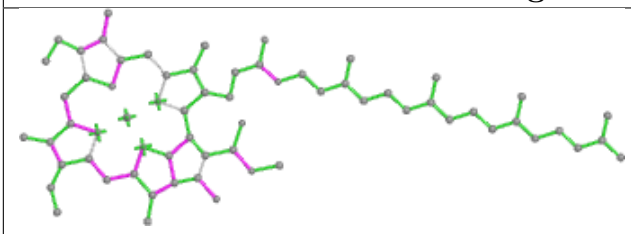


Rings

Ligand CLA b 611



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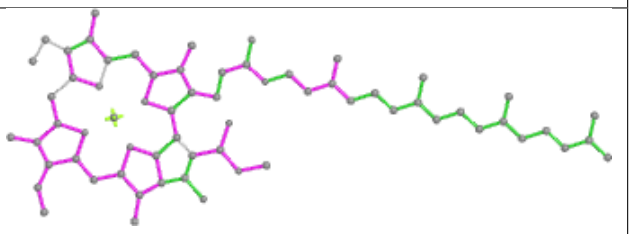
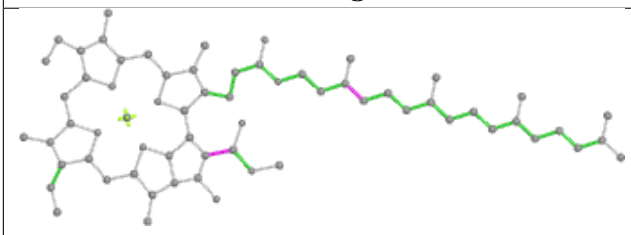


Bond angles



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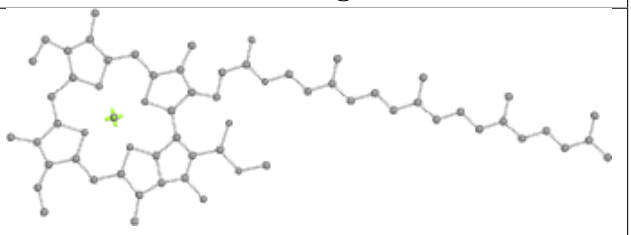
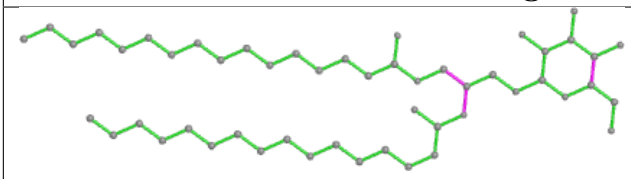


Rings

Ligand LMG b 622



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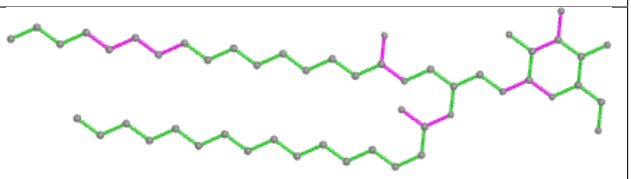
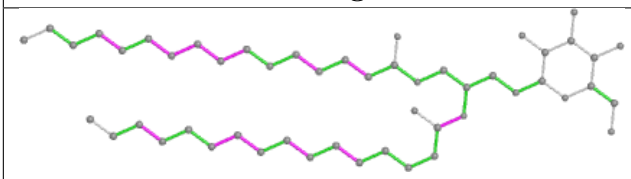


Bond angles



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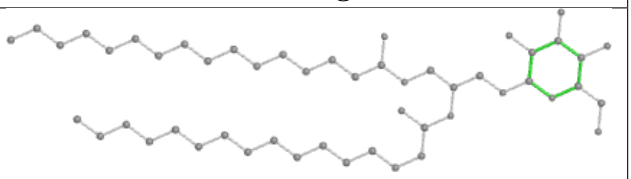
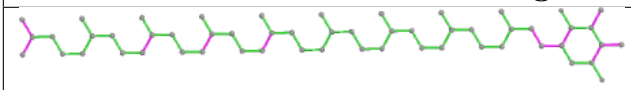
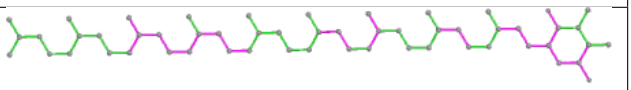


Rings

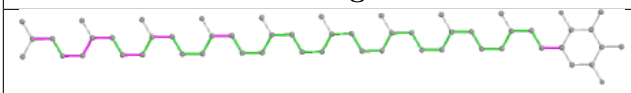
Ligand PL9 d 407



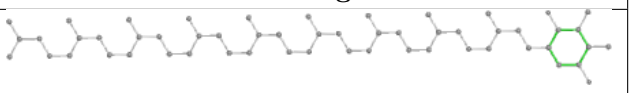
Bond lengths



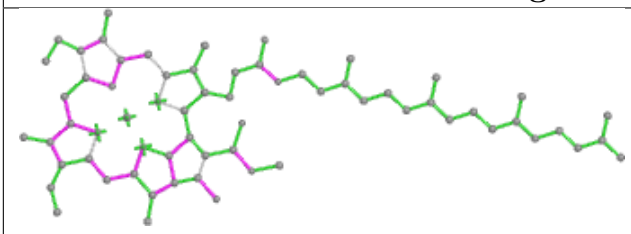
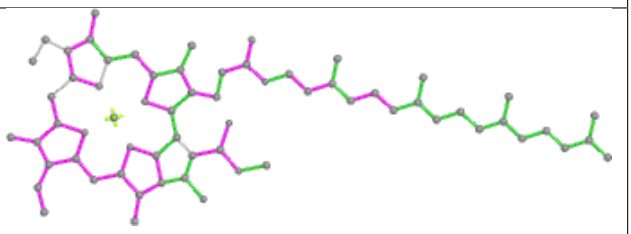
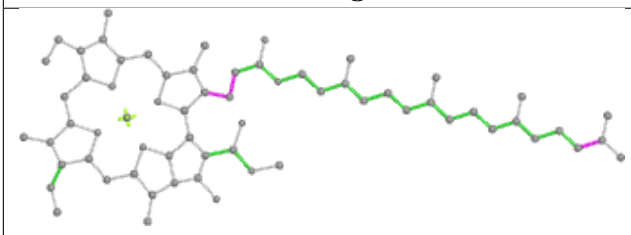
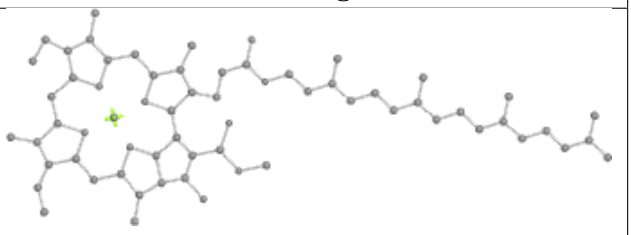
Bond angles

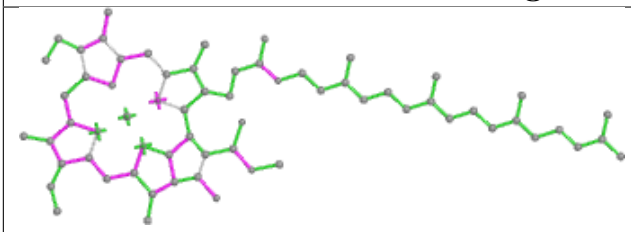
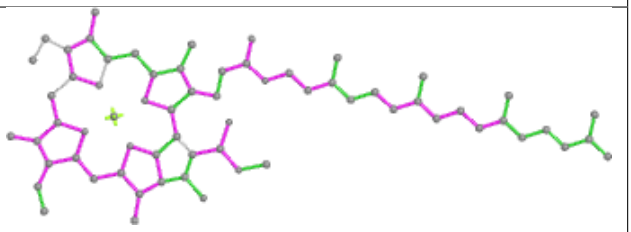
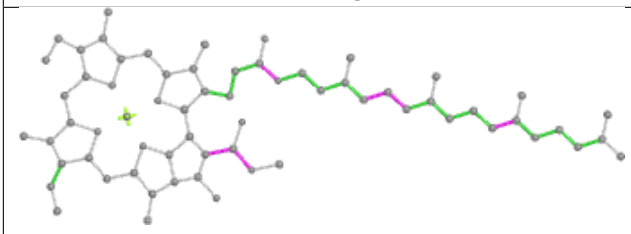
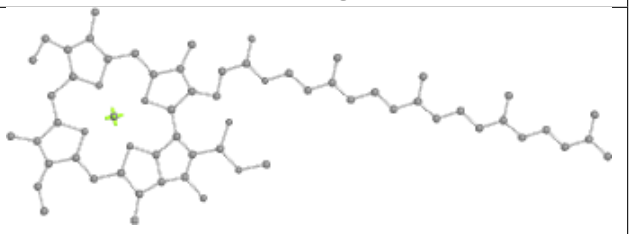


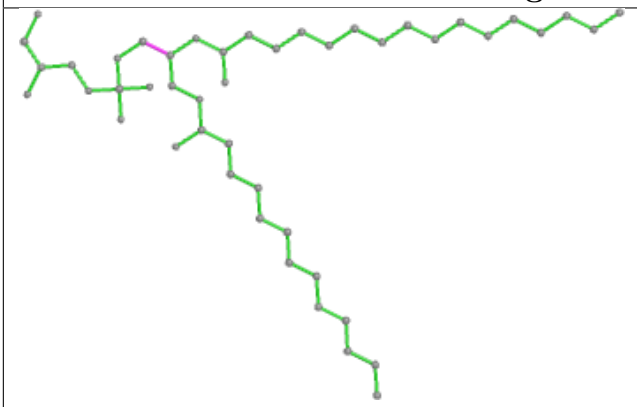
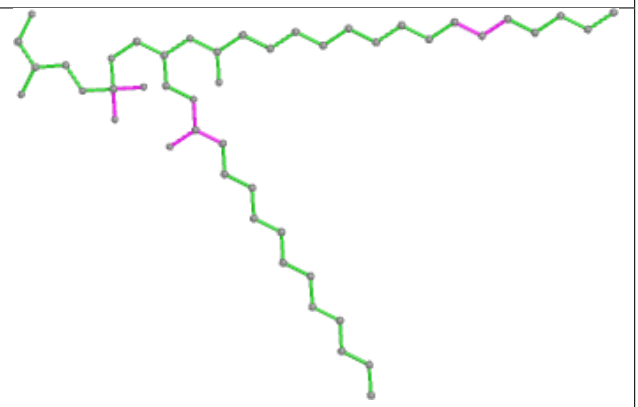
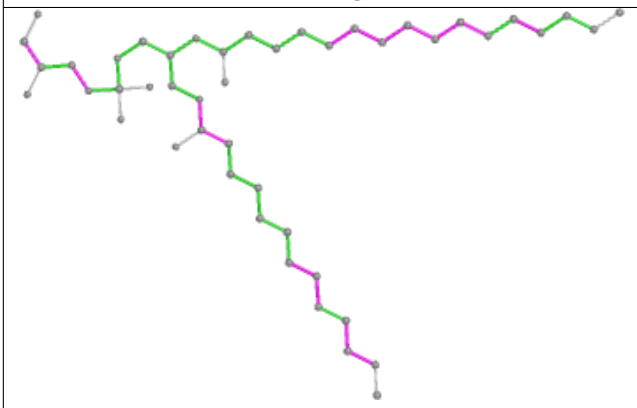
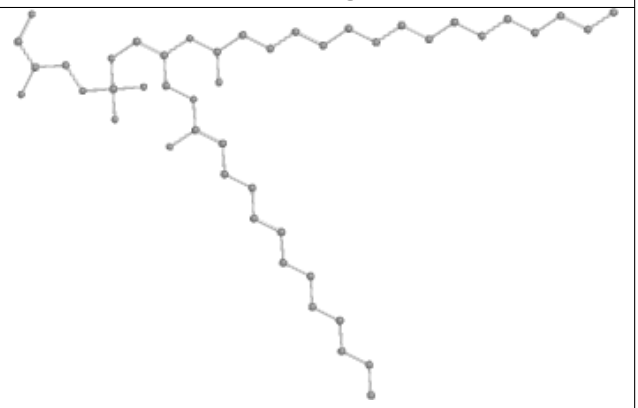
Torsions



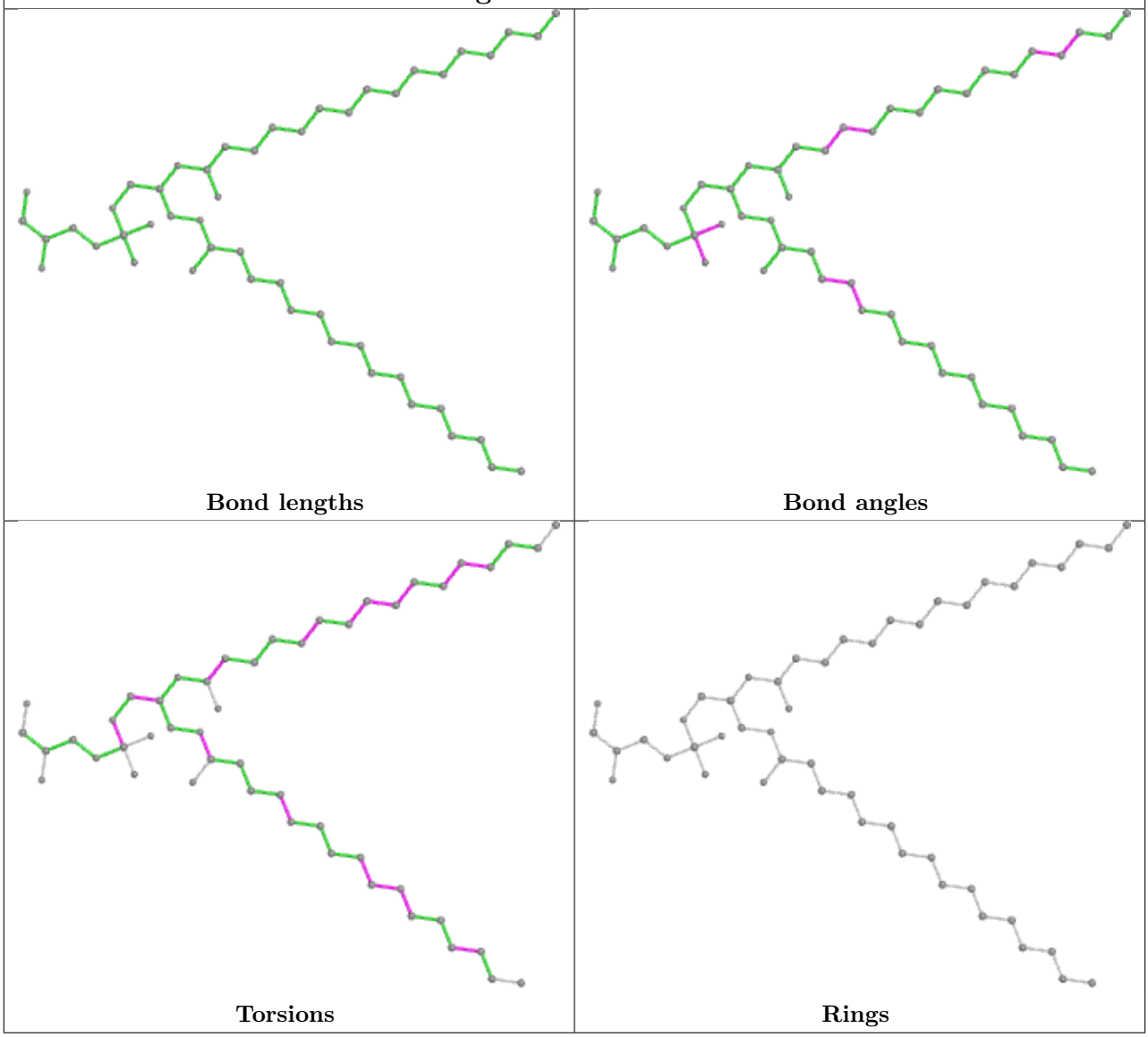
Rings

Ligand CLA c 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

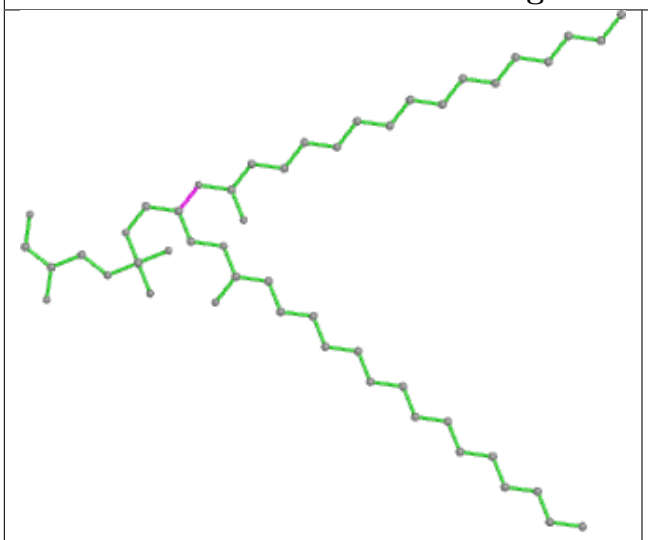
Ligand CLA B 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG d 410	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

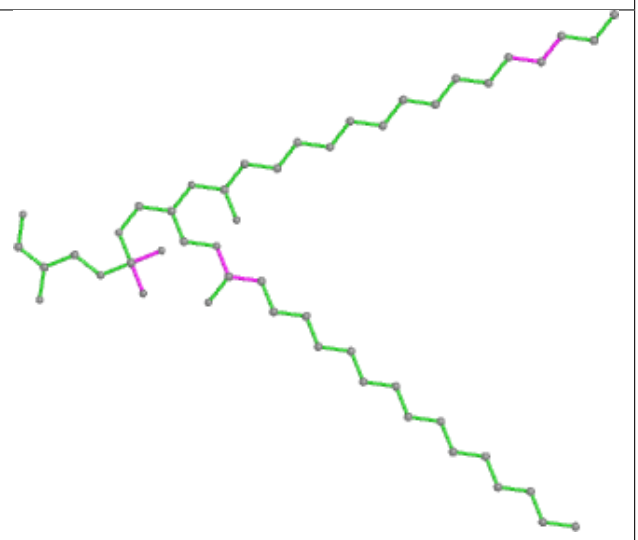
Ligand LHG l 101



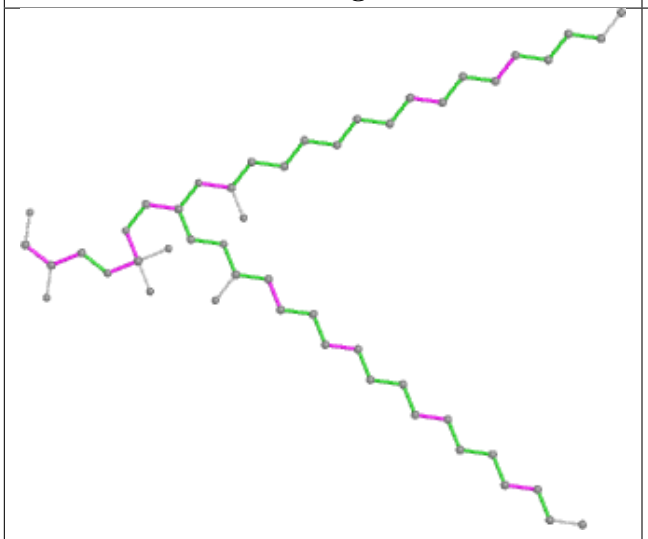
Ligand LHG d 409



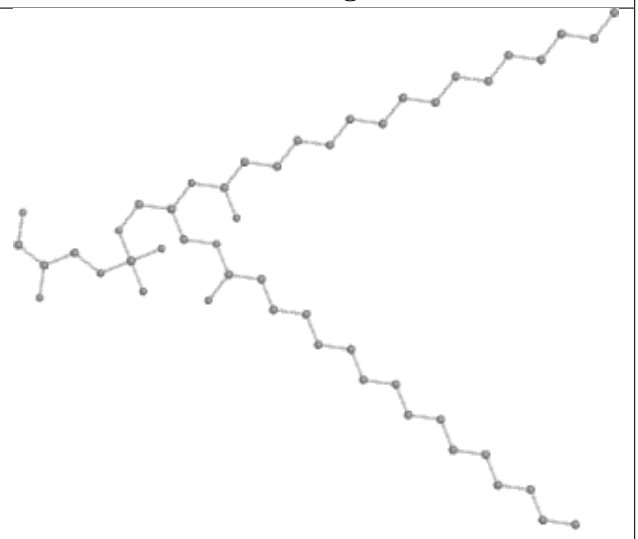
Bond lengths



Bond angles

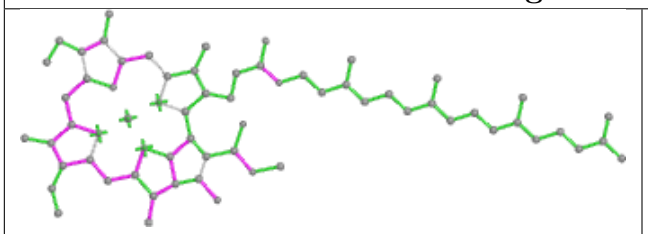


Torsions

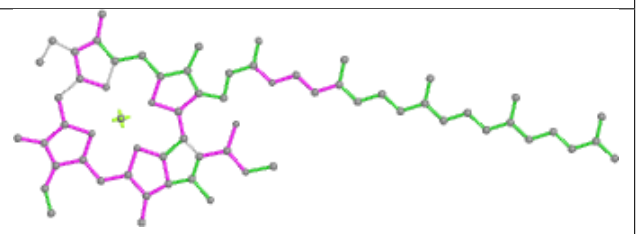


Rings

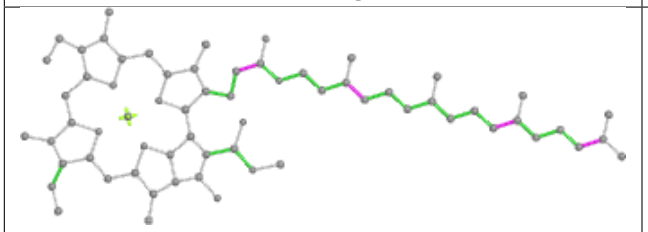
Ligand CLA C 506



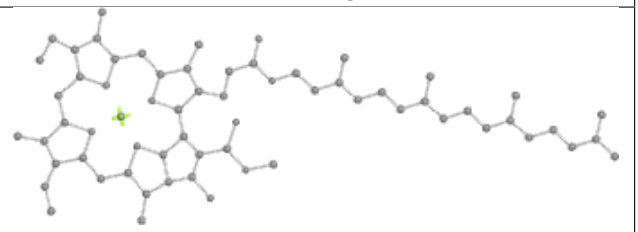
Bond lengths



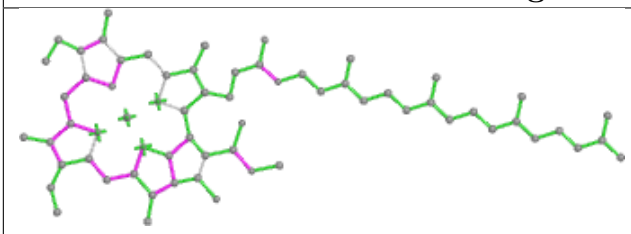
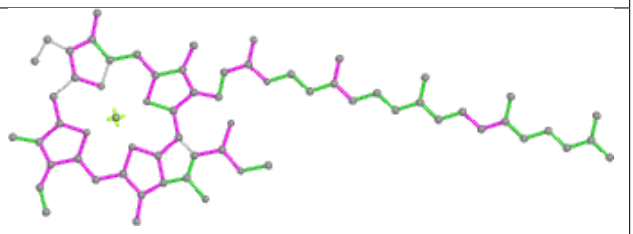
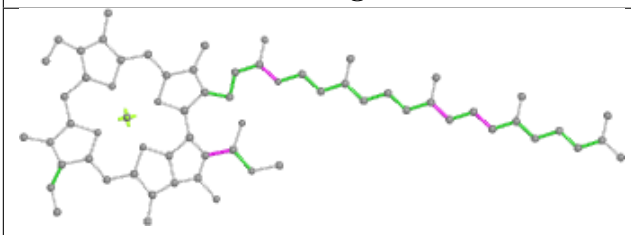
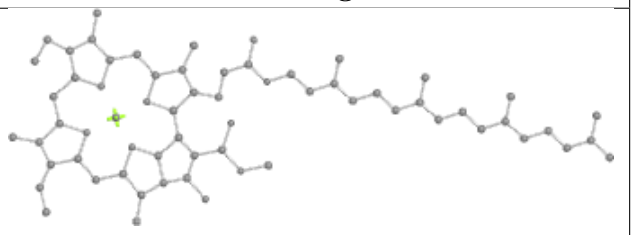
Bond angles



Torsions



Rings

Ligand CLA b 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

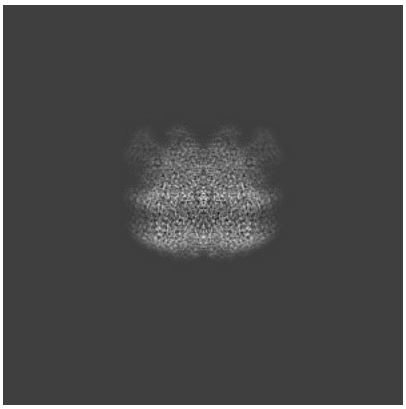
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30547. These allow visual inspection of the internal detail of the map and identification of artifacts.

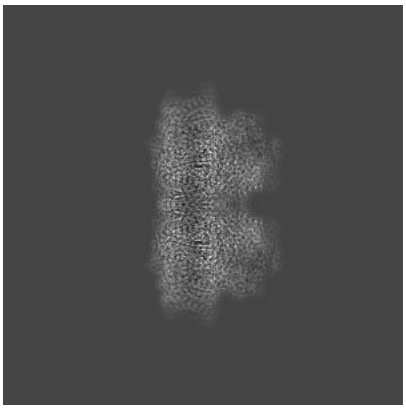
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

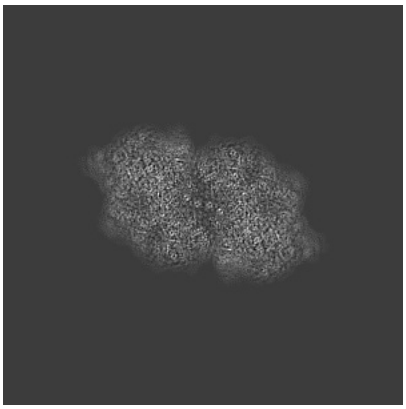
6.1.1 Primary map



X

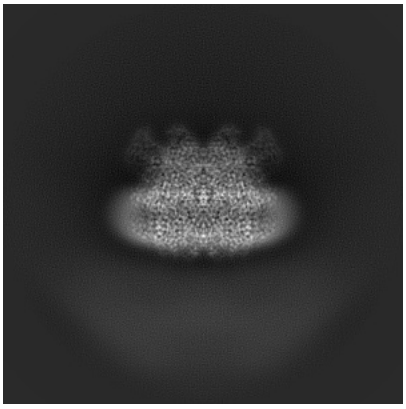


Y

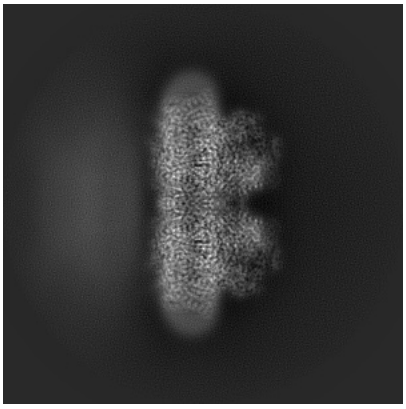


Z

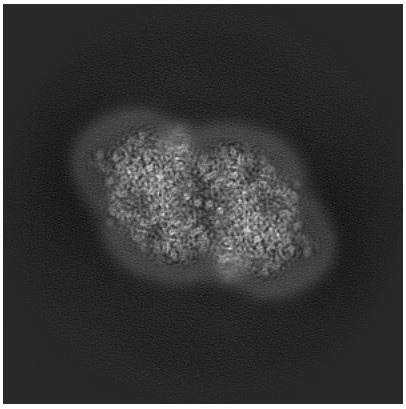
6.1.2 Raw map



X



Y

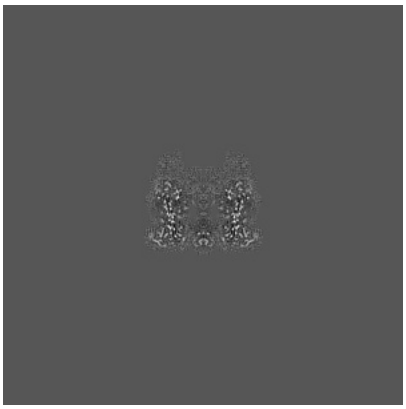


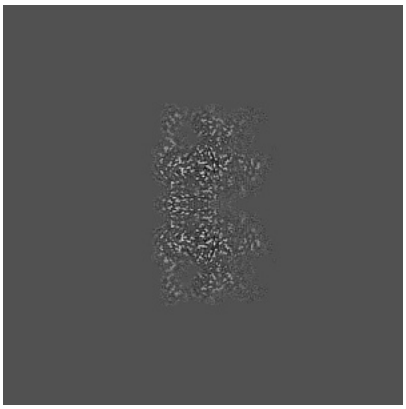
Z

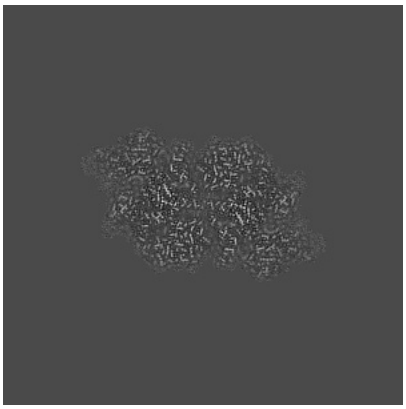
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

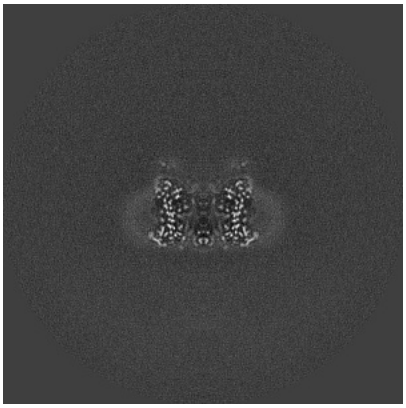
6.2.1 Primary map

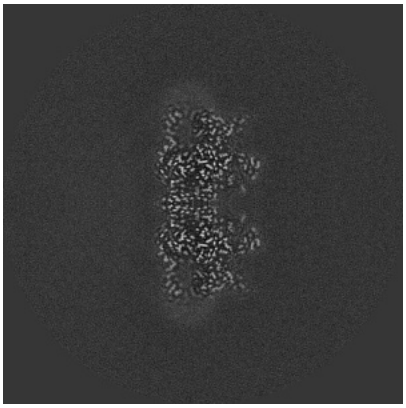

X Index: 200

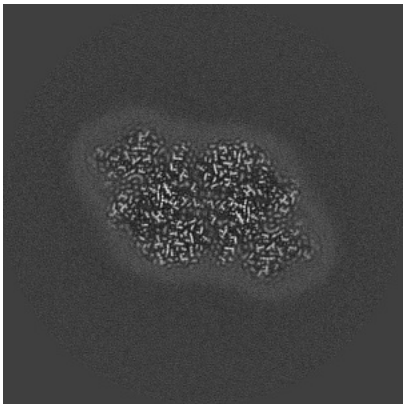

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

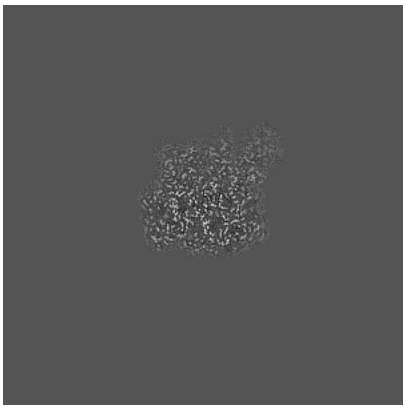

Y Index: 200


Z Index: 200

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

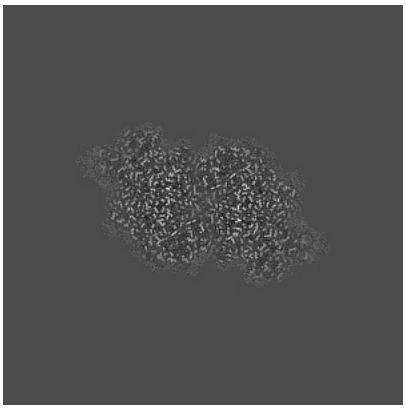
6.3 Largest variance slices (i)

6.3.1 Primary map



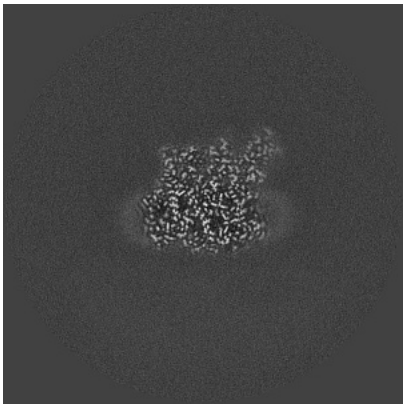
X Index: 167

Y Index: 218



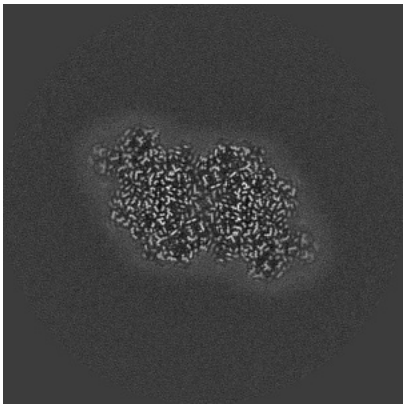
Z Index: 207

6.3.2 Raw map



X Index: 167

Y Index: 218

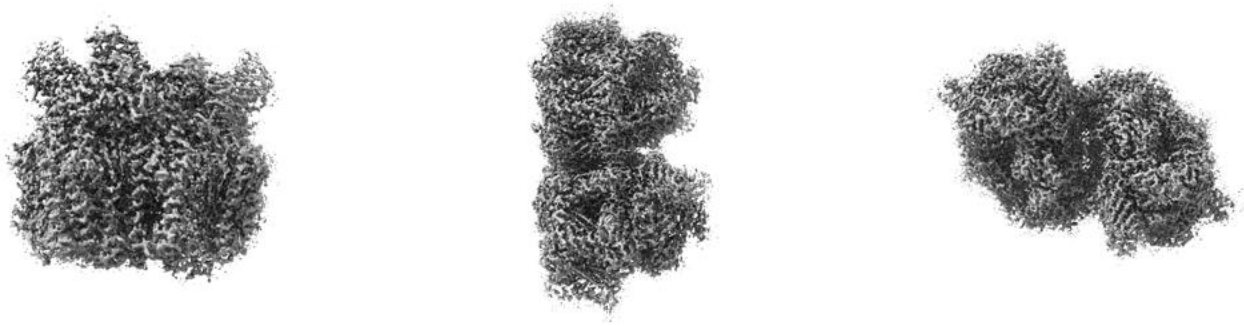


Z Index: 207

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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.

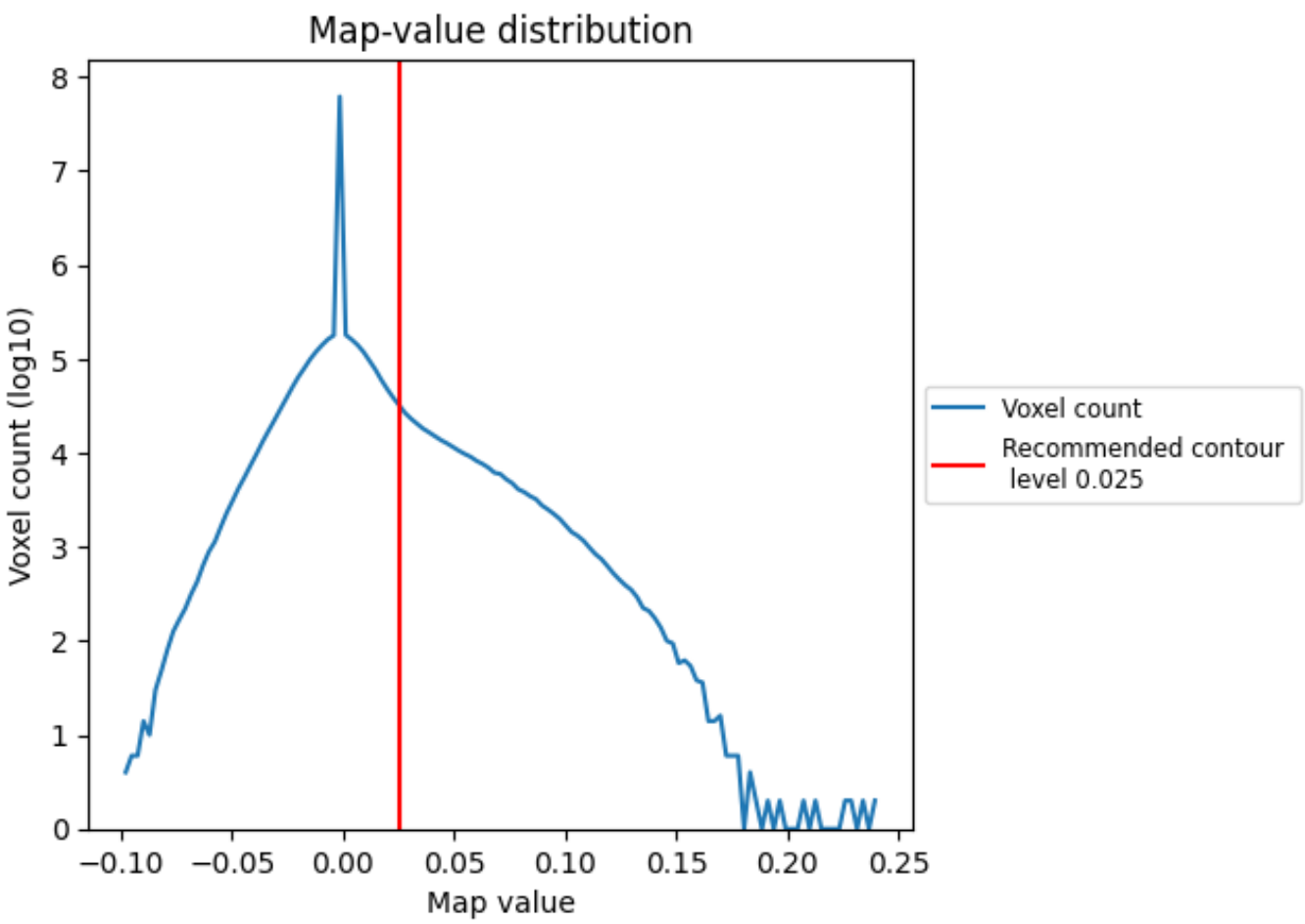
6.5 Mask visualisation (i)

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

7 Map analysis (i)

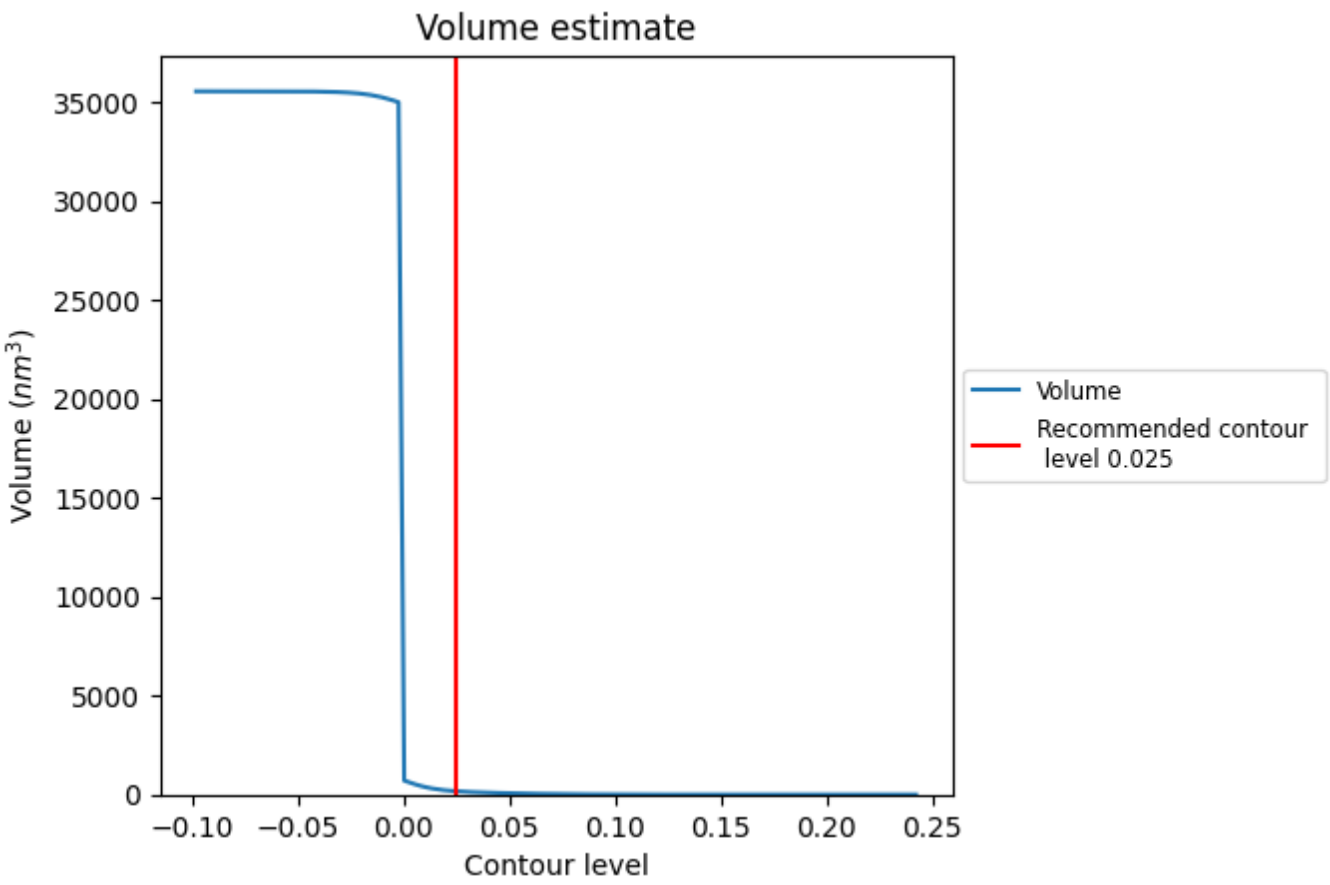
This section contains the results of statistical analysis of the map.

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.

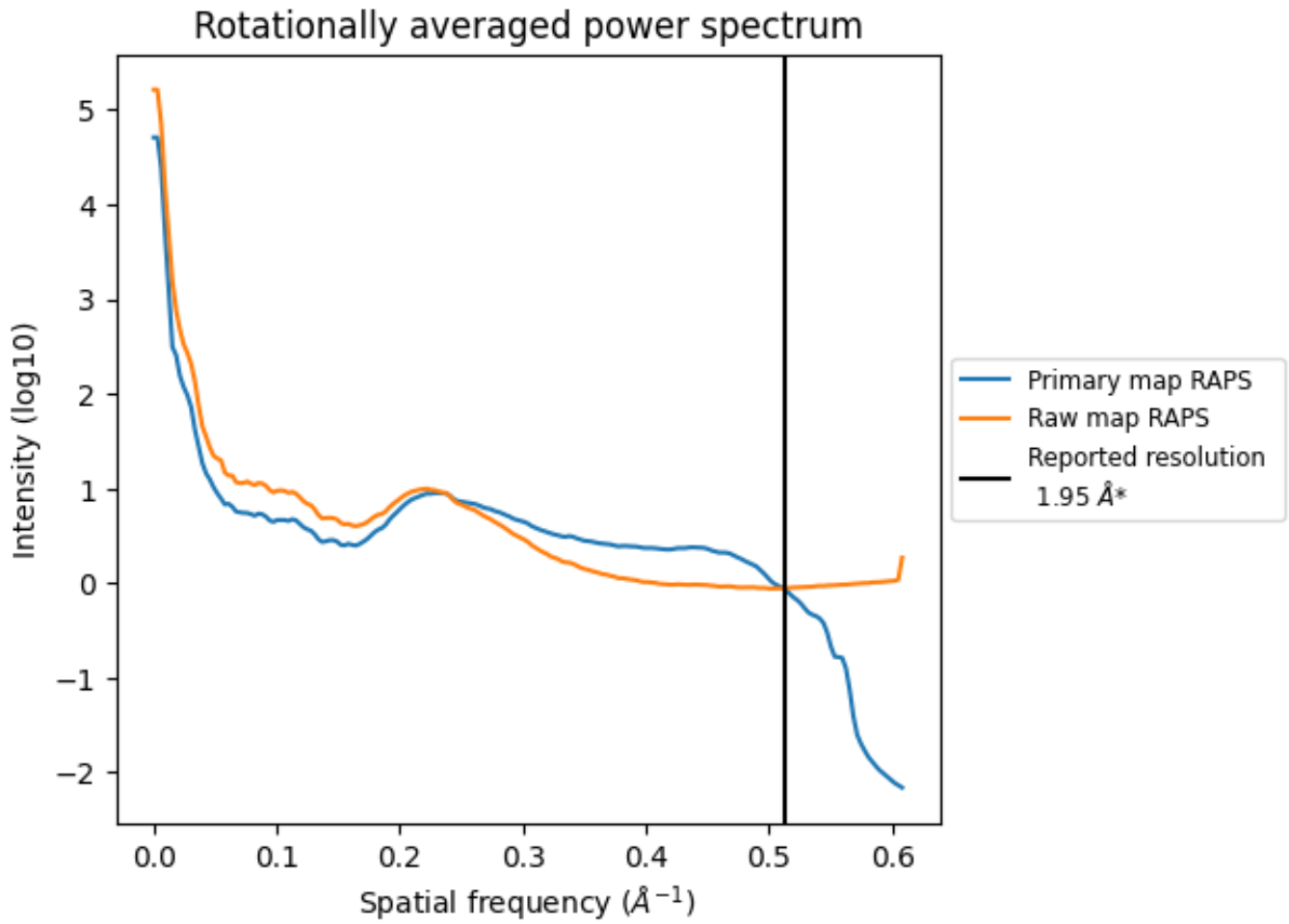
7.2 Volume estimate (i)



The volume at the recommended contour level is 169 nm^3; this corresponds to an approximate mass of 152 kDa.

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

7.3 Rotationally averaged power spectrum (i)

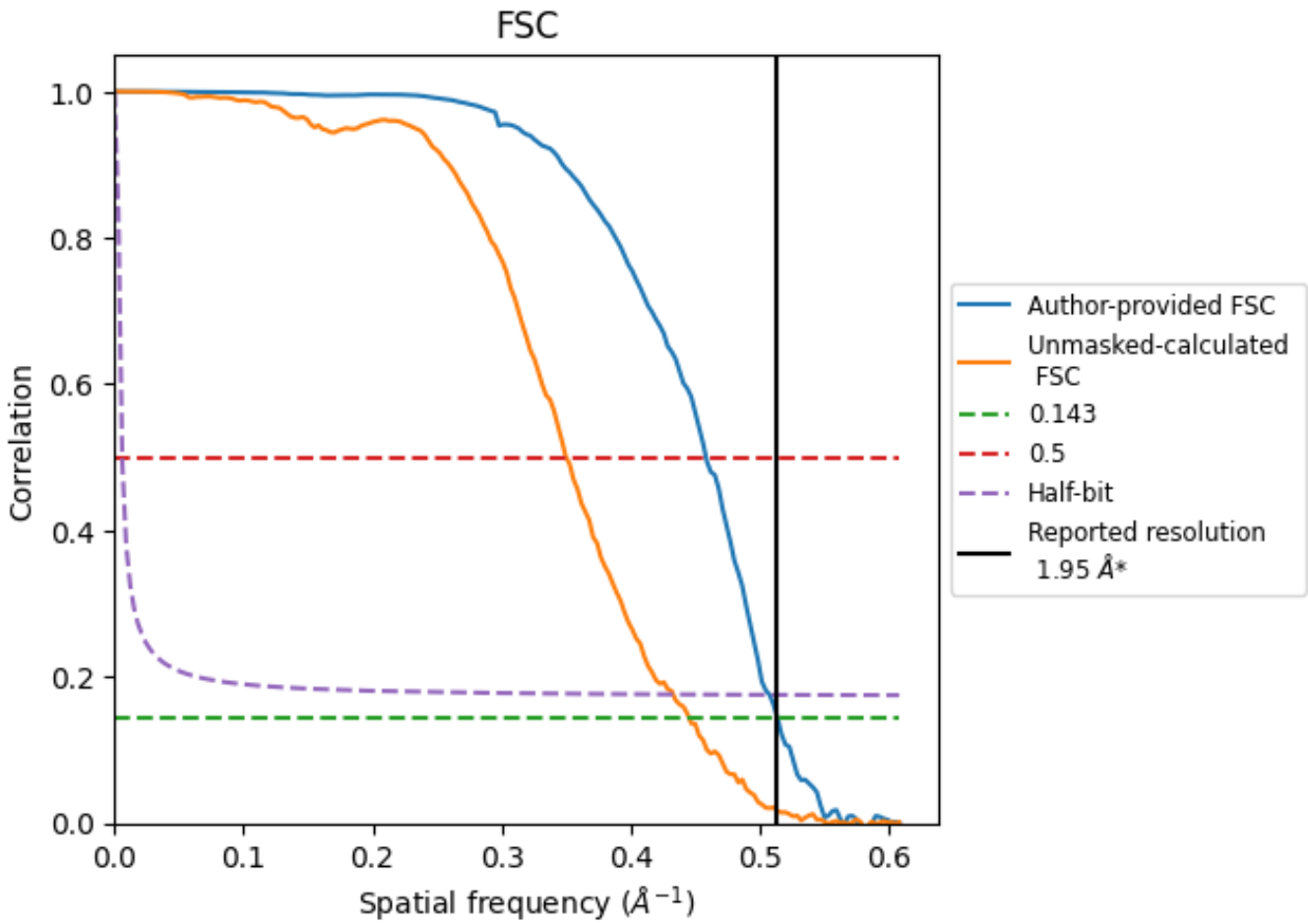


*Reported resolution corresponds to spatial frequency of 0.513 Å^{-1}

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 0.513 Å^{-1}

8.2 Resolution estimates (i)

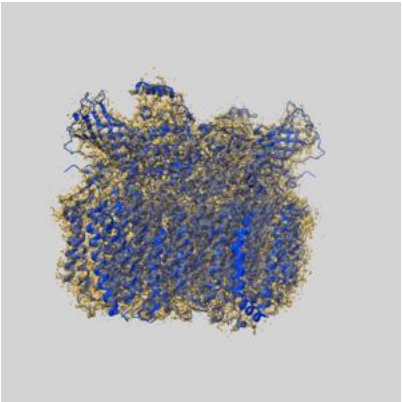
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.95	-	-
Author-provided FSC curve	1.95	2.18	1.97
Unmasked-calculated*	2.24	2.86	2.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.24 differs from the reported value 1.95 by more than 10 %

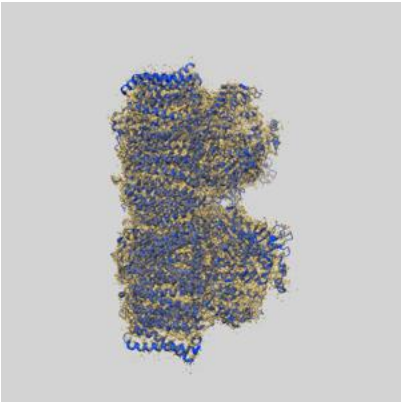
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30547 and PDB model 7D1T. Per-residue inclusion information can be found in section 3 on page 29.

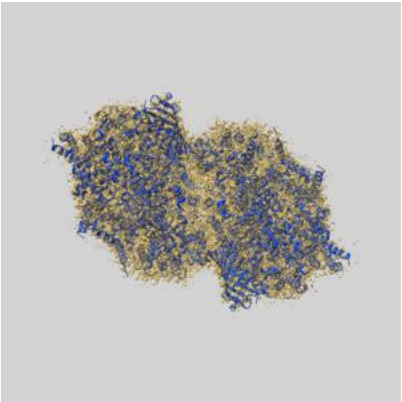
9.1 Map-model overlay (i)



X



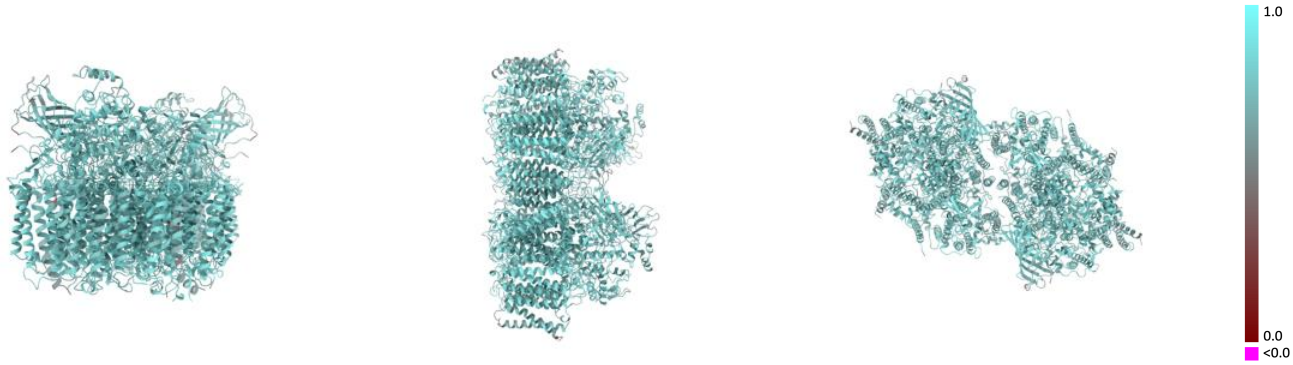
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

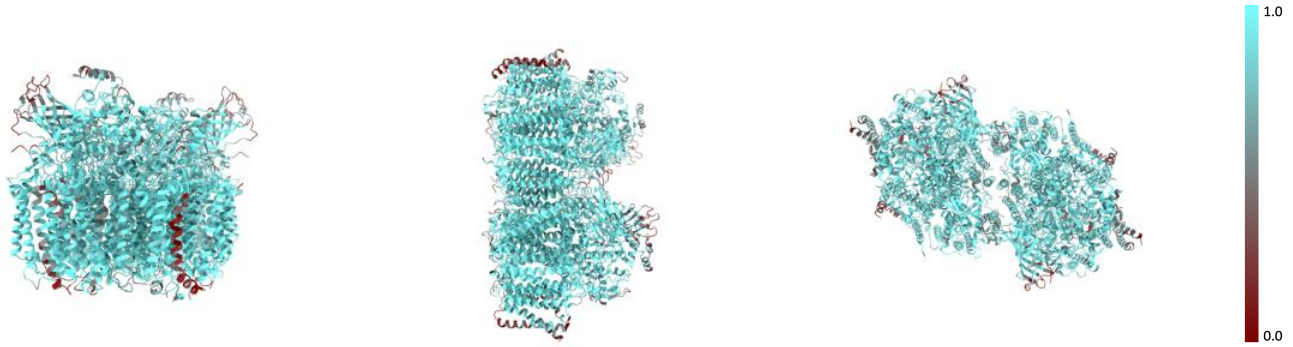
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

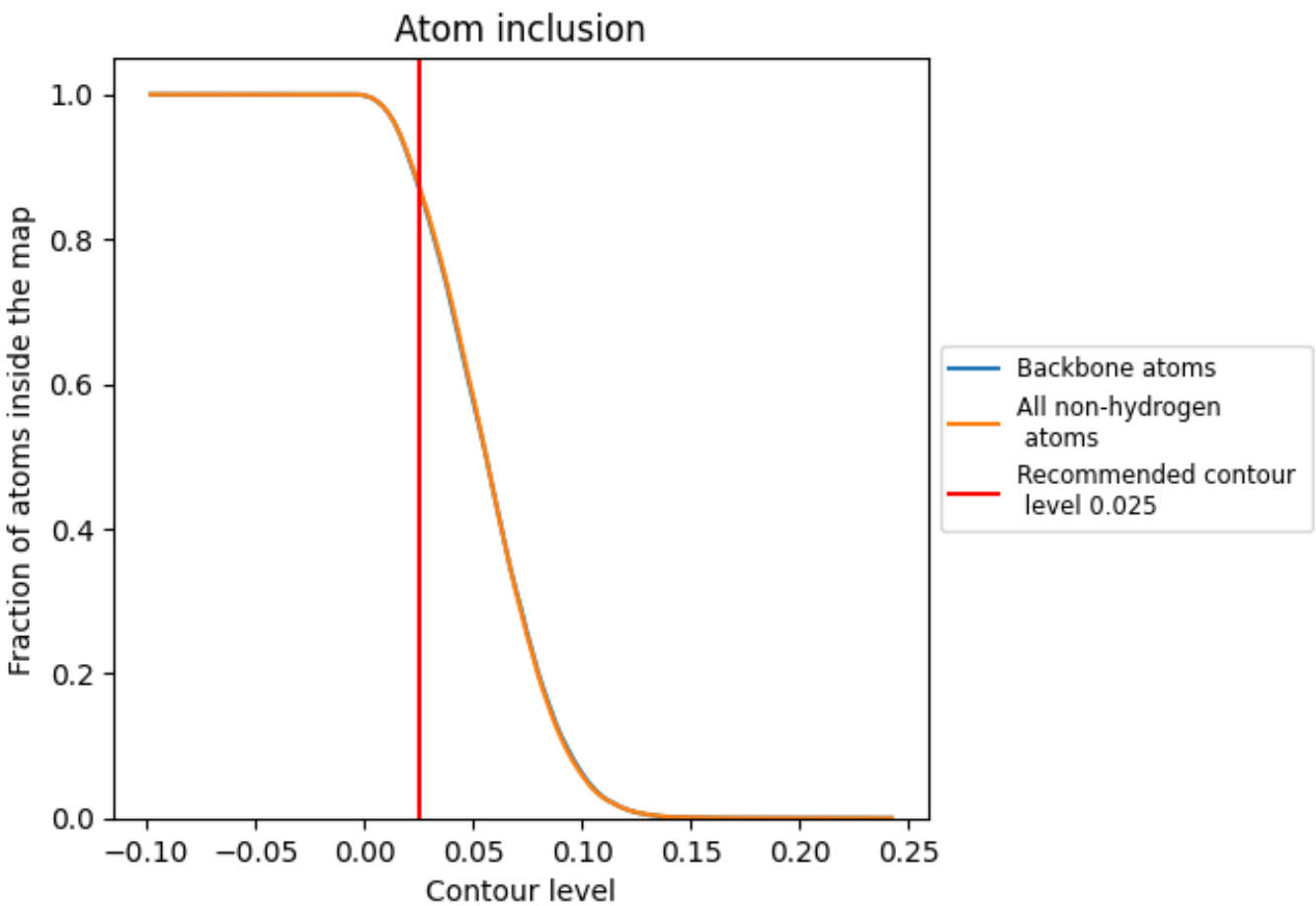
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8752	0.7760
A	0.9331	0.8060
B	0.9182	0.7910
C	0.9010	0.7770
D	0.9445	0.8080
E	0.8345	0.7550
F	0.8599	0.7660
H	0.9199	0.7810
I	0.8994	0.7730
J	0.8410	0.7630
K	0.8080	0.7400
L	0.8828	0.7850
M	0.8750	0.7860
O	0.7411	0.7210
R	0.1992	0.6150
T	0.8997	0.7970
U	0.7842	0.7400
V	0.8656	0.7580
X	0.8727	0.7610
Y	0.6684	0.6940
Z	0.5481	0.6450
a	0.9331	0.8070
b	0.9216	0.7920
c	0.9012	0.7780
d	0.9445	0.8080
e	0.8345	0.7550
f	0.8599	0.7660
h	0.9199	0.7820
i	0.8994	0.7780
j	0.8410	0.7630
k	0.8080	0.7410
l	0.9280	0.8030
m	0.8750	0.7870
o	0.7411	0.7210
r	0.1992	0.6080

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
t	0.8997	0.7970
u	0.7842	0.7410
v	0.8656	0.7610
x	0.8727	0.7590
y	0.6684	0.6900
z	0.5481	0.6410