Full wwPDB EM Validation Report

Sep 14, 2026 – 01:57 PM JST

PDB ID	:	7YMI / pdb_00007ymi
EMDB ID	:	EMD-33929
Title	:	PSII-Pcb Dimer of Acaryochloris Marina
Authors	:	Shen, L.L.; Gao, Y.Z.; Wang, W.D.; Zhang, X.; Shen, J.R.; Wang, P.Y.; Han, G.Y.
Deposited on	:	2022-07-28
Resolution	:	3.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

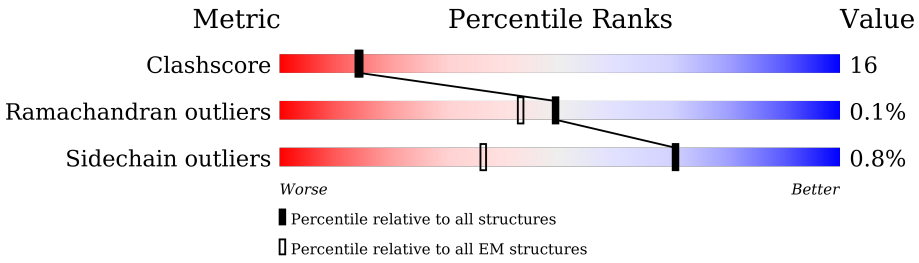
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

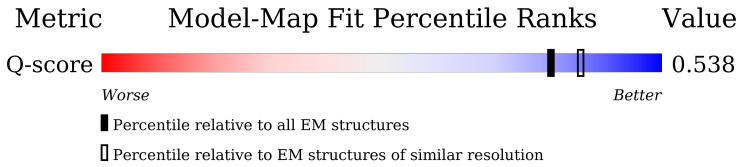
1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 Å.

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





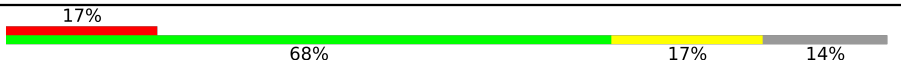
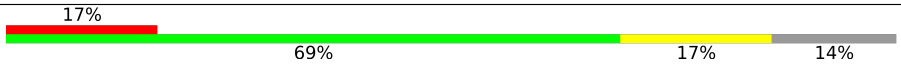
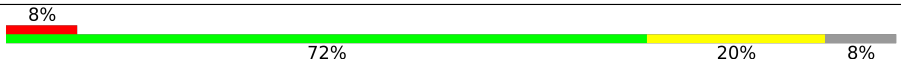
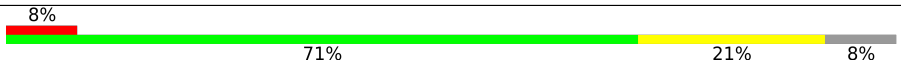
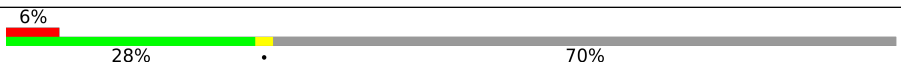
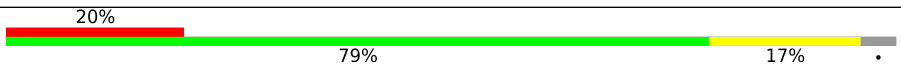
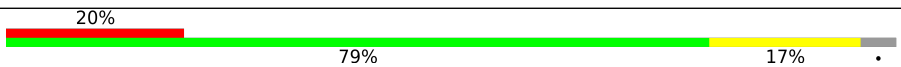
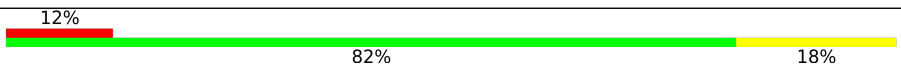
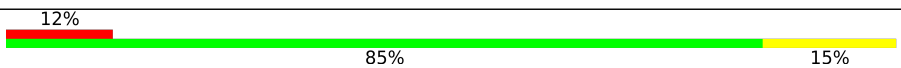
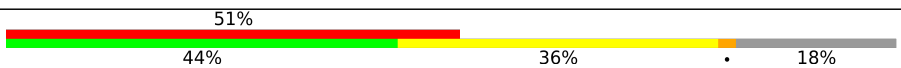
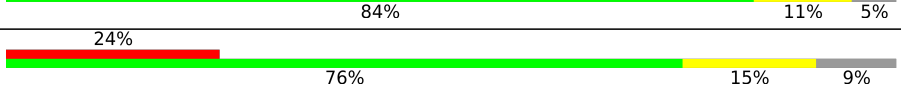
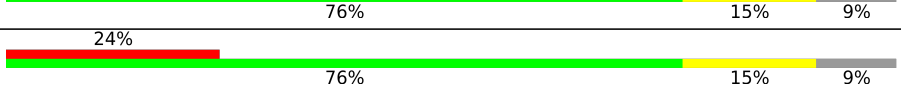
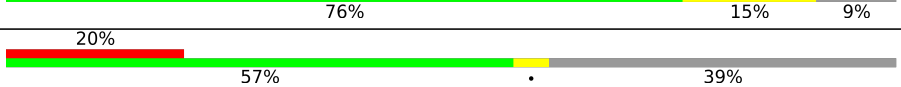
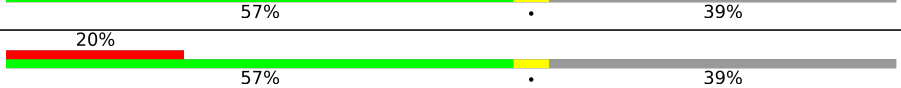
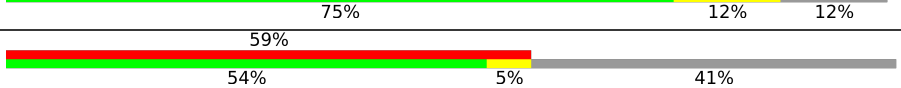
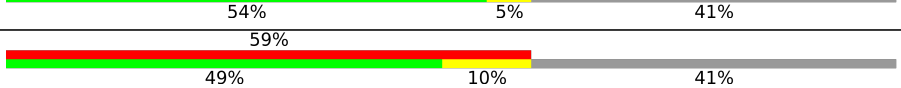
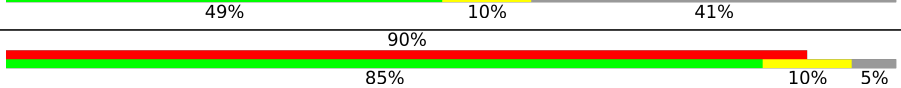
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	360	8% 61% 18% 21%
1	a	360	8% 59% 20% 21%
2	B	506	12% 77% 18% 5%
2	b	506	12% 77% 17% 5%

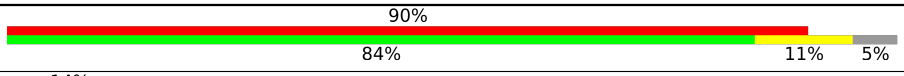
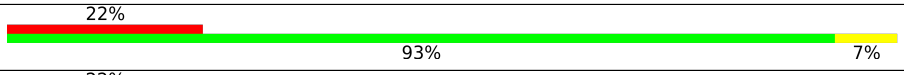
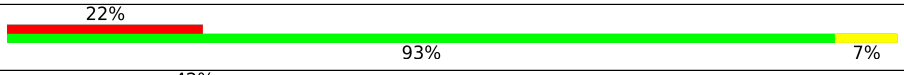
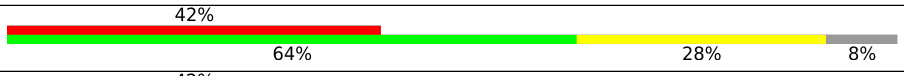
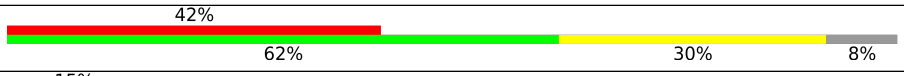
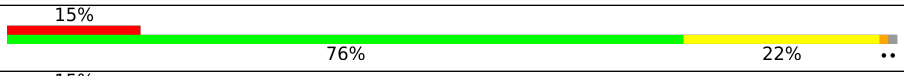
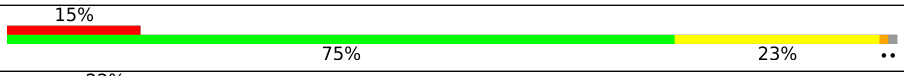
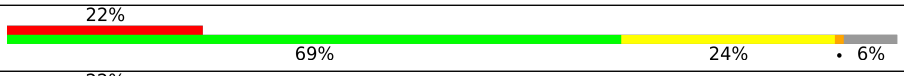
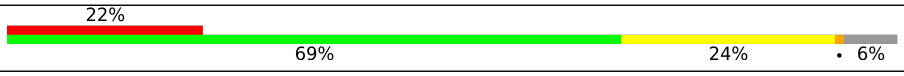
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Mol	Chain	Length	Quality of chain
3	C	490	
3	c	490	
4	D	351	
4	d	351	
5	E	83	
5	e	83	
6	F	99	
6	f	99	
7	H	71	
7	h	71	
8	I	34	
8	i	34	
9	K	45	
9	k	45	
10	L	38	
10	l	38	
11	M	34	
11	m	34	
12	T	46	
12	t	46	
13	X	40	
13	x	40	
14	Y	39	
14	y	39	
15	Z	62	

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Mol	Chain	Length	Quality of chain
15	z	62	
16	2	352	
16	6	352	
17	G	41	
17	g	41	
18	1	356	
18	5	356	
19	3	349	
19	7	349	
20	4	353	
20	8	353	

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
21	CL7	1	402	X	-	-	-
21	CL7	1	403	X	-	-	-
21	CL7	1	404	X	-	-	-
21	CL7	1	405	X	-	-	-
21	CL7	1	406	X	-	-	-
21	CL7	1	407	X	-	-	-
21	CL7	1	408	X	-	-	-
21	CL7	1	409	X	-	-	-
21	CL7	1	410	X	-	-	-
21	CL7	1	411	X	-	-	-
21	CL7	1	412	X	-	-	-
21	CL7	1	413	X	-	-	-
21	CL7	1	414	X	-	-	-
21	CL7	1	415	X	-	-	-
21	CL7	1	416	X	-	-	-
21	CL7	1	417	X	-	-	-
21	CL7	1	418	X	-	-	-
21	CL7	1	419	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	1	420	X	-	-	-
21	CL7	2	501	X	-	-	-
21	CL7	2	502	X	-	-	-
21	CL7	2	503	X	-	-	-
21	CL7	2	504	X	-	-	-
21	CL7	2	505	X	-	-	-
21	CL7	2	506	X	-	-	-
21	CL7	2	507	X	-	-	-
21	CL7	2	508	X	-	-	-
21	CL7	2	509	X	-	-	-
21	CL7	2	510	X	-	-	-
21	CL7	2	511	X	-	-	-
21	CL7	2	512	X	-	-	-
21	CL7	2	513	X	-	-	-
21	CL7	2	514	X	-	-	-
21	CL7	2	515	X	-	-	-
21	CL7	2	516	X	-	-	-
21	CL7	2	517	X	-	-	-
21	CL7	2	518	X	-	-	-
21	CL7	3	501	X	-	-	-
21	CL7	3	502	X	-	-	-
21	CL7	3	503	X	-	-	-
21	CL7	3	504	X	-	-	-
21	CL7	3	505	X	-	-	-
21	CL7	3	506	X	-	-	-
21	CL7	3	507	X	-	-	-
21	CL7	3	508	X	-	-	-
21	CL7	3	509	X	-	-	-
21	CL7	3	510	X	-	-	-
21	CL7	3	511	X	-	-	-
21	CL7	3	512	X	-	-	-
21	CL7	3	513	X	-	-	-
21	CL7	3	514	X	-	-	-
21	CL7	3	515	X	-	-	-
21	CL7	3	516	X	-	-	-
21	CL7	3	517	X	-	-	-
21	CL7	3	518	X	-	-	-
21	CL7	4	404	X	-	-	-
21	CL7	4	405	X	-	-	-
21	CL7	4	406	X	-	-	-
21	CL7	4	407	X	-	-	-
21	CL7	4	408	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	4	409	X	-	-	-
21	CL7	4	410	X	-	-	-
21	CL7	4	411	X	-	-	-
21	CL7	4	412	X	-	-	-
21	CL7	4	413	X	-	-	-
21	CL7	4	414	X	-	-	-
21	CL7	4	415	X	-	-	-
21	CL7	4	416	X	-	-	-
21	CL7	4	417	X	-	-	-
21	CL7	5	402	X	-	-	-
21	CL7	5	403	X	-	-	-
21	CL7	5	404	X	-	-	-
21	CL7	5	405	X	-	-	-
21	CL7	5	406	X	-	-	-
21	CL7	5	407	X	-	-	-
21	CL7	5	408	X	-	-	-
21	CL7	5	409	X	-	-	-
21	CL7	5	410	X	-	-	-
21	CL7	5	411	X	-	-	-
21	CL7	5	412	X	-	-	-
21	CL7	5	413	X	-	-	-
21	CL7	5	414	X	-	-	-
21	CL7	5	415	X	-	-	-
21	CL7	5	416	X	-	-	-
21	CL7	5	417	X	-	-	-
21	CL7	5	418	X	-	-	-
21	CL7	5	419	X	-	-	-
21	CL7	5	420	X	-	-	-
21	CL7	6	501	X	-	-	-
21	CL7	6	502	X	-	-	-
21	CL7	6	503	X	-	-	-
21	CL7	6	504	X	-	-	-
21	CL7	6	505	X	-	-	-
21	CL7	6	506	X	-	-	-
21	CL7	6	507	X	-	-	-
21	CL7	6	508	X	-	-	-
21	CL7	6	509	X	-	-	-
21	CL7	6	510	X	-	-	-
21	CL7	6	511	X	-	-	-
21	CL7	6	512	X	-	-	-
21	CL7	6	513	X	-	-	-
21	CL7	6	514	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	6	515	X	-	-	-
21	CL7	6	516	X	-	-	-
21	CL7	6	517	X	-	-	-
21	CL7	6	518	X	-	-	-
21	CL7	7	501	X	-	-	-
21	CL7	7	502	X	-	-	-
21	CL7	7	503	X	-	-	-
21	CL7	7	504	X	-	-	-
21	CL7	7	505	X	-	-	-
21	CL7	7	506	X	-	-	-
21	CL7	7	507	X	-	-	-
21	CL7	7	508	X	-	-	-
21	CL7	7	509	X	-	-	-
21	CL7	7	510	X	-	-	-
21	CL7	7	511	X	-	-	-
21	CL7	7	512	X	-	-	-
21	CL7	7	513	X	-	-	-
21	CL7	7	514	X	-	-	-
21	CL7	7	515	X	-	-	-
21	CL7	7	516	X	-	-	-
21	CL7	7	517	X	-	-	-
21	CL7	7	518	X	-	-	-
21	CL7	8	404	X	-	-	-
21	CL7	8	405	X	-	-	-
21	CL7	8	406	X	-	-	-
21	CL7	8	407	X	-	-	-
21	CL7	8	408	X	-	-	-
21	CL7	8	409	X	-	-	-
21	CL7	8	410	X	-	-	-
21	CL7	8	411	X	-	-	-
21	CL7	8	412	X	-	-	-
21	CL7	8	413	X	-	-	-
21	CL7	8	414	X	-	-	-
21	CL7	8	415	X	-	-	-
21	CL7	8	416	X	-	-	-
21	CL7	8	417	X	-	-	-
21	CL7	A	401	X	-	-	-
21	CL7	A	403	X	-	-	-
21	CL7	A	406	X	-	-	-
21	CL7	B	601	X	-	-	-
21	CL7	B	602	X	-	-	-
21	CL7	B	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	B	604	X	-	-	-
21	CL7	B	605	X	-	-	-
21	CL7	B	606	X	-	-	-
21	CL7	B	607	X	-	-	-
21	CL7	B	608	X	-	-	-
21	CL7	B	609	X	-	-	-
21	CL7	B	610	X	-	-	-
21	CL7	B	611	X	-	-	-
21	CL7	B	612	X	-	-	-
21	CL7	B	613	X	-	-	-
21	CL7	B	614	X	-	-	-
21	CL7	B	615	X	-	-	-
21	CL7	B	616	X	-	-	-
21	CL7	B	622	X	-	-	-
21	CL7	C	502	X	-	-	-
21	CL7	C	503	X	-	-	-
21	CL7	C	504	X	-	-	-
21	CL7	C	505	X	-	-	-
21	CL7	C	506	X	-	-	-
21	CL7	C	507	X	-	-	-
21	CL7	C	508	X	-	-	-
21	CL7	C	509	X	-	-	-
21	CL7	C	510	X	-	-	-
21	CL7	C	511	X	-	-	-
21	CL7	C	512	X	-	-	-
21	CL7	C	513	X	-	-	-
21	CL7	C	514	X	-	-	-
21	CL7	C	518	X	-	-	-
21	CL7	D	402	X	-	-	-
21	CL7	D	404	X	-	-	-
21	CL7	D	405	X	-	-	-
21	CL7	a	401	X	-	-	-
21	CL7	a	403	X	-	-	-
21	CL7	a	405	X	-	-	-
21	CL7	b	602	X	-	-	-
21	CL7	b	603	X	-	-	-
21	CL7	b	604	X	-	-	-
21	CL7	b	605	X	-	-	-
21	CL7	b	606	X	-	-	-
21	CL7	b	607	X	-	-	-
21	CL7	b	608	X	-	-	-
21	CL7	b	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	b	610	X	-	-	-
21	CL7	b	611	X	-	-	-
21	CL7	b	612	X	-	-	-
21	CL7	b	613	X	-	-	-
21	CL7	b	614	X	-	-	-
21	CL7	b	615	X	-	-	-
21	CL7	b	616	X	-	-	-
21	CL7	b	617	X	-	-	-
21	CL7	b	623	X	-	-	-
21	CL7	c	502	X	-	-	-
21	CL7	c	503	X	-	-	-
21	CL7	c	504	X	-	-	-
21	CL7	c	505	X	-	-	-
21	CL7	c	506	X	-	-	-
21	CL7	c	507	X	-	-	-
21	CL7	c	508	X	-	-	-
21	CL7	c	509	X	-	-	-
21	CL7	c	510	X	-	-	-
21	CL7	c	511	X	-	-	-
21	CL7	c	512	X	-	-	-
21	CL7	c	513	X	-	-	-
21	CL7	c	514	X	-	-	-
21	CL7	c	518	X	-	-	-
21	CL7	d	402	X	-	-	-
21	CL7	d	404	X	-	-	-
21	CL7	d	405	X	-	-	-
32	ZEX	1	422	-	-	X	-
32	ZEX	2	520	-	-	X	-
32	ZEX	2	521	-	-	X	-
32	ZEX	3	522	-	-	X	-
32	ZEX	3	525	-	-	X	-
32	ZEX	4	403	-	-	X	-
32	ZEX	5	422	-	-	X	-
32	ZEX	6	520	-	-	X	-
32	ZEX	7	522	-	-	X	-
32	ZEX	8	403	-	-	X	-

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 68428 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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	284	Total	C	N	O	S	0	0
			2209	1450	361	381	17		
1	a	284	Total	C	N	O	S	0	0
			2209	1450	361	381	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	479	Total	C	N	O	S	0	0
			3794	2472	637	671	14		
2	b	479	Total	C	N	O	S	0	0
			3794	2472	637	671	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	420	Total	C	N	O	S	0	0
			3313	2173	556	570	14		
3	c	420	Total	C	N	O	S	0	0
			3313	2173	556	570	14		

- Molecule 4 is a protein called Photosystem II D2 protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	323	Total	C	N	O	S	0	0
			2583	1713	420	439	11		
4	d	323	Total	C	N	O	S	0	0
			2583	1713	420	439	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	65	Total	C	N	O	S	0	0
			538	354	87	96	1		
5	e	65	Total	C	N	O	S	0	0
			538	354	87	96	1		

- Molecule 6 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	30	Total	C	N	O	S	0	0
			242	166	39	36	1		
6	f	30	Total	C	N	O	S	0	0
			242	166	39	36	1		

- Molecule 7 is a protein called Photosystem II 10 kDa phosphoprotein PsbH.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	68	Total	C	N	O	S	0	0
			519	342	83	91	3		
7	h	68	Total	C	N	O	S	0	0
			519	342	83	91	3		

- Molecule 8 is a protein called Photosystem II protein PsbI.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	34	Total	C	N	O	S	0	0
			281	194	41	45	1		
8	i	34	Total	C	N	O	S	0	0
			281	194	41	45	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	37	Total	C	N	O	S	0	0
			292	205	41	45	1		
9	k	37	Total	C	N	O	S	0	0
			292	205	41	45	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	36	Total	C	N	O	0	0
			288	194	45	49		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	l	36	Total 288	C 194	N 45	O 49	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total 232	C 156	N 36	O 39	S 1	0	0
11	m	31	Total 232	C 156	N 36	O 39	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	28	Total 231	C 163	N 32	O 34	S 2	0	0
12	t	28	Total 231	C 163	N 32	O 34	S 2	0	0

- Molecule 13 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	X	35	Total 269	C 185	N 39	O 45	0	0
13	x	35	Total 269	C 185	N 39	O 45	0	0

- Molecule 14 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Y	23	Total 164	C 111	N 27	O 25	S 1	0	0
14	y	23	Total 164	C 111	N 27	O 25	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Z	59	Total 429	C 290	N 64	O 73	S 2	0	0
15	z	59	Total 429	C 290	N 64	O 73	S 2	0	0

- Molecule 16 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2	349	Total	C	N	O	S	0	0
			2734	1811	442	473	8		
16	6	349	Total	C	N	O	S	0	0
			2734	1811	442	473	8		

- Molecule 17 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	G	41	Total	C	N	O	0	0
			205	123	41	41		
17	g	41	Total	C	N	O	0	0
			205	123	41	41		

- Molecule 18 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1	329	Total	C	N	O	S	0	0
			2567	1715	400	445	7		
18	5	329	Total	C	N	O	S	0	0
			2567	1715	400	445	7		

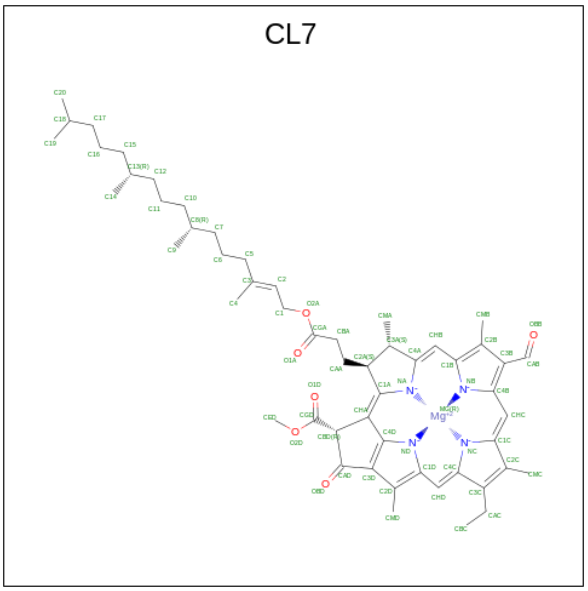
- Molecule 19 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3	344	Total	C	N	O	S	0	0
			2715	1794	444	468	9		
19	7	344	Total	C	N	O	S	0	0
			2715	1794	444	468	9		

- Molecule 20 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	4	331	Total	C	N	O	S	0	0
			2514	1638	412	448	16		
20	8	331	Total	C	N	O	S	0	0
			2514	1638	412	448	16		

- Molecule 21 is CHLOROPHYLL D (CCD ID: CL7) (formula: $C_{54}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	A	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	C	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	D	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	D	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	D	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			60	49	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	1	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	1	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	3	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	3	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	4	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			60	49	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	4	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	4	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	a	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	a	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	a	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	b	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	b	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	c	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	c	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			41	32	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
21	d	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	d	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	d	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	5	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	5	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	5	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	5	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	5	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	5	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			58	47	1	4	6	

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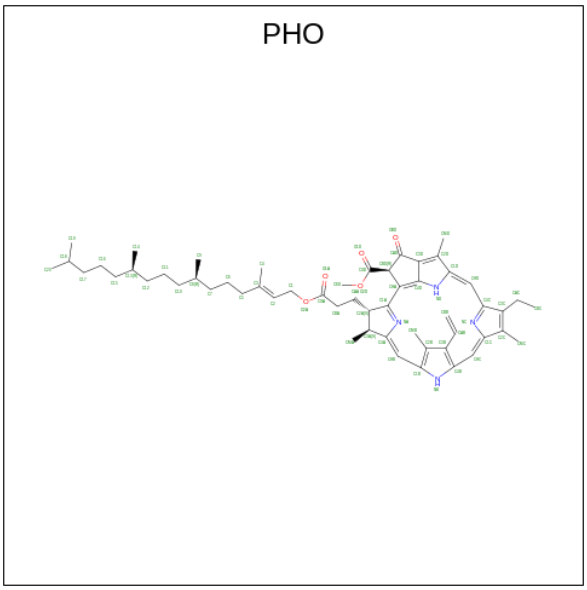
Mol	Chain	Residues	Atoms					AltConf
21	7	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	7	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	8	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	8	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	8	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 22 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



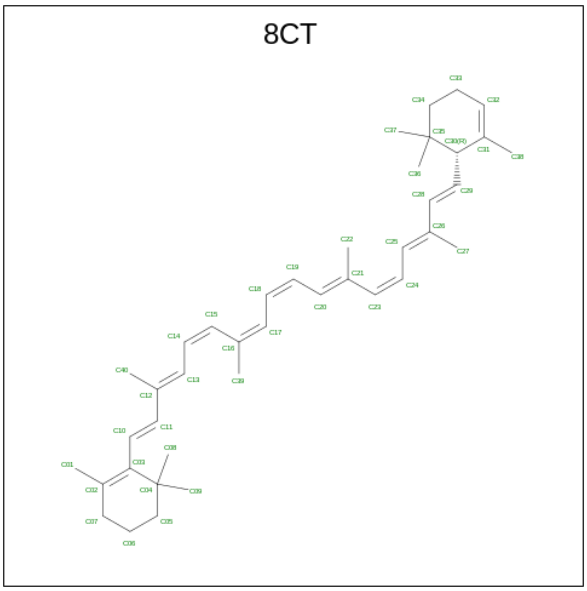
Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	N	O	0
			64	55	4	5	
22	D	1	Total	C	N	O	0
			64	55	4	5	

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

- Molecule 23 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



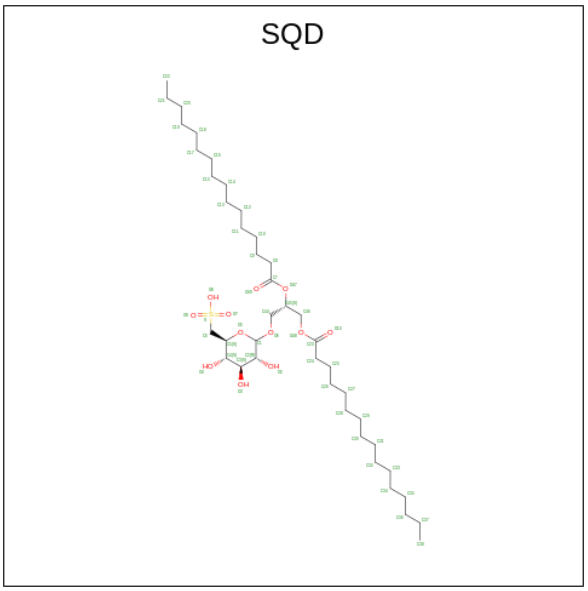
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	C	1	Total C 40 40	0
23	C	1	Total C 40 40	0
23	C	1	Total C 40 40	0
23	D	1	Total C 40 40	0

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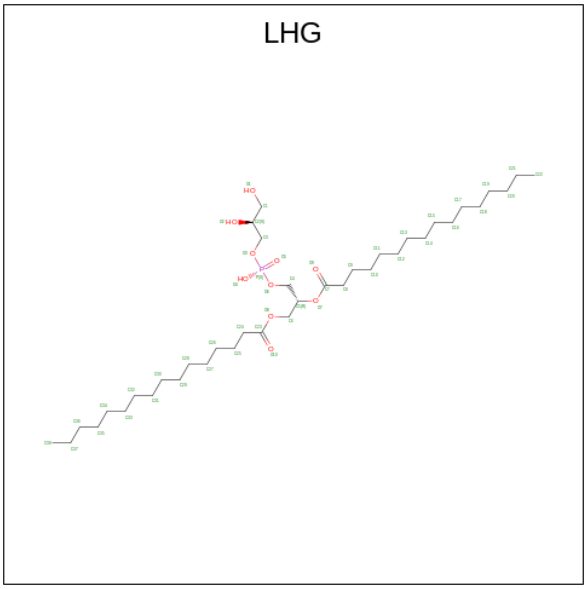
Mol	Chain	Residues	Atoms	AltConf
23	K	1	Total C 40 40	0
23	4	1	Total C 40 40	0
23	a	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	c	1	Total C 40 40	0
23	c	1	Total C 40 40	0
23	c	1	Total C 40 40	0
23	d	1	Total C 40 40	0
23	k	1	Total C 40 40	0
23	8	1	Total C 40 40	0

- Molecule 24 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



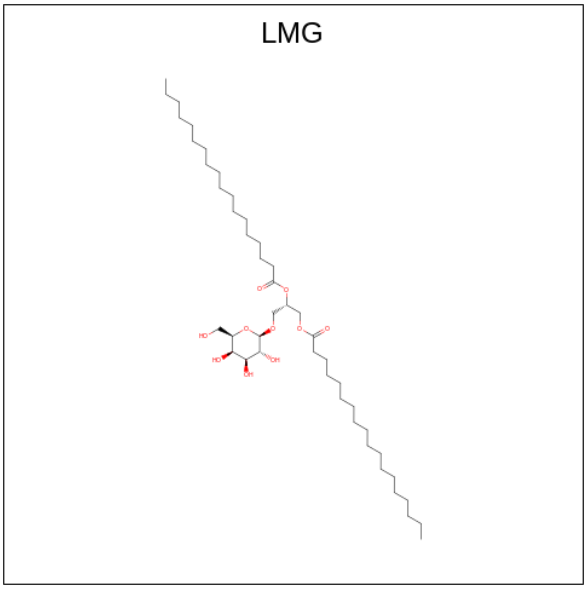
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	S	0
			34	21	12	1	
24	B	1	Total	C	O	S	0
			54	41	12	1	
24	B	1	Total	C	O	S	0
			34	21	12	1	
24	2	1	Total	C	O	S	0
			50	37	12	1	
24	2	1	Total	C	O	S	0
			41	28	12	1	
24	1	1	Total	C	O	S	0
			32	19	12	1	
24	3	1	Total	C	O	S	0
			46	33	12	1	
24	3	1	Total	C	O	S	0
			50	37	12	1	
24	b	1	Total	C	O	S	0
			54	41	12	1	
24	6	1	Total	C	O	S	0
			50	37	12	1	
24	6	1	Total	C	O	S	0
			41	28	12	1	
24	5	1	Total	C	O	S	0
			32	19	12	1	
24	7	1	Total	C	O	S	0
			46	33	12	1	
24	7	1	Total	C	O	S	0
			50	37	12	1	

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



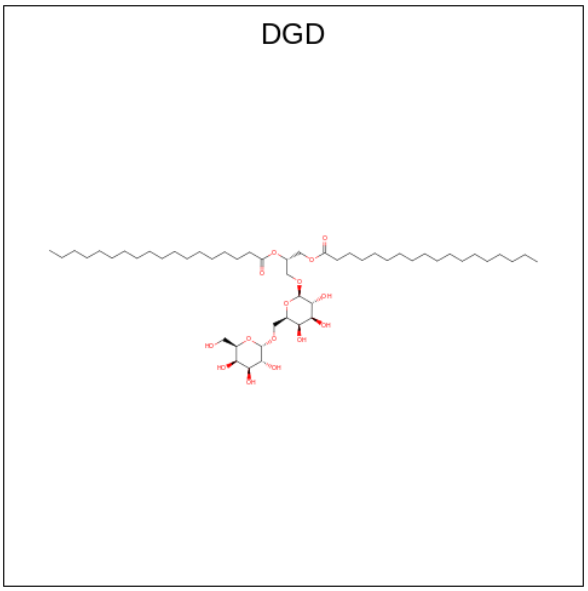
Mol	Chain	Residues	Atoms				AltConf
25	A	1	Total	C	O	P	0
			46	35	10	1	
25	B	1	Total	C	O	P	0
			45	34	10	1	
25	B	1	Total	C	O	P	0
			49	38	10	1	
25	D	1	Total	C	O	P	0
			49	38	10	1	
25	3	1	Total	C	O	P	0
			36	25	10	1	
25	4	1	Total	C	O	P	0
			49	38	10	1	
25	a	1	Total	C	O	P	0
			46	35	10	1	
25	b	1	Total	C	O	P	0
			45	34	10	1	
25	b	1	Total	C	O	P	0
			49	38	10	1	
25	d	1	Total	C	O	P	0
			49	38	10	1	
25	7	1	Total	C	O	P	0
			36	25	10	1	
25	8	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
26	B	1	Total C O 51 41 10	0
26	C	1	Total C O 50 40 10	0
26	D	1	Total C O 33 23 10	0
26	1	1	Total C O 51 41 10	0
26	b	1	Total C O 51 41 10	0
26	c	1	Total C O 50 40 10	0
26	d	1	Total C O 33 23 10	0
26	5	1	Total C O 51 41 10	0

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).

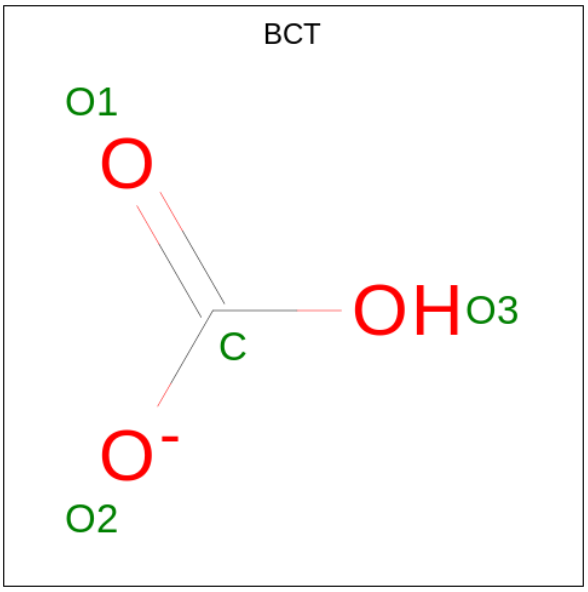


Mol	Chain	Residues	Atoms	AltConf
27	B	1	Total C O 62 47 15	0
27	C	1	Total C O 62 47 15	0
27	b	1	Total C O 62 47 15	0
27	c	1	Total C O 62 47 15	0

- Molecule 28 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

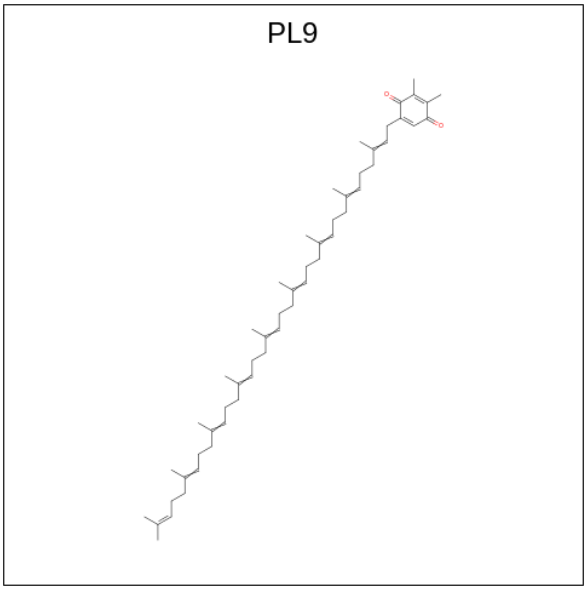
Mol	Chain	Residues	Atoms	AltConf
28	D	1	Total Fe 1 1	0
28	d	1	Total Fe 1 1	0

- Molecule 29 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



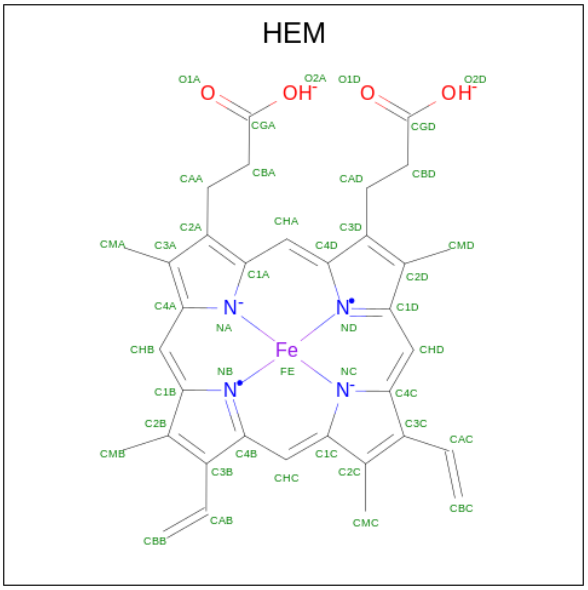
Mol	Chain	Residues	Atoms			AltConf
29	D	1	Total	C	O	0
			4	1	3	
29	d	1	Total	C	O	0
			4	1	3	

- Molecule 30 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



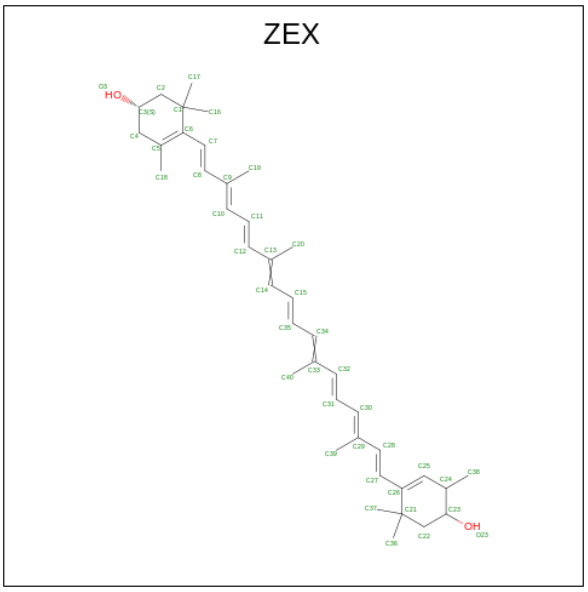
Mol	Chain	Residues	Atoms			AltConf
30	D	1	Total	C	O	0
			55	53	2	
30	d	1	Total	C	O	0
			55	53	2	

- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 32 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (CCD ID: ZEX) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
32	2	1	Total	C	O	0
			42	40	2	
32	2	1	Total	C	O	0
			42	40	2	
32	2	1	Total	C	O	0
			42	40	2	
32	2	1	Total	C	O	0
			42	40	2	
32	2	1	Total	C	O	0
			42	40	2	
32	1	1	Total	C	O	0
			42	40	2	
32	1	1	Total	C	O	0
			42	40	2	
32	3	1	Total	C	O	0
			42	40	2	
32	3	1	Total	C	O	0
			42	40	2	
32	3	1	Total	C	O	0
			42	40	2	
32	3	1	Total	C	O	0
			42	40	2	
32	4	1	Total	C	O	0
			42	40	2	
32	4	1	Total	C	O	0
			42	40	2	
32	4	1	Total	C	O	0
			42	40	2	

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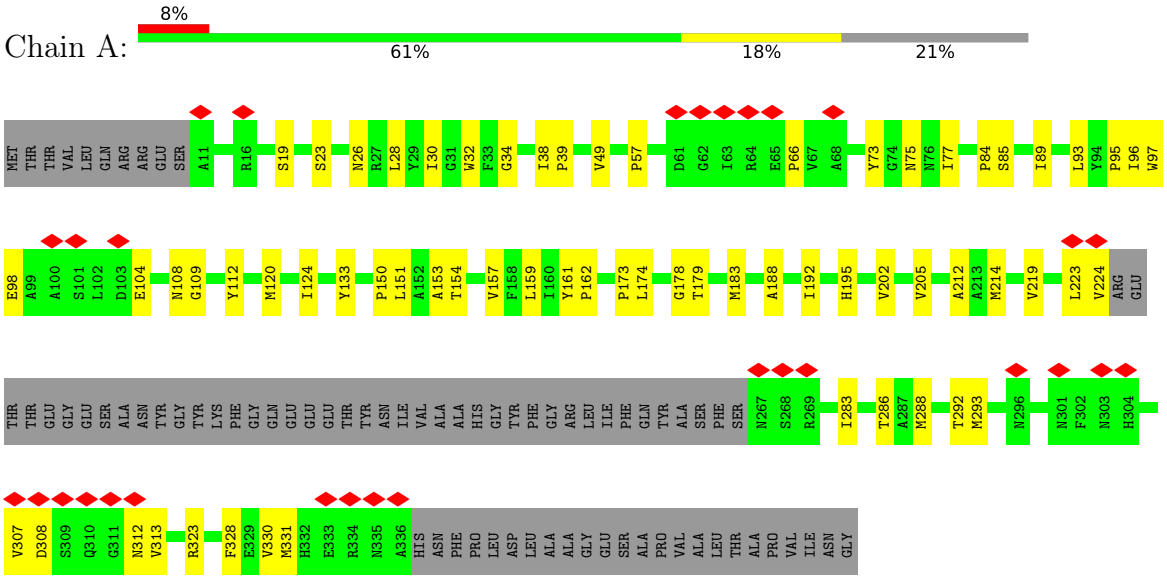
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Mol	Chain	Residues	Atoms	AltConf
32	4	1	Total C O 42 40 2	0
32	6	1	Total C O 42 40 2	0
32	6	1	Total C O 42 40 2	0
32	6	1	Total C O 42 40 2	0
32	6	1	Total C O 42 40 2	0
32	5	1	Total C O 42 40 2	0
32	5	1	Total C O 42 40 2	0
32	7	1	Total C O 42 40 2	0
32	7	1	Total C O 42 40 2	0
32	7	1	Total C O 42 40 2	0
32	8	1	Total C O 42 40 2	0
32	8	1	Total C O 42 40 2	0
32	8	1	Total C O 42 40 2	0
32	8	1	Total C O 42 40 2	0

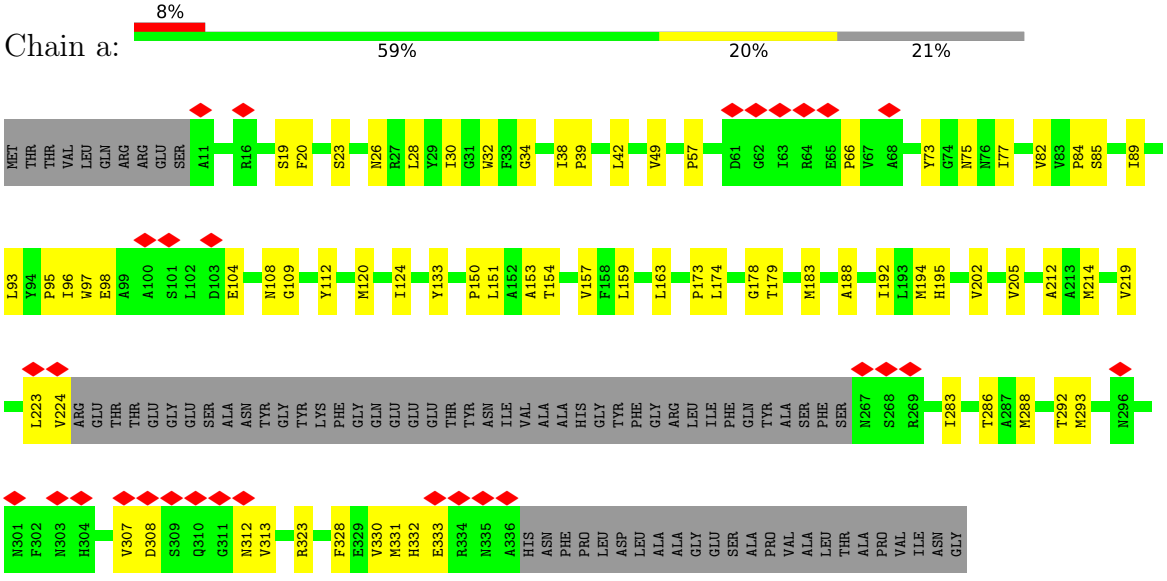
3 Residue-property plots (i)

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 2

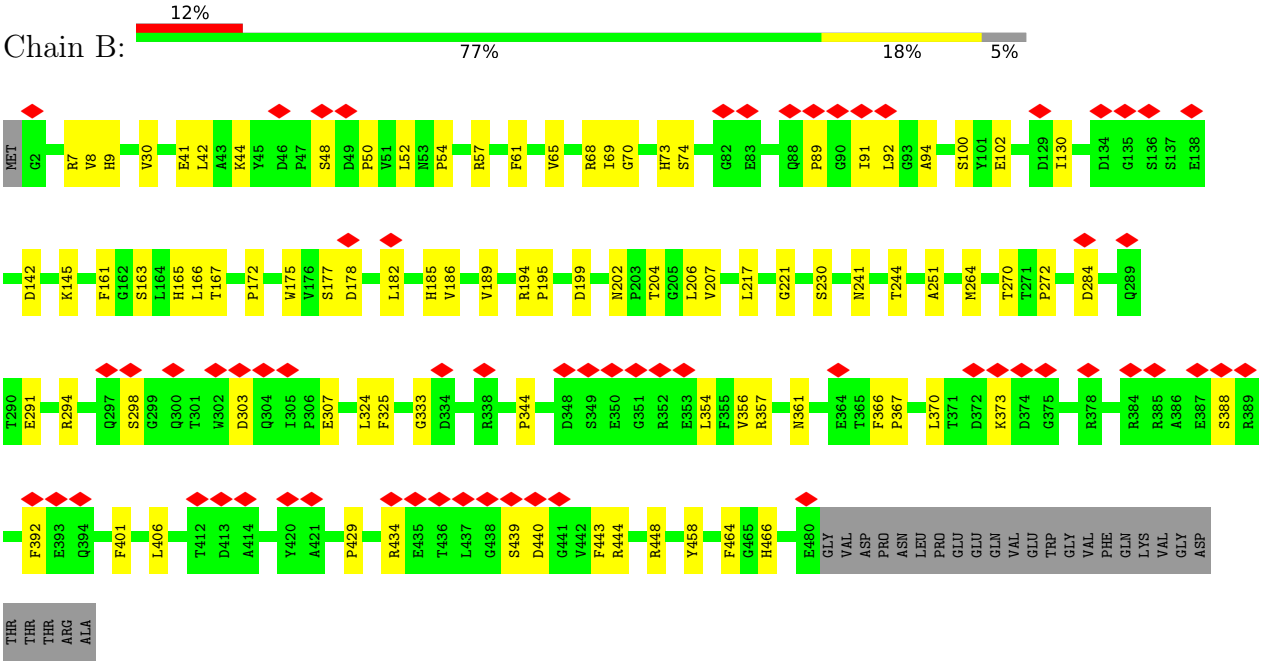


• Molecule 1: Photosystem II protein D1 2



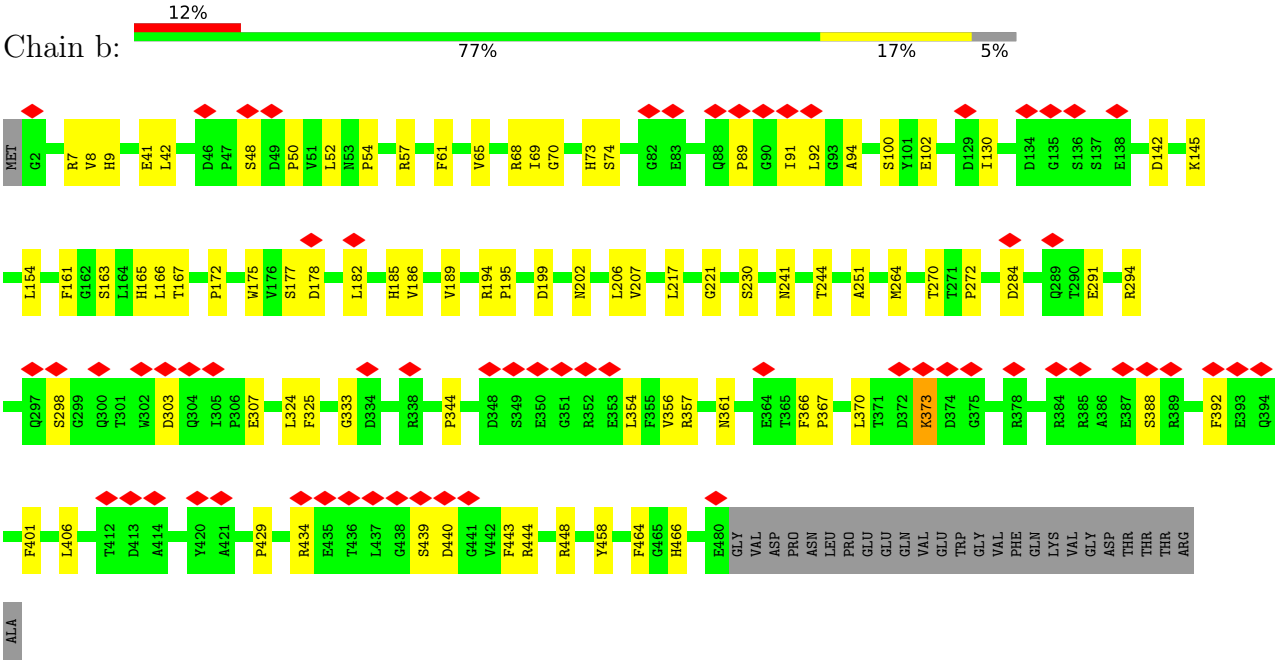
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



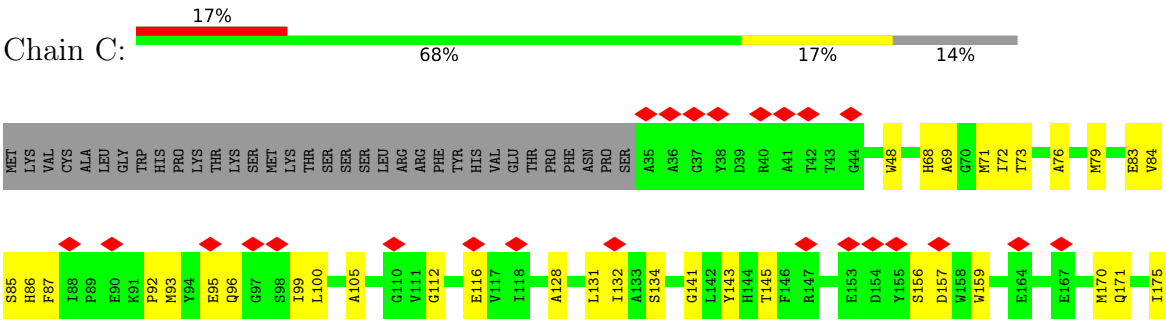
• Molecule 2: Photosystem II CP47 reaction center protein

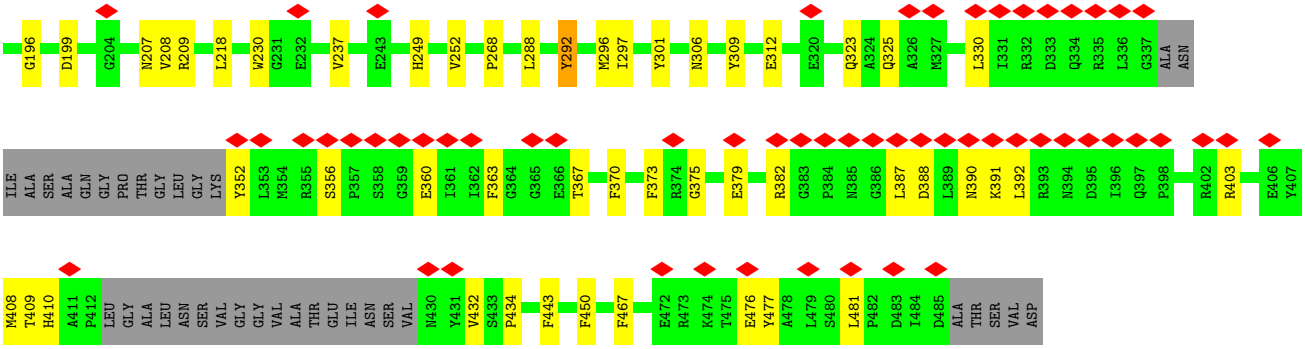
Chain b:



• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:

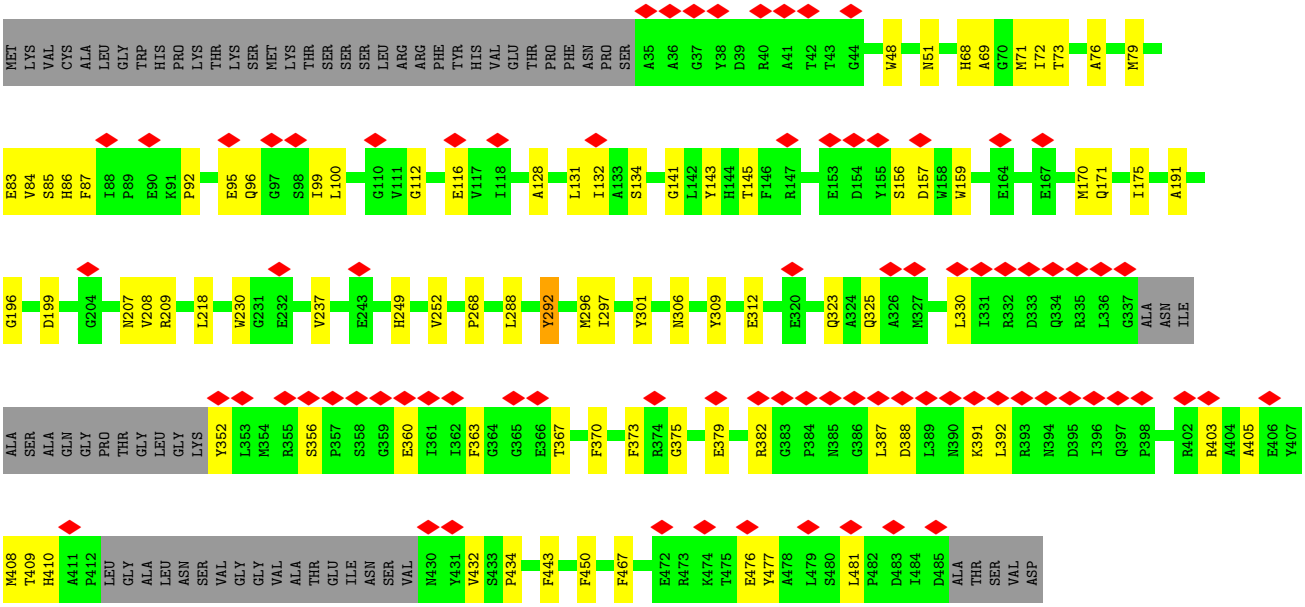




• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:

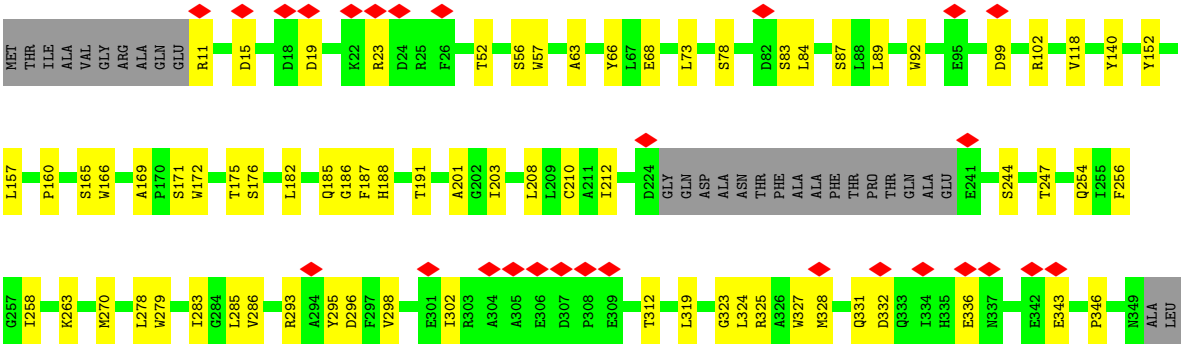




• Molecule 4: Photosystem II D2 protein 1

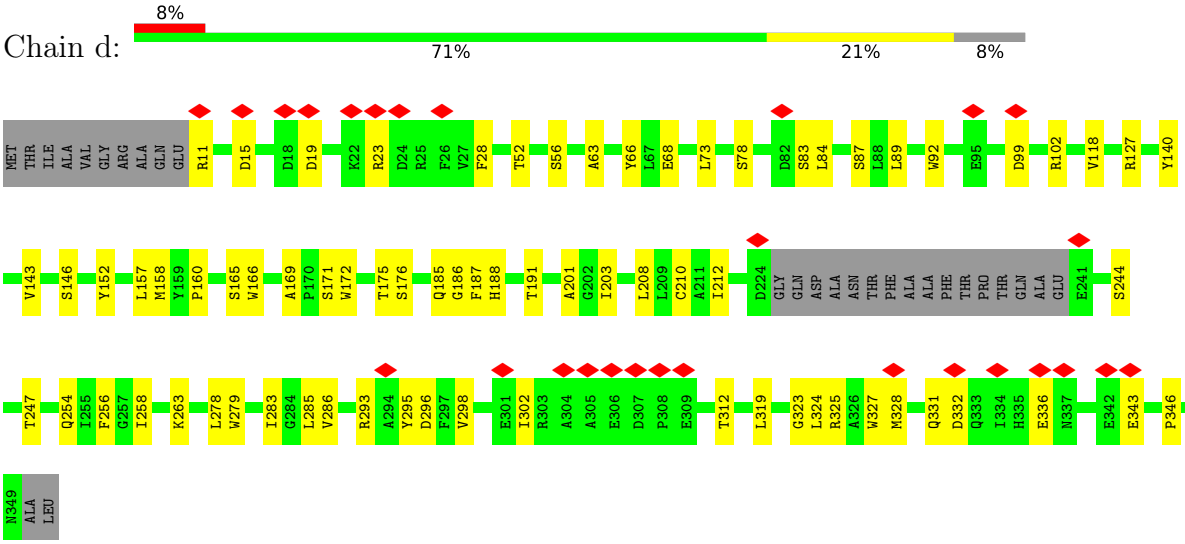
Chain D:





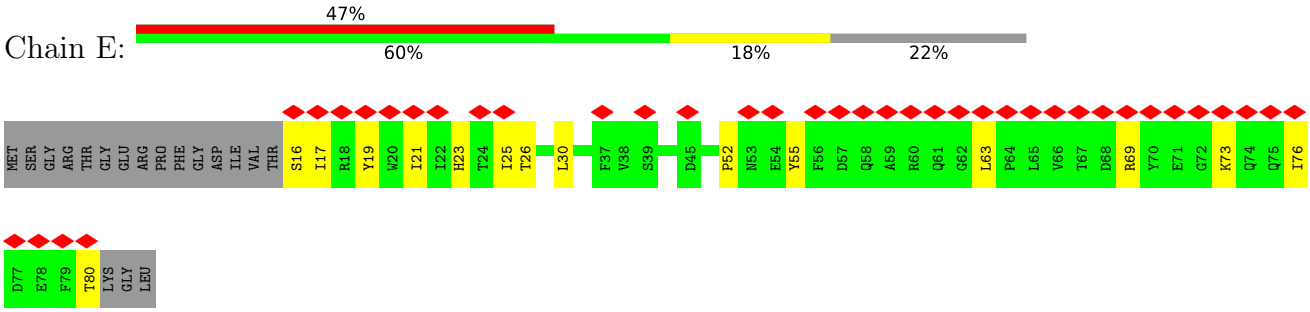
• Molecule 4: Photosystem II D2 protein 1

Chain d:



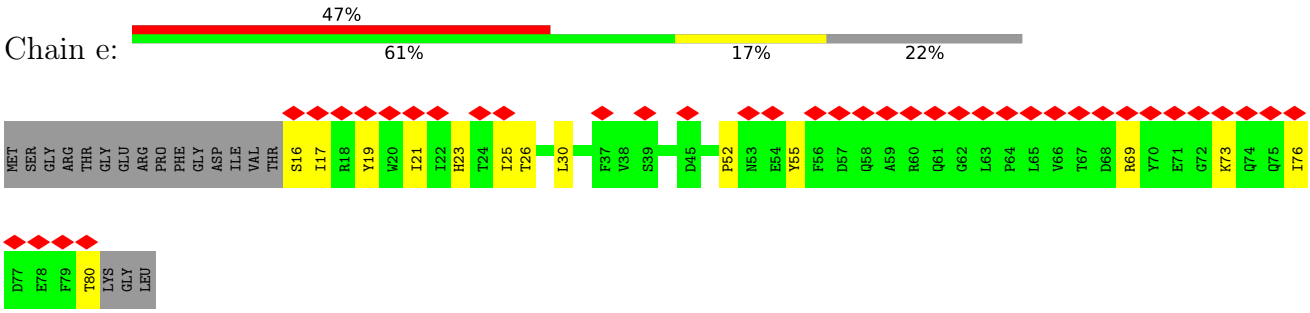
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



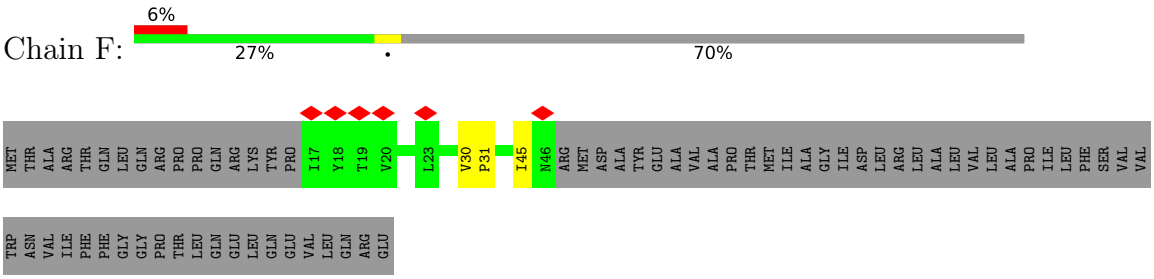
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



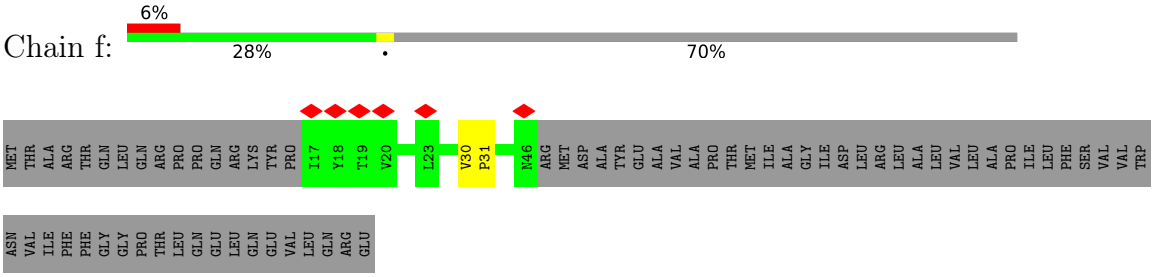
• Molecule 6: Photosystem II protein Y

Chain F:



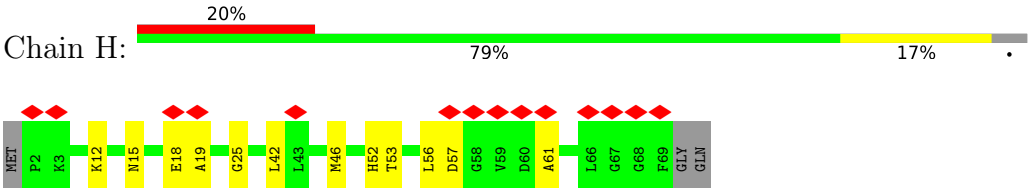
• Molecule 6: Photosystem II protein Y

Chain f:



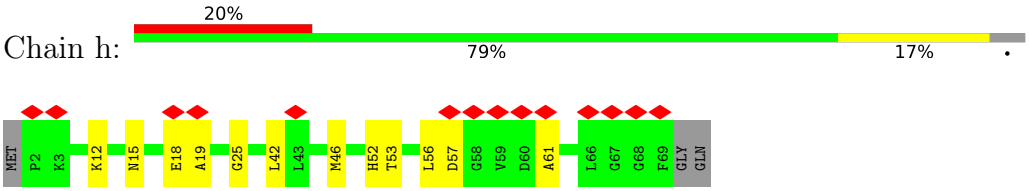
• Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH

Chain H:



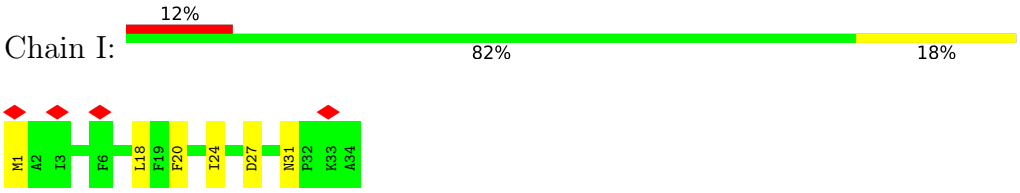
• Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH

Chain h:



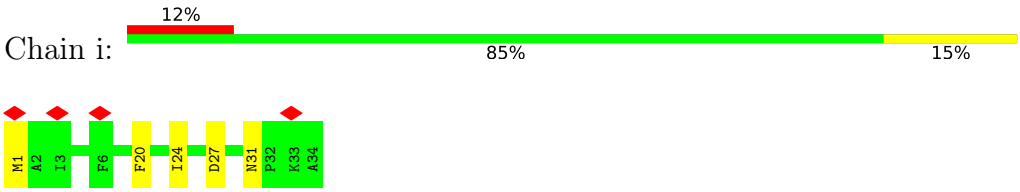
• Molecule 8: Photosystem II protein PsbI

Chain I:



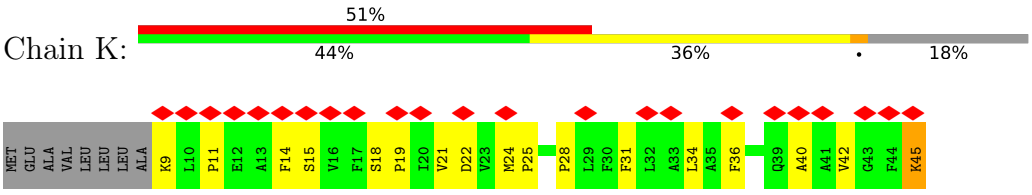
• Molecule 8: Photosystem II protein PsbI

Chain i:



• Molecule 9: Photosystem II reaction center protein K

Chain K:



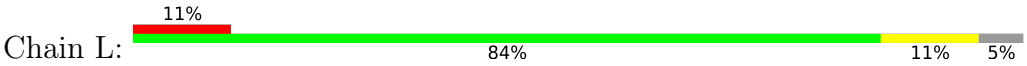
• Molecule 9: Photosystem II reaction center protein K

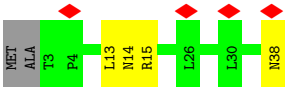
Chain k:



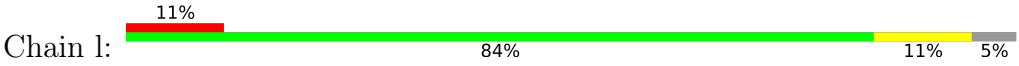


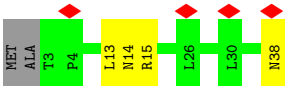
• Molecule 10: Photosystem II reaction center protein L



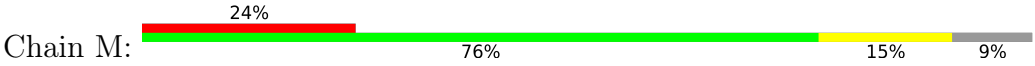


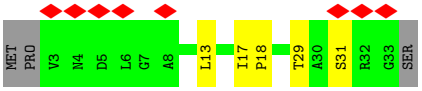
• Molecule 10: Photosystem II reaction center protein L



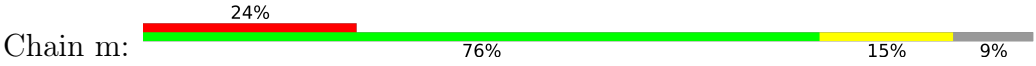


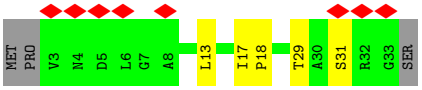
• Molecule 11: Photosystem II reaction center protein M





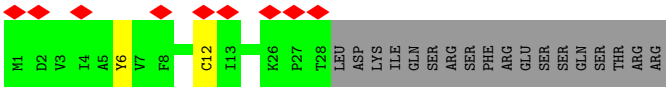
• Molecule 11: Photosystem II reaction center protein M





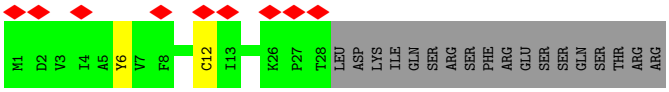
• Molecule 12: Photosystem II reaction center protein T





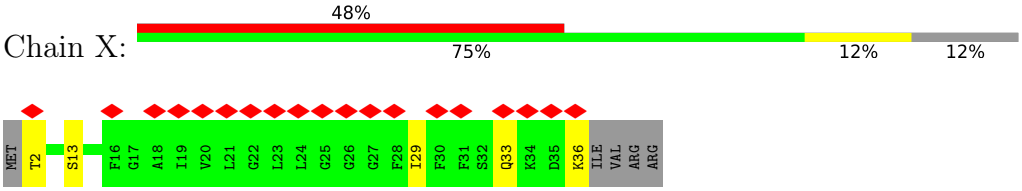
• Molecule 12: Photosystem II reaction center protein T





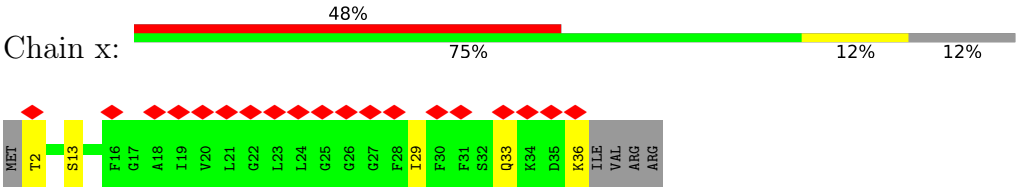
• Molecule 13: Photosystem II reaction center X protein

Chain X:



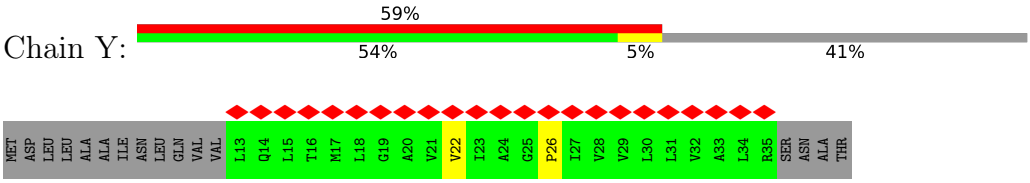
• Molecule 13: Photosystem II reaction center X protein

Chain x:



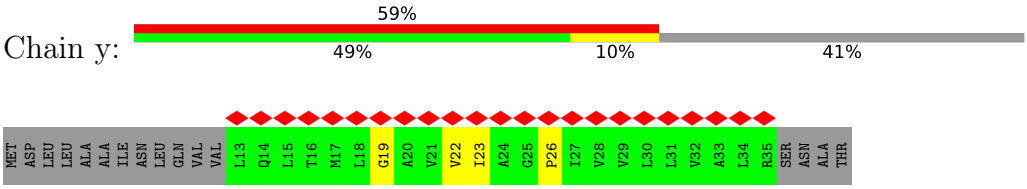
• Molecule 14: Photosystem II reaction center protein Ycf12

Chain Y:



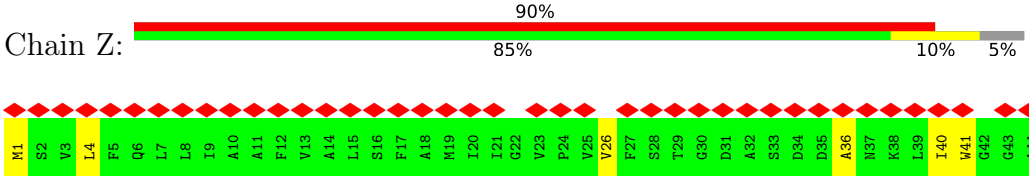
• Molecule 14: Photosystem II reaction center protein Ycf12

Chain y:



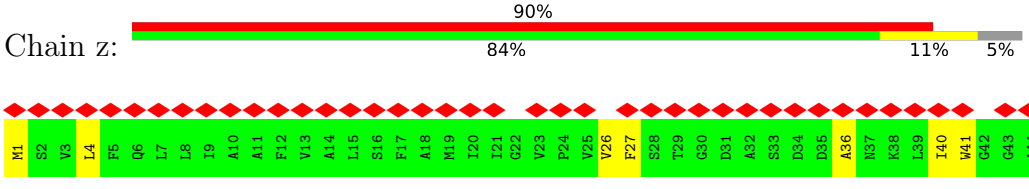
• Molecule 15: Photosystem II reaction center protein Z

Chain Z:



• Molecule 15: Photosystem II reaction center protein Z

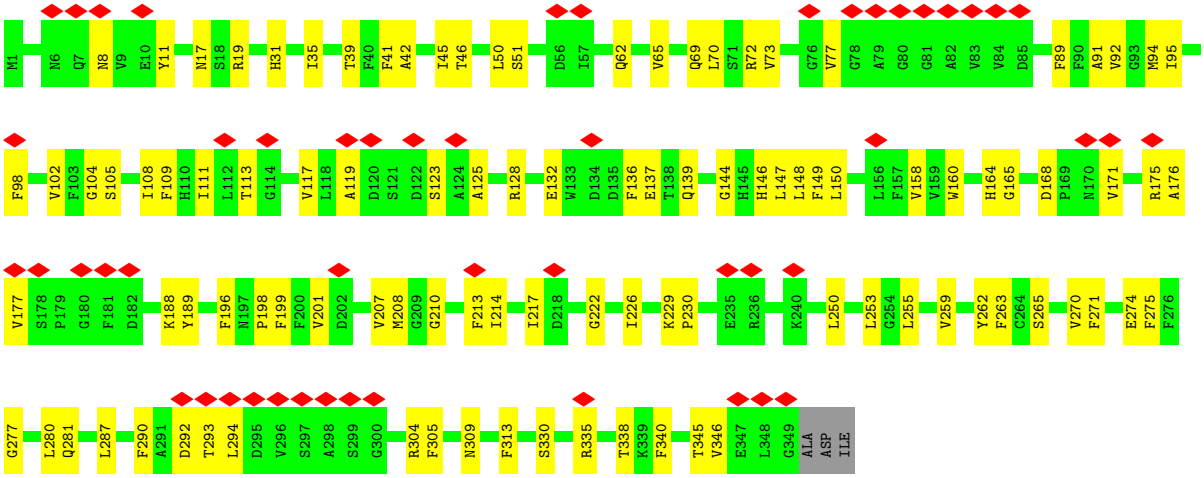
Chain z:



• Molecule 16: High light inducible protein

Chain 2:

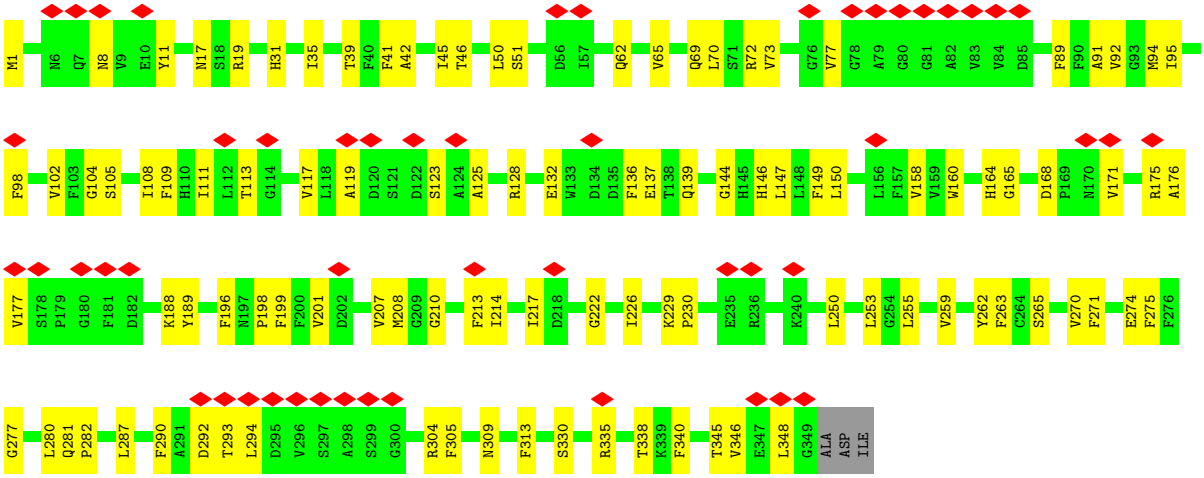




• Molecule 16: High light inducible protein

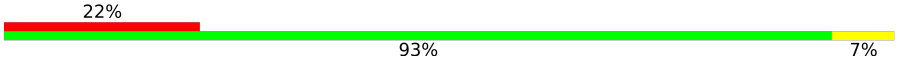
Chain 6:

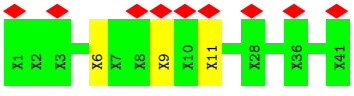




• Molecule 17: Unknown protein

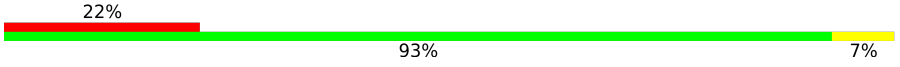
Chain G:

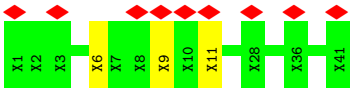




• Molecule 17: Unknown protein

Chain g:

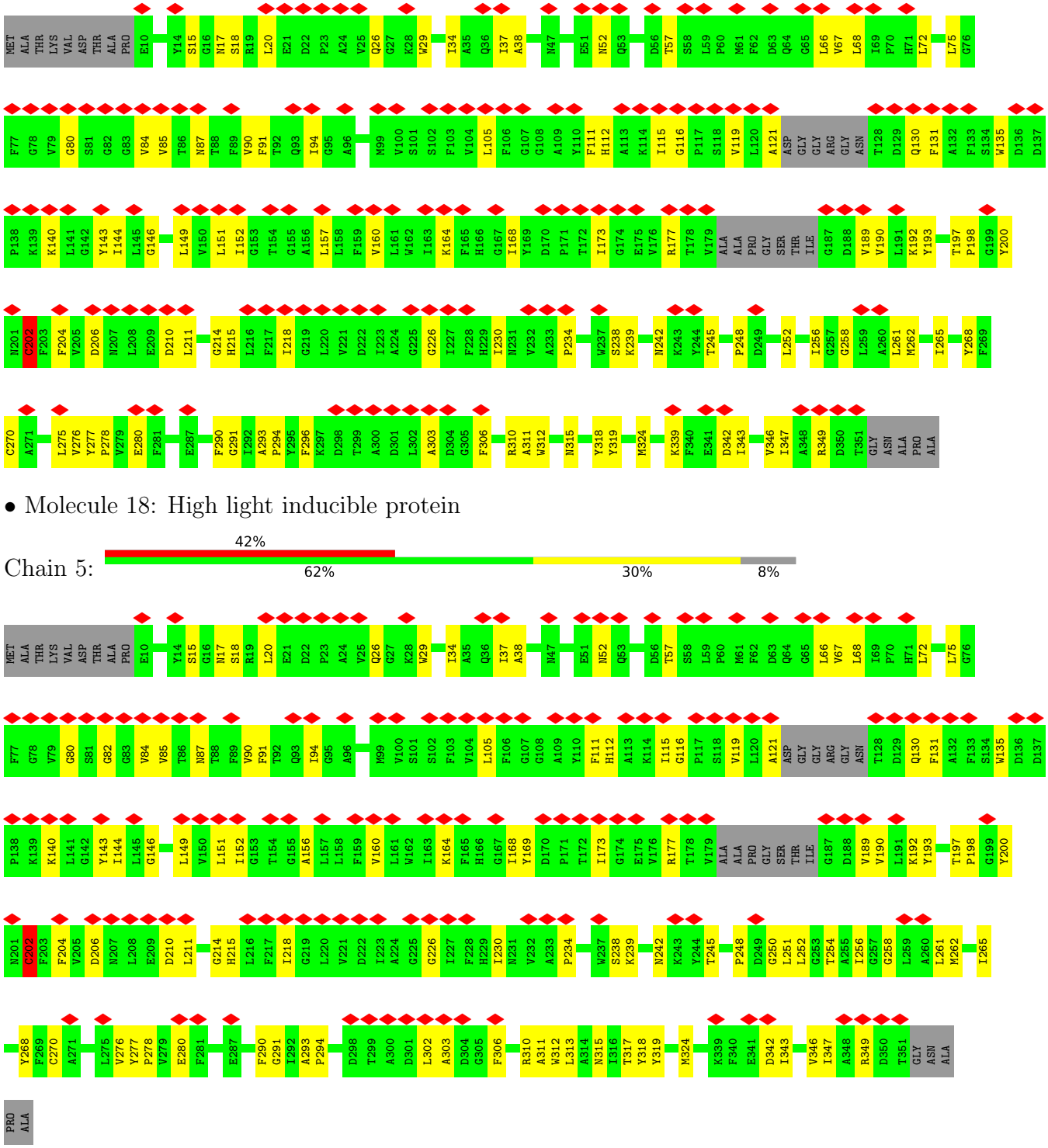




• Molecule 18: High light inducible protein

Chain 1:



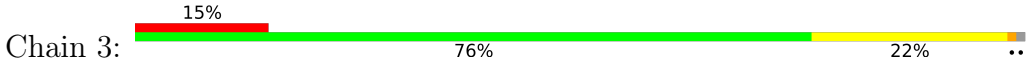


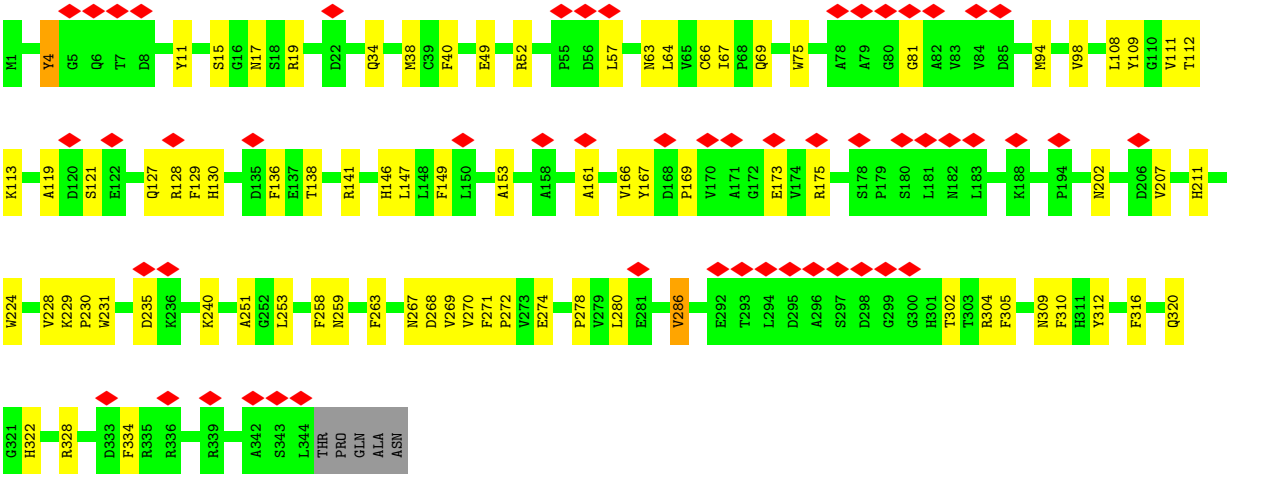
• Molecule 18: High light inducible protein

Chain 5:

• Molecule 19: High light inducible protein

Chain 3:

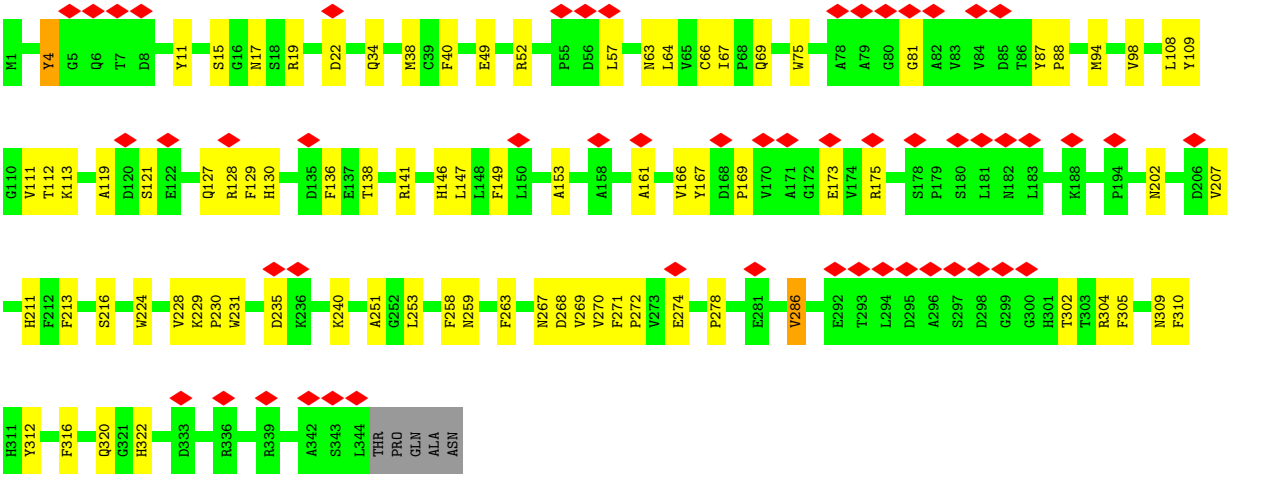




• Molecule 19: High light inducible protein

Chain 7:

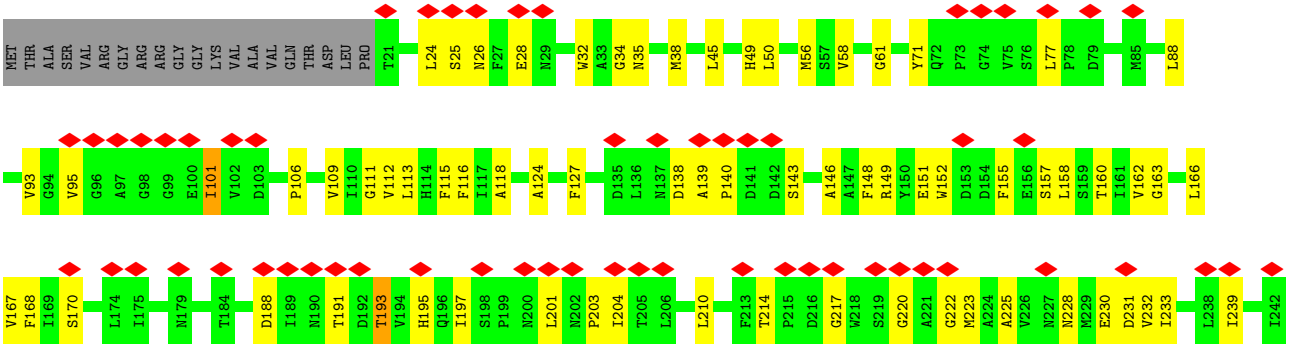


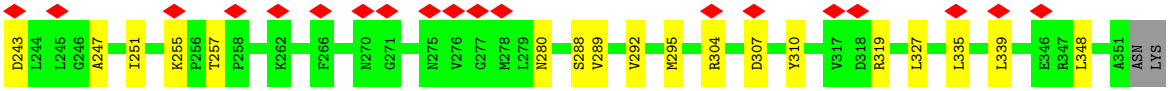


• Molecule 20: High light inducible protein

Chain 4:



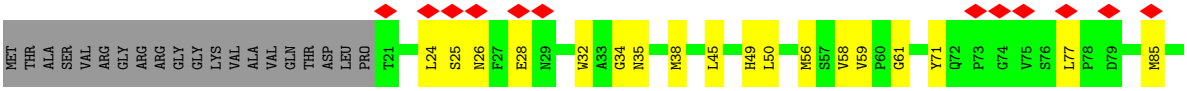


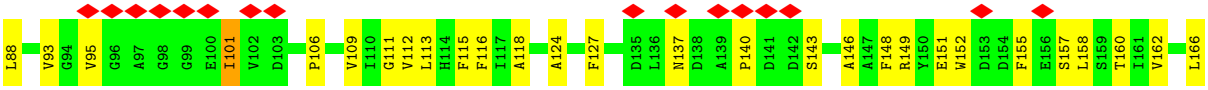


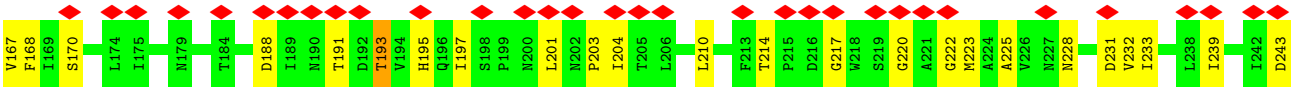
• Molecule 20: High light inducible protein

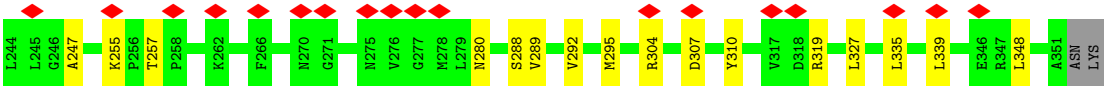
Chain 8:











4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	132346	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0188	Depositor
Map size (Å)	513.60004, 513.60004, 513.60004	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, FE2, CL7, LMG, 8CT, DGD, PL9, PHO, BCT, ZEX, SQD, HEM

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	0.39	0/2280	0.41	0/3112
1	a	0.39	0/2280	0.41	0/3112
2	B	0.37	0/3929	0.42	0/5360
2	b	0.37	0/3929	0.42	0/5360
3	C	0.34	0/3431	0.41	0/4669
3	c	0.34	0/3431	0.41	0/4669
4	D	0.38	0/2672	0.40	0/3641
4	d	0.38	0/2672	0.40	0/3641
5	E	0.25	0/555	0.38	0/757
5	e	0.25	0/555	0.38	0/757
6	F	0.33	0/250	0.39	0/343
6	f	0.33	0/250	0.39	0/343
7	H	0.32	0/534	0.49	1/729 (0.1%)
7	h	0.32	0/534	0.49	1/729 (0.1%)
8	I	0.39	0/290	0.37	0/391
8	i	0.39	0/290	0.37	0/391
9	K	0.26	0/303	0.39	0/413
9	k	0.26	0/303	0.39	0/413
10	L	0.37	0/295	0.38	0/401
10	l	0.37	0/295	0.38	0/401
11	M	0.33	0/236	0.44	0/322
11	m	0.33	0/236	0.44	0/322
12	T	0.31	0/238	0.35	0/321
12	t	0.31	0/238	0.35	0/321
13	X	0.25	0/276	0.29	0/370
13	x	0.25	0/276	0.29	0/370
14	Y	0.17	0/164	0.33	0/224
14	y	0.17	0/164	0.33	0/224
15	Z	0.19	0/438	0.29	0/599
15	z	0.20	0/438	0.29	0/599
16	2	0.35	0/2830	0.42	0/3855
16	6	0.35	0/2830	0.42	0/3855

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
18	1	0.28	0/2652	0.41	0/3618
18	5	0.28	0/2652	0.41	0/3618
19	3	0.38	0/2814	0.46	1/3841 (0.0%)
19	7	0.38	0/2814	0.46	1/3841 (0.0%)
20	4	0.33	0/2590	0.43	0/3537
20	8	0.33	0/2590	0.43	0/3537
All	All	0.35	0/53554	0.42	4/73006 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	53	THR	N-CA-C	-7.25	101.89	111.24
7	h	53	THR	N-CA-C	-7.25	101.89	111.24
19	3	286	VAL	N-CA-C	-6.78	102.78	112.35
19	7	286	VAL	N-CA-C	-6.78	102.78	112.35

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2209	0	2142	60	0
1	a	2209	0	2142	65	0
2	B	3794	0	3626	65	0
2	b	3794	0	3626	66	0
3	C	3313	0	3162	58	0
3	c	3313	0	3162	58	0
4	D	2583	0	2493	65	0
4	d	2583	0	2493	66	0
5	E	538	0	520	14	0
5	e	538	0	520	13	0
6	F	242	0	249	2	0
6	f	242	0	249	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	519	0	518	10	0
7	h	519	0	518	10	0
8	I	281	0	289	6	0
8	i	281	0	289	5	0
9	K	292	0	302	9	0
9	k	292	0	302	9	0
10	L	288	0	301	7	0
10	l	288	0	301	7	0
11	M	232	0	243	4	0
11	m	232	0	243	4	0
12	T	231	0	240	2	0
12	t	231	0	240	2	0
13	X	269	0	275	4	0
13	x	269	0	275	4	0
14	Y	164	0	197	1	0
14	y	164	0	197	2	0
15	Z	429	0	450	3	0
15	z	429	0	450	4	0
16	2	2734	0	2611	105	0
16	6	2734	0	2611	106	0
17	G	205	0	46	2	0
17	g	205	0	46	2	0
18	1	2567	0	2508	100	0
18	5	2567	0	2508	104	0
19	3	2715	0	2580	80	0
19	7	2715	0	2580	83	0
20	4	2514	0	2436	76	0
20	8	2514	0	2436	76	0
21	1	972	0	822	80	0
21	2	1065	0	1050	104	0
21	3	1024	0	962	118	0
21	4	757	0	681	60	0
21	5	972	0	822	83	0
21	6	1065	0	1050	110	0
21	7	1024	0	962	118	0
21	8	757	0	681	64	0
21	A	185	0	187	24	0
21	B	991	0	947	59	0
21	C	799	0	763	39	0
21	D	153	0	121	8	0
21	a	185	0	187	26	0
21	b	991	0	947	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	c	799	0	763	38	0
21	d	153	0	121	8	0
22	A	64	0	74	2	0
22	D	64	0	74	7	0
22	a	64	0	74	2	0
22	d	64	0	74	7	0
23	4	40	0	0	0	0
23	8	40	0	0	0	0
23	A	40	0	0	0	0
23	B	160	0	0	0	0
23	C	120	0	0	2	0
23	D	40	0	0	0	0
23	K	40	0	0	0	0
23	a	40	0	0	0	0
23	b	160	0	0	0	0
23	c	120	0	0	2	0
23	d	40	0	0	0	0
23	k	40	0	0	0	0
24	1	32	0	28	1	0
24	2	91	0	113	2	0
24	3	96	0	123	6	0
24	5	32	0	28	1	0
24	6	91	0	113	1	0
24	7	96	0	123	6	0
24	A	34	0	32	2	0
24	B	88	0	110	5	0
24	b	54	0	78	3	0
25	3	36	0	42	1	0
25	4	49	0	74	2	0
25	7	36	0	42	1	0
25	8	49	0	74	2	0
25	A	46	0	65	0	0
25	B	94	0	137	8	0
25	D	49	0	74	3	0
25	a	46	0	65	0	0
25	b	94	0	137	7	0
25	d	49	0	74	4	0
26	1	51	0	72	2	0
26	5	51	0	72	2	0
26	B	51	0	72	6	0
26	C	50	0	70	0	0
26	D	33	0	36	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	b	51	0	72	6	0
26	c	50	0	70	0	0
26	d	33	0	36	1	0
27	B	62	0	82	2	0
27	C	62	0	82	4	0
27	b	62	0	82	2	0
27	c	62	0	82	4	0
28	D	1	0	0	0	0
28	d	1	0	0	0	0
29	D	4	0	0	0	0
29	d	4	0	0	0	0
30	D	55	0	80	7	0
30	d	55	0	80	6	0
31	F	43	0	30	3	0
31	f	43	0	30	3	0
32	1	84	0	112	35	0
32	2	210	0	280	91	0
32	3	168	0	224	78	0
32	4	168	0	224	47	0
32	5	84	0	112	36	0
32	6	168	0	224	69	0
32	7	126	0	168	52	0
32	8	168	0	224	51	0
All	All	68428	0	65886	2083	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (2083) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:5:315:ASN:HB3	32:5:421:ZEX:C36	1.32	1.59
18:1:315:ASN:HB3	32:1:421:ZEX:C36	1.32	1.59
18:5:315:ASN:CB	32:5:421:ZEX:C36	1.81	1.58
18:1:315:ASN:CB	32:1:421:ZEX:C36	1.81	1.58
21:3:508:CL7:H42C	32:3:519:ZEX:C17	1.38	1.53
21:7:508:CL7:H42C	32:7:519:ZEX:C17	1.38	1.51
18:1:315:ASN:CG	32:1:421:ZEX:H362	1.43	1.43
18:5:315:ASN:CG	32:5:421:ZEX:C36	1.91	1.41
18:1:315:ASN:CG	32:1:421:ZEX:C36	1.91	1.40
21:3:505:CL7:C14	32:4:403:ZEX:C39	2.00	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:5:315:ASN:CG	32:5:421:ZEX:H362	1.43	1.39
21:7:505:CL7:C14	32:8:403:ZEX:C39	2.00	1.39
16:2:94:MET:SD	32:2:525:ZEX:C36	2.13	1.37
16:6:94:MET:SD	32:6:524:ZEX:C36	2.13	1.37
21:7:508:CL7:C4	32:7:519:ZEX:H173	1.59	1.32
16:2:210:GLY:HA3	32:2:521:ZEX:C36	1.60	1.29
21:3:508:CL7:C4	32:3:519:ZEX:H173	1.59	1.29
16:6:210:GLY:HA3	32:6:520:ZEX:C36	1.61	1.28
18:5:315:ASN:CB	32:5:421:ZEX:H362	1.52	1.27
21:3:508:CL7:C4	32:3:519:ZEX:C17	2.11	1.27
21:7:508:CL7:C4	32:7:519:ZEX:C17	2.11	1.25
21:7:505:CL7:C14	32:8:403:ZEX:H393	1.65	1.24
16:6:201:VAL:HG21	32:6:520:ZEX:O23	1.38	1.23
16:2:201:VAL:HG21	32:2:521:ZEX:O23	1.38	1.23
21:3:505:CL7:C14	32:4:403:ZEX:H393	1.65	1.22
21:3:505:CL7:H141	32:4:403:ZEX:C39	1.61	1.22
21:7:505:CL7:H141	32:8:403:ZEX:C39	1.61	1.19
16:2:210:GLY:CA	32:2:521:ZEX:H363	1.72	1.18
16:6:210:GLY:CA	32:6:520:ZEX:H363	1.72	1.17
18:1:315:ASN:CB	32:1:421:ZEX:H362	1.52	1.15
21:3:508:CL7:H43C	32:3:519:ZEX:H173	1.30	1.14
16:6:94:MET:SD	32:6:524:ZEX:H363	1.84	1.14
21:7:508:CL7:H43C	32:7:519:ZEX:H173	1.29	1.12
18:1:315:ASN:CG	32:1:421:ZEX:H361	1.75	1.12
19:3:111:VAL:HG21	32:3:525:ZEX:H42	1.28	1.11
21:7:513:CL7:NB	32:7:522:ZEX:H171	1.66	1.10
18:5:315:ASN:CG	32:5:421:ZEX:H361	1.75	1.10
21:7:513:CL7:C4B	32:7:522:ZEX:C17	2.30	1.10
21:3:513:CL7:C4B	32:3:522:ZEX:C17	2.30	1.09
21:7:513:CL7:NB	32:7:522:ZEX:C17	2.16	1.09
16:2:94:MET:SD	32:2:525:ZEX:H363	1.84	1.08
21:3:513:CL7:NB	32:3:522:ZEX:C17	2.16	1.08
21:3:513:CL7:NB	32:3:522:ZEX:H171	1.66	1.08
21:7:505:CL7:H142	32:8:403:ZEX:C39	1.75	1.08
21:3:508:CL7:H42C	32:3:519:ZEX:H171	1.30	1.07
32:2:520:ZEX:H42	19:7:111:VAL:HG21	1.29	1.06
21:7:508:CL7:H42C	32:7:519:ZEX:H171	1.30	1.06
21:3:513:CL7:C4B	32:3:522:ZEX:H172	1.85	1.06
16:6:210:GLY:HA3	32:6:520:ZEX:H363	1.06	1.05
21:7:513:CL7:C4B	32:7:522:ZEX:H172	1.85	1.04
32:2:525:ZEX:H193	21:1:418:CL7:H8	1.41	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:210:GLY:HA3	32:2:521:ZEX:H363	1.06	1.03
16:6:94:MET:SD	32:6:524:ZEX:H362	1.95	1.02
32:2:520:ZEX:C36	19:7:94:MET:CE	2.40	1.00
21:7:505:CL7:H141	32:8:403:ZEX:H391	1.00	1.00
32:6:524:ZEX:H193	21:5:418:CL7:H8	1.40	0.99
16:2:94:MET:SD	32:2:525:ZEX:H362	1.95	0.99
21:7:505:CL7:C14	32:8:403:ZEX:H391	1.80	0.98
19:3:94:MET:CE	32:3:525:ZEX:C36	2.41	0.98
21:3:505:CL7:H141	32:4:403:ZEX:H391	1.00	0.97
21:3:505:CL7:H142	32:4:403:ZEX:H393	0.99	0.96
21:7:505:CL7:H142	32:8:403:ZEX:H393	0.99	0.96
21:7:516:CL7:H3A	21:7:516:CL7:H11C	1.47	0.96
21:3:505:CL7:H142	32:4:403:ZEX:C39	1.75	0.96
19:7:309:ASN:OD1	32:7:519:ZEX:H363	1.66	0.96
18:5:315:ASN:OD1	32:5:421:ZEX:H361	1.66	0.95
18:1:315:ASN:OD1	32:1:421:ZEX:H361	1.66	0.95
19:3:94:MET:CE	32:3:525:ZEX:H362	1.97	0.95
21:6:505:CL7:H11C	32:6:520:ZEX:H172	1.48	0.95
19:3:94:MET:HE1	32:3:525:ZEX:H363	1.49	0.94
18:5:315:ASN:CB	32:5:421:ZEX:H363	1.63	0.94
32:2:520:ZEX:H363	19:7:94:MET:HE1	1.49	0.94
32:2:520:ZEX:H362	19:7:94:MET:CE	1.96	0.94
21:3:516:CL7:H11C	21:3:516:CL7:H3A	1.47	0.94
21:2:505:CL7:H11C	32:2:521:ZEX:H172	1.48	0.94
19:3:309:ASN:OD1	32:3:519:ZEX:H363	1.66	0.92
32:2:520:ZEX:C36	19:7:94:MET:HE1	1.99	0.92
18:1:315:ASN:CB	32:1:421:ZEX:H363	1.63	0.92
18:1:315:ASN:ND2	32:1:421:ZEX:H362	1.85	0.91
16:2:214:ILE:HD11	32:2:521:ZEX:H392	1.52	0.91
18:1:276:VAL:HG11	21:1:402:CL7:HAA2	1.53	0.91
16:6:214:ILE:HD11	32:6:520:ZEX:H392	1.52	0.90
4:D:185:GLN:HB2	21:D:404:CL7:HBC1	1.53	0.90
18:5:276:VAL:HG11	21:5:402:CL7:HAA2	1.53	0.90
21:7:513:CL7:C1B	32:7:522:ZEX:C17	2.50	0.90
18:5:315:ASN:ND2	32:5:421:ZEX:H362	1.85	0.90
16:2:210:GLY:CA	32:2:521:ZEX:C36	2.42	0.90
19:3:94:MET:HE1	32:3:525:ZEX:C36	1.99	0.90
21:2:512:CL7:H61C	32:2:523:ZEX:H202	1.52	0.90
32:3:522:ZEX:H363	21:6:518:CL7:CMA	2.02	0.89
4:d:185:GLN:HB2	21:d:404:CL7:HBC1	1.53	0.89
20:4:304:ARG:HG3	32:4:418:ZEX:H373	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:3:513:CL7:C1B	32:3:522:ZEX:C17	2.50	0.89
21:6:512:CL7:H61C	32:6:522:ZEX:H202	1.52	0.89
20:8:115:PHE:CE2	32:8:403:ZEX:H363	2.08	0.89
16:6:210:GLY:CA	32:6:520:ZEX:C36	2.43	0.88
20:8:304:ARG:HG3	32:8:418:ZEX:H373	1.52	0.88
20:4:115:PHE:CE2	32:4:403:ZEX:H363	2.08	0.88
32:2:520:ZEX:C36	19:7:94:MET:SD	2.61	0.88
32:2:520:ZEX:C4	19:7:111:VAL:HG21	2.03	0.88
16:6:210:GLY:HA3	32:6:520:ZEX:H362	1.56	0.88
19:3:111:VAL:HG21	32:3:525:ZEX:C4	2.03	0.88
16:2:210:GLY:HA3	32:2:521:ZEX:H362	1.56	0.87
21:2:518:CL7:CMA	32:7:522:ZEX:H363	2.04	0.87
19:3:94:MET:SD	32:3:525:ZEX:C36	2.63	0.86
16:6:201:VAL:HG21	32:6:520:ZEX:H1	1.41	0.86
16:2:207:VAL:HA	32:2:521:ZEX:H382	1.58	0.85
32:4:403:ZEX:O3	21:4:413:CL7:O2A	1.94	0.85
16:6:207:VAL:HA	32:6:520:ZEX:H382	1.58	0.84
21:6:505:CL7:O1A	32:6:520:ZEX:H171	1.77	0.84
32:8:403:ZEX:O3	21:8:413:CL7:O2A	1.94	0.84
16:2:201:VAL:HG21	32:2:521:ZEX:H1	1.42	0.84
21:A:401:CL7:H41C	21:A:406:CL7:CAB	2.09	0.83
21:2:505:CL7:O1A	32:2:521:ZEX:H171	1.77	0.83
21:a:401:CL7:H41C	21:a:405:CL7:CAB	2.09	0.82
18:1:211:LEU:HD12	32:1:422:ZEX:C38	2.10	0.82
21:6:513:CL7:C1B	32:6:522:ZEX:H41	2.09	0.82
18:5:211:LEU:HD12	32:5:422:ZEX:C38	2.10	0.82
21:7:505:CL7:HBA2	20:8:127:PHE:HB2	1.62	0.82
21:3:505:CL7:HBA2	20:4:127:PHE:HB2	1.62	0.81
32:3:525:ZEX:O23	16:6:290:PHE:CZ	2.33	0.81
21:2:513:CL7:C1B	32:2:523:ZEX:H41	2.09	0.81
18:5:214:GLY:HA3	32:5:422:ZEX:H362	1.63	0.81
21:7:508:CL7:H42C	32:7:519:ZEX:H172	1.59	0.81
18:1:214:GLY:HA3	32:1:422:ZEX:H362	1.63	0.81
21:6:502:CL7:H2	21:6:503:CL7:H12C	1.62	0.81
16:2:290:PHE:CZ	32:2:520:ZEX:O23	2.33	0.81
21:2:517:CL7:H42C	32:2:520:ZEX:H203	1.63	0.80
16:6:69:GLN:HE22	21:6:502:CL7:HAA1	1.47	0.80
21:2:502:CL7:H2	21:2:503:CL7:H12C	1.62	0.80
16:6:94:MET:HB3	32:6:522:ZEX:H25	1.63	0.80
3:C:296:MET:HE2	27:C:517:DGD:HB81	1.64	0.80
16:2:94:MET:HB3	32:2:523:ZEX:H25	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:613:CL7:H43C	25:B:623:LHG:H362	1.65	0.79
18:1:315:ASN:ND2	32:1:421:ZEX:H382	1.97	0.79
18:5:315:ASN:ND2	32:5:421:ZEX:H382	1.97	0.79
32:2:520:ZEX:H172	21:7:511:CL7:C1B	2.13	0.79
16:2:69:GLN:HE22	21:2:502:CL7:HAA1	1.47	0.79
21:3:513:CL7:C1B	32:3:522:ZEX:H173	2.13	0.78
32:3:525:ZEX:H203	21:6:517:CL7:H42C	1.63	0.78
21:b:614:CL7:H43C	25:b:624:LHG:H362	1.65	0.78
21:6:505:CL7:C1	32:6:520:ZEX:H172	2.13	0.78
3:c:296:MET:HE2	27:c:517:DGD:HB81	1.64	0.78
21:7:513:CL7:C1B	32:7:522:ZEX:H173	2.13	0.78
21:2:505:CL7:C1	32:2:521:ZEX:H172	2.13	0.78
1:A:133:TYR:OH	4:D:254:GLN:OE1	2.01	0.78
18:1:149:LEU:HD21	21:1:407:CL7:HAB	1.66	0.77
18:1:315:ASN:HB2	32:1:421:ZEX:H362	1.63	0.77
21:7:503:CL7:H143	21:7:509:CL7:H2	1.67	0.77
21:3:503:CL7:H143	21:3:509:CL7:H2	1.66	0.77
1:a:133:TYR:OH	4:d:254:GLN:OE1	2.01	0.77
20:8:239:ILE:HD11	32:8:419:ZEX:C30	2.15	0.77
20:4:239:ILE:HD11	32:4:419:ZEX:C30	2.15	0.76
21:3:508:CL7:H42C	32:3:519:ZEX:H172	1.59	0.76
21:3:513:CL7:C1B	32:3:522:ZEX:H171	2.15	0.76
21:c:502:CL7:H142	21:c:508:CL7:H71C	1.68	0.76
18:5:149:LEU:HD21	21:5:407:CL7:HAB	1.66	0.76
4:D:278:LEU:CD1	22:D:408:PHO:HBC3	2.16	0.76
21:b:603:CL7:H42C	27:b:625:DGD:HB51	1.68	0.75
16:2:109:PHE:HB2	21:1:406:CL7:HBA2	1.69	0.75
4:d:278:LEU:HD12	22:d:408:PHO:HBC3	1.68	0.75
21:A:401:CL7:H42C	21:A:406:CL7:CHC	2.16	0.75
21:a:401:CL7:H42C	21:a:405:CL7:CHC	2.16	0.75
21:7:512:CL7:H91C	32:7:522:ZEX:H182	1.69	0.75
21:7:505:CL7:H2	21:8:415:CL7:HBC1	1.69	0.75
21:7:513:CL7:C1B	32:7:522:ZEX:H171	2.15	0.75
21:3:511:CL7:C1B	32:3:525:ZEX:H172	2.15	0.75
16:6:109:PHE:HB2	21:5:406:CL7:HBA2	1.69	0.75
18:5:315:ASN:HB2	32:5:421:ZEX:H362	1.63	0.75
21:C:502:CL7:H142	21:C:508:CL7:H71C	1.68	0.74
19:3:129:PHE:CZ	32:3:522:ZEX:O3	2.41	0.74
2:B:130:ILE:O	7:H:15:ASN:ND2	2.20	0.74
4:D:278:LEU:HD12	22:D:408:PHO:HBC3	1.68	0.74
21:8:404:CL7:H41C	21:8:404:CL7:H92C	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:602:CL7:H42C	27:B:624:DGD:HB51	1.68	0.74
21:c:504:CL7:HBD	21:c:504:CL7:HBA2	1.70	0.74
4:d:278:LEU:CD1	22:d:408:PHO:HBC3	2.16	0.74
18:1:315:ASN:HB3	32:1:421:ZEX:H363	0.74	0.73
21:4:404:CL7:H92C	21:4:404:CL7:H41C	1.70	0.73
21:c:506:CL7:H41C	21:c:506:CL7:H92C	1.70	0.73
21:C:504:CL7:HBD	21:C:504:CL7:HBA2	1.70	0.73
18:5:315:ASN:HB3	32:5:421:ZEX:H363	0.74	0.73
21:3:505:CL7:H2	21:4:415:CL7:HBC1	1.69	0.73
21:3:512:CL7:H91C	32:3:522:ZEX:H182	1.69	0.73
2:b:130:ILE:O	7:h:15:ASN:ND2	2.20	0.73
21:C:506:CL7:H41C	21:C:506:CL7:H92C	1.70	0.73
4:D:191:THR:HG23	21:D:404:CL7:HBC2	1.71	0.73
19:7:129:PHE:CZ	32:7:522:ZEX:O3	2.41	0.73
32:2:520:ZEX:H362	19:7:94:MET:HE2	1.71	0.72
21:3:513:CL7:C2B	32:3:522:ZEX:H173	2.18	0.72
21:7:505:CL7:HMD2	21:7:507:CL7:HAB	1.71	0.72
2:b:163:SER:O	2:b:167:THR:OG1	2.08	0.72
21:7:513:CL7:C2B	32:7:522:ZEX:H173	2.18	0.72
32:2:520:ZEX:H363	19:7:94:MET:CE	2.14	0.72
1:a:153:ALA:CB	21:a:401:CL7:HED1	2.19	0.72
3:c:476:GLU:OE2	4:d:244:SER:OG	2.08	0.72
2:B:163:SER:O	2:B:167:THR:OG1	2.08	0.72
19:3:94:MET:HE2	32:3:525:ZEX:H362	1.72	0.72
1:A:153:ALA:CB	21:A:401:CL7:HED1	2.19	0.71
21:3:505:CL7:HMD2	21:3:507:CL7:HAB	1.71	0.71
4:d:191:THR:HG23	21:d:404:CL7:HBC2	1.71	0.71
18:5:130:GLN:O	18:5:140:LYS:NZ	2.23	0.71
16:6:17:ASN:ND2	21:6:509:CL7:OBB	2.24	0.70
16:2:17:ASN:ND2	21:2:509:CL7:OBB	2.24	0.70
18:1:130:GLN:O	18:1:140:LYS:NZ	2.23	0.70
21:1:402:CL7:HMA2	32:1:422:ZEX:H383	1.72	0.70
2:b:284:ASP:OD1	2:b:361:ASN:ND2	2.24	0.70
19:3:312:TYR:OH	21:3:517:CL7:OBB	2.10	0.70
16:6:158:VAL:HA	16:6:208:MET:HE1	1.74	0.70
21:5:402:CL7:HMA2	32:5:422:ZEX:H383	1.72	0.70
3:C:476:GLU:OE2	4:D:244:SER:OG	2.08	0.70
21:3:518:CL7:HMA1	32:4:420:ZEX:H372	1.73	0.70
21:a:401:CL7:C4	21:a:405:CL7:CAB	2.70	0.69
21:A:401:CL7:C4	21:A:406:CL7:CAB	2.70	0.69
21:3:505:CL7:C14	32:4:403:ZEX:H391	1.80	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:ASP:OD1	2:B:361:ASN:ND2	2.24	0.69
19:7:312:TYR:OH	21:7:517:CL7:OBB	2.10	0.69
3:C:288:LEU:HD21	21:C:509:CL7:HAB	1.74	0.69
16:6:335:ARG:NH2	24:6:521:SQD:O7	2.26	0.69
16:2:335:ARG:NH2	24:2:522:SQD:O7	2.26	0.69
1:A:153:ALA:HB1	21:A:401:CL7:HED1	1.75	0.69
19:7:66:CYS:HA	21:7:503:CL7:HED1	1.75	0.69
21:7:518:CL7:HMA1	32:8:420:ZEX:H372	1.73	0.69
20:8:220:GLY:O	21:8:417:CL7:OBD	2.11	0.69
16:2:158:VAL:HA	16:2:208:MET:HE1	1.74	0.69
21:3:513:CL7:CHC	32:3:522:ZEX:H172	2.23	0.69
16:6:98:PHE:CD1	32:6:522:ZEX:H31	2.28	0.68
32:2:523:ZEX:C36	21:1:420:CL7:HMA1	2.23	0.68
16:2:98:PHE:CD1	32:2:523:ZEX:H31	2.28	0.68
16:2:147:LEU:HD21	21:2:506:CL7:HAB	1.74	0.68
21:6:505:CL7:H11C	32:6:520:ZEX:C17	2.22	0.68
19:7:81:GLY:HA3	19:7:274:GLU:HG3	1.75	0.68
21:7:513:CL7:CHC	32:7:522:ZEX:H172	2.23	0.68
20:8:304:ARG:HG3	32:8:418:ZEX:C37	2.24	0.68
20:4:220:GLY:O	21:4:417:CL7:OBD	2.11	0.68
16:6:94:MET:SD	32:6:524:ZEX:H361	2.29	0.68
16:6:147:LEU:HD21	21:6:506:CL7:HAB	1.74	0.68
16:6:150:LEU:HD13	21:6:507:CL7:H43C	1.76	0.67
3:c:288:LEU:HD21	21:c:509:CL7:HAB	1.74	0.67
19:3:66:CYS:HA	21:3:503:CL7:HED1	1.75	0.67
16:6:137:GLU:HG2	16:6:229:LYS:HG3	1.76	0.67
32:6:522:ZEX:C36	21:5:420:CL7:HMA1	2.23	0.67
21:2:501:CL7:H121	21:2:507:CL7:H61C	1.77	0.67
1:a:153:ALA:HB1	21:a:401:CL7:HED1	1.75	0.67
16:2:98:PHE:CD1	32:2:523:ZEX:C31	2.78	0.67
19:3:81:GLY:HA3	19:3:274:GLU:HG3	1.75	0.67
21:3:508:CL7:C4	32:3:519:ZEX:H171	2.03	0.67
16:6:214:ILE:CD1	32:6:520:ZEX:H392	2.24	0.67
18:5:131:PHE:CD2	21:5:414:CL7:H3A	2.29	0.67
16:2:201:VAL:CG2	32:2:521:ZEX:O23	2.30	0.67
21:2:505:CL7:H41C	21:2:505:CL7:H101	1.76	0.67
21:2:518:CL7:HMA2	32:7:522:ZEX:H363	1.76	0.67
16:6:98:PHE:CD1	32:6:522:ZEX:C31	2.78	0.67
21:6:501:CL7:H121	21:6:507:CL7:H61C	1.77	0.67
21:6:505:CL7:H101	21:6:505:CL7:H41C	1.76	0.67
18:1:131:PHE:CD2	21:1:414:CL7:H3A	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:94:MET:CE	32:3:525:ZEX:H363	2.14	0.67
21:3:512:CL7:OBB	21:3:514:CL7:O1D	2.13	0.67
2:b:70:GLY:HA2	2:b:186:VAL:HG11	1.77	0.67
16:2:290:PHE:HZ	32:2:520:ZEX:O23	1.78	0.66
20:4:166:LEU:HD21	21:4:408:CL7:HAB	1.75	0.66
16:2:150:LEU:HD13	21:2:507:CL7:H43C	1.76	0.66
19:3:94:MET:HG3	32:3:522:ZEX:H24	1.77	0.66
32:3:525:ZEX:O23	16:6:290:PHE:HZ	1.78	0.66
3:c:476:GLU:OE2	4:d:247:THR:OG1	2.13	0.66
16:2:94:MET:SD	32:2:525:ZEX:H361	2.29	0.66
19:7:153:ALA:HB2	21:7:502:CL7:H101	1.77	0.66
20:8:166:LEU:HD21	21:8:408:CL7:HAB	1.75	0.66
20:8:232:VAL:HA	32:8:419:ZEX:O23	1.96	0.66
20:8:280:ASN:HD21	20:8:348:LEU:HD23	1.60	0.66
16:6:201:VAL:CG2	32:6:520:ZEX:O23	2.30	0.66
16:2:132:GLU:O	16:2:139:GLN:NE2	2.28	0.66
20:4:232:VAL:HA	32:4:419:ZEX:O23	1.95	0.66
16:6:132:GLU:O	16:6:139:GLN:NE2	2.28	0.66
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.78	0.66
16:2:137:GLU:HG2	16:2:229:LYS:HG3	1.77	0.66
16:2:175:ARG:HH11	16:2:177:VAL:HG22	1.61	0.66
16:2:214:ILE:CD1	32:2:521:ZEX:H392	2.24	0.66
32:3:522:ZEX:H363	21:6:518:CL7:HMA2	1.74	0.66
16:6:175:ARG:HH11	16:6:177:VAL:HG22	1.60	0.66
21:5:402:CL7:HMA2	32:5:422:ZEX:C38	2.26	0.66
21:7:512:CL7:OBB	21:7:514:CL7:O1D	2.13	0.66
19:7:94:MET:HG3	32:7:522:ZEX:H24	1.77	0.66
3:C:476:GLU:OE2	4:D:247:THR:OG1	2.13	0.66
21:2:517:CL7:OBB	32:2:520:ZEX:H392	1.96	0.65
21:2:505:CL7:H11C	32:2:521:ZEX:C17	2.22	0.65
21:6:505:CL7:C1	32:6:520:ZEX:C17	2.73	0.65
21:2:505:CL7:C1	32:2:521:ZEX:C17	2.73	0.65
21:4:404:CL7:HMB2	32:4:419:ZEX:H24	1.79	0.65
18:5:218:ILE:HG22	32:5:422:ZEX:H392	1.79	0.65
2:B:70:GLY:HA2	2:B:186:VAL:HG11	1.77	0.65
2:b:264:MET:O	2:b:448:ARG:NH1	2.30	0.65
2:B:264:MET:O	2:B:448:ARG:NH1	2.30	0.65
18:1:218:ILE:HG22	32:1:422:ZEX:H392	1.78	0.65
16:2:207:VAL:HG13	32:2:521:ZEX:C38	2.27	0.65
1:a:89:ILE:HD11	1:a:108:ASN:HB3	1.78	0.65
24:B:620:SQD:H241	10:l:15:ARG:HD2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1:190:VAL:HG22	32:1:422:ZEX:C36	2.27	0.65
19:3:207:VAL:HA	32:3:520:ZEX:O23	1.97	0.65
1:A:57:PRO:HB2	1:A:66:PRO:HB2	1.78	0.64
32:3:525:ZEX:H392	21:6:517:CL7:OBB	1.96	0.64
19:7:207:VAL:HA	32:7:520:ZEX:O23	1.97	0.64
1:A:153:ALA:HB1	21:A:401:CL7:CED	2.28	0.64
2:B:68:ARG:HH12	21:B:604:CL7:HED1	1.62	0.64
21:1:402:CL7:HMA2	32:1:422:ZEX:C38	2.26	0.64
20:4:304:ARG:HG3	32:4:418:ZEX:C37	2.24	0.64
16:2:262:TYR:HB2	32:2:520:ZEX:H383	1.80	0.64
1:a:57:PRO:HB2	1:a:66:PRO:HB2	1.78	0.64
19:3:153:ALA:HB2	21:3:502:CL7:H101	1.77	0.64
1:a:153:ALA:HB1	21:a:401:CL7:CED	2.28	0.64
4:d:102:ARG:HG3	5:e:73:LYS:HB2	1.79	0.64
18:5:119:VAL:HG22	18:5:121:ALA:H	1.62	0.64
1:A:95:PRO:HD2	1:A:98:GLU:HB2	1.80	0.64
32:2:520:ZEX:H361	19:7:94:MET:SD	2.35	0.64
4:D:102:ARG:HG3	5:E:73:LYS:HB2	1.79	0.64
10:L:15:ARG:HD2	24:b:621:SQD:H241	1.78	0.64
16:2:207:VAL:HG13	32:2:521:ZEX:H381	1.79	0.64
32:3:525:ZEX:H383	16:6:262:TYR:HB2	1.80	0.64
18:5:15:SER:O	18:5:18:SER:OG	2.15	0.64
19:3:94:MET:SD	32:3:525:ZEX:H361	2.37	0.64
3:c:306:ASN:N	27:c:517:DGD:O5E	2.28	0.64
21:7:518:CL7:HMA2	32:8:420:ZEX:H27	1.80	0.64
21:8:404:CL7:HMB2	32:8:419:ZEX:H24	1.79	0.64
21:2:517:CL7:H92C	32:2:520:ZEX:H193	1.80	0.64
2:b:68:ARG:HH12	21:b:605:CL7:HED1	1.62	0.64
21:5:403:CL7:HMB2	21:5:405:CL7:HHC	1.80	0.64
2:B:356:VAL:HG22	2:B:370:LEU:HG	1.79	0.64
32:2:521:ZEX:C10	24:7:523:SQD:H221	2.28	0.64
21:1:403:CL7:HMB2	21:1:405:CL7:HHC	1.80	0.64
20:4:115:PHE:CE2	32:4:403:ZEX:C36	2.80	0.64
20:4:280:ASN:HD21	20:4:348:LEU:HD23	1.60	0.64
16:6:207:VAL:HG13	32:6:520:ZEX:C38	2.27	0.64
2:b:356:VAL:HG22	2:b:370:LEU:HG	1.79	0.63
21:7:512:CL7:H91C	32:7:522:ZEX:C18	2.28	0.63
21:3:518:CL7:CMA	32:4:420:ZEX:H372	2.28	0.63
16:6:210:GLY:HA2	32:6:520:ZEX:H363	1.78	0.63
20:8:115:PHE:CE2	32:8:403:ZEX:C36	2.80	0.63
21:3:512:CL7:H91C	32:3:522:ZEX:C18	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:3:513:CL7:C3B	32:3:522:ZEX:C17	2.77	0.63
3:c:312:GLU:OE1	3:c:312:GLU:N	2.31	0.63
21:6:501:CL7:HMA1	32:6:520:ZEX:H24	1.80	0.63
3:C:312:GLU:N	3:C:312:GLU:OE1	2.31	0.63
18:5:190:VAL:HG22	32:5:422:ZEX:C36	2.28	0.63
21:2:518:CL7:HMA3	32:7:522:ZEX:H372	1.81	0.63
21:3:512:CL7:C9	32:3:522:ZEX:H182	2.28	0.63
32:3:525:ZEX:H193	21:6:517:CL7:H92C	1.80	0.63
21:b:615:CL7:CBD	21:b:615:CL7:HBA2	2.29	0.63
16:6:207:VAL:HG13	32:6:520:ZEX:H381	1.79	0.63
21:7:512:CL7:C9	32:7:522:ZEX:H182	2.28	0.63
3:C:312:GLU:HG3	3:C:403:ARG:HH12	1.64	0.63
21:5:402:CL7:HMB2	21:5:402:CL7:H43C	1.80	0.63
21:7:505:CL7:CMD	21:7:507:CL7:HAB	2.29	0.63
3:c:323:GLN:OE1	3:c:367:THR:OG1	2.16	0.63
15:Z:26:VAL:HG13	15:Z:36:ALA:HB1	1.81	0.62
32:2:520:ZEX:H172	21:7:511:CL7:CHB	2.29	0.62
18:1:119:VAL:HG22	18:1:121:ALA:H	1.62	0.62
20:8:307:ASP:HB3	20:8:319:ARG:HH22	1.64	0.62
21:3:505:CL7:HMD3	32:3:520:ZEX:C17	2.29	0.62
21:3:513:CL7:C3B	32:3:522:ZEX:H173	2.29	0.62
32:3:522:ZEX:H372	21:6:518:CL7:HMA3	1.81	0.62
21:7:513:CL7:C3B	32:7:522:ZEX:H173	2.29	0.62
1:A:124:ILE:HD12	1:A:151:LEU:HD21	1.82	0.62
3:C:323:GLN:OE1	3:C:367:THR:OG1	2.15	0.62
16:2:265:SER:HB2	16:2:280:LEU:HB2	1.80	0.62
19:3:17:ASN:ND2	21:3:509:CL7:OBB	2.33	0.62
3:c:312:GLU:HG3	3:c:403:ARG:HH12	1.64	0.62
21:7:518:CL7:CMA	32:8:420:ZEX:H372	2.28	0.62
21:5:406:CL7:C4	32:5:422:ZEX:H192	2.29	0.62
21:1:402:CL7:HMB2	21:1:402:CL7:H43C	1.80	0.62
21:3:505:CL7:CMD	21:3:507:CL7:HAB	2.29	0.62
21:3:518:CL7:HMA2	32:4:420:ZEX:H27	1.80	0.62
20:4:307:ASP:HB3	20:4:319:ARG:HH22	1.64	0.62
1:a:95:PRO:HD2	1:a:98:GLU:HB2	1.80	0.62
32:6:524:ZEX:H35	21:5:417:CL7:HBA2	1.81	0.62
20:8:34:GLY:HA3	21:8:413:CL7:HMD2	1.81	0.62
21:1:406:CL7:C4	32:1:422:ZEX:H192	2.29	0.62
1:a:124:ILE:HD12	1:a:151:LEU:HD21	1.82	0.62
1:a:308:ASP:N	1:a:312:ASN:O	2.30	0.62
16:6:165:GLY:HA2	16:6:176:ALA:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:7:173:GLU:OE1	19:7:175:ARG:NH2	2.32	0.62
21:7:505:CL7:HMD3	32:7:520:ZEX:C17	2.29	0.62
21:2:501:CL7:HMA1	32:2:521:ZEX:H24	1.81	0.62
19:3:121:SER:O	19:3:127:GLN:NE2	2.33	0.62
4:d:187:PHE:O	4:d:293:ARG:NH2	2.33	0.62
13:x:33:GLN:OE1	13:x:36:LYS:NZ	2.26	0.62
21:7:513:CL7:C3B	32:7:522:ZEX:C17	2.77	0.62
20:4:34:GLY:HA3	21:4:413:CL7:HMD2	1.81	0.62
20:4:77:LEU:HD11	20:4:101:ILE:HD11	1.82	0.62
3:C:306:ASN:N	27:C:517:DGD:O5E	2.28	0.62
3:c:79:MET:HB3	3:c:100:LEU:HD12	1.82	0.62
21:B:614:CL7:HBA2	21:B:614:CL7:CBD	2.29	0.61
3:C:84:VAL:O	9:K:9:LYS:N	2.33	0.61
4:D:187:PHE:O	4:D:293:ARG:NH2	2.33	0.61
32:2:525:ZEX:H35	21:1:417:CL7:HBA2	1.81	0.61
18:1:15:SER:O	18:1:18:SER:OG	2.15	0.61
19:7:17:ASN:ND2	21:7:509:CL7:OBB	2.33	0.61
19:7:121:SER:O	19:7:127:GLN:NE2	2.33	0.61
1:A:26:ASN:O	4:D:254:GLN:NE2	2.33	0.61
24:7:521:SQD:H172	21:8:413:CL7:H143	1.82	0.61
16:2:165:GLY:HA2	16:2:176:ALA:HA	1.81	0.61
21:1:406:CL7:H43C	32:1:422:ZEX:H7	1.82	0.61
3:c:356:SER:OG	3:c:360:GLU:N	2.31	0.61
4:d:118:VAL:HG21	4:d:157:LEU:HD11	1.82	0.61
15:z:26:VAL:HG13	15:z:36:ALA:HB1	1.81	0.61
21:7:508:CL7:C4	32:7:519:ZEX:H171	2.03	0.61
16:2:72:ARG:NH2	21:2:501:CL7:OBD	2.33	0.61
16:2:146:HIS:ND1	21:2:507:CL7:OBD	2.31	0.61
24:3:521:SQD:H172	21:4:413:CL7:H143	1.82	0.61
32:3:522:ZEX:H363	21:6:518:CL7:HMA3	1.83	0.61
24:3:523:SQD:H221	32:6:520:ZEX:C10	2.30	0.61
21:C:503:CL7:HBD	21:C:504:CL7:H43C	1.83	0.61
3:c:84:VAL:O	9:k:9:LYS:N	2.33	0.61
19:7:305:PHE:CZ	32:7:519:ZEX:H362	2.36	0.61
20:8:35:ASN:ND2	21:8:410:CL7:O1A	2.33	0.61
21:8:411:CL7:HBD	21:8:411:CL7:HBA1	1.83	0.61
21:3:501:CL7:H191	21:3:507:CL7:H172	1.83	0.61
21:4:412:CL7:HBD	21:4:412:CL7:HBA1	1.82	0.61
1:a:26:ASN:O	4:d:254:GLN:NE2	2.33	0.61
16:6:265:SER:HB2	16:6:280:LEU:HB2	1.80	0.61
21:8:412:CL7:HBD	21:8:412:CL7:HBA1	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:118:VAL:HG21	4:D:157:LEU:HD11	1.82	0.61
19:3:267:ASN:O	19:3:304:ARG:NH1	2.34	0.61
19:7:64:LEU:HD23	19:7:67:ILE:HB	1.83	0.61
21:C:514:CL7:H2A	21:C:514:CL7:HED3	1.83	0.60
18:1:318:TYR:OH	21:1:418:CL7:OBB	2.19	0.60
21:3:511:CL7:CHB	32:3:525:ZEX:H172	2.30	0.60
20:4:214:THR:OG1	20:4:217:GLY:O	2.16	0.60
20:8:77:LEU:HD11	20:8:101:ILE:HD11	1.82	0.60
2:B:161:PHE:HB2	21:B:606:CL7:HAB	1.83	0.60
16:6:117:VAL:HG12	16:6:119:ALA:H	1.66	0.60
18:5:26:GLN:O	18:5:29:TRP:HB3	2.02	0.60
18:5:318:TYR:OH	21:5:418:CL7:OBB	2.19	0.60
20:8:214:THR:OG1	20:8:217:GLY:O	2.16	0.60
19:3:173:GLU:OE1	19:3:175:ARG:NH2	2.32	0.60
16:6:72:ARG:NH2	21:6:501:CL7:OBD	2.34	0.60
21:5:406:CL7:H43C	32:5:422:ZEX:H7	1.82	0.60
18:1:242:ASN:HB3	18:1:245:THR:HG22	1.83	0.60
19:3:64:LEU:HD23	19:3:67:ILE:HB	1.83	0.60
19:3:305:PHE:CZ	32:3:519:ZEX:H362	2.36	0.60
21:4:411:CL7:HBD	21:4:411:CL7:HBA1	1.83	0.60
3:c:143:TYR:OH	21:c:514:CL7:O1D	2.19	0.60
19:7:267:ASN:O	19:7:304:ARG:NH1	2.34	0.60
19:7:235:ASP:OD1	19:7:240:LYS:NZ	2.28	0.60
18:1:211:LEU:CD1	32:1:422:ZEX:C38	2.80	0.60
18:5:211:LEU:CD1	32:5:422:ZEX:C38	2.80	0.60
18:1:26:GLN:O	18:1:29:TRP:HB3	2.02	0.60
2:b:161:PHE:HB2	21:b:607:CL7:HAB	1.83	0.60
17:g:9:UNK:O	17:g:11:UNK:N	2.35	0.60
18:5:280:GLU:OE1	18:5:280:GLU:N	2.30	0.60
3:C:79:MET:HB3	3:C:100:LEU:HD12	1.82	0.60
16:2:345:THR:HG22	19:7:19:ARG:HD3	1.84	0.60
21:2:505:CL7:HBC2	32:2:521:ZEX:H191	1.84	0.60
21:c:503:CL7:HBD	21:c:504:CL7:H43C	1.83	0.60
3:C:143:TYR:OH	21:C:514:CL7:O1D	2.19	0.60
16:2:98:PHE:CG	32:2:523:ZEX:C31	2.85	0.60
17:G:9:UNK:O	17:G:11:UNK:N	2.35	0.60
16:6:136:PHE:HB3	16:6:230:PRO:HG2	1.83	0.60
16:2:136:PHE:HB3	16:2:230:PRO:HG2	1.83	0.59
16:6:146:HIS:ND1	21:6:507:CL7:OBD	2.31	0.59
18:5:189:VAL:HG22	18:5:192:LYS:HB2	1.83	0.59
18:5:242:ASN:HB3	18:5:245:THR:HG22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ASP:N	1:A:312:ASN:O	2.30	0.59
4:D:11:ARG:NH2	4:D:19:ASP:OD2	2.36	0.59
16:2:210:GLY:HA2	32:2:521:ZEX:H363	1.78	0.59
21:2:508:CL7:HAC2	21:2:516:CL7:HBC3	1.85	0.59
16:6:98:PHE:CG	32:6:522:ZEX:C31	2.85	0.59
21:6:508:CL7:HAC2	21:6:516:CL7:HBC3	1.85	0.59
21:8:406:CL7:HAA2	21:8:406:CL7:HBD	1.85	0.59
21:c:511:CL7:HBD	21:c:511:CL7:HBA1	1.85	0.59
21:C:511:CL7:HBA1	21:C:511:CL7:HBD	1.85	0.59
19:3:52:ARG:NH1	17:g:6:UNK:O	2.35	0.59
18:5:311:ALA:O	18:5:315:ASN:ND2	2.35	0.59
32:2:520:ZEX:C17	21:7:511:CL7:CHB	2.79	0.59
20:4:168:PHE:CE1	21:4:414:CL7:HHB	2.38	0.59
2:b:73:HIS:CE1	2:b:100:SER:HB3	2.37	0.59
21:4:407:CL7:CAD	32:4:419:ZEX:H163	2.33	0.59
21:c:514:CL7:H2A	21:c:514:CL7:HED3	1.83	0.59
9:k:36:PHE:O	9:k:40:ALA:N	2.35	0.59
16:6:11:TYR:O	16:6:19:ARG:NH2	2.36	0.59
2:B:73:HIS:CE1	2:B:100:SER:HB3	2.37	0.59
2:B:291:GLU:OE2	2:B:294:ARG:NH2	2.36	0.59
21:7:501:CL7:H191	21:7:507:CL7:H172	1.83	0.59
16:2:117:VAL:HG12	16:2:119:ALA:H	1.66	0.59
20:4:228:ASN:ND2	20:4:231:ASP:OD2	2.36	0.59
21:2:518:CL7:HMA3	32:7:522:ZEX:H363	1.85	0.58
18:1:311:ALA:O	18:1:315:ASN:ND2	2.35	0.58
18:5:315:ASN:HD22	32:5:421:ZEX:H382	1.68	0.58
14:Y:22:VAL:O	14:Y:26:PRO:HD2	2.03	0.58
20:4:327:LEU:HD22	32:4:418:ZEX:C36	2.33	0.58
19:7:267:ASN:OD1	19:7:268:ASP:N	2.36	0.58
9:K:36:PHE:O	9:K:40:ALA:N	2.35	0.58
18:1:189:VAL:HG22	18:1:192:LYS:HB2	1.83	0.58
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.85	0.58
4:d:11:ARG:NH2	4:d:19:ASP:OD2	2.36	0.58
20:8:193:THR:HG23	20:8:195:HIS:CE1	2.38	0.58
20:8:228:ASN:ND2	20:8:231:ASP:OD2	2.36	0.58
20:8:327:LEU:HD22	32:8:418:ZEX:C36	2.33	0.58
1:A:188:ALA:HB2	1:A:328:PHE:HB3	1.85	0.58
21:4:406:CL7:HAA2	21:4:406:CL7:HBD	1.85	0.58
2:b:91:ILE:HG23	2:b:92:LEU:O	2.04	0.58
4:d:172:TRP:CH2	22:d:408:PHO:H101	2.38	0.58
32:2:520:ZEX:H363	19:7:94:MET:SD	2.43	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:3:511:CL7:CHB	32:3:525:ZEX:C17	2.81	0.58
20:4:222:GLY:N	21:4:417:CL7:OBD	2.37	0.58
1:a:188:ALA:HB2	1:a:328:PHE:HB3	1.85	0.58
19:3:19:ARG:HD3	16:6:345:THR:HG22	1.85	0.58
19:3:267:ASN:OD1	19:3:268:ASP:N	2.36	0.58
14:y:22:VAL:O	14:y:26:PRO:HD2	2.03	0.58
20:8:115:PHE:HE2	32:8:403:ZEX:C36	2.17	0.58
20:4:193:THR:HG23	20:4:195:HIS:CE1	2.38	0.58
17:G:6:UNK:O	19:7:52:ARG:NH1	2.36	0.58
20:4:115:PHE:HE2	32:4:403:ZEX:C36	2.17	0.58
20:8:168:PHE:CE1	21:8:414:CL7:HHB	2.38	0.58
21:6:505:CL7:HBC2	32:6:520:ZEX:H191	1.84	0.58
4:D:172:TRP:CH2	22:D:408:PHO:H101	2.39	0.57
21:c:505:CL7:HBD	21:c:505:CL7:HBA2	1.86	0.57
21:8:407:CL7:CAD	32:8:419:ZEX:H163	2.33	0.57
18:1:17:ASN:HB2	21:1:409:CL7:HBA2	1.86	0.57
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.85	0.57
19:7:310:PHE:HA	32:7:519:ZEX:H393	1.86	0.57
16:2:11:TYR:O	16:2:19:ARG:NH2	2.36	0.57
21:3:513:CL7:C4B	32:3:522:ZEX:H173	2.33	0.57
18:5:17:ASN:HB2	21:5:409:CL7:HBA2	1.86	0.57
21:3:515:CL7:CAB	32:4:420:ZEX:H401	2.35	0.57
19:7:211:HIS:CE1	32:7:520:ZEX:H383	2.39	0.57
2:B:91:ILE:HG23	2:B:92:LEU:O	2.04	0.57
18:1:315:ASN:HD22	32:1:421:ZEX:H382	1.68	0.57
21:1:406:CL7:HAA2	21:1:406:CL7:HBD	1.86	0.57
21:7:508:CL7:HAA2	21:7:508:CL7:HBD	1.86	0.57
21:2:505:CL7:HBA2	19:7:109:TYR:HB2	1.86	0.57
32:2:523:ZEX:H363	21:1:420:CL7:HMA1	1.85	0.57
18:1:280:GLU:OE1	18:1:280:GLU:N	2.30	0.57
19:3:211:HIS:CE1	32:3:520:ZEX:H383	2.39	0.57
21:C:505:CL7:HBD	21:C:505:CL7:HBA2	1.86	0.57
21:3:502:CL7:C2B	21:3:504:CL7:HAB	2.35	0.57
21:3:508:CL7:HAA2	21:3:508:CL7:HBD	1.86	0.57
16:2:199:PHE:CE2	32:7:522:ZEX:H382	2.39	0.57
19:3:235:ASP:OD1	19:3:240:LYS:NZ	2.28	0.57
20:8:115:PHE:HE2	32:8:403:ZEX:H363	1.69	0.57
1:A:153:ALA:CB	21:A:401:CL7:CED	2.83	0.57
1:A:307:VAL:HG12	1:A:313:VAL:HG22	1.86	0.57
21:B:602:CL7:HBD	21:B:602:CL7:HAA1	1.87	0.57
27:B:624:DGD:O5D	27:B:624:DGD:O4D	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:502:CL7:HAA2	21:2:502:CL7:HBD	1.87	0.57
20:4:335:LEU:O	20:4:339:LEU:HB2	2.05	0.57
21:6:505:CL7:O1A	32:6:520:ZEX:C17	2.51	0.57
21:5:406:CL7:HAA2	21:5:406:CL7:HBD	1.87	0.57
19:7:211:HIS:CE1	32:7:520:ZEX:C38	2.88	0.57
16:2:41:PHE:CE2	16:2:45:ILE:HG13	2.39	0.56
7:h:57:ASP:OD2	13:x:2:THR:OG1	2.23	0.56
32:6:522:ZEX:H363	21:5:420:CL7:HMA1	1.85	0.56
20:8:112:VAL:HG11	32:8:420:ZEX:H24	1.86	0.56
19:3:211:HIS:CE1	32:3:520:ZEX:C38	2.88	0.56
2:b:89:PRO:HB3	2:b:94:ALA:HB1	1.87	0.56
2:b:291:GLU:OE2	2:b:294:ARG:NH2	2.36	0.56
20:8:335:LEU:O	20:8:339:LEU:HB2	2.05	0.56
16:2:98:PHE:CE1	32:2:523:ZEX:H31	2.41	0.56
16:2:168:ASP:OD2	16:2:171:VAL:N	2.30	0.56
20:4:112:VAL:HG11	32:4:420:ZEX:H24	1.86	0.56
4:d:73:LEU:O	4:d:175:THR:OG1	2.16	0.56
16:6:41:PHE:CE2	16:6:45:ILE:HG13	2.39	0.56
16:6:105:SER:HB2	21:5:406:CL7:H2	1.86	0.56
21:7:510:CL7:H42C	32:7:519:ZEX:H172	1.87	0.56
20:8:222:GLY:N	21:8:417:CL7:OBD	2.36	0.56
21:B:607:CL7:H11C	26:B:621:LMG:H152	1.88	0.56
19:3:149:PHE:CE2	21:3:512:CL7:HHB	2.40	0.56
19:7:149:PHE:CE2	21:7:512:CL7:HHB	2.40	0.56
21:7:515:CL7:CAB	32:8:420:ZEX:H401	2.35	0.56
16:2:105:SER:HB2	21:1:406:CL7:H2	1.86	0.56
18:1:215:HIS:HA	18:1:218:ILE:HG12	1.87	0.56
19:3:310:PHE:HA	32:3:519:ZEX:H393	1.86	0.56
1:a:307:VAL:HG12	1:a:313:VAL:HG22	1.86	0.56
21:6:513:CL7:C1B	32:6:522:ZEX:C4	2.84	0.56
20:8:288:SER:O	20:8:292:VAL:HG23	2.06	0.56
32:3:525:ZEX:H392	21:6:517:CL7:CAB	2.35	0.56
18:5:160:VAL:HG12	18:5:164:LYS:HE3	1.87	0.56
19:7:309:ASN:OD1	32:7:519:ZEX:C36	2.49	0.56
20:8:45:LEU:HG	20:8:49:HIS:CE1	2.41	0.56
7:H:57:ASP:OD2	13:X:2:THR:OG1	2.23	0.56
21:2:517:CL7:CAB	32:2:520:ZEX:H392	2.35	0.56
18:1:20:LEU:HD11	21:1:412:CL7:HMA2	1.88	0.56
20:4:45:LEU:HG	20:4:49:HIS:CE1	2.41	0.56
1:a:77:ILE:HD11	12:t:6:TYR:HB3	1.88	0.56
21:6:502:CL7:HAA2	21:6:502:CL7:HBD	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:8:404:CL7:H2	21:8:406:CL7:H41C	1.87	0.56
21:2:507:CL7:H111	32:2:521:ZEX:H402	1.88	0.56
32:2:523:ZEX:H363	21:1:420:CL7:CMA	2.36	0.56
18:1:211:LEU:CD1	32:1:422:ZEX:H383	2.36	0.56
21:A:406:CL7:HED1	30:D:407:PL9:H362	1.88	0.56
4:D:73:LEU:O	4:D:175:THR:OG1	2.16	0.56
19:3:94:MET:SD	32:3:525:ZEX:H363	2.45	0.56
20:4:257:THR:HG23	21:4:408:CL7:HED2	1.88	0.56
20:4:288:SER:O	20:4:292:VAL:HG23	2.06	0.56
21:5:402:CL7:HBA2	21:5:402:CL7:CHA	2.35	0.56
20:8:257:THR:HG23	21:8:408:CL7:HED2	1.88	0.56
2:B:89:PRO:HB3	2:B:94:ALA:HB1	1.87	0.56
21:4:404:CL7:H2	21:4:406:CL7:H41C	1.87	0.56
25:b:624:LHG:O4	4:d:140:TYR:OH	2.19	0.56
27:b:625:DGD:O5D	27:b:625:DGD:O4D	2.18	0.56
16:6:1:MET:HE1	21:6:508:CL7:HMA3	1.88	0.56
25:B:623:LHG:H172	30:D:407:PL9:H303	1.88	0.55
1:a:153:ALA:CB	21:a:401:CL7:CED	2.83	0.55
21:a:405:CL7:HED1	30:d:407:PL9:H362	1.88	0.55
16:6:305:PHE:O	16:6:309:ASN:ND2	2.39	0.55
16:2:305:PHE:O	16:2:309:ASN:ND2	2.39	0.55
21:3:510:CL7:H42C	32:3:519:ZEX:H172	1.87	0.55
3:C:323:GLN:NE2	3:C:370:PHE:O	2.40	0.55
32:3:522:ZEX:H382	16:6:199:PHE:CE2	2.41	0.55
21:b:608:CL7:H11C	26:b:622:LMG:H152	1.88	0.55
16:6:98:PHE:CE1	32:6:522:ZEX:H31	2.41	0.55
21:7:502:CL7:C2B	21:7:504:CL7:HAB	2.35	0.55
25:B:623:LHG:O4	4:D:140:TYR:OH	2.19	0.55
19:3:109:TYR:HB2	21:6:505:CL7:HBA2	1.87	0.55
32:6:522:ZEX:H363	21:5:420:CL7:CMA	2.36	0.55
20:8:25:SER:OG	20:8:26:ASN:N	2.38	0.55
21:2:511:CL7:CHB	32:2:525:ZEX:C17	2.85	0.55
19:3:63:ASN:HB3	21:3:504:CL7:HAA2	1.88	0.55
21:b:603:CL7:HBD	21:b:603:CL7:HAA1	1.87	0.55
18:5:211:LEU:CD1	32:5:422:ZEX:H383	2.36	0.55
21:4:407:CL7:HHB	32:4:418:ZEX:H172	1.88	0.55
21:4:411:CL7:HBA1	21:4:411:CL7:HED3	1.89	0.55
3:c:99:ILE:HG22	3:c:434:PRO:HB3	1.89	0.55
18:5:215:HIS:HA	18:5:218:ILE:HG12	1.87	0.55
2:B:74:SER:OG	2:B:102:GLU:OE2	2.19	0.55
2:B:100:SER:OG	2:B:102:GLU:OE1	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:513:CL7:C1B	32:2:523:ZEX:C4	2.84	0.55
1:a:286:THR:OG1	21:a:401:CL7:O1D	2.23	0.55
32:6:522:ZEX:O23	18:5:268:TYR:CE2	2.60	0.55
1:A:77:ILE:HD11	12:T:6:TYR:HB3	1.88	0.55
21:B:615:CL7:HAA2	21:B:615:CL7:HBD	1.89	0.55
18:1:160:VAL:HG12	18:1:164:LYS:HE3	1.87	0.55
20:4:223:MET:HE3	21:4:417:CL7:H3A	1.89	0.55
2:B:217:LEU:O	2:B:221:GLY:N	2.38	0.55
16:2:77:VAL:HG21	16:2:275:PHE:HZ	1.71	0.55
32:2:525:ZEX:C19	21:1:418:CL7:H8	2.28	0.55
18:1:151:LEU:HD12	21:1:413:CL7:H3A	1.89	0.55
21:5:410:CL7:H143	21:5:410:CL7:HAA1	1.89	0.55
21:8:411:CL7:HBA1	21:8:411:CL7:HED3	1.89	0.55
21:B:613:CL7:H12C	21:B:613:CL7:HED3	1.89	0.55
21:4:405:CL7:H111	21:4:414:CL7:H12C	1.88	0.55
21:8:405:CL7:H111	21:8:414:CL7:H12C	1.88	0.55
32:2:523:ZEX:O23	18:1:268:TYR:CE2	2.60	0.54
21:3:516:CL7:HED1	32:4:403:ZEX:H10	1.89	0.54
20:4:239:ILE:HD11	32:4:419:ZEX:C29	2.36	0.54
21:b:614:CL7:H12C	21:b:614:CL7:HED3	1.89	0.54
3:c:196:GLY:HA3	3:c:209:ARG:O	2.07	0.54
18:5:151:LEU:HD12	21:5:413:CL7:H3A	1.89	0.54
21:5:406:CL7:H41C	32:5:422:ZEX:H192	1.89	0.54
3:C:356:SER:OG	3:C:360:GLU:N	2.31	0.54
20:4:295:MET:HG2	21:4:404:CL7:H93C	1.89	0.54
21:4:405:CL7:H42C	21:4:406:CL7:H72C	1.90	0.54
21:6:507:CL7:H111	32:6:520:ZEX:H402	1.88	0.54
3:C:196:GLY:HA3	3:C:209:ARG:O	2.07	0.54
21:1:406:CL7:H41C	32:1:422:ZEX:H192	1.89	0.54
21:3:504:CL7:H161	21:3:510:CL7:H41C	1.89	0.54
4:d:66:TYR:O	26:d:410:LMG:O5	2.15	0.54
18:5:346:VAL:HG13	18:5:349:ARG:HH11	1.72	0.54
19:7:63:ASN:HB3	21:7:504:CL7:HAA2	1.88	0.54
21:7:516:CL7:HED1	32:8:403:ZEX:H10	1.89	0.54
18:1:312:TRP:CZ2	21:1:405:CL7:HBA2	2.43	0.54
21:1:410:CL7:H143	21:1:410:CL7:HAA1	1.89	0.54
25:4:401:LHG:HC81	21:4:405:CL7:HMA1	1.90	0.54
25:b:624:LHG:H172	30:d:407:PL9:H303	1.88	0.54
3:c:159:TRP:NE1	21:c:514:CL7:O2A	2.41	0.54
32:6:522:ZEX:C36	21:5:420:CL7:CMA	2.86	0.54
20:8:239:ILE:HD11	32:8:419:ZEX:C29	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:99:ILE:HG22	3:C:434:PRO:HB3	1.89	0.54
21:1:402:CL7:HBA2	21:1:402:CL7:CHA	2.35	0.54
19:3:34:GLN:HE21	21:3:509:CL7:HMB3	1.73	0.54
18:5:20:LEU:HD11	21:5:412:CL7:HMA2	1.88	0.54
21:8:405:CL7:H42C	21:8:406:CL7:H72C	1.90	0.54
21:2:505:CL7:O1A	32:2:521:ZEX:C17	2.51	0.54
18:1:206:ASP:OD1	18:1:206:ASP:N	2.41	0.54
25:b:624:LHG:H101	25:b:624:LHG:H352	1.90	0.54
3:c:323:GLN:NE2	3:c:370:PHE:O	2.40	0.54
7:h:42:LEU:HD11	7:h:46:MET:HE3	1.89	0.54
21:7:504:CL7:HBA2	21:7:504:CL7:HBD	1.90	0.54
20:8:295:MET:HG2	21:8:404:CL7:H93C	1.89	0.54
21:8:407:CL7:HHB	32:8:418:ZEX:H172	1.88	0.54
1:A:219:VAL:O	1:A:223:LEU:HB2	2.07	0.54
18:1:197:THR:HB	18:1:200:TYR:HD2	1.71	0.54
21:6:511:CL7:CHB	32:6:524:ZEX:C17	2.85	0.54
21:7:501:CL7:H41C	21:7:501:CL7:H92C	1.90	0.54
21:8:407:CL7:CAD	32:8:419:ZEX:C16	2.86	0.54
16:2:277:GLY:O	16:2:304:ARG:NH1	2.41	0.54
18:1:346:VAL:HG13	18:1:349:ARG:HH11	1.72	0.54
21:3:504:CL7:HBD	21:3:504:CL7:HBA2	1.90	0.54
20:4:310:TYR:CE2	21:4:404:CL7:HBA2	2.43	0.54
21:4:407:CL7:CMD	21:4:409:CL7:HAB	2.38	0.54
21:b:605:CL7:H2	21:b:606:CL7:H12C	1.90	0.54
21:b:616:CL7:HAA2	21:b:616:CL7:HBD	1.89	0.54
16:6:77:VAL:HG21	16:6:275:PHE:HZ	1.71	0.54
18:5:197:THR:HB	18:5:200:TYR:HD2	1.71	0.54
20:8:115:PHE:CD2	32:8:403:ZEX:H363	2.43	0.54
25:8:401:LHG:HC81	21:8:405:CL7:HMA1	1.90	0.54
2:B:166:LEU:HB3	2:B:207:VAL:HG22	1.90	0.54
21:B:604:CL7:H2	21:B:605:CL7:H12C	1.90	0.54
3:C:159:TRP:NE1	21:C:514:CL7:O2A	2.41	0.54
1:a:124:ILE:HG21	21:c:506:CL7:H122	1.89	0.54
1:a:219:VAL:O	1:a:223:LEU:HB2	2.08	0.54
1:a:283:ILE:HG13	22:a:402:PHO:HBC3	1.90	0.54
3:c:69:ALA:O	3:c:73:THR:HG22	2.08	0.54
16:6:277:GLY:O	16:6:304:ARG:NH1	2.41	0.54
4:D:66:TYR:O	26:D:410:LMG:O5	2.15	0.54
16:6:51:SER:OG	18:5:290:PHE:N	2.41	0.54
16:6:213:PHE:O	16:6:217:ILE:HG12	2.08	0.54
21:8:407:CL7:CMD	21:8:409:CL7:HAB	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:42:LEU:HD11	7:H:46:MET:HE3	1.89	0.53
20:4:25:SER:OG	20:4:26:ASN:N	2.38	0.53
21:b:608:CL7:H121	26:b:622:LMG:H362	1.91	0.53
16:6:105:SER:CB	21:5:406:CL7:H2	2.38	0.53
20:8:45:LEU:HG	20:8:49:HIS:HE1	1.73	0.53
20:8:223:MET:HE3	21:8:417:CL7:H3A	1.89	0.53
21:1:408:CL7:HMD2	21:1:410:CL7:H193	1.89	0.53
21:3:501:CL7:H41C	21:3:501:CL7:H92C	1.90	0.53
4:d:160:PRO:HB3	4:d:169:ALA:HB2	1.90	0.53
21:6:513:CL7:HBA2	21:6:513:CL7:CHA	2.38	0.53
18:5:312:TRP:CZ2	21:5:405:CL7:HBA2	2.43	0.53
18:1:270:CYS:O	18:1:310:ARG:NH1	2.40	0.53
19:3:278:PRO:HD2	19:3:302:THR:HG21	1.91	0.53
6:f:30:VAL:HB	6:f:31:PRO:HD3	1.91	0.53
18:5:315:ASN:HB2	32:5:421:ZEX:C36	2.20	0.53
1:A:283:ILE:HG13	22:A:402:PHO:HBC3	1.90	0.53
3:C:69:ALA:O	3:C:73:THR:HG22	2.08	0.53
16:2:51:SER:OG	18:1:290:PHE:N	2.41	0.53
18:1:234:PRO:HA	21:1:407:CL7:HED3	1.91	0.53
21:4:407:CL7:CAD	32:4:419:ZEX:C16	2.86	0.53
2:b:344:PRO:HG3	2:b:429:PRO:HG3	1.90	0.53
18:5:270:CYS:O	18:5:310:ARG:NH1	2.40	0.53
1:A:57:PRO:HD3	1:A:73:TYR:CE1	2.44	0.53
1:A:124:ILE:HG21	21:C:506:CL7:H122	1.89	0.53
25:B:623:LHG:H101	25:B:623:LHG:H352	1.90	0.53
32:2:523:ZEX:C36	21:1:420:CL7:CMA	2.86	0.53
20:4:35:ASN:ND2	21:4:410:CL7:O1A	2.33	0.53
1:a:205:VAL:HG21	21:a:401:CL7:HHB	1.89	0.53
4:d:52:THR:HA	4:d:66:TYR:HD2	1.74	0.53
19:7:34:GLN:HE21	21:7:509:CL7:HMB3	1.73	0.53
2:B:458:TYR:HB3	21:B:604:CL7:HBC2	1.91	0.53
4:D:160:PRO:HB3	4:D:169:ALA:HB2	1.90	0.53
16:2:213:PHE:O	16:2:217:ILE:HG12	2.08	0.53
21:3:508:CL7:H51C	21:3:511:CL7:HAC1	1.90	0.53
4:d:84:LEU:HA	5:e:69:ARG:HB2	1.91	0.53
21:5:406:CL7:HBC2	32:5:422:ZEX:H191	1.90	0.53
2:B:344:PRO:HG3	2:B:429:PRO:HG3	1.90	0.53
21:B:607:CL7:H121	26:B:621:LMG:H362	1.91	0.53
16:2:35:ILE:O	16:2:39:THR:HG22	2.09	0.53
18:1:262:MET:HG2	21:1:402:CL7:H102	1.91	0.53
21:1:412:CL7:HBA2	21:1:412:CL7:HBD	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4:58:VAL:HG23	20:4:118:ALA:HB1	1.90	0.53
21:6:511:CL7:CHB	32:6:524:ZEX:H173	2.39	0.53
20:4:45:LEU:HG	20:4:49:HIS:HE1	1.73	0.53
2:b:166:LEU:HB3	2:b:207:VAL:HG22	1.90	0.53
21:6:511:CL7:C1B	32:6:524:ZEX:H172	2.39	0.53
18:5:146:GLY:HA3	18:5:230:ILE:HG13	1.91	0.53
18:5:276:VAL:O	18:5:278:PRO:HD3	2.09	0.53
20:8:58:VAL:HG23	20:8:118:ALA:HB1	1.90	0.53
20:8:310:TYR:CE2	21:8:404:CL7:HBA2	2.43	0.53
2:B:294:ARG:O	2:B:298:SER:OG	2.23	0.53
2:b:217:LEU:O	2:b:221:GLY:N	2.38	0.53
21:5:408:CL7:HMD2	21:5:410:CL7:H193	1.89	0.53
18:1:276:VAL:O	18:1:278:PRO:HD3	2.09	0.53
2:b:100:SER:OG	2:b:102:GLU:OE1	2.20	0.53
3:c:83:GLU:HG2	21:c:505:CL7:HED1	1.91	0.53
16:6:168:ASP:OD2	16:6:171:VAL:N	2.30	0.53
18:5:238:SER:O	18:5:242:ASN:ND2	2.37	0.53
18:5:303:ALA:HB3	18:5:306:PHE:HD2	1.74	0.53
21:5:412:CL7:HBD	21:5:412:CL7:HBA2	1.91	0.53
21:7:504:CL7:H161	21:7:510:CL7:H41C	1.89	0.53
1:A:205:VAL:HG21	21:A:401:CL7:HHB	1.89	0.52
4:D:84:LEU:HA	5:E:69:ARG:HB2	1.91	0.52
21:2:511:CL7:C1B	32:2:525:ZEX:H172	2.39	0.52
18:1:146:GLY:HA2	18:1:226:GLY:HA2	1.92	0.52
18:1:214:GLY:CA	32:1:422:ZEX:H362	2.37	0.52
18:1:303:ALA:HB3	18:1:306:PHE:HD2	1.74	0.52
1:a:57:PRO:HD3	1:a:73:TYR:CE1	2.43	0.52
3:c:230:TRP:CE3	27:c:517:DGD:HA21	2.44	0.52
16:6:92:VAL:HG22	21:6:512:CL7:H201	1.91	0.52
21:7:501:CL7:H101	21:7:507:CL7:H41C	1.92	0.52
4:D:298:VAL:HG22	10:L:38:ASN:OXT	2.09	0.52
21:D:404:CL7:HAA2	21:D:404:CL7:HBD	1.90	0.52
21:2:507:CL7:HMD3	21:2:509:CL7:H171	1.91	0.52
21:2:511:CL7:CHB	32:2:525:ZEX:H173	2.39	0.52
25:3:524:LHG:H242	21:4:413:CL7:C3D	2.40	0.52
3:c:141:GLY:O	3:c:145:THR:OG1	2.20	0.52
18:5:206:ASP:N	18:5:206:ASP:OD1	2.41	0.52
18:5:262:MET:HG2	21:5:402:CL7:H102	1.91	0.52
20:8:58:VAL:HG21	32:8:403:ZEX:H15	1.91	0.52
21:B:603:CL7:O1A	21:B:603:CL7:H3A	2.09	0.52
21:C:511:CL7:OBD	21:C:512:CL7:OBB	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:105:SER:CB	21:1:406:CL7:H2	2.38	0.52
20:4:56:MET:HE1	21:4:411:CL7:H12C	1.91	0.52
1:a:32:TRP:NE1	8:i:27:ASP:OD1	2.43	0.52
1:a:283:ILE:HA	1:a:286:THR:HG22	1.91	0.52
21:b:608:CL7:H101	26:b:622:LMG:H351	1.90	0.52
21:c:511:CL7:OBD	21:c:512:CL7:OBB	2.27	0.52
3:C:230:TRP:CE3	27:C:517:DGD:HA21	2.44	0.52
3:C:388:ASP:HB3	3:C:391:LYS:HG2	1.91	0.52
18:1:37:ILE:HG22	18:1:105:LEU:HD13	1.92	0.52
18:1:146:GLY:HA3	18:1:230:ILE:HG13	1.91	0.52
19:3:309:ASN:OD1	32:3:519:ZEX:C36	2.49	0.52
21:3:501:CL7:H101	21:3:507:CL7:H41C	1.91	0.52
21:3:507:CL7:O2D	21:3:507:CL7:H2A	2.09	0.52
21:4:414:CL7:HMA1	32:4:420:ZEX:H162	1.91	0.52
21:a:405:CL7:H41C	30:d:407:PL9:H211	1.91	0.52
20:8:292:VAL:HG13	21:8:406:CL7:H141	1.91	0.52
1:A:283:ILE:HA	1:A:286:THR:HG22	1.91	0.52
32:6:524:ZEX:C19	21:5:418:CL7:H8	2.28	0.52
21:7:508:CL7:H51C	21:7:511:CL7:HAC1	1.90	0.52
25:7:524:LHG:H242	21:8:413:CL7:C3D	2.40	0.52
21:8:414:CL7:HMA1	32:8:420:ZEX:H162	1.91	0.52
21:B:603:CL7:H3A	21:B:603:CL7:CGA	2.40	0.52
20:4:151:GLU:OE2	20:4:152:TRP:N	2.42	0.52
21:4:408:CL7:O1A	21:4:409:CL7:OBB	2.28	0.52
2:b:458:TYR:HB3	21:b:605:CL7:HBC2	1.91	0.52
4:d:298:VAL:HG22	10:l:38:ASN:OXT	2.09	0.52
21:d:404:CL7:HAA2	21:d:404:CL7:HBD	1.90	0.52
16:6:35:ILE:O	16:6:39:THR:HG22	2.09	0.52
21:5:408:CL7:H13	32:5:422:ZEX:H402	1.92	0.52
21:B:607:CL7:H101	26:B:621:LMG:H351	1.90	0.52
3:C:83:GLU:HG2	21:C:505:CL7:HED1	1.91	0.52
6:F:30:VAL:HB	6:F:31:PRO:HD3	1.91	0.52
20:4:115:PHE:CD2	32:4:403:ZEX:H363	2.43	0.52
3:c:363:PHE:CE2	3:c:387:LEU:HD11	2.45	0.52
18:5:111:PHE:O	18:5:116:GLY:N	2.37	0.52
21:7:510:CL7:HBD	21:7:510:CL7:HBA1	1.92	0.52
21:1:406:CL7:HBC2	32:1:422:ZEX:H191	1.90	0.52
21:3:508:CL7:H8	21:6:516:CL7:H201	1.92	0.52
18:5:80:GLY:H	18:5:84:VAL:HB	1.75	0.52
19:7:278:PRO:HD2	19:7:302:THR:HG21	1.91	0.52
21:A:406:CL7:H41C	30:D:407:PL9:H211	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:501:CL7:HMD2	21:2:503:CL7:O2A	2.10	0.52
21:3:510:CL7:HBD	21:3:510:CL7:HBA1	1.92	0.52
4:D:52:THR:HA	4:D:66:TYR:HD2	1.74	0.52
13:X:33:GLN:OE1	13:X:36:LYS:NZ	2.26	0.52
21:2:505:CL7:HMD3	32:2:521:ZEX:C16	2.40	0.52
21:2:516:CL7:H201	21:7:508:CL7:H8	1.91	0.52
18:1:111:PHE:O	18:1:116:GLY:N	2.37	0.52
19:3:108:LEU:O	19:3:112:THR:HG22	2.10	0.52
3:c:388:ASP:HB3	3:c:391:LYS:HG2	1.91	0.52
4:d:143:VAL:O	4:d:146:SER:OG	2.21	0.52
4:d:258:ILE:HD13	25:d:409:LHG:HC82	1.92	0.52
21:6:512:CL7:C6	32:6:522:ZEX:H202	2.34	0.52
24:5:423:SQD:O7	24:5:423:SQD:O4	2.28	0.52
20:8:56:MET:HE1	21:8:411:CL7:H12C	1.91	0.52
21:2:513:CL7:HBA2	21:2:513:CL7:CHA	2.38	0.51
4:d:258:ILE:HG21	25:d:409:LHG:H262	1.92	0.51
18:5:37:ILE:HG22	18:5:105:LEU:HD13	1.92	0.51
19:7:108:LEU:O	19:7:112:THR:HG22	2.10	0.51
1:A:32:TRP:NE1	8:I:27:ASP:OD1	2.43	0.51
3:C:409:THR:OG1	3:C:410:HIS:ND1	2.35	0.51
24:3:521:SQD:H271	24:3:521:SQD:H141	1.92	0.51
21:4:407:CL7:C3D	32:4:419:ZEX:H163	2.40	0.51
18:5:146:GLY:HA2	18:5:226:GLY:HA2	1.92	0.51
21:8:415:CL7:HBD	21:8:415:CL7:HAA2	1.93	0.51
3:C:363:PHE:CE2	3:C:387:LEU:HD11	2.45	0.51
16:2:92:VAL:HG22	21:2:512:CL7:H201	1.91	0.51
21:1:408:CL7:H13	32:1:422:ZEX:H402	1.92	0.51
21:6:505:CL7:HMD3	32:6:520:ZEX:C16	2.40	0.51
20:8:93:VAL:HG13	20:8:106:PRO:HB2	1.92	0.51
18:1:197:THR:HB	18:1:200:TYR:CD2	2.46	0.51
19:3:271:PHE:O	19:3:304:ARG:NH2	2.43	0.51
21:4:415:CL7:HAA2	21:4:415:CL7:HBD	1.93	0.51
21:b:604:CL7:H3A	21:b:604:CL7:CGA	2.40	0.51
21:B:607:CL7:H12C	26:B:621:LMG:H132	1.92	0.51
4:D:258:ILE:HD13	25:D:409:LHG:HC82	1.92	0.51
24:1:423:SQD:O7	24:1:423:SQD:O4	2.28	0.51
21:6:507:CL7:HMD3	21:6:509:CL7:H171	1.91	0.51
11:M:31:SER:OG	11:m:31:SER:OG	2.29	0.51
16:2:250:LEU:HD21	21:2:508:CL7:HAB	1.92	0.51
20:4:58:VAL:HG21	32:4:403:ZEX:H15	1.91	0.51
18:5:234:PRO:HA	21:5:407:CL7:HED3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:7:515:CL7:HMC2	32:8:420:ZEX:H391	1.92	0.51
21:8:408:CL7:O1A	21:8:409:CL7:OBB	2.28	0.51
21:3:515:CL7:HMC2	32:4:420:ZEX:H391	1.92	0.51
21:b:604:CL7:H3A	21:b:604:CL7:O1A	2.09	0.51
4:d:186:GLY:HA3	4:d:324:LEU:HD22	1.93	0.51
18:5:214:GLY:CA	32:5:422:ZEX:H362	2.37	0.51
20:8:304:ARG:HG3	32:8:418:ZEX:H23	1.93	0.51
2:B:65:VAL:HG11	21:B:604:CL7:HAA1	1.91	0.51
24:B:626:SQD:H112	1:a:28:LEU:HD12	1.93	0.51
7:H:52:HIS:NE2	7:H:61:ALA:O	2.40	0.51
16:2:262:TYR:HB2	32:2:520:ZEX:C38	2.41	0.51
2:b:65:VAL:HG11	21:b:605:CL7:HAA1	1.91	0.51
18:5:197:THR:HB	18:5:200:TYR:CD2	2.46	0.51
2:B:251:ALA:HB2	2:B:466:HIS:CG	2.46	0.51
4:D:186:GLY:HA3	4:D:324:LEU:HD22	1.93	0.51
32:3:525:ZEX:C38	16:6:262:TYR:HB2	2.41	0.51
20:4:109:VAL:O	20:4:113:LEU:HG	2.11	0.51
20:4:116:PHE:CD2	32:4:420:ZEX:H32	2.46	0.51
20:4:304:ARG:HG3	32:4:418:ZEX:H23	1.93	0.51
1:a:195:HIS:CD2	1:a:293:MET:HE2	2.46	0.51
2:b:251:ALA:HB2	2:b:466:HIS:CG	2.46	0.51
8:i:20:PHE:O	8:i:24:ILE:HG23	2.11	0.51
18:5:258:GLY:O	18:5:262:MET:HG3	2.11	0.51
19:7:147:LEU:HD21	21:7:506:CL7:HAB	1.93	0.51
21:7:507:CL7:O2D	21:7:507:CL7:H2A	2.09	0.51
1:A:19:SER:O	1:A:23:SER:HB3	2.11	0.50
4:D:171:SER:HB2	4:D:176:SER:HB2	1.94	0.50
19:3:147:LEU:HD21	21:3:506:CL7:HAB	1.93	0.50
2:b:91:ILE:HG12	2:b:92:LEU:H	1.76	0.50
2:b:294:ARG:O	2:b:298:SER:OG	2.23	0.50
21:b:608:CL7:H12C	26:b:622:LMG:H132	1.92	0.50
3:c:477:TYR:CZ	3:c:481:LEU:HD21	2.46	0.50
16:2:280:LEU:HD13	16:2:290:PHE:HB3	1.92	0.50
20:4:93:VAL:HG13	20:4:106:PRO:HB2	1.93	0.50
21:a:401:CL7:H41C	21:a:405:CL7:OBB	2.11	0.50
16:6:340:PHE:HA	16:6:346:VAL:HG21	1.94	0.50
8:I:20:PHE:O	8:I:24:ILE:HG23	2.11	0.50
16:2:207:VAL:HA	32:2:521:ZEX:C38	2.37	0.50
20:4:292:VAL:HG13	21:4:406:CL7:H141	1.92	0.50
21:8:407:CL7:C3D	32:8:419:ZEX:H163	2.40	0.50
1:A:84:PRO:HA	1:A:112:TYR:CG	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:ASP:HB2	7:H:19:ALA:HA	1.92	0.50
2:B:344:PRO:HB3	2:B:401:PHE:CE1	2.47	0.50
18:1:68:LEU:HB3	21:1:404:CL7:HED1	1.94	0.50
3:c:87:PHE:HA	3:c:96:GLN:NE2	2.27	0.50
21:5:417:CL7:CGA	21:5:417:CL7:H3A	2.39	0.50
20:8:151:GLU:OE2	20:8:152:TRP:N	2.42	0.50
4:D:63:ALA:HB1	4:D:68:GLU:HB3	1.93	0.50
18:1:80:GLY:H	18:1:84:VAL:HB	1.75	0.50
21:1:417:CL7:CGA	21:1:417:CL7:H3A	2.39	0.50
1:a:84:PRO:HA	1:a:112:TYR:CG	2.46	0.50
2:B:54:PRO:HD2	2:B:57:ARG:HG3	1.94	0.50
4:D:11:ARG:HG3	4:D:15:ASP:HB2	1.94	0.50
21:a:401:CL7:H141	21:a:405:CL7:H152	1.94	0.50
2:b:344:PRO:HB3	2:b:401:PHE:CE1	2.47	0.50
21:b:604:CL7:H101	21:b:606:CL7:H193	1.94	0.50
21:5:408:CL7:C14	32:5:422:ZEX:H402	2.41	0.50
19:7:271:PHE:O	19:7:304:ARG:NH2	2.43	0.50
24:7:521:SQD:H141	24:7:521:SQD:H271	1.92	0.50
20:8:109:VAL:O	20:8:113:LEU:HG	2.11	0.50
3:C:477:TYR:CZ	3:C:481:LEU:HD21	2.46	0.50
4:D:258:ILE:HG21	25:D:409:LHG:H262	1.92	0.50
21:2:513:CL7:NB	32:2:523:ZEX:H41	2.26	0.50
18:1:190:VAL:HG22	32:1:422:ZEX:H361	1.94	0.50
18:1:258:GLY:O	18:1:262:MET:HG3	2.11	0.50
1:a:19:SER:O	1:a:23:SER:HB3	2.11	0.50
16:6:250:LEU:HD21	21:6:508:CL7:HAB	1.92	0.50
16:6:280:LEU:HD13	16:6:290:PHE:HB3	1.93	0.50
21:6:501:CL7:HMD2	21:6:503:CL7:O2A	2.10	0.50
18:5:68:LEU:HB3	21:5:404:CL7:HED1	1.94	0.50
2:B:7:ARG:NH2	25:B:623:LHG:O5	2.35	0.50
20:8:210:LEU:HD21	21:8:417:CL7:C1B	2.42	0.50
21:B:603:CL7:H101	21:B:605:CL7:H193	1.94	0.50
25:B:625:LHG:HC11	10:L:13:LEU:HA	1.93	0.50
19:3:34:GLN:HG3	19:3:38:MET:HE3	1.94	0.50
2:b:142:ASP:HB2	7:h:19:ALA:HA	1.92	0.50
4:d:171:SER:HB2	4:d:176:SER:HB2	1.94	0.50
1:A:28:LEU:HD12	24:A:405:SQD:H112	1.93	0.49
21:A:401:CL7:H141	21:A:406:CL7:H152	1.94	0.49
2:b:7:ARG:NH2	25:b:624:LHG:O5	2.35	0.49
16:6:69:GLN:NE2	21:6:502:CL7:HAA1	2.23	0.49
21:6:513:CL7:NB	32:6:522:ZEX:H41	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4:210:LEU:HD21	21:4:417:CL7:C1B	2.42	0.49
2:b:54:PRO:HD2	2:b:57:ARG:HG3	1.94	0.49
4:d:63:ALA:HB1	4:d:68:GLU:HB3	1.93	0.49
21:6:502:CL7:C2B	21:6:504:CL7:HAB	2.42	0.49
18:5:152:ILE:HG21	21:5:408:CL7:H43C	1.93	0.49
19:7:259:ASN:HB3	21:7:501:CL7:H42C	1.95	0.49
2:B:333:GLY:O	2:B:439:SER:HB3	2.13	0.49
3:C:268:PRO:HA	21:C:507:CL7:HED2	1.93	0.49
4:D:283:ILE:HA	4:D:286:VAL:HG12	1.94	0.49
16:2:340:PHE:HA	16:2:346:VAL:HG21	1.94	0.49
18:1:152:ILE:HG21	21:1:408:CL7:H43C	1.94	0.49
21:1:408:CL7:C14	32:1:422:ZEX:H402	2.41	0.49
19:3:259:ASN:HB3	21:3:501:CL7:H42C	1.94	0.49
25:b:626:LHG:HC11	10:l:13:LEU:HA	1.93	0.49
4:d:11:ARG:HG3	4:d:15:ASP:HB2	1.94	0.49
21:6:518:CL7:HBD	21:6:518:CL7:HAA2	1.93	0.49
19:7:305:PHE:HZ	32:7:519:ZEX:H362	1.77	0.49
5:E:16:SER:OG	5:E:17:ILE:N	2.45	0.49
18:1:238:SER:O	18:1:242:ASN:ND2	2.37	0.49
3:c:268:PRO:HA	21:c:507:CL7:HED2	1.93	0.49
21:6:502:CL7:HMD2	21:6:503:CL7:H141	1.94	0.49
18:5:190:VAL:HG22	32:5:422:ZEX:H361	1.93	0.49
1:A:195:HIS:CD2	1:A:293:MET:HE2	2.46	0.49
21:A:401:CL7:H41C	21:A:406:CL7:OBB	2.11	0.49
2:B:270:THR:O	2:B:272:PRO:HD3	2.13	0.49
1:a:174:LEU:HD22	22:a:402:PHO:H143	1.95	0.49
20:8:116:PHE:CD2	32:8:420:ZEX:H32	2.46	0.49
19:3:305:PHE:HZ	32:3:519:ZEX:H362	1.77	0.49
1:a:49:VAL:HG22	30:d:407:PL9:H503	1.94	0.49
7:h:52:HIS:NE2	7:h:61:ALA:O	2.40	0.49
21:5:418:CL7:H2A	21:5:418:CL7:CED	2.43	0.49
19:7:149:PHE:HE2	21:7:512:CL7:HHB	1.78	0.49
3:C:87:PHE:HA	3:C:96:GLN:NE2	2.27	0.49
20:4:61:GLY:HA2	20:4:111:GLY:HA2	1.94	0.49
1:A:331:MET:CG	4:D:323:GLY:HA3	2.43	0.49
16:2:69:GLN:NE2	21:2:502:CL7:HAA1	2.23	0.49
21:2:510:CL7:H2A	21:2:510:CL7:O2A	2.12	0.49
21:1:402:CL7:C2D	21:1:404:CL7:H42C	2.43	0.49
20:4:188:ASP:HB3	20:4:191:THR:OG1	2.13	0.49
3:c:323:GLN:HG3	3:c:373:PHE:CD2	2.48	0.49
21:5:402:CL7:C2D	21:5:404:CL7:H42C	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:ILE:HG12	2:B:92:LEU:H	1.76	0.49
21:2:502:CL7:C2B	21:2:504:CL7:HAB	2.42	0.49
2:b:333:GLY:O	2:b:439:SER:HB3	2.13	0.49
21:2:518:CL7:HAA2	21:2:518:CL7:HBD	1.93	0.49
2:b:241:ASN:O	2:b:244:THR:HG22	2.13	0.49
21:6:510:CL7:O2A	21:6:510:CL7:H2A	2.12	0.49
1:A:49:VAL:HG22	30:D:407:PL9:H503	1.94	0.48
21:2:516:CL7:HBA1	21:2:516:CL7:H3A	1.55	0.48
21:2:518:CL7:H201	21:7:502:CL7:H51C	1.95	0.48
20:4:115:PHE:HE2	32:4:403:ZEX:H363	1.69	0.48
1:a:288:MET:O	1:a:292:THR:HG23	2.13	0.48
21:c:502:CL7:H202	21:c:502:CL7:H162	1.70	0.48
4:d:118:VAL:HG23	4:d:152:TYR:HE1	1.78	0.48
20:8:61:GLY:HA2	20:8:111:GLY:HA2	1.94	0.48
2:B:206:LEU:HD13	21:B:603:CL7:HED3	1.95	0.48
3:C:323:GLN:HG3	3:C:373:PHE:CD2	2.48	0.48
21:3:509:CL7:H111	21:3:509:CL7:H142	1.63	0.48
21:7:505:CL7:H71C	32:7:520:ZEX:C19	2.43	0.48
21:8:406:CL7:H41C	21:8:406:CL7:H62C	1.51	0.48
2:B:241:ASN:O	2:B:244:THR:HG22	2.13	0.48
16:2:8:ASN:O	16:2:8:ASN:ND2	2.46	0.48
19:7:34:GLN:HG3	19:7:38:MET:HE3	1.94	0.48
21:B:607:CL7:HBD	21:B:607:CL7:HED3	1.66	0.48
21:1:418:CL7:CED	21:1:418:CL7:H2A	2.43	0.48
3:c:71:MET:HE3	23:c:519:8CT:C40	2.43	0.48
4:d:283:ILE:HA	4:d:286:VAL:HG12	1.94	0.48
16:6:42:ALA:O	16:6:46:THR:OG1	2.30	0.48
21:C:502:CL7:HBA1	21:C:502:CL7:H3A	1.59	0.48
21:3:505:CL7:H71C	32:3:520:ZEX:C19	2.43	0.48
32:4:403:ZEX:H15	32:4:403:ZEX:H201	1.65	0.48
2:b:270:THR:O	2:b:272:PRO:HD3	2.12	0.48
4:d:256:PHE:O	25:d:409:LHG:H321	2.14	0.48
16:6:270:VAL:HG23	16:6:271:PHE:CD2	2.48	0.48
19:7:69:GLN:HB2	21:7:503:CL7:HED2	1.96	0.48
2:B:195:PRO:HB2	7:H:56:LEU:HD13	1.95	0.48
21:B:612:CL7:H62C	21:B:615:CL7:HMB3	1.95	0.48
18:1:256:ILE:HG23	18:1:324:MET:HE3	1.96	0.48
20:4:327:LEU:HD22	32:4:418:ZEX:H362	1.94	0.48
1:a:212:ALA:HB2	4:d:210:CYS:HB2	1.95	0.48
1:a:331:MET:CG	4:d:323:GLY:HA3	2.43	0.48
16:6:335:ARG:O	16:6:338:THR:OG1	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:5:211:LEU:HD12	32:5:422:ZEX:H382	1.93	0.48
1:A:202:VAL:HG22	21:A:401:CL7:C1B	2.44	0.48
21:B:614:CL7:H41C	21:B:614:CL7:H62C	1.50	0.48
3:C:71:MET:HE3	23:C:519:8CT:C40	2.43	0.48
5:E:26:THR:HG21	31:F:101:HEM:HMB2	1.96	0.48
16:2:271:PHE:O	16:2:304:ARG:NH2	2.47	0.48
21:3:502:CL7:H51C	21:6:518:CL7:H201	1.94	0.48
24:3:521:SQD:H45	24:3:521:SQD:H81	1.52	0.48
1:a:202:VAL:HG22	21:a:401:CL7:C1B	2.44	0.48
2:b:74:SER:OG	2:b:102:GLU:OE2	2.19	0.48
4:d:84:LEU:HD23	5:e:69:ARG:HA	1.96	0.48
20:8:95:VAL:HG12	20:8:101:ILE:HA	1.95	0.48
1:A:288:MET:O	1:A:292:THR:HG23	2.13	0.48
4:D:256:PHE:O	25:D:409:LHG:H321	2.14	0.48
21:2:502:CL7:HMD2	21:2:503:CL7:H141	1.94	0.48
21:2:510:CL7:H41C	21:2:510:CL7:H61C	1.54	0.48
21:1:420:CL7:O2D	21:1:420:CL7:H2A	2.14	0.48
21:b:605:CL7:HBA2	21:b:606:CL7:CAD	2.44	0.48
21:c:510:CL7:H3A	21:c:510:CL7:HBA2	1.63	0.48
18:5:291:GLY:HA3	26:5:401:LMG:HC72	1.96	0.48
20:8:188:ASP:HB3	20:8:191:THR:OG1	2.13	0.48
16:2:270:VAL:HG23	16:2:271:PHE:CD2	2.48	0.48
16:2:330:SER:HB2	19:7:113:LYS:HG3	1.95	0.48
16:2:335:ARG:O	16:2:338:THR:OG1	2.30	0.48
21:3:507:CL7:H62C	21:3:507:CL7:H101	1.64	0.48
3:c:199:ASP:OD2	3:c:209:ARG:NH2	2.36	0.48
5:e:26:THR:HG21	31:f:101:HEM:HMB2	1.96	0.48
16:6:77:VAL:HG21	16:6:275:PHE:CZ	2.49	0.48
16:6:207:VAL:HA	32:6:520:ZEX:C38	2.37	0.48
21:6:512:CL7:HMA2	21:6:512:CL7:H2	1.96	0.48
21:7:504:CL7:H93C	21:7:504:CL7:H111	1.74	0.48
20:8:170:SER:HB3	20:8:243:ASP:HB3	1.96	0.48
21:2:512:CL7:C6	32:2:523:ZEX:H202	2.34	0.47
4:d:295:TYR:OH	4:d:325:ARG:NH1	2.32	0.47
16:6:8:ASN:O	16:6:8:ASN:ND2	2.46	0.47
21:5:420:CL7:H2A	21:5:420:CL7:O2D	2.14	0.47
20:8:327:LEU:HD22	32:8:418:ZEX:H362	1.94	0.47
21:8:404:CL7:H3A	21:8:404:CL7:HBA1	1.27	0.47
1:A:174:LEU:HD22	22:A:402:PHO:H143	1.95	0.47
19:3:49:GLU:CD	19:3:66:CYS:H	2.22	0.47
21:3:506:CL7:HBA2	21:3:506:CL7:CHA	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:206:LEU:HD13	21:b:604:CL7:HED3	1.95	0.47
21:b:613:CL7:H62C	21:b:616:CL7:HMB3	1.95	0.47
16:6:271:PHE:O	16:6:304:ARG:NH2	2.47	0.47
21:6:514:CL7:HBA1	21:6:514:CL7:H3A	1.69	0.47
19:7:253:LEU:HD12	21:7:509:CL7:HED3	1.96	0.47
19:7:271:PHE:CZ	21:7:501:CL7:HBA2	2.50	0.47
2:B:189:VAL:HB	2:B:207:VAL:HG21	1.96	0.47
21:B:604:CL7:HBA2	21:B:605:CL7:CAD	2.44	0.47
21:C:506:CL7:H42C	21:C:506:CL7:C1C	2.45	0.47
4:D:84:LEU:HD23	5:E:69:ARG:HA	1.96	0.47
16:2:113:THR:HG21	21:2:513:CL7:HED1	1.96	0.47
19:3:113:LYS:HG3	16:6:330:SER:HB2	1.97	0.47
21:3:502:CL7:CGA	21:3:503:CL7:H12C	2.45	0.47
21:3:505:CL7:H43C	32:3:520:ZEX:H8	1.97	0.47
20:4:214:THR:HG21	20:4:225:ALA:HB3	1.96	0.47
32:4:403:ZEX:H11	32:4:403:ZEX:H191	1.76	0.47
18:5:57:THR:HG23	18:5:85:VAL:HB	1.97	0.47
21:5:409:CL7:OBD	32:5:421:ZEX:O3	2.25	0.47
1:A:223:LEU:O	1:A:224:VAL:C	2.56	0.47
4:D:118:VAL:HG23	4:D:152:TYR:HE1	1.78	0.47
19:3:69:GLN:HB2	21:3:503:CL7:HED2	1.96	0.47
19:3:253:LEU:HD12	21:3:509:CL7:HED3	1.96	0.47
20:4:95:VAL:HG12	20:4:101:ILE:HA	1.95	0.47
21:4:405:CL7:CGA	21:4:406:CL7:H12C	2.44	0.47
2:b:195:PRO:HB2	7:h:56:LEU:HD13	1.95	0.47
4:d:201:ALA:HB2	30:d:407:PL9:H353	1.97	0.47
21:7:503:CL7:H72C	21:7:503:CL7:H112	1.52	0.47
1:A:212:ALA:HB2	4:D:210:CYS:HB2	1.95	0.47
21:B:608:CL7:H3A	21:B:608:CL7:HBA1	1.54	0.47
3:C:325:GLN:HB2	3:C:408:MET:HG3	1.95	0.47
21:3:506:CL7:O1D	21:3:506:CL7:H2A	2.15	0.47
21:a:401:CL7:H41C	21:a:401:CL7:H62C	1.48	0.47
3:c:301:TYR:HB3	3:c:309:TYR:HE2	1.79	0.47
16:6:113:THR:HG21	21:6:513:CL7:HED1	1.96	0.47
19:7:229:LYS:HG2	19:7:230:PRO:HD2	1.97	0.47
21:7:506:CL7:HBA2	21:7:506:CL7:CHA	2.45	0.47
21:7:507:CL7:H101	21:7:507:CL7:H62C	1.64	0.47
21:8:405:CL7:CGA	21:8:406:CL7:H12C	2.44	0.47
2:B:41:GLU:OE2	2:B:61:PHE:N	2.35	0.47
16:2:77:VAL:HG21	16:2:275:PHE:CZ	2.49	0.47
20:4:170:SER:HB3	20:4:243:ASP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:145:LYS:NZ	7:h:18:GLU:OE1	2.40	0.47
9:k:15:SER:O	9:k:18:SER:OG	2.20	0.47
21:5:406:CL7:H12C	32:5:422:ZEX:H3	1.96	0.47
2:B:42:LEU:HD23	2:B:42:LEU:HA	1.73	0.47
21:B:603:CL7:H203	21:B:603:CL7:H161	1.75	0.47
3:C:112:GLY:N	3:C:116:GLU:O	2.48	0.47
3:C:301:TYR:HB3	3:C:309:TYR:HE2	1.79	0.47
4:D:201:ALA:HB2	30:D:407:PL9:H353	1.97	0.47
16:2:65:VAL:HG13	21:2:504:CL7:HMA2	1.96	0.47
16:2:102:VAL:O	16:2:105:SER:OG	2.29	0.47
19:3:63:ASN:O	19:3:64:LEU:HD12	2.15	0.47
21:b:610:CL7:H3A	21:b:610:CL7:HBA1	1.50	0.47
3:c:325:GLN:HB2	3:c:408:MET:HG3	1.95	0.47
21:c:507:CL7:H121	21:c:508:CL7:H192	1.97	0.47
21:6:511:CL7:H61C	21:6:511:CL7:H41C	1.58	0.47
19:7:146:HIS:ND1	21:7:507:CL7:OBD	2.48	0.47
20:8:214:THR:HG21	20:8:225:ALA:HB3	1.96	0.47
21:C:511:CL7:H111	21:C:511:CL7:H72C	1.48	0.47
9:K:19:PRO:O	9:K:22:ASP:HB2	2.15	0.47
16:2:287:LEU:HD23	21:2:517:CL7:HBC2	1.97	0.47
21:4:406:CL7:HBA1	21:4:406:CL7:H3A	1.62	0.47
21:4:411:CL7:H162	21:4:411:CL7:H141	1.70	0.47
21:4:415:CL7:H3A	21:4:415:CL7:HBA1	1.41	0.47
1:a:154:THR:HG22	21:a:401:CL7:H43C	1.97	0.47
1:a:223:LEU:O	1:a:224:VAL:C	2.56	0.47
2:b:189:VAL:HB	2:b:207:VAL:HG21	1.96	0.47
3:c:409:THR:OG1	3:c:410:HIS:ND1	2.35	0.47
21:c:506:CL7:H42C	21:c:506:CL7:C1C	2.45	0.47
21:A:406:CL7:HMD1	21:D:404:CL7:HAB	1.97	0.47
21:B:611:CL7:H141	21:B:611:CL7:H161	1.66	0.47
18:1:57:THR:HG23	18:1:85:VAL:HB	1.97	0.47
18:1:211:LEU:HD12	32:1:422:ZEX:H382	1.93	0.47
19:3:136:PHE:HB3	19:3:230:PRO:HG3	1.96	0.47
21:3:508:CL7:H62C	21:3:508:CL7:H102	1.52	0.47
21:b:616:CL7:HBA1	21:b:616:CL7:H3A	1.45	0.47
3:c:112:GLY:N	3:c:116:GLU:O	2.48	0.47
21:6:510:CL7:H61C	21:6:510:CL7:H41C	1.54	0.47
19:7:63:ASN:O	19:7:64:LEU:HD12	2.15	0.47
21:7:507:CL7:H41C	21:7:507:CL7:H61C	1.63	0.47
3:C:76:ALA:HB2	21:C:504:CL7:HMD2	1.97	0.47
18:1:291:GLY:HA3	26:1:401:LMG:HC72	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:409:CL7:HBD	21:1:409:CL7:HAA2	1.97	0.47
19:3:229:LYS:HG2	19:3:230:PRO:HD2	1.97	0.47
21:3:503:CL7:H112	21:3:503:CL7:H72C	1.52	0.47
9:k:31:PHE:O	9:k:34:LEU:HB3	2.15	0.47
18:5:256:ILE:HG23	18:5:324:MET:HE3	1.96	0.47
21:7:516:CL7:H11C	21:7:516:CL7:HBA1	1.54	0.47
21:B:611:CL7:H141	21:B:611:CL7:H203	1.97	0.46
21:B:612:CL7:H142	21:B:612:CL7:H111	1.73	0.46
21:C:510:CL7:H62C	21:C:510:CL7:H41C	1.60	0.46
5:E:21:ILE:O	5:E:25:ILE:HG12	2.16	0.46
21:2:512:CL7:HMA2	21:2:512:CL7:H2	1.96	0.46
21:1:406:CL7:H12C	32:1:422:ZEX:H3	1.96	0.46
19:3:119:ALA:HB2	19:3:130:HIS:CG	2.50	0.46
5:e:21:ILE:O	5:e:25:ILE:HG12	2.16	0.46
21:6:517:CL7:H162	21:6:517:CL7:H193	1.69	0.46
18:5:303:ALA:HB3	18:5:306:PHE:CD2	2.50	0.46
21:7:504:CL7:H92C	21:7:504:CL7:H61C	1.71	0.46
21:7:508:CL7:H61C	21:7:508:CL7:H41C	1.52	0.46
2:B:202:ASN:OD1	2:B:204:THR:OG1	2.27	0.46
21:C:504:CL7:H151	21:C:504:CL7:H112	1.75	0.46
11:M:13:LEU:HD12	11:M:13:LEU:HA	1.80	0.46
16:2:109:PHE:O	16:2:113:THR:OG1	2.22	0.46
21:1:409:CL7:OBB	21:1:411:CL7:HHB	2.16	0.46
19:3:271:PHE:CZ	21:3:501:CL7:HBA2	2.50	0.46
21:5:409:CL7:HAA2	21:5:409:CL7:HBD	1.97	0.46
1:A:157:VAL:HG11	21:A:406:CL7:HMC2	1.97	0.46
21:C:510:CL7:H202	21:C:513:CL7:HAC1	1.97	0.46
16:2:253:LEU:HD12	21:2:509:CL7:HED3	1.97	0.46
21:2:517:CL7:H62C	21:2:517:CL7:H41C	1.42	0.46
1:a:157:VAL:HG11	21:a:405:CL7:HMC2	1.97	0.46
1:a:331:MET:HG3	4:d:323:GLY:HA3	1.98	0.46
3:c:76:ALA:HB2	21:c:504:CL7:HMD2	1.96	0.46
19:7:49:GLU:CD	19:7:66:CYS:H	2.22	0.46
19:7:167:TYR:OH	19:7:274:GLU:OE2	2.28	0.46
21:7:516:CL7:CED	32:8:403:ZEX:H172	2.45	0.46
20:8:166:LEU:HD23	20:8:166:LEU:HA	1.78	0.46
21:8:407:CL7:HHB	32:8:418:ZEX:C17	2.46	0.46
2:B:8:VAL:HG23	2:B:9:HIS:CD2	2.50	0.46
2:b:41:GLU:OE2	2:b:61:PHE:N	2.35	0.46
21:c:504:CL7:H162	21:c:504:CL7:H141	1.62	0.46
16:6:65:VAL:HG13	21:6:504:CL7:HMA2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:5:409:CL7:OBB	21:5:411:CL7:HHB	2.16	0.46
19:7:119:ALA:HB2	19:7:130:HIS:CG	2.50	0.46
1:A:104:GLU:O	1:A:108:ASN:ND2	2.48	0.46
2:B:324:LEU:O	21:B:607:CL7:H43C	2.16	0.46
21:2:506:CL7:H143	21:2:518:CL7:HED1	1.98	0.46
21:1:416:CL7:HED3	21:1:416:CL7:HBD	1.71	0.46
32:4:403:ZEX:H28	32:4:403:ZEX:H25	1.65	0.46
1:a:20:PHE:O	1:a:23:SER:OG	2.29	0.46
21:b:613:CL7:H62C	21:b:613:CL7:H102	1.71	0.46
21:b:615:CL7:H62C	21:b:615:CL7:H41C	1.50	0.46
16:6:91:ALA:O	16:6:95:ILE:HG13	2.16	0.46
21:6:506:CL7:H143	21:6:518:CL7:HED1	1.98	0.46
32:6:522:ZEX:H15	32:6:522:ZEX:H201	1.74	0.46
21:7:502:CL7:CGA	21:7:503:CL7:H12C	2.45	0.46
21:B:604:CL7:H41C	21:B:604:CL7:H93C	1.98	0.46
21:C:510:CL7:HBA2	21:C:510:CL7:H3A	1.63	0.46
21:D:405:CL7:HBA1	21:D:405:CL7:H3A	1.58	0.46
21:2:513:CL7:NB	32:2:523:ZEX:C4	2.79	0.46
21:1:410:CL7:H51C	21:1:410:CL7:H8	1.63	0.46
21:3:508:CL7:H61C	21:3:508:CL7:H41C	1.53	0.46
20:4:158:LEU:O	20:4:162:VAL:HG23	2.16	0.46
2:b:230:SER:OG	7:h:25:GLY:O	2.33	0.46
4:d:208:LEU:O	4:d:212:ILE:HG23	2.15	0.46
21:5:418:CL7:H3A	21:5:418:CL7:HBA1	1.59	0.46
21:7:505:CL7:H43C	32:7:520:ZEX:H8	1.97	0.46
20:8:197:ILE:HD11	20:8:233:ILE:HG13	1.97	0.46
21:8:406:CL7:H121	21:8:406:CL7:H162	1.73	0.46
32:8:418:ZEX:H15	32:8:418:ZEX:H201	1.61	0.46
21:C:507:CL7:H121	21:C:508:CL7:H192	1.97	0.46
4:D:208:LEU:O	4:D:212:ILE:HG23	2.15	0.46
9:K:31:PHE:O	9:K:34:LEU:HB3	2.15	0.46
32:2:521:ZEX:C11	24:7:523:SQD:H221	2.46	0.46
19:3:167:TYR:OH	19:3:274:GLU:OE2	2.28	0.46
25:4:401:LHG:HC92	21:4:405:CL7:C1B	2.46	0.46
21:a:401:CL7:C14	21:a:405:CL7:H152	2.46	0.46
2:b:8:VAL:HG23	2:b:9:HIS:CD2	2.50	0.46
21:c:502:CL7:H3A	21:c:502:CL7:HBA1	1.59	0.46
2:B:145:LYS:NZ	7:H:18:GLU:OE1	2.40	0.46
2:B:230:SER:OG	7:H:25:GLY:O	2.33	0.46
21:B:612:CL7:H62C	21:B:612:CL7:H102	1.71	0.46
19:3:231:TRP:NE1	21:3:506:CL7:OBD	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:3:511:CL7:H62C	21:3:511:CL7:H41C	1.63	0.46
2:b:324:LEU:O	21:b:608:CL7:H43C	2.16	0.46
2:b:366:PHE:CD1	2:b:367:PRO:HD2	2.51	0.46
21:b:612:CL7:H161	21:b:612:CL7:H141	1.66	0.46
21:c:510:CL7:H202	21:c:513:CL7:HAC1	1.97	0.46
9:k:19:PRO:O	9:k:22:ASP:HB2	2.15	0.46
21:6:503:CL7:HAA2	21:6:503:CL7:HBD	1.98	0.46
21:5:417:CL7:H3A	21:5:417:CL7:HBA1	1.70	0.46
19:7:316:PHE:O	19:7:320:GLN:HG2	2.16	0.46
24:7:521:SQD:H81	24:7:521:SQD:H45	1.52	0.46
21:B:605:CL7:HAA2	21:B:605:CL7:HBD	1.98	0.46
3:C:92:PRO:HD2	3:C:95:GLU:HB3	1.97	0.46
22:D:408:PHO:HBC2	22:D:408:PHO:HHD	1.98	0.46
19:3:146:HIS:ND1	21:3:507:CL7:OBD	2.48	0.46
21:3:516:CL7:CED	32:4:403:ZEX:H172	2.45	0.46
21:4:406:CL7:H152	21:4:411:CL7:H43C	1.98	0.46
21:b:603:CL7:HBD	21:b:603:CL7:H12C	1.98	0.46
22:d:408:PHO:HBC2	22:d:408:PHO:HHD	1.98	0.46
16:2:91:ALA:O	16:2:95:ILE:HG13	2.16	0.46
32:2:523:ZEX:H201	32:2:523:ZEX:H15	1.74	0.46
21:d:404:CL7:H112	22:d:408:PHO:CHB	2.46	0.46
18:5:234:PRO:O	18:5:239:LYS:NZ	2.49	0.46
21:5:406:CL7:H142	21:5:406:CL7:H111	1.76	0.46
19:7:136:PHE:HB3	19:7:230:PRO:HG3	1.96	0.46
21:7:506:CL7:H2A	21:7:506:CL7:O1D	2.15	0.46
21:7:513:CL7:HBA2	21:7:513:CL7:CHA	2.46	0.46
15:Z:1:MET:HE3	15:Z:4:LEU:HD23	1.98	0.45
21:2:502:CL7:H2	21:2:503:CL7:C1	2.42	0.45
18:1:234:PRO:O	18:1:239:LYS:NZ	2.49	0.45
18:1:277:TYR:CE1	21:1:403:CL7:HED1	2.51	0.45
21:3:501:CL7:H142	32:3:520:ZEX:C31	2.46	0.45
21:b:606:CL7:HAA2	21:b:606:CL7:HBD	1.98	0.45
16:6:287:LEU:HD23	21:6:517:CL7:HBC2	1.97	0.45
1:A:154:THR:HG22	21:A:401:CL7:H43C	1.97	0.45
21:A:401:CL7:C14	21:A:406:CL7:H152	2.46	0.45
21:B:609:CL7:H3A	21:B:609:CL7:HBA1	1.50	0.45
21:2:510:CL7:HMA3	21:2:510:CL7:H51C	1.99	0.45
19:3:138:THR:HG22	19:3:141:ARG:HH21	1.81	0.45
19:3:316:PHE:O	19:3:320:GLN:HG2	2.16	0.45
21:3:504:CL7:H142	21:3:504:CL7:H112	1.77	0.45
20:4:197:ILE:HD11	20:4:233:ILE:HG13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:4:407:CL7:HHB	32:4:418:ZEX:C17	2.46	0.45
2:b:130:ILE:HG13	7:h:12:LYS:HA	1.99	0.45
21:b:612:CL7:H141	21:b:612:CL7:H203	1.97	0.45
16:6:94:MET:CE	32:6:524:ZEX:H362	2.47	0.45
21:6:510:CL7:HMA3	21:6:510:CL7:H51C	1.99	0.45
18:5:277:TYR:CE1	21:5:403:CL7:HED1	2.51	0.45
21:8:406:CL7:H162	21:8:406:CL7:H202	1.73	0.45
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.51	0.45
21:a:405:CL7:HMD1	21:d:404:CL7:HAB	1.97	0.45
32:7:520:ZEX:H11	32:7:520:ZEX:H191	1.52	0.45
21:B:602:CL7:HBD	21:B:602:CL7:H12C	1.98	0.45
21:B:611:CL7:H143	26:B:621:LMG:H411	1.99	0.45
21:2:515:CL7:H3A	21:2:515:CL7:HBA2	1.79	0.45
18:1:135:TRP:CD1	18:1:248:PRO:HG3	2.52	0.45
19:3:149:PHE:HE2	21:3:512:CL7:HHB	1.78	0.45
20:4:124:ALA:HB2	21:4:415:CL7:C2C	2.47	0.45
21:b:605:CL7:H41C	21:b:605:CL7:H93C	1.98	0.45
21:c:510:CL7:H41C	21:c:510:CL7:H62C	1.60	0.45
16:6:253:LEU:HD12	21:6:509:CL7:HED3	1.97	0.45
21:6:510:CL7:H162	21:6:510:CL7:H141	1.61	0.45
18:5:135:TRP:CD1	18:5:248:PRO:HG3	2.51	0.45
25:8:401:LHG:HC92	21:8:405:CL7:C1B	2.46	0.45
3:C:85:SER:OG	3:C:86:HIS:ND1	2.46	0.45
16:2:149:PHE:CE2	21:2:512:CL7:HHB	2.51	0.45
19:3:129:PHE:HZ	32:3:522:ZEX:O3	1.95	0.45
20:4:230:GLU:OE1	20:4:230:GLU:N	2.37	0.45
3:c:249:HIS:HA	3:c:252:VAL:HG22	1.98	0.45
5:e:19:TYR:HD1	5:e:23:HIS:CD2	2.35	0.45
18:5:215:HIS:HE1	21:5:402:CL7:NC	2.15	0.45
21:8:412:CL7:H121	21:8:412:CL7:H8	1.81	0.45
5:E:30:LEU:HD21	31:F:101:HEM:HBB1	1.98	0.45
16:2:42:ALA:O	16:2:46:THR:OG1	2.30	0.45
21:2:508:CL7:HAA2	21:2:508:CL7:HBD	1.98	0.45
18:1:151:LEU:HD23	18:1:151:LEU:HA	1.71	0.45
21:3:504:CL7:H93C	21:3:504:CL7:H111	1.74	0.45
20:4:88:LEU:HD23	20:4:88:LEU:HA	1.75	0.45
21:b:609:CL7:HBA1	21:b:609:CL7:H3A	1.54	0.45
4:d:99:ASP:OD2	4:d:102:ARG:HG2	2.17	0.45
5:e:30:LEU:HD21	31:f:101:HEM:HBB1	1.98	0.45
16:6:108:ILE:O	16:6:111:ILE:HG22	2.17	0.45
16:6:149:PHE:CE2	21:6:512:CL7:HHB	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:6:513:CL7:NB	32:6:522:ZEX:C4	2.79	0.45
21:6:516:CL7:H162	21:6:516:CL7:H193	1.75	0.45
20:8:157:SER:O	20:8:160:THR:HG22	2.17	0.45
2:B:303:ASP:N	2:B:303:ASP:OD1	2.49	0.45
21:B:615:CL7:HBA1	21:B:615:CL7:H3A	1.45	0.45
21:D:404:CL7:H61C	21:D:404:CL7:H41C	1.67	0.45
16:2:189:TYR:O	16:2:198:PRO:HG3	2.16	0.45
18:1:75:LEU:HA	18:1:168:ILE:HG22	1.99	0.45
18:1:303:ALA:HB3	18:1:306:PHE:CD2	2.50	0.45
19:3:258:PHE:HB3	21:3:505:CL7:H203	1.98	0.45
20:4:148:PHE:CZ	32:4:420:ZEX:O3	2.70	0.45
2:b:178:ASP:OD1	2:b:182:LEU:N	2.38	0.45
3:c:92:PRO:HD2	3:c:95:GLU:HB3	1.97	0.45
3:c:387:LEU:HD12	3:c:392:LEU:HD21	1.98	0.45
21:6:505:CL7:H41C	21:6:505:CL7:H62C	1.49	0.45
18:5:75:LEU:HA	18:5:168:ILE:HG22	1.99	0.45
21:7:509:CL7:H12C	21:7:509:CL7:HBA1	1.68	0.45
4:D:87:SER:HB3	5:E:69:ARG:CZ	2.46	0.45
21:a:405:CL7:H3A	21:a:405:CL7:HBA1	1.55	0.45
21:b:612:CL7:H143	26:b:622:LMG:H411	1.99	0.45
3:c:85:SER:OG	3:c:86:HIS:ND1	2.46	0.45
15:z:1:MET:HE3	15:z:4:LEU:HD23	1.98	0.45
21:6:515:CL7:H3A	21:6:515:CL7:HBA2	1.79	0.45
21:5:404:CL7:H202	21:5:411:CL7:HAB	1.99	0.45
1:A:331:MET:HG3	4:D:323:GLY:HA3	1.98	0.45
5:E:19:TYR:HD1	5:E:23:HIS:CD2	2.35	0.45
21:2:516:CL7:HBA1	21:2:516:CL7:H12C	1.71	0.45
21:1:405:CL7:H3A	21:1:405:CL7:HBA1	1.71	0.45
21:3:512:CL7:H41C	21:3:512:CL7:H62C	1.78	0.45
21:4:404:CL7:H3A	21:4:404:CL7:HBA1	1.27	0.45
2:b:303:ASP:OD1	2:b:303:ASP:N	2.49	0.45
3:c:191:ALA:HA	3:c:196:GLY:HA2	1.99	0.45
16:6:102:VAL:O	16:6:105:SER:OG	2.29	0.45
18:5:193:TYR:OH	18:5:210:ASP:OD2	2.35	0.45
19:7:128:ARG:HB3	21:7:514:CL7:HED1	1.99	0.45
20:8:71:TYR:OH	20:8:101:ILE:HB	2.17	0.45
20:8:158:LEU:O	20:8:162:VAL:HG23	2.16	0.45
16:2:31:HIS:ND1	21:2:509:CL7:H142	2.32	0.45
21:4:406:CL7:H61C	21:4:406:CL7:H101	1.53	0.45
2:b:291:GLU:CD	2:b:294:ARG:HH21	2.24	0.45
19:7:138:THR:HG22	19:7:141:ARG:HH21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:7:258:PHE:HB3	21:7:505:CL7:H203	1.98	0.45
20:8:148:PHE:CZ	32:8:420:ZEX:O3	2.70	0.45
16:2:94:MET:CE	32:2:525:ZEX:H362	2.47	0.44
21:1:403:CL7:HAA2	21:1:403:CL7:HBD	1.99	0.44
32:1:422:ZEX:H27	32:1:422:ZEX:H391	1.76	0.44
19:3:112:THR:HG23	19:3:113:LYS:H	1.82	0.44
20:4:88:LEU:HG	21:4:406:CL7:HED3	1.99	0.44
21:4:404:CL7:H91C	21:4:404:CL7:H112	1.85	0.44
21:4:406:CL7:H41C	21:4:406:CL7:H62C	1.51	0.44
18:5:67:VAL:HG13	21:5:405:CL7:HMA1	1.99	0.44
21:5:404:CL7:H193	21:5:404:CL7:H162	1.83	0.44
21:5:408:CL7:C13	32:5:422:ZEX:H402	2.47	0.44
21:7:501:CL7:H142	32:7:520:ZEX:C31	2.46	0.44
21:7:507:CL7:H143	21:7:507:CL7:H162	1.81	0.44
32:7:522:ZEX:H191	32:7:522:ZEX:H11	1.48	0.44
3:C:387:LEU:HD12	3:C:392:LEU:HD21	1.98	0.44
21:C:506:CL7:H3A	21:C:506:CL7:HBA1	1.63	0.44
9:K:21:VAL:HA	9:K:24:MET:HG3	1.98	0.44
18:1:215:HIS:HE1	21:1:402:CL7:NC	2.15	0.44
21:1:404:CL7:H202	21:1:411:CL7:HAB	1.99	0.44
19:3:128:ARG:HB3	21:3:514:CL7:HED1	1.99	0.44
19:3:251:ALA:HB2	19:3:322:HIS:CD2	2.52	0.44
19:3:270:VAL:O	19:3:272:PRO:HD3	2.17	0.44
32:3:519:ZEX:H191	32:3:519:ZEX:H11	1.61	0.44
20:4:157:SER:O	20:4:160:THR:HG22	2.17	0.44
21:a:405:CL7:HBD	21:a:405:CL7:HAA2	2.00	0.44
22:d:408:PHO:NC	22:d:408:PHO:ND	2.65	0.44
16:6:189:TYR:O	16:6:198:PRO:HG3	2.16	0.44
21:7:505:CL7:H3A	21:7:505:CL7:HBA1	1.79	0.44
21:8:406:CL7:H152	21:8:411:CL7:H43C	1.98	0.44
32:8:420:ZEX:H15	32:8:420:ZEX:H201	1.81	0.44
21:B:604:CL7:H162	21:B:604:CL7:H121	1.77	0.44
27:C:517:DGD:HB72	27:C:517:DGD:HB42	1.58	0.44
18:1:67:VAL:HG13	21:1:405:CL7:HMA1	1.99	0.44
18:1:111:PHE:HD1	18:1:115:ILE:HD12	1.83	0.44
21:4:412:CL7:H61C	21:4:412:CL7:H41C	1.76	0.44
21:c:503:CL7:CBD	21:c:504:CL7:H43C	2.47	0.44
9:k:21:VAL:HA	9:k:24:MET:HG3	1.98	0.44
21:5:403:CL7:HAA2	21:5:403:CL7:HBD	2.00	0.44
19:7:251:ALA:HB2	19:7:322:HIS:CD2	2.52	0.44
20:8:88:LEU:HG	21:8:406:CL7:HED3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:8:124:ALA:HB2	21:8:415:CL7:C2C	2.47	0.44
24:B:620:SQD:C24	10:l:15:ARG:HD2	2.46	0.44
3:C:249:HIS:HA	3:C:252:VAL:HG22	1.98	0.44
21:2:505:CL7:CMD	32:2:521:ZEX:H163	2.47	0.44
21:2:511:CL7:H41C	21:2:511:CL7:H61C	1.58	0.44
21:2:517:CL7:H3A	21:2:517:CL7:HBA1	1.48	0.44
18:1:140:LYS:O	18:1:144:ILE:HG13	2.17	0.44
18:1:193:TYR:OH	18:1:210:ASP:OD2	2.35	0.44
21:1:404:CL7:H62C	21:1:404:CL7:H41C	1.62	0.44
24:3:521:SQD:H161	24:3:521:SQD:H291	1.99	0.44
20:4:155:PHE:CZ	21:4:408:CL7:HED3	2.53	0.44
21:b:607:CL7:H3A	21:b:607:CL7:HBA2	1.70	0.44
16:6:123:SER:C	16:6:125:ALA:H	2.26	0.44
21:6:501:CL7:H92C	21:6:501:CL7:H61C	1.75	0.44
21:6:503:CL7:HBD	21:6:503:CL7:O1A	2.17	0.44
21:6:508:CL7:HBD	21:6:508:CL7:HAA2	1.98	0.44
21:6:517:CL7:H111	21:6:517:CL7:H142	1.80	0.44
18:5:111:PHE:HD1	18:5:115:ILE:HD12	1.83	0.44
19:7:112:THR:HG23	19:7:113:LYS:H	1.82	0.44
21:7:510:CL7:H101	21:7:510:CL7:H62C	1.82	0.44
20:8:155:PHE:CZ	21:8:408:CL7:HED3	2.53	0.44
2:B:130:ILE:HG13	7:H:12:LYS:HA	1.99	0.44
21:B:605:CL7:H3A	21:B:605:CL7:HBA1	1.78	0.44
3:C:141:GLY:O	3:C:145:THR:OG1	2.20	0.44
21:C:503:CL7:CBD	21:C:504:CL7:H43C	2.47	0.44
21:2:503:CL7:HAA2	21:2:503:CL7:HBD	1.98	0.44
21:1:408:CL7:H121	21:1:408:CL7:H161	1.87	0.44
21:1:417:CL7:H3A	21:1:417:CL7:HBA1	1.70	0.44
21:4:412:CL7:O2A	21:4:412:CL7:H2A	2.18	0.44
21:b:605:CL7:HAA2	21:b:605:CL7:HBD	1.99	0.44
21:b:607:CL7:H41C	21:b:607:CL7:H62C	1.65	0.44
21:c:503:CL7:O1A	21:c:504:CL7:H2	2.17	0.44
4:d:87:SER:HB3	5:e:69:ARG:CZ	2.46	0.44
16:6:188:LYS:HB3	16:6:196:PHE:CD2	2.53	0.44
19:7:274:GLU:OE1	19:7:274:GLU:N	2.36	0.44
21:7:509:CL7:H2A	21:7:509:CL7:O1A	2.16	0.44
24:7:521:SQD:H291	24:7:521:SQD:H161	1.99	0.44
21:8:406:CL7:H3A	21:8:406:CL7:HBA1	1.62	0.44
3:C:48:TRP:O	21:C:509:CL7:H2	2.17	0.44
3:C:191:ALA:HA	3:C:196:GLY:HA2	1.99	0.44
4:D:99:ASP:OD2	4:D:102:ARG:HG2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D:408:PHO:NC	22:D:408:PHO:ND	2.65	0.44
19:3:224:TRP:CZ3	19:3:228:VAL:HG21	2.53	0.44
2:b:52:LEU:HD21	2:b:307:GLU:HG2	2.00	0.44
21:b:604:CL7:H203	21:b:610:CL7:H102	2.00	0.44
4:d:328:MET:HG2	4:d:332:ASP:HB2	2.00	0.44
21:6:516:CL7:H41C	21:6:516:CL7:H61C	1.33	0.44
21:6:516:CL7:HBA1	21:6:516:CL7:H3A	1.55	0.44
21:5:404:CL7:H62C	21:5:404:CL7:H41C	1.63	0.44
21:5:410:CL7:H8	21:5:410:CL7:H51C	1.63	0.44
4:D:263:LYS:HE3	4:D:263:LYS:HB2	1.86	0.44
32:2:525:ZEX:H15	32:2:525:ZEX:H201	1.81	0.44
32:4:403:ZEX:H401	32:4:403:ZEX:H31	1.75	0.44
21:6:503:CL7:H62C	21:6:503:CL7:H41C	1.78	0.44
21:6:505:CL7:CMD	32:6:520:ZEX:H163	2.47	0.44
18:5:152:ILE:HD11	21:5:410:CL7:H61C	2.00	0.44
21:7:504:CL7:H62C	21:7:504:CL7:H41C	1.36	0.44
32:7:519:ZEX:H191	32:7:519:ZEX:H11	1.61	0.44
20:8:38:MET:HB2	20:8:38:MET:HE3	1.71	0.44
2:B:69:ILE:HD11	21:B:605:CL7:HBA1	1.99	0.44
21:2:509:CL7:H161	21:2:509:CL7:H141	1.49	0.44
21:2:510:CL7:H162	21:2:510:CL7:H141	1.61	0.44
1:a:104:GLU:O	1:a:108:ASN:ND2	2.48	0.44
2:b:443:PHE:O	2:b:444:ARG:HG3	2.18	0.44
21:b:605:CL7:H121	21:b:605:CL7:H162	1.77	0.44
21:b:608:CL7:HBD	21:b:608:CL7:HED3	1.66	0.44
21:b:609:CL7:HBC3	21:b:609:CL7:HHD	2.00	0.44
4:d:296:ASP:N	4:d:296:ASP:OD1	2.50	0.44
20:8:85:MET:HE2	20:8:85:MET:HB3	1.91	0.44
20:8:167:VAL:HG23	20:8:247:ALA:HB1	2.00	0.44
2:B:52:LEU:HD21	2:B:307:GLU:HG2	2.00	0.44
4:D:92:TRP:NE1	13:X:13:SER:HB3	2.33	0.44
16:2:108:ILE:O	16:2:111:ILE:HG22	2.17	0.44
16:2:144:GLY:HA3	16:2:226:ILE:HG13	2.00	0.44
21:2:512:CL7:O1D	21:2:512:CL7:HBA1	2.18	0.44
21:1:418:CL7:HBA1	21:1:418:CL7:H3A	1.59	0.44
21:3:503:CL7:H101	21:3:503:CL7:H13	1.74	0.44
21:4:406:CL7:H121	21:4:406:CL7:H162	1.73	0.44
4:d:28:PHE:O	4:d:127:ARG:NH1	2.47	0.44
4:d:92:TRP:NE1	13:x:13:SER:HB3	2.33	0.44
16:6:313:PHE:CD2	32:6:519:ZEX:H30	2.53	0.44
21:6:517:CL7:H62C	21:6:517:CL7:H41C	1.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:5:140:LYS:O	18:5:144:ILE:HG13	2.17	0.44
19:7:224:TRP:CZ3	19:7:228:VAL:HG21	2.53	0.44
20:8:289:VAL:HG22	21:8:410:CL7:HAB	1.99	0.44
21:8:404:CL7:H91C	21:8:404:CL7:H112	1.85	0.44
21:B:603:CL7:H93C	21:B:603:CL7:H111	1.78	0.43
21:C:504:CL7:H162	21:C:504:CL7:H141	1.62	0.43
19:3:161:ALA:HA	19:3:166:VAL:HG13	2.00	0.43
2:b:69:ILE:HD11	21:b:606:CL7:HBA1	1.99	0.43
16:6:144:GLY:HA3	16:6:226:ILE:HG13	2.00	0.43
21:6:512:CL7:O1D	21:6:512:CL7:HBA1	2.18	0.43
21:5:405:CL7:H3A	21:5:405:CL7:HBA1	1.71	0.43
21:8:412:CL7:H2A	21:8:412:CL7:O2A	2.18	0.43
1:A:202:VAL:HG22	21:A:401:CL7:C2B	2.48	0.43
1:A:214:MET:SD	22:D:408:PHO:CED	3.07	0.43
2:B:401:PHE:HB2	2:B:406:LEU:O	2.18	0.43
2:B:443:PHE:O	2:B:444:ARG:HG3	2.18	0.43
3:C:131:LEU:O	3:C:134:SER:OG	2.27	0.43
3:C:199:ASP:OD2	3:C:209:ARG:NH2	2.36	0.43
4:D:203:ILE:HD13	4:D:203:ILE:HA	1.80	0.43
32:2:520:ZEX:H15	32:2:520:ZEX:H201	1.85	0.43
18:1:90:VAL:O	18:1:94:ILE:HG12	2.18	0.43
21:1:404:CL7:H13	21:1:404:CL7:H102	1.51	0.43
21:1:406:CL7:H121	21:1:406:CL7:H162	1.83	0.43
20:4:71:TYR:OH	20:4:101:ILE:HB	2.17	0.43
21:4:405:CL7:H2	21:4:406:CL7:H11C	2.00	0.43
21:4:406:CL7:H143	21:4:406:CL7:H111	1.80	0.43
21:b:613:CL7:H3A	21:b:613:CL7:HBA1	1.60	0.43
27:c:517:DGD:HB72	27:c:517:DGD:HB42	1.58	0.43
5:e:16:SER:OG	5:e:17:ILE:N	2.45	0.43
11:m:13:LEU:HD12	11:m:13:LEU:HA	1.80	0.43
21:8:406:CL7:H61C	21:8:406:CL7:H101	1.53	0.43
1:A:96:ILE:HG22	8:I:1:MET:HE1	2.00	0.43
1:A:330:VAL:HG21	4:D:327:TRP:CE2	2.53	0.43
21:B:606:CL7:C4A	21:B:606:CL7:HBA2	2.46	0.43
21:D:405:CL7:HAA2	21:D:405:CL7:HBD	2.01	0.43
21:2:503:CL7:H3A	21:2:503:CL7:HBA1	1.85	0.43
21:1:410:CL7:HBA2	21:1:410:CL7:H11C	1.89	0.43
21:3:509:CL7:H12C	21:3:509:CL7:HBA1	1.68	0.43
21:3:509:CL7:O1A	21:3:509:CL7:H2A	2.16	0.43
21:3:513:CL7:CHA	21:3:513:CL7:HBA2	2.46	0.43
2:b:175:TRP:HA	2:b:185:HIS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:401:PHE:HB2	2:b:406:LEU:O	2.18	0.43
16:6:31:HIS:ND1	21:6:509:CL7:H142	2.32	0.43
21:6:502:CL7:H2	21:6:503:CL7:C1	2.42	0.43
18:5:90:VAL:O	18:5:94:ILE:HG12	2.19	0.43
19:7:253:LEU:HD23	19:7:253:LEU:HA	1.82	0.43
21:C:503:CL7:O1A	21:C:504:CL7:H2	2.17	0.43
21:C:507:CL7:H3A	21:C:507:CL7:HBA1	1.76	0.43
4:D:295:TYR:OH	4:D:325:ARG:NH1	2.32	0.43
21:2:503:CL7:HBD	21:2:503:CL7:O1A	2.17	0.43
21:2:514:CL7:H3A	21:2:514:CL7:HBA1	1.69	0.43
21:2:518:CL7:H2A	21:2:518:CL7:O1D	2.19	0.43
18:1:152:ILE:HD11	21:1:410:CL7:H61C	2.00	0.43
19:3:75:TRP:HH2	21:6:518:CL7:H121	1.83	0.43
19:3:109:TYR:HB2	21:6:505:CL7:CBA	2.49	0.43
32:3:519:ZEX:H27	32:3:519:ZEX:H30	1.76	0.43
21:c:505:CL7:HBA2	21:c:505:CL7:CHA	2.49	0.43
4:d:323:GLY:O	4:d:327:TRP:HD1	2.02	0.43
21:d:405:CL7:HAA2	21:d:405:CL7:HBD	2.01	0.43
18:5:144:ILE:HG12	21:5:413:CL7:HMC2	2.00	0.43
19:7:112:THR:HG23	19:7:113:LYS:N	2.33	0.43
19:7:270:VAL:O	19:7:272:PRO:HD3	2.17	0.43
21:7:501:CL7:H193	21:7:501:CL7:H162	1.83	0.43
21:7:503:CL7:H121	21:7:509:CL7:H43C	2.00	0.43
32:8:418:ZEX:H31	32:8:418:ZEX:H401	1.87	0.43
2:B:291:GLU:CD	2:B:294:ARG:HH21	2.24	0.43
21:B:604:CL7:HAA2	21:B:604:CL7:HBD	1.99	0.43
21:C:505:CL7:HBA2	21:C:505:CL7:CHA	2.48	0.43
16:2:188:LYS:HB3	16:2:196:PHE:CD2	2.53	0.43
32:2:525:ZEX:H1	18:1:296:PHE:HZ	1.66	0.43
21:1:408:CL7:C13	32:1:422:ZEX:H402	2.47	0.43
1:a:202:VAL:HG22	21:a:401:CL7:C2B	2.48	0.43
3:c:48:TRP:O	21:c:509:CL7:H2	2.17	0.43
21:7:503:CL7:H13	21:7:503:CL7:H101	1.74	0.43
32:8:420:ZEX:H11	32:8:420:ZEX:H191	1.89	0.43
3:C:68:HIS:CE1	3:C:72:ILE:HD11	2.54	0.43
21:2:511:CL7:H91C	21:2:511:CL7:H111	1.81	0.43
24:3:523:SQD:H221	32:6:520:ZEX:C11	2.48	0.43
20:4:167:VAL:HG23	20:4:247:ALA:HB1	2.00	0.43
20:4:289:VAL:HG22	21:4:410:CL7:HAB	2.00	0.43
21:b:607:CL7:HBA2	21:b:607:CL7:C4A	2.46	0.43
11:m:17:ILE:HB	11:m:18:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:6:94:MET:CE	32:6:524:ZEX:C36	2.95	0.43
21:6:509:CL7:H3A	21:6:509:CL7:HBA2	1.87	0.43
21:6:512:CL7:H161	21:6:512:CL7:H141	1.75	0.43
21:7:509:CL7:H93C	21:7:509:CL7:H62C	1.78	0.43
20:8:148:PHE:HZ	32:8:420:ZEX:HO3	1.64	0.43
21:8:412:CL7:H61C	21:8:412:CL7:H41C	1.76	0.43
21:B:610:CL7:OBD	21:B:612:CL7:H172	2.19	0.43
4:D:323:GLY:O	4:D:327:TRP:HD1	2.02	0.43
6:F:45:ILE:HD13	6:F:45:ILE:HA	1.87	0.43
21:2:505:CL7:H101	21:2:505:CL7:H62C	1.69	0.43
18:1:52:ASN:HD21	18:1:91:PHE:HD1	1.67	0.43
21:1:410:CL7:H62C	21:1:410:CL7:H41C	1.76	0.43
21:4:411:CL7:HED3	21:4:411:CL7:CGA	2.48	0.43
3:c:170:MET:HG3	3:c:268:PRO:HG3	2.01	0.43
3:c:207:ASN:OD1	3:c:208:VAL:N	2.52	0.43
16:6:168:ASP:HB3	16:6:171:VAL:HB	2.01	0.43
21:6:505:CL7:H101	21:6:505:CL7:H62C	1.69	0.43
18:5:151:LEU:HD23	18:5:151:LEU:HA	1.71	0.43
21:5:402:CL7:HBA2	21:5:402:CL7:HBD	2.01	0.43
21:5:410:CL7:H122	21:5:413:CL7:C3D	2.49	0.43
32:7:520:ZEX:H15	32:7:520:ZEX:H201	1.75	0.43
11:M:17:ILE:HB	11:M:18:PRO:HD3	2.00	0.43
16:2:123:SER:C	16:2:125:ALA:H	2.26	0.43
16:2:253:LEU:HD23	16:2:253:LEU:HA	1.82	0.43
16:2:313:PHE:CD2	32:2:519:ZEX:H30	2.53	0.43
21:1:406:CL7:H11C	32:1:422:ZEX:H173	2.00	0.43
19:3:11:TYR:HB3	19:3:15:SER:O	2.19	0.43
19:3:63:ASN:HB3	21:3:504:CL7:H2A	2.00	0.43
1:a:96:ILE:HG22	8:i:1:MET:HE1	2.00	0.43
2:b:434:ARG:HG2	2:b:439:SER:HB2	2.01	0.43
21:b:604:CL7:H93C	21:b:604:CL7:H111	1.78	0.43
21:b:612:CL7:HBC2	25:b:624:LHG:H342	2.01	0.43
3:c:68:HIS:CE1	3:c:72:ILE:HD11	2.54	0.43
21:c:509:CL7:H61C	21:c:509:CL7:H41C	1.41	0.43
2:B:175:TRP:HA	2:B:185:HIS:O	2.18	0.43
3:C:207:ASN:OD1	3:C:208:VAL:N	2.52	0.43
21:C:506:CL7:HAA2	21:C:506:CL7:CBD	2.49	0.43
21:C:507:CL7:H11C	21:C:507:CL7:HBA2	1.74	0.43
16:2:168:ASP:HB3	16:2:171:VAL:HB	2.01	0.43
21:2:502:CL7:H3A	21:2:502:CL7:HBA1	1.84	0.43
18:1:144:ILE:HG12	21:1:413:CL7:HMC2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:112:THR:HG23	19:3:113:LYS:N	2.33	0.43
1:a:330:VAL:HG21	4:d:327:TRP:CE2	2.53	0.43
3:c:131:LEU:O	3:c:134:SER:OG	2.27	0.43
21:c:508:CL7:H61C	21:c:508:CL7:H41C	1.77	0.43
16:6:35:ILE:HG12	21:6:512:CL7:O1D	2.19	0.43
16:6:128:ARG:HB3	21:6:514:CL7:HED1	2.00	0.43
16:6:144:GLY:HA2	16:6:222:GLY:HA2	2.01	0.43
21:6:518:CL7:H2A	21:6:518:CL7:O1D	2.19	0.43
19:7:161:ALA:HA	19:7:166:VAL:HG13	2.00	0.43
21:8:411:CL7:HED3	21:8:411:CL7:CGA	2.48	0.43
21:8:415:CL7:HBA1	21:8:415:CL7:H3A	1.41	0.43
21:B:606:CL7:H62C	21:B:606:CL7:H41C	1.65	0.43
21:B:612:CL7:H192	21:B:612:CL7:H162	1.85	0.43
24:B:620:SQD:H383	12:t:12:CYS:HB3	2.01	0.43
5:E:26:THR:HB	31:F:101:HEM:HAB	2.01	0.43
21:2:509:CL7:H3A	21:2:509:CL7:HBA2	1.87	0.43
21:3:503:CL7:H121	21:3:509:CL7:H43C	2.00	0.43
21:3:510:CL7:H41C	21:3:510:CL7:H61C	1.87	0.43
1:a:85:SER:HA	1:a:109:GLY:HA3	2.01	0.43
2:b:199:ASP:OD1	7:h:61:ALA:HA	2.18	0.43
2:b:357:ARG:NH2	4:d:336:GLU:O	2.49	0.43
21:b:611:CL7:OBD	21:b:613:CL7:H172	2.19	0.43
21:6:503:CL7:HBA1	21:6:503:CL7:H3A	1.85	0.43
21:5:406:CL7:H11C	32:5:422:ZEX:H173	2.00	0.43
21:5:410:CL7:H62C	21:5:410:CL7:H41C	1.76	0.43
21:5:413:CL7:O1D	21:5:413:CL7:H2A	2.19	0.43
21:7:502:CL7:H2	21:7:503:CL7:H193	2.01	0.43
21:7:505:CL7:H192	21:7:505:CL7:H162	1.75	0.43
21:A:406:CL7:HBD	21:A:406:CL7:HAA2	2.00	0.42
21:B:603:CL7:H203	21:B:609:CL7:H102	2.00	0.42
3:C:297:ILE:HB	21:C:502:CL7:H43C	2.01	0.42
3:C:476:GLU:CD	4:D:244:SER:HG	2.18	0.42
16:2:50:LEU:HD11	16:2:89:PHE:HB2	2.01	0.42
32:3:522:ZEX:H11	32:3:522:ZEX:H191	1.48	0.42
32:3:525:ZEX:H15	32:3:525:ZEX:H201	1.85	0.42
20:4:146:ALA:HA	20:4:149:ARG:HG3	2.00	0.42
21:4:412:CL7:H8	21:4:412:CL7:H121	1.81	0.42
21:b:606:CL7:HBA1	21:b:606:CL7:H3A	1.78	0.42
3:c:297:ILE:HB	21:c:502:CL7:H43C	2.01	0.42
9:k:42:VAL:HB	9:k:45:LYS:HE2	2.01	0.42
18:5:251:LEU:HD23	18:5:251:LEU:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:5:405:CL7:HAA2	21:5:405:CL7:HBD	2.01	0.42
21:5:407:CL7:HMA3	21:5:408:CL7:C2C	2.49	0.42
19:7:63:ASN:HB3	21:7:504:CL7:H2A	2.00	0.42
21:7:503:CL7:HAA2	21:7:503:CL7:HBD	2.01	0.42
32:8:403:ZEX:H11	32:8:403:ZEX:H191	1.76	0.42
1:A:97:TRP:CD1	1:A:98:GLU:HG2	2.54	0.42
2:B:199:ASP:OD2	2:B:202:ASN:N	2.53	0.42
3:C:170:MET:HG3	3:C:268:PRO:HG3	2.01	0.42
3:C:171:GLN:O	3:C:175:ILE:HG13	2.18	0.42
4:D:328:MET:HG2	4:D:332:ASP:HB2	2.00	0.42
10:L:15:ARG:HD2	24:b:621:SQD:C24	2.45	0.42
21:2:505:CL7:CBA	19:7:109:TYR:HB2	2.47	0.42
32:1:422:ZEX:H15	32:1:422:ZEX:H201	1.83	0.42
21:3:508:CL7:C2D	32:3:519:ZEX:H162	2.49	0.42
2:b:388:SER:HA	4:d:343:GLU:OE2	2.19	0.42
21:b:603:CL7:H142	21:b:603:CL7:H112	1.83	0.42
3:c:171:GLN:O	3:c:175:ILE:HG13	2.18	0.42
3:c:292:TYR:CD1	3:c:450:PHE:HB2	2.54	0.42
4:d:203:ILE:HD13	4:d:203:ILE:HA	1.80	0.42
10:l:14:ASN:OD1	10:l:14:ASN:N	2.52	0.42
16:6:164:HIS:ND1	16:6:164:HIS:O	2.52	0.42
18:5:72:LEU:HD11	21:5:404:CL7:HED3	2.01	0.42
19:7:202:ASN:HA	19:7:269:VAL:HG21	2.01	0.42
21:7:502:CL7:O1A	21:7:503:CL7:H12C	2.19	0.42
32:7:522:ZEX:H15	32:7:522:ZEX:H201	1.85	0.42
1:A:331:MET:SD	4:D:346:PRO:HB2	2.59	0.42
2:B:48:SER:O	2:B:50:PRO:HD3	2.19	0.42
2:B:199:ASP:OD1	7:H:61:ALA:HA	2.18	0.42
21:2:511:CL7:C1B	32:2:525:ZEX:C17	2.97	0.42
18:1:293:ALA:HB3	26:1:401:LMG:H122	2.01	0.42
21:1:406:CL7:H8	21:1:406:CL7:H52C	1.90	0.42
21:1:418:CL7:H2A	21:1:418:CL7:HED3	2.01	0.42
21:3:501:CL7:H193	21:3:501:CL7:H162	1.83	0.42
21:3:503:CL7:HAA2	21:3:503:CL7:HBD	2.01	0.42
20:4:140:PRO:HD2	20:4:143:SER:OG	2.19	0.42
1:a:93:LEU:HD21	21:a:403:CL7:HAA1	2.00	0.42
1:a:104:GLU:HG2	1:a:108:ASN:HD21	1.85	0.42
21:b:616:CL7:HBA2	21:b:616:CL7:H11C	1.71	0.42
4:d:188:HIS:HA	4:d:293:ARG:HD2	2.01	0.42
16:6:70:LEU:HD23	16:6:70:LEU:HA	1.86	0.42
21:6:511:CL7:C1B	32:6:524:ZEX:C17	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:6:516:CL7:HBA1	21:6:516:CL7:H12C	1.71	0.42
18:5:34:ILE:HA	21:5:413:CL7:HED1	2.01	0.42
20:8:140:PRO:HD2	20:8:143:SER:OG	2.19	0.42
2:B:177:SER:OG	2:B:178:ASP:N	2.52	0.42
21:B:603:CL7:H192	21:B:609:CL7:H122	2.01	0.42
21:B:611:CL7:HBC2	25:B:623:LHG:H342	2.01	0.42
3:C:467:PHE:HE2	8:I:31:ASN:HB2	1.85	0.42
16:2:35:ILE:HG12	21:2:512:CL7:O1D	2.19	0.42
16:2:73:VAL:HG12	16:2:160:TRP:CZ3	2.54	0.42
21:3:502:CL7:H2	21:3:503:CL7:H193	2.01	0.42
21:3:507:CL7:H41C	21:3:507:CL7:H61C	1.63	0.42
32:3:522:ZEX:H27	32:3:522:ZEX:H391	1.82	0.42
21:b:613:CL7:H142	21:b:613:CL7:H111	1.73	0.42
3:c:382:ARG:HD3	3:c:382:ARG:HA	1.87	0.42
5:e:26:THR:HB	31:f:101:HEM:HAB	2.01	0.42
16:6:348:LEU:HA	16:6:348:LEU:HD23	1.64	0.42
18:5:38:ALA:HB2	18:5:105:LEU:HB2	2.01	0.42
21:5:418:CL7:H2A	21:5:418:CL7:HED3	2.01	0.42
19:7:169:PRO:HB3	19:7:272:PRO:HB3	2.02	0.42
32:8:403:ZEX:H15	32:8:403:ZEX:H201	1.65	0.42
2:B:194:ARG:HB3	2:B:195:PRO:HD2	2.01	0.42
3:C:237:VAL:HG13	3:C:301:TYR:HA	2.01	0.42
15:Z:40:ILE:HG23	15:Z:41:TRP:HD1	1.84	0.42
20:4:35:ASN:CG	21:4:411:CL7:HAB	2.45	0.42
1:a:331:MET:SD	4:d:346:PRO:HB2	2.59	0.42
2:b:177:SER:OG	2:b:178:ASP:N	2.52	0.42
2:b:373:LYS:HE2	2:b:373:LYS:HB2	1.88	0.42
15:z:27:PHE:HD2	15:z:27:PHE:HA	1.76	0.42
16:6:292:ASP:O	16:6:293:THR:OG1	2.38	0.42
21:6:511:CL7:C2B	32:6:524:ZEX:H172	2.49	0.42
18:5:262:MET:HB3	21:5:402:CL7:H61C	2.01	0.42
18:5:313:LEU:O	18:5:317:THR:OG1	2.23	0.42
20:8:28:GLU:H	20:8:28:GLU:CD	2.28	0.42
20:8:146:ALA:HA	20:8:149:ARG:HG3	2.00	0.42
21:8:405:CL7:H2	21:8:406:CL7:H11C	2.00	0.42
1:A:93:LEU:HD21	21:A:403:CL7:HAA1	2.00	0.42
2:B:434:ARG:HG2	2:B:439:SER:HB2	2.01	0.42
21:B:608:CL7:HBC3	21:B:608:CL7:HHD	2.00	0.42
21:2:505:CL7:H151	19:7:98:VAL:HG22	2.01	0.42
19:3:253:LEU:HD23	19:3:253:LEU:HA	1.82	0.42
21:3:504:CL7:H61C	21:3:504:CL7:H92C	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:3:509:CL7:H62C	21:3:509:CL7:H93C	1.78	0.42
32:3:522:ZEX:H173	32:3:522:ZEX:H3	1.69	0.42
21:4:405:CL7:H62C	21:4:405:CL7:H41C	1.73	0.42
3:c:296:MET:HE1	3:c:443:PHE:CD1	2.55	0.42
16:6:73:VAL:HG12	16:6:160:TRP:CZ3	2.54	0.42
21:6:509:CL7:H93C	21:6:509:CL7:H62C	1.63	0.42
18:5:290:PHE:CE2	18:5:294:PRO:HG3	2.55	0.42
19:7:11:TYR:HB3	19:7:15:SER:O	2.19	0.42
23:C:516:8CT:C08	8:I:24:ILE:HG22	2.50	0.42
4:D:296:ASP:OD1	4:D:296:ASP:N	2.50	0.42
12:T:12:CYS:HB3	24:b:621:SQD:H383	2.02	0.42
16:2:70:LEU:HD23	16:2:70:LEU:HA	1.86	0.42
21:2:511:CL7:C2B	32:2:525:ZEX:H172	2.49	0.42
18:1:198:PRO:HD3	21:1:420:CL7:HAB	2.02	0.42
21:3:512:CL7:H12C	21:3:512:CL7:H52C	1.86	0.42
32:3:522:ZEX:H31	32:3:522:ZEX:H401	1.88	0.42
20:4:304:ARG:CG	32:4:418:ZEX:H373	2.37	0.42
16:6:111:ILE:HD12	16:6:111:ILE:HA	1.80	0.42
21:7:505:CL7:OBB	32:8:403:ZEX:H403	2.19	0.42
21:A:403:CL7:HBA2	21:A:403:CL7:H3A	1.95	0.42
2:B:165:HIS:CD2	2:B:165:HIS:C	2.98	0.42
21:B:612:CL7:HBA1	21:B:612:CL7:H3A	1.60	0.42
3:C:296:MET:HE1	3:C:443:PHE:CD1	2.55	0.42
21:C:509:CL7:H61C	21:C:509:CL7:H41C	1.41	0.42
4:D:19:ASP:O	4:D:23:ARG:HG3	2.20	0.42
10:L:14:ASN:OD1	10:L:14:ASN:N	2.52	0.42
16:2:128:ARG:HB3	21:2:514:CL7:HED1	2.01	0.42
16:2:164:HIS:ND1	16:2:164:HIS:O	2.52	0.42
18:1:38:ALA:HB2	18:1:105:LEU:HB2	2.01	0.42
18:1:151:LEU:CD1	21:1:413:CL7:H3A	2.50	0.42
18:1:290:PHE:CE2	18:1:294:PRO:HG3	2.55	0.42
21:1:402:CL7:HBA2	21:1:402:CL7:HBD	2.01	0.42
21:1:410:CL7:H122	21:1:413:CL7:C3D	2.49	0.42
19:3:169:PRO:HB3	19:3:272:PRO:HB3	2.02	0.42
1:a:97:TRP:CD1	1:a:98:GLU:HG2	2.54	0.42
1:a:154:THR:HG22	21:a:401:CL7:C4	2.50	0.42
21:a:401:CL7:H91C	21:a:401:CL7:H111	1.69	0.42
13:x:29:ILE:O	13:x:33:GLN:HG2	2.20	0.42
16:6:208:MET:HE3	16:6:208:MET:HB3	1.85	0.42
18:5:198:PRO:HD3	21:5:420:CL7:HAB	2.02	0.42
18:5:343:ILE:O	18:5:347:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:7:231:TRP:NE1	21:7:506:CL7:OBD	2.47	0.42
20:8:304:ARG:CG	32:8:418:ZEX:H373	2.37	0.42
4:D:165:SER:OG	4:D:166:TRP:N	2.53	0.42
21:2:509:CL7:H93C	21:2:509:CL7:H62C	1.63	0.42
32:2:520:ZEX:H173	21:7:511:CL7:CHB	2.50	0.42
18:1:342:ASP:O	18:1:346:VAL:HG23	2.19	0.42
21:1:405:CL7:HAA2	21:1:405:CL7:HBD	2.01	0.42
21:1:407:CL7:HMA3	21:1:408:CL7:C2C	2.49	0.42
32:4:418:ZEX:H201	32:4:418:ZEX:H15	1.61	0.42
3:c:237:VAL:HG13	3:c:301:TYR:HA	2.01	0.42
21:c:503:CL7:H62C	21:c:503:CL7:H41C	1.74	0.42
16:6:255:LEU:O	16:6:259:VAL:HG23	2.20	0.42
18:5:112:HIS:HE1	21:5:414:CL7:NC	2.18	0.42
20:8:35:ASN:CG	21:8:411:CL7:HAB	2.45	0.42
1:A:104:GLU:HG2	1:A:108:ASN:HD21	1.85	0.42
4:D:188:HIS:HA	4:D:293:ARG:HD2	2.01	0.42
13:X:29:ILE:O	13:X:33:GLN:HG2	2.20	0.42
21:2:515:CL7:HMB1	32:2:521:ZEX:H202	2.01	0.42
21:2:517:CL7:H142	21:2:517:CL7:H111	1.80	0.42
32:2:525:ZEX:H7	21:1:417:CL7:HED1	2.02	0.42
21:3:505:CL7:OBB	32:4:403:ZEX:H403	2.19	0.42
21:3:516:CL7:H11C	21:3:516:CL7:C3A	2.35	0.42
20:4:32:TRP:CD1	20:4:32:TRP:H	2.36	0.42
2:b:48:SER:O	2:b:50:PRO:HD3	2.20	0.42
21:c:507:CL7:HBC2	21:c:508:CL7:H201	2.02	0.42
4:d:83:SER:O	5:e:69:ARG:HB2	2.20	0.42
16:6:281:GLN:HG2	16:6:293:THR:HG22	2.01	0.42
32:6:520:ZEX:H27	32:6:520:ZEX:H391	1.75	0.42
21:7:508:CL7:H62C	21:7:508:CL7:H102	1.52	0.42
2:B:388:SER:HA	4:D:343:GLU:OE2	2.19	0.41
21:B:604:CL7:H92C	21:B:604:CL7:H62C	1.86	0.41
21:B:608:CL7:CHD	21:B:609:CL7:H93C	2.50	0.41
21:C:507:CL7:HBC2	21:C:508:CL7:H201	2.02	0.41
16:2:45:ILE:HD13	16:2:45:ILE:HA	1.92	0.41
16:2:104:GLY:O	16:2:108:ILE:HG13	2.20	0.41
16:2:208:MET:HE3	16:2:208:MET:HB3	1.85	0.41
16:2:262:TYR:CE2	32:7:522:ZEX:H383	2.55	0.41
26:b:622:LMG:H292	26:b:622:LMG:HC91	1.71	0.41
21:c:511:CL7:H72C	21:c:511:CL7:H111	1.48	0.41
15:z:40:ILE:HG23	15:z:41:TRP:HD1	1.84	0.41
16:6:104:GLY:O	16:6:108:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:5:406:CL7:H121	21:5:406:CL7:H162	1.83	0.41
21:B:602:CL7:H92C	21:B:602:CL7:H61C	1.88	0.41
21:C:503:CL7:H41C	21:C:503:CL7:H62C	1.74	0.41
9:K:15:SER:O	9:K:18:SER:OG	2.20	0.41
18:1:339:LYS:HE3	18:1:339:LYS:HB2	1.93	0.41
18:1:343:ILE:O	18:1:347:ILE:HG13	2.20	0.41
21:3:504:CL7:H62C	21:3:504:CL7:H41C	1.36	0.41
2:b:194:ARG:HB3	2:b:195:PRO:HD2	2.01	0.41
2:b:199:ASP:OD2	2:b:202:ASN:N	2.53	0.41
3:c:128:ALA:O	3:c:132:ILE:HG12	2.20	0.41
21:c:506:CL7:HAA2	21:c:506:CL7:CBD	2.49	0.41
5:e:76:ILE:O	5:e:80:THR:N	2.54	0.41
32:6:524:ZEX:C35	21:5:417:CL7:HBA2	2.49	0.41
18:5:293:ALA:HB3	26:5:401:LMG:H122	2.01	0.41
18:5:294:PRO:O	18:5:319:TYR:OH	2.28	0.41
21:5:403:CL7:H51C	21:5:404:CL7:H43C	2.02	0.41
19:7:129:PHE:HZ	32:7:522:ZEX:O3	1.95	0.41
21:7:508:CL7:C2D	32:7:519:ZEX:H162	2.49	0.41
32:7:519:ZEX:H30	32:7:519:ZEX:H27	1.76	0.41
1:A:38:ILE:HB	1:A:39:PRO:HD3	2.02	0.41
1:A:85:SER:HA	1:A:109:GLY:HA3	2.01	0.41
1:A:150:PRO:O	1:A:154:THR:HG23	2.20	0.41
3:C:292:TYR:CD1	3:C:450:PHE:HB2	2.55	0.41
3:C:388:ASP:OD1	3:C:390:ASN:N	2.45	0.41
21:C:508:CL7:H61C	21:C:508:CL7:H92C	1.81	0.41
21:D:404:CL7:H112	22:D:408:PHO:CHB	2.49	0.41
18:1:34:ILE:HA	21:1:413:CL7:HED1	2.01	0.41
18:1:112:HIS:HE1	21:1:414:CL7:NC	2.18	0.41
2:b:42:LEU:HD23	2:b:42:LEU:HA	1.73	0.41
3:c:467:PHE:HE2	8:i:31:ASN:HB2	1.85	0.41
4:d:89:LEU:HD23	4:d:89:LEU:HA	1.88	0.41
4:d:165:SER:OG	4:d:166:TRP:N	2.53	0.41
21:6:503:CL7:H102	21:6:503:CL7:H13	1.67	0.41
21:6:515:CL7:HMB1	32:6:520:ZEX:H202	2.01	0.41
18:5:52:ASN:HD21	18:5:91:PHE:HD1	1.67	0.41
21:8:406:CL7:H93C	21:8:406:CL7:H112	1.89	0.41
1:A:154:THR:HG22	21:A:401:CL7:C4	2.50	0.41
1:A:173:PRO:HB2	1:A:178:GLY:HA3	2.02	0.41
1:A:323:ARG:HG3	4:D:331:GLN:OE1	2.21	0.41
21:A:401:CL7:H91C	21:A:401:CL7:H111	1.69	0.41
2:B:172:PRO:HG3	21:B:606:CL7:O1D	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:621:LMG:H292	26:B:621:LMG:HC91	1.71	0.41
3:C:382:ARG:HA	3:C:382:ARG:HD3	1.87	0.41
4:D:83:SER:O	5:E:69:ARG:HB2	2.20	0.41
16:2:94:MET:CE	32:2:525:ZEX:C36	2.95	0.41
21:2:510:CL7:HBD	21:2:510:CL7:HBA1	2.03	0.41
18:1:72:LEU:HD11	21:1:404:CL7:HED3	2.01	0.41
18:1:252:LEU:O	18:1:256:ILE:HG13	2.19	0.41
18:1:262:MET:HB3	21:1:402:CL7:H61C	2.01	0.41
21:3:510:CL7:H42C	32:3:519:ZEX:C17	2.51	0.41
20:4:50:LEU:HD13	20:4:124:ALA:HB1	2.02	0.41
1:a:38:ILE:HB	1:a:39:PRO:HD3	2.02	0.41
1:a:150:PRO:O	1:a:154:THR:HG23	2.20	0.41
1:a:194:MET:HE2	1:a:194:MET:HB3	1.85	0.41
21:b:604:CL7:H203	21:b:604:CL7:H161	1.75	0.41
21:c:504:CL7:H151	21:c:504:CL7:H112	1.75	0.41
4:d:19:ASP:O	4:d:23:ARG:HG3	2.20	0.41
16:6:281:GLN:HA	16:6:282:PRO:HD3	1.93	0.41
32:6:524:ZEX:H7	21:5:417:CL7:HED1	2.02	0.41
18:5:252:LEU:O	18:5:256:ILE:HG13	2.19	0.41
19:7:57:LEU:HD23	19:7:57:LEU:HA	1.92	0.41
21:B:612:CL7:H51C	21:B:612:CL7:H12C	1.92	0.41
4:D:298:VAL:CG2	10:L:38:ASN:OXT	2.68	0.41
5:E:76:ILE:O	5:E:80:THR:N	2.54	0.41
16:2:281:GLN:HG2	16:2:293:THR:HG22	2.01	0.41
21:2:510:CL7:C2	32:2:519:ZEX:H181	2.51	0.41
24:2:522:SQD:O47	24:2:522:SQD:H1	2.21	0.41
21:3:501:CL7:H161	21:3:506:CL7:HMC1	2.02	0.41
20:4:28:GLU:H	20:4:28:GLU:CD	2.28	0.41
2:b:154:LEU:HD23	2:b:154:LEU:HA	1.87	0.41
21:b:605:CL7:H62C	21:b:605:CL7:H92C	1.86	0.41
21:b:609:CL7:CHD	21:b:610:CL7:H93C	2.50	0.41
4:d:298:VAL:CG2	10:l:38:ASN:OXT	2.68	0.41
2:B:464:PHE:HB2	4:D:279:TRP:CZ2	2.56	0.41
5:E:52:PRO:HA	5:E:55:TYR:CE2	2.56	0.41
9:K:42:VAL:HB	9:K:45:LYS:HE2	2.01	0.41
21:2:517:CL7:H2	19:7:40:PHE:CD1	2.55	0.41
19:3:40:PHE:CD1	21:6:517:CL7:H2	2.55	0.41
32:3:520:ZEX:H11	32:3:520:ZEX:H191	1.52	0.41
20:4:255:LYS:HD2	20:4:255:LYS:HA	1.91	0.41
2:b:91:ILE:O	2:b:94:ALA:HB3	2.21	0.41
2:b:165:HIS:CD2	2:b:165:HIS:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:476:GLU:CD	4:d:244:SER:HG	2.22	0.41
21:d:404:CL7:H61C	21:d:404:CL7:H41C	1.67	0.41
16:6:50:LEU:HD11	16:6:89:PHE:HB2	2.01	0.41
18:5:82:GLY:HA2	18:5:169:TYR:HE1	1.86	0.41
18:5:342:ASP:O	18:5:346:VAL:HG23	2.19	0.41
21:5:408:CL7:H162	21:5:408:CL7:H193	1.87	0.41
21:7:502:CL7:C2D	21:7:503:CL7:H151	2.51	0.41
21:8:411:CL7:H162	21:8:411:CL7:H141	1.70	0.41
21:C:510:CL7:H141	21:C:510:CL7:H162	1.70	0.41
16:2:98:PHE:CG	32:2:523:ZEX:H31	2.53	0.41
16:2:144:GLY:HA2	16:2:222:GLY:HA2	2.01	0.41
16:2:255:LEU:O	16:2:259:VAL:HG23	2.20	0.41
18:1:168:ILE:H	18:1:168:ILE:HG13	1.73	0.41
18:1:294:PRO:O	18:1:319:TYR:OH	2.28	0.41
21:1:413:CL7:H2A	21:1:413:CL7:O1D	2.19	0.41
21:3:502:CL7:O1A	21:3:503:CL7:H12C	2.19	0.41
1:a:75:ASN:HD21	4:d:312:THR:HG21	1.86	0.41
2:b:464:PHE:HB2	4:d:279:TRP:CZ2	2.56	0.41
23:c:516:8CT:C08	8:i:24:ILE:HG22	2.50	0.41
25:d:409:LHG:H301	25:d:409:LHG:H332	1.91	0.41
21:6:518:CL7:H52C	21:6:518:CL7:H8	1.84	0.41
21:5:418:CL7:H52C	21:5:418:CL7:H11C	1.82	0.41
21:7:505:CL7:H41C	32:7:520:ZEX:H193	2.03	0.41
20:8:32:TRP:CD1	20:8:32:TRP:H	2.36	0.41
3:C:48:TRP:CD1	3:C:48:TRP:H	2.39	0.41
10:L:13:LEU:H	11:M:29:THR:HG21	1.86	0.41
16:2:292:ASP:O	16:2:293:THR:OG1	2.38	0.41
18:1:157:LEU:HD23	18:1:157:LEU:HA	1.83	0.41
19:3:98:VAL:HG22	21:6:505:CL7:H151	2.03	0.41
20:4:138:ASP:OD1	20:4:138:ASP:N	2.53	0.41
1:a:42:LEU:HD23	1:a:42:LEU:HA	1.87	0.41
21:b:604:CL7:H62C	21:b:604:CL7:H41C	1.73	0.41
4:d:263:LYS:HE3	4:d:263:LYS:HB2	1.86	0.41
21:d:405:CL7:H3A	21:d:405:CL7:HBA1	1.59	0.41
21:6:501:CL7:H192	21:6:501:CL7:H162	1.76	0.41
18:5:343:ILE:HD13	18:5:343:ILE:HA	1.86	0.41
19:7:213:PHE:O	19:7:216:SER:OG	2.35	0.41
1:A:30:ILE:O	1:A:34:GLY:HA3	2.21	0.41
1:A:75:ASN:HD21	4:D:312:THR:HG21	1.86	0.41
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.03	0.41
21:A:406:CL7:C4	30:D:407:PL9:H211	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:ILE:O	2:B:94:ALA:HB3	2.21	0.41
2:B:325:PHE:HA	21:B:607:CL7:H43C	2.02	0.41
2:B:440:ASP:OD1	4:D:302:ILE:HD11	2.21	0.41
25:B:625:LHG:H202	30:D:407:PL9:H212	2.03	0.41
21:C:502:CL7:H72C	21:C:502:CL7:HMB3	2.02	0.41
4:D:89:LEU:HD23	4:D:89:LEU:HA	1.88	0.41
8:I:18:LEU:HD23	8:I:18:LEU:HA	1.73	0.41
21:2:518:CL7:HBA1	21:2:518:CL7:H3A	1.73	0.41
21:2:518:CL7:H8	21:2:518:CL7:H52C	1.84	0.41
32:2:523:ZEX:H162	32:2:523:ZEX:O3	2.21	0.41
19:3:202:ASN:HA	19:3:269:VAL:HG21	2.01	0.41
21:3:505:CL7:H41C	32:3:520:ZEX:H193	2.03	0.41
21:3:510:CL7:H101	21:3:510:CL7:H62C	1.82	0.41
21:4:416:CL7:HHD	21:4:416:CL7:HAC1	1.93	0.41
1:a:163:LEU:HD23	1:a:163:LEU:HA	1.87	0.41
2:b:41:GLU:CD	2:b:61:PHE:H	2.26	0.41
2:b:172:PRO:HG3	21:b:607:CL7:O1D	2.20	0.41
2:b:325:PHE:HA	21:b:608:CL7:H43C	2.02	0.41
21:b:604:CL7:H192	21:b:610:CL7:H122	2.01	0.41
21:b:613:CL7:H162	21:b:613:CL7:H192	1.85	0.41
3:c:48:TRP:CD1	3:c:48:TRP:H	2.39	0.41
9:k:11:PRO:HB2	9:k:14:PHE:HD2	1.86	0.41
10:l:13:LEU:H	11:m:29:THR:HG21	1.86	0.41
18:5:151:LEU:CD1	21:5:413:CL7:H3A	2.50	0.41
18:5:173:ILE:HG13	18:5:177:ARG:HD2	2.02	0.41
21:5:416:CL7:HED3	21:5:416:CL7:HBD	1.71	0.41
21:7:516:CL7:H11C	21:7:516:CL7:C3A	2.35	0.41
20:8:50:LEU:HD13	20:8:124:ALA:HB1	2.02	0.41
21:8:404:CL7:H12C	21:8:404:CL7:H52C	1.94	0.41
21:8:414:CL7:H62C	32:8:420:ZEX:H192	2.03	0.41
21:8:415:CL7:HHD	21:8:415:CL7:HAC2	1.93	0.41
2:B:357:ARG:NH2	4:D:336:GLU:O	2.49	0.41
3:C:93:MET:HE1	3:C:105:ALA:HB2	2.03	0.41
4:D:182:LEU:HD23	4:D:182:LEU:HA	1.80	0.41
21:2:501:CL7:H41C	21:2:501:CL7:H72C	2.03	0.41
21:2:502:CL7:CMB	21:2:504:CL7:HAB	2.51	0.41
21:2:518:CL7:H121	19:7:75:TRP:HH2	1.85	0.41
20:4:38:MET:HE3	20:4:38:MET:HB2	1.71	0.41
1:a:82:VAL:HB	1:a:174:LEU:HB2	2.03	0.41
1:a:323:ARG:HG3	4:d:331:GLN:OE1	2.21	0.41
21:6:502:CL7:CMB	21:6:504:CL7:HAB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:6:505:CL7:HHD	21:6:505:CL7:HAC2	1.91	0.41
18:5:261:LEU:O	18:5:265:ILE:HG13	2.21	0.41
21:7:504:CL7:H162	21:7:504:CL7:H141	1.79	0.41
21:7:508:CL7:H3A	21:7:508:CL7:HBA2	1.77	0.41
20:8:201:LEU:O	20:8:203:PRO:HD3	2.21	0.41
1:A:120:MET:SD	1:A:159:LEU:HB2	2.61	0.40
21:B:610:CL7:H202	21:B:610:CL7:H162	1.73	0.40
4:D:56:SER:HB3	4:D:78:SER:HB3	2.03	0.40
4:D:270:MET:HE2	4:D:270:MET:HB3	1.96	0.40
21:1:403:CL7:H51C	21:1:404:CL7:H43C	2.02	0.40
19:3:328:ARG:HG2	19:3:334:PHE:HE2	1.86	0.40
21:3:501:CL7:H13	32:3:520:ZEX:H402	2.03	0.40
1:a:30:ILE:O	1:a:34:GLY:HA3	2.21	0.40
1:a:173:PRO:HB2	1:a:178:GLY:HA3	2.02	0.40
1:a:323:ARG:NH2	4:d:327:TRP:O	2.40	0.40
2:b:440:ASP:OD1	4:d:302:ILE:HD11	2.21	0.40
3:c:405:ALA:O	3:c:409:THR:HG23	2.21	0.40
21:c:502:CL7:H72C	21:c:502:CL7:HMB3	2.03	0.40
16:6:207:VAL:HG22	32:6:520:ZEX:H383	2.03	0.40
21:6:511:CL7:C1C	21:5:418:CL7:H161	2.51	0.40
18:5:202:CYS:C	18:5:204:PHE:H	2.29	0.40
18:5:277:TYR:HE1	21:5:403:CL7:HED1	1.87	0.40
18:5:302:LEU:HD12	18:5:302:LEU:HA	1.92	0.40
19:7:268:ASP:N	19:7:268:ASP:OD1	2.54	0.40
21:7:516:CL7:HED2	32:8:403:ZEX:H172	2.02	0.40
1:A:323:ARG:NH2	4:D:327:TRP:O	2.40	0.40
24:B:626:SQD:H102	1:a:28:LEU:HB2	2.03	0.40
3:C:128:ALA:O	3:C:132:ILE:HG12	2.20	0.40
21:2:503:CL7:H13	21:2:503:CL7:H102	1.67	0.40
21:2:503:CL7:H41C	21:2:503:CL7:H62C	1.78	0.40
18:1:173:ILE:HG13	18:1:177:ARG:HD2	2.02	0.40
21:3:516:CL7:HED2	32:4:403:ZEX:H172	2.02	0.40
1:a:214:MET:SD	22:d:408:PHO:CED	3.09	0.40
1:a:332:HIS:CG	1:a:333:GLU:H	2.39	0.40
21:a:405:CL7:C4	30:d:407:PL9:H211	2.51	0.40
4:d:78:SER:HA	4:d:171:SER:HB3	2.03	0.40
9:k:25:PRO:O	9:k:28:PRO:HD2	2.21	0.40
21:6:505:CL7:C4B	21:6:505:CL7:H43C	2.51	0.40
18:5:87:ASN:OD1	18:5:87:ASN:N	2.54	0.40
21:7:517:CL7:H3A	21:7:517:CL7:HBA2	1.69	0.40
32:8:403:ZEX:H25	32:8:403:ZEX:H28	1.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LEU:HB2	24:A:405:SQD:H102	2.03	0.40
1:A:331:MET:HE2	4:D:319:LEU:HB3	2.02	0.40
3:C:375:GLY:O	3:C:379:GLU:HB2	2.21	0.40
9:K:11:PRO:HB2	9:K:14:PHE:HD2	1.86	0.40
16:2:148:LEU:HD23	16:2:148:LEU:HA	1.95	0.40
21:2:511:CL7:C1C	21:1:418:CL7:H161	2.51	0.40
18:1:87:ASN:OD1	18:1:87:ASN:N	2.54	0.40
18:1:206:ASP:HA	18:1:275:LEU:HB2	2.04	0.40
18:1:261:LEU:O	18:1:265:ILE:HG13	2.21	0.40
19:3:280:LEU:HD11	19:3:305:PHE:HA	2.04	0.40
21:3:502:CL7:C2D	21:3:503:CL7:H151	2.51	0.40
1:a:331:MET:HE2	4:d:319:LEU:HB3	2.02	0.40
3:c:330:LEU:HD12	3:c:352:TYR:N	2.37	0.40
3:c:375:GLY:O	3:c:379:GLU:HB2	2.21	0.40
4:d:56:SER:HB3	4:d:78:SER:HB3	2.04	0.40
16:6:70:LEU:HG	21:6:503:CL7:CED	2.52	0.40
16:6:98:PHE:CG	32:6:522:ZEX:H31	2.54	0.40
21:6:511:CL7:H91C	21:6:511:CL7:H111	1.81	0.40
32:5:422:ZEX:H27	32:5:422:ZEX:H391	1.76	0.40
19:7:87:TYR:N	19:7:88:PRO:HD2	2.37	0.40
20:8:255:LYS:HA	20:8:255:LYS:HD2	1.91	0.40
1:A:179:THR:O	1:A:183:MET:HG3	2.22	0.40
2:B:30:VAL:HG12	21:B:605:CL7:HHD	2.03	0.40
2:B:44:LYS:HE2	2:B:44:LYS:HB3	1.92	0.40
2:B:178:ASP:OD1	2:B:182:LEU:N	2.38	0.40
3:C:156:SER:OG	3:C:157:ASP:N	2.54	0.40
3:C:330:LEU:HD12	3:C:352:TYR:N	2.36	0.40
4:D:57:TRP:CH2	5:E:63:LEU:HD22	2.57	0.40
21:2:516:CL7:H162	21:2:516:CL7:H193	1.75	0.40
18:1:202:CYS:C	18:1:204:PHE:H	2.29	0.40
21:c:506:CL7:H42C	21:c:506:CL7:NC	2.36	0.40
4:d:158:MET:HE2	4:d:158:MET:HB3	1.91	0.40
21:6:510:CL7:HBD	21:6:510:CL7:HBA1	2.03	0.40
21:6:510:CL7:C2	32:6:519:ZEX:H181	2.51	0.40
21:6:511:CL7:H43C	32:6:524:ZEX:H3	2.03	0.40
18:5:156:ALA:O	18:5:160:VAL:HG23	2.22	0.40
18:5:250:GLY:O	18:5:254:THR:HG23	2.21	0.40
19:7:22:ASP:N	19:7:22:ASP:OD1	2.54	0.40
21:7:507:CL7:H142	21:7:507:CL7:H111	1.85	0.40
32:7:519:ZEX:H201	32:7:519:ZEX:H15	1.68	0.40
20:8:137:ASN:O	20:8:149:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:PRO:CB	1:A:66:PRO:HB2	2.49	0.40
21:B:610:CL7:HBA2	21:B:610:CL7:H11C	1.81	0.40
9:K:25:PRO:O	9:K:28:PRO:HD2	2.21	0.40
16:2:70:LEU:HG	21:2:503:CL7:CED	2.52	0.40
19:3:57:LEU:HD23	19:3:57:LEU:HA	1.92	0.40
32:3:520:ZEX:H401	32:3:520:ZEX:H31	1.79	0.40
20:4:45:LEU:HD12	20:4:45:LEU:HA	1.96	0.40
20:4:139:ALA:HA	20:4:140:PRO:HD3	1.88	0.40
20:4:163:GLY:HA3	20:4:251:ILE:HG13	2.04	0.40
20:4:201:LEU:O	20:4:203:PRO:HD3	2.21	0.40
1:a:120:MET:SD	1:a:159:LEU:HB2	2.61	0.40
1:a:179:THR:O	1:a:183:MET:HG3	2.22	0.40
2:b:464:PHE:HD2	21:b:612:CL7:HAC2	1.87	0.40
3:c:51:ASN:N	21:c:509:CL7:O1A	2.53	0.40
3:c:156:SER:OG	3:c:157:ASP:N	2.54	0.40
5:e:52:PRO:HA	5:e:55:TYR:CE2	2.56	0.40
14:y:19:GLY:O	14:y:23:ILE:HG12	2.22	0.40
16:6:271:PHE:CB	16:6:304:ARG:HH21	2.35	0.40
21:6:501:CL7:H72C	21:6:501:CL7:H41C	2.03	0.40
32:6:522:ZEX:H162	32:6:522:ZEX:O3	2.21	0.40
21:7:501:CL7:H161	21:7:506:CL7:HMC1	2.02	0.40
20:8:59:VAL:HG21	21:8:412:CL7:HAC2	2.03	0.40
20:8:152:TRP:HH2	21:8:411:CL7:H18	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	280/360 (78%)	269 (96%)	11 (4%)	0	100	100
1	a	280/360 (78%)	269 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	477/506 (94%)	452 (95%)	25 (5%)	0	100	100
2	b	477/506 (94%)	451 (94%)	26 (6%)	0	100	100
3	C	414/490 (84%)	398 (96%)	16 (4%)	0	100	100
3	c	414/490 (84%)	398 (96%)	16 (4%)	0	100	100
4	D	319/351 (91%)	309 (97%)	10 (3%)	0	100	100
4	d	319/351 (91%)	310 (97%)	9 (3%)	0	100	100
5	E	63/83 (76%)	59 (94%)	4 (6%)	0	100	100
5	e	63/83 (76%)	59 (94%)	4 (6%)	0	100	100
6	F	28/99 (28%)	27 (96%)	1 (4%)	0	100	100
6	f	28/99 (28%)	27 (96%)	1 (4%)	0	100	100
7	H	66/71 (93%)	62 (94%)	4 (6%)	0	100	100
7	h	66/71 (93%)	62 (94%)	4 (6%)	0	100	100
8	I	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
8	i	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
9	K	35/45 (78%)	35 (100%)	0	0	100	100
9	k	35/45 (78%)	35 (100%)	0	0	100	100
10	L	34/38 (90%)	34 (100%)	0	0	100	100
10	l	34/38 (90%)	34 (100%)	0	0	100	100
11	M	29/34 (85%)	29 (100%)	0	0	100	100
11	m	29/34 (85%)	29 (100%)	0	0	100	100
12	T	26/46 (56%)	26 (100%)	0	0	100	100
12	t	26/46 (56%)	26 (100%)	0	0	100	100
13	X	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
13	x	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
14	Y	21/39 (54%)	20 (95%)	1 (5%)	0	100	100
14	y	21/39 (54%)	20 (95%)	1 (5%)	0	100	100
15	Z	57/62 (92%)	57 (100%)	0	0	100	100
15	z	57/62 (92%)	57 (100%)	0	0	100	100
16	2	347/352 (99%)	325 (94%)	22 (6%)	0	100	100
16	6	347/352 (99%)	325 (94%)	22 (6%)	0	100	100
18	1	323/356 (91%)	307 (95%)	15 (5%)	1 (0%)	36	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
18	5	323/356 (91%)	307 (95%)	15 (5%)	1 (0%)	36 65
19	3	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	36 65
19	7	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	36 65
20	4	329/353 (93%)	306 (93%)	23 (7%)	0	100 100
20	8	329/353 (93%)	306 (93%)	23 (7%)	0	100 100
All	All	6510/7416 (88%)	6206 (95%)	300 (5%)	4 (0%)	49 75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	3	4	TYR
19	7	4	TYR
18	1	202	CYS
18	5	202	CYS

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	232/292 (80%)	232 (100%)	0	100 100
1	a	232/292 (80%)	232 (100%)	0	100 100
2	B	395/418 (94%)	392 (99%)	3 (1%)	73 79
2	b	395/418 (94%)	392 (99%)	3 (1%)	73 79
3	C	322/378 (85%)	319 (99%)	3 (1%)	70 78
3	c	322/378 (85%)	319 (99%)	3 (1%)	70 78
4	D	265/284 (93%)	264 (100%)	1 (0%)	84 84
4	d	265/284 (93%)	264 (100%)	1 (0%)	84 84
5	E	57/71 (80%)	57 (100%)	0	100 100
5	e	57/71 (80%)	57 (100%)	0	100 100
6	F	25/84 (30%)	25 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	f	25/84 (30%)	25 (100%)	0	100	100
7	H	55/57 (96%)	55 (100%)	0	100	100
7	h	55/57 (96%)	55 (100%)	0	100	100
8	I	30/30 (100%)	30 (100%)	0	100	100
8	i	30/30 (100%)	30 (100%)	0	100	100
9	K	31/37 (84%)	30 (97%)	1 (3%)	34	60
9	k	31/37 (84%)	30 (97%)	1 (3%)	34	60
10	L	33/34 (97%)	33 (100%)	0	100	100
10	l	33/34 (97%)	33 (100%)	0	100	100
11	M	24/27 (89%)	24 (100%)	0	100	100
11	m	24/27 (89%)	24 (100%)	0	100	100
12	T	24/42 (57%)	24 (100%)	0	100	100
12	t	24/42 (57%)	24 (100%)	0	100	100
13	X	28/33 (85%)	28 (100%)	0	100	100
13	x	28/33 (85%)	28 (100%)	0	100	100
14	Y	18/31 (58%)	18 (100%)	0	100	100
14	y	18/31 (58%)	18 (100%)	0	100	100
15	Z	43/46 (94%)	43 (100%)	0	100	100
15	z	43/46 (94%)	43 (100%)	0	100	100
16	2	276/278 (99%)	272 (99%)	4 (1%)	59	73
16	6	276/278 (99%)	272 (99%)	4 (1%)	59	73
18	1	262/278 (94%)	259 (99%)	3 (1%)	65	76
18	5	262/278 (94%)	259 (99%)	3 (1%)	65	76
19	3	269/273 (98%)	266 (99%)	3 (1%)	65	76
19	7	269/273 (98%)	266 (99%)	3 (1%)	65	76
20	4	260/277 (94%)	256 (98%)	4 (2%)	57	72
20	8	260/277 (94%)	256 (98%)	4 (2%)	57	72
All	All	5298/5940 (89%)	5254 (99%)	44 (1%)	70	79

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	354	LEU

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Mol	Chain	Res	Type
2	B	373	LYS
2	B	392	PHE
3	C	218	LEU
3	C	292	TYR
3	C	432	VAL
4	D	285	LEU
9	K	45	LYS
16	2	62	GLN
16	2	263	PHE
16	2	274	GLU
16	2	294	LEU
18	1	66	LEU
18	1	143	TYR
18	1	202	CYS
19	3	4	TYR
19	3	263	PHE
19	3	286	VAL
20	4	24	LEU
20	4	101	ILE
20	4	193	THR
20	4	204	ILE
2	b	354	LEU
2	b	373	LYS
2	b	392	PHE
3	c	218	LEU
3	c	292	TYR
3	c	432	VAL
4	d	285	LEU
9	k	45	LYS
16	6	62	GLN
16	6	263	PHE
16	6	274	GLU
16	6	294	LEU
18	5	66	LEU
18	5	143	TYR
18	5	202	CYS
19	7	4	TYR
19	7	263	PHE
19	7	286	VAL
20	8	24	LEU
20	8	101	ILE
20	8	193	THR

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Mol	Chain	Res	Type
20	8	204	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	108	ASN
1	A	303	ASN
1	A	335	ASN
2	B	9	HIS
2	B	26	HIS
2	B	187	GLN
2	B	224	HIS
2	B	289	GLN
2	B	394	GLN
3	C	68	HIS
4	D	128	GLN
4	D	196	HIS
4	D	337	ASN
4	D	349	ASN
5	E	23	HIS
8	I	31	ASN
10	L	7	ASN
16	2	62	GLN
18	1	166	HIS
18	1	331	HIS
19	3	2	GLN
19	3	34	GLN
20	4	195	HIS
20	4	227	ASN
20	4	280	ASN
1	a	108	ASN
1	a	303	ASN
1	a	335	ASN
2	b	9	HIS
2	b	26	HIS
2	b	122	HIS
2	b	224	HIS
2	b	289	GLN
2	b	394	GLN
3	c	68	HIS
4	d	196	HIS

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Mol	Chain	Res	Type
4	d	337	ASN
4	d	349	ASN
5	e	23	HIS
16	6	62	GLN
19	7	2	GLN
19	7	34	GLN
19	7	54	ASN
19	7	320	GLN
20	8	195	HIS
20	8	227	ASN
20	8	280	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 312 ligands modelled in this entry, 2 are monoatomic - leaving 310 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	SQD	B	626	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
21	CL7	8	405	-	71,73,73	1.69	16 (22%)	80,113,113	2.45	25 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	2	515	-	51,53,73	1.94	16 (31%)	56,89,113	2.71	19 (33%)
21	CL7	1	420	18	51,53,73	1.95	14 (27%)	56,89,113	2.79	22 (39%)
21	CL7	3	501	19	71,73,73	1.69	18 (25%)	80,113,113	2.39	23 (28%)
21	CL7	2	514	-	51,53,73	1.98	16 (31%)	56,89,113	2.72	19 (33%)
25	LHG	8	401	-	48,48,48	0.28	0	51,54,54	0.34	0
21	CL7	6	503	-	71,73,73	1.69	18 (25%)	80,113,113	2.51	25 (31%)
21	CL7	b	605	2	71,73,73	1.68	18 (25%)	80,113,113	2.33	23 (28%)
21	CL7	C	502	3	71,73,73	1.68	16 (22%)	80,113,113	2.36	22 (27%)
21	CL7	2	518	16	71,73,73	1.68	13 (18%)	80,113,113	2.33	23 (28%)
32	ZEX	4	403	-	42,43,43	1.01	4 (9%)	55,60,60	2.56	19 (34%)
21	CL7	7	512	19	61,63,73	1.84	18 (29%)	68,101,113	2.59	23 (33%)
32	ZEX	5	422	-	42,43,43	0.95	1 (2%)	55,60,60	2.24	18 (32%)
21	CL7	4	406	20	71,73,73	1.70	15 (21%)	80,113,113	2.35	21 (26%)
21	CL7	4	412	20	71,73,73	1.69	16 (22%)	80,113,113	2.38	24 (30%)
21	CL7	2	509	-	71,73,73	1.69	18 (25%)	80,113,113	2.31	20 (25%)
21	CL7	7	508	19	71,73,73	1.70	18 (25%)	80,113,113	2.31	21 (26%)
24	SQD	5	423	-	31,32,54	0.48	1 (3%)	40,43,65	0.60	1 (2%)
23	8CT	C	515	-	40,41,41	4.64	21 (52%)	50,56,56	2.40	23 (46%)
21	CL7	5	404	-	71,73,73	1.70	14 (19%)	80,113,113	2.39	21 (26%)
21	CL7	2	504	-	51,53,73	1.98	17 (33%)	56,89,113	2.77	19 (33%)
21	CL7	2	516	16	71,73,73	1.69	17 (23%)	80,113,113	2.39	23 (28%)
24	SQD	2	522	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	8	412	20	71,73,73	1.69	17 (23%)	80,113,113	2.37	25 (31%)
21	CL7	3	514	-	51,53,73	1.98	16 (31%)	56,89,113	2.83	19 (33%)
21	CL7	c	504	3	71,73,73	1.68	16 (22%)	80,113,113	2.40	21 (26%)
21	CL7	4	416	20	47,49,73	1.97	14 (29%)	51,84,113	2.85	18 (35%)
23	8CT	c	515	-	40,41,41	4.64	22 (55%)	50,56,56	2.40	23 (46%)
21	CL7	1	418	18	71,73,73	1.67	16 (22%)	80,113,113	2.46	23 (28%)
21	CL7	1	406	18	68,70,73	1.73	18 (26%)	76,109,113	2.42	20 (26%)
21	CL7	C	504	3	71,73,73	1.68	16 (22%)	80,113,113	2.39	21 (26%)
21	CL7	3	507	-	71,73,73	1.68	15 (21%)	80,113,113	2.40	23 (28%)
26	LMG	D	410	-	33,33,55	0.28	0	41,41,63	0.33	0
21	CL7	b	615	2	66,68,73	1.79	18 (27%)	74,107,113	2.50	24 (32%)
21	CL7	b	603	2	66,68,73	1.78	17 (25%)	74,107,113	2.51	22 (29%)
21	CL7	b	614	2	61,63,73	1.83	19 (31%)	68,101,113	2.47	18 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	SQD	6	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
21	CL7	4	410	20	51,53,73	1.98	17 (33%)	56,89,113	2.69	19 (33%)
24	SQD	7	521	-	45,46,54	0.42	1 (2%)	54,57,65	0.48	0
21	CL7	a	405	-	71,73,73	1.68	17 (23%)	80,113,113	2.44	21 (26%)
21	CL7	2	506	16	71,73,73	1.71	19 (26%)	80,113,113	2.38	23 (28%)
21	CL7	7	510	-	71,73,73	1.68	17 (23%)	80,113,113	2.38	24 (30%)
21	CL7	b	608	-	66,68,73	1.76	17 (25%)	74,107,113	2.48	20 (27%)
21	CL7	3	505	19	71,73,73	1.69	16 (22%)	80,113,113	2.39	21 (26%)
21	CL7	c	506	3	71,73,73	1.70	19 (26%)	80,113,113	2.36	23 (28%)
32	ZEX	1	421	-	42,43,43	0.92	1 (2%)	55,60,60	2.23	20 (36%)
25	LHG	b	626	-	48,48,48	0.30	0	51,54,54	0.34	0
21	CL7	5	420	18	51,53,73	1.95	14 (27%)	56,89,113	2.80	21 (37%)
32	ZEX	2	521	-	42,43,43	0.98	3 (7%)	55,60,60	2.19	17 (30%)
21	CL7	3	510	-	71,73,73	1.68	17 (23%)	80,113,113	2.37	24 (30%)
21	CL7	5	412	18	51,53,73	1.96	16 (31%)	56,89,113	2.76	20 (35%)
21	CL7	b	611	-	71,73,73	1.68	17 (23%)	80,113,113	2.46	22 (27%)
32	ZEX	8	420	-	42,43,43	1.02	3 (7%)	55,60,60	2.20	19 (34%)
32	ZEX	8	419	-	42,43,43	0.99	3 (7%)	55,60,60	2.43	25 (45%)
21	CL7	5	413	-	47,49,73	1.94	12 (25%)	51,84,113	2.97	22 (43%)
21	CL7	4	414	20	59,61,73	1.84	17 (28%)	65,98,113	2.66	21 (32%)
23	8CT	8	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.78	21 (42%)
25	LHG	A	407	-	45,45,48	0.31	0	48,51,54	0.43	0
21	CL7	B	610	-	71,73,73	1.69	17 (23%)	80,113,113	2.46	22 (27%)
21	CL7	2	510	16	71,73,73	1.68	17 (23%)	80,113,113	2.38	22 (27%)
21	CL7	6	509	-	71,73,73	1.69	18 (25%)	80,113,113	2.31	20 (25%)
21	CL7	6	513	16	51,53,73	1.96	14 (27%)	56,89,113	2.84	21 (37%)
32	ZEX	7	520	-	42,43,43	0.93	2 (4%)	55,60,60	2.65	22 (40%)
26	LMG	c	501	-	50,50,55	0.91	2 (4%)	58,58,63	1.21	5 (8%)
21	CL7	8	413	20	66,68,73	1.77	18 (27%)	74,107,113	2.43	21 (28%)
21	CL7	6	515	-	51,53,73	1.94	16 (31%)	56,89,113	2.71	19 (33%)
26	LMG	C	501	-	50,50,55	0.92	2 (4%)	58,58,63	1.22	5 (8%)
25	LHG	d	409	-	48,48,48	0.30	0	51,54,54	0.37	0
32	ZEX	6	522	-	42,43,43	1.05	4 (9%)	55,60,60	2.47	16 (29%)
25	LHG	7	524	-	35,35,48	0.34	0	38,41,54	0.47	0
32	ZEX	3	519	-	42,43,43	1.02	4 (9%)	55,60,60	2.58	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	4	415	-	51,53,73	1.96	20 (39%)	56,89,113	2.88	21 (37%)
32	ZEX	8	403	-	42,43,43	1.01	4 (9%)	55,60,60	2.56	19 (34%)
21	CL7	4	407	-	47,49,73	1.95	14 (29%)	51,84,113	2.82	20 (39%)
21	CL7	4	409	-	66,68,73	1.77	19 (28%)	74,107,113	2.67	25 (33%)
21	CL7	2	512	16	71,73,73	1.68	14 (19%)	80,113,113	2.42	21 (26%)
23	8CT	d	406	-	40,41,41	4.62	23 (57%)	50,56,56	2.99	19 (38%)
21	CL7	1	405	-	51,53,73	1.97	18 (35%)	56,89,113	2.71	19 (33%)
21	CL7	A	403	1	61,63,73	1.86	19 (31%)	68,101,113	2.62	23 (33%)
21	CL7	3	512	19	61,63,73	1.84	18 (29%)	68,101,113	2.59	23 (33%)
21	CL7	8	416	20	47,49,73	1.97	14 (29%)	51,84,113	2.85	18 (35%)
21	CL7	3	504	-	71,73,73	1.69	17 (23%)	80,113,113	2.40	21 (26%)
21	CL7	6	507	-	71,73,73	1.71	17 (23%)	80,113,113	2.43	21 (26%)
21	CL7	C	518	3	47,49,73	1.92	13 (27%)	51,84,113	2.87	19 (37%)
24	SQD	3	523	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
32	ZEX	3	520	-	42,43,43	0.94	2 (4%)	55,60,60	2.65	22 (40%)
21	CL7	d	402	-	56,58,73	1.89	15 (26%)	62,95,113	2.59	20 (32%)
21	CL7	C	509	3	71,73,73	1.70	16 (22%)	80,113,113	2.38	26 (32%)
22	PHO	D	408	-	58,69,69	2.52	12 (20%)	56,99,99	2.99	16 (28%)
21	CL7	4	405	-	71,73,73	1.69	16 (22%)	80,113,113	2.46	25 (31%)
21	CL7	5	411	-	51,53,73	1.97	16 (31%)	56,89,113	2.72	18 (32%)
32	ZEX	6	524	-	42,43,43	1.03	4 (9%)	55,60,60	2.51	17 (30%)
21	CL7	2	502	16	71,73,73	1.68	17 (23%)	80,113,113	2.36	23 (28%)
21	CL7	6	517	16	71,73,73	1.69	15 (21%)	80,113,113	2.36	21 (26%)
32	ZEX	7	519	-	42,43,43	1.02	3 (7%)	55,60,60	2.58	17 (30%)
21	CL7	c	511	3	71,73,73	1.69	15 (21%)	80,113,113	2.38	20 (25%)
23	8CT	c	519	-	40,41,41	4.66	21 (52%)	50,56,56	2.71	21 (42%)
21	CL7	1	416	-	47,49,73	1.95	12 (25%)	51,84,113	2.87	19 (37%)
21	CL7	4	413	20	66,68,73	1.77	18 (27%)	74,107,113	2.43	21 (28%)
23	8CT	c	516	-	40,41,41	4.65	20 (50%)	50,56,56	3.06	21 (42%)
21	CL7	c	509	3	71,73,73	1.70	16 (22%)	80,113,113	2.38	26 (32%)
21	CL7	1	407	18	47,49,73	1.94	15 (31%)	51,84,113	2.87	20 (39%)
26	LMG	B	621	-	51,51,55	0.25	0	59,59,63	0.33	0
21	CL7	7	503	-	71,73,73	1.68	15 (21%)	80,113,113	2.47	24 (30%)
21	CL7	b	623	2	51,53,73	1.97	15 (29%)	56,89,113	2.78	17 (30%)
32	ZEX	5	421	-	42,43,43	0.92	1 (2%)	55,60,60	2.23	20 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	B	605	2	71,73,73	1.67	18 (25%)	80,113,113	2.40	20 (25%)
21	CL7	1	403	-	66,68,73	1.75	17 (25%)	74,107,113	2.52	22 (29%)
21	CL7	C	511	3	71,73,73	1.69	15 (21%)	80,113,113	2.38	20 (25%)
21	CL7	4	417	20	48,50,73	1.93	13 (27%)	51,85,113	2.94	18 (35%)
22	PHO	a	402	-	58,69,69	0.84	3 (5%)	56,99,99	1.08	4 (7%)
32	ZEX	3	525	-	42,43,43	1.17	5 (11%)	55,60,60	2.43	18 (32%)
21	CL7	1	404	-	71,73,73	1.70	14 (19%)	80,113,113	2.39	21 (26%)
32	ZEX	3	522	-	42,43,43	1.00	4 (9%)	55,60,60	2.40	17 (30%)
23	8CT	C	516	-	40,41,41	4.65	20 (50%)	50,56,56	3.06	21 (42%)
21	CL7	b	606	2	71,73,73	1.67	18 (25%)	80,113,113	2.40	21 (26%)
23	8CT	B	627	-	40,41,41	4.70	24 (60%)	50,56,56	3.25	21 (42%)
21	CL7	2	505	16	71,73,73	1.72	18 (25%)	80,113,113	2.48	25 (31%)
27	DGD	B	624	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
21	CL7	2	503	-	71,73,73	1.68	18 (25%)	80,113,113	2.50	25 (31%)
23	8CT	B	617	-	40,41,41	4.65	24 (60%)	50,56,56	2.75	19 (38%)
27	DGD	C	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
21	CL7	B	612	2	71,73,73	1.68	18 (25%)	80,113,113	2.38	23 (28%)
21	CL7	B	616	2	51,53,73	1.97	18 (35%)	56,89,113	2.70	18 (32%)
21	CL7	1	415	-	47,49,73	1.94	11 (23%)	51,84,113	2.97	19 (37%)
21	CL7	4	404	20	71,73,73	1.71	19 (26%)	80,113,113	2.34	21 (26%)
23	8CT	a	404	-	40,41,41	4.63	21 (52%)	50,56,56	2.97	20 (40%)
21	CL7	b	616	2	56,58,73	1.89	17 (30%)	62,95,113	2.69	20 (32%)
21	CL7	B	615	2	56,58,73	1.89	17 (30%)	62,95,113	2.69	20 (32%)
21	CL7	C	506	3	71,73,73	1.70	19 (26%)	80,113,113	2.36	23 (28%)
21	CL7	c	518	3	47,49,73	1.92	13 (27%)	51,84,113	2.88	19 (37%)
25	LHG	b	624	-	44,44,48	0.31	0	47,50,54	0.39	0
21	CL7	C	514	3	51,53,73	1.95	14 (27%)	56,89,113	2.90	19 (33%)
21	CL7	C	503	3	66,68,73	1.77	17 (25%)	74,107,113	2.45	19 (25%)
24	SQD	7	523	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
23	8CT	B	618	-	40,41,41	4.69	21 (52%)	50,56,56	2.67	20 (40%)
21	CL7	b	604	2	71,73,73	1.69	18 (25%)	80,113,113	2.36	21 (26%)
21	CL7	1	408	-	71,73,73	1.67	15 (21%)	80,113,113	2.50	23 (28%)
32	ZEX	2	523	-	42,43,43	1.04	4 (9%)	55,60,60	2.47	16 (29%)
31	HEM	F	101	-	50,50,50	1.62	9 (18%)	66,82,82	1.82	15 (22%)
21	CL7	D	402	-	56,58,73	1.88	15 (26%)	62,95,113	2.60	20 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	7	501	19	71,73,73	1.69	17 (23%)	80,113,113	2.38	23 (28%)
23	8CT	b	619	-	40,41,41	4.69	20 (50%)	50,56,56	2.67	20 (40%)
21	CL7	B	613	2	61,63,73	1.83	19 (31%)	68,101,113	2.48	18 (26%)
21	CL7	2	501	16	71,73,73	1.68	16 (22%)	80,113,113	2.42	21 (26%)
21	CL7	1	419	-	51,53,73	1.97	15 (29%)	56,89,113	2.78	18 (32%)
21	CL7	5	407	18	47,49,73	1.94	15 (31%)	51,84,113	2.86	21 (41%)
21	CL7	8	409	-	66,68,73	1.77	18 (27%)	74,107,113	2.67	25 (33%)
21	CL7	8	417	20	48,50,73	1.93	13 (27%)	51,85,113	2.94	18 (35%)
21	CL7	7	502	19	64,66,73	1.78	17 (26%)	71,104,113	2.41	22 (30%)
21	CL7	1	409	18	51,53,73	1.95	16 (31%)	56,89,113	2.71	20 (35%)
26	LMG	d	410	-	33,33,55	0.28	0	41,41,63	0.33	0
21	CL7	2	508	16	51,53,73	1.97	18 (35%)	56,89,113	2.64	19 (33%)
32	ZEX	4	418	-	42,43,43	0.85	1 (2%)	55,60,60	2.33	16 (29%)
21	CL7	6	511	16	66,68,73	1.78	17 (25%)	74,107,113	2.40	21 (28%)
21	CL7	B	604	2	71,73,73	1.68	18 (25%)	80,113,113	2.33	23 (28%)
21	CL7	c	508	-	71,73,73	1.68	18 (25%)	80,113,113	2.47	23 (28%)
21	CL7	6	516	16	71,73,73	1.69	17 (23%)	80,113,113	2.39	23 (28%)
21	CL7	d	404	4	64,66,73	1.78	20 (31%)	71,104,113	2.49	22 (30%)
23	8CT	b	618	-	40,41,41	4.65	24 (60%)	50,56,56	2.75	19 (38%)
21	CL7	1	412	18	51,53,73	1.96	16 (31%)	56,89,113	2.76	20 (35%)
21	CL7	C	512	3	48,50,73	1.95	14 (29%)	51,85,113	2.84	18 (35%)
21	CL7	C	508	-	71,73,73	1.68	18 (25%)	80,113,113	2.47	23 (28%)
21	CL7	1	410	-	71,73,73	1.70	17 (23%)	80,113,113	2.33	23 (28%)
21	CL7	7	504	-	71,73,73	1.69	16 (22%)	80,113,113	2.40	21 (26%)
21	CL7	7	517	19	56,58,73	1.89	16 (28%)	62,95,113	2.65	20 (32%)
26	LMG	b	622	-	51,51,55	0.25	0	59,59,63	0.33	0
21	CL7	8	404	20	71,73,73	1.71	19 (26%)	80,113,113	2.33	21 (26%)
26	LMG	1	401	-	51,51,55	0.22	0	59,59,63	0.41	1 (1%)
25	LHG	D	409	-	48,48,48	0.30	0	51,54,54	0.37	0
21	CL7	c	512	3	48,50,73	1.95	14 (29%)	51,85,113	2.84	18 (35%)
21	CL7	2	513	16	51,53,73	1.96	14 (27%)	56,89,113	2.84	21 (37%)
21	CL7	6	506	16	71,73,73	1.71	19 (26%)	80,113,113	2.38	22 (27%)
21	CL7	7	514	-	51,53,73	1.98	16 (31%)	56,89,113	2.83	19 (33%)
21	CL7	c	513	3	47,49,73	1.92	14 (29%)	51,84,113	2.98	20 (39%)
27	DGD	c	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	ZEX	2	520	-	42,43,43	1.17	5 (11%)	55,60,60	2.43	18 (32%)
21	CL7	8	406	20	71,73,73	1.70	16 (22%)	80,113,113	2.35	21 (26%)
24	SQD	3	521	-	45,46,54	0.42	1 (2%)	54,57,65	0.48	0
21	CL7	2	511	16	66,68,73	1.78	17 (25%)	74,107,113	2.40	21 (28%)
21	CL7	7	507	-	71,73,73	1.68	15 (21%)	80,113,113	2.39	23 (28%)
21	CL7	3	517	19	56,58,73	1.88	16 (28%)	62,95,113	2.65	20 (32%)
23	8CT	k	101	-	40,41,41	4.75	24 (60%)	50,56,56	2.65	16 (32%)
21	CL7	1	411	-	51,53,73	1.97	16 (31%)	56,89,113	2.72	18 (32%)
21	CL7	b	612	2	71,73,73	1.69	18 (25%)	80,113,113	2.35	20 (25%)
21	CL7	6	505	16	71,73,73	1.72	19 (26%)	80,113,113	2.47	25 (31%)
21	CL7	C	510	3	71,73,73	1.72	19 (26%)	80,113,113	2.35	21 (26%)
21	CL7	8	414	20	59,61,73	1.84	19 (32%)	65,98,113	2.66	21 (32%)
21	CL7	c	502	3	71,73,73	1.68	16 (22%)	80,113,113	2.36	21 (26%)
21	CL7	B	609	2	71,73,73	1.69	17 (23%)	80,113,113	2.32	20 (25%)
21	CL7	3	511	19	71,73,73	1.69	17 (23%)	80,113,113	2.55	24 (30%)
21	CL7	a	401	1	71,73,73	1.73	14 (19%)	80,113,113	2.47	25 (31%)
21	CL7	2	507	-	71,73,73	1.71	17 (23%)	80,113,113	2.43	21 (26%)
21	CL7	1	414	18	47,49,73	1.95	12 (25%)	51,84,113	2.97	20 (39%)
32	ZEX	4	419	-	42,43,43	0.99	3 (7%)	55,60,60	2.43	25 (45%)
21	CL7	4	411	20	71,73,73	1.68	14 (19%)	80,113,113	2.40	23 (28%)
32	ZEX	6	519	-	42,43,43	1.05	3 (7%)	55,60,60	2.50	16 (29%)
23	8CT	b	601	-	40,41,41	4.70	24 (60%)	50,56,56	3.25	21 (42%)
25	LHG	B	625	-	48,48,48	0.30	0	51,54,54	0.34	0
21	CL7	5	418	18	71,73,73	1.67	16 (22%)	80,113,113	2.46	23 (28%)
21	CL7	8	407	-	47,49,73	1.94	13 (27%)	51,84,113	2.81	20 (39%)
21	CL7	3	509	19	71,73,73	1.69	15 (21%)	80,113,113	2.33	22 (27%)
21	CL7	D	404	4	64,66,73	1.78	20 (31%)	71,104,113	2.48	22 (30%)
24	SQD	b	621	-	53,54,54	0.39	1 (1%)	62,65,65	0.54	1 (1%)
21	CL7	6	501	16	71,73,73	1.68	16 (22%)	80,113,113	2.42	21 (26%)
24	SQD	1	423	-	31,32,54	0.48	1 (3%)	40,43,65	0.60	1 (2%)
32	ZEX	8	418	-	42,43,43	0.86	1 (2%)	55,60,60	2.33	16 (29%)
32	ZEX	2	525	-	42,43,43	1.02	3 (7%)	55,60,60	2.51	17 (30%)
21	CL7	5	403	-	66,68,73	1.75	17 (25%)	74,107,113	2.51	22 (29%)
30	PL9	D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
32	ZEX	1	422	-	42,43,43	0.95	1 (2%)	55,60,60	2.24	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	3	515	-	47,49,73	1.94	11 (23%)	51,84,113	2.93	21 (41%)
21	CL7	8	415	-	51,53,73	1.97	20 (39%)	56,89,113	2.88	22 (39%)
27	DGD	b	625	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
25	LHG	3	524	-	35,35,48	0.34	0	38,41,54	0.47	0
23	8CT	b	620	-	40,41,41	4.59	22 (55%)	50,56,56	2.92	18 (36%)
21	CL7	B	601	-	47,49,73	1.94	13 (27%)	51,84,113	2.86	18 (35%)
21	CL7	5	402	18	66,68,73	1.78	15 (22%)	74,107,113	2.50	19 (25%)
21	CL7	6	508	16	51,53,73	1.97	18 (35%)	56,89,113	2.64	19 (33%)
21	CL7	6	514	-	51,53,73	1.98	17 (33%)	56,89,113	2.72	19 (33%)
21	CL7	a	403	1	61,63,73	1.87	19 (31%)	68,101,113	2.61	23 (33%)
21	CL7	b	609	2	71,73,73	1.69	18 (25%)	80,113,113	2.30	19 (23%)
32	ZEX	2	519	-	42,43,43	1.06	3 (7%)	55,60,60	2.50	16 (29%)
23	8CT	K	101	-	40,41,41	4.76	24 (60%)	50,56,56	2.65	16 (32%)
21	CL7	c	507	3	66,68,73	1.76	17 (25%)	74,107,113	2.51	23 (31%)
21	CL7	C	505	-	61,63,73	1.85	17 (27%)	68,101,113	2.54	19 (27%)
21	CL7	A	401	1	71,73,73	1.74	14 (19%)	80,113,113	2.47	25 (31%)
22	PHO	d	408	-	58,69,69	2.53	12 (20%)	56,99,99	2.99	16 (28%)
21	CL7	5	406	18	68,70,73	1.73	18 (26%)	76,109,113	2.42	20 (26%)
21	CL7	C	513	3	47,49,73	1.92	13 (27%)	51,84,113	2.98	20 (39%)
21	CL7	1	402	18	66,68,73	1.78	15 (22%)	74,107,113	2.50	19 (25%)
21	CL7	c	503	3	66,68,73	1.77	17 (25%)	74,107,113	2.45	19 (25%)
21	CL7	B	603	2	71,73,73	1.69	18 (25%)	80,113,113	2.36	21 (26%)
21	CL7	3	518	19	51,53,73	1.98	13 (25%)	56,89,113	2.74	20 (35%)
23	8CT	A	404	-	40,41,41	4.63	21 (52%)	50,56,56	2.97	20 (40%)
21	CL7	6	512	16	71,73,73	1.68	14 (19%)	80,113,113	2.43	21 (26%)
29	BCT	D	403	28	2,3,3	1.00	0	2,3,3	1.67	1 (50%)
21	CL7	d	405	4	51,53,73	1.95	17 (33%)	56,89,113	2.77	22 (39%)
21	CL7	5	416	-	47,49,73	1.95	12 (25%)	51,84,113	2.88	19 (37%)
21	CL7	c	505	-	61,63,73	1.85	18 (29%)	68,101,113	2.54	19 (27%)
24	SQD	6	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	7	515	-	47,49,73	1.94	12 (25%)	51,84,113	2.93	21 (41%)
21	CL7	6	510	16	71,73,73	1.68	17 (23%)	80,113,113	2.38	22 (27%)
21	CL7	3	502	19	64,66,73	1.77	16 (25%)	71,104,113	2.41	22 (30%)
21	CL7	b	610	2	71,73,73	1.69	17 (23%)	80,113,113	2.32	20 (25%)
21	CL7	1	417	18	61,63,73	1.81	16 (26%)	68,101,113	2.57	20 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	LHG	B	623	-	44,44,48	0.32	0	47,50,54	0.39	0
32	ZEX	4	420	-	42,43,43	1.02	3 (7%)	55,60,60	2.20	19 (34%)
21	CL7	A	406	-	71,73,73	1.68	17 (23%)	80,113,113	2.44	21 (26%)
21	CL7	3	516	19	61,63,73	1.81	17 (27%)	68,101,113	2.56	25 (36%)
23	8CT	4	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.78	21 (42%)
21	CL7	8	411	20	71,73,73	1.68	15 (21%)	80,113,113	2.40	23 (28%)
21	CL7	8	408	20	51,53,73	1.97	17 (33%)	56,89,113	2.70	21 (37%)
21	CL7	5	419	-	51,53,73	1.98	15 (29%)	56,89,113	2.77	18 (32%)
21	CL7	B	611	2	71,73,73	1.69	18 (25%)	80,113,113	2.35	21 (26%)
21	CL7	1	413	-	47,49,73	1.94	12 (25%)	51,84,113	2.98	22 (43%)
21	CL7	7	509	19	71,73,73	1.68	15 (21%)	80,113,113	2.33	22 (27%)
21	CL7	7	513	-	51,53,73	1.98	18 (35%)	56,89,113	2.72	18 (32%)
21	CL7	7	506	19	51,53,73	1.97	17 (33%)	56,89,113	2.76	19 (33%)
21	CL7	7	511	19	71,73,73	1.69	17 (23%)	80,113,113	2.55	24 (30%)
23	8CT	B	619	-	40,41,41	4.59	22 (55%)	50,56,56	2.91	18 (36%)
21	CL7	5	417	18	61,63,73	1.81	16 (26%)	68,101,113	2.56	20 (29%)
23	8CT	D	406	-	40,41,41	4.62	23 (57%)	50,56,56	2.99	19 (38%)
29	BCT	d	403	28	2,3,3	1.00	0	2,3,3	1.67	1 (50%)
21	CL7	2	517	16	71,73,73	1.69	15 (21%)	80,113,113	2.36	21 (26%)
21	CL7	B	608	2	71,73,73	1.69	18 (25%)	80,113,113	2.30	19 (23%)
21	CL7	7	516	19	61,63,73	1.81	17 (27%)	68,101,113	2.56	25 (36%)
24	SQD	A	405	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
21	CL7	3	508	19	71,73,73	1.70	18 (25%)	80,113,113	2.31	21 (26%)
31	HEM	f	101	-	50,50,50	1.62	9 (18%)	66,82,82	1.82	15 (22%)
32	ZEX	6	520	-	42,43,43	0.98	3 (7%)	55,60,60	2.19	17 (30%)
32	ZEX	7	522	-	42,43,43	1.00	4 (9%)	55,60,60	2.40	17 (30%)
21	CL7	c	514	3	51,53,73	1.95	14 (27%)	56,89,113	2.90	19 (33%)
21	CL7	b	602	-	47,49,73	1.94	13 (27%)	51,84,113	2.87	18 (35%)
25	LHG	a	406	-	45,45,48	0.31	0	48,51,54	0.43	0
21	CL7	3	506	19	51,53,73	1.97	17 (33%)	56,89,113	2.75	19 (33%)
21	CL7	B	607	-	66,68,73	1.76	17 (25%)	74,107,113	2.48	20 (27%)
23	8CT	C	519	-	40,41,41	4.66	21 (52%)	50,56,56	2.71	21 (42%)
21	CL7	7	518	19	51,53,73	1.98	13 (25%)	56,89,113	2.74	20 (35%)
21	CL7	3	503	-	71,73,73	1.68	15 (21%)	80,113,113	2.47	24 (30%)
30	PL9	d	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.62	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	5	408	-	71,73,73	1.66	15 (21%)	80,113,113	2.51	23 (28%)
24	SQD	B	620	-	53,54,54	0.39	1 (1%)	62,65,65	0.54	1 (1%)
26	LMG	5	401	-	51,51,55	0.22	0	59,59,63	0.41	1 (1%)
22	PHO	A	402	-	58,69,69	0.84	3 (5%)	56,99,99	1.07	4 (7%)
25	LHG	4	401	-	48,48,48	0.28	0	51,54,54	0.34	0
21	CL7	6	504	-	51,53,73	1.98	17 (33%)	56,89,113	2.77	19 (33%)
21	CL7	6	502	16	71,73,73	1.68	17 (23%)	80,113,113	2.36	22 (27%)
21	CL7	B	606	2	61,63,73	1.81	16 (26%)	68,101,113	2.64	21 (30%)
21	CL7	3	513	-	51,53,73	1.98	18 (35%)	56,89,113	2.73	18 (32%)
21	CL7	8	410	20	51,53,73	1.98	17 (33%)	56,89,113	2.70	19 (33%)
21	CL7	B	614	2	66,68,73	1.79	18 (27%)	74,107,113	2.50	24 (32%)
21	CL7	c	510	3	71,73,73	1.72	19 (26%)	80,113,113	2.35	21 (26%)
21	CL7	4	408	20	51,53,73	1.97	17 (33%)	56,89,113	2.70	20 (35%)
21	CL7	5	414	18	47,49,73	1.95	12 (25%)	51,84,113	2.97	20 (39%)
21	CL7	5	410	-	71,73,73	1.70	17 (23%)	80,113,113	2.33	23 (28%)
21	CL7	5	415	-	47,49,73	1.94	11 (23%)	51,84,113	2.97	19 (37%)
21	CL7	B	602	2	66,68,73	1.78	17 (25%)	74,107,113	2.51	22 (29%)
21	CL7	b	613	2	71,73,73	1.68	18 (25%)	80,113,113	2.38	23 (28%)
21	CL7	5	409	18	51,53,73	1.95	16 (31%)	56,89,113	2.72	20 (35%)
21	CL7	5	405	-	51,53,73	1.97	18 (35%)	56,89,113	2.71	19 (33%)
21	CL7	D	405	4	51,53,73	1.95	17 (33%)	56,89,113	2.77	22 (39%)
21	CL7	C	507	3	66,68,73	1.77	17 (25%)	74,107,113	2.51	23 (31%)
21	CL7	7	505	19	71,73,73	1.70	17 (23%)	80,113,113	2.39	21 (26%)
21	CL7	b	607	2	61,63,73	1.81	16 (26%)	68,101,113	2.64	21 (30%)
24	SQD	2	524	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
21	CL7	B	622	2	51,53,73	1.97	15 (29%)	56,89,113	2.79	17 (30%)
21	CL7	b	617	2	51,53,73	1.97	18 (35%)	56,89,113	2.70	18 (32%)
21	CL7	6	518	16	71,73,73	1.68	13 (18%)	80,113,113	2.33	22 (27%)

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	SQD	B	626	-	-	3/29/49/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	8	405	-	2/2/15/20	18/39/115/115	-
21	CL7	2	515	-	2/2/11/20	8/15/91/115	-
21	CL7	1	420	18	2/2/11/20	6/15/91/115	-
21	CL7	3	501	19	2/2/15/20	21/39/115/115	-
21	CL7	2	514	-	2/2/11/20	9/15/91/115	-
25	LHG	8	401	-	-	8/53/53/53	-
21	CL7	6	503	-	2/2/15/20	17/39/115/115	-
21	CL7	b	605	2	2/2/15/20	17/39/115/115	-
21	CL7	C	502	3	2/2/15/20	20/39/115/115	-
21	CL7	2	518	16	2/2/15/20	12/39/115/115	-
32	ZEX	4	403	-	-	10/29/67/67	0/2/2/2
21	CL7	7	512	19	2/2/13/20	12/27/103/115	-
32	ZEX	5	422	-	-	6/29/67/67	0/2/2/2
21	CL7	4	406	20	2/2/15/20	24/39/115/115	-
21	CL7	4	412	20	2/2/15/20	17/39/115/115	-
21	CL7	2	509	-	2/2/15/20	16/39/115/115	-
21	CL7	7	508	19	2/2/15/20	16/39/115/115	-
24	SQD	5	423	-	-	3/27/47/69	0/1/1/1
23	8CT	C	515	-	-	14/29/63/63	0/2/2/2
21	CL7	5	404	-	2/2/15/20	15/39/115/115	-
21	CL7	2	504	-	2/2/11/20	6/15/91/115	-
21	CL7	2	516	16	2/2/15/20	16/39/115/115	-
24	SQD	2	522	-	-	7/45/65/69	0/1/1/1
21	CL7	8	412	20	2/2/15/20	17/39/115/115	-
21	CL7	3	514	-	2/2/11/20	5/15/91/115	-
21	CL7	c	504	3	2/2/15/20	19/39/115/115	-
21	CL7	4	416	20	2/2/10/20	7/10/86/115	-
23	8CT	c	515	-	-	14/29/63/63	0/2/2/2
21	CL7	1	418	18	2/2/15/20	22/39/115/115	-
21	CL7	1	406	18	2/2/14/20	13/36/112/115	-
21	CL7	C	504	3	2/2/15/20	19/39/115/115	-
21	CL7	3	507	-	2/2/15/20	15/39/115/115	-
26	LMG	D	410	-	-	6/28/48/70	0/1/1/1
21	CL7	b	615	2	2/2/14/20	14/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	b	603	2	2/2/14/20	9/33/109/115	-
21	CL7	b	614	2	2/2/13/20	5/27/103/115	-
24	SQD	6	523	-	-	0/36/56/69	0/1/1/1
21	CL7	4	410	20	2/2/11/20	9/15/91/115	-
24	SQD	7	521	-	-	3/41/61/69	0/1/1/1
21	CL7	a	405	-	2/2/15/20	16/39/115/115	-
21	CL7	2	506	16	2/2/15/20	14/39/115/115	-
21	CL7	7	510	-	2/2/15/20	15/39/115/115	-
21	CL7	b	608	-	2/2/14/20	11/33/109/115	-
21	CL7	3	505	19	2/2/15/20	14/39/115/115	-
21	CL7	c	506	3	2/2/15/20	16/39/115/115	-
32	ZEX	1	421	-	-	14/29/67/67	0/2/2/2
25	LHG	b	626	-	-	6/53/53/53	-
21	CL7	5	420	18	2/2/11/20	6/15/91/115	-
32	ZEX	2	521	-	-	6/29/67/67	0/2/2/2
21	CL7	3	510	-	2/2/15/20	15/39/115/115	-
21	CL7	5	412	18	2/2/11/20	10/15/91/115	-
21	CL7	b	611	-	2/2/15/20	11/39/115/115	-
32	ZEX	8	420	-	-	12/29/67/67	0/2/2/2
32	ZEX	8	419	-	-	9/29/67/67	0/2/2/2
21	CL7	5	413	-	2/2/10/20	2/10/86/115	-
21	CL7	4	414	20	2/2/12/20	8/25/101/115	-
23	8CT	8	402	-	-	4/29/63/63	0/2/2/2
25	LHG	A	407	-	-	5/50/50/53	-
21	CL7	B	610	-	2/2/15/20	11/39/115/115	-
21	CL7	2	510	16	2/2/15/20	20/39/115/115	-
21	CL7	6	509	-	2/2/15/20	16/39/115/115	-
21	CL7	6	513	16	2/2/11/20	8/15/91/115	-
32	ZEX	7	520	-	-	10/29/67/67	0/2/2/2
26	LMG	c	501	-	-	16/45/65/70	0/1/1/1
21	CL7	8	413	20	2/2/14/20	7/33/109/115	-
21	CL7	6	515	-	2/2/11/20	8/15/91/115	-
26	LMG	C	501	-	-	16/45/65/70	0/1/1/1
25	LHG	d	409	-	-	7/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	ZEX	6	522	-	-	6/29/67/67	0/2/2/2
25	LHG	7	524	-	-	3/40/40/53	-
32	ZEX	3	519	-	-	10/29/67/67	0/2/2/2
21	CL7	4	415	-	2/2/11/20	11/15/91/115	-
32	ZEX	8	403	-	-	10/29/67/67	0/2/2/2
21	CL7	4	407	-	2/2/10/20	3/10/86/115	-
21	CL7	4	409	-	2/2/14/20	17/33/109/115	-
21	CL7	2	512	16	2/2/15/20	18/39/115/115	-
23	8CT	d	406	-	-	10/29/63/63	0/2/2/2
21	CL7	1	405	-	2/2/11/20	10/15/91/115	-
21	CL7	A	403	1	2/2/13/20	9/27/103/115	-
21	CL7	3	512	19	2/2/13/20	12/27/103/115	-
21	CL7	8	416	20	2/2/10/20	7/10/86/115	-
21	CL7	3	504	-	2/2/15/20	16/39/115/115	-
21	CL7	6	507	-	2/2/15/20	20/39/115/115	-
21	CL7	C	518	3	2/2/10/20	5/10/86/115	-
24	SQD	3	523	-	-	7/45/65/69	0/1/1/1
32	ZEX	3	520	-	-	10/29/67/67	0/2/2/2
21	CL7	d	402	-	2/2/12/20	9/21/97/115	-
21	CL7	C	509	3	2/2/15/20	17/39/115/115	-
22	PHO	D	408	-	-	4/37/103/103	0/5/6/6
21	CL7	4	405	-	2/2/15/20	18/39/115/115	-
21	CL7	5	411	-	2/2/11/20	7/15/91/115	-
32	ZEX	6	524	-	-	11/29/67/67	0/2/2/2
21	CL7	2	502	16	2/2/15/20	17/39/115/115	-
21	CL7	6	517	16	2/2/15/20	21/39/115/115	-
32	ZEX	7	519	-	-	10/29/67/67	0/2/2/2
21	CL7	c	511	3	2/2/15/20	22/39/115/115	-
23	8CT	c	519	-	-	8/29/63/63	0/2/2/2
21	CL7	1	416	-	2/2/10/20	4/10/86/115	-
21	CL7	4	413	20	2/2/14/20	7/33/109/115	-
23	8CT	c	516	-	-	10/29/63/63	0/2/2/2
21	CL7	c	509	3	2/2/15/20	17/39/115/115	-
21	CL7	1	407	18	2/2/10/20	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LMG	B	621	-	-	7/46/66/70	0/1/1/1
21	CL7	7	503	-	2/2/15/20	20/39/115/115	-
21	CL7	b	623	2	2/2/11/20	8/15/91/115	-
32	ZEX	5	421	-	-	14/29/67/67	0/2/2/2
21	CL7	B	605	2	2/2/15/20	18/39/115/115	-
21	CL7	1	403	-	2/2/14/20	11/33/109/115	-
21	CL7	C	511	3	2/2/15/20	22/39/115/115	-
21	CL7	4	417	20	2/2/10/20	6/12/88/115	-
22	PHO	a	402	-	-	3/37/103/103	0/5/6/6
32	ZEX	3	525	-	-	7/29/67/67	0/2/2/2
21	CL7	1	404	-	2/2/15/20	15/39/115/115	-
32	ZEX	3	522	-	-	5/29/67/67	0/2/2/2
23	8CT	C	516	-	-	10/29/63/63	0/2/2/2
21	CL7	b	606	2	2/2/15/20	18/39/115/115	-
23	8CT	B	627	-	-	10/29/63/63	0/2/2/2
21	CL7	2	505	16	2/2/15/20	18/39/115/115	-
27	DGD	B	624	-	-	7/51/91/95	0/2/2/2
21	CL7	2	503	-	2/2/15/20	17/39/115/115	-
23	8CT	B	617	-	-	7/29/63/63	0/2/2/2
27	DGD	C	517	-	-	9/51/91/95	0/2/2/2
21	CL7	B	612	2	2/2/15/20	17/39/115/115	-
21	CL7	B	616	2	2/2/11/20	4/15/91/115	-
21	CL7	1	415	-	2/2/10/20	7/10/86/115	-
21	CL7	4	404	20	2/2/15/20	14/39/115/115	-
23	8CT	a	404	-	-	5/29/63/63	0/2/2/2
21	CL7	b	616	2	2/2/12/20	8/21/97/115	-
21	CL7	B	615	2	2/2/12/20	8/21/97/115	-
21	CL7	C	506	3	2/2/15/20	16/39/115/115	-
21	CL7	c	518	3	2/2/10/20	5/10/86/115	-
25	LHG	b	624	-	-	3/49/49/53	-
21	CL7	C	514	3	2/2/11/20	8/15/91/115	-
21	CL7	C	503	3	2/2/14/20	12/33/109/115	-
24	SQD	7	523	-	-	7/45/65/69	0/1/1/1
23	8CT	B	618	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	b	604	2	2/2/15/20	12/39/115/115	-
21	CL7	1	408	-	2/2/15/20	16/39/115/115	-
32	ZEX	2	523	-	-	6/29/67/67	0/2/2/2
31	HEM	F	101	-	-	8/14/54/54	-
21	CL7	D	402	-	2/2/12/20	9/21/97/115	-
21	CL7	7	501	19	2/2/15/20	21/39/115/115	-
23	8CT	b	619	-	-	10/29/63/63	0/2/2/2
21	CL7	B	613	2	2/2/13/20	5/27/103/115	-
21	CL7	2	501	16	2/2/15/20	17/39/115/115	-
21	CL7	1	419	-	2/2/11/20	9/15/91/115	-
21	CL7	5	407	18	2/2/10/20	4/10/86/115	-
21	CL7	8	409	-	2/2/14/20	17/33/109/115	-
21	CL7	8	417	20	2/2/10/20	6/12/88/115	-
21	CL7	7	502	19	2/2/13/20	12/31/107/115	-
21	CL7	1	409	18	2/2/11/20	6/15/91/115	-
26	LMG	d	410	-	-	6/28/48/70	0/1/1/1
21	CL7	2	508	16	2/2/11/20	5/15/91/115	-
32	ZEX	4	418	-	-	9/29/67/67	0/2/2/2
21	CL7	6	511	16	2/2/14/20	16/33/109/115	-
21	CL7	B	604	2	2/2/15/20	17/39/115/115	-
21	CL7	c	508	-	2/2/15/20	17/39/115/115	-
21	CL7	6	516	16	2/2/15/20	16/39/115/115	-
21	CL7	d	404	4	2/2/13/20	13/31/107/115	-
23	8CT	b	618	-	-	7/29/63/63	0/2/2/2
21	CL7	1	412	18	2/2/11/20	10/15/91/115	-
21	CL7	C	512	3	2/2/10/20	5/12/88/115	-
21	CL7	C	508	-	2/2/15/20	17/39/115/115	-
21	CL7	1	410	-	2/2/15/20	17/39/115/115	-
21	CL7	7	504	-	2/2/15/20	16/39/115/115	-
21	CL7	7	517	19	2/2/12/20	9/21/97/115	-
26	LMG	b	622	-	-	7/46/66/70	0/1/1/1
21	CL7	8	404	20	2/2/15/20	14/39/115/115	-
26	LMG	1	401	-	-	5/46/66/70	0/1/1/1
25	LHG	D	409	-	-	7/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	c	512	3	2/2/10/20	5/12/88/115	-
21	CL7	2	513	16	2/2/11/20	8/15/91/115	-
21	CL7	6	506	16	2/2/15/20	14/39/115/115	-
21	CL7	7	514	-	2/2/11/20	5/15/91/115	-
21	CL7	c	513	3	2/2/10/20	4/10/86/115	-
27	DGD	c	517	-	-	9/51/91/95	0/2/2/2
32	ZEX	2	520	-	-	7/29/67/67	0/2/2/2
21	CL7	8	406	20	2/2/15/20	24/39/115/115	-
24	SQD	3	521	-	-	3/41/61/69	0/1/1/1
21	CL7	2	511	16	2/2/14/20	16/33/109/115	-
21	CL7	7	507	-	2/2/15/20	15/39/115/115	-
21	CL7	3	517	19	2/2/12/20	9/21/97/115	-
23	8CT	k	101	-	-	10/29/63/63	0/2/2/2
21	CL7	1	411	-	2/2/11/20	7/15/91/115	-
21	CL7	b	612	2	2/2/15/20	17/39/115/115	-
21	CL7	6	505	16	2/2/15/20	18/39/115/115	-
21	CL7	C	510	3	2/2/15/20	20/39/115/115	-
21	CL7	8	414	20	2/2/12/20	8/25/101/115	-
21	CL7	c	502	3	2/2/15/20	20/39/115/115	-
21	CL7	B	609	2	2/2/15/20	14/39/115/115	-
21	CL7	3	511	19	2/2/15/20	19/39/115/115	-
21	CL7	a	401	1	2/2/15/20	18/39/115/115	-
21	CL7	2	507	-	2/2/15/20	20/39/115/115	-
21	CL7	1	414	18	2/2/10/20	3/10/86/115	-
32	ZEX	4	419	-	-	9/29/67/67	0/2/2/2
21	CL7	4	411	20	2/2/15/20	14/39/115/115	-
32	ZEX	6	519	-	-	11/29/67/67	0/2/2/2
23	8CT	b	601	-	-	10/29/63/63	0/2/2/2
25	LHG	B	625	-	-	6/53/53/53	-
21	CL7	5	418	18	2/2/15/20	22/39/115/115	-
21	CL7	8	407	-	2/2/10/20	3/10/86/115	-
21	CL7	3	509	19	2/2/15/20	17/39/115/115	-
21	CL7	D	404	4	2/2/13/20	13/31/107/115	-
24	SQD	b	621	-	-	5/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	6	501	16	2/2/15/20	17/39/115/115	-
24	SQD	1	423	-	-	3/27/47/69	0/1/1/1
32	ZEX	8	418	-	-	9/29/67/67	0/2/2/2
32	ZEX	2	525	-	-	11/29/67/67	0/2/2/2
21	CL7	5	403	-	2/2/14/20	11/33/109/115	-
30	PL9	D	407	-	-	9/53/73/73	0/1/1/1
32	ZEX	1	422	-	-	6/29/67/67	0/2/2/2
21	CL7	3	515	-	2/2/10/20	0/10/86/115	-
21	CL7	8	415	-	2/2/11/20	11/15/91/115	-
27	DGD	b	625	-	-	7/51/91/95	0/2/2/2
25	LHG	3	524	-	-	3/40/40/53	-
23	8CT	b	620	-	-	4/29/63/63	0/2/2/2
21	CL7	B	601	-	2/2/10/20	4/10/86/115	-
21	CL7	5	402	18	2/2/14/20	16/33/109/115	-
21	CL7	6	508	16	2/2/11/20	5/15/91/115	-
21	CL7	6	514	-	2/2/11/20	9/15/91/115	-
21	CL7	a	403	1	2/2/13/20	9/27/103/115	-
21	CL7	b	609	2	2/2/15/20	15/39/115/115	-
32	ZEX	2	519	-	-	11/29/67/67	0/2/2/2
23	8CT	K	101	-	-	10/29/63/63	0/2/2/2
21	CL7	c	507	3	2/2/14/20	15/33/109/115	-
21	CL7	C	505	-	2/2/13/20	13/27/103/115	-
21	CL7	A	401	1	2/2/15/20	18/39/115/115	-
22	PHO	d	408	-	-	4/37/103/103	0/5/6/6
21	CL7	5	406	18	2/2/14/20	13/36/112/115	-
21	CL7	C	513	3	2/2/10/20	4/10/86/115	-
21	CL7	1	402	18	2/2/14/20	16/33/109/115	-
21	CL7	c	503	3	2/2/14/20	12/33/109/115	-
21	CL7	B	603	2	2/2/15/20	12/39/115/115	-
21	CL7	3	518	19	2/2/11/20	7/15/91/115	-
23	8CT	A	404	-	-	5/29/63/63	0/2/2/2
21	CL7	6	512	16	2/2/15/20	18/39/115/115	-
21	CL7	d	405	4	2/2/11/20	8/15/91/115	-
21	CL7	5	416	-	2/2/10/20	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	c	505	-	2/2/13/20	13/27/103/115	-
24	SQD	6	521	-	-	7/45/65/69	0/1/1/1
21	CL7	7	515	-	2/2/10/20	0/10/86/115	-
21	CL7	6	510	16	2/2/15/20	20/39/115/115	-
21	CL7	3	502	19	2/2/13/20	12/31/107/115	-
21	CL7	b	610	2	2/2/15/20	14/39/115/115	-
21	CL7	1	417	18	2/2/13/20	9/27/103/115	-
25	LHG	B	623	-	-	3/49/49/53	-
32	ZEX	4	420	-	-	12/29/67/67	0/2/2/2
21	CL7	A	406	-	2/2/15/20	16/39/115/115	-
21	CL7	3	516	19	2/2/13/20	16/27/103/115	-
23	8CT	4	402	-	-	4/29/63/63	0/2/2/2
21	CL7	8	411	20	2/2/15/20	14/39/115/115	-
21	CL7	8	408	20	2/2/11/20	4/15/91/115	-
21	CL7	5	419	-	2/2/11/20	9/15/91/115	-
21	CL7	B	611	2	2/2/15/20	17/39/115/115	-
21	CL7	1	413	-	2/2/10/20	2/10/86/115	-
21	CL7	7	509	19	2/2/15/20	17/39/115/115	-
21	CL7	7	513	-	2/2/11/20	9/15/91/115	-
21	CL7	7	506	19	2/2/11/20	13/15/91/115	-
21	CL7	7	511	19	2/2/15/20	19/39/115/115	-
23	8CT	B	619	-	-	4/29/63/63	0/2/2/2
21	CL7	5	417	18	2/2/13/20	9/27/103/115	-
23	8CT	D	406	-	-	10/29/63/63	0/2/2/2
21	CL7	2	517	16	2/2/15/20	21/39/115/115	-
21	CL7	B	608	2	2/2/15/20	15/39/115/115	-
21	CL7	7	516	19	2/2/13/20	16/27/103/115	-
24	SQD	A	405	-	-	3/29/49/69	0/1/1/1
21	CL7	3	508	19	2/2/15/20	16/39/115/115	-
31	HEM	f	101	-	-	8/14/54/54	-
32	ZEX	6	520	-	-	6/29/67/67	0/2/2/2
32	ZEX	7	522	-	-	5/29/67/67	0/2/2/2
21	CL7	c	514	3	2/2/11/20	8/15/91/115	-
21	CL7	b	602	-	2/2/10/20	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LHG	a	406	-	-	5/50/50/53	-
21	CL7	3	506	19	2/2/11/20	13/15/91/115	-
21	CL7	B	607	-	2/2/14/20	11/33/109/115	-
23	8CT	C	519	-	-	8/29/63/63	0/2/2/2
21	CL7	7	518	19	2/2/11/20	7/15/91/115	-
21	CL7	3	503	-	2/2/15/20	20/39/115/115	-
30	PL9	d	407	-	-	9/53/73/73	0/1/1/1
21	CL7	5	408	-	2/2/15/20	16/39/115/115	-
24	SQD	B	620	-	-	5/49/69/69	0/1/1/1
26	LMG	5	401	-	-	5/46/66/70	0/1/1/1
22	PHO	A	402	-	-	3/37/103/103	0/5/6/6
25	LHG	4	401	-	-	8/53/53/53	-
21	CL7	6	504	-	2/2/11/20	6/15/91/115	-
21	CL7	6	502	16	2/2/15/20	17/39/115/115	-
21	CL7	B	606	2	2/2/13/20	5/27/103/115	-
21	CL7	3	513	-	2/2/11/20	9/15/91/115	-
21	CL7	8	410	20	2/2/11/20	9/15/91/115	-
21	CL7	B	614	2	2/2/14/20	14/33/109/115	-
21	CL7	c	510	3	2/2/15/20	20/39/115/115	-
21	CL7	4	408	20	2/2/11/20	4/15/91/115	-
21	CL7	5	414	18	2/2/10/20	3/10/86/115	-
21	CL7	5	410	-	2/2/15/20	17/39/115/115	-
21	CL7	5	415	-	2/2/10/20	7/10/86/115	-
21	CL7	B	602	2	2/2/14/20	9/33/109/115	-
21	CL7	b	613	2	2/2/15/20	17/39/115/115	-
21	CL7	5	409	18	2/2/11/20	6/15/91/115	-
21	CL7	5	405	-	2/2/11/20	10/15/91/115	-
21	CL7	D	405	4	2/2/11/20	8/15/91/115	-
21	CL7	C	507	3	2/2/14/20	15/33/109/115	-
21	CL7	7	505	19	2/2/15/20	14/39/115/115	-
21	CL7	b	607	2	2/2/13/20	5/27/103/115	-
24	SQD	2	524	-	-	0/36/56/69	0/1/1/1
21	CL7	B	622	2	2/2/11/20	8/15/91/115	-
21	CL7	b	617	2	2/2/11/20	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	6	518	16	2/2/15/20	12/39/115/115	-

All (4084) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	627	8CT	C02-C03	14.81	1.60	1.34
23	b	601	8CT	C02-C03	14.81	1.60	1.34
23	B	618	8CT	C02-C03	14.76	1.60	1.34
23	b	619	8CT	C02-C03	14.76	1.60	1.34
23	C	519	8CT	C02-C03	14.59	1.59	1.34
23	c	519	8CT	C02-C03	14.59	1.59	1.34
23	A	404	8CT	C02-C03	14.51	1.59	1.34
23	a	404	8CT	C02-C03	14.51	1.59	1.34
23	C	515	8CT	C02-C03	14.50	1.59	1.34
23	c	515	8CT	C02-C03	14.50	1.59	1.34
23	K	101	8CT	C02-C03	14.49	1.59	1.34
23	k	101	8CT	C02-C03	14.49	1.59	1.34
23	8	402	8CT	C02-C03	14.44	1.59	1.34
23	4	402	8CT	C02-C03	14.43	1.59	1.34
23	b	618	8CT	C02-C03	14.26	1.59	1.34
23	B	617	8CT	C02-C03	14.25	1.59	1.34
23	B	619	8CT	C02-C03	14.25	1.59	1.34
23	b	620	8CT	C02-C03	14.25	1.59	1.34
23	D	406	8CT	C02-C03	14.24	1.59	1.34
23	d	406	8CT	C02-C03	14.24	1.59	1.34
23	C	516	8CT	C02-C03	14.04	1.58	1.34
23	c	516	8CT	C02-C03	14.04	1.58	1.34
23	K	101	8CT	C32-C31	13.72	1.59	1.32
23	k	101	8CT	C32-C31	13.70	1.59	1.32
23	D	406	8CT	C32-C31	13.46	1.59	1.32
23	a	404	8CT	C32-C31	13.45	1.59	1.32
23	B	618	8CT	C32-C31	13.44	1.59	1.32
23	b	619	8CT	C32-C31	13.44	1.59	1.32
23	d	406	8CT	C32-C31	13.43	1.59	1.32
23	c	519	8CT	C32-C31	13.42	1.59	1.32
23	C	519	8CT	C32-C31	13.42	1.59	1.32
23	A	404	8CT	C32-C31	13.41	1.59	1.32
23	B	627	8CT	C32-C31	13.35	1.59	1.32
23	b	601	8CT	C32-C31	13.33	1.58	1.32
23	C	515	8CT	C32-C31	13.32	1.58	1.32
23	c	515	8CT	C32-C31	13.32	1.58	1.32
23	C	516	8CT	C32-C31	13.30	1.58	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	516	8CT	C32-C31	13.30	1.58	1.32
23	B	617	8CT	C32-C31	13.27	1.58	1.32
23	b	618	8CT	C32-C31	13.25	1.58	1.32
23	B	619	8CT	C32-C31	13.20	1.58	1.32
23	b	620	8CT	C32-C31	13.20	1.58	1.32
23	4	402	8CT	C32-C31	13.19	1.58	1.32
23	8	402	8CT	C32-C31	13.16	1.58	1.32
23	B	617	8CT	C34-C35	-9.92	1.33	1.54
23	b	618	8CT	C34-C35	-9.92	1.33	1.54
23	C	516	8CT	C34-C35	-9.78	1.34	1.54
23	c	516	8CT	C34-C35	-9.78	1.34	1.54
23	C	515	8CT	C34-C35	-9.74	1.34	1.54
23	c	515	8CT	C34-C35	-9.74	1.34	1.54
23	A	404	8CT	C34-C35	-9.53	1.34	1.54
23	a	404	8CT	C34-C35	-9.52	1.34	1.54
22	D	408	PHO	C1D-C2D	9.52	1.50	1.39
22	d	408	PHO	C1D-C2D	9.48	1.50	1.39
23	b	620	8CT	C34-C35	-9.37	1.34	1.54
23	C	519	8CT	C34-C35	-9.36	1.34	1.54
23	c	519	8CT	C34-C35	-9.36	1.34	1.54
23	K	101	8CT	C34-C35	-9.33	1.35	1.54
23	b	601	8CT	C34-C35	-9.33	1.35	1.54
23	B	619	8CT	C34-C35	-9.32	1.35	1.54
23	B	627	8CT	C34-C35	-9.31	1.35	1.54
23	k	101	8CT	C34-C35	-9.29	1.35	1.54
23	B	618	8CT	C34-C35	-9.27	1.35	1.54
23	b	619	8CT	C34-C35	-9.24	1.35	1.54
23	D	406	8CT	C34-C35	-9.19	1.35	1.54
23	d	406	8CT	C34-C35	-9.19	1.35	1.54
23	8	402	8CT	C34-C35	-9.19	1.35	1.54
23	4	402	8CT	C34-C35	-9.19	1.35	1.54
23	C	516	8CT	C04-C03	-7.99	1.42	1.53
23	c	516	8CT	C04-C03	-7.99	1.42	1.53
23	B	618	8CT	C04-C03	-7.92	1.42	1.53
23	b	619	8CT	C04-C03	-7.92	1.42	1.53
23	4	402	8CT	C04-C03	-7.70	1.43	1.53
23	8	402	8CT	C04-C03	-7.70	1.43	1.53
23	A	404	8CT	C04-C03	-7.63	1.43	1.53
23	a	404	8CT	C04-C03	-7.63	1.43	1.53
23	B	617	8CT	C04-C03	-7.63	1.43	1.53
23	b	618	8CT	C04-C03	-7.63	1.43	1.53
23	C	519	8CT	C04-C03	-7.62	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	519	8CT	C04-C03	-7.62	1.43	1.53
23	B	619	8CT	C04-C03	-7.49	1.43	1.53
23	b	620	8CT	C04-C03	-7.49	1.43	1.53
22	d	408	PHO	C1B-C2B	7.46	1.47	1.39
23	K	101	8CT	C04-C03	-7.45	1.43	1.53
23	k	101	8CT	C04-C03	-7.45	1.43	1.53
22	D	408	PHO	C1B-C2B	7.43	1.47	1.39
23	C	515	8CT	C04-C03	-7.27	1.43	1.53
23	c	515	8CT	C04-C03	-7.27	1.43	1.53
23	D	406	8CT	C04-C03	-7.01	1.44	1.53
23	d	406	8CT	C04-C03	-7.01	1.44	1.53
23	B	627	8CT	C04-C03	-6.80	1.44	1.53
23	b	601	8CT	C04-C03	-6.80	1.44	1.53
23	8	402	8CT	C05-C06	-6.76	1.35	1.52
23	4	402	8CT	C05-C06	-6.72	1.36	1.52
23	b	620	8CT	C05-C06	-6.57	1.36	1.52
23	B	619	8CT	C05-C06	-6.54	1.36	1.52
23	C	515	8CT	C05-C06	-6.53	1.36	1.52
23	c	515	8CT	C05-C06	-6.53	1.36	1.52
23	C	516	8CT	C05-C06	-6.51	1.36	1.52
23	c	516	8CT	C05-C06	-6.51	1.36	1.52
23	a	404	8CT	C05-C06	-6.50	1.36	1.52
23	A	404	8CT	C05-C06	-6.50	1.36	1.52
23	B	627	8CT	C05-C06	-6.48	1.36	1.52
23	b	601	8CT	C05-C06	-6.48	1.36	1.52
23	B	618	8CT	C05-C06	-6.48	1.36	1.52
23	b	619	8CT	C05-C06	-6.48	1.36	1.52
23	D	406	8CT	C05-C06	-6.47	1.36	1.52
23	d	406	8CT	C05-C06	-6.47	1.36	1.52
23	k	101	8CT	C05-C06	-6.45	1.36	1.52
23	B	617	8CT	C05-C06	-6.45	1.36	1.52
23	b	618	8CT	C05-C06	-6.45	1.36	1.52
23	K	101	8CT	C05-C06	-6.41	1.36	1.52
22	d	408	PHO	C4D-CHA	6.41	1.49	1.39
22	D	408	PHO	C4D-CHA	6.37	1.49	1.39
23	C	519	8CT	C05-C06	-6.33	1.36	1.52
23	c	519	8CT	C05-C06	-6.29	1.37	1.52
23	k	101	8CT	C15-C16	5.94	1.58	1.45
23	K	101	8CT	C15-C16	5.94	1.58	1.45
23	B	627	8CT	C15-C16	5.84	1.58	1.45
23	b	601	8CT	C15-C16	5.84	1.58	1.45
23	B	617	8CT	C15-C16	5.83	1.58	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	618	8CT	C15-C16	5.83	1.58	1.45
22	D	408	PHO	C3B-C2B	5.79	1.48	1.40
22	d	408	PHO	C3B-C2B	5.79	1.48	1.40
23	C	516	8CT	C15-C16	5.69	1.58	1.45
23	c	516	8CT	C15-C16	5.66	1.58	1.45
23	b	619	8CT	C15-C16	5.65	1.58	1.45
23	C	515	8CT	C15-C16	5.62	1.58	1.45
23	c	515	8CT	C15-C16	5.62	1.58	1.45
23	B	618	8CT	C15-C16	5.61	1.58	1.45
23	C	519	8CT	C15-C16	5.61	1.58	1.45
23	D	406	8CT	C15-C16	5.59	1.58	1.45
23	d	406	8CT	C15-C16	5.59	1.58	1.45
23	c	519	8CT	C15-C16	5.58	1.57	1.45
23	B	619	8CT	C15-C16	5.58	1.57	1.45
23	b	620	8CT	C15-C16	5.58	1.57	1.45
23	B	618	8CT	C11-C12	5.45	1.57	1.45
23	b	619	8CT	C11-C12	5.42	1.57	1.45
23	A	404	8CT	C15-C16	5.40	1.57	1.45
23	a	404	8CT	C15-C16	5.40	1.57	1.45
23	8	402	8CT	C34-C33	5.37	1.65	1.52
23	4	402	8CT	C34-C33	5.36	1.65	1.52
23	8	402	8CT	C15-C16	5.34	1.57	1.45
23	4	402	8CT	C15-C16	5.32	1.57	1.45
30	d	407	PL9	C3-C4	-5.29	1.40	1.49
23	B	627	8CT	C05-C04	5.29	1.66	1.54
23	b	601	8CT	C05-C04	5.29	1.66	1.54
23	K	101	8CT	C11-C12	5.27	1.57	1.45
23	k	101	8CT	C11-C12	5.27	1.57	1.45
30	D	407	PL9	C3-C4	-5.27	1.40	1.49
21	B	606	CL7	CHD-C4C	5.27	1.48	1.38
21	b	607	CL7	CHD-C4C	5.27	1.48	1.38
21	5	414	CL7	CHD-C4C	5.25	1.48	1.38
23	B	627	8CT	C35-C30	5.23	1.71	1.56
23	b	601	8CT	C35-C30	5.23	1.71	1.56
21	1	414	CL7	CHD-C4C	5.22	1.48	1.38
21	d	402	CL7	CHD-C4C	5.19	1.48	1.38
23	k	101	8CT	C05-C04	5.19	1.66	1.54
21	D	402	CL7	CHD-C4C	5.18	1.48	1.38
23	B	618	8CT	C34-C33	5.17	1.64	1.52
23	b	619	8CT	C34-C33	5.17	1.64	1.52
23	K	101	8CT	C05-C04	5.17	1.66	1.54
23	b	601	8CT	C11-C12	5.16	1.57	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	627	8CT	C11-C12	5.16	1.57	1.45
23	B	619	8CT	C34-C33	5.16	1.64	1.52
23	b	620	8CT	C34-C33	5.16	1.64	1.52
23	D	406	8CT	C34-C33	5.14	1.64	1.52
23	d	406	8CT	C34-C33	5.14	1.64	1.52
21	2	513	CL7	CHD-C4C	5.10	1.48	1.38
21	6	513	CL7	CHD-C4C	5.10	1.48	1.38
21	1	416	CL7	CHD-C4C	5.10	1.48	1.38
21	A	401	CL7	CHC-C1C	5.10	1.48	1.38
21	a	401	CL7	CHC-C1C	5.10	1.48	1.38
21	5	416	CL7	CHD-C4C	5.08	1.48	1.38
23	k	101	8CT	C35-C30	5.05	1.70	1.56
21	B	622	CL7	CHD-C4C	5.04	1.48	1.38
21	b	623	CL7	CHD-C4C	5.04	1.48	1.38
23	K	101	8CT	C35-C30	5.04	1.70	1.56
21	1	404	CL7	CHD-C4C	5.03	1.48	1.38
21	5	404	CL7	CHD-C4C	5.03	1.48	1.38
21	6	514	CL7	CHD-C4C	5.03	1.48	1.38
21	3	518	CL7	CHD-C4C	5.03	1.48	1.38
21	7	518	CL7	CHD-C4C	5.03	1.48	1.38
23	A	404	8CT	C34-C33	5.02	1.64	1.52
23	C	519	8CT	C11-C12	5.02	1.56	1.45
23	c	519	8CT	C11-C12	5.02	1.56	1.45
23	D	406	8CT	C05-C04	5.02	1.65	1.54
23	d	406	8CT	C05-C04	5.02	1.65	1.54
23	a	404	8CT	C34-C33	5.02	1.64	1.52
21	4	411	CL7	CHD-C4C	5.02	1.48	1.38
21	2	515	CL7	CHD-C4C	5.01	1.48	1.38
21	B	622	CL7	CHC-C1C	5.01	1.48	1.38
21	3	506	CL7	CHD-C4C	5.01	1.48	1.38
21	7	506	CL7	CHD-C4C	5.01	1.48	1.38
21	5	419	CL7	CHC-C1C	5.01	1.48	1.38
21	3	516	CL7	CHD-C4C	5.00	1.48	1.38
21	3	517	CL7	CHD-C4C	5.00	1.48	1.38
21	7	516	CL7	CHD-C4C	5.00	1.48	1.38
23	B	617	8CT	C05-C04	5.00	1.65	1.54
23	b	618	8CT	C05-C04	5.00	1.65	1.54
21	7	517	CL7	CHD-C4C	4.99	1.48	1.38
21	4	417	CL7	CHB-C1B	4.99	1.50	1.39
21	8	417	CL7	CHB-C1B	4.99	1.50	1.39
21	8	411	CL7	CHD-C4C	4.99	1.48	1.38
21	6	515	CL7	CHD-C4C	4.99	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	514	CL7	CHD-C4C	4.99	1.48	1.38
21	3	518	CL7	CHC-C1C	4.99	1.48	1.38
21	1	419	CL7	CHC-C1C	4.98	1.48	1.38
21	a	401	CL7	CHD-C4C	4.98	1.48	1.38
23	b	620	8CT	C05-C04	4.98	1.65	1.54
21	1	408	CL7	CHD-C4C	4.98	1.48	1.38
21	5	408	CL7	CHD-C4C	4.98	1.48	1.38
23	K	101	8CT	C14-C13	4.98	1.58	1.43
23	k	101	8CT	C14-C13	4.97	1.58	1.43
21	b	623	CL7	CHC-C1C	4.97	1.48	1.38
21	A	401	CL7	CHD-C4C	4.97	1.48	1.38
21	1	411	CL7	CHD-C4C	4.97	1.48	1.38
23	B	619	8CT	C05-C04	4.97	1.65	1.54
21	1	410	CL7	CHD-C4C	4.97	1.48	1.38
23	C	519	8CT	C05-C04	4.96	1.65	1.54
21	B	601	CL7	CHD-C4C	4.96	1.48	1.38
21	C	518	CL7	CHD-C4C	4.96	1.48	1.38
21	b	602	CL7	CHD-C4C	4.96	1.48	1.38
21	c	518	CL7	CHD-C4C	4.96	1.48	1.38
21	B	609	CL7	CHD-C4C	4.96	1.48	1.38
21	b	610	CL7	CHD-C4C	4.96	1.48	1.38
21	7	518	CL7	CHC-C1C	4.96	1.48	1.38
21	1	420	CL7	CHC-C1C	4.96	1.48	1.38
21	5	420	CL7	CHC-C1C	4.96	1.48	1.38
21	3	502	CL7	CHD-C4C	4.95	1.48	1.38
21	7	502	CL7	CHD-C4C	4.95	1.48	1.38
21	1	415	CL7	CHC-C1C	4.95	1.48	1.38
21	5	415	CL7	CHC-C1C	4.95	1.48	1.38
21	1	419	CL7	CHD-C4C	4.95	1.48	1.38
21	2	518	CL7	CHD-C4C	4.94	1.48	1.38
21	6	518	CL7	CHD-C4C	4.94	1.48	1.38
23	B	627	8CT	C34-C33	4.94	1.64	1.52
23	b	601	8CT	C34-C33	4.94	1.64	1.52
21	1	417	CL7	CHD-C4C	4.94	1.48	1.38
21	5	417	CL7	CHD-C4C	4.94	1.48	1.38
21	5	411	CL7	CHD-C4C	4.93	1.48	1.38
23	c	519	8CT	C05-C04	4.93	1.65	1.54
21	1	415	CL7	CHD-C4C	4.93	1.48	1.38
21	5	415	CL7	CHD-C4C	4.93	1.48	1.38
21	C	511	CL7	CHD-C4C	4.92	1.48	1.38
21	c	511	CL7	CHD-C4C	4.92	1.48	1.38
21	5	410	CL7	CHD-C4C	4.92	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	412	CL7	CHD-C4C	4.91	1.47	1.38
23	C	519	8CT	C34-C33	4.91	1.64	1.52
23	c	519	8CT	C34-C33	4.91	1.64	1.52
21	a	405	CL7	CHD-C4C	4.91	1.47	1.38
21	C	506	CL7	CHD-C4C	4.91	1.47	1.38
21	C	512	CL7	CHC-C1C	4.90	1.47	1.38
21	1	416	CL7	CHC-C1C	4.90	1.47	1.38
21	5	416	CL7	CHC-C1C	4.90	1.47	1.38
21	5	419	CL7	CHD-C4C	4.90	1.47	1.38
21	2	504	CL7	CHD-C4C	4.90	1.47	1.38
21	4	408	CL7	CHD-C4C	4.90	1.47	1.38
21	8	408	CL7	CHD-C4C	4.90	1.47	1.38
23	K	101	8CT	C28-C26	4.90	1.56	1.45
23	k	101	8CT	C28-C26	4.90	1.56	1.45
21	4	416	CL7	CHC-C1C	4.90	1.47	1.38
21	6	504	CL7	CHD-C4C	4.90	1.47	1.38
21	8	412	CL7	CHD-C4C	4.90	1.47	1.38
21	8	416	CL7	CHC-C1C	4.90	1.47	1.38
21	1	405	CL7	CHD-C4C	4.90	1.47	1.38
21	B	607	CL7	CHD-C4C	4.89	1.47	1.38
21	b	608	CL7	CHD-C4C	4.89	1.47	1.38
21	c	507	CL7	CHD-C4C	4.89	1.47	1.38
21	3	501	CL7	CHD-C4C	4.89	1.47	1.38
21	7	501	CL7	CHD-C4C	4.89	1.47	1.38
23	8	402	8CT	C05-C04	4.89	1.65	1.54
21	5	417	CL7	CHC-C1C	4.88	1.47	1.38
21	c	512	CL7	CHC-C1C	4.88	1.47	1.38
21	C	505	CL7	CHD-C4C	4.88	1.47	1.38
21	1	417	CL7	CHC-C1C	4.88	1.47	1.38
21	c	505	CL7	CHD-C4C	4.88	1.47	1.38
23	4	402	8CT	C05-C04	4.88	1.65	1.54
21	C	514	CL7	CHD-C4C	4.88	1.47	1.38
21	c	514	CL7	CHD-C4C	4.88	1.47	1.38
21	A	406	CL7	CHD-C4C	4.88	1.47	1.38
21	4	409	CL7	CHD-C4C	4.87	1.47	1.38
21	8	409	CL7	CHD-C4C	4.87	1.47	1.38
23	B	618	8CT	C05-C04	4.87	1.65	1.54
23	b	619	8CT	C05-C04	4.87	1.65	1.54
23	A	404	8CT	C05-C04	4.87	1.65	1.54
23	a	404	8CT	C05-C04	4.87	1.65	1.54
21	C	507	CL7	CHD-C4C	4.87	1.47	1.38
21	1	414	CL7	CHC-C1C	4.87	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	414	CL7	CHC-C1C	4.87	1.47	1.38
23	B	617	8CT	C11-C12	4.87	1.56	1.45
31	F	101	HEM	FE-NB	4.87	2.09	1.94
21	1	404	CL7	CHC-C1C	4.87	1.47	1.38
21	5	404	CL7	CHC-C1C	4.87	1.47	1.38
21	c	506	CL7	CHD-C4C	4.87	1.47	1.38
21	3	513	CL7	CHD-C4C	4.86	1.47	1.38
21	5	405	CL7	CHD-C4C	4.85	1.47	1.38
23	B	627	8CT	C14-C13	4.85	1.58	1.43
23	b	601	8CT	C14-C13	4.85	1.58	1.43
21	2	507	CL7	CHD-C4C	4.85	1.47	1.38
21	6	507	CL7	CHD-C4C	4.85	1.47	1.38
21	5	415	CL7	CHB-C1B	4.85	1.50	1.39
31	f	101	HEM	FE-NB	4.85	2.09	1.94
23	C	515	8CT	C05-C04	4.84	1.65	1.54
21	1	415	CL7	CHB-C1B	4.84	1.50	1.39
21	C	505	CL7	CHC-C1C	4.84	1.47	1.38
21	c	505	CL7	CHC-C1C	4.84	1.47	1.38
21	3	514	CL7	CHD-C4C	4.84	1.47	1.38
21	4	405	CL7	CHD-C4C	4.84	1.47	1.38
21	8	405	CL7	CHD-C4C	4.84	1.47	1.38
21	2	508	CL7	CHD-C4C	4.84	1.47	1.38
21	6	508	CL7	CHD-C4C	4.84	1.47	1.38
21	5	413	CL7	CHB-C1B	4.84	1.50	1.39
21	B	616	CL7	CHD-C4C	4.84	1.47	1.38
21	b	617	CL7	CHD-C4C	4.84	1.47	1.38
21	7	502	CL7	CHC-C1C	4.84	1.47	1.38
21	7	513	CL7	CHD-C4C	4.83	1.47	1.38
23	b	618	8CT	C11-C12	4.83	1.56	1.45
21	1	413	CL7	CHB-C1B	4.83	1.50	1.39
23	c	515	8CT	C05-C04	4.83	1.65	1.54
21	1	411	CL7	CHC-C1C	4.83	1.47	1.38
21	5	411	CL7	CHC-C1C	4.83	1.47	1.38
21	1	412	CL7	CHB-C1B	4.83	1.50	1.39
21	4	417	CL7	CHC-C1C	4.83	1.47	1.38
21	8	417	CL7	CHC-C1C	4.83	1.47	1.38
21	1	409	CL7	CHD-C4C	4.82	1.47	1.38
21	5	409	CL7	CHD-C4C	4.82	1.47	1.38
21	B	616	CL7	CHC-C1C	4.82	1.47	1.38
21	1	402	CL7	CHD-C4C	4.82	1.47	1.38
21	3	509	CL7	CHC-C1C	4.82	1.47	1.38
21	b	617	CL7	CHC-C1C	4.82	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	509	CL7	CHC-C1C	4.82	1.47	1.38
21	7	514	CL7	CHD-C4C	4.82	1.47	1.38
21	4	416	CL7	CHD-C4C	4.82	1.47	1.38
23	C	516	8CT	C05-C04	4.82	1.65	1.54
23	c	516	8CT	C05-C04	4.82	1.65	1.54
21	7	515	CL7	CHD-C4C	4.82	1.47	1.38
23	k	101	8CT	C34-C33	4.81	1.63	1.52
23	c	516	8CT	C14-C13	4.81	1.58	1.43
21	5	402	CL7	CHD-C4C	4.81	1.47	1.38
21	C	511	CL7	CHC-C1C	4.81	1.47	1.38
21	c	511	CL7	CHC-C1C	4.81	1.47	1.38
21	2	518	CL7	CHC-C1C	4.81	1.47	1.38
21	6	518	CL7	CHC-C1C	4.81	1.47	1.38
23	K	101	8CT	C34-C33	4.80	1.63	1.52
21	1	407	CL7	CHD-C4C	4.80	1.47	1.38
21	5	407	CL7	CHD-C4C	4.80	1.47	1.38
21	B	613	CL7	CHD-C4C	4.79	1.47	1.38
21	b	614	CL7	CHD-C4C	4.79	1.47	1.38
21	5	412	CL7	CHB-C1B	4.79	1.50	1.39
23	C	516	8CT	C14-C13	4.79	1.58	1.43
21	D	404	CL7	CHD-C4C	4.79	1.47	1.38
21	d	404	CL7	CHD-C4C	4.79	1.47	1.38
21	6	506	CL7	CHD-C4C	4.79	1.47	1.38
21	3	502	CL7	CHC-C1C	4.79	1.47	1.38
21	3	508	CL7	CHD-C4C	4.79	1.47	1.38
21	7	508	CL7	CHD-C4C	4.79	1.47	1.38
21	5	410	CL7	CHC-C1C	4.79	1.47	1.38
21	2	506	CL7	CHD-C4C	4.79	1.47	1.38
21	B	601	CL7	CHC-C1C	4.79	1.47	1.38
21	b	602	CL7	CHC-C1C	4.79	1.47	1.38
21	5	418	CL7	CHD-C4C	4.79	1.47	1.38
21	8	416	CL7	CHD-C4C	4.79	1.47	1.38
21	1	418	CL7	CHD-C4C	4.78	1.47	1.38
21	3	515	CL7	CHD-C4C	4.78	1.47	1.38
21	2	502	CL7	CHB-C1B	4.78	1.50	1.39
21	6	502	CL7	CHB-C1B	4.78	1.50	1.39
21	C	514	CL7	CHC-C1C	4.78	1.47	1.38
23	C	516	8CT	C11-C12	4.78	1.56	1.45
23	c	516	8CT	C11-C12	4.78	1.56	1.45
21	2	501	CL7	CHD-C4C	4.78	1.47	1.38
23	d	406	8CT	C14-C13	4.78	1.58	1.43
21	A	403	CL7	CHC-C1C	4.78	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	511	CL7	CHD-C4C	4.78	1.47	1.38
21	a	403	CL7	CHC-C1C	4.78	1.47	1.38
21	6	511	CL7	CHD-C4C	4.78	1.47	1.38
21	5	412	CL7	CHD-C4C	4.78	1.47	1.38
21	3	515	CL7	CHC-C1C	4.78	1.47	1.38
21	7	515	CL7	CHC-C1C	4.78	1.47	1.38
23	C	519	8CT	C35-C30	4.78	1.69	1.56
23	c	519	8CT	C35-C30	4.78	1.69	1.56
21	4	408	CL7	CHC-C1C	4.77	1.47	1.38
21	2	509	CL7	CHC-C1C	4.77	1.47	1.38
23	B	617	8CT	C14-C13	4.77	1.58	1.43
23	b	618	8CT	C14-C13	4.77	1.58	1.43
21	8	408	CL7	CHC-C1C	4.77	1.47	1.38
21	1	420	CL7	CHD-C4C	4.77	1.47	1.38
21	5	420	CL7	CHD-C4C	4.77	1.47	1.38
21	6	501	CL7	CHD-C4C	4.77	1.47	1.38
21	C	512	CL7	CHD-C4C	4.77	1.47	1.38
21	1	409	CL7	CHC-C1C	4.77	1.47	1.38
21	5	409	CL7	CHC-C1C	4.77	1.47	1.38
21	3	513	CL7	CHC-C1C	4.77	1.47	1.38
23	D	406	8CT	C11-C12	4.77	1.56	1.45
21	b	604	CL7	CHC-C1C	4.77	1.47	1.38
23	B	617	8CT	C35-C30	4.76	1.69	1.56
23	b	618	8CT	C35-C30	4.76	1.69	1.56
21	1	412	CL7	CHD-C4C	4.76	1.47	1.38
23	D	406	8CT	C14-C13	4.76	1.58	1.43
23	C	515	8CT	C34-C33	4.76	1.63	1.52
23	c	515	8CT	C34-C33	4.76	1.63	1.52
21	1	410	CL7	CHC-C1C	4.76	1.47	1.38
23	c	519	8CT	C14-C13	4.76	1.58	1.43
21	7	513	CL7	CHC-C1C	4.75	1.47	1.38
21	B	603	CL7	CHD-C4C	4.75	1.47	1.38
21	1	402	CL7	CHC-C1C	4.75	1.47	1.38
21	b	604	CL7	CHD-C4C	4.75	1.47	1.38
21	c	512	CL7	CHD-C4C	4.75	1.47	1.38
21	5	402	CL7	CHC-C1C	4.75	1.47	1.38
21	4	417	CL7	CHD-C4C	4.75	1.47	1.38
21	8	417	CL7	CHD-C4C	4.75	1.47	1.38
23	c	515	8CT	C11-C12	4.75	1.56	1.45
21	c	514	CL7	CHC-C1C	4.75	1.47	1.38
21	B	608	CL7	CHD-C4C	4.75	1.47	1.38
21	b	609	CL7	CHD-C4C	4.75	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	413	CL7	CHD-C4C	4.75	1.47	1.38
21	5	413	CL7	CHD-C4C	4.75	1.47	1.38
23	C	515	8CT	C35-C30	4.75	1.69	1.56
23	c	515	8CT	C35-C30	4.75	1.69	1.56
21	4	404	CL7	CHD-C4C	4.75	1.47	1.38
21	4	406	CL7	CHC-C1C	4.75	1.47	1.38
21	4	404	CL7	CHC-C1C	4.74	1.47	1.38
21	8	404	CL7	CHC-C1C	4.74	1.47	1.38
21	5	403	CL7	CHD-C4C	4.74	1.47	1.38
23	d	406	8CT	C11-C12	4.74	1.56	1.45
21	8	411	CL7	CHC-C1C	4.74	1.47	1.38
21	8	404	CL7	CHD-C4C	4.74	1.47	1.38
23	C	515	8CT	C11-C12	4.74	1.56	1.45
23	D	406	8CT	C35-C30	4.73	1.69	1.56
23	d	406	8CT	C35-C30	4.73	1.69	1.56
23	C	519	8CT	C14-C13	4.73	1.58	1.43
21	B	603	CL7	CHC-C1C	4.73	1.47	1.38
21	C	508	CL7	CHD-C4C	4.73	1.47	1.38
21	c	508	CL7	CHD-C4C	4.73	1.47	1.38
23	B	619	8CT	C11-C12	4.73	1.56	1.45
23	b	620	8CT	C11-C12	4.73	1.56	1.45
21	4	413	CL7	CHD-C4C	4.73	1.47	1.38
21	8	413	CL7	CHD-C4C	4.73	1.47	1.38
21	2	502	CL7	CHD-C4C	4.73	1.47	1.38
21	6	502	CL7	CHD-C4C	4.73	1.47	1.38
21	6	509	CL7	CHC-C1C	4.72	1.47	1.38
21	2	510	CL7	CHD-C4C	4.72	1.47	1.38
21	6	510	CL7	CHD-C4C	4.72	1.47	1.38
21	4	407	CL7	CHC-C1C	4.72	1.47	1.38
21	3	503	CL7	CHC-C1C	4.72	1.47	1.38
21	1	403	CL7	CHD-C4C	4.72	1.47	1.38
21	1	408	CL7	CHC-C1C	4.72	1.47	1.38
21	5	408	CL7	CHC-C1C	4.72	1.47	1.38
21	B	614	CL7	CHD-C4C	4.72	1.47	1.38
21	b	615	CL7	CHD-C4C	4.72	1.47	1.38
21	C	502	CL7	CHC-C1C	4.71	1.47	1.38
21	c	502	CL7	CHC-C1C	4.71	1.47	1.38
21	5	416	CL7	CHB-C1B	4.71	1.50	1.39
21	C	507	CL7	CHC-C1C	4.71	1.47	1.38
21	2	509	CL7	CHD-C4C	4.71	1.47	1.38
21	2	512	CL7	CHC-C1C	4.71	1.47	1.38
21	c	507	CL7	CHC-C1C	4.71	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	509	CL7	CHD-C4C	4.71	1.47	1.38
21	6	512	CL7	CHC-C1C	4.71	1.47	1.38
21	B	602	CL7	CHD-C4C	4.71	1.47	1.38
21	3	504	CL7	CHC-C1C	4.71	1.47	1.38
21	b	603	CL7	CHD-C4C	4.71	1.47	1.38
21	7	504	CL7	CHC-C1C	4.71	1.47	1.38
21	c	503	CL7	CHD-C4C	4.71	1.47	1.38
21	1	407	CL7	CHC-C1C	4.71	1.47	1.38
21	4	415	CL7	CHC-C1C	4.71	1.47	1.38
21	8	415	CL7	CHC-C1C	4.71	1.47	1.38
21	8	406	CL7	CHC-C1C	4.70	1.47	1.38
21	2	511	CL7	CHC-C1C	4.70	1.47	1.38
21	6	511	CL7	CHC-C1C	4.70	1.47	1.38
21	3	512	CL7	CHD-C4C	4.70	1.47	1.38
21	7	512	CL7	CHD-C4C	4.70	1.47	1.38
21	C	503	CL7	CHD-C4C	4.70	1.47	1.38
21	1	405	CL7	CHC-C1C	4.70	1.47	1.38
21	1	412	CL7	CHC-C1C	4.70	1.47	1.38
21	3	507	CL7	CHD-C4C	4.70	1.47	1.38
21	4	411	CL7	CHC-C1C	4.70	1.47	1.38
21	5	405	CL7	CHC-C1C	4.70	1.47	1.38
21	5	412	CL7	CHC-C1C	4.70	1.47	1.38
21	7	507	CL7	CHD-C4C	4.70	1.47	1.38
21	A	406	CL7	CHC-C1C	4.70	1.47	1.38
21	B	615	CL7	CHD-C4C	4.70	1.47	1.38
21	a	405	CL7	CHC-C1C	4.70	1.47	1.38
21	b	616	CL7	CHD-C4C	4.70	1.47	1.38
21	c	504	CL7	CHC-C1C	4.70	1.47	1.38
21	1	416	CL7	CHB-C1B	4.70	1.49	1.39
21	1	419	CL7	CHB-C1B	4.70	1.49	1.39
21	2	503	CL7	CHC-C1C	4.69	1.47	1.38
21	6	503	CL7	CHC-C1C	4.69	1.47	1.38
21	2	504	CL7	CHC-C1C	4.69	1.47	1.38
21	6	504	CL7	CHC-C1C	4.69	1.47	1.38
21	4	405	CL7	CHC-C1C	4.69	1.47	1.38
21	4	405	CL7	CHB-C1B	4.69	1.49	1.39
21	2	517	CL7	CHC-C1C	4.69	1.47	1.38
21	6	517	CL7	CHC-C1C	4.69	1.47	1.38
21	5	419	CL7	CHB-C1B	4.69	1.49	1.39
23	A	404	8CT	C11-C12	4.69	1.56	1.45
21	2	516	CL7	CHC-C1C	4.68	1.47	1.38
21	6	516	CL7	CHC-C1C	4.68	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	407	CL7	CHC-C1C	4.68	1.47	1.38
21	C	504	CL7	CHD-C4C	4.68	1.47	1.38
21	B	602	CL7	CHC-C1C	4.68	1.47	1.38
21	b	603	CL7	CHC-C1C	4.68	1.47	1.38
21	8	409	CL7	CHB-C1B	4.68	1.49	1.39
21	7	503	CL7	CHC-C1C	4.67	1.47	1.38
22	d	408	PHO	OBD-CAD	4.67	1.28	1.22
21	1	404	CL7	CHB-C1B	4.67	1.49	1.39
21	D	402	CL7	CHC-C1C	4.67	1.47	1.38
21	8	405	CL7	CHB-C1B	4.67	1.49	1.39
21	B	614	CL7	CHC-C1C	4.67	1.47	1.38
21	C	503	CL7	CHC-C1C	4.67	1.47	1.38
21	b	615	CL7	CHC-C1C	4.67	1.47	1.38
21	c	503	CL7	CHC-C1C	4.67	1.47	1.38
21	3	501	CL7	CHC-C1C	4.67	1.47	1.38
21	7	501	CL7	CHC-C1C	4.67	1.47	1.38
21	5	407	CL7	CHC-C1C	4.67	1.47	1.38
21	7	514	CL7	CHC-C1C	4.67	1.47	1.38
21	2	515	CL7	CHB-C1B	4.67	1.49	1.39
21	6	515	CL7	CHB-C1B	4.67	1.49	1.39
21	1	420	CL7	CHB-C1B	4.66	1.49	1.39
21	5	420	CL7	CHB-C1B	4.66	1.49	1.39
21	c	504	CL7	CHD-C4C	4.66	1.47	1.38
21	C	504	CL7	CHC-C1C	4.66	1.47	1.38
21	2	505	CL7	CHB-C1B	4.66	1.49	1.39
21	4	409	CL7	CHB-C1B	4.66	1.49	1.39
21	B	611	CL7	CHD-C4C	4.66	1.47	1.38
21	D	405	CL7	CHD-C4C	4.66	1.47	1.38
21	b	612	CL7	CHD-C4C	4.66	1.47	1.38
21	d	405	CL7	CHD-C4C	4.66	1.47	1.38
21	8	405	CL7	CHC-C1C	4.66	1.47	1.38
21	3	510	CL7	CHD-C4C	4.66	1.47	1.38
21	3	516	CL7	CHC-C1C	4.66	1.47	1.38
21	4	412	CL7	CHC-C1C	4.66	1.47	1.38
21	7	510	CL7	CHD-C4C	4.66	1.47	1.38
21	8	412	CL7	CHC-C1C	4.66	1.47	1.38
21	2	512	CL7	CHB-C1B	4.66	1.49	1.39
21	6	512	CL7	CHB-C1B	4.66	1.49	1.39
21	4	407	CL7	CHB-C1B	4.65	1.49	1.39
23	a	404	8CT	C11-C12	4.65	1.55	1.45
21	4	406	CL7	CHD-C4C	4.65	1.47	1.38
21	8	406	CL7	CHD-C4C	4.65	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	K	101	8CT	C24-C25	4.65	1.57	1.43
23	k	101	8CT	C24-C25	4.65	1.57	1.43
21	6	505	CL7	CHB-C1B	4.65	1.49	1.39
21	B	605	CL7	CHD-C4C	4.65	1.47	1.38
21	C	509	CL7	CHD-C4C	4.65	1.47	1.38
21	c	509	CL7	CHD-C4C	4.65	1.47	1.38
22	D	408	PHO	OBD-CAD	4.65	1.28	1.22
21	2	516	CL7	CHD-C4C	4.65	1.47	1.38
21	b	605	CL7	CHD-C4C	4.65	1.47	1.38
21	6	516	CL7	CHD-C4C	4.65	1.47	1.38
21	1	413	CL7	CHC-C1C	4.65	1.47	1.38
21	4	415	CL7	CHD-C4C	4.65	1.47	1.38
21	d	402	CL7	CHC-C1C	4.65	1.47	1.38
21	4	410	CL7	CHD-C4C	4.65	1.47	1.38
21	4	406	CL7	CHB-C1B	4.64	1.49	1.39
21	8	406	CL7	CHB-C1B	4.64	1.49	1.39
21	B	604	CL7	CHD-C4C	4.64	1.47	1.38
21	B	607	CL7	CHC-C1C	4.64	1.47	1.38
21	B	606	CL7	CHC-C1C	4.64	1.47	1.38
21	b	607	CL7	CHC-C1C	4.64	1.47	1.38
21	4	407	CL7	CHD-C4C	4.64	1.47	1.38
21	C	510	CL7	CHD-C4C	4.64	1.47	1.38
21	c	510	CL7	CHD-C4C	4.64	1.47	1.38
21	8	415	CL7	CHD-C4C	4.64	1.47	1.38
21	8	407	CL7	CHB-C1B	4.64	1.49	1.39
21	2	513	CL7	CHC-C1C	4.64	1.47	1.38
21	2	505	CL7	CHC-C1C	4.63	1.47	1.38
21	6	505	CL7	CHC-C1C	4.63	1.47	1.38
23	C	516	8CT	C34-C33	4.63	1.63	1.52
23	c	516	8CT	C34-C33	4.63	1.63	1.52
23	C	516	8CT	C24-C25	4.63	1.57	1.43
23	c	516	8CT	C24-C25	4.63	1.57	1.43
21	5	413	CL7	CHC-C1C	4.63	1.47	1.38
21	3	517	CL7	CHC-C1C	4.63	1.47	1.38
21	7	517	CL7	CHC-C1C	4.63	1.47	1.38
21	1	406	CL7	CHC-C1C	4.63	1.47	1.38
21	5	406	CL7	CHC-C1C	4.63	1.47	1.38
21	2	508	CL7	CHB-C1B	4.63	1.49	1.39
21	5	404	CL7	CHB-C1B	4.63	1.49	1.39
23	B	617	8CT	C34-C33	4.63	1.63	1.52
21	b	606	CL7	CHD-C4C	4.63	1.47	1.38
21	B	604	CL7	CHB-C1B	4.63	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	605	CL7	CHB-C1B	4.63	1.49	1.39
21	B	605	CL7	CHC-C1C	4.63	1.47	1.38
21	1	403	CL7	CHB-C1B	4.62	1.49	1.39
21	4	414	CL7	CHD-C4C	4.62	1.47	1.38
21	8	414	CL7	CHD-C4C	4.62	1.47	1.38
21	3	514	CL7	CHC-C1C	4.62	1.47	1.38
21	1	406	CL7	CHD-C4C	4.62	1.47	1.38
21	3	505	CL7	CHC-C1C	4.62	1.47	1.38
21	b	608	CL7	CHC-C1C	4.62	1.47	1.38
21	7	505	CL7	CHC-C1C	4.62	1.47	1.38
21	B	601	CL7	CHB-C1B	4.62	1.49	1.39
21	b	602	CL7	CHB-C1B	4.62	1.49	1.39
21	3	510	CL7	CHC-C1C	4.61	1.47	1.38
21	5	406	CL7	CHD-C4C	4.61	1.47	1.38
21	7	510	CL7	CHC-C1C	4.61	1.47	1.38
21	8	410	CL7	CHC-C1C	4.61	1.47	1.38
21	B	613	CL7	CHC-C1C	4.61	1.47	1.38
21	2	517	CL7	CHD-C4C	4.61	1.47	1.38
21	7	516	CL7	CHC-C1C	4.61	1.47	1.38
21	C	513	CL7	CHD-C4C	4.61	1.47	1.38
21	c	513	CL7	CHD-C4C	4.61	1.47	1.38
21	8	410	CL7	CHD-C4C	4.61	1.47	1.38
21	4	410	CL7	CHC-C1C	4.61	1.47	1.38
21	3	504	CL7	CHD-C4C	4.60	1.47	1.38
21	7	504	CL7	CHD-C4C	4.60	1.47	1.38
21	5	403	CL7	CHB-C1B	4.60	1.49	1.39
23	b	618	8CT	C34-C33	4.60	1.63	1.52
21	8	407	CL7	CHD-C4C	4.60	1.47	1.38
21	6	513	CL7	CHC-C1C	4.60	1.47	1.38
21	3	511	CL7	CHD-C4C	4.60	1.47	1.38
21	7	511	CL7	CHD-C4C	4.60	1.47	1.38
21	3	509	CL7	CHD-C4C	4.60	1.47	1.38
21	7	509	CL7	CHD-C4C	4.60	1.47	1.38
21	6	517	CL7	CHD-C4C	4.60	1.47	1.38
21	3	515	CL7	CHB-C1B	4.60	1.49	1.39
21	7	515	CL7	CHB-C1B	4.60	1.49	1.39
21	4	416	CL7	CHB-C1B	4.60	1.49	1.39
21	8	416	CL7	CHB-C1B	4.60	1.49	1.39
21	1	406	CL7	CHB-C1B	4.60	1.49	1.39
21	5	406	CL7	CHB-C1B	4.60	1.49	1.39
21	b	606	CL7	CHC-C1C	4.60	1.47	1.38
21	c	502	CL7	CHB-C1B	4.59	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	614	CL7	CHC-C1C	4.59	1.47	1.38
21	3	514	CL7	CHB-C1B	4.59	1.49	1.39
21	7	514	CL7	CHB-C1B	4.59	1.49	1.39
21	B	615	CL7	CHB-C1B	4.59	1.49	1.39
21	b	616	CL7	CHB-C1B	4.59	1.49	1.39
21	6	508	CL7	CHB-C1B	4.59	1.49	1.39
21	2	518	CL7	CHB-C1B	4.59	1.49	1.39
21	6	518	CL7	CHB-C1B	4.59	1.49	1.39
21	B	612	CL7	CHD-C4C	4.59	1.47	1.38
21	d	402	CL7	CHB-C1B	4.59	1.49	1.39
21	b	613	CL7	CHD-C4C	4.59	1.47	1.38
21	A	401	CL7	CHB-C1B	4.58	1.49	1.39
21	C	502	CL7	CHB-C1B	4.58	1.49	1.39
21	a	401	CL7	CHB-C1B	4.58	1.49	1.39
23	A	404	8CT	C14-C13	4.58	1.57	1.43
23	a	404	8CT	C14-C13	4.58	1.57	1.43
21	1	402	CL7	CHB-C1B	4.58	1.49	1.39
21	5	402	CL7	CHB-C1B	4.58	1.49	1.39
21	C	514	CL7	CHB-C1B	4.58	1.49	1.39
21	c	514	CL7	CHB-C1B	4.58	1.49	1.39
23	B	618	8CT	C35-C30	4.58	1.69	1.56
23	b	619	8CT	C35-C30	4.58	1.69	1.56
21	c	518	CL7	CHB-C1B	4.58	1.49	1.39
21	b	610	CL7	CHC-C1C	4.58	1.47	1.38
21	D	402	CL7	CHB-C1B	4.57	1.49	1.39
21	C	512	CL7	CHB-C1B	4.57	1.49	1.39
21	c	512	CL7	CHB-C1B	4.57	1.49	1.39
21	4	413	CL7	CHC-C1C	4.57	1.47	1.38
21	8	413	CL7	CHC-C1C	4.57	1.47	1.38
23	b	619	8CT	C14-C13	4.57	1.57	1.43
21	2	507	CL7	CHB-C1B	4.57	1.49	1.39
21	c	508	CL7	CHC-C1C	4.57	1.47	1.38
23	C	515	8CT	C14-C13	4.57	1.57	1.43
23	c	515	8CT	C14-C13	4.57	1.57	1.43
21	3	503	CL7	CHD-C4C	4.57	1.47	1.38
21	7	503	CL7	CHD-C4C	4.57	1.47	1.38
21	1	405	CL7	CHB-C1B	4.57	1.49	1.39
21	5	405	CL7	CHB-C1B	4.57	1.49	1.39
21	C	504	CL7	CHB-C1B	4.57	1.49	1.39
21	c	504	CL7	CHB-C1B	4.57	1.49	1.39
21	3	511	CL7	CHC-C1C	4.57	1.47	1.38
23	C	516	8CT	C35-C30	4.56	1.69	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	516	8CT	C35-C30	4.56	1.69	1.56
21	3	512	CL7	CHC-C1C	4.56	1.47	1.38
21	7	512	CL7	CHC-C1C	4.56	1.47	1.38
21	6	507	CL7	CHB-C1B	4.56	1.49	1.39
21	C	509	CL7	CHC-C1C	4.56	1.47	1.38
21	3	507	CL7	CHB-C1B	4.56	1.49	1.39
21	2	506	CL7	CHC-C1C	4.56	1.47	1.38
21	6	506	CL7	CHC-C1C	4.56	1.47	1.38
21	3	505	CL7	CHD-C4C	4.56	1.47	1.38
21	7	505	CL7	CHD-C4C	4.56	1.47	1.38
21	B	610	CL7	CHC-C1C	4.56	1.47	1.38
21	2	501	CL7	CHC-C1C	4.56	1.47	1.38
21	6	501	CL7	CHC-C1C	4.56	1.47	1.38
21	2	510	CL7	CHC-C1C	4.55	1.47	1.38
21	3	506	CL7	CHB-C1B	4.55	1.49	1.39
21	7	506	CL7	CHB-C1B	4.55	1.49	1.39
21	7	511	CL7	CHC-C1C	4.55	1.47	1.38
23	A	404	8CT	C35-C30	4.55	1.69	1.56
21	3	508	CL7	CHB-C1B	4.55	1.49	1.39
21	7	508	CL7	CHB-C1B	4.55	1.49	1.39
23	B	618	8CT	C14-C13	4.55	1.57	1.43
21	6	510	CL7	CHC-C1C	4.54	1.47	1.38
23	a	404	8CT	C35-C30	4.54	1.69	1.56
21	c	509	CL7	CHC-C1C	4.54	1.47	1.38
21	C	508	CL7	CHC-C1C	4.54	1.47	1.38
21	C	518	CL7	CHB-C1B	4.54	1.49	1.39
23	4	402	8CT	C14-C13	4.54	1.57	1.43
23	8	402	8CT	C14-C13	4.54	1.57	1.43
21	B	611	CL7	CHB-C1B	4.53	1.49	1.39
21	B	605	CL7	CHB-C1B	4.53	1.49	1.39
21	b	606	CL7	CHB-C1B	4.53	1.49	1.39
21	1	414	CL7	CHB-C1B	4.53	1.49	1.39
21	C	510	CL7	CHC-C1C	4.53	1.47	1.38
21	c	510	CL7	CHC-C1C	4.53	1.47	1.38
21	B	609	CL7	CHC-C1C	4.53	1.47	1.38
21	D	405	CL7	CHB-C1B	4.53	1.49	1.39
21	d	405	CL7	CHB-C1B	4.53	1.49	1.39
21	7	507	CL7	CHB-C1B	4.53	1.49	1.39
21	4	410	CL7	CHB-C1B	4.52	1.49	1.39
21	b	612	CL7	CHB-C1B	4.52	1.49	1.39
21	8	410	CL7	CHB-C1B	4.52	1.49	1.39
21	5	418	CL7	CHC-C1C	4.52	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	4	402	8CT	C35-C30	4.52	1.69	1.56
23	8	402	8CT	C35-C30	4.52	1.69	1.56
21	2	515	CL7	CHC-C1C	4.52	1.47	1.38
21	6	515	CL7	CHC-C1C	4.52	1.47	1.38
21	5	414	CL7	CHB-C1B	4.52	1.49	1.39
21	B	610	CL7	CHD-C4C	4.52	1.47	1.38
21	b	611	CL7	CHC-C1C	4.52	1.47	1.38
21	2	505	CL7	CHD-C4C	4.52	1.47	1.38
21	4	414	CL7	CHB-C1B	4.52	1.49	1.39
21	8	414	CL7	CHB-C1B	4.52	1.49	1.39
21	a	403	CL7	CHD-C4C	4.52	1.47	1.38
21	2	516	CL7	CHB-C1B	4.52	1.49	1.39
21	6	516	CL7	CHB-C1B	4.52	1.49	1.39
21	b	611	CL7	CHD-C4C	4.52	1.47	1.38
21	6	506	CL7	CHB-C1B	4.52	1.49	1.39
21	3	503	CL7	CHB-C1B	4.52	1.49	1.39
21	7	503	CL7	CHB-C1B	4.52	1.49	1.39
21	5	411	CL7	CHB-C1B	4.51	1.49	1.39
21	4	408	CL7	CHB-C1B	4.51	1.49	1.39
21	8	408	CL7	CHB-C1B	4.51	1.49	1.39
21	B	608	CL7	CHC-C1C	4.51	1.47	1.38
21	b	609	CL7	CHC-C1C	4.51	1.47	1.38
21	A	403	CL7	CHD-C4C	4.51	1.47	1.38
21	6	503	CL7	CHD-C4C	4.51	1.47	1.38
23	k	101	8CT	C18-C17	4.51	1.57	1.43
21	A	406	CL7	CHB-C1B	4.51	1.49	1.39
21	1	409	CL7	CHB-C1B	4.51	1.49	1.39
21	5	409	CL7	CHB-C1B	4.51	1.49	1.39
21	3	505	CL7	CHB-C1B	4.51	1.49	1.39
21	7	505	CL7	CHB-C1B	4.51	1.49	1.39
23	b	620	8CT	C14-C13	4.51	1.57	1.43
21	B	608	CL7	CHB-C1B	4.50	1.49	1.39
21	2	511	CL7	CHB-C1B	4.50	1.49	1.39
21	6	511	CL7	CHB-C1B	4.50	1.49	1.39
21	b	609	CL7	CHB-C1B	4.50	1.49	1.39
21	1	403	CL7	CHC-C1C	4.50	1.47	1.38
21	5	403	CL7	CHC-C1C	4.50	1.47	1.38
21	C	509	CL7	CHB-C1B	4.50	1.49	1.39
21	2	514	CL7	CHB-C1B	4.50	1.49	1.39
21	c	509	CL7	CHB-C1B	4.50	1.49	1.39
21	6	514	CL7	CHB-C1B	4.50	1.49	1.39
23	B	619	8CT	C14-C13	4.50	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	411	CL7	CHB-C1B	4.49	1.49	1.39
21	c	513	CL7	CHB-C1B	4.49	1.49	1.39
21	C	513	CL7	CHB-C1B	4.49	1.49	1.39
21	1	408	CL7	CHB-C1B	4.49	1.49	1.39
21	5	408	CL7	CHB-C1B	4.49	1.49	1.39
21	4	414	CL7	CHC-C1C	4.49	1.47	1.38
21	C	506	CL7	CHC-C1C	4.49	1.47	1.38
21	c	506	CL7	CHC-C1C	4.49	1.47	1.38
23	K	101	8CT	C18-C17	4.49	1.57	1.43
21	1	418	CL7	CHB-C1B	4.48	1.49	1.39
21	6	505	CL7	CHD-C4C	4.48	1.47	1.38
21	2	513	CL7	CHB-C1B	4.48	1.49	1.39
21	6	513	CL7	CHB-C1B	4.48	1.49	1.39
21	C	506	CL7	CHB-C1B	4.48	1.49	1.39
21	c	506	CL7	CHB-C1B	4.48	1.49	1.39
21	1	418	CL7	CHC-C1C	4.48	1.47	1.38
21	4	415	CL7	CHB-C1B	4.48	1.49	1.39
21	8	415	CL7	CHB-C1B	4.48	1.49	1.39
23	B	627	8CT	C24-C25	4.48	1.57	1.43
23	b	601	8CT	C24-C25	4.48	1.57	1.43
21	B	602	CL7	CHB-C1B	4.48	1.49	1.39
21	b	603	CL7	CHB-C1B	4.48	1.49	1.39
21	2	506	CL7	CHB-C1B	4.48	1.49	1.39
21	5	418	CL7	CHB-C1B	4.47	1.49	1.39
21	a	401	CL7	O2D-CGD	4.47	1.44	1.33
21	2	502	CL7	CHC-C1C	4.46	1.47	1.38
21	2	503	CL7	CHD-C4C	4.46	1.47	1.38
21	6	502	CL7	CHC-C1C	4.46	1.47	1.38
21	2	517	CL7	CHB-C1B	4.46	1.49	1.39
21	6	517	CL7	CHB-C1B	4.46	1.49	1.39
21	a	405	CL7	CHB-C1B	4.46	1.49	1.39
21	C	505	CL7	CHB-C1B	4.46	1.49	1.39
21	c	505	CL7	CHB-C1B	4.46	1.49	1.39
21	3	501	CL7	CHB-C1B	4.46	1.49	1.39
21	7	501	CL7	CHB-C1B	4.46	1.49	1.39
21	4	412	CL7	CHB-C1B	4.46	1.49	1.39
21	8	412	CL7	CHB-C1B	4.46	1.49	1.39
21	C	513	CL7	CHC-C1C	4.46	1.47	1.38
21	c	513	CL7	CHC-C1C	4.46	1.47	1.38
21	c	502	CL7	CHD-C4C	4.46	1.47	1.38
21	A	401	CL7	O2D-CGD	4.46	1.44	1.33
23	4	402	8CT	C11-C12	4.45	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	8	402	8CT	C11-C12	4.45	1.55	1.45
21	D	404	CL7	CHB-C1B	4.45	1.49	1.39
21	d	404	CL7	CHB-C1B	4.45	1.49	1.39
21	2	514	CL7	CHC-C1C	4.45	1.47	1.38
21	C	503	CL7	CHB-C1B	4.45	1.49	1.39
21	c	503	CL7	CHB-C1B	4.45	1.49	1.39
21	c	511	CL7	CHB-C1B	4.45	1.49	1.39
21	b	610	CL7	CHB-C1B	4.45	1.49	1.39
21	3	518	CL7	CHB-C1B	4.45	1.49	1.39
21	7	518	CL7	CHB-C1B	4.45	1.49	1.39
21	C	518	CL7	CHC-C1C	4.45	1.47	1.38
21	c	518	CL7	CHC-C1C	4.45	1.47	1.38
21	D	405	CL7	CHC-C1C	4.45	1.47	1.38
21	d	405	CL7	CHC-C1C	4.45	1.47	1.38
23	D	406	8CT	C24-C25	4.45	1.57	1.43
23	d	406	8CT	C24-C25	4.45	1.57	1.43
21	3	508	CL7	CHC-C1C	4.44	1.47	1.38
21	7	508	CL7	CHC-C1C	4.44	1.47	1.38
21	8	414	CL7	CHC-C1C	4.44	1.47	1.38
21	6	514	CL7	CHC-C1C	4.44	1.47	1.38
21	3	513	CL7	CHB-C1B	4.44	1.49	1.39
21	7	513	CL7	CHB-C1B	4.44	1.49	1.39
21	3	504	CL7	CHB-C1B	4.43	1.49	1.39
21	7	504	CL7	CHB-C1B	4.43	1.49	1.39
21	C	502	CL7	CHD-C4C	4.43	1.47	1.38
21	2	504	CL7	CHB-C1B	4.43	1.49	1.39
21	6	504	CL7	CHB-C1B	4.43	1.49	1.39
21	2	503	CL7	CHB-C1B	4.43	1.49	1.39
21	6	503	CL7	CHB-C1B	4.43	1.49	1.39
21	C	511	CL7	CHB-C1B	4.43	1.49	1.39
21	4	409	CL7	CHC-C1C	4.43	1.47	1.38
21	8	409	CL7	CHC-C1C	4.43	1.47	1.38
21	B	610	CL7	CHB-C1B	4.43	1.49	1.39
21	B	609	CL7	CHB-C1B	4.43	1.49	1.39
21	2	510	CL7	CHB-C1B	4.42	1.49	1.39
21	6	510	CL7	CHB-C1B	4.42	1.49	1.39
23	B	619	8CT	C35-C30	4.42	1.68	1.56
23	b	620	8CT	C35-C30	4.42	1.68	1.56
21	1	407	CL7	CHB-C1B	4.42	1.49	1.39
21	1	410	CL7	CHB-C1B	4.42	1.49	1.39
21	2	509	CL7	CHB-C1B	4.41	1.49	1.39
21	6	509	CL7	CHB-C1B	4.41	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	519	8CT	C24-C25	4.41	1.57	1.43
23	c	519	8CT	C24-C25	4.41	1.57	1.43
21	b	617	CL7	CHB-C1B	4.41	1.49	1.39
21	A	403	CL7	CHB-C1B	4.41	1.49	1.39
21	a	403	CL7	CHB-C1B	4.41	1.49	1.39
21	5	407	CL7	CHB-C1B	4.41	1.49	1.39
21	2	507	CL7	CHC-C1C	4.41	1.46	1.38
21	6	507	CL7	CHC-C1C	4.41	1.46	1.38
21	b	611	CL7	CHB-C1B	4.40	1.49	1.39
21	3	516	CL7	CHB-C1B	4.40	1.49	1.39
21	7	516	CL7	CHB-C1B	4.40	1.49	1.39
21	7	507	CL7	CHC-C1C	4.40	1.46	1.38
23	D	406	8CT	C28-C26	4.40	1.55	1.45
23	d	406	8CT	C28-C26	4.40	1.55	1.45
21	C	507	CL7	CHB-C1B	4.40	1.49	1.39
21	c	507	CL7	CHB-C1B	4.40	1.49	1.39
21	3	507	CL7	CHC-C1C	4.39	1.46	1.38
21	C	510	CL7	CHB-C1B	4.39	1.49	1.39
21	c	510	CL7	CHB-C1B	4.39	1.49	1.39
21	2	501	CL7	CHB-C1B	4.39	1.49	1.39
21	6	501	CL7	CHB-C1B	4.39	1.49	1.39
21	B	616	CL7	CHB-C1B	4.38	1.49	1.39
21	3	509	CL7	CHB-C1B	4.38	1.49	1.39
21	5	410	CL7	CHB-C1B	4.38	1.49	1.39
21	2	508	CL7	CHC-C1C	4.38	1.46	1.38
21	6	508	CL7	CHC-C1C	4.38	1.46	1.38
21	2	512	CL7	CHD-C4C	4.37	1.46	1.38
21	6	512	CL7	CHD-C4C	4.37	1.46	1.38
21	3	511	CL7	CHB-C1B	4.37	1.49	1.39
21	1	417	CL7	CHB-C1B	4.36	1.49	1.39
21	5	417	CL7	CHB-C1B	4.36	1.49	1.39
21	D	404	CL7	CHC-C1C	4.36	1.46	1.38
21	d	404	CL7	CHC-C1C	4.36	1.46	1.38
21	3	512	CL7	CHB-C1B	4.36	1.49	1.39
23	B	627	8CT	C18-C17	4.36	1.57	1.43
23	b	601	8CT	C18-C17	4.36	1.57	1.43
21	7	509	CL7	CHB-C1B	4.36	1.49	1.39
21	B	611	CL7	CHC-C1C	4.35	1.46	1.38
21	b	612	CL7	CHC-C1C	4.35	1.46	1.38
21	4	413	CL7	CHB-C1B	4.35	1.49	1.39
21	8	413	CL7	CHB-C1B	4.35	1.49	1.39
21	7	517	CL7	CHB-C1B	4.35	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	404	CL7	CHB-C1B	4.34	1.49	1.39
21	8	404	CL7	CHB-C1B	4.34	1.49	1.39
21	3	517	CL7	CHB-C1B	4.34	1.49	1.39
21	7	511	CL7	CHB-C1B	4.33	1.49	1.39
21	B	622	CL7	CHB-C1B	4.33	1.49	1.39
21	b	623	CL7	CHB-C1B	4.33	1.49	1.39
21	b	613	CL7	CHB-C1B	4.33	1.49	1.39
21	7	502	CL7	CHB-C1B	4.32	1.49	1.39
21	7	510	CL7	CHB-C1B	4.32	1.49	1.39
23	a	404	8CT	C24-C25	4.32	1.56	1.43
21	B	604	CL7	CHC-C1C	4.32	1.46	1.38
21	b	605	CL7	CHC-C1C	4.32	1.46	1.38
21	7	512	CL7	CHB-C1B	4.32	1.49	1.39
21	B	612	CL7	CHB-C1B	4.32	1.49	1.39
23	A	404	8CT	C24-C25	4.31	1.56	1.43
23	4	402	8CT	C24-C25	4.31	1.56	1.43
23	8	402	8CT	C24-C25	4.31	1.56	1.43
23	C	515	8CT	C24-C25	4.31	1.56	1.43
23	c	515	8CT	C24-C25	4.31	1.56	1.43
21	3	510	CL7	CHB-C1B	4.30	1.49	1.39
21	B	607	CL7	CHB-C1B	4.29	1.49	1.39
21	b	608	CL7	CHB-C1B	4.29	1.49	1.39
23	C	516	8CT	C28-C26	4.29	1.55	1.45
23	B	619	8CT	C24-C25	4.29	1.56	1.43
23	b	620	8CT	C24-C25	4.29	1.56	1.43
23	B	618	8CT	C28-C26	4.28	1.55	1.45
23	b	619	8CT	C28-C26	4.28	1.55	1.45
21	B	603	CL7	CHB-C1B	4.28	1.49	1.39
23	B	618	8CT	C24-C25	4.27	1.56	1.43
23	b	619	8CT	C24-C25	4.27	1.56	1.43
23	c	516	8CT	C18-C17	4.27	1.56	1.43
21	3	502	CL7	CHB-C1B	4.27	1.49	1.39
21	B	612	CL7	CHC-C1C	4.26	1.46	1.38
21	b	613	CL7	CHC-C1C	4.26	1.46	1.38
21	b	604	CL7	CHB-C1B	4.26	1.49	1.39
23	C	516	8CT	C18-C17	4.26	1.56	1.43
23	c	516	8CT	C28-C26	4.25	1.55	1.45
23	B	627	8CT	C28-C26	4.24	1.55	1.45
23	b	601	8CT	C28-C26	4.24	1.55	1.45
23	B	617	8CT	C24-C25	4.24	1.56	1.43
23	b	618	8CT	C24-C25	4.24	1.56	1.43
21	C	508	CL7	CHB-C1B	4.24	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	c	508	CL7	CHB-C1B	4.24	1.48	1.39
21	B	606	CL7	CHB-C1B	4.23	1.48	1.39
21	b	607	CL7	CHB-C1B	4.23	1.48	1.39
21	B	613	CL7	CHB-C1B	4.22	1.48	1.39
21	b	614	CL7	CHB-C1B	4.22	1.48	1.39
23	D	406	8CT	C18-C17	4.22	1.56	1.43
23	B	618	8CT	C18-C17	4.20	1.56	1.43
23	b	619	8CT	C18-C17	4.20	1.56	1.43
23	d	406	8CT	C18-C17	4.20	1.56	1.43
23	8	402	8CT	C28-C26	4.19	1.54	1.45
21	B	614	CL7	CHB-C1B	4.19	1.48	1.39
21	b	615	CL7	CHB-C1B	4.19	1.48	1.39
21	7	506	CL7	CHC-C1C	4.18	1.46	1.38
23	C	519	8CT	C28-C26	4.18	1.54	1.45
23	c	519	8CT	C28-C26	4.18	1.54	1.45
21	3	506	CL7	CHC-C1C	4.18	1.46	1.38
23	C	515	8CT	C28-C26	4.18	1.54	1.45
23	c	515	8CT	C28-C26	4.18	1.54	1.45
23	4	402	8CT	C28-C26	4.18	1.54	1.45
23	B	617	8CT	C18-C17	4.17	1.56	1.43
23	b	618	8CT	C18-C17	4.17	1.56	1.43
23	c	519	8CT	C18-C17	4.16	1.56	1.43
23	c	515	8CT	C18-C17	4.14	1.56	1.43
23	C	515	8CT	C18-C17	4.14	1.56	1.43
21	B	615	CL7	CHC-C1C	4.14	1.46	1.38
21	b	616	CL7	CHC-C1C	4.14	1.46	1.38
23	C	519	8CT	C18-C17	4.14	1.56	1.43
26	C	501	LMG	O8-C28	4.14	1.45	1.33
22	d	408	PHO	C3B-C4B	4.12	1.46	1.41
23	a	404	8CT	C18-C17	4.11	1.56	1.43
23	B	617	8CT	C28-C26	4.11	1.54	1.45
23	b	618	8CT	C28-C26	4.11	1.54	1.45
23	C	519	8CT	C06-C07	4.11	1.65	1.52
23	c	519	8CT	C06-C07	4.11	1.65	1.52
23	B	619	8CT	C28-C26	4.11	1.54	1.45
23	b	620	8CT	C28-C26	4.11	1.54	1.45
23	A	404	8CT	C28-C26	4.10	1.54	1.45
23	a	404	8CT	C28-C26	4.10	1.54	1.45
23	A	404	8CT	C18-C17	4.09	1.56	1.43
23	4	402	8CT	C18-C17	4.09	1.56	1.43
23	8	402	8CT	C18-C17	4.09	1.56	1.43
22	D	408	PHO	C3B-C4B	4.08	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	501	LMG	O8-C28	4.07	1.45	1.33
27	B	624	DGD	O1G-C1A	4.07	1.45	1.33
27	b	625	DGD	O1G-C1A	4.07	1.45	1.33
23	b	620	8CT	C18-C17	4.04	1.56	1.43
23	B	619	8CT	C18-C17	4.03	1.55	1.43
27	c	517	DGD	O1G-C1A	4.00	1.45	1.33
27	C	517	DGD	O2G-C1B	3.99	1.45	1.34
27	c	517	DGD	O2G-C1B	3.99	1.45	1.34
27	C	517	DGD	O1G-C1A	3.98	1.45	1.33
23	A	404	8CT	C06-C07	3.96	1.64	1.52
22	d	408	PHO	C3D-C4D	-3.95	1.35	1.41
23	a	404	8CT	C06-C07	3.95	1.64	1.52
21	b	603	CL7	O2A-CGA	3.93	1.44	1.33
23	b	618	8CT	C06-C07	3.93	1.64	1.52
22	D	408	PHO	C3D-C4D	-3.92	1.35	1.41
22	D	408	PHO	C3D-C2D	3.92	1.46	1.39
21	4	411	CL7	CHB-C1B	3.91	1.48	1.39
21	8	411	CL7	CHB-C1B	3.91	1.48	1.39
22	d	408	PHO	C3D-C2D	3.91	1.46	1.39
23	c	516	8CT	C06-C07	3.91	1.64	1.52
21	B	602	CL7	O2A-CGA	3.91	1.44	1.33
23	C	516	8CT	C06-C07	3.91	1.64	1.52
23	K	101	8CT	C23-C21	3.90	1.54	1.45
23	B	617	8CT	C06-C07	3.90	1.64	1.52
23	B	618	8CT	C06-C07	3.88	1.64	1.52
23	k	101	8CT	C23-C21	3.88	1.54	1.45
23	B	627	8CT	C06-C07	3.87	1.64	1.52
23	b	601	8CT	C06-C07	3.87	1.64	1.52
22	d	408	PHO	C3C-C2C	3.87	1.44	1.36
23	C	516	8CT	C23-C21	3.87	1.54	1.45
23	c	516	8CT	C23-C21	3.87	1.54	1.45
23	D	406	8CT	C06-C07	3.86	1.64	1.52
23	d	406	8CT	C06-C07	3.86	1.64	1.52
23	b	619	8CT	C06-C07	3.86	1.64	1.52
22	D	408	PHO	C3C-C2C	3.86	1.44	1.36
21	A	401	CL7	O2A-CGA	3.85	1.44	1.33
21	a	401	CL7	O2A-CGA	3.85	1.44	1.33
22	d	408	PHO	O2D-CGD	3.85	1.42	1.33
23	K	101	8CT	C06-C07	3.85	1.64	1.52
23	k	101	8CT	C06-C07	3.85	1.64	1.52
22	D	408	PHO	O2D-CGD	3.84	1.42	1.33
23	b	620	8CT	C06-C07	3.83	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	401	CL7	C2A-C1A	3.82	1.56	1.50
21	a	401	CL7	C2A-C1A	3.82	1.56	1.50
26	C	501	LMG	O7-C10	3.81	1.45	1.34
23	4	402	8CT	C06-C07	3.80	1.64	1.52
23	8	402	8CT	C06-C07	3.80	1.64	1.52
23	c	515	8CT	C06-C07	3.80	1.64	1.52
31	f	101	HEM	FE-NC	3.79	2.08	1.95
21	C	505	CL7	C2A-C1A	3.79	1.56	1.50
23	B	619	8CT	C06-C07	3.79	1.64	1.52
23	b	601	8CT	C23-C21	3.78	1.54	1.45
23	C	515	8CT	C06-C07	3.78	1.64	1.52
26	c	501	LMG	O7-C10	3.77	1.44	1.34
31	F	101	HEM	FE-NC	3.77	2.07	1.95
23	B	627	8CT	C23-C21	3.77	1.54	1.45
31	F	101	HEM	C1B-NB	-3.76	1.33	1.40
31	f	101	HEM	C1B-NB	-3.76	1.33	1.40
23	d	406	8CT	C23-C21	3.74	1.54	1.45
21	c	505	CL7	C2A-C1A	3.73	1.56	1.50
23	4	402	8CT	C23-C21	3.72	1.53	1.45
23	8	402	8CT	C23-C21	3.72	1.53	1.45
27	B	624	DGD	O2G-C1B	3.71	1.44	1.34
23	D	406	8CT	C23-C21	3.71	1.53	1.45
31	f	101	HEM	C4D-ND	-3.69	1.33	1.40
27	b	625	DGD	O2G-C1B	3.68	1.44	1.34
31	F	101	HEM	C4D-ND	-3.68	1.34	1.40
21	1	411	CL7	O2A-CGA	3.68	1.43	1.30
21	5	411	CL7	O2A-CGA	3.67	1.43	1.30
21	1	420	CL7	O2A-CGA	3.63	1.42	1.30
21	5	420	CL7	O2A-CGA	3.63	1.42	1.30
21	5	402	CL7	C2A-C1A	3.62	1.56	1.50
21	b	623	CL7	O2A-CGA	3.61	1.42	1.30
21	3	518	CL7	O2A-CGA	3.61	1.42	1.30
21	1	419	CL7	O2A-CGA	3.60	1.42	1.30
21	5	419	CL7	O2A-CGA	3.60	1.42	1.30
21	7	518	CL7	O2A-CGA	3.60	1.42	1.30
21	1	412	CL7	O2A-CGA	3.60	1.42	1.30
21	5	412	CL7	O2A-CGA	3.60	1.42	1.30
21	1	402	CL7	C2A-C1A	3.59	1.56	1.50
21	B	614	CL7	O2A-CGA	3.59	1.43	1.33
21	b	615	CL7	O2A-CGA	3.59	1.43	1.33
21	2	515	CL7	O2A-CGA	3.59	1.42	1.30
21	6	515	CL7	O2A-CGA	3.59	1.42	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	622	CL7	O2A-CGA	3.59	1.42	1.30
21	2	514	CL7	O2A-CGA	3.58	1.42	1.30
21	6	514	CL7	O2A-CGA	3.58	1.42	1.30
21	2	508	CL7	O2A-CGA	3.58	1.42	1.30
23	C	519	8CT	C23-C21	3.58	1.53	1.45
23	c	519	8CT	C23-C21	3.58	1.53	1.45
21	7	514	CL7	O2A-CGA	3.57	1.42	1.30
21	3	513	CL7	O2A-CGA	3.57	1.42	1.30
21	7	513	CL7	O2A-CGA	3.57	1.42	1.30
21	1	405	CL7	O2A-CGA	3.57	1.42	1.30
21	5	405	CL7	O2A-CGA	3.57	1.42	1.30
21	4	408	CL7	O2A-CGA	3.56	1.42	1.30
21	8	408	CL7	O2A-CGA	3.56	1.42	1.30
21	6	508	CL7	O2A-CGA	3.56	1.42	1.30
21	3	514	CL7	O2A-CGA	3.56	1.42	1.30
23	C	515	8CT	C23-C21	3.55	1.53	1.45
23	c	515	8CT	C23-C21	3.55	1.53	1.45
21	2	504	CL7	O2A-CGA	3.54	1.42	1.30
21	6	504	CL7	O2A-CGA	3.54	1.42	1.30
21	1	409	CL7	O2A-CGA	3.53	1.42	1.30
21	5	409	CL7	O2A-CGA	3.53	1.42	1.30
21	B	616	CL7	O2A-CGA	3.53	1.42	1.30
21	4	410	CL7	O2A-CGA	3.53	1.42	1.30
21	8	410	CL7	O2A-CGA	3.53	1.42	1.30
23	A	404	8CT	C23-C21	3.52	1.53	1.45
23	a	404	8CT	C23-C21	3.52	1.53	1.45
21	4	417	CL7	O2D-CGD	3.52	1.41	1.33
21	D	405	CL7	O2A-CGA	3.52	1.42	1.30
21	d	405	CL7	O2A-CGA	3.52	1.42	1.30
21	b	617	CL7	O2A-CGA	3.51	1.42	1.30
21	A	403	CL7	O2A-CGA	3.51	1.43	1.33
21	a	403	CL7	O2A-CGA	3.51	1.43	1.33
21	1	419	CL7	O2D-CGD	3.50	1.41	1.33
21	5	419	CL7	O2D-CGD	3.50	1.41	1.33
21	8	417	CL7	O2D-CGD	3.50	1.41	1.33
21	C	514	CL7	O2A-CGA	3.50	1.42	1.30
21	c	514	CL7	O2A-CGA	3.50	1.42	1.30
21	4	415	CL7	O2A-CGA	3.49	1.42	1.30
21	8	415	CL7	O2A-CGA	3.49	1.42	1.30
21	3	514	CL7	C2A-C1A	3.49	1.56	1.50
21	7	514	CL7	C2A-C1A	3.49	1.56	1.50
21	1	412	CL7	C2A-C1A	3.48	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	408	CL7	C2A-C1A	3.47	1.56	1.50
21	8	408	CL7	C2A-C1A	3.47	1.56	1.50
21	3	506	CL7	O2A-CGA	3.47	1.42	1.30
21	5	412	CL7	C2A-C1A	3.47	1.56	1.50
21	B	614	CL7	C2A-C1A	3.46	1.56	1.50
21	b	615	CL7	C2A-C1A	3.46	1.56	1.50
21	5	415	CL7	O2D-CGD	3.46	1.41	1.33
21	4	416	CL7	O2D-CGD	3.46	1.41	1.33
21	8	416	CL7	O2D-CGD	3.46	1.41	1.33
21	1	416	CL7	O2D-CGD	3.45	1.41	1.33
21	5	416	CL7	O2D-CGD	3.45	1.41	1.33
21	7	506	CL7	O2A-CGA	3.45	1.42	1.30
21	1	415	CL7	O2D-CGD	3.44	1.41	1.33
21	1	411	CL7	O2D-CGD	3.44	1.41	1.33
21	5	411	CL7	O2D-CGD	3.44	1.41	1.33
21	C	509	CL7	O2A-CGA	3.44	1.43	1.33
21	c	509	CL7	O2A-CGA	3.44	1.43	1.33
21	2	513	CL7	O2A-CGA	3.44	1.42	1.30
21	7	513	CL7	C2A-C1A	3.43	1.56	1.50
21	6	513	CL7	O2A-CGA	3.42	1.42	1.30
21	6	512	CL7	C4C-C3C	-3.42	1.39	1.45
23	b	620	8CT	C23-C21	3.41	1.53	1.45
23	B	619	8CT	C23-C21	3.41	1.53	1.45
21	1	407	CL7	O2D-CGD	3.41	1.41	1.33
21	2	512	CL7	C4C-C3C	-3.40	1.39	1.45
32	4	420	ZEX	C21-C26	-3.40	1.49	1.53
23	B	618	8CT	C23-C21	3.40	1.53	1.45
23	b	619	8CT	C23-C21	3.40	1.53	1.45
21	B	601	CL7	O2D-CGD	3.39	1.41	1.33
21	3	513	CL7	C2A-C1A	3.39	1.55	1.50
21	b	602	CL7	O2D-CGD	3.38	1.41	1.33
21	1	412	CL7	O2D-CGD	3.38	1.41	1.33
21	5	407	CL7	O2D-CGD	3.38	1.41	1.33
21	5	412	CL7	O2D-CGD	3.38	1.41	1.33
21	5	402	CL7	O2A-CGA	3.38	1.43	1.33
21	3	518	CL7	O2D-CGD	3.37	1.41	1.33
21	7	518	CL7	O2D-CGD	3.37	1.41	1.33
21	1	402	CL7	O2A-CGA	3.36	1.43	1.33
21	C	514	CL7	O2D-CGD	3.36	1.41	1.33
21	5	417	CL7	O2A-CGA	3.36	1.43	1.33
32	8	420	ZEX	C21-C26	-3.36	1.49	1.53
21	c	514	CL7	O2D-CGD	3.36	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	514	CL7	O2D-CGD	3.36	1.41	1.33
21	6	514	CL7	O2D-CGD	3.36	1.41	1.33
21	1	417	CL7	O2A-CGA	3.35	1.43	1.33
21	3	506	CL7	C2A-C1A	3.35	1.55	1.50
21	7	506	CL7	C2A-C1A	3.35	1.55	1.50
21	1	414	CL7	O2D-CGD	3.35	1.41	1.33
21	5	414	CL7	O2D-CGD	3.35	1.41	1.33
21	4	413	CL7	C2A-C1A	3.33	1.55	1.50
21	c	505	CL7	O2D-CGD	3.33	1.41	1.33
21	B	612	CL7	C4C-C3C	-3.33	1.39	1.45
21	b	613	CL7	C4C-C3C	-3.33	1.39	1.45
21	1	413	CL7	O2D-CGD	3.33	1.41	1.33
21	C	505	CL7	O2D-CGD	3.32	1.41	1.33
21	2	511	CL7	O2A-CGA	3.32	1.43	1.33
21	6	511	CL7	O2A-CGA	3.32	1.43	1.33
21	7	512	CL7	C2A-C1A	3.32	1.55	1.50
21	3	517	CL7	O2D-CGD	3.32	1.41	1.33
21	7	517	CL7	O2D-CGD	3.32	1.41	1.33
21	5	420	CL7	O2D-CGD	3.31	1.41	1.33
21	3	512	CL7	O2A-CGA	3.31	1.43	1.33
21	7	512	CL7	O2A-CGA	3.31	1.43	1.33
21	B	622	CL7	O2D-CGD	3.31	1.41	1.33
21	b	623	CL7	O2D-CGD	3.31	1.41	1.33
21	4	405	CL7	O2A-CGA	3.31	1.43	1.33
21	8	405	CL7	O2A-CGA	3.31	1.43	1.33
21	2	501	CL7	O2D-CGD	3.31	1.41	1.33
21	6	501	CL7	O2D-CGD	3.31	1.41	1.33
21	3	510	CL7	O2D-CGD	3.31	1.41	1.33
21	7	510	CL7	O2D-CGD	3.31	1.41	1.33
21	2	518	CL7	O2A-CGA	3.30	1.43	1.33
21	6	518	CL7	O2A-CGA	3.30	1.43	1.33
21	4	409	CL7	C2A-C1A	3.30	1.55	1.50
21	8	409	CL7	C2A-C1A	3.30	1.55	1.50
21	1	402	CL7	O2D-CGD	3.30	1.41	1.33
21	5	402	CL7	O2D-CGD	3.30	1.41	1.33
21	1	410	CL7	O2D-CGD	3.30	1.41	1.33
21	5	410	CL7	O2D-CGD	3.30	1.41	1.33
21	4	404	CL7	O2A-CGA	3.30	1.43	1.33
21	8	404	CL7	O2A-CGA	3.30	1.43	1.33
21	6	510	CL7	O2D-CGD	3.30	1.41	1.33
21	5	413	CL7	O2D-CGD	3.30	1.41	1.33
21	8	413	CL7	O2D-CGD	3.30	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	413	CL7	O2D-CGD	3.29	1.41	1.33
21	3	503	CL7	C4C-C3C	-3.29	1.39	1.45
21	7	503	CL7	C4C-C3C	-3.29	1.39	1.45
21	3	512	CL7	C2A-C1A	3.29	1.55	1.50
21	2	506	CL7	O2D-CGD	3.29	1.41	1.33
21	1	420	CL7	O2D-CGD	3.29	1.41	1.33
21	C	503	CL7	O2D-CGD	3.29	1.41	1.33
21	c	503	CL7	O2D-CGD	3.29	1.41	1.33
21	6	506	CL7	O2D-CGD	3.29	1.41	1.33
21	8	413	CL7	C2A-C1A	3.29	1.55	1.50
21	6	505	CL7	C4C-C3C	-3.29	1.39	1.45
21	C	505	CL7	O2A-CGA	3.29	1.42	1.33
21	c	505	CL7	O2A-CGA	3.29	1.42	1.33
21	5	410	CL7	O2A-CGA	3.28	1.42	1.33
21	2	510	CL7	O2D-CGD	3.28	1.41	1.33
21	3	515	CL7	O2D-CGD	3.28	1.41	1.33
21	7	515	CL7	O2D-CGD	3.28	1.41	1.33
21	D	402	CL7	O2D-CGD	3.28	1.41	1.33
21	d	402	CL7	O2D-CGD	3.28	1.41	1.33
21	1	418	CL7	C4C-C3C	-3.28	1.39	1.45
21	5	418	CL7	C4C-C3C	-3.28	1.39	1.45
21	5	404	CL7	O2D-CGD	3.28	1.41	1.33
21	1	410	CL7	O2A-CGA	3.28	1.42	1.33
21	6	507	CL7	O2A-CGA	3.28	1.42	1.33
21	4	406	CL7	O2A-CGA	3.28	1.42	1.33
21	6	502	CL7	O2A-CGA	3.28	1.42	1.33
21	8	406	CL7	O2A-CGA	3.28	1.42	1.33
21	1	409	CL7	O2D-CGD	3.27	1.41	1.33
21	5	409	CL7	O2D-CGD	3.27	1.41	1.33
21	2	511	CL7	C2A-C1A	3.27	1.55	1.50
21	6	511	CL7	C2A-C1A	3.27	1.55	1.50
21	c	512	CL7	O2D-CGD	3.27	1.41	1.33
21	1	410	CL7	C2A-C1A	3.27	1.55	1.50
21	5	410	CL7	C2A-C1A	3.27	1.55	1.50
21	2	505	CL7	C4C-C3C	-3.27	1.39	1.45
21	4	404	CL7	O2D-CGD	3.27	1.41	1.33
21	8	404	CL7	O2D-CGD	3.27	1.41	1.33
21	C	504	CL7	O2A-CGA	3.26	1.42	1.33
21	c	504	CL7	O2A-CGA	3.26	1.42	1.33
21	8	406	CL7	C2A-C1A	3.26	1.55	1.50
21	3	518	CL7	C2A-C1A	3.26	1.55	1.50
21	7	518	CL7	C2A-C1A	3.26	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	502	CL7	O2A-CGA	3.26	1.42	1.33
21	1	405	CL7	O2D-CGD	3.26	1.41	1.33
21	5	405	CL7	O2D-CGD	3.26	1.41	1.33
23	B	617	8CT	C23-C21	3.26	1.52	1.45
23	b	618	8CT	C23-C21	3.26	1.52	1.45
21	2	507	CL7	O2A-CGA	3.26	1.42	1.33
21	C	512	CL7	O2D-CGD	3.26	1.41	1.33
21	3	509	CL7	O2D-CGD	3.26	1.41	1.33
21	4	407	CL7	O2D-CGD	3.26	1.41	1.33
21	7	509	CL7	O2D-CGD	3.26	1.41	1.33
21	8	407	CL7	O2D-CGD	3.26	1.41	1.33
32	2	523	ZEX	C1-C6	-3.26	1.49	1.53
32	6	522	ZEX	C1-C6	-3.26	1.49	1.53
21	D	402	CL7	C2A-C1A	3.25	1.55	1.50
21	d	402	CL7	C2A-C1A	3.25	1.55	1.50
21	C	511	CL7	O2D-CGD	3.25	1.41	1.33
21	c	511	CL7	O2D-CGD	3.25	1.41	1.33
21	2	513	CL7	C2A-C1A	3.25	1.55	1.50
21	3	504	CL7	C2A-C1A	3.25	1.55	1.50
21	7	504	CL7	C2A-C1A	3.25	1.55	1.50
21	1	404	CL7	O2D-CGD	3.25	1.41	1.33
21	2	511	CL7	O2D-CGD	3.25	1.41	1.33
21	6	511	CL7	O2D-CGD	3.25	1.41	1.33
21	6	513	CL7	C2A-C1A	3.25	1.55	1.50
21	1	420	CL7	C2A-C1A	3.24	1.55	1.50
21	2	504	CL7	O2D-CGD	3.24	1.41	1.33
21	6	504	CL7	O2D-CGD	3.24	1.41	1.33
21	c	511	CL7	O2A-CGA	3.24	1.42	1.33
21	2	517	CL7	O2A-CGA	3.24	1.42	1.33
21	6	517	CL7	O2A-CGA	3.23	1.42	1.33
21	4	405	CL7	O2D-CGD	3.23	1.41	1.33
21	8	405	CL7	O2D-CGD	3.23	1.41	1.33
21	C	511	CL7	O2A-CGA	3.23	1.42	1.33
21	2	518	CL7	O2D-CGD	3.23	1.41	1.33
21	6	518	CL7	O2D-CGD	3.23	1.41	1.33
21	C	503	CL7	O2A-CGA	3.23	1.42	1.33
21	c	503	CL7	O2A-CGA	3.23	1.42	1.33
21	3	506	CL7	O2D-CGD	3.23	1.41	1.33
21	7	506	CL7	O2D-CGD	3.23	1.41	1.33
21	C	508	CL7	C4C-C3C	-3.23	1.39	1.45
21	4	410	CL7	C2A-C1A	3.23	1.55	1.50
21	6	505	CL7	O2D-CGD	3.23	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	505	CL7	O2D-CGD	3.23	1.41	1.33
21	2	506	CL7	O2A-CGA	3.22	1.42	1.33
21	6	506	CL7	O2A-CGA	3.22	1.42	1.33
21	A	406	CL7	C4C-C3C	-3.22	1.39	1.45
21	a	405	CL7	C4C-C3C	-3.22	1.39	1.45
21	3	517	CL7	O2A-CGA	3.22	1.42	1.33
21	7	517	CL7	O2A-CGA	3.22	1.42	1.33
21	B	613	CL7	C4C-C3C	-3.22	1.39	1.45
21	b	614	CL7	C4C-C3C	-3.22	1.39	1.45
21	C	502	CL7	O2A-CGA	3.22	1.42	1.33
21	c	502	CL7	O2A-CGA	3.22	1.42	1.33
21	5	420	CL7	C2A-C1A	3.22	1.55	1.50
21	3	501	CL7	O2D-CGD	3.22	1.41	1.33
21	7	501	CL7	O2D-CGD	3.22	1.41	1.33
21	B	607	CL7	C4C-C3C	-3.21	1.39	1.45
21	b	608	CL7	C4C-C3C	-3.21	1.39	1.45
21	6	511	CL7	C4C-C3C	-3.21	1.39	1.45
21	5	419	CL7	C2A-C1A	3.21	1.55	1.50
21	B	622	CL7	C2A-C1A	3.21	1.55	1.50
21	b	623	CL7	C2A-C1A	3.21	1.55	1.50
21	B	610	CL7	O2A-CGA	3.21	1.42	1.33
21	b	611	CL7	O2A-CGA	3.21	1.42	1.33
21	C	506	CL7	O2D-CGD	3.21	1.41	1.33
21	c	506	CL7	O2D-CGD	3.21	1.41	1.33
21	2	503	CL7	C4C-C3C	-3.21	1.39	1.45
21	6	503	CL7	C4C-C3C	-3.21	1.39	1.45
21	2	511	CL7	C4C-C3C	-3.21	1.39	1.45
21	1	408	CL7	O2D-CGD	3.21	1.41	1.33
21	1	403	CL7	C2A-C1A	3.20	1.55	1.50
21	4	413	CL7	O2A-CGA	3.20	1.42	1.33
21	2	515	CL7	O2D-CGD	3.20	1.41	1.33
21	6	515	CL7	O2D-CGD	3.20	1.41	1.33
21	4	406	CL7	C2A-C1A	3.20	1.55	1.50
21	7	508	CL7	O2A-CGA	3.20	1.42	1.33
21	2	509	CL7	O2D-CGD	3.20	1.41	1.33
21	6	509	CL7	O2D-CGD	3.20	1.41	1.33
21	B	609	CL7	O2D-CGD	3.20	1.41	1.33
21	b	610	CL7	O2D-CGD	3.20	1.41	1.33
21	1	406	CL7	O2D-CGD	3.20	1.41	1.33
21	5	406	CL7	O2D-CGD	3.20	1.41	1.33
21	6	516	CL7	O2A-CGA	3.20	1.42	1.33
21	2	501	CL7	C2A-C1A	3.20	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	501	CL7	C2A-C1A	3.20	1.55	1.50
21	B	604	CL7	C4C-C3C	-3.20	1.39	1.45
21	b	605	CL7	C4C-C3C	-3.20	1.39	1.45
21	3	516	CL7	O2A-CGA	3.20	1.42	1.33
21	7	516	CL7	O2A-CGA	3.20	1.42	1.33
21	4	412	CL7	O2A-CGA	3.20	1.42	1.33
21	2	516	CL7	O2A-CGA	3.20	1.42	1.33
21	2	508	CL7	O2D-CGD	3.20	1.41	1.33
21	6	508	CL7	O2D-CGD	3.20	1.41	1.33
21	3	514	CL7	O2D-CGD	3.20	1.41	1.33
21	7	514	CL7	O2D-CGD	3.19	1.41	1.33
21	2	503	CL7	C2A-C1A	3.19	1.55	1.50
21	6	503	CL7	C2A-C1A	3.19	1.55	1.50
23	B	619	8CT	C07-C02	-3.19	1.44	1.51
23	b	620	8CT	C07-C02	-3.19	1.44	1.51
23	c	515	8CT	C07-C02	-3.19	1.44	1.51
21	C	518	CL7	O2D-CGD	3.19	1.41	1.33
21	2	513	CL7	O2D-CGD	3.19	1.41	1.33
21	6	513	CL7	O2D-CGD	3.19	1.41	1.33
21	5	408	CL7	O2D-CGD	3.19	1.41	1.33
21	B	610	CL7	C4C-C3C	-3.19	1.39	1.45
21	b	611	CL7	C4C-C3C	-3.19	1.39	1.45
21	c	508	CL7	C4C-C3C	-3.19	1.39	1.45
21	1	403	CL7	O2D-CGD	3.19	1.41	1.33
21	5	403	CL7	O2D-CGD	3.19	1.41	1.33
21	3	508	CL7	O2A-CGA	3.19	1.42	1.33
21	3	504	CL7	C4C-C3C	-3.19	1.39	1.45
21	7	504	CL7	C4C-C3C	-3.19	1.39	1.45
21	8	413	CL7	O2A-CGA	3.19	1.42	1.33
21	5	403	CL7	C2A-C1A	3.19	1.55	1.50
21	8	410	CL7	C2A-C1A	3.19	1.55	1.50
32	2	520	ZEX	C1-C6	-3.18	1.49	1.53
21	D	402	CL7	O2A-CGA	3.18	1.42	1.33
21	d	402	CL7	O2A-CGA	3.18	1.42	1.33
21	B	615	CL7	O2A-CGA	3.18	1.42	1.33
21	b	616	CL7	O2A-CGA	3.18	1.42	1.33
21	C	510	CL7	O2D-CGD	3.18	1.41	1.33
21	3	502	CL7	C2A-C1A	3.18	1.55	1.50
21	1	403	CL7	O2A-CGA	3.18	1.42	1.33
21	B	615	CL7	O2D-CGD	3.18	1.41	1.33
21	b	616	CL7	O2D-CGD	3.18	1.41	1.33
21	B	614	CL7	O2D-CGD	3.18	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	615	CL7	O2D-CGD	3.18	1.41	1.33
21	8	412	CL7	O2A-CGA	3.18	1.42	1.33
21	1	419	CL7	C2A-C1A	3.18	1.55	1.50
21	4	414	CL7	O2A-CGA	3.18	1.42	1.33
21	8	414	CL7	O2A-CGA	3.18	1.42	1.33
21	4	411	CL7	O2D-CGD	3.18	1.41	1.33
21	c	518	CL7	O2D-CGD	3.17	1.40	1.33
21	7	507	CL7	O2A-CGA	3.17	1.42	1.33
21	8	411	CL7	O2D-CGD	3.17	1.40	1.33
21	4	412	CL7	C4C-C3C	-3.16	1.39	1.45
21	8	412	CL7	C4C-C3C	-3.16	1.39	1.45
21	3	502	CL7	O2A-CGA	3.16	1.42	1.33
21	7	502	CL7	O2A-CGA	3.16	1.42	1.33
21	C	502	CL7	C4C-C3C	-3.16	1.39	1.45
21	B	608	CL7	O2A-CGA	3.16	1.42	1.33
21	b	609	CL7	O2A-CGA	3.16	1.42	1.33
21	B	605	CL7	O2D-CGD	3.16	1.40	1.33
21	1	408	CL7	O2A-CGA	3.16	1.42	1.33
21	5	408	CL7	O2A-CGA	3.16	1.42	1.33
21	5	403	CL7	O2A-CGA	3.16	1.42	1.33
21	A	406	CL7	O2D-CGD	3.16	1.40	1.33
21	a	405	CL7	O2D-CGD	3.16	1.40	1.33
21	3	507	CL7	O2A-CGA	3.16	1.42	1.33
21	1	406	CL7	O2A-CGA	3.16	1.42	1.33
21	5	406	CL7	O2A-CGA	3.16	1.42	1.33
23	C	515	8CT	C07-C02	-3.15	1.44	1.51
21	3	510	CL7	O2A-CGA	3.15	1.42	1.33
21	7	510	CL7	O2A-CGA	3.15	1.42	1.33
21	c	510	CL7	O2D-CGD	3.15	1.40	1.33
23	B	617	8CT	C07-C02	-3.15	1.44	1.51
23	b	618	8CT	C07-C02	-3.15	1.44	1.51
23	B	627	8CT	C19-C20	3.15	1.53	1.43
23	b	601	8CT	C19-C20	3.15	1.53	1.43
21	2	512	CL7	O2A-CGA	3.15	1.42	1.33
21	6	512	CL7	O2A-CGA	3.15	1.42	1.33
21	B	605	CL7	C4C-C3C	-3.15	1.39	1.45
21	b	606	CL7	C4C-C3C	-3.15	1.39	1.45
21	b	609	CL7	O2D-CGD	3.15	1.40	1.33
21	3	504	CL7	O2D-CGD	3.15	1.40	1.33
21	7	504	CL7	O2D-CGD	3.15	1.40	1.33
21	b	606	CL7	O2D-CGD	3.15	1.40	1.33
21	2	516	CL7	O2D-CGD	3.15	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	4	419	ZEX	C21-C26	-3.15	1.49	1.53
21	B	608	CL7	O2D-CGD	3.15	1.40	1.33
21	c	502	CL7	C4C-C3C	-3.14	1.39	1.45
21	c	506	CL7	O2A-CGA	3.14	1.42	1.33
21	C	506	CL7	O2A-CGA	3.14	1.42	1.33
21	2	514	CL7	C2A-C1A	3.14	1.55	1.50
21	1	404	CL7	O2A-CGA	3.14	1.42	1.33
21	4	414	CL7	C4C-C3C	-3.14	1.39	1.45
21	8	414	CL7	C4C-C3C	-3.14	1.39	1.45
21	5	417	CL7	O2D-CGD	3.13	1.40	1.33
21	5	404	CL7	O2A-CGA	3.13	1.42	1.33
21	C	504	CL7	O2D-CGD	3.13	1.40	1.33
21	c	504	CL7	O2D-CGD	3.13	1.40	1.33
21	B	602	CL7	O2D-CGD	3.13	1.40	1.33
21	7	502	CL7	C2A-C1A	3.13	1.55	1.50
21	B	607	CL7	O2A-CGA	3.13	1.42	1.33
21	b	608	CL7	O2A-CGA	3.13	1.42	1.33
21	3	510	CL7	C4C-C3C	-3.13	1.39	1.45
21	7	510	CL7	C4C-C3C	-3.13	1.39	1.45
21	1	417	CL7	O2D-CGD	3.13	1.40	1.33
21	6	516	CL7	O2D-CGD	3.13	1.40	1.33
32	3	525	ZEX	C1-C6	-3.13	1.49	1.53
21	1	418	CL7	O2A-CGA	3.13	1.42	1.33
21	5	418	CL7	O2A-CGA	3.13	1.42	1.33
21	B	614	CL7	C4C-C3C	-3.12	1.39	1.45
21	b	615	CL7	C4C-C3C	-3.12	1.39	1.45
21	7	501	CL7	C4C-C3C	-3.12	1.39	1.45
21	3	513	CL7	O2D-CGD	3.12	1.40	1.33
21	7	513	CL7	O2D-CGD	3.12	1.40	1.33
21	C	510	CL7	C4C-C3C	-3.12	1.39	1.45
21	c	510	CL7	C4C-C3C	-3.12	1.39	1.45
21	4	410	CL7	O2D-CGD	3.12	1.40	1.33
21	4	414	CL7	O2D-CGD	3.12	1.40	1.33
21	8	410	CL7	O2D-CGD	3.12	1.40	1.33
21	8	414	CL7	O2D-CGD	3.12	1.40	1.33
21	B	610	CL7	C4C-NC	-3.12	1.34	1.37
21	b	611	CL7	C4C-NC	-3.12	1.34	1.37
21	B	603	CL7	O2D-CGD	3.12	1.40	1.33
21	b	604	CL7	O2D-CGD	3.12	1.40	1.33
21	4	409	CL7	O2A-CGA	3.11	1.42	1.33
32	8	419	ZEX	C21-C26	-3.11	1.49	1.53
21	2	504	CL7	C2A-C1A	3.11	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	512	CL7	C2A-C1A	3.11	1.55	1.50
21	6	504	CL7	C2A-C1A	3.11	1.55	1.50
21	6	512	CL7	C2A-C1A	3.11	1.55	1.50
21	3	511	CL7	C4C-C3C	-3.11	1.39	1.45
21	7	511	CL7	C4C-C3C	-3.11	1.39	1.45
23	K	101	8CT	C19-C20	3.11	1.53	1.43
23	k	101	8CT	C19-C20	3.11	1.53	1.43
21	8	409	CL7	O2A-CGA	3.11	1.42	1.33
21	6	514	CL7	C2A-C1A	3.11	1.55	1.50
21	2	518	CL7	C2A-C1A	3.10	1.55	1.50
23	4	402	8CT	C07-C02	-3.10	1.44	1.51
23	8	402	8CT	C07-C02	-3.10	1.44	1.51
21	3	511	CL7	O2D-CGD	3.10	1.40	1.33
21	7	511	CL7	O2D-CGD	3.10	1.40	1.33
21	3	501	CL7	C4C-C3C	-3.10	1.39	1.45
21	b	612	CL7	C4C-C3C	-3.10	1.39	1.45
23	K	101	8CT	C07-C02	-3.10	1.44	1.51
23	k	101	8CT	C07-C02	-3.10	1.44	1.51
21	b	603	CL7	O2D-CGD	3.10	1.40	1.33
21	B	610	CL7	O2D-CGD	3.10	1.40	1.33
21	b	612	CL7	C4C-NC	-3.09	1.34	1.37
21	B	616	CL7	O2D-CGD	3.09	1.40	1.33
21	b	617	CL7	O2D-CGD	3.09	1.40	1.33
21	b	611	CL7	O2D-CGD	3.09	1.40	1.33
21	B	609	CL7	O2A-CGA	3.09	1.42	1.33
21	b	610	CL7	O2A-CGA	3.09	1.42	1.33
21	3	503	CL7	O2A-CGA	3.09	1.42	1.33
21	7	503	CL7	O2A-CGA	3.09	1.42	1.33
21	C	512	CL7	C4C-C3C	-3.09	1.39	1.45
21	c	512	CL7	C4C-C3C	-3.09	1.39	1.45
21	C	507	CL7	C4C-C3C	-3.09	1.39	1.45
21	c	507	CL7	C4C-C3C	-3.09	1.39	1.45
21	4	415	CL7	O2D-CGD	3.09	1.40	1.33
21	8	415	CL7	O2D-CGD	3.09	1.40	1.33
21	B	606	CL7	O2A-CGA	3.09	1.42	1.33
21	b	607	CL7	O2A-CGA	3.09	1.42	1.33
21	B	611	CL7	C4C-C3C	-3.08	1.39	1.45
21	C	509	CL7	C4C-C3C	-3.08	1.39	1.45
21	4	406	CL7	C4C-C3C	-3.08	1.39	1.45
21	c	509	CL7	C4C-C3C	-3.08	1.39	1.45
21	8	406	CL7	C4C-C3C	-3.08	1.39	1.45
21	5	406	CL7	C2A-C1A	3.08	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	511	CL7	O2A-CGA	3.08	1.42	1.33
21	7	511	CL7	O2A-CGA	3.08	1.42	1.33
21	C	502	CL7	O2D-CGD	3.08	1.40	1.33
21	3	502	CL7	O2D-CGD	3.08	1.40	1.33
21	c	502	CL7	O2D-CGD	3.08	1.40	1.33
21	7	502	CL7	O2D-CGD	3.08	1.40	1.33
21	2	517	CL7	O2D-CGD	3.08	1.40	1.33
21	6	517	CL7	O2D-CGD	3.08	1.40	1.33
21	c	513	CL7	O2D-CGD	3.08	1.40	1.33
21	2	506	CL7	C2A-C1A	3.08	1.55	1.50
21	6	506	CL7	C2A-C1A	3.08	1.55	1.50
21	D	404	CL7	C4C-C3C	-3.07	1.39	1.45
21	d	404	CL7	C4C-C3C	-3.07	1.39	1.45
21	B	603	CL7	O2A-CGA	3.07	1.42	1.33
21	b	604	CL7	O2A-CGA	3.07	1.42	1.33
21	B	611	CL7	C4C-NC	-3.07	1.34	1.37
21	1	409	CL7	C2A-C1A	3.07	1.55	1.50
21	5	409	CL7	C2A-C1A	3.07	1.55	1.50
23	C	516	8CT	C07-C02	-3.07	1.44	1.51
23	c	516	8CT	C07-C02	-3.07	1.44	1.51
21	3	509	CL7	O2A-CGA	3.07	1.42	1.33
21	7	509	CL7	O2A-CGA	3.07	1.42	1.33
21	4	410	CL7	C4C-C3C	-3.07	1.39	1.45
21	C	513	CL7	O2D-CGD	3.06	1.40	1.33
21	C	509	CL7	C4C-NC	-3.06	1.34	1.37
21	c	509	CL7	C4C-NC	-3.06	1.34	1.37
21	B	604	CL7	O2A-CGA	3.06	1.42	1.33
21	b	605	CL7	O2A-CGA	3.06	1.42	1.33
21	B	613	CL7	O2A-CGA	3.06	1.42	1.33
21	b	614	CL7	O2A-CGA	3.06	1.42	1.33
21	4	411	CL7	C4C-C3C	-3.06	1.39	1.45
21	8	411	CL7	C4C-C3C	-3.06	1.39	1.45
21	C	514	CL7	C2A-C1A	3.05	1.55	1.50
21	2	515	CL7	C2A-C1A	3.05	1.55	1.50
21	6	515	CL7	C2A-C1A	3.05	1.55	1.50
21	2	510	CL7	C4C-C3C	-3.05	1.39	1.45
21	6	510	CL7	C4C-C3C	-3.05	1.39	1.45
21	C	507	CL7	O2A-CGA	3.05	1.42	1.33
21	c	507	CL7	O2A-CGA	3.05	1.42	1.33
21	6	518	CL7	C2A-C1A	3.05	1.55	1.50
21	2	516	CL7	C4C-C3C	-3.05	1.39	1.45
21	3	512	CL7	C4C-C3C	-3.05	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	516	CL7	C4C-C3C	-3.05	1.39	1.45
21	7	512	CL7	C4C-C3C	-3.05	1.39	1.45
21	4	412	CL7	O2D-CGD	3.05	1.40	1.33
21	8	412	CL7	O2D-CGD	3.05	1.40	1.33
23	B	618	8CT	C07-C02	-3.05	1.45	1.51
21	C	510	CL7	O2A-CGA	3.05	1.42	1.33
21	c	510	CL7	O2A-CGA	3.05	1.42	1.33
21	c	514	CL7	C2A-C1A	3.05	1.55	1.50
21	4	408	CL7	O2D-CGD	3.04	1.40	1.33
21	8	408	CL7	O2D-CGD	3.04	1.40	1.33
21	C	511	CL7	C4C-C3C	-3.04	1.39	1.45
21	c	511	CL7	C4C-C3C	-3.04	1.39	1.45
21	B	605	CL7	O2A-CGA	3.04	1.42	1.33
22	A	402	PHO	C3A-C2A	-3.04	1.51	1.54
22	a	402	PHO	C3A-C2A	-3.04	1.51	1.54
21	1	406	CL7	C2A-C1A	3.03	1.55	1.50
21	a	403	CL7	O2D-CGD	3.03	1.40	1.33
23	C	516	8CT	C19-C20	3.03	1.52	1.43
23	c	516	8CT	C19-C20	3.03	1.52	1.43
21	3	504	CL7	O2A-CGA	3.03	1.42	1.33
21	7	504	CL7	O2A-CGA	3.03	1.42	1.33
21	3	503	CL7	C2A-C1A	3.03	1.55	1.50
21	B	612	CL7	O2A-CGA	3.03	1.42	1.33
21	B	606	CL7	O2D-CGD	3.03	1.40	1.33
21	8	406	CL7	O2D-CGD	3.03	1.40	1.33
21	B	613	CL7	O2D-CGD	3.03	1.40	1.33
32	2	519	ZEX	C1-C6	-3.03	1.49	1.53
32	6	519	ZEX	C1-C6	-3.03	1.49	1.53
21	C	507	CL7	O2D-CGD	3.03	1.40	1.33
21	c	507	CL7	O2D-CGD	3.03	1.40	1.33
23	B	618	8CT	C19-C20	3.02	1.52	1.43
23	b	619	8CT	C19-C20	3.02	1.52	1.43
21	7	503	CL7	C2A-C1A	3.02	1.55	1.50
21	6	505	CL7	O2A-CGA	3.02	1.42	1.33
21	2	510	CL7	O2A-CGA	3.02	1.42	1.33
21	6	510	CL7	O2A-CGA	3.02	1.42	1.33
21	2	509	CL7	O2A-CGA	3.02	1.42	1.33
21	6	509	CL7	O2A-CGA	3.02	1.42	1.33
21	4	407	CL7	C4C-C3C	-3.02	1.39	1.45
21	2	505	CL7	O2A-CGA	3.02	1.42	1.33
21	b	613	CL7	O2A-CGA	3.02	1.42	1.33
21	B	612	CL7	O2D-CGD	3.02	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	613	CL7	O2D-CGD	3.02	1.40	1.33
21	3	508	CL7	O2D-CGD	3.01	1.40	1.33
21	7	508	CL7	O2D-CGD	3.01	1.40	1.33
21	b	606	CL7	O2A-CGA	3.01	1.42	1.33
21	b	605	CL7	O2D-CGD	3.01	1.40	1.33
21	D	404	CL7	O2A-CGA	3.01	1.42	1.33
21	d	404	CL7	O2A-CGA	3.01	1.42	1.33
21	1	408	CL7	C2A-C1A	3.01	1.55	1.50
21	5	408	CL7	C2A-C1A	3.01	1.55	1.50
21	2	508	CL7	C4C-C3C	-3.01	1.39	1.45
21	6	508	CL7	C4C-C3C	-3.01	1.39	1.45
21	6	509	CL7	C4C-C3C	-3.01	1.39	1.45
21	3	507	CL7	C4C-C3C	-3.01	1.39	1.45
21	7	507	CL7	C4C-C3C	-3.01	1.39	1.45
21	3	505	CL7	O2A-CGA	3.01	1.42	1.33
21	7	505	CL7	O2A-CGA	3.01	1.42	1.33
21	3	505	CL7	O2D-CGD	3.01	1.40	1.33
21	7	505	CL7	O2D-CGD	3.01	1.40	1.33
21	3	507	CL7	C2A-C1A	3.01	1.55	1.50
21	7	507	CL7	C2A-C1A	3.01	1.55	1.50
21	2	501	CL7	O2A-CGA	3.01	1.42	1.33
21	6	501	CL7	O2A-CGA	3.01	1.42	1.33
21	2	501	CL7	C4C-C3C	-3.00	1.39	1.45
21	3	505	CL7	C4C-C3C	-3.00	1.39	1.45
21	6	501	CL7	C4C-C3C	-3.00	1.39	1.45
21	7	505	CL7	C4C-C3C	-3.00	1.39	1.45
21	4	409	CL7	O2D-CGD	3.00	1.40	1.33
21	2	507	CL7	C2A-C1A	3.00	1.55	1.50
21	6	507	CL7	C2A-C1A	3.00	1.55	1.50
23	b	619	8CT	C07-C02	-3.00	1.45	1.51
21	B	616	CL7	C4C-C3C	-3.00	1.39	1.45
21	b	617	CL7	C4C-C3C	-3.00	1.39	1.45
21	b	614	CL7	O2D-CGD	3.00	1.40	1.33
21	7	501	CL7	O2A-CGA	3.00	1.42	1.33
21	3	516	CL7	O2D-CGD	3.00	1.40	1.33
21	b	607	CL7	O2D-CGD	3.00	1.40	1.33
21	7	516	CL7	O2D-CGD	3.00	1.40	1.33
21	3	516	CL7	C4C-C3C	-3.00	1.39	1.45
21	7	516	CL7	C4C-C3C	-3.00	1.39	1.45
21	B	604	CL7	O2D-CGD	3.00	1.40	1.33
21	2	509	CL7	C4C-C3C	-3.00	1.39	1.45
21	8	409	CL7	O2D-CGD	2.99	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	403	CL7	O2D-CGD	2.99	1.40	1.33
21	2	502	CL7	C4C-C3C	-2.99	1.39	1.45
21	6	502	CL7	C4C-C3C	-2.99	1.39	1.45
21	4	413	CL7	C4C-C3C	-2.99	1.39	1.45
21	8	413	CL7	C4C-C3C	-2.99	1.39	1.45
21	4	411	CL7	O2A-CGA	2.99	1.42	1.33
21	8	411	CL7	O2A-CGA	2.99	1.42	1.33
21	B	607	CL7	O2D-CGD	2.99	1.40	1.33
21	b	608	CL7	O2D-CGD	2.99	1.40	1.33
21	8	410	CL7	C4C-C3C	-2.99	1.39	1.45
21	1	406	CL7	C4C-C3C	-2.99	1.39	1.45
21	5	406	CL7	C4C-C3C	-2.99	1.39	1.45
21	3	501	CL7	O2A-CGA	2.99	1.42	1.33
21	D	404	CL7	O2D-CGD	2.98	1.40	1.33
21	d	404	CL7	O2D-CGD	2.98	1.40	1.33
21	2	512	CL7	O2D-CGD	2.98	1.40	1.33
21	6	512	CL7	O2D-CGD	2.98	1.40	1.33
23	D	406	8CT	C19-C20	2.98	1.52	1.43
23	d	406	8CT	C19-C20	2.98	1.52	1.43
21	8	407	CL7	C4C-C3C	-2.98	1.39	1.45
21	C	512	CL7	C2A-C1A	2.98	1.55	1.50
21	c	512	CL7	C2A-C1A	2.98	1.55	1.50
21	8	405	CL7	C2A-C1A	2.98	1.55	1.50
21	8	414	CL7	C4C-NC	-2.98	1.34	1.37
21	4	406	CL7	O2D-CGD	2.98	1.40	1.33
21	1	418	CL7	O2D-CGD	2.97	1.40	1.33
21	5	418	CL7	O2D-CGD	2.97	1.40	1.33
23	D	406	8CT	C07-C02	-2.97	1.45	1.51
23	d	406	8CT	C07-C02	-2.97	1.45	1.51
21	3	512	CL7	O2D-CGD	2.97	1.40	1.33
21	7	512	CL7	O2D-CGD	2.97	1.40	1.33
21	d	405	CL7	O2D-CGD	2.97	1.40	1.33
21	D	405	CL7	O2D-CGD	2.97	1.40	1.33
21	A	403	CL7	C4C-C3C	-2.97	1.39	1.45
21	a	403	CL7	C4C-C3C	-2.97	1.39	1.45
21	1	404	CL7	C2A-C1A	2.97	1.55	1.50
21	5	404	CL7	C2A-C1A	2.97	1.55	1.50
21	B	615	CL7	C4C-NC	-2.97	1.34	1.37
21	b	616	CL7	C4C-NC	-2.97	1.34	1.37
21	B	604	CL7	C4C-NC	-2.96	1.34	1.37
21	b	605	CL7	C4C-NC	-2.96	1.34	1.37
21	2	507	CL7	O2D-CGD	2.96	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	507	CL7	O2D-CGD	2.96	1.40	1.33
21	C	503	CL7	C2A-C1A	2.96	1.55	1.50
21	c	503	CL7	C2A-C1A	2.96	1.55	1.50
21	b	612	CL7	O2A-CGA	2.95	1.42	1.33
21	B	611	CL7	O2D-CGD	2.95	1.40	1.33
21	1	405	CL7	C4C-C3C	-2.95	1.40	1.45
21	5	405	CL7	C4C-C3C	-2.95	1.40	1.45
21	B	611	CL7	O2A-CGA	2.95	1.42	1.33
21	2	506	CL7	C4C-C3C	-2.95	1.40	1.45
21	6	506	CL7	C4C-C3C	-2.95	1.40	1.45
21	C	505	CL7	C4C-C3C	-2.95	1.40	1.45
21	c	505	CL7	C4C-C3C	-2.95	1.40	1.45
21	B	606	CL7	C2A-C1A	2.95	1.55	1.50
21	b	607	CL7	C2A-C1A	2.95	1.55	1.50
21	3	508	CL7	C4C-C3C	-2.94	1.40	1.45
21	6	505	CL7	C4C-NC	-2.94	1.34	1.37
21	5	403	CL7	C4C-C3C	-2.94	1.40	1.45
21	A	403	CL7	C2A-C1A	2.94	1.55	1.50
21	a	403	CL7	C2A-C1A	2.94	1.55	1.50
21	C	504	CL7	C4C-C3C	-2.94	1.40	1.45
21	3	515	CL7	C4C-C3C	-2.94	1.40	1.45
21	c	504	CL7	C4C-C3C	-2.94	1.40	1.45
21	7	515	CL7	C4C-C3C	-2.94	1.40	1.45
21	4	405	CL7	C2A-C1A	2.94	1.55	1.50
21	B	603	CL7	C4C-C3C	-2.94	1.40	1.45
21	b	604	CL7	C4C-C3C	-2.94	1.40	1.45
21	C	509	CL7	O2D-CGD	2.94	1.40	1.33
21	4	417	CL7	C2A-C1A	2.94	1.55	1.50
21	8	417	CL7	C2A-C1A	2.94	1.55	1.50
21	2	512	CL7	C4C-NC	-2.93	1.34	1.37
21	6	512	CL7	C4C-NC	-2.93	1.34	1.37
21	C	513	CL7	C4C-C3C	-2.93	1.40	1.45
21	c	513	CL7	C4C-C3C	-2.93	1.40	1.45
21	b	612	CL7	O2D-CGD	2.93	1.40	1.33
21	c	508	CL7	C4C-NC	-2.93	1.34	1.37
23	B	627	8CT	C07-C02	-2.93	1.45	1.51
23	b	601	8CT	C07-C02	-2.93	1.45	1.51
21	2	502	CL7	O2D-CGD	2.93	1.40	1.33
21	6	502	CL7	O2D-CGD	2.93	1.40	1.33
21	1	402	CL7	C4C-C3C	-2.93	1.40	1.45
21	3	513	CL7	C4C-C3C	-2.93	1.40	1.45
21	5	402	CL7	C4C-C3C	-2.93	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	513	CL7	C4C-C3C	-2.93	1.40	1.45
21	2	505	CL7	C4C-NC	-2.93	1.34	1.37
21	2	517	CL7	C4C-C3C	-2.93	1.40	1.45
21	6	517	CL7	C4C-C3C	-2.93	1.40	1.45
21	3	510	CL7	C2A-C1A	2.93	1.55	1.50
21	7	510	CL7	C2A-C1A	2.93	1.55	1.50
21	7	508	CL7	C4C-C3C	-2.93	1.40	1.45
23	A	404	8CT	C19-C20	2.93	1.52	1.43
21	B	613	CL7	C4C-NC	-2.93	1.34	1.37
21	b	614	CL7	C4C-NC	-2.93	1.34	1.37
22	A	402	PHO	CBD-CGD	-2.93	1.48	1.52
22	a	402	PHO	CBD-CGD	-2.93	1.48	1.52
21	c	509	CL7	O2D-CGD	2.92	1.40	1.33
21	3	510	CL7	C4C-NC	-2.92	1.34	1.37
21	7	510	CL7	C4C-NC	-2.92	1.34	1.37
21	1	403	CL7	C4C-C3C	-2.92	1.40	1.45
21	D	404	CL7	C4C-NC	-2.92	1.34	1.37
21	d	404	CL7	C4C-NC	-2.92	1.34	1.37
23	a	404	8CT	C19-C20	2.92	1.52	1.43
21	4	414	CL7	C4C-NC	-2.92	1.34	1.37
21	B	615	CL7	C4C-C3C	-2.92	1.40	1.45
21	1	413	CL7	C4C-C3C	-2.92	1.40	1.45
21	b	616	CL7	C4C-C3C	-2.92	1.40	1.45
21	5	413	CL7	C4C-C3C	-2.92	1.40	1.45
21	c	518	CL7	C4C-C3C	-2.92	1.40	1.45
21	B	602	CL7	C4C-C3C	-2.91	1.40	1.45
21	b	603	CL7	C4C-C3C	-2.91	1.40	1.45
21	4	404	CL7	C4C-C3C	-2.91	1.40	1.45
21	8	404	CL7	C4C-C3C	-2.91	1.40	1.45
21	2	516	CL7	C4C-NC	-2.91	1.34	1.37
21	6	516	CL7	C4C-NC	-2.91	1.34	1.37
21	3	508	CL7	C2A-C1A	2.91	1.55	1.50
21	7	508	CL7	C2A-C1A	2.91	1.55	1.50
21	3	503	CL7	O2D-CGD	2.90	1.40	1.33
21	7	503	CL7	O2D-CGD	2.90	1.40	1.33
21	1	417	CL7	C4C-C3C	-2.90	1.40	1.45
21	5	417	CL7	C4C-C3C	-2.90	1.40	1.45
21	C	518	CL7	C4C-C3C	-2.90	1.40	1.45
32	2	525	ZEX	C21-C26	-2.90	1.49	1.53
32	6	524	ZEX	C21-C26	-2.90	1.49	1.53
21	b	614	CL7	C1B-C2B	-2.90	1.36	1.43
21	D	405	CL7	C4C-C3C	-2.90	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	d	405	CL7	C4C-C3C	-2.90	1.40	1.45
21	B	613	CL7	C1B-C2B	-2.90	1.36	1.43
21	A	406	CL7	C4C-NC	-2.89	1.34	1.37
21	a	405	CL7	C4C-NC	-2.89	1.34	1.37
22	d	408	PHO	O2A-CGA	2.89	1.41	1.33
21	1	418	CL7	C4C-NC	-2.89	1.34	1.37
21	C	508	CL7	O2A-CGA	2.88	1.41	1.33
23	C	519	8CT	C19-C20	2.88	1.52	1.43
23	c	519	8CT	C19-C20	2.88	1.52	1.43
21	2	502	CL7	C4C-NC	-2.88	1.34	1.37
21	6	502	CL7	C4C-NC	-2.88	1.34	1.37
21	c	508	CL7	O2A-CGA	2.88	1.41	1.33
21	7	505	CL7	C2A-C1A	2.88	1.55	1.50
21	2	510	CL7	C4C-NC	-2.88	1.34	1.37
21	6	510	CL7	C4C-NC	-2.88	1.34	1.37
21	C	502	CL7	C4C-NC	-2.87	1.34	1.37
21	c	502	CL7	C4C-NC	-2.87	1.34	1.37
21	C	510	CL7	C4C-NC	-2.87	1.34	1.37
21	c	510	CL7	C4C-NC	-2.87	1.34	1.37
21	3	517	CL7	C2A-C1A	2.87	1.55	1.50
21	7	517	CL7	C2A-C1A	2.87	1.55	1.50
21	8	408	CL7	C4C-C3C	-2.87	1.40	1.45
32	2	520	ZEX	C21-C26	-2.87	1.49	1.53
32	3	525	ZEX	C21-C26	-2.87	1.49	1.53
23	4	402	8CT	C19-C20	2.87	1.52	1.43
23	8	402	8CT	C19-C20	2.87	1.52	1.43
21	3	507	CL7	O2D-CGD	2.87	1.40	1.33
21	7	507	CL7	O2D-CGD	2.87	1.40	1.33
21	B	602	CL7	C4C-NC	-2.87	1.34	1.37
21	b	603	CL7	C4C-NC	-2.87	1.34	1.37
23	B	617	8CT	C19-C20	2.86	1.52	1.43
23	b	618	8CT	C19-C20	2.86	1.52	1.43
21	c	503	CL7	C4C-C3C	-2.86	1.40	1.45
22	D	408	PHO	O2A-CGA	2.86	1.41	1.33
23	C	515	8CT	C19-C20	2.86	1.52	1.43
23	c	515	8CT	C19-C20	2.86	1.52	1.43
21	C	508	CL7	C4C-NC	-2.86	1.34	1.37
21	C	508	CL7	O2D-CGD	2.86	1.40	1.33
21	c	508	CL7	O2D-CGD	2.86	1.40	1.33
21	d	405	CL7	C2A-C1A	2.86	1.55	1.50
21	3	517	CL7	C4C-C3C	-2.86	1.40	1.45
21	7	517	CL7	C4C-C3C	-2.86	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	408	CL7	C4C-C3C	-2.86	1.40	1.45
21	2	517	CL7	C2A-C1A	2.86	1.55	1.50
21	6	517	CL7	C2A-C1A	2.86	1.55	1.50
21	2	503	CL7	O2A-CGA	2.85	1.41	1.33
21	6	503	CL7	O2A-CGA	2.85	1.41	1.33
21	A	406	CL7	O2A-CGA	2.85	1.41	1.33
21	a	405	CL7	O2A-CGA	2.85	1.41	1.33
23	A	404	8CT	C07-C02	-2.85	1.45	1.51
23	a	404	8CT	C07-C02	-2.85	1.45	1.51
21	5	405	CL7	C2A-C1A	2.85	1.55	1.50
21	3	509	CL7	C4C-C3C	-2.85	1.40	1.45
21	3	511	CL7	C2A-C1A	2.85	1.55	1.50
21	4	405	CL7	C4C-C3C	-2.84	1.40	1.45
21	8	405	CL7	C4C-C3C	-2.84	1.40	1.45
21	3	516	CL7	C4C-NC	-2.84	1.34	1.37
21	7	516	CL7	C4C-NC	-2.84	1.34	1.37
21	5	418	CL7	C4C-NC	-2.84	1.34	1.37
21	C	510	CL7	C2A-C1A	2.84	1.55	1.50
21	D	405	CL7	C2A-C1A	2.84	1.55	1.50
21	4	406	CL7	C4C-NC	-2.84	1.34	1.37
21	B	615	CL7	C2A-C1A	2.84	1.55	1.50
21	3	505	CL7	C2A-C1A	2.84	1.55	1.50
21	b	616	CL7	C2A-C1A	2.84	1.55	1.50
21	C	502	CL7	C2A-C1A	2.83	1.55	1.50
21	c	502	CL7	C2A-C1A	2.83	1.55	1.50
21	C	503	CL7	C4C-C3C	-2.83	1.40	1.45
21	3	518	CL7	C4C-C3C	-2.83	1.40	1.45
21	7	518	CL7	C4C-C3C	-2.83	1.40	1.45
21	8	415	CL7	C4C-C3C	-2.83	1.40	1.45
23	B	619	8CT	C19-C20	2.82	1.52	1.43
21	1	405	CL7	C2A-C1A	2.82	1.55	1.50
21	7	511	CL7	C2A-C1A	2.82	1.55	1.50
21	c	510	CL7	C2A-C1A	2.82	1.55	1.50
23	b	620	8CT	C19-C20	2.82	1.52	1.43
21	8	415	CL7	C2A-C1A	2.82	1.55	1.50
21	B	608	CL7	C4C-C3C	-2.81	1.40	1.45
21	b	609	CL7	C4C-C3C	-2.81	1.40	1.45
21	B	603	CL7	C4C-NC	-2.81	1.34	1.37
21	b	604	CL7	C4C-NC	-2.81	1.34	1.37
21	3	508	CL7	C4C-NC	-2.80	1.34	1.37
21	7	508	CL7	C4C-NC	-2.80	1.34	1.37
21	B	606	CL7	C4C-C3C	-2.80	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	607	CL7	C4C-C3C	-2.80	1.40	1.45
21	1	420	CL7	C4C-C3C	-2.80	1.40	1.45
21	7	509	CL7	C4C-C3C	-2.80	1.40	1.45
21	4	410	CL7	C4C-NC	-2.80	1.34	1.37
21	8	410	CL7	C4C-NC	-2.80	1.34	1.37
21	1	407	CL7	C4C-C3C	-2.80	1.40	1.45
31	F	101	HEM	C1C-C2C	-2.80	1.39	1.45
21	B	612	CL7	C4C-NC	-2.79	1.34	1.37
21	b	613	CL7	C4C-NC	-2.79	1.34	1.37
32	2	523	ZEX	C21-C26	-2.79	1.49	1.53
32	6	522	ZEX	C21-C26	-2.79	1.49	1.53
31	f	101	HEM	C1C-C2C	-2.79	1.39	1.45
21	c	514	CL7	C4C-C3C	-2.79	1.40	1.45
21	4	415	CL7	C2A-C1A	2.79	1.55	1.50
21	4	404	CL7	C4C-NC	-2.79	1.34	1.37
21	8	404	CL7	C4C-NC	-2.79	1.34	1.37
21	6	504	CL7	C4C-C3C	-2.79	1.40	1.45
21	3	501	CL7	C4C-NC	-2.79	1.34	1.37
21	7	501	CL7	C4C-NC	-2.79	1.34	1.37
21	2	504	CL7	C4C-C3C	-2.78	1.40	1.45
21	C	504	CL7	C2A-C1A	2.78	1.55	1.50
21	c	504	CL7	C2A-C1A	2.78	1.55	1.50
21	1	409	CL7	C4C-C3C	-2.78	1.40	1.45
21	5	409	CL7	C4C-C3C	-2.78	1.40	1.45
21	1	411	CL7	C2A-C1A	2.78	1.55	1.50
21	2	501	CL7	C4C-NC	-2.78	1.34	1.37
21	6	501	CL7	C4C-NC	-2.78	1.34	1.37
21	4	411	CL7	C1B-C2B	-2.78	1.36	1.43
21	8	411	CL7	C1B-C2B	-2.78	1.36	1.43
21	6	503	CL7	C4C-NC	-2.78	1.34	1.37
21	7	504	CL7	C4C-NC	-2.78	1.34	1.37
31	F	101	HEM	FE-ND	-2.78	1.86	1.94
31	f	101	HEM	FE-ND	-2.78	1.86	1.94
21	3	511	CL7	C4C-NC	-2.78	1.34	1.37
21	7	511	CL7	C4C-NC	-2.78	1.34	1.37
21	4	415	CL7	C4C-C3C	-2.78	1.40	1.45
32	2	519	ZEX	C21-C26	-2.77	1.50	1.53
21	B	612	CL7	MG-ND	-2.77	2.00	2.05
21	b	613	CL7	MG-ND	-2.77	2.00	2.05
21	C	510	CL7	MG-ND	-2.77	2.00	2.05
21	c	510	CL7	MG-ND	-2.77	2.00	2.05
21	5	407	CL7	C4C-C3C	-2.77	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	412	CL7	C2A-C1A	2.77	1.55	1.50
21	8	412	CL7	C2A-C1A	2.77	1.55	1.50
21	C	514	CL7	C4C-C3C	-2.77	1.40	1.45
21	5	420	CL7	C4C-C3C	-2.77	1.40	1.45
21	3	502	CL7	C4C-C3C	-2.76	1.40	1.45
21	7	502	CL7	C4C-C3C	-2.76	1.40	1.45
21	B	622	CL7	C4C-C3C	-2.76	1.40	1.45
21	b	623	CL7	C4C-C3C	-2.76	1.40	1.45
21	3	517	CL7	C4C-NC	-2.76	1.34	1.37
21	6	517	CL7	C4C-NC	-2.76	1.34	1.37
21	2	507	CL7	C3B-C4B	-2.76	1.36	1.42
21	b	610	CL7	C4C-C3C	-2.76	1.40	1.45
21	b	607	CL7	C4C-NC	-2.76	1.34	1.37
21	5	411	CL7	C2A-C1A	2.76	1.55	1.50
21	B	603	CL7	C2A-C1A	2.75	1.55	1.50
21	8	406	CL7	C4C-NC	-2.75	1.34	1.37
21	4	404	CL7	C2A-C1A	2.75	1.55	1.50
21	8	404	CL7	C2A-C1A	2.75	1.55	1.50
21	1	403	CL7	C4C-NC	-2.75	1.34	1.37
21	5	403	CL7	C4C-NC	-2.75	1.34	1.37
21	B	607	CL7	C1B-C2B	-2.75	1.36	1.43
21	b	608	CL7	C1B-C2B	-2.75	1.36	1.43
21	3	504	CL7	C4C-NC	-2.75	1.34	1.37
21	7	512	CL7	C4C-NC	-2.75	1.34	1.37
21	5	411	CL7	C4C-C3C	-2.74	1.40	1.45
21	4	411	CL7	C2A-C1A	2.74	1.55	1.50
21	8	411	CL7	C2A-C1A	2.74	1.55	1.50
23	C	519	8CT	C07-C02	-2.74	1.45	1.51
23	c	519	8CT	C07-C02	-2.74	1.45	1.51
21	C	503	CL7	C4C-NC	-2.74	1.34	1.37
21	c	503	CL7	C4C-NC	-2.74	1.34	1.37
21	6	507	CL7	C3B-C4B	-2.74	1.36	1.42
21	D	405	CL7	C4C-NC	-2.74	1.34	1.37
21	d	405	CL7	C4C-NC	-2.74	1.34	1.37
21	7	517	CL7	C4C-NC	-2.74	1.34	1.37
21	C	504	CL7	C4C-NC	-2.74	1.34	1.37
21	c	504	CL7	C4C-NC	-2.74	1.34	1.37
21	3	502	CL7	C1B-C2B	-2.74	1.36	1.43
21	7	502	CL7	C1B-C2B	-2.74	1.36	1.43
21	4	415	CL7	C4C-NC	-2.74	1.34	1.37
21	8	415	CL7	C4C-NC	-2.74	1.34	1.37
21	2	517	CL7	C4C-NC	-2.74	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	609	CL7	C4C-C3C	-2.73	1.40	1.45
21	1	410	CL7	C4C-C3C	-2.73	1.40	1.45
21	5	410	CL7	C4C-C3C	-2.73	1.40	1.45
32	6	519	ZEX	C21-C26	-2.73	1.50	1.53
21	6	507	CL7	C4C-C3C	-2.73	1.40	1.45
21	b	612	CL7	C2A-C1A	2.73	1.54	1.50
21	C	506	CL7	C2A-C1A	2.73	1.54	1.50
21	B	616	CL7	C1B-C2B	-2.73	1.36	1.43
21	b	617	CL7	C1B-C2B	-2.73	1.36	1.43
21	B	605	CL7	C4C-NC	-2.72	1.34	1.37
21	b	606	CL7	C4C-NC	-2.72	1.34	1.37
21	1	411	CL7	C4C-C3C	-2.72	1.40	1.45
21	2	503	CL7	C4C-NC	-2.72	1.34	1.37
21	4	416	CL7	C4C-C3C	-2.72	1.40	1.45
21	8	416	CL7	C4C-C3C	-2.72	1.40	1.45
21	B	606	CL7	C4C-NC	-2.71	1.34	1.37
21	B	616	CL7	C4C-NC	-2.71	1.34	1.37
21	b	617	CL7	C4C-NC	-2.71	1.34	1.37
21	3	508	CL7	C1B-C2B	-2.71	1.36	1.43
21	7	508	CL7	C1B-C2B	-2.71	1.36	1.43
21	2	516	CL7	C2A-C1A	2.71	1.54	1.50
21	B	622	CL7	CHC-C4B	2.71	1.45	1.39
21	b	623	CL7	CHC-C4B	2.71	1.45	1.39
21	B	608	CL7	C2A-C1A	2.71	1.54	1.50
21	b	609	CL7	C2A-C1A	2.71	1.54	1.50
21	B	604	CL7	C2A-C1A	2.71	1.54	1.50
21	b	605	CL7	C2A-C1A	2.71	1.54	1.50
21	b	604	CL7	C2A-C1A	2.70	1.54	1.50
21	3	512	CL7	C4C-NC	-2.70	1.34	1.37
21	A	401	CL7	CHC-C4B	2.70	1.45	1.39
21	a	401	CL7	CHC-C4B	2.70	1.45	1.39
21	2	518	CL7	C4C-C3C	-2.70	1.40	1.45
21	6	518	CL7	C4C-C3C	-2.70	1.40	1.45
21	2	507	CL7	C4C-C3C	-2.70	1.40	1.45
21	C	507	CL7	C1B-C2B	-2.70	1.36	1.43
21	c	507	CL7	C1B-C2B	-2.70	1.36	1.43
21	1	405	CL7	C4C-NC	-2.69	1.34	1.37
21	2	507	CL7	MG-ND	-2.69	2.00	2.05
21	6	507	CL7	MG-ND	-2.69	2.00	2.05
21	B	615	CL7	MG-ND	-2.69	2.00	2.05
21	b	616	CL7	MG-ND	-2.69	2.00	2.05
21	2	508	CL7	C2A-C1A	2.69	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	508	CL7	C2A-C1A	2.69	1.54	1.50
21	7	505	CL7	C4C-NC	-2.69	1.34	1.37
21	C	507	CL7	C4C-NC	-2.69	1.34	1.37
21	1	407	CL7	C4C-NC	-2.69	1.34	1.37
21	A	403	CL7	C4C-NC	-2.69	1.34	1.37
21	C	506	CL7	C4C-NC	-2.69	1.34	1.37
21	c	506	CL7	C4C-NC	-2.69	1.34	1.37
21	6	509	CL7	C4C-NC	-2.69	1.34	1.37
21	3	503	CL7	C4C-NC	-2.69	1.34	1.37
21	7	503	CL7	C4C-NC	-2.69	1.34	1.37
21	C	511	CL7	C4C-NC	-2.69	1.34	1.37
21	6	518	CL7	C4C-NC	-2.69	1.34	1.37
21	4	417	CL7	C4C-C3C	-2.69	1.40	1.45
21	8	417	CL7	C4C-C3C	-2.69	1.40	1.45
21	a	403	CL7	MG-ND	-2.68	2.00	2.05
21	B	611	CL7	C2A-C1A	2.68	1.54	1.50
21	6	516	CL7	C2A-C1A	2.68	1.54	1.50
21	c	506	CL7	C2A-C1A	2.68	1.54	1.50
21	3	505	CL7	MG-ND	-2.67	2.00	2.05
21	7	505	CL7	MG-ND	-2.67	2.00	2.05
21	4	414	CL7	C2A-C1A	2.67	1.54	1.50
21	8	414	CL7	C2A-C1A	2.67	1.54	1.50
21	c	511	CL7	C4C-NC	-2.67	1.34	1.37
21	4	412	CL7	C4C-NC	-2.67	1.34	1.37
21	2	508	CL7	C4C-NC	-2.66	1.34	1.37
21	6	508	CL7	C4C-NC	-2.66	1.34	1.37
21	1	415	CL7	CHC-C4B	2.66	1.45	1.39
21	5	415	CL7	CHC-C4B	2.66	1.45	1.39
21	c	507	CL7	C4C-NC	-2.66	1.34	1.37
21	a	403	CL7	C4C-NC	-2.66	1.34	1.37
21	1	406	CL7	C4C-NC	-2.66	1.34	1.37
21	5	406	CL7	C4C-NC	-2.66	1.34	1.37
21	C	506	CL7	MG-ND	-2.66	2.00	2.05
21	c	506	CL7	MG-ND	-2.66	2.00	2.05
21	B	606	CL7	C1B-C2B	-2.66	1.37	1.43
21	b	607	CL7	C1B-C2B	-2.66	1.37	1.43
21	6	510	CL7	MG-ND	-2.65	2.00	2.05
21	b	612	CL7	C1B-C2B	-2.65	1.37	1.43
21	3	507	CL7	MG-ND	-2.65	2.00	2.05
21	7	507	CL7	MG-ND	-2.65	2.00	2.05
21	1	413	CL7	C4C-NC	-2.65	1.34	1.37
21	5	413	CL7	C4C-NC	-2.65	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	510	CL7	MG-ND	-2.65	2.00	2.05
21	C	506	CL7	C4C-C3C	-2.65	1.40	1.45
32	8	420	ZEX	C1-C6	-2.65	1.50	1.53
21	2	509	CL7	MG-ND	-2.65	2.00	2.05
21	1	404	CL7	C4C-C3C	-2.65	1.40	1.45
21	5	404	CL7	C4C-C3C	-2.65	1.40	1.45
21	3	505	CL7	C4C-NC	-2.65	1.34	1.37
21	3	509	CL7	C2A-C1A	2.64	1.54	1.50
21	C	507	CL7	C2A-C1A	2.64	1.54	1.50
21	c	507	CL7	C2A-C1A	2.64	1.54	1.50
21	C	518	CL7	MG-ND	-2.64	2.00	2.05
32	2	520	ZEX	C30-C29	-2.64	1.32	1.35
32	3	525	ZEX	C30-C29	-2.64	1.32	1.35
21	A	403	CL7	MG-ND	-2.64	2.00	2.05
21	C	511	CL7	C1B-C2B	-2.64	1.37	1.43
21	c	511	CL7	C1B-C2B	-2.64	1.37	1.43
21	6	509	CL7	MG-ND	-2.64	2.00	2.05
21	b	608	CL7	C4C-NC	-2.64	1.34	1.37
21	5	407	CL7	C4C-NC	-2.64	1.34	1.37
21	B	616	CL7	C2A-C1A	2.64	1.54	1.50
21	b	617	CL7	C2A-C1A	2.64	1.54	1.50
21	3	514	CL7	C4C-C3C	-2.63	1.40	1.45
21	7	514	CL7	C4C-C3C	-2.63	1.40	1.45
21	2	509	CL7	C4C-NC	-2.63	1.34	1.37
21	b	623	CL7	C1B-C2B	-2.63	1.37	1.43
21	B	611	CL7	C1B-C2B	-2.63	1.37	1.43
21	C	508	CL7	C1B-C2B	-2.63	1.37	1.43
21	c	508	CL7	C1B-C2B	-2.63	1.37	1.43
21	B	612	CL7	C3B-C4B	-2.63	1.36	1.42
21	b	613	CL7	C3B-C4B	-2.63	1.36	1.42
21	2	515	CL7	C4C-C3C	-2.63	1.40	1.45
21	6	515	CL7	C4C-C3C	-2.63	1.40	1.45
21	B	612	CL7	C1B-C2B	-2.63	1.37	1.43
21	b	613	CL7	C1B-C2B	-2.63	1.37	1.43
21	5	405	CL7	C4C-NC	-2.62	1.34	1.37
21	3	511	CL7	C1B-C2B	-2.62	1.37	1.43
21	7	511	CL7	C1B-C2B	-2.62	1.37	1.43
21	C	507	CL7	MG-ND	-2.62	2.00	2.05
21	c	507	CL7	MG-ND	-2.62	2.00	2.05
21	6	504	CL7	MG-ND	-2.62	2.00	2.05
21	3	506	CL7	C4C-C3C	-2.62	1.40	1.45
21	7	506	CL7	C4C-C3C	-2.62	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	622	CL7	C1B-C2B	-2.62	1.37	1.43
21	B	609	CL7	C4C-NC	-2.62	1.34	1.37
21	b	610	CL7	C4C-NC	-2.62	1.34	1.37
21	6	517	CL7	MG-ND	-2.62	2.00	2.05
21	2	505	CL7	C2A-C1A	2.62	1.54	1.50
21	6	505	CL7	C2A-C1A	2.62	1.54	1.50
21	2	511	CL7	C4C-NC	-2.62	1.34	1.37
21	2	518	CL7	C4C-NC	-2.62	1.34	1.37
21	3	517	CL7	MG-ND	-2.62	2.00	2.05
21	7	517	CL7	MG-ND	-2.62	2.00	2.05
21	B	607	CL7	C4C-NC	-2.62	1.34	1.37
21	5	414	CL7	CHC-C4B	2.62	1.45	1.39
21	3	512	CL7	MG-ND	-2.62	2.00	2.05
21	7	512	CL7	MG-ND	-2.62	2.00	2.05
21	2	504	CL7	MG-ND	-2.62	2.00	2.05
23	C	519	8CT	C01-C02	2.62	1.55	1.50
21	8	412	CL7	C4C-NC	-2.62	1.34	1.37
21	B	610	CL7	C1B-C2B	-2.61	1.37	1.43
21	b	611	CL7	C1B-C2B	-2.61	1.37	1.43
21	1	414	CL7	CHC-C4B	2.61	1.45	1.39
32	4	420	ZEX	C1-C6	-2.61	1.50	1.53
21	B	602	CL7	C2A-C1A	2.61	1.54	1.50
21	B	604	CL7	C3B-C4B	-2.61	1.36	1.42
21	b	605	CL7	C3B-C4B	-2.61	1.36	1.42
21	3	509	CL7	C1B-C2B	-2.61	1.37	1.43
21	1	417	CL7	CHC-C4B	2.61	1.45	1.39
21	5	417	CL7	CHC-C4B	2.61	1.45	1.39
21	B	601	CL7	C4C-C3C	-2.61	1.40	1.45
21	b	602	CL7	C4C-C3C	-2.61	1.40	1.45
21	2	503	CL7	CBD-CGD	-2.61	1.44	1.52
21	6	503	CL7	CBD-CGD	-2.61	1.44	1.52
21	D	404	CL7	C2A-C1A	2.61	1.54	1.50
21	7	509	CL7	C1B-C2B	-2.60	1.37	1.43
21	C	513	CL7	C4C-NC	-2.60	1.34	1.37
21	c	513	CL7	C4C-NC	-2.60	1.34	1.37
21	c	506	CL7	C4C-C3C	-2.60	1.40	1.45
21	1	415	CL7	C4C-C3C	-2.60	1.40	1.45
21	5	415	CL7	C4C-C3C	-2.60	1.40	1.45
32	3	519	ZEX	C21-C26	-2.60	1.50	1.53
21	4	413	CL7	C4C-NC	-2.60	1.34	1.37
21	8	413	CL7	C4C-NC	-2.60	1.34	1.37
23	B	627	8CT	C01-C02	2.60	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	601	8CT	C01-C02	2.60	1.55	1.50
21	2	513	CL7	C4C-C3C	-2.60	1.40	1.45
21	6	513	CL7	C4C-C3C	-2.60	1.40	1.45
21	c	518	CL7	MG-ND	-2.59	2.00	2.05
21	3	505	CL7	MG-NB	-2.59	2.00	2.05
21	4	409	CL7	MG-ND	-2.59	2.00	2.05
21	8	409	CL7	MG-ND	-2.59	2.00	2.05
21	5	412	CL7	C4C-NC	-2.59	1.34	1.37
21	7	509	CL7	MG-ND	-2.59	2.00	2.05
21	b	603	CL7	C2A-C1A	2.59	1.54	1.50
21	1	418	CL7	C2A-C1A	2.59	1.54	1.50
21	5	418	CL7	C2A-C1A	2.59	1.54	1.50
21	2	504	CL7	C4C-NC	-2.59	1.34	1.37
21	6	504	CL7	C4C-NC	-2.59	1.34	1.37
21	D	404	CL7	C1B-C2B	-2.59	1.37	1.43
21	d	404	CL7	C1B-C2B	-2.59	1.37	1.43
21	4	413	CL7	MG-ND	-2.59	2.00	2.05
21	8	413	CL7	MG-ND	-2.59	2.00	2.05
21	3	512	CL7	C1B-C2B	-2.59	1.37	1.43
21	7	512	CL7	C1B-C2B	-2.59	1.37	1.43
21	3	507	CL7	C4C-NC	-2.58	1.34	1.37
21	7	507	CL7	C4C-NC	-2.58	1.34	1.37
21	B	607	CL7	C2A-C1A	2.58	1.54	1.50
21	b	608	CL7	C2A-C1A	2.58	1.54	1.50
21	5	419	CL7	CHC-C4B	2.58	1.45	1.39
21	1	419	CL7	C4C-C3C	-2.58	1.40	1.45
21	5	419	CL7	C4C-C3C	-2.58	1.40	1.45
21	B	615	CL7	C3B-C4B	-2.58	1.36	1.42
21	b	616	CL7	C3B-C4B	-2.58	1.36	1.42
21	b	611	CL7	MG-ND	-2.58	2.00	2.05
21	4	411	CL7	C4C-NC	-2.58	1.34	1.37
21	6	511	CL7	C4C-NC	-2.58	1.34	1.37
21	8	411	CL7	C4C-NC	-2.58	1.34	1.37
21	7	509	CL7	C2A-C1A	2.58	1.54	1.50
21	1	412	CL7	C4C-NC	-2.58	1.34	1.37
21	c	512	CL7	C4C-NC	-2.58	1.34	1.37
21	3	509	CL7	MG-ND	-2.58	2.00	2.05
23	K	101	8CT	C22-C21	2.58	1.56	1.50
21	2	517	CL7	MG-ND	-2.58	2.00	2.05
21	3	518	CL7	CHC-C4B	2.58	1.45	1.39
21	7	518	CL7	CHC-C4B	2.58	1.45	1.39
21	A	401	CL7	C4C-C3C	-2.58	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	401	CL7	C4C-C3C	-2.58	1.40	1.45
21	C	508	CL7	C3B-C4B	-2.58	1.36	1.42
23	k	101	8CT	C22-C21	2.58	1.56	1.50
21	1	419	CL7	CHC-C4B	2.58	1.45	1.39
22	d	408	PHO	CBD-CGD	-2.57	1.49	1.52
23	c	519	8CT	C01-C02	2.57	1.55	1.50
23	B	627	8CT	C22-C21	2.57	1.56	1.50
21	D	402	CL7	C4C-C3C	-2.57	1.40	1.45
21	C	506	CL7	C3B-C4B	-2.57	1.36	1.42
21	c	506	CL7	C3B-C4B	-2.57	1.36	1.42
21	3	510	CL7	C1B-C2B	-2.57	1.37	1.43
21	7	510	CL7	C1B-C2B	-2.57	1.37	1.43
21	C	505	CL7	C4C-NC	-2.57	1.34	1.37
21	c	505	CL7	C4C-NC	-2.57	1.34	1.37
21	3	510	CL7	MG-ND	-2.57	2.00	2.05
21	7	510	CL7	MG-ND	-2.57	2.00	2.05
21	C	508	CL7	C2A-C1A	2.57	1.54	1.50
21	c	508	CL7	C2A-C1A	2.57	1.54	1.50
21	8	412	CL7	MG-ND	-2.57	2.00	2.05
21	C	510	CL7	C1B-C2B	-2.57	1.37	1.43
21	C	518	CL7	C4C-NC	-2.57	1.34	1.37
21	c	518	CL7	C4C-NC	-2.57	1.34	1.37
32	3	520	ZEX	C21-C26	-2.57	1.50	1.53
21	B	610	CL7	MG-ND	-2.57	2.00	2.05
21	7	505	CL7	MG-NB	-2.57	2.00	2.05
21	1	412	CL7	C4C-C3C	-2.57	1.40	1.45
21	5	412	CL7	C4C-C3C	-2.57	1.40	1.45
21	3	507	CL7	C3B-C4B	-2.57	1.36	1.42
21	1	420	CL7	CHC-C4B	2.56	1.45	1.39
21	5	420	CL7	CHC-C4B	2.56	1.45	1.39
22	D	408	PHO	CBD-CGD	-2.56	1.49	1.52
21	B	602	CL7	C1B-C2B	-2.56	1.37	1.43
21	b	603	CL7	C1B-C2B	-2.56	1.37	1.43
21	C	513	CL7	MG-ND	-2.56	2.00	2.05
21	3	518	CL7	C4C-NC	-2.56	1.34	1.37
21	7	518	CL7	C4C-NC	-2.56	1.34	1.37
21	1	416	CL7	CHC-C4B	2.56	1.45	1.39
21	5	416	CL7	CHC-C4B	2.56	1.45	1.39
21	B	609	CL7	C2A-C1A	2.56	1.54	1.50
21	b	610	CL7	C2A-C1A	2.56	1.54	1.50
21	4	405	CL7	C4C-NC	-2.56	1.34	1.37
21	5	420	CL7	C4C-NC	-2.56	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	405	CL7	C4C-NC	-2.56	1.34	1.37
21	d	402	CL7	C4C-C3C	-2.56	1.40	1.45
21	4	411	CL7	MG-ND	-2.56	2.00	2.05
32	4	419	ZEX	C1-C6	-2.56	1.50	1.53
21	2	510	CL7	C2A-C1A	2.56	1.54	1.50
21	6	510	CL7	C2A-C1A	2.56	1.54	1.50
21	4	412	CL7	MG-ND	-2.55	2.00	2.05
21	2	502	CL7	C2A-C1A	2.55	1.54	1.50
21	6	502	CL7	C2A-C1A	2.55	1.54	1.50
21	1	417	CL7	C4C-NC	-2.55	1.34	1.37
21	5	417	CL7	C4C-NC	-2.55	1.34	1.37
21	3	502	CL7	MG-ND	-2.55	2.00	2.05
21	c	508	CL7	C3B-C4B	-2.55	1.36	1.42
21	6	506	CL7	C4C-NC	-2.55	1.34	1.37
21	7	502	CL7	MG-ND	-2.55	2.00	2.05
21	5	416	CL7	C4C-C3C	-2.55	1.40	1.45
21	b	615	CL7	C1B-C2B	-2.55	1.37	1.43
23	B	619	8CT	C01-C02	2.55	1.55	1.50
23	b	620	8CT	C01-C02	2.55	1.55	1.50
21	C	512	CL7	C4C-NC	-2.55	1.34	1.37
21	B	603	CL7	C1B-C2B	-2.54	1.37	1.43
21	b	604	CL7	C1B-C2B	-2.54	1.37	1.43
21	B	614	CL7	C4C-NC	-2.54	1.34	1.37
21	b	615	CL7	C4C-NC	-2.54	1.34	1.37
23	b	601	8CT	C22-C21	2.54	1.56	1.50
21	C	508	CL7	MG-ND	-2.54	2.00	2.05
21	c	508	CL7	MG-ND	-2.54	2.00	2.05
21	d	404	CL7	C2A-C1A	2.54	1.54	1.50
21	3	502	CL7	C4C-NC	-2.54	1.34	1.37
21	B	609	CL7	C1B-C2B	-2.54	1.37	1.43
21	B	614	CL7	C1B-C2B	-2.54	1.37	1.43
21	b	610	CL7	C1B-C2B	-2.54	1.37	1.43
21	6	502	CL7	MG-ND	-2.54	2.00	2.05
21	2	509	CL7	C1B-C2B	-2.54	1.37	1.43
21	B	603	CL7	CHC-C4B	2.54	1.45	1.39
21	b	604	CL7	CHC-C4B	2.54	1.45	1.39
21	2	502	CL7	MG-ND	-2.53	2.00	2.05
21	c	511	CL7	MG-ND	-2.53	2.00	2.05
21	4	409	CL7	C4C-NC	-2.53	1.34	1.37
21	8	409	CL7	C4C-NC	-2.53	1.34	1.37
21	b	609	CL7	MG-ND	-2.53	2.00	2.05
21	8	413	CL7	C1B-C2B	-2.53	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	515	8CT	C01-C02	2.53	1.55	1.50
21	4	413	CL7	C1B-C2B	-2.53	1.37	1.43
21	c	510	CL7	C1B-C2B	-2.53	1.37	1.43
21	6	509	CL7	C1B-C2B	-2.53	1.37	1.43
21	7	507	CL7	C3B-C4B	-2.53	1.36	1.42
21	C	511	CL7	MG-ND	-2.53	2.00	2.05
21	4	410	CL7	C1B-C2B	-2.53	1.37	1.43
21	8	410	CL7	C1B-C2B	-2.53	1.37	1.43
21	D	404	CL7	MG-ND	-2.53	2.00	2.05
21	d	404	CL7	MG-ND	-2.53	2.00	2.05
21	c	509	CL7	C1B-C2B	-2.53	1.37	1.43
21	4	404	CL7	C1B-C2B	-2.53	1.37	1.43
21	8	404	CL7	C1B-C2B	-2.53	1.37	1.43
32	7	520	ZEX	C21-C26	-2.53	1.50	1.53
21	1	416	CL7	C4C-C3C	-2.52	1.40	1.45
21	4	407	CL7	CHC-C4B	2.52	1.45	1.39
21	8	407	CL7	CHC-C4B	2.52	1.45	1.39
32	5	421	ZEX	C21-C26	-2.52	1.50	1.53
21	3	509	CL7	C4C-NC	-2.52	1.34	1.37
21	7	509	CL7	C4C-NC	-2.52	1.34	1.37
21	8	406	CL7	MG-ND	-2.52	2.00	2.05
21	c	509	CL7	MG-ND	-2.52	2.00	2.05
21	c	513	CL7	MG-ND	-2.52	2.00	2.05
21	5	418	CL7	MG-ND	-2.52	2.00	2.05
21	B	608	CL7	C1B-C2B	-2.52	1.37	1.43
21	3	501	CL7	C2A-C1A	2.52	1.54	1.50
21	7	501	CL7	C2A-C1A	2.52	1.54	1.50
21	3	517	CL7	C1B-C2B	-2.52	1.37	1.43
21	7	517	CL7	C1B-C2B	-2.52	1.37	1.43
21	2	506	CL7	C4C-NC	-2.52	1.34	1.37
21	3	502	CL7	CHC-C4B	2.52	1.45	1.39
21	7	502	CL7	CHC-C4B	2.52	1.45	1.39
21	B	608	CL7	MG-ND	-2.52	2.00	2.05
21	1	404	CL7	CHC-C4B	2.52	1.45	1.39
23	B	627	8CT	C30-C29	2.52	1.54	1.50
23	b	601	8CT	C30-C29	2.52	1.54	1.50
21	6	501	CL7	MG-ND	-2.52	2.00	2.05
21	C	502	CL7	C1B-C2B	-2.52	1.37	1.43
21	c	502	CL7	C1B-C2B	-2.52	1.37	1.43
32	8	419	ZEX	C1-C6	-2.52	1.50	1.53
21	4	408	CL7	C4C-NC	-2.52	1.34	1.37
21	8	408	CL7	C4C-NC	-2.52	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	411	CL7	MG-ND	-2.51	2.00	2.05
21	B	612	CL7	C1C-NC	-2.51	1.34	1.37
21	b	613	CL7	C1C-NC	-2.51	1.34	1.37
32	1	421	ZEX	C21-C26	-2.51	1.50	1.53
21	C	509	CL7	C1B-C2B	-2.51	1.37	1.43
21	b	609	CL7	C1B-C2B	-2.51	1.37	1.43
32	7	519	ZEX	C21-C26	-2.51	1.50	1.53
21	1	411	CL7	C4C-NC	-2.51	1.34	1.37
21	5	411	CL7	C4C-NC	-2.51	1.34	1.37
21	C	509	CL7	MG-ND	-2.51	2.00	2.05
21	1	418	CL7	MG-ND	-2.51	2.00	2.05
21	6	514	CL7	MG-ND	-2.51	2.00	2.05
21	C	514	CL7	CHC-C4B	2.51	1.45	1.39
21	B	613	CL7	MG-ND	-2.50	2.00	2.05
32	8	403	ZEX	C21-C26	-2.50	1.50	1.53
21	1	420	CL7	C4C-NC	-2.50	1.34	1.37
21	1	414	CL7	C4C-C3C	-2.50	1.40	1.45
21	5	414	CL7	C4C-C3C	-2.50	1.40	1.45
21	C	510	CL7	MG-NB	-2.50	2.00	2.05
21	c	510	CL7	MG-NB	-2.50	2.00	2.05
21	C	511	CL7	CHC-C4B	2.50	1.45	1.39
21	c	511	CL7	CHC-C4B	2.50	1.45	1.39
21	B	606	CL7	C1C-NC	-2.50	1.34	1.37
21	b	607	CL7	C1C-NC	-2.50	1.34	1.37
21	2	517	CL7	C1B-C2B	-2.50	1.37	1.43
21	5	404	CL7	CHC-C4B	2.50	1.45	1.39
21	2	508	CL7	C1B-C2B	-2.50	1.37	1.43
21	2	514	CL7	C4C-NC	-2.50	1.34	1.37
21	6	514	CL7	C4C-NC	-2.50	1.34	1.37
21	4	409	CL7	C4C-C3C	-2.50	1.40	1.45
21	8	409	CL7	C4C-C3C	-2.50	1.40	1.45
21	6	517	CL7	C1B-C2B	-2.50	1.37	1.43
23	C	515	8CT	C22-C21	2.50	1.56	1.50
23	c	515	8CT	C22-C21	2.50	1.56	1.50
21	3	507	CL7	MG-NB	-2.49	2.00	2.05
21	3	504	CL7	C1B-C2B	-2.49	1.37	1.43
21	7	504	CL7	C1B-C2B	-2.49	1.37	1.43
21	2	516	CL7	MG-ND	-2.49	2.00	2.05
21	6	516	CL7	MG-ND	-2.49	2.00	2.05
21	4	414	CL7	MG-ND	-2.49	2.00	2.05
21	8	414	CL7	MG-ND	-2.49	2.00	2.05
21	1	407	CL7	C1B-C2B	-2.49	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	608	CL7	C4C-NC	-2.49	1.34	1.37
21	b	609	CL7	C4C-NC	-2.49	1.34	1.37
21	B	604	CL7	MG-ND	-2.49	2.00	2.05
21	2	511	CL7	MG-ND	-2.49	2.00	2.05
21	b	605	CL7	MG-ND	-2.49	2.00	2.05
21	6	511	CL7	MG-ND	-2.49	2.00	2.05
21	A	406	CL7	C2A-C1A	2.49	1.54	1.50
21	a	405	CL7	C2A-C1A	2.49	1.54	1.50
21	2	501	CL7	MG-ND	-2.49	2.00	2.05
21	2	514	CL7	MG-ND	-2.49	2.00	2.05
21	C	511	CL7	C2A-C1A	2.49	1.54	1.50
32	1	422	ZEX	C21-C26	-2.49	1.50	1.53
32	3	520	ZEX	C1-C6	-2.49	1.50	1.53
21	D	404	CL7	C1C-C2C	-2.49	1.40	1.45
21	d	404	CL7	C1C-C2C	-2.49	1.40	1.45
21	c	504	CL7	MG-ND	-2.49	2.00	2.05
21	7	502	CL7	C4C-NC	-2.48	1.34	1.37
21	8	416	CL7	MG-ND	-2.48	2.00	2.05
21	B	607	CL7	MG-ND	-2.48	2.00	2.05
21	b	608	CL7	MG-ND	-2.48	2.00	2.05
21	4	406	CL7	MG-ND	-2.48	2.00	2.05
21	7	507	CL7	MG-NB	-2.48	2.00	2.05
32	4	403	ZEX	C21-C26	-2.48	1.50	1.53
21	2	518	CL7	CHC-C4B	2.48	1.45	1.39
21	6	518	CL7	CHC-C4B	2.48	1.45	1.39
21	3	505	CL7	C1C-NC	-2.48	1.34	1.37
21	7	505	CL7	C1C-NC	-2.48	1.34	1.37
21	3	514	CL7	CHC-C4B	2.48	1.45	1.39
21	7	514	CL7	CHC-C4B	2.48	1.45	1.39
21	6	513	CL7	C4C-NC	-2.48	1.34	1.37
23	C	515	8CT	C01-C02	2.47	1.55	1.50
21	c	514	CL7	CHC-C4B	2.47	1.45	1.39
21	3	503	CL7	MG-ND	-2.47	2.00	2.05
21	7	503	CL7	MG-ND	-2.47	2.00	2.05
21	6	508	CL7	C1B-C2B	-2.47	1.37	1.43
21	3	507	CL7	C1B-C2B	-2.47	1.37	1.43
21	5	407	CL7	C1B-C2B	-2.47	1.37	1.43
21	1	409	CL7	CHC-C4B	2.47	1.44	1.39
21	5	409	CL7	CHC-C4B	2.47	1.44	1.39
21	1	410	CL7	C4C-NC	-2.47	1.34	1.37
21	5	410	CL7	C4C-NC	-2.47	1.34	1.37
21	A	403	CL7	C1B-C2B	-2.47	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	403	CL7	C1B-C2B	-2.47	1.37	1.43
21	1	402	CL7	C4C-NC	-2.47	1.34	1.37
21	5	402	CL7	C4C-NC	-2.47	1.34	1.37
21	2	507	CL7	C4C-NC	-2.47	1.34	1.37
21	3	513	CL7	C4C-NC	-2.47	1.34	1.37
21	6	507	CL7	C4C-NC	-2.47	1.34	1.37
21	7	513	CL7	C4C-NC	-2.47	1.34	1.37
21	8	417	CL7	CHC-C4B	2.47	1.44	1.39
21	6	516	CL7	CHC-C4B	2.46	1.44	1.39
21	3	505	CL7	C1B-C2B	-2.46	1.37	1.43
21	7	505	CL7	C1B-C2B	-2.46	1.37	1.43
21	6	503	CL7	O2D-CGD	2.46	1.39	1.33
21	D	402	CL7	CHD-C1D	2.46	1.44	1.39
21	d	402	CL7	CHD-C1D	2.46	1.44	1.39
21	2	503	CL7	MG-ND	-2.46	2.00	2.05
21	3	506	CL7	MG-ND	-2.46	2.00	2.05
21	6	503	CL7	MG-ND	-2.46	2.00	2.05
21	7	506	CL7	MG-ND	-2.46	2.00	2.05
21	C	503	CL7	C1B-C2B	-2.46	1.37	1.43
21	c	503	CL7	C1B-C2B	-2.46	1.37	1.43
21	1	415	CL7	CAB-C3B	2.46	1.50	1.45
21	5	415	CL7	CAB-C3B	2.46	1.50	1.45
21	4	417	CL7	CHC-C4B	2.46	1.44	1.39
21	C	504	CL7	MG-ND	-2.46	2.00	2.05
21	2	506	CL7	MG-ND	-2.46	2.00	2.05
21	6	506	CL7	MG-ND	-2.46	2.00	2.05
21	1	403	CL7	MG-ND	-2.46	2.00	2.05
21	5	403	CL7	MG-ND	-2.46	2.00	2.05
21	d	402	CL7	C4C-NC	-2.46	1.34	1.37
21	C	508	CL7	MG-NB	-2.46	2.00	2.05
21	3	516	CL7	C1C-NC	-2.46	1.34	1.37
21	7	516	CL7	C1C-NC	-2.46	1.34	1.37
21	6	505	CL7	C3B-C4B	-2.46	1.37	1.42
21	4	407	CL7	MG-ND	-2.46	2.00	2.05
21	b	614	CL7	MG-ND	-2.46	2.00	2.05
21	c	508	CL7	MG-NB	-2.45	2.00	2.05
21	7	507	CL7	C1B-C2B	-2.45	1.37	1.43
21	c	511	CL7	C2A-C1A	2.45	1.54	1.50
21	3	515	CL7	CHC-C4B	2.45	1.44	1.39
21	2	505	CL7	C3B-C4B	-2.45	1.37	1.42
21	1	408	CL7	C4C-C3C	-2.45	1.40	1.45
21	4	416	CL7	MG-ND	-2.45	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	416	CL7	CHC-C4B	2.45	1.44	1.39
21	8	416	CL7	CHC-C4B	2.45	1.44	1.39
21	5	408	CL7	C4C-C3C	-2.45	1.40	1.45
21	2	514	CL7	C4C-C3C	-2.45	1.40	1.45
21	6	514	CL7	C4C-C3C	-2.45	1.40	1.45
21	1	418	CL7	C1B-C2B	-2.45	1.37	1.43
21	5	418	CL7	C1B-C2B	-2.45	1.37	1.43
21	A	403	CL7	C1C-NC	-2.45	1.34	1.37
21	a	403	CL7	C1C-NC	-2.45	1.34	1.37
21	5	408	CL7	CHC-C4B	2.45	1.44	1.39
21	b	613	CL7	MG-NB	-2.45	2.00	2.05
21	2	510	CL7	C1B-C2B	-2.45	1.37	1.43
21	6	510	CL7	C1B-C2B	-2.45	1.37	1.43
21	b	607	CL7	MG-ND	-2.45	2.00	2.05
21	B	614	CL7	MG-ND	-2.45	2.00	2.05
21	b	615	CL7	MG-ND	-2.45	2.00	2.05
21	A	406	CL7	C1B-C2B	-2.45	1.37	1.43
21	2	504	CL7	C1B-C2B	-2.45	1.37	1.43
21	6	504	CL7	C1B-C2B	-2.45	1.37	1.43
32	7	520	ZEX	C1-C6	-2.45	1.50	1.53
21	B	611	CL7	C1C-C2C	-2.45	1.40	1.45
21	2	512	CL7	MG-ND	-2.45	2.00	2.05
21	6	512	CL7	MG-ND	-2.45	2.00	2.05
21	1	417	CL7	C1B-C2B	-2.45	1.37	1.43
21	5	417	CL7	C1B-C2B	-2.45	1.37	1.43
21	2	503	CL7	C1B-C2B	-2.45	1.37	1.43
21	4	411	CL7	CHC-C4B	2.45	1.44	1.39
21	8	411	CL7	CHC-C4B	2.45	1.44	1.39
21	3	506	CL7	C4C-NC	-2.45	1.34	1.37
21	3	515	CL7	C4C-NC	-2.45	1.34	1.37
21	7	506	CL7	C4C-NC	-2.45	1.34	1.37
21	7	515	CL7	C4C-NC	-2.45	1.34	1.37
21	3	508	CL7	MG-ND	-2.44	2.00	2.05
21	1	413	CL7	CAB-C3B	2.44	1.50	1.45
21	5	413	CL7	CAB-C3B	2.44	1.50	1.45
21	B	606	CL7	MG-ND	-2.44	2.00	2.05
21	2	516	CL7	C1B-C2B	-2.44	1.37	1.43
21	6	516	CL7	C1B-C2B	-2.44	1.37	1.43
32	5	422	ZEX	C21-C26	-2.44	1.50	1.53
21	B	608	CL7	MG-NB	-2.44	2.00	2.05
21	B	613	CL7	C1B-NB	-2.44	1.34	1.37
21	b	614	CL7	C1B-NB	-2.44	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	505	CL7	MG-ND	-2.44	2.00	2.05
21	7	516	CL7	MG-ND	-2.44	2.00	2.05
21	B	615	CL7	C1C-C2C	-2.44	1.40	1.45
21	b	616	CL7	C1C-C2C	-2.44	1.40	1.45
21	B	612	CL7	MG-NB	-2.44	2.01	2.05
21	7	514	CL7	MG-ND	-2.44	2.01	2.05
21	c	514	CL7	C4C-NC	-2.44	1.34	1.37
21	1	411	CL7	CHC-C4B	2.44	1.44	1.39
21	5	411	CL7	CHC-C4B	2.44	1.44	1.39
21	4	415	CL7	MG-ND	-2.44	2.01	2.05
21	8	415	CL7	MG-ND	-2.44	2.01	2.05
21	3	508	CL7	C1C-C2C	-2.44	1.40	1.45
21	7	506	CL7	C1C-C2C	-2.44	1.40	1.45
21	7	508	CL7	C1C-C2C	-2.44	1.40	1.45
21	4	412	CL7	CHC-C4B	2.44	1.44	1.39
21	8	412	CL7	CHC-C4B	2.44	1.44	1.39
23	K	101	8CT	C30-C29	2.44	1.53	1.50
23	k	101	8CT	C30-C29	2.44	1.53	1.50
21	2	516	CL7	CHC-C4B	2.44	1.44	1.39
21	B	601	CL7	C4C-NC	-2.44	1.34	1.37
21	b	602	CL7	C4C-NC	-2.44	1.34	1.37
21	C	514	CL7	CHD-C1D	2.43	1.44	1.39
21	2	513	CL7	C4C-NC	-2.43	1.34	1.37
21	A	403	CL7	MG-NB	-2.43	2.01	2.05
21	2	503	CL7	O2D-CGD	2.43	1.39	1.33
21	B	608	CL7	C3B-C4B	-2.43	1.37	1.42
21	b	609	CL7	C3B-C4B	-2.43	1.37	1.42
21	7	511	CL7	MG-ND	-2.43	2.01	2.05
21	8	407	CL7	MG-ND	-2.43	2.01	2.05
21	1	408	CL7	CHC-C4B	2.43	1.44	1.39
32	3	522	ZEX	C21-C26	-2.43	1.50	1.53
32	7	522	ZEX	C21-C26	-2.43	1.50	1.53
21	a	405	CL7	C1B-C2B	-2.43	1.37	1.43
21	C	503	CL7	MG-ND	-2.43	2.01	2.05
21	1	406	CL7	MG-ND	-2.43	2.01	2.05
21	c	503	CL7	MG-ND	-2.43	2.01	2.05
21	3	517	CL7	C3B-C4B	-2.43	1.37	1.42
21	D	402	CL7	CHC-C4B	2.43	1.44	1.39
21	d	402	CL7	CHC-C4B	2.43	1.44	1.39
21	1	411	CL7	MG-ND	-2.43	2.01	2.05
21	4	409	CL7	C3B-C4B	-2.43	1.37	1.42
21	c	514	CL7	CHD-C1D	2.43	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	508	CL7	C3B-C4B	-2.43	1.37	1.42
21	b	612	CL7	C3B-C4B	-2.43	1.37	1.42
21	6	508	CL7	C3B-C4B	-2.43	1.37	1.42
21	5	406	CL7	MG-ND	-2.43	2.01	2.05
21	2	514	CL7	C3B-C4B	-2.43	1.37	1.42
21	3	505	CL7	C3B-C4B	-2.43	1.37	1.42
21	6	514	CL7	C3B-C4B	-2.43	1.37	1.42
21	7	505	CL7	C3B-C4B	-2.43	1.37	1.42
21	4	415	CL7	C1C-NC	-2.43	1.34	1.37
21	8	415	CL7	C1C-NC	-2.43	1.34	1.37
21	7	508	CL7	C3B-C4B	-2.43	1.37	1.42
21	b	609	CL7	MG-NB	-2.43	2.01	2.05
21	4	408	CL7	CHC-C4B	2.43	1.44	1.39
21	C	502	CL7	MG-ND	-2.42	2.01	2.05
21	3	501	CL7	MG-ND	-2.42	2.01	2.05
21	c	502	CL7	MG-ND	-2.42	2.01	2.05
21	c	510	CL7	C3B-C4B	-2.42	1.37	1.42
21	1	419	CL7	CHD-C1D	2.42	1.44	1.39
21	5	419	CL7	CHD-C1D	2.42	1.44	1.39
21	B	604	CL7	C1B-C2B	-2.42	1.37	1.43
21	b	605	CL7	C1B-C2B	-2.42	1.37	1.43
21	1	417	CL7	MG-ND	-2.42	2.01	2.05
21	b	613	CL7	C2A-C1A	2.42	1.54	1.50
21	D	405	CL7	MG-ND	-2.42	2.01	2.05
21	a	403	CL7	MG-NB	-2.42	2.01	2.05
21	d	405	CL7	MG-ND	-2.42	2.01	2.05
21	6	507	CL7	MG-NB	-2.42	2.01	2.05
21	7	515	CL7	CHC-C4B	2.42	1.44	1.39
21	3	514	CL7	MG-ND	-2.42	2.01	2.05
21	B	609	CL7	MG-NB	-2.42	2.01	2.05
21	2	514	CL7	MG-NB	-2.42	2.01	2.05
21	b	610	CL7	MG-NB	-2.42	2.01	2.05
21	4	414	CL7	C1B-C2B	-2.42	1.37	1.43
21	8	414	CL7	C1B-C2B	-2.42	1.37	1.43
21	B	612	CL7	C2A-C1A	2.42	1.54	1.50
21	1	410	CL7	C1B-C2B	-2.42	1.37	1.43
21	5	410	CL7	C1B-C2B	-2.42	1.37	1.43
21	C	512	CL7	CHC-C4B	2.42	1.44	1.39
21	c	512	CL7	CHC-C4B	2.42	1.44	1.39
22	A	402	PHO	C4D-CHA	2.42	1.43	1.39
22	a	402	PHO	C4D-CHA	2.42	1.43	1.39
21	C	503	CL7	MG-NB	-2.42	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	c	503	CL7	MG-NB	-2.42	2.01	2.05
21	7	517	CL7	C3B-C4B	-2.42	1.37	1.42
21	6	505	CL7	MG-ND	-2.42	2.01	2.05
21	b	612	CL7	C1C-C2C	-2.42	1.40	1.45
21	C	510	CL7	C3B-C4B	-2.42	1.37	1.42
21	3	514	CL7	CAB-C3B	2.42	1.50	1.45
21	7	514	CL7	CAB-C3B	2.42	1.50	1.45
21	B	603	CL7	MG-ND	-2.42	2.01	2.05
21	b	604	CL7	MG-ND	-2.42	2.01	2.05
21	B	609	CL7	MG-ND	-2.42	2.01	2.05
21	b	610	CL7	MG-ND	-2.42	2.01	2.05
21	5	411	CL7	MG-ND	-2.42	2.01	2.05
21	2	512	CL7	CHC-C4B	2.41	1.44	1.39
21	6	512	CL7	CHC-C4B	2.41	1.44	1.39
21	3	506	CL7	C3B-C4B	-2.41	1.37	1.42
21	7	506	CL7	C3B-C4B	-2.41	1.37	1.42
21	3	515	CL7	MG-ND	-2.41	2.01	2.05
21	4	417	CL7	MG-ND	-2.41	2.01	2.05
21	7	515	CL7	MG-ND	-2.41	2.01	2.05
21	8	417	CL7	MG-ND	-2.41	2.01	2.05
21	3	506	CL7	C1C-C2C	-2.41	1.40	1.45
21	D	402	CL7	C4C-NC	-2.41	1.34	1.37
21	3	509	CL7	C3B-C4B	-2.41	1.37	1.42
21	7	509	CL7	C3B-C4B	-2.41	1.37	1.42
23	K	101	8CT	C28-C29	2.41	1.38	1.32
23	k	101	8CT	C28-C29	2.41	1.38	1.32
21	8	409	CL7	C3B-C4B	-2.41	1.37	1.42
21	2	511	CL7	C1B-C2B	-2.41	1.37	1.43
21	6	511	CL7	C1B-C2B	-2.41	1.37	1.43
21	3	509	CL7	MG-NB	-2.41	2.01	2.05
21	7	509	CL7	MG-NB	-2.41	2.01	2.05
21	2	511	CL7	CHC-C4B	2.41	1.44	1.39
21	3	513	CL7	CHC-C4B	2.41	1.44	1.39
21	7	513	CL7	CHC-C4B	2.41	1.44	1.39
21	D	404	CL7	C1B-NB	-2.41	1.34	1.37
21	6	503	CL7	C1B-C2B	-2.41	1.37	1.43
21	5	406	CL7	CHC-C4B	2.41	1.44	1.39
21	4	410	CL7	MG-ND	-2.41	2.01	2.05
21	B	611	CL7	C3B-C4B	-2.41	1.37	1.42
21	4	408	CL7	C1B-C2B	-2.41	1.37	1.43
21	8	408	CL7	C1B-C2B	-2.41	1.37	1.43
21	1	411	CL7	C1B-C2B	-2.41	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	411	CL7	C1B-C2B	-2.41	1.37	1.43
21	3	516	CL7	C1B-C2B	-2.41	1.37	1.43
21	7	516	CL7	C1B-C2B	-2.41	1.37	1.43
21	B	611	CL7	MG-NB	-2.41	2.01	2.05
21	3	508	CL7	C3B-C4B	-2.41	1.37	1.42
21	2	506	CL7	C1B-C2B	-2.41	1.37	1.43
21	6	506	CL7	C1B-C2B	-2.41	1.37	1.43
21	d	404	CL7	C1B-NB	-2.41	1.34	1.37
21	2	507	CL7	MG-NB	-2.41	2.01	2.05
21	6	518	CL7	MG-ND	-2.41	2.01	2.05
21	3	511	CL7	MG-ND	-2.40	2.01	2.05
21	7	508	CL7	MG-ND	-2.40	2.01	2.05
23	8	402	8CT	C22-C21	2.40	1.55	1.50
21	5	404	CL7	CAB-C3B	2.40	1.50	1.45
21	B	605	CL7	C1C-NC	-2.40	1.34	1.37
21	b	606	CL7	C1C-NC	-2.40	1.34	1.37
21	5	417	CL7	MG-ND	-2.40	2.01	2.05
21	c	505	CL7	CHC-C4B	2.40	1.44	1.39
21	2	508	CL7	C1C-C2C	-2.40	1.40	1.45
21	6	508	CL7	C1C-C2C	-2.40	1.40	1.45
21	B	613	CL7	C3B-C4B	-2.40	1.37	1.42
21	7	501	CL7	MG-ND	-2.40	2.01	2.05
23	K	101	8CT	C01-C02	2.40	1.54	1.50
23	k	101	8CT	C01-C02	2.40	1.54	1.50
21	C	514	CL7	C4C-NC	-2.40	1.34	1.37
21	1	402	CL7	CHC-C4B	2.40	1.44	1.39
21	6	511	CL7	CHC-C4B	2.40	1.44	1.39
23	A	404	8CT	C01-C02	2.40	1.54	1.50
21	B	611	CL7	MG-ND	-2.40	2.01	2.05
21	4	416	CL7	C1B-C2B	-2.40	1.37	1.43
21	8	416	CL7	C1B-C2B	-2.40	1.37	1.43
21	8	408	CL7	CHC-C4B	2.40	1.44	1.39
21	b	606	CL7	CHC-C4B	2.40	1.44	1.39
21	2	508	CL7	MG-ND	-2.40	2.01	2.05
21	6	508	CL7	MG-ND	-2.40	2.01	2.05
21	1	414	CL7	CHD-C1D	2.40	1.44	1.39
21	5	414	CL7	CHD-C1D	2.40	1.44	1.39
21	3	516	CL7	MG-ND	-2.40	2.01	2.05
21	8	413	CL7	C1B-NB	-2.40	1.34	1.37
21	6	509	CL7	C3B-C4B	-2.39	1.37	1.42
21	B	613	CL7	C2A-C1A	2.39	1.54	1.50
21	b	614	CL7	C2A-C1A	2.39	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	509	CL7	C3B-C4B	-2.39	1.37	1.42
21	2	505	CL7	CHC-C4B	2.39	1.44	1.39
21	6	505	CL7	CHC-C4B	2.39	1.44	1.39
21	1	407	CL7	MG-ND	-2.39	2.01	2.05
21	5	407	CL7	MG-ND	-2.39	2.01	2.05
21	D	404	CL7	C3B-C4B	-2.39	1.37	1.42
21	5	418	CL7	C1C-NC	-2.39	1.34	1.37
21	b	602	CL7	CHC-C4B	2.39	1.44	1.39
21	2	505	CL7	C1B-C2B	-2.39	1.37	1.43
21	4	407	CL7	C4C-NC	-2.39	1.34	1.37
21	8	407	CL7	C4C-NC	-2.39	1.34	1.37
21	3	513	CL7	C1B-C2B	-2.39	1.37	1.43
21	7	513	CL7	C1B-C2B	-2.39	1.37	1.43
21	1	412	CL7	CAB-C3B	2.39	1.50	1.45
21	5	412	CL7	CAB-C3B	2.39	1.50	1.45
21	4	404	CL7	MG-ND	-2.39	2.01	2.05
21	8	404	CL7	MG-ND	-2.39	2.01	2.05
21	1	410	CL7	MG-ND	-2.39	2.01	2.05
21	5	410	CL7	MG-ND	-2.39	2.01	2.05
21	C	513	CL7	C1B-C2B	-2.39	1.37	1.43
21	c	513	CL7	C1B-C2B	-2.39	1.37	1.43
21	C	505	CL7	CHC-C4B	2.39	1.44	1.39
21	4	404	CL7	CHC-C4B	2.39	1.44	1.39
21	8	404	CL7	CHC-C4B	2.39	1.44	1.39
21	c	505	CL7	C1B-C2B	-2.39	1.37	1.43
21	B	605	CL7	CHC-C4B	2.38	1.44	1.39
21	5	413	CL7	CHC-C4B	2.38	1.44	1.39
21	2	518	CL7	MG-ND	-2.38	2.01	2.05
21	B	613	CL7	C1C-NC	-2.38	1.34	1.37
21	b	614	CL7	C1C-NC	-2.38	1.34	1.37
21	b	612	CL7	MG-ND	-2.38	2.01	2.05
21	B	615	CL7	C1B-C2B	-2.38	1.37	1.43
21	2	516	CL7	C1C-NC	-2.38	1.34	1.37
21	6	516	CL7	C1C-NC	-2.38	1.34	1.37
21	1	406	CL7	CHC-C4B	2.38	1.44	1.39
21	8	410	CL7	MG-ND	-2.38	2.01	2.05
21	7	518	CL7	CHD-C1D	2.38	1.44	1.39
21	4	408	CL7	MG-ND	-2.38	2.01	2.05
21	3	507	CL7	CHC-C4B	2.38	1.44	1.39
21	7	507	CL7	CHC-C4B	2.38	1.44	1.39
21	3	501	CL7	CHC-C4B	2.38	1.44	1.39
21	7	501	CL7	CHC-C4B	2.38	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	514	CL7	C4C-NC	-2.38	1.34	1.37
21	7	514	CL7	C4C-NC	-2.38	1.34	1.37
23	a	404	8CT	C01-C02	2.37	1.54	1.50
21	6	508	CL7	MG-NB	-2.37	2.01	2.05
21	2	503	CL7	CHC-C4B	2.37	1.44	1.39
21	6	503	CL7	CHC-C4B	2.37	1.44	1.39
21	d	404	CL7	C3B-C4B	-2.37	1.37	1.42
21	B	610	CL7	MG-NB	-2.37	2.01	2.05
21	b	611	CL7	MG-NB	-2.37	2.01	2.05
21	A	401	CL7	CHD-C1D	2.37	1.44	1.39
21	3	508	CL7	MG-NB	-2.37	2.01	2.05
21	7	508	CL7	MG-NB	-2.37	2.01	2.05
21	C	505	CL7	C1B-C2B	-2.37	1.37	1.43
21	B	601	CL7	CHC-C4B	2.37	1.44	1.39
21	1	404	CL7	CAB-C3B	2.37	1.50	1.45
21	6	514	CL7	MG-NB	-2.37	2.01	2.05
21	2	509	CL7	CHC-C4B	2.37	1.44	1.39
21	6	509	CL7	CHC-C4B	2.37	1.44	1.39
21	1	417	CL7	C2A-C1A	2.37	1.54	1.50
21	5	417	CL7	C2A-C1A	2.37	1.54	1.50
21	B	602	CL7	MG-ND	-2.37	2.01	2.05
21	c	506	CL7	MG-NB	-2.37	2.01	2.05
21	1	409	CL7	C1B-C2B	-2.37	1.37	1.43
21	5	409	CL7	C1B-C2B	-2.37	1.37	1.43
21	C	507	CL7	CHC-C4B	2.37	1.44	1.39
21	c	507	CL7	CHC-C4B	2.37	1.44	1.39
21	4	406	CL7	C1B-C2B	-2.37	1.37	1.43
21	8	406	CL7	C1B-C2B	-2.37	1.37	1.43
21	c	502	CL7	CHC-C4B	2.37	1.44	1.39
21	4	416	CL7	C4C-NC	-2.37	1.34	1.37
21	8	416	CL7	C4C-NC	-2.37	1.34	1.37
21	5	402	CL7	CHC-C4B	2.37	1.44	1.39
21	1	409	CL7	C4C-NC	-2.37	1.34	1.37
21	5	409	CL7	C4C-NC	-2.37	1.34	1.37
21	B	610	CL7	C2A-C1A	2.37	1.54	1.50
21	4	415	CL7	C1B-C2B	-2.37	1.37	1.43
21	8	415	CL7	C1B-C2B	-2.37	1.37	1.43
21	1	402	CL7	MG-ND	-2.37	2.01	2.05
21	4	406	CL7	MG-NB	-2.37	2.01	2.05
21	8	406	CL7	MG-NB	-2.37	2.01	2.05
21	1	408	CL7	CHD-C1D	2.37	1.44	1.39
21	5	408	CL7	CHD-C1D	2.37	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	401	CL7	CHD-C1D	2.37	1.44	1.39
21	4	404	CL7	MG-NB	-2.37	2.01	2.05
21	d	404	CL7	MG-NB	-2.37	2.01	2.05
21	8	404	CL7	MG-NB	-2.37	2.01	2.05
21	1	407	CL7	CHC-C4B	2.36	1.44	1.39
21	5	407	CL7	CHC-C4B	2.36	1.44	1.39
21	b	612	CL7	MG-NB	-2.36	2.01	2.05
23	4	402	8CT	C01-C02	2.36	1.54	1.50
23	8	402	8CT	C01-C02	2.36	1.54	1.50
21	B	607	CL7	CHC-C4B	2.36	1.44	1.39
21	b	608	CL7	CHC-C4B	2.36	1.44	1.39
21	2	518	CL7	CAB-C3B	2.36	1.50	1.45
21	6	518	CL7	CAB-C3B	2.36	1.50	1.45
21	6	505	CL7	C1B-C2B	-2.36	1.37	1.43
21	C	502	CL7	CHC-C4B	2.36	1.44	1.39
21	2	503	CL7	C1C-NC	-2.36	1.34	1.37
21	7	515	CL7	CAB-C3B	2.36	1.50	1.45
21	2	508	CL7	MG-NB	-2.36	2.01	2.05
21	2	502	CL7	C3B-C4B	-2.36	1.37	1.42
21	6	502	CL7	C3B-C4B	-2.36	1.37	1.42
23	4	402	8CT	C22-C21	2.36	1.55	1.50
21	4	405	CL7	MG-ND	-2.36	2.01	2.05
21	8	405	CL7	MG-ND	-2.36	2.01	2.05
21	b	616	CL7	C1B-C2B	-2.36	1.37	1.43
21	b	614	CL7	C3B-C4B	-2.36	1.37	1.42
21	b	611	CL7	C2A-C1A	2.36	1.54	1.50
21	4	412	CL7	C1B-C2B	-2.36	1.37	1.43
21	8	412	CL7	C1B-C2B	-2.36	1.37	1.43
21	3	511	CL7	MG-NB	-2.36	2.01	2.05
21	5	404	CL7	CHD-C1D	2.36	1.44	1.39
21	C	513	CL7	CHC-C4B	2.36	1.44	1.39
21	c	513	CL7	CHC-C4B	2.36	1.44	1.39
21	1	419	CL7	C4C-NC	-2.35	1.34	1.37
21	5	419	CL7	C4C-NC	-2.35	1.34	1.37
21	4	407	CL7	MG-NB	-2.35	2.01	2.05
21	8	408	CL7	MG-ND	-2.35	2.01	2.05
21	4	414	CL7	CHC-C4B	2.35	1.44	1.39
21	8	414	CL7	CHC-C4B	2.35	1.44	1.39
23	B	618	8CT	C22-C21	2.35	1.55	1.50
23	b	619	8CT	C22-C21	2.35	1.55	1.50
21	C	506	CL7	MG-NB	-2.35	2.01	2.05
21	2	509	CL7	C2A-C1A	2.35	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	509	CL7	C2A-C1A	2.35	1.54	1.50
21	1	404	CL7	CHD-C1D	2.35	1.44	1.39
21	5	416	CL7	CHD-C1D	2.35	1.44	1.39
21	1	420	CL7	CAB-C3B	2.35	1.50	1.45
21	5	420	CL7	CAB-C3B	2.35	1.50	1.45
21	3	515	CL7	CAB-C3B	2.35	1.50	1.45
21	1	405	CL7	CHC-C4B	2.35	1.44	1.39
21	5	405	CL7	CHC-C4B	2.35	1.44	1.39
21	2	515	CL7	MG-ND	-2.35	2.01	2.05
21	6	515	CL7	MG-ND	-2.35	2.01	2.05
21	2	513	CL7	CHD-C1D	2.35	1.44	1.39
21	C	507	CL7	C3B-C4B	-2.35	1.37	1.42
21	7	510	CL7	MG-NB	-2.35	2.01	2.05
21	6	513	CL7	CHD-C1D	2.35	1.44	1.39
21	D	405	CL7	C1B-C2B	-2.35	1.37	1.43
21	d	405	CL7	C1B-C2B	-2.35	1.37	1.43
23	D	406	8CT	C22-C21	2.35	1.55	1.50
23	d	406	8CT	C22-C21	2.35	1.55	1.50
21	b	603	CL7	MG-ND	-2.35	2.01	2.05
21	a	403	CL7	CHC-C4B	2.35	1.44	1.39
21	C	504	CL7	CHC-C4B	2.35	1.44	1.39
31	F	101	HEM	C4B-NB	-2.35	1.34	1.38
31	f	101	HEM	C4B-NB	-2.35	1.34	1.38
21	B	613	CL7	MG-NB	-2.35	2.01	2.05
21	b	614	CL7	MG-NB	-2.35	2.01	2.05
23	D	406	8CT	C01-C02	2.34	1.54	1.50
23	d	406	8CT	C01-C02	2.34	1.54	1.50
21	7	511	CL7	MG-NB	-2.34	2.01	2.05
21	2	501	CL7	C3B-C4B	-2.34	1.37	1.42
21	2	513	CL7	C1C-C2C	-2.34	1.40	1.45
21	6	513	CL7	C1C-C2C	-2.34	1.40	1.45
21	1	413	CL7	CHC-C4B	2.34	1.44	1.39
21	3	509	CL7	CHC-C4B	2.34	1.44	1.39
21	7	509	CL7	CHC-C4B	2.34	1.44	1.39
21	1	405	CL7	C1B-C2B	-2.34	1.37	1.43
21	5	405	CL7	C1B-C2B	-2.34	1.37	1.43
21	C	504	CL7	CAB-C3B	2.34	1.50	1.45
21	c	504	CL7	CAB-C3B	2.34	1.50	1.45
21	5	402	CL7	MG-ND	-2.34	2.01	2.05
21	3	514	CL7	C1C-NC	-2.34	1.34	1.37
21	7	514	CL7	C1C-NC	-2.34	1.34	1.37
21	B	603	CL7	MG-NB	-2.34	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	507	CL7	CHD-C1D	2.34	1.44	1.39
21	6	507	CL7	CHD-C1D	2.34	1.44	1.39
21	6	507	CL7	C1C-C2C	-2.34	1.40	1.45
21	4	413	CL7	C1B-NB	-2.34	1.34	1.37
21	3	518	CL7	CHD-C1D	2.34	1.44	1.39
21	B	622	CL7	CHD-C1D	2.33	1.44	1.39
21	2	513	CL7	CHC-C4B	2.33	1.44	1.39
21	3	503	CL7	CHC-C4B	2.33	1.44	1.39
21	6	513	CL7	CHC-C4B	2.33	1.44	1.39
21	7	503	CL7	CHC-C4B	2.33	1.44	1.39
21	4	409	CL7	MG-NB	-2.33	2.01	2.05
21	8	409	CL7	MG-NB	-2.33	2.01	2.05
21	c	507	CL7	C3B-C4B	-2.33	1.37	1.42
21	7	513	CL7	MG-ND	-2.33	2.01	2.05
21	8	407	CL7	MG-NB	-2.33	2.01	2.05
21	B	609	CL7	CHD-C1D	2.33	1.44	1.39
21	2	501	CL7	CHC-C4B	2.33	1.44	1.39
21	b	610	CL7	CHD-C1D	2.33	1.44	1.39
21	6	501	CL7	CHC-C4B	2.33	1.44	1.39
21	b	617	CL7	MG-ND	-2.33	2.01	2.05
21	4	410	CL7	C3B-C4B	-2.33	1.37	1.42
21	8	410	CL7	C3B-C4B	-2.33	1.37	1.42
21	C	508	CL7	C1C-C2C	-2.33	1.40	1.45
21	c	508	CL7	C1C-C2C	-2.33	1.40	1.45
21	2	517	CL7	CHC-C4B	2.33	1.44	1.39
21	6	517	CL7	CHC-C4B	2.33	1.44	1.39
21	C	512	CL7	C1B-C2B	-2.33	1.37	1.43
21	c	512	CL7	C1B-C2B	-2.33	1.37	1.43
21	4	405	CL7	CHC-C4B	2.33	1.44	1.39
21	8	405	CL7	CHC-C4B	2.33	1.44	1.39
21	3	510	CL7	MG-NB	-2.33	2.01	2.05
21	6	516	CL7	MG-NB	-2.33	2.01	2.05
21	c	504	CL7	CHC-C4B	2.33	1.44	1.39
21	5	402	CL7	CAB-C3B	2.33	1.50	1.45
21	D	404	CL7	MG-NB	-2.33	2.01	2.05
21	B	616	CL7	CHC-C4B	2.33	1.44	1.39
21	1	412	CL7	CHC-C4B	2.33	1.44	1.39
21	b	617	CL7	CHC-C4B	2.33	1.44	1.39
21	5	412	CL7	CHC-C4B	2.33	1.44	1.39
21	C	509	CL7	C3B-C4B	-2.33	1.37	1.42
21	c	509	CL7	C3B-C4B	-2.33	1.37	1.42
23	B	617	8CT	C01-C02	2.33	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	503	CL7	C1C-C2C	-2.33	1.40	1.45
21	c	503	CL7	C1C-C2C	-2.33	1.40	1.45
21	2	515	CL7	C4C-NC	-2.33	1.34	1.37
21	6	515	CL7	C4C-NC	-2.33	1.34	1.37
21	6	503	CL7	C1C-NC	-2.33	1.34	1.37
21	1	402	CL7	CAB-C3B	2.32	1.50	1.45
21	7	517	CL7	CHC-C4B	2.32	1.44	1.39
23	b	618	8CT	C01-C02	2.32	1.54	1.50
21	3	518	CL7	MG-ND	-2.32	2.01	2.05
21	2	507	CL7	C1C-C2C	-2.32	1.40	1.45
21	3	516	CL7	CHD-C1D	2.32	1.44	1.39
21	7	516	CL7	CHD-C1D	2.32	1.44	1.39
21	1	408	CL7	C3B-C4B	-2.32	1.37	1.42
21	5	408	CL7	C3B-C4B	-2.32	1.37	1.42
21	1	416	CL7	CHD-C1D	2.32	1.44	1.39
21	2	514	CL7	CHD-C1D	2.32	1.44	1.39
21	6	514	CL7	CHD-C1D	2.32	1.44	1.39
21	2	510	CL7	CHC-C4B	2.32	1.44	1.39
21	6	510	CL7	CHC-C4B	2.32	1.44	1.39
21	3	513	CL7	MG-ND	-2.32	2.01	2.05
21	3	511	CL7	C1B-NB	-2.32	1.34	1.37
21	7	511	CL7	C1B-NB	-2.32	1.34	1.37
21	B	609	CL7	CHC-C4B	2.32	1.44	1.39
21	4	407	CL7	C1B-C2B	-2.32	1.37	1.43
21	8	407	CL7	C1B-C2B	-2.32	1.37	1.43
21	6	503	CL7	MG-NB	-2.32	2.01	2.05
21	3	511	CL7	CHC-C4B	2.32	1.44	1.39
21	7	511	CL7	CHC-C4B	2.32	1.44	1.39
21	1	418	CL7	C1C-NC	-2.32	1.34	1.37
21	B	616	CL7	MG-ND	-2.32	2.01	2.05
21	A	403	CL7	CHC-C4B	2.31	1.44	1.39
21	1	413	CL7	MG-ND	-2.31	2.01	2.05
21	1	416	CL7	OBD-CAD	2.31	1.26	1.22
21	5	416	CL7	OBD-CAD	2.31	1.26	1.22
21	6	501	CL7	C3B-C4B	-2.31	1.37	1.42
21	3	504	CL7	MG-ND	-2.31	2.01	2.05
21	7	504	CL7	MG-ND	-2.31	2.01	2.05
21	2	504	CL7	C3B-C4B	-2.31	1.37	1.42
21	6	504	CL7	C3B-C4B	-2.31	1.37	1.42
21	B	607	CL7	CHD-C1D	2.31	1.44	1.39
21	b	608	CL7	CHD-C1D	2.31	1.44	1.39
21	3	517	CL7	CHC-C4B	2.31	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	408	CL7	MG-ND	-2.31	2.01	2.05
21	5	408	CL7	MG-ND	-2.31	2.01	2.05
21	2	506	CL7	C1C-NC	-2.31	1.34	1.37
21	6	506	CL7	C1C-NC	-2.31	1.34	1.37
21	2	516	CL7	MG-NB	-2.31	2.01	2.05
21	b	623	CL7	CHD-C1D	2.31	1.44	1.39
21	5	415	CL7	CHD-C1D	2.31	1.44	1.39
21	C	518	CL7	C3B-C4B	-2.31	1.37	1.42
21	c	518	CL7	C3B-C4B	-2.31	1.37	1.42
21	1	418	CL7	MG-NB	-2.31	2.01	2.05
21	b	604	CL7	MG-NB	-2.31	2.01	2.05
21	7	518	CL7	MG-ND	-2.31	2.01	2.05
21	C	509	CL7	MG-NB	-2.31	2.01	2.05
23	d	406	8CT	C38-C31	2.31	1.54	1.50
21	7	512	CL7	CHC-C4B	2.31	1.44	1.39
21	1	415	CL7	CHD-C1D	2.31	1.44	1.39
21	C	503	CL7	C1C-NC	-2.31	1.34	1.37
21	c	503	CL7	C1C-NC	-2.31	1.34	1.37
21	d	405	CL7	MG-NB	-2.30	2.01	2.05
21	6	512	CL7	MG-NB	-2.30	2.01	2.05
32	3	522	ZEX	C1-C6	-2.30	1.50	1.53
32	7	522	ZEX	C1-C6	-2.30	1.50	1.53
21	A	401	CL7	OBD-CAD	2.30	1.26	1.22
21	3	506	CL7	CHD-C1D	2.30	1.44	1.39
21	7	506	CL7	CHD-C1D	2.30	1.44	1.39
21	4	413	CL7	MG-NB	-2.30	2.01	2.05
21	8	413	CL7	MG-NB	-2.30	2.01	2.05
21	2	506	CL7	CHC-C4B	2.30	1.44	1.39
21	6	506	CL7	CHC-C4B	2.30	1.44	1.39
21	B	604	CL7	C1C-C2C	-2.30	1.40	1.45
21	b	605	CL7	C1C-C2C	-2.30	1.40	1.45
21	C	503	CL7	CHC-C4B	2.30	1.44	1.39
21	c	503	CL7	CHC-C4B	2.30	1.44	1.39
21	2	514	CL7	C1C-C2C	-2.30	1.40	1.45
21	1	410	CL7	CHD-C1D	2.30	1.44	1.39
21	5	410	CL7	CHD-C1D	2.30	1.44	1.39
21	1	406	CL7	C3B-C4B	-2.30	1.37	1.42
21	5	406	CL7	C3B-C4B	-2.30	1.37	1.42
21	B	610	CL7	C1C-NC	-2.30	1.35	1.37
21	b	611	CL7	C1C-NC	-2.30	1.35	1.37
21	3	512	CL7	C1B-NB	-2.30	1.35	1.37
23	C	516	8CT	C22-C21	2.30	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	516	8CT	C22-C21	2.30	1.55	1.50
21	5	418	CL7	MG-NB	-2.30	2.01	2.05
21	4	406	CL7	CHC-C4B	2.30	1.44	1.39
21	8	406	CL7	CHC-C4B	2.30	1.44	1.39
21	2	505	CL7	MG-NB	-2.30	2.01	2.05
21	6	505	CL7	MG-NB	-2.30	2.01	2.05
21	3	516	CL7	CHC-C4B	2.30	1.44	1.39
21	2	501	CL7	C1B-C2B	-2.30	1.37	1.43
21	6	501	CL7	C1B-C2B	-2.30	1.37	1.43
21	2	506	CL7	C3B-C4B	-2.30	1.37	1.42
21	6	506	CL7	C3B-C4B	-2.30	1.37	1.42
21	1	406	CL7	MG-NB	-2.30	2.01	2.05
21	2	503	CL7	MG-NB	-2.30	2.01	2.05
21	4	416	CL7	MG-NB	-2.30	2.01	2.05
21	8	416	CL7	MG-NB	-2.30	2.01	2.05
21	4	410	CL7	MG-NB	-2.29	2.01	2.05
21	A	406	CL7	CHC-C4B	2.29	1.44	1.39
21	4	411	CL7	CHD-C1D	2.29	1.44	1.39
21	a	405	CL7	CHC-C4B	2.29	1.44	1.39
21	8	411	CL7	CHD-C1D	2.29	1.44	1.39
21	B	615	CL7	C1C-NC	-2.29	1.35	1.37
21	b	616	CL7	C1C-NC	-2.29	1.35	1.37
32	3	522	ZEX	C10-C9	-2.29	1.32	1.35
32	7	522	ZEX	C10-C9	-2.29	1.32	1.35
21	b	615	CL7	C3B-C4B	-2.29	1.37	1.42
21	1	414	CL7	CAB-C3B	2.29	1.50	1.45
21	5	414	CL7	CAB-C3B	2.29	1.50	1.45
21	4	405	CL7	C1B-C2B	-2.29	1.37	1.43
21	2	518	CL7	C1B-C2B	-2.29	1.37	1.43
21	6	518	CL7	C1B-C2B	-2.29	1.37	1.43
21	B	611	CL7	C1C-NC	-2.29	1.35	1.37
21	b	612	CL7	C1C-NC	-2.29	1.35	1.37
21	3	501	CL7	C1B-C2B	-2.29	1.37	1.43
21	7	501	CL7	C1B-C2B	-2.29	1.37	1.43
21	C	509	CL7	CHC-C4B	2.29	1.44	1.39
21	2	507	CL7	C1B-C2B	-2.29	1.37	1.43
21	6	507	CL7	C1B-C2B	-2.29	1.37	1.43
21	B	614	CL7	C3B-C4B	-2.29	1.37	1.42
21	c	509	CL7	MG-NB	-2.29	2.01	2.05
21	c	504	CL7	C1B-C2B	-2.29	1.37	1.43
21	7	503	CL7	MG-NB	-2.29	2.01	2.05
21	7	502	CL7	CHD-C1D	2.29	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	618	8CT	C01-C02	2.29	1.54	1.50
23	b	619	8CT	C01-C02	2.29	1.54	1.50
21	D	405	CL7	MG-NB	-2.29	2.01	2.05
32	6	520	ZEX	C21-C26	-2.29	1.50	1.53
21	1	403	CL7	CHC-C4B	2.29	1.44	1.39
21	5	403	CL7	CHC-C4B	2.29	1.44	1.39
21	7	506	CL7	C1B-C2B	-2.29	1.37	1.43
21	a	401	CL7	OBD-CAD	2.29	1.26	1.22
21	B	606	CL7	CHC-C4B	2.29	1.44	1.39
21	2	504	CL7	CHC-C4B	2.29	1.44	1.39
21	2	515	CL7	CHC-C4B	2.29	1.44	1.39
21	3	512	CL7	CHC-C4B	2.29	1.44	1.39
21	b	607	CL7	CHC-C4B	2.29	1.44	1.39
21	6	504	CL7	CHC-C4B	2.29	1.44	1.39
21	6	515	CL7	CHC-C4B	2.29	1.44	1.39
21	D	405	CL7	C3B-C4B	-2.29	1.37	1.42
21	d	405	CL7	C3B-C4B	-2.29	1.37	1.42
21	1	405	CL7	MG-ND	-2.28	2.01	2.05
21	5	405	CL7	MG-ND	-2.28	2.01	2.05
21	8	416	CL7	CHD-C1D	2.28	1.44	1.39
21	3	516	CL7	C2A-C1A	2.28	1.54	1.50
21	7	516	CL7	C2A-C1A	2.28	1.54	1.50
21	3	514	CL7	C1B-C2B	-2.28	1.37	1.43
21	7	514	CL7	C1B-C2B	-2.28	1.37	1.43
21	C	506	CL7	C1C-C2C	-2.28	1.40	1.45
21	c	506	CL7	C1C-C2C	-2.28	1.40	1.45
21	b	610	CL7	CHC-C4B	2.28	1.44	1.39
21	1	411	CL7	CAB-C3B	2.28	1.50	1.45
21	C	506	CL7	C1B-C2B	-2.28	1.37	1.43
21	c	506	CL7	C1B-C2B	-2.28	1.37	1.43
21	7	516	CL7	CHC-C4B	2.28	1.44	1.39
21	4	404	CL7	C1C-C2C	-2.28	1.40	1.45
21	8	404	CL7	C1C-C2C	-2.28	1.40	1.45
21	A	403	CL7	C3B-C4B	-2.28	1.37	1.42
21	a	403	CL7	C3B-C4B	-2.28	1.37	1.42
21	5	406	CL7	MG-NB	-2.28	2.01	2.05
21	B	622	CL7	CAB-C3B	2.28	1.50	1.45
21	b	623	CL7	CAB-C3B	2.28	1.50	1.45
21	4	416	CL7	CHD-C1D	2.28	1.44	1.39
21	2	505	CL7	C1B-NB	-2.28	1.35	1.37
21	2	502	CL7	CHC-C4B	2.28	1.44	1.39
21	1	404	CL7	MG-ND	-2.28	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	404	CL7	MG-ND	-2.28	2.01	2.05
21	3	516	CL7	C3B-C4B	-2.28	1.37	1.42
21	7	516	CL7	C3B-C4B	-2.28	1.37	1.42
21	A	401	CL7	CAA-C2A	-2.28	1.49	1.54
21	6	505	CL7	C1B-NB	-2.28	1.35	1.37
21	B	610	CL7	CHC-C4B	2.28	1.44	1.39
21	b	611	CL7	CHC-C4B	2.28	1.44	1.39
21	3	511	CL7	C1C-C2C	-2.28	1.40	1.45
21	7	511	CL7	C1C-C2C	-2.28	1.40	1.45
21	A	403	CL7	CAB-C3B	2.28	1.50	1.45
21	a	403	CL7	CAB-C3B	2.28	1.50	1.45
21	2	512	CL7	MG-NB	-2.28	2.01	2.05
21	A	406	CL7	C1C-NC	-2.28	1.35	1.37
21	a	405	CL7	C1C-NC	-2.28	1.35	1.37
21	1	408	CL7	C1B-C2B	-2.28	1.37	1.43
21	a	401	CL7	CAA-C2A	-2.27	1.49	1.54
21	B	606	CL7	C1C-C2C	-2.27	1.40	1.45
21	b	607	CL7	C1C-C2C	-2.27	1.40	1.45
21	8	410	CL7	MG-NB	-2.27	2.01	2.05
21	B	602	CL7	MG-NB	-2.27	2.01	2.05
21	b	603	CL7	MG-NB	-2.27	2.01	2.05
21	B	606	CL7	CHD-C1D	2.27	1.44	1.39
21	b	607	CL7	CHD-C1D	2.27	1.44	1.39
21	7	518	CL7	C1B-C2B	-2.27	1.37	1.43
23	D	406	8CT	C38-C31	2.27	1.54	1.50
21	4	415	CL7	CHC-C4B	2.27	1.44	1.39
21	8	415	CL7	CHC-C4B	2.27	1.44	1.39
21	C	504	CL7	C1B-C2B	-2.27	1.37	1.43
21	3	516	CL7	C1C-C2C	-2.27	1.40	1.45
21	7	516	CL7	C1C-C2C	-2.27	1.40	1.45
21	1	404	CL7	C1B-C2B	-2.27	1.37	1.43
21	5	404	CL7	C1B-C2B	-2.27	1.37	1.43
21	2	504	CL7	CHD-C1D	2.27	1.44	1.39
21	6	504	CL7	CHD-C1D	2.27	1.44	1.39
21	3	510	CL7	C1C-NC	-2.27	1.35	1.37
21	3	501	CL7	C3B-C4B	-2.27	1.37	1.42
21	7	501	CL7	C3B-C4B	-2.27	1.37	1.42
21	5	413	CL7	MG-ND	-2.27	2.01	2.05
21	1	402	CL7	C1B-C2B	-2.27	1.37	1.43
21	5	402	CL7	C1B-C2B	-2.27	1.37	1.43
21	C	505	CL7	CHD-C1D	2.27	1.44	1.39
21	c	505	CL7	CHD-C1D	2.27	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	3	519	ZEX	C10-C9	-2.27	1.32	1.35
32	7	519	ZEX	C10-C9	-2.27	1.32	1.35
21	3	502	CL7	CHD-C1D	2.27	1.44	1.39
21	B	605	CL7	C1C-C2C	-2.27	1.40	1.45
21	b	606	CL7	C1C-C2C	-2.27	1.40	1.45
21	3	506	CL7	C1B-C2B	-2.27	1.37	1.43
21	8	404	CL7	CAB-C3B	2.27	1.50	1.45
21	C	507	CL7	C1C-NC	-2.26	1.35	1.37
21	1	409	CL7	C1C-C2C	-2.26	1.40	1.45
21	5	409	CL7	C1C-C2C	-2.26	1.40	1.45
21	8	416	CL7	CAB-C3B	2.26	1.50	1.45
21	4	413	CL7	CHC-C4B	2.26	1.44	1.39
21	8	413	CL7	CHC-C4B	2.26	1.44	1.39
21	4	412	CL7	C1C-NC	-2.26	1.35	1.37
21	6	512	CL7	CAB-C3B	2.26	1.50	1.45
32	8	418	ZEX	C21-C26	-2.26	1.50	1.53
21	4	405	CL7	CAB-C3B	2.26	1.50	1.45
21	8	405	CL7	CAB-C3B	2.26	1.50	1.45
21	B	613	CL7	CHC-C4B	2.26	1.44	1.39
21	b	614	CL7	CHC-C4B	2.26	1.44	1.39
21	2	512	CL7	C1B-C2B	-2.26	1.37	1.43
21	6	512	CL7	C1B-C2B	-2.26	1.37	1.43
21	D	405	CL7	CAB-C3B	2.26	1.49	1.45
21	d	405	CL7	CAB-C3B	2.26	1.49	1.45
21	7	510	CL7	C1C-NC	-2.26	1.35	1.37
21	1	410	CL7	CHC-C4B	2.26	1.44	1.39
21	5	410	CL7	CHC-C4B	2.26	1.44	1.39
21	1	405	CL7	CHD-C1D	2.26	1.44	1.39
21	5	405	CL7	CHD-C1D	2.26	1.44	1.39
21	8	405	CL7	C1B-C2B	-2.26	1.37	1.43
21	2	514	CL7	CHC-C4B	2.26	1.44	1.39
21	6	514	CL7	CHC-C4B	2.26	1.44	1.39
23	d	406	8CT	C30-C29	2.26	1.53	1.50
21	c	509	CL7	CHC-C4B	2.26	1.44	1.39
21	6	514	CL7	C1C-C2C	-2.26	1.40	1.45
21	3	515	CL7	C1B-C2B	-2.26	1.37	1.43
21	7	515	CL7	C1B-C2B	-2.26	1.37	1.43
21	B	605	CL7	C2A-C1A	2.26	1.54	1.50
21	b	606	CL7	C2A-C1A	2.26	1.54	1.50
21	1	414	CL7	C4C-NC	-2.26	1.35	1.37
21	5	414	CL7	C4C-NC	-2.26	1.35	1.37
21	3	518	CL7	C1B-C2B	-2.26	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	503	CL7	MG-NB	-2.26	2.01	2.05
21	2	509	CL7	C1C-NC	-2.26	1.35	1.37
21	5	417	CL7	CHD-C1D	2.26	1.44	1.39
21	3	504	CL7	CHC-C4B	2.25	1.44	1.39
21	6	506	CL7	CHD-C1D	2.25	1.44	1.39
21	7	504	CL7	CHC-C4B	2.25	1.44	1.39
21	8	410	CL7	CHC-C4B	2.25	1.44	1.39
21	3	503	CL7	C1B-C2B	-2.25	1.37	1.43
21	2	502	CL7	MG-NB	-2.25	2.01	2.05
21	1	419	CL7	MG-ND	-2.25	2.01	2.05
21	5	419	CL7	MG-ND	-2.25	2.01	2.05
21	3	504	CL7	C1C-NC	-2.25	1.35	1.37
21	3	506	CL7	C1C-NC	-2.25	1.35	1.37
21	7	504	CL7	C1C-NC	-2.25	1.35	1.37
21	7	506	CL7	C1C-NC	-2.25	1.35	1.37
21	6	502	CL7	CHC-C4B	2.25	1.44	1.39
21	c	514	CL7	C1B-C2B	-2.25	1.38	1.43
21	1	417	CL7	CHD-C1D	2.25	1.44	1.39
21	3	501	CL7	C1C-NC	-2.25	1.35	1.37
21	1	418	CL7	C3B-C4B	-2.25	1.37	1.42
21	5	418	CL7	C3B-C4B	-2.25	1.37	1.42
21	1	418	CL7	CHC-C4B	2.25	1.44	1.39
21	5	418	CL7	CHC-C4B	2.25	1.44	1.39
21	6	513	CL7	C1B-C2B	-2.25	1.38	1.43
21	b	602	CL7	C3B-C4B	-2.25	1.37	1.42
21	C	512	CL7	CHD-C1D	2.25	1.44	1.39
21	B	602	CL7	C3B-C4B	-2.25	1.37	1.42
21	b	603	CL7	C3B-C4B	-2.25	1.37	1.42
21	B	614	CL7	C1C-C2C	-2.25	1.40	1.45
21	D	402	CL7	MG-ND	-2.25	2.01	2.05
21	d	402	CL7	MG-ND	-2.25	2.01	2.05
21	6	502	CL7	MG-NB	-2.25	2.01	2.05
21	C	518	CL7	CHC-C4B	2.25	1.44	1.39
21	c	518	CL7	CHC-C4B	2.25	1.44	1.39
21	4	404	CL7	CAB-C3B	2.25	1.49	1.45
21	2	506	CL7	C1C-C2C	-2.25	1.40	1.45
21	6	506	CL7	C1C-C2C	-2.25	1.40	1.45
21	5	411	CL7	CAB-C3B	2.25	1.49	1.45
21	7	517	CL7	CHD-C1D	2.25	1.44	1.39
21	1	402	CL7	C1C-NC	-2.24	1.35	1.37
21	5	402	CL7	C1C-NC	-2.24	1.35	1.37
21	2	510	CL7	MG-NB	-2.24	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	510	CL7	MG-NB	-2.24	2.01	2.05
23	D	406	8CT	C30-C29	2.24	1.53	1.50
21	B	607	CL7	MG-NB	-2.24	2.01	2.05
21	b	608	CL7	MG-NB	-2.24	2.01	2.05
21	c	512	CL7	CHD-C1D	2.24	1.44	1.39
21	1	415	CL7	OBD-CAD	2.24	1.26	1.22
21	1	407	CL7	CHD-C1D	2.24	1.44	1.39
21	5	407	CL7	CHD-C1D	2.24	1.44	1.39
21	B	601	CL7	CAB-C3B	2.24	1.49	1.45
21	1	419	CL7	CAB-C3B	2.24	1.49	1.45
21	b	602	CL7	CAB-C3B	2.24	1.49	1.45
21	5	419	CL7	CAB-C3B	2.24	1.49	1.45
21	4	409	CL7	CHD-C1D	2.24	1.44	1.39
21	8	409	CL7	CHD-C1D	2.24	1.44	1.39
21	7	512	CL7	C1B-NB	-2.24	1.35	1.37
21	C	502	CL7	C3B-C4B	-2.24	1.37	1.42
21	c	502	CL7	C3B-C4B	-2.24	1.37	1.42
21	B	608	CL7	CHC-C4B	2.24	1.44	1.39
21	b	609	CL7	CHC-C4B	2.24	1.44	1.39
21	A	403	CL7	C1B-NB	-2.24	1.35	1.37
21	a	403	CL7	C1B-NB	-2.24	1.35	1.37
21	4	414	CL7	C3B-C4B	-2.24	1.37	1.42
21	2	514	CL7	C1B-C2B	-2.24	1.38	1.43
21	6	514	CL7	C1B-C2B	-2.24	1.38	1.43
21	7	503	CL7	C1B-C2B	-2.24	1.38	1.43
21	c	518	CL7	C1B-C2B	-2.24	1.38	1.43
21	C	513	CL7	CAB-C3B	2.24	1.49	1.45
21	c	513	CL7	CAB-C3B	2.24	1.49	1.45
21	1	406	CL7	C1B-C2B	-2.24	1.38	1.43
21	D	405	CL7	CHC-C4B	2.24	1.44	1.39
21	d	405	CL7	CHC-C4B	2.24	1.44	1.39
21	5	408	CL7	C1B-C2B	-2.24	1.38	1.43
21	3	503	CL7	C3B-C4B	-2.24	1.37	1.42
21	4	415	CL7	C3B-C4B	-2.24	1.37	1.42
21	7	503	CL7	C3B-C4B	-2.24	1.37	1.42
21	B	615	CL7	CHD-C1D	2.24	1.44	1.39
21	A	406	CL7	C3B-C4B	-2.24	1.37	1.42
21	B	601	CL7	C3B-C4B	-2.24	1.37	1.42
21	5	407	CL7	CAB-C3B	2.24	1.49	1.45
21	2	507	CL7	C1C-NC	-2.24	1.35	1.37
21	A	401	CL7	C1B-C2B	-2.24	1.38	1.43
21	C	511	CL7	CHD-C1D	2.24	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	409	CL7	CHD-C1D	2.24	1.44	1.39
21	c	511	CL7	CHD-C1D	2.24	1.44	1.39
21	5	409	CL7	CHD-C1D	2.24	1.44	1.39
21	3	512	CL7	C1C-NC	-2.24	1.35	1.37
21	7	512	CL7	C1C-NC	-2.24	1.35	1.37
21	B	622	CL7	MG-ND	-2.24	2.01	2.05
21	2	517	CL7	C3B-C4B	-2.24	1.37	1.42
32	2	521	ZEX	C21-C26	-2.23	1.50	1.53
21	3	517	CL7	CHD-C1D	2.23	1.44	1.39
21	1	403	CL7	CAB-C3B	2.23	1.49	1.45
21	5	403	CL7	CAB-C3B	2.23	1.49	1.45
21	2	512	CL7	CAB-C3B	2.23	1.49	1.45
21	c	513	CL7	MG-NB	-2.23	2.01	2.05
21	B	605	CL7	C1B-C2B	-2.23	1.38	1.43
21	b	606	CL7	C1B-C2B	-2.23	1.38	1.43
32	2	520	ZEX	C14-C13	-2.23	1.32	1.35
32	3	525	ZEX	C14-C13	-2.23	1.32	1.35
21	1	409	CL7	CAB-C3B	2.23	1.49	1.45
21	3	510	CL7	C3B-C4B	-2.23	1.37	1.42
21	2	507	CL7	CHC-C4B	2.23	1.44	1.39
21	6	507	CL7	CHC-C4B	2.23	1.44	1.39
21	4	404	CL7	C1C-NC	-2.23	1.35	1.37
21	8	404	CL7	C1C-NC	-2.23	1.35	1.37
23	c	519	8CT	C38-C31	2.23	1.54	1.50
21	C	510	CL7	CHC-C4B	2.23	1.44	1.39
21	c	510	CL7	CHC-C4B	2.23	1.44	1.39
21	8	416	CL7	OBD-CAD	2.23	1.26	1.22
21	B	602	CL7	CHC-C4B	2.23	1.44	1.39
21	B	614	CL7	CHC-C4B	2.23	1.44	1.39
21	b	603	CL7	CHC-C4B	2.23	1.44	1.39
21	b	615	CL7	CHC-C4B	2.23	1.44	1.39
21	a	405	CL7	C3B-C4B	-2.23	1.37	1.42
21	2	515	CL7	CHD-C1D	2.23	1.44	1.39
21	6	515	CL7	CHD-C1D	2.23	1.44	1.39
21	2	502	CL7	C1B-C2B	-2.23	1.38	1.43
21	6	502	CL7	C1B-C2B	-2.23	1.38	1.43
21	4	416	CL7	CAB-C3B	2.23	1.49	1.45
21	4	413	CL7	C3B-C4B	-2.23	1.37	1.42
21	7	510	CL7	C3B-C4B	-2.23	1.37	1.42
21	1	409	CL7	MG-ND	-2.23	2.01	2.05
21	5	409	CL7	MG-ND	-2.23	2.01	2.05
21	A	406	CL7	MG-NB	-2.23	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	405	CL7	MG-NB	-2.23	2.01	2.05
21	2	513	CL7	C1B-C2B	-2.23	1.38	1.43
21	C	514	CL7	C1B-C2B	-2.23	1.38	1.43
21	8	415	CL7	C3B-C4B	-2.23	1.37	1.42
21	3	511	CL7	C1C-NC	-2.23	1.35	1.37
21	7	511	CL7	C1C-NC	-2.23	1.35	1.37
21	A	406	CL7	C1C-C2C	-2.23	1.40	1.45
21	a	405	CL7	C1C-C2C	-2.23	1.40	1.45
21	2	507	CL7	CBD-CGD	-2.22	1.45	1.52
21	6	507	CL7	CBD-CGD	-2.22	1.45	1.52
21	3	508	CL7	CHD-C1D	2.22	1.44	1.39
23	B	619	8CT	C22-C21	2.22	1.55	1.50
23	b	620	8CT	C22-C21	2.22	1.55	1.50
21	2	503	CL7	C3B-C4B	-2.22	1.37	1.42
21	6	503	CL7	C3B-C4B	-2.22	1.37	1.42
21	8	414	CL7	C3B-C4B	-2.22	1.37	1.42
21	c	511	CL7	C3B-C4B	-2.22	1.37	1.42
21	6	513	CL7	C3B-C4B	-2.22	1.37	1.42
21	5	409	CL7	CAB-C3B	2.22	1.49	1.45
21	4	410	CL7	CHC-C4B	2.22	1.44	1.39
21	B	603	CL7	C3B-C4B	-2.22	1.37	1.42
21	b	604	CL7	C3B-C4B	-2.22	1.37	1.42
21	B	611	CL7	CHC-C4B	2.22	1.44	1.39
21	b	612	CL7	CHC-C4B	2.22	1.44	1.39
21	d	405	CL7	C1C-C2C	-2.22	1.40	1.45
21	7	504	CL7	C1C-C2C	-2.22	1.40	1.45
21	C	507	CL7	CHD-C1D	2.22	1.44	1.39
21	4	409	CL7	CHC-C4B	2.22	1.44	1.39
21	8	409	CL7	CHC-C4B	2.22	1.44	1.39
21	2	513	CL7	C3B-C4B	-2.22	1.37	1.42
21	C	511	CL7	C3B-C4B	-2.22	1.37	1.42
21	b	615	CL7	C1C-C2C	-2.22	1.41	1.45
21	2	506	CL7	CHD-C1D	2.22	1.44	1.39
21	b	616	CL7	CHD-C1D	2.22	1.44	1.39
21	3	510	CL7	CHC-C4B	2.21	1.44	1.39
21	7	510	CL7	CHC-C4B	2.21	1.44	1.39
23	A	404	8CT	C22-C21	2.21	1.55	1.50
21	8	413	CL7	C3B-C4B	-2.21	1.37	1.42
21	b	605	CL7	MG-NB	-2.21	2.01	2.05
21	3	515	CL7	CHD-C1D	2.21	1.44	1.39
21	7	508	CL7	CHD-C1D	2.21	1.44	1.39
21	7	515	CL7	CHD-C1D	2.21	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	415	CL7	CAB-C3B	2.21	1.49	1.45
21	C	518	CL7	C1B-C2B	-2.21	1.38	1.43
21	1	411	CL7	CHD-C1D	2.21	1.44	1.39
21	5	411	CL7	CHD-C1D	2.21	1.44	1.39
21	B	614	CL7	C1C-NC	-2.21	1.35	1.37
21	C	510	CL7	C1C-NC	-2.21	1.35	1.37
21	b	615	CL7	C1C-NC	-2.21	1.35	1.37
21	c	510	CL7	C1C-NC	-2.21	1.35	1.37
21	B	604	CL7	MG-NB	-2.21	2.01	2.05
21	C	502	CL7	MG-NB	-2.21	2.01	2.05
32	4	418	ZEX	C21-C26	-2.21	1.50	1.53
21	c	507	CL7	C1C-NC	-2.21	1.35	1.37
21	2	516	CL7	C1C-C2C	-2.21	1.41	1.45
21	6	516	CL7	C1C-C2C	-2.21	1.41	1.45
21	C	508	CL7	CHC-C4B	2.21	1.44	1.39
21	C	518	CL7	CHD-C1D	2.21	1.44	1.39
21	c	508	CL7	CHC-C4B	2.21	1.44	1.39
21	c	518	CL7	CHD-C1D	2.21	1.44	1.39
21	a	401	CL7	C1B-C2B	-2.21	1.38	1.43
21	7	501	CL7	C1C-NC	-2.21	1.35	1.37
21	2	504	CL7	C1C-C2C	-2.21	1.41	1.45
21	1	419	CL7	C1B-C2B	-2.21	1.38	1.43
21	5	419	CL7	C1B-C2B	-2.21	1.38	1.43
32	2	525	ZEX	C1-C6	-2.21	1.50	1.53
32	6	524	ZEX	C1-C6	-2.21	1.50	1.53
21	B	605	CL7	MG-ND	-2.21	2.01	2.05
21	b	606	CL7	MG-ND	-2.21	2.01	2.05
21	6	507	CL7	C1C-NC	-2.21	1.35	1.37
23	a	404	8CT	C22-C21	2.21	1.55	1.50
21	3	514	CL7	MG-NB	-2.21	2.01	2.05
21	7	514	CL7	MG-NB	-2.21	2.01	2.05
21	3	511	CL7	C3B-C4B	-2.21	1.37	1.42
21	7	511	CL7	C3B-C4B	-2.21	1.37	1.42
21	3	512	CL7	CAB-C3B	2.21	1.49	1.45
21	7	512	CL7	CAB-C3B	2.21	1.49	1.45
21	5	406	CL7	C1B-C2B	-2.21	1.38	1.43
23	B	617	8CT	C22-C21	2.21	1.55	1.50
23	b	618	8CT	C22-C21	2.21	1.55	1.50
21	4	406	CL7	CAB-C3B	2.21	1.49	1.45
21	8	406	CL7	CAB-C3B	2.21	1.49	1.45
21	A	406	CL7	MG-ND	-2.21	2.01	2.05
21	B	601	CL7	MG-ND	-2.21	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	405	CL7	MG-ND	-2.21	2.01	2.05
21	b	602	CL7	MG-ND	-2.21	2.01	2.05
21	6	517	CL7	C3B-C4B	-2.21	1.37	1.42
21	4	416	CL7	OBD-CAD	2.21	1.26	1.22
21	c	502	CL7	MG-NB	-2.20	2.01	2.05
21	3	504	CL7	C1C-C2C	-2.20	1.41	1.45
21	2	510	CL7	C1C-NC	-2.20	1.35	1.37
21	6	510	CL7	C1C-NC	-2.20	1.35	1.37
21	2	509	CL7	MG-NB	-2.20	2.01	2.05
21	6	509	CL7	MG-NB	-2.20	2.01	2.05
21	B	616	CL7	CAB-C3B	2.20	1.49	1.45
21	b	617	CL7	CAB-C3B	2.20	1.49	1.45
21	1	408	CL7	C4C-NC	-2.20	1.35	1.37
21	5	408	CL7	C4C-NC	-2.20	1.35	1.37
21	D	402	CL7	C1B-C2B	-2.20	1.38	1.43
21	d	402	CL7	C1B-C2B	-2.20	1.38	1.43
21	B	612	CL7	CHC-C4B	2.20	1.44	1.39
21	4	405	CL7	CHD-C1D	2.20	1.44	1.39
21	b	613	CL7	CHC-C4B	2.20	1.44	1.39
21	8	405	CL7	CHD-C1D	2.20	1.44	1.39
23	C	519	8CT	C38-C31	2.20	1.54	1.50
21	8	412	CL7	C1C-NC	-2.20	1.35	1.37
21	3	510	CL7	C1C-C2C	-2.20	1.41	1.45
21	7	510	CL7	C1C-C2C	-2.20	1.41	1.45
21	5	415	CL7	OBD-CAD	2.20	1.26	1.22
21	b	623	CL7	MG-ND	-2.20	2.01	2.05
21	1	407	CL7	CAB-C3B	2.20	1.49	1.45
21	B	610	CL7	C3B-C4B	-2.20	1.37	1.42
21	b	611	CL7	C3B-C4B	-2.20	1.37	1.42
21	C	513	CL7	MG-NB	-2.20	2.01	2.05
21	c	506	CL7	CHD-C1D	2.20	1.44	1.39
21	D	405	CL7	C1C-NC	-2.20	1.35	1.37
21	D	404	CL7	CHC-C4B	2.20	1.44	1.39
21	d	404	CL7	CHC-C4B	2.20	1.44	1.39
21	1	416	CL7	C4C-NC	-2.20	1.35	1.37
21	1	402	CL7	CHD-C1D	2.20	1.44	1.39
21	5	402	CL7	CHD-C1D	2.20	1.44	1.39
21	2	502	CL7	C1C-C2C	-2.20	1.41	1.45
21	6	502	CL7	C1C-C2C	-2.20	1.41	1.45
21	1	403	CL7	C3B-C4B	-2.20	1.37	1.42
21	5	403	CL7	C3B-C4B	-2.20	1.37	1.42
21	B	616	CL7	MG-NB	-2.20	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	617	CL7	MG-NB	-2.20	2.01	2.05
21	b	602	CL7	CHD-C1D	2.20	1.44	1.39
21	3	505	CL7	CHC-C4B	2.20	1.44	1.39
21	1	403	CL7	C1B-C2B	-2.20	1.38	1.43
21	4	410	CL7	C1C-C2C	-2.20	1.41	1.45
21	D	402	CL7	CAB-C3B	2.20	1.49	1.45
21	d	402	CL7	CAB-C3B	2.20	1.49	1.45
21	C	505	CL7	MG-ND	-2.20	2.01	2.05
21	1	412	CL7	C1B-C2B	-2.20	1.38	1.43
21	5	412	CL7	C1B-C2B	-2.20	1.38	1.43
21	c	507	CL7	CHD-C1D	2.20	1.44	1.39
21	B	605	CL7	C3B-C4B	-2.20	1.37	1.42
21	b	606	CL7	C3B-C4B	-2.20	1.37	1.42
21	B	603	CL7	C1C-C2C	-2.20	1.41	1.45
21	b	604	CL7	C1C-C2C	-2.20	1.41	1.45
21	c	505	CL7	MG-ND	-2.19	2.01	2.05
21	B	613	CL7	CHD-C1D	2.19	1.44	1.39
21	b	614	CL7	CHD-C1D	2.19	1.44	1.39
21	4	412	CL7	C3B-C4B	-2.19	1.37	1.42
21	8	412	CL7	C3B-C4B	-2.19	1.37	1.42
21	C	504	CL7	MG-NB	-2.19	2.01	2.05
21	B	605	CL7	C3D-C4D	-2.19	1.34	1.39
21	b	606	CL7	C3D-C4D	-2.19	1.34	1.39
21	5	411	CL7	MG-NB	-2.19	2.01	2.05
21	C	502	CL7	C1B-NB	-2.19	1.35	1.37
21	3	503	CL7	C1C-NC	-2.19	1.35	1.37
21	7	503	CL7	C1C-NC	-2.19	1.35	1.37
21	3	505	CL7	C1B-NB	-2.19	1.35	1.37
21	7	505	CL7	C1B-NB	-2.19	1.35	1.37
32	4	403	ZEX	C14-C13	-2.19	1.32	1.35
21	C	505	CL7	CAB-C3B	2.19	1.49	1.45
21	c	505	CL7	CAB-C3B	2.19	1.49	1.45
21	3	514	CL7	CHD-C1D	2.19	1.44	1.39
21	B	604	CL7	CHD-C1D	2.19	1.44	1.39
21	C	506	CL7	C1B-NB	-2.19	1.35	1.37
21	c	506	CL7	C1B-NB	-2.19	1.35	1.37
21	5	414	CL7	MG-ND	-2.19	2.01	2.05
21	6	504	CL7	C1C-C2C	-2.19	1.41	1.45
21	7	514	CL7	CHD-C1D	2.19	1.44	1.39
21	b	609	CL7	C1C-C2C	-2.19	1.41	1.45
21	d	405	CL7	C1C-NC	-2.19	1.35	1.37
21	6	509	CL7	C1C-NC	-2.19	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	510	CL7	C1C-C2C	-2.19	1.41	1.45
21	6	510	CL7	C1C-C2C	-2.19	1.41	1.45
21	1	410	CL7	CAB-C3B	2.19	1.49	1.45
21	4	415	CL7	CAB-C3B	2.19	1.49	1.45
21	5	410	CL7	CAB-C3B	2.19	1.49	1.45
21	1	416	CL7	CAB-C3B	2.19	1.49	1.45
21	5	416	CL7	CAB-C3B	2.19	1.49	1.45
21	B	604	CL7	C1C-NC	-2.19	1.35	1.37
21	b	605	CL7	C1C-NC	-2.19	1.35	1.37
21	B	606	CL7	CAB-C3B	2.19	1.49	1.45
21	b	607	CL7	CAB-C3B	2.19	1.49	1.45
21	5	420	CL7	C1B-C2B	-2.19	1.38	1.43
21	4	409	CL7	C1C-C2C	-2.18	1.41	1.45
21	b	610	CL7	C1C-C2C	-2.18	1.41	1.45
21	8	409	CL7	C1C-C2C	-2.18	1.41	1.45
21	2	517	CL7	MG-NB	-2.18	2.01	2.05
21	6	517	CL7	MG-NB	-2.18	2.01	2.05
21	D	405	CL7	C1C-C2C	-2.18	1.41	1.45
21	2	513	CL7	MG-ND	-2.18	2.01	2.05
21	6	513	CL7	MG-ND	-2.18	2.01	2.05
21	C	509	CL7	C1C-C2C	-2.18	1.41	1.45
21	c	509	CL7	C1C-C2C	-2.18	1.41	1.45
21	B	602	CL7	CAB-C3B	2.18	1.49	1.45
21	2	503	CL7	CAB-C3B	2.18	1.49	1.45
21	b	603	CL7	CAB-C3B	2.18	1.49	1.45
21	6	503	CL7	CAB-C3B	2.18	1.49	1.45
21	c	504	CL7	MG-NB	-2.18	2.01	2.05
21	1	420	CL7	C1B-C2B	-2.18	1.38	1.43
21	5	403	CL7	C1B-C2B	-2.18	1.38	1.43
21	8	415	CL7	MG-NB	-2.18	2.01	2.05
21	4	412	CL7	CHD-C1D	2.18	1.44	1.39
21	B	608	CL7	C1C-C2C	-2.18	1.41	1.45
21	3	506	CL7	CAB-C3B	2.18	1.49	1.45
21	3	518	CL7	CAB-C3B	2.18	1.49	1.45
21	7	506	CL7	CAB-C3B	2.18	1.49	1.45
21	7	518	CL7	CAB-C3B	2.18	1.49	1.45
21	3	504	CL7	CHD-C1D	2.18	1.44	1.39
21	3	513	CL7	CHD-C1D	2.18	1.44	1.39
21	5	412	CL7	CHD-C1D	2.18	1.44	1.39
21	7	504	CL7	CHD-C1D	2.18	1.44	1.39
21	7	513	CL7	CHD-C1D	2.18	1.44	1.39
31	F	101	HEM	C1D-ND	-2.18	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	c	505	CL7	C3B-C4B	-2.18	1.37	1.42
21	b	615	CL7	CHD-C1D	2.18	1.44	1.39
21	3	504	CL7	MG-NB	-2.18	2.01	2.05
21	7	504	CL7	MG-NB	-2.18	2.01	2.05
21	B	616	CL7	C1C-NC	-2.18	1.35	1.37
21	b	617	CL7	C1C-NC	-2.18	1.35	1.37
21	B	612	CL7	C1C-C2C	-2.18	1.41	1.45
21	b	613	CL7	C1C-C2C	-2.18	1.41	1.45
21	1	408	CL7	MG-NB	-2.18	2.01	2.05
21	5	408	CL7	MG-NB	-2.18	2.01	2.05
21	b	605	CL7	CHD-C1D	2.17	1.44	1.39
21	4	413	CL7	C1C-NC	-2.17	1.35	1.37
21	8	413	CL7	C1C-NC	-2.17	1.35	1.37
23	C	516	8CT	C01-C02	2.17	1.54	1.50
23	c	516	8CT	C01-C02	2.17	1.54	1.50
21	A	401	CL7	CAB-C3B	2.17	1.49	1.45
21	a	401	CL7	CAB-C3B	2.17	1.49	1.45
21	1	414	CL7	MG-ND	-2.17	2.01	2.05
21	3	509	CL7	C1B-NB	-2.17	1.35	1.37
21	7	509	CL7	C1B-NB	-2.17	1.35	1.37
21	C	512	CL7	MG-ND	-2.17	2.01	2.05
21	c	512	CL7	MG-ND	-2.17	2.01	2.05
21	C	505	CL7	C3B-C4B	-2.17	1.37	1.42
21	8	412	CL7	CHD-C1D	2.17	1.44	1.39
21	B	613	CL7	CBD-CGD	-2.17	1.45	1.52
21	b	614	CL7	CBD-CGD	-2.17	1.45	1.52
31	f	101	HEM	C1D-ND	-2.17	1.34	1.38
21	7	505	CL7	CHC-C4B	2.17	1.44	1.39
21	1	420	CL7	MG-ND	-2.17	2.01	2.05
21	C	503	CL7	C3B-C4B	-2.17	1.37	1.42
21	c	503	CL7	C3B-C4B	-2.17	1.37	1.42
21	2	508	CL7	CHD-C1D	2.17	1.44	1.39
21	6	508	CL7	CHD-C1D	2.17	1.44	1.39
21	B	615	CL7	MG-NB	-2.17	2.01	2.05
21	2	515	CL7	C3B-C4B	-2.17	1.37	1.42
21	4	411	CL7	C1C-NC	-2.17	1.35	1.37
21	8	411	CL7	C1C-NC	-2.17	1.35	1.37
21	B	616	CL7	CHD-C1D	2.17	1.44	1.39
21	c	502	CL7	C1C-NC	-2.17	1.35	1.37
21	6	515	CL7	C3B-C4B	-2.16	1.37	1.42
23	B	617	8CT	C39-C16	2.16	1.55	1.50
23	b	618	8CT	C39-C16	2.16	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	508	CL7	C1B-NB	-2.16	1.35	1.37
21	C	509	CL7	C2A-C1A	2.16	1.54	1.50
21	6	505	CL7	C1C-C2C	-2.16	1.41	1.45
21	1	413	CL7	CHD-C1D	2.16	1.44	1.39
21	5	413	CL7	CHD-C1D	2.16	1.44	1.39
23	K	101	8CT	C10-C03	2.16	1.52	1.45
23	k	101	8CT	C10-C03	2.16	1.52	1.45
21	7	505	CL7	C1C-C2C	-2.16	1.41	1.45
21	1	407	CL7	C3B-C4B	-2.16	1.37	1.42
21	5	407	CL7	C3B-C4B	-2.16	1.37	1.42
21	8	410	CL7	C1C-C2C	-2.16	1.41	1.45
21	4	408	CL7	CHD-C1D	2.16	1.44	1.39
21	c	510	CL7	C1B-NB	-2.16	1.35	1.37
21	A	403	CL7	CHD-C1D	2.16	1.44	1.39
21	B	601	CL7	CHD-C1D	2.16	1.44	1.39
21	C	506	CL7	CHC-C4B	2.16	1.44	1.39
21	C	506	CL7	CHD-C1D	2.16	1.44	1.39
21	B	607	CL7	C3B-C4B	-2.16	1.37	1.42
21	b	608	CL7	C3B-C4B	-2.16	1.37	1.42
21	d	402	CL7	OBD-CAD	2.16	1.26	1.22
21	c	506	CL7	CHC-C4B	2.16	1.44	1.39
21	1	420	CL7	CHD-C1D	2.15	1.44	1.39
21	5	420	CL7	CHD-C1D	2.15	1.44	1.39
21	5	420	CL7	MG-ND	-2.15	2.01	2.05
21	2	506	CL7	MG-NB	-2.15	2.01	2.05
21	4	414	CL7	MG-NB	-2.15	2.01	2.05
21	8	414	CL7	MG-NB	-2.15	2.01	2.05
21	8	417	CL7	CAB-C3B	2.15	1.49	1.45
21	6	508	CL7	CHC-C4B	2.15	1.44	1.39
21	3	517	CL7	C1C-C2C	-2.15	1.41	1.45
21	7	517	CL7	C1C-C2C	-2.15	1.41	1.45
21	3	508	CL7	C1B-NB	-2.15	1.35	1.37
21	c	502	CL7	C1B-NB	-2.15	1.35	1.37
21	4	404	CL7	CHD-C1D	2.15	1.44	1.39
21	8	404	CL7	CHD-C1D	2.15	1.44	1.39
21	8	408	CL7	CHD-C1D	2.15	1.44	1.39
21	B	604	CL7	CAB-C3B	2.15	1.49	1.45
21	b	605	CL7	CAB-C3B	2.15	1.49	1.45
21	C	502	CL7	C1C-NC	-2.15	1.35	1.37
21	4	409	CL7	C1C-NC	-2.15	1.35	1.37
21	3	509	CL7	C3D-C4D	-2.15	1.34	1.39
21	7	509	CL7	C3D-C4D	-2.15	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	419	CL7	OBD-CAD	2.15	1.26	1.22
21	5	419	CL7	OBD-CAD	2.15	1.26	1.22
21	2	504	CL7	MG-NB	-2.15	2.01	2.05
21	3	512	CL7	MG-NB	-2.15	2.01	2.05
21	6	504	CL7	MG-NB	-2.15	2.01	2.05
21	2	505	CL7	C3D-C4D	-2.15	1.34	1.39
21	6	505	CL7	C3D-C4D	-2.15	1.34	1.39
21	B	603	CL7	C1B-NB	-2.15	1.35	1.37
21	2	518	CL7	CHD-C1D	2.15	1.44	1.39
21	6	518	CL7	CHD-C1D	2.15	1.44	1.39
21	B	603	CL7	CHD-C1D	2.15	1.44	1.39
21	b	604	CL7	CHD-C1D	2.15	1.44	1.39
21	b	616	CL7	MG-NB	-2.15	2.01	2.05
21	1	411	CL7	MG-NB	-2.15	2.01	2.05
21	2	510	CL7	C3B-C4B	-2.15	1.37	1.42
21	6	510	CL7	C3B-C4B	-2.15	1.37	1.42
21	B	607	CL7	C1C-NC	-2.15	1.35	1.37
21	5	416	CL7	C4C-NC	-2.15	1.35	1.37
21	1	416	CL7	C1B-C2B	-2.15	1.38	1.43
21	5	416	CL7	C1B-C2B	-2.15	1.38	1.43
21	B	612	CL7	C1B-NB	-2.15	1.35	1.37
21	b	613	CL7	C1B-NB	-2.15	1.35	1.37
23	k	101	8CT	C39-C16	2.14	1.55	1.50
21	B	609	CL7	C1C-C2C	-2.14	1.41	1.45
21	2	515	CL7	C1B-C2B	-2.14	1.38	1.43
21	6	515	CL7	C1B-C2B	-2.14	1.38	1.43
23	b	618	8CT	C38-C31	2.14	1.54	1.50
23	K	101	8CT	C39-C16	2.14	1.55	1.50
21	2	511	CL7	CHD-C1D	2.14	1.44	1.39
21	6	511	CL7	CHD-C1D	2.14	1.44	1.39
21	3	505	CL7	C1C-C2C	-2.14	1.41	1.45
21	b	611	CL7	CAB-C3B	2.14	1.49	1.45
21	C	514	CL7	MG-ND	-2.14	2.01	2.05
21	2	511	CL7	C1B-NB	-2.14	1.35	1.37
21	b	609	CL7	C1B-NB	-2.14	1.35	1.37
21	C	510	CL7	CHD-C1D	2.14	1.44	1.39
21	c	510	CL7	CHD-C1D	2.14	1.44	1.39
21	5	412	CL7	MG-ND	-2.14	2.01	2.05
21	2	508	CL7	CHC-C4B	2.14	1.44	1.39
21	1	417	CL7	C1C-NC	-2.14	1.35	1.37
21	5	417	CL7	C1C-NC	-2.14	1.35	1.37
21	3	513	CL7	MG-NB	-2.14	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	412	CL7	CHD-C1D	2.14	1.44	1.39
21	B	609	CL7	C3B-C4B	-2.14	1.37	1.42
21	4	405	CL7	C3B-C4B	-2.14	1.37	1.42
21	b	610	CL7	C3B-C4B	-2.14	1.37	1.42
21	8	405	CL7	C3B-C4B	-2.14	1.37	1.42
21	2	505	CL7	C1C-NC	-2.14	1.35	1.37
21	2	511	CL7	CAB-C3B	2.14	1.49	1.45
21	C	510	CL7	CBD-CGD	-2.14	1.45	1.52
21	c	510	CL7	CBD-CGD	-2.14	1.45	1.52
32	2	525	ZEX	C30-C29	-2.14	1.32	1.35
32	6	524	ZEX	C30-C29	-2.14	1.32	1.35
21	c	518	CL7	C1C-C2C	-2.14	1.41	1.45
21	B	622	CL7	C4C-NC	-2.14	1.35	1.37
23	B	617	8CT	C30-C29	2.14	1.53	1.50
23	b	618	8CT	C30-C29	2.14	1.53	1.50
21	b	608	CL7	C1C-NC	-2.14	1.35	1.37
21	B	614	CL7	CHD-C1D	2.14	1.44	1.39
21	8	408	CL7	CAB-C3B	2.14	1.49	1.45
21	2	502	CL7	CAB-C3B	2.14	1.49	1.45
21	6	502	CL7	CAB-C3B	2.14	1.49	1.45
21	B	613	CL7	C1C-C2C	-2.13	1.41	1.45
21	4	415	CL7	MG-NB	-2.13	2.01	2.05
32	2	520	ZEX	C10-C9	-2.13	1.33	1.35
32	3	525	ZEX	C10-C9	-2.13	1.33	1.35
21	6	511	CL7	C1B-NB	-2.13	1.35	1.37
21	4	411	CL7	C3B-C4B	-2.13	1.37	1.42
21	8	411	CL7	C3B-C4B	-2.13	1.37	1.42
21	B	602	CL7	CHD-C1D	2.13	1.44	1.39
21	b	603	CL7	CHD-C1D	2.13	1.44	1.39
21	C	506	CL7	CBD-CGD	-2.13	1.45	1.52
21	c	506	CL7	CBD-CGD	-2.13	1.45	1.52
21	b	604	CL7	C1B-NB	-2.13	1.35	1.37
21	5	414	CL7	OBD-CAD	2.13	1.26	1.22
21	3	501	CL7	CAB-C3B	2.13	1.49	1.45
21	7	501	CL7	CAB-C3B	2.13	1.49	1.45
21	6	506	CL7	MG-NB	-2.13	2.01	2.05
21	b	617	CL7	CHD-C1D	2.13	1.44	1.39
24	b	621	SQD	O8-S	2.13	1.55	1.47
21	a	403	CL7	CHD-C1D	2.13	1.44	1.39
21	2	505	CL7	C1C-C2C	-2.13	1.41	1.45
21	4	404	CL7	C1B-NB	-2.13	1.35	1.37
21	8	404	CL7	C1B-NB	-2.13	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	501	CL7	CHD-C1D	2.13	1.44	1.39
21	7	501	CL7	CHD-C1D	2.13	1.44	1.39
21	3	507	CL7	CBD-CGD	-2.13	1.45	1.52
21	7	507	CL7	CBD-CGD	-2.13	1.45	1.52
21	C	510	CL7	C3D-C4D	-2.13	1.34	1.39
21	c	510	CL7	C3D-C4D	-2.13	1.34	1.39
21	4	417	CL7	CAB-C3B	2.13	1.49	1.45
21	C	518	CL7	C1C-C2C	-2.13	1.41	1.45
32	2	523	ZEX	C34-C33	-2.13	1.33	1.35
32	6	522	ZEX	C34-C33	-2.13	1.33	1.35
21	4	417	CL7	C4C-NC	-2.13	1.35	1.37
21	8	417	CL7	C4C-NC	-2.13	1.35	1.37
21	1	412	CL7	MG-ND	-2.12	2.01	2.05
21	4	414	CL7	C1C-NC	-2.12	1.35	1.37
21	6	515	CL7	CAB-C3B	2.12	1.49	1.45
21	B	622	CL7	MG-NB	-2.12	2.01	2.05
21	3	506	CL7	CHC-C4B	2.12	1.44	1.39
21	7	506	CL7	CHC-C4B	2.12	1.44	1.39
21	B	601	CL7	C1B-C2B	-2.12	1.38	1.43
21	8	409	CL7	C1C-NC	-2.12	1.35	1.37
21	B	609	CL7	C3D-C4D	-2.12	1.34	1.39
21	b	610	CL7	C3D-C4D	-2.12	1.34	1.39
21	6	509	CL7	CHD-C1D	2.12	1.44	1.39
21	7	512	CL7	MG-NB	-2.12	2.01	2.05
21	1	405	CL7	CAB-C3B	2.12	1.49	1.45
21	5	405	CL7	CAB-C3B	2.12	1.49	1.45
21	1	414	CL7	OBD-CAD	2.12	1.26	1.22
21	B	608	CL7	C1B-NB	-2.12	1.35	1.37
21	4	417	CL7	C3B-C4B	-2.12	1.37	1.42
21	8	417	CL7	C3B-C4B	-2.12	1.37	1.42
21	B	614	CL7	MG-NB	-2.12	2.01	2.05
21	b	615	CL7	MG-NB	-2.12	2.01	2.05
21	5	419	CL7	MG-NB	-2.12	2.01	2.05
24	1	423	SQD	O8-S	2.12	1.55	1.47
21	2	506	CL7	C1B-NB	-2.12	1.35	1.37
21	6	506	CL7	C1B-NB	-2.12	1.35	1.37
21	D	402	CL7	OBD-CAD	2.12	1.26	1.22
21	3	501	CL7	C1C-C2C	-2.12	1.41	1.45
21	7	513	CL7	MG-NB	-2.12	2.01	2.05
21	C	512	CL7	OBD-CAD	2.12	1.26	1.22
21	c	512	CL7	OBD-CAD	2.12	1.26	1.22
21	2	504	CL7	C1B-NB	-2.12	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	504	CL7	C1B-NB	-2.12	1.35	1.37
21	6	505	CL7	C1C-NC	-2.12	1.35	1.37
21	3	513	CL7	C1C-C2C	-2.12	1.41	1.45
21	7	513	CL7	C1C-C2C	-2.12	1.41	1.45
21	b	623	CL7	MG-NB	-2.12	2.01	2.05
24	5	423	SQD	O8-S	2.12	1.55	1.47
21	7	501	CL7	C1C-C2C	-2.12	1.41	1.45
21	1	414	CL7	C1B-C2B	-2.12	1.38	1.43
21	5	414	CL7	C1B-C2B	-2.12	1.38	1.43
21	4	408	CL7	CAB-C3B	2.12	1.49	1.45
21	7	508	CL7	CHC-C4B	2.12	1.44	1.39
21	b	602	CL7	C1B-C2B	-2.12	1.38	1.43
21	4	408	CL7	C3B-C4B	-2.12	1.37	1.42
21	8	408	CL7	C3B-C4B	-2.12	1.37	1.42
21	2	514	CL7	C1B-NB	-2.12	1.35	1.37
21	6	514	CL7	C1B-NB	-2.12	1.35	1.37
21	2	502	CL7	C1C-NC	-2.11	1.35	1.37
21	6	502	CL7	C1C-NC	-2.11	1.35	1.37
21	4	406	CL7	C3B-C4B	-2.11	1.37	1.42
21	8	406	CL7	C3B-C4B	-2.11	1.37	1.42
24	B	620	SQD	O8-S	2.11	1.55	1.47
21	c	509	CL7	C2A-C1A	2.11	1.54	1.50
23	B	619	8CT	C38-C31	2.11	1.54	1.50
23	b	620	8CT	C38-C31	2.11	1.54	1.50
21	3	504	CL7	C3B-C4B	-2.11	1.37	1.42
21	7	504	CL7	C3B-C4B	-2.11	1.37	1.42
21	4	407	CL7	CAB-C3B	2.11	1.49	1.45
21	8	407	CL7	CAB-C3B	2.11	1.49	1.45
21	6	510	CL7	CHD-C1D	2.11	1.44	1.39
21	c	512	CL7	CAB-C3B	2.11	1.49	1.45
21	B	610	CL7	CAB-C3B	2.11	1.49	1.45
21	b	614	CL7	C1C-C2C	-2.11	1.41	1.45
21	c	509	CL7	CHD-C1D	2.11	1.44	1.39
21	1	405	CL7	C3B-C4B	-2.11	1.37	1.42
21	5	405	CL7	C3B-C4B	-2.11	1.37	1.42
21	c	514	CL7	MG-ND	-2.11	2.01	2.05
21	2	509	CL7	C1C-C2C	-2.11	1.41	1.45
21	6	509	CL7	C1C-C2C	-2.11	1.41	1.45
21	1	411	CL7	C3B-C4B	-2.11	1.37	1.42
21	5	411	CL7	C3B-C4B	-2.11	1.37	1.42
23	B	627	8CT	C39-C16	2.11	1.55	1.50
21	d	404	CL7	C1C-NC	-2.11	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	512	CL7	CAB-C3B	2.11	1.49	1.45
21	4	413	CL7	CAB-C3B	2.11	1.49	1.45
21	8	413	CL7	CAB-C3B	2.11	1.49	1.45
21	B	615	CL7	CAB-C3B	2.11	1.49	1.45
21	b	616	CL7	CAB-C3B	2.11	1.49	1.45
21	4	408	CL7	CBD-CGD	-2.11	1.45	1.52
21	8	408	CL7	CBD-CGD	-2.11	1.45	1.52
21	2	504	CL7	C1C-NC	-2.11	1.35	1.37
21	6	504	CL7	C1C-NC	-2.11	1.35	1.37
21	B	611	CL7	CBD-CGD	-2.11	1.45	1.52
21	b	612	CL7	CBD-CGD	-2.11	1.45	1.52
21	2	515	CL7	OBD-CAD	2.10	1.26	1.22
21	6	515	CL7	OBD-CAD	2.10	1.26	1.22
21	1	406	CL7	C1C-C2C	-2.10	1.41	1.45
21	5	406	CL7	C1C-C2C	-2.10	1.41	1.45
21	C	506	CL7	C1C-NC	-2.10	1.35	1.37
21	c	506	CL7	C1C-NC	-2.10	1.35	1.37
23	B	627	8CT	C10-C03	2.10	1.52	1.45
21	2	509	CL7	CHD-C1D	2.10	1.44	1.39
21	4	415	CL7	CBD-CGD	-2.10	1.45	1.52
21	8	415	CL7	CBD-CGD	-2.10	1.45	1.52
32	8	403	ZEX	C14-C13	-2.10	1.33	1.35
21	5	409	CL7	OBD-CAD	2.10	1.26	1.22
21	B	611	CL7	CHD-C1D	2.10	1.44	1.39
21	2	516	CL7	C3B-C4B	-2.10	1.37	1.42
21	b	623	CL7	C4C-NC	-2.10	1.35	1.37
21	4	417	CL7	MG-NB	-2.10	2.01	2.05
21	8	417	CL7	MG-NB	-2.10	2.01	2.05
21	C	514	CL7	OBD-CAD	2.10	1.26	1.22
21	c	514	CL7	OBD-CAD	2.10	1.26	1.22
24	A	405	SQD	O8-S	2.10	1.55	1.47
24	B	626	SQD	O8-S	2.10	1.55	1.47
23	b	601	8CT	C39-C16	2.10	1.55	1.50
21	4	407	CL7	C3B-C4B	-2.10	1.37	1.42
21	5	413	CL7	C3B-C4B	-2.10	1.37	1.42
21	5	409	CL7	C3B-C4B	-2.10	1.37	1.42
21	4	414	CL7	C1B-NB	-2.10	1.35	1.37
21	8	414	CL7	C1B-NB	-2.10	1.35	1.37
21	2	501	CL7	CHD-C1D	2.10	1.44	1.39
21	6	501	CL7	CHD-C1D	2.10	1.44	1.39
23	B	617	8CT	C38-C31	2.10	1.54	1.50
21	B	603	CL7	C1C-NC	-2.10	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	604	CL7	C1C-NC	-2.10	1.35	1.37
21	1	408	CL7	C1C-C2C	-2.10	1.41	1.45
21	3	514	CL7	C1C-C2C	-2.10	1.41	1.45
21	5	408	CL7	C1C-C2C	-2.10	1.41	1.45
21	7	514	CL7	C1C-C2C	-2.10	1.41	1.45
21	C	509	CL7	CHD-C1D	2.10	1.44	1.39
21	6	515	CL7	MG-NB	-2.10	2.01	2.05
21	a	405	CL7	C3D-C4D	-2.10	1.34	1.39
32	2	521	ZEX	C30-C29	-2.10	1.33	1.35
32	6	520	ZEX	C30-C29	-2.10	1.33	1.35
21	5	403	CL7	C1C-NC	-2.10	1.35	1.37
21	C	510	CL7	C1C-C2C	-2.09	1.41	1.45
21	c	510	CL7	C1C-C2C	-2.09	1.41	1.45
32	4	420	ZEX	C10-C9	-2.09	1.33	1.35
32	8	420	ZEX	C10-C9	-2.09	1.33	1.35
21	1	415	CL7	C4C-NC	-2.09	1.35	1.37
23	b	601	8CT	C10-C03	2.09	1.52	1.45
21	A	403	CL7	CBD-CGD	-2.09	1.45	1.52
21	A	406	CL7	CHD-C1D	2.09	1.44	1.39
21	a	405	CL7	CHD-C1D	2.09	1.44	1.39
21	C	508	CL7	C1C-NC	-2.09	1.35	1.37
21	2	508	CL7	C1C-NC	-2.09	1.35	1.37
21	c	508	CL7	C1C-NC	-2.09	1.35	1.37
21	6	508	CL7	C1C-NC	-2.09	1.35	1.37
21	4	410	CL7	CAB-C3B	2.09	1.49	1.45
21	8	410	CL7	CAB-C3B	2.09	1.49	1.45
21	b	612	CL7	CHD-C1D	2.09	1.44	1.39
21	B	610	CL7	C1B-NB	-2.09	1.35	1.37
21	b	611	CL7	C1B-NB	-2.09	1.35	1.37
21	1	405	CL7	MG-NB	-2.09	2.01	2.05
21	B	608	CL7	CAB-C3B	2.09	1.49	1.45
21	b	609	CL7	CAB-C3B	2.09	1.49	1.45
21	6	511	CL7	CAB-C3B	2.09	1.49	1.45
21	2	510	CL7	CHD-C1D	2.09	1.44	1.39
21	3	502	CL7	C1C-C2C	-2.09	1.41	1.45
21	7	502	CL7	C1C-C2C	-2.09	1.41	1.45
21	1	412	CL7	C3B-C4B	-2.09	1.38	1.42
21	5	412	CL7	C3B-C4B	-2.09	1.38	1.42
21	1	415	CL7	C3A-C2A	2.09	1.56	1.54
21	5	415	CL7	C3A-C2A	2.09	1.56	1.54
21	2	502	CL7	CHD-C1D	2.09	1.44	1.39
21	1	413	CL7	OBD-CAD	2.09	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	413	CL7	OBD-CAD	2.09	1.26	1.22
21	7	512	CL7	C1C-C2C	-2.09	1.41	1.45
23	C	519	8CT	C22-C21	2.09	1.55	1.50
23	c	519	8CT	C22-C21	2.09	1.55	1.50
21	a	403	CL7	CBD-CGD	-2.09	1.45	1.52
21	c	514	CL7	CAB-C3B	2.09	1.49	1.45
32	2	521	ZEX	C1-C6	-2.09	1.50	1.53
32	6	520	ZEX	C1-C6	-2.09	1.50	1.53
21	2	515	CL7	CAB-C3B	2.09	1.49	1.45
32	4	403	ZEX	C34-C33	-2.09	1.33	1.35
32	8	403	ZEX	C34-C33	-2.09	1.33	1.35
21	1	413	CL7	C3B-C4B	-2.09	1.38	1.42
21	B	622	CL7	OBD-CAD	2.09	1.26	1.22
21	b	623	CL7	OBD-CAD	2.09	1.26	1.22
21	1	407	CL7	C1C-C2C	-2.09	1.41	1.45
21	4	405	CL7	C1C-C2C	-2.09	1.41	1.45
21	5	407	CL7	C1C-C2C	-2.09	1.41	1.45
21	4	415	CL7	CHD-C1D	2.09	1.44	1.39
21	8	415	CL7	CHD-C1D	2.09	1.44	1.39
21	C	509	CL7	C1C-NC	-2.09	1.35	1.37
21	c	509	CL7	C1C-NC	-2.09	1.35	1.37
21	3	512	CL7	C1C-C2C	-2.09	1.41	1.45
21	1	409	CL7	OBD-CAD	2.09	1.26	1.22
21	C	510	CL7	C1B-NB	-2.08	1.35	1.37
21	4	410	CL7	CHD-C1D	2.08	1.44	1.39
21	1	406	CL7	CAB-C3B	2.08	1.49	1.45
21	4	416	CL7	C3B-C4B	-2.08	1.38	1.42
21	8	416	CL7	C3B-C4B	-2.08	1.38	1.42
21	2	501	CL7	MG-NB	-2.08	2.01	2.05
21	C	508	CL7	CHD-C1D	2.08	1.44	1.39
21	4	417	CL7	CHD-C1D	2.08	1.44	1.39
21	8	417	CL7	CHD-C1D	2.08	1.44	1.39
21	b	609	CL7	C1C-NC	-2.08	1.35	1.37
21	3	508	CL7	CHC-C4B	2.08	1.44	1.39
21	6	516	CL7	C3B-C4B	-2.08	1.38	1.42
21	C	512	CL7	MG-NB	-2.08	2.01	2.05
21	c	512	CL7	MG-NB	-2.08	2.01	2.05
21	5	415	CL7	C4C-NC	-2.08	1.35	1.37
21	2	515	CL7	MG-NB	-2.08	2.01	2.05
21	2	506	CL7	CAB-C3B	2.08	1.49	1.45
21	6	506	CL7	CAB-C3B	2.08	1.49	1.45
21	B	607	CL7	C1C-C2C	-2.08	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	608	CL7	C1C-C2C	-2.08	1.41	1.45
21	C	514	CL7	CAB-C3B	2.08	1.49	1.45
21	5	406	CL7	CAB-C3B	2.08	1.49	1.45
21	2	509	CL7	C3D-C4D	-2.08	1.34	1.39
21	D	405	CL7	C1B-NB	-2.08	1.35	1.37
21	6	509	CL7	C3D-C4D	-2.08	1.34	1.39
21	5	405	CL7	MG-NB	-2.08	2.01	2.05
21	B	605	CL7	CHD-C1D	2.08	1.44	1.39
21	b	606	CL7	CHD-C1D	2.08	1.44	1.39
21	6	516	CL7	CAB-C3B	2.08	1.49	1.45
21	C	506	CL7	C3D-C4D	-2.08	1.34	1.39
21	B	605	CL7	CAB-C3B	2.08	1.49	1.45
21	b	606	CL7	CAB-C3B	2.08	1.49	1.45
21	1	411	CL7	OBD-CAD	2.08	1.26	1.22
21	5	411	CL7	OBD-CAD	2.08	1.26	1.22
21	B	606	CL7	C3B-C4B	-2.08	1.38	1.42
21	b	607	CL7	C3B-C4B	-2.08	1.38	1.42
21	1	410	CL7	C3B-C4B	-2.07	1.38	1.42
21	5	410	CL7	C3B-C4B	-2.07	1.38	1.42
21	8	407	CL7	C3B-C4B	-2.07	1.38	1.42
21	B	616	CL7	CBD-CGD	-2.07	1.45	1.52
21	b	617	CL7	CBD-CGD	-2.07	1.45	1.52
21	B	607	CL7	C1B-NB	-2.07	1.35	1.37
21	b	608	CL7	C1B-NB	-2.07	1.35	1.37
21	1	416	CL7	MG-ND	-2.07	2.01	2.05
21	5	407	CL7	MG-NB	-2.07	2.01	2.05
21	5	416	CL7	MG-ND	-2.07	2.01	2.05
21	1	419	CL7	MG-NB	-2.07	2.01	2.05
21	C	508	CL7	CBD-CGD	-2.07	1.45	1.52
21	c	508	CL7	CBD-CGD	-2.07	1.45	1.52
21	B	602	CL7	C1C-NC	-2.07	1.35	1.37
21	2	508	CL7	C1B-NB	-2.07	1.35	1.37
21	6	508	CL7	C1B-NB	-2.07	1.35	1.37
21	8	409	CL7	CBD-CGD	-2.07	1.45	1.52
32	4	403	ZEX	C1-C6	-2.07	1.50	1.53
32	8	403	ZEX	C1-C6	-2.07	1.50	1.53
21	A	406	CL7	C3D-C4D	-2.07	1.34	1.39
21	B	608	CL7	C1C-NC	-2.07	1.35	1.37
21	C	503	CL7	CBD-CGD	-2.07	1.45	1.52
21	c	503	CL7	CBD-CGD	-2.07	1.45	1.52
21	3	516	CL7	C3D-C4D	-2.07	1.34	1.39
31	F	101	HEM	C3C-C4C	-2.07	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	f	101	HEM	C3C-C4C	-2.07	1.42	1.46
21	1	418	CL7	CHD-C1D	2.07	1.44	1.39
21	5	417	CL7	MG-NB	-2.07	2.01	2.05
21	8	407	CL7	CHD-C1D	2.07	1.44	1.39
21	d	405	CL7	C1B-NB	-2.07	1.35	1.37
32	8	419	ZEX	C34-C33	-2.07	1.33	1.35
21	8	410	CL7	CHD-C1D	2.07	1.44	1.39
21	c	508	CL7	CHD-C1D	2.07	1.44	1.39
21	1	406	CL7	OBD-CAD	2.07	1.26	1.22
21	5	406	CL7	OBD-CAD	2.07	1.26	1.22
21	2	511	CL7	MG-NB	-2.07	2.01	2.05
21	3	513	CL7	CBD-CGD	-2.06	1.45	1.52
21	7	513	CL7	CBD-CGD	-2.06	1.45	1.52
21	2	506	CL7	OBD-CAD	2.06	1.26	1.22
21	1	409	CL7	C3B-C4B	-2.06	1.38	1.42
21	C	508	CL7	C1B-NB	-2.06	1.35	1.37
21	c	508	CL7	C1B-NB	-2.06	1.35	1.37
23	B	627	8CT	C28-C29	2.06	1.37	1.32
23	b	601	8CT	C28-C29	2.06	1.37	1.32
21	8	414	CL7	C1C-NC	-2.06	1.35	1.37
32	3	519	ZEX	C30-C29	-2.06	1.33	1.35
32	7	519	ZEX	C30-C29	-2.06	1.33	1.35
21	7	516	CL7	C3D-C4D	-2.06	1.34	1.39
21	8	405	CL7	C1C-C2C	-2.06	1.41	1.45
23	B	617	8CT	C10-C03	2.06	1.52	1.45
23	b	618	8CT	C10-C03	2.06	1.52	1.45
21	C	507	CL7	C1B-NB	-2.06	1.35	1.37
21	c	507	CL7	C1B-NB	-2.06	1.35	1.37
21	D	404	CL7	CAB-C3B	2.06	1.49	1.45
21	d	404	CL7	CAB-C3B	2.06	1.49	1.45
21	4	414	CL7	C1C-C2C	-2.06	1.41	1.45
21	8	414	CL7	C1C-C2C	-2.06	1.41	1.45
24	2	524	SQD	O8-S	2.06	1.54	1.47
24	6	523	SQD	O8-S	2.06	1.54	1.47
21	1	404	CL7	C4C-NC	-2.06	1.35	1.37
21	5	404	CL7	C4C-NC	-2.06	1.35	1.37
23	C	515	8CT	C39-C16	2.06	1.55	1.50
23	c	515	8CT	C39-C16	2.06	1.55	1.50
21	7	517	CL7	MG-NB	-2.06	2.01	2.05
21	2	517	CL7	C1B-NB	-2.06	1.35	1.37
21	1	403	CL7	CHD-C1D	2.06	1.44	1.39
21	1	402	CL7	C1C-C2C	-2.06	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	402	CL7	C1C-C2C	-2.06	1.41	1.45
21	4	405	CL7	C1C-NC	-2.06	1.35	1.37
21	8	405	CL7	C1C-NC	-2.06	1.35	1.37
21	1	404	CL7	MG-NB	-2.06	2.01	2.05
21	5	404	CL7	MG-NB	-2.06	2.01	2.05
21	C	505	CL7	OBD-CAD	2.05	1.26	1.22
21	1	410	CL7	OBD-CAD	2.05	1.26	1.22
21	c	505	CL7	OBD-CAD	2.05	1.26	1.22
21	5	410	CL7	OBD-CAD	2.05	1.26	1.22
21	1	406	CL7	CHD-C1D	2.05	1.44	1.39
21	6	502	CL7	CHD-C1D	2.05	1.44	1.39
21	7	508	CL7	C1C-NC	-2.05	1.35	1.37
21	C	505	CL7	MG-NB	-2.05	2.01	2.05
21	4	409	CL7	CBD-CGD	-2.05	1.46	1.52
21	6	506	CL7	OBD-CAD	2.05	1.26	1.22
21	2	510	CL7	C1B-NB	-2.05	1.35	1.37
21	6	510	CL7	C1B-NB	-2.05	1.35	1.37
21	4	414	CL7	CAB-C3B	2.05	1.49	1.45
21	8	414	CL7	CAB-C3B	2.05	1.49	1.45
21	1	417	CL7	MG-NB	-2.05	2.01	2.05
32	2	519	ZEX	C10-C9	-2.05	1.33	1.35
32	6	519	ZEX	C10-C9	-2.05	1.33	1.35
21	2	508	CL7	CAB-C3B	2.05	1.49	1.45
21	6	508	CL7	CAB-C3B	2.05	1.49	1.45
21	B	608	CL7	C3D-C4D	-2.05	1.34	1.39
21	b	609	CL7	C3D-C4D	-2.05	1.34	1.39
21	2	501	CL7	C1C-C2C	-2.05	1.41	1.45
21	6	501	CL7	C1C-C2C	-2.05	1.41	1.45
21	B	614	CL7	C1B-NB	-2.05	1.35	1.37
21	b	615	CL7	C1B-NB	-2.05	1.35	1.37
21	C	507	CL7	MG-NB	-2.05	2.01	2.05
21	c	507	CL7	MG-NB	-2.05	2.01	2.05
21	2	516	CL7	CAB-C3B	2.05	1.49	1.45
21	2	509	CL7	CBD-CGD	-2.05	1.46	1.52
21	1	407	CL7	MG-NB	-2.05	2.01	2.05
21	B	616	CL7	C3B-C4B	-2.05	1.38	1.42
21	b	617	CL7	C3B-C4B	-2.05	1.38	1.42
21	1	405	CL7	C1C-C2C	-2.05	1.41	1.45
21	5	405	CL7	C1C-C2C	-2.05	1.41	1.45
21	1	412	CL7	OBD-CAD	2.05	1.26	1.22
21	5	412	CL7	OBD-CAD	2.05	1.26	1.22
21	4	409	CL7	C1B-C2B	-2.05	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	409	CL7	C1B-C2B	-2.05	1.38	1.43
21	3	506	CL7	C1B-NB	-2.05	1.35	1.37
21	7	506	CL7	C1B-NB	-2.05	1.35	1.37
21	B	616	CL7	C1C-C2C	-2.05	1.41	1.45
21	b	617	CL7	C1C-C2C	-2.05	1.41	1.45
21	6	517	CL7	C1B-NB	-2.05	1.35	1.37
21	b	605	CL7	CHC-C4B	2.05	1.44	1.39
21	6	501	CL7	MG-NB	-2.05	2.01	2.05
21	3	516	CL7	MG-NB	-2.05	2.01	2.05
21	7	516	CL7	MG-NB	-2.05	2.01	2.05
21	5	406	CL7	CHD-C1D	2.05	1.44	1.39
21	4	408	CL7	C1C-C2C	-2.05	1.41	1.45
21	8	408	CL7	C1C-C2C	-2.05	1.41	1.45
21	c	506	CL7	C3D-C4D	-2.05	1.34	1.39
21	6	511	CL7	MG-NB	-2.05	2.01	2.05
21	1	405	CL7	OBD-CAD	2.05	1.26	1.22
21	5	405	CL7	OBD-CAD	2.05	1.26	1.22
21	C	502	CL7	CAB-C3B	2.05	1.49	1.45
21	c	502	CL7	CAB-C3B	2.05	1.49	1.45
21	3	508	CL7	CBD-CGD	-2.05	1.46	1.52
21	7	508	CL7	CBD-CGD	-2.05	1.46	1.52
21	7	513	CL7	C1B-NB	-2.04	1.35	1.37
21	B	610	CL7	C1C-C2C	-2.04	1.41	1.45
21	2	503	CL7	C1C-C2C	-2.04	1.41	1.45
21	b	611	CL7	C1C-C2C	-2.04	1.41	1.45
21	6	503	CL7	C1C-C2C	-2.04	1.41	1.45
21	8	415	CL7	C1C-C2C	-2.04	1.41	1.45
21	4	407	CL7	CHD-C1D	2.04	1.44	1.39
21	3	512	CL7	C3B-C4B	-2.04	1.38	1.42
21	6	509	CL7	CBD-CGD	-2.04	1.46	1.52
21	D	404	CL7	C1C-NC	-2.04	1.35	1.37
21	5	418	CL7	CHD-C1D	2.04	1.44	1.39
21	b	603	CL7	C3D-C4D	-2.04	1.34	1.39
21	b	614	CL7	C3D-C4D	-2.04	1.34	1.39
21	C	504	CL7	C1C-NC	-2.04	1.35	1.37
21	c	504	CL7	C1C-NC	-2.04	1.35	1.37
21	c	513	CL7	CHD-C1D	2.04	1.44	1.39
21	C	518	CL7	MG-NB	-2.04	2.01	2.05
21	c	518	CL7	MG-NB	-2.04	2.01	2.05
21	2	505	CL7	CAB-C3B	2.04	1.49	1.45
21	6	505	CL7	CAB-C3B	2.04	1.49	1.45
21	3	510	CL7	C1B-NB	-2.04	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	612	CL7	C3D-C4D	-2.04	1.34	1.39
21	b	613	CL7	C3D-C4D	-2.04	1.34	1.39
21	5	403	CL7	MG-NB	-2.04	2.01	2.05
21	C	505	CL7	C1B-NB	-2.04	1.35	1.37
21	c	505	CL7	C1B-NB	-2.04	1.35	1.37
21	2	501	CL7	CAB-C3B	2.04	1.49	1.45
21	B	603	CL7	C3D-C4D	-2.04	1.34	1.39
21	b	604	CL7	C3D-C4D	-2.04	1.34	1.39
21	D	404	CL7	CBD-CGD	-2.04	1.46	1.52
21	d	404	CL7	CBD-CGD	-2.04	1.46	1.52
21	5	417	CL7	C3B-C4B	-2.04	1.38	1.42
21	C	513	CL7	CHD-C1D	2.04	1.44	1.39
21	b	610	CL7	C1C-NC	-2.04	1.35	1.37
21	6	501	CL7	CAB-C3B	2.04	1.49	1.45
21	C	511	CL7	MG-NB	-2.04	2.01	2.05
21	c	511	CL7	MG-NB	-2.04	2.01	2.05
21	B	615	CL7	CBD-CGD	-2.04	1.46	1.52
21	b	616	CL7	CBD-CGD	-2.04	1.46	1.52
21	1	420	CL7	OBD-CAD	2.04	1.26	1.22
21	5	420	CL7	OBD-CAD	2.04	1.26	1.22
21	5	403	CL7	CHD-C1D	2.04	1.44	1.39
21	D	402	CL7	C3B-C4B	-2.04	1.38	1.42
21	d	402	CL7	C3B-C4B	-2.04	1.38	1.42
32	2	523	ZEX	C10-C9	-2.04	1.33	1.35
32	6	522	ZEX	C10-C9	-2.04	1.33	1.35
21	1	412	CL7	MG-NB	-2.04	2.01	2.05
21	5	412	CL7	MG-NB	-2.04	2.01	2.05
21	3	517	CL7	C1C-NC	-2.04	1.35	1.37
21	4	415	CL7	C1B-NB	-2.04	1.35	1.37
21	7	502	CL7	C3B-C4B	-2.04	1.38	1.42
21	B	604	CL7	CHC-C4B	2.04	1.44	1.39
21	B	612	CL7	CHD-C1D	2.04	1.44	1.39
21	b	613	CL7	CHD-C1D	2.04	1.44	1.39
21	2	516	CL7	C1B-NB	-2.04	1.35	1.37
21	1	403	CL7	C1C-NC	-2.04	1.35	1.37
21	6	516	CL7	C1B-NB	-2.04	1.35	1.37
21	D	404	CL7	C3D-C4D	-2.03	1.34	1.39
21	3	513	CL7	C3B-C4B	-2.03	1.38	1.42
21	7	513	CL7	C3B-C4B	-2.03	1.38	1.42
23	B	618	8CT	C30-C29	2.03	1.53	1.50
21	2	512	CL7	C3B-C4B	-2.03	1.38	1.42
21	6	512	CL7	C3B-C4B	-2.03	1.38	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	512	CL7	C3B-C4B	-2.03	1.38	1.42
21	2	503	CL7	C1B-NB	-2.03	1.35	1.37
21	4	408	CL7	C1C-NC	-2.03	1.35	1.37
21	6	503	CL7	C1B-NB	-2.03	1.35	1.37
21	b	612	CL7	C3D-C4D	-2.03	1.34	1.39
21	1	410	CL7	MG-NB	-2.03	2.01	2.05
21	3	508	CL7	C1C-NC	-2.03	1.35	1.37
21	3	503	CL7	CBD-CGD	-2.03	1.46	1.52
21	7	503	CL7	CBD-CGD	-2.03	1.46	1.52
21	7	517	CL7	C1C-NC	-2.03	1.35	1.37
21	1	406	CL7	C3D-C4D	-2.03	1.34	1.39
21	5	406	CL7	C3D-C4D	-2.03	1.34	1.39
21	2	511	CL7	C3B-C4B	-2.03	1.38	1.42
21	c	504	CL7	CBD-CGD	-2.03	1.46	1.52
21	B	613	CL7	C3D-C4D	-2.03	1.34	1.39
21	3	502	CL7	C3B-C4B	-2.03	1.38	1.42
21	4	412	CL7	CAB-C3B	2.03	1.49	1.45
21	8	412	CL7	CAB-C3B	2.03	1.49	1.45
21	3	504	CL7	CAB-C3B	2.03	1.49	1.45
21	b	606	CL7	MG-NB	-2.03	2.01	2.05
21	D	404	CL7	CHD-C1D	2.03	1.44	1.39
21	d	404	CL7	CHD-C1D	2.03	1.44	1.39
21	B	614	CL7	CBD-CGD	-2.03	1.46	1.52
21	b	615	CL7	CBD-CGD	-2.03	1.46	1.52
21	C	507	CL7	CBD-CGD	-2.03	1.46	1.52
21	4	415	CL7	OBD-CAD	2.03	1.26	1.22
21	8	415	CL7	OBD-CAD	2.03	1.26	1.22
21	3	511	CL7	CBD-CGD	-2.03	1.46	1.52
21	7	511	CL7	CBD-CGD	-2.03	1.46	1.52
21	3	512	CL7	CHD-C1D	2.03	1.44	1.39
21	7	512	CL7	CHD-C1D	2.03	1.44	1.39
21	7	510	CL7	C1B-NB	-2.03	1.35	1.37
21	a	403	CL7	C1C-C2C	-2.03	1.41	1.45
21	c	507	CL7	CBD-CGD	-2.03	1.46	1.52
21	1	403	CL7	MG-NB	-2.03	2.01	2.05
32	3	519	ZEX	C34-C33	-2.03	1.33	1.35
21	4	413	CL7	C1C-C2C	-2.03	1.41	1.45
21	8	413	CL7	C1C-C2C	-2.03	1.41	1.45
21	8	411	CL7	MG-NB	-2.02	2.01	2.05
32	3	522	ZEX	C30-C29	-2.02	1.33	1.35
32	7	522	ZEX	C30-C29	-2.02	1.33	1.35
21	3	513	CL7	C1C-NC	-2.02	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	513	CL7	C1C-NC	-2.02	1.35	1.37
21	C	504	CL7	CBD-CGD	-2.02	1.46	1.52
21	B	601	CL7	C1C-C2C	-2.02	1.41	1.45
21	b	602	CL7	C1C-C2C	-2.02	1.41	1.45
21	b	603	CL7	C1C-NC	-2.02	1.35	1.37
21	B	602	CL7	C3D-C4D	-2.02	1.34	1.39
21	d	404	CL7	C3D-C4D	-2.02	1.34	1.39
21	4	409	CL7	CAB-C3B	2.02	1.49	1.45
21	8	409	CL7	CAB-C3B	2.02	1.49	1.45
21	7	515	CL7	MG-NB	-2.02	2.01	2.05
21	C	513	CL7	C1B-NB	-2.02	1.35	1.37
21	c	513	CL7	C1B-NB	-2.02	1.35	1.37
21	6	514	CL7	C1C-NC	-2.02	1.35	1.37
21	1	410	CL7	C1C-C2C	-2.02	1.41	1.45
21	5	410	CL7	C1C-C2C	-2.02	1.41	1.45
21	3	501	CL7	MG-NB	-2.02	2.01	2.05
21	7	501	CL7	MG-NB	-2.02	2.01	2.05
21	1	417	CL7	C3B-C4B	-2.02	1.38	1.42
21	3	507	CL7	C1C-C2C	-2.02	1.41	1.45
21	7	507	CL7	C1C-C2C	-2.02	1.41	1.45
21	3	501	CL7	OBD-CAD	2.02	1.26	1.22
21	4	404	CL7	OBD-CAD	2.02	1.26	1.22
21	8	404	CL7	OBD-CAD	2.02	1.26	1.22
21	4	410	CL7	C1B-NB	-2.02	1.35	1.37
21	8	410	CL7	C1B-NB	-2.02	1.35	1.37
21	B	611	CL7	C3D-C4D	-2.02	1.34	1.39
21	8	412	CL7	C1C-C2C	-2.02	1.41	1.45
21	3	517	CL7	MG-NB	-2.02	2.01	2.05
21	4	415	CL7	C1C-C2C	-2.02	1.41	1.45
21	A	403	CL7	C1C-C2C	-2.02	1.41	1.45
21	8	406	CL7	CBD-CGD	-2.02	1.46	1.52
21	c	505	CL7	C1C-C2C	-2.02	1.41	1.45
21	3	502	CL7	C3D-C4D	-2.02	1.34	1.39
21	7	502	CL7	C3D-C4D	-2.02	1.34	1.39
21	7	502	CL7	MG-NB	-2.01	2.01	2.05
21	1	407	CL7	OBD-CAD	2.01	1.25	1.22
21	5	407	CL7	OBD-CAD	2.01	1.25	1.22
21	c	513	CL7	C1C-NC	-2.01	1.35	1.37
21	6	505	CL7	CHD-C1D	2.01	1.43	1.39
24	2	522	SQD	O8-S	2.01	1.54	1.47
24	6	521	SQD	O8-S	2.01	1.54	1.47
21	2	511	CL7	OBD-CAD	2.01	1.25	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	407	CL7	OBD-CAD	2.01	1.25	1.22
21	6	511	CL7	OBD-CAD	2.01	1.25	1.22
21	1	417	CL7	CBD-CGD	-2.01	1.46	1.52
21	5	417	CL7	CBD-CGD	-2.01	1.46	1.52
32	6	524	ZEX	C14-C13	-2.01	1.33	1.35
23	D	406	8CT	C39-C16	2.01	1.55	1.50
23	d	406	8CT	C39-C16	2.01	1.55	1.50
21	A	401	CL7	C4C-NC	-2.01	1.35	1.37
21	a	401	CL7	C4C-NC	-2.01	1.35	1.37
21	8	414	CL7	CHD-C1D	2.01	1.43	1.39
21	4	404	CL7	C3B-C4B	-2.01	1.38	1.42
21	8	404	CL7	C3B-C4B	-2.01	1.38	1.42
21	1	405	CL7	C1B-NB	-2.01	1.35	1.37
21	5	405	CL7	C1B-NB	-2.01	1.35	1.37
21	5	410	CL7	MG-NB	-2.01	2.01	2.05
23	B	619	8CT	C39-C16	2.01	1.55	1.50
23	b	620	8CT	C39-C16	2.01	1.55	1.50
21	7	505	CL7	CAB-C3B	2.01	1.49	1.45
21	3	510	CL7	CHD-C1D	2.01	1.43	1.39
21	C	503	CL7	CAB-C3B	2.01	1.49	1.45
21	c	503	CL7	CAB-C3B	2.01	1.49	1.45
21	B	604	CL7	C1B-NB	-2.01	1.35	1.37
21	b	605	CL7	C1B-NB	-2.01	1.35	1.37
21	1	418	CL7	CAB-C3B	2.01	1.49	1.45
21	5	418	CL7	CAB-C3B	2.01	1.49	1.45
21	C	511	CL7	C3D-C4D	-2.01	1.34	1.39
21	c	511	CL7	C3D-C4D	-2.01	1.34	1.39
21	4	412	CL7	MG-NB	-2.01	2.01	2.05
21	8	412	CL7	MG-NB	-2.01	2.01	2.05
21	c	505	CL7	MG-NB	-2.01	2.01	2.05
21	4	406	CL7	C1C-C2C	-2.01	1.41	1.45
32	4	419	ZEX	C34-C33	-2.01	1.33	1.35
21	8	408	CL7	C1C-NC	-2.01	1.35	1.37
21	3	502	CL7	MG-NB	-2.01	2.01	2.05
21	2	517	CL7	C1C-NC	-2.01	1.35	1.37
21	6	517	CL7	C1C-NC	-2.01	1.35	1.37
21	6	511	CL7	C3B-C4B	-2.00	1.38	1.42
23	c	515	8CT	C30-C29	2.00	1.53	1.50
21	8	413	CL7	CBD-CGD	-2.00	1.46	1.52
24	3	521	SQD	O8-S	2.00	1.54	1.47
24	7	521	SQD	O8-S	2.00	1.54	1.47
21	B	605	CL7	MG-NB	-2.00	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	504	CL7	CHD-C1D	2.00	1.43	1.39
21	c	504	CL7	CHD-C1D	2.00	1.43	1.39
21	1	403	CL7	C1C-C2C	-2.00	1.41	1.45
21	5	403	CL7	C1C-C2C	-2.00	1.41	1.45
21	B	609	CL7	C1C-NC	-2.00	1.35	1.37
21	4	409	CL7	C1B-NB	-2.00	1.35	1.37
21	7	502	CL7	C1B-NB	-2.00	1.35	1.37
23	A	404	8CT	C39-C16	2.00	1.55	1.50
23	a	404	8CT	C39-C16	2.00	1.55	1.50
21	8	415	CL7	C1B-NB	-2.00	1.35	1.37
21	4	413	CL7	CBD-CGD	-2.00	1.46	1.52
21	8	406	CL7	C1C-C2C	-2.00	1.41	1.45
21	8	414	CL7	CBD-CGD	-2.00	1.46	1.52
21	7	510	CL7	CHD-C1D	2.00	1.43	1.39
21	3	513	CL7	C1B-NB	-2.00	1.35	1.37

All (5533) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	d	408	PHO	C2D-C1D-ND	10.75	116.95	109.53
22	D	408	PHO	C2D-C1D-ND	10.73	116.94	109.53
21	A	403	CL7	C3C-C4C-NC	10.55	117.83	110.18
21	a	403	CL7	C3C-C4C-NC	10.50	117.79	110.18
22	D	408	PHO	C2B-C1B-NB	10.40	116.71	109.53
22	d	408	PHO	C2B-C1B-NB	10.37	116.69	109.53
21	7	505	CL7	C3C-C4C-NC	10.29	117.64	110.18
21	3	505	CL7	C3C-C4C-NC	10.28	117.63	110.18
23	8	402	8CT	C33-C32-C31	-10.15	115.12	124.85
23	4	402	8CT	C33-C32-C31	-10.12	115.15	124.85
21	3	514	CL7	C3C-C4C-NC	10.01	117.43	110.18
21	7	514	CL7	C3C-C4C-NC	10.01	117.43	110.18
21	8	415	CL7	C3C-C4C-NC	9.96	117.40	110.18
21	4	415	CL7	C3C-C4C-NC	9.95	117.39	110.18
21	1	415	CL7	C3C-C4C-NC	9.82	117.29	110.18
21	3	511	CL7	C3C-C4C-NC	9.81	117.29	110.18
21	5	415	CL7	C3C-C4C-NC	9.81	117.29	110.18
21	7	511	CL7	C3C-C4C-NC	9.81	117.29	110.18
21	4	416	CL7	C3C-C4C-NC	9.76	117.25	110.18
21	8	416	CL7	C3C-C4C-NC	9.76	117.25	110.18
23	b	620	8CT	C33-C32-C31	-9.72	115.53	124.85
21	6	512	CL7	C3C-C4C-NC	9.71	117.22	110.18
21	1	414	CL7	C3C-C4C-NC	9.69	117.20	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	414	CL7	C3C-C4C-NC	9.69	117.20	110.18
21	2	512	CL7	C3C-C4C-NC	9.68	117.19	110.18
23	B	619	8CT	C33-C32-C31	-9.68	115.57	124.85
23	D	406	8CT	C33-C32-C31	-9.66	115.58	124.85
23	d	406	8CT	C33-C32-C31	-9.65	115.59	124.85
21	4	417	CL7	C3C-C4C-NC	9.65	117.17	110.18
21	5	420	CL7	C3C-C4C-NC	9.65	117.17	110.18
21	8	417	CL7	C3C-C4C-NC	9.65	117.17	110.18
21	1	420	CL7	C3C-C4C-NC	9.64	117.17	110.18
21	3	503	CL7	C3C-C4C-NC	9.62	117.15	110.18
21	7	503	CL7	C3C-C4C-NC	9.62	117.15	110.18
21	6	503	CL7	C3C-C4C-NC	9.58	117.12	110.18
21	2	503	CL7	C3C-C4C-NC	9.55	117.10	110.18
21	1	413	CL7	C3C-C4C-NC	9.54	117.09	110.18
21	5	413	CL7	C3C-C4C-NC	9.54	117.09	110.18
21	4	407	CL7	C3C-C4C-NC	9.53	117.09	110.18
23	a	404	8CT	C33-C32-C31	-9.52	115.72	124.85
23	A	404	8CT	C33-C32-C31	-9.50	115.74	124.85
21	8	407	CL7	C3C-C4C-NC	9.47	117.04	110.18
21	4	409	CL7	C3C-C4C-NC	9.47	117.04	110.18
21	8	409	CL7	C3C-C4C-NC	9.47	117.04	110.18
21	c	502	CL7	C3C-C4C-NC	9.44	117.02	110.18
21	7	512	CL7	C3C-C4C-NC	9.42	117.01	110.18
21	1	417	CL7	C3C-C4C-NC	9.41	117.00	110.18
21	5	417	CL7	C3C-C4C-NC	9.41	117.00	110.18
21	C	502	CL7	C3C-C4C-NC	9.39	116.99	110.18
21	B	610	CL7	C3C-C4C-NC	9.39	116.99	110.18
21	b	611	CL7	C3C-C4C-NC	9.39	116.99	110.18
21	3	512	CL7	C3C-C4C-NC	9.39	116.98	110.18
21	C	503	CL7	C3C-C4C-NC	9.36	116.96	110.18
21	3	515	CL7	C3C-C4C-NC	9.35	116.96	110.18
21	7	515	CL7	C3C-C4C-NC	9.35	116.96	110.18
21	c	503	CL7	C3C-C4C-NC	9.35	116.95	110.18
21	8	414	CL7	C3C-C4C-NC	9.29	116.91	110.18
21	4	413	CL7	C3C-C4C-NC	9.27	116.89	110.18
21	8	413	CL7	C3C-C4C-NC	9.27	116.89	110.18
21	4	408	CL7	C3C-C4C-NC	9.26	116.89	110.18
32	2	519	ZEX	C27-C28-C29	-9.26	112.24	126.23
32	6	519	ZEX	C27-C28-C29	-9.26	112.24	126.23
21	4	414	CL7	C3C-C4C-NC	9.25	116.88	110.18
21	3	513	CL7	C3C-C4C-NC	9.25	116.88	110.18
21	7	513	CL7	C3C-C4C-NC	9.25	116.88	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	402	CL7	C3C-C4C-NC	9.23	116.86	110.18
21	5	402	CL7	C3C-C4C-NC	9.23	116.86	110.18
21	B	613	CL7	C3C-C4C-NC	9.22	116.86	110.18
21	b	614	CL7	C3C-C4C-NC	9.22	116.86	110.18
21	2	517	CL7	C3C-C4C-NC	9.22	116.86	110.18
21	C	513	CL7	C3C-C4C-NC	9.21	116.85	110.18
21	c	507	CL7	C3C-C4C-NC	9.21	116.85	110.18
21	c	513	CL7	C3C-C4C-NC	9.21	116.85	110.18
21	8	408	CL7	C3C-C4C-NC	9.21	116.85	110.18
21	6	517	CL7	C3C-C4C-NC	9.21	116.85	110.18
21	3	507	CL7	C3C-C4C-NC	9.19	116.84	110.18
21	7	507	CL7	C3C-C4C-NC	9.19	116.84	110.18
21	C	507	CL7	C3C-C4C-NC	9.16	116.82	110.18
21	1	406	CL7	C3C-C4C-NC	9.15	116.81	110.18
21	5	406	CL7	C3C-C4C-NC	9.15	116.81	110.18
21	2	510	CL7	C3C-C4C-NC	9.13	116.80	110.18
21	6	510	CL7	C3C-C4C-NC	9.13	116.80	110.18
21	7	509	CL7	C3C-C4C-NC	9.13	116.79	110.18
21	A	401	CL7	C3C-C4C-NC	9.12	116.79	110.18
21	a	401	CL7	C3C-C4C-NC	9.12	116.79	110.18
21	C	510	CL7	C3C-C4C-NC	9.12	116.79	110.18
21	c	510	CL7	C3C-C4C-NC	9.12	116.79	110.18
21	2	514	CL7	C3C-C4C-NC	9.11	116.78	110.18
21	6	514	CL7	C3C-C4C-NC	9.11	116.78	110.18
21	1	418	CL7	C3C-C4C-NC	9.11	116.78	110.18
32	2	520	ZEX	C28-C27-C26	-9.11	111.53	127.09
32	3	525	ZEX	C28-C27-C26	-9.11	111.53	127.09
21	3	509	CL7	C3C-C4C-NC	9.11	116.78	110.18
21	B	612	CL7	C3C-C4C-NC	9.10	116.77	110.18
21	b	613	CL7	C3C-C4C-NC	9.10	116.77	110.18
21	5	403	CL7	C3C-C4C-NC	9.07	116.75	110.18
21	5	418	CL7	C3C-C4C-NC	9.06	116.75	110.18
21	1	403	CL7	C3C-C4C-NC	9.05	116.74	110.18
21	2	505	CL7	C3C-C4C-NC	9.05	116.73	110.18
23	B	627	8CT	C33-C32-C31	-9.04	116.18	124.85
21	1	404	CL7	C3C-C4C-NC	9.04	116.73	110.18
21	5	404	CL7	C3C-C4C-NC	9.04	116.73	110.18
21	B	602	CL7	C3C-C4C-NC	9.03	116.73	110.18
21	b	603	CL7	C3C-C4C-NC	9.03	116.73	110.18
21	5	411	CL7	C3C-C4C-NC	9.03	116.72	110.18
21	1	411	CL7	C3C-C4C-NC	9.02	116.71	110.18
23	b	601	8CT	C33-C32-C31	-9.01	116.21	124.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	614	CL7	C3C-C4C-NC	8.99	116.69	110.18
21	b	615	CL7	C3C-C4C-NC	8.99	116.69	110.18
21	8	406	CL7	C3C-C4C-NC	8.98	116.69	110.18
21	4	406	CL7	C3C-C4C-NC	8.96	116.67	110.18
21	7	504	CL7	C3C-C4C-NC	8.96	116.67	110.18
21	3	504	CL7	C3C-C4C-NC	8.96	116.67	110.18
21	2	502	CL7	C3C-C4C-NC	8.95	116.66	110.18
21	6	502	CL7	C3C-C4C-NC	8.95	116.66	110.18
21	5	412	CL7	C3C-C4C-NC	8.95	116.66	110.18
23	c	519	8CT	C33-C32-C31	-8.94	116.28	124.85
21	1	412	CL7	C3C-C4C-NC	8.94	116.66	110.18
21	6	505	CL7	C3C-C4C-NC	8.94	116.66	110.18
21	3	518	CL7	C3C-C4C-NC	8.93	116.65	110.18
21	7	518	CL7	C3C-C4C-NC	8.93	116.65	110.18
23	C	519	8CT	C33-C32-C31	-8.92	116.30	124.85
21	D	405	CL7	C3C-C4C-NC	8.91	116.64	110.18
21	d	405	CL7	C3C-C4C-NC	8.91	116.64	110.18
21	2	515	CL7	C3C-C4C-NC	8.90	116.63	110.18
21	6	515	CL7	C3C-C4C-NC	8.90	116.63	110.18
21	C	504	CL7	C3C-C4C-NC	8.86	116.60	110.18
21	C	514	CL7	C3C-C4C-NC	8.86	116.60	110.18
21	c	504	CL7	C3C-C4C-NC	8.86	116.60	110.18
21	B	616	CL7	C3C-C4C-NC	8.85	116.59	110.18
21	b	617	CL7	C3C-C4C-NC	8.85	116.59	110.18
21	c	514	CL7	C3C-C4C-NC	8.84	116.59	110.18
21	B	615	CL7	C3C-C4C-NC	8.83	116.58	110.18
21	b	616	CL7	C3C-C4C-NC	8.83	116.58	110.18
21	2	511	CL7	C3C-C4C-NC	8.83	116.58	110.18
21	4	410	CL7	C3C-C4C-NC	8.82	116.57	110.18
21	1	419	CL7	C3C-C4C-NC	8.82	116.57	110.18
21	5	419	CL7	C3C-C4C-NC	8.82	116.57	110.18
21	B	608	CL7	C3C-C4C-NC	8.81	116.57	110.18
21	b	609	CL7	C3C-C4C-NC	8.81	116.57	110.18
21	3	510	CL7	C3C-C4C-NC	8.81	116.56	110.18
21	7	510	CL7	C3C-C4C-NC	8.81	116.56	110.18
21	7	517	CL7	C3C-C4C-NC	8.81	116.56	110.18
21	8	410	CL7	C3C-C4C-NC	8.81	116.56	110.18
21	3	517	CL7	C3C-C4C-NC	8.80	116.56	110.18
21	6	511	CL7	C3C-C4C-NC	8.80	116.56	110.18
21	5	408	CL7	C3C-C4C-NC	8.80	116.56	110.18
21	B	609	CL7	C3C-C4C-NC	8.79	116.55	110.18
21	b	608	CL7	C3C-C4C-NC	8.79	116.55	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	507	CL7	C3C-C4C-NC	8.79	116.55	110.18
21	1	407	CL7	C3C-C4C-NC	8.78	116.54	110.18
21	2	501	CL7	C3C-C4C-NC	8.77	116.54	110.18
21	6	501	CL7	C3C-C4C-NC	8.77	116.54	110.18
21	1	408	CL7	C3C-C4C-NC	8.77	116.53	110.18
21	7	506	CL7	C2C-C1C-NC	8.77	116.56	110.10
21	2	507	CL7	C3C-C4C-NC	8.76	116.53	110.18
21	5	407	CL7	C3C-C4C-NC	8.75	116.52	110.18
21	b	610	CL7	C3C-C4C-NC	8.74	116.52	110.18
21	C	506	CL7	C3C-C4C-NC	8.74	116.51	110.18
21	5	416	CL7	C3C-C4C-NC	8.74	116.51	110.18
21	5	412	CL7	C2C-C1C-NC	8.73	116.54	110.10
21	B	607	CL7	C3C-C4C-NC	8.73	116.50	110.18
21	1	416	CL7	C3C-C4C-NC	8.73	116.50	110.18
21	2	518	CL7	C3C-C4C-NC	8.73	116.50	110.18
21	B	615	CL7	C2C-C1C-NC	8.72	116.53	110.10
21	b	616	CL7	C2C-C1C-NC	8.72	116.53	110.10
21	1	412	CL7	C2C-C1C-NC	8.72	116.53	110.10
21	c	506	CL7	C3C-C4C-NC	8.72	116.50	110.18
21	3	506	CL7	C2C-C1C-NC	8.72	116.53	110.10
21	4	404	CL7	C3C-C4C-NC	8.71	116.49	110.18
21	6	518	CL7	C3C-C4C-NC	8.71	116.49	110.18
21	8	404	CL7	C3C-C4C-NC	8.71	116.49	110.18
21	3	501	CL7	C3C-C4C-NC	8.70	116.48	110.18
21	3	506	CL7	C3C-C4C-NC	8.69	116.47	110.18
21	7	506	CL7	C3C-C4C-NC	8.69	116.47	110.18
21	6	513	CL7	C3C-C4C-NC	8.69	116.47	110.18
21	B	622	CL7	C3C-C4C-NC	8.68	116.47	110.18
21	c	508	CL7	C3C-C4C-NC	8.67	116.47	110.18
21	C	512	CL7	C3C-C4C-NC	8.67	116.46	110.18
21	2	516	CL7	C3C-C4C-NC	8.67	116.46	110.18
21	c	512	CL7	C3C-C4C-NC	8.67	116.46	110.18
21	6	516	CL7	C3C-C4C-NC	8.67	116.46	110.18
21	A	406	CL7	C3C-C4C-NC	8.67	116.46	110.18
21	a	405	CL7	C3C-C4C-NC	8.67	116.46	110.18
21	2	506	CL7	C3C-C4C-NC	8.67	116.46	110.18
21	6	509	CL7	C3C-C4C-NC	8.66	116.46	110.18
21	C	505	CL7	C3C-C4C-NC	8.66	116.45	110.18
21	C	508	CL7	C3C-C4C-NC	8.66	116.45	110.18
21	c	505	CL7	C3C-C4C-NC	8.66	116.45	110.18
21	B	611	CL7	C2C-C1C-NC	8.66	116.48	110.10
21	2	513	CL7	C3C-C4C-NC	8.65	116.45	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	7	501	CL7	C3C-C4C-NC	8.65	116.45	110.18
21	b	623	CL7	C3C-C4C-NC	8.63	116.44	110.18
21	B	605	CL7	C3C-C4C-NC	8.63	116.43	110.18
21	b	606	CL7	C3C-C4C-NC	8.63	116.43	110.18
21	2	509	CL7	C3C-C4C-NC	8.62	116.43	110.18
21	6	506	CL7	C3C-C4C-NC	8.62	116.43	110.18
21	1	403	CL7	C2C-C1C-NC	8.60	116.44	110.10
21	b	612	CL7	C2C-C1C-NC	8.59	116.44	110.10
21	B	601	CL7	C3C-C4C-NC	8.59	116.40	110.18
21	b	602	CL7	C3C-C4C-NC	8.59	116.40	110.18
21	1	409	CL7	C3C-C4C-NC	8.59	116.40	110.18
21	5	409	CL7	C3C-C4C-NC	8.59	116.40	110.18
21	6	507	CL7	C2C-C1C-NC	8.58	116.43	110.10
21	2	507	CL7	C2C-C1C-NC	8.57	116.42	110.10
21	5	403	CL7	C2C-C1C-NC	8.57	116.42	110.10
21	4	412	CL7	C3C-C4C-NC	8.57	116.39	110.18
21	c	511	CL7	C3C-C4C-NC	8.56	116.39	110.18
21	7	508	CL7	C2C-C1C-NC	8.54	116.40	110.10
21	1	405	CL7	C3C-C4C-NC	8.53	116.36	110.18
21	8	412	CL7	C3C-C4C-NC	8.53	116.36	110.18
21	8	409	CL7	C2C-C1C-NC	8.52	116.38	110.10
21	2	508	CL7	C3C-C4C-NC	8.52	116.35	110.18
21	6	508	CL7	C3C-C4C-NC	8.52	116.35	110.18
21	4	409	CL7	C2C-C1C-NC	8.51	116.38	110.10
21	C	511	CL7	C3C-C4C-NC	8.51	116.35	110.18
21	5	405	CL7	C3C-C4C-NC	8.51	116.34	110.18
23	B	627	8CT	C19-C20-C21	-8.50	115.17	127.31
23	b	601	8CT	C19-C20-C21	-8.50	115.17	127.31
21	1	410	CL7	C3C-C4C-NC	8.50	116.34	110.18
21	5	410	CL7	C3C-C4C-NC	8.50	116.34	110.18
23	C	516	8CT	C33-C32-C31	-8.50	116.70	124.85
23	c	516	8CT	C33-C32-C31	-8.50	116.70	124.85
21	3	508	CL7	C2C-C1C-NC	8.49	116.36	110.10
21	4	411	CL7	C3C-C4C-NC	8.48	116.33	110.18
21	8	411	CL7	C3C-C4C-NC	8.48	116.33	110.18
21	C	509	CL7	C3C-C4C-NC	8.48	116.32	110.18
21	c	509	CL7	C3C-C4C-NC	8.48	116.32	110.18
21	B	606	CL7	C3C-C4C-NC	8.47	116.32	110.18
21	d	402	CL7	C3C-C4C-NC	8.47	116.32	110.18
21	B	603	CL7	C3C-C4C-NC	8.47	116.32	110.18
21	b	604	CL7	C3C-C4C-NC	8.47	116.32	110.18
21	B	601	CL7	C2C-C1C-NC	8.47	116.34	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	602	CL7	C2C-C1C-NC	8.47	116.34	110.10
23	b	618	8CT	C33-C32-C31	-8.46	116.74	124.85
21	D	402	CL7	C3C-C4C-NC	8.44	116.30	110.18
21	b	607	CL7	C3C-C4C-NC	8.44	116.30	110.18
21	B	611	CL7	C3C-C4C-NC	8.43	116.29	110.18
23	B	617	8CT	C33-C32-C31	-8.43	116.77	124.85
23	C	516	8CT	C14-C13-C12	-8.42	115.29	127.31
21	B	604	CL7	C3C-C4C-NC	8.42	116.28	110.18
21	b	605	CL7	C3C-C4C-NC	8.42	116.28	110.18
21	2	501	CL7	C2C-C1C-NC	8.42	116.31	110.10
21	6	501	CL7	C2C-C1C-NC	8.42	116.31	110.10
23	c	516	8CT	C14-C13-C12	-8.41	115.31	127.31
21	b	612	CL7	C3C-C4C-NC	8.40	116.27	110.18
23	B	627	8CT	C24-C25-C26	-8.39	115.33	127.31
22	d	408	PHO	C4D-ND-C1D	-8.38	100.31	108.83
21	2	514	CL7	C2C-C1C-NC	8.37	116.27	110.10
21	6	514	CL7	C2C-C1C-NC	8.37	116.27	110.10
23	D	406	8CT	C19-C20-C21	-8.37	115.37	127.31
23	b	601	8CT	C24-C25-C26	-8.37	115.37	127.31
22	D	408	PHO	C4D-ND-C1D	-8.36	100.32	108.83
21	7	508	CL7	C3C-C4C-NC	8.36	116.23	110.18
21	2	502	CL7	C2C-C1C-NC	8.35	116.26	110.10
21	6	502	CL7	C2C-C1C-NC	8.35	116.26	110.10
23	d	406	8CT	C19-C20-C21	-8.35	115.39	127.31
21	c	507	CL7	C2C-C1C-NC	8.35	116.25	110.10
21	c	518	CL7	C3C-C4C-NC	8.33	116.22	110.18
21	C	518	CL7	C3C-C4C-NC	8.33	116.22	110.18
21	C	507	CL7	C2C-C1C-NC	8.32	116.23	110.10
21	6	504	CL7	C3C-C4C-NC	8.31	116.20	110.18
21	3	508	CL7	C3C-C4C-NC	8.31	116.20	110.18
21	2	508	CL7	C2C-C1C-NC	8.30	116.22	110.10
21	6	508	CL7	C2C-C1C-NC	8.30	116.22	110.10
21	4	405	CL7	C3C-C4C-NC	8.30	116.19	110.18
21	8	405	CL7	C3C-C4C-NC	8.30	116.19	110.18
21	2	506	CL7	C2C-C1C-NC	8.29	116.22	110.10
21	6	506	CL7	C2C-C1C-NC	8.29	116.22	110.10
32	3	522	ZEX	C11-C10-C9	-8.29	115.48	127.31
32	7	522	ZEX	C11-C10-C9	-8.29	115.48	127.31
21	C	514	CL7	C2C-C1C-NC	8.27	116.20	110.10
21	4	409	CL7	C4D-C3D-CAD	-8.26	101.86	107.42
21	8	409	CL7	C4D-C3D-CAD	-8.26	101.86	107.42
21	2	504	CL7	C3C-C4C-NC	8.26	116.16	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	8	410	CL7	C2C-C1C-NC	8.23	116.17	110.10
21	B	605	CL7	C2C-C1C-NC	8.23	116.17	110.10
21	b	606	CL7	C2C-C1C-NC	8.23	116.17	110.10
21	C	506	CL7	C2C-C1C-NC	8.22	116.16	110.10
21	c	506	CL7	C2C-C1C-NC	8.22	116.16	110.10
21	2	513	CL7	C2C-C1C-NC	8.22	116.16	110.10
23	C	515	8CT	C33-C32-C31	-8.21	116.97	124.85
23	c	515	8CT	C33-C32-C31	-8.21	116.97	124.85
21	1	402	CL7	C2C-C1C-NC	8.21	116.16	110.10
21	5	402	CL7	C2C-C1C-NC	8.21	116.16	110.10
21	c	514	CL7	C2C-C1C-NC	8.20	116.15	110.10
21	3	507	CL7	C2C-C1C-NC	8.20	116.15	110.10
21	D	404	CL7	C3C-C4C-NC	8.20	116.12	110.18
21	d	404	CL7	C3C-C4C-NC	8.20	116.12	110.18
21	6	513	CL7	C2C-C1C-NC	8.19	116.14	110.10
21	C	512	CL7	C2C-C1C-NC	8.19	116.14	110.10
21	1	413	CL7	C2C-C1C-NC	8.19	116.14	110.10
21	5	413	CL7	C2C-C1C-NC	8.19	116.14	110.10
21	C	508	CL7	C4D-C3D-CAD	-8.16	101.92	107.42
21	c	508	CL7	C4D-C3D-CAD	-8.16	101.92	107.42
21	c	505	CL7	C2C-C1C-NC	8.16	116.12	110.10
21	c	512	CL7	C2C-C1C-NC	8.16	116.12	110.10
21	5	405	CL7	C2C-C1C-NC	8.16	116.12	110.10
21	C	518	CL7	C2C-C1C-NC	8.16	116.12	110.10
21	7	504	CL7	C2C-C1C-NC	8.16	116.12	110.10
21	4	410	CL7	C2C-C1C-NC	8.16	116.12	110.10
21	c	504	CL7	C2C-C1C-NC	8.16	116.12	110.10
21	c	518	CL7	C2C-C1C-NC	8.15	116.11	110.10
21	3	502	CL7	C3C-C4C-NC	8.15	116.09	110.18
21	7	507	CL7	C2C-C1C-NC	8.15	116.11	110.10
21	3	504	CL7	C2C-C1C-NC	8.15	116.11	110.10
21	7	517	CL7	C2C-C1C-NC	8.14	116.11	110.10
21	1	409	CL7	C2C-C1C-NC	8.14	116.10	110.10
21	5	409	CL7	C2C-C1C-NC	8.14	116.10	110.10
21	3	517	CL7	C2C-C1C-NC	8.13	116.09	110.10
21	2	510	CL7	C2C-C1C-NC	8.13	116.09	110.10
21	1	406	CL7	C2C-C1C-NC	8.13	116.09	110.10
21	6	510	CL7	C2C-C1C-NC	8.13	116.09	110.10
21	5	406	CL7	C2C-C1C-NC	8.13	116.09	110.10
21	B	603	CL7	C2C-C1C-NC	8.12	116.09	110.10
21	C	505	CL7	C2C-C1C-NC	8.12	116.09	110.10
21	b	604	CL7	C2C-C1C-NC	8.12	116.09	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	405	CL7	C2C-C1C-NC	8.12	116.09	110.10
21	B	604	CL7	C2C-C1C-NC	8.12	116.09	110.10
21	b	605	CL7	C2C-C1C-NC	8.12	116.09	110.10
21	D	402	CL7	C2C-C1C-NC	8.12	116.08	110.10
21	d	402	CL7	C2C-C1C-NC	8.12	116.08	110.10
21	C	504	CL7	C2C-C1C-NC	8.11	116.08	110.10
21	7	502	CL7	C3C-C4C-NC	8.11	116.06	110.18
21	7	515	CL7	C2C-C1C-NC	8.10	116.08	110.10
21	3	515	CL7	C2C-C1C-NC	8.09	116.07	110.10
21	c	513	CL7	C2C-C1C-NC	8.09	116.07	110.10
21	d	405	CL7	C2C-C1C-NC	8.09	116.06	110.10
21	4	416	CL7	C2C-C1C-NC	8.08	116.06	110.10
21	8	416	CL7	C2C-C1C-NC	8.08	116.06	110.10
21	C	513	CL7	C2C-C1C-NC	8.08	116.06	110.10
23	B	618	8CT	C33-C32-C31	-8.07	117.11	124.85
21	2	515	CL7	C2C-C1C-NC	8.06	116.04	110.10
21	6	515	CL7	C2C-C1C-NC	8.06	116.04	110.10
21	8	415	CL7	C2C-C1C-NC	8.05	116.04	110.10
21	2	504	CL7	C2C-C1C-NC	8.05	116.04	110.10
21	D	405	CL7	C2C-C1C-NC	8.04	116.03	110.10
21	4	405	CL7	C2C-C1C-NC	8.03	116.03	110.10
21	5	408	CL7	C4D-C3D-CAD	-8.03	102.01	107.42
23	b	619	8CT	C33-C32-C31	-8.03	117.15	124.85
21	1	407	CL7	C2C-C1C-NC	8.02	116.02	110.10
21	5	407	CL7	C2C-C1C-NC	8.02	116.02	110.10
21	3	516	CL7	C3C-C4C-NC	8.02	115.99	110.18
21	7	516	CL7	C3C-C4C-NC	8.02	115.99	110.18
21	4	413	CL7	C2C-C1C-NC	8.02	116.01	110.10
21	8	413	CL7	C2C-C1C-NC	8.02	116.01	110.10
21	8	405	CL7	C2C-C1C-NC	8.01	116.01	110.10
21	4	415	CL7	C2C-C1C-NC	8.01	116.01	110.10
21	6	504	CL7	C2C-C1C-NC	8.00	116.00	110.10
21	2	516	CL7	C2C-C1C-NC	7.99	115.99	110.10
21	6	516	CL7	C2C-C1C-NC	7.99	115.99	110.10
21	5	418	CL7	C2C-C1C-NC	7.99	115.99	110.10
21	3	501	CL7	C2C-C1C-NC	7.98	115.99	110.10
23	a	404	8CT	C24-C25-C26	-7.98	115.93	127.31
21	4	404	CL7	C2C-C1C-NC	7.97	115.98	110.10
21	8	404	CL7	C2C-C1C-NC	7.97	115.98	110.10
21	C	514	CL7	C4D-C3D-CAD	-7.97	102.06	107.42
21	1	408	CL7	C4D-C3D-CAD	-7.97	102.06	107.42
21	c	514	CL7	C4D-C3D-CAD	-7.97	102.06	107.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	418	CL7	C2C-C1C-NC	7.96	115.97	110.10
21	3	518	CL7	C2C-C1C-NC	7.96	115.97	110.10
21	7	518	CL7	C2C-C1C-NC	7.96	115.97	110.10
21	B	606	CL7	C2C-C1C-NC	7.94	115.96	110.10
21	b	607	CL7	C2C-C1C-NC	7.94	115.96	110.10
21	1	410	CL7	C2C-C1C-NC	7.94	115.96	110.10
21	5	410	CL7	C2C-C1C-NC	7.94	115.96	110.10
21	2	503	CL7	C2C-C1C-NC	7.94	115.95	110.10
21	5	408	CL7	C2C-C1C-NC	7.94	115.95	110.10
21	7	501	CL7	C2C-C1C-NC	7.93	115.95	110.10
23	A	404	8CT	C24-C25-C26	-7.93	116.00	127.31
21	B	612	CL7	C2C-C1C-NC	7.92	115.94	110.10
21	b	613	CL7	C2C-C1C-NC	7.92	115.94	110.10
32	3	520	ZEX	C11-C10-C9	-7.92	116.01	127.31
32	7	520	ZEX	C11-C10-C9	-7.92	116.01	127.31
21	6	503	CL7	C2C-C1C-NC	7.92	115.94	110.10
21	7	510	CL7	C2C-C1C-NC	7.92	115.94	110.10
21	1	408	CL7	C2C-C1C-NC	7.91	115.93	110.10
21	4	408	CL7	C2C-C1C-NC	7.89	115.92	110.10
21	C	510	CL7	C2C-C1C-NC	7.89	115.92	110.10
21	c	510	CL7	C2C-C1C-NC	7.89	115.92	110.10
21	3	510	CL7	C2C-C1C-NC	7.88	115.91	110.10
21	4	417	CL7	C2C-C1C-NC	7.88	115.91	110.10
21	8	417	CL7	C2C-C1C-NC	7.88	115.91	110.10
21	B	602	CL7	C2C-C1C-NC	7.88	115.91	110.10
21	b	615	CL7	C2C-C1C-NC	7.88	115.91	110.10
21	A	406	CL7	C2C-C1C-NC	7.88	115.91	110.10
21	4	414	CL7	C2C-C1C-NC	7.88	115.91	110.10
21	a	405	CL7	C2C-C1C-NC	7.88	115.91	110.10
21	b	603	CL7	C2C-C1C-NC	7.87	115.90	110.10
21	5	416	CL7	C2C-C1C-NC	7.86	115.89	110.10
21	2	509	CL7	C2C-C1C-NC	7.85	115.89	110.10
21	8	414	CL7	C2C-C1C-NC	7.84	115.88	110.10
21	B	614	CL7	C2C-C1C-NC	7.84	115.88	110.10
21	8	408	CL7	C2C-C1C-NC	7.84	115.88	110.10
32	5	421	ZEX	C31-C30-C29	-7.83	116.13	127.31
21	C	509	CL7	C2C-C1C-NC	7.83	115.87	110.10
21	c	509	CL7	C2C-C1C-NC	7.83	115.87	110.10
21	6	509	CL7	C2C-C1C-NC	7.82	115.87	110.10
21	1	416	CL7	C2C-C1C-NC	7.81	115.86	110.10
21	1	419	CL7	C2C-C1C-NC	7.81	115.86	110.10
21	5	419	CL7	C2C-C1C-NC	7.81	115.86	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1	421	ZEX	C31-C30-C29	-7.81	116.17	127.31
21	1	415	CL7	C2C-C1C-NC	7.81	115.86	110.10
21	5	415	CL7	C2C-C1C-NC	7.80	115.85	110.10
21	b	609	CL7	C2C-C1C-NC	7.79	115.84	110.10
21	7	512	CL7	C2C-C1C-NC	7.78	115.84	110.10
21	4	407	CL7	C2C-C1C-NC	7.78	115.84	110.10
21	3	514	CL7	C2C-C1C-NC	7.77	115.83	110.10
21	7	514	CL7	C2C-C1C-NC	7.77	115.83	110.10
21	4	406	CL7	C2C-C1C-NC	7.76	115.82	110.10
21	B	608	CL7	C2C-C1C-NC	7.76	115.82	110.10
21	d	404	CL7	C2C-C1C-NC	7.76	115.82	110.10
21	D	404	CL7	C2C-C1C-NC	7.74	115.81	110.10
21	3	513	CL7	C2C-C1C-NC	7.74	115.81	110.10
21	7	513	CL7	C2C-C1C-NC	7.74	115.81	110.10
21	8	407	CL7	C2C-C1C-NC	7.74	115.81	110.10
21	3	512	CL7	C2C-C1C-NC	7.74	115.81	110.10
21	1	420	CL7	C2C-C1C-NC	7.73	115.80	110.10
21	8	406	CL7	C2C-C1C-NC	7.73	115.80	110.10
21	C	508	CL7	C2C-C1C-NC	7.73	115.80	110.10
21	c	508	CL7	C2C-C1C-NC	7.73	115.80	110.10
21	5	420	CL7	C2C-C1C-NC	7.71	115.79	110.10
21	2	505	CL7	C2C-C1C-NC	7.69	115.77	110.10
32	3	519	ZEX	C31-C30-C29	-7.69	116.34	127.31
32	7	519	ZEX	C31-C30-C29	-7.69	116.34	127.31
21	7	509	CL7	C2C-C1C-NC	7.68	115.76	110.10
21	c	511	CL7	C2C-C1C-NC	7.65	115.75	110.10
21	C	511	CL7	C2C-C1C-NC	7.62	115.72	110.10
21	b	610	CL7	C2C-C1C-NC	7.62	115.72	110.10
21	7	505	CL7	C2C-C1C-NC	7.61	115.71	110.10
21	2	518	CL7	C2C-C1C-NC	7.61	115.71	110.10
21	6	518	CL7	C2C-C1C-NC	7.61	115.71	110.10
21	B	609	CL7	C2C-C1C-NC	7.60	115.71	110.10
21	3	516	CL7	C2C-C1C-NC	7.60	115.71	110.10
21	7	516	CL7	C2C-C1C-NC	7.60	115.71	110.10
21	6	505	CL7	C2C-C1C-NC	7.60	115.70	110.10
21	7	502	CL7	C2C-C1C-NC	7.60	115.70	110.10
21	B	616	CL7	C2C-C1C-NC	7.59	115.70	110.10
21	b	617	CL7	C2C-C1C-NC	7.59	115.70	110.10
21	3	509	CL7	C2C-C1C-NC	7.59	115.69	110.10
21	3	505	CL7	C2C-C1C-NC	7.59	115.69	110.10
21	B	606	CL7	C2B-C1B-NB	7.58	115.31	110.23
21	b	607	CL7	C2B-C1B-NB	7.58	115.31	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	c	502	CL7	C2C-C1C-NC	7.56	115.68	110.10
21	2	517	CL7	C2C-C1C-NC	7.56	115.68	110.10
21	6	517	CL7	C2C-C1C-NC	7.56	115.68	110.10
21	3	503	CL7	C2C-C1C-NC	7.55	115.67	110.10
21	3	511	CL7	C2C-C1C-NC	7.55	115.67	110.10
21	7	503	CL7	C2C-C1C-NC	7.55	115.67	110.10
21	7	511	CL7	C2C-C1C-NC	7.55	115.67	110.10
21	B	607	CL7	C2C-C1C-NC	7.53	115.65	110.10
21	1	411	CL7	C2C-C1C-NC	7.53	115.65	110.10
21	5	411	CL7	C2C-C1C-NC	7.53	115.65	110.10
21	2	511	CL7	C2C-C1C-NC	7.53	115.65	110.10
21	3	502	CL7	C2C-C1C-NC	7.53	115.65	110.10
21	C	502	CL7	C2C-C1C-NC	7.52	115.65	110.10
21	B	622	CL7	C2C-C1C-NC	7.52	115.64	110.10
21	6	511	CL7	C2C-C1C-NC	7.51	115.64	110.10
21	b	608	CL7	C2C-C1C-NC	7.50	115.63	110.10
21	C	503	CL7	C2C-C1C-NC	7.48	115.62	110.10
21	c	503	CL7	C2C-C1C-NC	7.48	115.62	110.10
21	B	610	CL7	C2C-C1C-NC	7.47	115.61	110.10
21	B	613	CL7	C2C-C1C-NC	7.47	115.61	110.10
21	b	611	CL7	C2C-C1C-NC	7.47	115.61	110.10
21	b	614	CL7	C2C-C1C-NC	7.46	115.61	110.10
21	b	623	CL7	C2C-C1C-NC	7.45	115.60	110.10
23	8	402	8CT	C30-C31-C32	-7.42	112.34	121.47
23	4	402	8CT	C30-C31-C32	-7.42	112.34	121.47
32	4	403	ZEX	C31-C30-C29	-7.42	116.72	127.31
32	8	403	ZEX	C31-C30-C29	-7.42	116.72	127.31
21	1	414	CL7	C2C-C1C-NC	7.41	115.57	110.10
21	5	414	CL7	C2C-C1C-NC	7.41	115.57	110.10
21	1	404	CL7	C2C-C1C-NC	7.41	115.56	110.10
21	5	404	CL7	C2C-C1C-NC	7.41	115.56	110.10
21	4	411	CL7	C2B-C1B-NB	7.39	115.19	110.23
21	8	411	CL7	C2B-C1B-NB	7.39	115.19	110.23
32	3	520	ZEX	C31-C30-C29	-7.33	116.84	127.31
32	2	519	ZEX	C31-C30-C29	-7.33	116.85	127.31
32	6	519	ZEX	C31-C30-C29	-7.33	116.85	127.31
32	7	520	ZEX	C31-C30-C29	-7.32	116.86	127.31
21	2	512	CL7	C2C-C1C-NC	7.31	115.49	110.10
21	A	403	CL7	C2C-C1C-NC	7.30	115.48	110.10
21	6	512	CL7	C2C-C1C-NC	7.29	115.48	110.10
21	4	412	CL7	C2C-C1C-NC	7.29	115.48	110.10
21	4	411	CL7	C2C-C1C-NC	7.27	115.46	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	8	411	CL7	C2C-C1C-NC	7.27	115.46	110.10
21	A	401	CL7	C2C-C1C-NC	7.26	115.45	110.10
21	a	401	CL7	C2C-C1C-NC	7.26	115.45	110.10
32	2	525	ZEX	C31-C30-C29	-7.25	116.97	127.31
32	6	524	ZEX	C31-C30-C29	-7.25	116.97	127.31
21	8	412	CL7	C2C-C1C-NC	7.25	115.44	110.10
21	a	403	CL7	C2C-C1C-NC	7.24	115.44	110.10
32	1	422	ZEX	C7-C8-C9	-7.20	115.35	126.23
32	5	422	ZEX	C7-C8-C9	-7.20	115.35	126.23
32	2	523	ZEX	C35-C34-C33	-7.16	117.09	127.31
32	6	522	ZEX	C35-C34-C33	-7.16	117.09	127.31
32	4	419	ZEX	C28-C27-C26	-7.16	114.86	127.09
32	8	419	ZEX	C28-C27-C26	-7.16	114.86	127.09
23	C	519	8CT	C24-C25-C26	-7.15	117.10	127.31
23	c	519	8CT	C24-C25-C26	-7.14	117.12	127.31
32	2	525	ZEX	C28-C27-C26	-7.07	115.01	127.09
32	6	524	ZEX	C28-C27-C26	-7.07	115.01	127.09
32	4	403	ZEX	C28-C27-C26	-7.01	115.11	127.09
32	2	525	ZEX	C7-C8-C9	-7.01	115.64	126.23
32	6	524	ZEX	C7-C8-C9	-7.01	115.64	126.23
32	8	403	ZEX	C28-C27-C26	-6.99	115.14	127.09
21	1	419	CL7	C4D-C3D-CAD	-6.99	102.72	107.42
32	4	419	ZEX	C15-C14-C13	-6.99	117.34	127.31
21	2	513	CL7	C4D-C3D-CAD	-6.98	102.72	107.42
32	4	418	ZEX	C31-C30-C29	-6.97	117.36	127.31
32	8	418	ZEX	C31-C30-C29	-6.97	117.36	127.31
32	8	419	ZEX	C15-C14-C13	-6.97	117.36	127.31
21	B	622	CL7	C2B-C1B-NB	6.95	114.89	110.23
21	6	513	CL7	C4D-C3D-CAD	-6.94	102.75	107.42
21	b	623	CL7	C4D-C3D-CAD	-6.93	102.75	107.42
21	5	419	CL7	C4D-C3D-CAD	-6.91	102.77	107.42
32	4	420	ZEX	C28-C27-C26	-6.90	115.29	127.09
32	8	420	ZEX	C28-C27-C26	-6.90	115.29	127.09
21	b	623	CL7	C2B-C1B-NB	6.90	114.86	110.23
21	B	622	CL7	C4D-C3D-CAD	-6.89	102.78	107.42
21	7	502	CL7	C2B-C1B-NB	6.89	114.85	110.23
21	1	402	CL7	C1A-NA-C4A	6.86	110.46	106.30
21	1	410	CL7	C2B-C1B-NB	6.85	114.83	110.23
21	3	502	CL7	C2B-C1B-NB	6.85	114.82	110.23
21	5	402	CL7	C1A-NA-C4A	6.83	110.43	106.30
21	5	410	CL7	C2B-C1B-NB	6.82	114.80	110.23
21	b	615	CL7	C2B-C1B-NB	6.81	114.80	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	7	518	CL7	C2B-C1B-NB	6.81	114.80	110.23
23	K	101	8CT	C33-C32-C31	-6.80	118.33	124.85
21	B	614	CL7	C2B-C1B-NB	6.80	114.79	110.23
21	C	513	CL7	C4D-C3D-CAD	-6.79	102.85	107.42
21	3	518	CL7	C2B-C1B-NB	6.79	114.78	110.23
21	3	512	CL7	C2B-C1B-NB	6.78	114.78	110.23
21	A	401	CL7	C2B-C1B-NB	6.77	114.77	110.23
32	2	523	ZEX	C28-C27-C26	-6.76	115.54	127.09
23	k	101	8CT	C33-C32-C31	-6.76	118.37	124.85
23	B	619	8CT	C24-C25-C26	-6.75	117.67	127.31
23	b	620	8CT	C24-C25-C26	-6.75	117.67	127.31
32	6	522	ZEX	C28-C27-C26	-6.75	115.56	127.09
21	7	512	CL7	C2B-C1B-NB	6.74	114.75	110.23
21	c	513	CL7	C4D-C3D-CAD	-6.74	102.88	107.42
21	7	517	CL7	C2B-C1B-NB	6.73	114.75	110.23
21	6	511	CL7	C2B-C1B-NB	6.73	114.75	110.23
21	a	401	CL7	C2B-C1B-NB	6.73	114.74	110.23
21	1	417	CL7	C2C-C1C-NC	6.73	115.06	110.10
21	5	417	CL7	C2C-C1C-NC	6.73	115.06	110.10
21	7	516	CL7	C2B-C1B-NB	6.72	114.74	110.23
23	B	627	8CT	C14-C13-C12	-6.69	117.76	127.31
32	6	520	ZEX	C7-C8-C9	-6.68	116.14	126.23
21	1	414	CL7	C2B-C1B-NB	6.68	114.71	110.23
21	5	414	CL7	C2B-C1B-NB	6.68	114.71	110.23
21	3	516	CL7	C2B-C1B-NB	6.67	114.71	110.23
21	3	517	CL7	C2B-C1B-NB	6.67	114.71	110.23
21	2	511	CL7	C2B-C1B-NB	6.67	114.70	110.23
32	2	521	ZEX	C7-C8-C9	-6.67	116.16	126.23
23	b	601	8CT	C14-C13-C12	-6.65	117.81	127.31
23	d	406	8CT	C19-C18-C17	-6.63	109.89	123.47
23	D	406	8CT	C19-C18-C17	-6.62	109.91	123.47
23	A	404	8CT	C19-C20-C21	-6.62	117.86	127.31
21	D	402	CL7	C2B-C1B-NB	6.62	114.67	110.23
21	d	402	CL7	C2B-C1B-NB	6.62	114.67	110.23
23	a	404	8CT	C19-C20-C21	-6.62	117.86	127.31
21	8	417	CL7	C4D-C3D-CAD	-6.62	102.97	107.42
21	6	513	CL7	C2B-C1B-NB	6.62	114.67	110.23
21	4	417	CL7	C4D-C3D-CAD	-6.60	102.97	107.42
21	8	413	CL7	C2B-C1B-NB	6.59	114.65	110.23
21	2	513	CL7	C2B-C1B-NB	6.57	114.64	110.23
21	6	518	CL7	C2B-C1B-NB	6.57	114.64	110.23
21	B	607	CL7	C2B-C1B-NB	6.57	114.63	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	608	CL7	C2B-C1B-NB	6.57	114.63	110.23
21	4	412	CL7	C2B-C1B-NB	6.56	114.63	110.23
21	8	412	CL7	C2B-C1B-NB	6.56	114.63	110.23
32	6	522	ZEX	C7-C8-C9	-6.56	116.33	126.23
21	2	518	CL7	C2B-C1B-NB	6.56	114.63	110.23
23	C	516	8CT	C10-C11-C12	-6.56	116.33	126.23
23	c	516	8CT	C10-C11-C12	-6.56	116.33	126.23
21	B	616	CL7	C2B-C1B-NB	6.55	114.62	110.23
21	4	413	CL7	C2B-C1B-NB	6.55	114.62	110.23
21	b	617	CL7	C2B-C1B-NB	6.55	114.62	110.23
21	B	615	CL7	C1A-NA-C4A	6.55	110.27	106.30
21	b	616	CL7	C1A-NA-C4A	6.55	110.27	106.30
32	2	523	ZEX	C7-C8-C9	-6.54	116.36	126.23
21	1	417	CL7	C2B-C1B-NB	6.53	114.61	110.23
21	5	417	CL7	C2B-C1B-NB	6.51	114.60	110.23
21	2	507	CL7	C4D-C3D-CAD	-6.50	103.04	107.42
21	6	507	CL7	C4D-C3D-CAD	-6.50	103.04	107.42
21	B	603	CL7	C2B-C1B-NB	6.48	114.58	110.23
21	4	404	CL7	C2B-C1B-NB	6.48	114.58	110.23
21	8	404	CL7	C2B-C1B-NB	6.48	114.58	110.23
23	b	601	8CT	C10-C11-C12	-6.47	116.45	126.23
21	c	511	CL7	C2B-C1B-NB	6.47	114.57	110.23
21	b	611	CL7	C1A-NA-C4A	6.47	110.22	106.30
21	3	511	CL7	C1A-NA-C4A	6.47	110.22	106.30
21	4	405	CL7	C1A-NA-C4A	6.47	110.22	106.30
21	8	405	CL7	C1A-NA-C4A	6.47	110.22	106.30
21	2	504	CL7	C2B-C1B-NB	6.46	114.56	110.23
21	6	504	CL7	C2B-C1B-NB	6.46	114.56	110.23
21	C	511	CL7	C2B-C1B-NB	6.45	114.56	110.23
23	B	627	8CT	C10-C11-C12	-6.45	116.49	126.23
21	C	505	CL7	C2B-C1B-NB	6.45	114.56	110.23
21	7	511	CL7	C1A-NA-C4A	6.44	110.20	106.30
21	1	407	CL7	C2B-C1B-NB	6.43	114.55	110.23
21	c	505	CL7	C2B-C1B-NB	6.43	114.54	110.23
21	2	503	CL7	C1A-NA-C4A	6.43	110.19	106.30
21	6	503	CL7	C1A-NA-C4A	6.43	110.19	106.30
21	b	604	CL7	C2B-C1B-NB	6.42	114.54	110.23
21	6	517	CL7	C2B-C1B-NB	6.41	114.53	110.23
21	c	514	CL7	C2B-C1B-NB	6.41	114.53	110.23
21	2	505	CL7	C1A-NA-C4A	6.39	110.17	106.30
21	6	505	CL7	C1A-NA-C4A	6.39	110.17	106.30
21	7	510	CL7	C2B-C1B-NB	6.39	114.52	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	407	CL7	C2B-C1B-NB	6.39	114.51	110.23
21	3	513	CL7	C2B-C1B-NB	6.37	114.50	110.23
32	4	418	ZEX	C15-C14-C13	-6.37	118.22	127.31
32	8	418	ZEX	C15-C14-C13	-6.37	118.22	127.31
21	C	514	CL7	C2B-C1B-NB	6.36	114.50	110.23
21	d	405	CL7	C2B-C1B-NB	6.36	114.50	110.23
21	3	503	CL7	C1A-NA-C4A	6.36	110.15	106.30
21	B	610	CL7	C1A-NA-C4A	6.35	110.15	106.30
21	7	503	CL7	C1A-NA-C4A	6.35	110.15	106.30
21	A	406	CL7	C1A-NA-C4A	6.35	110.15	106.30
32	2	520	ZEX	C31-C30-C29	-6.35	118.25	127.31
32	3	525	ZEX	C31-C30-C29	-6.35	118.25	127.31
21	3	511	CL7	C2B-C1B-NB	6.35	114.49	110.23
21	7	511	CL7	C2B-C1B-NB	6.35	114.49	110.23
21	B	613	CL7	C2B-C1B-NB	6.34	114.48	110.23
21	7	513	CL7	C2B-C1B-NB	6.34	114.48	110.23
21	1	413	CL7	C1A-NA-C4A	6.34	110.14	106.30
21	1	405	CL7	C2B-C1B-NB	6.34	114.48	110.23
21	5	405	CL7	C2B-C1B-NB	6.34	114.48	110.23
21	2	504	CL7	C4D-C3D-CAD	-6.34	103.16	107.42
21	6	504	CL7	C4D-C3D-CAD	-6.34	103.16	107.42
21	b	608	CL7	C4D-C3D-CAD	-6.33	103.16	107.42
21	2	517	CL7	C2B-C1B-NB	6.32	114.47	110.23
32	3	519	ZEX	C15-C14-C13	-6.32	118.29	127.31
32	7	519	ZEX	C15-C14-C13	-6.32	118.29	127.31
21	B	604	CL7	C1A-NA-C4A	6.32	110.13	106.30
21	b	605	CL7	C1A-NA-C4A	6.32	110.13	106.30
21	3	501	CL7	C2B-C1B-NB	6.32	114.47	110.23
21	7	501	CL7	C2B-C1B-NB	6.32	114.47	110.23
21	b	614	CL7	C2B-C1B-NB	6.31	114.46	110.23
21	7	505	CL7	C1A-NA-C4A	6.31	110.12	106.30
21	3	505	CL7	C1A-NA-C4A	6.31	110.12	106.30
21	b	609	CL7	C2B-C1B-NB	6.30	114.46	110.23
21	a	405	CL7	C1A-NA-C4A	6.30	110.11	106.30
21	B	608	CL7	C2B-C1B-NB	6.30	114.45	110.23
21	3	510	CL7	C2B-C1B-NB	6.30	114.45	110.23
21	D	405	CL7	C2B-C1B-NB	6.30	114.45	110.23
21	4	417	CL7	C1A-NA-C4A	6.29	110.11	106.30
21	8	417	CL7	C1A-NA-C4A	6.29	110.11	106.30
21	5	413	CL7	C1A-NA-C4A	6.29	110.11	106.30
32	7	519	ZEX	C27-C28-C29	-6.28	116.74	126.23
32	3	519	ZEX	C27-C28-C29	-6.28	116.75	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	c	518	CL7	C2B-C1B-NB	6.28	114.44	110.23
21	1	418	CL7	C2B-C1B-NB	6.28	114.44	110.23
21	5	418	CL7	C2B-C1B-NB	6.28	114.44	110.23
21	7	506	CL7	C1A-NA-C4A	6.27	110.10	106.30
21	4	415	CL7	C2B-C1B-NB	6.26	114.43	110.23
21	B	615	CL7	C2B-C1B-NB	6.26	114.43	110.23
21	5	420	CL7	C2B-C1B-NB	6.26	114.43	110.23
21	8	415	CL7	C2B-C1B-NB	6.25	114.42	110.23
22	d	408	PHO	C3D-C4D-ND	6.25	116.24	107.72
21	d	404	CL7	C2B-C1B-NB	6.25	114.42	110.23
32	4	403	ZEX	C7-C8-C9	-6.25	116.79	126.23
21	1	420	CL7	C2B-C1B-NB	6.24	114.42	110.23
21	c	504	CL7	C2B-C1B-NB	6.24	114.42	110.23
21	B	607	CL7	C4D-C3D-CAD	-6.24	103.22	107.42
21	C	508	CL7	C2B-C1B-NB	6.23	114.41	110.23
21	c	508	CL7	C2B-C1B-NB	6.23	114.41	110.23
21	B	609	CL7	C2B-C1B-NB	6.23	114.41	110.23
21	b	610	CL7	C2B-C1B-NB	6.23	114.41	110.23
21	C	518	CL7	C2B-C1B-NB	6.23	114.41	110.23
22	D	408	PHO	C3D-C4D-ND	6.23	116.21	107.72
21	3	506	CL7	C1A-NA-C4A	6.23	110.07	106.30
21	B	610	CL7	C2B-C1B-NB	6.22	114.40	110.23
21	b	611	CL7	C2B-C1B-NB	6.22	114.40	110.23
21	2	516	CL7	C2B-C1B-NB	6.22	114.40	110.23
21	6	516	CL7	C2B-C1B-NB	6.22	114.40	110.23
21	A	406	CL7	C2B-C1B-NB	6.21	114.40	110.23
21	B	601	CL7	C2B-C1B-NB	6.21	114.40	110.23
21	D	404	CL7	C2B-C1B-NB	6.21	114.39	110.23
32	8	403	ZEX	C7-C8-C9	-6.20	116.86	126.23
21	2	506	CL7	C2B-C1B-NB	6.20	114.39	110.23
21	6	506	CL7	C2B-C1B-NB	6.20	114.39	110.23
21	2	510	CL7	C2B-C1B-NB	6.19	114.38	110.23
21	6	510	CL7	C2B-C1B-NB	6.19	114.38	110.23
21	4	414	CL7	C1A-NA-C4A	6.19	110.05	106.30
21	C	511	CL7	C4D-C3D-CAD	-6.19	103.25	107.42
21	c	511	CL7	C4D-C3D-CAD	-6.19	103.25	107.42
21	8	414	CL7	C1A-NA-C4A	6.19	110.05	106.30
23	B	618	8CT	C30-C31-C32	-6.19	113.86	121.47
23	b	619	8CT	C30-C31-C32	-6.19	113.86	121.47
21	C	504	CL7	C2B-C1B-NB	6.19	114.38	110.23
21	B	602	CL7	C2B-C1B-NB	6.18	114.38	110.23
21	b	603	CL7	C2B-C1B-NB	6.18	114.38	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	616	CL7	C2B-C1B-NB	6.18	114.38	110.23
21	5	409	CL7	C2B-C1B-NB	6.17	114.37	110.23
21	A	403	CL7	C2B-C1B-NB	6.17	114.36	110.23
21	a	403	CL7	C2B-C1B-NB	6.17	114.36	110.23
21	6	503	CL7	C2B-C1B-NB	6.16	114.36	110.23
21	b	602	CL7	C2B-C1B-NB	6.16	114.36	110.23
21	C	513	CL7	C2B-C1B-NB	6.15	114.36	110.23
21	c	513	CL7	C2B-C1B-NB	6.15	114.36	110.23
21	4	408	CL7	C2B-C1B-NB	6.15	114.36	110.23
21	8	408	CL7	C2B-C1B-NB	6.15	114.36	110.23
21	a	405	CL7	C2B-C1B-NB	6.15	114.35	110.23
21	2	503	CL7	C2B-C1B-NB	6.14	114.35	110.23
21	1	418	CL7	C4D-C3D-CAD	-6.14	103.29	107.42
21	5	418	CL7	C4D-C3D-CAD	-6.14	103.29	107.42
21	4	414	CL7	C2B-C1B-NB	6.14	114.35	110.23
21	8	414	CL7	C2B-C1B-NB	6.14	114.35	110.23
21	1	409	CL7	C2B-C1B-NB	6.14	114.34	110.23
21	1	419	CL7	C2B-C1B-NB	6.13	114.34	110.23
21	5	419	CL7	C2B-C1B-NB	6.13	114.34	110.23
21	B	612	CL7	C2B-C1B-NB	6.13	114.34	110.23
21	b	613	CL7	C2B-C1B-NB	6.13	114.34	110.23
21	B	605	CL7	C1A-NA-C4A	6.13	110.01	106.30
21	1	416	CL7	C2B-C1B-NB	6.12	114.34	110.23
21	5	416	CL7	C2B-C1B-NB	6.12	114.34	110.23
21	b	606	CL7	C1A-NA-C4A	6.12	110.01	106.30
32	3	520	ZEX	C35-C34-C33	-6.11	118.58	127.31
32	7	520	ZEX	C35-C34-C33	-6.11	118.58	127.31
21	1	404	CL7	C2B-C1B-NB	6.10	114.32	110.23
21	1	403	CL7	C1A-NA-C4A	6.10	109.99	106.30
32	2	525	ZEX	C11-C10-C9	-6.10	118.61	127.31
32	6	524	ZEX	C11-C10-C9	-6.10	118.61	127.31
21	6	501	CL7	C4D-C3D-CAD	-6.09	103.32	107.42
21	5	411	CL7	C2B-C1B-NB	6.09	114.32	110.23
23	b	619	8CT	C19-C18-C17	-6.09	111.00	123.47
21	4	406	CL7	C2B-C1B-NB	6.09	114.31	110.23
21	8	406	CL7	C2B-C1B-NB	6.09	114.31	110.23
21	3	515	CL7	C2B-C1B-NB	6.08	114.31	110.23
21	7	515	CL7	C2B-C1B-NB	6.08	114.31	110.23
21	2	512	CL7	C2B-C1B-NB	6.08	114.31	110.23
21	6	512	CL7	C2B-C1B-NB	6.08	114.31	110.23
23	B	618	8CT	C19-C18-C17	-6.08	111.03	123.47
21	5	403	CL7	C1A-NA-C4A	6.07	109.98	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	415	CL7	C1A-NA-C4A	6.07	109.97	106.30
21	1	415	CL7	C1A-NA-C4A	6.07	109.97	106.30
21	1	411	CL7	C2B-C1B-NB	6.06	114.30	110.23
21	1	408	CL7	C2B-C1B-NB	6.06	114.29	110.23
21	5	420	CL7	C1A-NA-C4A	6.06	109.97	106.30
21	3	504	CL7	C2B-C1B-NB	6.06	114.29	110.23
21	5	404	CL7	C2B-C1B-NB	6.06	114.29	110.23
21	7	504	CL7	C2B-C1B-NB	6.06	114.29	110.23
32	3	519	ZEX	C11-C10-C9	-6.06	118.67	127.31
21	2	501	CL7	C4D-C3D-CAD	-6.06	103.34	107.42
21	3	509	CL7	C2B-C1B-NB	6.05	114.29	110.23
21	4	407	CL7	C2B-C1B-NB	6.04	114.28	110.23
21	5	408	CL7	C2B-C1B-NB	6.04	114.28	110.23
21	8	407	CL7	C2B-C1B-NB	6.04	114.28	110.23
21	8	410	CL7	C1A-NA-C4A	6.04	109.96	106.30
32	7	519	ZEX	C11-C10-C9	-6.04	118.70	127.31
21	C	510	CL7	C2B-C1B-NB	6.03	114.28	110.23
21	1	402	CL7	C2B-C1B-NB	6.03	114.28	110.23
21	5	402	CL7	C2B-C1B-NB	6.03	114.28	110.23
21	4	415	CL7	C1A-NA-C4A	6.02	109.94	106.30
21	C	512	CL7	C2B-C1B-NB	6.02	114.27	110.23
21	1	403	CL7	C2B-C1B-NB	6.02	114.27	110.23
21	c	512	CL7	C2B-C1B-NB	6.02	114.27	110.23
21	c	510	CL7	C2B-C1B-NB	6.01	114.26	110.23
21	4	410	CL7	C1A-NA-C4A	6.01	109.94	106.30
21	2	509	CL7	C2B-C1B-NB	6.01	114.26	110.23
21	C	502	CL7	C1A-NA-C4A	6.01	109.94	106.30
21	c	502	CL7	C1A-NA-C4A	6.01	109.94	106.30
21	8	415	CL7	C1A-NA-C4A	6.00	109.94	106.30
21	6	509	CL7	C2B-C1B-NB	6.00	114.25	110.23
21	1	415	CL7	C2B-C1B-NB	6.00	114.25	110.23
21	5	403	CL7	C2B-C1B-NB	6.00	114.25	110.23
21	1	420	CL7	C1A-NA-C4A	5.99	109.93	106.30
21	7	509	CL7	C2B-C1B-NB	5.99	114.25	110.23
21	C	503	CL7	C2B-C1B-NB	5.98	114.24	110.23
21	3	505	CL7	C2B-C1B-NB	5.98	114.24	110.23
21	c	503	CL7	C2B-C1B-NB	5.98	114.24	110.23
21	7	505	CL7	C2B-C1B-NB	5.98	114.24	110.23
21	1	413	CL7	C2B-C1B-NB	5.97	114.23	110.23
21	5	415	CL7	C2B-C1B-NB	5.97	114.23	110.23
21	C	502	CL7	C2B-C1B-NB	5.97	114.23	110.23
21	b	604	CL7	C1A-NA-C4A	5.97	109.91	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	603	CL7	C1A-NA-C4A	5.95	109.90	106.30
23	B	619	8CT	C19-C20-C21	-5.95	118.82	127.31
21	d	405	CL7	C1A-NA-C4A	5.94	109.90	106.30
21	4	405	CL7	C2B-C1B-NB	5.94	114.21	110.23
21	3	504	CL7	C1A-NA-C4A	5.94	109.90	106.30
21	8	405	CL7	C2B-C1B-NB	5.94	114.21	110.23
21	b	602	CL7	C1A-NA-C4A	5.94	109.89	106.30
21	5	406	CL7	C2B-C1B-NB	5.94	114.21	110.23
21	D	404	CL7	C1A-NA-C4A	5.93	109.89	106.30
21	d	404	CL7	C1A-NA-C4A	5.93	109.89	106.30
21	2	514	CL7	C2B-C1B-NB	5.93	114.21	110.23
21	6	514	CL7	C2B-C1B-NB	5.93	114.21	110.23
23	b	620	8CT	C19-C20-C21	-5.93	118.85	127.31
21	5	413	CL7	C2B-C1B-NB	5.92	114.20	110.23
21	c	502	CL7	C2B-C1B-NB	5.92	114.20	110.23
21	1	406	CL7	C1A-NA-C4A	5.92	109.88	106.30
21	4	409	CL7	C1A-NA-C4A	5.92	109.88	106.30
21	8	409	CL7	C1A-NA-C4A	5.92	109.88	106.30
21	1	406	CL7	C2B-C1B-NB	5.92	114.20	110.23
21	B	601	CL7	C1A-NA-C4A	5.90	109.87	106.30
21	C	506	CL7	C1A-NA-C4A	5.90	109.87	106.30
21	7	504	CL7	C1A-NA-C4A	5.90	109.87	106.30
21	6	501	CL7	C1A-NA-C4A	5.89	109.87	106.30
23	A	404	8CT	C10-C11-C12	-5.88	117.34	126.23
21	6	513	CL7	C1A-NA-C4A	5.88	109.86	106.30
21	C	506	CL7	C2B-C1B-NB	5.88	114.17	110.23
21	c	506	CL7	C2B-C1B-NB	5.88	114.17	110.23
21	D	405	CL7	C1A-NA-C4A	5.88	109.86	106.30
21	c	506	CL7	C1A-NA-C4A	5.88	109.86	106.30
21	7	510	CL7	C1A-NA-C4A	5.88	109.86	106.30
21	1	412	CL7	C1A-NA-C4A	5.87	109.86	106.30
21	2	501	CL7	C1A-NA-C4A	5.87	109.85	106.30
21	5	412	CL7	C1A-NA-C4A	5.87	109.85	106.30
23	a	404	8CT	C10-C11-C12	-5.87	117.37	126.23
21	8	406	CL7	C1A-NA-C4A	5.86	109.85	106.30
21	5	406	CL7	C1A-NA-C4A	5.85	109.84	106.30
21	3	514	CL7	C1A-NA-C4A	5.84	109.84	106.30
21	7	514	CL7	C1A-NA-C4A	5.84	109.84	106.30
21	2	501	CL7	C2B-C1B-NB	5.84	114.15	110.23
21	6	501	CL7	C2B-C1B-NB	5.84	114.15	110.23
21	3	503	CL7	C2B-C1B-NB	5.84	114.15	110.23
32	7	522	ZEX	C28-C27-C26	-5.83	117.13	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	7	513	CL7	C1A-NA-C4A	5.83	109.83	106.30
21	3	514	CL7	C2B-C1B-NB	5.82	114.14	110.23
21	7	514	CL7	C2B-C1B-NB	5.82	114.14	110.23
21	7	503	CL7	C2B-C1B-NB	5.82	114.13	110.23
21	3	510	CL7	C1A-NA-C4A	5.82	109.82	106.30
32	3	522	ZEX	C28-C27-C26	-5.82	117.15	127.09
21	7	506	CL7	C2B-C1B-NB	5.81	114.13	110.23
21	5	418	CL7	C1A-NA-C4A	5.81	109.82	106.30
23	c	516	8CT	C04-C03-C02	-5.81	114.43	122.61
21	3	516	CL7	C1A-NA-C4A	5.81	109.82	106.30
21	C	512	CL7	C1A-NA-C4A	5.80	109.81	106.30
21	4	406	CL7	C1A-NA-C4A	5.80	109.81	106.30
21	c	512	CL7	C1A-NA-C4A	5.80	109.81	106.30
23	C	516	8CT	C04-C03-C02	-5.80	114.44	122.61
21	C	505	CL7	C1A-NA-C4A	5.79	109.81	106.30
21	4	410	CL7	C2B-C1B-NB	5.79	114.11	110.23
21	8	410	CL7	C2B-C1B-NB	5.79	114.11	110.23
32	1	421	ZEX	C28-C27-C26	-5.79	117.20	127.09
32	5	421	ZEX	C28-C27-C26	-5.79	117.20	127.09
21	C	518	CL7	C4D-C3D-CAD	-5.78	103.53	107.42
21	c	518	CL7	C4D-C3D-CAD	-5.78	103.53	107.42
21	3	513	CL7	C1A-NA-C4A	5.78	109.80	106.30
21	1	418	CL7	C1A-NA-C4A	5.77	109.79	106.30
21	3	506	CL7	C2B-C1B-NB	5.77	114.10	110.23
23	B	619	8CT	C14-C13-C12	-5.77	119.08	127.31
21	2	513	CL7	C1A-NA-C4A	5.76	109.79	106.30
21	C	509	CL7	C1A-NA-C4A	5.76	109.79	106.30
21	c	509	CL7	C1A-NA-C4A	5.76	109.79	106.30
21	6	502	CL7	C1A-NA-C4A	5.75	109.78	106.30
31	f	101	HEM	CHC-C4B-NB	5.75	130.66	124.42
21	6	507	CL7	C2B-C1B-NB	5.75	114.09	110.23
31	F	101	HEM	CHC-C4B-NB	5.75	130.66	124.42
21	c	505	CL7	C1A-NA-C4A	5.74	109.78	106.30
21	2	515	CL7	C1A-NA-C4A	5.74	109.77	106.30
21	6	515	CL7	C1A-NA-C4A	5.74	109.77	106.30
21	7	516	CL7	C1A-NA-C4A	5.74	109.77	106.30
23	K	101	8CT	C19-C20-C21	-5.73	119.13	127.31
23	k	101	8CT	C19-C20-C21	-5.73	119.13	127.31
23	b	620	8CT	C14-C13-C12	-5.73	119.13	127.31
32	4	403	ZEX	C15-C14-C13	-5.73	119.13	127.31
21	C	513	CL7	C1A-NA-C4A	5.73	109.77	106.30
21	c	513	CL7	C1A-NA-C4A	5.73	109.77	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	614	CL7	C1A-NA-C4A	5.73	109.77	106.30
21	2	508	CL7	C1A-NA-C4A	5.73	109.77	106.30
21	b	615	CL7	C1A-NA-C4A	5.73	109.77	106.30
21	6	516	CL7	C1A-NA-C4A	5.73	109.77	106.30
23	b	619	8CT	C18-C17-C16	-5.73	119.14	127.31
21	6	508	CL7	C1A-NA-C4A	5.72	109.76	106.30
21	B	611	CL7	C1A-NA-C4A	5.71	109.76	106.30
32	8	403	ZEX	C15-C14-C13	-5.71	119.16	127.31
21	2	502	CL7	C1A-NA-C4A	5.71	109.75	106.30
23	B	618	8CT	C18-C17-C16	-5.70	119.17	127.31
21	2	507	CL7	C2B-C1B-NB	5.70	114.06	110.23
21	8	413	CL7	C1A-NA-C4A	5.70	109.75	106.30
21	6	505	CL7	C2B-C1B-NB	5.70	114.05	110.23
23	C	516	8CT	C35-C30-C29	-5.70	105.50	112.70
21	4	404	CL7	C1A-NA-C4A	5.70	109.75	106.30
21	B	608	CL7	C1A-NA-C4A	5.70	109.75	106.30
21	c	514	CL7	C1A-NA-C4A	5.70	109.75	106.30
21	C	503	CL7	C4D-C3D-CAD	-5.69	103.59	107.42
21	c	503	CL7	C4D-C3D-CAD	-5.69	103.59	107.42
21	4	413	CL7	C1A-NA-C4A	5.69	109.74	106.30
21	2	506	CL7	C4D-C3D-CAD	-5.68	103.59	107.42
21	2	516	CL7	C1A-NA-C4A	5.68	109.74	106.30
21	3	508	CL7	C1A-NA-C4A	5.68	109.74	106.30
21	7	508	CL7	C1A-NA-C4A	5.68	109.74	106.30
21	2	505	CL7	C1-C2-C3	5.68	135.86	126.04
21	6	505	CL7	C1-C2-C3	5.68	135.86	126.04
21	B	612	CL7	C1A-NA-C4A	5.68	109.74	106.30
21	3	507	CL7	C1A-NA-C4A	5.68	109.74	106.30
21	b	613	CL7	C1A-NA-C4A	5.68	109.74	106.30
21	7	507	CL7	C1A-NA-C4A	5.68	109.74	106.30
23	c	516	8CT	C35-C30-C29	-5.68	105.53	112.70
21	1	409	CL7	C1A-NA-C4A	5.68	109.74	106.30
21	5	409	CL7	C1A-NA-C4A	5.68	109.74	106.30
21	c	508	CL7	C1A-NA-C4A	5.67	109.74	106.30
21	b	609	CL7	C1A-NA-C4A	5.67	109.73	106.30
21	2	505	CL7	C2B-C1B-NB	5.67	114.03	110.23
21	B	605	CL7	C2B-C1B-NB	5.65	114.02	110.23
21	b	606	CL7	C2B-C1B-NB	5.65	114.02	110.23
21	b	612	CL7	C1A-NA-C4A	5.65	109.72	106.30
21	C	514	CL7	C1A-NA-C4A	5.64	109.72	106.30
21	1	407	CL7	C1A-NA-C4A	5.64	109.72	106.30
21	c	504	CL7	C1A-NA-C4A	5.64	109.72	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	416	CL7	C4D-C3D-CAD	-5.64	103.63	107.42
21	6	507	CL7	C1A-NA-C4A	5.64	109.71	106.30
21	8	404	CL7	C1A-NA-C4A	5.64	109.71	106.30
21	6	506	CL7	C4D-C3D-CAD	-5.63	103.63	107.42
21	C	508	CL7	C1A-NA-C4A	5.63	109.71	106.30
21	2	512	CL7	C1A-NA-C4A	5.63	109.71	106.30
21	6	512	CL7	C1A-NA-C4A	5.63	109.71	106.30
21	2	514	CL7	C1A-NA-C4A	5.63	109.71	106.30
21	6	514	CL7	C1A-NA-C4A	5.63	109.71	106.30
21	8	408	CL7	C1A-NA-C4A	5.62	109.71	106.30
21	2	504	CL7	C1A-NA-C4A	5.62	109.70	106.30
21	4	408	CL7	C1A-NA-C4A	5.62	109.70	106.30
32	2	523	ZEX	C27-C28-C29	-5.61	117.75	126.23
32	6	522	ZEX	C27-C28-C29	-5.61	117.75	126.23
23	B	617	8CT	C18-C17-C16	-5.61	119.30	127.31
23	b	618	8CT	C18-C17-C16	-5.61	119.30	127.31
21	C	504	CL7	C1A-NA-C4A	5.61	109.70	106.30
21	1	408	CL7	C1A-NA-C4A	5.61	109.70	106.30
21	5	407	CL7	C1A-NA-C4A	5.61	109.70	106.30
21	7	506	CL7	C4D-C3D-CAD	-5.60	103.65	107.42
21	1	404	CL7	C1A-NA-C4A	5.60	109.69	106.30
21	6	504	CL7	C1A-NA-C4A	5.60	109.69	106.30
21	5	404	CL7	C1A-NA-C4A	5.60	109.69	106.30
21	1	416	CL7	C4D-C3D-CAD	-5.60	103.65	107.42
21	2	507	CL7	C1A-NA-C4A	5.59	109.69	106.30
21	3	506	CL7	C4D-C3D-CAD	-5.59	103.66	107.42
21	C	507	CL7	C2B-C1B-NB	5.58	113.98	110.23
21	c	507	CL7	C2B-C1B-NB	5.58	113.98	110.23
21	4	405	CL7	C4D-C3D-CAD	-5.58	103.66	107.42
21	1	405	CL7	C1A-NA-C4A	5.58	109.68	106.30
21	5	405	CL7	C1A-NA-C4A	5.58	109.68	106.30
21	5	408	CL7	C1A-NA-C4A	5.58	109.68	106.30
21	2	510	CL7	C1A-NA-C4A	5.58	109.68	106.30
21	6	510	CL7	C1A-NA-C4A	5.58	109.68	106.30
21	4	416	CL7	C2B-C1B-NB	5.57	113.96	110.23
21	8	416	CL7	C2B-C1B-NB	5.57	113.96	110.23
21	C	503	CL7	C1A-NA-C4A	5.56	109.67	106.30
21	c	503	CL7	C1A-NA-C4A	5.56	109.67	106.30
23	C	516	8CT	C24-C25-C26	-5.56	119.37	127.31
23	c	516	8CT	C24-C25-C26	-5.56	119.37	127.31
21	3	507	CL7	C4D-C3D-CAD	-5.56	103.68	107.42
21	8	405	CL7	C4D-C3D-CAD	-5.56	103.68	107.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	7	507	CL7	C4D-C3D-CAD	-5.55	103.68	107.42
21	1	412	CL7	C2B-C1B-NB	5.55	113.95	110.23
21	5	412	CL7	C2B-C1B-NB	5.55	113.95	110.23
21	6	515	CL7	C2B-C1B-NB	5.54	113.95	110.23
21	2	515	CL7	C2B-C1B-NB	5.54	113.95	110.23
21	7	507	CL7	C2B-C1B-NB	5.54	113.94	110.23
21	3	515	CL7	C1A-NA-C4A	5.52	109.64	106.30
21	3	507	CL7	C2B-C1B-NB	5.51	113.93	110.23
21	5	416	CL7	C1A-NA-C4A	5.51	109.64	106.30
23	4	402	8CT	C19-C20-C21	-5.51	119.45	127.31
21	C	518	CL7	C1A-NA-C4A	5.50	109.63	106.30
21	c	518	CL7	C1A-NA-C4A	5.50	109.63	106.30
21	C	507	CL7	C4D-C3D-CAD	-5.50	103.72	107.42
21	c	507	CL7	C4D-C3D-CAD	-5.50	103.72	107.42
23	8	402	8CT	C19-C20-C21	-5.49	119.48	127.31
21	1	416	CL7	C1A-NA-C4A	5.48	109.62	106.30
21	8	409	CL7	C2B-C1B-NB	5.48	113.91	110.23
21	3	509	CL7	C1A-NA-C4A	5.48	109.62	106.30
23	C	519	8CT	C19-C20-C21	-5.47	119.50	127.31
23	c	519	8CT	C19-C20-C21	-5.47	119.50	127.31
21	c	507	CL7	C1A-NA-C4A	5.47	109.61	106.30
21	1	415	CL7	C4D-C3D-CAD	-5.46	103.74	107.42
21	5	415	CL7	C4D-C3D-CAD	-5.46	103.74	107.42
21	1	410	CL7	C1A-NA-C4A	5.46	109.61	106.30
21	5	410	CL7	C1A-NA-C4A	5.46	109.61	106.30
21	7	509	CL7	C1A-NA-C4A	5.46	109.61	106.30
21	4	407	CL7	C1A-NA-C4A	5.45	109.60	106.30
21	8	407	CL7	C1A-NA-C4A	5.45	109.60	106.30
21	7	517	CL7	C1A-NA-C4A	5.45	109.60	106.30
21	2	511	CL7	C1A-NA-C4A	5.43	109.59	106.30
21	6	511	CL7	C1A-NA-C4A	5.43	109.59	106.30
23	K	101	8CT	C07-C02-C03	-5.43	114.85	122.73
23	k	101	8CT	C07-C02-C03	-5.43	114.85	122.73
21	B	603	CL7	CMD-C2D-C1D	5.42	133.63	125.37
21	b	604	CL7	CMD-C2D-C1D	5.42	133.63	125.37
21	2	506	CL7	C1A-NA-C4A	5.42	109.58	106.30
21	6	506	CL7	C1A-NA-C4A	5.42	109.58	106.30
21	C	507	CL7	C1A-NA-C4A	5.42	109.58	106.30
21	b	607	CL7	CMD-C2D-C1D	5.41	133.61	125.37
21	4	409	CL7	C2B-C1B-NB	5.41	113.86	110.23
21	3	501	CL7	C1A-NA-C4A	5.40	109.57	106.30
21	4	416	CL7	C1A-NA-C4A	5.40	109.57	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	404	8CT	C14-C13-C12	-5.40	119.61	127.31
23	a	404	8CT	C14-C13-C12	-5.40	119.61	127.31
21	7	515	CL7	C1A-NA-C4A	5.40	109.57	106.30
21	2	508	CL7	C2B-C1B-NB	5.39	113.85	110.23
21	B	606	CL7	CMD-C2D-C1D	5.39	133.57	125.37
21	8	416	CL7	C1A-NA-C4A	5.38	109.56	106.30
21	A	403	CL7	C1A-NA-C4A	5.38	109.56	106.30
21	a	403	CL7	C1A-NA-C4A	5.38	109.56	106.30
21	3	517	CL7	C1A-NA-C4A	5.38	109.56	106.30
23	k	101	8CT	C14-C13-C12	-5.37	119.64	127.31
21	c	505	CL7	C4D-C3D-CAD	-5.37	103.81	107.42
21	B	606	CL7	C1A-NA-C4A	5.37	109.55	106.30
21	b	607	CL7	C1A-NA-C4A	5.37	109.55	106.30
21	C	505	CL7	C4D-C3D-CAD	-5.36	103.81	107.42
21	a	401	CL7	C1A-NA-C4A	5.36	109.55	106.30
23	K	101	8CT	C14-C13-C12	-5.36	119.67	127.31
21	1	419	CL7	C1A-NA-C4A	5.35	109.54	106.30
21	5	419	CL7	C1A-NA-C4A	5.35	109.54	106.30
32	2	519	ZEX	C35-C34-C33	-5.35	119.67	127.31
32	6	519	ZEX	C35-C34-C33	-5.35	119.67	127.31
21	6	508	CL7	C2B-C1B-NB	5.35	113.82	110.23
21	7	501	CL7	C1A-NA-C4A	5.34	109.53	106.30
23	D	406	8CT	C18-C17-C16	-5.33	119.70	127.31
21	c	510	CL7	C1A-NA-C4A	5.33	109.53	106.30
23	d	406	8CT	C18-C17-C16	-5.33	119.71	127.31
21	B	604	CL7	C2B-C1B-NB	5.33	113.80	110.23
21	b	605	CL7	C2B-C1B-NB	5.33	113.80	110.23
21	C	510	CL7	C1A-NA-C4A	5.32	109.52	106.30
21	3	516	CL7	CMD-C2D-C1D	5.30	133.44	125.37
21	7	516	CL7	CMD-C2D-C1D	5.30	133.44	125.37
21	A	406	CL7	CMD-C2D-C1D	5.29	133.43	125.37
21	a	405	CL7	CMD-C2D-C1D	5.29	133.43	125.37
32	2	520	ZEX	C35-C34-C33	-5.29	119.75	127.31
21	A	401	CL7	C1A-NA-C4A	5.29	109.50	106.30
32	3	525	ZEX	C35-C34-C33	-5.29	119.77	127.31
21	3	518	CL7	C1A-NA-C4A	5.28	109.50	106.30
21	7	518	CL7	C1A-NA-C4A	5.28	109.50	106.30
21	B	602	CL7	C1A-NA-C4A	5.28	109.50	106.30
21	2	509	CL7	C1A-NA-C4A	5.28	109.50	106.30
23	D	406	8CT	C01-C02-C03	-5.28	118.60	124.53
23	d	406	8CT	C01-C02-C03	-5.28	118.60	124.53
21	b	603	CL7	C1A-NA-C4A	5.28	109.50	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	616	CL7	C1A-NA-C4A	5.28	109.50	106.30
21	2	518	CL7	C1A-NA-C4A	5.28	109.50	106.30
23	B	617	8CT	C30-C31-C32	-5.27	114.99	121.47
21	B	609	CL7	C1A-NA-C4A	5.25	109.48	106.30
32	3	522	ZEX	C35-C34-C33	-5.24	119.83	127.31
32	7	522	ZEX	C35-C34-C33	-5.24	119.83	127.31
21	C	509	CL7	C2B-C1B-NB	5.24	113.75	110.23
32	2	521	ZEX	C27-C28-C29	-5.24	118.32	126.23
32	6	520	ZEX	C27-C28-C29	-5.24	118.32	126.23
23	b	618	8CT	C30-C31-C32	-5.23	115.03	121.47
21	6	509	CL7	C1A-NA-C4A	5.23	109.47	106.30
32	2	519	ZEX	C15-C14-C13	-5.22	119.86	127.31
21	b	617	CL7	C1A-NA-C4A	5.22	109.46	106.30
21	6	518	CL7	C1A-NA-C4A	5.22	109.46	106.30
32	3	520	ZEX	C27-C28-C29	-5.21	118.37	126.23
32	7	520	ZEX	C27-C28-C29	-5.21	118.37	126.23
21	5	403	CL7	C4D-C3D-CAD	-5.21	103.92	107.42
32	6	519	ZEX	C15-C14-C13	-5.20	119.88	127.31
21	B	605	CL7	CMD-C2D-C1D	5.20	133.29	125.37
21	b	606	CL7	CMD-C2D-C1D	5.20	133.29	125.37
21	2	517	CL7	C1A-NA-C4A	5.20	109.45	106.30
21	1	417	CL7	C1A-NA-C4A	5.20	109.45	106.30
21	4	412	CL7	C1A-NA-C4A	5.19	109.45	106.30
21	b	610	CL7	C1A-NA-C4A	5.19	109.45	106.30
21	8	412	CL7	C1A-NA-C4A	5.19	109.45	106.30
21	c	509	CL7	C2B-C1B-NB	5.19	113.71	110.23
23	D	406	8CT	C30-C31-C32	-5.19	115.09	121.47
21	B	611	CL7	C2B-C1B-NB	5.19	113.71	110.23
21	5	411	CL7	C1A-NA-C4A	5.18	109.44	106.30
21	1	412	CL7	C4D-C3D-CAD	-5.18	103.93	107.42
21	5	412	CL7	C4D-C3D-CAD	-5.18	103.93	107.42
21	4	412	CL7	C4D-C3D-CAD	-5.18	103.94	107.42
21	8	412	CL7	C4D-C3D-CAD	-5.18	103.94	107.42
21	2	503	CL7	CMD-C2D-C1D	5.18	133.25	125.37
21	6	503	CL7	CMD-C2D-C1D	5.18	133.25	125.37
21	6	517	CL7	C1A-NA-C4A	5.17	109.43	106.30
21	6	512	CL7	C2D-C1D-ND	5.16	113.69	110.23
21	1	409	CL7	C4D-C3D-CAD	-5.16	103.95	107.42
21	5	409	CL7	C4D-C3D-CAD	-5.16	103.95	107.42
32	1	422	ZEX	C28-C27-C26	-5.15	118.28	127.09
21	1	403	CL7	C4D-C3D-CAD	-5.15	103.95	107.42
21	B	607	CL7	C1A-NA-C4A	5.15	109.42	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	516	8CT	C18-C17-C16	-5.15	119.97	127.31
21	b	612	CL7	C2B-C1B-NB	5.15	113.68	110.23
23	d	406	8CT	C30-C31-C32	-5.15	115.14	121.47
23	B	617	8CT	C01-C02-C03	-5.15	118.75	124.53
23	K	101	8CT	C04-C03-C02	-5.14	115.37	122.61
23	k	101	8CT	C04-C03-C02	-5.14	115.37	122.61
21	1	411	CL7	C1A-NA-C4A	5.14	109.42	106.30
32	5	422	ZEX	C28-C27-C26	-5.14	118.30	127.09
21	2	512	CL7	C2D-C1D-ND	5.14	113.68	110.23
21	5	417	CL7	C1A-NA-C4A	5.13	109.41	106.30
21	B	609	CL7	CMD-C2D-C1D	5.13	133.18	125.37
21	b	610	CL7	CMD-C2D-C1D	5.13	133.18	125.37
21	D	402	CL7	C4D-C3D-CAD	-5.13	103.97	107.42
21	d	402	CL7	C4D-C3D-CAD	-5.13	103.97	107.42
23	C	516	8CT	C18-C17-C16	-5.13	119.99	127.31
21	2	516	CL7	C4D-C3D-CAD	-5.13	103.97	107.42
21	6	516	CL7	C4D-C3D-CAD	-5.13	103.97	107.42
21	B	613	CL7	C1A-NA-C4A	5.12	109.40	106.30
21	b	614	CL7	C1A-NA-C4A	5.12	109.40	106.30
32	8	403	ZEX	C35-C34-C33	-5.12	120.00	127.31
32	4	403	ZEX	C35-C34-C33	-5.12	120.00	127.31
21	8	411	CL7	C1A-NA-C4A	5.12	109.40	106.30
21	b	608	CL7	C1A-NA-C4A	5.11	109.40	106.30
32	3	519	ZEX	C7-C8-C9	-5.11	118.51	126.23
32	7	519	ZEX	C7-C8-C9	-5.11	118.51	126.23
21	2	504	CL7	CMD-C2D-C1D	5.11	133.15	125.37
21	6	504	CL7	CMD-C2D-C1D	5.11	133.15	125.37
21	4	411	CL7	C1A-NA-C4A	5.11	109.39	106.30
21	d	404	CL7	CMD-C2D-C1D	5.11	133.14	125.37
32	2	523	ZEX	C15-C14-C13	-5.10	120.03	127.31
23	b	618	8CT	C01-C02-C03	-5.09	118.81	124.53
21	c	506	CL7	CMD-C2D-C1D	5.09	133.11	125.37
21	D	404	CL7	CMD-C2D-C1D	5.08	133.11	125.37
32	6	522	ZEX	C15-C14-C13	-5.08	120.05	127.31
21	3	515	CL7	C4D-C3D-CAD	-5.08	104.00	107.42
21	7	515	CL7	C4D-C3D-CAD	-5.08	104.00	107.42
21	1	417	CL7	CMD-C2D-C1D	5.08	133.10	125.37
21	5	417	CL7	CMD-C2D-C1D	5.08	133.10	125.37
21	7	512	CL7	C1A-NA-C4A	5.07	109.37	106.30
21	3	512	CL7	C1A-NA-C4A	5.06	109.36	106.30
23	K	101	8CT	C01-C02-C03	-5.06	118.85	124.53
23	k	101	8CT	C01-C02-C03	-5.06	118.85	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	506	CL7	CMD-C2D-C1D	5.05	133.06	125.37
21	1	414	CL7	C1A-NA-C4A	5.04	109.35	106.30
21	5	414	CL7	C1A-NA-C4A	5.04	109.35	106.30
21	D	402	CL7	C1A-NA-C4A	5.03	109.35	106.30
21	d	402	CL7	C1A-NA-C4A	5.03	109.35	106.30
21	2	502	CL7	C2B-C1B-NB	5.02	113.60	110.23
21	6	502	CL7	C2B-C1B-NB	5.02	113.60	110.23
26	C	501	LMG	O7-C10-C11	5.02	122.32	111.50
21	3	511	CL7	C4D-C3D-CAD	-5.02	104.04	107.42
21	7	511	CL7	C4D-C3D-CAD	-5.02	104.04	107.42
32	8	420	ZEX	C15-C14-C13	-5.02	120.15	127.31
21	1	410	CL7	CMD-C2D-C1D	5.01	133.00	125.37
21	5	410	CL7	CMD-C2D-C1D	5.01	133.00	125.37
23	b	620	8CT	C18-C17-C16	-5.01	120.17	127.31
21	3	508	CL7	C2B-C1B-NB	5.00	113.58	110.23
32	4	419	ZEX	C35-C34-C33	-5.00	120.18	127.31
32	4	420	ZEX	C15-C14-C13	-4.99	120.18	127.31
21	2	514	CL7	CMD-C2D-C1D	4.99	132.97	125.37
21	6	514	CL7	CMD-C2D-C1D	4.99	132.97	125.37
21	4	416	CL7	C4D-C3D-CAD	-4.99	104.06	107.42
21	8	416	CL7	C4D-C3D-CAD	-4.99	104.06	107.42
23	B	618	8CT	C14-C13-C12	-4.98	120.20	127.31
23	B	619	8CT	C18-C17-C16	-4.98	120.20	127.31
32	8	419	ZEX	C35-C34-C33	-4.98	120.21	127.31
32	7	519	ZEX	C28-C27-C26	-4.98	118.59	127.09
21	5	414	CL7	C4D-C3D-CAD	-4.97	104.07	107.42
32	3	519	ZEX	C28-C27-C26	-4.97	118.60	127.09
32	4	418	ZEX	C27-C28-C29	-4.97	118.73	126.23
23	B	617	8CT	C24-C25-C26	-4.97	120.22	127.31
23	b	618	8CT	C24-C25-C26	-4.97	120.22	127.31
23	c	516	8CT	C19-C20-C21	-4.97	120.22	127.31
23	k	101	8CT	C35-C30-C29	-4.97	106.42	112.70
23	b	619	8CT	C14-C13-C12	-4.97	120.22	127.31
21	6	511	CL7	CMD-C2D-C1D	4.97	132.93	125.37
21	4	411	CL7	CMD-C2D-C1D	4.96	132.93	125.37
21	8	411	CL7	CMD-C2D-C1D	4.96	132.93	125.37
23	C	516	8CT	C19-C20-C21	-4.96	120.23	127.31
21	7	508	CL7	C2B-C1B-NB	4.96	113.56	110.23
23	K	101	8CT	C10-C11-C12	-4.96	118.74	126.23
23	k	101	8CT	C10-C11-C12	-4.96	118.74	126.23
21	1	414	CL7	C4D-C3D-CAD	-4.96	104.08	107.42
21	2	511	CL7	CMD-C2D-C1D	4.96	132.92	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	K	101	8CT	C35-C30-C29	-4.95	106.44	112.70
21	3	503	CL7	C4D-C3D-CAD	-4.95	104.09	107.42
21	7	503	CL7	C4D-C3D-CAD	-4.95	104.09	107.42
32	8	418	ZEX	C27-C28-C29	-4.94	118.77	126.23
26	c	501	LMG	O7-C10-C11	4.94	122.16	111.50
21	3	517	CL7	C4D-C3D-CAD	-4.94	104.09	107.42
21	7	517	CL7	C4D-C3D-CAD	-4.94	104.09	107.42
23	a	404	8CT	C18-C17-C16	-4.94	120.26	127.31
23	c	519	8CT	C14-C13-C12	-4.93	120.27	127.31
23	C	519	8CT	C14-C13-C12	-4.92	120.28	127.31
23	A	404	8CT	C18-C17-C16	-4.92	120.29	127.31
21	7	510	CL7	C4D-C3D-CAD	-4.90	104.12	107.42
22	D	408	PHO	C1C-C2C-C3C	-4.89	104.54	108.61
23	B	627	8CT	C19-C18-C17	-4.88	113.47	123.47
21	c	510	CL7	CMD-C2D-C1D	4.88	132.80	125.37
21	3	510	CL7	C4D-C3D-CAD	-4.87	104.14	107.42
23	b	601	8CT	C19-C18-C17	-4.87	113.49	123.47
21	b	605	CL7	CMD-C2D-C1D	4.87	132.79	125.37
21	C	510	CL7	CMD-C2D-C1D	4.87	132.79	125.37
22	d	408	PHO	C1C-C2C-C3C	-4.87	104.56	108.61
21	6	512	CL7	C1D-ND-C4D	-4.86	102.88	106.33
21	1	407	CL7	C4D-C3D-CAD	-4.85	104.15	107.42
31	f	101	HEM	CHD-C1D-ND	4.85	129.69	124.42
21	B	614	CL7	C4D-C3D-CAD	-4.85	104.15	107.42
21	C	504	CL7	C1D-ND-C4D	-4.85	102.89	106.33
21	c	504	CL7	C1D-ND-C4D	-4.85	102.89	106.33
31	F	101	HEM	CHD-C1D-ND	4.85	129.69	124.42
21	2	510	CL7	C4D-C3D-CAD	-4.85	104.16	107.42
21	6	510	CL7	C4D-C3D-CAD	-4.85	104.16	107.42
21	B	604	CL7	CMD-C2D-C1D	4.84	132.75	125.37
21	5	407	CL7	C4D-C3D-CAD	-4.82	104.17	107.42
21	2	512	CL7	C1D-ND-C4D	-4.82	102.91	106.33
21	B	622	CL7	C1A-NA-C4A	4.82	109.22	106.30
21	b	623	CL7	C1A-NA-C4A	4.82	109.22	106.30
21	b	613	CL7	C4D-C3D-CAD	-4.81	104.18	107.42
21	6	501	CL7	CMD-C2D-C1D	4.81	132.70	125.37
23	B	619	8CT	C30-C31-C32	-4.81	115.55	121.47
23	b	620	8CT	C30-C31-C32	-4.81	115.55	121.47
21	B	612	CL7	C4D-C3D-CAD	-4.80	104.19	107.42
21	b	607	CL7	C4D-C3D-CAD	-4.80	104.19	107.42
21	2	503	CL7	C1D-ND-C4D	-4.80	102.92	106.33
21	6	503	CL7	C1D-ND-C4D	-4.80	102.92	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	610	CL7	CMD-C2D-C1D	4.80	132.68	125.37
21	b	611	CL7	CMD-C2D-C1D	4.80	132.68	125.37
21	5	415	CL7	C1D-ND-C4D	-4.80	102.92	106.33
21	b	615	CL7	C4D-C3D-CAD	-4.80	104.19	107.42
21	3	504	CL7	C4D-C3D-CAD	-4.80	104.19	107.42
23	B	619	8CT	C10-C11-C12	-4.80	118.98	126.23
23	b	620	8CT	C10-C11-C12	-4.80	118.98	126.23
32	7	520	ZEX	C15-C14-C13	-4.79	120.47	127.31
21	5	411	CL7	CMD-C2D-C1D	4.79	132.67	125.37
21	2	501	CL7	CMD-C2D-C1D	4.79	132.66	125.37
21	1	411	CL7	CMD-C2D-C1D	4.79	132.66	125.37
32	3	520	ZEX	C15-C14-C13	-4.79	120.48	127.31
21	7	504	CL7	C4D-C3D-CAD	-4.78	104.20	107.42
21	B	606	CL7	C4D-C3D-CAD	-4.78	104.20	107.42
21	B	616	CL7	CMD-C2D-C1D	4.78	132.64	125.37
21	b	617	CL7	CMD-C2D-C1D	4.78	132.64	125.37
21	b	606	CL7	C1D-ND-C4D	-4.77	102.94	106.33
21	3	508	CL7	C4D-C3D-CAD	-4.77	104.21	107.42
21	7	508	CL7	C4D-C3D-CAD	-4.77	104.21	107.42
21	B	605	CL7	C1D-ND-C4D	-4.76	102.95	106.33
32	4	418	ZEX	C35-C34-C33	-4.76	120.52	127.31
32	8	418	ZEX	C35-C34-C33	-4.76	120.52	127.31
32	2	525	ZEX	C35-C34-C33	-4.75	120.53	127.31
32	6	524	ZEX	C35-C34-C33	-4.75	120.53	127.31
21	c	502	CL7	C2D-C1D-ND	4.75	113.42	110.23
21	c	502	CL7	C1D-ND-C4D	-4.75	102.96	106.33
21	c	511	CL7	C1A-NA-C4A	4.75	109.17	106.30
21	1	415	CL7	C1D-ND-C4D	-4.74	102.97	106.33
21	3	501	CL7	C4D-C3D-CAD	-4.74	104.23	107.42
21	7	501	CL7	C4D-C3D-CAD	-4.74	104.23	107.42
21	7	502	CL7	CMD-C2D-C1D	4.72	132.56	125.37
21	5	404	CL7	C1D-ND-C4D	-4.72	102.98	106.33
21	1	404	CL7	C1D-ND-C4D	-4.72	102.98	106.33
21	1	411	CL7	C4D-C3D-CAD	-4.72	104.24	107.42
21	5	411	CL7	C4D-C3D-CAD	-4.72	104.24	107.42
21	C	511	CL7	C1A-NA-C4A	4.72	109.16	106.30
32	4	403	ZEX	C11-C10-C9	-4.71	120.58	127.31
21	3	502	CL7	CMD-C2D-C1D	4.71	132.54	125.37
21	8	406	CL7	CMD-C2D-C1D	4.71	132.54	125.37
32	1	422	ZEX	C27-C28-C29	-4.71	119.12	126.23
21	3	503	CL7	C2D-C1D-ND	4.71	113.39	110.23
21	7	503	CL7	C2D-C1D-ND	4.71	113.39	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	8	403	ZEX	C11-C10-C9	-4.70	120.60	127.31
21	3	511	CL7	CMD-C2D-C1D	4.70	132.53	125.37
21	C	502	CL7	C1D-ND-C4D	-4.70	103.00	106.33
21	4	415	CL7	CMD-C2D-C1D	4.70	132.53	125.37
21	8	415	CL7	CMD-C2D-C1D	4.70	132.53	125.37
21	C	502	CL7	C2D-C1D-ND	4.70	113.38	110.23
32	5	422	ZEX	C27-C28-C29	-4.70	119.14	126.23
23	A	404	8CT	C01-C02-C03	-4.70	119.25	124.53
21	a	405	CL7	C1D-ND-C4D	-4.70	103.00	106.33
21	C	514	CL7	C1D-ND-C4D	-4.69	103.00	106.33
21	c	514	CL7	C1D-ND-C4D	-4.69	103.00	106.33
21	7	511	CL7	CMD-C2D-C1D	4.69	132.51	125.37
21	4	406	CL7	CMD-C2D-C1D	4.69	132.51	125.37
21	7	510	CL7	CMD-C2D-C1D	4.69	132.51	125.37
21	B	610	CL7	C1D-ND-C4D	-4.68	103.01	106.33
21	4	417	CL7	C2B-C1B-NB	4.68	113.37	110.23
21	8	417	CL7	C2B-C1B-NB	4.68	113.37	110.23
23	a	404	8CT	C01-C02-C03	-4.68	119.27	124.53
21	3	510	CL7	CMD-C2D-C1D	4.68	132.50	125.37
21	B	601	CL7	CMD-C2D-C1D	4.68	132.49	125.37
21	1	413	CL7	CMD-C2D-C1D	4.67	132.49	125.37
21	5	413	CL7	CMD-C2D-C1D	4.67	132.49	125.37
23	b	618	8CT	C07-C02-C03	-4.67	115.94	122.73
21	c	505	CL7	CMD-C2D-C1D	4.67	132.48	125.37
21	C	505	CL7	CMD-C2D-C1D	4.67	132.48	125.37
21	A	406	CL7	C1D-ND-C4D	-4.67	103.02	106.33
21	4	404	CL7	CMD-C2D-C1D	4.67	132.48	125.37
21	8	404	CL7	CMD-C2D-C1D	4.67	132.48	125.37
23	B	617	8CT	C07-C02-C03	-4.67	115.96	122.73
23	C	515	8CT	C01-C02-C03	-4.66	119.29	124.53
23	c	515	8CT	C01-C02-C03	-4.66	119.29	124.53
21	b	602	CL7	CMD-C2D-C1D	4.66	132.46	125.37
21	1	419	CL7	CMD-C2D-C1D	4.66	132.46	125.37
21	1	405	CL7	C1D-ND-C4D	-4.66	103.03	106.33
21	b	611	CL7	C1D-ND-C4D	-4.66	103.03	106.33
21	5	405	CL7	C1D-ND-C4D	-4.66	103.03	106.33
32	8	420	ZEX	C11-C10-C9	-4.65	120.67	127.31
32	4	420	ZEX	C11-C10-C9	-4.65	120.68	127.31
21	3	503	CL7	C1D-ND-C4D	-4.65	103.03	106.33
21	7	503	CL7	C1D-ND-C4D	-4.65	103.03	106.33
21	1	413	CL7	C2D-C1D-ND	4.64	113.34	110.23
21	5	419	CL7	CMD-C2D-C1D	4.64	132.44	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	402	CL7	C4D-C3D-CAD	-4.64	104.30	107.42
21	8	412	CL7	CMD-C2D-C1D	4.63	132.42	125.37
21	5	413	CL7	C2D-C1D-ND	4.63	113.33	110.23
21	C	503	CL7	CMD-C2D-C1D	4.63	132.42	125.37
21	c	503	CL7	CMD-C2D-C1D	4.63	132.42	125.37
21	3	514	CL7	C4D-C3D-CAD	-4.62	104.31	107.42
23	B	627	8CT	C01-C02-C03	-4.62	119.34	124.53
23	b	601	8CT	C01-C02-C03	-4.62	119.34	124.53
21	4	412	CL7	CMD-C2D-C1D	4.62	132.40	125.37
21	B	609	CL7	C4D-C3D-CAD	-4.62	104.31	107.42
21	b	610	CL7	C4D-C3D-CAD	-4.62	104.31	107.42
21	4	415	CL7	O2D-CGD-CBD	4.62	119.47	111.27
21	8	415	CL7	O2D-CGD-CBD	4.62	119.47	111.27
21	1	404	CL7	CMD-C2D-C1D	4.61	132.40	125.37
21	5	404	CL7	CMD-C2D-C1D	4.61	132.40	125.37
21	6	518	CL7	CMD-C2D-C1D	4.61	132.40	125.37
21	7	514	CL7	C4D-C3D-CAD	-4.61	104.32	107.42
23	C	515	8CT	C19-C20-C21	-4.61	120.73	127.31
21	4	410	CL7	CMD-C2D-C1D	4.61	132.39	125.37
21	8	410	CL7	CMD-C2D-C1D	4.61	132.39	125.37
21	C	512	CL7	C1D-ND-C4D	-4.61	103.06	106.33
21	D	402	CL7	CMD-C2D-C1D	4.61	132.38	125.37
21	3	518	CL7	CMD-C2D-C1D	4.61	132.38	125.37
21	7	518	CL7	CMD-C2D-C1D	4.61	132.38	125.37
21	1	413	CL7	C1D-ND-C4D	-4.60	103.06	106.33
21	2	518	CL7	CMD-C2D-C1D	4.60	132.38	125.37
21	7	502	CL7	C4D-C3D-CAD	-4.60	104.33	107.42
21	3	501	CL7	C1D-ND-C4D	-4.60	103.07	106.33
23	c	515	8CT	C19-C20-C21	-4.60	120.75	127.31
21	4	408	CL7	CMD-C2D-C1D	4.59	132.36	125.37
21	8	408	CL7	CMD-C2D-C1D	4.59	132.36	125.37
21	b	611	CL7	C2D-C1D-ND	4.59	113.31	110.23
21	3	504	CL7	C1D-ND-C4D	-4.59	103.07	106.33
21	d	402	CL7	CMD-C2D-C1D	4.59	132.36	125.37
21	c	512	CL7	C1D-ND-C4D	-4.59	103.08	106.33
21	7	504	CL7	C1D-ND-C4D	-4.59	103.08	106.33
21	5	408	CL7	CMD-C2D-C1D	4.58	132.35	125.37
21	C	512	CL7	CMD-C2D-C1D	4.58	132.34	125.37
21	c	512	CL7	CMD-C2D-C1D	4.58	132.34	125.37
21	B	622	CL7	CMD-C2D-C1D	4.58	132.34	125.37
21	b	623	CL7	CMD-C2D-C1D	4.58	132.34	125.37
21	B	616	CL7	C4D-C3D-CAD	-4.58	104.34	107.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	502	CL7	C4D-C3D-CAD	-4.58	104.34	107.42
21	b	617	CL7	C4D-C3D-CAD	-4.58	104.34	107.42
21	b	603	CL7	CMD-C2D-C1D	4.58	132.34	125.37
21	4	413	CL7	CMD-C2D-C1D	4.57	132.34	125.37
21	8	413	CL7	CMD-C2D-C1D	4.57	132.34	125.37
21	B	610	CL7	C2D-C1D-ND	4.57	113.30	110.23
21	B	602	CL7	CMD-C2D-C1D	4.57	132.33	125.37
21	3	509	CL7	CMD-C2D-C1D	4.57	132.33	125.37
21	5	413	CL7	C1D-ND-C4D	-4.57	103.09	106.33
21	D	405	CL7	CMD-C2D-C1D	4.57	132.32	125.37
21	d	405	CL7	CMD-C2D-C1D	4.57	132.32	125.37
21	d	404	CL7	C1D-ND-C4D	-4.57	103.09	106.33
21	5	418	CL7	CMD-C2D-C1D	4.56	132.32	125.37
21	4	414	CL7	C4D-C3D-CAD	-4.56	104.35	107.42
21	7	509	CL7	CMD-C2D-C1D	4.56	132.31	125.37
23	b	601	8CT	C24-C23-C21	-4.56	113.61	126.42
21	1	402	CL7	C4D-C3D-CAD	-4.55	104.36	107.42
23	B	627	8CT	C24-C23-C21	-4.55	113.64	126.42
21	1	408	CL7	CMD-C2D-C1D	4.55	132.30	125.37
21	B	615	CL7	CMD-C2D-C1D	4.55	132.30	125.37
21	b	616	CL7	CMD-C2D-C1D	4.55	132.30	125.37
23	4	402	8CT	C01-C02-C03	-4.55	119.42	124.53
32	4	419	ZEX	C8-C7-C6	-4.54	114.44	127.20
21	1	414	CL7	CMD-C2D-C1D	4.54	132.29	125.37
21	1	418	CL7	CMD-C2D-C1D	4.54	132.29	125.37
21	5	414	CL7	CMD-C2D-C1D	4.54	132.29	125.37
21	7	501	CL7	C1D-ND-C4D	-4.54	103.11	106.33
21	8	414	CL7	C1D-ND-C4D	-4.54	103.11	106.33
21	1	420	CL7	CMD-C2D-C1D	4.53	132.27	125.37
21	5	420	CL7	CMD-C2D-C1D	4.53	132.27	125.37
23	8	402	8CT	C01-C02-C03	-4.53	119.44	124.53
21	2	517	CL7	C4D-C3D-CAD	-4.53	104.37	107.42
21	6	517	CL7	C4D-C3D-CAD	-4.53	104.37	107.42
21	4	414	CL7	C1D-ND-C4D	-4.53	103.12	106.33
32	8	419	ZEX	C8-C7-C6	-4.53	114.49	127.20
21	1	405	CL7	CMD-C2D-C1D	4.52	132.26	125.37
21	5	405	CL7	CMD-C2D-C1D	4.52	132.26	125.37
21	8	414	CL7	C4D-C3D-CAD	-4.52	104.38	107.42
21	C	511	CL7	CMD-C2D-C1D	4.52	132.25	125.37
21	B	616	CL7	C1D-ND-C4D	-4.52	103.12	106.33
21	c	511	CL7	CMD-C2D-C1D	4.52	132.25	125.37
21	D	404	CL7	C1D-ND-C4D	-4.51	103.13	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	512	CL7	CMD-C2D-C1D	4.51	132.24	125.37
21	7	512	CL7	CMD-C2D-C1D	4.51	132.24	125.37
21	1	402	CL7	CMD-C2D-C1D	4.51	132.24	125.37
21	5	402	CL7	CMD-C2D-C1D	4.51	132.24	125.37
21	1	404	CL7	C4D-C3D-CAD	-4.51	104.39	107.42
21	5	404	CL7	C4D-C3D-CAD	-4.51	104.39	107.42
23	C	519	8CT	C01-C02-C03	-4.51	119.47	124.53
21	4	414	CL7	C2D-C1D-ND	4.50	113.25	110.23
21	a	403	CL7	CMD-C2D-C1D	4.50	132.23	125.37
21	3	503	CL7	CMD-C2D-C1D	4.50	132.22	125.37
21	7	503	CL7	CMD-C2D-C1D	4.50	132.22	125.37
21	1	412	CL7	C1D-ND-C4D	-4.50	103.14	106.33
21	1	416	CL7	C1D-ND-C4D	-4.50	103.14	106.33
21	5	412	CL7	C1D-ND-C4D	-4.50	103.14	106.33
21	5	416	CL7	C1D-ND-C4D	-4.50	103.14	106.33
21	3	515	CL7	CMD-C2D-C1D	4.50	132.22	125.37
21	7	515	CL7	CMD-C2D-C1D	4.50	132.22	125.37
23	c	519	8CT	C01-C02-C03	-4.50	119.48	124.53
21	8	414	CL7	C2D-C1D-ND	4.50	113.25	110.23
21	5	413	CL7	C4D-C3D-CAD	-4.50	104.39	107.42
21	8	416	CL7	CMD-C2D-C1D	4.50	132.22	125.37
21	3	509	CL7	C4D-C3D-CAD	-4.50	104.39	107.42
21	7	509	CL7	C4D-C3D-CAD	-4.50	104.39	107.42
21	b	617	CL7	C1D-ND-C4D	-4.50	103.14	106.33
32	8	420	ZEX	C7-C8-C9	-4.50	119.44	126.23
21	1	413	CL7	C4D-C3D-CAD	-4.49	104.40	107.42
21	A	403	CL7	CMD-C2D-C1D	4.48	132.20	125.37
21	C	504	CL7	CMD-C2D-C1D	4.48	132.20	125.37
21	c	504	CL7	CMD-C2D-C1D	4.48	132.20	125.37
32	6	519	ZEX	C7-C8-C9	-4.48	119.46	126.23
32	4	420	ZEX	C7-C8-C9	-4.48	119.46	126.23
21	1	417	CL7	C4D-C3D-CAD	-4.48	104.40	107.42
21	5	417	CL7	C4D-C3D-CAD	-4.48	104.40	107.42
21	2	505	CL7	C1D-ND-C4D	-4.48	103.15	106.33
21	6	505	CL7	C1D-ND-C4D	-4.48	103.15	106.33
21	6	516	CL7	CMD-C2D-C1D	4.47	132.18	125.37
21	2	503	CL7	C2D-C1D-ND	4.47	113.23	110.23
21	6	503	CL7	C2D-C1D-ND	4.47	113.23	110.23
21	3	506	CL7	CMD-C2D-C1D	4.47	132.18	125.37
21	7	506	CL7	CMD-C2D-C1D	4.47	132.18	125.37
32	7	522	ZEX	C15-C14-C13	-4.47	120.93	127.31
21	2	506	CL7	CMD-C2D-C1D	4.47	132.18	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	506	CL7	CMD-C2D-C1D	4.47	132.18	125.37
21	4	416	CL7	CMD-C2D-C1D	4.47	132.18	125.37
32	8	418	ZEX	C11-C10-C9	-4.47	120.93	127.31
21	1	406	CL7	C1D-ND-C4D	-4.47	103.16	106.33
21	5	406	CL7	C1D-ND-C4D	-4.47	103.16	106.33
21	4	404	CL7	C4D-C3D-CAD	-4.47	104.42	107.42
21	2	516	CL7	CMD-C2D-C1D	4.46	132.17	125.37
32	3	522	ZEX	C15-C14-C13	-4.46	120.94	127.31
21	B	607	CL7	C1D-ND-C4D	-4.46	103.17	106.33
21	3	513	CL7	CMD-C2D-C1D	4.46	132.16	125.37
32	2	519	ZEX	C7-C8-C9	-4.46	119.49	126.23
21	b	612	CL7	CMD-C2D-C1D	4.46	132.16	125.37
21	B	611	CL7	CMD-C2D-C1D	4.46	132.16	125.37
21	8	406	CL7	C1D-ND-C4D	-4.46	103.17	106.33
21	2	505	CL7	O2A-C1-C2	-4.45	96.93	108.64
21	6	505	CL7	O2A-C1-C2	-4.45	96.93	108.64
21	b	602	CL7	C1D-ND-C4D	-4.45	103.17	106.33
21	8	404	CL7	C4D-C3D-CAD	-4.45	104.43	107.42
21	C	505	CL7	C1D-ND-C4D	-4.45	103.17	106.33
21	c	505	CL7	C1D-ND-C4D	-4.45	103.17	106.33
21	B	615	CL7	C4D-C3D-CAD	-4.45	104.43	107.42
21	b	616	CL7	C4D-C3D-CAD	-4.45	104.43	107.42
21	7	513	CL7	CMD-C2D-C1D	4.45	132.14	125.37
32	4	418	ZEX	C11-C10-C9	-4.44	120.97	127.31
21	B	605	CL7	C4D-C3D-CAD	-4.44	104.43	107.42
21	b	606	CL7	C4D-C3D-CAD	-4.44	104.43	107.42
21	1	411	CL7	C1D-ND-C4D	-4.44	103.18	106.33
21	4	405	CL7	CMD-C2D-C1D	4.43	132.12	125.37
21	B	607	CL7	CMD-C2D-C1D	4.43	132.12	125.37
21	b	608	CL7	CMD-C2D-C1D	4.43	132.12	125.37
21	1	415	CL7	C2D-C1D-ND	4.43	113.20	110.23
21	5	415	CL7	C2D-C1D-ND	4.43	113.20	110.23
21	B	601	CL7	C1D-ND-C4D	-4.43	103.19	106.33
21	2	511	CL7	C4D-C3D-CAD	-4.43	104.44	107.42
21	6	511	CL7	C4D-C3D-CAD	-4.43	104.44	107.42
21	6	505	CL7	CMD-C2D-C1D	4.43	132.11	125.37
21	3	515	CL7	C2D-C1D-ND	4.43	113.20	110.23
21	7	515	CL7	C2D-C1D-ND	4.43	113.20	110.23
21	4	406	CL7	C1D-ND-C4D	-4.43	103.19	106.33
21	8	407	CL7	CMD-C2D-C1D	4.42	132.11	125.37
21	1	419	CL7	C1D-ND-C4D	-4.42	103.19	106.33
21	5	419	CL7	C1D-ND-C4D	-4.42	103.19	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	614	CL7	CMD-C2D-C1D	4.42	132.10	125.37
21	C	507	CL7	CMD-C2D-C1D	4.42	132.10	125.37
21	c	507	CL7	CMD-C2D-C1D	4.42	132.10	125.37
21	3	515	CL7	C1D-ND-C4D	-4.42	103.20	106.33
21	7	515	CL7	C1D-ND-C4D	-4.42	103.20	106.33
21	b	615	CL7	CMD-C2D-C1D	4.42	132.09	125.37
21	8	405	CL7	CMD-C2D-C1D	4.41	132.09	125.37
21	2	505	CL7	CMD-C2D-C1D	4.41	132.09	125.37
32	2	520	ZEX	C27-C26-C25	-4.41	115.71	122.84
32	3	525	ZEX	C27-C26-C25	-4.41	115.71	122.84
21	C	509	CL7	C1D-ND-C4D	-4.41	103.20	106.33
21	c	509	CL7	C1D-ND-C4D	-4.41	103.20	106.33
23	B	618	8CT	C04-C03-C02	-4.41	116.41	122.61
23	b	619	8CT	C04-C03-C02	-4.41	116.41	122.61
21	b	608	CL7	C1D-ND-C4D	-4.41	103.20	106.33
21	5	411	CL7	C1D-ND-C4D	-4.41	103.20	106.33
21	2	515	CL7	C4D-C3D-CAD	-4.40	104.46	107.42
21	6	515	CL7	C4D-C3D-CAD	-4.40	104.46	107.42
21	4	417	CL7	C1D-ND-C4D	-4.40	103.21	106.33
21	2	502	CL7	C4D-C3D-CAD	-4.40	104.46	107.42
21	6	502	CL7	C4D-C3D-CAD	-4.40	104.46	107.42
21	6	513	CL7	C1D-ND-C4D	-4.40	103.21	106.33
21	4	407	CL7	CMD-C2D-C1D	4.40	132.07	125.37
32	2	525	ZEX	C15-C14-C13	-4.40	121.04	127.31
21	3	511	CL7	CAA-CBA-CGA	-4.40	100.41	113.25
21	7	511	CL7	CAA-CBA-CGA	-4.40	100.41	113.25
21	4	410	CL7	C1D-ND-C4D	-4.39	103.21	106.33
21	a	401	CL7	C1-C2-C3	-4.39	118.45	126.04
21	C	513	CL7	CMD-C2D-C1D	4.39	132.05	125.37
21	B	602	CL7	C1D-ND-C4D	-4.39	103.22	106.33
21	b	603	CL7	C1D-ND-C4D	-4.39	103.22	106.33
21	7	501	CL7	CMD-C2D-C1D	4.39	132.05	125.37
21	C	504	CL7	C2D-C1D-ND	4.38	113.17	110.23
21	c	504	CL7	C2D-C1D-ND	4.38	113.17	110.23
21	1	409	CL7	CMD-C2D-C1D	4.38	132.04	125.37
21	3	514	CL7	CMD-C2D-C1D	4.38	132.04	125.37
21	c	518	CL7	CMD-C2D-C1D	4.38	132.04	125.37
32	1	422	ZEX	C11-C10-C9	-4.38	121.06	127.31
32	5	422	ZEX	C11-C10-C9	-4.38	121.06	127.31
21	5	409	CL7	CMD-C2D-C1D	4.37	132.03	125.37
22	A	402	PHO	C4D-CHA-CBD	-4.37	106.54	108.52
22	a	402	PHO	C4D-CHA-CBD	-4.37	106.54	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	512	CL7	C4D-C3D-CAD	-4.37	104.48	107.42
21	3	501	CL7	CMD-C2D-C1D	4.37	132.02	125.37
21	2	502	CL7	C1D-ND-C4D	-4.37	103.23	106.33
21	6	502	CL7	C1D-ND-C4D	-4.37	103.23	106.33
21	A	401	CL7	C1-C2-C3	-4.36	118.50	126.04
21	c	513	CL7	CMD-C2D-C1D	4.36	132.01	125.37
32	1	421	ZEX	C35-C34-C33	-4.36	121.08	127.31
32	5	421	ZEX	C35-C34-C33	-4.36	121.08	127.31
21	C	518	CL7	CMD-C2D-C1D	4.36	132.01	125.37
21	3	504	CL7	CMD-C2D-C1D	4.36	132.01	125.37
21	7	504	CL7	CMD-C2D-C1D	4.36	132.01	125.37
21	B	611	CL7	C1D-ND-C4D	-4.36	103.24	106.33
21	b	612	CL7	C1D-ND-C4D	-4.36	103.24	106.33
21	8	410	CL7	C1D-ND-C4D	-4.36	103.24	106.33
21	7	514	CL7	CMD-C2D-C1D	4.36	132.01	125.37
21	B	613	CL7	C4D-C3D-CAD	-4.36	104.49	107.42
21	7	512	CL7	C4D-C3D-CAD	-4.35	104.49	107.42
21	7	514	CL7	C1D-ND-C4D	-4.35	103.24	106.33
21	2	513	CL7	C1D-ND-C4D	-4.35	103.25	106.33
21	C	514	CL7	CMD-C2D-C1D	4.34	131.99	125.37
21	2	515	CL7	CMD-C2D-C1D	4.34	131.98	125.37
21	6	515	CL7	CMD-C2D-C1D	4.34	131.98	125.37
21	1	420	CL7	C2D-C1D-ND	4.34	113.14	110.23
21	5	420	CL7	C2D-C1D-ND	4.34	113.14	110.23
21	c	514	CL7	CMD-C2D-C1D	4.33	131.97	125.37
21	b	614	CL7	C4D-C3D-CAD	-4.33	104.50	107.42
21	A	401	CL7	C2D-C1D-ND	4.33	113.14	110.23
21	a	401	CL7	C2D-C1D-ND	4.33	113.14	110.23
32	6	524	ZEX	C15-C14-C13	-4.33	121.13	127.31
21	8	417	CL7	C1D-ND-C4D	-4.33	103.26	106.33
21	B	608	CL7	C1D-ND-C4D	-4.33	103.26	106.33
21	b	609	CL7	C1D-ND-C4D	-4.33	103.26	106.33
21	1	420	CL7	C1D-ND-C4D	-4.33	103.26	106.33
21	5	420	CL7	C1D-ND-C4D	-4.33	103.26	106.33
21	7	502	CL7	C1A-NA-C4A	4.33	108.92	106.30
21	1	407	CL7	CMD-C2D-C1D	4.32	131.96	125.37
21	5	407	CL7	CMD-C2D-C1D	4.32	131.96	125.37
21	3	514	CL7	C1D-ND-C4D	-4.32	103.26	106.33
21	A	401	CL7	C1D-ND-C4D	-4.32	103.27	106.33
21	a	401	CL7	C1D-ND-C4D	-4.32	103.27	106.33
21	3	511	CL7	C1D-ND-C4D	-4.32	103.27	106.33
21	7	511	CL7	C1D-ND-C4D	-4.32	103.27	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	508	CL7	C4D-C3D-CAD	-4.31	104.52	107.42
21	8	409	CL7	O2D-CGD-CBD	4.31	118.93	111.27
21	6	507	CL7	CMD-C2D-C1D	4.31	131.94	125.37
32	3	519	ZEX	C18-C5-C6	-4.31	119.69	124.53
21	8	415	CL7	C1D-ND-C4D	-4.31	103.28	106.33
32	8	403	ZEX	C27-C28-C29	-4.30	119.73	126.23
21	C	509	CL7	CMD-C2D-C1D	4.30	131.93	125.37
21	c	509	CL7	CMD-C2D-C1D	4.30	131.93	125.37
21	2	507	CL7	CMD-C2D-C1D	4.30	131.91	125.37
21	2	509	CL7	CMD-C2D-C1D	4.30	131.91	125.37
21	6	509	CL7	CMD-C2D-C1D	4.30	131.91	125.37
21	6	508	CL7	C4D-C3D-CAD	-4.30	104.53	107.42
21	3	517	CL7	CMD-C2D-C1D	4.29	131.91	125.37
21	4	409	CL7	O2D-CGD-CBD	4.29	118.89	111.27
32	4	418	ZEX	C28-C27-C26	-4.29	119.76	127.09
32	8	418	ZEX	C28-C27-C26	-4.29	119.76	127.09
32	7	519	ZEX	C18-C5-C6	-4.29	119.71	124.53
32	4	403	ZEX	C27-C28-C29	-4.29	119.76	126.23
21	b	602	CL7	C2D-C1D-ND	4.29	113.11	110.23
21	3	507	CL7	O2D-CGD-CBD	4.29	118.89	111.27
21	7	507	CL7	O2D-CGD-CBD	4.29	118.89	111.27
21	C	513	CL7	C2D-C1D-ND	4.29	113.11	110.23
21	2	517	CL7	CMD-C2D-C1D	4.28	131.89	125.37
21	6	517	CL7	CMD-C2D-C1D	4.28	131.89	125.37
21	2	509	CL7	C4D-C3D-CAD	-4.28	104.54	107.42
21	5	414	CL7	C1D-ND-C4D	-4.28	103.29	106.33
21	b	614	CL7	CMD-C2D-C1D	4.28	131.89	125.37
21	1	420	CL7	O2D-CGD-CBD	4.28	118.87	111.27
21	7	517	CL7	CMD-C2D-C1D	4.28	131.88	125.37
21	2	512	CL7	C4D-C3D-CAD	-4.28	104.54	107.42
21	6	512	CL7	C4D-C3D-CAD	-4.28	104.54	107.42
21	3	502	CL7	C1A-NA-C4A	4.27	108.89	106.30
23	A	404	8CT	C30-C31-C32	-4.27	116.21	121.47
21	B	613	CL7	CMD-C2D-C1D	4.27	131.88	125.37
21	c	513	CL7	C2D-C1D-ND	4.27	113.09	110.23
32	6	520	ZEX	C35-C34-C33	-4.27	121.22	127.31
21	8	411	CL7	C3A-C4A-CHB	-4.27	117.36	123.70
21	1	414	CL7	C1D-ND-C4D	-4.27	103.30	106.33
21	C	504	CL7	C4D-C3D-CAD	-4.27	104.55	107.42
21	c	504	CL7	C4D-C3D-CAD	-4.27	104.55	107.42
21	5	420	CL7	O2D-CGD-CBD	4.27	118.85	111.27
23	C	519	8CT	C18-C17-C16	-4.26	121.22	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	411	CL7	C3A-C4A-CHB	-4.26	117.37	123.70
21	6	509	CL7	C4D-C3D-CAD	-4.26	104.55	107.42
23	a	404	8CT	C30-C31-C32	-4.26	116.22	121.47
21	2	508	CL7	CMD-C2D-C1D	4.26	131.85	125.37
21	6	508	CL7	CMD-C2D-C1D	4.26	131.85	125.37
21	4	415	CL7	C1D-ND-C4D	-4.26	103.31	106.33
21	2	513	CL7	CMD-C2D-C1D	4.26	131.85	125.37
21	B	622	CL7	C1D-ND-C4D	-4.25	103.31	106.33
21	b	623	CL7	C1D-ND-C4D	-4.25	103.31	106.33
23	c	519	8CT	C18-C17-C16	-4.25	121.24	127.31
21	B	604	CL7	C4D-C3D-CAD	-4.25	104.56	107.42
21	b	605	CL7	C4D-C3D-CAD	-4.25	104.56	107.42
21	1	415	CL7	CMD-C2D-C1D	4.24	131.83	125.37
21	6	513	CL7	CMD-C2D-C1D	4.24	131.83	125.37
32	2	521	ZEX	C35-C34-C33	-4.24	121.25	127.31
21	5	415	CL7	CMD-C2D-C1D	4.24	131.83	125.37
21	2	517	CL7	C2D-C1D-ND	4.24	113.08	110.23
21	6	517	CL7	C2D-C1D-ND	4.24	113.08	110.23
32	5	422	ZEX	C35-C34-C33	-4.24	121.26	127.31
21	2	507	CL7	O2D-CGD-CBD	4.24	118.80	111.27
21	6	507	CL7	O2D-CGD-CBD	4.24	118.80	111.27
21	c	503	CL7	C1D-ND-C4D	-4.24	103.33	106.33
23	4	402	8CT	C11-C10-C03	-4.24	115.31	127.20
32	7	520	ZEX	C18-C5-C6	-4.24	119.77	124.53
21	A	401	CL7	CMD-C2D-C1D	4.24	131.82	125.37
21	a	401	CL7	CMD-C2D-C1D	4.24	131.82	125.37
23	8	402	8CT	C11-C10-C03	-4.23	115.31	127.20
21	1	417	CL7	C1D-ND-C4D	-4.23	103.33	106.33
21	5	417	CL7	C1D-ND-C4D	-4.23	103.33	106.33
21	1	407	CL7	C1D-ND-C4D	-4.23	103.33	106.33
21	5	407	CL7	C1D-ND-C4D	-4.23	103.33	106.33
21	B	601	CL7	C2D-C1D-ND	4.23	113.06	110.23
21	B	603	CL7	C1D-ND-C4D	-4.23	103.33	106.33
21	2	515	CL7	C1D-ND-C4D	-4.23	103.33	106.33
21	b	604	CL7	C1D-ND-C4D	-4.23	103.33	106.33
23	B	618	8CT	C01-C02-C03	-4.22	119.78	124.53
23	b	619	8CT	C01-C02-C03	-4.22	119.78	124.53
21	1	416	CL7	CMD-C2D-C1D	4.22	131.80	125.37
21	B	614	CL7	C3A-C4A-CHB	-4.22	117.43	123.70
21	b	615	CL7	C3A-C4A-CHB	-4.22	117.43	123.70
21	1	412	CL7	C2D-C1D-ND	4.22	113.06	110.23
21	5	412	CL7	C2D-C1D-ND	4.22	113.06	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	619	8CT	C35-C30-C29	-4.22	107.37	112.70
32	1	422	ZEX	C35-C34-C33	-4.22	121.29	127.31
21	4	409	CL7	CMD-C2D-C1D	4.21	131.79	125.37
21	8	409	CL7	CMD-C2D-C1D	4.21	131.79	125.37
21	C	503	CL7	C1D-ND-C4D	-4.21	103.34	106.33
21	1	409	CL7	C1D-ND-C4D	-4.21	103.34	106.33
21	4	416	CL7	C1D-ND-C4D	-4.21	103.34	106.33
21	5	409	CL7	C1D-ND-C4D	-4.21	103.34	106.33
21	8	416	CL7	C1D-ND-C4D	-4.21	103.34	106.33
32	3	520	ZEX	C18-C5-C6	-4.21	119.80	124.53
21	b	603	CL7	C4D-C3D-CAD	-4.20	104.59	107.42
23	b	620	8CT	C35-C30-C29	-4.20	107.39	112.70
21	5	416	CL7	CMD-C2D-C1D	4.20	131.77	125.37
21	4	411	CL7	C1D-ND-C4D	-4.20	103.35	106.33
21	A	403	CL7	C4D-C3D-CAD	-4.20	104.59	107.42
21	a	403	CL7	C4D-C3D-CAD	-4.20	104.59	107.42
21	3	512	CL7	C1D-ND-C4D	-4.20	103.35	106.33
21	6	515	CL7	C1D-ND-C4D	-4.18	103.36	106.33
21	c	508	CL7	C1D-ND-C4D	-4.18	103.37	106.33
21	7	505	CL7	C1D-ND-C4D	-4.18	103.37	106.33
32	3	520	ZEX	C28-C27-C26	-4.18	119.95	127.09
32	7	520	ZEX	C28-C27-C26	-4.18	119.95	127.09
21	c	506	CL7	C4D-C3D-CAD	-4.17	104.61	107.42
21	8	415	CL7	C2D-C1D-ND	4.17	113.03	110.23
21	B	602	CL7	C4D-C3D-CAD	-4.17	104.61	107.42
32	8	418	ZEX	C7-C8-C9	-4.17	119.94	126.23
32	7	522	ZEX	C27-C28-C29	-4.17	119.94	126.23
21	D	405	CL7	C4D-C3D-CAD	-4.16	104.62	107.42
21	d	405	CL7	C4D-C3D-CAD	-4.16	104.62	107.42
21	8	411	CL7	C1D-ND-C4D	-4.16	103.38	106.33
21	2	518	CL7	C1D-ND-C4D	-4.16	103.38	106.33
21	6	518	CL7	C1D-ND-C4D	-4.16	103.38	106.33
21	7	512	CL7	C1D-ND-C4D	-4.16	103.38	106.33
21	c	513	CL7	C1D-ND-C4D	-4.16	103.38	106.33
32	4	418	ZEX	C7-C8-C9	-4.16	119.95	126.23
23	4	402	8CT	C13-C14-C15	-4.15	110.25	123.22
23	8	402	8CT	C13-C14-C15	-4.15	110.25	123.22
32	3	522	ZEX	C27-C28-C29	-4.15	119.96	126.23
21	4	407	CL7	C1D-ND-C4D	-4.15	103.38	106.33
21	2	501	CL7	C1D-ND-C4D	-4.15	103.39	106.33
21	6	501	CL7	C1D-ND-C4D	-4.15	103.39	106.33
21	a	401	CL7	C3A-C4A-CHB	-4.15	117.55	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	505	CL7	C1D-ND-C4D	-4.15	103.39	106.33
21	A	401	CL7	C3A-C4A-CHB	-4.14	117.55	123.70
21	3	512	CL7	C2D-C1D-ND	4.14	113.01	110.23
21	C	508	CL7	C1D-ND-C4D	-4.14	103.39	106.33
21	2	502	CL7	CMD-C2D-C1D	4.14	131.68	125.37
21	6	502	CL7	CMD-C2D-C1D	4.14	131.68	125.37
21	7	514	CL7	O2D-CGD-CBD	4.14	118.62	111.27
21	1	403	CL7	C1D-ND-C4D	-4.14	103.39	106.33
21	1	408	CL7	C1D-ND-C4D	-4.14	103.39	106.33
21	5	403	CL7	C1D-ND-C4D	-4.14	103.39	106.33
21	5	408	CL7	C1D-ND-C4D	-4.14	103.39	106.33
21	8	407	CL7	C1D-ND-C4D	-4.13	103.40	106.33
21	B	606	CL7	C3A-C4A-CHB	-4.13	117.58	123.70
21	b	607	CL7	C3A-C4A-CHB	-4.13	117.58	123.70
21	B	616	CL7	C2D-C1D-ND	4.13	113.00	110.23
21	b	617	CL7	C2D-C1D-ND	4.13	113.00	110.23
21	1	406	CL7	CMD-C2D-C1D	4.12	131.65	125.37
21	5	406	CL7	CMD-C2D-C1D	4.12	131.65	125.37
21	2	510	CL7	CMD-C2D-C1D	4.12	131.65	125.37
21	6	510	CL7	CMD-C2D-C1D	4.12	131.65	125.37
21	2	517	CL7	C1D-ND-C4D	-4.12	103.41	106.33
21	6	517	CL7	C1D-ND-C4D	-4.12	103.41	106.33
21	C	506	CL7	C4D-C3D-CAD	-4.12	104.65	107.42
21	C	513	CL7	C1D-ND-C4D	-4.12	103.41	106.33
21	4	417	CL7	CMD-C2D-C1D	4.12	131.64	125.37
21	8	417	CL7	CMD-C2D-C1D	4.12	131.64	125.37
21	4	415	CL7	C2D-C1D-ND	4.12	112.99	110.23
21	3	514	CL7	O2D-CGD-CBD	4.12	118.59	111.27
21	8	406	CL7	C2D-C1D-ND	4.12	112.99	110.23
21	D	402	CL7	C1D-ND-C4D	-4.11	103.41	106.33
21	1	412	CL7	CMD-C2D-C1D	4.11	131.63	125.37
21	5	412	CL7	CMD-C2D-C1D	4.11	131.63	125.37
21	4	405	CL7	C1D-ND-C4D	-4.11	103.41	106.33
21	8	405	CL7	C1D-ND-C4D	-4.11	103.41	106.33
21	6	509	CL7	C1D-ND-C4D	-4.11	103.42	106.33
21	3	518	CL7	C3A-C4A-CHB	-4.11	117.60	123.70
32	6	520	ZEX	C28-C27-C26	-4.11	120.07	127.09
21	1	405	CL7	C2D-C1D-ND	4.11	112.98	110.23
21	5	405	CL7	C2D-C1D-ND	4.11	112.98	110.23
21	7	518	CL7	C3A-C4A-CHB	-4.10	117.61	123.70
21	b	603	CL7	C2D-C1D-ND	4.10	112.98	110.23
21	3	518	CL7	C1D-ND-C4D	-4.10	103.42	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	505	CL7	O2D-CGD-CBD	4.10	118.55	111.27
21	a	405	CL7	C2D-C1D-ND	4.10	112.98	110.23
21	7	512	CL7	C2D-C1D-ND	4.10	112.98	110.23
21	1	402	CL7	C1D-ND-C4D	-4.10	103.42	106.33
21	2	509	CL7	C1D-ND-C4D	-4.10	103.42	106.33
21	3	508	CL7	CMD-C2D-C1D	4.10	131.61	125.37
21	6	505	CL7	O2D-CGD-CBD	4.10	118.55	111.27
21	B	612	CL7	C1D-ND-C4D	-4.09	103.43	106.33
21	b	613	CL7	C1D-ND-C4D	-4.09	103.43	106.33
21	c	509	CL7	C4D-C3D-CAD	-4.09	104.67	107.42
21	6	516	CL7	C1D-ND-C4D	-4.09	103.43	106.33
21	B	602	CL7	C2D-C1D-ND	4.09	112.97	110.23
21	C	502	CL7	CMD-C2D-C1D	4.09	131.60	125.37
21	c	502	CL7	CMD-C2D-C1D	4.09	131.60	125.37
21	7	518	CL7	C1D-ND-C4D	-4.09	103.43	106.33
32	2	521	ZEX	C28-C27-C26	-4.09	120.10	127.09
21	1	411	CL7	C2D-C1D-ND	4.09	112.97	110.23
21	D	405	CL7	C3A-C4A-CHB	-4.09	117.64	123.70
21	4	417	CL7	C2D-C1D-ND	4.09	112.97	110.23
21	7	508	CL7	CMD-C2D-C1D	4.08	131.59	125.37
21	2	514	CL7	C4D-C3D-CAD	-4.08	104.67	107.42
21	4	406	CL7	C2D-C1D-ND	4.08	112.97	110.23
21	2	518	CL7	C4D-C3D-CAD	-4.08	104.67	107.42
21	6	518	CL7	C4D-C3D-CAD	-4.08	104.67	107.42
23	b	619	8CT	C13-C14-C15	-4.08	110.49	123.22
23	B	618	8CT	C13-C14-C15	-4.08	110.49	123.22
32	3	522	ZEX	C18-C5-C6	-4.08	119.95	124.53
32	7	522	ZEX	C18-C5-C6	-4.08	119.95	124.53
21	A	401	CL7	CAA-C2A-C1A	-4.08	98.78	112.19
21	4	414	CL7	CMD-C2D-C1D	4.07	131.57	125.37
21	2	516	CL7	C1D-ND-C4D	-4.07	103.44	106.33
32	4	420	ZEX	C31-C30-C29	-4.07	121.50	127.31
32	8	420	ZEX	C31-C30-C29	-4.07	121.50	127.31
21	d	405	CL7	C3A-C4A-CHB	-4.07	117.66	123.70
21	C	508	CL7	CMD-C2D-C1D	4.07	131.56	125.37
21	c	508	CL7	CMD-C2D-C1D	4.07	131.56	125.37
21	1	418	CL7	O2D-CGD-CBD	4.07	118.50	111.27
21	5	418	CL7	O2D-CGD-CBD	4.07	118.50	111.27
21	C	506	CL7	C1D-ND-C4D	-4.07	103.45	106.33
21	3	513	CL7	C1D-ND-C4D	-4.07	103.45	106.33
21	4	409	CL7	C1D-ND-C4D	-4.07	103.45	106.33
21	c	506	CL7	C1D-ND-C4D	-4.07	103.45	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	d	402	CL7	C1D-ND-C4D	-4.07	103.45	106.33
21	7	513	CL7	C1D-ND-C4D	-4.07	103.45	106.33
21	8	409	CL7	C1D-ND-C4D	-4.07	103.45	106.33
21	4	411	CL7	C4D-C3D-CAD	-4.07	104.68	107.42
23	8	402	8CT	C07-C02-C03	-4.07	116.83	122.73
23	B	617	8CT	C14-C13-C12	-4.06	121.51	127.31
23	b	618	8CT	C14-C13-C12	-4.06	121.51	127.31
21	a	401	CL7	CAA-C2A-C1A	-4.06	98.82	112.19
21	1	404	CL7	O2D-CGD-CBD	4.06	118.48	111.27
21	c	507	CL7	C1D-ND-C4D	-4.06	103.45	106.33
21	C	502	CL7	C4D-C3D-CAD	-4.05	104.69	107.42
21	6	514	CL7	C4D-C3D-CAD	-4.05	104.69	107.42
21	1	410	CL7	C3A-C4A-CHB	-4.05	117.69	123.70
21	5	410	CL7	C3A-C4A-CHB	-4.05	117.69	123.70
21	5	402	CL7	C1D-ND-C4D	-4.05	103.46	106.33
21	8	414	CL7	CMD-C2D-C1D	4.05	131.54	125.37
23	C	519	8CT	C04-C03-C02	-4.05	116.91	122.61
23	c	519	8CT	C04-C03-C02	-4.05	116.91	122.61
21	5	404	CL7	O2D-CGD-CBD	4.05	118.47	111.27
21	8	411	CL7	C4D-C3D-CAD	-4.05	104.69	107.42
21	8	413	CL7	C4D-C3D-CAD	-4.05	104.69	107.42
21	b	602	CL7	C4D-C3D-CAD	-4.05	104.70	107.42
21	1	418	CL7	C1D-ND-C4D	-4.05	103.46	106.33
21	5	418	CL7	C1D-ND-C4D	-4.05	103.46	106.33
23	k	101	8CT	C19-C18-C17	-4.05	115.18	123.47
32	2	520	ZEX	C8-C7-C6	-4.05	115.83	127.20
32	3	525	ZEX	C8-C7-C6	-4.05	115.83	127.20
21	2	503	CL7	C3A-C4A-CHB	-4.05	117.69	123.70
21	C	511	CL7	C1D-ND-C4D	-4.05	103.46	106.33
23	4	402	8CT	C07-C02-C03	-4.05	116.86	122.73
21	C	507	CL7	C1D-ND-C4D	-4.05	103.46	106.33
21	6	503	CL7	C3A-C4A-CHB	-4.04	117.70	123.70
21	8	417	CL7	C2D-C1D-ND	4.04	112.94	110.23
21	c	502	CL7	C4D-C3D-CAD	-4.04	104.70	107.42
21	A	406	CL7	C2D-C1D-ND	4.04	112.94	110.23
21	5	411	CL7	C2D-C1D-ND	4.04	112.94	110.23
23	K	101	8CT	C19-C18-C17	-4.04	115.20	123.47
21	C	509	CL7	C4D-C3D-CAD	-4.04	104.70	107.42
21	3	510	CL7	C3A-C4A-CHB	-4.04	117.71	123.70
21	7	510	CL7	C3A-C4A-CHB	-4.04	117.71	123.70
21	6	514	CL7	C1D-ND-C4D	-4.04	103.47	106.33
21	D	405	CL7	C1D-ND-C4D	-4.04	103.47	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	d	405	CL7	C1D-ND-C4D	-4.04	103.47	106.33
21	C	512	CL7	C4D-C3D-CAD	-4.03	104.71	107.42
21	3	508	CL7	C1D-ND-C4D	-4.03	103.47	106.33
21	7	508	CL7	C1D-ND-C4D	-4.03	103.47	106.33
21	2	514	CL7	C1D-ND-C4D	-4.03	103.47	106.33
21	3	516	CL7	C1D-ND-C4D	-4.02	103.48	106.33
21	b	609	CL7	CMD-C2D-C1D	4.02	131.49	125.37
21	3	504	CL7	C3A-C4A-CHB	-4.02	117.73	123.70
21	4	413	CL7	C4D-C3D-CAD	-4.02	104.72	107.42
23	C	519	8CT	C07-C02-C03	-4.02	116.90	122.73
23	c	519	8CT	C07-C02-C03	-4.02	116.90	122.73
21	c	512	CL7	C4D-C3D-CAD	-4.01	104.72	107.42
21	B	606	CL7	CHD-C1D-ND	-4.01	120.01	124.26
21	b	607	CL7	CHD-C1D-ND	-4.01	120.01	124.26
21	A	403	CL7	C1D-ND-C4D	-4.01	103.49	106.33
21	a	403	CL7	C1D-ND-C4D	-4.01	103.49	106.33
21	c	510	CL7	C1D-ND-C4D	-4.00	103.49	106.33
21	7	504	CL7	C3A-C4A-CHB	-4.00	117.76	123.70
32	2	523	ZEX	C27-C26-C25	-4.00	116.37	122.84
21	4	404	CL7	C1D-ND-C4D	-4.00	103.49	106.33
21	7	516	CL7	C1D-ND-C4D	-4.00	103.49	106.33
23	D	406	8CT	C14-C13-C12	-4.00	121.60	127.31
21	3	505	CL7	O2D-CGD-CBD	4.00	118.37	111.27
21	3	511	CL7	C2D-C1D-ND	4.00	112.91	110.23
21	7	511	CL7	C2D-C1D-ND	4.00	112.91	110.23
21	B	608	CL7	CMD-C2D-C1D	4.00	131.46	125.37
21	C	510	CL7	C4D-C3D-CAD	-4.00	104.73	107.42
21	c	510	CL7	C4D-C3D-CAD	-4.00	104.73	107.42
21	7	505	CL7	O2D-CGD-CBD	3.99	118.37	111.27
32	7	519	ZEX	C35-C34-C33	-3.99	121.61	127.31
32	6	522	ZEX	C27-C26-C25	-3.99	116.39	122.84
32	8	403	ZEX	C27-C26-C25	-3.99	116.39	122.84
21	8	404	CL7	C1D-ND-C4D	-3.99	103.50	106.33
21	1	410	CL7	C1D-ND-C4D	-3.98	103.51	106.33
21	B	601	CL7	C4D-C3D-CAD	-3.98	104.74	107.42
21	4	410	CL7	C2D-C1D-ND	3.98	112.90	110.23
23	d	406	8CT	C14-C13-C12	-3.98	121.63	127.31
21	c	511	CL7	C1D-ND-C4D	-3.98	103.51	106.33
21	1	405	CL7	C4D-C3D-CAD	-3.98	104.74	107.42
21	b	604	CL7	C3A-C4A-CHB	-3.97	117.80	123.70
21	1	416	CL7	C2D-C1D-ND	3.97	112.89	110.23
21	5	416	CL7	C2D-C1D-ND	3.97	112.89	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	3	519	ZEX	C35-C34-C33	-3.97	121.64	127.31
21	5	405	CL7	C4D-C3D-CAD	-3.97	104.75	107.42
21	B	603	CL7	C3A-C4A-CHB	-3.97	117.81	123.70
21	1	402	CL7	C2D-C1D-ND	3.97	112.89	110.23
21	5	402	CL7	C2D-C1D-ND	3.97	112.89	110.23
21	b	612	CL7	C4D-C3D-CAD	-3.96	104.75	107.42
21	1	408	CL7	O2D-CGD-CBD	3.96	118.30	111.27
23	A	404	8CT	C35-C30-C29	-3.96	107.70	112.70
21	2	502	CL7	C2D-C1D-ND	3.96	112.88	110.23
21	c	503	CL7	C2D-C1D-ND	3.96	112.88	110.23
21	6	502	CL7	C2D-C1D-ND	3.96	112.88	110.23
21	B	609	CL7	C1D-ND-C4D	-3.96	103.53	106.33
21	C	510	CL7	C1D-ND-C4D	-3.96	103.53	106.33
21	b	610	CL7	C1D-ND-C4D	-3.96	103.53	106.33
21	A	406	CL7	C4D-C3D-CAD	-3.96	104.76	107.42
21	3	504	CL7	C2D-C1D-ND	3.95	112.88	110.23
21	B	606	CL7	O2D-CGD-CBD	3.95	118.29	111.27
32	4	403	ZEX	C27-C26-C25	-3.95	116.45	122.84
21	6	516	CL7	C2D-C1D-ND	3.95	112.88	110.23
21	7	504	CL7	C2D-C1D-ND	3.95	112.88	110.23
21	C	512	CL7	C2D-C1D-ND	3.95	112.88	110.23
21	1	403	CL7	C2D-C1D-ND	3.95	112.88	110.23
21	c	512	CL7	C2D-C1D-ND	3.95	112.88	110.23
21	5	403	CL7	C2D-C1D-ND	3.95	112.88	110.23
21	8	410	CL7	C2D-C1D-ND	3.95	112.88	110.23
21	6	518	CL7	C2D-C1D-ND	3.95	112.88	110.23
21	5	408	CL7	O2D-CGD-CBD	3.94	118.28	111.27
21	B	611	CL7	C4D-C3D-CAD	-3.94	104.77	107.42
21	7	513	CL7	C3A-C4A-CHB	-3.94	117.85	123.70
21	3	514	CL7	C2D-C1D-ND	3.94	112.87	110.23
21	B	613	CL7	C1D-ND-C4D	-3.94	103.54	106.33
21	7	516	CL7	C4D-C3D-CAD	-3.94	104.77	107.42
21	1	420	CL7	C4D-C3D-CAD	-3.94	104.77	107.42
21	5	420	CL7	C4D-C3D-CAD	-3.94	104.77	107.42
23	a	404	8CT	C35-C30-C29	-3.93	107.73	112.70
21	B	610	CL7	CAA-CBA-CGA	-3.93	101.75	113.25
21	1	407	CL7	C2D-C1D-ND	3.93	112.87	110.23
21	5	407	CL7	C2D-C1D-ND	3.93	112.87	110.23
21	C	510	CL7	C3A-C4A-CHB	-3.93	117.86	123.70
21	c	510	CL7	C3A-C4A-CHB	-3.93	117.86	123.70
21	3	513	CL7	C3A-C4A-CHB	-3.93	117.87	123.70
21	7	501	CL7	C2D-C1D-ND	3.93	112.87	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	503	CL7	C2D-C1D-ND	3.93	112.87	110.23
21	b	615	CL7	C2D-C1D-ND	3.93	112.87	110.23
21	b	611	CL7	CAA-CBA-CGA	-3.93	101.77	113.25
21	b	607	CL7	O2D-CGD-CBD	3.92	118.24	111.27
21	2	516	CL7	C2D-C1D-ND	3.92	112.86	110.23
21	2	518	CL7	C2D-C1D-ND	3.92	112.86	110.23
21	3	507	CL7	CMD-C2D-C1D	3.92	131.34	125.37
21	7	507	CL7	CMD-C2D-C1D	3.92	131.34	125.37
21	C	505	CL7	C3A-C4A-CHB	-3.92	117.88	123.70
21	c	505	CL7	C3A-C4A-CHB	-3.92	117.88	123.70
21	6	511	CL7	C2D-C1D-ND	3.92	112.86	110.23
21	7	514	CL7	C2D-C1D-ND	3.92	112.86	110.23
21	6	506	CL7	C1D-ND-C4D	-3.92	103.55	106.33
21	4	405	CL7	CAA-CBA-CGA	-3.92	101.81	113.25
21	8	405	CL7	CAA-CBA-CGA	-3.92	101.81	113.25
23	B	617	8CT	C10-C11-C12	-3.92	120.32	126.23
32	7	520	ZEX	C7-C8-C9	-3.91	120.32	126.23
21	B	608	CL7	C4D-C3D-CAD	-3.91	104.79	107.42
21	b	609	CL7	C4D-C3D-CAD	-3.91	104.79	107.42
21	2	511	CL7	C2D-C1D-ND	3.91	112.85	110.23
32	2	523	ZEX	C1-C6-C5	-3.91	117.11	122.61
32	6	522	ZEX	C1-C6-C5	-3.91	117.11	122.61
21	C	511	CL7	CAA-CBA-CGA	-3.91	101.83	113.25
21	c	511	CL7	CAA-CBA-CGA	-3.91	101.83	113.25
23	b	618	8CT	C10-C11-C12	-3.91	120.33	126.23
21	3	511	CL7	O2D-CGD-CBD	3.90	118.21	111.27
21	7	511	CL7	O2D-CGD-CBD	3.90	118.21	111.27
21	2	504	CL7	C3A-C4A-CHB	-3.90	117.91	123.70
21	6	504	CL7	C3A-C4A-CHB	-3.90	117.91	123.70
32	1	421	ZEX	C27-C28-C29	-3.90	120.34	126.23
32	5	421	ZEX	C27-C28-C29	-3.90	120.34	126.23
21	B	607	CL7	C2D-C1D-ND	3.90	112.85	110.23
21	8	408	CL7	C4D-C3D-CAD	-3.90	104.80	107.42
21	4	413	CL7	C1D-ND-C4D	-3.90	103.57	106.33
21	5	410	CL7	C1D-ND-C4D	-3.90	103.57	106.33
32	2	523	ZEX	C31-C30-C29	-3.90	121.75	127.31
32	6	522	ZEX	C31-C30-C29	-3.90	121.75	127.31
21	2	501	CL7	C2D-C1D-ND	3.89	112.84	110.23
21	6	501	CL7	C2D-C1D-ND	3.89	112.84	110.23
21	4	411	CL7	CHD-C1D-ND	-3.89	120.14	124.26
21	8	411	CL7	CHD-C1D-ND	-3.89	120.14	124.26
21	3	501	CL7	C2D-C1D-ND	3.89	112.84	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	3	520	ZEX	C7-C8-C9	-3.89	120.35	126.23
21	b	614	CL7	C1D-ND-C4D	-3.89	103.57	106.33
21	2	511	CL7	C1D-ND-C4D	-3.89	103.57	106.33
21	5	408	CL7	C3A-C4A-CHB	-3.88	117.94	123.70
21	3	513	CL7	C4D-C3D-CAD	-3.88	104.81	107.42
21	a	405	CL7	C4D-C3D-CAD	-3.88	104.81	107.42
21	6	511	CL7	C1D-ND-C4D	-3.88	103.58	106.33
21	4	413	CL7	C2D-C1D-ND	3.88	112.83	110.23
21	4	412	CL7	C1D-ND-C4D	-3.88	103.58	106.33
21	8	413	CL7	C1D-ND-C4D	-3.88	103.58	106.33
21	2	506	CL7	C1D-ND-C4D	-3.87	103.58	106.33
21	8	408	CL7	C1D-ND-C4D	-3.87	103.58	106.33
21	C	514	CL7	C2D-C1D-ND	3.87	112.83	110.23
21	c	514	CL7	C2D-C1D-ND	3.87	112.83	110.23
21	B	622	CL7	C2D-C1D-ND	3.87	112.83	110.23
21	b	623	CL7	C2D-C1D-ND	3.87	112.83	110.23
21	1	408	CL7	C3A-C4A-CHB	-3.87	117.96	123.70
21	6	512	CL7	CHD-C4C-C3C	-3.87	118.67	124.94
21	4	408	CL7	C4D-C3D-CAD	-3.86	104.82	107.42
21	1	417	CL7	C2D-C1D-ND	3.86	112.82	110.23
21	5	417	CL7	C2D-C1D-ND	3.86	112.82	110.23
21	6	503	CL7	CED-O2D-CGD	-3.86	107.20	115.94
21	4	408	CL7	C1D-ND-C4D	-3.86	103.59	106.33
23	d	406	8CT	C25-C24-C23	-3.86	111.18	123.22
21	8	413	CL7	C2D-C1D-ND	3.86	112.82	110.23
23	D	406	8CT	C25-C24-C23	-3.86	111.18	123.22
21	4	408	CL7	C2D-C1D-ND	3.86	112.82	110.23
21	8	408	CL7	C2D-C1D-ND	3.86	112.82	110.23
21	a	403	CL7	CHD-C4C-C3C	-3.86	118.69	124.94
21	2	512	CL7	CHD-C4C-C3C	-3.85	118.70	124.94
21	b	612	CL7	C2D-C1D-ND	3.85	112.81	110.23
21	2	508	CL7	C1D-ND-C4D	-3.85	103.60	106.33
21	6	508	CL7	C1D-ND-C4D	-3.85	103.60	106.33
21	3	512	CL7	C3A-C4A-CHB	-3.85	117.99	123.70
21	7	512	CL7	C3A-C4A-CHB	-3.85	117.99	123.70
21	B	611	CL7	C2D-C1D-ND	3.85	112.81	110.23
21	c	509	CL7	O2D-CGD-CBD	3.84	118.10	111.27
22	D	408	PHO	C4B-NB-C1B	-3.84	102.88	108.83
21	7	506	CL7	C3A-C4A-CHB	-3.84	118.00	123.70
21	3	517	CL7	C1D-ND-C4D	-3.84	103.61	106.33
21	7	517	CL7	C1D-ND-C4D	-3.84	103.61	106.33
21	b	608	CL7	C2D-C1D-ND	3.84	112.81	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	516	CL7	C4D-C3D-CAD	-3.84	104.83	107.42
21	B	614	CL7	CAA-C2A-C3A	-3.84	102.26	112.78
21	D	405	CL7	C2D-C1D-ND	3.84	112.81	110.23
21	d	405	CL7	C2D-C1D-ND	3.84	112.81	110.23
22	d	408	PHO	C4B-NB-C1B	-3.84	102.88	108.83
21	2	503	CL7	CED-O2D-CGD	-3.84	107.25	115.94
21	4	415	CL7	C4D-C3D-CAD	-3.84	104.84	107.42
23	C	516	8CT	C14-C15-C16	-3.84	115.63	126.42
21	A	403	CL7	CHD-C4C-C3C	-3.84	118.72	124.94
21	8	412	CL7	C1D-ND-C4D	-3.84	103.61	106.33
21	3	510	CL7	C2D-C1D-ND	3.84	112.80	110.23
21	7	510	CL7	C2D-C1D-ND	3.84	112.80	110.23
21	3	506	CL7	C3A-C4A-CHB	-3.84	118.01	123.70
21	2	512	CL7	O2D-CGD-CBD	3.84	118.08	111.27
21	6	512	CL7	O2D-CGD-CBD	3.84	118.08	111.27
21	2	515	CL7	C2D-C1D-ND	3.84	112.80	110.23
21	b	615	CL7	CAA-C2A-C3A	-3.83	102.28	112.78
21	6	513	CL7	C3A-C4A-CHB	-3.83	118.02	123.70
23	D	406	8CT	C10-C11-C12	-3.83	120.45	126.23
21	B	614	CL7	C2D-C1D-ND	3.83	112.80	110.23
21	2	510	CL7	C1D-ND-C4D	-3.83	103.61	106.33
21	6	510	CL7	C1D-ND-C4D	-3.83	103.61	106.33
21	2	513	CL7	C3A-C4A-CHB	-3.83	118.02	123.70
21	C	508	CL7	C3A-C4A-CHB	-3.83	118.02	123.70
21	7	513	CL7	C4D-C3D-CAD	-3.83	104.85	107.42
21	a	405	CL7	CHD-C1D-ND	-3.82	120.21	124.26
23	d	406	8CT	C10-C11-C12	-3.82	120.46	126.23
21	3	507	CL7	C1D-ND-C4D	-3.82	103.62	106.33
21	7	507	CL7	C1D-ND-C4D	-3.82	103.62	106.33
23	c	516	8CT	C14-C15-C16	-3.82	115.69	126.42
21	B	605	CL7	C2D-C1D-ND	3.82	112.79	110.23
21	C	503	CL7	C3A-C4A-CHB	-3.81	118.04	123.70
27	b	625	DGD	O2G-C1B-C2B	3.81	119.72	111.50
21	c	503	CL7	C3A-C4A-CHB	-3.81	118.04	123.70
32	2	520	ZEX	C15-C14-C13	-3.81	121.87	127.31
32	3	525	ZEX	C15-C14-C13	-3.81	121.87	127.31
21	C	509	CL7	O2D-CGD-CBD	3.81	118.04	111.27
21	C	509	CL7	C2D-C1D-ND	3.81	112.79	110.23
21	1	409	CL7	C2D-C1D-ND	3.81	112.79	110.23
21	c	509	CL7	C2D-C1D-ND	3.81	112.79	110.23
21	5	409	CL7	C2D-C1D-ND	3.81	112.79	110.23
21	C	508	CL7	O2D-CGD-CBD	3.81	118.04	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	c	508	CL7	O2D-CGD-CBD	3.81	118.04	111.27
21	3	509	CL7	C1D-ND-C4D	-3.81	103.63	106.33
21	b	606	CL7	C2D-C1D-ND	3.81	112.78	110.23
21	5	417	CL7	CHD-C1D-ND	-3.81	120.23	124.26
21	d	404	CL7	C2D-C1D-ND	3.81	112.78	110.23
32	5	422	ZEX	C15-C14-C13	-3.80	121.88	127.31
32	1	422	ZEX	C15-C14-C13	-3.80	121.88	127.31
21	B	606	CL7	C1D-ND-C4D	-3.80	103.63	106.33
21	b	607	CL7	C1D-ND-C4D	-3.80	103.63	106.33
23	B	617	8CT	C04-C03-C02	-3.80	117.26	122.61
21	c	508	CL7	C3A-C4A-CHB	-3.80	118.06	123.70
32	1	421	ZEX	C15-C14-C13	-3.80	121.89	127.31
21	B	622	CL7	C3A-C4A-CHB	-3.80	118.06	123.70
21	b	623	CL7	C3A-C4A-CHB	-3.80	118.06	123.70
27	B	624	DGD	O2G-C1B-C2B	3.80	119.68	111.50
21	4	412	CL7	C2D-C1D-ND	3.80	112.78	110.23
21	8	412	CL7	C2D-C1D-ND	3.80	112.78	110.23
21	6	507	CL7	C3A-C4A-CHB	-3.80	118.07	123.70
21	1	417	CL7	CHD-C1D-ND	-3.80	120.24	124.26
21	3	505	CL7	CMD-C2D-C1D	3.80	131.15	125.37
21	7	505	CL7	CMD-C2D-C1D	3.80	131.15	125.37
21	1	419	CL7	C2D-C1D-ND	3.79	112.78	110.23
21	3	509	CL7	C2D-C1D-ND	3.79	112.78	110.23
32	4	418	ZEX	C18-C5-C6	-3.79	120.27	124.53
32	8	418	ZEX	C18-C5-C6	-3.79	120.27	124.53
21	6	515	CL7	C2D-C1D-ND	3.79	112.77	110.23
21	2	507	CL7	C3A-C4A-CHB	-3.79	118.08	123.70
21	7	509	CL7	C1D-ND-C4D	-3.79	103.64	106.33
21	B	615	CL7	C1D-ND-C4D	-3.79	103.64	106.33
32	5	421	ZEX	C15-C14-C13	-3.79	121.90	127.31
21	8	410	CL7	C4D-C3D-CAD	-3.79	104.87	107.42
21	A	406	CL7	CHD-C1D-ND	-3.79	120.25	124.26
21	C	505	CL7	C2D-C1D-ND	3.78	112.77	110.23
21	c	505	CL7	C2D-C1D-ND	3.78	112.77	110.23
21	b	611	CL7	O2D-CGD-CBD	3.78	117.99	111.27
21	8	415	CL7	C4D-C3D-CAD	-3.78	104.88	107.42
31	F	101	HEM	C1B-NB-C4B	3.78	108.98	105.07
31	f	101	HEM	C1B-NB-C4B	3.78	108.98	105.07
23	b	618	8CT	C04-C03-C02	-3.78	117.29	122.61
21	8	404	CL7	C3A-C4A-CHB	-3.78	118.09	123.70
21	6	506	CL7	C2D-C1D-ND	3.78	112.77	110.23
21	C	507	CL7	C2D-C1D-ND	3.78	112.77	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	511	CL7	CHD-C1D-ND	-3.78	120.26	124.26
21	B	604	CL7	C1D-ND-C4D	-3.78	103.65	106.33
21	b	605	CL7	C1D-ND-C4D	-3.78	103.65	106.33
31	F	101	HEM	CHA-C4D-ND	3.78	129.03	124.37
31	f	101	HEM	CHA-C4D-ND	3.78	129.03	124.37
21	4	410	CL7	C4D-C3D-CAD	-3.78	104.88	107.42
21	1	414	CL7	C2D-C1D-ND	3.78	112.76	110.23
21	5	414	CL7	C2D-C1D-ND	3.78	112.76	110.23
21	7	509	CL7	C2D-C1D-ND	3.78	112.76	110.23
32	3	519	ZEX	C15-C35-C34	-3.77	115.75	123.47
32	7	519	ZEX	C15-C35-C34	-3.77	115.75	123.47
21	1	418	CL7	C2D-C1D-ND	3.77	112.76	110.23
21	5	418	CL7	C2D-C1D-ND	3.77	112.76	110.23
21	3	502	CL7	C3A-C4A-CHB	-3.77	118.11	123.70
21	7	502	CL7	C3A-C4A-CHB	-3.77	118.11	123.70
21	6	518	CL7	C3A-C4A-CHB	-3.77	118.11	123.70
21	B	610	CL7	O2D-CGD-CBD	3.76	117.96	111.27
21	4	413	CL7	C3A-C4A-CHB	-3.76	118.11	123.70
21	8	413	CL7	C3A-C4A-CHB	-3.76	118.11	123.70
21	3	503	CL7	CHD-C4C-C3C	-3.76	118.84	124.94
21	7	503	CL7	CHD-C4C-C3C	-3.76	118.84	124.94
21	1	406	CL7	C4D-C3D-CAD	-3.76	104.89	107.42
21	5	406	CL7	C4D-C3D-CAD	-3.76	104.89	107.42
21	c	507	CL7	C2D-C1D-ND	3.76	112.75	110.23
21	4	408	CL7	C3A-C4A-CHB	-3.76	118.12	123.70
21	D	404	CL7	C2D-C1D-ND	3.76	112.75	110.23
21	8	408	CL7	C3A-C4A-CHB	-3.76	118.12	123.70
21	4	404	CL7	C3A-C4A-CHB	-3.76	118.13	123.70
21	1	407	CL7	C3A-C4A-CHB	-3.75	118.13	123.70
21	5	407	CL7	C3A-C4A-CHB	-3.75	118.13	123.70
21	2	518	CL7	C3A-C4A-CHB	-3.75	118.13	123.70
32	4	420	ZEX	C35-C34-C33	-3.75	121.95	127.31
32	8	420	ZEX	C35-C34-C33	-3.75	121.95	127.31
21	1	404	CL7	C1-C2-C3	3.75	132.53	126.04
21	5	404	CL7	C1-C2-C3	3.75	132.53	126.04
21	B	604	CL7	O2D-CGD-CBD	3.75	117.93	111.27
23	B	627	8CT	C39-C16-C17	-3.75	117.67	122.92
23	b	620	8CT	C24-C23-C21	-3.74	115.90	126.42
21	1	414	CL7	C3A-C4A-CHB	-3.74	118.14	123.70
21	5	414	CL7	C3A-C4A-CHB	-3.74	118.14	123.70
21	b	616	CL7	C1D-ND-C4D	-3.74	103.68	106.33
21	B	608	CL7	C2D-C1D-ND	3.74	112.74	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	609	CL7	C2D-C1D-ND	3.74	112.74	110.23
21	5	419	CL7	C2D-C1D-ND	3.74	112.74	110.23
21	b	605	CL7	O2D-CGD-CBD	3.74	117.91	111.27
21	7	518	CL7	C4D-C3D-CAD	-3.74	104.91	107.42
21	4	405	CL7	C1-C2-C3	3.74	132.51	126.04
21	8	405	CL7	C1-C2-C3	3.74	132.51	126.04
23	c	515	8CT	C10-C11-C12	-3.74	120.59	126.23
21	1	402	CL7	C3A-C4A-CHB	-3.74	118.16	123.70
21	5	402	CL7	C3A-C4A-CHB	-3.74	118.16	123.70
21	2	503	CL7	CAA-CBA-CGA	-3.74	102.34	113.25
21	6	503	CL7	CAA-CBA-CGA	-3.74	102.34	113.25
21	3	517	CL7	C2D-C1D-ND	3.74	112.74	110.23
23	B	619	8CT	C01-C02-C03	-3.73	120.33	124.53
23	b	620	8CT	C01-C02-C03	-3.73	120.33	124.53
21	3	510	CL7	C1D-ND-C4D	-3.73	103.68	106.33
21	7	510	CL7	C1D-ND-C4D	-3.73	103.68	106.33
21	c	511	CL7	CHD-C1D-ND	-3.73	120.31	124.26
21	3	518	CL7	C4D-C3D-CAD	-3.73	104.91	107.42
21	2	506	CL7	C2D-C1D-ND	3.73	112.73	110.23
21	3	518	CL7	C2D-C1D-ND	3.73	112.73	110.23
21	7	518	CL7	C2D-C1D-ND	3.73	112.73	110.23
32	8	419	ZEX	C31-C30-C29	-3.73	121.99	127.31
21	6	503	CL7	CHD-C4C-C3C	-3.73	118.90	124.94
32	4	419	ZEX	C31-C30-C29	-3.72	121.99	127.31
23	b	601	8CT	C39-C16-C17	-3.72	117.71	122.92
21	4	412	CL7	CHD-C1D-ND	-3.72	120.32	124.26
21	3	507	CL7	C2D-C1D-ND	3.72	112.73	110.23
21	7	507	CL7	C2D-C1D-ND	3.72	112.73	110.23
21	C	507	CL7	C3A-C4A-CHB	-3.72	118.18	123.70
21	c	507	CL7	C3A-C4A-CHB	-3.72	118.18	123.70
23	C	515	8CT	C10-C11-C12	-3.72	120.61	126.23
23	K	101	8CT	C24-C25-C26	-3.72	122.00	127.31
23	k	101	8CT	C24-C25-C26	-3.72	122.00	127.31
21	2	510	CL7	C2D-C1D-ND	3.72	112.73	110.23
21	6	510	CL7	C2D-C1D-ND	3.72	112.73	110.23
23	B	619	8CT	C24-C23-C21	-3.72	115.97	126.42
21	2	503	CL7	CHD-C4C-C3C	-3.72	118.91	124.94
32	2	521	ZEX	C15-C14-C13	-3.72	122.00	127.31
32	2	523	ZEX	C31-C32-C33	-3.72	115.98	126.42
21	C	504	CL7	C3A-C4A-CHB	-3.72	118.19	123.70
21	c	504	CL7	C3A-C4A-CHB	-3.72	118.19	123.70
21	B	607	CL7	CHD-C1D-ND	-3.71	120.33	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	609	CL7	C3A-C4A-CHB	-3.71	118.19	123.70
21	b	610	CL7	C3A-C4A-CHB	-3.71	118.19	123.70
21	3	516	CL7	CHD-C1D-ND	-3.70	120.33	124.26
32	6	522	ZEX	C31-C32-C33	-3.70	116.01	126.42
23	k	101	8CT	C18-C17-C16	-3.70	122.02	127.31
21	7	517	CL7	C2D-C1D-ND	3.70	112.71	110.23
23	B	617	8CT	C19-C20-C21	-3.70	122.03	127.31
23	b	618	8CT	C19-C20-C21	-3.70	122.03	127.31
21	4	411	CL7	O2A-C1-C2	-3.70	98.91	108.64
21	8	411	CL7	O2A-C1-C2	-3.70	98.91	108.64
23	B	619	8CT	C11-C10-C03	-3.70	116.82	127.20
23	b	620	8CT	C11-C10-C03	-3.70	116.82	127.20
21	8	412	CL7	CHD-C1D-ND	-3.69	120.35	124.26
32	6	520	ZEX	C15-C14-C13	-3.69	122.04	127.31
21	B	612	CL7	O2D-CGD-CBD	3.69	117.83	111.27
21	B	622	CL7	O2D-CGD-CBD	3.69	117.83	111.27
21	b	613	CL7	O2D-CGD-CBD	3.69	117.83	111.27
21	b	623	CL7	O2D-CGD-CBD	3.69	117.83	111.27
21	2	517	CL7	C3A-C4A-CHB	-3.69	118.22	123.70
21	7	516	CL7	CHD-C1D-ND	-3.69	120.35	124.26
21	B	612	CL7	C2D-C1D-ND	3.69	112.70	110.23
21	b	613	CL7	C2D-C1D-ND	3.69	112.70	110.23
23	K	101	8CT	C18-C17-C16	-3.69	122.05	127.31
21	C	514	CL7	C3A-C4A-CHB	-3.69	118.23	123.70
21	3	516	CL7	C7-C6-C5	-3.68	103.37	113.36
21	7	516	CL7	C7-C6-C5	-3.68	103.37	113.36
21	6	512	CL7	CMD-C2D-C1D	3.68	130.97	125.37
21	C	502	CL7	CHD-C4C-C3C	-3.68	118.98	124.94
21	b	615	CL7	C1D-ND-C4D	-3.68	103.72	106.33
21	c	502	CL7	CHD-C4C-C3C	-3.68	118.98	124.94
21	b	608	CL7	CHD-C1D-ND	-3.67	120.37	124.26
21	4	405	CL7	C2D-C1D-ND	3.67	112.69	110.23
21	3	511	CL7	CHD-C4C-C3C	-3.67	118.99	124.94
21	7	511	CL7	CHD-C4C-C3C	-3.67	118.99	124.94
21	c	514	CL7	C3A-C4A-CHB	-3.67	118.25	123.70
21	7	508	CL7	C1-C2-C3	3.67	132.39	126.04
21	5	403	CL7	CMD-C2D-C1D	3.67	130.96	125.37
21	6	506	CL7	C3A-C4A-CHB	-3.67	118.26	123.70
21	4	409	CL7	C3A-C4A-CHB	-3.67	118.26	123.70
21	8	409	CL7	C3A-C4A-CHB	-3.67	118.26	123.70
21	1	411	CL7	C3A-C4A-CHB	-3.67	118.26	123.70
21	2	512	CL7	CMD-C2D-C1D	3.67	130.95	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	517	CL7	C3A-C4A-CHB	-3.67	118.26	123.70
21	4	412	CL7	O2D-CGD-CBD	3.66	117.78	111.27
21	8	412	CL7	O2D-CGD-CBD	3.66	117.78	111.27
21	D	404	CL7	O2D-CGD-CBD	3.66	117.77	111.27
21	d	404	CL7	O2D-CGD-CBD	3.66	117.77	111.27
21	1	403	CL7	CMD-C2D-C1D	3.66	130.94	125.37
21	4	411	CL7	C2D-C1D-ND	3.66	112.68	110.23
21	8	411	CL7	C2D-C1D-ND	3.66	112.68	110.23
21	3	506	CL7	C1D-ND-C4D	-3.66	103.74	106.33
21	1	420	CL7	C3A-C4A-CHB	-3.65	118.28	123.70
21	5	420	CL7	C3A-C4A-CHB	-3.65	118.28	123.70
21	1	411	CL7	CHD-C1D-ND	-3.65	120.39	124.26
21	2	506	CL7	C3A-C4A-CHB	-3.65	118.28	123.70
32	2	521	ZEX	C11-C10-C9	-3.65	122.09	127.31
21	3	508	CL7	C1-C2-C3	3.65	132.36	126.04
21	5	411	CL7	C3A-C4A-CHB	-3.65	118.29	123.70
21	6	511	CL7	C3A-C4A-CHB	-3.65	118.29	123.70
32	6	520	ZEX	C11-C10-C9	-3.64	122.11	127.31
21	B	613	CL7	C2D-C1D-ND	3.64	112.67	110.23
21	3	513	CL7	C2D-C1D-ND	3.64	112.67	110.23
21	2	504	CL7	C1D-ND-C4D	-3.64	103.75	106.33
21	6	504	CL7	C1D-ND-C4D	-3.64	103.75	106.33
21	2	511	CL7	C3A-C4A-CHB	-3.64	118.30	123.70
21	B	602	CL7	O2D-CGD-CBD	3.64	117.73	111.27
21	B	602	CL7	C3A-C4A-CHB	-3.64	118.30	123.70
21	b	603	CL7	C3A-C4A-CHB	-3.64	118.30	123.70
21	b	603	CL7	O2D-CGD-CBD	3.64	117.73	111.27
27	C	517	DGD	O2G-C1B-C2B	3.64	119.34	111.50
27	c	517	DGD	O2G-C1B-C2B	3.64	119.34	111.50
21	5	411	CL7	CHD-C1D-ND	-3.64	120.41	124.26
21	7	506	CL7	C1D-ND-C4D	-3.63	103.75	106.33
23	c	519	8CT	C10-C11-C12	-3.63	120.74	126.23
21	3	517	CL7	C3A-C4A-CHB	-3.63	118.31	123.70
21	7	517	CL7	C3A-C4A-CHB	-3.63	118.31	123.70
21	A	406	CL7	O2D-CGD-CBD	3.63	117.72	111.27
21	a	405	CL7	O2D-CGD-CBD	3.63	117.72	111.27
21	B	610	CL7	C4D-C3D-CAD	-3.63	104.98	107.42
21	1	406	CL7	C3A-C4A-CHB	-3.63	118.32	123.70
21	5	406	CL7	C3A-C4A-CHB	-3.63	118.32	123.70
21	8	405	CL7	C2D-C1D-ND	3.62	112.66	110.23
21	2	508	CL7	C2D-C1D-ND	3.62	112.66	110.23
21	6	508	CL7	C2D-C1D-ND	3.62	112.66	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	611	CL7	C4D-C3D-CAD	-3.62	104.99	107.42
21	3	503	CL7	C3A-C4A-CHB	-3.62	118.33	123.70
21	7	503	CL7	C3A-C4A-CHB	-3.62	118.33	123.70
23	C	519	8CT	C10-C11-C12	-3.62	120.77	126.23
21	1	417	CL7	CHD-C4C-C3C	-3.61	119.08	124.94
21	5	417	CL7	CHD-C4C-C3C	-3.61	119.08	124.94
21	b	614	CL7	C2D-C1D-ND	3.61	112.65	110.23
32	4	419	ZEX	C27-C28-C29	-3.61	120.78	126.23
32	8	419	ZEX	C27-C28-C29	-3.61	120.78	126.23
21	4	407	CL7	C3A-C4A-CHB	-3.61	118.34	123.70
21	8	407	CL7	C3A-C4A-CHB	-3.61	118.34	123.70
21	1	414	CL7	CAC-C3C-C4C	-3.61	119.00	124.68
21	5	414	CL7	CAC-C3C-C4C	-3.61	119.00	124.68
21	c	518	CL7	O2D-CGD-CBD	3.61	117.68	111.27
23	b	601	8CT	C30-C31-C32	-3.61	117.03	121.47
21	6	501	CL7	C3A-C4A-CHB	-3.61	118.34	123.70
21	8	406	CL7	C3A-C4A-CHB	-3.61	118.35	123.70
21	3	505	CL7	C7-C6-C5	-3.61	103.57	113.36
21	4	415	CL7	C3A-C4A-CHB	-3.60	118.35	123.70
21	7	513	CL7	C2D-C1D-ND	3.60	112.65	110.23
21	D	404	CL7	C3A-C4A-CHB	-3.60	118.35	123.70
21	A	406	CL7	O2A-C1-C2	-3.60	99.17	108.64
21	C	518	CL7	O2D-CGD-CBD	3.60	117.66	111.27
21	d	404	CL7	C3A-C4A-CHB	-3.60	118.36	123.70
21	A	403	CL7	C2D-C1D-ND	3.60	112.64	110.23
21	a	403	CL7	C2D-C1D-ND	3.60	112.64	110.23
21	7	505	CL7	C7-C6-C5	-3.59	103.60	113.36
21	4	406	CL7	C3A-C4A-CHB	-3.59	118.37	123.70
21	D	404	CL7	C4D-C3D-CAD	-3.59	105.00	107.42
21	2	501	CL7	C3A-C4A-CHB	-3.59	118.37	123.70
21	a	405	CL7	O2A-C1-C2	-3.59	99.20	108.64
21	5	418	CL7	C3A-C4A-CHB	-3.59	118.37	123.70
23	4	402	8CT	C24-C25-C26	-3.59	122.19	127.31
23	8	402	8CT	C24-C25-C26	-3.59	122.19	127.31
21	8	415	CL7	C3A-C4A-CHB	-3.59	118.37	123.70
21	3	515	CL7	O2D-CGD-CBD	3.59	117.64	111.27
21	7	515	CL7	O2D-CGD-CBD	3.59	117.64	111.27
23	B	627	8CT	C30-C31-C32	-3.58	117.06	121.47
21	1	418	CL7	C3A-C4A-CHB	-3.58	118.39	123.70
21	A	403	CL7	C4C-C3C-C2C	-3.58	102.46	107.13
21	a	403	CL7	C4C-C3C-C2C	-3.58	102.46	107.13
21	B	614	CL7	C1D-ND-C4D	-3.58	103.79	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2	521	ZEX	C35-C15-C14	-3.58	116.14	123.47
21	D	402	CL7	C3A-C4A-CHB	-3.58	118.39	123.70
21	d	402	CL7	C3A-C4A-CHB	-3.58	118.39	123.70
21	3	508	CL7	C2D-C1D-ND	3.58	112.63	110.23
21	4	416	CL7	C2D-C1D-ND	3.58	112.63	110.23
21	7	508	CL7	C2D-C1D-ND	3.58	112.63	110.23
21	8	416	CL7	C2D-C1D-ND	3.58	112.63	110.23
21	C	511	CL7	C2D-C1D-ND	3.58	112.63	110.23
21	b	612	CL7	CHD-C1D-ND	-3.58	120.47	124.26
21	2	510	CL7	C3A-C4A-CHB	-3.57	118.39	123.70
21	6	510	CL7	C3A-C4A-CHB	-3.57	118.39	123.70
21	1	414	CL7	CHD-C1D-ND	-3.57	120.47	124.26
21	5	414	CL7	CHD-C1D-ND	-3.57	120.47	124.26
21	C	518	CL7	C1D-ND-C4D	-3.57	103.80	106.33
21	3	501	CL7	CHD-C1D-ND	-3.57	120.48	124.26
21	7	501	CL7	CHD-C1D-ND	-3.57	120.48	124.26
21	B	610	CL7	C3A-C4A-CHB	-3.57	118.40	123.70
32	2	520	ZEX	C10-C11-C12	-3.57	112.08	123.22
21	1	417	CL7	C3A-C4A-CHB	-3.57	118.41	123.70
21	b	617	CL7	C3A-C4A-CHB	-3.57	118.41	123.70
21	c	513	CL7	C3A-C4A-CHB	-3.57	118.41	123.70
21	5	417	CL7	C3A-C4A-CHB	-3.57	118.41	123.70
32	3	525	ZEX	C10-C11-C12	-3.56	112.09	123.22
21	d	404	CL7	C4D-C3D-CAD	-3.56	105.02	107.42
21	C	513	CL7	C3A-C4A-CHB	-3.56	118.41	123.70
21	D	402	CL7	CHD-C1D-ND	-3.56	120.48	124.26
21	d	402	CL7	CHD-C1D-ND	-3.56	120.48	124.26
23	C	516	8CT	C07-C02-C03	-3.56	117.56	122.73
23	c	516	8CT	C07-C02-C03	-3.56	117.56	122.73
32	6	520	ZEX	C35-C15-C14	-3.56	116.17	123.47
23	C	516	8CT	C01-C02-C07	3.56	120.46	113.62
23	c	516	8CT	C01-C02-C07	3.56	120.46	113.62
21	B	613	CL7	C3A-C4A-CHB	-3.56	118.41	123.70
21	b	614	CL7	C3A-C4A-CHB	-3.56	118.41	123.70
21	1	416	CL7	O2D-CGD-CBD	3.56	117.60	111.27
21	5	416	CL7	O2D-CGD-CBD	3.56	117.60	111.27
21	1	404	CL7	C2D-C1D-ND	3.56	112.62	110.23
21	5	404	CL7	C2D-C1D-ND	3.56	112.62	110.23
21	B	616	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	5	420	CL7	CHD-C4C-C3C	-3.56	119.17	124.94
21	3	507	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	7	507	CL7	C3A-C4A-CHB	-3.56	118.42	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	410	CL7	C4D-C3D-CAD	-3.56	105.03	107.42
21	5	410	CL7	C4D-C3D-CAD	-3.56	105.03	107.42
21	C	502	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	c	502	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	b	611	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	1	409	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	3	512	CL7	O2D-CGD-CBD	3.55	117.58	111.27
21	7	512	CL7	O2D-CGD-CBD	3.55	117.58	111.27
21	1	416	CL7	C3A-C4A-CHB	-3.55	118.42	123.70
21	5	404	CL7	CHD-C1D-ND	-3.55	120.50	124.26
23	b	619	8CT	C07-C02-C03	-3.55	117.57	122.73
21	4	412	CL7	C3A-C4A-CHB	-3.55	118.43	123.70
21	c	518	CL7	C1D-ND-C4D	-3.55	103.81	106.33
21	1	415	CL7	CHD-C4C-C3C	-3.55	119.19	124.94
21	5	415	CL7	CHD-C4C-C3C	-3.55	119.19	124.94
21	1	420	CL7	CHD-C4C-C3C	-3.55	119.19	124.94
21	5	409	CL7	C3A-C4A-CHB	-3.55	118.44	123.70
21	3	505	CL7	CHD-C4C-C3C	-3.55	119.19	124.94
21	7	505	CL7	CHD-C4C-C3C	-3.55	119.19	124.94
21	1	418	CL7	CHD-C4C-C3C	-3.55	119.19	124.94
21	4	410	CL7	C3A-C4A-CHB	-3.54	118.44	123.70
21	8	410	CL7	C3A-C4A-CHB	-3.54	118.44	123.70
21	B	611	CL7	CHD-C1D-ND	-3.54	120.51	124.26
21	B	615	CL7	C2D-C1D-ND	3.54	112.61	110.23
21	c	518	CL7	C3A-C4A-CHB	-3.54	118.45	123.70
21	4	415	CL7	CHD-C4C-C3C	-3.54	119.20	124.94
23	B	618	8CT	C07-C02-C03	-3.54	117.59	122.73
21	A	403	CL7	CAC-C3C-C4C	-3.54	119.11	124.68
21	7	509	CL7	C3A-C4A-CHB	-3.54	118.45	123.70
21	1	403	CL7	C3A-C4A-CHB	-3.53	118.46	123.70
21	3	509	CL7	C3A-C4A-CHB	-3.53	118.46	123.70
21	5	403	CL7	C3A-C4A-CHB	-3.53	118.46	123.70
21	5	418	CL7	CHD-C4C-C3C	-3.53	119.22	124.94
21	6	509	CL7	C2D-C1D-ND	3.53	112.60	110.23
21	8	412	CL7	C3A-C4A-CHB	-3.53	118.46	123.70
21	1	419	CL7	CHD-C1D-ND	-3.53	120.52	124.26
21	5	419	CL7	CHD-C1D-ND	-3.53	120.52	124.26
22	a	402	PHO	C2B-C1B-NB	-3.52	107.09	109.53
21	1	410	CL7	C2D-C1D-ND	3.52	112.59	110.23
21	c	518	CL7	C2D-C1D-ND	3.52	112.59	110.23
21	C	518	CL7	C3A-C4A-CHB	-3.52	118.48	123.70
32	3	520	ZEX	C31-C32-C33	-3.52	116.53	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	7	520	ZEX	C31-C32-C33	-3.52	116.53	126.42
21	D	404	CL7	CHD-C1D-ND	-3.52	120.53	124.26
21	d	404	CL7	CHD-C1D-ND	-3.52	120.53	124.26
21	3	502	CL7	C1D-ND-C4D	-3.52	103.84	106.33
21	7	502	CL7	C1D-ND-C4D	-3.52	103.84	106.33
21	a	403	CL7	CAC-C3C-C4C	-3.52	119.14	124.68
21	7	515	CL7	C3A-C4A-CHB	-3.52	118.48	123.70
21	1	404	CL7	CHD-C1D-ND	-3.52	120.53	124.26
21	3	515	CL7	C3A-C4A-CHB	-3.51	118.48	123.70
21	5	416	CL7	C3A-C4A-CHB	-3.51	118.48	123.70
21	2	509	CL7	C2D-C1D-ND	3.51	112.59	110.23
21	8	415	CL7	CHD-C4C-C3C	-3.51	119.25	124.94
32	2	519	ZEX	C18-C5-C6	-3.51	120.59	124.53
32	6	519	ZEX	C18-C5-C6	-3.51	120.59	124.53
21	C	518	CL7	CMA-C3A-C2A	-3.50	107.92	116.10
21	2	507	CL7	C1D-ND-C4D	-3.50	103.85	106.33
21	2	513	CL7	O2D-CGD-CBD	3.50	117.49	111.27
21	6	513	CL7	O2D-CGD-CBD	3.50	117.49	111.27
21	b	608	CL7	C3A-C4A-CHB	-3.50	118.50	123.70
21	4	414	CL7	CHD-C4C-C3C	-3.50	119.26	124.94
21	8	414	CL7	CHD-C4C-C3C	-3.50	119.26	124.94
21	7	501	CL7	C3A-C4A-CHB	-3.50	118.50	123.70
21	C	518	CL7	C2D-C1D-ND	3.50	112.58	110.23
21	8	407	CL7	C2D-C1D-ND	3.50	112.58	110.23
21	3	514	CL7	CHD-C4C-C3C	-3.50	119.27	124.94
21	7	511	CL7	C3A-C4A-CHB	-3.50	118.51	123.70
21	4	407	CL7	CMA-C3A-C2A	-3.50	107.93	116.10
21	8	407	CL7	CMA-C3A-C2A	-3.50	107.93	116.10
21	4	416	CL7	CHD-C4C-C3C	-3.50	119.27	124.94
22	d	408	PHO	C1-C2-C3	-3.50	119.99	126.04
21	B	609	CL7	CHD-C1D-ND	-3.50	120.55	124.26
21	b	610	CL7	CHD-C1D-ND	-3.50	120.55	124.26
21	5	414	CL7	CHD-C4C-C3C	-3.50	119.27	124.94
32	2	525	ZEX	C27-C28-C29	-3.50	120.95	126.23
32	6	524	ZEX	C27-C28-C29	-3.50	120.95	126.23
21	4	409	CL7	C2D-C1D-ND	3.50	112.58	110.23
21	8	409	CL7	C2D-C1D-ND	3.50	112.58	110.23
21	7	514	CL7	CHD-C4C-C3C	-3.49	119.28	124.94
21	B	605	CL7	CHD-C1D-ND	-3.49	120.56	124.26
21	b	616	CL7	C2D-C1D-ND	3.49	112.57	110.23
21	8	416	CL7	CHD-C4C-C3C	-3.49	119.28	124.94
21	3	511	CL7	C3A-C4A-CHB	-3.49	118.52	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	402	PHO	C2B-C1B-NB	-3.49	107.12	109.53
21	B	607	CL7	C3A-C4A-CHB	-3.49	118.52	123.70
21	2	505	CL7	CHD-C4C-C3C	-3.49	119.29	124.94
21	b	606	CL7	CHD-C1D-ND	-3.49	120.56	124.26
21	c	518	CL7	CMA-C3A-C2A	-3.49	107.96	116.10
32	4	420	ZEX	C27-C28-C29	-3.48	120.97	126.23
32	8	420	ZEX	C27-C28-C29	-3.48	120.97	126.23
22	D	408	PHO	C1-C2-C3	-3.48	120.02	126.04
21	5	410	CL7	C2D-C1D-ND	3.48	112.57	110.23
21	6	505	CL7	CHD-C4C-C3C	-3.48	119.30	124.94
21	3	501	CL7	C3A-C4A-CHB	-3.48	118.53	123.70
21	3	505	CL7	C3A-C4A-CHB	-3.48	118.53	123.70
21	7	505	CL7	C3A-C4A-CHB	-3.48	118.53	123.70
21	1	414	CL7	CHD-C4C-C3C	-3.48	119.30	124.94
22	d	408	PHO	O2D-CGD-CBD	3.48	115.40	111.00
22	D	408	PHO	O2D-CGD-CBD	3.48	115.40	111.00
21	c	511	CL7	C2D-C1D-ND	3.47	112.56	110.23
21	4	407	CL7	CHD-C4C-C3C	-3.47	119.31	124.94
21	b	602	CL7	C3A-C4A-CHB	-3.47	118.55	123.70
21	B	608	CL7	O2D-CGD-CBD	3.47	117.43	111.27
21	B	601	CL7	C3A-C4A-CHB	-3.47	118.56	123.70
23	C	516	8CT	C01-C02-C03	-3.47	120.64	124.53
23	c	516	8CT	C01-C02-C03	-3.47	120.64	124.53
21	6	507	CL7	C1D-ND-C4D	-3.47	103.87	106.33
21	b	617	CL7	CHD-C1D-ND	-3.46	120.59	124.26
21	3	514	CL7	C3A-C4A-CHB	-3.46	118.56	123.70
21	4	407	CL7	C2D-C1D-ND	3.46	112.55	110.23
21	A	403	CL7	C3A-C4A-CHB	-3.46	118.57	123.70
21	a	403	CL7	C3A-C4A-CHB	-3.46	118.57	123.70
21	8	407	CL7	CHD-C4C-C3C	-3.46	119.33	124.94
32	2	519	ZEX	C2-C3-C4	3.45	115.03	110.30
21	7	514	CL7	C3A-C4A-CHB	-3.45	118.58	123.70
21	b	609	CL7	O2D-CGD-CBD	3.45	117.40	111.27
21	1	413	CL7	CHD-C4C-C3C	-3.45	119.35	124.94
21	4	417	CL7	CHD-C4C-C3C	-3.45	119.35	124.94
21	5	413	CL7	CHD-C4C-C3C	-3.45	119.35	124.94
21	8	417	CL7	CHD-C4C-C3C	-3.45	119.35	124.94
21	4	414	CL7	CHC-C1C-NC	-3.45	121.29	124.45
32	6	519	ZEX	C2-C3-C4	3.44	115.02	110.30
21	C	511	CL7	CHC-C1C-NC	-3.44	121.29	124.45
21	c	511	CL7	CHC-C1C-NC	-3.44	121.29	124.45
32	8	403	ZEX	C18-C5-C6	-3.44	120.66	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	512	CL7	O2D-CGD-CBD	3.44	117.38	111.27
21	c	512	CL7	O2D-CGD-CBD	3.44	117.38	111.27
21	4	412	CL7	CHD-C4C-C3C	-3.44	119.37	124.94
21	2	511	CL7	CHD-C4C-C3C	-3.44	119.37	124.94
21	3	512	CL7	CHD-C4C-C3C	-3.44	119.37	124.94
21	7	512	CL7	CHD-C4C-C3C	-3.44	119.37	124.94
32	8	419	ZEX	C18-C5-C4	3.44	120.72	114.36
21	8	414	CL7	CHC-C1C-NC	-3.43	121.30	124.45
21	A	401	CL7	C4-C3-C5	3.43	121.05	115.27
21	a	401	CL7	C4-C3-C5	3.43	121.05	115.27
21	C	510	CL7	C2D-C1D-ND	3.43	112.53	110.23
21	1	406	CL7	C2D-C1D-ND	3.43	112.53	110.23
21	c	510	CL7	C2D-C1D-ND	3.43	112.53	110.23
21	5	406	CL7	C2D-C1D-ND	3.43	112.53	110.23
21	1	405	CL7	CHD-C1D-ND	-3.43	120.62	124.26
21	5	405	CL7	CHD-C1D-ND	-3.43	120.62	124.26
21	1	403	CL7	O2D-CGD-CBD	3.43	117.37	111.27
21	1	414	CL7	O2D-CGD-CBD	3.43	117.37	111.27
21	5	403	CL7	O2D-CGD-CBD	3.43	117.37	111.27
21	5	414	CL7	O2D-CGD-CBD	3.43	117.37	111.27
21	B	616	CL7	CHD-C1D-ND	-3.43	120.62	124.26
32	4	419	ZEX	C18-C5-C4	3.43	120.71	114.36
21	3	516	CL7	C2D-C1D-ND	3.43	112.53	110.23
21	B	615	CL7	O2D-CGD-CBD	3.43	117.36	111.27
21	b	616	CL7	O2D-CGD-CBD	3.43	117.36	111.27
21	6	511	CL7	CHD-C4C-C3C	-3.43	119.39	124.94
23	4	402	8CT	C18-C17-C16	-3.42	122.42	127.31
21	B	604	CL7	C2D-C1D-ND	3.42	112.53	110.23
21	b	605	CL7	C2D-C1D-ND	3.42	112.53	110.23
23	B	619	8CT	C01-C02-C07	3.42	120.19	113.62
23	b	620	8CT	C01-C02-C07	3.42	120.19	113.62
21	2	516	CL7	C3A-C4A-CHB	-3.42	118.62	123.70
21	8	412	CL7	CHD-C4C-C3C	-3.42	119.39	124.94
21	5	413	CL7	CHB-C1B-NB	-3.42	120.64	124.26
21	b	612	CL7	O2D-CGD-CBD	3.42	117.35	111.27
23	A	404	8CT	C04-C03-C02	-3.42	117.80	122.61
23	a	404	8CT	C04-C03-C02	-3.42	117.80	122.61
32	4	403	ZEX	C18-C5-C6	-3.42	120.69	124.53
21	B	603	CL7	CHD-C1D-ND	-3.42	120.64	124.26
21	b	604	CL7	CHD-C1D-ND	-3.42	120.64	124.26
21	c	508	CL7	C2D-C1D-ND	3.42	112.52	110.23
21	3	505	CL7	C2D-C1D-ND	3.42	112.52	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	507	CL7	CHD-C4C-C3C	-3.41	119.40	124.94
21	b	623	CL7	CHD-C1D-ND	-3.41	120.64	124.26
21	B	615	CL7	C3A-C4A-CHB	-3.41	118.63	123.70
21	b	616	CL7	C3A-C4A-CHB	-3.41	118.63	123.70
32	7	520	ZEX	C11-C12-C13	-3.41	116.83	126.42
21	B	622	CL7	CHD-C1D-ND	-3.41	120.64	124.26
21	6	515	CL7	C3A-C4A-CHB	-3.41	118.64	123.70
21	1	415	CL7	C3A-C4A-CHB	-3.41	118.65	123.70
21	5	415	CL7	C3A-C4A-CHB	-3.41	118.65	123.70
32	3	520	ZEX	C11-C12-C13	-3.41	116.85	126.42
23	8	402	8CT	C18-C17-C16	-3.41	122.45	127.31
21	4	405	CL7	CHD-C1D-ND	-3.41	120.65	124.26
21	8	405	CL7	CHD-C1D-ND	-3.41	120.65	124.26
21	B	611	CL7	O2D-CGD-CBD	3.40	117.32	111.27
21	6	513	CL7	C2D-C1D-ND	3.40	112.51	110.23
21	7	516	CL7	C2D-C1D-ND	3.40	112.51	110.23
21	6	516	CL7	C3A-C4A-CHB	-3.40	118.65	123.70
21	b	613	CL7	C3A-C4A-CHB	-3.40	118.66	123.70
21	1	417	CL7	O2D-CGD-CBD	3.40	117.31	111.27
21	C	512	CL7	C3A-C4A-CHB	-3.40	118.66	123.70
21	c	512	CL7	C3A-C4A-CHB	-3.40	118.66	123.70
21	2	513	CL7	C2D-C1D-ND	3.40	112.51	110.23
21	c	507	CL7	CHD-C4C-C3C	-3.40	119.43	124.94
21	3	502	CL7	CHD-C1D-ND	-3.40	120.66	124.26
21	8	409	CL7	CHB-C1B-NB	-3.40	120.66	124.26
21	7	505	CL7	C2D-C1D-ND	3.40	112.51	110.23
21	1	402	CL7	CHD-C4C-C3C	-3.39	119.44	124.94
23	B	627	8CT	C15-C16-C17	3.39	124.15	118.94
23	b	601	8CT	C15-C16-C17	3.39	124.15	118.94
21	B	603	CL7	C4D-C3D-CAD	-3.39	105.14	107.42
21	b	604	CL7	C4D-C3D-CAD	-3.39	105.14	107.42
23	B	619	8CT	C07-C02-C03	-3.39	117.81	122.73
23	b	620	8CT	C07-C02-C03	-3.39	117.81	122.73
21	1	413	CL7	CHB-C1B-NB	-3.39	120.67	124.26
21	a	405	CL7	C3A-C4A-CHB	-3.39	118.68	123.70
23	B	617	8CT	C11-C10-C03	-3.38	117.70	127.20
23	b	618	8CT	C11-C10-C03	-3.38	117.70	127.20
21	A	406	CL7	C3A-C4A-CHB	-3.38	118.68	123.70
21	D	405	CL7	O2D-CGD-CBD	3.38	117.28	111.27
21	8	413	CL7	CHD-C4C-C3C	-3.38	119.46	124.94
21	4	406	CL7	C4D-C3D-CAD	-3.38	105.15	107.42
21	C	508	CL7	C2D-C1D-ND	3.38	112.50	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	402	CL7	CHD-C4C-C3C	-3.38	119.46	124.94
21	5	417	CL7	O2D-CGD-CBD	3.38	117.27	111.27
21	B	612	CL7	C3A-C4A-CHB	-3.38	118.69	123.70
23	b	601	8CT	C14-C15-C16	-3.37	116.94	126.42
32	3	522	ZEX	C19-C9-C10	-3.37	118.20	122.92
21	B	603	CL7	C2D-C1D-ND	3.37	112.49	110.23
21	b	604	CL7	C2D-C1D-ND	3.37	112.49	110.23
21	D	404	CL7	CAA-CBA-CGA	-3.37	103.40	113.25
21	2	515	CL7	C3A-C4A-CHB	-3.37	118.70	123.70
21	3	517	CL7	O2D-CGD-CBD	3.37	117.26	111.27
21	7	517	CL7	O2D-CGD-CBD	3.37	117.26	111.27
21	B	612	CL7	CHC-C1C-NC	-3.37	121.36	124.45
21	b	613	CL7	CHC-C1C-NC	-3.37	121.36	124.45
21	6	505	CL7	C2D-C1D-ND	3.37	112.49	110.23
21	C	504	CL7	CHD-C4C-C3C	-3.37	119.48	124.94
21	3	516	CL7	C3A-C4A-CHB	-3.37	118.70	123.70
21	4	413	CL7	CHD-C4C-C3C	-3.36	119.48	124.94
23	B	627	8CT	C14-C15-C16	-3.36	116.97	126.42
21	4	404	CL7	C2D-C1D-ND	3.36	112.49	110.23
21	3	514	CL7	C4C-C3C-C2C	-3.36	102.75	107.13
21	7	514	CL7	C4C-C3C-C2C	-3.36	102.75	107.13
21	c	504	CL7	CHD-C4C-C3C	-3.36	119.49	124.94
21	4	414	CL7	O2D-CGD-CBD	3.36	117.24	111.27
21	3	503	CL7	C7-C6-C5	-3.36	104.24	113.36
21	7	503	CL7	C7-C6-C5	-3.36	104.24	113.36
21	7	502	CL7	CHD-C1D-ND	-3.36	120.70	124.26
32	1	422	ZEX	C18-C5-C4	3.36	120.57	114.36
32	5	422	ZEX	C18-C5-C4	3.36	120.57	114.36
32	7	522	ZEX	C19-C9-C10	-3.35	118.22	122.92
21	7	516	CL7	C3A-C4A-CHB	-3.35	118.72	123.70
21	B	610	CL7	CHD-C4C-C3C	-3.35	119.50	124.94
21	d	404	CL7	CAA-CBA-CGA	-3.35	103.46	113.25
21	4	409	CL7	CHB-C1B-NB	-3.35	120.71	124.26
21	d	405	CL7	O2D-CGD-CBD	3.35	117.22	111.27
21	1	406	CL7	C7-C6-C5	-3.35	104.26	113.36
21	5	406	CL7	C7-C6-C5	-3.35	104.26	113.36
21	c	509	CL7	CHD-C1D-ND	-3.35	120.71	124.26
21	B	613	CL7	CHD-C4C-C3C	-3.35	119.51	124.94
21	b	614	CL7	CHD-C4C-C3C	-3.35	119.51	124.94
21	c	508	CL7	C7-C6-C5	-3.35	104.27	113.36
21	8	414	CL7	O2D-CGD-CBD	3.34	117.21	111.27
21	4	408	CL7	CHD-C4C-C3C	-3.34	119.52	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	c	513	CL7	CHC-C1C-NC	-3.34	121.38	124.45
23	C	515	8CT	C01-C02-C07	3.34	120.03	113.62
21	2	509	CL7	C3A-C4A-CHB	-3.34	118.74	123.70
21	B	612	CL7	CHD-C4C-C3C	-3.34	119.52	124.94
32	2	521	ZEX	C18-C5-C6	-3.34	120.78	124.53
21	1	407	CL7	CHD-C1D-ND	-3.34	120.72	124.26
21	5	407	CL7	CHD-C1D-ND	-3.34	120.72	124.26
32	6	520	ZEX	C18-C5-C6	-3.34	120.78	124.53
21	C	509	CL7	CHD-C1D-ND	-3.34	120.72	124.26
21	6	513	CL7	CHD-C1D-ND	-3.34	120.72	124.26
23	c	515	8CT	C35-C30-C29	-3.34	108.48	112.70
21	5	406	CL7	CHD-C4C-C3C	-3.34	119.53	124.94
21	2	505	CL7	C2D-C1D-ND	3.34	112.47	110.23
21	8	405	CL7	C3A-C4A-CHB	-3.33	118.75	123.70
21	b	613	CL7	CHD-C4C-C3C	-3.33	119.54	124.94
21	A	406	CL7	CHD-C4C-C3C	-3.33	119.54	124.94
21	8	404	CL7	C2D-C1D-ND	3.33	112.47	110.23
21	B	611	CL7	C3A-C4A-CHB	-3.33	118.75	123.70
21	b	612	CL7	C3A-C4A-CHB	-3.33	118.75	123.70
21	8	406	CL7	CHD-C1D-ND	-3.33	120.73	124.26
21	6	509	CL7	C3A-C4A-CHB	-3.33	118.76	123.70
21	1	406	CL7	CHD-C4C-C3C	-3.33	119.54	124.94
21	C	508	CL7	C7-C6-C5	-3.33	104.31	113.36
21	b	611	CL7	CHD-C4C-C3C	-3.33	119.54	124.94
23	D	406	8CT	C01-C02-C07	3.33	120.01	113.62
23	d	406	8CT	C01-C02-C07	3.33	120.01	113.62
21	C	513	CL7	CHC-C1C-NC	-3.33	121.40	124.45
31	f	101	HEM	CHB-C1B-NB	3.33	128.48	124.37
21	C	503	CL7	CHD-C4C-C3C	-3.33	119.55	124.94
32	7	520	ZEX	C18-C5-C4	3.33	120.52	114.36
21	5	416	CL7	CHD-C1D-ND	-3.32	120.74	124.26
21	3	507	CL7	CHC-C1C-NC	-3.32	121.40	124.45
21	1	413	CL7	CMA-C3A-C2A	-3.32	108.35	116.10
21	c	507	CL7	CHD-C1D-ND	-3.32	120.74	124.26
21	1	415	CL7	O2D-CGD-CBD	3.32	117.17	111.27
21	C	507	CL7	CHD-C1D-ND	-3.32	120.74	124.26
21	c	514	CL7	CHD-C1D-ND	-3.32	120.74	124.26
21	8	416	CL7	C3A-C4A-CHB	-3.32	118.77	123.70
21	5	413	CL7	CMA-C3A-C2A	-3.32	108.35	116.10
21	8	408	CL7	CHD-C4C-C3C	-3.32	119.56	124.94
23	C	515	8CT	C35-C30-C29	-3.32	108.51	112.70
21	B	610	CL7	C7-C6-C5	-3.32	104.35	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	611	CL7	C7-C6-C5	-3.32	104.35	113.36
21	7	518	CL7	CHD-C1D-ND	-3.32	120.75	124.26
21	8	406	CL7	C4D-C3D-CAD	-3.32	105.19	107.42
21	8	414	CL7	CHD-C1D-ND	-3.32	120.75	124.26
21	4	405	CL7	C3A-C4A-CHB	-3.31	118.78	123.70
21	a	405	CL7	CHD-C4C-C3C	-3.31	119.57	124.94
21	6	514	CL7	O2D-CGD-CBD	3.31	117.16	111.27
21	5	403	CL7	CHD-C4C-C3C	-3.31	119.57	124.94
32	3	520	ZEX	C18-C5-C4	3.31	120.49	114.36
21	4	406	CL7	CHD-C1D-ND	-3.31	120.75	124.26
21	B	608	CL7	C3A-C4A-CHB	-3.31	118.79	123.70
21	b	609	CL7	C3A-C4A-CHB	-3.31	118.79	123.70
21	1	403	CL7	CHD-C4C-C3C	-3.31	119.57	124.94
21	3	501	CL7	CHD-C4C-C3C	-3.31	119.57	124.94
21	c	503	CL7	CHD-C4C-C3C	-3.31	119.58	124.94
21	5	419	CL7	C3A-C4A-CHB	-3.31	118.79	123.70
21	B	602	CL7	CHD-C1D-ND	-3.31	120.75	124.26
21	b	603	CL7	CHD-C1D-ND	-3.31	120.75	124.26
30	d	407	PL9	C7-C3-C4	3.31	119.56	116.88
21	2	516	CL7	C7-C6-C5	-3.31	104.38	113.36
23	D	406	8CT	C11-C10-C03	-3.31	117.92	127.20
23	d	406	8CT	C11-C10-C03	-3.31	117.92	127.20
21	2	504	CL7	O2D-CGD-CBD	3.30	117.14	111.27
21	6	504	CL7	O2D-CGD-CBD	3.30	117.14	111.27
21	6	516	CL7	C7-C6-C5	-3.30	104.39	113.36
21	2	501	CL7	CHC-C1C-NC	-3.30	121.42	124.45
21	6	501	CL7	CHC-C1C-NC	-3.30	121.42	124.45
21	4	416	CL7	C3A-C4A-CHB	-3.30	118.80	123.70
23	c	515	8CT	C01-C02-C07	3.30	119.96	113.62
21	1	416	CL7	CHD-C1D-ND	-3.30	120.76	124.26
21	3	504	CL7	CHD-C1D-ND	-3.30	120.76	124.26
21	4	406	CL7	CHD-C4C-C3C	-3.30	119.59	124.94
21	8	406	CL7	CHD-C4C-C3C	-3.30	119.59	124.94
21	5	415	CL7	O2D-CGD-CBD	3.30	117.13	111.27
21	B	605	CL7	C3A-C4A-CHB	-3.30	118.81	123.70
21	b	606	CL7	C3A-C4A-CHB	-3.30	118.81	123.70
32	1	422	ZEX	C31-C30-C29	-3.30	122.60	127.31
21	4	417	CL7	CMB-C2B-C1B	3.30	130.39	125.37
21	8	417	CL7	CMB-C2B-C1B	3.30	130.39	125.37
31	F	101	HEM	CHB-C1B-NB	3.30	128.44	124.37
21	2	505	CL7	CHB-C1B-NB	-3.30	120.77	124.26
21	7	504	CL7	CHD-C1D-ND	-3.30	120.77	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	404	CL7	CHD-C4C-C3C	-3.30	119.60	124.94
21	5	404	CL7	CHD-C4C-C3C	-3.30	119.60	124.94
21	2	514	CL7	O2D-CGD-CBD	3.29	117.12	111.27
21	7	513	CL7	CHD-C4C-C3C	-3.29	119.60	124.94
21	B	612	CL7	CMD-C2D-C1D	3.29	130.39	125.37
21	b	613	CL7	CMD-C2D-C1D	3.29	130.39	125.37
23	A	404	8CT	C07-C02-C03	-3.29	117.95	122.73
23	a	404	8CT	C07-C02-C03	-3.29	117.95	122.73
30	D	407	PL9	C7-C3-C4	3.29	119.55	116.88
21	3	517	CL7	CHD-C1D-ND	-3.29	120.77	124.26
21	7	501	CL7	CHD-C4C-C3C	-3.29	119.61	124.94
21	7	515	CL7	CHD-C4C-C3C	-3.29	119.61	124.94
21	3	518	CL7	CHD-C1D-ND	-3.29	120.78	124.26
21	3	515	CL7	CHD-C4C-C3C	-3.29	119.61	124.94
21	2	508	CL7	C3A-C4A-CHB	-3.29	118.82	123.70
22	d	408	PHO	O2D-CGD-O1D	-3.29	117.41	123.84
21	1	419	CL7	C3A-C4A-CHB	-3.28	118.83	123.70
21	3	505	CL7	C4C-C3C-C2C	-3.28	102.85	107.13
21	7	505	CL7	C4C-C3C-C2C	-3.28	102.85	107.13
22	D	408	PHO	O2D-CGD-O1D	-3.28	117.42	123.84
21	5	405	CL7	C3A-C4A-CHB	-3.28	118.83	123.70
21	4	407	CL7	CHC-C1C-NC	-3.28	121.44	124.45
21	A	406	CL7	C7-C6-C5	-3.28	104.44	113.36
21	a	405	CL7	C7-C6-C5	-3.28	104.44	113.36
21	6	505	CL7	CHB-C1B-NB	-3.28	120.78	124.26
21	2	513	CL7	CHD-C1D-ND	-3.28	120.78	124.26
21	4	414	CL7	CHD-C1D-ND	-3.28	120.78	124.26
21	C	510	CL7	CHC-C1C-NC	-3.28	121.44	124.45
21	c	510	CL7	CHC-C1C-NC	-3.28	121.44	124.45
21	4	407	CL7	C4D-C3D-CAD	-3.28	105.21	107.42
21	8	407	CL7	C4D-C3D-CAD	-3.28	105.21	107.42
21	c	510	CL7	C7-C6-C5	-3.28	104.45	113.36
32	5	422	ZEX	C31-C30-C29	-3.28	122.63	127.31
22	d	408	PHO	C4-C3-C5	3.28	120.79	115.27
21	C	510	CL7	C7-C6-C5	-3.28	104.46	113.36
21	2	518	CL7	CHD-C1D-ND	-3.28	120.79	124.26
21	c	512	CL7	CHD-C1D-ND	-3.28	120.79	124.26
21	6	518	CL7	CHD-C1D-ND	-3.28	120.79	124.26
21	B	601	CL7	O2D-CGD-CBD	3.28	117.09	111.27
23	B	627	8CT	C35-C30-C29	3.28	116.84	112.70
23	b	601	8CT	C35-C30-C29	3.28	116.84	112.70
21	3	513	CL7	CHD-C4C-C3C	-3.28	119.63	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	7	522	ZEX	C35-C15-C14	-3.28	116.76	123.47
21	C	513	CL7	CHD-C4C-C3C	-3.28	119.63	124.94
21	c	513	CL7	CHD-C4C-C3C	-3.28	119.63	124.94
21	b	602	CL7	O2D-CGD-CBD	3.27	117.09	111.27
21	2	508	CL7	O2D-CGD-CBD	3.27	117.08	111.27
21	6	508	CL7	O2D-CGD-CBD	3.27	117.08	111.27
21	2	514	CL7	C3A-C4A-CHB	-3.27	118.84	123.70
21	C	512	CL7	CHD-C4C-C3C	-3.27	119.63	124.94
21	3	502	CL7	O2D-CGD-CBD	3.27	117.08	111.27
21	7	502	CL7	O2D-CGD-CBD	3.27	117.08	111.27
32	4	418	ZEX	C39-C29-C30	-3.27	118.34	122.92
32	3	522	ZEX	C35-C15-C14	-3.27	116.78	123.47
21	2	504	CL7	CHD-C1D-ND	-3.27	120.80	124.26
21	6	504	CL7	CHD-C1D-ND	-3.27	120.80	124.26
32	8	418	ZEX	C39-C29-C30	-3.27	118.35	122.92
21	C	514	CL7	CHD-C1D-ND	-3.27	120.80	124.26
21	b	602	CL7	CHD-C1D-ND	-3.27	120.80	124.26
21	C	510	CL7	CHD-C4C-C3C	-3.27	119.64	124.94
21	c	510	CL7	CHD-C4C-C3C	-3.27	119.64	124.94
21	B	605	CL7	CMB-C2B-C1B	3.27	130.34	125.37
21	b	606	CL7	CMB-C2B-C1B	3.27	130.34	125.37
22	D	408	PHO	C4-C3-C5	3.27	120.77	115.27
21	2	514	CL7	CHD-C1D-ND	-3.26	120.80	124.26
21	6	514	CL7	CHD-C1D-ND	-3.26	120.80	124.26
21	1	405	CL7	C3A-C4A-CHB	-3.26	118.86	123.70
21	6	508	CL7	C3A-C4A-CHB	-3.26	118.86	123.70
21	D	402	CL7	O2D-CGD-CBD	3.26	117.06	111.27
21	d	402	CL7	O2D-CGD-CBD	3.26	117.06	111.27
21	C	512	CL7	CHD-C1D-ND	-3.26	120.80	124.26
21	7	507	CL7	CHC-C1C-NC	-3.26	121.46	124.45
23	C	515	8CT	C11-C10-C03	-3.26	118.04	127.20
23	c	515	8CT	C11-C10-C03	-3.26	118.04	127.20
21	1	410	CL7	CHD-C1D-ND	-3.26	120.81	124.26
21	2	503	CL7	C4D-C3D-CAD	-3.26	105.23	107.42
21	6	503	CL7	C4D-C3D-CAD	-3.26	105.23	107.42
21	c	506	CL7	C3A-C4A-CHB	-3.26	118.86	123.70
32	2	520	ZEX	C27-C28-C29	-3.26	121.31	126.23
32	3	525	ZEX	C27-C28-C29	-3.26	121.31	126.23
21	7	508	CL7	C3A-C4A-CHB	-3.26	118.86	123.70
21	7	517	CL7	CHD-C1D-ND	-3.26	120.81	124.26
21	3	506	CL7	C2D-C1D-ND	3.25	112.41	110.23
21	c	512	CL7	CHD-C4C-C3C	-3.25	119.67	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	506	CL7	C3A-C4A-CHB	-3.25	118.88	123.70
21	D	405	CL7	CHD-C4C-C3C	-3.25	119.67	124.94
21	d	405	CL7	CHD-C4C-C3C	-3.25	119.67	124.94
21	B	622	CL7	CHD-C4C-C3C	-3.25	119.67	124.94
21	b	623	CL7	CHD-C4C-C3C	-3.25	119.67	124.94
21	c	507	CL7	CHC-C1C-NC	-3.25	121.47	124.45
21	3	504	CL7	CHD-C4C-C3C	-3.25	119.67	124.94
21	7	504	CL7	CHD-C4C-C3C	-3.25	119.67	124.94
21	8	407	CL7	CHC-C1C-NC	-3.25	121.47	124.45
21	6	514	CL7	C3A-C4A-CHB	-3.25	118.88	123.70
21	b	606	CL7	CHD-C4C-C3C	-3.25	119.68	124.94
32	2	521	ZEX	C31-C30-C29	-3.25	122.68	127.31
32	6	520	ZEX	C31-C30-C29	-3.25	122.68	127.31
22	D	408	PHO	CMB-C2B-C3B	3.24	130.75	124.68
21	C	514	CL7	O2D-CGD-CBD	3.24	117.03	111.27
21	C	506	CL7	O2D-CGD-CBD	3.24	117.03	111.27
21	c	506	CL7	O2D-CGD-CBD	3.24	117.03	111.27
21	B	601	CL7	CHD-C1D-ND	-3.24	120.83	124.26
22	d	408	PHO	CMB-C2B-C3B	3.24	130.74	124.68
21	C	504	CL7	CHD-C1D-ND	-3.24	120.83	124.26
21	c	504	CL7	CHD-C1D-ND	-3.24	120.83	124.26
21	C	505	CL7	CHD-C4C-C3C	-3.24	119.69	124.94
21	c	505	CL7	CHD-C4C-C3C	-3.24	119.69	124.94
21	C	511	CL7	C3A-C4A-CHB	-3.24	118.90	123.70
21	3	508	CL7	C3A-C4A-CHB	-3.24	118.90	123.70
21	c	511	CL7	C3A-C4A-CHB	-3.24	118.90	123.70
21	B	607	CL7	CHD-C4C-C3C	-3.24	119.69	124.94
21	b	608	CL7	CHD-C4C-C3C	-3.24	119.69	124.94
21	c	514	CL7	O2D-CGD-CBD	3.24	117.02	111.27
21	5	410	CL7	CHD-C1D-ND	-3.24	120.83	124.26
21	1	404	CL7	C3A-C4A-CHB	-3.24	118.90	123.70
21	5	404	CL7	C3A-C4A-CHB	-3.24	118.90	123.70
21	7	506	CL7	C2D-C1D-ND	3.23	112.40	110.23
21	4	414	CL7	C3A-C4A-CHB	-3.23	118.90	123.70
21	8	414	CL7	C3A-C4A-CHB	-3.23	118.90	123.70
21	a	401	CL7	CHD-C4C-C3C	-3.23	119.70	124.94
21	6	506	CL7	CHD-C1D-ND	-3.23	120.84	124.26
21	a	405	CL7	CAA-CBA-CGA	-3.23	103.81	113.25
21	1	418	CL7	CHC-C1C-NC	-3.23	121.48	124.45
21	8	412	CL7	CHC-C1C-NC	-3.23	121.49	124.45
21	1	411	CL7	O2D-CGD-CBD	3.23	117.00	111.27
21	4	404	CL7	O2D-CGD-CBD	3.23	117.00	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	411	CL7	O2D-CGD-CBD	3.23	117.00	111.27
21	8	404	CL7	O2D-CGD-CBD	3.23	117.00	111.27
21	4	411	CL7	CHC-C1C-NC	-3.23	121.49	124.45
32	3	522	ZEX	C1-C2-C3	-3.23	106.36	113.64
32	7	522	ZEX	C1-C2-C3	-3.23	106.36	113.64
21	C	507	CL7	CHC-C1C-NC	-3.23	121.49	124.45
21	5	418	CL7	CHC-C1C-NC	-3.23	121.49	124.45
21	B	605	CL7	CHD-C4C-C3C	-3.23	119.71	124.94
21	A	406	CL7	CAA-CBA-CGA	-3.22	103.83	113.25
21	2	511	CL7	CHD-C1D-ND	-3.22	120.84	124.26
21	4	406	CL7	O2D-CGD-CBD	3.22	117.00	111.27
21	b	611	CL7	CHD-C1D-ND	-3.22	120.84	124.26
21	3	518	CL7	CHD-C4C-C3C	-3.22	119.72	124.94
21	7	518	CL7	CHD-C4C-C3C	-3.22	119.72	124.94
21	A	401	CL7	CAA-CBA-CGA	-3.22	103.84	113.25
21	a	401	CL7	CAA-CBA-CGA	-3.22	103.84	113.25
21	1	413	CL7	C3A-C4A-CHB	-3.22	118.92	123.70
21	5	413	CL7	C3A-C4A-CHB	-3.22	118.92	123.70
21	6	511	CL7	CHD-C1D-ND	-3.22	120.85	124.26
23	B	617	8CT	C14-C15-C16	-3.21	117.39	126.42
23	b	618	8CT	C14-C15-C16	-3.21	117.39	126.42
21	2	518	CL7	CHD-C4C-C3C	-3.21	119.73	124.94
21	6	518	CL7	CHD-C4C-C3C	-3.21	119.73	124.94
21	8	411	CL7	CHC-C1C-NC	-3.21	121.50	124.45
21	2	515	CL7	O2D-CGD-CBD	3.21	116.97	111.27
21	6	515	CL7	O2D-CGD-CBD	3.21	116.97	111.27
21	1	414	CL7	C4C-C3C-C2C	-3.21	102.94	107.13
21	5	414	CL7	C4C-C3C-C2C	-3.21	102.94	107.13
21	A	401	CL7	CHD-C4C-C3C	-3.21	119.74	124.94
21	4	409	CL7	CMB-C2B-C1B	3.21	130.26	125.37
21	2	501	CL7	CHD-C1D-ND	-3.21	120.86	124.26
21	6	501	CL7	CHD-C1D-ND	-3.21	120.86	124.26
21	1	411	CL7	CHD-C4C-C3C	-3.21	119.74	124.94
21	4	412	CL7	CAA-CBA-CGA	-3.21	103.88	113.25
21	8	412	CL7	CAA-CBA-CGA	-3.21	103.88	113.25
21	8	406	CL7	O2D-CGD-CBD	3.21	116.97	111.27
21	4	412	CL7	CHC-C1C-NC	-3.21	121.51	124.45
21	2	518	CL7	C7-C6-C5	-3.20	104.66	113.36
21	3	510	CL7	CHD-C4C-C3C	-3.20	119.75	124.94
21	7	510	CL7	CHD-C4C-C3C	-3.20	119.75	124.94
21	5	412	CL7	C3A-C4A-CHB	-3.20	118.95	123.70
21	2	510	CL7	C7-C6-C5	-3.20	104.66	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	510	CL7	C7-C6-C5	-3.20	104.66	113.36
21	2	506	CL7	CHD-C1D-ND	-3.20	120.87	124.26
21	2	510	CL7	CHD-C4C-C3C	-3.20	119.75	124.94
21	6	510	CL7	CHD-C4C-C3C	-3.20	119.75	124.94
21	B	615	CL7	CHB-C1B-NB	-3.20	120.87	124.26
21	C	509	CL7	C3A-C4A-CHB	-3.20	118.95	123.70
21	c	509	CL7	C3A-C4A-CHB	-3.20	118.95	123.70
21	5	411	CL7	CHD-C4C-C3C	-3.20	119.76	124.94
21	6	512	CL7	C3A-C4A-CHB	-3.19	118.96	123.70
21	8	409	CL7	CMB-C2B-C1B	3.19	130.23	125.37
21	3	517	CL7	CHD-C4C-C3C	-3.19	119.76	124.94
21	6	518	CL7	C7-C6-C5	-3.19	104.69	113.36
21	1	402	CL7	CHC-C1C-NC	-3.19	121.52	124.45
21	5	402	CL7	CHC-C1C-NC	-3.19	121.52	124.45
21	1	412	CL7	C3A-C4A-CHB	-3.19	118.96	123.70
21	C	509	CL7	CHD-C4C-C3C	-3.19	119.77	124.94
21	c	509	CL7	CHD-C4C-C3C	-3.19	119.77	124.94
21	2	518	CL7	O2D-CGD-CBD	3.19	116.94	111.27
21	6	518	CL7	O2D-CGD-CBD	3.19	116.94	111.27
21	1	408	CL7	C7-C6-C5	-3.19	104.69	113.36
21	5	408	CL7	C7-C6-C5	-3.19	104.69	113.36
21	B	609	CL7	C2D-C1D-ND	3.19	112.37	110.23
21	b	607	CL7	C2D-C1D-ND	3.19	112.37	110.23
21	b	610	CL7	C2D-C1D-ND	3.19	112.37	110.23
21	1	408	CL7	CAA-CBA-CGA	-3.19	103.94	113.25
21	5	408	CL7	CAA-CBA-CGA	-3.19	103.94	113.25
21	8	409	CL7	CHC-C1C-NC	-3.19	121.53	124.45
21	7	517	CL7	CHD-C4C-C3C	-3.19	119.77	124.94
21	B	610	CL7	CHD-C1D-ND	-3.19	120.88	124.26
21	B	613	CL7	CHD-C1D-ND	-3.19	120.88	124.26
21	b	614	CL7	CHD-C1D-ND	-3.19	120.88	124.26
21	b	608	CL7	C7-C6-C5	-3.19	104.71	113.36
21	B	616	CL7	CHD-C4C-C3C	-3.18	119.78	124.94
21	b	617	CL7	CHD-C4C-C3C	-3.18	119.78	124.94
32	3	522	ZEX	C8-C7-C6	-3.18	118.26	127.20
23	B	627	8CT	C01-C02-C07	3.18	119.73	113.62
23	b	601	8CT	C01-C02-C07	3.18	119.73	113.62
21	b	612	CL7	C7-C6-C5	-3.18	104.72	113.36
21	4	409	CL7	CHC-C1C-NC	-3.18	121.53	124.45
21	2	512	CL7	C3A-C4A-CHB	-3.18	118.98	123.70
21	C	511	CL7	CHD-C4C-C3C	-3.18	119.78	124.94
21	c	511	CL7	CHD-C4C-C3C	-3.18	119.78	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	509	CL7	CHD-C1D-ND	-3.18	120.89	124.26
21	2	517	CL7	CHD-C4C-C3C	-3.18	119.79	124.94
21	B	607	CL7	C7-C6-C5	-3.18	104.73	113.36
21	2	502	CL7	CHD-C4C-C3C	-3.18	119.79	124.94
21	3	507	CL7	CHD-C4C-C3C	-3.18	119.79	124.94
21	6	502	CL7	CHD-C4C-C3C	-3.18	119.79	124.94
21	7	507	CL7	CHD-C4C-C3C	-3.18	119.79	124.94
21	B	611	CL7	C7-C6-C5	-3.18	104.73	113.36
21	B	606	CL7	C2D-C1D-ND	3.17	112.36	110.23
21	b	616	CL7	CHB-C1B-NB	-3.17	120.90	124.26
32	7	522	ZEX	C8-C7-C6	-3.17	118.30	127.20
21	3	508	CL7	C7-C6-C5	-3.17	104.75	113.36
21	2	501	CL7	CHD-C4C-C3C	-3.17	119.81	124.94
21	6	517	CL7	CHD-C4C-C3C	-3.17	119.81	124.94
23	B	617	8CT	C18-C19-C20	-3.16	116.99	123.47
23	b	618	8CT	C18-C19-C20	-3.16	116.99	123.47
21	7	508	CL7	C7-C6-C5	-3.16	104.77	113.36
21	2	503	CL7	CHD-C1D-ND	-3.16	120.91	124.26
21	6	503	CL7	CHD-C1D-ND	-3.16	120.91	124.26
23	c	519	8CT	C24-C23-C21	-3.16	117.53	126.42
21	B	606	CL7	CHD-C4C-C3C	-3.16	119.82	124.94
21	b	607	CL7	CHD-C4C-C3C	-3.16	119.82	124.94
21	6	506	CL7	C7-C6-C5	-3.16	104.78	113.36
21	c	503	CL7	CHD-C1D-ND	-3.16	120.91	124.26
23	C	519	8CT	C24-C23-C21	-3.15	117.55	126.42
21	6	515	CL7	CHD-C4C-C3C	-3.15	119.83	124.94
21	3	513	CL7	O2D-CGD-CBD	3.15	116.87	111.27
21	7	513	CL7	O2D-CGD-CBD	3.15	116.87	111.27
32	4	419	ZEX	C3-C4-C5	-3.15	105.58	111.85
21	2	515	CL7	CMB-C2B-C1B	3.15	130.17	125.37
21	6	515	CL7	CMB-C2B-C1B	3.15	130.17	125.37
21	2	506	CL7	C7-C6-C5	-3.15	104.80	113.36
21	3	516	CL7	O2D-CGD-CBD	3.15	116.87	111.27
21	1	402	CL7	CHD-C1D-ND	-3.15	120.92	124.26
21	5	402	CL7	CHD-C1D-ND	-3.15	120.92	124.26
21	6	501	CL7	CHD-C4C-C3C	-3.15	119.83	124.94
21	3	503	CL7	CMB-C2B-C1B	3.15	130.16	125.37
21	2	517	CL7	CHD-C1D-ND	-3.15	120.92	124.26
21	6	517	CL7	CHD-C1D-ND	-3.15	120.92	124.26
21	1	403	CL7	CHB-C1B-NB	-3.14	120.93	124.26
21	7	516	CL7	O2D-CGD-CBD	3.14	116.85	111.27
21	C	503	CL7	CHD-C1D-ND	-3.14	120.93	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	403	CL7	CHB-C1B-NB	-3.14	120.93	124.26
21	2	515	CL7	CHD-C4C-C3C	-3.14	119.85	124.94
32	8	419	ZEX	C3-C4-C5	-3.14	105.61	111.85
21	2	509	CL7	CHD-C1D-ND	-3.14	120.94	124.26
21	1	415	CL7	CHD-C1D-ND	-3.13	120.94	124.26
21	6	502	CL7	CHD-C1D-ND	-3.13	120.94	124.26
21	B	602	CL7	CHD-C4C-C3C	-3.13	119.86	124.94
21	b	603	CL7	CHD-C4C-C3C	-3.13	119.86	124.94
21	3	501	CL7	O2D-CGD-CBD	3.13	116.83	111.27
21	7	501	CL7	O2D-CGD-CBD	3.13	116.83	111.27
21	3	518	CL7	O2D-CGD-CBD	3.13	116.83	111.27
21	7	518	CL7	O2D-CGD-CBD	3.13	116.83	111.27
21	5	415	CL7	CHD-C1D-ND	-3.13	120.94	124.26
21	2	502	CL7	CHD-C1D-ND	-3.13	120.95	124.26
21	C	518	CL7	CHD-C1D-ND	-3.13	120.95	124.26
32	2	520	ZEX	C35-C15-C14	-3.13	117.07	123.47
23	B	618	8CT	C27-C26-C28	3.13	123.00	118.08
23	b	619	8CT	C27-C26-C28	3.13	123.00	118.08
21	2	509	CL7	CHC-C1C-NC	-3.12	121.58	124.45
21	7	503	CL7	CMB-C2B-C1B	3.12	130.13	125.37
21	4	410	CL7	CHD-C4C-C3C	-3.12	119.88	124.94
21	8	406	CL7	C7-C6-C5	-3.12	104.88	113.36
21	B	604	CL7	C3A-C4A-CHB	-3.12	119.07	123.70
21	4	410	CL7	O2D-CGD-CBD	3.12	116.81	111.27
21	1	403	CL7	CHC-C1C-NC	-3.12	121.59	124.45
21	4	406	CL7	C7-C6-C5	-3.12	104.89	113.36
21	c	508	CL7	CHD-C4C-C3C	-3.12	119.89	124.94
21	6	509	CL7	CHC-C1C-NC	-3.12	121.59	124.45
21	4	404	CL7	CHD-C1D-ND	-3.12	120.96	124.26
21	7	508	CL7	CHD-C1D-ND	-3.12	120.96	124.26
32	3	519	ZEX	C27-C26-C25	-3.11	117.81	122.84
21	c	518	CL7	CHD-C1D-ND	-3.11	120.96	124.26
21	8	408	CL7	CHD-C1D-ND	-3.11	120.96	124.26
32	3	525	ZEX	C35-C15-C14	-3.11	117.10	123.47
21	7	509	CL7	CHD-C4C-C3C	-3.11	119.90	124.94
32	2	519	ZEX	C11-C10-C9	-3.11	122.88	127.31
32	6	519	ZEX	C11-C10-C9	-3.11	122.88	127.31
21	6	509	CL7	CHD-C4C-C3C	-3.11	119.90	124.94
21	8	410	CL7	CHD-C4C-C3C	-3.11	119.90	124.94
21	B	603	CL7	C7-C6-C5	-3.11	104.92	113.36
21	b	604	CL7	C7-C6-C5	-3.11	104.92	113.36
21	3	511	CL7	O2A-C1-C2	-3.11	100.47	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	7	511	CL7	O2A-C1-C2	-3.11	100.47	108.64
21	b	605	CL7	C3A-C4A-CHB	-3.11	119.09	123.70
21	3	510	CL7	CHD-C1D-ND	-3.10	120.97	124.26
21	B	613	CL7	CHC-C1C-NC	-3.10	121.60	124.45
21	4	405	CL7	CHD-C4C-C3C	-3.10	119.91	124.94
21	8	405	CL7	CHD-C4C-C3C	-3.10	119.91	124.94
21	C	508	CL7	CHD-C4C-C3C	-3.10	119.91	124.94
21	8	410	CL7	O2D-CGD-CBD	3.10	116.78	111.27
21	3	509	CL7	CHD-C4C-C3C	-3.10	119.91	124.94
32	8	418	ZEX	C15-C35-C34	-3.10	117.13	123.47
32	7	519	ZEX	C27-C26-C25	-3.10	117.83	122.84
21	4	411	CL7	CHD-C4C-C3C	-3.10	119.92	124.94
21	C	505	CL7	CHD-C1D-ND	-3.10	120.98	124.26
21	c	505	CL7	CHD-C1D-ND	-3.10	120.98	124.26
21	8	404	CL7	CHD-C1D-ND	-3.10	120.98	124.26
21	2	505	CL7	C3A-C4A-CHB	-3.10	119.10	123.70
21	6	505	CL7	C3A-C4A-CHB	-3.10	119.10	123.70
21	b	606	CL7	O2D-CGD-CBD	3.10	116.77	111.27
21	2	503	CL7	CHC-C1C-NC	-3.10	121.61	124.45
21	5	403	CL7	CHC-C1C-NC	-3.10	121.61	124.45
21	1	405	CL7	CHD-C4C-C3C	-3.10	119.92	124.94
21	4	415	CL7	C4C-C3C-C2C	-3.09	103.09	107.13
32	4	418	ZEX	C15-C35-C34	-3.09	117.14	123.47
21	6	513	CL7	CMB-C2B-C1B	3.09	130.08	125.37
21	5	412	CL7	CHD-C4C-C3C	-3.09	119.93	124.94
21	2	509	CL7	CHD-C4C-C3C	-3.09	119.93	124.94
21	1	412	CL7	CHD-C4C-C3C	-3.09	119.93	124.94
21	2	516	CL7	CHD-C1D-ND	-3.09	120.98	124.26
21	6	516	CL7	CHD-C1D-ND	-3.09	120.98	124.26
21	8	416	CL7	CHD-C1D-ND	-3.09	120.99	124.26
21	8	411	CL7	CHD-C4C-C3C	-3.09	119.93	124.94
21	b	614	CL7	CHC-C1C-NC	-3.09	121.61	124.45
21	2	509	CL7	C7-C6-C5	-3.09	104.97	113.36
21	6	509	CL7	C7-C6-C5	-3.09	104.97	113.36
21	B	613	CL7	O2D-CGD-CBD	3.09	116.75	111.27
21	C	508	CL7	C3B-C2B-C1B	-3.09	103.44	107.16
21	c	508	CL7	C3B-C2B-C1B	-3.09	103.44	107.16
21	2	514	CL7	C2D-C1D-ND	3.09	112.30	110.23
21	6	514	CL7	C2D-C1D-ND	3.09	112.30	110.23
21	C	507	CL7	O2A-CGA-O1A	-3.09	115.81	123.59
21	c	507	CL7	O2A-CGA-O1A	-3.09	115.81	123.59
21	5	405	CL7	CHD-C4C-C3C	-3.08	119.94	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	611	CL7	CHC-C1C-NC	-3.08	121.62	124.45
21	3	508	CL7	CHD-C1D-ND	-3.08	120.99	124.26
32	3	522	ZEX	C30-C31-C32	-3.08	113.60	123.22
32	7	522	ZEX	C30-C31-C32	-3.08	113.60	123.22
21	8	415	CL7	C4C-C3C-C2C	-3.08	103.11	107.13
21	6	503	CL7	CHC-C1C-NC	-3.08	121.62	124.45
21	2	513	CL7	CHB-C1B-NB	-3.08	121.00	124.26
21	6	513	CL7	CHB-C1B-NB	-3.08	121.00	124.26
21	8	415	CL7	CHD-C1D-ND	-3.08	121.00	124.26
21	3	515	CL7	CHC-C1C-NC	-3.08	121.62	124.45
21	1	419	CL7	CHD-C4C-C3C	-3.08	119.95	124.94
32	7	520	ZEX	C1-C2-C3	-3.08	106.69	113.64
21	2	507	CL7	C3B-C2B-C1B	-3.08	103.45	107.16
21	6	507	CL7	C3B-C2B-C1B	-3.08	103.45	107.16
26	C	501	LMG	C8-O7-C10	-3.08	110.21	117.79
21	B	605	CL7	O2D-CGD-CBD	3.08	116.74	111.27
32	3	520	ZEX	C1-C2-C3	-3.08	106.69	113.64
21	4	408	CL7	CHD-C1D-ND	-3.08	121.00	124.26
21	2	502	CL7	C3A-C4A-CHB	-3.08	119.14	123.70
21	3	506	CL7	CHD-C1D-ND	-3.08	121.00	124.26
21	C	508	CL7	CAA-CBA-CGA	-3.08	104.27	113.25
21	c	508	CL7	CAA-CBA-CGA	-3.08	104.27	113.25
21	3	510	CL7	C7-C6-C5	-3.07	105.01	113.36
21	7	510	CL7	C7-C6-C5	-3.07	105.01	113.36
21	6	502	CL7	C3A-C4A-CHB	-3.07	119.14	123.70
21	2	513	CL7	CMB-C2B-C1B	3.07	130.05	125.37
21	B	604	CL7	CHD-C1D-ND	-3.07	121.00	124.26
21	6	516	CL7	O2D-CGD-CBD	3.07	116.73	111.27
21	5	419	CL7	CHD-C4C-C3C	-3.07	119.96	124.94
32	4	403	ZEX	C31-C32-C33	-3.07	117.79	126.42
32	8	403	ZEX	C31-C32-C33	-3.07	117.79	126.42
21	8	413	CL7	O2D-CGD-CBD	3.07	116.72	111.27
21	7	510	CL7	CHD-C1D-ND	-3.07	121.01	124.26
32	4	419	ZEX	C11-C10-C9	-3.07	122.93	127.31
21	2	516	CL7	CHD-C4C-C3C	-3.07	119.96	124.94
21	6	516	CL7	CHD-C4C-C3C	-3.07	119.96	124.94
21	B	605	CL7	CHB-C1B-NB	-3.07	121.01	124.26
21	b	606	CL7	CHB-C1B-NB	-3.07	121.01	124.26
21	4	413	CL7	O2D-CGD-CBD	3.07	116.72	111.27
21	C	518	CL7	CHC-C1C-NC	-3.07	121.63	124.45
21	c	518	CL7	CHC-C1C-NC	-3.07	121.63	124.45
21	B	601	CL7	CHB-C1B-NB	-3.07	121.01	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	602	CL7	CHB-C1B-NB	-3.07	121.01	124.26
21	3	515	CL7	CHD-C1D-ND	-3.07	121.01	124.26
21	7	515	CL7	CHD-C1D-ND	-3.07	121.01	124.26
23	D	406	8CT	C07-C02-C03	-3.07	118.28	122.73
23	d	406	8CT	C07-C02-C03	-3.07	118.28	122.73
21	1	403	CL7	CHD-C1D-ND	-3.07	121.01	124.26
21	6	501	CL7	CMB-C2B-C1B	3.07	130.04	125.37
21	4	417	CL7	CHC-C1C-NC	-3.07	121.64	124.45
21	8	417	CL7	CHC-C1C-NC	-3.07	121.64	124.45
21	b	614	CL7	O2D-CGD-CBD	3.06	116.71	111.27
23	4	402	8CT	C05-C04-C03	3.06	115.20	110.48
21	C	510	CL7	CHD-C1D-ND	-3.06	121.02	124.26
21	4	416	CL7	CHD-C1D-ND	-3.06	121.02	124.26
21	c	510	CL7	CHD-C1D-ND	-3.06	121.02	124.26
21	7	506	CL7	CHD-C1D-ND	-3.06	121.02	124.26
21	B	610	CL7	CHC-C1C-NC	-3.06	121.64	124.45
21	7	515	CL7	CHC-C1C-NC	-3.06	121.64	124.45
21	8	410	CL7	CHD-C1D-ND	-3.06	121.02	124.26
21	B	614	CL7	CHD-C4C-C3C	-3.06	119.98	124.94
21	b	615	CL7	CHD-C4C-C3C	-3.06	119.98	124.94
21	1	415	CL7	CHC-C1C-NC	-3.06	121.64	124.45
21	5	415	CL7	CHC-C1C-NC	-3.06	121.64	124.45
21	C	513	CL7	O2D-CGD-CBD	3.06	116.70	111.27
21	3	502	CL7	C2D-C1D-ND	3.06	112.28	110.23
21	7	502	CL7	C2D-C1D-ND	3.06	112.28	110.23
21	4	410	CL7	CHD-C1D-ND	-3.06	121.02	124.26
21	1	407	CL7	CHD-C4C-C3C	-3.06	119.98	124.94
26	c	501	LMG	C8-O7-C10	-3.06	110.27	117.79
21	5	403	CL7	CHD-C1D-ND	-3.05	121.02	124.26
23	c	519	8CT	C11-C10-C03	-3.05	118.62	127.20
21	C	514	CL7	CHD-C4C-C3C	-3.05	119.99	124.94
32	8	419	ZEX	C11-C10-C9	-3.05	122.95	127.31
21	C	502	CL7	O2D-CGD-CBD	3.05	116.69	111.27
23	C	515	8CT	C25-C24-C23	-3.05	113.70	123.22
32	3	522	ZEX	C11-C12-C13	-3.05	117.85	126.42
32	7	522	ZEX	C11-C12-C13	-3.05	117.85	126.42
21	7	514	CL7	CHD-C1D-ND	-3.05	121.03	124.26
31	F	101	HEM	CBA-CAA-C2A	-3.05	104.16	112.63
31	f	101	HEM	CBA-CAA-C2A	-3.05	104.16	112.63
21	1	408	CL7	C2D-C1D-ND	3.05	112.28	110.23
21	5	408	CL7	C2D-C1D-ND	3.05	112.28	110.23
21	2	516	CL7	O2D-CGD-CBD	3.05	116.68	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	415	CL7	CHD-C1D-ND	-3.05	121.03	124.26
32	1	422	ZEX	C21-C22-C23	-3.05	107.09	113.69
21	C	509	CL7	CAA-CBA-CGA	-3.05	104.35	113.25
21	c	509	CL7	CAA-CBA-CGA	-3.05	104.35	113.25
21	3	509	CL7	C7-C6-C5	-3.05	105.09	113.36
21	7	509	CL7	C7-C6-C5	-3.05	105.09	113.36
32	4	420	ZEX	C30-C31-C32	-3.04	113.72	123.22
21	3	501	CL7	CHC-C1C-NC	-3.04	121.66	124.45
21	2	501	CL7	CMB-C2B-C1B	3.04	130.00	125.37
23	8	402	8CT	C05-C04-C03	3.04	115.17	110.48
21	B	604	CL7	CHD-C4C-C3C	-3.04	120.00	124.94
21	1	412	CL7	O2D-CGD-CBD	3.04	116.68	111.27
21	5	412	CL7	O2D-CGD-CBD	3.04	116.68	111.27
21	6	504	CL7	CAA-CBA-CGA	-3.04	104.43	112.51
23	c	515	8CT	C25-C24-C23	-3.04	113.72	123.22
21	1	406	CL7	CHB-C1B-NB	-3.04	121.04	124.26
21	B	608	CL7	CHD-C4C-C3C	-3.04	120.01	124.94
21	b	609	CL7	CHD-C4C-C3C	-3.04	120.01	124.94
21	5	407	CL7	CHD-C4C-C3C	-3.04	120.01	124.94
21	b	603	CL7	O2A-CGA-CBA	3.04	121.45	111.91
21	c	513	CL7	O2D-CGD-CBD	3.04	116.67	111.27
21	b	605	CL7	CHD-C1D-ND	-3.04	121.04	124.26
21	C	509	CL7	CMB-C2B-C1B	3.04	130.00	125.37
21	2	504	CL7	CAA-CBA-CGA	-3.04	104.45	112.51
23	C	519	8CT	C11-C10-C03	-3.04	118.67	127.20
26	C	501	LMG	O8-C28-C29	3.04	121.44	111.91
21	4	408	CL7	CHC-C1C-NC	-3.04	121.66	124.45
21	c	514	CL7	CHD-C4C-C3C	-3.04	120.02	124.94
21	6	506	CL7	CHD-C4C-C3C	-3.04	120.02	124.94
21	5	418	CL7	C7-C6-C5	-3.03	105.12	113.36
21	8	408	CL7	CHC-C1C-NC	-3.03	121.67	124.45
32	8	420	ZEX	C30-C31-C32	-3.03	113.75	123.22
21	B	602	CL7	O2A-CGA-CBA	3.03	121.43	111.91
21	7	501	CL7	CHC-C1C-NC	-3.03	121.67	124.45
21	c	502	CL7	O2D-CGD-CBD	3.03	116.65	111.27
21	c	513	CL7	CHD-C1D-ND	-3.03	121.05	124.26
21	4	411	CL7	C3B-C2B-C1B	-3.03	103.50	107.16
21	8	411	CL7	C3B-C2B-C1B	-3.03	103.50	107.16
21	D	402	CL7	C2D-C1D-ND	3.03	112.26	110.23
21	b	605	CL7	CHD-C4C-C3C	-3.03	120.03	124.94
21	1	414	CL7	CHC-C1C-NC	-3.03	121.67	124.45
21	5	414	CL7	CHC-C1C-NC	-3.03	121.67	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	418	CL7	C7-C6-C5	-3.03	105.14	113.36
21	5	406	CL7	CHB-C1B-NB	-3.03	121.05	124.26
32	2	521	ZEX	C30-C31-C32	-3.02	113.78	123.22
32	6	520	ZEX	C30-C31-C32	-3.02	113.78	123.22
21	2	509	CL7	CAA-CBA-CGA	-3.02	104.42	113.25
21	6	509	CL7	CAA-CBA-CGA	-3.02	104.42	113.25
21	3	512	CL7	CHD-C1D-ND	-3.02	121.06	124.26
32	8	420	ZEX	C10-C11-C12	-3.02	113.78	123.22
21	2	506	CL7	CHD-C4C-C3C	-3.02	120.04	124.94
21	1	409	CL7	O2D-CGD-CBD	3.02	116.64	111.27
21	5	409	CL7	O2D-CGD-CBD	3.02	116.64	111.27
21	3	503	CL7	CHC-C1C-NC	-3.02	121.68	124.45
21	c	509	CL7	CMB-C2B-C1B	3.02	129.97	125.37
26	c	501	LMG	O8-C28-C29	3.02	121.38	111.91
32	4	420	ZEX	C10-C11-C12	-3.02	113.80	123.22
32	1	422	ZEX	C3-C4-C5	-3.02	105.84	111.85
32	5	422	ZEX	C3-C4-C5	-3.02	105.84	111.85
21	1	417	CL7	C4C-C3C-C2C	-3.02	103.19	107.13
21	5	417	CL7	C4C-C3C-C2C	-3.02	103.19	107.13
32	1	421	ZEX	C11-C10-C9	-3.02	123.00	127.31
32	5	421	ZEX	C11-C10-C9	-3.02	123.00	127.31
32	5	422	ZEX	C21-C22-C23	-3.02	107.16	113.69
21	1	419	CL7	CHC-C1C-NC	-3.01	121.68	124.45
21	2	508	CL7	CHD-C1D-ND	-3.01	121.07	124.26
21	6	508	CL7	CHD-C1D-ND	-3.01	121.07	124.26
21	6	514	CL7	CHD-C4C-C3C	-3.01	120.06	124.94
21	B	615	CL7	CHD-C1D-ND	-3.01	121.07	124.26
21	1	402	CL7	CHB-C1B-NB	-3.01	121.07	124.26
21	3	514	CL7	CHD-C1D-ND	-3.01	121.07	124.26
21	5	402	CL7	CHB-C1B-NB	-3.01	121.07	124.26
32	2	521	ZEX	C1-C2-C3	-3.01	106.84	113.64
21	D	405	CL7	CHD-C1D-ND	-3.01	121.07	124.26
21	d	405	CL7	CHD-C1D-ND	-3.01	121.07	124.26
23	4	402	8CT	C19-C18-C17	-3.01	117.31	123.47
23	8	402	8CT	C19-C18-C17	-3.01	117.31	123.47
21	B	613	CL7	CAA-CBA-CGA	-3.01	104.47	113.25
21	b	614	CL7	CAA-CBA-CGA	-3.01	104.47	113.25
21	B	603	CL7	CHD-C4C-C3C	-3.01	120.07	124.94
21	2	508	CL7	CHD-C4C-C3C	-3.01	120.07	124.94
21	b	604	CL7	CHD-C4C-C3C	-3.01	120.07	124.94
21	6	508	CL7	CHD-C4C-C3C	-3.01	120.07	124.94
21	7	510	CL7	CHC-C1C-NC	-3.01	121.69	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	415	CL7	CHB-C1B-NB	-3.00	121.08	124.26
32	6	520	ZEX	C1-C2-C3	-3.00	106.86	113.64
21	5	419	CL7	CHC-C1C-NC	-3.00	121.69	124.45
21	B	601	CL7	CHD-C4C-C3C	-3.00	120.07	124.94
21	b	602	CL7	CHD-C4C-C3C	-3.00	120.07	124.94
21	7	511	CL7	C7-C6-C5	-3.00	105.20	113.36
21	C	504	CL7	CHC-C1C-NC	-3.00	121.69	124.45
21	3	503	CL7	CHD-C1D-ND	-3.00	121.08	124.26
21	7	503	CL7	CHD-C1D-ND	-3.00	121.08	124.26
21	b	603	CL7	CAA-C2A-C1A	-3.00	102.32	112.19
32	2	521	ZEX	C3-C4-C5	-3.00	105.88	111.85
31	F	101	HEM	C4C-NC-C1C	3.00	108.28	105.35
31	f	101	HEM	C4C-NC-C1C	3.00	108.28	105.35
21	c	518	CL7	CHD-C4C-C3C	-3.00	120.08	124.94
21	B	604	CL7	C4-C3-C5	3.00	120.31	115.27
21	b	605	CL7	C4-C3-C5	3.00	120.31	115.27
21	6	505	CL7	C4D-C3D-CAD	-3.00	105.40	107.42
21	C	518	CL7	CHD-C4C-C3C	-3.00	120.08	124.94
21	2	514	CL7	CHD-C4C-C3C	-3.00	120.08	124.94
21	2	515	CL7	CHD-C1D-ND	-3.00	121.08	124.26
21	C	508	CL7	CHD-C1D-ND	-3.00	121.08	124.26
21	6	512	CL7	CHC-C1C-NC	-3.00	121.70	124.45
21	c	508	CL7	CHD-C1D-ND	-3.00	121.09	124.26
21	7	512	CL7	CHD-C1D-ND	-3.00	121.09	124.26
21	2	517	CL7	O2D-CGD-CBD	2.99	116.59	111.27
21	6	517	CL7	O2D-CGD-CBD	2.99	116.59	111.27
21	3	511	CL7	C7-C6-C5	-2.99	105.23	113.36
21	D	402	CL7	CHC-C1C-NC	-2.99	121.70	124.45
21	3	505	CL7	C4D-C3D-CAD	-2.99	105.41	107.42
21	7	505	CL7	C4D-C3D-CAD	-2.99	105.41	107.42
23	B	617	8CT	C01-C02-C07	2.99	119.36	113.62
21	8	417	CL7	O2D-CGD-CBD	2.99	116.58	111.27
21	1	412	CL7	CHD-C1D-ND	-2.99	121.09	124.26
21	d	402	CL7	C2D-C1D-ND	2.99	112.24	110.23
21	B	602	CL7	CAA-C2A-C1A	-2.99	102.36	112.19
21	B	609	CL7	CHD-C4C-C3C	-2.99	120.10	124.94
21	1	413	CL7	CHD-C1D-ND	-2.99	121.09	124.26
21	7	517	CL7	CHC-C1C-NC	-2.99	121.71	124.45
21	2	502	CL7	O2D-CGD-CBD	2.99	116.57	111.27
21	6	502	CL7	O2D-CGD-CBD	2.99	116.57	111.27
21	3	511	CL7	C4C-C3C-C2C	-2.99	103.24	107.13
21	7	511	CL7	C4C-C3C-C2C	-2.99	103.24	107.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	3	522	ZEX	C7-C8-C9	-2.98	121.72	126.23
32	7	522	ZEX	C7-C8-C9	-2.98	121.72	126.23
32	1	421	ZEX	C27-C26-C25	-2.98	118.02	122.84
32	5	421	ZEX	C27-C26-C25	-2.98	118.02	122.84
23	c	516	8CT	C40-C12-C13	-2.98	118.74	122.92
21	3	506	CL7	CHB-C1B-NB	-2.98	121.10	124.26
21	7	506	CL7	CHB-C1B-NB	-2.98	121.10	124.26
21	3	514	CL7	CHC-C1C-NC	-2.98	121.71	124.45
21	4	417	CL7	O2D-CGD-CBD	2.98	116.57	111.27
21	2	512	CL7	CHC-C1C-NC	-2.98	121.71	124.45
21	d	402	CL7	CHC-C1C-NC	-2.98	121.71	124.45
21	2	502	CL7	C7-C6-C5	-2.98	105.26	113.36
21	6	502	CL7	C7-C6-C5	-2.98	105.26	113.36
21	A	401	CL7	CHD-C1D-ND	-2.98	121.10	124.26
21	1	412	CL7	CHC-C1C-NC	-2.98	121.72	124.45
21	5	412	CL7	CHC-C1C-NC	-2.98	121.72	124.45
21	7	503	CL7	CHC-C1C-NC	-2.98	121.72	124.45
21	7	514	CL7	CHC-C1C-NC	-2.98	121.72	124.45
21	2	505	CL7	C4D-C3D-CAD	-2.98	105.42	107.42
21	5	415	CL7	CHB-C1B-NB	-2.98	121.10	124.26
21	1	409	CL7	CHD-C1D-ND	-2.98	121.10	124.26
21	a	401	CL7	CHD-C1D-ND	-2.98	121.10	124.26
21	5	409	CL7	CHD-C1D-ND	-2.98	121.10	124.26
21	3	510	CL7	CHC-C1C-NC	-2.98	121.72	124.45
21	C	513	CL7	CHD-C1D-ND	-2.98	121.11	124.26
21	B	622	CL7	CHC-C1C-NC	-2.98	121.72	124.45
21	C	503	CL7	C4C-C3C-C2C	-2.98	103.25	107.13
21	3	512	CL7	CHC-C1C-NC	-2.98	121.72	124.45
21	7	512	CL7	CHC-C1C-NC	-2.98	121.72	124.45
21	3	517	CL7	CHC-C1C-NC	-2.97	121.72	124.45
21	7	504	CL7	O2D-CGD-CBD	2.97	116.55	111.27
23	b	618	8CT	C01-C02-C07	2.97	119.33	113.62
21	C	506	CL7	CHB-C1B-NB	-2.97	121.11	124.26
21	c	506	CL7	CHB-C1B-NB	-2.97	121.11	124.26
21	5	412	CL7	CHD-C1D-ND	-2.97	121.11	124.26
23	B	627	8CT	C07-C02-C03	-2.97	118.42	122.73
23	b	601	8CT	C07-C02-C03	-2.97	118.42	122.73
32	6	520	ZEX	C3-C4-C5	-2.97	105.94	111.85
21	4	414	CL7	CHB-C1B-NB	-2.97	121.11	124.26
21	6	515	CL7	CHD-C1D-ND	-2.97	121.11	124.26
21	8	414	CL7	CHB-C1B-NB	-2.97	121.11	124.26
21	2	502	CL7	CHB-C1B-NB	-2.97	121.11	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	502	CL7	CHB-C1B-NB	-2.97	121.11	124.26
21	7	503	CL7	CHB-C1B-NB	-2.97	121.11	124.26
21	1	410	CL7	CHD-C4C-C3C	-2.97	120.13	124.94
21	8	411	CL7	O2D-CGD-CBD	2.97	116.54	111.27
21	b	610	CL7	CHD-C4C-C3C	-2.97	120.13	124.94
23	C	516	8CT	C40-C12-C13	-2.96	118.77	122.92
21	1	416	CL7	CHD-C4C-C3C	-2.96	120.14	124.94
21	b	616	CL7	CHD-C1D-ND	-2.96	121.12	124.26
21	5	417	CL7	CHC-C1C-NC	-2.96	121.73	124.45
21	8	404	CL7	CHD-C4C-C3C	-2.96	120.14	124.94
21	5	413	CL7	CHD-C1D-ND	-2.96	121.12	124.26
21	B	603	CL7	CHC-C1C-NC	-2.96	121.73	124.45
21	5	410	CL7	CHD-C4C-C3C	-2.96	120.14	124.94
21	5	408	CL7	C3B-C2B-C1B	-2.96	103.59	107.16
21	4	411	CL7	O2D-CGD-CBD	2.96	116.53	111.27
21	5	410	CL7	C7-C6-C5	-2.96	105.33	113.36
21	2	510	CL7	CHC-C1C-NC	-2.96	121.74	124.45
21	8	406	CL7	CAA-CBA-CGA	-2.96	104.61	113.25
21	b	604	CL7	CHC-C1C-NC	-2.96	121.74	124.45
21	2	501	CL7	O2D-CGD-CBD	2.96	116.52	111.27
21	3	504	CL7	O2D-CGD-CBD	2.96	116.52	111.27
21	c	504	CL7	CHC-C1C-NC	-2.95	121.74	124.45
21	c	503	CL7	C4C-C3C-C2C	-2.95	103.28	107.13
21	B	611	CL7	CHC-C1C-NC	-2.95	121.74	124.45
21	b	612	CL7	CHC-C1C-NC	-2.95	121.74	124.45
21	3	513	CL7	CHD-C1D-ND	-2.95	121.13	124.26
21	7	513	CL7	CHD-C1D-ND	-2.95	121.13	124.26
21	4	404	CL7	CHD-C4C-C3C	-2.95	120.16	124.94
21	C	509	CL7	O2A-CGA-CBA	2.95	121.16	111.91
21	c	509	CL7	O2A-CGA-CBA	2.95	121.16	111.91
21	a	401	CL7	O2D-CGD-CBD	2.95	116.51	111.27
21	B	615	CL7	CHD-C4C-C3C	-2.95	120.16	124.94
21	b	616	CL7	CHD-C4C-C3C	-2.95	120.16	124.94
21	4	406	CL7	CAA-CBA-CGA	-2.95	104.64	113.25
21	8	406	CL7	CHC-C1C-NC	-2.95	121.75	124.45
21	1	410	CL7	C7-C6-C5	-2.94	105.36	113.36
21	3	503	CL7	CHB-C1B-NB	-2.94	121.14	124.26
21	4	406	CL7	CHC-C1C-NC	-2.94	121.75	124.45
21	1	408	CL7	C3B-C2B-C1B	-2.94	103.61	107.16
21	7	516	CL7	CHD-C4C-C3C	-2.94	120.17	124.94
21	3	517	CL7	C3B-C2B-C1B	-2.94	103.61	107.16
21	7	517	CL7	C3B-C2B-C1B	-2.94	103.61	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	501	CL7	O2D-CGD-CBD	2.94	116.49	111.27
21	6	510	CL7	CHC-C1C-NC	-2.94	121.75	124.45
21	A	401	CL7	O2D-CGD-CBD	2.94	116.49	111.27
21	a	403	CL7	O2D-CGD-CBD	2.94	116.48	111.27
21	4	405	CL7	O2D-CGD-CBD	2.94	116.48	111.27
21	8	405	CL7	O2D-CGD-CBD	2.94	116.48	111.27
21	3	507	CL7	C7-C6-C5	-2.93	105.39	113.36
21	7	518	CL7	CHC-C1C-NC	-2.93	121.76	124.45
21	A	403	CL7	O2D-CGD-CBD	2.93	116.48	111.27
21	7	507	CL7	C7-C6-C5	-2.93	105.40	113.36
32	6	520	ZEX	C2-C3-C4	-2.93	106.29	110.30
21	B	609	CL7	O2D-CGD-CBD	2.93	116.47	111.27
21	b	610	CL7	O2D-CGD-CBD	2.93	116.47	111.27
21	4	412	CL7	C7-C6-C5	-2.93	105.41	113.36
21	8	412	CL7	C7-C6-C5	-2.93	105.41	113.36
21	1	419	CL7	CHB-C1B-NB	-2.93	121.16	124.26
21	2	505	CL7	CHC-C1C-NC	-2.93	121.76	124.45
21	b	623	CL7	CHC-C1C-NC	-2.93	121.76	124.45
21	3	504	CL7	C7-C6-C5	-2.93	105.41	113.36
21	5	416	CL7	CHD-C4C-C3C	-2.93	120.20	124.94
21	7	504	CL7	C7-C6-C5	-2.93	105.41	113.36
21	2	501	CL7	CHB-C1B-NB	-2.93	121.16	124.26
21	6	501	CL7	CHB-C1B-NB	-2.93	121.16	124.26
21	3	516	CL7	CHD-C4C-C3C	-2.93	120.20	124.94
21	c	509	CL7	C1-C2-C3	2.93	131.10	126.04
21	B	607	CL7	CHC-C1C-NC	-2.92	121.77	124.45
21	B	616	CL7	O2D-CGD-CBD	2.92	116.46	111.27
21	b	617	CL7	O2D-CGD-CBD	2.92	116.46	111.27
21	5	407	CL7	O2D-CGD-CBD	2.92	116.46	111.27
21	B	604	CL7	CMB-C2B-C1B	2.92	129.82	125.37
21	b	605	CL7	CMB-C2B-C1B	2.92	129.82	125.37
32	2	521	ZEX	C2-C3-C4	-2.92	106.30	110.30
32	1	421	ZEX	C18-C5-C6	-2.92	121.25	124.53
32	5	421	ZEX	C18-C5-C6	-2.92	121.25	124.53
32	1	421	ZEX	C39-C29-C30	-2.92	118.83	122.92
21	1	417	CL7	CHC-C1C-NC	-2.92	121.77	124.45
21	2	512	CL7	CHD-C1D-ND	-2.92	121.17	124.26
21	6	512	CL7	CHD-C1D-ND	-2.92	121.17	124.26
21	1	407	CL7	O2D-CGD-CBD	2.92	116.46	111.27
21	2	504	CL7	CMB-C2B-C1B	2.92	129.81	125.37
21	6	504	CL7	CMB-C2B-C1B	2.92	129.81	125.37
21	7	513	CL7	CHC-C1C-NC	-2.92	121.77	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	619	8CT	C25-C24-C23	-2.92	114.11	123.22
32	5	421	ZEX	C39-C29-C30	-2.92	118.84	122.92
21	B	608	CL7	C3B-C2B-C1B	-2.92	103.64	107.16
21	4	405	CL7	CHC-C1C-NC	-2.92	121.77	124.45
21	b	615	CL7	C3B-C2B-C1B	-2.91	103.64	107.16
21	2	507	CL7	C2D-C1D-ND	2.91	112.19	110.23
21	6	507	CL7	C2D-C1D-ND	2.91	112.19	110.23
23	b	620	8CT	C19-C18-C17	-2.91	117.50	123.47
21	c	506	CL7	CHD-C4C-C3C	-2.91	120.22	124.94
21	B	607	CL7	O2D-CGD-CBD	2.91	116.44	111.27
32	2	525	ZEX	C1-C6-C5	-2.91	118.51	122.61
31	F	101	HEM	CHD-C1D-C2D	-2.91	120.43	124.98
31	f	101	HEM	CHD-C1D-C2D	-2.91	120.43	124.98
23	B	618	8CT	C25-C24-C23	-2.91	114.13	123.22
21	2	511	CL7	CHC-C1C-NC	-2.91	121.78	124.45
21	6	511	CL7	CHC-C1C-NC	-2.91	121.78	124.45
21	C	506	CL7	CHD-C4C-C3C	-2.91	120.22	124.94
27	B	624	DGD	O1G-C1A-C2A	2.91	121.03	111.91
32	2	523	ZEX	C18-C5-C4	2.91	119.74	114.36
32	6	522	ZEX	C18-C5-C4	2.91	119.74	114.36
21	C	509	CL7	C1-C2-C3	2.91	131.07	126.04
21	6	505	CL7	CHD-C1D-ND	-2.91	121.18	124.26
21	8	405	CL7	CHC-C1C-NC	-2.91	121.78	124.45
32	6	524	ZEX	C1-C6-C5	-2.91	118.52	122.61
21	B	614	CL7	C3B-C2B-C1B	-2.90	103.66	107.16
21	6	507	CL7	CHC-C1C-NC	-2.90	121.78	124.45
21	b	608	CL7	O2D-CGD-CBD	2.90	116.43	111.27
21	4	417	CL7	CHD-C1D-ND	-2.90	121.18	124.26
21	2	515	CL7	CHC-C1C-NC	-2.90	121.79	124.45
21	6	515	CL7	CHC-C1C-NC	-2.90	121.79	124.45
21	7	509	CL7	CHC-C1C-NC	-2.90	121.79	124.45
21	C	504	CL7	CHB-C1B-NB	-2.90	121.19	124.26
21	c	504	CL7	CHB-C1B-NB	-2.90	121.19	124.26
21	3	518	CL7	CHC-C1C-NC	-2.90	121.79	124.45
23	B	619	8CT	C19-C18-C17	-2.90	117.53	123.47
21	c	506	CL7	C2D-C1D-ND	2.90	112.17	110.23
27	b	625	DGD	O1G-C1A-C2A	2.90	121.00	111.91
21	2	505	CL7	CHD-C1D-ND	-2.90	121.19	124.26
21	b	616	CL7	CAA-CBA-CGA	-2.90	104.79	113.25
21	C	511	CL7	C7-C6-C5	-2.90	105.49	113.36
21	1	410	CL7	O2D-CGD-CBD	2.90	116.41	111.27
21	3	513	CL7	CHC-C1C-NC	-2.90	121.79	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	510	CL7	O2D-CGD-CBD	2.89	116.41	111.27
21	B	615	CL7	CAA-CBA-CGA	-2.89	104.80	113.25
21	6	517	CL7	CMB-C2B-C1B	2.89	129.78	125.37
21	1	420	CL7	CHD-C1D-ND	-2.89	121.19	124.26
21	5	419	CL7	CHB-C1B-NB	-2.89	121.19	124.26
21	5	420	CL7	CHD-C1D-ND	-2.89	121.19	124.26
21	5	410	CL7	O2D-CGD-CBD	2.89	116.41	111.27
21	b	608	CL7	CHC-C1C-NC	-2.89	121.80	124.45
21	4	409	CL7	CHD-C1D-ND	-2.89	121.19	124.26
21	8	409	CL7	CHD-C1D-ND	-2.89	121.19	124.26
21	b	609	CL7	C3B-C2B-C1B	-2.89	103.67	107.16
21	c	514	CL7	CMB-C2B-C1B	2.89	129.77	125.37
21	5	407	CL7	CHC-C1C-NC	-2.89	121.80	124.45
21	1	419	CL7	O2D-CGD-CBD	2.89	116.40	111.27
21	c	511	CL7	C7-C6-C5	-2.89	105.52	113.36
21	6	505	CL7	CHC-C1C-NC	-2.88	121.80	124.45
21	5	419	CL7	O2D-CGD-CBD	2.88	116.39	111.27
21	2	517	CL7	CMB-C2B-C1B	2.88	129.76	125.37
21	2	517	CL7	CHC-C1C-NC	-2.88	121.81	124.45
21	6	517	CL7	CHC-C1C-NC	-2.88	121.81	124.45
21	4	409	CL7	CHD-C4C-C3C	-2.88	120.27	124.94
21	8	409	CL7	CHD-C4C-C3C	-2.88	120.27	124.94
21	3	507	CL7	CMB-C2B-C1B	2.88	129.76	125.37
21	b	615	CL7	CHD-C1D-ND	-2.88	121.21	124.26
21	b	612	CL7	CHD-C4C-C3C	-2.88	120.27	124.94
21	6	513	CL7	C3B-C2B-C1B	-2.88	103.69	107.16
21	c	507	CL7	CMB-C2B-C1B	2.88	129.75	125.37
21	8	417	CL7	CHD-C1D-ND	-2.88	121.21	124.26
21	1	407	CL7	CHC-C1C-NC	-2.88	121.81	124.45
21	B	606	CL7	C3B-C2B-C1B	-2.88	103.69	107.16
21	b	607	CL7	C3B-C2B-C1B	-2.88	103.69	107.16
21	4	416	CL7	CMA-C3A-C2A	-2.87	109.39	116.10
32	4	403	ZEX	C15-C35-C34	-2.87	117.59	123.47
32	8	403	ZEX	C15-C35-C34	-2.87	117.59	123.47
21	2	510	CL7	O2D-CGD-CBD	2.87	116.37	111.27
21	C	514	CL7	CMB-C2B-C1B	2.87	129.74	125.37
21	C	512	CL7	CMB-C2B-C1B	2.87	129.74	125.37
21	c	512	CL7	CMB-C2B-C1B	2.87	129.74	125.37
21	4	408	CL7	CAA-CBA-CGA	-2.87	104.89	112.51
21	8	408	CL7	CAA-CBA-CGA	-2.87	104.89	112.51
21	7	507	CL7	CMB-C2B-C1B	2.87	129.74	125.37
21	4	413	CL7	CHC-C1C-NC	-2.87	121.82	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	8	413	CL7	CHC-C1C-NC	-2.87	121.82	124.45
21	B	611	CL7	CHD-C4C-C3C	-2.87	120.29	124.94
21	C	507	CL7	CMB-C2B-C1B	2.87	129.74	125.37
21	1	406	CL7	O2D-CGD-CBD	2.87	116.36	111.27
21	5	406	CL7	O2D-CGD-CBD	2.87	116.36	111.27
21	B	603	CL7	CHB-C1B-NB	-2.87	121.22	124.26
21	2	512	CL7	CHB-C1B-NB	-2.87	121.22	124.26
21	6	512	CL7	CHB-C1B-NB	-2.87	121.22	124.26
21	2	507	CL7	CHC-C1C-NC	-2.86	121.82	124.45
21	1	418	CL7	CHD-C1D-ND	-2.86	121.22	124.26
21	A	403	CL7	CHC-C1C-NC	-2.86	121.82	124.45
21	a	403	CL7	CHC-C1C-NC	-2.86	121.82	124.45
21	1	409	CL7	CHD-C4C-C3C	-2.86	120.30	124.94
21	5	409	CL7	CHD-C4C-C3C	-2.86	120.30	124.94
21	C	514	CL7	CHB-C1B-NB	-2.86	121.23	124.26
21	c	514	CL7	CHB-C1B-NB	-2.86	121.23	124.26
21	3	511	CL7	O2A-CGA-O1A	-2.86	116.37	123.59
21	7	511	CL7	O2A-CGA-O1A	-2.86	116.37	123.59
21	3	508	CL7	O2D-CGD-CBD	2.86	116.35	111.27
21	7	508	CL7	O2D-CGD-CBD	2.86	116.35	111.27
21	5	405	CL7	O2D-CGD-CBD	2.86	116.35	111.27
21	7	508	CL7	CHD-C4C-C3C	-2.86	120.30	124.94
21	4	416	CL7	CHC-C1C-NC	-2.86	121.83	124.45
21	8	416	CL7	CHC-C1C-NC	-2.86	121.83	124.45
21	8	416	CL7	CMA-C3A-C2A	-2.86	109.42	116.10
21	b	604	CL7	CHB-C1B-NB	-2.86	121.23	124.26
32	4	420	ZEX	C1-C6-C5	-2.86	118.58	122.61
23	B	617	8CT	C35-C30-C29	-2.86	109.09	112.70
23	b	618	8CT	C35-C30-C29	-2.86	109.09	112.70
21	3	512	CL7	C7-C6-C5	-2.86	105.59	113.36
21	7	512	CL7	C7-C6-C5	-2.86	105.59	113.36
21	2	502	CL7	CHC-C1C-NC	-2.86	121.83	124.45
21	6	502	CL7	CHC-C1C-NC	-2.86	121.83	124.45
21	4	414	CL7	CMB-C2B-C1B	2.86	129.72	125.37
21	8	414	CL7	CMB-C2B-C1B	2.86	129.72	125.37
32	4	419	ZEX	C27-C26-C25	-2.86	118.22	122.84
21	3	505	CL7	CHC-C1C-NC	-2.86	121.83	124.45
21	7	505	CL7	CHC-C1C-NC	-2.86	121.83	124.45
32	8	420	ZEX	C1-C6-C5	-2.86	118.59	122.61
21	2	503	CL7	C7-C6-C5	-2.85	105.61	113.36
21	2	513	CL7	C3B-C2B-C1B	-2.85	103.72	107.16
27	B	624	DGD	C2G-O2G-C1B	-2.85	110.76	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	415	CL7	CHB-C1B-NB	-2.85	121.24	124.26
21	1	404	CL7	C7-C6-C5	-2.85	105.61	113.36
21	B	614	CL7	O2D-CGD-CBD	2.85	116.33	111.27
21	b	615	CL7	O2D-CGD-CBD	2.85	116.33	111.27
21	8	415	CL7	CHB-C1B-NB	-2.85	121.24	124.26
32	8	419	ZEX	C27-C26-C25	-2.85	118.24	122.84
27	b	625	DGD	C2G-O2G-C1B	-2.85	110.78	117.79
21	4	417	CL7	CHB-C1B-NB	-2.85	121.24	124.26
21	8	417	CL7	CHB-C1B-NB	-2.85	121.24	124.26
21	3	516	CL7	C3B-C2B-C1B	-2.85	103.72	107.16
21	6	517	CL7	C3B-C2B-C1B	-2.85	103.72	107.16
21	7	516	CL7	C3B-C2B-C1B	-2.85	103.72	107.16
21	2	509	CL7	O2D-CGD-CBD	2.85	116.33	111.27
21	d	405	CL7	CHB-C1B-NB	-2.85	121.24	124.26
21	6	515	CL7	CHB-C1B-NB	-2.85	121.25	124.26
21	2	515	CL7	CHB-C1B-NB	-2.84	121.25	124.26
21	2	510	CL7	CHD-C1D-ND	-2.84	121.25	124.26
21	6	503	CL7	C7-C6-C5	-2.84	105.64	113.36
21	5	404	CL7	C7-C6-C5	-2.84	105.64	113.36
21	6	509	CL7	O2D-CGD-CBD	2.84	116.32	111.27
21	7	506	CL7	C3B-C4B-NB	2.84	113.15	110.52
21	d	402	CL7	CHD-C4C-C3C	-2.84	120.33	124.94
21	2	516	CL7	CHB-C1B-NB	-2.84	121.25	124.26
21	6	516	CL7	CHB-C1B-NB	-2.84	121.25	124.26
21	3	508	CL7	CHD-C4C-C3C	-2.84	120.34	124.94
21	3	511	CL7	CHD-C1D-ND	-2.84	121.25	124.26
21	7	511	CL7	CHD-C1D-ND	-2.84	121.25	124.26
21	1	405	CL7	O2D-CGD-CBD	2.84	116.31	111.27
32	1	422	ZEX	C30-C31-C32	-2.84	114.36	123.22
23	C	516	8CT	C30-C31-C32	-2.84	117.98	121.47
23	c	516	8CT	C30-C31-C32	-2.84	117.98	121.47
23	d	406	8CT	C22-C21-C20	-2.84	118.95	122.92
32	4	420	ZEX	C35-C15-C14	-2.84	117.66	123.47
32	8	420	ZEX	C35-C15-C14	-2.84	117.66	123.47
21	5	420	CL7	CHB-C1B-NB	-2.84	121.25	124.26
21	6	510	CL7	CHD-C1D-ND	-2.84	121.25	124.26
23	C	515	8CT	C19-C18-C17	-2.83	117.67	123.47
21	B	614	CL7	CHD-C1D-ND	-2.83	121.26	124.26
21	C	512	CL7	CHC-C1C-NC	-2.83	121.85	124.45
21	c	510	CL7	O2D-CGD-CBD	2.83	116.31	111.27
21	3	507	CL7	C3B-C2B-C1B	-2.83	103.74	107.16
32	5	422	ZEX	C30-C31-C32	-2.83	114.37	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	517	CL7	C3B-C2B-C1B	-2.83	103.74	107.16
21	5	418	CL7	CHD-C1D-ND	-2.83	121.26	124.26
21	B	602	CL7	CHC-C1C-NC	-2.83	121.85	124.45
21	B	604	CL7	CHB-C1B-NB	-2.83	121.26	124.26
21	b	605	CL7	CHB-C1B-NB	-2.83	121.26	124.26
32	3	520	ZEX	C19-C9-C10	-2.83	118.96	122.92
32	7	520	ZEX	C19-C9-C10	-2.83	118.96	122.92
21	2	504	CL7	CHB-C1B-NB	-2.83	121.26	124.26
21	6	504	CL7	CHB-C1B-NB	-2.83	121.26	124.26
21	4	417	CL7	C4C-C3C-C2C	-2.83	103.44	107.13
21	8	417	CL7	C4C-C3C-C2C	-2.83	103.44	107.13
21	3	506	CL7	C3B-C4B-NB	2.83	113.14	110.52
21	C	505	CL7	CHB-C1B-NB	-2.83	121.27	124.26
21	4	405	CL7	CHB-C1B-NB	-2.83	121.27	124.26
21	c	505	CL7	CHB-C1B-NB	-2.83	121.27	124.26
21	C	510	CL7	O2D-CGD-CBD	2.83	116.29	111.27
21	2	516	CL7	CHC-C1C-NC	-2.83	121.86	124.45
21	3	509	CL7	CHC-C1C-NC	-2.83	121.86	124.45
21	6	516	CL7	CHC-C1C-NC	-2.83	121.86	124.45
21	c	506	CL7	CHD-C1D-ND	-2.82	121.27	124.26
21	b	603	CL7	CHC-C1C-NC	-2.82	121.86	124.45
23	c	515	8CT	C19-C18-C17	-2.82	117.69	123.47
21	C	509	CL7	O2A-CGA-O1A	-2.82	116.47	123.59
21	c	509	CL7	O2A-CGA-O1A	-2.82	116.47	123.59
32	4	419	ZEX	C18-C5-C6	-2.82	121.36	124.53
21	1	411	CL7	CHC-C1C-NC	-2.82	121.86	124.45
21	5	411	CL7	CHC-C1C-NC	-2.82	121.86	124.45
21	c	504	CL7	C7-C6-C5	-2.82	105.70	113.36
21	5	409	CL7	CHB-C1B-NB	-2.82	121.27	124.26
21	1	408	CL7	CHD-C1D-ND	-2.82	121.27	124.26
21	c	502	CL7	CHD-C1D-ND	-2.82	121.27	124.26
21	5	408	CL7	CHD-C1D-ND	-2.82	121.27	124.26
21	7	507	CL7	C3B-C2B-C1B	-2.82	103.76	107.16
21	4	416	CL7	O2D-CGD-CBD	2.82	116.28	111.27
21	8	416	CL7	O2D-CGD-CBD	2.82	116.28	111.27
21	5	418	CL7	CHB-C1B-NB	-2.82	121.27	124.26
21	3	505	CL7	C3B-C2B-C1B	-2.82	103.76	107.16
21	7	505	CL7	C3B-C2B-C1B	-2.82	103.76	107.16
23	D	406	8CT	C22-C21-C20	-2.82	118.97	122.92
21	B	609	CL7	C7-C6-C5	-2.82	105.71	113.36
21	2	506	CL7	CHB-C1B-NB	-2.82	121.28	124.26
21	6	506	CL7	CHB-C1B-NB	-2.82	121.28	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	416	CL7	CMB-C2B-C1B	2.82	129.66	125.37
21	D	402	CL7	CHD-C4C-C3C	-2.82	120.37	124.94
21	C	506	CL7	C2D-C1D-ND	2.82	112.12	110.23
21	3	509	CL7	O2D-CGD-CBD	2.82	116.27	111.27
21	7	509	CL7	O2D-CGD-CBD	2.82	116.27	111.27
21	C	504	CL7	C7-C6-C5	-2.82	105.71	113.36
21	b	610	CL7	C7-C6-C5	-2.81	105.72	113.36
21	B	612	CL7	CHB-C1B-NB	-2.81	121.28	124.26
21	C	506	CL7	CHD-C1D-ND	-2.81	121.28	124.26
21	1	404	CL7	CHC-C1C-NC	-2.81	121.87	124.45
21	5	404	CL7	CHC-C1C-NC	-2.81	121.87	124.45
21	1	418	CL7	CHB-C1B-NB	-2.81	121.28	124.26
21	3	506	CL7	CHD-C4C-C3C	-2.81	120.38	124.94
21	7	506	CL7	CHD-C4C-C3C	-2.81	120.38	124.94
23	D	406	8CT	C04-C03-C02	-2.81	118.66	122.61
23	d	406	8CT	C04-C03-C02	-2.81	118.66	122.61
21	C	514	CL7	CHC-C1C-NC	-2.81	121.87	124.45
21	1	416	CL7	CHB-C1B-NB	-2.81	121.28	124.26
21	c	518	CL7	CHB-C1B-NB	-2.81	121.28	124.26
21	3	502	CL7	CHD-C4C-C3C	-2.81	120.39	124.94
21	7	502	CL7	CHD-C4C-C3C	-2.81	120.39	124.94
21	c	512	CL7	CHC-C1C-NC	-2.81	121.87	124.45
21	b	613	CL7	CAA-CBA-CGA	-2.81	105.05	113.25
21	1	406	CL7	CHC-C1C-NC	-2.81	121.87	124.45
21	5	406	CL7	CHC-C1C-NC	-2.81	121.87	124.45
21	D	405	CL7	CHB-C1B-NB	-2.81	121.29	124.26
21	1	405	CL7	CHB-C1B-NB	-2.81	121.29	124.26
21	6	507	CL7	CHB-C1B-NB	-2.81	121.29	124.26
21	5	405	CL7	CHB-C1B-NB	-2.81	121.29	124.26
21	1	406	CL7	C4-C3-C5	2.81	119.99	115.27
21	b	613	CL7	CHB-C1B-NB	-2.80	121.29	124.26
21	8	405	CL7	CHB-C1B-NB	-2.80	121.29	124.26
21	2	507	CL7	CHB-C1B-NB	-2.80	121.29	124.26
32	3	520	ZEX	C8-C7-C6	-2.80	119.33	127.20
21	2	504	CL7	C2D-C1D-ND	2.80	112.11	110.23
21	6	504	CL7	C2D-C1D-ND	2.80	112.11	110.23
32	7	520	ZEX	C8-C7-C6	-2.80	119.33	127.20
21	B	612	CL7	C3B-C2B-C1B	-2.80	103.78	107.16
21	b	613	CL7	C3B-C2B-C1B	-2.80	103.78	107.16
21	5	406	CL7	CHD-C1D-ND	-2.80	121.29	124.26
21	d	405	CL7	C3B-C2B-C1B	-2.80	103.78	107.16
21	B	601	CL7	CHC-C1C-NC	-2.80	121.88	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	602	CL7	CHC-C1C-NC	-2.80	121.88	124.45
21	2	514	CL7	C4C-C3C-C2C	-2.80	103.48	107.13
21	6	514	CL7	C4C-C3C-C2C	-2.80	103.48	107.13
21	C	504	CL7	O2D-CGD-CBD	2.80	116.24	111.27
21	C	505	CL7	O2D-CGD-CBD	2.80	116.24	111.27
21	5	406	CL7	C4-C3-C5	2.80	119.98	115.27
21	1	420	CL7	CHB-C1B-NB	-2.80	121.30	124.26
21	B	604	CL7	CHC-C1C-NC	-2.80	121.88	124.45
21	b	605	CL7	CHC-C1C-NC	-2.80	121.88	124.45
21	1	409	CL7	CHB-C1B-NB	-2.80	121.30	124.26
21	B	603	CL7	C3B-C2B-C1B	-2.80	103.79	107.16
21	D	404	CL7	CHD-C4C-C3C	-2.80	120.41	124.94
21	d	404	CL7	CHD-C4C-C3C	-2.80	120.41	124.94
21	5	416	CL7	CMB-C2B-C1B	2.80	129.63	125.37
21	c	504	CL7	O2D-CGD-CBD	2.79	116.23	111.27
21	3	513	CL7	CHB-C1B-NB	-2.79	121.30	124.26
21	d	404	CL7	CHB-C1B-NB	-2.79	121.30	124.26
23	B	627	8CT	C23-C21-C20	2.79	123.23	118.94
32	3	519	ZEX	C19-C9-C10	-2.79	119.01	122.92
32	7	519	ZEX	C19-C9-C10	-2.79	119.01	122.92
21	4	409	CL7	C4C-C3C-C2C	-2.79	103.49	107.13
21	2	502	CL7	CAA-CBA-CGA	-2.79	105.09	113.25
21	6	502	CL7	CAA-CBA-CGA	-2.79	105.09	113.25
21	3	511	CL7	O2A-CGA-CBA	2.79	120.67	111.91
21	7	511	CL7	O2A-CGA-CBA	2.79	120.67	111.91
21	b	609	CL7	CHC-C1C-NC	-2.79	121.89	124.45
21	C	502	CL7	CHD-C1D-ND	-2.79	121.30	124.26
23	4	402	8CT	C14-C13-C12	-2.79	123.33	127.31
23	8	402	8CT	C14-C13-C12	-2.79	123.33	127.31
21	D	402	CL7	C3B-C2B-C1B	-2.79	103.80	107.16
21	d	402	CL7	C3B-C2B-C1B	-2.79	103.80	107.16
23	b	601	8CT	C27-C26-C25	-2.78	119.02	122.92
21	3	501	CL7	CHB-C1B-NB	-2.78	121.31	124.26
21	7	501	CL7	CHB-C1B-NB	-2.78	121.31	124.26
23	C	515	8CT	C18-C17-C16	-2.78	123.34	127.31
21	3	510	CL7	O2D-CGD-CBD	2.78	116.22	111.27
21	7	510	CL7	O2D-CGD-CBD	2.78	116.22	111.27
32	8	419	ZEX	C18-C5-C6	-2.78	121.40	124.53
21	7	510	CL7	C3B-C2B-C1B	-2.78	103.80	107.16
21	7	503	CL7	CAA-CBA-CGA	-2.78	105.12	113.25
21	7	512	CL7	CHB-C1B-NB	-2.78	121.31	124.26
21	8	409	CL7	C4C-C3C-C2C	-2.78	103.50	107.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	616	CL7	C3B-C2B-C1B	-2.78	103.80	107.16
21	B	612	CL7	CAA-CBA-CGA	-2.78	105.12	113.25
21	6	507	CL7	CAA-CBA-CGA	-2.78	105.12	113.25
21	7	502	CL7	CHC-C1C-NC	-2.78	121.90	124.45
21	5	416	CL7	CHB-C1B-NB	-2.78	121.31	124.26
21	B	606	CL7	CAA-C2A-C3A	-2.78	105.17	112.78
21	b	607	CL7	CAA-C2A-C3A	-2.78	105.17	112.78
23	b	601	8CT	C23-C21-C20	2.78	123.21	118.94
21	B	608	CL7	CHC-C1C-NC	-2.78	121.90	124.45
21	B	615	CL7	C3B-C2B-C1B	-2.78	103.81	107.16
21	1	414	CL7	C3B-C2B-C1B	-2.78	103.81	107.16
21	5	414	CL7	C3B-C2B-C1B	-2.78	103.81	107.16
21	c	505	CL7	O2D-CGD-CBD	2.78	116.20	111.27
21	6	512	CL7	CAC-C3C-C2C	2.78	132.28	127.53
21	b	604	CL7	C3B-C2B-C1B	-2.78	103.81	107.16
32	1	422	ZEX	C35-C15-C14	-2.77	117.79	123.47
23	C	515	8CT	C07-C02-C03	-2.77	118.70	122.73
21	3	512	CL7	CHB-C1B-NB	-2.77	121.32	124.26
21	7	516	CL7	CHB-C1B-NB	-2.77	121.32	124.26
32	5	422	ZEX	C35-C15-C14	-2.77	117.79	123.47
21	c	518	CL7	CMB-C2B-C1B	2.77	129.59	125.37
21	2	512	CL7	CAC-C3C-C2C	2.77	132.27	127.53
21	2	510	CL7	CMB-C2B-C1B	2.77	129.59	125.37
21	6	510	CL7	CMB-C2B-C1B	2.77	129.59	125.37
21	2	506	CL7	O2D-CGD-CBD	2.77	116.19	111.27
21	2	507	CL7	CAA-CBA-CGA	-2.77	105.15	113.25
21	D	405	CL7	C3B-C2B-C1B	-2.77	103.81	107.16
21	3	503	CL7	CAA-CBA-CGA	-2.77	105.15	113.25
21	1	403	CL7	C7-C6-C5	-2.77	105.83	113.36
21	5	403	CL7	C7-C6-C5	-2.77	105.83	113.36
21	7	513	CL7	CHB-C1B-NB	-2.77	121.33	124.26
21	5	420	CL7	CHC-C1C-NC	-2.77	121.91	124.45
21	C	518	CL7	CHB-C1B-NB	-2.77	121.33	124.26
21	D	404	CL7	CHB-C1B-NB	-2.77	121.33	124.26
21	4	408	CL7	O2D-CGD-CBD	2.77	116.19	111.27
21	8	408	CL7	O2D-CGD-CBD	2.77	116.19	111.27
21	6	506	CL7	C4-C3-C5	2.77	119.93	115.27
21	1	420	CL7	CHC-C1C-NC	-2.77	121.91	124.45
21	1	406	CL7	CHD-C1D-ND	-2.76	121.33	124.26
21	c	514	CL7	CHC-C1C-NC	-2.76	121.92	124.45
21	2	509	CL7	CMB-C2B-C1B	2.76	129.57	125.37
21	5	406	CL7	C3B-C2B-C1B	-2.76	103.83	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	404	CL7	C4C-C3C-C2C	-2.76	103.53	107.13
21	5	404	CL7	C4C-C3C-C2C	-2.76	103.53	107.13
21	3	503	CL7	O2D-CGD-CBD	2.76	116.17	111.27
21	7	503	CL7	O2D-CGD-CBD	2.76	116.17	111.27
21	4	417	CL7	C3A-C4A-CHB	-2.76	119.61	123.70
21	8	417	CL7	C3A-C4A-CHB	-2.76	119.61	123.70
21	B	616	CL7	C3B-C2B-C1B	-2.76	103.83	107.16
23	B	627	8CT	C27-C26-C25	-2.76	119.06	122.92
23	B	627	8CT	C05-C04-C03	2.76	114.73	110.48
23	b	601	8CT	C05-C04-C03	2.76	114.73	110.48
23	A	404	8CT	C24-C23-C21	-2.76	118.67	126.42
23	a	404	8CT	C24-C23-C21	-2.76	118.67	126.42
21	1	415	CL7	C4C-C3C-C2C	-2.76	103.53	107.13
21	4	416	CL7	C4C-C3C-C2C	-2.76	103.53	107.13
21	5	415	CL7	C4C-C3C-C2C	-2.76	103.53	107.13
21	8	416	CL7	C4C-C3C-C2C	-2.76	103.53	107.13
21	2	514	CL7	C3B-C2B-C1B	-2.75	103.84	107.16
21	6	514	CL7	C3B-C2B-C1B	-2.75	103.84	107.16
23	B	617	8CT	C25-C24-C23	-2.75	114.62	123.22
21	3	504	CL7	CMB-C2B-C1B	2.75	129.56	125.37
21	6	509	CL7	CMB-C2B-C1B	2.75	129.56	125.37
21	1	416	CL7	CHC-C1C-NC	-2.75	121.92	124.45
21	5	416	CL7	CHC-C1C-NC	-2.75	121.92	124.45
23	b	618	8CT	C25-C24-C23	-2.75	114.63	123.22
21	3	514	CL7	CMB-C2B-C1B	2.75	129.56	125.37
21	7	514	CL7	CMB-C2B-C1B	2.75	129.56	125.37
21	2	502	CL7	CMB-C2B-C1B	2.75	129.56	125.37
21	6	502	CL7	CMB-C2B-C1B	2.75	129.56	125.37
21	3	516	CL7	CHB-C1B-NB	-2.75	121.35	124.26
21	4	415	CL7	CHC-C1C-NC	-2.75	121.93	124.45
21	8	415	CL7	CHC-C1C-NC	-2.75	121.93	124.45
21	1	402	CL7	CMB-C2B-C1B	2.75	129.55	125.37
21	5	402	CL7	CMB-C2B-C1B	2.75	129.55	125.37
21	6	506	CL7	O2D-CGD-CBD	2.75	116.15	111.27
21	2	506	CL7	C4-C3-C5	2.75	119.89	115.27
21	2	512	CL7	C7-C6-C5	-2.74	105.90	113.36
21	6	512	CL7	C7-C6-C5	-2.74	105.90	113.36
21	1	410	CL7	C3B-C2B-C1B	-2.74	103.85	107.16
21	5	410	CL7	C3B-C2B-C1B	-2.74	103.85	107.16
21	A	406	CL7	C3B-C2B-C1B	-2.74	103.85	107.16
21	1	417	CL7	C7-C6-C5	-2.74	105.91	113.36
21	5	417	CL7	C7-C6-C5	-2.74	105.91	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	515	8CT	C18-C17-C16	-2.74	123.40	127.31
21	B	614	CL7	CHB-C1B-NB	-2.74	121.35	124.26
21	b	615	CL7	CHB-C1B-NB	-2.74	121.35	124.26
21	3	502	CL7	CHC-C1C-NC	-2.74	121.93	124.45
21	8	413	CL7	C3B-C2B-C1B	-2.74	103.85	107.16
21	c	502	CL7	CHC-C1C-NC	-2.74	121.94	124.45
21	D	402	CL7	CHB-C1B-NB	-2.74	121.36	124.26
21	8	413	CL7	CHB-C1B-NB	-2.74	121.36	124.26
21	2	504	CL7	C3B-C2B-C1B	-2.74	103.85	107.16
21	6	504	CL7	C3B-C2B-C1B	-2.74	103.85	107.16
21	6	507	CL7	CHD-C4C-C3C	-2.74	120.50	124.94
21	A	403	CL7	CHD-C1D-ND	-2.74	121.36	124.26
21	2	518	CL7	CHC-C1C-NC	-2.74	121.94	124.45
21	6	518	CL7	CHC-C1C-NC	-2.74	121.94	124.45
21	B	616	CL7	CAA-CBA-CGA	-2.74	105.24	112.51
21	b	617	CL7	CAA-CBA-CGA	-2.74	105.24	112.51
21	4	413	CL7	CHB-C1B-NB	-2.74	121.36	124.26
21	1	406	CL7	C3B-C2B-C1B	-2.74	103.86	107.16
21	3	504	CL7	CHB-C1B-NB	-2.74	121.36	124.26
21	6	518	CL7	CHB-C1B-NB	-2.74	121.36	124.26
21	7	504	CL7	CHB-C1B-NB	-2.74	121.36	124.26
23	C	519	8CT	C19-C18-C17	-2.74	117.87	123.47
21	a	401	CL7	CAA-C2A-C3A	-2.74	105.29	112.78
21	3	503	CL7	C3B-C2B-C1B	-2.74	103.86	107.16
21	c	518	CL7	C3B-C2B-C1B	-2.73	103.86	107.16
21	c	505	CL7	C7-C6-C5	-2.73	105.94	113.36
23	c	515	8CT	C07-C02-C03	-2.73	118.76	122.73
21	4	413	CL7	C3B-C2B-C1B	-2.73	103.86	107.16
32	4	419	ZEX	C15-C35-C34	-2.73	117.88	123.47
32	8	419	ZEX	C15-C35-C34	-2.73	117.88	123.47
21	1	402	CL7	O2D-CGD-CBD	2.73	116.12	111.27
21	5	402	CL7	O2D-CGD-CBD	2.73	116.12	111.27
21	c	504	CL7	CMB-C2B-C1B	2.73	129.53	125.37
21	C	518	CL7	CMB-C2B-C1B	2.73	129.53	125.37
21	7	504	CL7	CMB-C2B-C1B	2.73	129.53	125.37
21	7	503	CL7	C3B-C2B-C1B	-2.73	103.87	107.16
21	4	407	CL7	C3B-C2B-C1B	-2.73	103.87	107.16
21	A	406	CL7	CHC-C1C-NC	-2.73	121.95	124.45
21	a	405	CL7	CHC-C1C-NC	-2.73	121.95	124.45
21	C	506	CL7	C3B-C2B-C1B	-2.73	103.87	107.16
21	c	506	CL7	C3B-C2B-C1B	-2.73	103.87	107.16
21	A	401	CL7	CAA-C2A-C3A	-2.73	105.31	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	518	CL7	CHB-C1B-NB	-2.73	121.37	124.26
23	c	519	8CT	C19-C18-C17	-2.73	117.89	123.47
21	2	507	CL7	CHD-C4C-C3C	-2.73	120.52	124.94
21	b	617	CL7	C3B-C2B-C1B	-2.73	103.87	107.16
21	2	513	CL7	CHD-C4C-C3C	-2.73	120.52	124.94
21	6	513	CL7	CHD-C4C-C3C	-2.73	120.52	124.94
21	3	508	CL7	CMB-C2B-C1B	2.72	129.52	125.37
21	7	508	CL7	CMB-C2B-C1B	2.72	129.52	125.37
23	C	515	8CT	C39-C16-C15	2.72	122.37	118.08
23	c	515	8CT	C39-C16-C15	2.72	122.37	118.08
21	C	518	CL7	C3B-C2B-C1B	-2.72	103.87	107.16
21	3	510	CL7	C3B-C2B-C1B	-2.72	103.87	107.16
21	3	501	CL7	C7-C6-C5	-2.72	105.96	113.36
21	1	418	CL7	C3B-C2B-C1B	-2.72	103.87	107.16
21	5	418	CL7	C3B-C2B-C1B	-2.72	103.87	107.16
21	A	401	CL7	CHB-C1B-NB	-2.72	121.37	124.26
21	C	505	CL7	C7-C6-C5	-2.72	105.96	113.36
21	A	401	CL7	CHC-C1C-NC	-2.72	121.95	124.45
21	a	401	CL7	CHC-C1C-NC	-2.72	121.95	124.45
21	B	602	CL7	CHB-C1B-NB	-2.72	121.38	124.26
21	b	603	CL7	CHB-C1B-NB	-2.72	121.38	124.26
21	B	614	CL7	C7-C6-C5	-2.72	105.97	113.36
21	4	415	CL7	C3B-C2B-C1B	-2.72	103.88	107.16
21	8	415	CL7	C3B-C2B-C1B	-2.72	103.88	107.16
21	C	508	CL7	CHC-C1C-NC	-2.72	121.95	124.45
21	7	518	CL7	CHB-C1B-NB	-2.72	121.38	124.26
21	3	515	CL7	CMB-C2B-C1B	2.72	129.51	125.37
21	7	515	CL7	CMB-C2B-C1B	2.72	129.51	125.37
21	A	401	CL7	C3B-C2B-C1B	-2.72	103.88	107.16
21	3	509	CL7	CHD-C1D-ND	-2.72	121.38	124.26
21	7	509	CL7	CHD-C1D-ND	-2.72	121.38	124.26
21	6	510	CL7	O2A-C1-C2	-2.71	101.50	108.64
32	1	421	ZEX	C18-C5-C4	2.71	119.38	114.36
32	5	421	ZEX	C18-C5-C4	2.71	119.38	114.36
21	C	509	CL7	C7-C6-C5	-2.71	105.99	113.36
21	b	615	CL7	C7-C6-C5	-2.71	105.99	113.36
21	a	401	CL7	C3B-C2B-C1B	-2.71	103.89	107.16
24	3	523	SQD	O8-S-C6	-2.71	101.42	105.74
24	7	523	SQD	O8-S-C6	-2.71	101.42	105.74
32	2	525	ZEX	C18-C5-C4	2.71	119.38	114.36
32	6	524	ZEX	C18-C5-C4	2.71	119.38	114.36
21	B	614	CL7	CHC-C1C-NC	-2.71	121.96	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	404	CL7	CHC-C1C-NC	-2.71	121.96	124.45
21	b	615	CL7	CHC-C1C-NC	-2.71	121.96	124.45
21	8	404	CL7	CHC-C1C-NC	-2.71	121.96	124.45
21	c	510	CL7	C3B-C2B-C1B	-2.71	103.89	107.16
21	8	409	CL7	C3B-C2B-C1B	-2.71	103.89	107.16
21	a	403	CL7	CHD-C1D-ND	-2.71	121.39	124.26
21	7	501	CL7	C7-C6-C5	-2.71	105.99	113.36
21	7	507	CL7	CHB-C1B-NB	-2.71	121.39	124.26
26	C	501	LMG	O7-C10-O9	-2.71	117.16	123.70
21	5	405	CL7	CHC-C1C-NC	-2.71	121.97	124.45
21	5	414	CL7	CHB-C1B-NB	-2.71	121.39	124.26
21	3	518	CL7	CHB-C1B-NB	-2.71	121.39	124.26
21	3	509	CL7	C3B-C2B-C1B	-2.71	103.89	107.16
21	8	407	CL7	C3B-C2B-C1B	-2.71	103.89	107.16
21	6	514	CL7	CHB-C1B-NB	-2.71	121.39	124.26
21	C	502	CL7	CHC-C1C-NC	-2.71	121.97	124.45
21	c	509	CL7	C7-C6-C5	-2.70	106.01	113.36
21	B	610	CL7	C3B-C2B-C1B	-2.70	103.90	107.16
21	b	611	CL7	C3B-C2B-C1B	-2.70	103.90	107.16
21	C	506	CL7	CHC-C1C-NC	-2.70	121.97	124.45
21	c	506	CL7	CHC-C1C-NC	-2.70	121.97	124.45
21	5	408	CL7	CHD-C4C-C3C	-2.70	120.56	124.94
21	C	510	CL7	C3B-C2B-C1B	-2.70	103.90	107.16
21	C	502	CL7	CHB-C1B-NB	-2.70	121.40	124.26
21	a	405	CL7	C3B-C2B-C1B	-2.70	103.90	107.16
32	7	522	ZEX	C27-C26-C25	-2.70	118.48	122.84
21	a	401	CL7	CHB-C1B-NB	-2.70	121.40	124.26
21	c	507	CL7	O2D-CGD-CBD	2.70	116.06	111.27
21	3	513	CL7	C3B-C2B-C1B	-2.70	103.90	107.16
21	7	513	CL7	C3B-C2B-C1B	-2.70	103.90	107.16
21	C	504	CL7	CMB-C2B-C1B	2.70	129.48	125.37
21	C	511	CL7	C3B-C2B-C1B	-2.70	103.91	107.16
21	c	511	CL7	C3B-C2B-C1B	-2.70	103.91	107.16
23	b	619	8CT	C40-C12-C13	-2.70	119.15	122.92
21	2	510	CL7	O2A-C1-C2	-2.70	101.55	108.64
21	6	503	CL7	C3B-C2B-C1B	-2.69	103.91	107.16
21	B	615	CL7	C3B-C4B-NB	2.69	113.01	110.52
21	8	405	CL7	CMB-C2B-C1B	2.69	129.47	125.37
21	2	507	CL7	CHD-C1D-ND	-2.69	121.41	124.26
21	d	402	CL7	CHB-C1B-NB	-2.69	121.41	124.26
21	6	507	CL7	CHD-C1D-ND	-2.69	121.41	124.26
21	1	408	CL7	CHD-C4C-C3C	-2.69	120.58	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	603	CL7	O2D-CGD-CBD	2.69	116.05	111.27
21	B	612	CL7	CHD-C1D-ND	-2.69	121.41	124.26
21	b	613	CL7	CHD-C1D-ND	-2.69	121.41	124.26
21	b	610	CL7	C3B-C2B-C1B	-2.69	103.92	107.16
23	c	516	8CT	C19-C18-C17	-2.69	117.97	123.47
21	5	413	CL7	CHC-C1C-NC	-2.69	121.99	124.45
21	b	604	CL7	O2D-CGD-CBD	2.69	116.04	111.27
21	2	503	CL7	C3B-C2B-C1B	-2.69	103.92	107.16
21	B	609	CL7	C3B-C2B-C1B	-2.68	103.92	107.16
21	3	512	CL7	C3B-C2B-C1B	-2.68	103.92	107.16
21	4	409	CL7	C3B-C2B-C1B	-2.68	103.92	107.16
21	7	512	CL7	C3B-C2B-C1B	-2.68	103.92	107.16
21	2	512	CL7	C3B-C2B-C1B	-2.68	103.92	107.16
21	6	512	CL7	C3B-C2B-C1B	-2.68	103.92	107.16
21	2	503	CL7	CHB-C1B-NB	-2.68	121.42	124.26
21	6	503	CL7	CHB-C1B-NB	-2.68	121.42	124.26
21	3	512	CL7	C4C-C3C-C2C	-2.68	103.63	107.13
21	7	512	CL7	C4C-C3C-C2C	-2.68	103.63	107.13
21	C	507	CL7	O2D-CGD-CBD	2.68	116.03	111.27
32	3	522	ZEX	C27-C26-C25	-2.68	118.51	122.84
21	1	412	CL7	CHB-C1B-NB	-2.68	121.42	124.26
21	3	518	CL7	C3B-C2B-C1B	-2.68	103.93	107.16
21	b	616	CL7	C3B-C4B-NB	2.68	113.00	110.52
21	B	601	CL7	C3B-C2B-C1B	-2.68	103.93	107.16
21	B	613	CL7	C3B-C2B-C1B	-2.67	103.93	107.16
21	1	408	CL7	CHB-C1B-NB	-2.67	121.43	124.26
21	5	408	CL7	CHB-C1B-NB	-2.67	121.43	124.26
21	7	518	CL7	CAA-CBA-CGA	-2.67	105.41	112.51
21	4	415	CL7	CAC-C3C-C4C	-2.67	120.47	124.68
21	1	414	CL7	CHB-C1B-NB	-2.67	121.43	124.26
21	4	405	CL7	CMB-C2B-C1B	2.67	129.44	125.37
21	7	509	CL7	C3B-C2B-C1B	-2.67	103.94	107.16
21	1	405	CL7	CHC-C1C-NC	-2.67	122.00	124.45
21	5	412	CL7	C1C-C2C-C3C	-2.67	103.04	106.94
23	C	516	8CT	C19-C18-C17	-2.67	118.00	123.47
21	1	414	CL7	CMB-C2B-C1B	2.67	129.44	125.37
21	5	414	CL7	CMB-C2B-C1B	2.67	129.44	125.37
21	2	514	CL7	CHB-C1B-NB	-2.67	121.43	124.26
21	1	413	CL7	CHC-C1C-NC	-2.67	122.00	124.45
23	B	618	8CT	C40-C12-C13	-2.67	119.19	122.92
21	a	403	CL7	C7-C6-C5	-2.67	106.11	113.36
21	2	510	CL7	CHB-C1B-NB	-2.67	121.43	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	510	CL7	CHB-C1B-NB	-2.67	121.43	124.26
21	7	516	CL7	CHC-C1C-NC	-2.67	122.00	124.45
21	C	503	CL7	O2D-CGD-CBD	2.67	116.00	111.27
21	c	503	CL7	O2D-CGD-CBD	2.67	116.00	111.27
21	B	607	CL7	C3B-C2B-C1B	-2.67	103.94	107.16
21	b	608	CL7	C3B-C2B-C1B	-2.67	103.94	107.16
21	1	412	CL7	C1C-C2C-C3C	-2.67	103.05	106.94
21	c	508	CL7	CHC-C1C-NC	-2.66	122.00	124.45
21	7	513	CL7	CMB-C2B-C1B	2.66	129.43	125.37
21	3	516	CL7	CHC-C1C-NC	-2.66	122.01	124.45
21	4	413	CL7	CHD-C1D-ND	-2.66	121.44	124.26
21	1	413	CL7	C3B-C2B-C1B	-2.66	103.95	107.16
21	3	518	CL7	CAA-CBA-CGA	-2.66	105.44	112.51
21	3	507	CL7	CHB-C1B-NB	-2.66	121.44	124.26
21	6	504	CL7	CHD-C4C-C3C	-2.66	120.63	124.94
22	d	408	PHO	CBA-CAA-C2A	-2.66	106.04	113.81
32	2	523	ZEX	C7-C6-C5	2.66	127.90	121.46
32	6	522	ZEX	C7-C6-C5	2.66	127.90	121.46
21	B	612	CL7	C7-C6-C5	-2.66	106.14	113.36
21	b	613	CL7	C7-C6-C5	-2.66	106.14	113.36
32	6	524	ZEX	C11-C12-C13	-2.66	118.95	126.42
32	8	418	ZEX	C27-C26-C25	-2.66	118.55	122.84
21	3	505	CL7	CAA-CBA-CGA	-2.66	105.49	113.25
21	b	614	CL7	C3B-C2B-C1B	-2.66	103.95	107.16
21	B	602	CL7	C7-C6-C5	-2.66	106.14	113.36
21	b	603	CL7	C7-C6-C5	-2.66	106.14	113.36
21	b	609	CL7	CHD-C1D-ND	-2.66	121.44	124.26
21	B	605	CL7	CHC-C1C-NC	-2.66	122.01	124.45
21	5	405	CL7	C3B-C2B-C1B	-2.66	103.96	107.16
22	D	408	PHO	CBA-CAA-C2A	-2.66	106.05	113.81
21	5	412	CL7	CHB-C1B-NB	-2.66	121.45	124.26
21	A	403	CL7	C7-C6-C5	-2.65	106.15	113.36
21	3	501	CL7	C3B-C2B-C1B	-2.65	103.96	107.16
21	7	501	CL7	C3B-C2B-C1B	-2.65	103.96	107.16
21	1	417	CL7	C3B-C2B-C1B	-2.65	103.96	107.16
21	5	417	CL7	C3B-C2B-C1B	-2.65	103.96	107.16
23	b	601	8CT	C28-C26-C25	2.65	123.01	118.94
21	8	415	CL7	CAC-C3C-C4C	-2.65	120.50	124.68
21	7	518	CL7	C3B-C2B-C1B	-2.65	103.96	107.16
21	3	505	CL7	CHB-C1B-NB	-2.65	121.45	124.26
21	7	505	CL7	CHB-C1B-NB	-2.65	121.45	124.26
32	6	519	ZEX	C28-C29-C30	2.65	123.01	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	606	CL7	CHC-C1C-NC	-2.65	122.02	124.45
32	2	525	ZEX	C11-C12-C13	-2.65	118.97	126.42
21	7	506	CL7	CHC-C1C-NC	-2.65	122.02	124.45
21	C	512	CL7	C1C-C2C-C3C	-2.65	103.07	106.94
21	c	512	CL7	C1C-C2C-C3C	-2.65	103.07	106.94
21	8	413	CL7	CHD-C1D-ND	-2.65	121.45	124.26
32	2	519	ZEX	C28-C29-C30	2.65	123.01	118.94
23	A	404	8CT	C13-C14-C15	-2.65	114.95	123.22
23	a	404	8CT	C13-C14-C15	-2.65	114.95	123.22
21	4	411	CL7	CAA-C2A-C3A	-2.65	105.53	112.78
21	8	411	CL7	CAA-C2A-C3A	-2.65	105.53	112.78
21	7	505	CL7	CAA-CBA-CGA	-2.65	105.52	113.25
21	D	405	CL7	O2D-CGD-O1D	-2.65	118.66	123.84
21	7	511	CL7	CHC-C1C-NC	-2.65	122.02	124.45
22	D	408	PHO	CED-O2D-CGD	2.65	121.92	115.94
32	4	418	ZEX	C27-C26-C25	-2.65	118.56	122.84
21	b	602	CL7	C3B-C2B-C1B	-2.64	103.97	107.16
21	4	412	CL7	C3B-C2B-C1B	-2.64	103.97	107.16
21	c	514	CL7	C3B-C2B-C1B	-2.64	103.97	107.16
21	8	412	CL7	C3B-C2B-C1B	-2.64	103.97	107.16
21	c	502	CL7	CHB-C1B-NB	-2.64	121.46	124.26
21	2	504	CL7	CHD-C4C-C3C	-2.64	120.66	124.94
21	3	513	CL7	CMB-C2B-C1B	2.64	129.39	125.37
21	3	515	CL7	CHB-C1B-NB	-2.64	121.46	124.26
21	7	515	CL7	CHB-C1B-NB	-2.64	121.46	124.26
32	4	419	ZEX	C7-C8-C9	-2.64	122.25	126.23
21	c	513	CL7	CHB-C1B-NB	-2.64	121.46	124.26
21	3	511	CL7	CHC-C1C-NC	-2.64	122.03	124.45
21	5	407	CL7	CMA-C3A-C2A	-2.64	109.94	116.10
21	2	507	CL7	CMB-C2B-C1B	2.64	129.39	125.37
21	6	507	CL7	CMB-C2B-C1B	2.64	129.39	125.37
22	d	408	PHO	CED-O2D-CGD	2.64	121.90	115.94
23	c	519	8CT	C01-C02-C07	2.64	118.68	113.62
21	5	406	CL7	CMB-C2B-C1B	2.64	129.38	125.37
21	C	512	CL7	CHB-C1B-NB	-2.64	121.47	124.26
21	c	512	CL7	CHB-C1B-NB	-2.64	121.47	124.26
32	8	419	ZEX	C7-C8-C9	-2.64	122.25	126.23
23	C	519	8CT	C01-C02-C07	2.64	118.68	113.62
21	5	413	CL7	C3B-C2B-C1B	-2.63	103.98	107.16
21	1	407	CL7	CMA-C3A-C2A	-2.63	109.95	116.10
21	b	612	CL7	C1C-C2C-C3C	-2.63	103.10	106.94
21	2	516	CL7	CMB-C2B-C1B	2.63	129.38	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	516	CL7	CMB-C2B-C1B	2.63	129.38	125.37
21	1	420	CL7	C4C-C3C-C2C	-2.63	103.70	107.13
21	A	401	CL7	CMB-C2B-C1B	2.63	129.37	125.37
23	B	627	8CT	C28-C26-C25	2.63	122.97	118.94
21	4	414	CL7	CAC-C3C-C2C	2.63	132.03	127.53
21	B	610	CL7	CHB-C1B-NB	-2.63	121.47	124.26
21	a	401	CL7	CMB-C2B-C1B	2.63	129.37	125.37
21	8	414	CL7	CAC-C3C-C2C	2.63	132.02	127.53
32	4	418	ZEX	C11-C12-C13	-2.63	119.03	126.42
32	8	418	ZEX	C11-C12-C13	-2.63	119.03	126.42
23	c	515	8CT	C40-C12-C11	2.63	122.22	118.08
27	c	517	DGD	C3G-C2G-C1G	-2.63	105.58	111.79
21	B	611	CL7	C1C-C2C-C3C	-2.63	103.11	106.94
21	1	406	CL7	CMB-C2B-C1B	2.63	129.37	125.37
21	1	407	CL7	CMB-C2B-C1B	2.63	129.37	125.37
26	c	501	LMG	O7-C10-O9	-2.63	117.36	123.70
21	B	602	CL7	C3B-C2B-C1B	-2.62	103.99	107.16
21	b	603	CL7	C3B-C2B-C1B	-2.62	103.99	107.16
21	2	505	CL7	C7-C6-C5	-2.62	106.23	113.36
21	6	505	CL7	C7-C6-C5	-2.62	106.23	113.36
21	1	405	CL7	C3B-C2B-C1B	-2.62	104.00	107.16
21	5	420	CL7	C4C-C3C-C2C	-2.62	103.71	107.13
21	C	510	CL7	CHB-C1B-NB	-2.62	121.48	124.26
21	A	403	CL7	C1-C2-C3	2.62	130.58	126.04
21	6	510	CL7	C3B-C2B-C1B	-2.62	104.00	107.16
21	C	514	CL7	C3B-C2B-C1B	-2.62	104.00	107.16
21	2	509	CL7	C3B-C2B-C1B	-2.62	104.00	107.16
21	1	415	CL7	C3B-C2B-C1B	-2.62	104.00	107.16
21	4	408	CL7	C4C-C3C-C2C	-2.62	103.71	107.13
21	2	510	CL7	C3B-C2B-C1B	-2.62	104.00	107.16
21	3	509	CL7	C4-C3-C5	2.62	119.68	115.27
21	3	511	CL7	CHB-C1B-NB	-2.62	121.48	124.26
23	C	515	8CT	C18-C19-C20	-2.62	118.11	123.47
23	c	515	8CT	C18-C19-C20	-2.62	118.11	123.47
32	2	525	ZEX	C27-C26-C25	-2.62	118.61	122.84
32	6	524	ZEX	C27-C26-C25	-2.62	118.61	122.84
27	C	517	DGD	C3G-C2G-C1G	-2.62	105.60	111.79
21	d	404	CL7	C7-C6-C5	-2.62	106.25	113.36
21	8	407	CL7	CHB-C1B-NB	-2.62	121.49	124.26
21	7	506	CL7	CMB-C2B-C1B	2.62	129.35	125.37
21	1	410	CL7	CHB-C1B-NB	-2.62	121.49	124.26
32	4	419	ZEX	C30-C31-C32	-2.62	115.06	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	420	CL7	C3B-C2B-C1B	-2.61	104.00	107.16
21	a	403	CL7	C1-C2-C3	2.61	130.56	126.04
32	2	519	ZEX	C10-C11-C12	-2.61	115.06	123.22
32	6	519	ZEX	C10-C11-C12	-2.61	115.06	123.22
32	8	419	ZEX	C30-C31-C32	-2.61	115.06	123.22
21	1	416	CL7	C3B-C2B-C1B	-2.61	104.01	107.16
21	1	420	CL7	C3B-C2B-C1B	-2.61	104.01	107.16
21	c	504	CL7	C3B-C2B-C1B	-2.61	104.01	107.16
21	5	416	CL7	C3B-C2B-C1B	-2.61	104.01	107.16
21	4	410	CL7	CMB-C2B-C1B	2.61	129.35	125.37
21	8	410	CL7	CMB-C2B-C1B	2.61	129.35	125.37
21	4	407	CL7	O2D-CGD-CBD	2.61	115.91	111.27
21	8	407	CL7	O2D-CGD-CBD	2.61	115.91	111.27
21	4	409	CL7	C7-C6-C5	-2.61	106.27	113.36
21	8	409	CL7	C7-C6-C5	-2.61	106.27	113.36
21	6	509	CL7	C3B-C2B-C1B	-2.61	104.01	107.16
21	C	510	CL7	CMB-C2B-C1B	2.61	129.34	125.37
21	C	504	CL7	C3B-C2B-C1B	-2.61	104.01	107.16
21	C	513	CL7	CHB-C1B-NB	-2.61	121.49	124.26
21	3	513	CL7	C4C-C3C-C2C	-2.61	103.72	107.13
21	7	513	CL7	C4C-C3C-C2C	-2.61	103.72	107.13
21	B	608	CL7	CHD-C1D-ND	-2.61	121.50	124.26
21	d	405	CL7	O2D-CGD-O1D	-2.61	118.74	123.84
21	5	410	CL7	CHB-C1B-NB	-2.61	121.50	124.26
21	b	611	CL7	CHB-C1B-NB	-2.61	121.50	124.26
21	3	506	CL7	CMB-C2B-C1B	2.61	129.34	125.37
21	B	622	CL7	C3B-C2B-C1B	-2.61	104.02	107.16
21	1	407	CL7	C3B-C2B-C1B	-2.61	104.02	107.16
21	5	408	CL7	CHC-C1C-NC	-2.61	122.06	124.45
21	2	518	CL7	C3B-C2B-C1B	-2.61	104.02	107.16
21	6	518	CL7	C3B-C2B-C1B	-2.61	104.02	107.16
21	B	609	CL7	CAA-CBA-CGA	-2.60	105.64	113.25
23	C	515	8CT	C40-C12-C11	2.60	122.18	118.08
21	c	510	CL7	CMB-C2B-C1B	2.60	129.34	125.37
21	5	407	CL7	CMB-C2B-C1B	2.60	129.34	125.37
21	D	404	CL7	C7-C6-C5	-2.60	106.29	113.36
21	2	501	CL7	C1C-C2C-C3C	-2.60	103.14	106.94
21	6	501	CL7	C1C-C2C-C3C	-2.60	103.14	106.94
32	2	519	ZEX	C8-C7-C6	-2.60	119.89	127.20
32	6	519	ZEX	C8-C7-C6	-2.60	119.89	127.20
21	3	504	CL7	CHC-C1C-NC	-2.60	122.06	124.45
21	7	504	CL7	CHC-C1C-NC	-2.60	122.06	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	417	CL7	CMB-C2B-C1B	2.60	129.33	125.37
21	5	417	CL7	CMB-C2B-C1B	2.60	129.33	125.37
21	A	403	CL7	C3B-C2B-C1B	-2.60	104.02	107.16
21	b	610	CL7	CAA-CBA-CGA	-2.60	105.65	113.25
21	7	509	CL7	C4-C3-C5	2.60	119.65	115.27
31	F	101	HEM	CHD-C4C-NC	2.60	127.25	124.44
21	4	412	CL7	CHB-C1B-NB	-2.60	121.50	124.26
21	8	412	CL7	CHB-C1B-NB	-2.60	121.50	124.26
21	c	510	CL7	CHB-C1B-NB	-2.60	121.51	124.26
21	3	514	CL7	CHB-C1B-NB	-2.60	121.51	124.26
21	7	511	CL7	CHB-C1B-NB	-2.60	121.51	124.26
21	7	514	CL7	CHB-C1B-NB	-2.60	121.51	124.26
21	D	404	CL7	C3B-C2B-C1B	-2.60	104.03	107.16
21	d	404	CL7	C3B-C2B-C1B	-2.60	104.03	107.16
21	1	403	CL7	CMB-C2B-C1B	2.60	129.32	125.37
21	5	412	CL7	CAA-CBA-CGA	-2.60	105.61	112.51
21	B	608	CL7	CHB-C1B-NB	-2.60	121.51	124.26
21	2	510	CL7	CAA-CBA-CGA	-2.60	105.67	113.25
21	6	510	CL7	CAA-CBA-CGA	-2.60	105.67	113.25
21	5	408	CL7	C4C-C3C-C2C	-2.60	103.74	107.13
21	4	407	CL7	CHB-C1B-NB	-2.59	121.51	124.26
21	3	506	CL7	CHC-C1C-NC	-2.59	122.07	124.45
21	2	511	CL7	C3B-C2B-C1B	-2.59	104.03	107.16
21	6	511	CL7	C3B-C2B-C1B	-2.59	104.03	107.16
21	5	415	CL7	C3B-C2B-C1B	-2.59	104.03	107.16
21	1	412	CL7	CAA-CBA-CGA	-2.59	105.63	112.51
21	8	408	CL7	C4C-C3C-C2C	-2.59	103.75	107.13
21	B	606	CL7	C7-C6-C5	-2.59	106.32	113.36
21	b	607	CL7	C7-C6-C5	-2.59	106.32	113.36
21	a	403	CL7	C3B-C2B-C1B	-2.59	104.03	107.16
21	7	517	CL7	CHB-C1B-NB	-2.59	121.52	124.26
21	2	506	CL7	CHC-C1C-NC	-2.59	122.07	124.45
21	6	506	CL7	CHC-C1C-NC	-2.59	122.07	124.45
21	6	511	CL7	O2D-CGD-CBD	2.59	115.87	111.27
21	7	516	CL7	C4-C3-C5	2.59	119.63	115.27
21	5	407	CL7	C3B-C2B-C1B	-2.59	104.04	107.16
21	B	603	CL7	O2A-C1-C2	-2.59	101.83	108.64
21	b	604	CL7	O2A-C1-C2	-2.59	101.83	108.64
21	5	403	CL7	CMB-C2B-C1B	2.59	129.31	125.37
21	4	414	CL7	C3B-C2B-C1B	-2.59	104.04	107.16
21	3	502	CL7	C3B-C2B-C1B	-2.59	104.04	107.16
21	7	502	CL7	C3B-C2B-C1B	-2.59	104.04	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	511	CL7	O2D-CGD-CBD	2.59	115.86	111.27
21	3	517	CL7	CHB-C1B-NB	-2.59	121.52	124.26
21	1	403	CL7	C1C-C2C-C3C	-2.59	103.17	106.94
21	1	408	CL7	CHC-C1C-NC	-2.59	122.08	124.45
21	3	503	CL7	C4C-C3C-C2C	-2.59	103.76	107.13
21	7	503	CL7	C4C-C3C-C2C	-2.59	103.76	107.13
32	2	525	ZEX	C39-C29-C30	-2.58	119.31	122.92
32	6	524	ZEX	C39-C29-C30	-2.58	119.31	122.92
21	3	510	CL7	CAA-C2A-C3A	-2.58	105.71	112.78
21	C	513	CL7	CMB-C2B-C1B	2.58	129.30	125.37
21	c	513	CL7	CMB-C2B-C1B	2.58	129.30	125.37
21	2	503	CL7	C4C-C3C-C2C	-2.58	103.77	107.13
21	1	402	CL7	C4C-C3C-C2C	-2.58	103.77	107.13
21	1	408	CL7	C4C-C3C-C2C	-2.58	103.77	107.13
21	5	402	CL7	C4C-C3C-C2C	-2.58	103.77	107.13
23	4	402	8CT	C35-C30-C29	-2.58	109.44	112.70
23	8	402	8CT	C35-C30-C29	-2.58	109.44	112.70
21	C	505	CL7	C3B-C2B-C1B	-2.58	104.05	107.16
21	b	623	CL7	C3B-C2B-C1B	-2.58	104.05	107.16
21	C	504	CL7	CAA-CBA-CGA	-2.58	105.72	113.25
21	c	504	CL7	CAA-CBA-CGA	-2.58	105.72	113.25
21	6	503	CL7	C4C-C3C-C2C	-2.58	103.77	107.13
21	8	414	CL7	C3B-C2B-C1B	-2.58	104.05	107.16
21	3	516	CL7	C4-C3-C5	2.58	119.60	115.27
21	B	613	CL7	C4C-C3C-C2C	-2.57	103.77	107.13
21	C	503	CL7	C3B-C2B-C1B	-2.57	104.06	107.16
21	c	503	CL7	C3B-C2B-C1B	-2.57	104.06	107.16
21	3	509	CL7	C4C-C3C-C2C	-2.57	103.77	107.13
31	f	101	HEM	CHD-C4C-NC	2.57	127.22	124.44
21	b	612	CL7	CMB-C2B-C1B	2.57	129.28	125.37
21	5	403	CL7	C1C-C2C-C3C	-2.57	103.19	106.94
21	7	510	CL7	CAA-C2A-C3A	-2.57	105.74	112.78
21	1	415	CL7	CMB-C2B-C1B	2.57	129.28	125.37
21	5	415	CL7	CMB-C2B-C1B	2.57	129.28	125.37
23	K	101	8CT	C40-C12-C13	-2.57	119.33	122.92
21	3	509	CL7	CHB-C1B-NB	-2.57	121.54	124.26
21	1	411	CL7	C4C-C3C-C2C	-2.57	103.78	107.13
21	B	611	CL7	CMB-C2B-C1B	2.57	129.28	125.37
21	2	508	CL7	CHC-C1C-NC	-2.56	122.10	124.45
21	6	508	CL7	CHC-C1C-NC	-2.56	122.10	124.45
21	4	410	CL7	CHB-C1B-NB	-2.56	121.54	124.26
21	8	410	CL7	CHB-C1B-NB	-2.56	121.54	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	616	CL7	CHC-C1C-NC	-2.56	122.10	124.45
21	b	617	CL7	CHC-C1C-NC	-2.56	122.10	124.45
21	c	505	CL7	C3B-C2B-C1B	-2.56	104.07	107.16
21	3	502	CL7	C4-C3-C5	2.56	119.58	115.27
21	7	502	CL7	C4-C3-C5	2.56	119.58	115.27
21	B	615	CL7	CHC-C1C-NC	-2.56	122.10	124.45
21	b	616	CL7	CHC-C1C-NC	-2.56	122.10	124.45
21	c	502	CL7	C4C-C3C-C2C	-2.56	103.79	107.13
21	6	511	CL7	CHB-C1B-NB	-2.56	121.55	124.26
21	5	411	CL7	C4C-C3C-C2C	-2.56	103.79	107.13
21	B	610	CL7	C4C-C3C-C2C	-2.56	103.79	107.13
21	4	407	CL7	C4C-C3C-C2C	-2.56	103.79	107.13
21	b	611	CL7	C4C-C3C-C2C	-2.56	103.79	107.13
21	b	614	CL7	C4C-C3C-C2C	-2.56	103.79	107.13
21	1	417	CL7	CHB-C1B-NB	-2.56	121.55	124.26
21	2	517	CL7	C4C-C3C-C2C	-2.56	103.79	107.13
21	4	410	CL7	CHC-C1C-NC	-2.56	122.10	124.45
21	1	403	CL7	C3B-C2B-C1B	-2.56	104.08	107.16
21	6	505	CL7	C3B-C2B-C1B	-2.56	104.08	107.16
32	3	519	ZEX	C11-C12-C13	-2.56	119.23	126.42
21	5	403	CL7	C3B-C2B-C1B	-2.56	104.08	107.16
21	b	609	CL7	CHB-C1B-NB	-2.56	121.55	124.26
21	2	504	CL7	CHC-C1C-NC	-2.55	122.11	124.45
21	6	504	CL7	CHC-C1C-NC	-2.55	122.11	124.45
21	6	517	CL7	CHB-C1B-NB	-2.55	121.55	124.26
21	8	410	CL7	CHC-C1C-NC	-2.55	122.11	124.45
21	C	502	CL7	CAA-CBA-CGA	-2.55	105.79	113.25
21	7	509	CL7	C4C-C3C-C2C	-2.55	103.80	107.13
21	1	419	CL7	C3B-C2B-C1B	-2.55	104.08	107.16
21	6	511	CL7	C7-C6-C5	-2.55	106.43	113.36
21	7	508	CL7	O2A-C1-C2	-2.55	101.93	108.64
21	3	511	CL7	C3B-C2B-C1B	-2.55	104.08	107.16
21	7	511	CL7	C3B-C2B-C1B	-2.55	104.08	107.16
21	3	509	CL7	CMB-C2B-C1B	2.55	129.25	125.37
32	7	519	ZEX	C11-C12-C13	-2.55	119.25	126.42
21	8	407	CL7	C4C-C3C-C2C	-2.55	103.80	107.13
21	c	502	CL7	CAA-CBA-CGA	-2.55	105.80	113.25
21	8	411	CL7	CMB-C2B-C1B	2.55	129.25	125.37
21	5	417	CL7	CHB-C1B-NB	-2.55	121.56	124.26
21	7	510	CL7	CHB-C1B-NB	-2.55	121.56	124.26
21	6	517	CL7	C4C-C3C-C2C	-2.55	103.81	107.13
32	1	421	ZEX	C7-C8-C9	-2.55	122.39	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	5	421	ZEX	C7-C8-C9	-2.55	122.39	126.23
21	c	509	CL7	CHC-C1C-NC	-2.55	122.11	124.45
23	C	515	8CT	C35-C30-C31	2.55	115.98	111.42
23	c	515	8CT	C35-C30-C31	2.55	115.98	111.42
21	5	413	CL7	C3B-C4B-NB	2.54	112.88	110.52
21	3	505	CL7	C4-C3-C5	2.54	119.55	115.27
23	k	101	8CT	C40-C12-C13	-2.54	119.36	122.92
21	7	509	CL7	CHB-C1B-NB	-2.54	121.56	124.26
21	c	513	CL7	CMA-C3A-C2A	-2.54	110.16	116.10
21	5	407	CL7	CHB-C1B-NB	-2.54	121.56	124.26
27	C	517	DGD	C4E-C3E-C2E	-2.54	106.39	110.82
21	5	419	CL7	C3B-C2B-C1B	-2.54	104.09	107.16
21	4	405	CL7	O2A-CGA-CBA	2.54	119.88	111.91
21	8	405	CL7	O2A-CGA-CBA	2.54	119.88	111.91
21	2	507	CL7	CED-O2D-CGD	-2.54	110.19	115.94
21	6	507	CL7	CED-O2D-CGD	-2.54	110.19	115.94
21	7	509	CL7	CMB-C2B-C1B	2.54	129.24	125.37
21	2	501	CL7	C3B-C2B-C1B	-2.54	104.09	107.16
21	6	501	CL7	C3B-C2B-C1B	-2.54	104.09	107.16
21	4	409	CL7	C1-C2-C3	-2.54	121.65	126.04
21	8	409	CL7	C1-C2-C3	-2.54	121.65	126.04
21	C	502	CL7	C4C-C3C-C2C	-2.54	103.82	107.13
21	C	502	CL7	C7-C6-C5	-2.54	106.46	113.36
21	5	411	CL7	CHB-C1B-NB	-2.54	121.57	124.26
21	2	511	CL7	C7-C6-C5	-2.54	106.47	113.36
24	b	621	SQD	O8-S-C6	-2.54	101.70	105.74
21	1	413	CL7	C4C-C3C-C2C	-2.54	103.82	107.13
21	5	413	CL7	C4C-C3C-C2C	-2.54	103.82	107.13
21	2	517	CL7	CAA-CBA-CGA	-2.54	105.84	113.25
21	c	506	CL7	CMB-C2B-C1B	2.53	129.23	125.37
23	b	619	8CT	C01-C02-C07	2.53	118.48	113.62
32	4	420	ZEX	C15-C35-C34	-2.53	118.29	123.47
32	8	420	ZEX	C15-C35-C34	-2.53	118.29	123.47
21	C	503	CL7	CHC-C1C-NC	-2.53	122.13	124.45
21	c	503	CL7	CHC-C1C-NC	-2.53	122.13	124.45
21	B	609	CL7	C4C-C3C-C2C	-2.53	103.83	107.13
21	2	505	CL7	C3B-C2B-C1B	-2.53	104.11	107.16
21	3	508	CL7	O2A-C1-C2	-2.53	101.98	108.64
24	B	620	SQD	O8-S-C6	-2.53	101.71	105.74
21	C	513	CL7	CMA-C3A-C2A	-2.53	110.19	116.10
21	c	502	CL7	C7-C6-C5	-2.53	106.49	113.36
21	4	411	CL7	CMB-C2B-C1B	2.53	129.22	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	406	8CT	C13-C14-C15	-2.53	115.33	123.22
21	B	606	CL7	C4C-C3C-C2C	-2.53	103.83	107.13
21	7	505	CL7	C4-C3-C5	2.52	119.52	115.27
21	6	517	CL7	CAA-CBA-CGA	-2.52	105.88	113.25
23	B	618	8CT	C01-C02-C07	2.52	118.46	113.62
32	2	520	ZEX	C7-C8-C9	-2.52	122.42	126.23
32	3	525	ZEX	C7-C8-C9	-2.52	122.42	126.23
21	2	511	CL7	CHB-C1B-NB	-2.52	121.59	124.26
27	c	517	DGD	C4E-C3E-C2E	-2.52	106.42	110.82
21	1	407	CL7	CHB-C1B-NB	-2.52	121.59	124.26
21	2	514	CL7	CHC-C1C-NC	-2.52	122.14	124.45
23	d	406	8CT	C13-C14-C15	-2.52	115.35	123.22
21	b	610	CL7	C4C-C3C-C2C	-2.52	103.84	107.13
21	2	506	CL7	CMB-C2B-C1B	2.52	129.20	125.37
21	6	506	CL7	CMB-C2B-C1B	2.52	129.20	125.37
21	b	602	CL7	C3B-C4B-NB	2.52	112.85	110.52
21	C	505	CL7	C1C-C2C-C3C	-2.52	103.27	106.94
21	4	406	CL7	C3B-C2B-C1B	-2.52	104.12	107.16
21	8	406	CL7	C3B-C2B-C1B	-2.52	104.12	107.16
21	2	514	CL7	CMB-C2B-C1B	2.51	129.20	125.37
21	6	514	CL7	CMB-C2B-C1B	2.51	129.20	125.37
21	2	517	CL7	CHB-C1B-NB	-2.51	121.59	124.26
21	b	610	CL7	CHC-C1C-NC	-2.51	122.14	124.45
21	3	510	CL7	CHB-C1B-NB	-2.51	121.60	124.26
21	3	506	CL7	O2D-CGD-CBD	2.51	115.73	111.27
21	7	506	CL7	O2D-CGD-CBD	2.51	115.73	111.27
21	1	411	CL7	CHB-C1B-NB	-2.51	121.60	124.26
21	d	405	CL7	CHC-C1C-NC	-2.51	122.14	124.45
21	c	505	CL7	C1C-C2C-C3C	-2.51	103.27	106.94
23	C	515	8CT	C13-C14-C15	-2.51	115.38	123.22
23	c	515	8CT	C13-C14-C15	-2.51	115.38	123.22
21	1	413	CL7	C3B-C4B-NB	2.51	112.84	110.52
23	C	516	8CT	C11-C10-C03	-2.51	120.15	127.20
23	c	516	8CT	C11-C10-C03	-2.51	120.15	127.20
21	B	609	CL7	CHC-C1C-NC	-2.51	122.15	124.45
21	B	608	CL7	C4C-C3C-C2C	-2.51	103.86	107.13
21	b	609	CL7	C4C-C3C-C2C	-2.51	103.86	107.13
21	3	502	CL7	C7-C6-C5	-2.51	106.54	113.36
21	C	506	CL7	CMB-C2B-C1B	2.51	129.19	125.37
21	3	508	CL7	C1C-C2C-C3C	-2.51	103.28	106.94
21	7	508	CL7	C1C-C2C-C3C	-2.51	103.28	106.94
21	5	410	CL7	CHC-C1C-NC	-2.51	122.15	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	401	CL7	C6-C5-C3	-2.51	106.89	113.45
22	D	408	PHO	CAC-C3C-C4C	2.50	130.62	124.27
21	2	507	CL7	C7-C6-C5	-2.50	106.56	113.36
21	1	404	CL7	CHB-C1B-NB	-2.50	121.61	124.26
21	3	512	CL7	CMB-C2B-C1B	2.50	129.18	125.37
21	7	502	CL7	C7-C6-C5	-2.50	106.56	113.36
21	B	606	CL7	CHB-C1B-NB	-2.50	121.61	124.26
21	b	607	CL7	CHB-C1B-NB	-2.50	121.61	124.26
21	1	404	CL7	C3B-C2B-C1B	-2.50	104.14	107.16
21	5	404	CL7	C3B-C2B-C1B	-2.50	104.14	107.16
21	b	607	CL7	C4C-C3C-C2C	-2.50	103.87	107.13
21	7	512	CL7	CMB-C2B-C1B	2.50	129.17	125.37
21	6	507	CL7	C7-C6-C5	-2.50	106.58	113.36
21	b	609	CL7	C7-C6-C5	-2.50	106.58	113.36
21	4	413	CL7	C4C-C3C-C2C	-2.50	103.87	107.13
21	8	413	CL7	C4C-C3C-C2C	-2.50	103.87	107.13
22	d	408	PHO	CAC-C3C-C4C	2.50	130.60	124.27
21	C	509	CL7	CHC-C1C-NC	-2.49	122.16	124.45
21	6	514	CL7	CHC-C1C-NC	-2.49	122.16	124.45
21	B	608	CL7	C7-C6-C5	-2.49	106.59	113.36
21	c	505	CL7	CHC-C1C-NC	-2.49	122.17	124.45
21	2	506	CL7	C3B-C2B-C1B	-2.49	104.16	107.16
21	6	506	CL7	C3B-C2B-C1B	-2.49	104.16	107.16
23	k	101	8CT	C22-C21-C20	-2.49	119.44	122.92
21	a	401	CL7	C6-C5-C3	-2.49	106.93	113.45
21	c	506	CL7	C4C-C3C-C2C	-2.49	103.88	107.13
21	1	410	CL7	CHC-C1C-NC	-2.49	122.17	124.45
21	B	605	CL7	C3B-C2B-C1B	-2.49	104.16	107.16
21	b	606	CL7	C3B-C2B-C1B	-2.49	104.16	107.16
21	5	414	CL7	CMA-C3A-C2A	-2.49	110.29	116.10
21	b	603	CL7	O2A-CGA-O1A	-2.49	117.31	123.59
21	2	513	CL7	C4C-C3C-C2C	-2.49	103.89	107.13
21	6	513	CL7	C4C-C3C-C2C	-2.49	103.89	107.13
21	b	611	CL7	C4-C3-C5	2.49	119.45	115.27
21	7	517	CL7	C4-C3-C5	2.49	120.09	114.60
21	D	405	CL7	C4C-C3C-C2C	-2.49	103.89	107.13
21	d	405	CL7	C4C-C3C-C2C	-2.49	103.89	107.13
21	2	516	CL7	C3B-C2B-C1B	-2.48	104.16	107.16
21	B	603	CL7	C1-C2-C3	2.48	130.34	126.04
21	b	604	CL7	C1-C2-C3	2.48	130.34	126.04
21	1	403	CL7	C4-C3-C5	2.48	119.45	115.27
21	5	403	CL7	C4-C3-C5	2.48	119.45	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	504	CL7	C3B-C2B-C1B	-2.48	104.17	107.16
21	7	504	CL7	C3B-C2B-C1B	-2.48	104.17	107.16
21	B	609	CL7	CMB-C2B-C1B	2.48	129.15	125.37
21	5	404	CL7	CHB-C1B-NB	-2.48	121.63	124.26
21	1	418	CL7	C1C-C2C-C3C	-2.48	103.32	106.94
21	5	418	CL7	C1C-C2C-C3C	-2.48	103.32	106.94
21	B	610	CL7	C4-C3-C5	2.48	119.44	115.27
21	D	405	CL7	CHC-C1C-NC	-2.48	122.17	124.45
23	B	618	8CT	C19-C20-C21	-2.48	123.77	127.31
21	B	601	CL7	C3B-C4B-NB	2.48	112.81	110.52
21	C	507	CL7	C1C-C2C-C3C	-2.48	103.32	106.94
21	c	507	CL7	C1C-C2C-C3C	-2.48	103.32	106.94
26	1	401	LMG	O1-C7-C8	-2.48	104.92	110.90
26	5	401	LMG	O1-C7-C8	-2.48	104.92	110.90
21	A	403	CL7	CHB-C1B-NB	-2.48	121.63	124.26
21	a	403	CL7	CHB-C1B-NB	-2.48	121.63	124.26
21	A	403	CL7	CAA-CBA-CGA	-2.48	106.01	113.25
21	a	403	CL7	CAA-CBA-CGA	-2.48	106.01	113.25
21	C	506	CL7	C4C-C3C-C2C	-2.48	103.90	107.13
21	C	507	CL7	CHB-C1B-NB	-2.48	121.64	124.26
21	c	507	CL7	CHB-C1B-NB	-2.48	121.64	124.26
21	6	512	CL7	C4C-C3C-C2C	-2.48	103.90	107.13
32	4	419	ZEX	C38-C24-C25	-2.48	106.93	110.87
21	C	502	CL7	C3B-C2B-C1B	-2.47	104.17	107.16
21	1	414	CL7	CMA-C3A-C2A	-2.47	110.32	116.10
21	B	602	CL7	O2A-CGA-O1A	-2.47	117.35	123.59
32	8	419	ZEX	C38-C24-C25	-2.47	106.93	110.87
21	6	516	CL7	C3B-C2B-C1B	-2.47	104.18	107.16
21	4	409	CL7	CAA-CBA-CGA	-2.47	106.03	113.25
21	B	614	CL7	C4C-C3C-C2C	-2.47	103.91	107.13
21	1	408	CL7	C4-C3-C5	2.47	119.43	115.27
21	5	408	CL7	C4-C3-C5	2.47	119.43	115.27
32	7	520	ZEX	C2-C3-C4	-2.47	106.92	110.30
21	3	517	CL7	C4-C3-C5	2.47	120.06	114.60
21	b	614	CL7	C7-C6-C5	-2.47	106.65	113.36
21	3	509	CL7	O2A-CGA-O1A	-2.47	117.36	123.59
21	7	509	CL7	O2A-CGA-O1A	-2.47	117.36	123.59
21	B	613	CL7	C7-C6-C5	-2.47	106.66	113.36
23	C	515	8CT	C27-C26-C28	2.47	121.97	118.08
23	c	515	8CT	C27-C26-C28	2.47	121.97	118.08
21	8	409	CL7	CAA-CBA-CGA	-2.47	106.04	113.25
21	7	506	CL7	C4C-C3C-C2C	-2.47	103.91	107.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	502	CL7	CMB-C2B-C1B	2.47	129.13	125.37
21	1	409	CL7	CMB-C2B-C1B	2.47	129.13	125.37
21	c	502	CL7	CMB-C2B-C1B	2.47	129.13	125.37
32	4	419	ZEX	C11-C12-C13	-2.47	119.49	126.42
32	8	419	ZEX	C11-C12-C13	-2.47	119.49	126.42
21	4	404	CL7	C3B-C2B-C1B	-2.47	104.19	107.16
21	8	404	CL7	C3B-C2B-C1B	-2.47	104.19	107.16
21	8	405	CL7	C3B-C2B-C1B	-2.47	104.19	107.16
21	2	507	CL7	C4C-C3C-C2C	-2.47	103.91	107.13
21	c	504	CL7	C1C-C2C-C3C	-2.47	103.34	106.94
23	b	601	8CT	C22-C21-C20	-2.47	119.47	122.92
21	c	509	CL7	CHB-C1B-NB	-2.46	121.65	124.26
23	B	627	8CT	C22-C21-C20	-2.46	119.47	122.92
21	c	502	CL7	C3B-C2B-C1B	-2.46	104.19	107.16
21	C	509	CL7	CHB-C1B-NB	-2.46	121.65	124.26
23	D	406	8CT	C05-C04-C03	2.46	114.27	110.48
23	d	406	8CT	C05-C04-C03	2.46	114.27	110.48
21	5	405	CL7	C1C-C2C-C3C	-2.46	103.35	106.94
21	5	409	CL7	CMB-C2B-C1B	2.46	129.12	125.37
21	2	502	CL7	C4-C3-C5	2.46	119.41	115.27
21	6	502	CL7	C4-C3-C5	2.46	119.41	115.27
32	3	520	ZEX	C2-C3-C4	-2.46	106.94	110.30
23	b	619	8CT	C19-C20-C21	-2.46	123.80	127.31
21	C	510	CL7	C1-C2-C3	2.46	130.30	126.04
21	c	510	CL7	C1-C2-C3	2.46	130.30	126.04
21	8	411	CL7	C4-C3-C5	2.46	119.41	115.27
21	3	506	CL7	C4C-C3C-C2C	-2.46	103.92	107.13
21	4	414	CL7	C4C-C3C-C2C	-2.46	103.92	107.13
21	8	414	CL7	C4C-C3C-C2C	-2.46	103.92	107.13
21	b	610	CL7	CMB-C2B-C1B	2.46	129.11	125.37
23	K	101	8CT	C22-C21-C20	-2.46	119.48	122.92
21	5	409	CL7	C3B-C2B-C1B	-2.46	104.20	107.16
21	1	405	CL7	C1C-C2C-C3C	-2.45	103.36	106.94
21	8	407	CL7	CMB-C2B-C1B	2.45	129.11	125.37
21	C	511	CL7	O2D-CGD-CBD	2.45	115.63	111.27
21	c	511	CL7	O2D-CGD-CBD	2.45	115.63	111.27
21	2	512	CL7	C4C-C3C-C2C	-2.45	103.93	107.13
21	B	601	CL7	C1C-C2C-C3C	-2.45	103.36	106.94
21	b	602	CL7	C1C-C2C-C3C	-2.45	103.36	106.94
21	8	411	CL7	C7-C6-C5	-2.45	106.70	113.36
21	6	507	CL7	C4C-C3C-C2C	-2.45	103.93	107.13
21	4	407	CL7	CMB-C2B-C1B	2.45	129.10	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	c	503	CL7	CMB-C2B-C1B	2.45	129.10	125.37
21	C	518	CL7	C1C-C2C-C3C	-2.45	103.36	106.94
21	A	401	CL7	C4C-C3C-C2C	-2.45	103.94	107.13
21	a	401	CL7	C4C-C3C-C2C	-2.45	103.94	107.13
21	1	404	CL7	CMB-C2B-C1B	2.45	129.10	125.37
21	5	404	CL7	CMB-C2B-C1B	2.45	129.10	125.37
21	7	511	CL7	CMB-C2B-C1B	2.45	129.10	125.37
21	c	512	CL7	C3B-C2B-C1B	-2.45	104.21	107.16
21	C	504	CL7	C1C-C2C-C3C	-2.45	103.37	106.94
21	b	615	CL7	C4C-C3C-C2C	-2.45	103.94	107.13
21	7	501	CL7	C4-C3-C5	2.45	119.39	115.27
32	3	520	ZEX	C35-C15-C14	-2.45	118.47	123.47
21	c	518	CL7	C1C-C2C-C3C	-2.44	103.37	106.94
22	D	408	PHO	C16-C15-C13	-2.44	108.02	115.92
21	5	411	CL7	C3B-C2B-C1B	-2.44	104.21	107.16
21	5	412	CL7	CMB-C2B-C1B	2.44	129.09	125.37
21	D	405	CL7	CAA-CBA-CGA	-2.44	106.02	112.51
21	d	405	CL7	CAA-CBA-CGA	-2.44	106.02	112.51
21	4	411	CL7	C7-C6-C5	-2.44	106.73	113.36
21	2	515	CL7	C3B-C2B-C1B	-2.44	104.21	107.16
21	6	515	CL7	C3B-C2B-C1B	-2.44	104.21	107.16
21	C	505	CL7	CHC-C1C-NC	-2.44	122.21	124.45
23	A	404	8CT	C11-C10-C03	-2.44	120.35	127.20
21	2	512	CL7	O2D-CGD-O1D	-2.44	119.07	123.84
21	6	512	CL7	O2D-CGD-O1D	-2.44	119.07	123.84
21	4	411	CL7	C4-C3-C5	2.44	119.37	115.27
21	4	404	CL7	CHB-C1B-NB	-2.44	121.68	124.26
21	8	404	CL7	CHB-C1B-NB	-2.44	121.68	124.26
21	C	503	CL7	CMB-C2B-C1B	2.44	129.08	125.37
23	b	601	8CT	C40-C12-C13	-2.44	119.51	122.92
21	4	413	CL7	C7-C6-C5	-2.44	106.74	113.36
21	8	413	CL7	C7-C6-C5	-2.44	106.74	113.36
22	d	408	PHO	C16-C15-C13	-2.44	108.04	115.92
21	6	517	CL7	C7-C6-C5	-2.44	106.74	113.36
21	2	515	CL7	C4C-C3C-C2C	-2.44	103.95	107.13
21	6	515	CL7	C4C-C3C-C2C	-2.44	103.95	107.13
21	2	517	CL7	C7-C6-C5	-2.44	106.75	113.36
21	5	402	CL7	C3B-C2B-C1B	-2.44	104.22	107.16
21	8	410	CL7	C1C-C2C-C3C	-2.44	103.39	106.94
21	B	604	CL7	C1C-C2C-C3C	-2.43	103.39	106.94
21	C	509	CL7	C1C-C2C-C3C	-2.43	103.39	106.94
21	b	605	CL7	C1C-C2C-C3C	-2.43	103.39	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	c	509	CL7	C1C-C2C-C3C	-2.43	103.39	106.94
32	3	525	ZEX	C31-C32-C33	-2.43	119.58	126.42
21	4	406	CL7	CHB-C1B-NB	-2.43	121.68	124.26
21	8	406	CL7	CHB-C1B-NB	-2.43	121.68	124.26
32	7	520	ZEX	C35-C15-C14	-2.43	118.49	123.47
23	C	515	8CT	C14-C13-C12	-2.43	123.84	127.31
23	c	515	8CT	C14-C13-C12	-2.43	123.84	127.31
21	B	615	CL7	C4-C3-C5	2.43	119.98	114.60
21	b	616	CL7	C4-C3-C5	2.43	119.98	114.60
21	B	615	CL7	C1C-C2C-C3C	-2.43	103.39	106.94
21	b	616	CL7	C1C-C2C-C3C	-2.43	103.39	106.94
32	3	522	ZEX	C31-C30-C29	-2.43	123.84	127.31
32	7	522	ZEX	C31-C30-C29	-2.43	123.84	127.31
21	3	501	CL7	C4-C3-C5	2.43	119.36	115.27
21	6	503	CL7	C4-C3-C5	2.43	119.36	115.27
21	1	411	CL7	C3B-C2B-C1B	-2.43	104.23	107.16
32	6	519	ZEX	C28-C27-C26	-2.43	122.93	127.09
21	2	510	CL7	C4C-C3C-C2C	-2.43	103.96	107.13
21	6	510	CL7	C4C-C3C-C2C	-2.43	103.96	107.13
21	2	512	CL7	C4-C3-C5	2.43	119.36	115.27
21	C	512	CL7	C3B-C2B-C1B	-2.43	104.23	107.16
21	c	513	CL7	C4C-C3C-C2C	-2.43	103.96	107.13
21	B	609	CL7	CHB-C1B-NB	-2.43	121.69	124.26
21	B	605	CL7	C1C-C2C-C3C	-2.43	103.39	106.94
21	b	606	CL7	C1C-C2C-C3C	-2.43	103.39	106.94
21	4	409	CL7	O2A-C1-C2	2.43	115.02	108.64
21	8	409	CL7	O2A-C1-C2	2.43	115.02	108.64
21	4	404	CL7	C7-C6-C5	-2.43	106.77	113.36
32	2	520	ZEX	C31-C32-C33	-2.43	119.60	126.42
21	b	610	CL7	CHB-C1B-NB	-2.43	121.69	124.26
32	4	403	ZEX	C39-C29-C30	-2.43	119.52	122.92
32	8	403	ZEX	C39-C29-C30	-2.43	119.52	122.92
23	a	404	8CT	C11-C10-C03	-2.43	120.39	127.20
32	1	421	ZEX	C8-C7-C6	-2.43	120.39	127.20
32	5	421	ZEX	C8-C7-C6	-2.43	120.39	127.20
21	1	408	CL7	O2D-CGD-O1D	-2.43	119.10	123.84
21	2	510	CL7	C4-C3-C5	2.43	119.35	115.27
21	6	510	CL7	C4-C3-C5	2.43	119.35	115.27
21	3	515	CL7	C3B-C2B-C1B	-2.43	104.23	107.16
21	7	515	CL7	C3B-C2B-C1B	-2.43	104.23	107.16
21	3	511	CL7	CMB-C2B-C1B	2.42	129.06	125.37
21	A	406	CL7	CHB-C1B-NB	-2.42	121.69	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	509	CL7	CHB-C1B-NB	-2.42	121.69	124.26
21	6	509	CL7	CHB-C1B-NB	-2.42	121.69	124.26
21	1	409	CL7	C3B-C2B-C1B	-2.42	104.24	107.16
23	A	404	8CT	C22-C21-C20	-2.42	119.53	122.92
21	1	412	CL7	CMB-C2B-C1B	2.42	129.06	125.37
21	C	513	CL7	C4C-C3C-C2C	-2.42	103.97	107.13
21	8	404	CL7	C7-C6-C5	-2.42	106.78	113.36
21	a	405	CL7	CHB-C1B-NB	-2.42	121.69	124.26
21	4	405	CL7	C3B-C2B-C1B	-2.42	104.24	107.16
32	1	421	ZEX	C31-C32-C33	-2.42	119.62	126.42
32	5	421	ZEX	C31-C32-C33	-2.42	119.62	126.42
21	C	510	CL7	CAA-CBA-CGA	-2.42	106.18	113.25
21	2	503	CL7	C4-C3-C5	2.42	119.34	115.27
21	C	514	CL7	C1C-C2C-C3C	-2.42	103.41	106.94
21	c	514	CL7	C1C-C2C-C3C	-2.42	103.41	106.94
21	2	516	CL7	CAA-CBA-CGA	-2.42	106.19	113.25
21	3	501	CL7	C1C-C2C-C3C	-2.42	103.41	106.94
21	7	501	CL7	C1C-C2C-C3C	-2.42	103.41	106.94
21	4	404	CL7	C4C-C3C-C2C	-2.42	103.97	107.13
21	8	404	CL7	C4C-C3C-C2C	-2.42	103.97	107.13
21	2	505	CL7	CGD-CBD-CAD	2.42	118.56	110.73
32	2	519	ZEX	C28-C27-C26	-2.42	122.96	127.09
21	4	410	CL7	C1C-C2C-C3C	-2.42	103.41	106.94
21	B	611	CL7	C4-C3-C5	2.41	119.33	115.27
21	b	612	CL7	C4-C3-C5	2.41	119.33	115.27
21	c	510	CL7	CAA-CBA-CGA	-2.41	106.20	113.25
21	2	503	CL7	O2D-CGD-CBD	2.41	115.55	111.27
21	1	416	CL7	C4C-C3C-C2C	-2.41	103.98	107.13
21	6	505	CL7	CGD-CBD-CAD	2.41	118.55	110.73
21	2	502	CL7	C1C-C2C-C3C	-2.41	103.42	106.94
21	6	502	CL7	C1C-C2C-C3C	-2.41	103.42	106.94
21	5	408	CL7	O2D-CGD-O1D	-2.41	119.12	123.84
23	B	627	8CT	C40-C12-C13	-2.41	119.55	122.92
21	3	501	CL7	C3B-C4B-NB	2.41	112.75	110.52
21	7	501	CL7	C3B-C4B-NB	2.41	112.75	110.52
21	6	512	CL7	C4-C3-C5	2.41	119.32	115.27
23	B	618	8CT	C28-C26-C25	-2.41	115.25	118.94
23	b	619	8CT	C28-C26-C25	-2.41	115.25	118.94
21	1	413	CL7	O2D-CGD-CBD	2.41	115.55	111.27
21	6	516	CL7	CAA-CBA-CGA	-2.41	106.22	113.25
32	7	520	ZEX	C1-C6-C5	-2.40	119.23	122.61
23	C	519	8CT	C18-C19-C20	-2.40	118.55	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	519	8CT	C18-C19-C20	-2.40	118.55	123.47
21	1	402	CL7	C3B-C2B-C1B	-2.40	104.26	107.16
21	c	513	CL7	C3B-C2B-C1B	-2.40	104.26	107.16
21	1	418	CL7	CAC-C3C-C2C	2.40	131.64	127.53
21	5	418	CL7	CAC-C3C-C2C	2.40	131.64	127.53
21	A	403	CL7	O2A-CGA-CBA	2.40	119.45	111.91
21	a	403	CL7	O2A-CGA-CBA	2.40	119.45	111.91
21	B	603	CL7	C1C-C2C-C3C	-2.40	103.44	106.94
21	b	604	CL7	C1C-C2C-C3C	-2.40	103.44	106.94
32	3	519	ZEX	C39-C29-C30	-2.40	119.56	122.92
32	7	519	ZEX	C39-C29-C30	-2.40	119.56	122.92
21	C	503	CL7	C7-C6-C5	-2.40	106.84	113.36
32	4	419	ZEX	C1-C6-C5	-2.40	119.23	122.61
21	c	511	CL7	C1C-C2C-C3C	-2.40	103.44	106.94
32	8	419	ZEX	C1-C6-C5	-2.40	119.24	122.61
21	4	411	CL7	CHB-C1B-NB	-2.40	121.72	124.26
21	1	408	CL7	CMB-C2B-C1B	2.40	129.02	125.37
21	5	413	CL7	O2D-CGD-CBD	2.40	115.52	111.27
21	3	516	CL7	CAA-C2A-C1A	-2.39	104.31	112.19
32	3	520	ZEX	C1-C6-C5	-2.39	119.24	122.61
21	3	503	CL7	C4-C3-C5	2.39	119.30	115.27
21	b	612	CL7	CHB-C1B-NB	-2.39	121.72	124.26
21	1	406	CL7	C4C-C3C-C2C	-2.39	104.01	107.13
21	5	406	CL7	C4C-C3C-C2C	-2.39	104.01	107.13
23	a	404	8CT	C22-C21-C20	-2.39	119.57	122.92
21	7	516	CL7	CAA-C2A-C1A	-2.39	104.32	112.19
23	C	516	8CT	C27-C26-C25	-2.39	119.57	122.92
23	c	516	8CT	C27-C26-C25	-2.39	119.57	122.92
21	3	518	CL7	C4C-C3C-C2C	-2.39	104.01	107.13
21	7	518	CL7	C4C-C3C-C2C	-2.39	104.01	107.13
21	B	611	CL7	CHB-C1B-NB	-2.39	121.73	124.26
21	B	604	CL7	C7-C6-C5	-2.39	106.87	113.36
21	b	605	CL7	C7-C6-C5	-2.39	106.87	113.36
21	3	508	CL7	CBA-CAA-C2A	-2.39	106.81	113.86
21	7	508	CL7	CBA-CAA-C2A	-2.39	106.81	113.86
21	1	419	CL7	C4C-C3C-C2C	-2.39	104.01	107.13
21	5	419	CL7	C4C-C3C-C2C	-2.39	104.01	107.13
21	5	408	CL7	CMB-C2B-C1B	2.39	129.00	125.37
21	5	416	CL7	C4C-C3C-C2C	-2.39	104.02	107.13
21	8	414	CL7	CAA-CBA-CGA	-2.39	106.28	113.25
21	c	503	CL7	C7-C6-C5	-2.39	106.88	113.36
21	B	602	CL7	C4C-C3C-C2C	-2.39	104.02	107.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	515	CL7	C4C-C3C-C2C	-2.39	104.02	107.13
21	7	515	CL7	C4C-C3C-C2C	-2.39	104.02	107.13
21	4	417	CL7	CAA-C2A-C3A	2.39	120.22	114.26
21	8	417	CL7	CAA-C2A-C3A	2.39	120.22	114.26
21	c	507	CL7	C7-C6-C5	-2.39	106.88	113.36
21	1	416	CL7	CMA-C3A-C2A	-2.39	110.53	116.10
21	5	416	CL7	CMA-C3A-C2A	-2.39	110.53	116.10
21	C	513	CL7	C3B-C2B-C1B	-2.38	104.28	107.16
21	6	503	CL7	O2D-CGD-CBD	2.38	115.50	111.27
21	C	511	CL7	C1C-C2C-C3C	-2.38	103.46	106.94
21	3	501	CL7	CAA-C2A-C1A	-2.38	104.36	112.19
21	7	501	CL7	CAA-C2A-C1A	-2.38	104.36	112.19
23	A	404	8CT	C18-C19-C20	-2.38	118.60	123.47
32	2	523	ZEX	C21-C26-C27	2.38	122.51	115.78
21	b	603	CL7	C4C-C3C-C2C	-2.38	104.03	107.13
21	4	414	CL7	CAA-CBA-CGA	-2.38	106.30	113.25
21	4	405	CL7	O2A-CGA-O1A	-2.38	117.59	123.59
21	8	405	CL7	O2A-CGA-O1A	-2.38	117.59	123.59
21	C	514	CL7	CAA-CBA-CGA	-2.38	106.20	112.51
21	c	514	CL7	CAA-CBA-CGA	-2.38	106.20	112.51
21	7	504	CL7	C1C-C2C-C3C	-2.38	103.47	106.94
21	C	507	CL7	C7-C6-C5	-2.38	106.91	113.36
23	a	404	8CT	C18-C19-C20	-2.38	118.61	123.47
21	8	411	CL7	CHB-C1B-NB	-2.38	121.74	124.26
21	4	405	CL7	C1C-C2C-C3C	-2.38	103.47	106.94
21	8	405	CL7	C1C-C2C-C3C	-2.38	103.47	106.94
21	7	508	CL7	CHC-C1C-NC	-2.37	122.27	124.45
21	B	606	CL7	CHC-C1C-NC	-2.37	122.27	124.45
21	b	607	CL7	CHC-C1C-NC	-2.37	122.27	124.45
21	2	518	CL7	C4C-C3C-C2C	-2.37	104.04	107.13
32	1	421	ZEX	C1-C6-C5	-2.37	119.27	122.61
32	5	421	ZEX	C1-C6-C5	-2.37	119.27	122.61
32	6	522	ZEX	C21-C26-C27	2.37	122.48	115.78
21	8	407	CL7	CHD-C1D-ND	-2.37	121.75	124.26
21	2	513	CL7	CHC-C1C-NC	-2.37	122.28	124.45
21	C	510	CL7	C4C-C3C-C2C	-2.37	104.04	107.13
21	c	510	CL7	C4C-C3C-C2C	-2.37	104.04	107.13
32	3	525	ZEX	C1-C6-C5	-2.37	119.28	122.61
31	f	101	HEM	C4D-ND-C1D	2.37	107.52	105.07
21	3	504	CL7	C1C-C2C-C3C	-2.37	103.48	106.94
21	A	403	CL7	O2A-CGA-O1A	-2.37	117.62	123.59
21	a	403	CL7	O2A-CGA-O1A	-2.37	117.62	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	501	CL7	CMB-C2B-C1B	2.37	128.97	125.37
23	B	617	8CT	C04-C03-C10	2.37	122.47	115.78
23	b	618	8CT	C04-C03-C10	2.37	122.47	115.78
31	F	101	HEM	C4D-ND-C1D	2.37	107.52	105.07
21	7	503	CL7	C4-C3-C5	2.37	119.25	115.27
21	1	418	CL7	C4-C3-C5	2.37	119.25	115.27
21	5	418	CL7	C4-C3-C5	2.37	119.25	115.27
21	b	613	CL7	O2D-CGD-O1D	-2.37	119.21	123.84
21	B	612	CL7	C4C-C3C-C2C	-2.37	104.04	107.13
21	b	613	CL7	C4C-C3C-C2C	-2.37	104.04	107.13
21	6	513	CL7	CHC-C1C-NC	-2.36	122.28	124.45
21	4	405	CL7	C7-C6-C5	-2.36	106.95	113.36
21	8	405	CL7	C7-C6-C5	-2.36	106.95	113.36
21	3	507	CL7	CHD-C1D-ND	-2.36	121.76	124.26
21	7	507	CL7	CHD-C1D-ND	-2.36	121.76	124.26
21	C	508	CL7	CHB-C1B-NB	-2.36	121.76	124.26
21	c	508	CL7	CHB-C1B-NB	-2.36	121.76	124.26
32	2	520	ZEX	C1-C6-C5	-2.36	119.29	122.61
23	K	101	8CT	C27-C26-C25	-2.36	119.62	122.92
23	k	101	8CT	C27-C26-C25	-2.36	119.62	122.92
23	a	404	8CT	C19-C18-C17	-2.35	118.65	123.47
21	4	407	CL7	CHD-C1D-ND	-2.35	121.77	124.26
21	B	616	CL7	C4C-C3C-C2C	-2.35	104.06	107.13
21	b	617	CL7	C4C-C3C-C2C	-2.35	104.06	107.13
32	6	520	ZEX	C17-C1-C6	-2.35	106.49	110.30
21	b	611	CL7	CMB-C2B-C1B	2.35	128.95	125.37
21	1	409	CL7	C4C-C3C-C2C	-2.35	104.06	107.13
21	5	409	CL7	C4C-C3C-C2C	-2.35	104.06	107.13
21	B	609	CL7	C4-C3-C5	2.35	119.22	115.27
21	b	610	CL7	C4-C3-C5	2.35	119.22	115.27
21	A	406	CL7	C1C-C2C-C3C	-2.35	103.51	106.94
21	a	405	CL7	C1C-C2C-C3C	-2.35	103.51	106.94
21	6	518	CL7	C4C-C3C-C2C	-2.35	104.07	107.13
21	B	607	CL7	C4-C3-C5	2.35	119.22	115.27
21	7	501	CL7	CMB-C2B-C1B	2.35	128.94	125.37
21	8	413	CL7	CAA-CBA-CGA	-2.35	106.40	113.25
21	8	411	CL7	CAA-CBA-CGA	-2.34	106.40	113.25
21	7	518	CL7	CMB-C2B-C1B	2.34	128.94	125.37
23	B	619	8CT	C14-C15-C16	-2.34	119.83	126.42
23	b	620	8CT	C14-C15-C16	-2.34	119.83	126.42
21	C	507	CL7	C4-C3-C5	2.34	119.21	115.27
23	C	516	8CT	C35-C30-C31	2.34	115.61	111.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	516	8CT	C35-C30-C31	2.34	115.61	111.42
23	A	404	8CT	C19-C18-C17	-2.34	118.68	123.47
21	5	407	CL7	C4C-C3C-C2C	-2.34	104.08	107.13
21	2	516	CL7	C1C-C2C-C3C	-2.34	103.52	106.94
21	6	516	CL7	C1C-C2C-C3C	-2.34	103.52	106.94
21	B	612	CL7	O2D-CGD-O1D	-2.34	119.26	123.84
32	2	521	ZEX	C17-C1-C6	-2.34	106.50	110.30
21	3	507	CL7	C4-C3-C5	2.34	119.20	115.27
21	4	413	CL7	C4-C3-C5	2.34	119.20	115.27
21	8	413	CL7	C4-C3-C5	2.34	119.20	115.27
21	2	508	CL7	C1C-C2C-C3C	-2.34	103.53	106.94
21	3	507	CL7	C1C-C2C-C3C	-2.34	103.53	106.94
21	6	508	CL7	C1C-C2C-C3C	-2.34	103.53	106.94
21	7	515	CL7	C1C-C2C-C3C	-2.34	103.53	106.94
21	c	507	CL7	O2A-CGA-CBA	2.34	119.24	111.91
21	4	413	CL7	CAA-CBA-CGA	-2.34	106.42	113.25
21	3	518	CL7	CMB-C2B-C1B	2.34	128.93	125.37
21	4	408	CL7	C3B-C2B-C1B	-2.34	104.34	107.16
21	8	408	CL7	C3B-C2B-C1B	-2.34	104.34	107.16
21	C	507	CL7	C4C-C3C-C2C	-2.34	104.08	107.13
21	c	507	CL7	C4C-C3C-C2C	-2.34	104.08	107.13
21	c	511	CL7	C4-C3-C5	2.34	119.20	115.27
21	C	513	CL7	C1C-C2C-C3C	-2.34	103.53	106.94
21	4	411	CL7	CAA-CBA-CGA	-2.33	106.43	113.25
21	3	508	CL7	CHC-C1C-NC	-2.33	122.31	124.45
21	B	610	CL7	CMB-C2B-C1B	2.33	128.92	125.37
21	1	407	CL7	C4C-C3C-C2C	-2.33	104.09	107.13
32	7	522	ZEX	C21-C22-C23	-2.33	108.64	113.69
21	c	507	CL7	C4-C3-C5	2.33	119.19	115.27
21	7	510	CL7	C4-C3-C5	2.33	119.19	115.27
21	c	513	CL7	C1C-C2C-C3C	-2.33	103.54	106.94
32	2	519	ZEX	C15-C35-C34	-2.33	118.70	123.47
32	6	519	ZEX	C15-C35-C34	-2.33	118.70	123.47
21	4	414	CL7	C1C-C2C-C3C	-2.33	103.54	106.94
21	8	414	CL7	C1C-C2C-C3C	-2.33	103.54	106.94
21	3	517	CL7	C4C-C3C-C2C	-2.33	104.09	107.13
21	7	517	CL7	C4C-C3C-C2C	-2.33	104.09	107.13
21	3	517	CL7	C1C-C2C-C3C	-2.33	103.54	106.94
21	7	517	CL7	C1C-C2C-C3C	-2.33	103.54	106.94
21	1	412	CL7	C3B-C2B-C1B	-2.33	104.35	107.16
21	5	412	CL7	C3B-C2B-C1B	-2.33	104.35	107.16
21	C	507	CL7	O2A-CGA-CBA	2.33	119.21	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	608	CL7	C4-C3-C5	2.33	119.18	115.27
21	1	413	CL7	C1C-C2C-C3C	-2.32	103.55	106.94
21	5	413	CL7	C1C-C2C-C3C	-2.32	103.55	106.94
21	3	510	CL7	C4-C3-C5	2.32	119.18	115.27
32	2	525	ZEX	C1-C6-C7	2.32	122.35	115.78
32	6	524	ZEX	C1-C6-C7	2.32	122.35	115.78
21	6	506	CL7	C1C-C2C-C3C	-2.32	103.55	106.94
21	C	508	CL7	CMB-C2B-C1B	2.32	128.91	125.37
21	c	508	CL7	CMB-C2B-C1B	2.32	128.91	125.37
21	3	515	CL7	C1C-C2C-C3C	-2.32	103.55	106.94
21	4	406	CL7	C1C-C2C-C3C	-2.32	103.55	106.94
27	c	517	DGD	O3G-C3G-C2G	-2.32	105.30	110.90
21	2	502	CL7	C3B-C4B-NB	2.32	112.67	110.52
21	6	502	CL7	C3B-C4B-NB	2.32	112.67	110.52
21	2	505	CL7	C4C-C3C-C2C	-2.32	104.10	107.13
21	1	406	CL7	C1C-C2C-C3C	-2.32	103.56	106.94
21	5	406	CL7	C1C-C2C-C3C	-2.32	103.56	106.94
21	4	410	CL7	C3B-C2B-C1B	-2.32	104.36	107.16
21	8	410	CL7	C3B-C2B-C1B	-2.32	104.36	107.16
27	C	517	DGD	O3G-C3G-C2G	-2.32	105.31	110.90
32	8	419	ZEX	C1-C6-C7	2.32	122.34	115.78
32	7	520	ZEX	C39-C29-C30	-2.32	119.68	122.92
32	3	522	ZEX	C21-C22-C23	-2.32	108.67	113.69
32	2	523	ZEX	C39-C29-C28	2.32	121.73	118.08
32	6	522	ZEX	C39-C29-C28	2.32	121.73	118.08
32	1	422	ZEX	C15-C35-C34	-2.32	118.73	123.47
32	5	422	ZEX	C15-C35-C34	-2.32	118.73	123.47
21	2	506	CL7	C4C-C3C-C2C	-2.32	104.11	107.13
21	4	408	CL7	CHB-C1B-NB	-2.32	121.81	124.26
21	8	408	CL7	CHB-C1B-NB	-2.32	121.81	124.26
21	1	407	CL7	C1C-C2C-C3C	-2.32	103.56	106.94
23	4	402	8CT	C25-C24-C23	-2.31	116.00	123.22
23	8	402	8CT	C25-C24-C23	-2.31	116.00	123.22
32	4	419	ZEX	C1-C6-C7	2.31	122.33	115.78
21	b	603	CL7	C1C-C2C-C3C	-2.31	103.56	106.94
21	D	402	CL7	C3B-C4B-NB	2.31	112.66	110.52
21	d	402	CL7	C3B-C4B-NB	2.31	112.66	110.52
21	C	511	CL7	C4-C3-C5	2.31	119.16	115.27
23	c	519	8CT	C27-C26-C25	-2.31	119.68	122.92
21	7	507	CL7	C1C-C2C-C3C	-2.31	103.56	106.94
21	2	516	CL7	C4C-C3C-C2C	-2.31	104.11	107.13
21	6	516	CL7	C4C-C3C-C2C	-2.31	104.11	107.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2	525	ZEX	C15-C35-C34	-2.31	118.74	123.47
32	6	524	ZEX	C15-C35-C34	-2.31	118.74	123.47
21	2	517	CL7	C1-C2-C3	2.31	130.04	126.04
21	3	516	CL7	C3B-C4B-NB	2.31	112.66	110.52
21	7	516	CL7	C3B-C4B-NB	2.31	112.66	110.52
21	2	510	CL7	C1C-C2C-C3C	-2.31	103.57	106.94
21	6	510	CL7	C1C-C2C-C3C	-2.31	103.57	106.94
21	3	507	CL7	CAA-CBA-CGA	-2.31	106.51	113.25
32	4	419	ZEX	C40-C33-C32	2.31	121.71	118.08
32	8	419	ZEX	C40-C33-C32	2.31	121.71	118.08
21	7	507	CL7	C4-C3-C5	2.31	119.15	115.27
23	b	620	8CT	C05-C04-C03	2.31	114.03	110.48
32	3	520	ZEX	C39-C29-C30	-2.31	119.69	122.92
21	B	602	CL7	C1C-C2C-C3C	-2.31	103.57	106.94
21	2	511	CL7	CMB-C2B-C1B	2.31	128.88	125.37
21	6	511	CL7	CMB-C2B-C1B	2.31	128.88	125.37
23	C	519	8CT	C27-C26-C25	-2.30	119.69	122.92
21	4	416	CL7	C3B-C2B-C1B	-2.30	104.38	107.16
21	3	504	CL7	C4C-C3C-C2C	-2.30	104.12	107.13
21	7	504	CL7	C4C-C3C-C2C	-2.30	104.12	107.13
21	7	507	CL7	C4C-C3C-C2C	-2.30	104.12	107.13
32	4	420	ZEX	C20-C13-C12	2.30	121.70	118.08
32	8	420	ZEX	C20-C13-C12	2.30	121.70	118.08
21	C	505	CL7	C4-C3-C5	2.30	119.14	115.27
21	7	507	CL7	CAA-CBA-CGA	-2.30	106.53	113.25
23	B	619	8CT	C05-C04-C03	2.30	114.02	110.48
23	A	404	8CT	C27-C26-C25	-2.30	119.70	122.92
21	1	420	CL7	CMB-C2B-C1B	2.30	128.87	125.37
21	3	514	CL7	C3B-C2B-C1B	-2.30	104.39	107.16
21	2	506	CL7	C1C-C2C-C3C	-2.30	103.58	106.94
21	B	606	CL7	C3B-C4B-NB	2.30	112.65	110.52
21	b	607	CL7	C3B-C4B-NB	2.30	112.65	110.52
21	1	410	CL7	C1C-C2C-C3C	-2.30	103.59	106.94
21	5	410	CL7	C1C-C2C-C3C	-2.30	103.59	106.94
21	1	409	CL7	CAA-CBA-CGA	-2.30	106.41	112.51
21	1	403	CL7	C3B-C4B-NB	2.29	112.64	110.52
21	5	403	CL7	C3B-C4B-NB	2.29	112.64	110.52
21	2	509	CL7	C4C-C3C-C2C	-2.29	104.14	107.13
21	b	609	CL7	O2D-CGD-O1D	-2.29	119.35	123.84
32	3	519	ZEX	C2-C3-C4	-2.29	107.17	110.30
21	6	505	CL7	C4C-C3C-C2C	-2.29	104.14	107.13
21	4	405	CL7	O2A-C1-C2	-2.29	102.61	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	8	405	CL7	O2A-C1-C2	-2.29	102.61	108.64
21	C	506	CL7	C7-C6-C5	-2.29	107.13	113.36
21	c	506	CL7	C7-C6-C5	-2.29	107.13	113.36
21	5	407	CL7	C1C-C2C-C3C	-2.29	103.59	106.94
21	c	505	CL7	C4-C3-C5	2.29	119.12	115.27
21	2	504	CL7	C1C-C2C-C3C	-2.29	103.60	106.94
21	4	412	CL7	CAC-C3C-C2C	2.29	131.45	127.53
21	8	412	CL7	CAC-C3C-C2C	2.29	131.45	127.53
21	7	502	CL7	CHB-C1B-NB	-2.29	121.83	124.26
21	B	608	CL7	O2D-CGD-O1D	-2.29	119.36	123.84
21	6	506	CL7	C4C-C3C-C2C	-2.29	104.14	107.13
21	2	508	CL7	CHB-C1B-NB	-2.29	121.83	124.26
21	7	514	CL7	C3B-C2B-C1B	-2.29	104.40	107.16
21	5	409	CL7	CAA-CBA-CGA	-2.29	106.44	112.51
21	3	502	CL7	CHB-C1B-NB	-2.29	121.84	124.26
21	6	517	CL7	C1-C2-C3	2.29	130.00	126.04
21	6	508	CL7	CHB-C1B-NB	-2.28	121.84	124.26
21	4	411	CL7	C4C-C3C-C2C	-2.28	104.15	107.13
21	4	412	CL7	C4C-C3C-C2C	-2.28	104.15	107.13
21	6	509	CL7	C4C-C3C-C2C	-2.28	104.15	107.13
21	8	411	CL7	C4C-C3C-C2C	-2.28	104.15	107.13
21	8	412	CL7	C4C-C3C-C2C	-2.28	104.15	107.13
21	8	416	CL7	C3B-C2B-C1B	-2.28	104.41	107.16
21	3	513	CL7	CAA-CBA-CGA	-2.28	106.45	112.51
21	3	518	CL7	C1C-C2C-C3C	-2.28	103.61	106.94
21	7	518	CL7	C1C-C2C-C3C	-2.28	103.61	106.94
21	B	615	CL7	C4C-C3C-C2C	-2.28	104.15	107.13
21	b	616	CL7	C4C-C3C-C2C	-2.28	104.15	107.13
21	6	511	CL7	C1C-C2C-C3C	-2.28	103.61	106.94
23	D	406	8CT	C18-C19-C20	2.28	128.14	123.47
23	d	406	8CT	C18-C19-C20	2.28	128.14	123.47
21	B	612	CL7	CMB-C2B-C1B	2.28	128.84	125.37
21	b	613	CL7	CMB-C2B-C1B	2.28	128.84	125.37
21	D	405	CL7	C3B-C4B-NB	2.28	112.63	110.52
21	d	405	CL7	C3B-C4B-NB	2.28	112.63	110.52
21	b	608	CL7	C4C-C3C-C2C	-2.28	104.16	107.13
21	B	612	CL7	CAC-C3C-C2C	2.28	131.42	127.53
21	b	613	CL7	CAC-C3C-C2C	2.28	131.42	127.53
21	8	406	CL7	C1C-C2C-C3C	-2.28	103.62	106.94
21	3	507	CL7	C4C-C3C-C2C	-2.27	104.16	107.13
23	4	402	8CT	C01-C02-C07	2.27	117.98	113.62
23	8	402	8CT	C01-C02-C07	2.27	117.98	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	7	510	CL7	C1C-C2C-C3C	-2.27	103.62	106.94
23	B	619	8CT	C04-C03-C02	-2.27	119.41	122.61
23	b	620	8CT	C04-C03-C02	-2.27	119.41	122.61
21	2	505	CL7	C1C-C2C-C3C	-2.27	103.62	106.94
21	1	417	CL7	CAC-C3C-C4C	-2.27	121.10	124.68
21	5	417	CL7	CAC-C3C-C4C	-2.27	121.10	124.68
21	B	604	CL7	C3B-C2B-C1B	-2.27	104.42	107.16
21	b	605	CL7	C3B-C2B-C1B	-2.27	104.42	107.16
31	F	101	HEM	C4C-CHD-C1D	-2.27	121.16	126.06
21	4	408	CL7	CMB-C2B-C1B	2.27	128.83	125.37
21	8	408	CL7	CMB-C2B-C1B	2.27	128.83	125.37
21	7	513	CL7	CAA-CBA-CGA	-2.27	106.48	112.51
21	1	415	CL7	CMA-C3A-C2A	-2.27	110.80	116.10
21	5	415	CL7	CMA-C3A-C2A	-2.27	110.80	116.10
21	b	613	CL7	O2A-CGA-O1A	-2.27	117.87	123.59
21	D	402	CL7	C1C-C2C-C3C	-2.27	103.63	106.94
21	d	402	CL7	C1C-C2C-C3C	-2.27	103.63	106.94
21	B	604	CL7	C3B-C4B-NB	2.27	112.62	110.52
21	b	605	CL7	C3B-C4B-NB	2.27	112.62	110.52
21	6	504	CL7	C1C-C2C-C3C	-2.27	103.63	106.94
32	7	519	ZEX	C2-C3-C4	-2.27	107.20	110.30
21	2	508	CL7	C3B-C4B-NB	2.26	112.62	110.52
21	6	508	CL7	C3B-C4B-NB	2.26	112.62	110.52
21	b	605	CL7	CAA-CBA-CGA	-2.26	106.64	113.25
21	2	511	CL7	C1C-C2C-C3C	-2.26	103.64	106.94
22	A	402	PHO	CMA-C3A-C4A	-2.26	109.42	114.38
32	1	422	ZEX	C18-C5-C6	-2.26	121.99	124.53
21	6	509	CL7	C1C-C2C-C3C	-2.26	103.64	106.94
21	3	510	CL7	C4C-C3C-C2C	-2.26	104.18	107.13
23	D	406	8CT	C24-C25-C26	-2.26	124.08	127.31
23	d	406	8CT	C24-C25-C26	-2.26	124.08	127.31
32	4	418	ZEX	C20-C13-C14	-2.26	119.76	122.92
32	8	418	ZEX	C20-C13-C14	-2.26	119.76	122.92
21	6	507	CL7	C1C-C2C-C3C	-2.26	103.64	106.94
21	3	510	CL7	C1C-C2C-C3C	-2.26	103.64	106.94
31	f	101	HEM	C4C-CHD-C1D	-2.26	121.18	126.06
32	3	520	ZEX	C3-C4-C5	-2.26	107.36	111.85
21	2	503	CL7	CAA-C2A-C1A	2.26	119.61	112.19
21	6	503	CL7	CAA-C2A-C1A	2.26	119.61	112.19
21	3	501	CL7	C4C-C3C-C2C	-2.26	104.18	107.13
21	5	420	CL7	CMB-C2B-C1B	2.26	128.81	125.37
23	B	618	8CT	C24-C25-C26	-2.26	124.09	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	619	8CT	C24-C25-C26	-2.26	124.09	127.31
32	8	419	ZEX	C35-C15-C14	-2.26	118.85	123.47
21	1	402	CL7	C1C-C2C-C3C	-2.26	103.65	106.94
21	5	402	CL7	C1C-C2C-C3C	-2.26	103.65	106.94
22	a	402	PHO	CMA-C3A-C4A	-2.26	109.44	114.38
21	C	514	CL7	C4C-C3C-C2C	-2.26	104.19	107.13
23	c	519	8CT	C40-C12-C13	-2.26	119.76	122.92
32	2	520	ZEX	C19-C9-C8	2.26	121.63	118.08
32	3	525	ZEX	C19-C9-C8	2.26	121.63	118.08
21	2	503	CL7	C4D-C3D-C2D	2.25	110.24	107.30
21	6	503	CL7	C4D-C3D-C2D	2.25	110.24	107.30
23	C	519	8CT	C40-C12-C13	-2.25	119.77	122.92
32	4	403	ZEX	C35-C15-C14	-2.25	118.86	123.47
32	8	403	ZEX	C35-C15-C14	-2.25	118.86	123.47
23	B	619	8CT	C18-C19-C20	-2.25	118.86	123.47
21	2	507	CL7	C1C-C2C-C3C	-2.25	103.65	106.94
21	6	505	CL7	C1C-C2C-C3C	-2.25	103.65	106.94
21	B	604	CL7	CAA-CBA-CGA	-2.25	106.67	113.25
21	2	509	CL7	C1C-C2C-C3C	-2.25	103.65	106.94
21	C	506	CL7	C3B-C4B-NB	2.25	112.61	110.52
21	c	506	CL7	C3B-C4B-NB	2.25	112.61	110.52
21	3	502	CL7	CGD-CBD-CAD	2.25	118.03	110.73
21	7	502	CL7	CGD-CBD-CAD	2.25	118.03	110.73
31	f	101	HEM	CHA-C4D-C3D	-2.25	121.10	125.33
32	4	419	ZEX	C35-C15-C14	-2.25	118.86	123.47
21	2	506	CL7	CAA-CBA-CGA	-2.25	106.68	113.25
21	6	506	CL7	CAA-CBA-CGA	-2.25	106.68	113.25
31	F	101	HEM	CHA-C4D-C3D	-2.25	121.10	125.33
21	B	606	CL7	O2D-CGD-O1D	-2.25	119.44	123.84
23	a	404	8CT	C27-C26-C25	-2.25	119.77	122.92
21	B	607	CL7	C4C-C3C-C2C	-2.25	104.20	107.13
27	c	517	DGD	O1G-C1A-C2A	2.25	118.96	111.91
21	4	409	CL7	C4-C3-C5	2.25	119.05	115.27
27	C	517	DGD	O1G-C1A-C2A	2.25	118.96	111.91
21	B	622	CL7	C4C-C3C-C2C	-2.25	104.20	107.13
21	3	515	CL7	CAC-C3C-C2C	2.25	131.37	127.53
21	7	515	CL7	CAC-C3C-C2C	2.25	131.37	127.53
31	f	101	HEM	C1A-CHA-C4D	-2.25	121.01	126.34
21	7	510	CL7	C4C-C3C-C2C	-2.25	104.20	107.13
26	c	501	LMG	C30-C29-C28	-2.25	105.45	113.62
32	2	525	ZEX	C35-C15-C14	-2.25	118.87	123.47
21	D	405	CL7	CMB-C2B-C1B	2.25	128.79	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	d	405	CL7	CMB-C2B-C1B	2.25	128.79	125.37
32	1	421	ZEX	C3-C4-C5	-2.25	107.38	111.85
32	5	421	ZEX	C3-C4-C5	-2.25	107.38	111.85
23	C	516	8CT	C22-C21-C20	-2.24	119.78	122.92
21	d	405	CL7	C1C-C2C-C3C	-2.24	103.66	106.94
21	8	409	CL7	C4-C3-C5	2.24	119.05	115.27
31	F	101	HEM	C1A-CHA-C4D	-2.24	121.02	126.34
21	3	511	CL7	C1-C2-C3	2.24	129.92	126.04
21	c	508	CL7	C4C-C3C-C2C	-2.24	104.20	107.13
21	C	510	CL7	C1C-C2C-C3C	-2.24	103.67	106.94
21	c	510	CL7	C1C-C2C-C3C	-2.24	103.67	106.94
21	B	612	CL7	O2A-CGA-O1A	-2.24	117.94	123.59
21	D	405	CL7	C1C-C2C-C3C	-2.24	103.67	106.94
23	b	620	8CT	C18-C19-C20	-2.24	118.89	123.47
23	c	516	8CT	C22-C21-C20	-2.24	119.79	122.92
21	8	406	CL7	C4C-C3C-C2C	-2.24	104.21	107.13
21	b	607	CL7	O2D-CGD-O1D	-2.24	119.47	123.84
21	2	511	CL7	C4D-C3D-C2D	2.23	110.21	107.30
21	6	511	CL7	C4D-C3D-C2D	2.23	110.21	107.30
32	4	403	ZEX	C10-C11-C12	-2.23	116.25	123.22
32	8	403	ZEX	C10-C11-C12	-2.23	116.25	123.22
21	3	516	CL7	C1C-C2C-C3C	-2.23	103.68	106.94
21	7	506	CL7	C1C-C2C-C3C	-2.23	103.68	106.94
21	7	516	CL7	C1C-C2C-C3C	-2.23	103.68	106.94
21	3	503	CL7	CED-O2D-CGD	-2.23	110.89	115.94
21	2	502	CL7	C4C-C3C-C2C	-2.23	104.22	107.13
21	6	502	CL7	C4C-C3C-C2C	-2.23	104.22	107.13
21	1	419	CL7	C1C-C2C-C3C	-2.23	103.68	106.94
21	5	419	CL7	C1C-C2C-C3C	-2.23	103.68	106.94
21	7	506	CL7	C3B-C2B-C1B	-2.23	104.47	107.16
21	c	514	CL7	C4C-C3C-C2C	-2.23	104.22	107.13
21	1	403	CL7	CAA-CBA-CGA	-2.23	106.73	113.25
21	B	605	CL7	C4C-C3C-C2C	-2.23	104.22	107.13
21	b	606	CL7	C4C-C3C-C2C	-2.23	104.22	107.13
21	7	511	CL7	C1-C2-C3	2.23	129.90	126.04
32	6	524	ZEX	C35-C15-C14	-2.23	118.91	123.47
32	5	422	ZEX	C18-C5-C6	-2.23	122.02	124.53
21	2	501	CL7	C1-C2-C3	2.23	129.90	126.04
21	5	410	CL7	C3B-C4B-NB	2.23	112.58	110.52
21	5	403	CL7	CAA-CBA-CGA	-2.23	106.74	113.25
32	7	520	ZEX	C3-C4-C5	-2.23	107.42	111.85
21	6	501	CL7	C1-C2-C3	2.23	129.90	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	7	503	CL7	CED-O2D-CGD	-2.23	110.90	115.94
21	C	508	CL7	C1C-C2C-C3C	-2.23	103.69	106.94
21	c	508	CL7	C1C-C2C-C3C	-2.23	103.69	106.94
21	4	412	CL7	C3B-C4B-NB	2.23	112.58	110.52
21	8	412	CL7	C3B-C4B-NB	2.23	112.58	110.52
21	B	622	CL7	CHB-C1B-NB	-2.23	121.90	124.26
21	b	623	CL7	CHB-C1B-NB	-2.23	121.90	124.26
21	B	612	CL7	C1C-C2C-C3C	-2.23	103.69	106.94
21	b	613	CL7	C1C-C2C-C3C	-2.23	103.69	106.94
26	C	501	LMG	C30-C29-C28	-2.23	105.52	113.62
21	2	516	CL7	C1-C2-C3	2.23	129.89	126.04
21	6	516	CL7	C1-C2-C3	2.23	129.89	126.04
21	2	506	CL7	C3B-C4B-NB	2.23	112.58	110.52
21	6	506	CL7	C3B-C4B-NB	2.23	112.58	110.52
21	7	504	CL7	CAA-CBA-CGA	-2.23	106.75	113.25
21	3	517	CL7	CMB-C2B-C1B	2.22	128.76	125.37
21	3	504	CL7	CAA-CBA-CGA	-2.22	106.76	113.25
21	C	508	CL7	C4C-C3C-C2C	-2.22	104.23	107.13
21	b	623	CL7	C4C-C3C-C2C	-2.22	104.23	107.13
21	d	402	CL7	C4C-C3C-C2C	-2.22	104.23	107.13
21	1	410	CL7	O2A-CGA-O1A	-2.22	117.98	123.59
21	B	622	CL7	C1C-C2C-C3C	-2.22	103.70	106.94
21	1	410	CL7	C4C-C3C-C2C	-2.22	104.23	107.13
21	5	410	CL7	C4C-C3C-C2C	-2.22	104.23	107.13
32	6	519	ZEX	C39-C29-C30	-2.22	119.81	122.92
21	3	511	CL7	C4-C3-C5	2.22	119.01	115.27
21	7	511	CL7	C4-C3-C5	2.22	119.01	115.27
21	7	517	CL7	CMB-C2B-C1B	2.22	128.75	125.37
21	b	606	CL7	CAA-CBA-CGA	-2.22	106.77	113.25
32	2	519	ZEX	C39-C29-C30	-2.22	119.81	122.92
23	4	402	8CT	C10-C11-C12	-2.22	122.88	126.23
23	C	519	8CT	C13-C14-C15	-2.22	116.30	123.22
32	2	519	ZEX	C31-C32-C33	-2.22	120.19	126.42
32	6	519	ZEX	C31-C32-C33	-2.22	120.19	126.42
21	7	516	CL7	CMB-C2B-C1B	2.22	128.75	125.37
32	2	521	ZEX	C40-C33-C32	2.22	121.57	118.08
21	3	506	CL7	C1C-C2C-C3C	-2.22	103.70	106.94
22	A	402	PHO	C1C-C2C-C3C	-2.22	106.77	108.61
21	5	410	CL7	O2A-CGA-O1A	-2.22	118.00	123.59
23	b	619	8CT	C40-C12-C11	2.22	121.57	118.08
22	a	402	PHO	C1C-C2C-C3C	-2.22	106.77	108.61
21	7	501	CL7	C4C-C3C-C2C	-2.21	104.24	107.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	K	101	8CT	C25-C24-C23	-2.21	116.31	123.22
23	k	101	8CT	C25-C24-C23	-2.21	116.31	123.22
21	B	605	CL7	CAA-CBA-CGA	-2.21	106.79	113.25
23	c	519	8CT	C13-C14-C15	-2.21	116.31	123.22
23	B	618	8CT	C40-C12-C11	2.21	121.56	118.08
21	5	403	CL7	C4C-C3C-C2C	-2.21	104.25	107.13
21	2	518	CL7	CMB-C2B-C1B	2.21	128.74	125.37
21	6	518	CL7	CMB-C2B-C1B	2.21	128.74	125.37
21	2	503	CL7	CAA-C2A-C3A	2.21	118.83	112.78
21	6	503	CL7	CAA-C2A-C3A	2.21	118.83	112.78
21	6	504	CL7	C4C-C3C-C2C	-2.21	104.25	107.13
21	b	623	CL7	C1C-C2C-C3C	-2.21	103.71	106.94
21	B	616	CL7	CHB-C1B-NB	-2.21	121.92	124.26
21	b	607	CL7	C1C-C2C-C3C	-2.21	103.72	106.94
21	D	402	CL7	C4C-C3C-C2C	-2.21	104.25	107.13
21	D	402	CL7	C4-C3-C5	2.21	119.48	114.60
21	d	402	CL7	C4-C3-C5	2.21	119.48	114.60
23	A	404	8CT	C14-C15-C16	-2.21	120.22	126.42
23	a	404	8CT	C14-C15-C16	-2.21	120.22	126.42
21	3	506	CL7	C3B-C2B-C1B	-2.21	104.50	107.16
21	C	503	CL7	CHB-C1B-NB	-2.21	121.92	124.26
21	c	503	CL7	CHB-C1B-NB	-2.21	121.92	124.26
21	c	511	CL7	CHB-C1B-NB	-2.21	121.92	124.26
21	D	404	CL7	C1C-C2C-C3C	-2.21	103.72	106.94
21	4	406	CL7	C4C-C3C-C2C	-2.21	104.25	107.13
23	4	402	8CT	C18-C19-C20	-2.21	118.95	123.47
23	8	402	8CT	C18-C19-C20	-2.21	118.95	123.47
32	5	421	ZEX	C10-C11-C12	-2.20	116.34	123.22
21	3	516	CL7	CMB-C2B-C1B	2.20	128.73	125.37
21	2	512	CL7	C1C-C2C-C3C	-2.20	103.72	106.94
29	D	403	BCT	O2-C-O1	2.20	125.26	119.55
29	d	403	BCT	O2-C-O1	2.20	125.26	119.55
21	4	404	CL7	C1C-C2C-C3C	-2.20	103.72	106.94
21	8	404	CL7	C1C-C2C-C3C	-2.20	103.72	106.94
32	1	421	ZEX	C10-C11-C12	-2.20	116.34	123.22
21	C	506	CL7	CBA-CAA-C2A	-2.20	107.36	113.86
32	6	520	ZEX	C40-C33-C32	2.20	121.55	118.08
21	b	617	CL7	CHB-C1B-NB	-2.20	121.93	124.26
32	3	520	ZEX	C40-C33-C34	-2.20	119.84	122.92
32	7	520	ZEX	C40-C33-C34	-2.20	119.84	122.92
21	C	511	CL7	CHB-C1B-NB	-2.20	121.93	124.26
21	2	515	CL7	C1C-C2C-C3C	-2.20	103.73	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	515	CL7	C1C-C2C-C3C	-2.20	103.73	106.94
21	4	404	CL7	CAC-C3C-C2C	2.20	131.29	127.53
21	1	410	CL7	C3B-C4B-NB	2.20	112.56	110.52
32	6	524	ZEX	C30-C31-C32	-2.20	116.36	123.22
21	4	410	CL7	C4C-C3C-C2C	-2.20	104.26	107.13
23	C	515	8CT	C22-C21-C23	2.20	121.54	118.08
23	c	515	8CT	C22-C21-C23	2.20	121.54	118.08
21	1	418	CL7	C4C-C3C-C2C	-2.20	104.26	107.13
21	5	418	CL7	C4C-C3C-C2C	-2.20	104.26	107.13
21	d	404	CL7	C1C-C2C-C3C	-2.20	103.73	106.94
23	C	516	8CT	C24-C23-C21	-2.20	120.25	126.42
23	c	516	8CT	C24-C23-C21	-2.20	120.25	126.42
21	A	406	CL7	C4C-C3C-C2C	-2.20	104.26	107.13
21	a	405	CL7	C4C-C3C-C2C	-2.20	104.26	107.13
23	8	402	8CT	C10-C11-C12	-2.20	122.92	126.23
21	8	404	CL7	CAC-C3C-C2C	2.19	131.28	127.53
32	2	525	ZEX	C30-C31-C32	-2.19	116.37	123.22
21	C	512	CL7	CAC-C3C-C2C	2.19	131.28	127.53
21	c	512	CL7	CAC-C3C-C2C	2.19	131.28	127.53
21	c	506	CL7	CBA-CAA-C2A	-2.19	107.39	113.86
21	4	414	CL7	C4-C3-C5	2.19	118.95	115.27
21	8	414	CL7	C4-C3-C5	2.19	118.95	115.27
21	4	413	CL7	C1C-C2C-C3C	-2.19	103.75	106.94
21	8	413	CL7	C1C-C2C-C3C	-2.19	103.75	106.94
32	3	520	ZEX	C27-C26-C25	-2.19	119.31	122.84
32	7	520	ZEX	C27-C26-C25	-2.19	119.31	122.84
32	3	520	ZEX	C1-C6-C7	2.19	121.97	115.78
21	c	508	CL7	CED-O2D-CGD	-2.19	110.99	115.94
21	1	410	CL7	C4-C3-C5	2.19	118.95	115.27
21	5	410	CL7	C4-C3-C5	2.19	118.95	115.27
21	c	504	CL7	C4C-C3C-C2C	-2.19	104.28	107.13
21	8	410	CL7	C4C-C3C-C2C	-2.19	104.28	107.13
21	B	606	CL7	C1C-C2C-C3C	-2.19	103.75	106.94
21	4	416	CL7	CHB-C1B-NB	-2.18	121.94	124.26
21	8	416	CL7	CHB-C1B-NB	-2.18	121.94	124.26
21	3	510	CL7	C4D-C3D-C2D	2.18	110.14	107.30
21	7	510	CL7	C4D-C3D-C2D	2.18	110.14	107.30
21	3	516	CL7	C4C-C3C-C2C	-2.18	104.28	107.13
21	7	516	CL7	C4C-C3C-C2C	-2.18	104.28	107.13
21	B	607	CL7	CHB-C1B-NB	-2.18	121.94	124.26
21	b	608	CL7	CHB-C1B-NB	-2.18	121.94	124.26
21	1	403	CL7	C4C-C3C-C2C	-2.18	104.28	107.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	512	CL7	C1C-C2C-C3C	-2.18	103.75	106.94
21	C	508	CL7	CED-O2D-CGD	-2.18	111.00	115.94
32	2	520	ZEX	C8-C9-C10	-2.18	115.59	118.94
32	3	525	ZEX	C8-C9-C10	-2.18	115.59	118.94
21	C	504	CL7	C4C-C3C-C2C	-2.18	104.28	107.13
21	1	405	CL7	C3B-C4B-NB	2.18	112.54	110.52
21	1	409	CL7	C1C-C2C-C3C	-2.18	103.76	106.94
21	4	416	CL7	C1C-C2C-C3C	-2.18	103.76	106.94
21	5	409	CL7	C1C-C2C-C3C	-2.18	103.76	106.94
21	8	416	CL7	C1C-C2C-C3C	-2.18	103.76	106.94
21	2	504	CL7	C4C-C3C-C2C	-2.18	104.28	107.13
23	B	617	8CT	C39-C16-C17	-2.18	119.87	122.92
23	b	618	8CT	C39-C16-C17	-2.18	119.87	122.92
21	A	401	CL7	C4D-C3D-CAD	-2.18	105.96	107.42
21	a	401	CL7	C4D-C3D-CAD	-2.18	105.96	107.42
21	C	508	CL7	O2D-CGD-O1D	-2.18	119.58	123.84
21	c	508	CL7	O2D-CGD-O1D	-2.18	119.58	123.84
21	2	511	CL7	C4C-C3C-C2C	-2.18	104.29	107.13
21	B	614	CL7	C4D-C3D-C2D	2.18	110.14	107.30
21	3	505	CL7	CMB-C2B-C1B	2.18	128.68	125.37
21	7	505	CL7	CMB-C2B-C1B	2.18	128.68	125.37
21	5	417	CL7	C4-C3-C5	2.18	118.93	115.27
21	2	508	CL7	C4C-C3C-C2C	-2.18	104.29	107.13
21	6	508	CL7	C4C-C3C-C2C	-2.18	104.29	107.13
23	C	515	8CT	C15-C16-C17	-2.18	115.60	118.94
21	3	502	CL7	C4C-C3C-C2C	-2.17	104.29	107.13
21	B	607	CL7	C1C-C2C-C3C	-2.17	103.77	106.94
32	7	520	ZEX	C1-C6-C7	2.17	121.93	115.78
21	A	401	CL7	O2A-CGA-CBA	2.17	118.73	111.91
21	a	401	CL7	O2A-CGA-CBA	2.17	118.73	111.91
21	D	402	CL7	CMB-C2B-C1B	2.17	128.68	125.37
21	d	402	CL7	CMB-C2B-C1B	2.17	128.68	125.37
32	2	520	ZEX	C23-C24-C25	-2.17	106.24	109.33
23	B	618	8CT	C08-C04-C03	-2.17	106.78	110.30
23	b	619	8CT	C08-C04-C03	-2.17	106.78	110.30
21	C	506	CL7	C1C-C2C-C3C	-2.17	103.77	106.94
21	7	507	CL7	CAC-C3C-C2C	2.17	131.24	127.53
21	B	611	CL7	O2A-CGA-O1A	-2.17	118.12	123.59
32	5	422	ZEX	C27-C26-C25	-2.17	119.34	122.84
23	B	617	8CT	C36-C35-C30	2.16	112.82	109.55
23	b	618	8CT	C36-C35-C30	2.16	112.82	109.55
21	4	412	CL7	C1C-C2C-C3C	-2.16	103.78	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	503	CL7	C4-C3-C5	2.16	118.91	115.27
21	c	503	CL7	C4-C3-C5	2.16	118.91	115.27
21	8	407	CL7	CAC-C3C-C2C	2.16	131.23	127.53
21	b	612	CL7	O2A-CGA-O1A	-2.16	118.13	123.59
23	A	404	8CT	C01-C02-C07	2.16	117.77	113.62
23	a	404	8CT	C01-C02-C07	2.16	117.77	113.62
21	4	415	CL7	C3B-C4B-NB	2.16	112.52	110.52
21	D	404	CL7	O2A-CGA-O1A	-2.16	118.14	123.59
21	d	404	CL7	O2A-CGA-O1A	-2.16	118.14	123.59
21	1	412	CL7	C3B-C4B-NB	2.16	112.52	110.52
21	5	412	CL7	C3B-C4B-NB	2.16	112.52	110.52
21	8	417	CL7	C3B-C2B-C1B	-2.16	104.55	107.16
21	6	518	CL7	C1C-C2C-C3C	-2.16	103.79	106.94
32	4	403	ZEX	C1-C6-C7	2.16	121.89	115.78
32	8	403	ZEX	C1-C6-C7	2.16	121.89	115.78
23	c	515	8CT	C15-C16-C17	-2.16	115.63	118.94
23	c	519	8CT	C39-C16-C15	2.16	121.48	118.08
21	6	503	CL7	C1C-C2C-C3C	-2.16	103.79	106.94
21	C	518	CL7	C3B-C4B-NB	2.16	112.52	110.52
21	c	518	CL7	C3B-C4B-NB	2.16	112.52	110.52
21	3	509	CL7	C4D-C3D-C2D	2.16	110.11	107.30
21	7	509	CL7	C4D-C3D-C2D	2.16	110.11	107.30
21	2	505	CL7	CAC-C3C-C2C	2.16	131.22	127.53
21	2	503	CL7	C1C-C2C-C3C	-2.16	103.79	106.94
21	7	502	CL7	C4C-C3C-C2C	-2.16	104.32	107.13
32	4	419	ZEX	C21-C26-C27	2.16	121.88	115.78
21	2	514	CL7	C3B-C4B-NB	2.16	112.52	110.52
21	6	514	CL7	C3B-C4B-NB	2.16	112.52	110.52
21	5	409	CL7	C3B-C4B-NB	2.16	112.52	110.52
21	5	404	CL7	C3D-C4D-ND	2.16	113.26	110.17
32	8	403	ZEX	C20-C13-C12	2.16	121.47	118.08
21	1	404	CL7	C3D-C4D-ND	2.15	113.26	110.17
23	4	402	8CT	C40-C12-C11	2.15	121.47	118.08
23	8	402	8CT	C40-C12-C11	2.15	121.47	118.08
21	5	420	CL7	C1C-C2C-C3C	-2.15	103.80	106.94
21	1	417	CL7	C4-C3-C5	2.15	118.89	115.27
21	1	413	CL7	CMB-C2B-C1B	2.15	128.65	125.37
21	3	515	CL7	CMA-C3A-C2A	-2.15	111.07	116.10
21	7	502	CL7	C1C-C2C-C3C	-2.15	103.80	106.94
32	8	403	ZEX	C20-C13-C14	-2.15	119.91	122.92
21	b	612	CL7	C3B-C2B-C1B	-2.15	104.56	107.16
21	7	515	CL7	CMA-C3A-C2A	-2.15	111.08	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	8	404	CL7	CMB-C2B-C1B	2.15	128.64	125.37
21	3	515	CL7	C4D-C3D-C2D	2.15	110.10	107.30
21	7	515	CL7	C4D-C3D-C2D	2.15	110.10	107.30
32	3	525	ZEX	C23-C24-C25	-2.15	106.27	109.33
21	b	608	CL7	C1C-C2C-C3C	-2.15	103.80	106.94
21	d	404	CL7	C3B-C4B-NB	2.15	112.51	110.52
21	c	506	CL7	C1C-C2C-C3C	-2.15	103.81	106.94
21	b	615	CL7	C4D-C3D-C2D	2.15	110.10	107.30
21	8	415	CL7	C3B-C4B-NB	2.15	112.51	110.52
23	4	402	8CT	C22-C21-C23	2.15	121.46	118.08
32	1	422	ZEX	C27-C26-C25	-2.15	119.37	122.84
21	3	507	CL7	CAC-C3C-C2C	2.15	131.20	127.53
31	F	101	HEM	CBD-CAD-C3D	-2.15	106.67	112.63
31	f	101	HEM	CBD-CAD-C3D	-2.15	106.67	112.63
21	1	420	CL7	C1C-C2C-C3C	-2.15	103.81	106.94
21	B	611	CL7	C3B-C2B-C1B	-2.15	104.57	107.16
21	4	407	CL7	CAC-C3C-C2C	2.15	131.20	127.53
32	8	419	ZEX	C21-C26-C27	2.14	121.84	115.78
21	6	501	CL7	C4-C3-C5	2.14	118.88	115.27
32	4	403	ZEX	C20-C13-C12	2.14	121.45	118.08
31	F	101	HEM	C4A-NA-C1A	2.14	107.45	105.35
31	f	101	HEM	C4A-NA-C1A	2.14	107.45	105.35
21	B	601	CL7	C4C-C3C-C2C	-2.14	104.33	107.13
21	b	602	CL7	C4C-C3C-C2C	-2.14	104.33	107.13
21	1	402	CL7	CAA-C2A-C3A	-2.14	106.91	112.78
32	4	419	ZEX	C10-C11-C12	-2.14	116.54	123.22
32	8	419	ZEX	C10-C11-C12	-2.14	116.54	123.22
21	A	406	CL7	CMB-C2B-C1B	2.14	128.63	125.37
21	c	505	CL7	C3B-C4B-NB	2.14	112.50	110.52
21	5	405	CL7	C3B-C4B-NB	2.14	112.50	110.52
21	6	515	CL7	CAA-CBA-CGA	-2.14	106.83	112.51
21	7	514	CL7	O2D-CGD-O1D	-2.14	119.66	123.84
23	8	402	8CT	C22-C21-C23	2.14	121.45	118.08
21	6	511	CL7	C4C-C3C-C2C	-2.14	104.34	107.13
21	4	404	CL7	CMB-C2B-C1B	2.14	128.62	125.37
21	6	505	CL7	CAC-C3C-C2C	2.14	131.19	127.53
21	2	518	CL7	C1C-C2C-C3C	-2.14	103.82	106.94
21	b	615	CL7	CBA-CAA-C2A	2.14	120.17	113.86
21	C	502	CL7	C1C-C2C-C3C	-2.14	103.82	106.94
21	c	502	CL7	C1C-C2C-C3C	-2.14	103.82	106.94
21	2	508	CL7	C3B-C2B-C1B	-2.14	104.58	107.16
21	4	417	CL7	C3B-C2B-C1B	-2.14	104.58	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	502	CL7	C1C-C2C-C3C	-2.14	103.82	106.94
32	7	519	ZEX	C21-C26-C27	2.13	121.81	115.78
21	2	501	CL7	C4-C3-C5	2.13	118.86	115.27
21	3	512	CL7	CED-O2D-CGD	-2.13	111.11	115.94
32	8	418	ZEX	C31-C32-C33	-2.13	120.42	126.42
21	b	609	CL7	CAA-CBA-CGA	-2.13	107.02	113.25
21	3	512	CL7	C4-C3-C5	2.13	118.86	115.27
21	3	505	CL7	CHD-C1D-ND	-2.13	122.00	124.26
21	5	402	CL7	CAA-C2A-C3A	-2.13	106.94	112.78
21	5	413	CL7	CMB-C2B-C1B	2.13	128.61	125.37
23	C	519	8CT	C39-C16-C15	2.13	121.43	118.08
21	B	614	CL7	CBA-CAA-C2A	2.13	120.15	113.86
32	4	403	ZEX	C20-C13-C14	-2.13	119.94	122.92
21	2	515	CL7	CAA-CBA-CGA	-2.13	106.86	112.51
21	8	406	CL7	C4-C3-C5	2.13	118.85	115.27
21	c	502	CL7	CAC-C3C-C2C	2.13	131.17	127.53
21	4	406	CL7	C4-C3-C5	2.13	118.85	115.27
21	5	419	CL7	CMB-C2B-C1B	2.13	128.61	125.37
21	8	412	CL7	C1C-C2C-C3C	-2.13	103.83	106.94
21	D	404	CL7	C3B-C4B-NB	2.13	112.49	110.52
21	1	411	CL7	CAA-CBA-CGA	-2.13	106.87	112.51
21	5	411	CL7	CAA-CBA-CGA	-2.13	106.87	112.51
24	2	524	SQD	O8-S-C6	-2.13	102.35	105.74
21	7	512	CL7	C4-C3-C5	2.13	118.85	115.27
21	b	615	CL7	C1C-C2C-C3C	-2.13	103.84	106.94
21	4	408	CL7	C3B-C4B-NB	2.12	112.49	110.52
21	8	408	CL7	C3B-C4B-NB	2.12	112.49	110.52
23	C	515	8CT	C05-C04-C03	2.12	113.75	110.48
21	6	508	CL7	C3B-C2B-C1B	-2.12	104.60	107.16
32	3	519	ZEX	C21-C26-C27	2.12	121.79	115.78
23	8	402	8CT	C39-C16-C15	2.12	121.42	118.08
21	2	511	CL7	CAC-C3C-C2C	2.12	131.16	127.53
21	c	504	CL7	C4-C3-C5	2.12	118.84	115.27
21	d	404	CL7	C4C-C3C-C2C	-2.12	104.36	107.13
32	4	418	ZEX	C31-C32-C33	-2.12	120.45	126.42
32	3	519	ZEX	C20-C13-C14	-2.12	119.95	122.92
32	7	519	ZEX	C20-C13-C14	-2.12	119.95	122.92
21	a	403	CL7	C3B-C4B-NB	2.12	112.48	110.52
21	7	505	CL7	CHD-C1D-ND	-2.12	122.01	124.26
21	B	608	CL7	CAA-CBA-CGA	-2.12	107.06	113.25
21	3	514	CL7	O2D-CGD-O1D	-2.12	119.69	123.84
21	7	512	CL7	CED-O2D-CGD	-2.12	111.14	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	409	CL7	CHC-C1C-NC	-2.12	122.51	124.45
21	5	409	CL7	CHC-C1C-NC	-2.12	122.51	124.45
21	1	419	CL7	CMB-C2B-C1B	2.12	128.60	125.37
21	4	415	CL7	CMB-C2B-C1B	2.12	128.60	125.37
21	8	415	CL7	CMB-C2B-C1B	2.12	128.60	125.37
23	C	516	8CT	C11-C12-C13	2.12	122.19	118.94
23	c	516	8CT	C11-C12-C13	2.12	122.19	118.94
23	C	519	8CT	C22-C21-C20	-2.12	119.96	122.92
23	c	519	8CT	C22-C21-C20	-2.12	119.96	122.92
24	6	523	SQD	O8-S-C6	-2.12	102.36	105.74
23	4	402	8CT	C39-C16-C15	2.12	121.41	118.08
21	3	510	CL7	CAC-C3C-C2C	2.12	131.15	127.53
22	D	408	PHO	O2A-CGA-O1A	-2.11	118.26	123.59
21	5	418	CL7	CAA-CBA-CGA	-2.11	107.08	113.25
21	B	603	CL7	C4C-C3C-C2C	-2.11	104.37	107.13
21	b	604	CL7	C4C-C3C-C2C	-2.11	104.37	107.13
21	C	505	CL7	C3B-C4B-NB	2.11	112.48	110.52
21	C	513	CL7	C3B-C4B-NB	2.11	112.48	110.52
21	D	404	CL7	C4C-C3C-C2C	-2.11	104.37	107.13
32	2	520	ZEX	C20-C13-C12	2.11	121.40	118.08
32	3	525	ZEX	C20-C13-C12	2.11	121.40	118.08
22	d	408	PHO	O2A-CGA-O1A	-2.11	118.26	123.59
21	d	404	CL7	CHC-C1C-NC	-2.11	122.51	124.45
21	1	420	CL7	C4D-C3D-C2D	2.11	110.05	107.30
21	5	420	CL7	C4D-C3D-C2D	2.11	110.05	107.30
21	C	502	CL7	CAC-C3C-C2C	2.11	131.14	127.53
21	4	411	CL7	C1C-C2C-C3C	-2.11	103.86	106.94
21	8	411	CL7	C1C-C2C-C3C	-2.11	103.86	106.94
21	1	418	CL7	CAA-CBA-CGA	-2.11	107.09	113.25
21	7	516	CL7	CBC-CAC-C3C	-2.11	106.61	112.43
21	1	409	CL7	C3B-C4B-NB	2.11	112.47	110.52
32	2	520	ZEX	C18-C5-C4	2.11	118.26	114.36
32	3	525	ZEX	C18-C5-C4	2.11	118.26	114.36
21	B	603	CL7	C4-C3-C5	2.11	118.81	115.27
21	7	510	CL7	CAC-C3C-C2C	2.11	131.13	127.53
21	C	509	CL7	C4C-C3C-C2C	-2.11	104.38	107.13
21	c	509	CL7	C4C-C3C-C2C	-2.11	104.38	107.13
21	1	418	CL7	CED-O2D-CGD	-2.11	111.17	115.94
21	5	418	CL7	CED-O2D-CGD	-2.11	111.17	115.94
21	a	405	CL7	CMB-C2B-C1B	2.11	128.58	125.37
23	c	515	8CT	C05-C04-C03	2.10	113.72	110.48
21	C	504	CL7	C4-C3-C5	2.10	118.81	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	511	CL7	C2A-C1A-CHA	-2.10	122.16	126.36
21	4	405	CL7	C3B-C4B-NB	2.10	112.47	110.52
23	d	406	8CT	C27-C26-C28	2.10	121.39	118.08
21	c	511	CL7	C2A-C1A-CHA	-2.10	122.16	126.36
21	D	404	CL7	CHC-C1C-NC	-2.10	122.52	124.45
21	B	604	CL7	O2D-CGD-O1D	-2.10	119.73	123.84
21	c	513	CL7	C3B-C4B-NB	2.10	112.46	110.52
21	3	508	CL7	CHB-C1B-NB	-2.10	122.03	124.26
21	b	604	CL7	C4-C3-C5	2.10	118.80	115.27
21	7	517	CL7	C3B-C4B-NB	2.10	112.46	110.52
21	6	511	CL7	CAC-C3C-C2C	2.10	131.12	127.53
21	1	408	CL7	C1-O2A-CGA	-2.10	110.94	116.44
21	2	518	CL7	C3B-C4B-NB	2.10	112.46	110.52
32	3	522	ZEX	C8-C9-C10	2.10	122.16	118.94
32	7	522	ZEX	C8-C9-C10	2.10	122.16	118.94
21	4	413	CL7	C3B-C4B-NB	2.10	112.46	110.52
21	3	505	CL7	CED-O2D-CGD	-2.10	111.20	115.94
21	7	505	CL7	CED-O2D-CGD	-2.10	111.20	115.94
21	4	407	CL7	C1C-C2C-C3C	-2.10	103.88	106.94
21	B	607	CL7	CED-O2D-CGD	-2.10	111.20	115.94
32	4	420	ZEX	C18-C5-C4	2.10	118.24	114.36
32	8	420	ZEX	C18-C5-C4	2.10	118.24	114.36
21	6	505	CL7	CMB-C2B-C1B	2.10	128.56	125.37
32	4	403	ZEX	C7-C6-C5	-2.10	116.39	121.46
32	8	403	ZEX	C7-C6-C5	-2.10	116.39	121.46
21	2	513	CL7	C1C-C2C-C3C	-2.09	103.88	106.94
21	6	513	CL7	C1C-C2C-C3C	-2.09	103.88	106.94
21	6	518	CL7	C3B-C4B-NB	2.09	112.46	110.52
32	1	421	ZEX	C15-C35-C34	-2.09	119.18	123.47
32	5	421	ZEX	C15-C35-C34	-2.09	119.18	123.47
21	4	405	CL7	C4C-C3C-C2C	-2.09	104.40	107.13
21	3	516	CL7	CBC-CAC-C3C	-2.09	106.66	112.43
21	3	514	CL7	CAC-C3C-C4C	-2.09	121.38	124.68
21	7	514	CL7	CAC-C3C-C4C	-2.09	121.38	124.68
21	b	605	CL7	O2D-CGD-O1D	-2.09	119.75	123.84
21	c	509	CL7	O2D-CGD-O1D	-2.09	119.75	123.84
32	1	421	ZEX	C37-C21-C26	-2.09	106.91	110.30
32	5	421	ZEX	C37-C21-C26	-2.09	106.91	110.30
21	2	505	CL7	O2D-CGD-O1D	-2.09	119.75	123.84
32	4	403	ZEX	C40-C33-C34	-2.09	120.00	122.92
32	4	420	ZEX	C38-C24-C23	-2.09	108.97	112.20
21	2	513	CL7	O2D-CGD-O1D	-2.09	119.75	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	403	CL7	C3B-C4B-NB	2.09	112.45	110.52
21	B	616	CL7	C1C-C2C-C3C	-2.09	103.89	106.94
21	b	617	CL7	C1C-C2C-C3C	-2.09	103.89	106.94
21	7	512	CL7	C1C-C2C-C3C	-2.09	103.89	106.94
32	8	403	ZEX	C40-C33-C34	-2.09	120.00	122.92
32	2	523	ZEX	C4-C5-C6	-2.09	116.20	120.85
32	6	522	ZEX	C4-C5-C6	-2.09	116.20	120.85
21	4	412	CL7	C4-C3-C5	2.09	118.78	115.27
21	8	412	CL7	C4-C3-C5	2.09	118.78	115.27
21	B	610	CL7	C1C-C2C-C3C	-2.09	103.89	106.94
21	b	611	CL7	C1C-C2C-C3C	-2.09	103.89	106.94
21	1	410	CL7	CAA-CBA-CGA	-2.09	107.16	113.25
21	c	507	CL7	C1-C2-C3	2.08	129.65	126.04
23	D	406	8CT	C27-C26-C28	2.08	121.36	118.08
21	b	608	CL7	CED-O2D-CGD	-2.08	111.22	115.94
21	5	408	CL7	C1-O2A-CGA	-2.08	110.98	116.44
21	C	506	CL7	C1-O2A-CGA	-2.08	110.98	116.44
21	B	614	CL7	C1C-C2C-C3C	-2.08	103.90	106.94
32	8	418	ZEX	C1-C2-C3	-2.08	108.94	113.64
21	A	401	CL7	CAC-C3C-C2C	2.08	131.09	127.53
21	a	401	CL7	CAC-C3C-C2C	2.08	131.09	127.53
21	7	508	CL7	C4C-C3C-C2C	-2.08	104.41	107.13
24	5	423	SQD	O8-S-C6	-2.08	102.42	105.74
21	2	508	CL7	CMB-C2B-C1B	2.08	128.54	125.37
21	5	416	CL7	C1C-C2C-C3C	-2.08	103.90	106.94
21	4	410	CL7	C3B-C4B-NB	2.08	112.44	110.52
21	8	410	CL7	C3B-C4B-NB	2.08	112.44	110.52
21	8	405	CL7	C4C-C3C-C2C	-2.08	104.42	107.13
21	3	512	CL7	O2D-CGD-O1D	-2.08	119.77	123.84
21	7	512	CL7	O2D-CGD-O1D	-2.08	119.77	123.84
21	5	411	CL7	C1C-C2C-C3C	-2.08	103.90	106.94
21	7	508	CL7	CHB-C1B-NB	-2.08	122.06	124.26
21	1	404	CL7	CAA-CBA-CGA	-2.08	107.18	113.25
21	5	404	CL7	CAA-CBA-CGA	-2.08	107.18	113.25
32	8	420	ZEX	C38-C24-C23	-2.08	108.99	112.20
21	4	408	CL7	C1C-C2C-C3C	-2.08	103.91	106.94
21	8	408	CL7	C1C-C2C-C3C	-2.08	103.91	106.94
21	6	513	CL7	C3D-C4D-ND	2.08	113.15	110.17
21	1	420	CL7	O2D-CGD-O1D	-2.08	119.78	123.84
21	5	410	CL7	CAA-CBA-CGA	-2.08	107.18	113.25
21	C	509	CL7	CAC-C3C-C2C	2.08	131.08	127.53
21	c	509	CL7	CAC-C3C-C2C	2.08	131.08	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	4	418	ZEX	C19-C9-C10	-2.08	120.01	122.92
21	3	516	CL7	CBA-CAA-C2A	-2.08	107.73	113.86
21	d	405	CL7	CED-O2D-CGD	-2.08	111.24	115.94
23	B	618	8CT	C18-C19-C20	2.08	127.73	123.47
21	6	513	CL7	O2D-CGD-O1D	-2.08	119.78	123.84
21	3	503	CL7	C1C-C2C-C3C	-2.08	103.91	106.94
21	7	503	CL7	C1C-C2C-C3C	-2.08	103.91	106.94
32	5	422	ZEX	C1-C2-C3	-2.08	108.95	113.64
21	2	518	CL7	O2D-CGD-O1D	-2.08	119.78	123.84
21	6	518	CL7	O2D-CGD-O1D	-2.08	119.78	123.84
21	7	516	CL7	CBA-CAA-C2A	-2.08	107.74	113.86
21	2	505	CL7	CMB-C2B-C1B	2.07	128.53	125.37
21	8	407	CL7	C1C-C2C-C3C	-2.07	103.91	106.94
21	c	506	CL7	C1-O2A-CGA	-2.07	111.00	116.44
21	C	509	CL7	O2D-CGD-O1D	-2.07	119.78	123.84
21	8	413	CL7	C3B-C4B-NB	2.07	112.44	110.52
21	6	517	CL7	C1C-C2C-C3C	-2.07	103.92	106.94
21	2	502	CL7	C3B-C2B-C1B	-2.07	104.66	107.16
21	6	502	CL7	C3B-C2B-C1B	-2.07	104.66	107.16
21	4	404	CL7	C3B-C4B-NB	2.07	112.44	110.52
21	8	404	CL7	C3B-C4B-NB	2.07	112.44	110.52
21	b	615	CL7	C4-C3-C5	2.07	118.75	115.27
32	4	418	ZEX	C1-C2-C3	-2.07	108.97	113.64
21	1	415	CL7	C1C-C2C-C3C	-2.07	103.92	106.94
21	8	406	CL7	CED-O2D-CGD	-2.07	111.25	115.94
21	2	513	CL7	C3B-C4B-NB	2.07	112.44	110.52
32	8	418	ZEX	C19-C9-C10	-2.07	120.02	122.92
32	1	421	ZEX	C1-C2-C3	-2.07	108.97	113.64
32	5	421	ZEX	C1-C2-C3	-2.07	108.97	113.64
21	1	411	CL7	C1C-C2C-C3C	-2.07	103.92	106.94
21	6	514	CL7	C1C-C2C-C3C	-2.07	103.92	106.94
21	5	415	CL7	C1C-C2C-C3C	-2.07	103.92	106.94
32	1	422	ZEX	C1-C2-C3	-2.07	108.97	113.64
24	2	522	SQD	O8-S-C6	-2.07	102.45	105.74
24	6	521	SQD	O8-S-C6	-2.07	102.45	105.74
32	4	420	ZEX	C40-C33-C32	2.07	121.33	118.08
32	8	420	ZEX	C40-C33-C32	2.07	121.33	118.08
21	4	415	CL7	O1D-CGD-CBD	-2.07	120.26	124.48
32	2	525	ZEX	C21-C26-C27	2.07	121.62	115.78
32	6	524	ZEX	C21-C26-C27	2.07	121.62	115.78
21	5	420	CL7	O2D-CGD-O1D	-2.07	119.80	123.84
21	1	412	CL7	C4C-C3C-C2C	-2.07	104.43	107.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	412	CL7	C4C-C3C-C2C	-2.07	104.43	107.13
21	8	405	CL7	C3B-C4B-NB	2.07	112.43	110.52
21	3	512	CL7	C1C-C2C-C3C	-2.06	103.93	106.94
21	C	509	CL7	C3B-C2B-C1B	-2.06	104.67	107.16
32	4	420	ZEX	C39-C29-C28	2.06	121.33	118.08
32	8	420	ZEX	C39-C29-C28	2.06	121.33	118.08
21	2	501	CL7	C3B-C4B-NB	2.06	112.43	110.52
21	C	506	CL7	C9-C8-C7	-2.06	103.82	111.29
21	2	517	CL7	C1C-C2C-C3C	-2.06	103.93	106.94
21	6	508	CL7	CMB-C2B-C1B	2.06	128.51	125.37
23	b	619	8CT	C18-C19-C20	2.06	127.69	123.47
21	6	505	CL7	O2D-CGD-O1D	-2.06	119.81	123.84
21	D	405	CL7	CED-O2D-CGD	-2.06	111.28	115.94
21	B	614	CL7	C3B-C4B-NB	2.06	112.42	110.52
23	4	402	8CT	C08-C04-C03	-2.06	106.96	110.30
21	3	510	CL7	CMB-C2B-C1B	2.06	128.50	125.37
21	7	510	CL7	CMB-C2B-C1B	2.06	128.50	125.37
21	C	509	CL7	CED-O2D-CGD	-2.06	111.28	115.94
21	d	404	CL7	C4-C3-C5	2.06	118.73	115.27
21	3	517	CL7	C3B-C4B-NB	2.06	112.42	110.52
24	1	423	SQD	O8-S-C6	-2.06	102.46	105.74
21	1	416	CL7	C1C-C2C-C3C	-2.06	103.94	106.94
21	3	502	CL7	CMB-C2B-C1B	2.06	128.50	125.37
21	7	502	CL7	CMB-C2B-C1B	2.06	128.50	125.37
21	7	501	CL7	C2A-C1A-CHA	-2.06	122.25	126.36
21	2	513	CL7	C3D-C4D-ND	2.06	113.12	110.17
23	C	519	8CT	C35-C30-C31	2.06	115.10	111.42
21	3	508	CL7	C4C-C3C-C2C	-2.06	104.45	107.13
23	c	515	8CT	C11-C12-C13	-2.05	115.79	118.94
21	2	501	CL7	C4C-C3C-C2C	-2.05	104.45	107.13
21	6	501	CL7	C4C-C3C-C2C	-2.05	104.45	107.13
23	b	619	8CT	C11-C10-C03	-2.05	121.44	127.20
21	2	514	CL7	C1C-C2C-C3C	-2.05	103.94	106.94
21	7	516	CL7	CED-O2D-CGD	-2.05	111.29	115.94
21	C	507	CL7	C1-C2-C3	2.05	129.59	126.04
21	c	506	CL7	C9-C8-C7	-2.05	103.86	111.29
21	5	408	CL7	O2A-CGA-O1A	-2.05	118.42	123.59
21	4	409	CL7	C3B-C4B-NB	2.05	112.42	110.52
21	4	409	CL7	CBC-CAC-C3C	-2.05	106.78	112.43
21	8	409	CL7	CBC-CAC-C3C	-2.05	106.78	112.43
21	7	518	CL7	C3B-C4B-NB	2.05	112.42	110.52
21	3	516	CL7	CED-O2D-CGD	-2.05	111.30	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	614	CL7	C1C-C2C-C3C	-2.05	103.95	106.94
21	8	415	CL7	O1D-CGD-CBD	-2.05	120.29	124.48
21	3	501	CL7	C2A-C1A-CHA	-2.05	122.27	126.36
21	4	406	CL7	CED-O2D-CGD	-2.05	111.31	115.94
32	4	419	ZEX	C20-C13-C14	-2.05	120.06	122.92
32	8	419	ZEX	C20-C13-C14	-2.05	120.06	122.92
32	4	419	ZEX	C1-C2-C3	-2.05	109.02	113.64
23	8	402	8CT	C08-C04-C03	-2.04	106.98	110.30
21	2	518	CL7	C4-C3-C5	2.04	118.71	115.27
21	b	615	CL7	C3B-C4B-NB	2.04	112.41	110.52
21	1	408	CL7	O2A-CGA-O1A	-2.04	118.44	123.59
21	b	615	CL7	CMB-C2B-C1B	2.04	128.48	125.37
23	C	515	8CT	C24-C25-C26	-2.04	124.40	127.31
23	c	515	8CT	C24-C25-C26	-2.04	124.40	127.31
21	2	516	CL7	CAC-C3C-C2C	2.04	131.02	127.53
21	6	516	CL7	CAC-C3C-C2C	2.04	131.02	127.53
32	2	521	ZEX	C11-C12-C13	-2.04	120.69	126.42
32	6	520	ZEX	C11-C12-C13	-2.04	120.69	126.42
21	3	518	CL7	C3B-C4B-NB	2.04	112.41	110.52
21	6	501	CL7	C3B-C4B-NB	2.04	112.41	110.52
23	c	519	8CT	C35-C30-C31	2.04	115.07	111.42
21	c	509	CL7	C3B-C2B-C1B	-2.04	104.70	107.16
21	B	613	CL7	C1C-C2C-C3C	-2.04	103.97	106.94
21	7	510	CL7	O2A-CGA-CBA	2.04	118.30	111.91
21	B	614	CL7	C4-C3-C5	2.04	118.70	115.27
21	D	404	CL7	C4-C3-C5	2.04	118.70	115.27
21	7	512	CL7	C4D-C3D-C2D	2.04	109.95	107.30
21	6	516	CL7	O2A-C1-C2	-2.04	103.28	108.64
21	7	509	CL7	C1C-C2C-C3C	-2.04	103.97	106.94
21	4	412	CL7	O2D-CGD-O1D	-2.04	119.86	123.84
21	6	503	CL7	C3B-C4B-NB	2.04	112.40	110.52
21	c	509	CL7	CED-O2D-CGD	-2.03	111.34	115.94
23	K	101	8CT	C05-C04-C03	2.03	113.61	110.48
21	B	614	CL7	CMB-C2B-C1B	2.03	128.47	125.37
21	8	408	CL7	C4D-C3D-C2D	2.03	109.95	107.30
23	C	515	8CT	C11-C12-C13	-2.03	115.82	118.94
23	k	101	8CT	C05-C04-C03	2.03	113.61	110.48
21	1	418	CL7	CMB-C2B-C1B	2.03	128.46	125.37
21	5	418	CL7	CMB-C2B-C1B	2.03	128.46	125.37
23	B	618	8CT	C11-C10-C03	-2.03	121.50	127.20
21	C	507	CL7	C3B-C2B-C1B	-2.03	104.71	107.16
21	1	413	CL7	C4D-C3D-C2D	2.03	109.95	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	415	CL7	C4D-C3D-C2D	2.03	109.95	107.30
21	5	413	CL7	C4D-C3D-C2D	2.03	109.95	107.30
32	8	419	ZEX	C1-C2-C3	-2.03	109.06	113.64
21	6	513	CL7	C3B-C4B-NB	2.03	112.40	110.52
21	1	413	CL7	O2D-CGD-O1D	-2.03	119.87	123.84
21	3	502	CL7	C1-C2-C3	2.03	129.55	126.04
21	7	502	CL7	C1-C2-C3	2.03	129.55	126.04
21	7	503	CL7	CAC-C3C-C2C	2.03	131.00	127.53
21	2	516	CL7	O2A-C1-C2	-2.03	103.31	108.64
21	3	507	CL7	O2D-CGD-O1D	-2.03	119.87	123.84
21	7	507	CL7	O2D-CGD-O1D	-2.03	119.87	123.84
21	3	512	CL7	C4D-C3D-C2D	2.03	109.94	107.30
21	3	510	CL7	O2A-CGA-CBA	2.03	118.27	111.91
32	2	519	ZEX	C18-C5-C4	2.03	118.11	114.36
32	6	519	ZEX	C18-C5-C4	2.03	118.11	114.36
21	6	518	CL7	C4-C3-C5	2.03	118.68	115.27
21	1	405	CL7	C4C-C3C-C2C	-2.03	104.49	107.13
32	2	520	ZEX	C21-C26-C27	2.02	121.51	115.78
32	3	525	ZEX	C21-C26-C27	2.02	121.51	115.78
21	1	420	CL7	CAA-CBA-CGA	-2.02	107.14	112.51
21	B	610	CL7	C4D-C3D-C2D	2.02	109.93	107.30
21	C	502	CL7	C4D-C3D-C2D	2.02	109.93	107.30
21	b	611	CL7	C4D-C3D-C2D	2.02	109.93	107.30
32	1	422	ZEX	C10-C11-C12	-2.02	116.91	123.22
21	b	605	CL7	CED-O2D-CGD	-2.02	111.36	115.94
21	1	420	CL7	C3B-C4B-NB	2.02	112.39	110.52
32	2	521	ZEX	C10-C11-C12	-2.02	116.91	123.22
21	b	606	CL7	C4D-C3D-C2D	2.02	109.93	107.30
32	6	520	ZEX	C10-C11-C12	-2.02	116.91	123.22
21	2	505	CL7	C4-C3-C2	-2.02	118.50	123.68
21	c	507	CL7	C3B-C2B-C1B	-2.02	104.72	107.16
21	8	412	CL7	O2D-CGD-O1D	-2.02	119.89	123.84
21	8	412	CL7	C4D-C3D-C2D	2.02	109.93	107.30
21	1	405	CL7	CMB-C2B-C1B	2.02	128.44	125.37
21	5	405	CL7	CMB-C2B-C1B	2.02	128.44	125.37
32	8	419	ZEX	C19-C9-C8	2.02	121.26	118.08
21	3	504	CL7	CBA-CAA-C2A	2.02	119.82	113.86
21	7	504	CL7	CBA-CAA-C2A	2.02	119.82	113.86
32	1	422	ZEX	C1-C6-C7	2.02	121.49	115.78
32	5	422	ZEX	C1-C6-C7	2.02	121.49	115.78
21	5	413	CL7	O2D-CGD-O1D	-2.02	119.89	123.84
21	2	518	CL7	CAC-C3C-C2C	2.02	130.98	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	503	CL7	CAC-C3C-C2C	2.02	130.98	127.53
21	5	405	CL7	C4C-C3C-C2C	-2.02	104.50	107.13
23	C	519	8CT	C35-C30-C29	-2.02	110.15	112.70
23	c	519	8CT	C35-C30-C29	-2.02	110.15	112.70
32	3	519	ZEX	C31-C32-C33	-2.02	120.75	126.42
27	B	624	DGD	O1G-C1A-O1A	-2.02	118.50	123.59
21	8	415	CL7	C1C-C2C-C3C	-2.02	104.00	106.94
32	5	422	ZEX	C10-C11-C12	-2.02	116.93	123.22
21	3	503	CL7	C4D-C3D-C2D	2.02	109.92	107.30
21	7	503	CL7	C4D-C3D-C2D	2.02	109.92	107.30
21	C	508	CL7	C4-C3-C5	2.02	118.66	115.27
21	c	508	CL7	C4-C3-C5	2.02	118.66	115.27
32	4	419	ZEX	C19-C9-C8	2.02	121.25	118.08
21	5	420	CL7	CAA-CBA-CGA	-2.01	107.16	112.51
21	5	407	CL7	CAC-C3C-C2C	2.01	130.97	127.53
21	2	506	CL7	C4D-C3D-C2D	2.01	109.92	107.30
21	4	412	CL7	CMB-C2B-C1B	2.01	128.44	125.37
21	8	412	CL7	CMB-C2B-C1B	2.01	128.44	125.37
32	8	420	ZEX	C37-C21-C26	-2.01	107.03	110.30
21	B	602	CL7	O2D-CGD-O1D	-2.01	119.90	123.84
21	8	409	CL7	C1C-C2C-C3C	-2.01	104.00	106.94
32	4	420	ZEX	C37-C21-C26	-2.01	107.04	110.30
32	2	523	ZEX	C10-C11-C12	-2.01	116.94	123.22
32	6	522	ZEX	C10-C11-C12	-2.01	116.94	123.22
21	b	603	CL7	O2D-CGD-O1D	-2.01	119.91	123.84
21	B	604	CL7	CED-O2D-CGD	-2.01	111.39	115.94
32	4	420	ZEX	C1-C2-C3	-2.01	109.11	113.64
32	8	420	ZEX	C1-C2-C3	-2.01	109.11	113.64
21	3	509	CL7	C1C-C2C-C3C	-2.01	104.01	106.94
21	6	505	CL7	C4-C3-C2	-2.01	118.53	123.68
32	7	519	ZEX	C31-C32-C33	-2.01	120.78	126.42
21	5	414	CL7	CGD-CBD-CAD	2.01	117.23	110.73
21	1	410	CL7	CMB-C2B-C1B	2.01	128.43	125.37
21	5	410	CL7	CMB-C2B-C1B	2.01	128.43	125.37
21	2	502	CL7	CAC-C3C-C2C	2.01	130.96	127.53
32	2	523	ZEX	C28-C29-C30	-2.01	115.86	118.94
32	6	522	ZEX	C28-C29-C30	-2.01	115.86	118.94
21	1	407	CL7	C3B-C4B-NB	2.00	112.38	110.52
21	5	407	CL7	C3B-C4B-NB	2.00	112.38	110.52
21	8	409	CL7	C3B-C4B-NB	2.00	112.38	110.52
32	1	421	ZEX	C40-C33-C34	-2.00	120.11	122.92
32	5	421	ZEX	C40-C33-C34	-2.00	120.11	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	b	625	DGD	O1G-C1A-O1A	-2.00	118.54	123.59
21	4	409	CL7	C1C-C2C-C3C	-2.00	104.02	106.94
21	B	611	CL7	C4C-C3C-C2C	-2.00	104.52	107.13
21	B	605	CL7	C3B-C4B-NB	2.00	112.37	110.52
21	b	606	CL7	C3B-C4B-NB	2.00	112.37	110.52
21	2	503	CL7	C3B-C4B-NB	2.00	112.37	110.52
21	8	415	CL7	C4D-C3D-C2D	2.00	109.91	107.30
21	1	414	CL7	CGD-CBD-CAD	2.00	117.22	110.73

All (424) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	401	CL7	NA
21	A	401	CL7	NC
21	A	403	CL7	NA
21	A	403	CL7	NC
21	A	406	CL7	NA
21	A	406	CL7	NC
21	B	601	CL7	NA
21	B	601	CL7	NC
21	B	602	CL7	NA
21	B	602	CL7	NC
21	B	603	CL7	NA
21	B	603	CL7	NC
21	B	604	CL7	NA
21	B	604	CL7	NC
21	B	605	CL7	NA
21	B	605	CL7	NC
21	B	606	CL7	NA
21	B	606	CL7	NC
21	B	607	CL7	NA
21	B	607	CL7	NC
21	B	608	CL7	NA
21	B	608	CL7	NC
21	B	609	CL7	NA
21	B	609	CL7	NC
21	B	610	CL7	NA
21	B	610	CL7	NC
21	B	611	CL7	NA
21	B	611	CL7	NC
21	B	612	CL7	NA
21	B	612	CL7	NC

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Mol	Chain	Res	Type	Atom
21	B	613	CL7	NA
21	B	613	CL7	NC
21	B	614	CL7	NA
21	B	614	CL7	NC
21	B	615	CL7	NA
21	B	615	CL7	NC
21	B	616	CL7	NA
21	B	616	CL7	NC
21	B	622	CL7	NA
21	B	622	CL7	NC
21	C	502	CL7	NA
21	C	502	CL7	NC
21	C	503	CL7	NA
21	C	503	CL7	NC
21	C	504	CL7	NA
21	C	504	CL7	NC
21	C	505	CL7	NA
21	C	505	CL7	NC
21	C	506	CL7	NA
21	C	506	CL7	NC
21	C	507	CL7	NA
21	C	507	CL7	NC
21	C	508	CL7	NA
21	C	508	CL7	NC
21	C	509	CL7	NA
21	C	509	CL7	NC
21	C	510	CL7	NA
21	C	510	CL7	NC
21	C	511	CL7	NA
21	C	511	CL7	NC
21	C	512	CL7	NA
21	C	512	CL7	NC
21	C	513	CL7	NA
21	C	513	CL7	NC
21	C	514	CL7	NA
21	C	514	CL7	NC
21	C	518	CL7	NA
21	C	518	CL7	NC
21	D	402	CL7	NA
21	D	402	CL7	NC
21	D	404	CL7	NA
21	D	404	CL7	NC

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Mol	Chain	Res	Type	Atom
21	D	405	CL7	NA
21	D	405	CL7	NC
21	2	501	CL7	NA
21	2	501	CL7	NC
21	2	502	CL7	NA
21	2	502	CL7	NC
21	2	503	CL7	NA
21	2	503	CL7	NC
21	2	504	CL7	NA
21	2	504	CL7	NC
21	2	505	CL7	NA
21	2	505	CL7	NC
21	2	506	CL7	NA
21	2	506	CL7	NC
21	2	507	CL7	NA
21	2	507	CL7	NC
21	2	508	CL7	NA
21	2	508	CL7	NC
21	2	509	CL7	NA
21	2	509	CL7	NC
21	2	510	CL7	NA
21	2	510	CL7	NC
21	2	511	CL7	NA
21	2	511	CL7	NC
21	2	512	CL7	NA
21	2	512	CL7	NC
21	2	513	CL7	NA
21	2	513	CL7	NC
21	2	514	CL7	NA
21	2	514	CL7	NC
21	2	515	CL7	NA
21	2	515	CL7	NC
21	2	516	CL7	NA
21	2	516	CL7	NC
21	2	517	CL7	NA
21	2	517	CL7	NC
21	2	518	CL7	NA
21	2	518	CL7	NC
21	1	402	CL7	NA
21	1	402	CL7	NC
21	1	403	CL7	NA
21	1	403	CL7	NC

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Mol	Chain	Res	Type	Atom
21	1	404	CL7	NA
21	1	404	CL7	NC
21	1	405	CL7	NA
21	1	405	CL7	NC
21	1	406	CL7	NA
21	1	406	CL7	NC
21	1	407	CL7	NA
21	1	407	CL7	NC
21	1	408	CL7	NA
21	1	408	CL7	NC
21	1	409	CL7	NA
21	1	409	CL7	NC
21	1	410	CL7	NA
21	1	410	CL7	NC
21	1	411	CL7	NA
21	1	411	CL7	NC
21	1	412	CL7	NA
21	1	412	CL7	NC
21	1	413	CL7	NA
21	1	413	CL7	NC
21	1	414	CL7	NA
21	1	414	CL7	NC
21	1	415	CL7	NA
21	1	415	CL7	NC
21	1	416	CL7	NA
21	1	416	CL7	NC
21	1	417	CL7	NA
21	1	417	CL7	NC
21	1	418	CL7	NA
21	1	418	CL7	NC
21	1	419	CL7	NA
21	1	419	CL7	NC
21	1	420	CL7	NA
21	1	420	CL7	NC
21	3	501	CL7	NA
21	3	501	CL7	NC
21	3	502	CL7	NA
21	3	502	CL7	NC
21	3	503	CL7	NA
21	3	503	CL7	NC
21	3	504	CL7	NA
21	3	504	CL7	NC

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Mol	Chain	Res	Type	Atom
21	3	505	CL7	NA
21	3	505	CL7	NC
21	3	506	CL7	NA
21	3	506	CL7	NC
21	3	507	CL7	NA
21	3	507	CL7	NC
21	3	508	CL7	NA
21	3	508	CL7	NC
21	3	509	CL7	NA
21	3	509	CL7	NC
21	3	510	CL7	NA
21	3	510	CL7	NC
21	3	511	CL7	NA
21	3	511	CL7	NC
21	3	512	CL7	NA
21	3	512	CL7	NC
21	3	513	CL7	NA
21	3	513	CL7	NC
21	3	514	CL7	NA
21	3	514	CL7	NC
21	3	515	CL7	NA
21	3	515	CL7	NC
21	3	516	CL7	NA
21	3	516	CL7	NC
21	3	517	CL7	NA
21	3	517	CL7	NC
21	3	518	CL7	NA
21	3	518	CL7	NC
21	4	404	CL7	NA
21	4	404	CL7	NC
21	4	405	CL7	NA
21	4	405	CL7	NC
21	4	406	CL7	NA
21	4	406	CL7	NC
21	4	407	CL7	NA
21	4	407	CL7	NC
21	4	408	CL7	NA
21	4	408	CL7	NC
21	4	409	CL7	NA
21	4	409	CL7	NC
21	4	410	CL7	NA
21	4	410	CL7	NC

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Mol	Chain	Res	Type	Atom
21	4	411	CL7	NA
21	4	411	CL7	NC
21	4	412	CL7	NA
21	4	412	CL7	NC
21	4	413	CL7	NA
21	4	413	CL7	NC
21	4	414	CL7	NA
21	4	414	CL7	NC
21	4	415	CL7	NA
21	4	415	CL7	NC
21	4	416	CL7	NA
21	4	416	CL7	NC
21	4	417	CL7	NA
21	4	417	CL7	NC
21	a	401	CL7	NA
21	a	401	CL7	NC
21	a	403	CL7	NA
21	a	403	CL7	NC
21	a	405	CL7	NA
21	a	405	CL7	NC
21	b	602	CL7	NA
21	b	602	CL7	NC
21	b	603	CL7	NA
21	b	603	CL7	NC
21	b	604	CL7	NA
21	b	604	CL7	NC
21	b	605	CL7	NA
21	b	605	CL7	NC
21	b	606	CL7	NA
21	b	606	CL7	NC
21	b	607	CL7	NA
21	b	607	CL7	NC
21	b	608	CL7	NA
21	b	608	CL7	NC
21	b	609	CL7	NA
21	b	609	CL7	NC
21	b	610	CL7	NA
21	b	610	CL7	NC
21	b	611	CL7	NA
21	b	611	CL7	NC
21	b	612	CL7	NA
21	b	612	CL7	NC

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Mol	Chain	Res	Type	Atom
21	b	613	CL7	NA
21	b	613	CL7	NC
21	b	614	CL7	NA
21	b	614	CL7	NC
21	b	615	CL7	NA
21	b	615	CL7	NC
21	b	616	CL7	NA
21	b	616	CL7	NC
21	b	617	CL7	NA
21	b	617	CL7	NC
21	b	623	CL7	NA
21	b	623	CL7	NC
21	c	502	CL7	NA
21	c	502	CL7	NC
21	c	503	CL7	NA
21	c	503	CL7	NC
21	c	504	CL7	NA
21	c	504	CL7	NC
21	c	505	CL7	NA
21	c	505	CL7	NC
21	c	506	CL7	NA
21	c	506	CL7	NC
21	c	507	CL7	NA
21	c	507	CL7	NC
21	c	508	CL7	NA
21	c	508	CL7	NC
21	c	509	CL7	NA
21	c	509	CL7	NC
21	c	510	CL7	NA
21	c	510	CL7	NC
21	c	511	CL7	NA
21	c	511	CL7	NC
21	c	512	CL7	NA
21	c	512	CL7	NC
21	c	513	CL7	NA
21	c	513	CL7	NC
21	c	514	CL7	NA
21	c	514	CL7	NC
21	c	518	CL7	NA
21	c	518	CL7	NC
21	d	402	CL7	NA
21	d	402	CL7	NC

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Mol	Chain	Res	Type	Atom
21	d	404	CL7	NA
21	d	404	CL7	NC
21	d	405	CL7	NA
21	d	405	CL7	NC
21	6	501	CL7	NA
21	6	501	CL7	NC
21	6	502	CL7	NA
21	6	502	CL7	NC
21	6	503	CL7	NA
21	6	503	CL7	NC
21	6	504	CL7	NA
21	6	504	CL7	NC
21	6	505	CL7	NA
21	6	505	CL7	NC
21	6	506	CL7	NA
21	6	506	CL7	NC
21	6	507	CL7	NA
21	6	507	CL7	NC
21	6	508	CL7	NA
21	6	508	CL7	NC
21	6	509	CL7	NA
21	6	509	CL7	NC
21	6	510	CL7	NA
21	6	510	CL7	NC
21	6	511	CL7	NA
21	6	511	CL7	NC
21	6	512	CL7	NA
21	6	512	CL7	NC
21	6	513	CL7	NA
21	6	513	CL7	NC
21	6	514	CL7	NA
21	6	514	CL7	NC
21	6	515	CL7	NA
21	6	515	CL7	NC
21	6	516	CL7	NA
21	6	516	CL7	NC
21	6	517	CL7	NA
21	6	517	CL7	NC
21	6	518	CL7	NA
21	6	518	CL7	NC
21	5	402	CL7	NA
21	5	402	CL7	NC

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Mol	Chain	Res	Type	Atom
21	5	403	CL7	NA
21	5	403	CL7	NC
21	5	404	CL7	NA
21	5	404	CL7	NC
21	5	405	CL7	NA
21	5	405	CL7	NC
21	5	406	CL7	NA
21	5	406	CL7	NC
21	5	407	CL7	NA
21	5	407	CL7	NC
21	5	408	CL7	NA
21	5	408	CL7	NC
21	5	409	CL7	NA
21	5	409	CL7	NC
21	5	410	CL7	NA
21	5	410	CL7	NC
21	5	411	CL7	NA
21	5	411	CL7	NC
21	5	412	CL7	NA
21	5	412	CL7	NC
21	5	413	CL7	NA
21	5	413	CL7	NC
21	5	414	CL7	NA
21	5	414	CL7	NC
21	5	415	CL7	NA
21	5	415	CL7	NC
21	5	416	CL7	NA
21	5	416	CL7	NC
21	5	417	CL7	NA
21	5	417	CL7	NC
21	5	418	CL7	NA
21	5	418	CL7	NC
21	5	419	CL7	NA
21	5	419	CL7	NC
21	5	420	CL7	NA
21	5	420	CL7	NC
21	7	501	CL7	NA
21	7	501	CL7	NC
21	7	502	CL7	NA
21	7	502	CL7	NC
21	7	503	CL7	NA
21	7	503	CL7	NC

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Mol	Chain	Res	Type	Atom
21	7	504	CL7	NA
21	7	504	CL7	NC
21	7	505	CL7	NA
21	7	505	CL7	NC
21	7	506	CL7	NA
21	7	506	CL7	NC
21	7	507	CL7	NA
21	7	507	CL7	NC
21	7	508	CL7	NA
21	7	508	CL7	NC
21	7	509	CL7	NA
21	7	509	CL7	NC
21	7	510	CL7	NA
21	7	510	CL7	NC
21	7	511	CL7	NA
21	7	511	CL7	NC
21	7	512	CL7	NA
21	7	512	CL7	NC
21	7	513	CL7	NA
21	7	513	CL7	NC
21	7	514	CL7	NA
21	7	514	CL7	NC
21	7	515	CL7	NA
21	7	515	CL7	NC
21	7	516	CL7	NA
21	7	516	CL7	NC
21	7	517	CL7	NA
21	7	517	CL7	NC
21	7	518	CL7	NA
21	7	518	CL7	NC
21	8	404	CL7	NA
21	8	404	CL7	NC
21	8	405	CL7	NA
21	8	405	CL7	NC
21	8	406	CL7	NA
21	8	406	CL7	NC
21	8	407	CL7	NA
21	8	407	CL7	NC
21	8	408	CL7	NA
21	8	408	CL7	NC
21	8	409	CL7	NA
21	8	409	CL7	NC

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Mol	Chain	Res	Type	Atom
21	8	410	CL7	NA
21	8	410	CL7	NC
21	8	411	CL7	NA
21	8	411	CL7	NC
21	8	412	CL7	NA
21	8	412	CL7	NC
21	8	413	CL7	NA
21	8	413	CL7	NC
21	8	414	CL7	NA
21	8	414	CL7	NC
21	8	415	CL7	NA
21	8	415	CL7	NC
21	8	416	CL7	NA
21	8	416	CL7	NC
21	8	417	CL7	NA
21	8	417	CL7	NC

All (3294) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	401	CL7	C2B-C3B-CAB-OBB
21	A	401	CL7	C4B-C3B-CAB-OBB
21	A	403	CL7	O1A-CGA-O2A-C1
21	A	403	CL7	CBA-CGA-O2A-C1
21	A	403	CL7	C1A-C2A-CAA-CBA
21	A	403	CL7	C3A-C2A-CAA-CBA
21	A	406	CL7	C1A-C2A-CAA-CBA
21	A	406	CL7	C3A-C2A-CAA-CBA
21	A	406	CL7	C2B-C3B-CAB-OBB
21	A	406	CL7	C4B-C3B-CAB-OBB
21	B	602	CL7	O1A-CGA-O2A-C1
21	B	602	CL7	CBA-CGA-O2A-C1
21	B	602	CL7	C2-C3-C5-C6
21	B	602	CL7	C4-C3-C5-C6
21	B	602	CL7	C2B-C3B-CAB-OBB
21	B	602	CL7	C4B-C3B-CAB-OBB
21	B	604	CL7	C1A-C2A-CAA-CBA
21	B	604	CL7	C3A-C2A-CAA-CBA
21	B	604	CL7	C2B-C3B-CAB-OBB
21	B	604	CL7	C4B-C3B-CAB-OBB
21	B	605	CL7	C1A-C2A-CAA-CBA
21	B	605	CL7	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	B	607	CL7	C1A-C2A-CAA-CBA
21	B	607	CL7	C3A-C2A-CAA-CBA
21	B	607	CL7	CBD-CGD-O2D-CED
21	B	607	CL7	C2B-C3B-CAB-OBB
21	B	607	CL7	C4B-C3B-CAB-OBB
21	B	608	CL7	C4-C3-C5-C6
21	B	608	CL7	C1A-C2A-CAA-CBA
21	B	608	CL7	C3A-C2A-CAA-CBA
21	B	609	CL7	C3A-C2A-CAA-CBA
21	B	609	CL7	C2B-C3B-CAB-OBB
21	B	609	CL7	C4B-C3B-CAB-OBB
21	B	610	CL7	O1A-CGA-O2A-C1
21	B	610	CL7	CBA-CGA-O2A-C1
21	B	611	CL7	C2B-C3B-CAB-OBB
21	B	611	CL7	C4B-C3B-CAB-OBB
21	B	612	CL7	C6-C7-C8-C10
21	B	612	CL7	C3A-C2A-CAA-CBA
21	B	612	CL7	C2B-C3B-CAB-OBB
21	B	612	CL7	C4B-C3B-CAB-OBB
21	B	614	CL7	C4-C3-C5-C6
21	B	614	CL7	CHA-CBD-CGD-O2D
21	B	614	CL7	CHA-CBD-CGD-O1D
21	B	614	CL7	CAD-CBD-CGD-O1D
21	B	614	CL7	C4B-C3B-CAB-OBB
21	B	615	CL7	O1A-CGA-O2A-C1
21	B	615	CL7	CBA-CGA-O2A-C1
21	B	615	CL7	C1A-C2A-CAA-CBA
21	B	615	CL7	C3A-C2A-CAA-CBA
21	B	622	CL7	CBD-CGD-O2D-CED
21	B	622	CL7	C2B-C3B-CAB-OBB
21	B	622	CL7	C4B-C3B-CAB-OBB
21	C	502	CL7	C1A-C2A-CAA-CBA
21	C	502	CL7	C3A-C2A-CAA-CBA
21	C	502	CL7	C4B-C3B-CAB-OBB
21	C	503	CL7	C2-C3-C5-C6
21	C	503	CL7	C4-C3-C5-C6
21	C	503	CL7	CBD-CGD-O2D-CED
21	C	503	CL7	C2B-C3B-CAB-OBB
21	C	503	CL7	C4B-C3B-CAB-OBB
21	C	504	CL7	C2-C3-C5-C6
21	C	504	CL7	C4-C3-C5-C6
21	C	504	CL7	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	C	505	CL7	C1A-C2A-CAA-CBA
21	C	505	CL7	C2B-C3B-CAB-OBB
21	C	505	CL7	C4B-C3B-CAB-OBB
21	C	506	CL7	C14-C13-C15-C16
21	C	506	CL7	C2B-C3B-CAB-OBB
21	C	506	CL7	C4B-C3B-CAB-OBB
21	C	507	CL7	O1A-CGA-O2A-C1
21	C	507	CL7	CBA-CGA-O2A-C1
21	C	507	CL7	C1A-C2A-CAA-CBA
21	C	507	CL7	C3A-C2A-CAA-CBA
21	C	507	CL7	CHA-CBD-CGD-O2D
21	C	507	CL7	CHA-CBD-CGD-O1D
21	C	507	CL7	C2B-C3B-CAB-OBB
21	C	507	CL7	C4B-C3B-CAB-OBB
21	C	508	CL7	C2-C3-C5-C6
21	C	508	CL7	C4-C3-C5-C6
21	C	508	CL7	C2B-C3B-CAB-OBB
21	C	508	CL7	C4B-C3B-CAB-OBB
21	C	509	CL7	O1A-CGA-O2A-C1
21	C	509	CL7	CBA-CGA-O2A-C1
21	C	509	CL7	C2B-C3B-CAB-OBB
21	C	509	CL7	C4B-C3B-CAB-OBB
21	C	510	CL7	O2A-C1-C2-C3
21	C	510	CL7	C2-C3-C5-C6
21	C	510	CL7	C4-C3-C5-C6
21	C	510	CL7	C14-C13-C15-C16
21	C	510	CL7	C1A-C2A-CAA-CBA
21	C	510	CL7	C2B-C3B-CAB-OBB
21	C	510	CL7	C4B-C3B-CAB-OBB
21	C	511	CL7	C3A-C2A-CAA-CBA
21	C	511	CL7	C4B-C3B-CAB-OBB
21	C	512	CL7	C1A-C2A-CAA-CBA
21	C	512	CL7	C2B-C3B-CAB-OBB
21	C	512	CL7	C4B-C3B-CAB-OBB
21	C	513	CL7	CBD-CGD-O2D-CED
21	C	514	CL7	CHA-CBD-CGD-O2D
21	C	514	CL7	CHA-CBD-CGD-O1D
21	C	514	CL7	CBD-CGD-O2D-CED
21	C	514	CL7	C2B-C3B-CAB-OBB
21	C	514	CL7	C4B-C3B-CAB-OBB
21	C	518	CL7	C2B-C3B-CAB-OBB
21	C	518	CL7	C4B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
21	D	402	CL7	CHA-CBD-CGD-O2D
21	D	402	CL7	CHA-CBD-CGD-O1D
21	D	402	CL7	C2B-C3B-CAB-OBB
21	D	402	CL7	C4B-C3B-CAB-OBB
21	D	404	CL7	C2-C3-C5-C6
21	D	404	CL7	C4-C3-C5-C6
21	D	404	CL7	C4B-C3B-CAB-OBB
21	D	405	CL7	C1A-C2A-CAA-CBA
21	D	405	CL7	C3A-C2A-CAA-CBA
21	D	405	CL7	CAD-CBD-CGD-O2D
21	D	405	CL7	CAD-CBD-CGD-O1D
21	D	405	CL7	C2B-C3B-CAB-OBB
21	D	405	CL7	C4B-C3B-CAB-OBB
21	2	501	CL7	C2B-C3B-CAB-OBB
21	2	501	CL7	C4B-C3B-CAB-OBB
21	2	502	CL7	C1A-C2A-CAA-CBA
21	2	502	CL7	C3A-C2A-CAA-CBA
21	2	502	CL7	C2B-C3B-CAB-OBB
21	2	502	CL7	C4B-C3B-CAB-OBB
21	2	503	CL7	C1A-C2A-CAA-CBA
21	2	504	CL7	C1A-C2A-CAA-CBA
21	2	504	CL7	CBD-CGD-O2D-CED
21	2	504	CL7	C2B-C3B-CAB-OBB
21	2	504	CL7	C4B-C3B-CAB-OBB
21	2	505	CL7	C4B-C3B-CAB-OBB
21	2	506	CL7	C2B-C3B-CAB-OBB
21	2	506	CL7	C4B-C3B-CAB-OBB
21	2	507	CL7	C2B-C3B-CAB-OBB
21	2	507	CL7	C4B-C3B-CAB-OBB
21	2	508	CL7	C4B-C3B-CAB-OBB
21	2	509	CL7	C11-C12-C13-C15
21	2	509	CL7	C2B-C3B-CAB-OBB
21	2	509	CL7	C4B-C3B-CAB-OBB
21	2	510	CL7	C2-C3-C5-C6
21	2	510	CL7	C4-C3-C5-C6
21	2	511	CL7	C2-C3-C5-C6
21	2	511	CL7	C4-C3-C5-C6
21	2	511	CL7	CBD-CGD-O2D-CED
21	2	511	CL7	C4B-C3B-CAB-OBB
21	2	512	CL7	C4B-C3B-CAB-OBB
21	2	513	CL7	C1A-C2A-CAA-CBA
21	2	513	CL7	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	2	513	CL7	C2B-C3B-CAB-OBB
21	2	513	CL7	C4B-C3B-CAB-OBB
21	2	514	CL7	C1A-C2A-CAA-CBA
21	2	514	CL7	C3A-C2A-CAA-CBA
21	2	514	CL7	CBD-CGD-O2D-CED
21	2	514	CL7	C2B-C3B-CAB-OBB
21	2	514	CL7	C4B-C3B-CAB-OBB
21	2	515	CL7	CHA-CBD-CGD-O2D
21	2	515	CL7	CHA-CBD-CGD-O1D
21	2	515	CL7	CAD-CBD-CGD-O1D
21	2	515	CL7	C2B-C3B-CAB-OBB
21	2	515	CL7	C4B-C3B-CAB-OBB
21	2	516	CL7	O1A-CGA-O2A-C1
21	2	516	CL7	CBA-CGA-O2A-C1
21	2	516	CL7	C3A-C2A-CAA-CBA
21	2	516	CL7	C4B-C3B-CAB-OBB
21	2	517	CL7	C1A-C2A-CAA-CBA
21	2	517	CL7	C3A-C2A-CAA-CBA
21	2	517	CL7	C2B-C3B-CAB-OBB
21	2	517	CL7	C4B-C3B-CAB-OBB
21	2	518	CL7	C1A-C2A-CAA-CBA
21	2	518	CL7	C3A-C2A-CAA-CBA
21	2	518	CL7	C4B-C3B-CAB-OBB
21	1	402	CL7	C1A-C2A-CAA-CBA
21	1	402	CL7	C3A-C2A-CAA-CBA
21	1	403	CL7	C2B-C3B-CAB-OBB
21	1	403	CL7	C4B-C3B-CAB-OBB
21	1	404	CL7	O2A-C1-C2-C3
21	1	404	CL7	C2-C3-C5-C6
21	1	404	CL7	C4-C3-C5-C6
21	1	404	CL7	C2B-C3B-CAB-OBB
21	1	404	CL7	C4B-C3B-CAB-OBB
21	1	406	CL7	C2B-C3B-CAB-OBB
21	1	406	CL7	C4B-C3B-CAB-OBB
21	1	407	CL7	C2B-C3B-CAB-OBB
21	1	407	CL7	C4B-C3B-CAB-OBB
21	1	408	CL7	C1A-C2A-CAA-CBA
21	1	408	CL7	C3A-C2A-CAA-CBA
21	1	408	CL7	C2B-C3B-CAB-OBB
21	1	408	CL7	C4B-C3B-CAB-OBB
21	1	409	CL7	CBD-CGD-O2D-CED
21	1	409	CL7	C2B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
21	1	409	CL7	C4B-C3B-CAB-OBB
21	1	410	CL7	O1A-CGA-O2A-C1
21	1	410	CL7	CBA-CGA-O2A-C1
21	1	410	CL7	C1A-C2A-CAA-CBA
21	1	410	CL7	C3A-C2A-CAA-CBA
21	1	410	CL7	C2B-C3B-CAB-OBB
21	1	410	CL7	C4B-C3B-CAB-OBB
21	1	411	CL7	CBD-CGD-O2D-CED
21	1	411	CL7	C4B-C3B-CAB-OBB
21	1	412	CL7	C1A-C2A-CAA-CBA
21	1	412	CL7	C2B-C3B-CAB-OBB
21	1	412	CL7	C4B-C3B-CAB-OBB
21	1	413	CL7	CAD-CBD-CGD-O2D
21	1	413	CL7	CAD-CBD-CGD-O1D
21	1	414	CL7	C2B-C3B-CAB-OBB
21	1	414	CL7	C4B-C3B-CAB-OBB
21	1	415	CL7	CHA-CBD-CGD-O2D
21	1	415	CL7	CHA-CBD-CGD-O1D
21	1	415	CL7	C2B-C3B-CAB-OBB
21	1	415	CL7	C4B-C3B-CAB-OBB
21	1	416	CL7	CBD-CGD-O2D-CED
21	1	416	CL7	C2B-C3B-CAB-OBB
21	1	416	CL7	C4B-C3B-CAB-OBB
21	1	417	CL7	O1A-CGA-O2A-C1
21	1	417	CL7	CBA-CGA-O2A-C1
21	1	417	CL7	C3A-C2A-CAA-CBA
21	1	417	CL7	C2B-C3B-CAB-OBB
21	1	417	CL7	C4B-C3B-CAB-OBB
21	1	418	CL7	CHA-CBD-CGD-O2D
21	1	418	CL7	CHA-CBD-CGD-O1D
21	1	418	CL7	C2B-C3B-CAB-OBB
21	1	418	CL7	C4B-C3B-CAB-OBB
21	1	419	CL7	CBD-CGD-O2D-CED
21	1	419	CL7	C2B-C3B-CAB-OBB
21	1	419	CL7	C4B-C3B-CAB-OBB
21	1	420	CL7	C2B-C3B-CAB-OBB
21	1	420	CL7	C4B-C3B-CAB-OBB
21	3	501	CL7	C1A-C2A-CAA-CBA
21	3	501	CL7	C2B-C3B-CAB-OBB
21	3	501	CL7	C4B-C3B-CAB-OBB
21	3	502	CL7	CBD-CGD-O2D-CED
21	3	502	CL7	C2B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
21	3	502	CL7	C4B-C3B-CAB-OBB
21	3	503	CL7	CBD-CGD-O2D-CED
21	3	503	CL7	C2B-C3B-CAB-OBB
21	3	503	CL7	C4B-C3B-CAB-OBB
21	3	504	CL7	C1A-C2A-CAA-CBA
21	3	504	CL7	C2B-C3B-CAB-OBB
21	3	504	CL7	C4B-C3B-CAB-OBB
21	3	506	CL7	C1A-C2A-CAA-CBA
21	3	506	CL7	C3A-C2A-CAA-CBA
21	3	506	CL7	CHA-CBD-CGD-O1D
21	3	506	CL7	CAD-CBD-CGD-O2D
21	3	506	CL7	CAD-CBD-CGD-O1D
21	3	506	CL7	C4B-C3B-CAB-OBB
21	3	507	CL7	C2-C3-C5-C6
21	3	507	CL7	C4-C3-C5-C6
21	3	507	CL7	C2B-C3B-CAB-OBB
21	3	507	CL7	C4B-C3B-CAB-OBB
21	3	508	CL7	C2-C3-C5-C6
21	3	508	CL7	C4-C3-C5-C6
21	3	508	CL7	C2B-C3B-CAB-OBB
21	3	508	CL7	C4B-C3B-CAB-OBB
21	3	509	CL7	O1A-CGA-O2A-C1
21	3	509	CL7	CBA-CGA-O2A-C1
21	3	509	CL7	C2B-C3B-CAB-OBB
21	3	509	CL7	C4B-C3B-CAB-OBB
21	3	510	CL7	C1A-C2A-CAA-CBA
21	3	510	CL7	CBD-CGD-O2D-CED
21	3	510	CL7	C2B-C3B-CAB-OBB
21	3	510	CL7	C4B-C3B-CAB-OBB
21	3	511	CL7	O1A-CGA-O2A-C1
21	3	511	CL7	CBA-CGA-O2A-C1
21	3	511	CL7	C2B-C3B-CAB-OBB
21	3	511	CL7	C4B-C3B-CAB-OBB
21	3	513	CL7	C1A-C2A-CAA-CBA
21	3	513	CL7	C2B-C3B-CAB-OBB
21	3	513	CL7	C4B-C3B-CAB-OBB
21	3	516	CL7	O1A-CGA-O2A-C1
21	3	516	CL7	CBA-CGA-O2A-C1
21	3	516	CL7	C3A-C2A-CAA-CBA
21	3	516	CL7	C2B-C3B-CAB-OBB
21	3	516	CL7	C4B-C3B-CAB-OBB
21	3	517	CL7	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	3	517	CL7	C3A-C2A-CAA-CBA
21	3	517	CL7	C4B-C3B-CAB-OBB
21	3	518	CL7	C2B-C3B-CAB-OBB
21	3	518	CL7	C4B-C3B-CAB-OBB
21	4	404	CL7	C3A-C2A-CAA-CBA
21	4	405	CL7	O1A-CGA-O2A-C1
21	4	405	CL7	CBA-CGA-O2A-C1
21	4	405	CL7	C2-C3-C5-C6
21	4	405	CL7	C4-C3-C5-C6
21	4	405	CL7	C4B-C3B-CAB-OBB
21	4	406	CL7	C1A-C2A-CAA-CBA
21	4	406	CL7	C3A-C2A-CAA-CBA
21	4	406	CL7	C4B-C3B-CAB-OBB
21	4	407	CL7	C2B-C3B-CAB-OBB
21	4	407	CL7	C4B-C3B-CAB-OBB
21	4	408	CL7	C4B-C3B-CAB-OBB
21	4	409	CL7	C1A-C2A-CAA-CBA
21	4	409	CL7	C3A-C2A-CAA-CBA
21	4	409	CL7	C2B-C3B-CAB-OBB
21	4	409	CL7	C4B-C3B-CAB-OBB
21	4	410	CL7	C1A-C2A-CAA-CBA
21	4	410	CL7	C2B-C3B-CAB-OBB
21	4	410	CL7	C4B-C3B-CAB-OBB
21	4	411	CL7	C1A-C2A-CAA-CBA
21	4	411	CL7	CBD-CGD-O2D-CED
21	4	411	CL7	C2B-C3B-CAB-OBB
21	4	411	CL7	C4B-C3B-CAB-OBB
21	4	412	CL7	C1A-C2A-CAA-CBA
21	4	414	CL7	C2B-C3B-CAB-OBB
21	4	414	CL7	C4B-C3B-CAB-OBB
21	4	415	CL7	C1A-C2A-CAA-CBA
21	4	415	CL7	C3A-C2A-CAA-CBA
21	4	415	CL7	CAD-CBD-CGD-O2D
21	4	416	CL7	CHA-CBD-CGD-O2D
21	4	416	CL7	CHA-CBD-CGD-O1D
21	4	416	CL7	C2B-C3B-CAB-OBB
21	4	416	CL7	C4B-C3B-CAB-OBB
21	4	417	CL7	C1A-C2A-CAA-CBA
21	4	417	CL7	C2B-C3B-CAB-OBB
21	4	417	CL7	C4B-C3B-CAB-OBB
21	a	401	CL7	C2B-C3B-CAB-OBB
21	a	401	CL7	C4B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
21	a	403	CL7	O1A-CGA-O2A-C1
21	a	403	CL7	CBA-CGA-O2A-C1
21	a	403	CL7	C1A-C2A-CAA-CBA
21	a	403	CL7	C3A-C2A-CAA-CBA
21	a	405	CL7	C1A-C2A-CAA-CBA
21	a	405	CL7	C3A-C2A-CAA-CBA
21	a	405	CL7	C2B-C3B-CAB-OBB
21	a	405	CL7	C4B-C3B-CAB-OBB
21	b	603	CL7	O1A-CGA-O2A-C1
21	b	603	CL7	CBA-CGA-O2A-C1
21	b	603	CL7	C2-C3-C5-C6
21	b	603	CL7	C4-C3-C5-C6
21	b	603	CL7	C2B-C3B-CAB-OBB
21	b	603	CL7	C4B-C3B-CAB-OBB
21	b	605	CL7	C1A-C2A-CAA-CBA
21	b	605	CL7	C3A-C2A-CAA-CBA
21	b	605	CL7	C2B-C3B-CAB-OBB
21	b	605	CL7	C4B-C3B-CAB-OBB
21	b	606	CL7	C1A-C2A-CAA-CBA
21	b	606	CL7	C3A-C2A-CAA-CBA
21	b	608	CL7	C1A-C2A-CAA-CBA
21	b	608	CL7	C3A-C2A-CAA-CBA
21	b	608	CL7	CBD-CGD-O2D-CED
21	b	608	CL7	C2B-C3B-CAB-OBB
21	b	608	CL7	C4B-C3B-CAB-OBB
21	b	609	CL7	C4-C3-C5-C6
21	b	609	CL7	C1A-C2A-CAA-CBA
21	b	609	CL7	C3A-C2A-CAA-CBA
21	b	610	CL7	C3A-C2A-CAA-CBA
21	b	610	CL7	C2B-C3B-CAB-OBB
21	b	610	CL7	C4B-C3B-CAB-OBB
21	b	611	CL7	O1A-CGA-O2A-C1
21	b	611	CL7	CBA-CGA-O2A-C1
21	b	612	CL7	C2B-C3B-CAB-OBB
21	b	612	CL7	C4B-C3B-CAB-OBB
21	b	613	CL7	C6-C7-C8-C10
21	b	613	CL7	C3A-C2A-CAA-CBA
21	b	613	CL7	C2B-C3B-CAB-OBB
21	b	613	CL7	C4B-C3B-CAB-OBB
21	b	615	CL7	C4-C3-C5-C6
21	b	615	CL7	CHA-CBD-CGD-O2D
21	b	615	CL7	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	b	615	CL7	CAD-CBD-CGD-O1D
21	b	615	CL7	C4B-C3B-CAB-OBB
21	b	616	CL7	O1A-CGA-O2A-C1
21	b	616	CL7	CBA-CGA-O2A-C1
21	b	616	CL7	C1A-C2A-CAA-CBA
21	b	616	CL7	C3A-C2A-CAA-CBA
21	b	623	CL7	CBD-CGD-O2D-CED
21	b	623	CL7	C2B-C3B-CAB-OBB
21	b	623	CL7	C4B-C3B-CAB-OBB
21	c	502	CL7	C1A-C2A-CAA-CBA
21	c	502	CL7	C3A-C2A-CAA-CBA
21	c	502	CL7	C4B-C3B-CAB-OBB
21	c	503	CL7	C2-C3-C5-C6
21	c	503	CL7	C4-C3-C5-C6
21	c	503	CL7	CBD-CGD-O2D-CED
21	c	503	CL7	C2B-C3B-CAB-OBB
21	c	503	CL7	C4B-C3B-CAB-OBB
21	c	504	CL7	C2-C3-C5-C6
21	c	504	CL7	C4-C3-C5-C6
21	c	504	CL7	C1A-C2A-CAA-CBA
21	c	505	CL7	C1A-C2A-CAA-CBA
21	c	505	CL7	C2B-C3B-CAB-OBB
21	c	505	CL7	C4B-C3B-CAB-OBB
21	c	506	CL7	C14-C13-C15-C16
21	c	506	CL7	C2B-C3B-CAB-OBB
21	c	506	CL7	C4B-C3B-CAB-OBB
21	c	507	CL7	O1A-CGA-O2A-C1
21	c	507	CL7	CBA-CGA-O2A-C1
21	c	507	CL7	C1A-C2A-CAA-CBA
21	c	507	CL7	C3A-C2A-CAA-CBA
21	c	507	CL7	CHA-CBD-CGD-O2D
21	c	507	CL7	CHA-CBD-CGD-O1D
21	c	507	CL7	C2B-C3B-CAB-OBB
21	c	507	CL7	C4B-C3B-CAB-OBB
21	c	508	CL7	C2-C3-C5-C6
21	c	508	CL7	C4-C3-C5-C6
21	c	508	CL7	C2B-C3B-CAB-OBB
21	c	508	CL7	C4B-C3B-CAB-OBB
21	c	509	CL7	O1A-CGA-O2A-C1
21	c	509	CL7	CBA-CGA-O2A-C1
21	c	509	CL7	C2B-C3B-CAB-OBB
21	c	509	CL7	C4B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
21	c	510	CL7	O2A-C1-C2-C3
21	c	510	CL7	C2-C3-C5-C6
21	c	510	CL7	C4-C3-C5-C6
21	c	510	CL7	C14-C13-C15-C16
21	c	510	CL7	C1A-C2A-CAA-CBA
21	c	510	CL7	C2B-C3B-CAB-OBB
21	c	510	CL7	C4B-C3B-CAB-OBB
21	c	511	CL7	C3A-C2A-CAA-CBA
21	c	511	CL7	C4B-C3B-CAB-OBB
21	c	512	CL7	C1A-C2A-CAA-CBA
21	c	512	CL7	C2B-C3B-CAB-OBB
21	c	512	CL7	C4B-C3B-CAB-OBB
21	c	513	CL7	CBD-CGD-O2D-CED
21	c	514	CL7	CHA-CBD-CGD-O2D
21	c	514	CL7	CHA-CBD-CGD-O1D
21	c	514	CL7	CBD-CGD-O2D-CED
21	c	514	CL7	C2B-C3B-CAB-OBB
21	c	514	CL7	C4B-C3B-CAB-OBB
21	c	518	CL7	C2B-C3B-CAB-OBB
21	c	518	CL7	C4B-C3B-CAB-OBB
21	d	402	CL7	CHA-CBD-CGD-O2D
21	d	402	CL7	CHA-CBD-CGD-O1D
21	d	402	CL7	C2B-C3B-CAB-OBB
21	d	402	CL7	C4B-C3B-CAB-OBB
21	d	404	CL7	C2-C3-C5-C6
21	d	404	CL7	C4-C3-C5-C6
21	d	404	CL7	C4B-C3B-CAB-OBB
21	d	405	CL7	C1A-C2A-CAA-CBA
21	d	405	CL7	C3A-C2A-CAA-CBA
21	d	405	CL7	CAD-CBD-CGD-O2D
21	d	405	CL7	CAD-CBD-CGD-O1D
21	d	405	CL7	C2B-C3B-CAB-OBB
21	d	405	CL7	C4B-C3B-CAB-OBB
21	6	501	CL7	C2B-C3B-CAB-OBB
21	6	501	CL7	C4B-C3B-CAB-OBB
21	6	502	CL7	C1A-C2A-CAA-CBA
21	6	502	CL7	C3A-C2A-CAA-CBA
21	6	502	CL7	C2B-C3B-CAB-OBB
21	6	502	CL7	C4B-C3B-CAB-OBB
21	6	503	CL7	C1A-C2A-CAA-CBA
21	6	504	CL7	C1A-C2A-CAA-CBA
21	6	504	CL7	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	6	504	CL7	C2B-C3B-CAB-OBB
21	6	504	CL7	C4B-C3B-CAB-OBB
21	6	505	CL7	C4B-C3B-CAB-OBB
21	6	506	CL7	C2B-C3B-CAB-OBB
21	6	506	CL7	C4B-C3B-CAB-OBB
21	6	507	CL7	C2B-C3B-CAB-OBB
21	6	507	CL7	C4B-C3B-CAB-OBB
21	6	508	CL7	C4B-C3B-CAB-OBB
21	6	509	CL7	C11-C12-C13-C15
21	6	509	CL7	C2B-C3B-CAB-OBB
21	6	509	CL7	C4B-C3B-CAB-OBB
21	6	510	CL7	C2-C3-C5-C6
21	6	510	CL7	C4-C3-C5-C6
21	6	511	CL7	C2-C3-C5-C6
21	6	511	CL7	C4-C3-C5-C6
21	6	511	CL7	CBD-CGD-O2D-CED
21	6	511	CL7	C4B-C3B-CAB-OBB
21	6	512	CL7	C4B-C3B-CAB-OBB
21	6	513	CL7	C1A-C2A-CAA-CBA
21	6	513	CL7	CHA-CBD-CGD-O1D
21	6	513	CL7	C2B-C3B-CAB-OBB
21	6	513	CL7	C4B-C3B-CAB-OBB
21	6	514	CL7	C1A-C2A-CAA-CBA
21	6	514	CL7	C3A-C2A-CAA-CBA
21	6	514	CL7	CBD-CGD-O2D-CED
21	6	514	CL7	C2B-C3B-CAB-OBB
21	6	514	CL7	C4B-C3B-CAB-OBB
21	6	515	CL7	CHA-CBD-CGD-O2D
21	6	515	CL7	CHA-CBD-CGD-O1D
21	6	515	CL7	CAD-CBD-CGD-O1D
21	6	515	CL7	C2B-C3B-CAB-OBB
21	6	515	CL7	C4B-C3B-CAB-OBB
21	6	516	CL7	O1A-CGA-O2A-C1
21	6	516	CL7	CBA-CGA-O2A-C1
21	6	516	CL7	C3A-C2A-CAA-CBA
21	6	516	CL7	C4B-C3B-CAB-OBB
21	6	517	CL7	C1A-C2A-CAA-CBA
21	6	517	CL7	C3A-C2A-CAA-CBA
21	6	517	CL7	C2B-C3B-CAB-OBB
21	6	517	CL7	C4B-C3B-CAB-OBB
21	6	518	CL7	C1A-C2A-CAA-CBA
21	6	518	CL7	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	6	518	CL7	C4B-C3B-CAB-OBB
21	5	402	CL7	C1A-C2A-CAA-CBA
21	5	402	CL7	C3A-C2A-CAA-CBA
21	5	403	CL7	C2B-C3B-CAB-OBB
21	5	403	CL7	C4B-C3B-CAB-OBB
21	5	404	CL7	O2A-C1-C2-C3
21	5	404	CL7	C2-C3-C5-C6
21	5	404	CL7	C4-C3-C5-C6
21	5	404	CL7	C2B-C3B-CAB-OBB
21	5	404	CL7	C4B-C3B-CAB-OBB
21	5	406	CL7	C2B-C3B-CAB-OBB
21	5	406	CL7	C4B-C3B-CAB-OBB
21	5	407	CL7	C2B-C3B-CAB-OBB
21	5	407	CL7	C4B-C3B-CAB-OBB
21	5	408	CL7	C1A-C2A-CAA-CBA
21	5	408	CL7	C3A-C2A-CAA-CBA
21	5	408	CL7	C2B-C3B-CAB-OBB
21	5	408	CL7	C4B-C3B-CAB-OBB
21	5	409	CL7	CBD-CGD-O2D-CED
21	5	409	CL7	C2B-C3B-CAB-OBB
21	5	409	CL7	C4B-C3B-CAB-OBB
21	5	410	CL7	O1A-CGA-O2A-C1
21	5	410	CL7	CBA-CGA-O2A-C1
21	5	410	CL7	C1A-C2A-CAA-CBA
21	5	410	CL7	C3A-C2A-CAA-CBA
21	5	410	CL7	C2B-C3B-CAB-OBB
21	5	410	CL7	C4B-C3B-CAB-OBB
21	5	411	CL7	CBD-CGD-O2D-CED
21	5	411	CL7	C4B-C3B-CAB-OBB
21	5	412	CL7	C1A-C2A-CAA-CBA
21	5	412	CL7	C2B-C3B-CAB-OBB
21	5	412	CL7	C4B-C3B-CAB-OBB
21	5	413	CL7	CAD-CBD-CGD-O2D
21	5	413	CL7	CAD-CBD-CGD-O1D
21	5	414	CL7	C2B-C3B-CAB-OBB
21	5	414	CL7	C4B-C3B-CAB-OBB
21	5	415	CL7	CHA-CBD-CGD-O2D
21	5	415	CL7	CHA-CBD-CGD-O1D
21	5	415	CL7	C2B-C3B-CAB-OBB
21	5	415	CL7	C4B-C3B-CAB-OBB
21	5	416	CL7	CBD-CGD-O2D-CED
21	5	416	CL7	C2B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
21	5	416	CL7	C4B-C3B-CAB-OBB
21	5	417	CL7	O1A-CGA-O2A-C1
21	5	417	CL7	CBA-CGA-O2A-C1
21	5	417	CL7	C3A-C2A-CAA-CBA
21	5	417	CL7	C2B-C3B-CAB-OBB
21	5	417	CL7	C4B-C3B-CAB-OBB
21	5	418	CL7	CHA-CBD-CGD-O2D
21	5	418	CL7	CHA-CBD-CGD-O1D
21	5	418	CL7	C2B-C3B-CAB-OBB
21	5	418	CL7	C4B-C3B-CAB-OBB
21	5	419	CL7	CBD-CGD-O2D-CED
21	5	419	CL7	C2B-C3B-CAB-OBB
21	5	419	CL7	C4B-C3B-CAB-OBB
21	5	420	CL7	C2B-C3B-CAB-OBB
21	5	420	CL7	C4B-C3B-CAB-OBB
21	7	501	CL7	C1A-C2A-CAA-CBA
21	7	501	CL7	C2B-C3B-CAB-OBB
21	7	501	CL7	C4B-C3B-CAB-OBB
21	7	502	CL7	CBD-CGD-O2D-CED
21	7	502	CL7	C2B-C3B-CAB-OBB
21	7	502	CL7	C4B-C3B-CAB-OBB
21	7	503	CL7	CBD-CGD-O2D-CED
21	7	503	CL7	C2B-C3B-CAB-OBB
21	7	503	CL7	C4B-C3B-CAB-OBB
21	7	504	CL7	C1A-C2A-CAA-CBA
21	7	504	CL7	C2B-C3B-CAB-OBB
21	7	504	CL7	C4B-C3B-CAB-OBB
21	7	506	CL7	C1A-C2A-CAA-CBA
21	7	506	CL7	C3A-C2A-CAA-CBA
21	7	506	CL7	CHA-CBD-CGD-O1D
21	7	506	CL7	CAD-CBD-CGD-O2D
21	7	506	CL7	CAD-CBD-CGD-O1D
21	7	506	CL7	C4B-C3B-CAB-OBB
21	7	507	CL7	C2-C3-C5-C6
21	7	507	CL7	C4-C3-C5-C6
21	7	507	CL7	C2B-C3B-CAB-OBB
21	7	507	CL7	C4B-C3B-CAB-OBB
21	7	508	CL7	C2-C3-C5-C6
21	7	508	CL7	C4-C3-C5-C6
21	7	508	CL7	C2B-C3B-CAB-OBB
21	7	508	CL7	C4B-C3B-CAB-OBB
21	7	509	CL7	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	7	509	CL7	CBA-CGA-O2A-C1
21	7	509	CL7	C2B-C3B-CAB-OBB
21	7	509	CL7	C4B-C3B-CAB-OBB
21	7	510	CL7	C1A-C2A-CAA-CBA
21	7	510	CL7	CBD-CGD-O2D-CED
21	7	510	CL7	C2B-C3B-CAB-OBB
21	7	510	CL7	C4B-C3B-CAB-OBB
21	7	511	CL7	O1A-CGA-O2A-C1
21	7	511	CL7	CBA-CGA-O2A-C1
21	7	511	CL7	C2B-C3B-CAB-OBB
21	7	511	CL7	C4B-C3B-CAB-OBB
21	7	513	CL7	C1A-C2A-CAA-CBA
21	7	513	CL7	C2B-C3B-CAB-OBB
21	7	513	CL7	C4B-C3B-CAB-OBB
21	7	516	CL7	O1A-CGA-O2A-C1
21	7	516	CL7	CBA-CGA-O2A-C1
21	7	516	CL7	C3A-C2A-CAA-CBA
21	7	516	CL7	C2B-C3B-CAB-OBB
21	7	516	CL7	C4B-C3B-CAB-OBB
21	7	517	CL7	C1A-C2A-CAA-CBA
21	7	517	CL7	C3A-C2A-CAA-CBA
21	7	517	CL7	C4B-C3B-CAB-OBB
21	7	518	CL7	C2B-C3B-CAB-OBB
21	7	518	CL7	C4B-C3B-CAB-OBB
21	8	404	CL7	C3A-C2A-CAA-CBA
21	8	405	CL7	O1A-CGA-O2A-C1
21	8	405	CL7	CBA-CGA-O2A-C1
21	8	405	CL7	C2-C3-C5-C6
21	8	405	CL7	C4-C3-C5-C6
21	8	405	CL7	C4B-C3B-CAB-OBB
21	8	406	CL7	C1A-C2A-CAA-CBA
21	8	406	CL7	C3A-C2A-CAA-CBA
21	8	406	CL7	C4B-C3B-CAB-OBB
21	8	407	CL7	C2B-C3B-CAB-OBB
21	8	407	CL7	C4B-C3B-CAB-OBB
21	8	408	CL7	C4B-C3B-CAB-OBB
21	8	409	CL7	C1A-C2A-CAA-CBA
21	8	409	CL7	C3A-C2A-CAA-CBA
21	8	409	CL7	C2B-C3B-CAB-OBB
21	8	409	CL7	C4B-C3B-CAB-OBB
21	8	410	CL7	C1A-C2A-CAA-CBA
21	8	410	CL7	C2B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
21	8	410	CL7	C4B-C3B-CAB-OBB
21	8	411	CL7	C1A-C2A-CAA-CBA
21	8	411	CL7	CBD-CGD-O2D-CED
21	8	411	CL7	C2B-C3B-CAB-OBB
21	8	411	CL7	C4B-C3B-CAB-OBB
21	8	412	CL7	C1A-C2A-CAA-CBA
21	8	414	CL7	C2B-C3B-CAB-OBB
21	8	414	CL7	C4B-C3B-CAB-OBB
21	8	415	CL7	C1A-C2A-CAA-CBA
21	8	415	CL7	C3A-C2A-CAA-CBA
21	8	415	CL7	CAD-CBD-CGD-O2D
21	8	416	CL7	CHA-CBD-CGD-O2D
21	8	416	CL7	CHA-CBD-CGD-O1D
21	8	416	CL7	C2B-C3B-CAB-OBB
21	8	416	CL7	C4B-C3B-CAB-OBB
21	8	417	CL7	C1A-C2A-CAA-CBA
21	8	417	CL7	C2B-C3B-CAB-OBB
21	8	417	CL7	C4B-C3B-CAB-OBB
23	A	404	8CT	C25-C26-C28-C29
23	A	404	8CT	C27-C26-C28-C29
23	B	617	8CT	C14-C15-C16-C17
23	B	617	8CT	C14-C15-C16-C39
23	B	618	8CT	C25-C26-C28-C29
23	B	618	8CT	C27-C26-C28-C29
23	B	619	8CT	C10-C11-C12-C13
23	B	619	8CT	C10-C11-C12-C40
23	B	627	8CT	C14-C15-C16-C17
23	B	627	8CT	C14-C15-C16-C39
23	B	627	8CT	C28-C29-C30-C35
23	C	515	8CT	C02-C03-C10-C11
23	C	515	8CT	C10-C11-C12-C13
23	C	515	8CT	C10-C11-C12-C40
23	C	515	8CT	C16-C17-C18-C19
23	C	515	8CT	C27-C26-C28-C29
23	C	515	8CT	C28-C29-C30-C35
23	C	516	8CT	C02-C03-C10-C11
23	C	516	8CT	C10-C11-C12-C13
23	C	516	8CT	C10-C11-C12-C40
23	C	516	8CT	C14-C15-C16-C17
23	C	516	8CT	C14-C15-C16-C39
23	C	516	8CT	C27-C26-C28-C29
23	C	519	8CT	C25-C26-C28-C29

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Mol	Chain	Res	Type	Atoms
23	C	519	8CT	C27-C26-C28-C29
23	C	519	8CT	C28-C29-C30-C31
23	C	519	8CT	C28-C29-C30-C35
23	D	406	8CT	C10-C11-C12-C13
23	D	406	8CT	C10-C11-C12-C40
23	D	406	8CT	C16-C17-C18-C19
23	D	406	8CT	C25-C26-C28-C29
23	D	406	8CT	C27-C26-C28-C29
23	K	101	8CT	C20-C21-C23-C24
23	K	101	8CT	C22-C21-C23-C24
23	K	101	8CT	C25-C26-C28-C29
23	K	101	8CT	C27-C26-C28-C29
23	K	101	8CT	C28-C29-C30-C35
23	a	404	8CT	C25-C26-C28-C29
23	a	404	8CT	C27-C26-C28-C29
23	b	601	8CT	C14-C15-C16-C17
23	b	601	8CT	C14-C15-C16-C39
23	b	601	8CT	C28-C29-C30-C35
23	b	618	8CT	C14-C15-C16-C17
23	b	618	8CT	C14-C15-C16-C39
23	b	619	8CT	C25-C26-C28-C29
23	b	619	8CT	C27-C26-C28-C29
23	b	620	8CT	C10-C11-C12-C13
23	b	620	8CT	C10-C11-C12-C40
23	c	515	8CT	C02-C03-C10-C11
23	c	515	8CT	C10-C11-C12-C13
23	c	515	8CT	C10-C11-C12-C40
23	c	515	8CT	C16-C17-C18-C19
23	c	515	8CT	C27-C26-C28-C29
23	c	515	8CT	C28-C29-C30-C35
23	c	516	8CT	C02-C03-C10-C11
23	c	516	8CT	C10-C11-C12-C13
23	c	516	8CT	C10-C11-C12-C40
23	c	516	8CT	C14-C15-C16-C17
23	c	516	8CT	C14-C15-C16-C39
23	c	516	8CT	C27-C26-C28-C29
23	c	519	8CT	C04-C03-C10-C11
23	c	519	8CT	C25-C26-C28-C29
23	c	519	8CT	C27-C26-C28-C29
23	c	519	8CT	C28-C29-C30-C31
23	c	519	8CT	C28-C29-C30-C35
23	d	406	8CT	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	d	406	8CT	C10-C11-C12-C40
23	d	406	8CT	C16-C17-C18-C19
23	d	406	8CT	C25-C26-C28-C29
23	d	406	8CT	C27-C26-C28-C29
23	k	101	8CT	C20-C21-C23-C24
23	k	101	8CT	C22-C21-C23-C24
23	k	101	8CT	C25-C26-C28-C29
23	k	101	8CT	C27-C26-C28-C29
23	k	101	8CT	C28-C29-C30-C35
24	2	522	SQD	O49-C7-O47-C45
24	2	522	SQD	C8-C7-O47-C45
24	2	522	SQD	O5-C5-C6-S
24	3	521	SQD	O49-C7-O47-C45
24	3	521	SQD	C8-C7-O47-C45
24	3	523	SQD	O5-C5-C6-S
24	6	521	SQD	O49-C7-O47-C45
24	6	521	SQD	C8-C7-O47-C45
24	6	521	SQD	O5-C5-C6-S
24	7	521	SQD	O49-C7-O47-C45
24	7	521	SQD	C8-C7-O47-C45
24	7	523	SQD	O5-C5-C6-S
25	A	407	LHG	C2-C3-O3-P
25	D	409	LHG	C3-O3-P-O6
25	D	409	LHG	C4-O6-P-O3
25	4	401	LHG	C2-C3-O3-P
25	4	401	LHG	C4-O6-P-O3
25	a	406	LHG	C2-C3-O3-P
25	d	409	LHG	C3-O3-P-O6
25	d	409	LHG	C4-O6-P-O3
25	8	401	LHG	C2-C3-O3-P
25	8	401	LHG	C4-O6-P-O3
26	B	621	LMG	C29-C28-O8-C9
26	C	501	LMG	O6-C1-O1-C7
26	b	622	LMG	C29-C28-O8-C9
26	c	501	LMG	O6-C1-O1-C7
30	D	407	PL9	C39-C41-C42-C43
30	d	407	PL9	C39-C41-C42-C43
31	F	101	HEM	C2B-C3B-CAB-CBB
31	F	101	HEM	C2C-C3C-CAC-CBC
31	f	101	HEM	C2B-C3B-CAB-CBB
31	f	101	HEM	C2C-C3C-CAC-CBC
32	2	519	ZEX	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
32	2	519	ZEX	C25-C26-C27-C28
32	2	519	ZEX	C7-C8-C9-C19
32	2	519	ZEX	C7-C8-C9-C10
32	2	519	ZEX	C11-C12-C13-C20
32	2	519	ZEX	C11-C12-C13-C14
32	2	519	ZEX	C27-C28-C29-C30
32	2	519	ZEX	C27-C28-C29-C39
32	2	520	ZEX	C31-C32-C33-C34
32	2	520	ZEX	C31-C32-C33-C40
32	2	520	ZEX	C27-C28-C29-C30
32	2	520	ZEX	C27-C28-C29-C39
32	2	521	ZEX	C25-C26-C27-C28
32	2	523	ZEX	C25-C26-C27-C28
32	2	523	ZEX	C31-C32-C33-C40
32	2	523	ZEX	C27-C28-C29-C30
32	2	523	ZEX	C27-C28-C29-C39
32	2	525	ZEX	C25-C26-C27-C28
32	2	525	ZEX	C31-C32-C33-C34
32	2	525	ZEX	C31-C32-C33-C40
32	2	525	ZEX	C27-C28-C29-C30
32	1	421	ZEX	C25-C26-C27-C28
32	1	421	ZEX	C7-C8-C9-C19
32	1	421	ZEX	C7-C8-C9-C10
32	1	421	ZEX	C11-C12-C13-C20
32	1	421	ZEX	C11-C12-C13-C14
32	1	421	ZEX	C31-C32-C33-C34
32	1	421	ZEX	C31-C32-C33-C40
32	1	421	ZEX	C27-C28-C29-C30
32	1	421	ZEX	C27-C28-C29-C39
32	1	422	ZEX	C25-C26-C27-C28
32	1	422	ZEX	C9-C10-C11-C12
32	3	519	ZEX	C25-C26-C27-C28
32	3	519	ZEX	C31-C32-C33-C34
32	3	519	ZEX	C31-C32-C33-C40
32	3	520	ZEX	C25-C26-C27-C28
32	3	522	ZEX	C1-C6-C7-C8
32	3	522	ZEX	C25-C26-C27-C28
32	3	525	ZEX	C31-C32-C33-C34
32	3	525	ZEX	C31-C32-C33-C40
32	3	525	ZEX	C27-C28-C29-C30
32	3	525	ZEX	C27-C28-C29-C39
32	4	403	ZEX	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
32	4	403	ZEX	C7-C8-C9-C19
32	4	403	ZEX	C7-C8-C9-C10
32	4	418	ZEX	C7-C8-C9-C19
32	4	418	ZEX	C7-C8-C9-C10
32	4	419	ZEX	C13-C14-C15-C35
32	4	419	ZEX	C27-C28-C29-C30
32	4	419	ZEX	C27-C28-C29-C39
32	4	420	ZEX	C27-C28-C29-C30
32	4	420	ZEX	C27-C28-C29-C39
32	6	519	ZEX	C1-C6-C7-C8
32	6	519	ZEX	C25-C26-C27-C28
32	6	519	ZEX	C7-C8-C9-C19
32	6	519	ZEX	C7-C8-C9-C10
32	6	519	ZEX	C11-C12-C13-C20
32	6	519	ZEX	C11-C12-C13-C14
32	6	519	ZEX	C27-C28-C29-C30
32	6	519	ZEX	C27-C28-C29-C39
32	6	520	ZEX	C25-C26-C27-C28
32	6	522	ZEX	C25-C26-C27-C28
32	6	522	ZEX	C31-C32-C33-C40
32	6	522	ZEX	C27-C28-C29-C30
32	6	522	ZEX	C27-C28-C29-C39
32	6	524	ZEX	C25-C26-C27-C28
32	6	524	ZEX	C31-C32-C33-C34
32	6	524	ZEX	C31-C32-C33-C40
32	6	524	ZEX	C27-C28-C29-C30
32	5	421	ZEX	C25-C26-C27-C28
32	5	421	ZEX	C7-C8-C9-C19
32	5	421	ZEX	C7-C8-C9-C10
32	5	421	ZEX	C11-C12-C13-C20
32	5	421	ZEX	C11-C12-C13-C14
32	5	421	ZEX	C31-C32-C33-C34
32	5	421	ZEX	C31-C32-C33-C40
32	5	421	ZEX	C27-C28-C29-C30
32	5	421	ZEX	C27-C28-C29-C39
32	5	422	ZEX	C25-C26-C27-C28
32	5	422	ZEX	C9-C10-C11-C12
32	7	519	ZEX	C25-C26-C27-C28
32	7	519	ZEX	C31-C32-C33-C34
32	7	519	ZEX	C31-C32-C33-C40
32	7	520	ZEX	C25-C26-C27-C28
32	7	522	ZEX	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
32	7	522	ZEX	C25-C26-C27-C28
32	8	403	ZEX	C5-C6-C7-C8
32	8	403	ZEX	C7-C8-C9-C19
32	8	403	ZEX	C7-C8-C9-C10
32	8	418	ZEX	C7-C8-C9-C19
32	8	418	ZEX	C7-C8-C9-C10
32	8	419	ZEX	C13-C14-C15-C35
32	8	419	ZEX	C27-C28-C29-C30
32	8	419	ZEX	C27-C28-C29-C39
32	8	420	ZEX	C27-C28-C29-C30
32	8	420	ZEX	C27-C28-C29-C39
21	A	401	CL7	O1D-CGD-O2D-CED
21	B	601	CL7	O1D-CGD-O2D-CED
21	B	607	CL7	O1D-CGD-O2D-CED
21	2	502	CL7	O1D-CGD-O2D-CED
21	2	514	CL7	O1D-CGD-O2D-CED
21	3	503	CL7	O1D-CGD-O2D-CED
21	a	401	CL7	O1D-CGD-O2D-CED
21	b	602	CL7	O1D-CGD-O2D-CED
21	b	608	CL7	O1D-CGD-O2D-CED
21	6	502	CL7	O1D-CGD-O2D-CED
21	6	514	CL7	O1D-CGD-O2D-CED
21	7	503	CL7	O1D-CGD-O2D-CED
21	A	403	CL7	C4C-C3C-CAC-CBC
21	a	403	CL7	C4C-C3C-CAC-CBC
21	C	503	CL7	O1D-CGD-O2D-CED
21	2	511	CL7	O1D-CGD-O2D-CED
21	1	409	CL7	O1D-CGD-O2D-CED
21	1	416	CL7	O1D-CGD-O2D-CED
21	1	419	CL7	O1D-CGD-O2D-CED
21	3	502	CL7	O1D-CGD-O2D-CED
21	4	417	CL7	O1D-CGD-O2D-CED
21	c	503	CL7	O1D-CGD-O2D-CED
21	6	511	CL7	O1D-CGD-O2D-CED
21	5	409	CL7	O1D-CGD-O2D-CED
21	5	416	CL7	O1D-CGD-O2D-CED
21	5	419	CL7	O1D-CGD-O2D-CED
21	7	502	CL7	O1D-CGD-O2D-CED
21	8	417	CL7	O1D-CGD-O2D-CED
21	A	401	CL7	CBD-CGD-O2D-CED
21	A	403	CL7	CBD-CGD-O2D-CED
21	B	601	CL7	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	B	605	CL7	CBD-CGD-O2D-CED
21	C	518	CL7	CBD-CGD-O2D-CED
21	2	502	CL7	CBD-CGD-O2D-CED
21	1	405	CL7	CBD-CGD-O2D-CED
21	1	407	CL7	CBD-CGD-O2D-CED
21	1	420	CL7	CBD-CGD-O2D-CED
21	3	506	CL7	CBD-CGD-O2D-CED
21	4	417	CL7	CBD-CGD-O2D-CED
21	a	401	CL7	CBD-CGD-O2D-CED
21	a	403	CL7	CBD-CGD-O2D-CED
21	b	602	CL7	CBD-CGD-O2D-CED
21	b	606	CL7	CBD-CGD-O2D-CED
21	c	518	CL7	CBD-CGD-O2D-CED
21	6	502	CL7	CBD-CGD-O2D-CED
21	5	405	CL7	CBD-CGD-O2D-CED
21	5	407	CL7	CBD-CGD-O2D-CED
21	5	420	CL7	CBD-CGD-O2D-CED
21	7	506	CL7	CBD-CGD-O2D-CED
21	8	417	CL7	CBD-CGD-O2D-CED
26	B	621	LMG	O10-C28-O8-C9
26	b	622	LMG	O10-C28-O8-C9
21	C	514	CL7	O1D-CGD-O2D-CED
21	1	407	CL7	O1D-CGD-O2D-CED
21	3	510	CL7	O1D-CGD-O2D-CED
21	c	514	CL7	O1D-CGD-O2D-CED
21	5	407	CL7	O1D-CGD-O2D-CED
21	7	510	CL7	O1D-CGD-O2D-CED
21	1	414	CL7	C4C-C3C-CAC-CBC
21	4	415	CL7	C4C-C3C-CAC-CBC
21	4	416	CL7	C4C-C3C-CAC-CBC
21	5	414	CL7	C4C-C3C-CAC-CBC
21	8	415	CL7	C4C-C3C-CAC-CBC
21	8	416	CL7	C4C-C3C-CAC-CBC
21	B	622	CL7	O1D-CGD-O2D-CED
21	4	411	CL7	O1D-CGD-O2D-CED
21	b	623	CL7	O1D-CGD-O2D-CED
21	8	411	CL7	O1D-CGD-O2D-CED
21	C	504	CL7	CBD-CGD-O2D-CED
21	C	510	CL7	CBD-CGD-O2D-CED
21	C	512	CL7	CBD-CGD-O2D-CED
21	2	510	CL7	CBD-CGD-O2D-CED
21	2	517	CL7	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	1	403	CL7	CBD-CGD-O2D-CED
21	1	410	CL7	CBD-CGD-O2D-CED
21	1	412	CL7	CBD-CGD-O2D-CED
21	1	418	CL7	CBD-CGD-O2D-CED
21	3	508	CL7	CBD-CGD-O2D-CED
21	3	509	CL7	CBD-CGD-O2D-CED
21	3	516	CL7	CBD-CGD-O2D-CED
21	3	518	CL7	CBD-CGD-O2D-CED
21	4	409	CL7	CBD-CGD-O2D-CED
21	4	410	CL7	CBD-CGD-O2D-CED
21	c	504	CL7	CBD-CGD-O2D-CED
21	c	510	CL7	CBD-CGD-O2D-CED
21	c	512	CL7	CBD-CGD-O2D-CED
21	6	510	CL7	CBD-CGD-O2D-CED
21	6	517	CL7	CBD-CGD-O2D-CED
21	5	403	CL7	CBD-CGD-O2D-CED
21	5	410	CL7	CBD-CGD-O2D-CED
21	5	412	CL7	CBD-CGD-O2D-CED
21	5	418	CL7	CBD-CGD-O2D-CED
21	7	508	CL7	CBD-CGD-O2D-CED
21	7	509	CL7	CBD-CGD-O2D-CED
21	7	516	CL7	CBD-CGD-O2D-CED
21	7	518	CL7	CBD-CGD-O2D-CED
21	8	409	CL7	CBD-CGD-O2D-CED
21	8	410	CL7	CBD-CGD-O2D-CED
21	C	513	CL7	O1D-CGD-O2D-CED
21	2	504	CL7	O1D-CGD-O2D-CED
21	c	513	CL7	O1D-CGD-O2D-CED
21	6	504	CL7	O1D-CGD-O2D-CED
21	1	411	CL7	O1D-CGD-O2D-CED
21	5	411	CL7	O1D-CGD-O2D-CED
21	B	611	CL7	CBD-CGD-O2D-CED
21	C	505	CL7	CBD-CGD-O2D-CED
21	2	509	CL7	CBD-CGD-O2D-CED
21	b	612	CL7	CBD-CGD-O2D-CED
21	c	505	CL7	CBD-CGD-O2D-CED
21	6	509	CL7	CBD-CGD-O2D-CED
21	1	404	CL7	C10-C11-C12-C13
21	5	404	CL7	C10-C11-C12-C13
21	B	602	CL7	C3-C5-C6-C7
21	B	605	CL7	C3-C5-C6-C7
21	B	609	CL7	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	B	613	CL7	C3-C5-C6-C7
21	B	614	CL7	C3-C5-C6-C7
21	C	502	CL7	C3-C5-C6-C7
21	C	508	CL7	C3-C5-C6-C7
21	C	509	CL7	C3-C5-C6-C7
21	C	510	CL7	C3-C5-C6-C7
21	2	506	CL7	C3-C5-C6-C7
21	2	507	CL7	C3-C5-C6-C7
21	2	516	CL7	C3-C5-C6-C7
21	1	408	CL7	C3-C5-C6-C7
21	3	501	CL7	C3-C5-C6-C7
21	3	504	CL7	C3-C5-C6-C7
21	3	505	CL7	C3-C5-C6-C7
21	3	508	CL7	C3-C5-C6-C7
21	4	404	CL7	C3-C5-C6-C7
21	4	405	CL7	C3-C5-C6-C7
21	4	413	CL7	C3-C5-C6-C7
21	b	603	CL7	C3-C5-C6-C7
21	b	606	CL7	C3-C5-C6-C7
21	b	610	CL7	C3-C5-C6-C7
21	b	614	CL7	C3-C5-C6-C7
21	b	615	CL7	C3-C5-C6-C7
21	c	502	CL7	C3-C5-C6-C7
21	c	508	CL7	C3-C5-C6-C7
21	c	509	CL7	C3-C5-C6-C7
21	c	510	CL7	C3-C5-C6-C7
21	6	506	CL7	C3-C5-C6-C7
21	6	507	CL7	C3-C5-C6-C7
21	6	516	CL7	C3-C5-C6-C7
21	5	408	CL7	C3-C5-C6-C7
21	7	501	CL7	C3-C5-C6-C7
21	7	504	CL7	C3-C5-C6-C7
21	7	505	CL7	C3-C5-C6-C7
21	7	508	CL7	C3-C5-C6-C7
21	8	404	CL7	C3-C5-C6-C7
21	8	405	CL7	C3-C5-C6-C7
21	8	413	CL7	C3-C5-C6-C7
21	C	518	CL7	O1D-CGD-O2D-CED
21	1	420	CL7	O1D-CGD-O2D-CED
21	c	518	CL7	O1D-CGD-O2D-CED
21	5	420	CL7	O1D-CGD-O2D-CED
21	D	402	CL7	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
21	2	514	CL7	C4C-C3C-CAC-CBC
21	d	402	CL7	C2C-C3C-CAC-CBC
21	6	514	CL7	C4C-C3C-CAC-CBC
21	B	606	CL7	C4-C3-C5-C6
21	C	502	CL7	C4-C3-C5-C6
21	1	410	CL7	C4-C3-C5-C6
21	3	512	CL7	C4-C3-C5-C6
21	4	412	CL7	C4-C3-C5-C6
21	b	607	CL7	C4-C3-C5-C6
21	c	502	CL7	C4-C3-C5-C6
21	5	410	CL7	C4-C3-C5-C6
21	7	512	CL7	C4-C3-C5-C6
21	8	412	CL7	C4-C3-C5-C6
21	B	606	CL7	C2-C3-C5-C6
21	C	502	CL7	C2-C3-C5-C6
21	4	412	CL7	C2-C3-C5-C6
21	b	607	CL7	C2-C3-C5-C6
21	c	502	CL7	C2-C3-C5-C6
21	8	412	CL7	C2-C3-C5-C6
21	2	506	CL7	CBD-CGD-O2D-CED
21	3	514	CL7	CBD-CGD-O2D-CED
21	6	506	CL7	CBD-CGD-O2D-CED
21	7	514	CL7	CBD-CGD-O2D-CED
21	B	604	CL7	C2A-CAA-CBA-CGA
21	B	607	CL7	C2A-CAA-CBA-CGA
21	B	610	CL7	C2A-CAA-CBA-CGA
21	C	514	CL7	C2A-CAA-CBA-CGA
21	2	502	CL7	C2A-CAA-CBA-CGA
21	1	409	CL7	C2A-CAA-CBA-CGA
21	3	516	CL7	C2A-CAA-CBA-CGA
21	3	518	CL7	C2A-CAA-CBA-CGA
21	4	409	CL7	C2A-CAA-CBA-CGA
21	b	605	CL7	C2A-CAA-CBA-CGA
21	b	608	CL7	C2A-CAA-CBA-CGA
21	b	611	CL7	C2A-CAA-CBA-CGA
21	c	514	CL7	C2A-CAA-CBA-CGA
21	6	502	CL7	C2A-CAA-CBA-CGA
21	5	409	CL7	C2A-CAA-CBA-CGA
21	7	516	CL7	C2A-CAA-CBA-CGA
21	7	518	CL7	C2A-CAA-CBA-CGA
21	8	409	CL7	C2A-CAA-CBA-CGA
21	C	505	CL7	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	C	506	CL7	C3-C5-C6-C7
21	2	512	CL7	C3-C5-C6-C7
21	4	406	CL7	C3-C5-C6-C7
21	c	505	CL7	C3-C5-C6-C7
21	c	506	CL7	C3-C5-C6-C7
21	6	512	CL7	C3-C5-C6-C7
21	8	406	CL7	C3-C5-C6-C7
21	B	605	CL7	O1D-CGD-O2D-CED
21	1	405	CL7	O1D-CGD-O2D-CED
21	3	506	CL7	O1D-CGD-O2D-CED
21	b	606	CL7	O1D-CGD-O2D-CED
21	5	405	CL7	O1D-CGD-O2D-CED
21	7	506	CL7	O1D-CGD-O2D-CED
23	C	515	8CT	C12-C13-C14-C15
23	c	515	8CT	C12-C13-C14-C15
32	2	519	ZEX	C29-C30-C31-C32
32	2	521	ZEX	C9-C10-C11-C12
32	4	418	ZEX	C9-C10-C11-C12
32	6	519	ZEX	C29-C30-C31-C32
32	6	520	ZEX	C9-C10-C11-C12
32	8	418	ZEX	C9-C10-C11-C12
21	A	406	CL7	CBD-CGD-O2D-CED
21	C	506	CL7	CBD-CGD-O2D-CED
21	D	402	CL7	CBD-CGD-O2D-CED
21	2	503	CL7	CBD-CGD-O2D-CED
21	a	405	CL7	CBD-CGD-O2D-CED
21	c	506	CL7	CBD-CGD-O2D-CED
21	d	402	CL7	CBD-CGD-O2D-CED
21	6	503	CL7	CBD-CGD-O2D-CED
25	B	625	LHG	O2-C2-C3-O3
25	b	626	LHG	O2-C2-C3-O3
21	A	401	CL7	C3-C5-C6-C7
21	C	504	CL7	C3-C5-C6-C7
21	1	406	CL7	C3-C5-C6-C7
21	1	417	CL7	C3-C5-C6-C7
21	1	418	CL7	C3-C5-C6-C7
21	a	401	CL7	C3-C5-C6-C7
21	c	504	CL7	C3-C5-C6-C7
21	5	406	CL7	C3-C5-C6-C7
21	5	417	CL7	C3-C5-C6-C7
21	5	418	CL7	C3-C5-C6-C7
26	c	501	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
21	C	511	CL7	C13-C15-C16-C17
21	C	511	CL7	CBD-CGD-O2D-CED
21	2	507	CL7	CBD-CGD-O2D-CED
21	4	412	CL7	CBD-CGD-O2D-CED
21	c	511	CL7	CBD-CGD-O2D-CED
21	6	507	CL7	CBD-CGD-O2D-CED
21	8	412	CL7	CBD-CGD-O2D-CED
21	3	514	CL7	C4C-C3C-CAC-CBC
21	7	514	CL7	C4C-C3C-CAC-CBC
21	3	509	CL7	C8-C10-C11-C12
21	c	511	CL7	C13-C15-C16-C17
21	7	509	CL7	C8-C10-C11-C12
21	A	403	CL7	O1D-CGD-O2D-CED
21	a	403	CL7	O1D-CGD-O2D-CED
21	C	503	CL7	C3-C5-C6-C7
21	c	503	CL7	C3-C5-C6-C7
26	C	501	LMG	C29-C28-O8-C9
21	A	401	CL7	C4-C3-C5-C6
21	B	603	CL7	C4-C3-C5-C6
21	C	509	CL7	C4-C3-C5-C6
21	2	505	CL7	C4-C3-C5-C6
21	2	516	CL7	C4-C3-C5-C6
21	2	517	CL7	C4-C3-C5-C6
21	1	403	CL7	C4-C3-C5-C6
21	3	504	CL7	C4-C3-C5-C6
21	3	510	CL7	C4-C3-C5-C6
21	3	511	CL7	C4-C3-C5-C6
21	4	406	CL7	C4-C3-C5-C6
21	a	401	CL7	C4-C3-C5-C6
21	b	604	CL7	C4-C3-C5-C6
21	c	509	CL7	C4-C3-C5-C6
21	6	505	CL7	C4-C3-C5-C6
21	6	516	CL7	C4-C3-C5-C6
21	6	517	CL7	C4-C3-C5-C6
21	5	403	CL7	C4-C3-C5-C6
21	7	504	CL7	C4-C3-C5-C6
21	7	510	CL7	C4-C3-C5-C6
21	7	511	CL7	C4-C3-C5-C6
21	8	406	CL7	C4-C3-C5-C6
21	A	401	CL7	C2-C3-C5-C6
21	B	603	CL7	C2-C3-C5-C6
21	B	608	CL7	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	B	614	CL7	C2-C3-C5-C6
21	C	509	CL7	C2-C3-C5-C6
21	2	505	CL7	C2-C3-C5-C6
21	2	516	CL7	C2-C3-C5-C6
21	2	517	CL7	C2-C3-C5-C6
21	1	403	CL7	C2-C3-C5-C6
21	3	504	CL7	C2-C3-C5-C6
21	3	510	CL7	C2-C3-C5-C6
21	3	511	CL7	C2-C3-C5-C6
21	4	406	CL7	C2-C3-C5-C6
21	a	401	CL7	C2-C3-C5-C6
21	b	604	CL7	C2-C3-C5-C6
21	b	609	CL7	C2-C3-C5-C6
21	b	615	CL7	C2-C3-C5-C6
21	c	509	CL7	C2-C3-C5-C6
21	6	505	CL7	C2-C3-C5-C6
21	6	516	CL7	C2-C3-C5-C6
21	6	517	CL7	C2-C3-C5-C6
21	5	403	CL7	C2-C3-C5-C6
21	7	504	CL7	C2-C3-C5-C6
21	7	510	CL7	C2-C3-C5-C6
21	7	511	CL7	C2-C3-C5-C6
21	8	406	CL7	C2-C3-C5-C6
21	B	622	CL7	C2A-CAA-CBA-CGA
21	1	405	CL7	C2A-CAA-CBA-CGA
21	3	503	CL7	C2A-CAA-CBA-CGA
21	3	512	CL7	C2A-CAA-CBA-CGA
21	4	404	CL7	C2A-CAA-CBA-CGA
21	b	623	CL7	C2A-CAA-CBA-CGA
21	5	405	CL7	C2A-CAA-CBA-CGA
21	7	503	CL7	C2A-CAA-CBA-CGA
21	7	512	CL7	C2A-CAA-CBA-CGA
21	8	404	CL7	C2A-CAA-CBA-CGA
21	A	406	CL7	C2C-C3C-CAC-CBC
21	a	405	CL7	C2C-C3C-CAC-CBC
21	4	414	CL7	CBD-CGD-O2D-CED
21	8	414	CL7	CBD-CGD-O2D-CED
26	c	501	LMG	O10-C28-O8-C9
21	1	410	CL7	O1D-CGD-O2D-CED
21	3	509	CL7	O1D-CGD-O2D-CED
21	3	516	CL7	O1D-CGD-O2D-CED
21	5	410	CL7	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	7	509	CL7	O1D-CGD-O2D-CED
21	7	516	CL7	O1D-CGD-O2D-CED
21	C	510	CL7	O1D-CGD-O2D-CED
26	C	501	LMG	O10-C28-O8-C9
21	2	510	CL7	C3-C5-C6-C7
21	6	510	CL7	C3-C5-C6-C7
21	C	504	CL7	O1D-CGD-O2D-CED
21	c	504	CL7	O1D-CGD-O2D-CED
21	c	510	CL7	O1D-CGD-O2D-CED
21	c	510	CL7	C13-C15-C16-C17
21	A	401	CL7	C2C-C3C-CAC-CBC
21	a	401	CL7	C2C-C3C-CAC-CBC
21	C	510	CL7	C13-C15-C16-C17
21	2	510	CL7	C8-C10-C11-C12
21	3	503	CL7	C5-C6-C7-C8
21	6	510	CL7	C8-C10-C11-C12
21	7	503	CL7	C5-C6-C7-C8
27	C	517	DGD	C4B-C5B-C6B-C7B
27	c	517	DGD	C4B-C5B-C6B-C7B
21	2	512	CL7	C5-C6-C7-C8
21	3	504	CL7	C8-C10-C11-C12
21	3	504	CL7	C13-C15-C16-C17
21	3	505	CL7	C15-C16-C17-C18
21	3	510	CL7	C5-C6-C7-C8
21	3	510	CL7	C10-C11-C12-C13
21	4	412	CL7	C10-C11-C12-C13
21	6	512	CL7	C5-C6-C7-C8
21	7	504	CL7	C8-C10-C11-C12
21	7	504	CL7	C13-C15-C16-C17
21	7	505	CL7	C15-C16-C17-C18
21	7	510	CL7	C5-C6-C7-C8
21	7	510	CL7	C10-C11-C12-C13
21	8	412	CL7	C10-C11-C12-C13
25	A	407	LHG	O2-C2-C3-O3
25	a	406	LHG	O2-C2-C3-O3
21	1	410	CL7	C2-C3-C5-C6
21	5	410	CL7	C2-C3-C5-C6
21	B	603	CL7	C11-C10-C8-C9
21	B	603	CL7	C14-C13-C15-C16
21	B	608	CL7	C11-C10-C8-C9
21	B	611	CL7	C11-C10-C8-C9
21	B	611	CL7	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	B	612	CL7	C11-C12-C13-C14
21	C	507	CL7	C11-C10-C8-C9
21	C	509	CL7	C11-C10-C8-C9
21	C	511	CL7	C11-C12-C13-C14
21	D	404	CL7	C11-C10-C8-C9
21	2	505	CL7	C14-C13-C15-C16
21	2	510	CL7	C11-C10-C8-C9
21	2	510	CL7	C11-C12-C13-C14
21	1	408	CL7	C11-C10-C8-C9
21	3	501	CL7	C11-C10-C8-C9
21	3	501	CL7	C11-C12-C13-C14
21	3	504	CL7	C11-C10-C8-C9
21	3	507	CL7	C11-C10-C8-C9
21	3	509	CL7	C14-C13-C15-C16
21	3	511	CL7	C11-C10-C8-C9
21	4	404	CL7	C11-C10-C8-C9
21	4	404	CL7	C14-C13-C15-C16
21	4	406	CL7	C11-C10-C8-C9
21	b	604	CL7	C11-C10-C8-C9
21	b	604	CL7	C14-C13-C15-C16
21	b	609	CL7	C11-C10-C8-C9
21	b	612	CL7	C11-C10-C8-C9
21	b	612	CL7	C11-C12-C13-C14
21	b	613	CL7	C11-C12-C13-C14
21	c	507	CL7	C11-C10-C8-C9
21	c	509	CL7	C11-C10-C8-C9
21	c	511	CL7	C11-C12-C13-C14
21	d	404	CL7	C11-C10-C8-C9
21	6	505	CL7	C14-C13-C15-C16
21	6	510	CL7	C11-C10-C8-C9
21	6	510	CL7	C11-C12-C13-C14
21	5	408	CL7	C11-C10-C8-C9
21	7	501	CL7	C11-C10-C8-C9
21	7	501	CL7	C11-C12-C13-C14
21	7	504	CL7	C11-C10-C8-C9
21	7	507	CL7	C11-C10-C8-C9
21	7	509	CL7	C14-C13-C15-C16
21	7	511	CL7	C11-C10-C8-C9
21	8	404	CL7	C11-C10-C8-C9
21	8	404	CL7	C14-C13-C15-C16
21	8	406	CL7	C11-C10-C8-C9
21	C	512	CL7	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	3	518	CL7	O1D-CGD-O2D-CED
21	c	512	CL7	O1D-CGD-O2D-CED
21	7	518	CL7	O1D-CGD-O2D-CED
21	D	404	CL7	CBD-CGD-O2D-CED
21	d	404	CL7	CBD-CGD-O2D-CED
21	5	419	CL7	C2A-CAA-CBA-CGA
23	B	618	8CT	C10-C11-C12-C40
23	C	515	8CT	C14-C15-C16-C39
23	C	515	8CT	C22-C21-C23-C24
23	C	519	8CT	C14-C15-C16-C39
23	b	619	8CT	C10-C11-C12-C40
23	c	515	8CT	C14-C15-C16-C39
23	c	515	8CT	C22-C21-C23-C24
23	c	519	8CT	C14-C15-C16-C39
32	2	525	ZEX	C27-C28-C29-C39
32	3	519	ZEX	C7-C8-C9-C19
32	3	519	ZEX	C27-C28-C29-C39
32	3	520	ZEX	C27-C28-C29-C39
32	3	522	ZEX	C7-C8-C9-C19
32	4	403	ZEX	C27-C28-C29-C39
32	4	418	ZEX	C27-C28-C29-C39
32	6	524	ZEX	C27-C28-C29-C39
32	7	519	ZEX	C7-C8-C9-C19
32	7	519	ZEX	C27-C28-C29-C39
32	7	520	ZEX	C27-C28-C29-C39
32	7	522	ZEX	C7-C8-C9-C19
32	8	403	ZEX	C27-C28-C29-C39
32	8	418	ZEX	C27-C28-C29-C39
23	B	618	8CT	C10-C11-C12-C13
23	C	515	8CT	C14-C15-C16-C17
23	C	519	8CT	C14-C15-C16-C17
23	b	619	8CT	C10-C11-C12-C13
23	c	515	8CT	C14-C15-C16-C17
23	c	519	8CT	C14-C15-C16-C17
32	2	521	ZEX	C7-C8-C9-C10
32	2	523	ZEX	C31-C32-C33-C34
32	1	422	ZEX	C7-C8-C9-C10
32	3	519	ZEX	C7-C8-C9-C10
32	3	519	ZEX	C27-C28-C29-C30
32	3	520	ZEX	C27-C28-C29-C30
32	3	522	ZEX	C7-C8-C9-C10
32	4	403	ZEX	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
32	4	418	ZEX	C27-C28-C29-C30
32	4	419	ZEX	C7-C8-C9-C10
32	6	520	ZEX	C7-C8-C9-C10
32	6	522	ZEX	C31-C32-C33-C34
32	5	422	ZEX	C7-C8-C9-C10
32	7	519	ZEX	C7-C8-C9-C10
32	7	519	ZEX	C27-C28-C29-C30
32	7	520	ZEX	C27-C28-C29-C30
32	7	522	ZEX	C7-C8-C9-C10
32	8	403	ZEX	C27-C28-C29-C30
32	8	418	ZEX	C27-C28-C29-C30
32	8	419	ZEX	C7-C8-C9-C10
21	2	510	CL7	C13-C15-C16-C17
21	2	511	CL7	C8-C10-C11-C12
21	1	404	CL7	C13-C15-C16-C17
21	1	408	CL7	C15-C16-C17-C18
21	3	501	CL7	C15-C16-C17-C18
21	6	510	CL7	C13-C15-C16-C17
21	6	511	CL7	C8-C10-C11-C12
21	5	404	CL7	C13-C15-C16-C17
21	5	408	CL7	C15-C16-C17-C18
21	7	501	CL7	C15-C16-C17-C18
21	1	418	CL7	O1D-CGD-O2D-CED
21	3	508	CL7	O1D-CGD-O2D-CED
21	5	418	CL7	O1D-CGD-O2D-CED
21	7	508	CL7	O1D-CGD-O2D-CED
21	1	419	CL7	C4C-C3C-CAC-CBC
21	5	419	CL7	C4C-C3C-CAC-CBC
21	6	510	CL7	O1D-CGD-O2D-CED
21	B	604	CL7	C3-C5-C6-C7
21	2	505	CL7	C3-C5-C6-C7
21	b	605	CL7	C3-C5-C6-C7
21	6	505	CL7	C3-C5-C6-C7
21	B	604	CL7	C15-C16-C17-C18
21	B	611	CL7	C5-C6-C7-C8
21	C	510	CL7	C5-C6-C7-C8
21	2	517	CL7	C5-C6-C7-C8
21	1	406	CL7	C10-C11-C12-C13
21	3	504	CL7	C5-C6-C7-C8
21	4	406	CL7	C13-C15-C16-C17
21	4	409	CL7	C8-C10-C11-C12
21	4	412	CL7	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	4	412	CL7	C15-C16-C17-C18
21	b	605	CL7	C15-C16-C17-C18
21	b	612	CL7	C5-C6-C7-C8
21	6	517	CL7	C5-C6-C7-C8
21	5	406	CL7	C10-C11-C12-C13
21	7	504	CL7	C5-C6-C7-C8
21	8	406	CL7	C13-C15-C16-C17
21	8	409	CL7	C8-C10-C11-C12
21	8	412	CL7	C8-C10-C11-C12
21	8	412	CL7	C15-C16-C17-C18
21	2	510	CL7	O1D-CGD-O2D-CED
21	A	401	CL7	C8-C10-C11-C12
21	B	605	CL7	C5-C6-C7-C8
21	B	608	CL7	C15-C16-C17-C18
21	C	502	CL7	C15-C16-C17-C18
21	C	510	CL7	C10-C11-C12-C13
21	2	502	CL7	C8-C10-C11-C12
21	2	510	CL7	C5-C6-C7-C8
21	1	404	CL7	C15-C16-C17-C18
21	3	511	CL7	C10-C11-C12-C13
21	3	512	CL7	C5-C6-C7-C8
21	4	405	CL7	C13-C15-C16-C17
21	4	409	CL7	C10-C11-C12-C13
21	a	401	CL7	C8-C10-C11-C12
21	b	606	CL7	C5-C6-C7-C8
21	b	609	CL7	C15-C16-C17-C18
21	c	502	CL7	C15-C16-C17-C18
21	c	510	CL7	C5-C6-C7-C8
21	c	510	CL7	C10-C11-C12-C13
21	6	502	CL7	C8-C10-C11-C12
21	6	510	CL7	C5-C6-C7-C8
21	5	404	CL7	C15-C16-C17-C18
21	7	511	CL7	C10-C11-C12-C13
21	7	512	CL7	C5-C6-C7-C8
21	8	405	CL7	C13-C15-C16-C17
21	8	409	CL7	C10-C11-C12-C13
21	1	412	CL7	O1D-CGD-O2D-CED
21	4	410	CL7	O1D-CGD-O2D-CED
21	5	412	CL7	O1D-CGD-O2D-CED
21	8	410	CL7	O1D-CGD-O2D-CED
24	2	522	SQD	C7-C8-C9-C10
24	6	521	SQD	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
21	3	517	CL7	CBD-CGD-O2D-CED
21	7	517	CL7	CBD-CGD-O2D-CED
21	A	406	CL7	C5-C6-C7-C8
21	B	603	CL7	C5-C6-C7-C8
21	B	605	CL7	C13-C15-C16-C17
21	2	503	CL7	C8-C10-C11-C12
21	2	512	CL7	C13-C15-C16-C17
21	3	509	CL7	C5-C6-C7-C8
21	3	509	CL7	C10-C11-C12-C13
21	a	405	CL7	C5-C6-C7-C8
21	b	604	CL7	C5-C6-C7-C8
21	b	606	CL7	C13-C15-C16-C17
21	6	503	CL7	C8-C10-C11-C12
21	6	512	CL7	C13-C15-C16-C17
21	7	509	CL7	C5-C6-C7-C8
21	7	509	CL7	C10-C11-C12-C13
21	B	608	CL7	C5-C6-C7-C8
21	3	505	CL7	C8-C10-C11-C12
21	4	406	CL7	C15-C16-C17-C18
21	b	609	CL7	C5-C6-C7-C8
21	7	505	CL7	C8-C10-C11-C12
21	8	406	CL7	C15-C16-C17-C18
21	1	415	CL7	CBD-CGD-O2D-CED
21	5	415	CL7	CBD-CGD-O2D-CED
21	1	406	CL7	C13-C15-C16-C17
21	5	406	CL7	C13-C15-C16-C17
21	2	501	CL7	C15-C16-C17-C18
21	6	501	CL7	C15-C16-C17-C18
21	B	603	CL7	C12-C13-C15-C16
21	C	504	CL7	C11-C12-C13-C15
21	C	508	CL7	C11-C10-C8-C7
21	2	512	CL7	C11-C12-C13-C15
21	1	406	CL7	C12-C13-C15-C16
21	1	408	CL7	C12-C13-C15-C16
21	1	418	CL7	C12-C13-C15-C16
21	3	501	CL7	C11-C10-C8-C7
21	3	503	CL7	C11-C10-C8-C7
21	3	503	CL7	C12-C13-C15-C16
21	3	508	CL7	C6-C7-C8-C10
21	3	510	CL7	C6-C7-C8-C10
21	3	511	CL7	C12-C13-C15-C16
21	4	406	CL7	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
21	4	406	CL7	C11-C10-C8-C7
21	4	406	CL7	C12-C13-C15-C16
21	b	604	CL7	C12-C13-C15-C16
21	c	504	CL7	C11-C12-C13-C15
21	c	508	CL7	C11-C10-C8-C7
21	6	512	CL7	C11-C12-C13-C15
21	5	406	CL7	C12-C13-C15-C16
21	5	408	CL7	C12-C13-C15-C16
21	5	418	CL7	C12-C13-C15-C16
21	7	501	CL7	C11-C10-C8-C7
21	7	503	CL7	C11-C10-C8-C7
21	7	503	CL7	C12-C13-C15-C16
21	7	508	CL7	C6-C7-C8-C10
21	7	510	CL7	C6-C7-C8-C10
21	7	511	CL7	C12-C13-C15-C16
21	8	406	CL7	C6-C7-C8-C10
21	8	406	CL7	C11-C10-C8-C7
21	8	406	CL7	C12-C13-C15-C16
21	B	610	CL7	C3-C5-C6-C7
21	2	509	CL7	C3-C5-C6-C7
21	3	502	CL7	C3-C5-C6-C7
21	b	611	CL7	C3-C5-C6-C7
21	6	509	CL7	C3-C5-C6-C7
21	7	502	CL7	C3-C5-C6-C7
23	B	617	8CT	C12-C13-C14-C15
23	B	618	8CT	C12-C13-C14-C15
23	B	618	8CT	C16-C17-C18-C19
23	B	618	8CT	C18-C19-C20-C21
23	C	516	8CT	C23-C24-C25-C26
23	C	519	8CT	C12-C13-C14-C15
23	b	618	8CT	C12-C13-C14-C15
23	b	619	8CT	C12-C13-C14-C15
23	b	619	8CT	C16-C17-C18-C19
23	b	619	8CT	C18-C19-C20-C21
23	c	516	8CT	C23-C24-C25-C26
23	c	519	8CT	C12-C13-C14-C15
32	2	520	ZEX	C33-C34-C35-C15
32	2	525	ZEX	C9-C10-C11-C12
32	3	519	ZEX	C29-C30-C31-C32
32	3	525	ZEX	C33-C34-C35-C15
32	4	420	ZEX	C29-C30-C31-C32
32	6	524	ZEX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
32	7	519	ZEX	C29-C30-C31-C32
32	8	420	ZEX	C29-C30-C31-C32
21	1	419	CL7	C2A-CAA-CBA-CGA
21	4	406	CL7	C2A-CAA-CBA-CGA
21	8	406	CL7	C2A-CAA-CBA-CGA
21	C	505	CL7	O1D-CGD-O2D-CED
21	2	509	CL7	O1D-CGD-O2D-CED
21	2	517	CL7	O1D-CGD-O2D-CED
21	1	403	CL7	O1D-CGD-O2D-CED
21	4	409	CL7	O1D-CGD-O2D-CED
21	c	505	CL7	O1D-CGD-O2D-CED
21	6	509	CL7	O1D-CGD-O2D-CED
21	6	517	CL7	O1D-CGD-O2D-CED
21	5	403	CL7	O1D-CGD-O2D-CED
21	8	409	CL7	O1D-CGD-O2D-CED
21	C	506	CL7	C5-C6-C7-C8
21	C	508	CL7	C5-C6-C7-C8
21	C	511	CL7	C10-C11-C12-C13
21	1	403	CL7	C5-C6-C7-C8
21	1	404	CL7	C8-C10-C11-C12
21	c	506	CL7	C5-C6-C7-C8
21	c	508	CL7	C5-C6-C7-C8
21	c	511	CL7	C10-C11-C12-C13
21	5	403	CL7	C5-C6-C7-C8
21	5	404	CL7	C8-C10-C11-C12
21	1	410	CL7	C8-C10-C11-C12
21	4	404	CL7	C5-C6-C7-C8
21	5	410	CL7	C8-C10-C11-C12
21	8	404	CL7	C5-C6-C7-C8
21	1	402	CL7	C3-C5-C6-C7
21	5	402	CL7	C3-C5-C6-C7
21	B	610	CL7	C8-C10-C11-C12
21	C	509	CL7	C5-C6-C7-C8
21	2	509	CL7	C13-C15-C16-C17
21	2	511	CL7	C5-C6-C7-C8
21	1	402	CL7	C10-C11-C12-C13
21	1	404	CL7	C5-C6-C7-C8
21	b	611	CL7	C8-C10-C11-C12
21	c	509	CL7	C5-C6-C7-C8
21	6	509	CL7	C13-C15-C16-C17
21	6	511	CL7	C5-C6-C7-C8
21	5	402	CL7	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	5	404	CL7	C5-C6-C7-C8
21	B	611	CL7	O1D-CGD-O2D-CED
21	b	612	CL7	O1D-CGD-O2D-CED
21	B	603	CL7	C8-C10-C11-C12
21	B	614	CL7	C8-C10-C11-C12
21	C	503	CL7	C8-C10-C11-C12
21	C	511	CL7	C8-C10-C11-C12
21	2	501	CL7	C8-C10-C11-C12
21	2	509	CL7	C5-C6-C7-C8
21	1	403	CL7	C8-C10-C11-C12
21	1	406	CL7	C8-C10-C11-C12
21	3	501	CL7	C13-C15-C16-C17
21	4	405	CL7	C5-C6-C7-C8
21	b	604	CL7	C8-C10-C11-C12
21	b	615	CL7	C8-C10-C11-C12
21	c	503	CL7	C8-C10-C11-C12
21	c	511	CL7	C8-C10-C11-C12
21	6	501	CL7	C8-C10-C11-C12
21	6	509	CL7	C5-C6-C7-C8
21	5	403	CL7	C8-C10-C11-C12
21	5	406	CL7	C8-C10-C11-C12
21	7	501	CL7	C13-C15-C16-C17
21	8	405	CL7	C5-C6-C7-C8
21	C	507	CL7	C5-C6-C7-C8
21	C	509	CL7	C15-C16-C17-C18
21	2	505	CL7	C15-C16-C17-C18
21	2	510	CL7	C15-C16-C17-C18
21	4	404	CL7	C8-C10-C11-C12
21	c	507	CL7	C5-C6-C7-C8
21	c	509	CL7	C15-C16-C17-C18
21	6	505	CL7	C15-C16-C17-C18
21	6	510	CL7	C15-C16-C17-C18
21	8	404	CL7	C8-C10-C11-C12
25	3	524	LHG	C3-O3-P-O6
25	7	524	LHG	C3-O3-P-O6
21	B	608	CL7	C3-C5-C6-C7
21	b	609	CL7	C3-C5-C6-C7
21	B	616	CL7	CBD-CGD-O2D-CED
21	b	617	CL7	CBD-CGD-O2D-CED
21	B	602	CL7	C5-C6-C7-C8
21	C	504	CL7	C10-C11-C12-C13
21	2	516	CL7	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
21	2	517	CL7	C8-C10-C11-C12
21	b	603	CL7	C5-C6-C7-C8
21	c	504	CL7	C10-C11-C12-C13
21	6	516	CL7	C15-C16-C17-C18
21	6	517	CL7	C8-C10-C11-C12
32	2	520	ZEX	C25-C26-C27-C28
32	3	525	ZEX	C25-C26-C27-C28
32	4	403	ZEX	C25-C26-C27-C28
32	4	418	ZEX	C25-C26-C27-C28
32	4	420	ZEX	C25-C26-C27-C28
32	8	403	ZEX	C25-C26-C27-C28
32	8	418	ZEX	C25-C26-C27-C28
32	8	420	ZEX	C25-C26-C27-C28
25	A	407	LHG	C1-C2-C3-O3
25	a	406	LHG	C1-C2-C3-O3
21	3	501	CL7	C4-C3-C5-C6
21	3	505	CL7	C4-C3-C5-C6
21	6	503	CL7	C4-C3-C5-C6
21	7	501	CL7	C4-C3-C5-C6
21	7	505	CL7	C4-C3-C5-C6
21	3	512	CL7	C2-C3-C5-C6
21	7	512	CL7	C2-C3-C5-C6
21	C	511	CL7	C15-C16-C17-C18
21	3	507	CL7	C13-C15-C16-C17
21	4	411	CL7	C13-C15-C16-C17
21	c	511	CL7	C15-C16-C17-C18
21	7	507	CL7	C13-C15-C16-C17
21	8	411	CL7	C13-C15-C16-C17
21	D	402	CL7	C2A-CAA-CBA-CGA
21	d	402	CL7	C2A-CAA-CBA-CGA
21	2	518	CL7	C16-C17-C18-C19
21	6	518	CL7	C16-C17-C18-C19
21	B	607	CL7	C3-C5-C6-C7
21	B	612	CL7	C3-C5-C6-C7
21	2	517	CL7	C3-C5-C6-C7
21	b	608	CL7	C3-C5-C6-C7
21	b	613	CL7	C3-C5-C6-C7
21	6	517	CL7	C3-C5-C6-C7
23	4	402	8CT	C12-C13-C14-C15
23	8	402	8CT	C12-C13-C14-C15
32	2	523	ZEX	C29-C30-C31-C32
32	4	403	ZEX	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
32	6	522	ZEX	C29-C30-C31-C32
32	8	403	ZEX	C29-C30-C31-C32
21	1	420	CL7	C4C-C3C-CAC-CBC
21	5	420	CL7	C4C-C3C-CAC-CBC
21	2	517	CL7	C10-C11-C12-C13
21	6	517	CL7	C10-C11-C12-C13
21	2	506	CL7	O1D-CGD-O2D-CED
21	6	506	CL7	O1D-CGD-O2D-CED
21	2	517	CL7	C15-C16-C17-C18
21	6	517	CL7	C15-C16-C17-C18
22	D	408	PHO	O1D-CGD-O2D-CED
22	d	408	PHO	O1D-CGD-O2D-CED
27	C	517	DGD	C3B-C4B-C5B-C6B
21	3	511	CL7	C3-C5-C6-C7
21	7	511	CL7	C3-C5-C6-C7
27	c	517	DGD	C3B-C4B-C5B-C6B
21	2	501	CL7	C5-C6-C7-C8
21	6	501	CL7	C5-C6-C7-C8
21	3	514	CL7	O1D-CGD-O2D-CED
21	7	514	CL7	O1D-CGD-O2D-CED
21	B	611	CL7	C4-C3-C5-C6
21	b	612	CL7	C4-C3-C5-C6
21	B	604	CL7	C11-C12-C13-C14
21	B	608	CL7	C6-C7-C8-C9
21	B	611	CL7	C6-C7-C8-C9
21	2	501	CL7	C11-C12-C13-C14
21	2	509	CL7	C6-C7-C8-C9
21	3	508	CL7	C11-C10-C8-C9
21	b	605	CL7	C11-C12-C13-C14
21	b	609	CL7	C6-C7-C8-C9
21	b	612	CL7	C6-C7-C8-C9
21	6	501	CL7	C11-C12-C13-C14
21	6	509	CL7	C6-C7-C8-C9
21	7	508	CL7	C11-C10-C8-C9
21	2	509	CL7	C8-C10-C11-C12
21	6	509	CL7	C8-C10-C11-C12
26	C	501	LMG	O6-C5-C6-O5
26	c	501	LMG	O6-C5-C6-O5
21	B	615	CL7	C2A-CAA-CBA-CGA
21	b	616	CL7	C2A-CAA-CBA-CGA
23	B	618	8CT	C14-C15-C16-C39
23	B	627	8CT	C10-C11-C12-C40

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Mol	Chain	Res	Type	Atoms
23	D	406	8CT	C22-C21-C23-C24
23	b	601	8CT	C10-C11-C12-C40
23	b	619	8CT	C14-C15-C16-C39
23	d	406	8CT	C22-C21-C23-C24
32	2	521	ZEX	C7-C8-C9-C19
32	1	422	ZEX	C7-C8-C9-C19
32	4	419	ZEX	C7-C8-C9-C19
32	4	420	ZEX	C31-C32-C33-C40
32	6	520	ZEX	C7-C8-C9-C19
32	5	422	ZEX	C7-C8-C9-C19
32	8	419	ZEX	C7-C8-C9-C19
32	8	420	ZEX	C31-C32-C33-C40
23	B	618	8CT	C14-C15-C16-C17
23	B	627	8CT	C10-C11-C12-C13
23	C	515	8CT	C25-C26-C28-C29
23	D	406	8CT	C20-C21-C23-C24
23	b	601	8CT	C10-C11-C12-C13
23	b	619	8CT	C14-C15-C16-C17
23	c	515	8CT	C25-C26-C28-C29
23	d	406	8CT	C20-C21-C23-C24
32	3	520	ZEX	C7-C8-C9-C10
32	4	420	ZEX	C31-C32-C33-C34
32	7	520	ZEX	C7-C8-C9-C10
32	8	420	ZEX	C31-C32-C33-C34
22	d	408	PHO	C2C-C3C-CAC-CBC
22	D	408	PHO	C2C-C3C-CAC-CBC
21	2	518	CL7	C16-C17-C18-C20
21	6	518	CL7	C16-C17-C18-C20
21	B	605	CL7	C10-C11-C12-C13
21	D	402	CL7	O1D-CGD-O2D-CED
21	4	406	CL7	CBD-CGD-O2D-CED
21	8	406	CL7	CBD-CGD-O2D-CED
21	A	406	CL7	O1D-CGD-O2D-CED
21	2	503	CL7	O1D-CGD-O2D-CED
21	a	405	CL7	O1D-CGD-O2D-CED
21	d	402	CL7	O1D-CGD-O2D-CED
21	B	612	CL7	C13-C15-C16-C17
21	1	402	CL7	C8-C10-C11-C12
21	b	606	CL7	C10-C11-C12-C13
21	b	613	CL7	C13-C15-C16-C17
21	5	402	CL7	C8-C10-C11-C12
21	C	506	CL7	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	c	506	CL7	O1D-CGD-O2D-CED
21	6	503	CL7	O1D-CGD-O2D-CED
21	B	614	CL7	C3A-C2A-CAA-CBA
21	C	504	CL7	C3A-C2A-CAA-CBA
21	C	505	CL7	C3A-C2A-CAA-CBA
21	2	507	CL7	C3A-C2A-CAA-CBA
21	2	510	CL7	C3A-C2A-CAA-CBA
21	2	512	CL7	C3A-C2A-CAA-CBA
21	2	513	CL7	C3A-C2A-CAA-CBA
21	3	504	CL7	C3A-C2A-CAA-CBA
21	3	512	CL7	C3A-C2A-CAA-CBA
21	4	412	CL7	C3A-C2A-CAA-CBA
21	4	414	CL7	C3A-C2A-CAA-CBA
21	b	615	CL7	C3A-C2A-CAA-CBA
21	c	504	CL7	C3A-C2A-CAA-CBA
21	c	505	CL7	C3A-C2A-CAA-CBA
21	6	507	CL7	C3A-C2A-CAA-CBA
21	6	510	CL7	C3A-C2A-CAA-CBA
21	6	512	CL7	C3A-C2A-CAA-CBA
21	6	513	CL7	C3A-C2A-CAA-CBA
21	7	504	CL7	C3A-C2A-CAA-CBA
21	7	512	CL7	C3A-C2A-CAA-CBA
21	8	412	CL7	C3A-C2A-CAA-CBA
21	8	414	CL7	C3A-C2A-CAA-CBA
23	C	516	8CT	C12-C13-C14-C15
23	c	516	8CT	C12-C13-C14-C15
21	C	502	CL7	C16-C17-C18-C19
21	c	502	CL7	C16-C17-C18-C19
27	C	517	DGD	CCB-CDB-CEB-CFB
27	c	517	DGD	CCB-CDB-CEB-CFB
21	C	507	CL7	O2A-C1-C2-C3
21	C	508	CL7	O2A-C1-C2-C3
21	c	507	CL7	O2A-C1-C2-C3
21	c	508	CL7	O2A-C1-C2-C3
21	A	406	CL7	C3-C5-C6-C7
21	a	405	CL7	C3-C5-C6-C7
21	C	506	CL7	C10-C11-C12-C13
21	c	506	CL7	C10-C11-C12-C13
21	2	503	CL7	C4-C3-C5-C6
26	C	501	LMG	C4-C5-C6-O5
26	C	501	LMG	C11-C10-O7-C8
26	c	501	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
27	C	517	DGD	C8A-C9A-CAA-CBA
27	c	517	DGD	C8A-C9A-CAA-CBA
21	4	405	CL7	C10-C11-C12-C13
21	8	405	CL7	C10-C11-C12-C13
21	6	503	CL7	C3-C5-C6-C7
26	c	501	LMG	C4-C5-C6-O5
21	A	401	CL7	C4C-C3C-CAC-CBC
21	a	401	CL7	C4C-C3C-CAC-CBC
27	C	517	DGD	O6E-C5E-C6E-O5E
27	c	517	DGD	O6E-C5E-C6E-O5E
26	C	501	LMG	O9-C10-O7-C8
26	c	501	LMG	O9-C10-O7-C8
21	2	518	CL7	C10-C11-C12-C13
21	6	518	CL7	C10-C11-C12-C13
21	2	503	CL7	C3-C5-C6-C7
23	B	627	8CT	C02-C03-C10-C11
23	C	515	8CT	C04-C03-C10-C11
23	C	519	8CT	C04-C03-C10-C11
23	D	406	8CT	C02-C03-C10-C11
23	K	101	8CT	C04-C03-C10-C11
23	b	601	8CT	C02-C03-C10-C11
23	c	515	8CT	C04-C03-C10-C11
23	d	406	8CT	C02-C03-C10-C11
23	k	101	8CT	C04-C03-C10-C11
32	2	519	ZEX	C5-C6-C7-C8
32	2	521	ZEX	C5-C6-C7-C8
32	2	525	ZEX	C1-C6-C7-C8
32	2	525	ZEX	C5-C6-C7-C8
32	1	421	ZEX	C1-C6-C7-C8
32	1	421	ZEX	C5-C6-C7-C8
32	1	422	ZEX	C1-C6-C7-C8
32	1	422	ZEX	C5-C6-C7-C8
32	3	519	ZEX	C1-C6-C7-C8
32	3	519	ZEX	C5-C6-C7-C8
32	3	522	ZEX	C5-C6-C7-C8
32	4	403	ZEX	C1-C6-C7-C8
32	6	519	ZEX	C5-C6-C7-C8
32	6	520	ZEX	C5-C6-C7-C8
32	6	524	ZEX	C1-C6-C7-C8
32	6	524	ZEX	C5-C6-C7-C8
32	5	421	ZEX	C1-C6-C7-C8
32	5	421	ZEX	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
32	5	422	ZEX	C1-C6-C7-C8
32	5	422	ZEX	C5-C6-C7-C8
32	7	519	ZEX	C1-C6-C7-C8
32	7	519	ZEX	C5-C6-C7-C8
32	7	522	ZEX	C5-C6-C7-C8
32	8	403	ZEX	C1-C6-C7-C8
21	3	508	CL7	C5-C6-C7-C8
21	4	406	CL7	C10-C11-C12-C13
21	8	406	CL7	C10-C11-C12-C13
21	A	406	CL7	C10-C11-C12-C13
21	a	405	CL7	C10-C11-C12-C13
21	7	508	CL7	C5-C6-C7-C8
21	B	608	CL7	C6-C7-C8-C10
21	B	611	CL7	C2-C3-C5-C6
21	B	611	CL7	C6-C7-C8-C10
21	B	612	CL7	C12-C13-C15-C16
21	C	509	CL7	C11-C10-C8-C7
21	C	511	CL7	C6-C7-C8-C10
21	C	511	CL7	C11-C10-C8-C7
21	2	505	CL7	C11-C12-C13-C15
21	2	505	CL7	C12-C13-C15-C16
21	2	511	CL7	C6-C7-C8-C10
21	2	517	CL7	C12-C13-C15-C16
21	1	418	CL7	C11-C10-C8-C7
21	3	504	CL7	C11-C10-C8-C7
21	3	508	CL7	C11-C10-C8-C7
21	b	609	CL7	C6-C7-C8-C10
21	b	612	CL7	C2-C3-C5-C6
21	b	612	CL7	C6-C7-C8-C10
21	b	613	CL7	C12-C13-C15-C16
21	c	509	CL7	C11-C10-C8-C7
21	c	511	CL7	C6-C7-C8-C10
21	c	511	CL7	C11-C10-C8-C7
21	6	505	CL7	C11-C12-C13-C15
21	6	505	CL7	C12-C13-C15-C16
21	6	511	CL7	C6-C7-C8-C10
21	6	517	CL7	C12-C13-C15-C16
21	5	418	CL7	C11-C10-C8-C7
21	7	504	CL7	C11-C10-C8-C7
21	7	508	CL7	C11-C10-C8-C7
21	2	506	CL7	C8-C10-C11-C12
21	2	507	CL7	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	6	506	CL7	C8-C10-C11-C12
32	2	525	ZEX	C29-C30-C31-C32
32	4	420	ZEX	C33-C34-C35-C15
32	6	524	ZEX	C29-C30-C31-C32
32	8	420	ZEX	C33-C34-C35-C15
21	C	511	CL7	O1D-CGD-O2D-CED
21	c	511	CL7	O1D-CGD-O2D-CED
21	2	513	CL7	C2A-CAA-CBA-CGA
21	4	410	CL7	C2A-CAA-CBA-CGA
21	4	415	CL7	C2A-CAA-CBA-CGA
21	6	513	CL7	C2A-CAA-CBA-CGA
21	8	410	CL7	C2A-CAA-CBA-CGA
21	8	415	CL7	C2A-CAA-CBA-CGA
21	B	603	CL7	C10-C11-C12-C13
21	C	502	CL7	C13-C15-C16-C17
21	1	403	CL7	C10-C11-C12-C13
21	b	604	CL7	C10-C11-C12-C13
21	c	502	CL7	C13-C15-C16-C17
21	5	403	CL7	C10-C11-C12-C13
21	C	507	CL7	C10-C11-C12-C13
21	c	507	CL7	C10-C11-C12-C13
21	4	412	CL7	O1D-CGD-O2D-CED
21	8	412	CL7	O1D-CGD-O2D-CED
21	1	418	CL7	C15-C16-C17-C18
21	6	507	CL7	C8-C10-C11-C12
21	5	418	CL7	C15-C16-C17-C18
21	2	507	CL7	O1D-CGD-O2D-CED
21	6	507	CL7	O1D-CGD-O2D-CED
31	F	101	HEM	C4B-C3B-CAB-CBB
31	F	101	HEM	C4C-C3C-CAC-CBC
31	f	101	HEM	C4B-C3B-CAB-CBB
31	f	101	HEM	C4C-C3C-CAC-CBC
21	4	412	CL7	C13-C15-C16-C17
21	4	416	CL7	CBD-CGD-O2D-CED
21	8	416	CL7	CBD-CGD-O2D-CED
21	8	412	CL7	C13-C15-C16-C17
21	4	414	CL7	O1D-CGD-O2D-CED
21	8	414	CL7	O1D-CGD-O2D-CED
21	2	505	CL7	C10-C11-C12-C13
21	2	516	CL7	C5-C6-C7-C8
21	3	510	CL7	C8-C10-C11-C12
21	6	505	CL7	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	6	516	CL7	C5-C6-C7-C8
21	7	510	CL7	C8-C10-C11-C12
21	3	501	CL7	C2-C3-C5-C6
21	3	505	CL7	C2-C3-C5-C6
21	7	501	CL7	C2-C3-C5-C6
21	7	505	CL7	C2-C3-C5-C6
21	A	406	CL7	C11-C10-C8-C9
21	B	605	CL7	C14-C13-C15-C16
21	B	612	CL7	C6-C7-C8-C9
21	C	504	CL7	C11-C10-C8-C9
21	2	505	CL7	C11-C12-C13-C14
21	2	509	CL7	C11-C12-C13-C14
21	2	510	CL7	C14-C13-C15-C16
21	1	408	CL7	C14-C13-C15-C16
21	3	507	CL7	C14-C13-C15-C16
21	a	405	CL7	C11-C10-C8-C9
21	b	606	CL7	C14-C13-C15-C16
21	b	613	CL7	C6-C7-C8-C9
21	c	504	CL7	C11-C10-C8-C9
21	6	505	CL7	C11-C12-C13-C14
21	6	509	CL7	C11-C12-C13-C14
21	6	510	CL7	C14-C13-C15-C16
21	5	408	CL7	C14-C13-C15-C16
21	7	507	CL7	C14-C13-C15-C16
21	3	512	CL7	C3-C5-C6-C7
21	7	512	CL7	C3-C5-C6-C7
21	3	501	CL7	C2A-CAA-CBA-CGA
21	7	501	CL7	C2A-CAA-CBA-CGA
21	B	608	CL7	C2C-C3C-CAC-CBC
21	b	609	CL7	C2C-C3C-CAC-CBC
32	3	520	ZEX	C7-C8-C9-C19
32	7	520	ZEX	C7-C8-C9-C19
21	1	410	CL7	C5-C6-C7-C8
21	5	410	CL7	C5-C6-C7-C8
23	C	516	8CT	C25-C26-C28-C29
23	c	516	8CT	C25-C26-C28-C29
21	B	609	CL7	C1A-C2A-CAA-CBA
21	B	612	CL7	C1A-C2A-CAA-CBA
21	B	614	CL7	C1A-C2A-CAA-CBA
21	C	509	CL7	C1A-C2A-CAA-CBA
21	C	511	CL7	C1A-C2A-CAA-CBA
21	C	514	CL7	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	D	402	CL7	C1A-C2A-CAA-CBA
21	2	501	CL7	C1A-C2A-CAA-CBA
21	2	507	CL7	C1A-C2A-CAA-CBA
21	2	510	CL7	C1A-C2A-CAA-CBA
21	2	511	CL7	C1A-C2A-CAA-CBA
21	2	512	CL7	C1A-C2A-CAA-CBA
21	2	516	CL7	C1A-C2A-CAA-CBA
21	1	417	CL7	C1A-C2A-CAA-CBA
21	1	418	CL7	C1A-C2A-CAA-CBA
21	3	503	CL7	C1A-C2A-CAA-CBA
21	3	514	CL7	C1A-C2A-CAA-CBA
21	3	516	CL7	C1A-C2A-CAA-CBA
21	4	404	CL7	C1A-C2A-CAA-CBA
21	4	414	CL7	C1A-C2A-CAA-CBA
21	b	610	CL7	C1A-C2A-CAA-CBA
21	b	613	CL7	C1A-C2A-CAA-CBA
21	b	615	CL7	C1A-C2A-CAA-CBA
21	c	511	CL7	C1A-C2A-CAA-CBA
21	c	514	CL7	C1A-C2A-CAA-CBA
21	d	402	CL7	C1A-C2A-CAA-CBA
21	6	501	CL7	C1A-C2A-CAA-CBA
21	6	507	CL7	C1A-C2A-CAA-CBA
21	6	510	CL7	C1A-C2A-CAA-CBA
21	6	511	CL7	C1A-C2A-CAA-CBA
21	6	512	CL7	C1A-C2A-CAA-CBA
21	6	516	CL7	C1A-C2A-CAA-CBA
21	5	417	CL7	C1A-C2A-CAA-CBA
21	5	418	CL7	C1A-C2A-CAA-CBA
21	7	503	CL7	C1A-C2A-CAA-CBA
21	7	514	CL7	C1A-C2A-CAA-CBA
21	7	516	CL7	C1A-C2A-CAA-CBA
21	8	404	CL7	C1A-C2A-CAA-CBA
21	8	414	CL7	C1A-C2A-CAA-CBA
21	C	504	CL7	C16-C17-C18-C20
21	c	504	CL7	C16-C17-C18-C20
25	B	625	LHG	C15-C16-C17-C18
25	b	626	LHG	C15-C16-C17-C18
23	K	101	8CT	C18-C19-C20-C21
23	k	101	8CT	C18-C19-C20-C21
21	1	408	CL7	C4C-C3C-CAC-CBC
21	5	408	CL7	C4C-C3C-CAC-CBC
21	C	511	CL7	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	c	511	CL7	C3-C5-C6-C7
21	3	507	CL7	C5-C6-C7-C8
21	7	507	CL7	C5-C6-C7-C8
26	D	410	LMG	O6-C5-C6-O5
26	d	410	LMG	O6-C5-C6-O5
32	4	419	ZEX	C25-C26-C27-C28
32	8	419	ZEX	C25-C26-C27-C28
26	b	622	LMG	C38-C39-C40-C41
26	B	621	LMG	C38-C39-C40-C41
27	B	624	DGD	C2A-C1A-O1G-C1G
27	b	625	DGD	C2A-C1A-O1G-C1G
21	1	402	CL7	C4-C3-C5-C6
21	5	402	CL7	C4-C3-C5-C6
21	2	503	CL7	C2-C3-C5-C6
21	4	417	CL7	C3A-C2A-CAA-CBA
21	6	503	CL7	C2-C3-C5-C6
21	8	417	CL7	C3A-C2A-CAA-CBA
21	2	517	CL7	C2A-CAA-CBA-CGA
21	6	517	CL7	C2A-CAA-CBA-CGA
21	3	507	CL7	C3-C5-C6-C7
26	B	621	LMG	C7-C8-C9-O8
26	b	622	LMG	C7-C8-C9-O8
24	3	523	SQD	C45-C44-O6-C1
24	7	523	SQD	C45-C44-O6-C1
21	1	415	CL7	C4C-C3C-CAC-CBC
21	5	415	CL7	C4C-C3C-CAC-CBC
21	4	414	CL7	C5-C6-C7-C8
21	8	414	CL7	C5-C6-C7-C8
21	d	404	CL7	O1D-CGD-O2D-CED
26	1	401	LMG	O6-C5-C6-O5
26	5	401	LMG	O6-C5-C6-O5
21	7	507	CL7	C3-C5-C6-C7
21	2	503	CL7	C10-C11-C12-C13
21	6	503	CL7	C10-C11-C12-C13
21	C	502	CL7	C2B-C3B-CAB-OBB
21	C	504	CL7	C2B-C3B-CAB-OBB
21	C	513	CL7	C2B-C3B-CAB-OBB
21	D	404	CL7	C2B-C3B-CAB-OBB
21	2	508	CL7	C2B-C3B-CAB-OBB
21	2	516	CL7	C2B-C3B-CAB-OBB
21	1	402	CL7	C2B-C3B-CAB-OBB
21	4	405	CL7	C2B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
21	c	502	CL7	C2B-C3B-CAB-OBB
21	c	504	CL7	C2B-C3B-CAB-OBB
21	c	513	CL7	C2B-C3B-CAB-OBB
21	d	404	CL7	C2B-C3B-CAB-OBB
21	6	508	CL7	C2B-C3B-CAB-OBB
21	6	516	CL7	C2B-C3B-CAB-OBB
21	5	402	CL7	C2B-C3B-CAB-OBB
21	8	405	CL7	C2B-C3B-CAB-OBB
21	D	404	CL7	O1D-CGD-O2D-CED
21	2	512	CL7	C10-C11-C12-C13
21	6	512	CL7	C10-C11-C12-C13
21	4	415	CL7	CBD-CGD-O2D-CED
21	8	415	CL7	CBD-CGD-O2D-CED
21	B	609	CL7	C13-C15-C16-C17
21	b	610	CL7	C13-C15-C16-C17
21	B	606	CL7	C4B-C3B-CAB-OBB
21	B	613	CL7	C4B-C3B-CAB-OBB
21	1	405	CL7	C4B-C3B-CAB-OBB
21	4	415	CL7	C4B-C3B-CAB-OBB
21	b	607	CL7	C4B-C3B-CAB-OBB
21	b	614	CL7	C4B-C3B-CAB-OBB
21	5	405	CL7	C4B-C3B-CAB-OBB
21	8	415	CL7	C4B-C3B-CAB-OBB
21	1	410	CL7	C15-C16-C17-C18
21	5	410	CL7	C15-C16-C17-C18
26	C	501	LMG	C12-C13-C14-C15
21	4	409	CL7	C5-C6-C7-C8
21	8	409	CL7	C5-C6-C7-C8
25	D	409	LHG	O6-C4-C5-O7
25	d	409	LHG	O6-C4-C5-O7
21	B	609	CL7	C16-C17-C18-C20
21	C	504	CL7	C16-C17-C18-C19
21	b	610	CL7	C16-C17-C18-C20
21	c	504	CL7	C16-C17-C18-C19
21	7	512	CL7	CBD-CGD-O2D-CED
21	B	607	CL7	C8-C10-C11-C12
21	b	608	CL7	C8-C10-C11-C12
21	1	415	CL7	O1D-CGD-O2D-CED
27	B	624	DGD	O1A-C1A-O1G-C1G
27	b	625	DGD	O1A-C1A-O1G-C1G
24	b	621	SQD	C32-C33-C34-C35
21	3	512	CL7	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	5	410	CL7	C10-C11-C12-C13
26	C	501	LMG	C2-C1-O1-C7
26	1	401	LMG	C2-C1-O1-C7
26	c	501	LMG	C2-C1-O1-C7
26	5	401	LMG	C2-C1-O1-C7
24	B	620	SQD	C32-C33-C34-C35
21	A	401	CL7	C10-C11-C12-C13
21	B	604	CL7	C8-C10-C11-C12
21	1	410	CL7	C10-C11-C12-C13
21	a	401	CL7	C10-C11-C12-C13
21	b	605	CL7	C8-C10-C11-C12
21	B	609	CL7	C16-C17-C18-C19
21	b	610	CL7	C16-C17-C18-C19
22	A	402	PHO	CHA-CBD-CGD-O1D
22	A	402	PHO	CHA-CBD-CGD-O2D
22	a	402	PHO	CHA-CBD-CGD-O1D
22	a	402	PHO	CHA-CBD-CGD-O2D
21	5	415	CL7	O1D-CGD-O2D-CED
21	2	507	CL7	C4-C3-C5-C6
21	6	507	CL7	C4-C3-C5-C6
21	7	502	CL7	C4-C3-C5-C6
21	B	603	CL7	C11-C10-C8-C7
21	B	604	CL7	C12-C13-C15-C16
21	B	605	CL7	C12-C13-C15-C16
21	B	609	CL7	C6-C7-C8-C10
21	B	612	CL7	C11-C10-C8-C7
21	C	504	CL7	C11-C10-C8-C7
21	C	506	CL7	C12-C13-C15-C16
21	C	507	CL7	C11-C10-C8-C7
21	C	511	CL7	C12-C13-C15-C16
21	2	503	CL7	C12-C13-C15-C16
21	2	507	CL7	C11-C10-C8-C7
21	2	510	CL7	C6-C7-C8-C10
21	2	510	CL7	C11-C10-C8-C7
21	1	408	CL7	C11-C10-C8-C7
21	3	501	CL7	C12-C13-C15-C16
21	3	507	CL7	C6-C7-C8-C10
21	4	411	CL7	C11-C12-C13-C15
21	b	604	CL7	C11-C10-C8-C7
21	b	605	CL7	C12-C13-C15-C16
21	b	606	CL7	C12-C13-C15-C16
21	b	610	CL7	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
21	b	613	CL7	C11-C10-C8-C7
21	c	504	CL7	C11-C10-C8-C7
21	c	506	CL7	C12-C13-C15-C16
21	c	507	CL7	C11-C10-C8-C7
21	c	511	CL7	C12-C13-C15-C16
21	6	503	CL7	C12-C13-C15-C16
21	6	507	CL7	C11-C10-C8-C7
21	6	510	CL7	C6-C7-C8-C10
21	6	510	CL7	C11-C10-C8-C7
21	5	408	CL7	C11-C10-C8-C7
21	7	501	CL7	C12-C13-C15-C16
21	7	507	CL7	C6-C7-C8-C10
21	8	411	CL7	C11-C12-C13-C15
21	3	516	CL7	C4C-C3C-CAC-CBC
21	B	612	CL7	C11-C10-C8-C9
21	C	511	CL7	C14-C13-C15-C16
21	2	501	CL7	C6-C7-C8-C9
21	2	503	CL7	C14-C13-C15-C16
21	2	505	CL7	C11-C10-C8-C9
21	2	512	CL7	C11-C10-C8-C9
21	1	402	CL7	C6-C7-C8-C9
21	1	406	CL7	C14-C13-C15-C16
21	1	418	CL7	C14-C13-C15-C16
21	3	501	CL7	C14-C13-C15-C16
21	3	503	CL7	C6-C7-C8-C9
21	3	503	CL7	C11-C10-C8-C9
21	3	504	CL7	C11-C12-C13-C14
21	3	509	CL7	C11-C10-C8-C9
21	3	511	CL7	C14-C13-C15-C16
21	b	613	CL7	C11-C10-C8-C9
21	c	511	CL7	C14-C13-C15-C16
21	6	501	CL7	C6-C7-C8-C9
21	6	503	CL7	C14-C13-C15-C16
21	6	505	CL7	C11-C10-C8-C9
21	6	512	CL7	C11-C10-C8-C9
21	5	402	CL7	C6-C7-C8-C9
21	5	406	CL7	C14-C13-C15-C16
21	5	418	CL7	C14-C13-C15-C16
21	7	501	CL7	C14-C13-C15-C16
21	7	503	CL7	C6-C7-C8-C9
21	7	503	CL7	C11-C10-C8-C9
21	7	504	CL7	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	7	509	CL7	C11-C10-C8-C9
21	7	511	CL7	C14-C13-C15-C16
21	7	516	CL7	C4C-C3C-CAC-CBC
21	1	402	CL7	C5-C6-C7-C8
21	4	413	CL7	C10-C11-C12-C13
21	5	402	CL7	C5-C6-C7-C8
21	8	413	CL7	C10-C11-C12-C13
21	3	517	CL7	O1D-CGD-O2D-CED
21	7	517	CL7	O1D-CGD-O2D-CED
23	K	101	8CT	C10-C11-C12-C40
23	k	101	8CT	C10-C11-C12-C40
32	3	520	ZEX	C31-C32-C33-C40
32	4	420	ZEX	C11-C12-C13-C20
32	7	520	ZEX	C31-C32-C33-C40
32	8	420	ZEX	C11-C12-C13-C20
23	B	619	8CT	C25-C26-C28-C29
23	K	101	8CT	C10-C11-C12-C13
23	b	620	8CT	C25-C26-C28-C29
23	k	101	8CT	C10-C11-C12-C13
32	2	525	ZEX	C7-C8-C9-C10
32	6	524	ZEX	C7-C8-C9-C10
21	3	504	CL7	C4C-C3C-CAC-CBC
21	7	504	CL7	C4C-C3C-CAC-CBC
21	3	502	CL7	C4-C3-C5-C6
21	2	518	CL7	C15-C16-C17-C18
21	6	518	CL7	C15-C16-C17-C18
26	c	501	LMG	C12-C13-C14-C15
21	B	616	CL7	O1D-CGD-O2D-CED
21	b	617	CL7	O1D-CGD-O2D-CED
21	C	506	CL7	C3A-C2A-CAA-CBA
21	C	510	CL7	C3A-C2A-CAA-CBA
21	2	503	CL7	C3A-C2A-CAA-CBA
21	2	515	CL7	C3A-C2A-CAA-CBA
21	1	405	CL7	C3A-C2A-CAA-CBA
21	1	418	CL7	C3A-C2A-CAA-CBA
21	3	501	CL7	C3A-C2A-CAA-CBA
21	3	503	CL7	C3A-C2A-CAA-CBA
21	4	411	CL7	C3A-C2A-CAA-CBA
21	c	506	CL7	C3A-C2A-CAA-CBA
21	c	510	CL7	C3A-C2A-CAA-CBA
21	6	503	CL7	C3A-C2A-CAA-CBA
21	6	515	CL7	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	5	405	CL7	C3A-C2A-CAA-CBA
21	5	418	CL7	C3A-C2A-CAA-CBA
21	7	501	CL7	C3A-C2A-CAA-CBA
21	7	503	CL7	C3A-C2A-CAA-CBA
21	8	411	CL7	C3A-C2A-CAA-CBA
23	A	404	8CT	C23-C24-C25-C26
23	a	404	8CT	C23-C24-C25-C26
21	C	502	CL7	CBD-CGD-O2D-CED
21	3	505	CL7	C2C-C3C-CAC-CBC
21	7	505	CL7	C2C-C3C-CAC-CBC
21	C	505	CL7	C6-C7-C8-C10
21	c	505	CL7	C6-C7-C8-C10
27	B	624	DGD	C6B-C7B-C8B-C9B
27	b	625	DGD	C6B-C7B-C8B-C9B
21	B	612	CL7	C10-C11-C12-C13
21	b	613	CL7	C10-C11-C12-C13
21	c	502	CL7	CBD-CGD-O2D-CED
22	A	402	PHO	O2A-C1-C2-C3
22	a	402	PHO	O2A-C1-C2-C3
21	3	503	CL7	C10-C11-C12-C13
21	7	503	CL7	C8-C10-C11-C12
21	7	503	CL7	C10-C11-C12-C13
21	2	511	CL7	C3-C5-C6-C7
21	6	511	CL7	C3-C5-C6-C7
21	3	503	CL7	C8-C10-C11-C12
21	B	613	CL7	C4-C3-C5-C6
21	b	614	CL7	C4-C3-C5-C6
25	A	407	LHG	C3-O3-P-O6
25	a	406	LHG	C3-O3-P-O6
21	C	503	CL7	C10-C11-C12-C13
21	c	503	CL7	C10-C11-C12-C13
21	C	506	CL7	C4C-C3C-CAC-CBC
21	c	506	CL7	C4C-C3C-CAC-CBC
25	B	625	LHG	C1-C2-C3-O3
25	b	626	LHG	C1-C2-C3-O3
21	2	501	CL7	C2-C1-O2A-CGA
21	2	509	CL7	C2-C1-O2A-CGA
21	1	402	CL7	C2-C1-O2A-CGA
21	1	417	CL7	C2-C1-O2A-CGA
21	6	501	CL7	C2-C1-O2A-CGA
21	6	509	CL7	C2-C1-O2A-CGA
21	5	402	CL7	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
21	5	417	CL7	C2-C1-O2A-CGA
21	B	604	CL7	C13-C15-C16-C17
21	B	607	CL7	C11-C10-C8-C9
21	C	508	CL7	C6-C7-C8-C9
21	C	508	CL7	C14-C13-C15-C16
21	2	503	CL7	C11-C10-C8-C9
21	2	509	CL7	C14-C13-C15-C16
21	2	511	CL7	C11-C10-C8-C9
21	2	518	CL7	C14-C13-C15-C16
21	3	503	CL7	C14-C13-C15-C16
21	3	508	CL7	C6-C7-C8-C9
21	3	508	CL7	C14-C13-C15-C16
21	b	608	CL7	C11-C10-C8-C9
21	c	508	CL7	C6-C7-C8-C9
21	c	508	CL7	C14-C13-C15-C16
21	6	503	CL7	C11-C10-C8-C9
21	6	509	CL7	C14-C13-C15-C16
21	6	511	CL7	C11-C10-C8-C9
21	6	518	CL7	C14-C13-C15-C16
21	7	503	CL7	C14-C13-C15-C16
21	7	508	CL7	C6-C7-C8-C9
21	7	508	CL7	C14-C13-C15-C16
26	c	501	LMG	C38-C39-C40-C41
27	B	624	DGD	CBB-CCB-CDB-CEB
27	b	625	DGD	CBB-CCB-CDB-CEB
21	1	408	CL7	C13-C15-C16-C17
21	b	605	CL7	C13-C15-C16-C17
21	5	408	CL7	C13-C15-C16-C17
32	4	403	ZEX	C21-C26-C27-C28
32	8	403	ZEX	C21-C26-C27-C28
26	C	501	LMG	C38-C39-C40-C41
21	C	502	CL7	C16-C17-C18-C20
21	c	502	CL7	C16-C17-C18-C20
23	B	618	8CT	C02-C03-C10-C11
23	B	627	8CT	C04-C03-C10-C11
23	4	402	8CT	C02-C03-C10-C11
23	b	601	8CT	C04-C03-C10-C11
23	b	619	8CT	C02-C03-C10-C11
23	8	402	8CT	C02-C03-C10-C11
32	2	521	ZEX	C1-C6-C7-C8
32	3	520	ZEX	C1-C6-C7-C8
32	3	520	ZEX	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
32	4	418	ZEX	C1-C6-C7-C8
32	4	418	ZEX	C5-C6-C7-C8
32	4	420	ZEX	C1-C6-C7-C8
32	4	420	ZEX	C5-C6-C7-C8
32	6	520	ZEX	C1-C6-C7-C8
32	7	520	ZEX	C1-C6-C7-C8
32	7	520	ZEX	C5-C6-C7-C8
32	8	418	ZEX	C1-C6-C7-C8
32	8	418	ZEX	C5-C6-C7-C8
32	8	420	ZEX	C1-C6-C7-C8
32	8	420	ZEX	C5-C6-C7-C8
21	8	406	CL7	O1D-CGD-O2D-CED
23	B	619	8CT	C27-C26-C28-C29
23	b	620	8CT	C27-C26-C28-C29
21	4	406	CL7	O1D-CGD-O2D-CED
21	4	416	CL7	O1D-CGD-O2D-CED
21	8	416	CL7	O1D-CGD-O2D-CED
23	C	515	8CT	C20-C21-C23-C24
23	c	515	8CT	C20-C21-C23-C24
21	3	511	CL7	C5-C6-C7-C8
21	7	511	CL7	C5-C6-C7-C8
30	d	407	PL9	C17-C18-C19-C20
21	4	405	CL7	C16-C17-C18-C19
21	8	405	CL7	C16-C17-C18-C19
25	4	401	LHG	O6-C4-C5-C6
25	8	401	LHG	O6-C4-C5-C6
21	B	608	CL7	C11-C10-C8-C7
21	C	502	CL7	C12-C13-C15-C16
21	C	510	CL7	C12-C13-C15-C16
21	D	404	CL7	C11-C10-C8-C7
21	2	512	CL7	C11-C10-C8-C7
21	1	402	CL7	C6-C7-C8-C10
21	1	404	CL7	C11-C12-C13-C15
21	3	503	CL7	C6-C7-C8-C10
21	3	508	CL7	C12-C13-C15-C16
21	3	509	CL7	C11-C10-C8-C7
21	3	511	CL7	C11-C10-C8-C7
21	4	404	CL7	C11-C10-C8-C7
21	b	609	CL7	C11-C10-C8-C7
21	c	502	CL7	C12-C13-C15-C16
21	c	510	CL7	C12-C13-C15-C16
21	d	404	CL7	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
21	6	512	CL7	C11-C10-C8-C7
21	5	402	CL7	C6-C7-C8-C10
21	5	404	CL7	C11-C12-C13-C15
21	7	503	CL7	C6-C7-C8-C10
21	7	508	CL7	C12-C13-C15-C16
21	7	509	CL7	C11-C10-C8-C7
21	7	511	CL7	C11-C10-C8-C7
21	8	404	CL7	C11-C10-C8-C7
21	4	406	CL7	C5-C6-C7-C8
21	8	406	CL7	C5-C6-C7-C8
23	C	516	8CT	C16-C17-C18-C19
23	c	516	8CT	C16-C17-C18-C19
21	2	517	CL7	C16-C17-C18-C19
21	6	517	CL7	C16-C17-C18-C19
21	3	516	CL7	C5-C6-C7-C8
21	7	516	CL7	C5-C6-C7-C8
21	1	403	CL7	C2A-CAA-CBA-CGA
21	3	514	CL7	C2A-CAA-CBA-CGA
21	5	403	CL7	C2A-CAA-CBA-CGA
21	7	514	CL7	C2A-CAA-CBA-CGA
27	C	517	DGD	C2A-C1A-O1G-C1G
27	c	517	DGD	C2A-C1A-O1G-C1G
26	C	501	LMG	C39-C40-C41-C42
21	B	603	CL7	CAD-CBD-CGD-O2D
21	B	604	CL7	CAD-CBD-CGD-O2D
21	B	612	CL7	CAD-CBD-CGD-O2D
21	B	613	CL7	CAD-CBD-CGD-O2D
21	B	622	CL7	CAD-CBD-CGD-O2D
21	C	502	CL7	CAD-CBD-CGD-O2D
21	C	503	CL7	CAD-CBD-CGD-O2D
21	C	506	CL7	CAD-CBD-CGD-O2D
21	2	505	CL7	CAD-CBD-CGD-O2D
21	2	509	CL7	CAD-CBD-CGD-O2D
21	2	515	CL7	CAD-CBD-CGD-O2D
21	1	404	CL7	CAD-CBD-CGD-O2D
21	1	410	CL7	CAD-CBD-CGD-O2D
21	1	411	CL7	CAD-CBD-CGD-O2D
21	1	412	CL7	CAD-CBD-CGD-O2D
21	3	504	CL7	CAD-CBD-CGD-O2D
21	3	509	CL7	CAD-CBD-CGD-O2D
21	3	510	CL7	CAD-CBD-CGD-O2D
21	4	411	CL7	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	a	401	CL7	CAD-CBD-CGD-O2D
21	b	604	CL7	CAD-CBD-CGD-O2D
21	b	605	CL7	CAD-CBD-CGD-O2D
21	b	613	CL7	CAD-CBD-CGD-O2D
21	b	614	CL7	CAD-CBD-CGD-O2D
21	b	623	CL7	CAD-CBD-CGD-O2D
21	c	502	CL7	CAD-CBD-CGD-O2D
21	c	503	CL7	CAD-CBD-CGD-O2D
21	c	506	CL7	CAD-CBD-CGD-O2D
21	6	505	CL7	CAD-CBD-CGD-O2D
21	6	509	CL7	CAD-CBD-CGD-O2D
21	6	515	CL7	CAD-CBD-CGD-O2D
21	5	404	CL7	CAD-CBD-CGD-O2D
21	5	410	CL7	CAD-CBD-CGD-O2D
21	5	411	CL7	CAD-CBD-CGD-O2D
21	5	412	CL7	CAD-CBD-CGD-O2D
21	7	504	CL7	CAD-CBD-CGD-O2D
21	7	509	CL7	CAD-CBD-CGD-O2D
21	7	510	CL7	CAD-CBD-CGD-O2D
21	8	411	CL7	CAD-CBD-CGD-O2D
22	D	408	PHO	CAD-CBD-CGD-O2D
22	d	408	PHO	CAD-CBD-CGD-O2D
30	D	407	PL9	C17-C18-C19-C20
21	B	606	CL7	C5-C6-C7-C8
21	3	507	CL7	C15-C16-C17-C18
21	4	406	CL7	C8-C10-C11-C12
21	b	607	CL7	C5-C6-C7-C8
21	7	507	CL7	C15-C16-C17-C18
21	8	406	CL7	C8-C10-C11-C12
21	C	505	CL7	C6-C7-C8-C9
21	2	507	CL7	C16-C17-C18-C19
21	c	505	CL7	C6-C7-C8-C9
21	6	507	CL7	C16-C17-C18-C19
26	D	410	LMG	O6-C1-O1-C7
26	d	410	LMG	O6-C1-O1-C7
21	3	507	CL7	C10-C11-C12-C13
21	7	507	CL7	C10-C11-C12-C13
25	3	524	LHG	C2-C3-O3-P
25	7	524	LHG	C2-C3-O3-P
25	4	401	LHG	O6-C4-C5-O7
25	8	401	LHG	O6-C4-C5-O7
21	1	418	CL7	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	5	418	CL7	C8-C10-C11-C12
21	B	616	CL7	C2A-CAA-CBA-CGA
21	b	617	CL7	C2A-CAA-CBA-CGA
21	B	605	CL7	CHA-CBD-CGD-O1D
21	B	608	CL7	CHA-CBD-CGD-O1D
21	B	610	CL7	CHA-CBD-CGD-O1D
21	B	615	CL7	CHA-CBD-CGD-O2D
21	B	615	CL7	CHA-CBD-CGD-O1D
21	C	505	CL7	CHA-CBD-CGD-O1D
21	C	510	CL7	CHA-CBD-CGD-O2D
21	C	510	CL7	CHA-CBD-CGD-O1D
21	2	502	CL7	CHA-CBD-CGD-O1D
21	2	506	CL7	CHA-CBD-CGD-O2D
21	2	506	CL7	CHA-CBD-CGD-O1D
21	2	513	CL7	CHA-CBD-CGD-O2D
21	1	408	CL7	CHA-CBD-CGD-O2D
21	1	408	CL7	CHA-CBD-CGD-O1D
21	3	502	CL7	CHA-CBD-CGD-O1D
21	3	506	CL7	CHA-CBD-CGD-O2D
21	4	409	CL7	CHA-CBD-CGD-O2D
21	4	409	CL7	CHA-CBD-CGD-O1D
21	b	606	CL7	CHA-CBD-CGD-O1D
21	b	609	CL7	CHA-CBD-CGD-O1D
21	b	611	CL7	CHA-CBD-CGD-O1D
21	b	616	CL7	CHA-CBD-CGD-O2D
21	b	616	CL7	CHA-CBD-CGD-O1D
21	c	505	CL7	CHA-CBD-CGD-O1D
21	c	510	CL7	CHA-CBD-CGD-O2D
21	c	510	CL7	CHA-CBD-CGD-O1D
21	6	502	CL7	CHA-CBD-CGD-O1D
21	6	506	CL7	CHA-CBD-CGD-O2D
21	6	506	CL7	CHA-CBD-CGD-O1D
21	6	513	CL7	CHA-CBD-CGD-O2D
21	5	408	CL7	CHA-CBD-CGD-O2D
21	5	408	CL7	CHA-CBD-CGD-O1D
21	7	502	CL7	CHA-CBD-CGD-O1D
21	7	506	CL7	CHA-CBD-CGD-O2D
21	8	409	CL7	CHA-CBD-CGD-O2D
21	8	409	CL7	CHA-CBD-CGD-O1D
21	4	415	CL7	O1D-CGD-O2D-CED
21	8	415	CL7	O1D-CGD-O2D-CED
21	A	401	CL7	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	a	401	CL7	O1A-CGA-O2A-C1
26	c	501	LMG	C39-C40-C41-C42
21	4	404	CL7	C16-C17-C18-C20
21	8	404	CL7	C16-C17-C18-C20
21	7	512	CL7	O1D-CGD-O2D-CED
21	C	508	CL7	C11-C10-C8-C9
21	C	511	CL7	C6-C7-C8-C9
21	c	508	CL7	C11-C10-C8-C9
21	c	511	CL7	C6-C7-C8-C9
21	3	512	CL7	O1D-CGD-O2D-CED
21	B	601	CL7	C4C-C3C-CAC-CBC
21	b	602	CL7	C4C-C3C-CAC-CBC
21	2	505	CL7	C8-C10-C11-C12
21	6	505	CL7	C8-C10-C11-C12
21	C	506	CL7	C2A-CAA-CBA-CGA
21	c	506	CL7	C2A-CAA-CBA-CGA
23	A	404	8CT	C22-C21-C23-C24
23	B	617	8CT	C10-C11-C12-C40
23	a	404	8CT	C22-C21-C23-C24
23	b	618	8CT	C10-C11-C12-C40
32	2	525	ZEX	C7-C8-C9-C19
32	6	524	ZEX	C7-C8-C9-C19
23	B	617	8CT	C10-C11-C12-C13
23	b	618	8CT	C10-C11-C12-C13
21	1	404	CL7	C1A-C2A-CAA-CBA
21	c	509	CL7	C1A-C2A-CAA-CBA
21	5	404	CL7	C1A-C2A-CAA-CBA
21	2	512	CL7	C16-C17-C18-C20
21	6	512	CL7	C16-C17-C18-C20
21	b	612	CL7	C10-C11-C12-C13
21	B	614	CL7	C2-C1-O2A-CGA
21	4	409	CL7	C2-C1-O2A-CGA
21	b	615	CL7	C2-C1-O2A-CGA
21	8	409	CL7	C2-C1-O2A-CGA
21	B	611	CL7	C10-C11-C12-C13
21	2	512	CL7	C4-C3-C5-C6
21	6	512	CL7	C4-C3-C5-C6
21	1	402	CL7	C2-C3-C5-C6
21	5	402	CL7	C2-C3-C5-C6
25	D	409	LHG	C3-O3-P-O4
25	D	409	LHG	C4-O6-P-O4
25	3	524	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
25	4	401	LHG	C4-O6-P-O4
25	d	409	LHG	C3-O3-P-O4
25	d	409	LHG	C4-O6-P-O4
25	7	524	LHG	C3-O3-P-O5
25	8	401	LHG	C4-O6-P-O4
25	b	624	LHG	C10-C11-C12-C13
21	C	506	CL7	C8-C10-C11-C12
21	c	506	CL7	C8-C10-C11-C12
21	2	508	CL7	C2A-CAA-CBA-CGA
21	6	508	CL7	C2A-CAA-CBA-CGA
25	B	623	LHG	C10-C11-C12-C13
21	2	503	CL7	C16-C17-C18-C19
21	6	503	CL7	C16-C17-C18-C19
21	B	601	CL7	CAD-CBD-CGD-O1D
21	2	502	CL7	CAD-CBD-CGD-O1D
21	2	506	CL7	CAD-CBD-CGD-O1D
21	2	511	CL7	CAD-CBD-CGD-O1D
21	2	513	CL7	CAD-CBD-CGD-O1D
21	1	409	CL7	CAD-CBD-CGD-O1D
21	b	602	CL7	CAD-CBD-CGD-O1D
21	6	502	CL7	CAD-CBD-CGD-O1D
21	6	506	CL7	CAD-CBD-CGD-O1D
21	6	511	CL7	CAD-CBD-CGD-O1D
21	6	513	CL7	CAD-CBD-CGD-O1D
21	5	409	CL7	CAD-CBD-CGD-O1D
24	B	620	SQD	O5-C5-C6-S
24	b	621	SQD	O5-C5-C6-S
21	2	505	CL7	C4C-C3C-CAC-CBC
21	6	505	CL7	C4C-C3C-CAC-CBC
21	C	510	CL7	C16-C17-C18-C19
21	c	510	CL7	C16-C17-C18-C19
21	B	604	CL7	CBD-CGD-O2D-CED
21	3	516	CL7	C4-C3-C5-C6
21	7	516	CL7	C4-C3-C5-C6
21	B	605	CL7	C6-C7-C8-C10
21	B	611	CL7	C11-C10-C8-C7
21	B	611	CL7	C11-C12-C13-C15
21	C	502	CL7	C11-C10-C8-C7
21	C	511	CL7	C11-C12-C13-C15
21	2	506	CL7	C11-C12-C13-C15
21	2	508	CL7	C3A-C2A-CAA-CBA
21	1	412	CL7	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	3	501	CL7	C6-C7-C8-C10
21	3	501	CL7	C11-C12-C13-C15
21	3	509	CL7	C12-C13-C15-C16
21	3	510	CL7	C3A-C2A-CAA-CBA
21	3	513	CL7	C3A-C2A-CAA-CBA
21	4	404	CL7	C6-C7-C8-C10
21	4	409	CL7	C11-C10-C8-C7
21	b	606	CL7	C6-C7-C8-C10
21	b	612	CL7	C11-C10-C8-C7
21	b	612	CL7	C11-C12-C13-C15
21	c	502	CL7	C11-C10-C8-C7
21	c	511	CL7	C11-C12-C13-C15
21	6	506	CL7	C11-C12-C13-C15
21	6	508	CL7	C3A-C2A-CAA-CBA
21	5	412	CL7	C3A-C2A-CAA-CBA
21	7	501	CL7	C6-C7-C8-C10
21	7	501	CL7	C11-C12-C13-C15
21	7	509	CL7	C12-C13-C15-C16
21	7	510	CL7	C3A-C2A-CAA-CBA
21	7	513	CL7	C3A-C2A-CAA-CBA
21	8	404	CL7	C6-C7-C8-C10
21	8	409	CL7	C11-C10-C8-C7
23	B	627	8CT	C28-C29-C30-C31
23	C	515	8CT	C28-C29-C30-C31
23	4	402	8CT	C28-C29-C30-C31
23	b	601	8CT	C28-C29-C30-C31
23	c	515	8CT	C28-C29-C30-C31
23	8	402	8CT	C28-C29-C30-C31
23	B	617	8CT	C16-C17-C18-C19
23	b	618	8CT	C16-C17-C18-C19
32	4	419	ZEX	C33-C34-C35-C15
32	8	419	ZEX	C33-C34-C35-C15
21	b	605	CL7	CBD-CGD-O2D-CED
24	7	523	SQD	C9-C10-C11-C12
21	4	411	CL7	C5-C6-C7-C8
21	4	412	CL7	C5-C6-C7-C8
21	8	412	CL7	C5-C6-C7-C8
24	3	523	SQD	C9-C10-C11-C12
27	c	517	DGD	O1A-C1A-O1G-C1G
21	8	411	CL7	C5-C6-C7-C8
21	A	406	CL7	C16-C17-C18-C19
21	2	517	CL7	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
21	a	405	CL7	C16-C17-C18-C19
27	C	517	DGD	O1A-C1A-O1G-C1G
24	2	522	SQD	O47-C45-C46-O48
24	6	521	SQD	O47-C45-C46-O48
26	B	621	LMG	O7-C8-C9-O8
26	b	622	LMG	O7-C8-C9-O8
24	2	522	SQD	C45-C44-O6-C1
24	3	521	SQD	C45-C44-O6-C1
24	6	521	SQD	C45-C44-O6-C1
24	7	521	SQD	C45-C44-O6-C1
21	B	614	CL7	C11-C12-C13-C15
21	b	615	CL7	C11-C12-C13-C15
21	6	517	CL7	C16-C17-C18-C20
21	6	503	CL7	C13-C15-C16-C17
21	C	502	CL7	O1D-CGD-O2D-CED
21	c	502	CL7	O1D-CGD-O2D-CED
21	2	503	CL7	C13-C15-C16-C17
30	D	407	PL9	C35-C34-C36-C37
30	D	407	PL9	C45-C44-C46-C47
30	d	407	PL9	C35-C34-C36-C37
30	d	407	PL9	C45-C44-C46-C47
21	A	401	CL7	CBA-CGA-O2A-C1
21	a	401	CL7	CBA-CGA-O2A-C1
24	B	620	SQD	C17-C18-C19-C20
24	A	405	SQD	C9-C10-C11-C12
24	B	626	SQD	C9-C10-C11-C12
24	b	621	SQD	C17-C18-C19-C20
21	B	609	CL7	C6-C7-C8-C9
21	C	502	CL7	C11-C10-C8-C9
21	C	502	CL7	C14-C13-C15-C16
21	C	503	CL7	C6-C7-C8-C9
21	2	501	CL7	C11-C10-C8-C9
21	2	502	CL7	C11-C10-C8-C9
21	2	507	CL7	C11-C10-C8-C9
21	2	507	CL7	C11-C12-C13-C14
21	2	511	CL7	C6-C7-C8-C9
21	1	404	CL7	C11-C12-C13-C14
21	3	509	CL7	C11-C12-C13-C14
21	3	510	CL7	C6-C7-C8-C9
21	3	511	CL7	C6-C7-C8-C9
21	4	405	CL7	C11-C12-C13-C14
21	4	406	CL7	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
21	4	409	CL7	C11-C10-C8-C9
21	4	411	CL7	C11-C12-C13-C14
21	b	610	CL7	C6-C7-C8-C9
21	c	502	CL7	C11-C10-C8-C9
21	c	502	CL7	C14-C13-C15-C16
21	c	503	CL7	C6-C7-C8-C9
21	6	501	CL7	C11-C10-C8-C9
21	6	502	CL7	C11-C10-C8-C9
21	6	507	CL7	C11-C10-C8-C9
21	6	507	CL7	C11-C12-C13-C14
21	6	511	CL7	C6-C7-C8-C9
21	5	404	CL7	C11-C12-C13-C14
21	7	509	CL7	C11-C12-C13-C14
21	7	510	CL7	C6-C7-C8-C9
21	7	511	CL7	C6-C7-C8-C9
21	8	405	CL7	C11-C12-C13-C14
21	8	406	CL7	C6-C7-C8-C9
21	8	409	CL7	C11-C10-C8-C9
21	8	411	CL7	C11-C12-C13-C14
21	3	505	CL7	C16-C17-C18-C19
21	7	505	CL7	C16-C17-C18-C19
21	B	614	CL7	C2B-C3B-CAB-OBB
21	C	511	CL7	C2B-C3B-CAB-OBB
21	2	505	CL7	C2B-C3B-CAB-OBB
21	2	511	CL7	C2B-C3B-CAB-OBB
21	2	512	CL7	C2B-C3B-CAB-OBB
21	2	518	CL7	C2B-C3B-CAB-OBB
21	1	411	CL7	C2B-C3B-CAB-OBB
21	3	506	CL7	C2B-C3B-CAB-OBB
21	3	517	CL7	C2B-C3B-CAB-OBB
21	4	406	CL7	C2B-C3B-CAB-OBB
21	4	408	CL7	C2B-C3B-CAB-OBB
21	b	615	CL7	C2B-C3B-CAB-OBB
21	c	511	CL7	C2B-C3B-CAB-OBB
21	6	505	CL7	C2B-C3B-CAB-OBB
21	6	511	CL7	C2B-C3B-CAB-OBB
21	6	512	CL7	C2B-C3B-CAB-OBB
21	6	518	CL7	C2B-C3B-CAB-OBB
21	5	411	CL7	C2B-C3B-CAB-OBB
21	7	506	CL7	C2B-C3B-CAB-OBB
21	7	517	CL7	C2B-C3B-CAB-OBB
21	8	406	CL7	C2B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
21	8	408	CL7	C2B-C3B-CAB-OBB
32	3	520	ZEX	C31-C32-C33-C34
32	7	520	ZEX	C31-C32-C33-C34
21	3	510	CL7	CAA-CBA-CGA-O2A
21	7	510	CL7	CAA-CBA-CGA-O2A
21	B	608	CL7	C8-C10-C11-C12
21	4	405	CL7	C16-C17-C18-C20
27	C	517	DGD	CDB-CEB-CFB-CGB
27	c	517	DGD	CDB-CEB-CFB-CGB
21	B	611	CL7	C13-C15-C16-C17
21	b	609	CL7	C8-C10-C11-C12
21	b	612	CL7	C13-C15-C16-C17
21	B	605	CL7	C4B-C3B-CAB-OBB
21	C	504	CL7	C4B-C3B-CAB-OBB
21	C	513	CL7	C4B-C3B-CAB-OBB
21	1	402	CL7	C4B-C3B-CAB-OBB
21	b	606	CL7	C4B-C3B-CAB-OBB
21	c	504	CL7	C4B-C3B-CAB-OBB
21	c	513	CL7	C4B-C3B-CAB-OBB
21	5	402	CL7	C4B-C3B-CAB-OBB
21	2	516	CL7	C2A-CAA-CBA-CGA
21	6	516	CL7	C2A-CAA-CBA-CGA
21	B	602	CL7	C2-C1-O2A-CGA
21	2	516	CL7	C2-C1-O2A-CGA
21	1	410	CL7	C2-C1-O2A-CGA
21	3	517	CL7	C2-C1-O2A-CGA
21	4	405	CL7	C2-C1-O2A-CGA
21	b	603	CL7	C2-C1-O2A-CGA
21	6	516	CL7	C2-C1-O2A-CGA
21	5	410	CL7	C2-C1-O2A-CGA
21	7	517	CL7	C2-C1-O2A-CGA
21	8	405	CL7	C2-C1-O2A-CGA
25	b	624	LHG	C28-C29-C30-C31
26	1	401	LMG	C37-C38-C39-C40
26	5	401	LMG	C37-C38-C39-C40
21	8	405	CL7	C16-C17-C18-C20
25	B	623	LHG	C28-C29-C30-C31
32	2	520	ZEX	C21-C26-C27-C28
32	3	525	ZEX	C21-C26-C27-C28
25	B	625	LHG	C11-C12-C13-C14
21	1	418	CL7	C4-C3-C5-C6
21	5	418	CL7	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	2	507	CL7	C2-C3-C5-C6
21	6	507	CL7	C2-C3-C5-C6
24	B	620	SQD	C14-C15-C16-C17
25	b	626	LHG	C11-C12-C13-C14
24	b	621	SQD	C14-C15-C16-C17
21	2	518	CL7	C2A-CAA-CBA-CGA
21	6	518	CL7	C2A-CAA-CBA-CGA
24	3	523	SQD	O47-C45-C46-O48
24	7	523	SQD	O47-C45-C46-O48
22	D	408	PHO	CHA-CBD-CGD-O1D
22	d	408	PHO	CHA-CBD-CGD-O1D
21	C	508	CL7	C12-C13-C15-C16
21	2	501	CL7	C11-C10-C8-C7
21	2	502	CL7	C6-C7-C8-C10
21	2	502	CL7	C11-C10-C8-C7
21	2	516	CL7	C12-C13-C15-C16
21	3	502	CL7	C2-C3-C5-C6
21	3	507	CL7	C11-C10-C8-C7
21	3	507	CL7	C12-C13-C15-C16
21	c	508	CL7	C12-C13-C15-C16
21	6	501	CL7	C11-C10-C8-C7
21	6	502	CL7	C6-C7-C8-C10
21	6	502	CL7	C11-C10-C8-C7
21	6	516	CL7	C12-C13-C15-C16
21	7	502	CL7	C2-C3-C5-C6
21	7	507	CL7	C11-C10-C8-C7
21	7	507	CL7	C12-C13-C15-C16
21	B	605	CL7	C6-C7-C8-C9
21	2	502	CL7	C6-C7-C8-C9
21	2	506	CL7	C11-C12-C13-C14
21	2	512	CL7	C11-C12-C13-C14
21	3	501	CL7	C6-C7-C8-C9
21	4	404	CL7	C6-C7-C8-C9
21	b	606	CL7	C6-C7-C8-C9
21	6	502	CL7	C6-C7-C8-C9
21	6	506	CL7	C11-C12-C13-C14
21	6	512	CL7	C11-C12-C13-C14
21	7	501	CL7	C6-C7-C8-C9
21	8	404	CL7	C6-C7-C8-C9
21	B	611	CL7	C15-C16-C17-C18
21	b	612	CL7	C15-C16-C17-C18
32	1	421	ZEX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
32	5	421	ZEX	C9-C10-C11-C12
21	B	603	CL7	C16-C17-C18-C20
21	b	604	CL7	C16-C17-C18-C20
27	B	624	DGD	CCA-CDA-CEA-CFA
21	3	505	CL7	C2A-CAA-CBA-CGA
21	7	505	CL7	C2A-CAA-CBA-CGA
26	B	621	LMG	C36-C37-C38-C39
27	b	625	DGD	CCA-CDA-CEA-CFA
26	b	622	LMG	C36-C37-C38-C39
21	3	503	CL7	C13-C15-C16-C17
21	7	503	CL7	C13-C15-C16-C17
21	4	404	CL7	C16-C17-C18-C19
21	8	404	CL7	C16-C17-C18-C19
27	B	624	DGD	C8B-C9B-CAB-CBB
27	b	625	DGD	C8B-C9B-CAB-CBB
21	C	504	CL7	CAA-CBA-CGA-O2A
21	1	418	CL7	CAA-CBA-CGA-O2A
21	c	504	CL7	CAA-CBA-CGA-O2A
21	5	418	CL7	CAA-CBA-CGA-O2A
21	3	509	CL7	C15-C16-C17-C18
21	7	509	CL7	C15-C16-C17-C18
21	1	402	CL7	CBD-CGD-O2D-CED
21	5	402	CL7	CBD-CGD-O2D-CED
21	4	411	CL7	C16-C17-C18-C20
21	8	411	CL7	C16-C17-C18-C20
32	1	421	ZEX	C33-C34-C35-C15
32	4	419	ZEX	C9-C10-C11-C12
32	4	420	ZEX	C9-C10-C11-C12
32	5	421	ZEX	C33-C34-C35-C15
32	8	419	ZEX	C9-C10-C11-C12
32	8	420	ZEX	C9-C10-C11-C12
30	D	407	PL9	C16-C17-C18-C19
30	d	407	PL9	C16-C17-C18-C19
21	4	408	CL7	CAA-CBA-CGA-O2A
21	8	408	CL7	CAA-CBA-CGA-O2A
21	C	503	CL7	C2-C1-O2A-CGA
21	1	403	CL7	C2-C1-O2A-CGA
21	4	412	CL7	C2-C1-O2A-CGA
21	c	503	CL7	C2-C1-O2A-CGA
21	5	403	CL7	C2-C1-O2A-CGA
21	8	412	CL7	C2-C1-O2A-CGA
21	D	405	CL7	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
21	d	405	CL7	C4C-C3C-CAC-CBC
21	B	614	CL7	C11-C12-C13-C14
21	2	507	CL7	C16-C17-C18-C20
21	b	615	CL7	C11-C12-C13-C14
21	6	507	CL7	C16-C17-C18-C20
21	3	513	CL7	C2A-CAA-CBA-CGA
21	7	513	CL7	C2A-CAA-CBA-CGA
21	b	605	CL7	O1D-CGD-O2D-CED
21	3	505	CL7	C3A-C2A-CAA-CBA
21	7	505	CL7	C3A-C2A-CAA-CBA
21	B	604	CL7	O1D-CGD-O2D-CED
21	B	606	CL7	C6-C7-C8-C9
21	1	418	CL7	C16-C17-C18-C19
21	5	418	CL7	C16-C17-C18-C19
32	4	403	ZEX	C33-C34-C35-C15
32	8	403	ZEX	C33-C34-C35-C15
21	3	506	CL7	C2C-C3C-CAC-CBC
21	A	401	CL7	C11-C10-C8-C9
21	B	611	CL7	C14-C13-C15-C16
21	2	506	CL7	C11-C10-C8-C9
21	1	406	CL7	C11-C12-C13-C14
21	3	502	CL7	C11-C10-C8-C9
21	4	406	CL7	C14-C13-C15-C16
21	4	413	CL7	C11-C10-C8-C9
21	a	401	CL7	C11-C10-C8-C9
21	b	612	CL7	C14-C13-C15-C16
21	6	506	CL7	C11-C10-C8-C9
21	5	406	CL7	C11-C12-C13-C14
21	7	502	CL7	C11-C10-C8-C9
21	8	406	CL7	C14-C13-C15-C16
21	8	413	CL7	C11-C10-C8-C9
21	1	417	CL7	C6-C7-C8-C9
21	1	418	CL7	C16-C17-C18-C20
21	b	607	CL7	C6-C7-C8-C9
21	5	417	CL7	C6-C7-C8-C9
21	5	418	CL7	C16-C17-C18-C20
21	7	506	CL7	C2C-C3C-CAC-CBC
21	3	506	CL7	CAA-CBA-CGA-O1A
21	7	506	CL7	CAA-CBA-CGA-O1A
21	2	505	CL7	C13-C15-C16-C17
21	6	505	CL7	C13-C15-C16-C17
23	B	627	8CT	C39-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	b	601	8CT	C39-C16-C17-C18
31	F	101	HEM	CAA-CBA-CGA-O1A
31	f	101	HEM	CAA-CBA-CGA-O1A
21	C	509	CL7	C16-C17-C18-C20
21	c	509	CL7	C16-C17-C18-C20
21	A	406	CL7	O2A-C1-C2-C3
21	C	511	CL7	O2A-C1-C2-C3
21	2	509	CL7	O2A-C1-C2-C3
21	a	405	CL7	O2A-C1-C2-C3
21	c	511	CL7	O2A-C1-C2-C3
21	6	509	CL7	O2A-C1-C2-C3
21	B	615	CL7	C2C-C3C-CAC-CBC
21	b	616	CL7	C2C-C3C-CAC-CBC
31	F	101	HEM	CAD-CBD-CGD-O1D
31	f	101	HEM	CAD-CBD-CGD-O1D
24	B	620	SQD	C46-C45-O47-C7
24	b	621	SQD	C46-C45-O47-C7
21	2	506	CL7	C1A-C2A-CAA-CBA
21	2	515	CL7	C1A-C2A-CAA-CBA
21	4	405	CL7	C1A-C2A-CAA-CBA
21	6	506	CL7	C1A-C2A-CAA-CBA
21	6	515	CL7	C1A-C2A-CAA-CBA
21	8	405	CL7	C1A-C2A-CAA-CBA
21	c	509	CL7	C16-C17-C18-C19
21	A	406	CL7	C11-C10-C8-C7
21	B	612	CL7	C11-C12-C13-C15
21	2	501	CL7	C11-C12-C13-C15
21	3	503	CL7	C11-C12-C13-C15
21	3	511	CL7	C11-C12-C13-C15
21	4	404	CL7	C12-C13-C15-C16
21	4	412	CL7	C12-C13-C15-C16
21	a	405	CL7	C11-C10-C8-C7
21	b	613	CL7	C11-C12-C13-C15
21	6	501	CL7	C11-C12-C13-C15
21	7	503	CL7	C11-C12-C13-C15
21	7	511	CL7	C11-C12-C13-C15
21	8	404	CL7	C12-C13-C15-C16
21	8	412	CL7	C12-C13-C15-C16
21	2	514	CL7	CAA-CBA-CGA-O2A
21	6	514	CL7	CAA-CBA-CGA-O2A
21	2	514	CL7	CAA-CBA-CGA-O1A
21	6	514	CL7	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
21	B	612	CL7	C5-C6-C7-C8
21	b	613	CL7	C5-C6-C7-C8
21	C	509	CL7	C16-C17-C18-C19
21	A	401	CL7	C2A-CAA-CBA-CGA
21	2	501	CL7	C2A-CAA-CBA-CGA
21	1	402	CL7	C2A-CAA-CBA-CGA
21	4	405	CL7	C2A-CAA-CBA-CGA
21	a	401	CL7	C2A-CAA-CBA-CGA
21	6	501	CL7	C2A-CAA-CBA-CGA
21	5	402	CL7	C2A-CAA-CBA-CGA
21	8	405	CL7	C2A-CAA-CBA-CGA
26	c	501	LMG	C33-C34-C35-C36
26	C	501	LMG	C33-C34-C35-C36
26	c	501	LMG	C11-C12-C13-C14
21	3	506	CL7	CAA-CBA-CGA-O2A
21	7	506	CL7	CAA-CBA-CGA-O2A
21	C	508	CL7	C8-C10-C11-C12
21	c	508	CL7	C8-C10-C11-C12
21	2	518	CL7	C3-C5-C6-C7
21	6	518	CL7	C3-C5-C6-C7
23	B	627	8CT	C15-C16-C17-C18
23	b	601	8CT	C15-C16-C17-C18
25	4	401	LHG	O7-C5-C6-O8
25	8	401	LHG	O7-C5-C6-O8
26	1	401	LMG	O7-C8-C9-O8
26	5	401	LMG	O7-C8-C9-O8
21	C	508	CL7	C13-C15-C16-C17
21	1	402	CL7	O1D-CGD-O2D-CED
21	4	410	CL7	CAA-CBA-CGA-O1A
21	8	410	CL7	CAA-CBA-CGA-O1A
31	F	101	HEM	CAA-CBA-CGA-O2A
21	c	508	CL7	C13-C15-C16-C17
21	5	402	CL7	O1D-CGD-O2D-CED
21	3	504	CL7	C16-C17-C18-C19
31	f	101	HEM	CAA-CBA-CGA-O2A
21	4	411	CL7	C4-C3-C5-C6
21	8	411	CL7	C4-C3-C5-C6
21	C	509	CL7	C2-C1-O2A-CGA
21	3	508	CL7	C2-C1-O2A-CGA
21	3	511	CL7	C2-C1-O2A-CGA
21	c	509	CL7	C2-C1-O2A-CGA
21	7	508	CL7	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
21	7	511	CL7	C2-C1-O2A-CGA
21	7	504	CL7	C16-C17-C18-C19
21	C	502	CL7	C11-C12-C13-C14
21	1	418	CL7	C11-C10-C8-C9
21	c	502	CL7	C11-C12-C13-C14
21	5	418	CL7	C11-C10-C8-C9
21	2	517	CL7	C13-C15-C16-C17
21	6	517	CL7	C13-C15-C16-C17
32	3	520	ZEX	C21-C26-C27-C28
32	7	520	ZEX	C21-C26-C27-C28
21	C	508	CL7	C15-C16-C17-C18
21	c	508	CL7	C15-C16-C17-C18
21	4	410	CL7	CAA-CBA-CGA-O2A
21	8	410	CL7	CAA-CBA-CGA-O2A
23	D	406	8CT	C04-C03-C10-C11
23	d	406	8CT	C04-C03-C10-C11
21	C	510	CL7	CAA-CBA-CGA-O2A
21	c	510	CL7	CAA-CBA-CGA-O2A
21	4	408	CL7	CAA-CBA-CGA-O1A
21	8	408	CL7	CAA-CBA-CGA-O1A
32	1	421	ZEX	C29-C30-C31-C32
32	4	418	ZEX	C29-C30-C31-C32
32	5	421	ZEX	C29-C30-C31-C32
32	8	418	ZEX	C29-C30-C31-C32
21	B	604	CL7	C4-C3-C5-C6
21	b	605	CL7	C4-C3-C5-C6
32	4	420	ZEX	C11-C12-C13-C14
32	8	420	ZEX	C11-C12-C13-C14
21	A	403	CL7	C6-C7-C8-C9
21	a	403	CL7	C6-C7-C8-C9
30	D	407	PL9	C33-C34-C36-C37
30	D	407	PL9	C43-C44-C46-C47
30	d	407	PL9	C33-C34-C36-C37
30	d	407	PL9	C43-C44-C46-C47
21	1	410	CL7	C3-C5-C6-C7
21	5	410	CL7	C3-C5-C6-C7
21	3	513	CL7	CAA-CBA-CGA-O2A
21	7	513	CL7	CAA-CBA-CGA-O2A
25	a	406	LHG	C9-C10-C11-C12
21	4	406	CL7	C16-C17-C18-C20
21	8	406	CL7	C16-C17-C18-C20
25	A	407	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	3	518	CL7	CAA-CBA-CGA-O2A
21	7	518	CL7	CAA-CBA-CGA-O2A
21	4	405	CL7	C8-C10-C11-C12
21	8	405	CL7	C8-C10-C11-C12
25	D	409	LHG	O6-C4-C5-C6
25	d	409	LHG	O6-C4-C5-C6
27	B	624	DGD	O2G-C1B-C2B-C3B
27	b	625	DGD	O2G-C1B-C2B-C3B
21	2	506	CL7	C4-C3-C5-C6
21	4	414	CL7	C4-C3-C5-C6
21	6	506	CL7	C4-C3-C5-C6
21	8	414	CL7	C4-C3-C5-C6
21	B	609	CL7	C12-C13-C15-C16
21	2	505	CL7	C6-C7-C8-C10
21	3	516	CL7	C2-C3-C5-C6
21	4	411	CL7	C2-C3-C5-C6
21	b	610	CL7	C12-C13-C15-C16
21	6	505	CL7	C6-C7-C8-C10
21	7	516	CL7	C2-C3-C5-C6
21	8	411	CL7	C2-C3-C5-C6
23	D	406	8CT	C18-C19-C20-C21
23	d	406	8CT	C18-C19-C20-C21
21	A	401	CL7	CAA-CBA-CGA-O2A
21	a	401	CL7	CAA-CBA-CGA-O2A
21	B	605	CL7	C2B-C3B-CAB-OBB
21	b	606	CL7	C2B-C3B-CAB-OBB
21	D	404	CL7	C2A-CAA-CBA-CGA
21	1	412	CL7	C2A-CAA-CBA-CGA
21	d	404	CL7	C2A-CAA-CBA-CGA
21	5	412	CL7	C2A-CAA-CBA-CGA
21	B	622	CL7	CAA-CBA-CGA-O2A
21	b	623	CL7	CAA-CBA-CGA-O2A
21	7	513	CL7	C2C-C3C-CAC-CBC
21	B	605	CL7	C4-C3-C5-C6
21	C	507	CL7	C4-C3-C5-C6
21	C	511	CL7	C4-C3-C5-C6
21	2	502	CL7	C4-C3-C5-C6
21	b	606	CL7	C4-C3-C5-C6
21	c	507	CL7	C4-C3-C5-C6
21	c	511	CL7	C4-C3-C5-C6
21	6	502	CL7	C4-C3-C5-C6
30	D	407	PL9	C20-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
30	d	407	PL9	C20-C19-C21-C22
21	3	513	CL7	C2C-C3C-CAC-CBC
21	4	415	CL7	CAA-CBA-CGA-O2A
21	5	412	CL7	CAA-CBA-CGA-O2A
21	8	415	CL7	CAA-CBA-CGA-O2A
21	B	613	CL7	C2-C3-C5-C6
21	2	512	CL7	C2-C3-C5-C6
21	b	614	CL7	C2-C3-C5-C6
21	6	512	CL7	C2-C3-C5-C6
21	B	605	CL7	C11-C12-C13-C14
21	C	504	CL7	C11-C12-C13-C14
21	2	507	CL7	C14-C13-C15-C16
21	4	412	CL7	C11-C10-C8-C9
21	4	412	CL7	C14-C13-C15-C16
21	b	606	CL7	C11-C12-C13-C14
21	c	504	CL7	C11-C12-C13-C14
21	6	507	CL7	C14-C13-C15-C16
21	8	412	CL7	C11-C10-C8-C9
21	8	412	CL7	C14-C13-C15-C16
21	1	412	CL7	CAA-CBA-CGA-O2A
21	2	504	CL7	C3A-C2A-CAA-CBA
21	1	419	CL7	C3A-C2A-CAA-CBA
21	6	504	CL7	C3A-C2A-CAA-CBA
21	5	419	CL7	C3A-C2A-CAA-CBA
21	1	411	CL7	CAA-CBA-CGA-O2A
21	5	411	CL7	CAA-CBA-CGA-O2A
21	A	401	CL7	CAD-CBD-CGD-O2D
21	B	609	CL7	CAD-CBD-CGD-O2D
21	C	504	CL7	CAD-CBD-CGD-O2D
21	C	509	CL7	CAD-CBD-CGD-O2D
21	C	518	CL7	CAD-CBD-CGD-O2D
21	D	404	CL7	CAD-CBD-CGD-O2D
21	2	508	CL7	CAD-CBD-CGD-O2D
21	1	420	CL7	CAD-CBD-CGD-O2D
21	3	501	CL7	CAD-CBD-CGD-O2D
21	3	503	CL7	CAD-CBD-CGD-O2D
21	3	507	CL7	CAD-CBD-CGD-O2D
21	3	508	CL7	CAD-CBD-CGD-O2D
21	3	511	CL7	CAD-CBD-CGD-O2D
21	3	512	CL7	CAD-CBD-CGD-O2D
21	3	513	CL7	CAD-CBD-CGD-O2D
21	b	610	CL7	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	c	504	CL7	CAD-CBD-CGD-O2D
21	c	509	CL7	CAD-CBD-CGD-O2D
21	c	518	CL7	CAD-CBD-CGD-O2D
21	d	404	CL7	CAD-CBD-CGD-O2D
21	6	508	CL7	CAD-CBD-CGD-O2D
21	5	420	CL7	CAD-CBD-CGD-O2D
21	7	501	CL7	CAD-CBD-CGD-O2D
21	7	503	CL7	CAD-CBD-CGD-O2D
21	7	507	CL7	CAD-CBD-CGD-O2D
21	7	508	CL7	CAD-CBD-CGD-O2D
21	7	511	CL7	CAD-CBD-CGD-O2D
21	7	512	CL7	CAD-CBD-CGD-O2D
21	7	513	CL7	CAD-CBD-CGD-O2D
26	C	501	LMG	C19-C20-C21-C22
21	1	419	CL7	CAA-CBA-CGA-O2A
21	5	419	CL7	CAA-CBA-CGA-O2A
31	F	101	HEM	CAD-CBD-CGD-O2D
31	f	101	HEM	CAD-CBD-CGD-O2D
26	C	501	LMG	C29-C30-C31-C32
21	4	406	CL7	CAA-CBA-CGA-O2A
21	8	406	CL7	CAA-CBA-CGA-O2A
21	C	504	CL7	C8-C10-C11-C12
21	c	504	CL7	C8-C10-C11-C12
21	2	516	CL7	C16-C17-C18-C19
21	6	516	CL7	C16-C17-C18-C19
21	1	405	CL7	CAA-CBA-CGA-O2A
21	3	513	CL7	CAA-CBA-CGA-O1A
21	5	405	CL7	CAA-CBA-CGA-O1A
21	5	405	CL7	CAA-CBA-CGA-O2A
21	7	513	CL7	CAA-CBA-CGA-O1A
21	2	501	CL7	CAA-CBA-CGA-O2A
21	6	501	CL7	CAA-CBA-CGA-O2A
23	A	404	8CT	C20-C21-C23-C24
23	a	404	8CT	C20-C21-C23-C24
24	2	522	SQD	C44-C45-C46-O48
24	6	521	SQD	C44-C45-C46-O48
21	1	405	CL7	CAA-CBA-CGA-O1A
26	c	501	LMG	C29-C30-C31-C32
21	6	503	CL7	C5-C6-C7-C8
21	B	609	CL7	CAA-CBA-CGA-O2A
21	3	518	CL7	CAA-CBA-CGA-O1A
21	B	610	CL7	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
21	C	506	CL7	O2A-C1-C2-C3
21	4	413	CL7	O2A-C1-C2-C3
21	b	611	CL7	O2A-C1-C2-C3
21	c	506	CL7	O2A-C1-C2-C3
21	8	413	CL7	O2A-C1-C2-C3
25	D	409	LHG	C31-C32-C33-C34
25	d	409	LHG	C31-C32-C33-C34
21	b	610	CL7	CAA-CBA-CGA-O2A
21	1	411	CL7	CAA-CBA-CGA-O1A
21	1	412	CL7	CAA-CBA-CGA-O1A
21	5	411	CL7	CAA-CBA-CGA-O1A
21	5	412	CL7	CAA-CBA-CGA-O1A
21	7	518	CL7	CAA-CBA-CGA-O1A
25	B	623	LHG	C25-C26-C27-C28
25	b	624	LHG	C25-C26-C27-C28
21	7	501	CL7	C5-C6-C7-C8
26	C	501	LMG	C11-C12-C13-C14
21	A	406	CL7	CHA-CBD-CGD-O2D
21	B	605	CL7	CHA-CBD-CGD-O2D
21	B	608	CL7	CHA-CBD-CGD-O2D
21	B	610	CL7	CHA-CBD-CGD-O2D
21	B	616	CL7	CHA-CBD-CGD-O2D
21	C	505	CL7	CHA-CBD-CGD-O2D
21	C	511	CL7	CHA-CBD-CGD-O1D
21	2	502	CL7	CHA-CBD-CGD-O2D
21	2	507	CL7	CHA-CBD-CGD-O2D
21	2	517	CL7	CHA-CBD-CGD-O2D
21	2	517	CL7	CHA-CBD-CGD-O1D
21	1	405	CL7	CHA-CBD-CGD-O2D
21	1	405	CL7	CHA-CBD-CGD-O1D
21	3	502	CL7	CHA-CBD-CGD-O2D
21	3	505	CL7	CHA-CBD-CGD-O2D
21	3	505	CL7	CHA-CBD-CGD-O1D
21	3	512	CL7	CHA-CBD-CGD-O1D
21	3	516	CL7	CHA-CBD-CGD-O2D
21	3	516	CL7	CHA-CBD-CGD-O1D
21	a	405	CL7	CHA-CBD-CGD-O2D
21	b	606	CL7	CHA-CBD-CGD-O2D
21	b	609	CL7	CHA-CBD-CGD-O2D
21	b	611	CL7	CHA-CBD-CGD-O2D
21	b	617	CL7	CHA-CBD-CGD-O2D
21	c	505	CL7	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	c	511	CL7	CHA-CBD-CGD-O1D
21	6	502	CL7	CHA-CBD-CGD-O2D
21	6	507	CL7	CHA-CBD-CGD-O2D
21	6	517	CL7	CHA-CBD-CGD-O2D
21	6	517	CL7	CHA-CBD-CGD-O1D
21	5	405	CL7	CHA-CBD-CGD-O2D
21	5	405	CL7	CHA-CBD-CGD-O1D
21	7	502	CL7	CHA-CBD-CGD-O2D
21	7	505	CL7	CHA-CBD-CGD-O2D
21	7	505	CL7	CHA-CBD-CGD-O1D
21	7	512	CL7	CHA-CBD-CGD-O1D
21	7	516	CL7	CHA-CBD-CGD-O2D
21	7	516	CL7	CHA-CBD-CGD-O1D
21	1	419	CL7	CAA-CBA-CGA-O1A
21	5	419	CL7	CAA-CBA-CGA-O1A
30	D	407	PL9	C17-C18-C19-C21
30	d	407	PL9	C17-C18-C19-C21
21	2	503	CL7	C5-C6-C7-C8
21	3	501	CL7	C5-C6-C7-C8
21	2	510	CL7	CAA-CBA-CGA-O2A
21	2	512	CL7	CAA-CBA-CGA-O2A
21	6	510	CL7	CAA-CBA-CGA-O2A
21	6	512	CL7	CAA-CBA-CGA-O2A
21	8	412	CL7	CAA-CBA-CGA-O2A
26	c	501	LMG	C28-C29-C30-C31
21	1	406	CL7	O1D-CGD-O2D-CED
21	5	406	CL7	O1D-CGD-O2D-CED
21	4	413	CL7	C8-C10-C11-C12
21	c	509	CL7	C8-C10-C11-C12
21	8	413	CL7	C8-C10-C11-C12
21	d	404	CL7	C3-C5-C6-C7
21	C	509	CL7	C8-C10-C11-C12
21	3	501	CL7	CAA-CBA-CGA-O2A
21	7	501	CL7	CAA-CBA-CGA-O2A
21	2	511	CL7	C11-C12-C13-C14
21	6	511	CL7	C11-C12-C13-C14
21	D	404	CL7	C3-C5-C6-C7
26	D	410	LMG	C11-C10-O7-C8
26	d	410	LMG	C11-C10-O7-C8
21	4	409	CL7	CAA-CBA-CGA-O2A
21	4	412	CL7	CAA-CBA-CGA-O2A
21	8	409	CL7	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	1	418	CL7	C6-C7-C8-C10
21	5	418	CL7	C6-C7-C8-C10
26	D	410	LMG	O7-C10-C11-C12
26	d	410	LMG	O7-C10-C11-C12
21	B	604	CL7	C14-C13-C15-C16
21	B	612	CL7	C14-C13-C15-C16
21	2	517	CL7	C14-C13-C15-C16
21	1	408	CL7	C11-C12-C13-C14
21	3	503	CL7	C11-C12-C13-C14
21	3	511	CL7	C11-C12-C13-C14
21	b	605	CL7	C14-C13-C15-C16
21	b	613	CL7	C14-C13-C15-C16
21	6	517	CL7	C14-C13-C15-C16
21	5	408	CL7	C11-C12-C13-C14
21	7	503	CL7	C11-C12-C13-C14
21	7	511	CL7	C11-C12-C13-C14
23	4	402	8CT	C23-C24-C25-C26
23	8	402	8CT	C23-C24-C25-C26
25	4	401	LHG	C15-C16-C17-C18
25	8	401	LHG	C15-C16-C17-C18
21	B	622	CL7	CAA-CBA-CGA-O1A
21	b	623	CL7	CAA-CBA-CGA-O1A
24	A	405	SQD	C4-C5-C6-S
24	B	626	SQD	C4-C5-C6-S
24	1	423	SQD	C4-C5-C6-S
24	5	423	SQD	C4-C5-C6-S
21	3	505	CL7	C16-C17-C18-C20
21	7	505	CL7	C16-C17-C18-C20
21	4	415	CL7	CAA-CBA-CGA-O1A
21	8	415	CL7	CAA-CBA-CGA-O1A
21	a	401	CL7	CAA-CBA-CGA-O1A
21	3	517	CL7	CAA-CBA-CGA-O2A
21	7	517	CL7	CAA-CBA-CGA-O2A
21	A	401	CL7	CAA-CBA-CGA-O1A
21	b	610	CL7	CAA-CBA-CGA-O1A
21	1	408	CL7	C10-C11-C12-C13
21	5	408	CL7	C10-C11-C12-C13
21	2	512	CL7	C16-C17-C18-C19
21	6	512	CL7	C16-C17-C18-C19
21	1	406	CL7	CBD-CGD-O2D-CED
21	5	406	CL7	CBD-CGD-O2D-CED
26	c	501	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
21	2	501	CL7	CAA-CBA-CGA-O1A
21	6	501	CL7	CAA-CBA-CGA-O1A
21	4	413	CL7	C5-C6-C7-C8
21	8	413	CL7	C5-C6-C7-C8
21	1	405	CL7	C1A-C2A-CAA-CBA
21	3	505	CL7	C1A-C2A-CAA-CBA
21	3	512	CL7	C1A-C2A-CAA-CBA
21	5	405	CL7	C1A-C2A-CAA-CBA
21	7	505	CL7	C1A-C2A-CAA-CBA
21	7	512	CL7	C1A-C2A-CAA-CBA
21	B	609	CL7	CAA-CBA-CGA-O1A
25	b	626	LHG	C14-C15-C16-C17
21	3	511	CL7	C15-C16-C17-C18
21	7	511	CL7	C15-C16-C17-C18
25	B	625	LHG	C14-C15-C16-C17
25	b	626	LHG	C17-C18-C19-C20
21	2	503	CL7	C2A-CAA-CBA-CGA
21	6	503	CL7	C2A-CAA-CBA-CGA
21	B	607	CL7	C11-C12-C13-C14
21	C	508	CL7	C16-C17-C18-C20
21	2	501	CL7	C16-C17-C18-C19
21	b	608	CL7	C11-C12-C13-C14
21	c	508	CL7	C16-C17-C18-C20
21	6	501	CL7	C16-C17-C18-C19
21	6	502	CL7	C10-C11-C12-C13
25	B	625	LHG	C17-C18-C19-C20
21	2	507	CL7	CAA-CBA-CGA-O2A
21	6	507	CL7	CAA-CBA-CGA-O2A
21	2	502	CL7	C10-C11-C12-C13
32	4	419	ZEX	C21-C26-C27-C28
32	8	419	ZEX	C21-C26-C27-C28
21	1	418	CL7	C2-C3-C5-C6
21	5	418	CL7	C2-C3-C5-C6
25	4	401	LHG	C3-O3-P-O5
25	8	401	LHG	C3-O3-P-O5
21	B	604	CL7	C16-C17-C18-C20
21	2	503	CL7	C16-C17-C18-C20
21	3	509	CL7	C16-C17-C18-C20
21	b	605	CL7	C16-C17-C18-C20
21	6	503	CL7	C16-C17-C18-C20
21	7	509	CL7	C16-C17-C18-C20
21	3	517	CL7	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
21	7	517	CL7	CAA-CBA-CGA-O1A
21	C	511	CL7	CAA-CBA-CGA-O2A
21	c	511	CL7	CAA-CBA-CGA-O2A
21	d	404	CL7	C10-C11-C12-C13
21	2	507	CL7	C13-C15-C16-C17
21	2	516	CL7	C13-C15-C16-C17
21	6	507	CL7	C13-C15-C16-C17
21	6	516	CL7	C13-C15-C16-C17
21	2	512	CL7	CAA-CBA-CGA-O1A
21	6	512	CL7	CAA-CBA-CGA-O1A
21	8	406	CL7	CAA-CBA-CGA-O1A
21	D	404	CL7	C10-C11-C12-C13
21	B	610	CL7	C16-C17-C18-C20
21	b	611	CL7	C16-C17-C18-C20
21	A	406	CL7	C2A-CAA-CBA-CGA
21	4	406	CL7	CAA-CBA-CGA-O1A
21	4	409	CL7	CAA-CBA-CGA-O1A
21	8	409	CL7	CAA-CBA-CGA-O1A
26	D	410	LMG	O9-C10-C11-C12
26	d	410	LMG	O9-C10-C11-C12
21	1	418	CL7	C10-C11-C12-C13
21	5	418	CL7	C10-C11-C12-C13
21	3	516	CL7	C6-C7-C8-C9
21	7	516	CL7	C6-C7-C8-C9
21	A	403	CL7	CAD-CBD-CGD-O1D
21	C	505	CL7	CAD-CBD-CGD-O1D
21	C	507	CL7	CAD-CBD-CGD-O1D
21	2	510	CL7	CAD-CBD-CGD-O1D
21	2	518	CL7	CAD-CBD-CGD-O1D
21	3	502	CL7	CAD-CBD-CGD-O1D
21	4	407	CL7	CAD-CBD-CGD-O1D
21	4	410	CL7	CAD-CBD-CGD-O1D
21	4	413	CL7	CAD-CBD-CGD-O1D
21	4	415	CL7	CAD-CBD-CGD-O1D
21	a	403	CL7	CAD-CBD-CGD-O1D
21	c	505	CL7	CAD-CBD-CGD-O1D
21	c	507	CL7	CAD-CBD-CGD-O1D
21	6	510	CL7	CAD-CBD-CGD-O1D
21	6	518	CL7	CAD-CBD-CGD-O1D
21	7	502	CL7	CAD-CBD-CGD-O1D
21	8	407	CL7	CAD-CBD-CGD-O1D
21	8	410	CL7	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	8	413	CL7	CAD-CBD-CGD-O1D
21	8	415	CL7	CAD-CBD-CGD-O1D
24	A	405	SQD	O5-C5-C6-S
24	B	626	SQD	O5-C5-C6-S
24	1	423	SQD	O5-C5-C6-S
24	3	523	SQD	C46-C45-O47-C7
24	5	423	SQD	O5-C5-C6-S
24	7	523	SQD	C46-C45-O47-C7
26	B	621	LMG	C35-C36-C37-C38
26	b	622	LMG	C35-C36-C37-C38
21	B	610	CL7	C14-C13-C15-C16
21	C	506	CL7	C11-C12-C13-C14
21	4	405	CL7	C6-C7-C8-C9
21	b	611	CL7	C14-C13-C15-C16
21	c	506	CL7	C11-C12-C13-C14
21	8	405	CL7	C6-C7-C8-C9
27	C	517	DGD	C1A-C2A-C3A-C4A
27	c	517	DGD	C1A-C2A-C3A-C4A
21	D	404	CL7	CAA-CBA-CGA-O2A
26	1	401	LMG	O7-C10-C11-C12
26	5	401	LMG	O7-C10-C11-C12
21	D	405	CL7	C2A-CAA-CBA-CGA
21	a	405	CL7	C2A-CAA-CBA-CGA
21	d	405	CL7	C2A-CAA-CBA-CGA
21	C	502	CL7	CAA-CBA-CGA-O2A
21	1	406	CL7	CAA-CBA-CGA-O2A
21	3	512	CL7	CAA-CBA-CGA-O2A
21	c	502	CL7	CAA-CBA-CGA-O2A
21	d	404	CL7	CAA-CBA-CGA-O2A
21	5	406	CL7	CAA-CBA-CGA-O2A
21	7	512	CL7	CAA-CBA-CGA-O2A
26	D	410	LMG	O9-C10-O7-C8
26	d	410	LMG	O9-C10-O7-C8
21	C	510	CL7	C16-C17-C18-C20
21	c	510	CL7	C16-C17-C18-C20
21	2	509	CL7	C4-C3-C5-C6
21	6	509	CL7	C4-C3-C5-C6
21	B	610	CL7	C11-C12-C13-C15
21	C	508	CL7	C11-C12-C13-C15
21	2	501	CL7	C6-C7-C8-C10
21	2	505	CL7	C11-C10-C8-C7
21	2	510	CL7	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
21	2	511	CL7	C11-C10-C8-C7
21	1	404	CL7	C12-C13-C15-C16
21	3	502	CL7	C11-C10-C8-C7
21	b	611	CL7	C11-C12-C13-C15
21	c	508	CL7	C11-C12-C13-C15
21	6	501	CL7	C6-C7-C8-C10
21	6	505	CL7	C11-C10-C8-C7
21	6	510	CL7	C11-C12-C13-C15
21	6	511	CL7	C11-C10-C8-C7
21	5	404	CL7	C12-C13-C15-C16
21	7	502	CL7	C11-C10-C8-C7
23	B	617	8CT	C28-C29-C30-C31
23	K	101	8CT	C28-C29-C30-C31
23	b	618	8CT	C28-C29-C30-C31
23	k	101	8CT	C28-C29-C30-C31
21	6	507	CL7	CAA-CBA-CGA-O1A
24	3	523	SQD	C11-C12-C13-C14
24	7	523	SQD	C11-C12-C13-C14
21	2	507	CL7	CAA-CBA-CGA-O1A
21	1	406	CL7	CAA-CBA-CGA-O1A
21	5	406	CL7	CAA-CBA-CGA-O1A
32	2	519	ZEX	C33-C34-C35-C15
32	6	519	ZEX	C33-C34-C35-C15
24	3	523	SQD	C13-C14-C15-C16
24	7	523	SQD	C13-C14-C15-C16
21	B	603	CL7	C16-C17-C18-C19
21	b	604	CL7	C16-C17-C18-C19
26	C	501	LMG	C32-C33-C34-C35
21	2	510	CL7	CAA-CBA-CGA-O1A
21	4	412	CL7	CAA-CBA-CGA-O1A
21	6	510	CL7	CAA-CBA-CGA-O1A
21	8	412	CL7	CAA-CBA-CGA-O1A
21	C	505	CL7	C4C-C3C-CAC-CBC
21	c	505	CL7	C4C-C3C-CAC-CBC
24	1	423	SQD	O48-C23-C24-C25
24	5	423	SQD	O48-C23-C24-C25
21	3	505	CL7	CAA-CBA-CGA-O2A
21	7	505	CL7	CAA-CBA-CGA-O2A

There are no ring outliers.

269 monomers are involved in 1314 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	626	SQD	2	0
21	8	405	CL7	6	0
21	2	515	CL7	2	0
21	1	420	CL7	6	0
21	3	501	CL7	9	0
21	2	514	CL7	2	0
25	8	401	LHG	2	0
21	6	503	CL7	10	0
21	b	605	CL7	9	0
21	C	502	CL7	4	0
21	2	518	CL7	11	0
32	4	403	ZEX	22	0
21	7	512	CL7	6	0
32	5	422	ZEX	21	0
21	4	406	CL7	13	0
21	4	412	CL7	4	0
21	2	509	CL7	7	0
21	7	508	CL7	14	0
24	5	423	SQD	1	0
21	5	404	CL7	7	0
21	2	504	CL7	3	0
21	2	516	CL7	5	0
24	2	522	SQD	2	0
21	8	412	CL7	5	0
21	3	514	CL7	2	0
21	c	504	CL7	7	0
21	4	416	CL7	1	0
21	1	418	CL7	7	0
21	1	406	CL7	12	0
21	C	504	CL7	7	0
21	3	507	CL7	8	0
26	D	410	LMG	1	0
21	b	615	CL7	2	0
21	b	603	CL7	4	0
21	b	614	CL7	2	0
21	4	410	CL7	2	0
24	7	521	SQD	4	0
21	a	405	CL7	13	0
21	2	506	CL7	2	0
21	7	510	CL7	4	0
21	b	608	CL7	7	0
21	3	505	CL7	17	0
21	c	506	CL7	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1	421	ZEX	13	0
25	b	626	LHG	1	0
21	5	420	CL7	6	0
32	2	521	ZEX	29	0
21	3	510	CL7	6	0
21	5	412	CL7	2	0
21	b	611	CL7	1	0
32	8	420	ZEX	13	0
32	8	419	ZEX	7	0
21	5	413	CL7	6	0
21	4	414	CL7	3	0
21	B	610	CL7	3	0
21	2	510	CL7	6	0
21	6	509	CL7	6	0
21	6	513	CL7	6	0
32	7	520	ZEX	10	0
21	8	413	CL7	4	0
21	6	515	CL7	2	0
25	d	409	LHG	4	0
32	6	522	ZEX	19	0
25	7	524	LHG	1	0
32	3	519	ZEX	17	0
21	4	415	CL7	4	0
32	8	403	ZEX	21	0
21	4	407	CL7	6	0
21	4	409	CL7	2	0
21	2	512	CL7	7	0
21	1	405	CL7	5	0
21	A	403	CL7	2	0
21	3	512	CL7	8	0
21	3	504	CL7	9	0
21	6	507	CL7	5	0
24	3	523	SQD	2	0
32	3	520	ZEX	11	0
21	C	509	CL7	3	0
22	D	408	PHO	7	0
21	4	405	CL7	7	0
21	5	411	CL7	2	0
32	6	524	ZEX	17	0
21	2	502	CL7	9	0
21	6	517	CL7	9	0
32	7	519	ZEX	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	c	511	CL7	3	0
23	c	519	8CT	1	0
21	1	416	CL7	1	0
21	4	413	CL7	4	0
23	c	516	8CT	1	0
21	c	509	CL7	4	0
21	1	407	CL7	3	0
26	B	621	LMG	6	0
21	7	503	CL7	11	0
32	5	421	ZEX	15	0
21	B	605	CL7	7	0
21	1	403	CL7	4	0
21	C	511	CL7	3	0
21	4	417	CL7	4	0
22	a	402	PHO	2	0
32	3	525	ZEX	23	0
21	1	404	CL7	7	0
32	3	522	ZEX	27	0
23	C	516	8CT	1	0
21	b	606	CL7	6	0
21	2	505	CL7	14	0
27	B	624	DGD	2	0
21	2	503	CL7	10	0
27	C	517	DGD	4	0
21	B	612	CL7	7	0
21	4	404	CL7	7	0
21	b	616	CL7	4	0
21	B	615	CL7	3	0
21	C	506	CL7	5	0
25	b	624	LHG	6	0
21	C	514	CL7	3	0
21	C	503	CL7	4	0
24	7	523	SQD	2	0
21	b	604	CL7	9	0
21	1	408	CL7	7	0
32	2	523	ZEX	19	0
31	F	101	HEM	3	0
21	7	501	CL7	8	0
21	B	613	CL7	2	0
21	2	501	CL7	5	0
21	5	407	CL7	3	0
21	8	409	CL7	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	8	417	CL7	4	0
21	7	502	CL7	7	0
21	1	409	CL7	3	0
26	d	410	LMG	1	0
21	2	508	CL7	3	0
32	4	418	ZEX	9	0
21	6	511	CL7	9	0
21	B	604	CL7	9	0
21	c	508	CL7	4	0
21	6	516	CL7	6	0
21	d	404	CL7	6	0
21	1	412	CL7	2	0
21	C	512	CL7	1	0
21	C	508	CL7	4	0
21	1	410	CL7	7	0
21	7	504	CL7	9	0
21	7	517	CL7	2	0
26	b	622	LMG	6	0
21	8	404	CL7	8	0
26	1	401	LMG	2	0
25	D	409	LHG	3	0
21	c	512	CL7	1	0
21	2	513	CL7	6	0
21	6	506	CL7	2	0
21	7	514	CL7	2	0
21	c	513	CL7	1	0
27	c	517	DGD	4	0
32	2	520	ZEX	24	0
21	8	406	CL7	14	0
24	3	521	SQD	4	0
21	2	511	CL7	8	0
21	7	507	CL7	10	0
21	3	517	CL7	1	0
21	1	411	CL7	2	0
21	b	612	CL7	5	0
21	6	505	CL7	17	0
21	C	510	CL7	4	0
21	8	414	CL7	4	0
21	c	502	CL7	5	0
21	B	609	CL7	4	0
21	3	511	CL7	5	0
21	a	401	CL7	18	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	2	507	CL7	5	0
21	1	414	CL7	2	0
32	4	419	ZEX	7	0
21	4	411	CL7	7	0
32	6	519	ZEX	2	0
25	B	625	LHG	2	0
21	5	418	CL7	8	0
21	8	407	CL7	6	0
21	3	509	CL7	9	0
21	D	404	CL7	6	0
24	b	621	SQD	3	0
21	6	501	CL7	7	0
24	1	423	SQD	1	0
32	8	418	ZEX	10	0
32	2	525	ZEX	17	0
21	5	403	CL7	5	0
30	D	407	PL9	7	0
32	1	422	ZEX	22	0
21	3	515	CL7	2	0
21	8	415	CL7	5	0
27	b	625	DGD	2	0
25	3	524	LHG	1	0
21	5	402	CL7	10	0
21	6	508	CL7	4	0
21	6	514	CL7	2	0
21	a	403	CL7	1	0
21	b	609	CL7	3	0
32	2	519	ZEX	2	0
21	c	507	CL7	3	0
21	C	505	CL7	3	0
21	A	401	CL7	16	0
22	d	408	PHO	7	0
21	5	406	CL7	12	0
21	C	513	CL7	1	0
21	1	402	CL7	10	0
21	c	503	CL7	4	0
21	B	603	CL7	8	0
21	3	518	CL7	3	0
21	6	512	CL7	8	0
21	d	405	CL7	2	0
21	5	416	CL7	1	0
21	c	505	CL7	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	6	521	SQD	1	0
21	7	515	CL7	2	0
21	6	510	CL7	6	0
21	3	502	CL7	7	0
21	b	610	CL7	4	0
21	1	417	CL7	4	0
25	B	623	LHG	6	0
32	4	420	ZEX	9	0
21	A	406	CL7	12	0
21	3	516	CL7	5	0
21	8	411	CL7	8	0
21	8	408	CL7	4	0
21	B	611	CL7	4	0
21	1	413	CL7	6	0
21	7	509	CL7	8	0
21	7	513	CL7	12	0
21	7	506	CL7	5	0
21	7	511	CL7	5	0
21	5	417	CL7	5	0
21	2	517	CL7	9	0
21	B	608	CL7	3	0
21	7	516	CL7	6	0
24	A	405	SQD	2	0
21	3	508	CL7	13	0
31	f	101	HEM	3	0
32	6	520	ZEX	31	0
32	7	522	ZEX	25	0
21	c	514	CL7	3	0
21	3	506	CL7	5	0
21	B	607	CL7	7	0
23	C	519	8CT	1	0
21	7	518	CL7	3	0
21	3	503	CL7	11	0
30	d	407	PL9	6	0
21	5	408	CL7	7	0
24	B	620	SQD	3	0
26	5	401	LMG	2	0
22	A	402	PHO	2	0
25	4	401	LHG	2	0
21	6	504	CL7	3	0
21	6	502	CL7	8	0
21	B	606	CL7	4	0

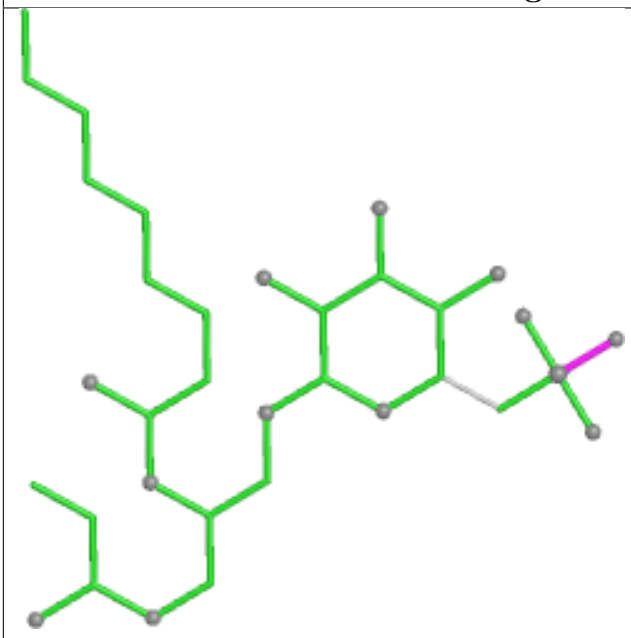
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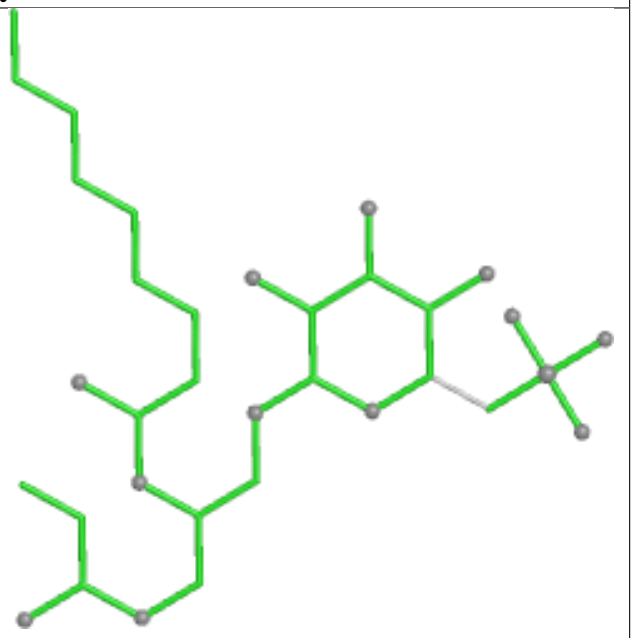
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	3	513	CL7	13	0
21	8	410	CL7	2	0
21	B	614	CL7	2	0
21	c	510	CL7	3	0
21	4	408	CL7	4	0
21	5	414	CL7	2	0
21	5	410	CL7	6	0
21	B	602	CL7	4	0
21	b	613	CL7	6	0
21	5	409	CL7	4	0
21	5	405	CL7	5	0
21	D	405	CL7	2	0
21	C	507	CL7	5	0
21	7	505	CL7	19	0
21	b	607	CL7	5	0
21	6	518	CL7	10	0

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

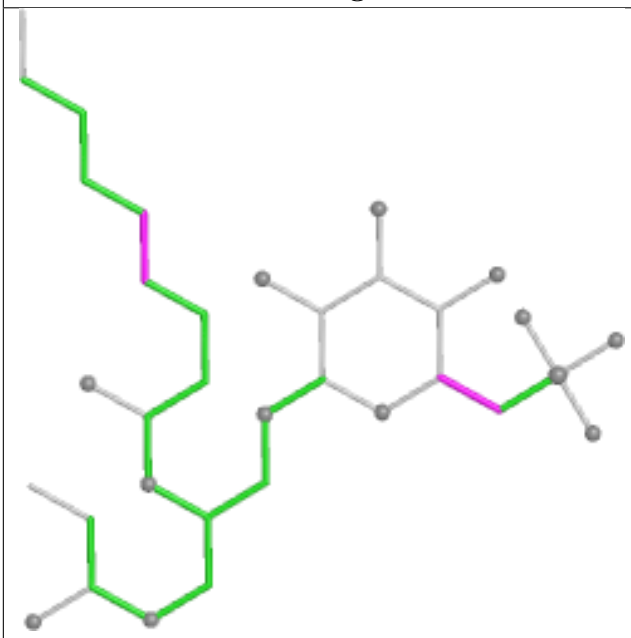
Ligand SQD B 626



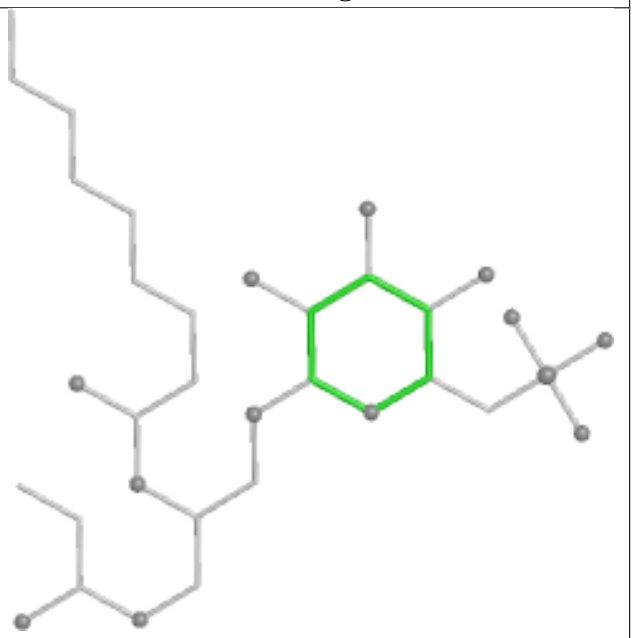
Bond lengths



Bond angles

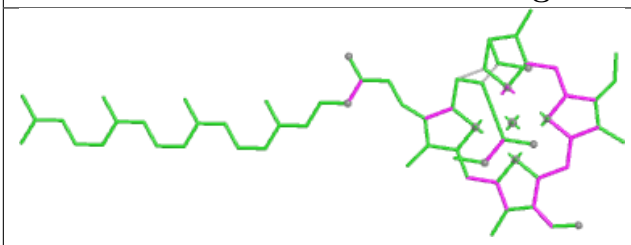


Torsions

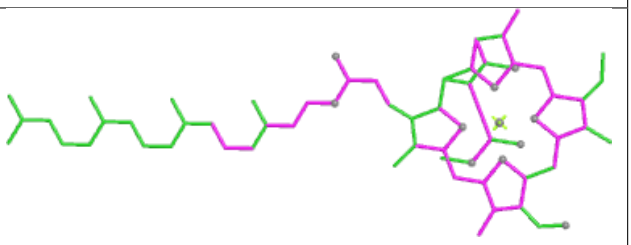


Rings

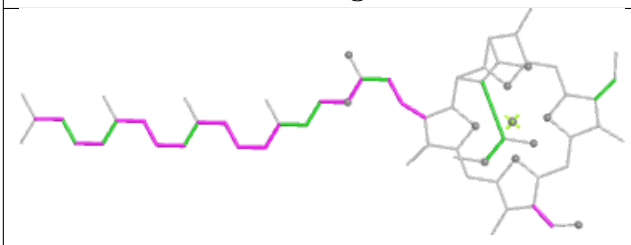
Ligand CL7 8 405



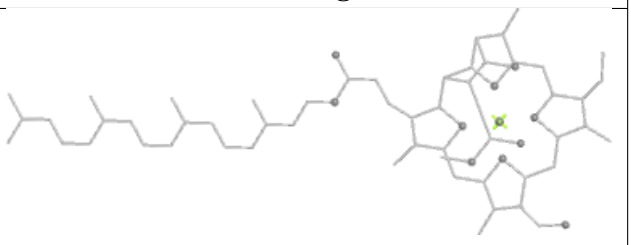
Bond lengths



Bond angles

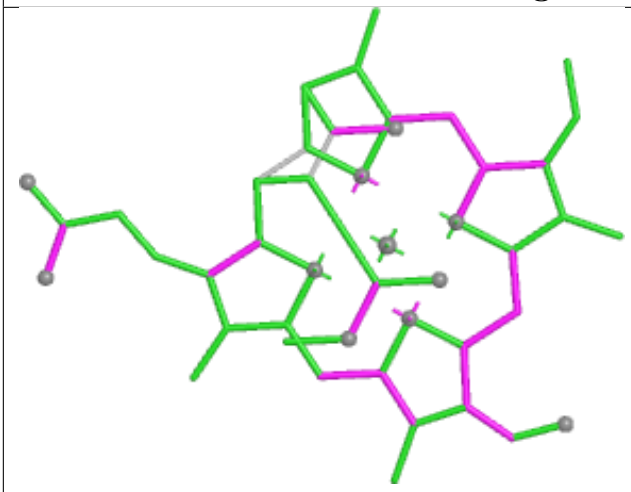


Torsions



Rings

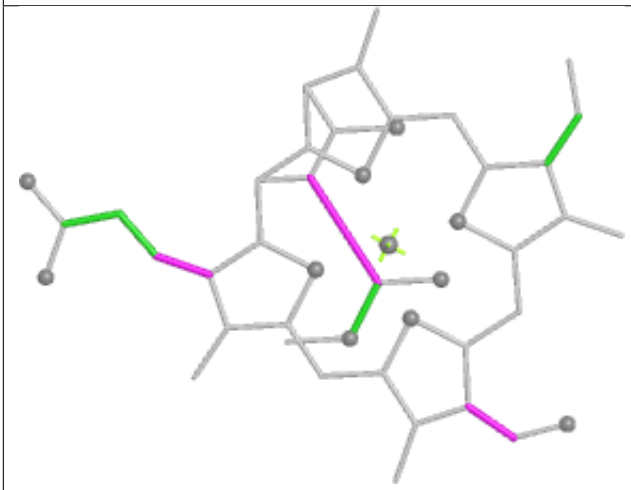
Ligand CL7 2 515



Bond lengths



Bond angles



Torsions

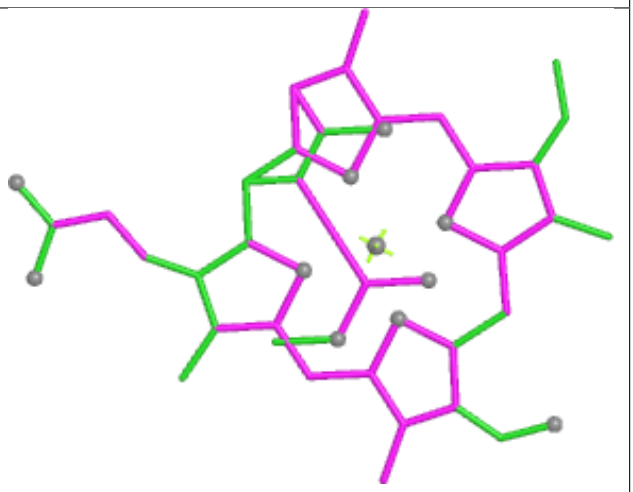


Rings

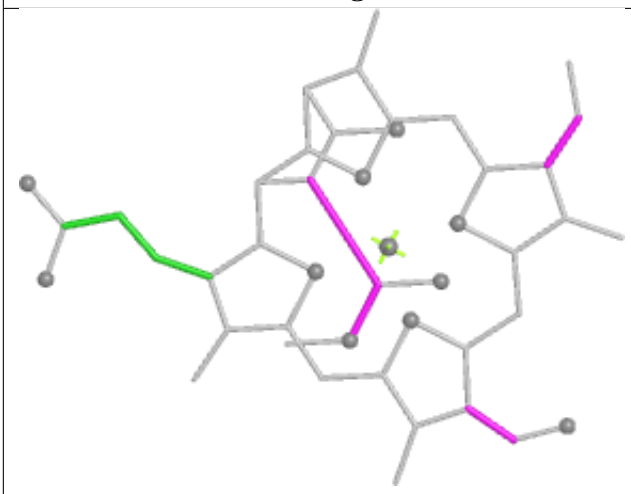
Ligand CL7 1 420



Bond lengths



Bond angles

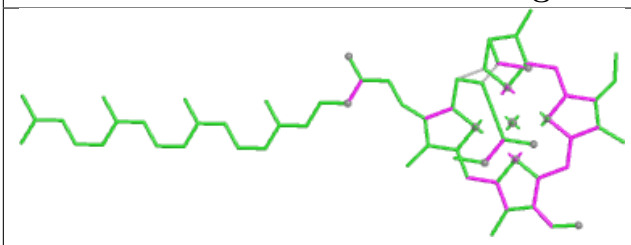


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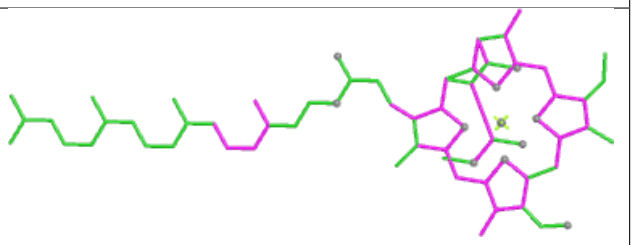


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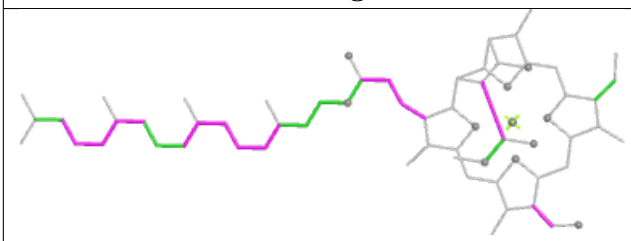
Ligand CL7 3 501



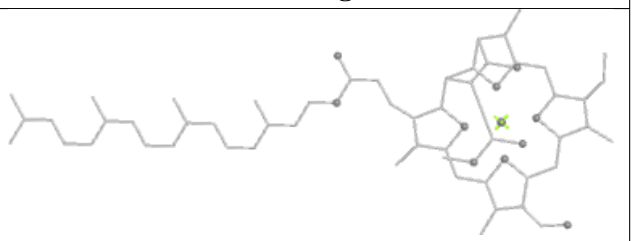
Bond lengths



Bond angles

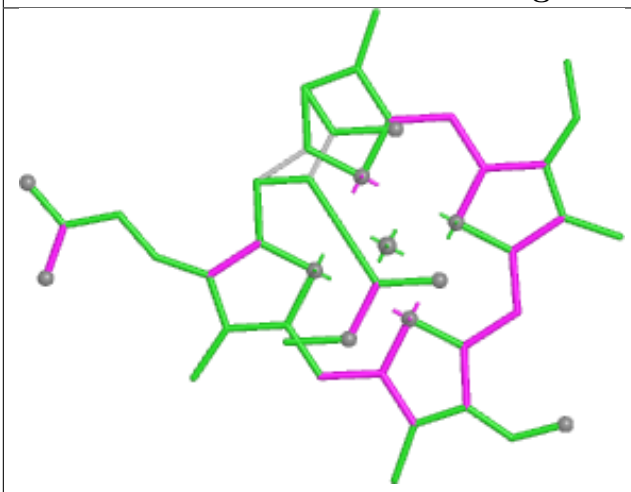


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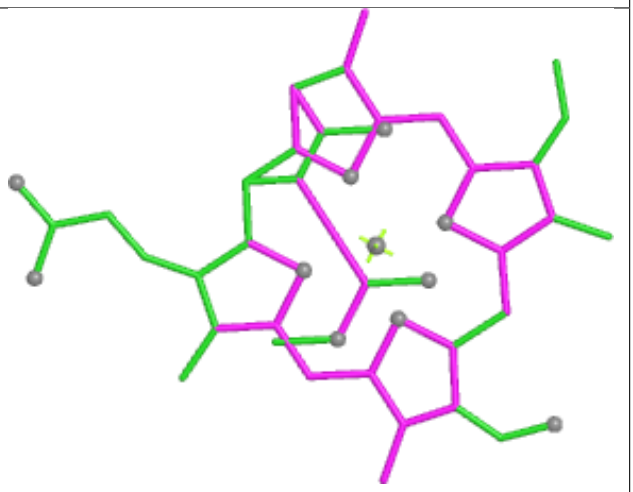


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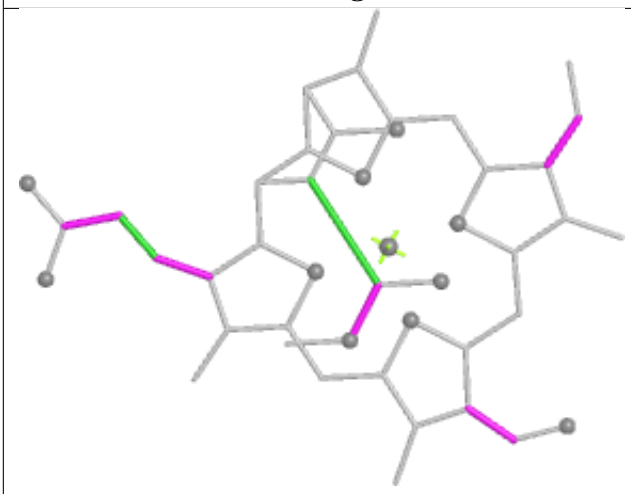
Ligand CL7 2 514



Bond lengths



Bond angles

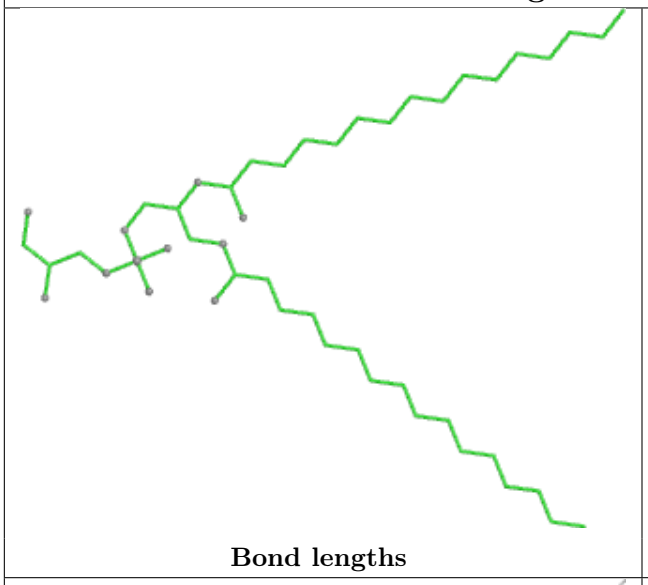


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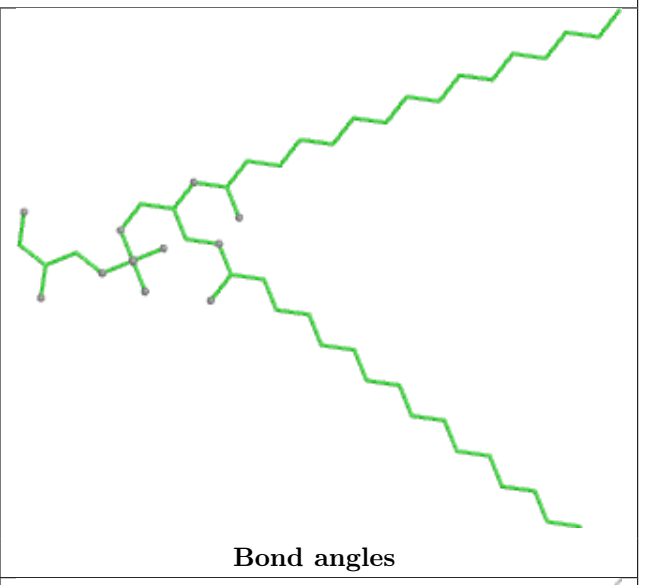


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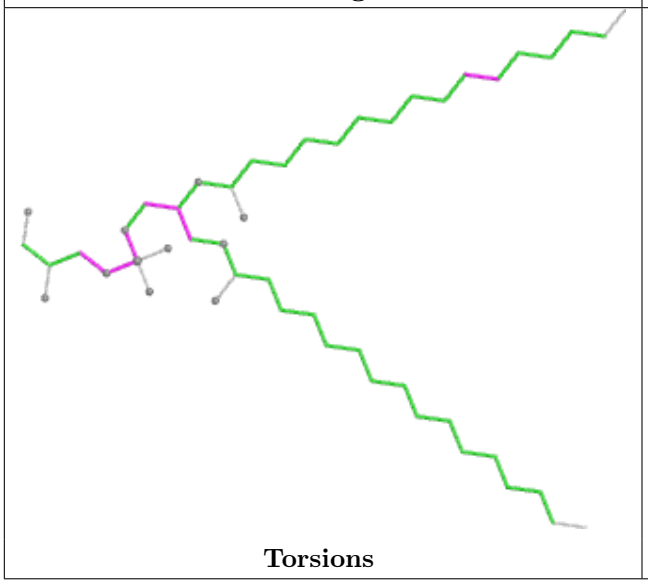
Ligand LHG 8 401



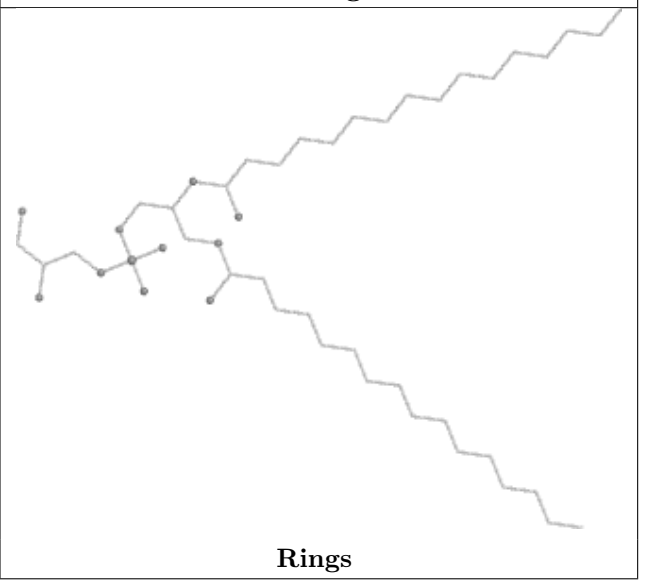
Bond lengths



Bond angles

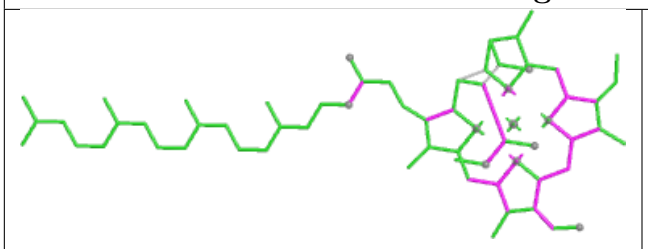


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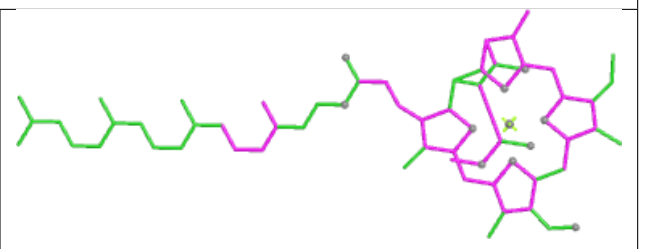


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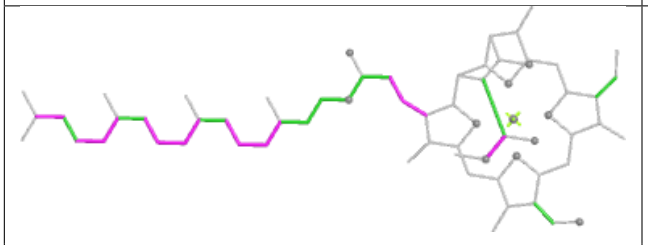
Ligand CL7 6 503



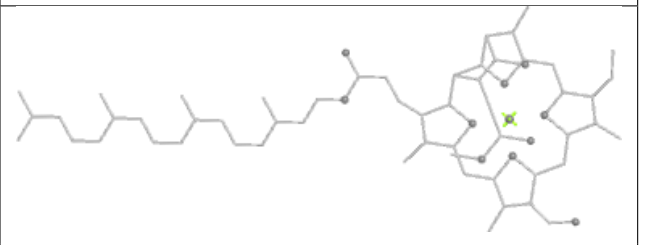
Bond lengths



Bond angles

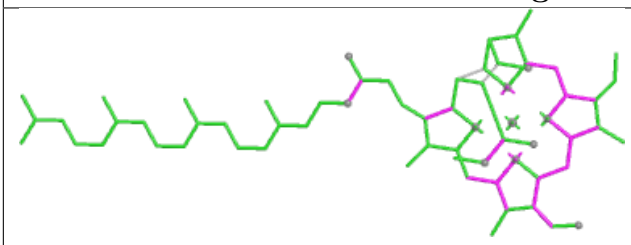


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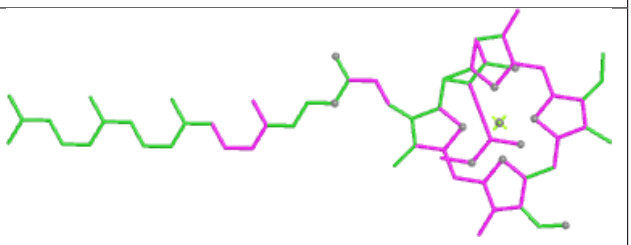


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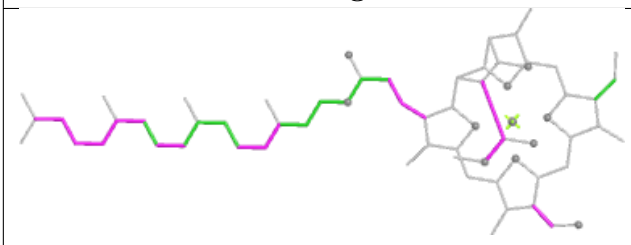
Ligand CL7 b 605



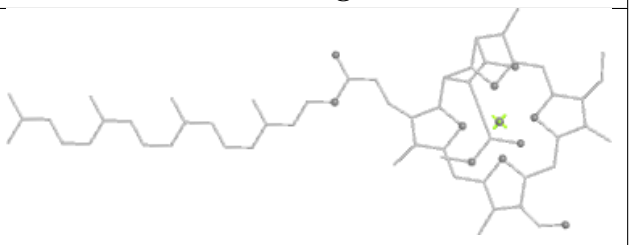
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Bond angles

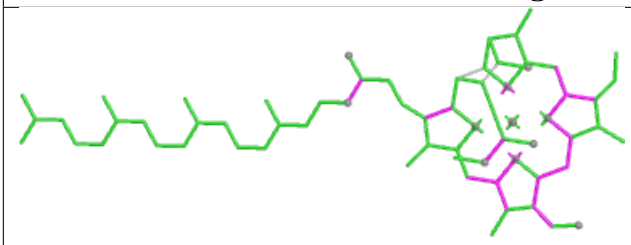


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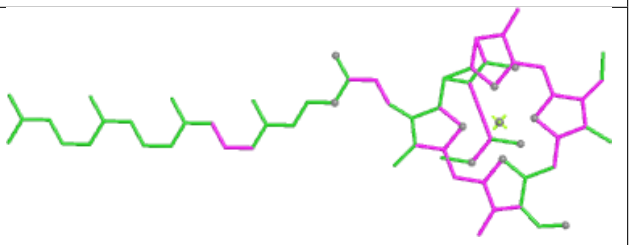


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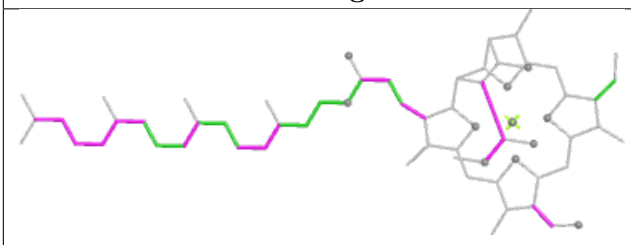
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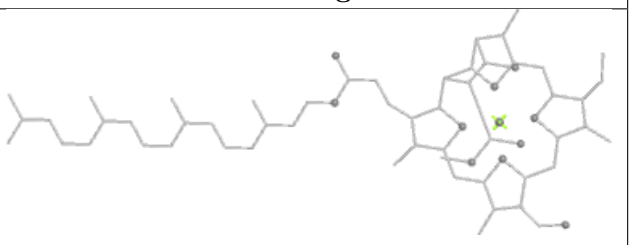
Bond lengths



Bond angles

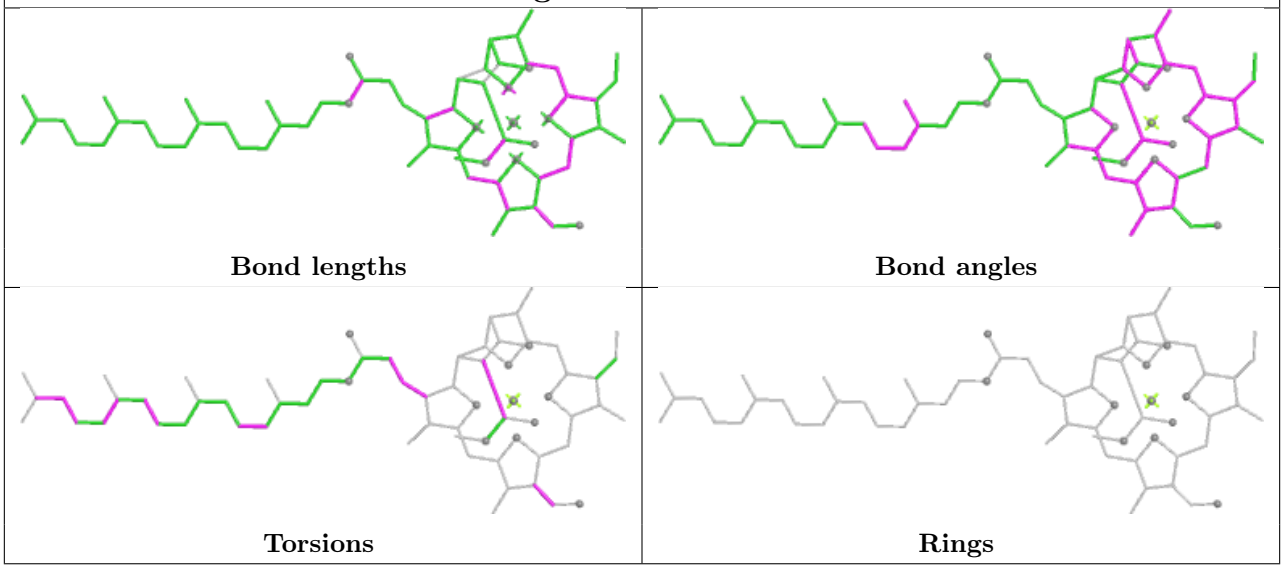


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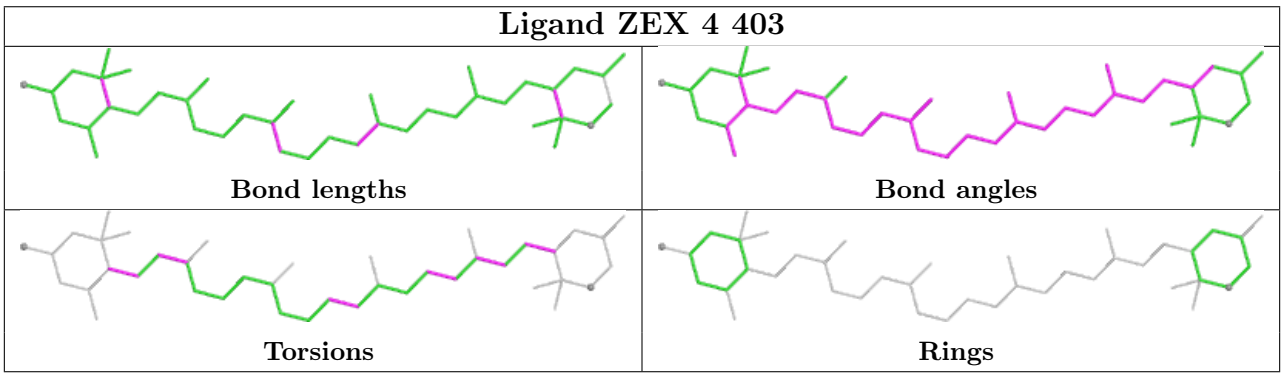


Rings

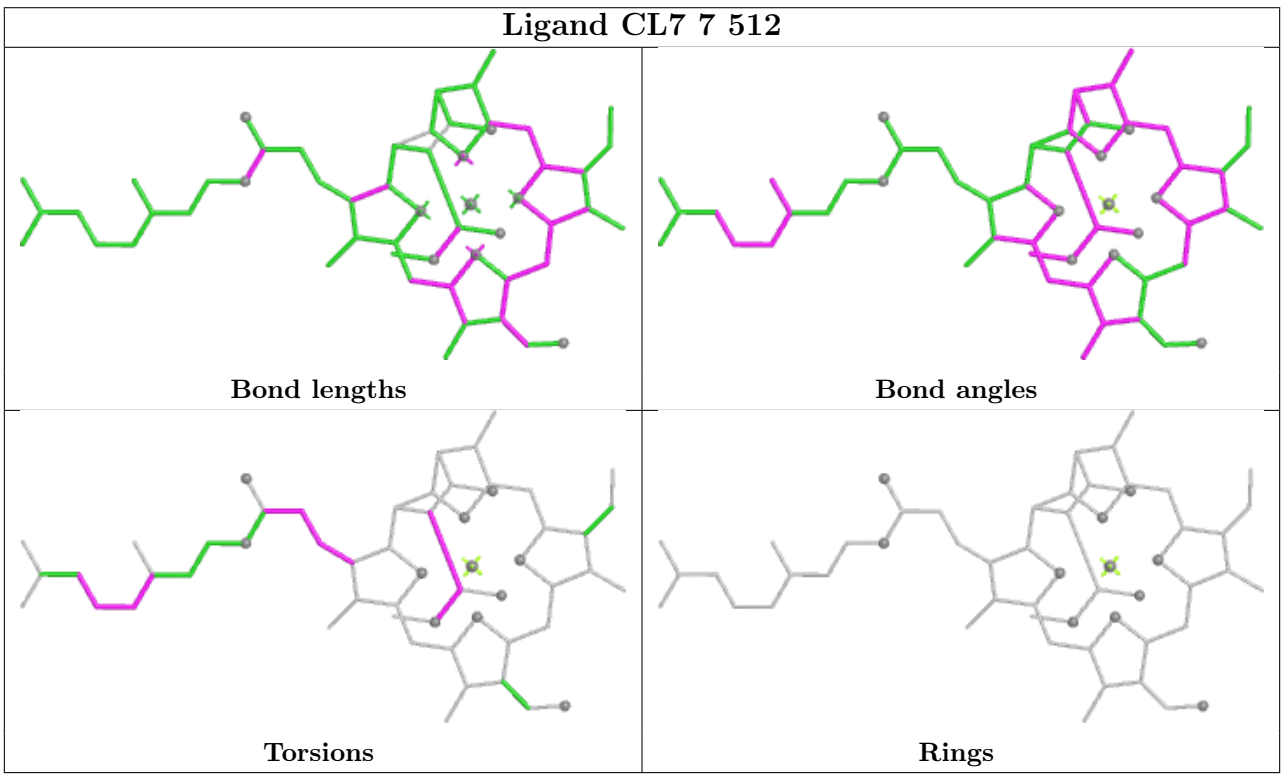
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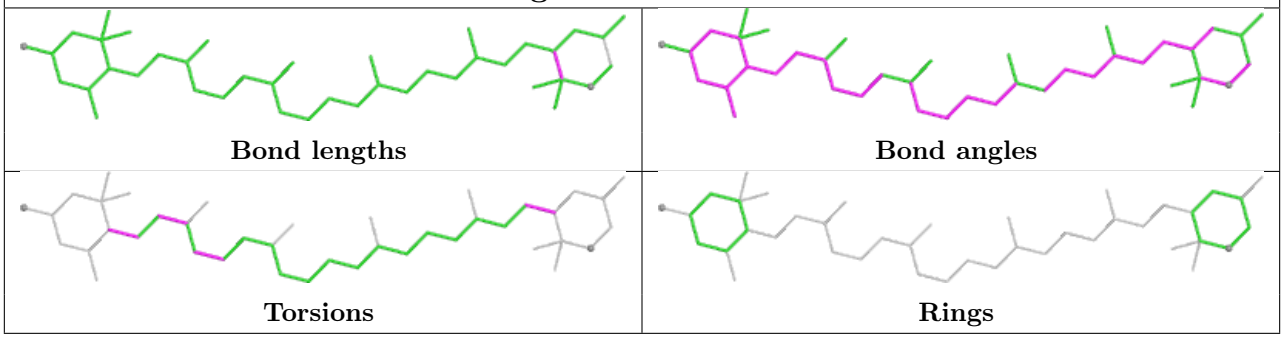
Ligand ZEX 4 403



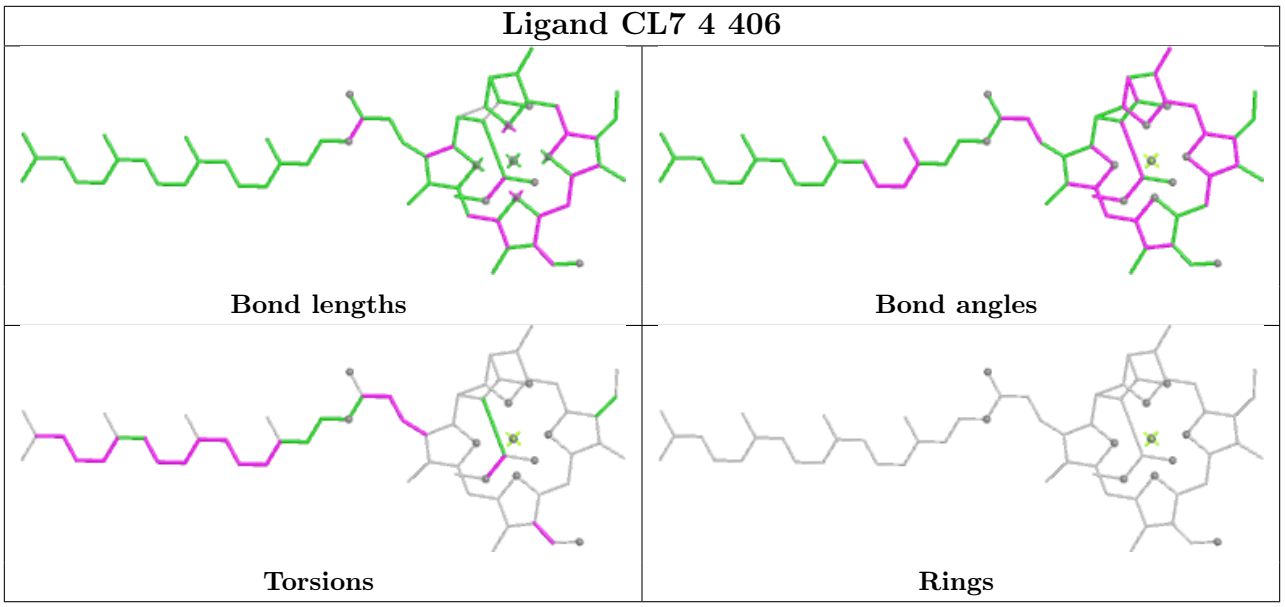
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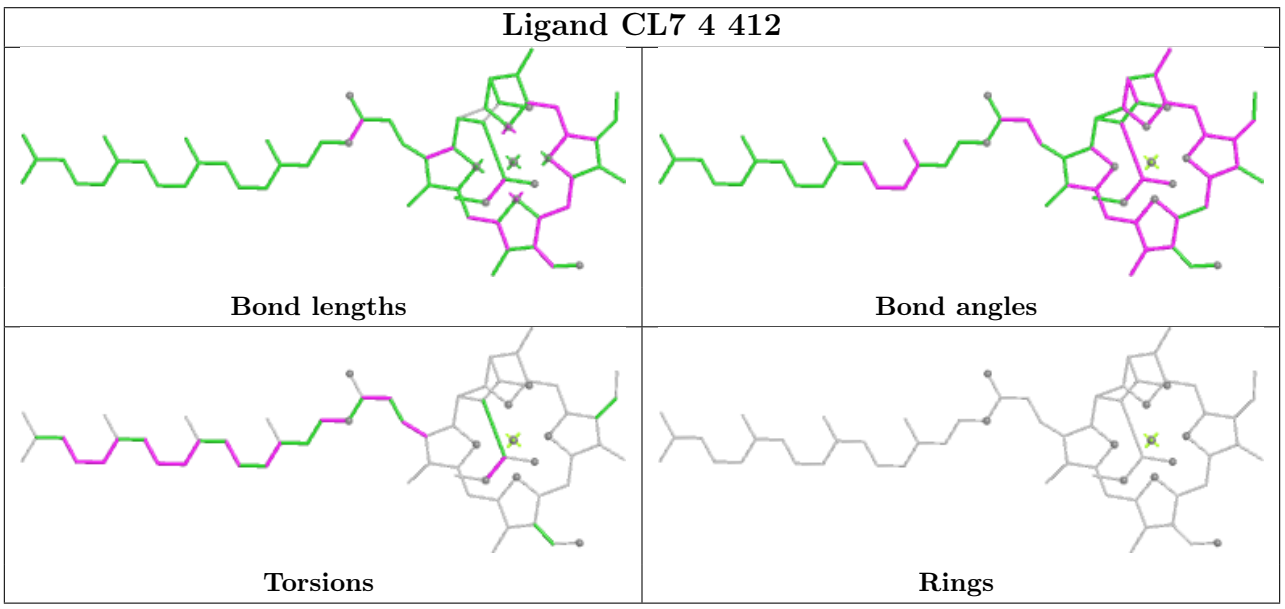
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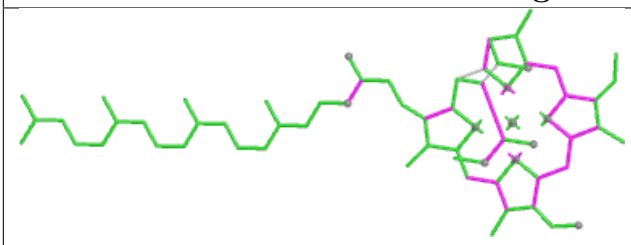
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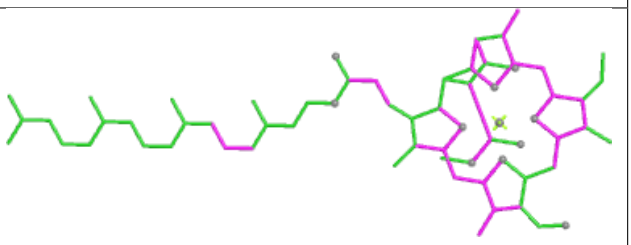
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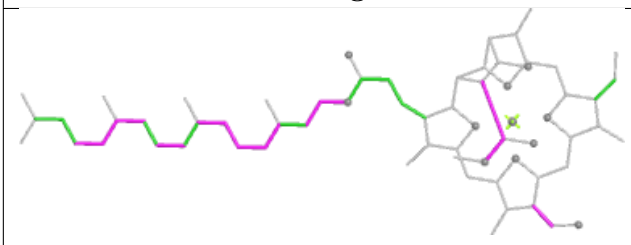
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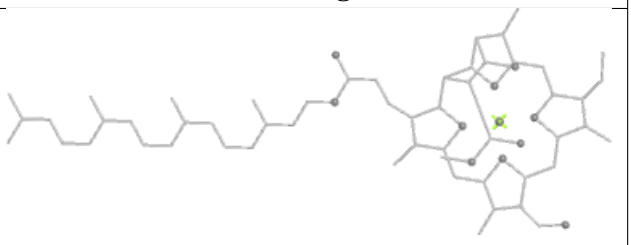
Bond lengths



Bond angles

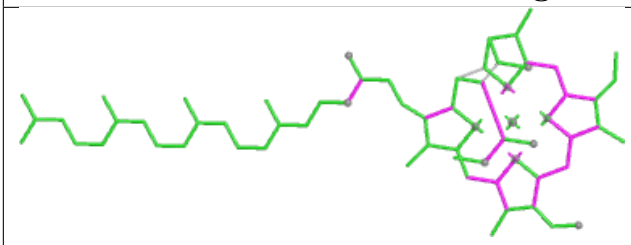


Torsions

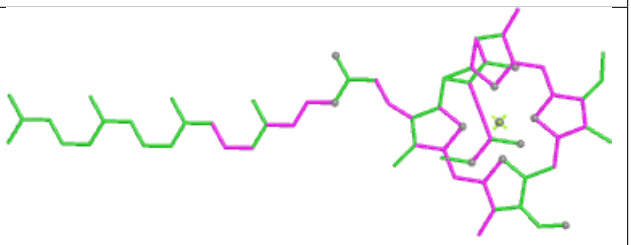


Rings

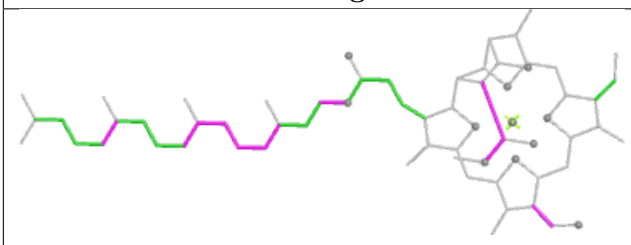
Ligand CL7 7 508



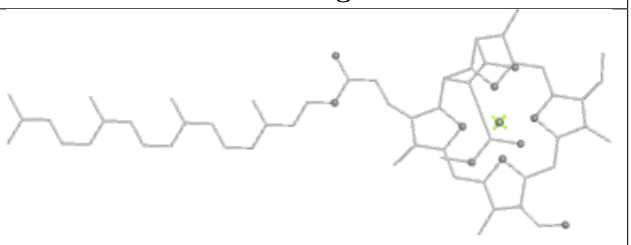
Bond lengths



Bond angles

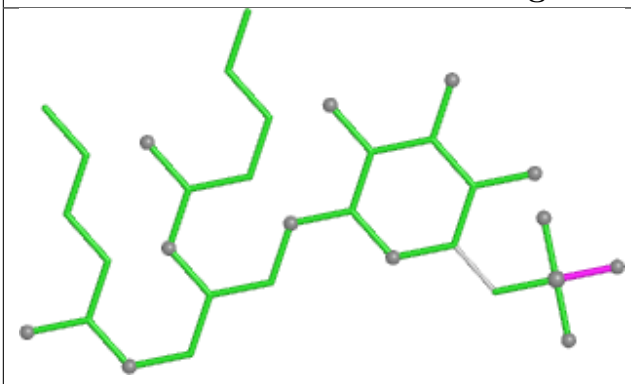


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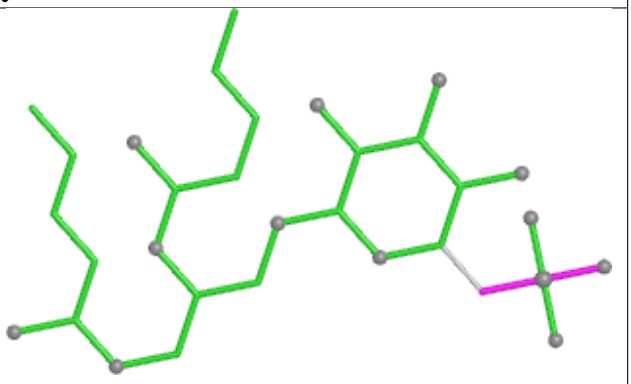


Rings

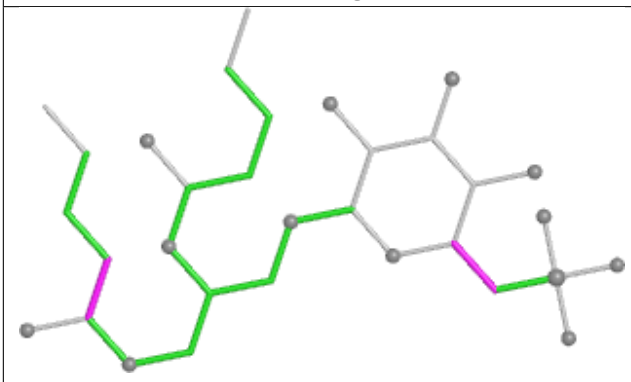
Ligand SQD 5 423



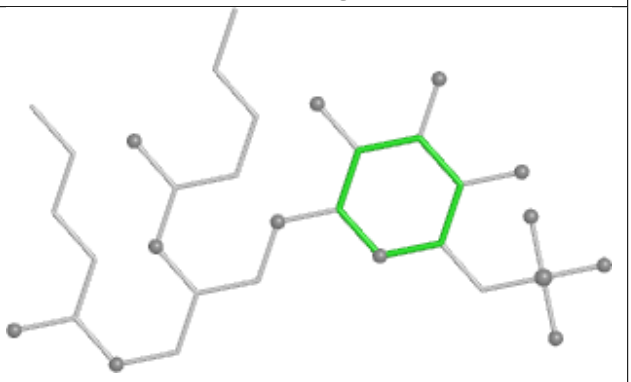
Bond lengths



Bond angles

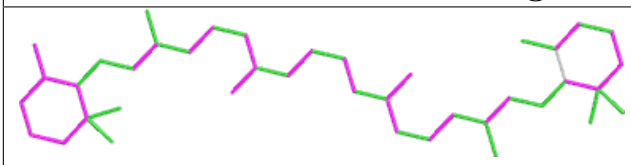


Torsions

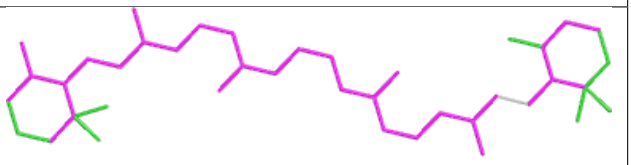


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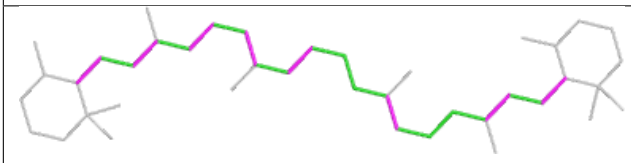
Ligand 8CT C 515



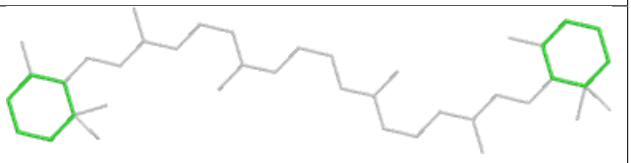
Bond lengths



Bond angles

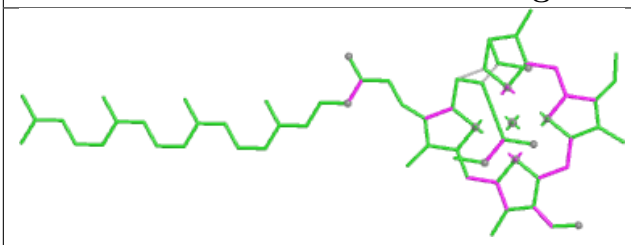


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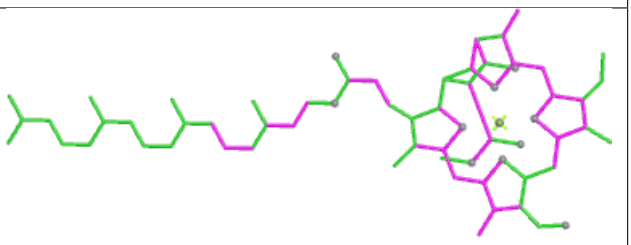


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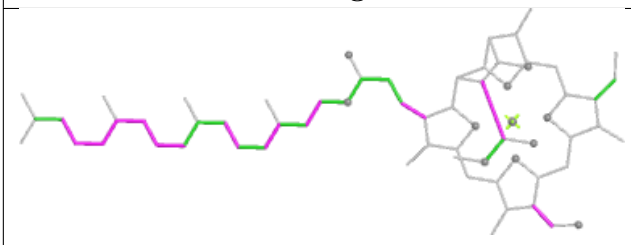
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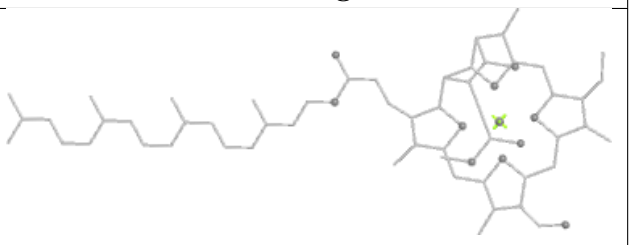
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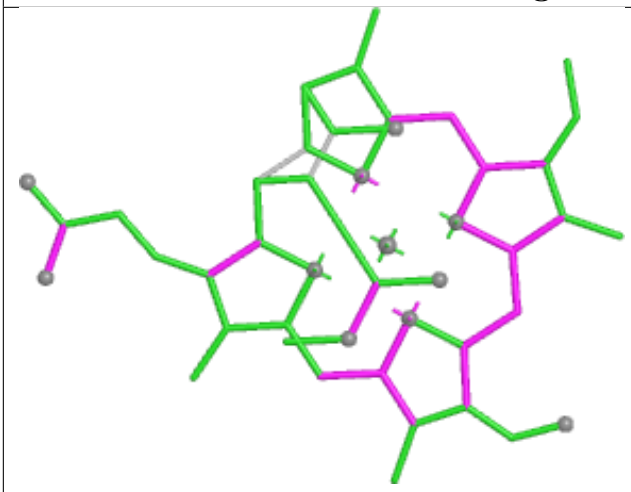


Torsions



Rings

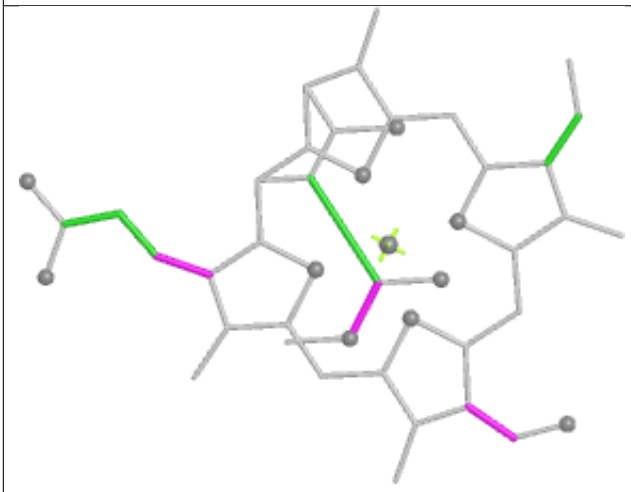
Ligand CL7 2 504



Bond lengths



Bond angles

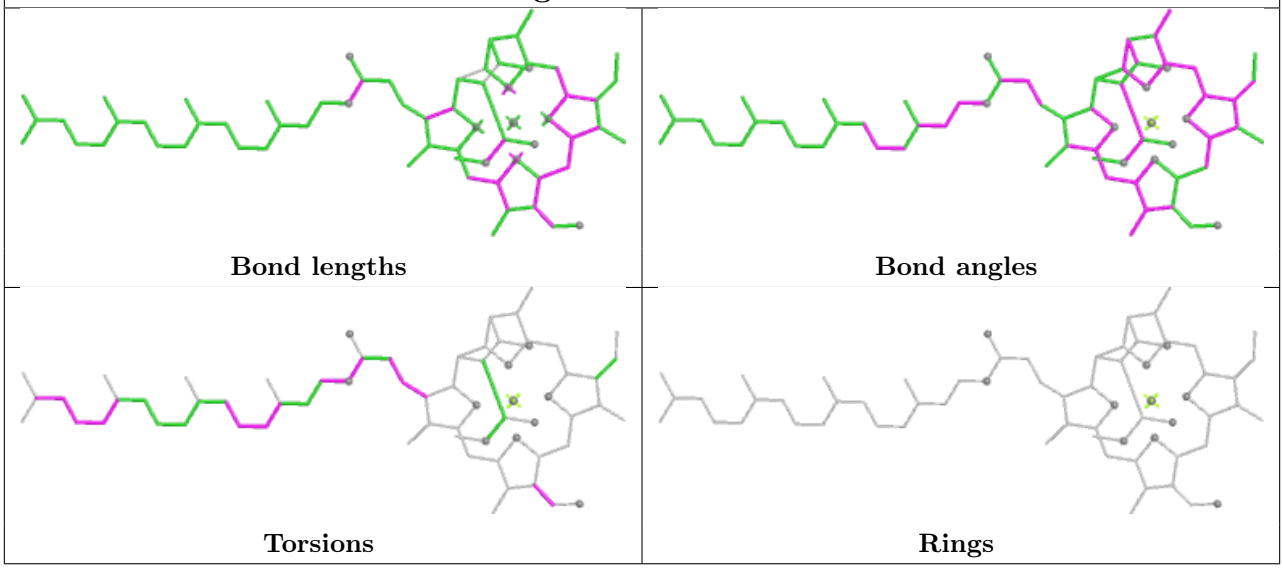


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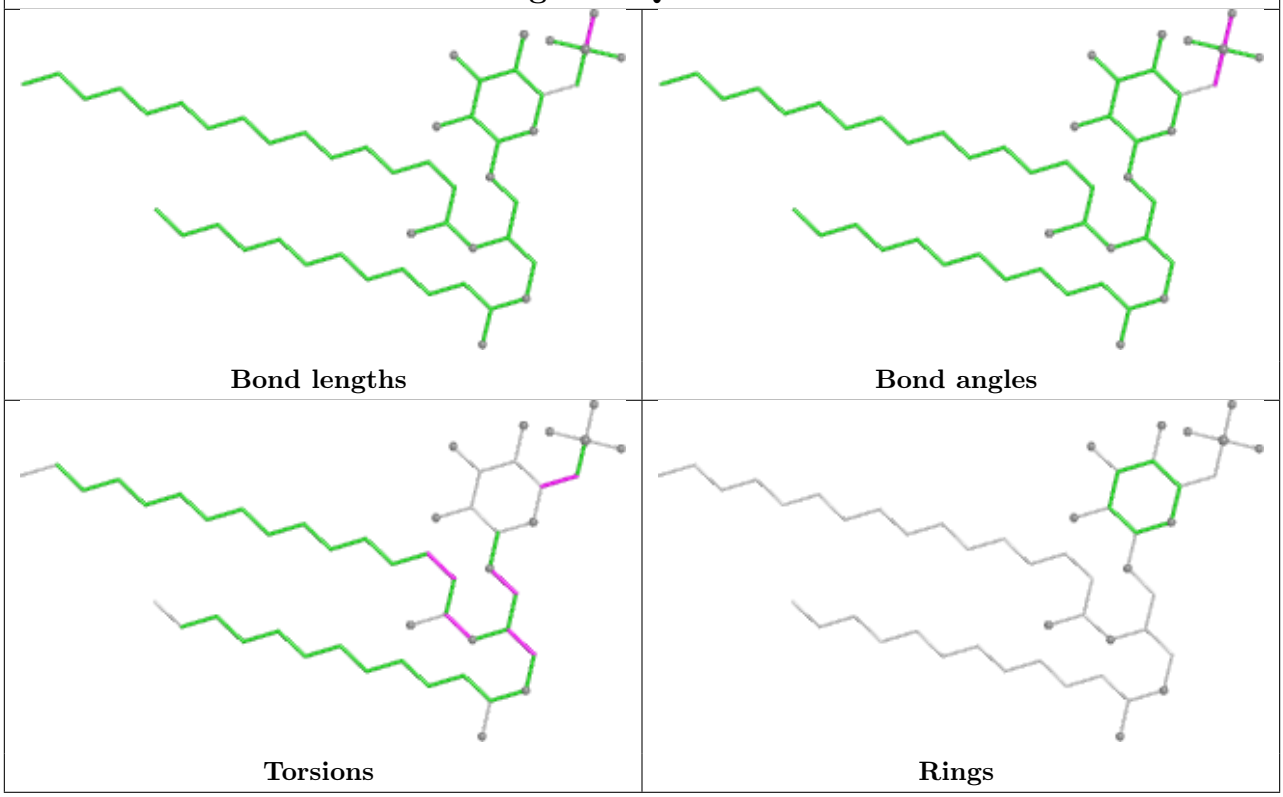


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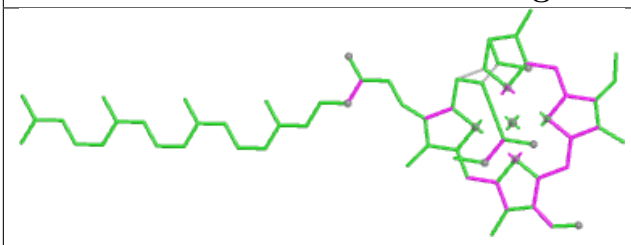
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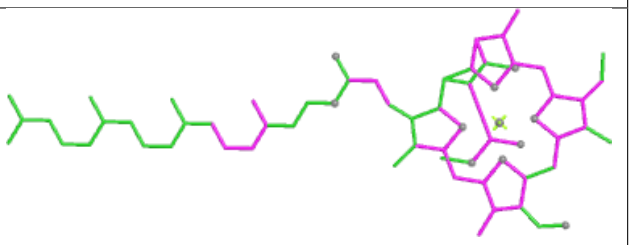
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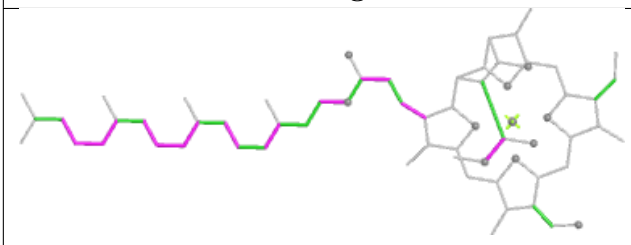
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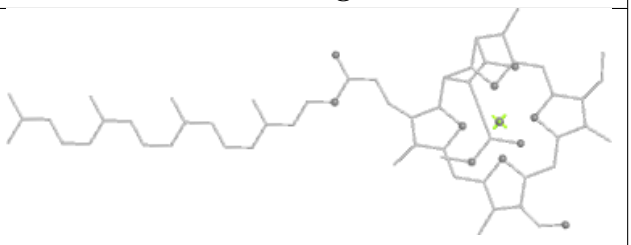
Bond lengths



Bond angles

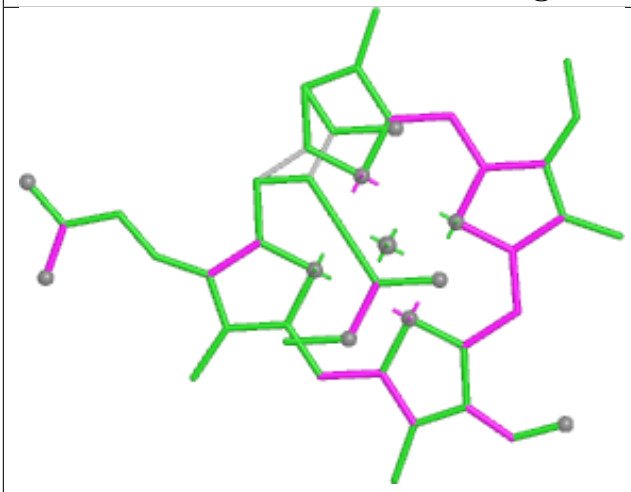


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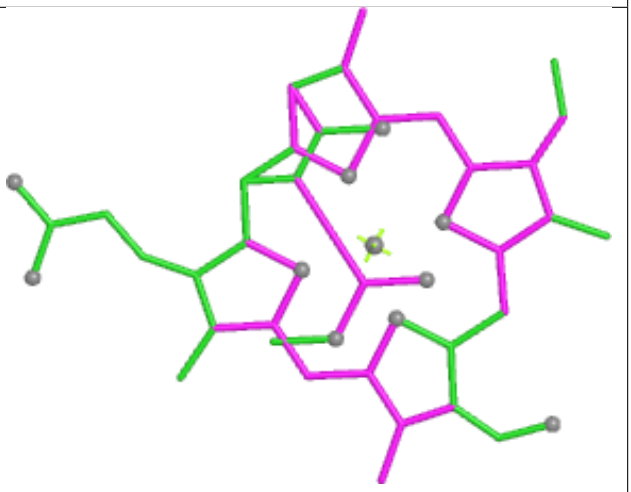


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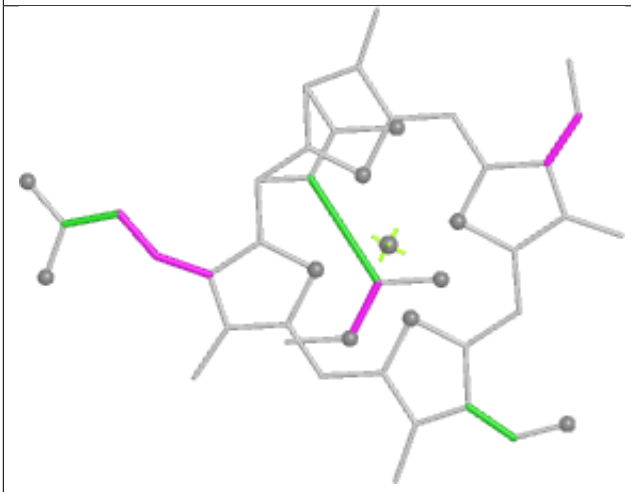
Ligand CL7 3 514



Bond lengths



Bond angles

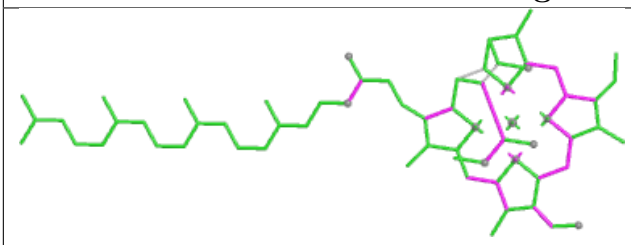


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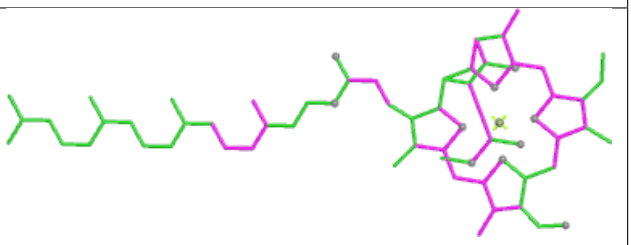


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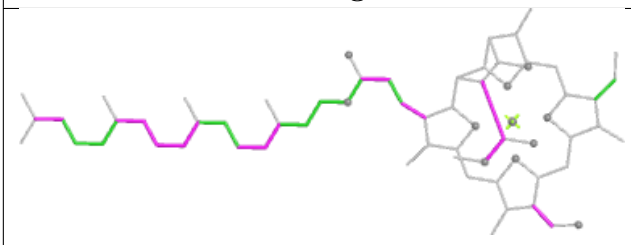
Ligand CL7 c 504



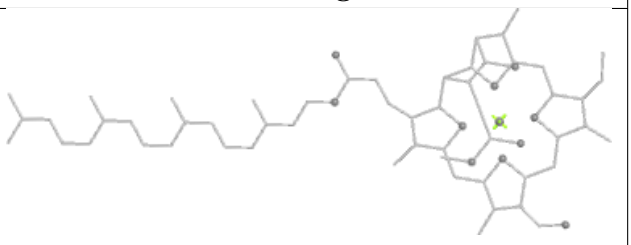
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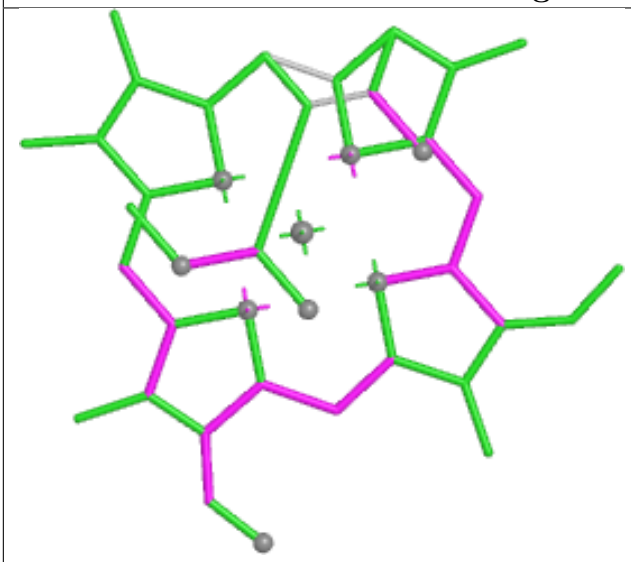


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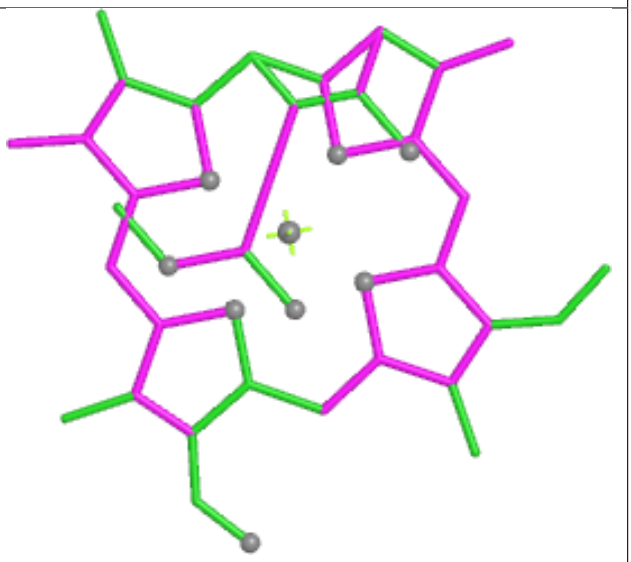


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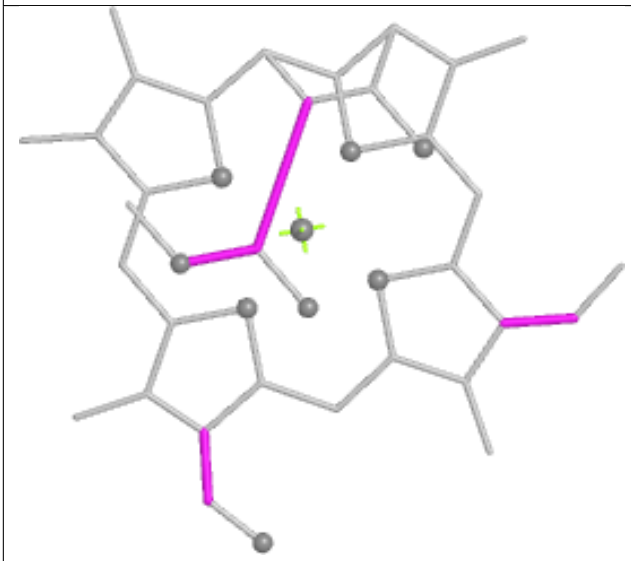
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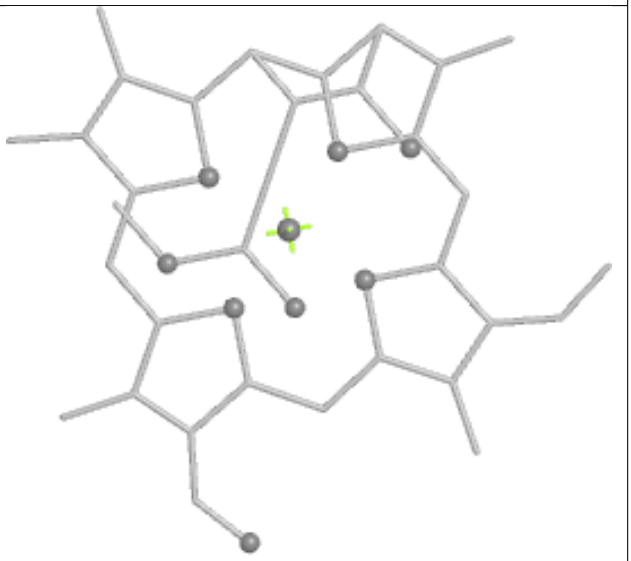
Bond lengths



Bond angles

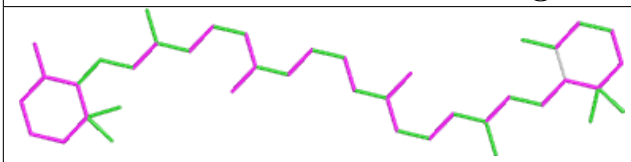


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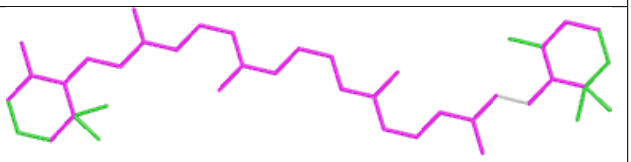


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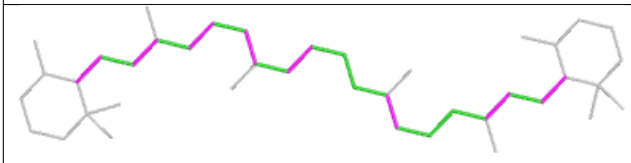
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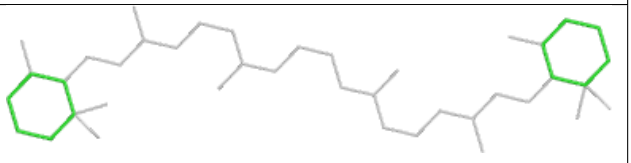
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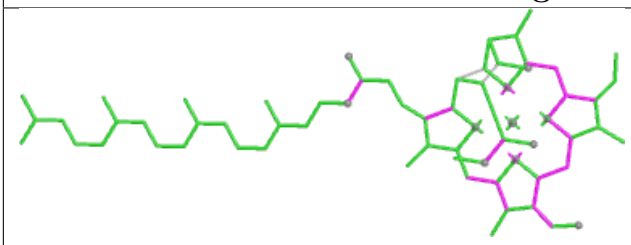


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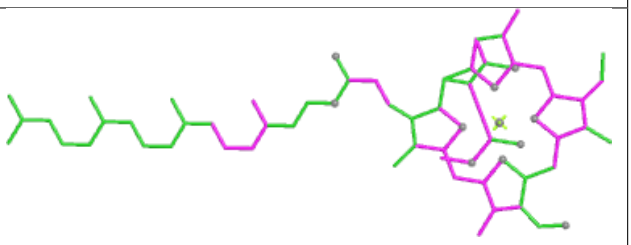


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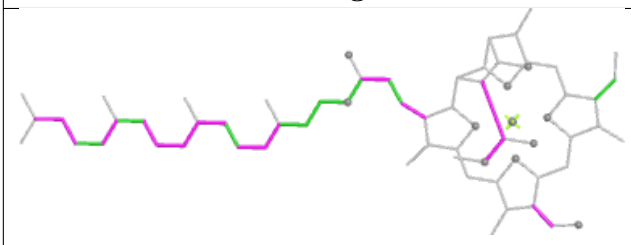
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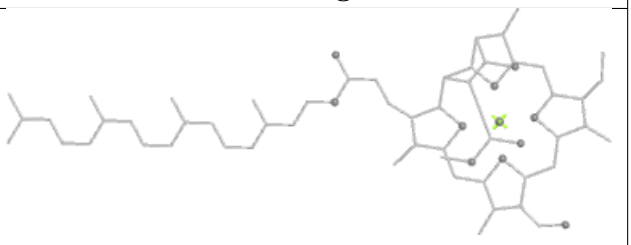
Bond lengths



Bond angles

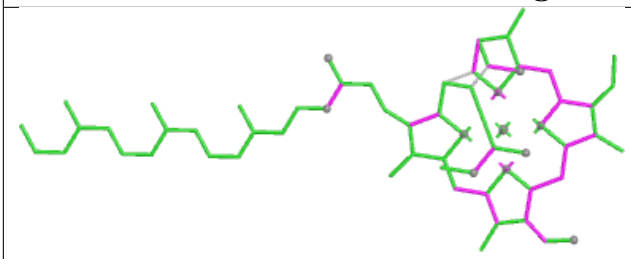


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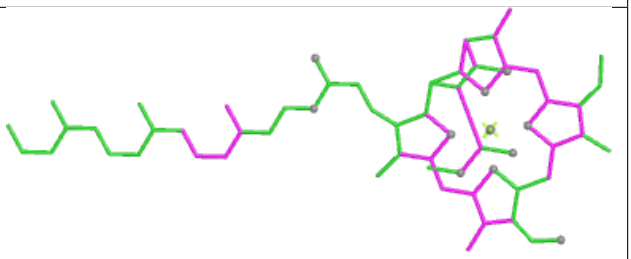


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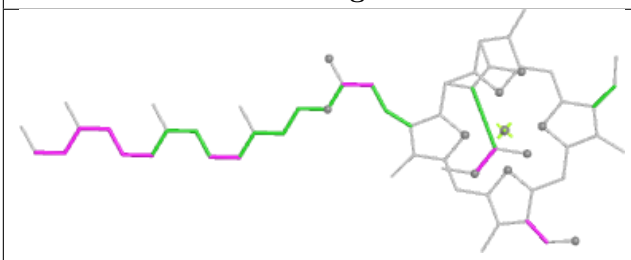
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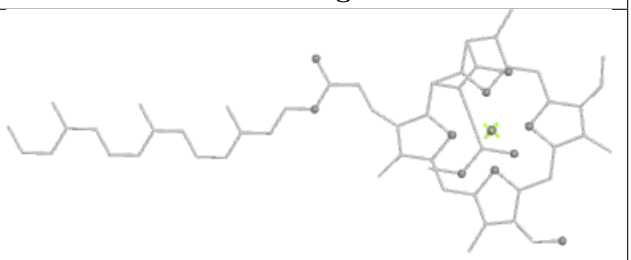
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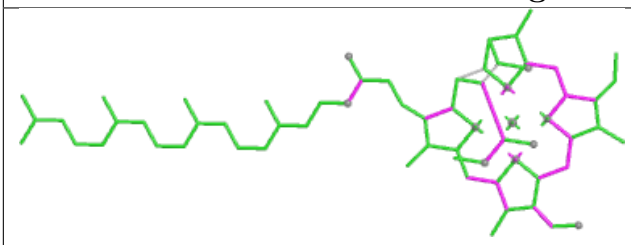


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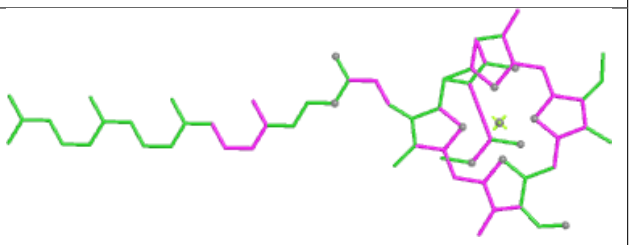


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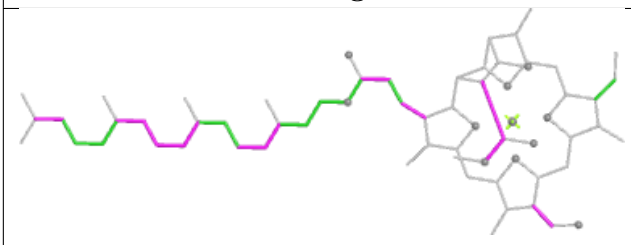
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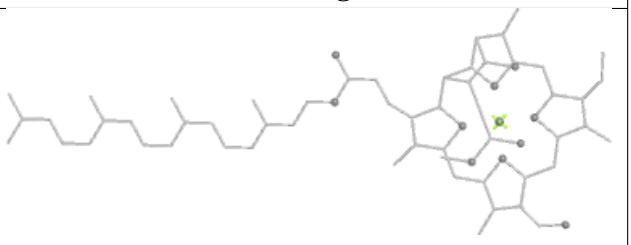
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Bond angles

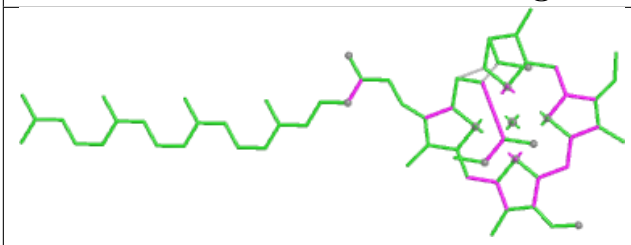


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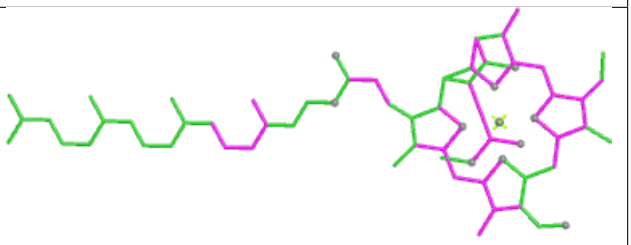


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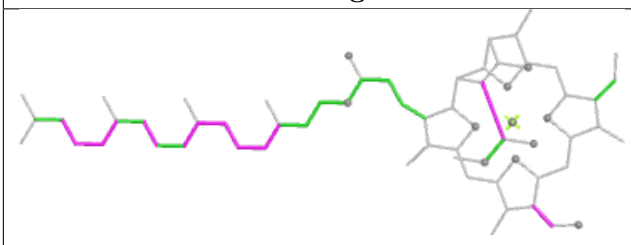
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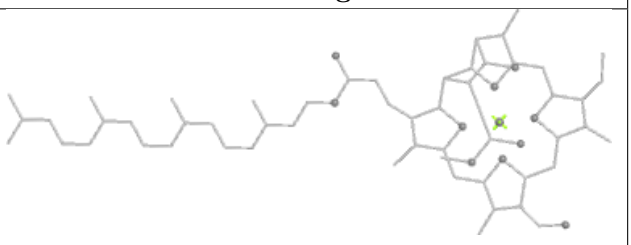
Bond lengths



Bond angles

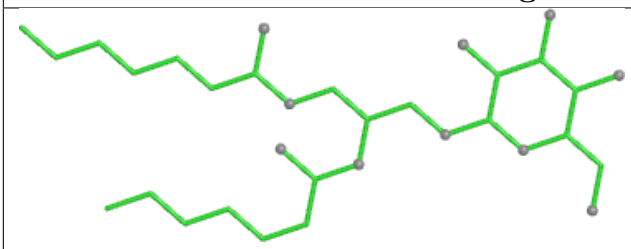


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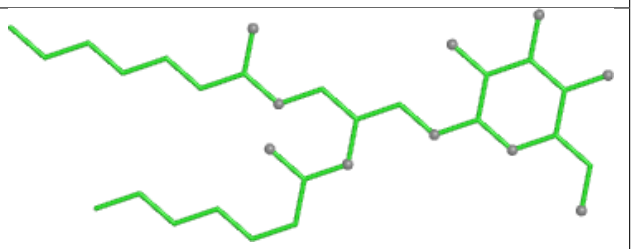


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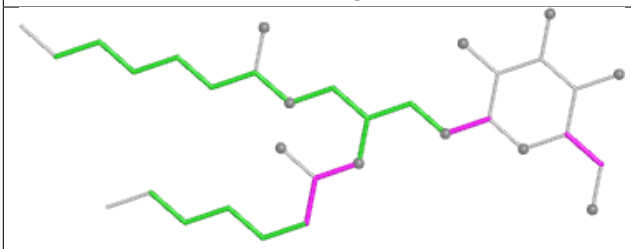
Ligand LMG D 410



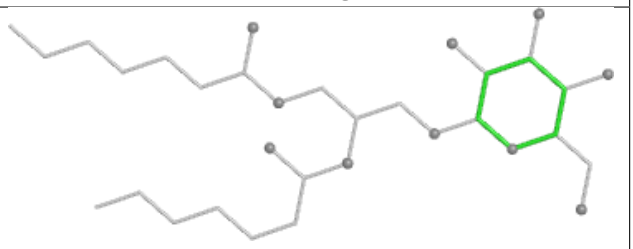
Bond lengths



Bond angles

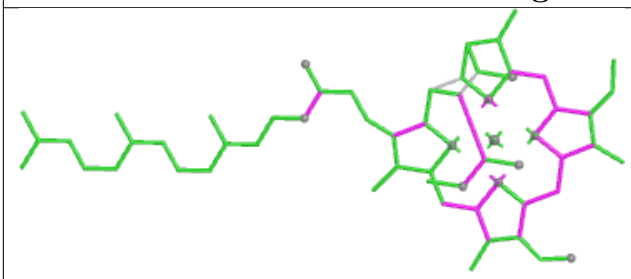


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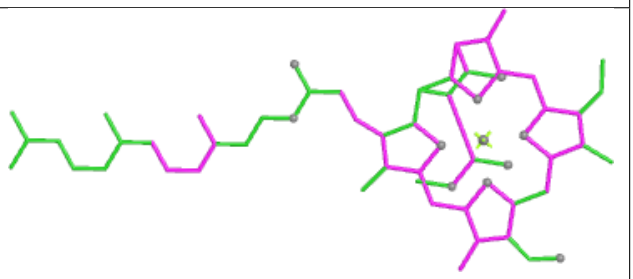


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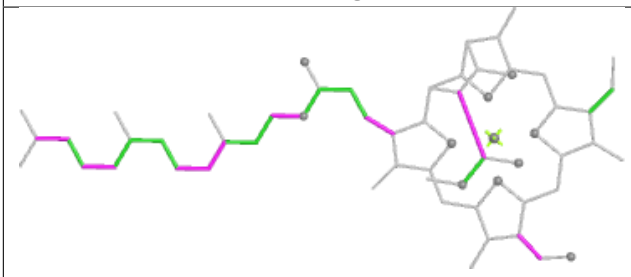
Ligand CL7 b 615



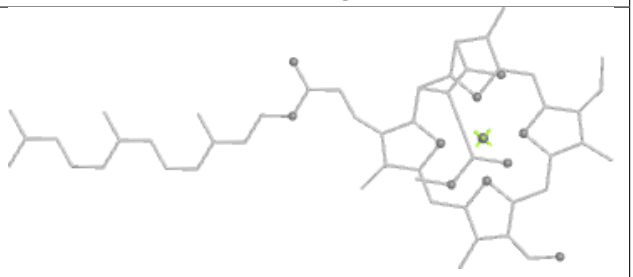
Bond lengths



Bond angles

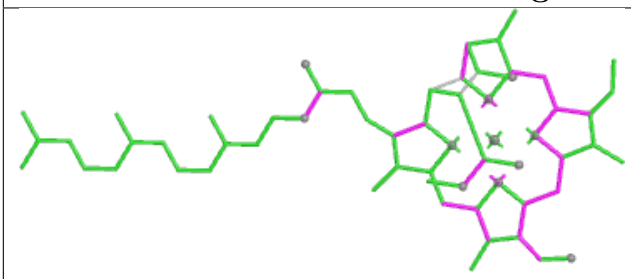


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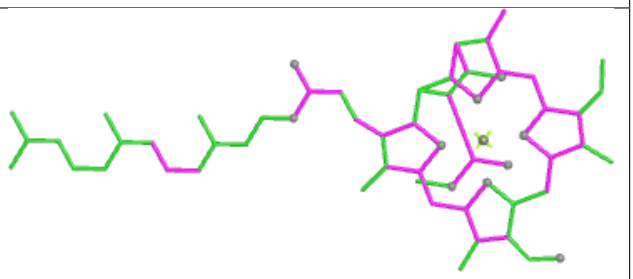


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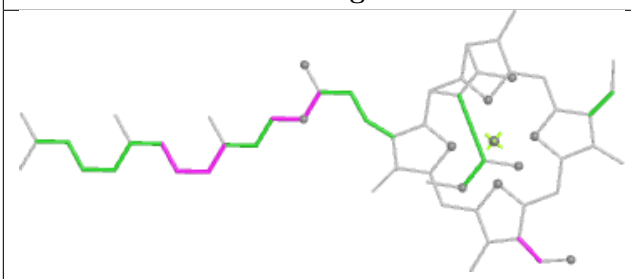
Ligand CL7 b 603



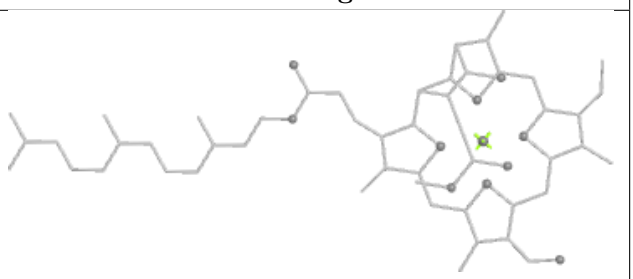
Bond lengths



Bond angles

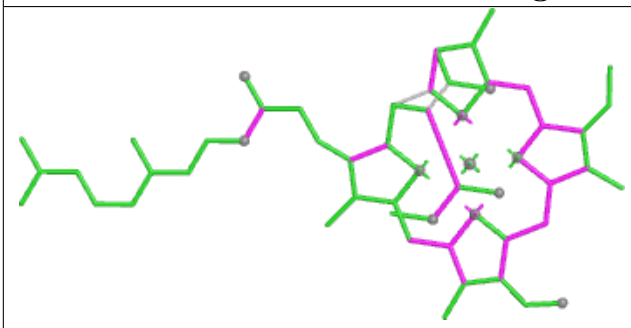


Torsions

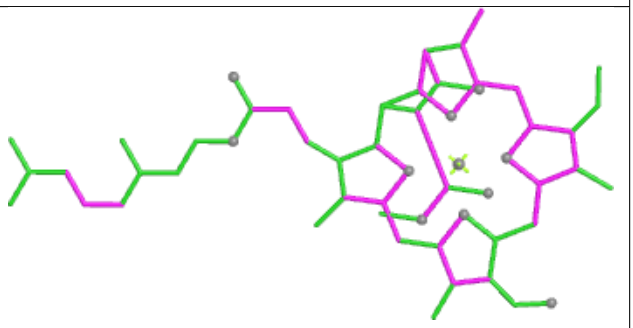


Rings

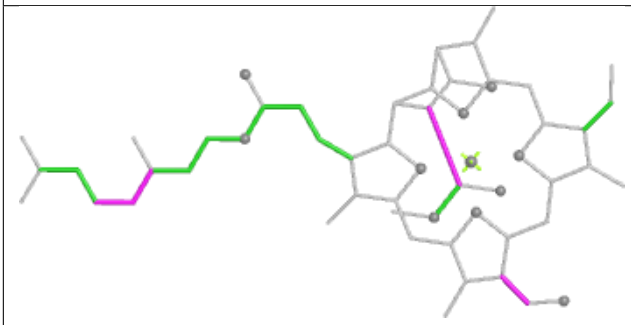
Ligand CL7 b 614



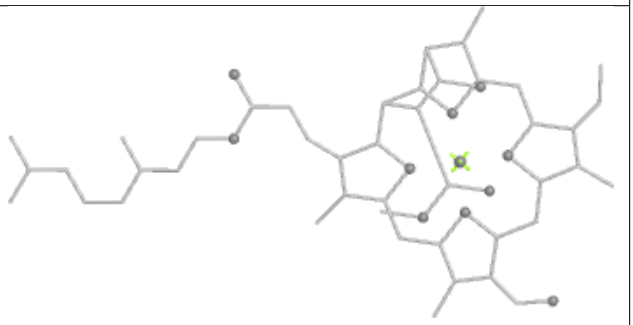
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Bond angles

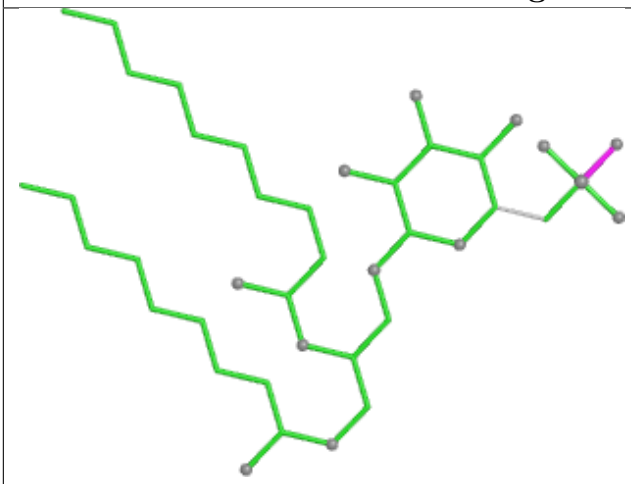


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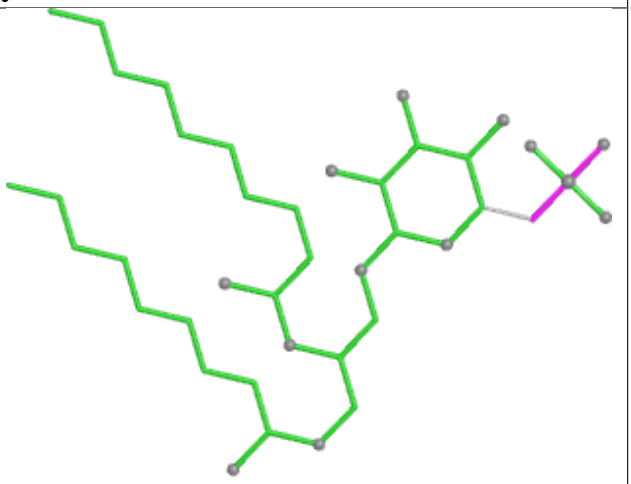


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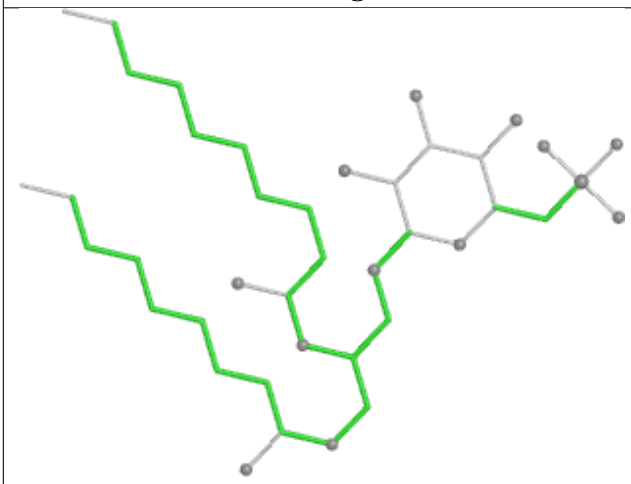
Ligand SQD 6 523



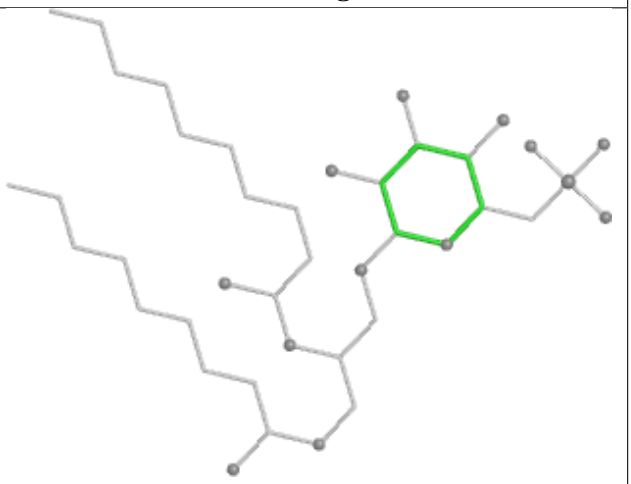
Bond lengths



Bond angles

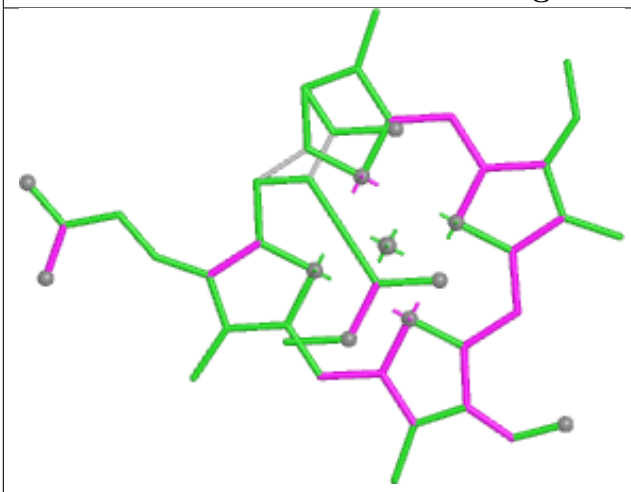


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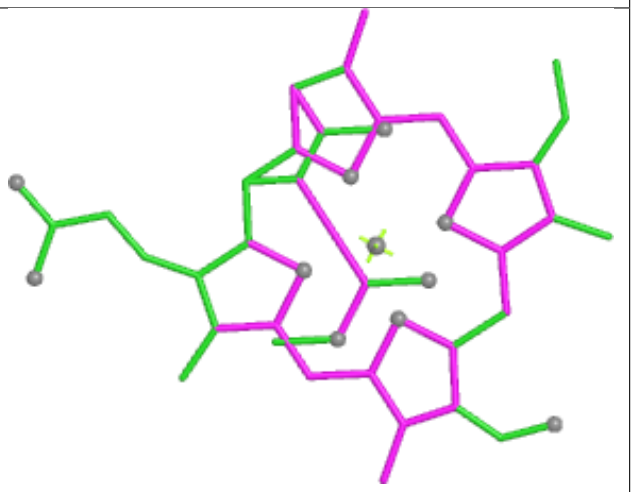


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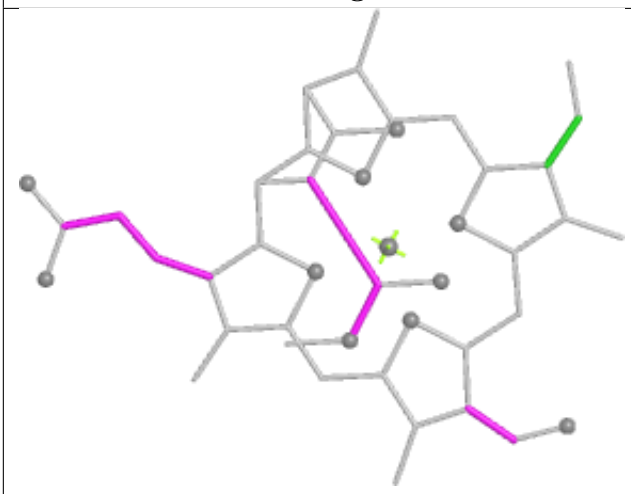
Ligand CL7 4 410



Bond lengths



Bond angles

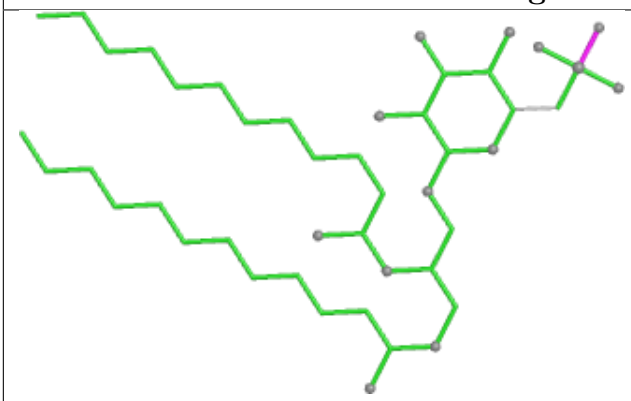


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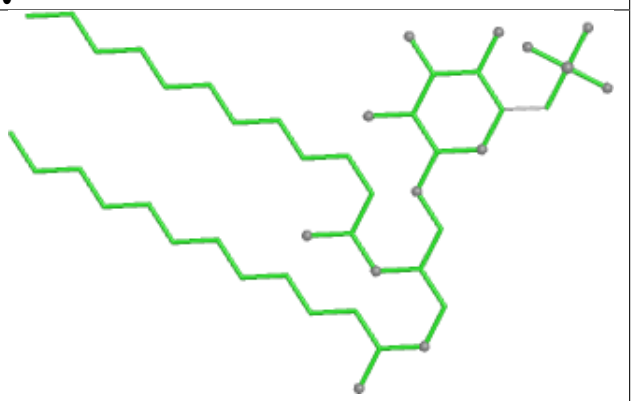


Rings

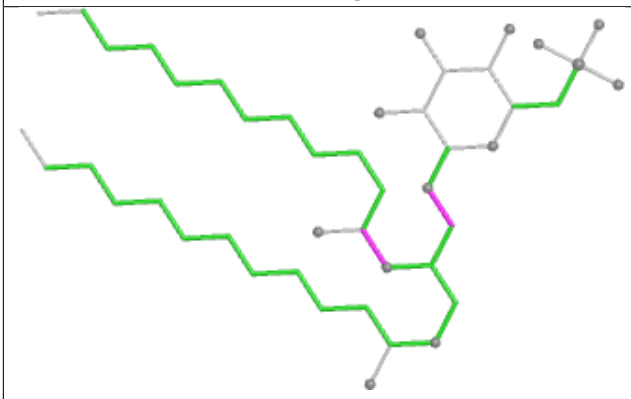
Ligand SQD 7 521



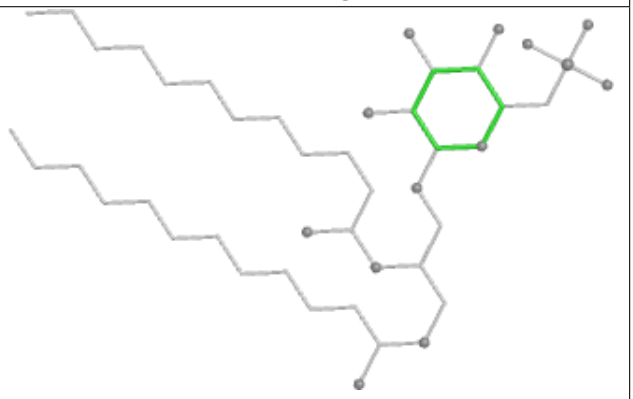
Bond lengths



Bond angles

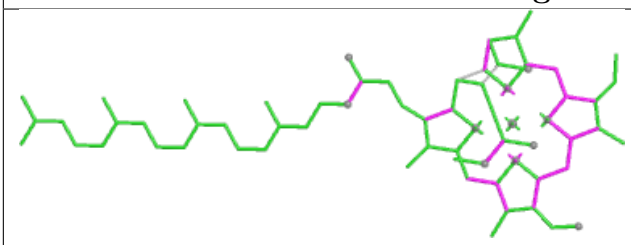


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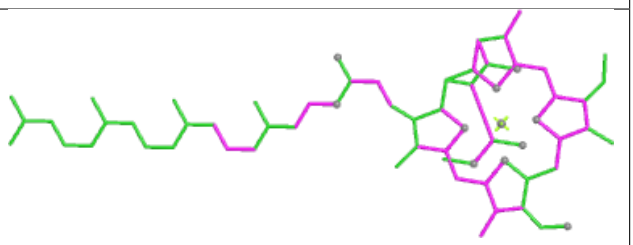


Rings

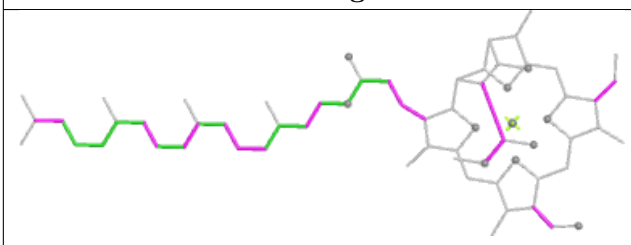
Ligand CL7 a 405



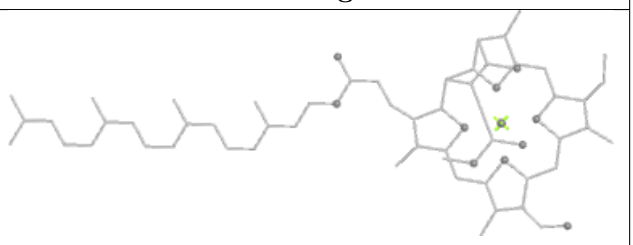
Bond lengths



Bond angles

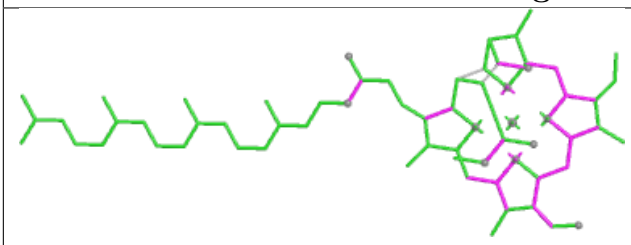


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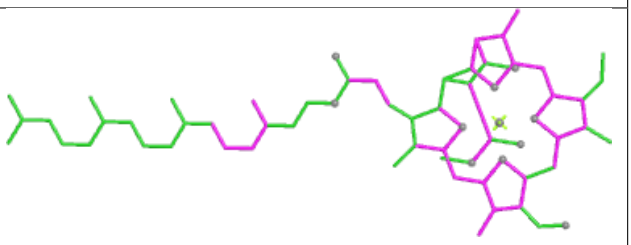


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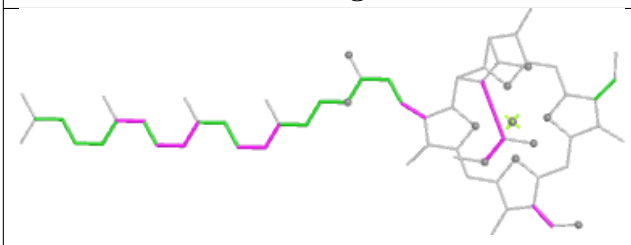
Ligand CL7 2 506



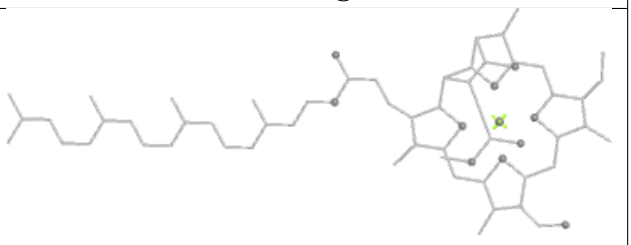
Bond lengths



Bond angles

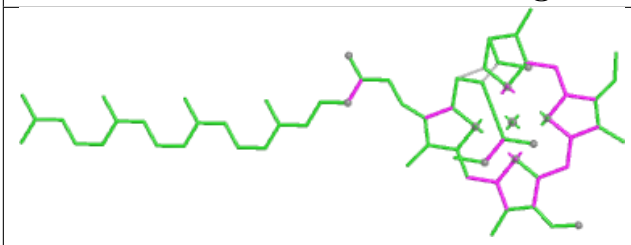


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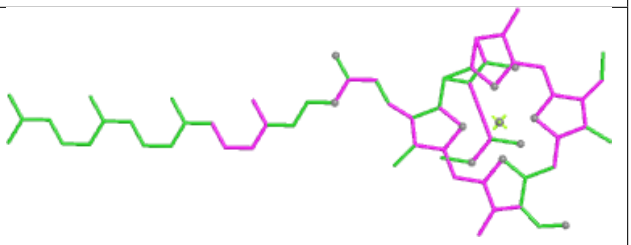


Rings

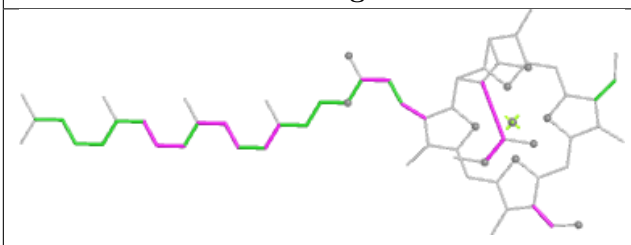
Ligand CL7 7 510



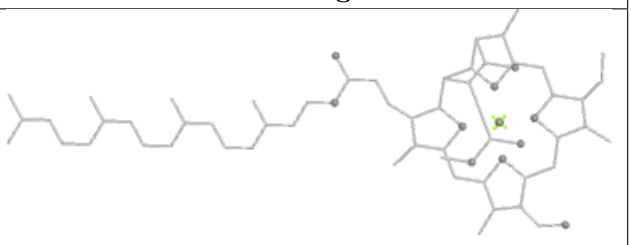
Bond lengths



Bond angles

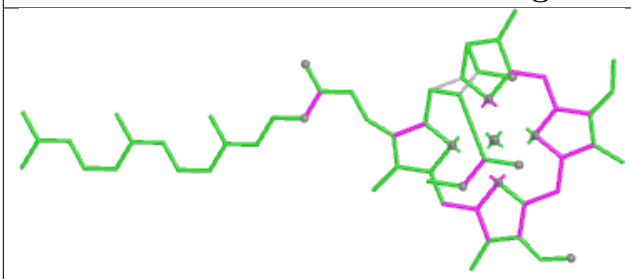


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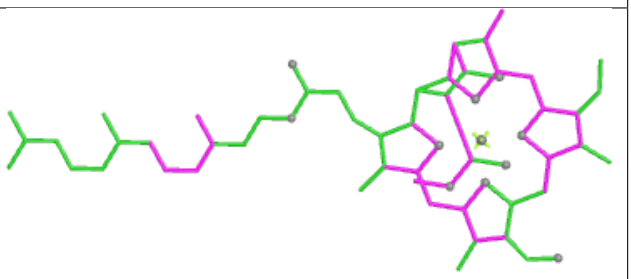


Rings

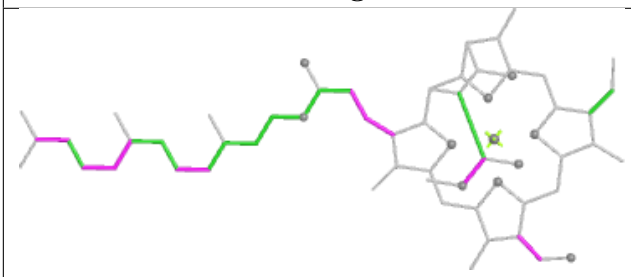
Ligand CL7 b 608



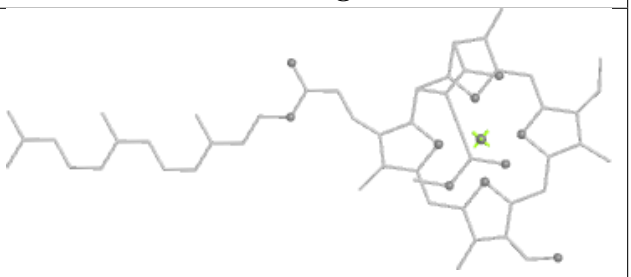
Bond lengths



Bond angles

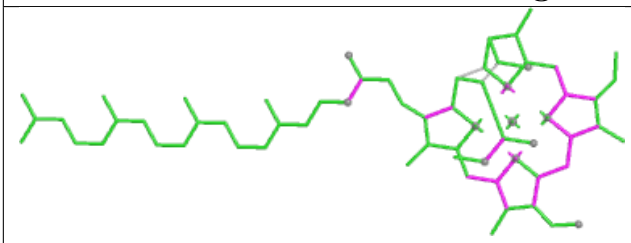


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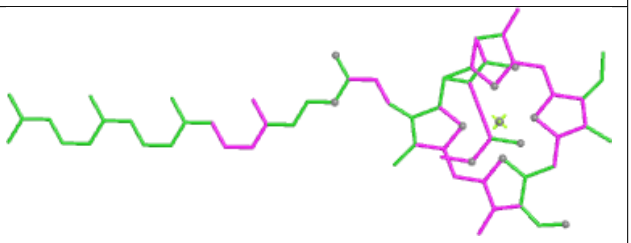


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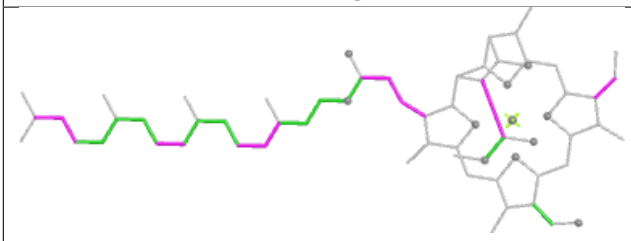
Ligand CL7 3 505



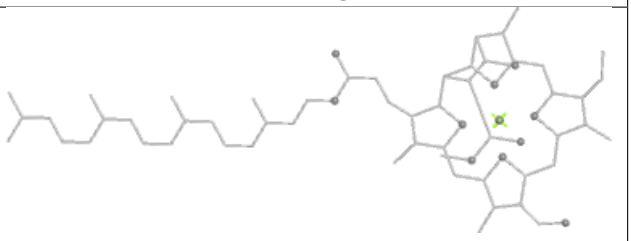
Bond lengths



Bond angles

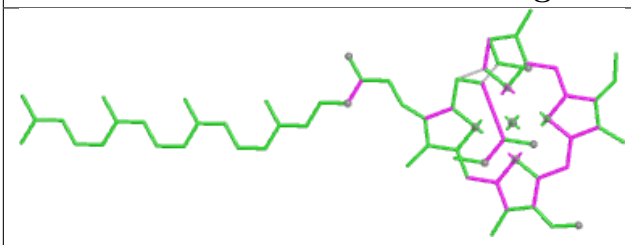


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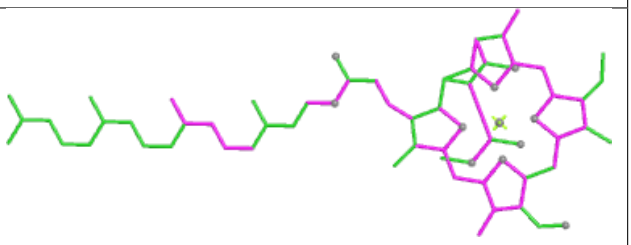


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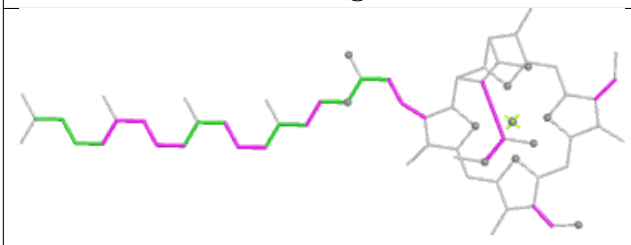
Ligand CL7 c 506



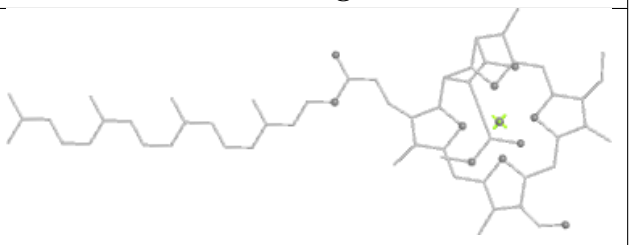
Bond lengths



Bond angles

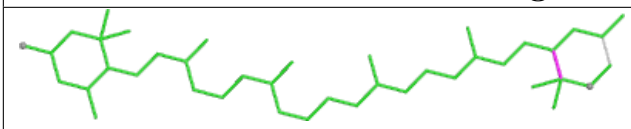


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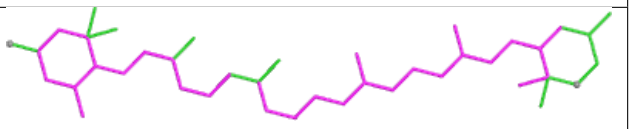


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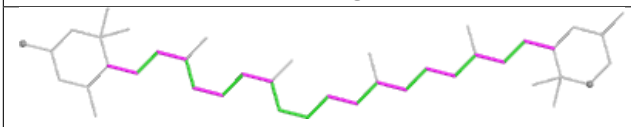
Ligand ZEX 1 421



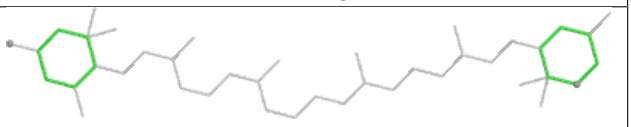
Bond lengths



Bond angles

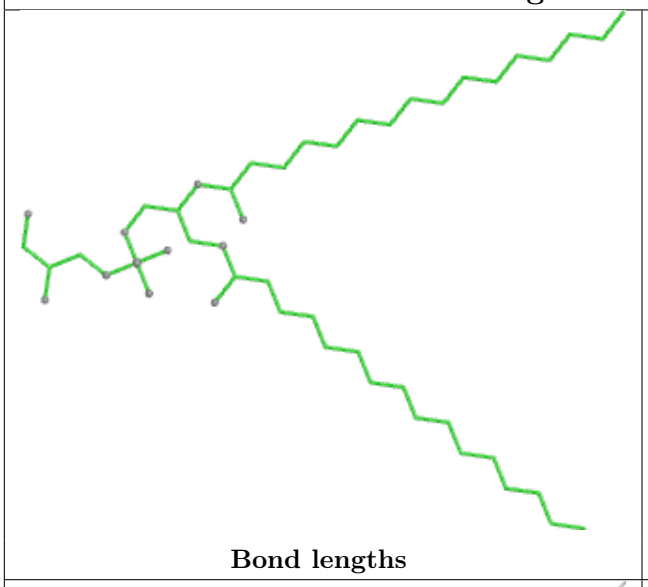


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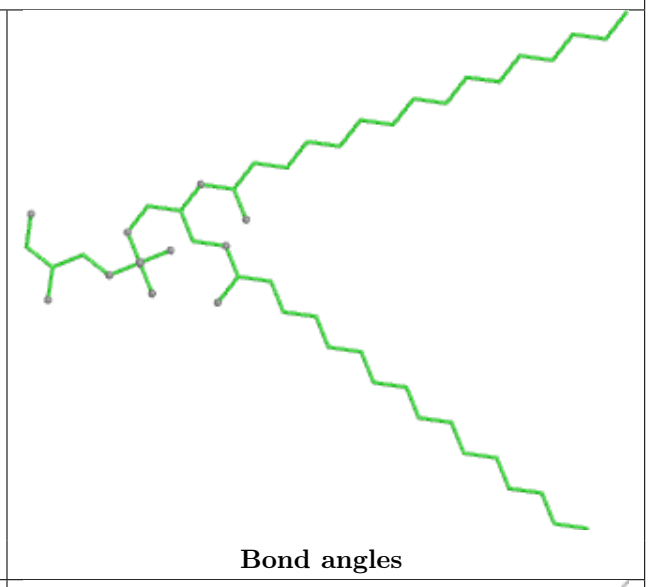


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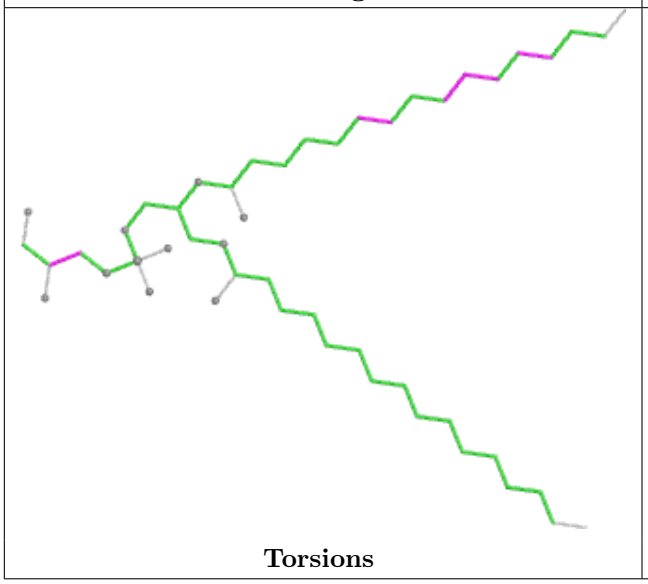
Ligand LHG b 626



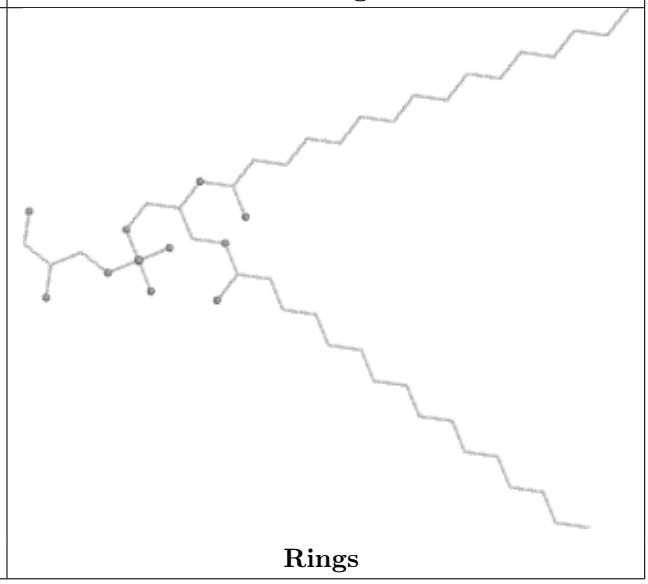
Bond lengths



Bond angles



Torsions

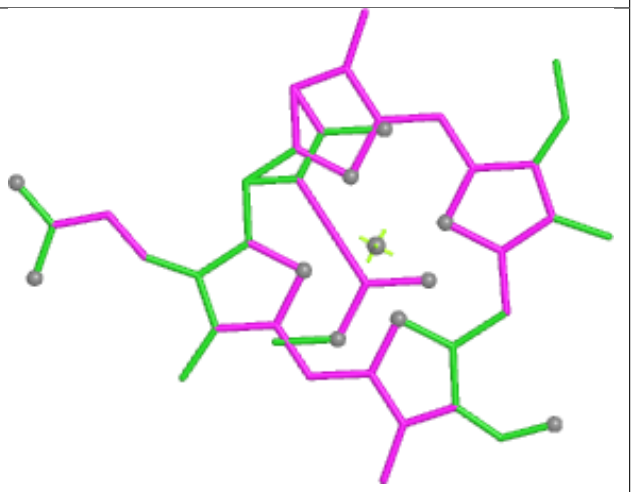


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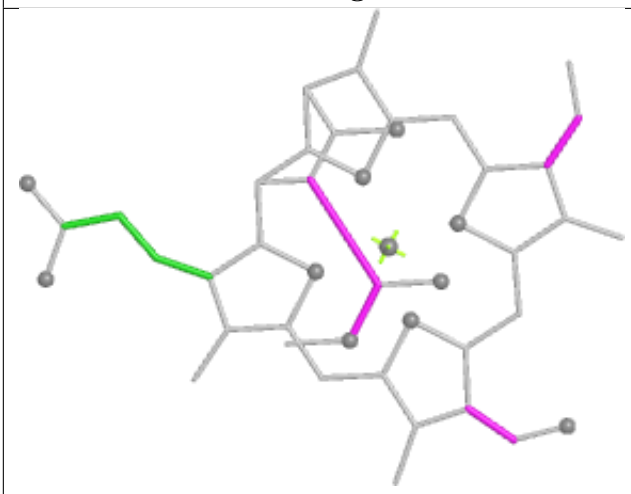
Ligand CL7 5 420



Bond lengths



Bond angles

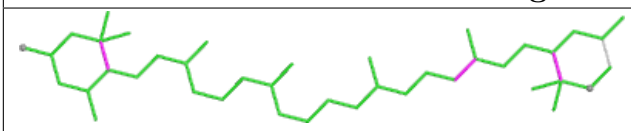


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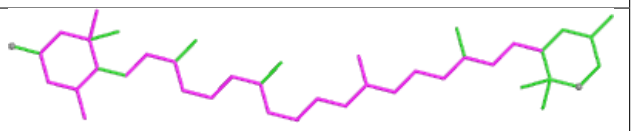


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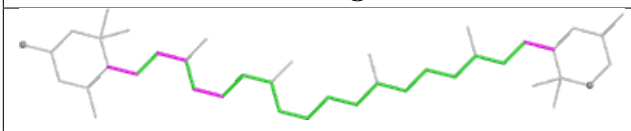
Ligand ZEX 2 521



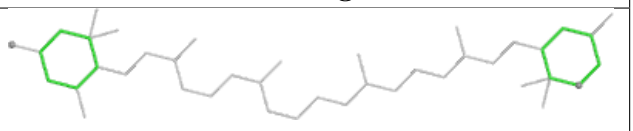
Bond lengths



Bond angles

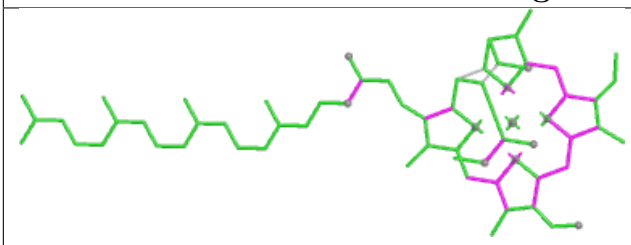


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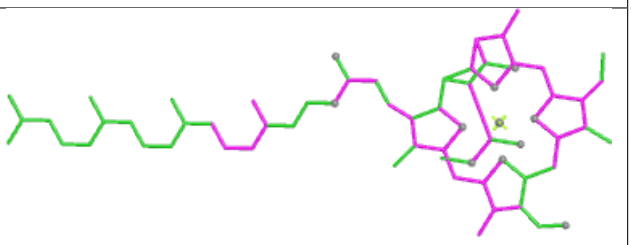


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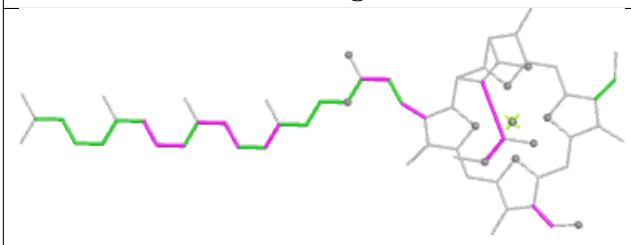
Ligand CL7 3 510



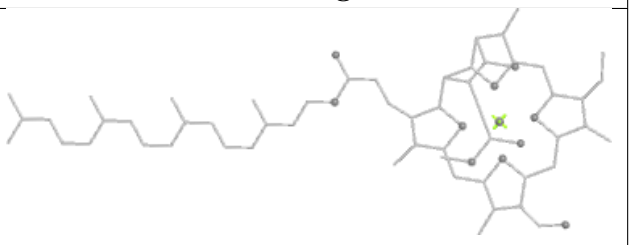
Bond lengths



Bond angles

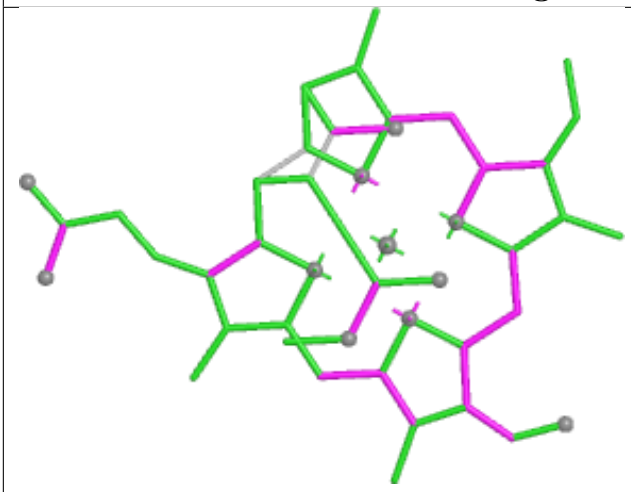


Torsions



Rings

Ligand CL7 5 412



Bond lengths



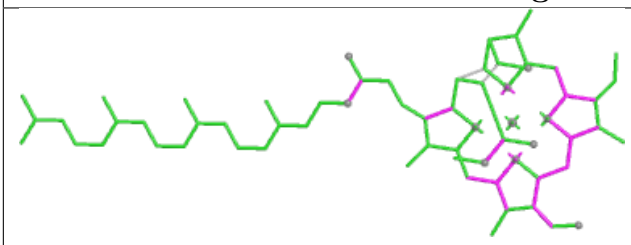
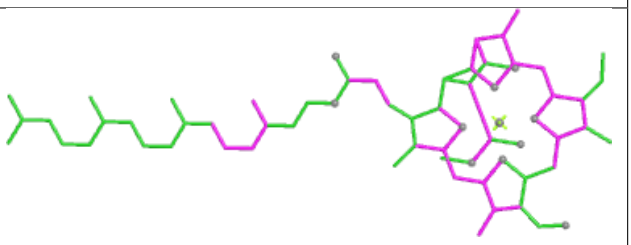
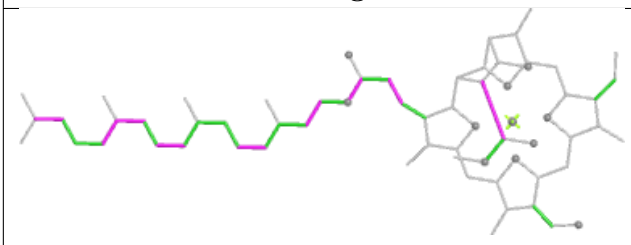
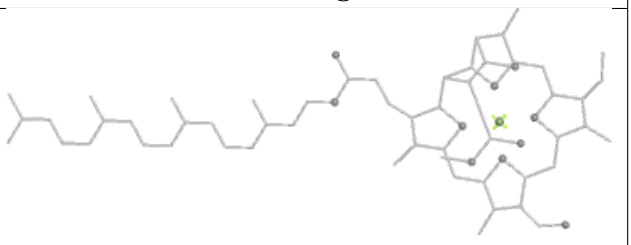
Bond angles

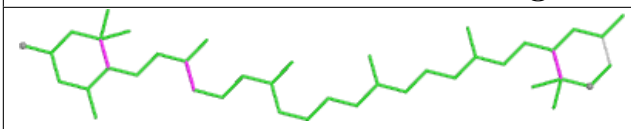
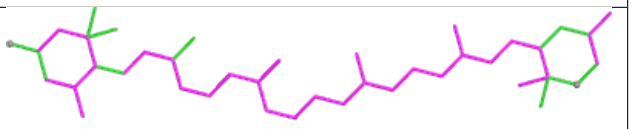
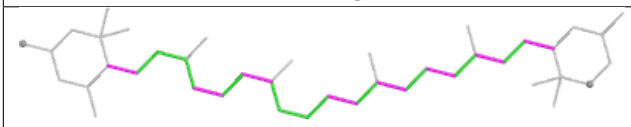
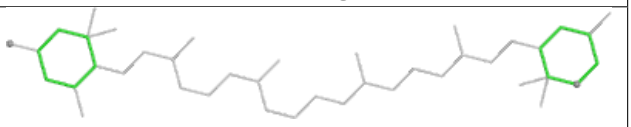


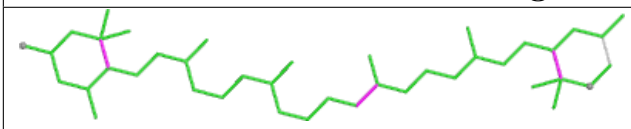
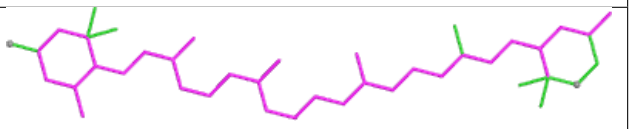
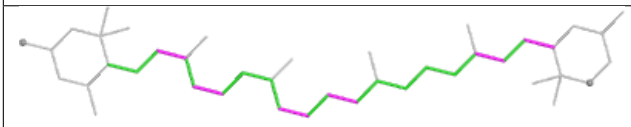
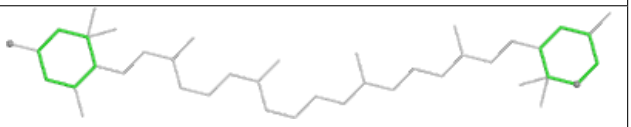
Torsions



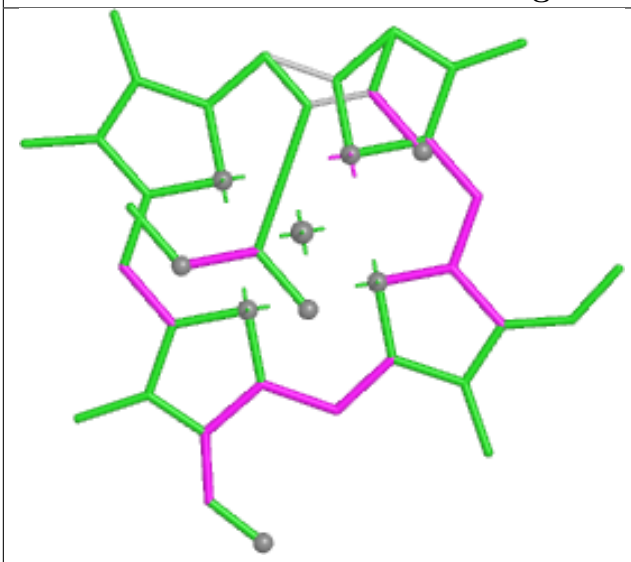
Rings

Ligand CL7 b 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

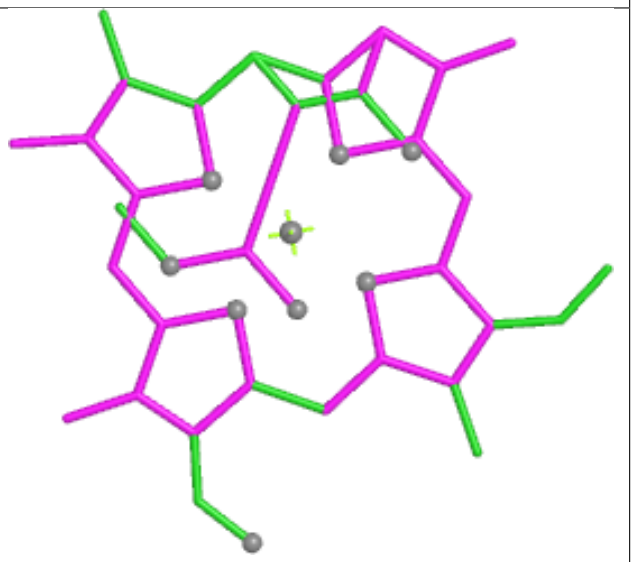
Ligand ZEX 8 420	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand ZEX 8 419	
	
Bond lengths	Bond angles
	
Torsions	Rings

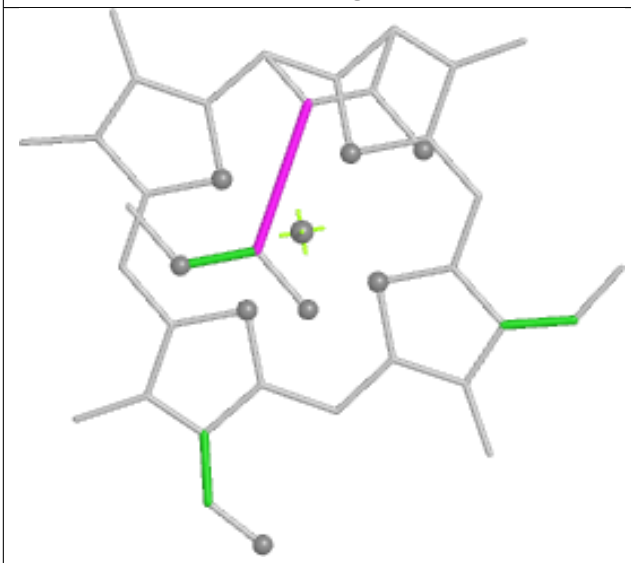
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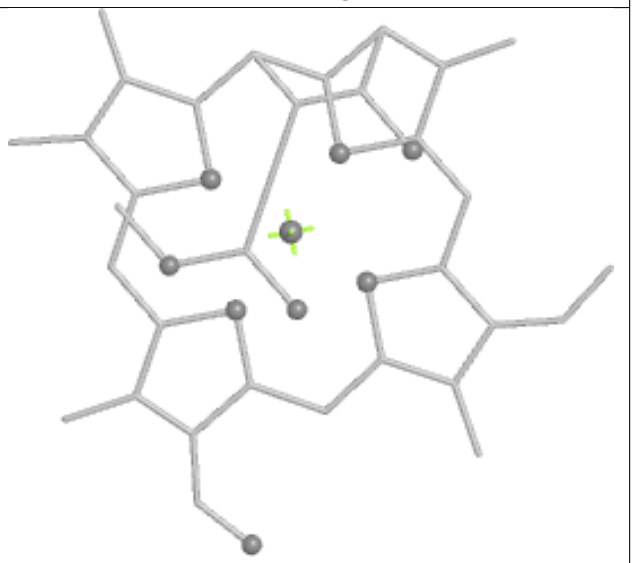
Bond lengths



Bond angles

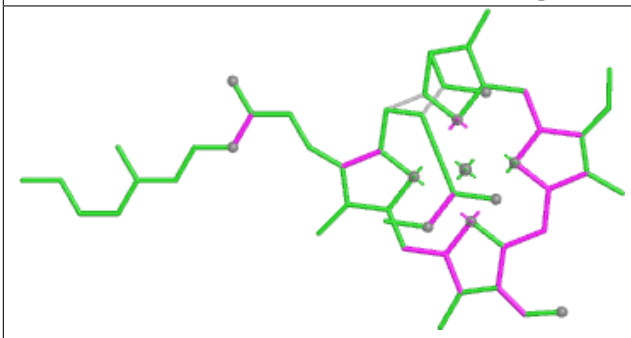


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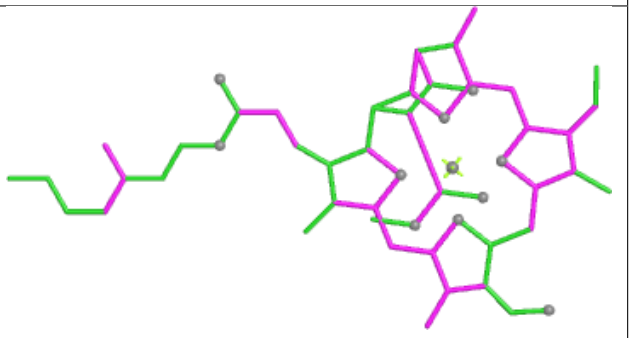


Rings

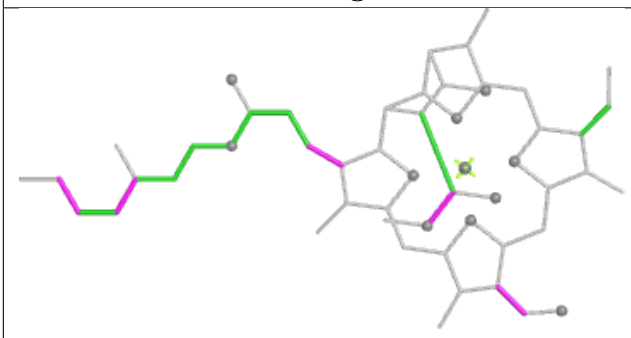
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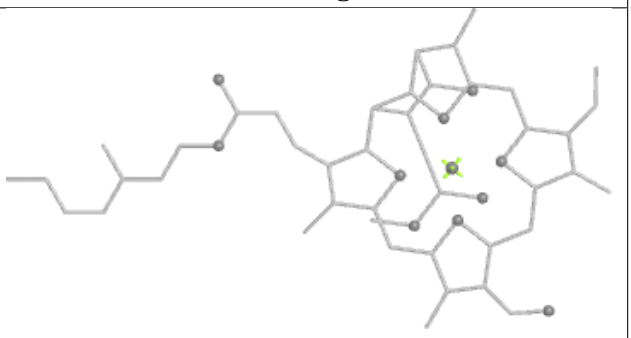
Bond lengths



Bond angles

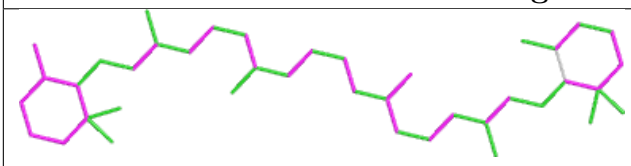


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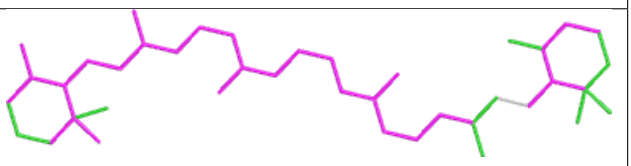


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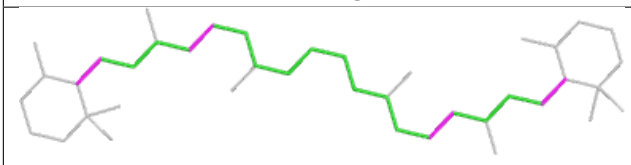
Ligand 8CT 8 402



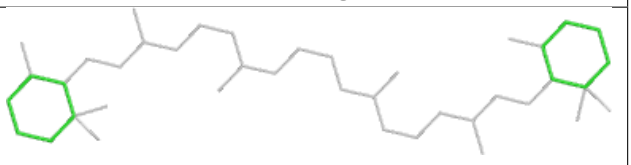
Bond lengths



Bond angles

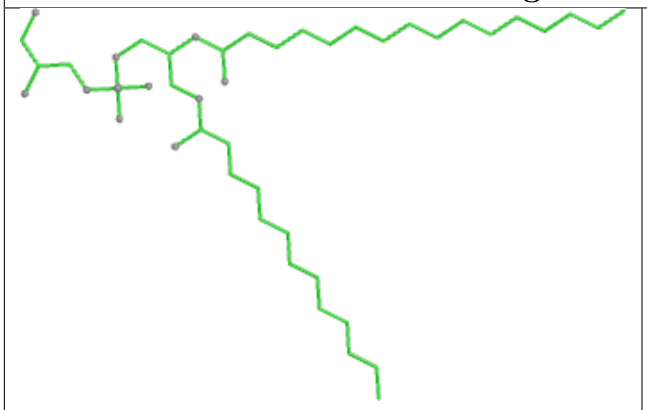


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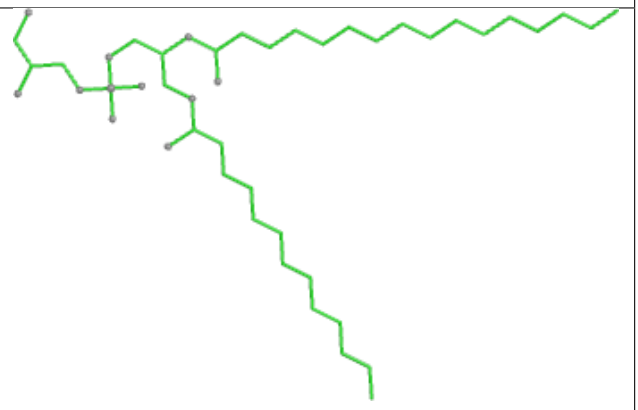


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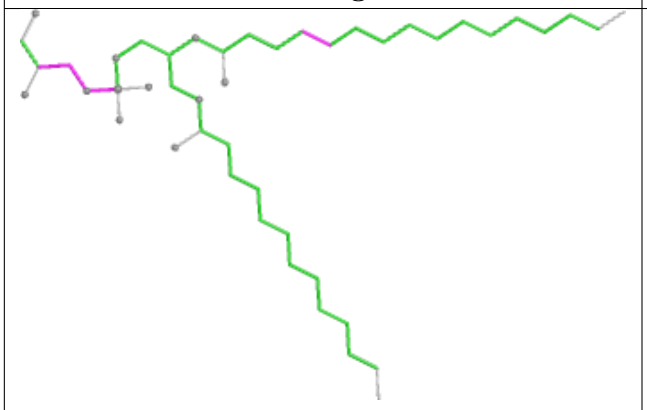
Ligand LHG A 407



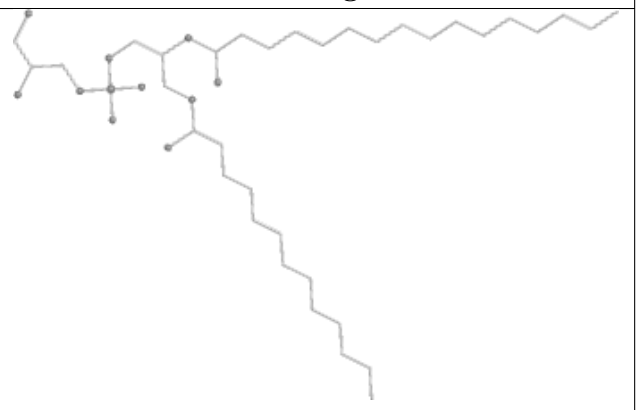
Bond lengths



Bond angles

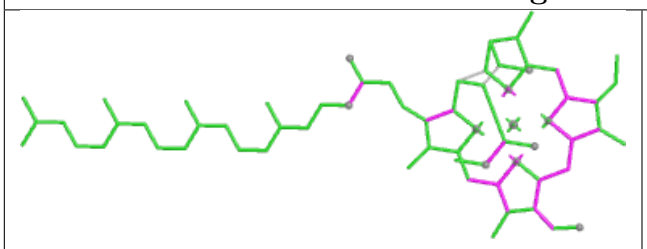


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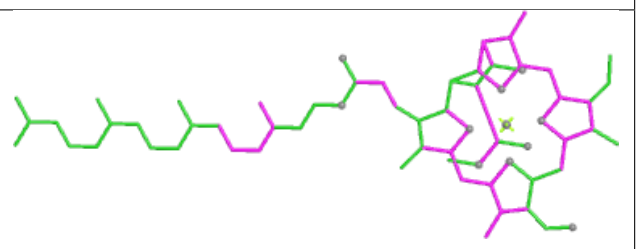


Rings

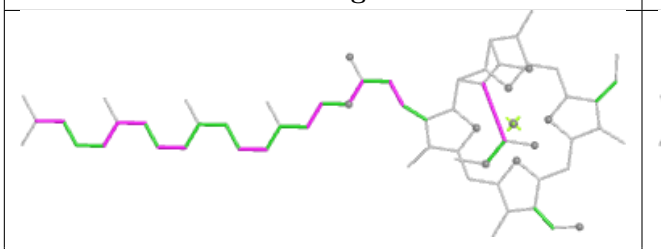
Ligand CL7 B 610



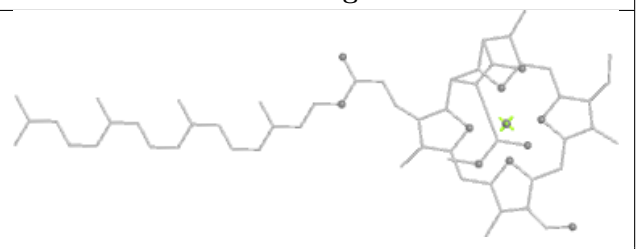
Bond lengths



Bond angles

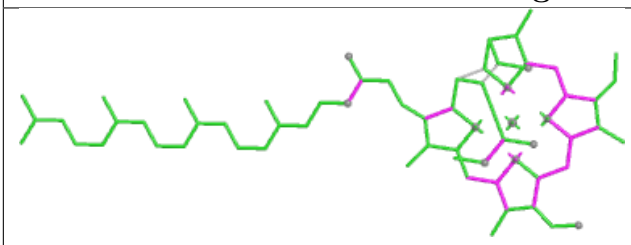


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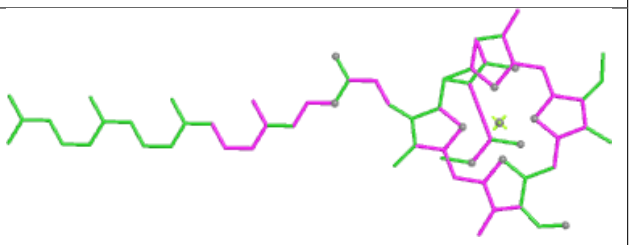


Rings

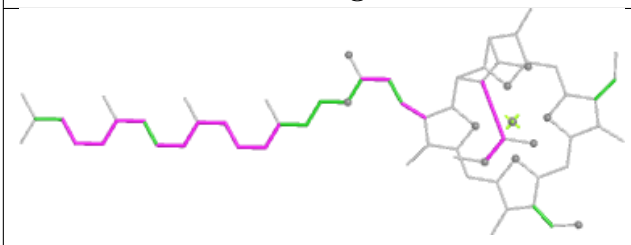
Ligand CL7 2 510



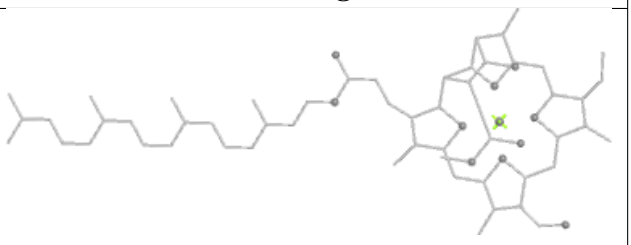
Bond lengths



Bond angles

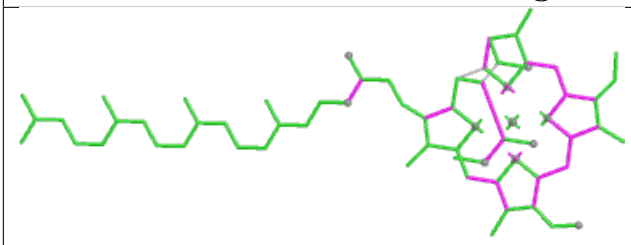


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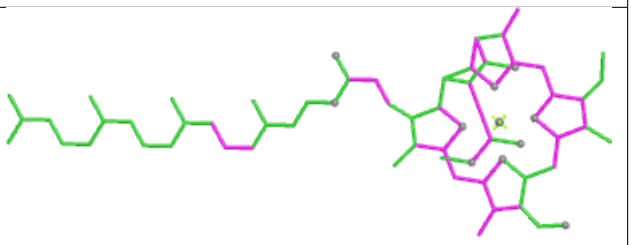


Rings

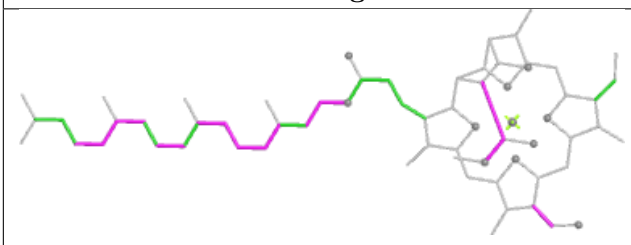
Ligand CL7 6 509



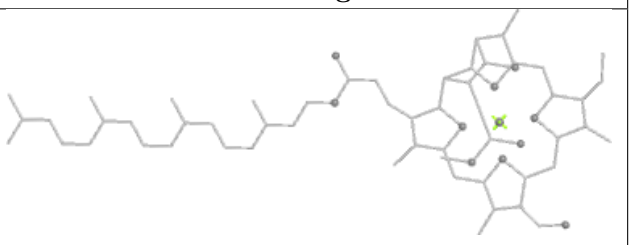
Bond lengths



Bond angles

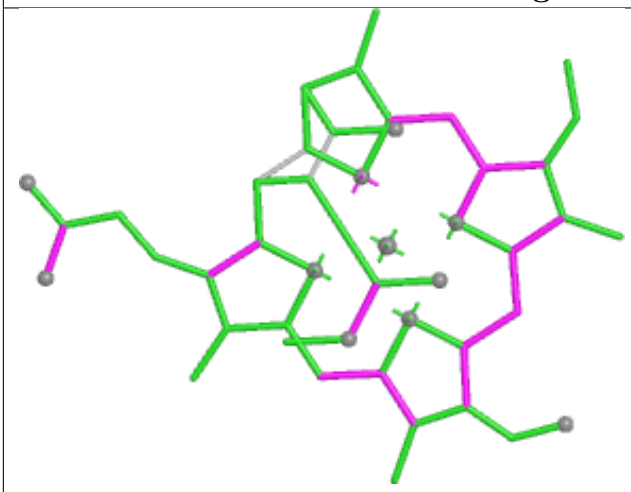


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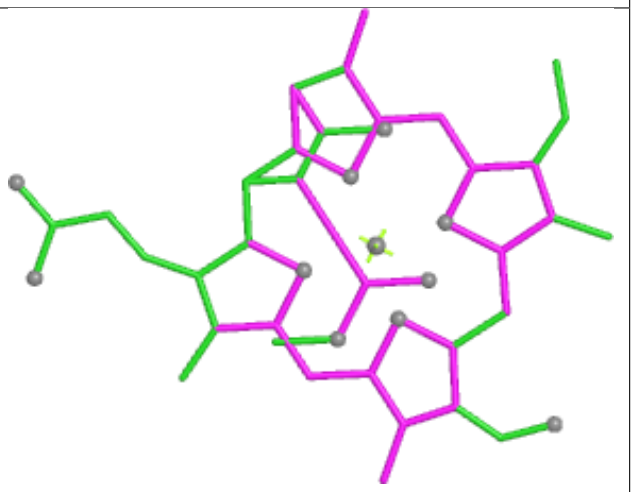


Rings

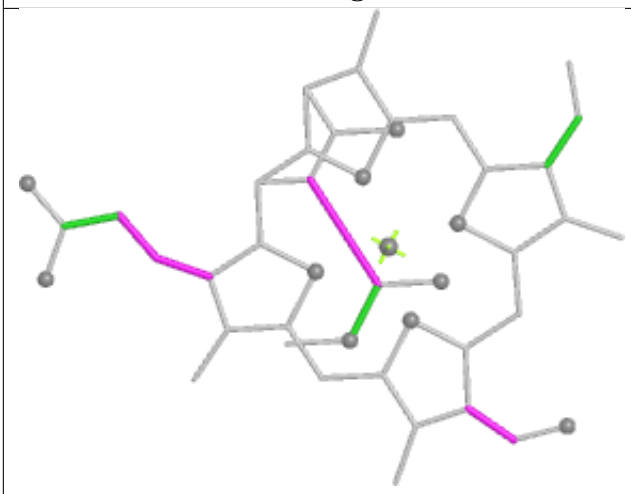
Ligand CL7 6 513



Bond lengths



Bond angles

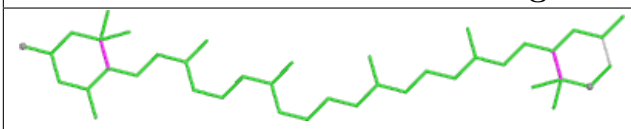


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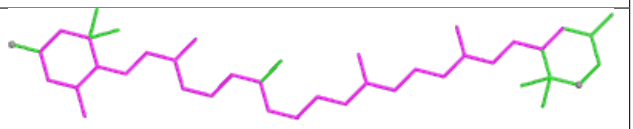


Rings

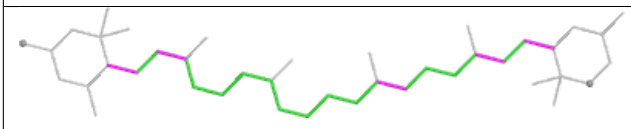
Ligand ZEX 7 520



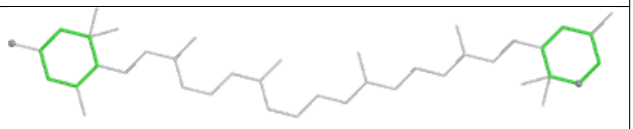
Bond lengths



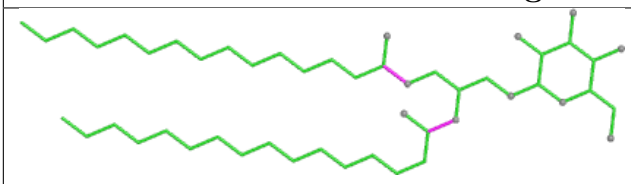
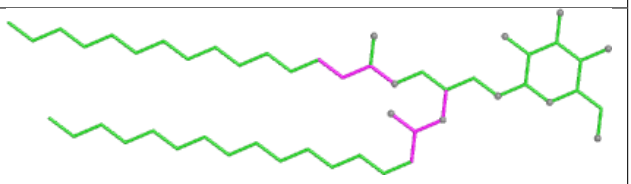
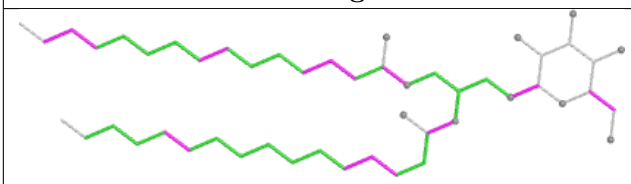
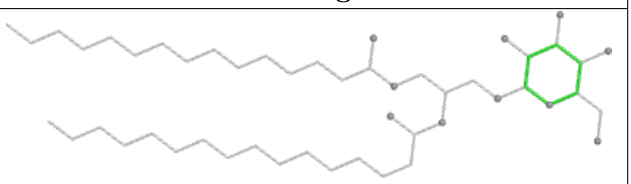
Bond angles

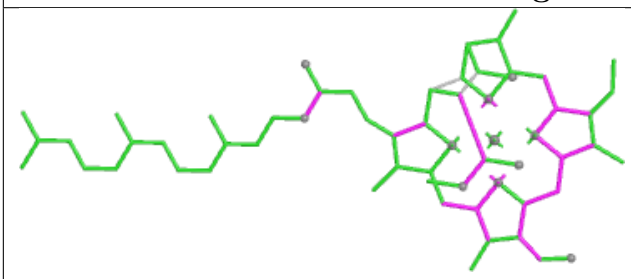
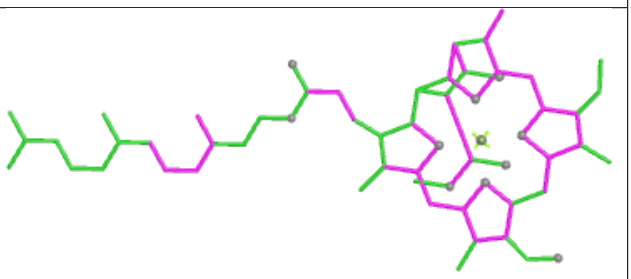
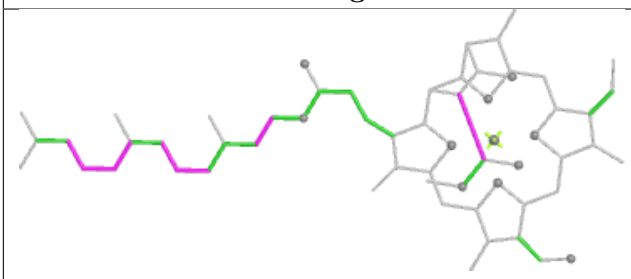
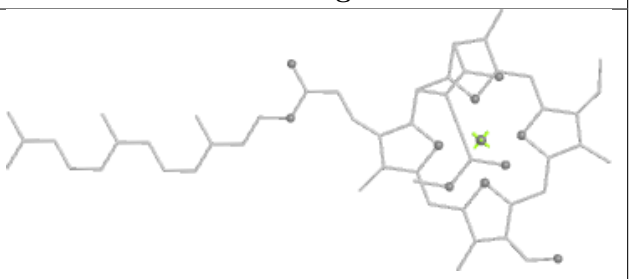


Torsions



Rings

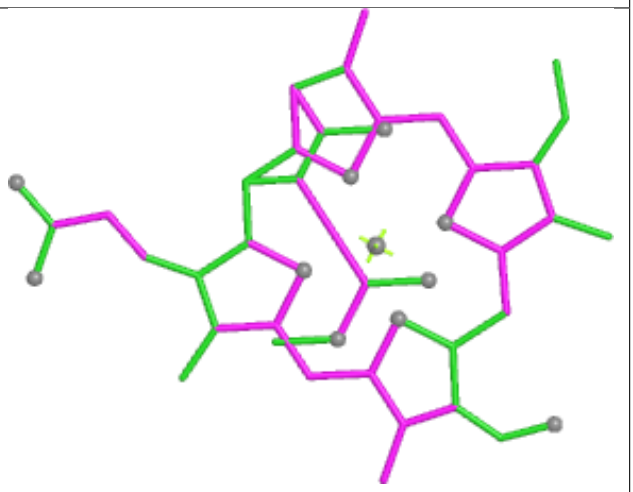
Ligand LMG c 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CL7 8 413	
 Bond lengths	 Bond angles
 Torsions	 Rings

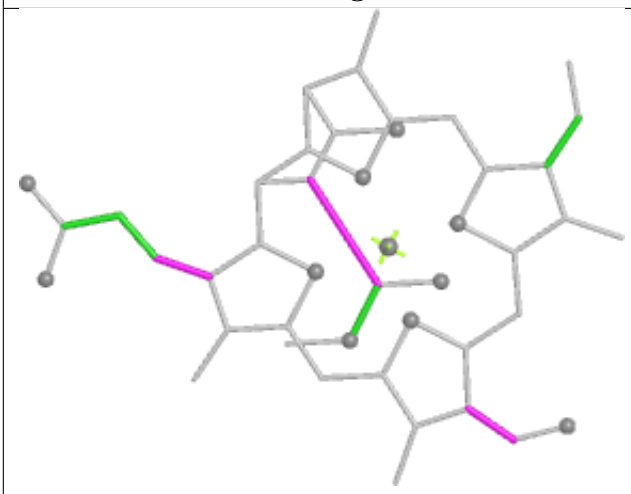
Ligand CL7 6 515



Bond lengths



Bond angles

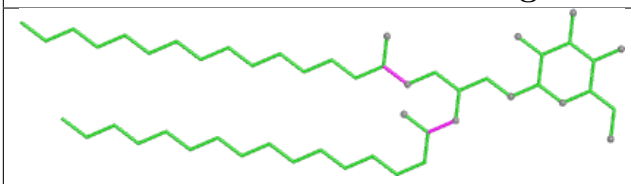


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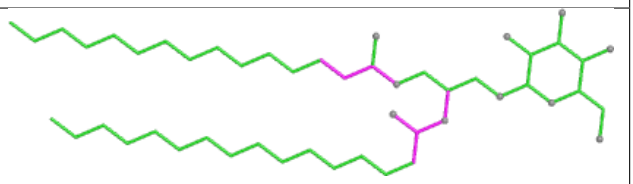


Rings

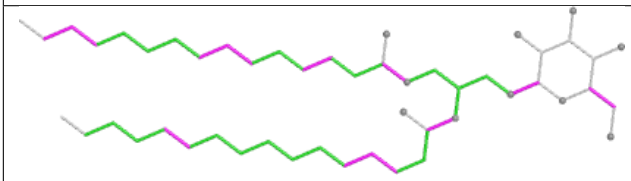
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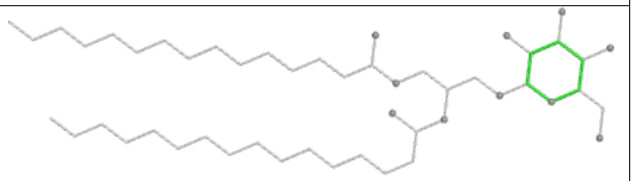
Bond lengths



Bond angles

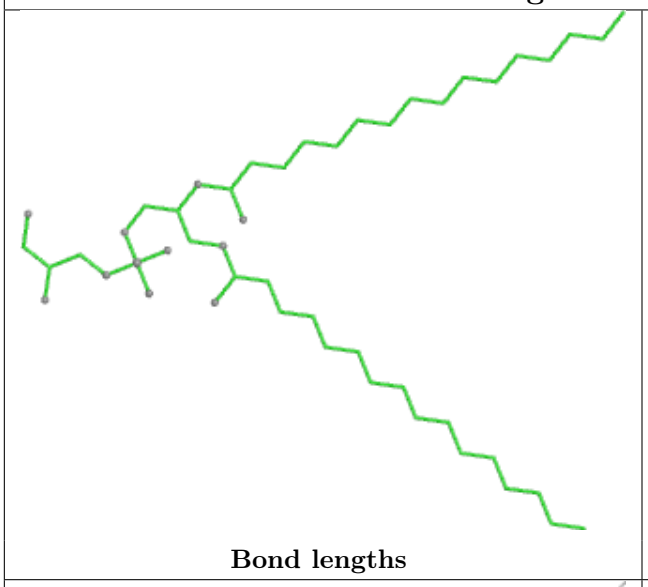


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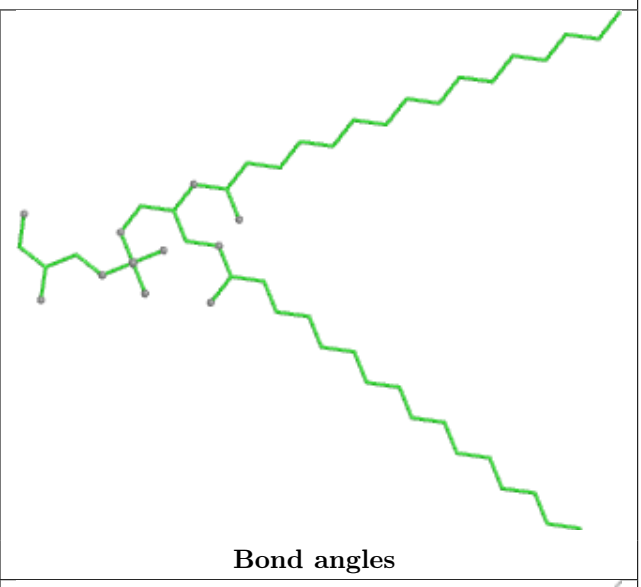


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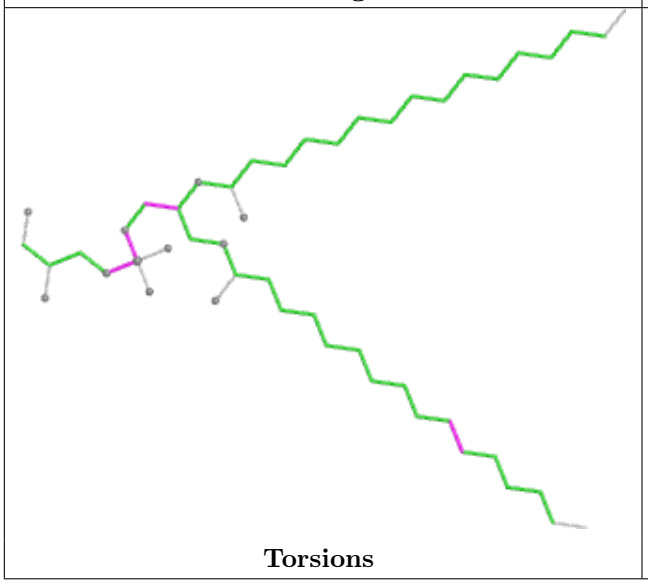
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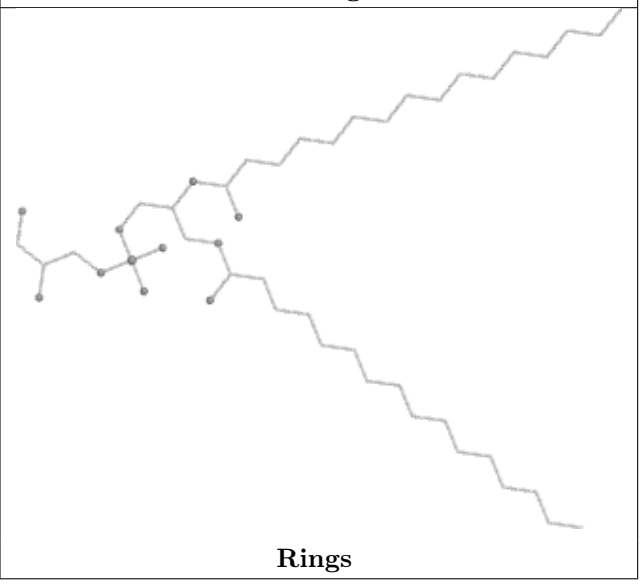
Bond lengths



Bond angles

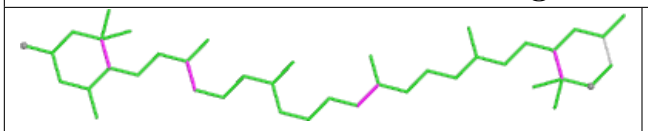


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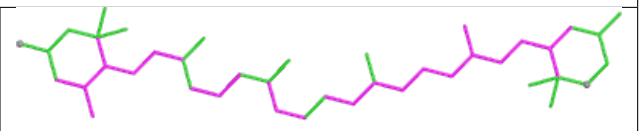


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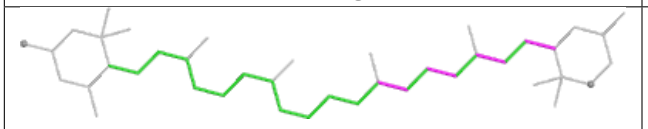
Ligand ZEX 6 522



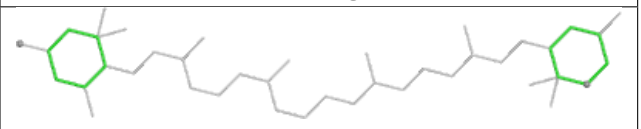
Bond lengths



Bond angles

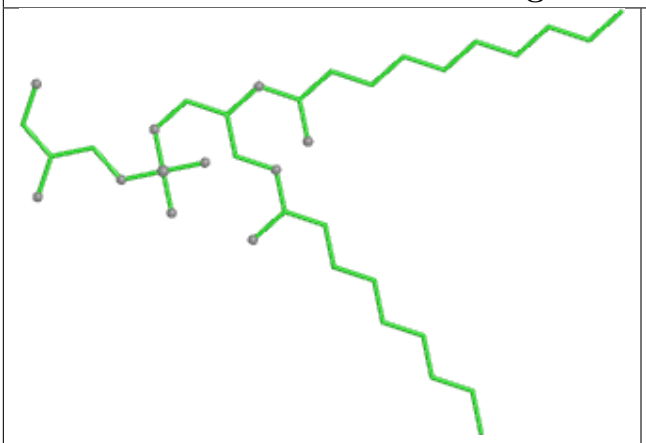


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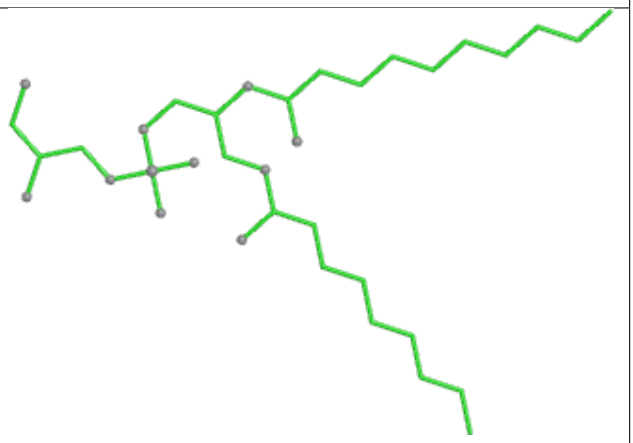


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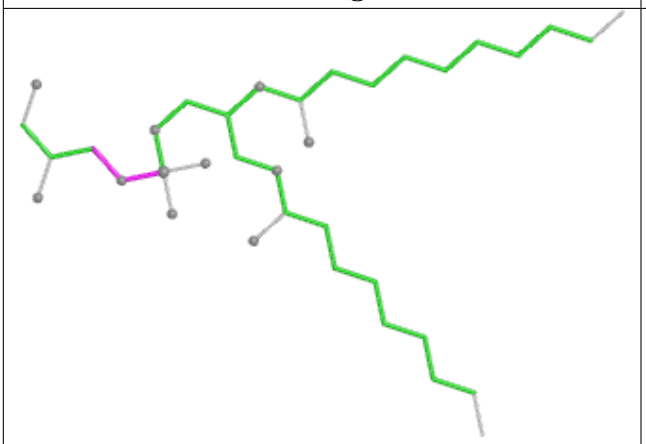
Ligand LHG 7 524



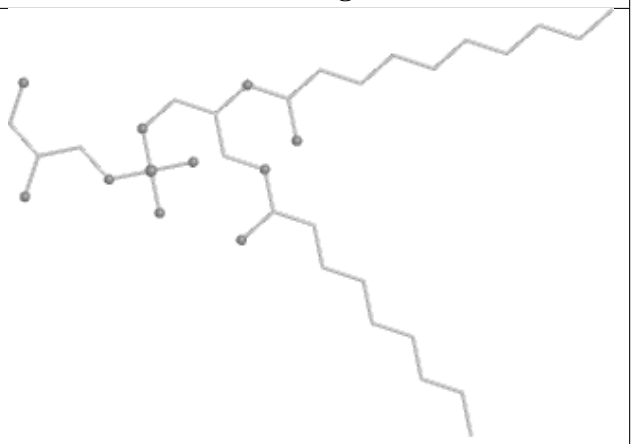
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Bond angles

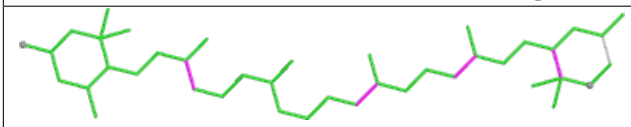


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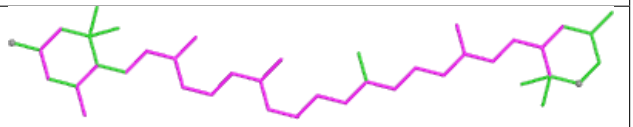


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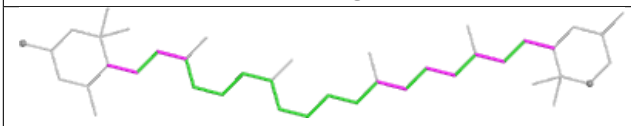
Ligand ZEX 3 519



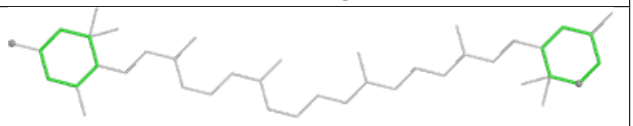
Bond lengths



Bond angles

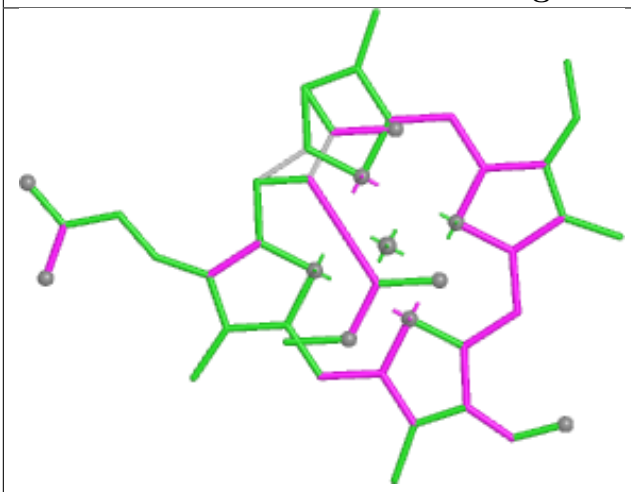


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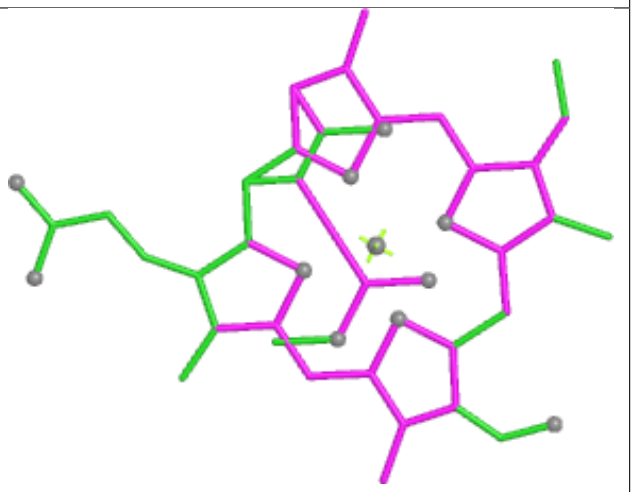


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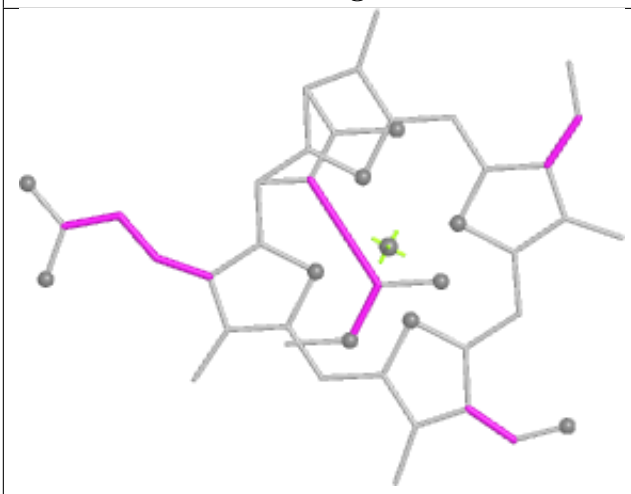
Ligand CL7 4 415



Bond lengths



Bond angles

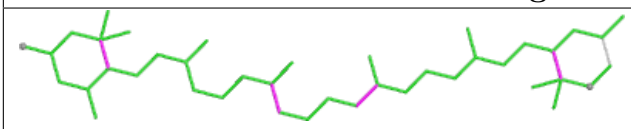


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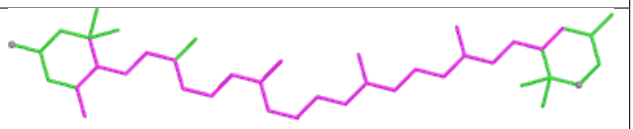


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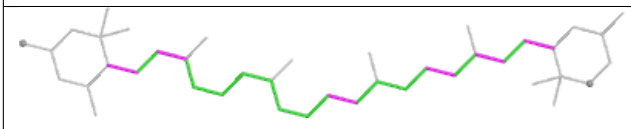
Ligand ZEX 8 403



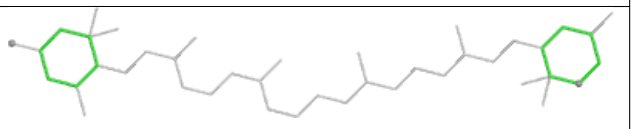
Bond lengths



Bond angles

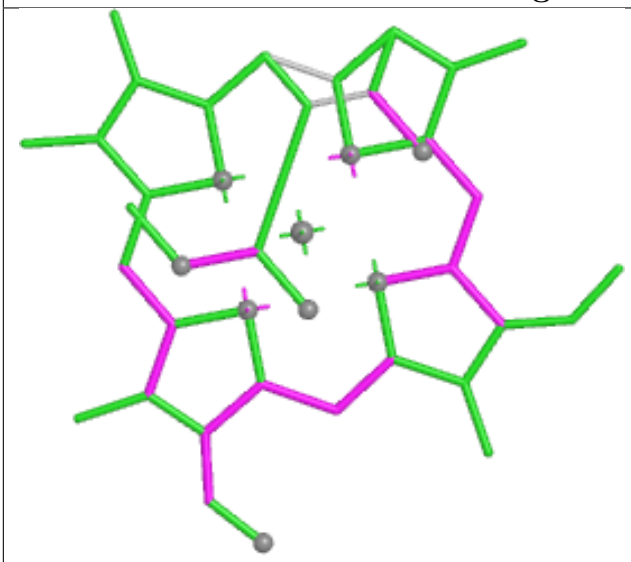


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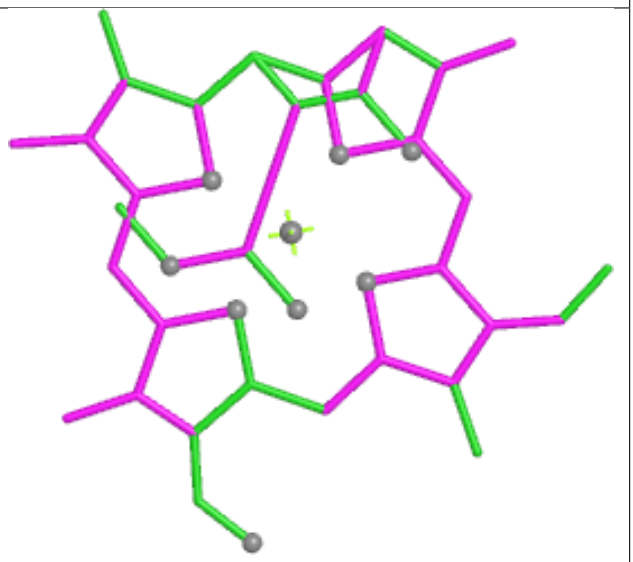


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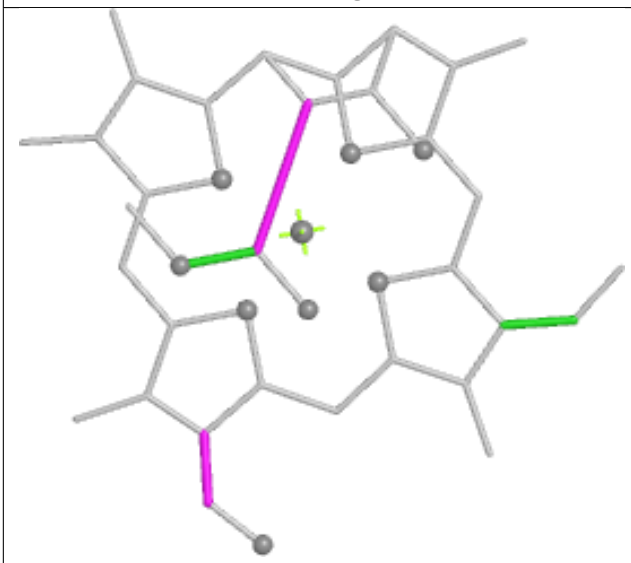
Ligand CL7 4 407



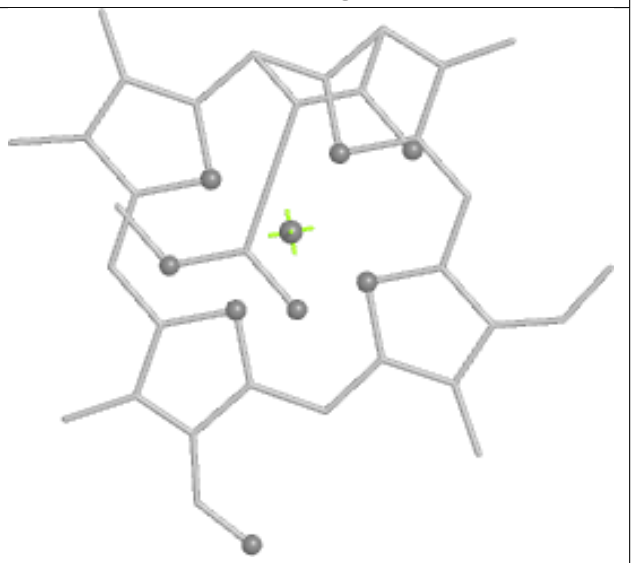
Bond lengths



Bond angles

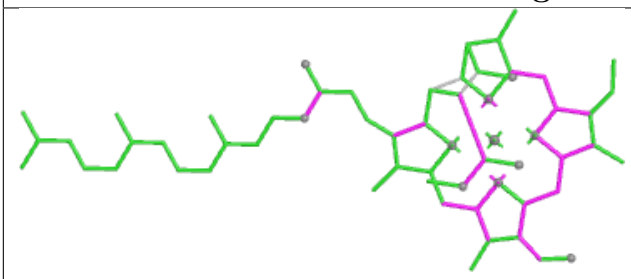


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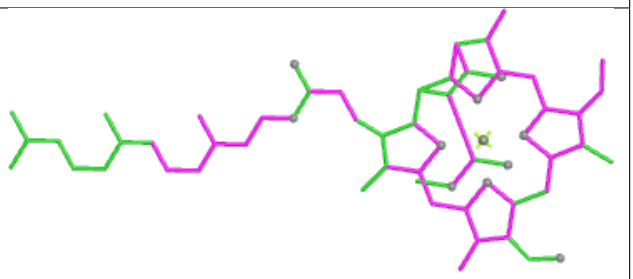


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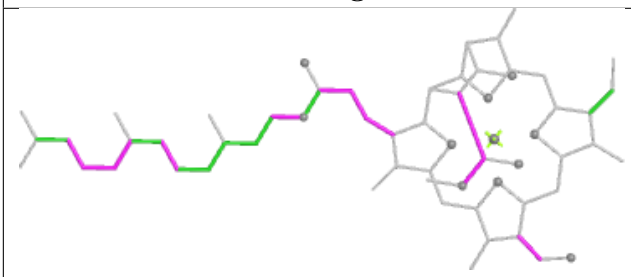
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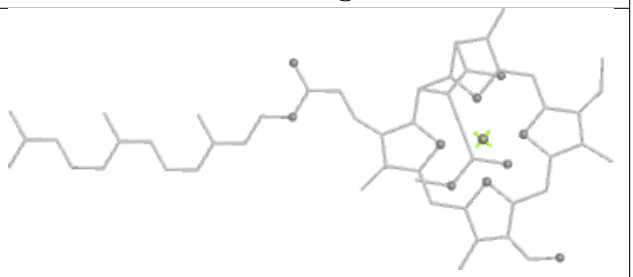
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Bond angles

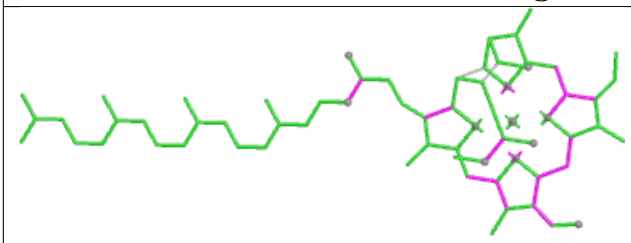


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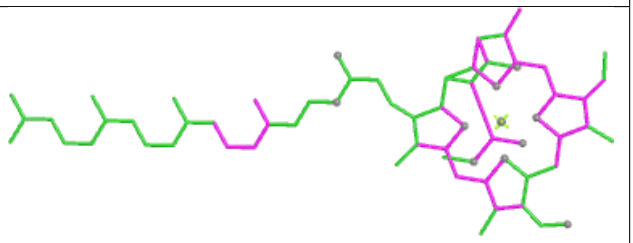


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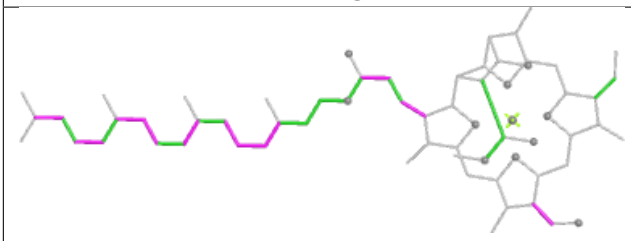
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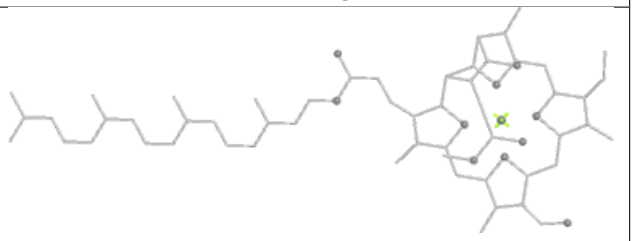
Bond lengths



Bond angles

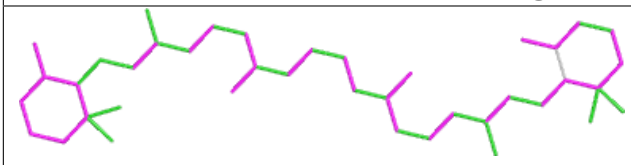


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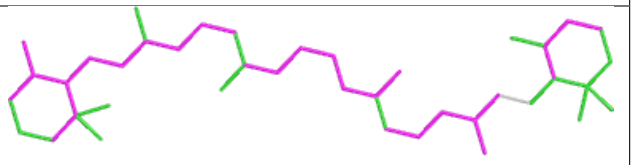


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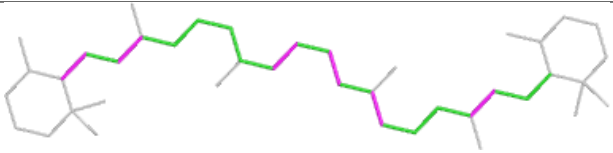
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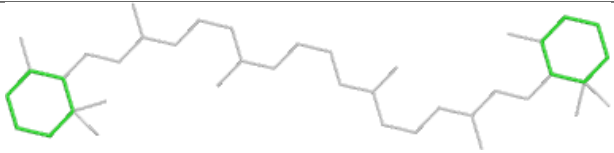
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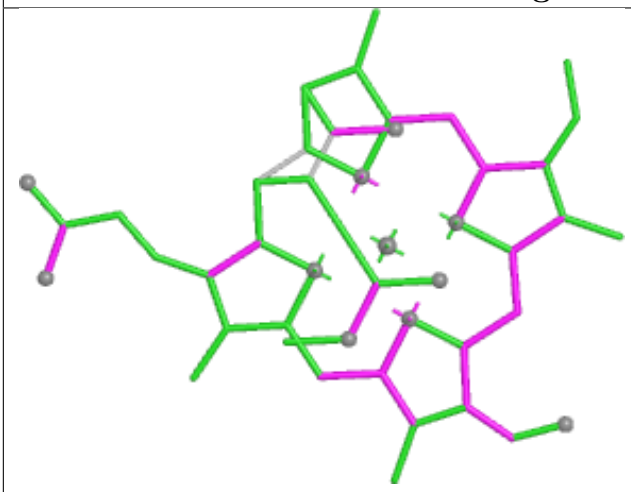


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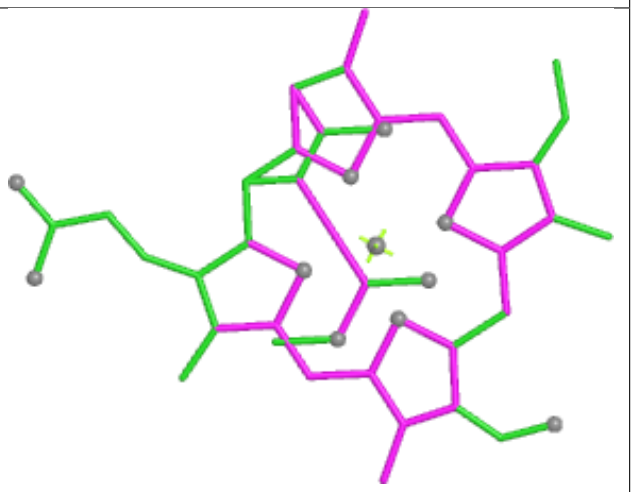


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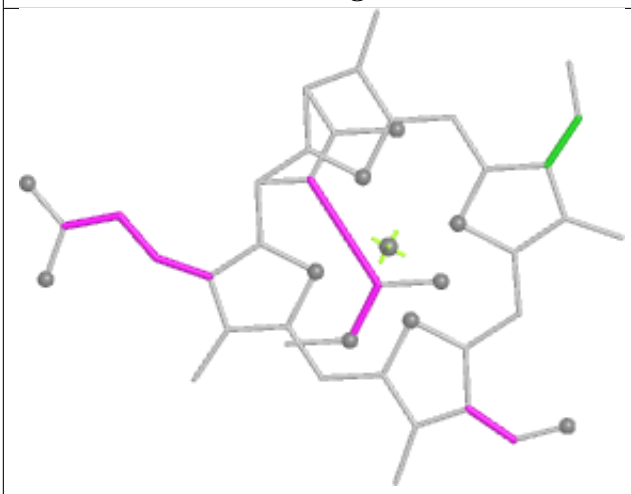
Ligand CL7 1 405



Bond lengths



Bond angles

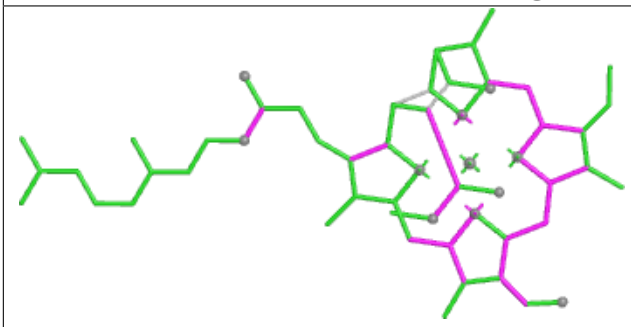


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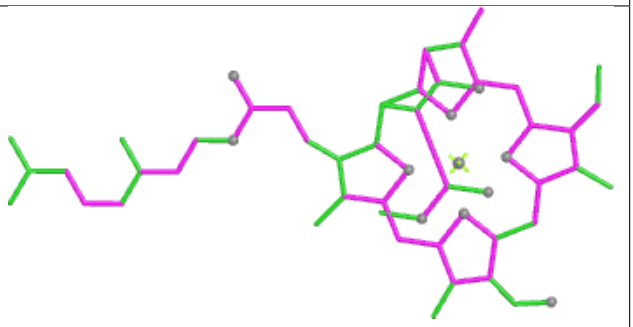


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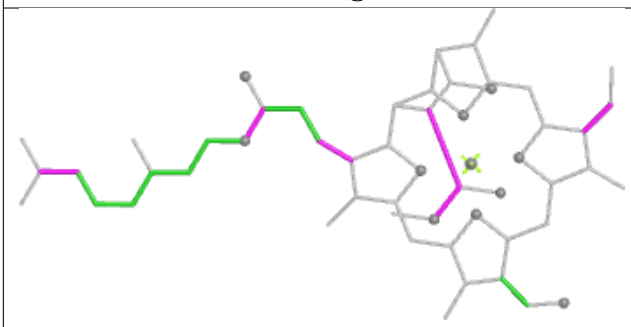
Ligand CL7 A 403



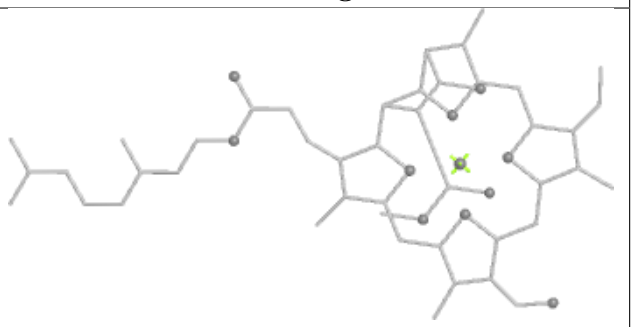
Bond lengths



Bond angles

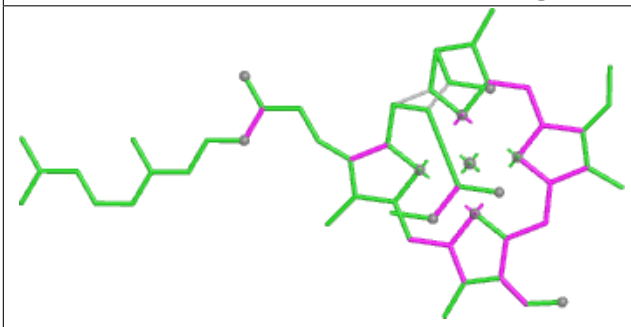


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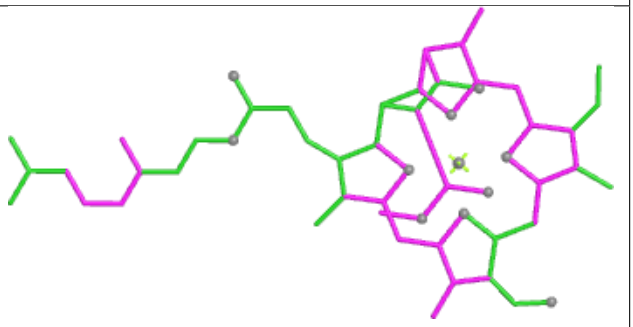


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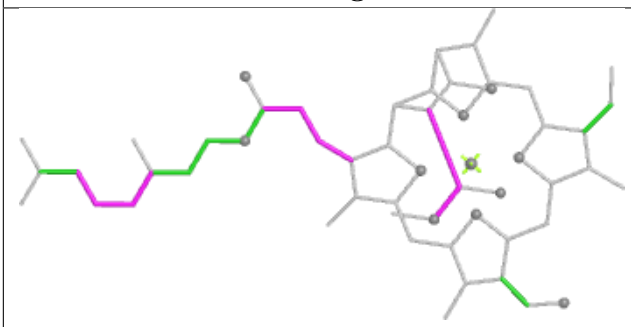
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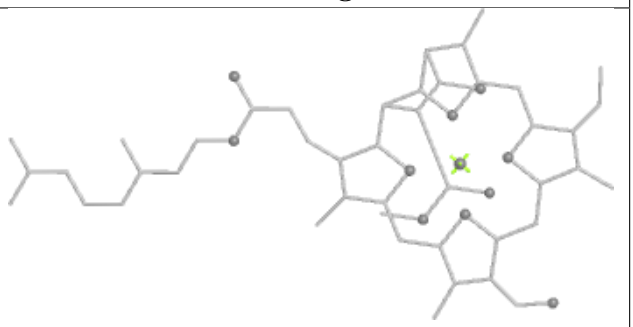
Bond lengths



Bond angles

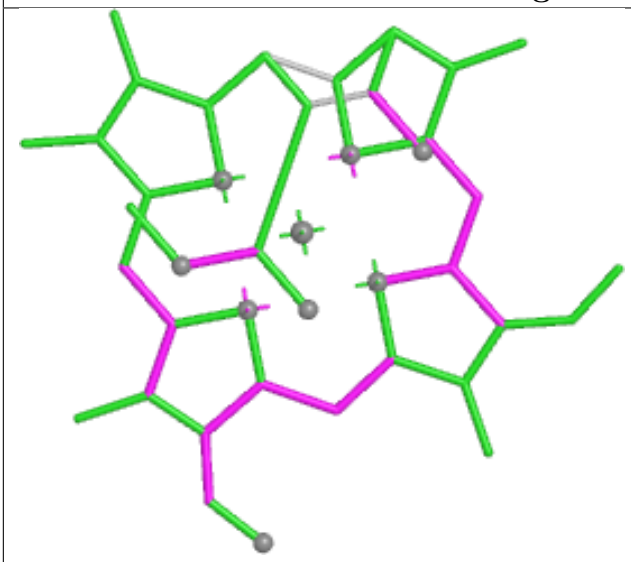


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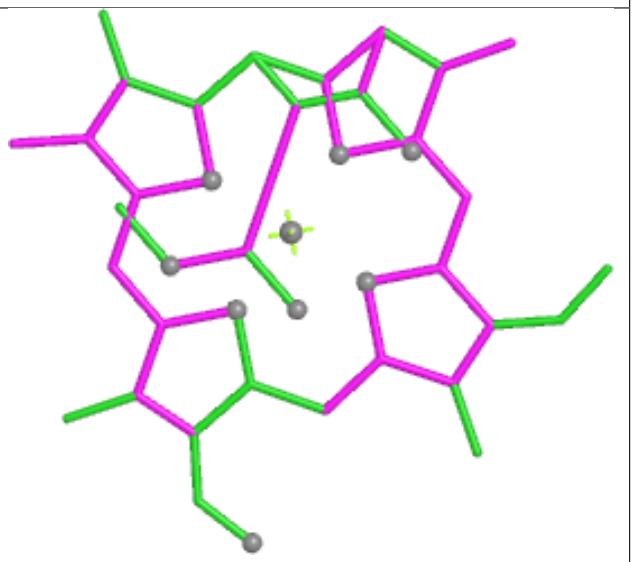


Rings

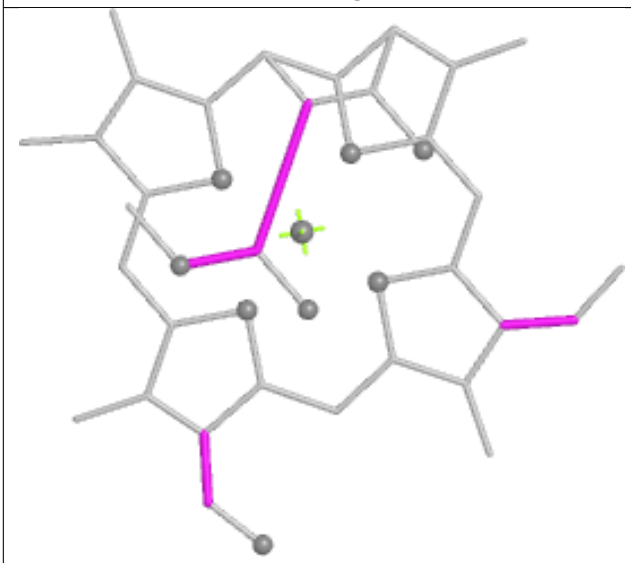
Ligand CL7 8 416



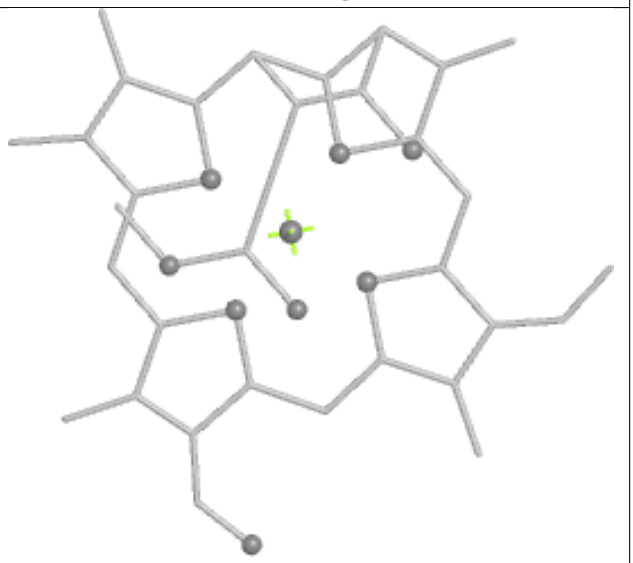
Bond lengths



Bond angles

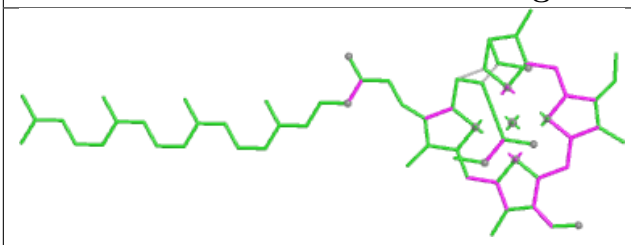


Torsions

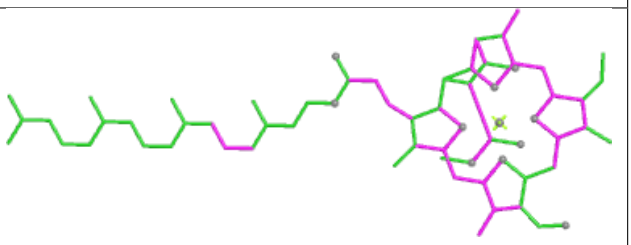


Rings

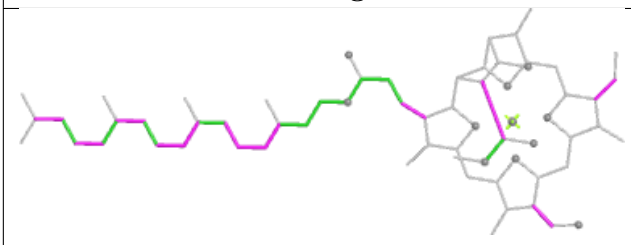
Ligand CL7 3 504



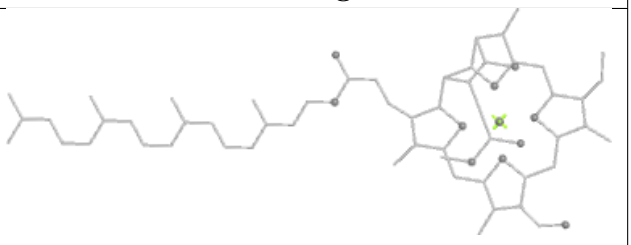
Bond lengths



Bond angles

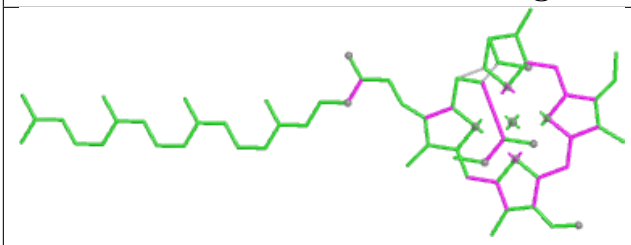


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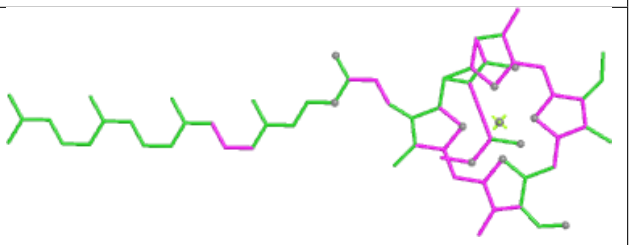


Rings

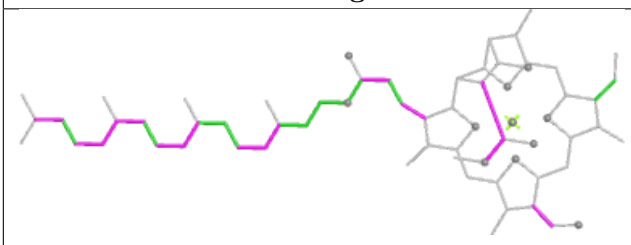
Ligand CL7 6 507



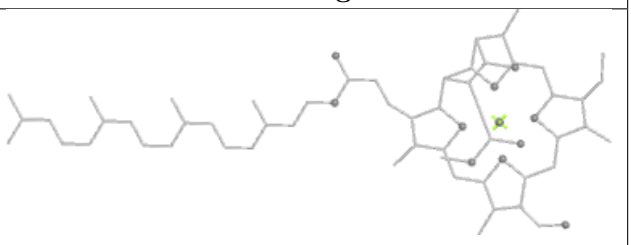
Bond lengths



Bond angles

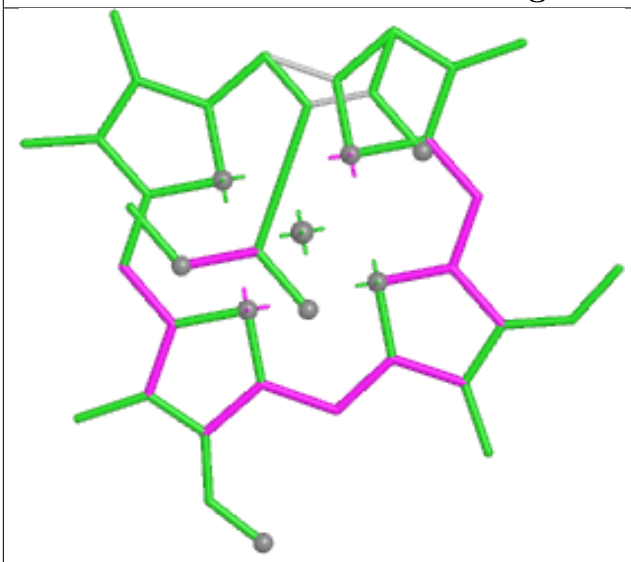


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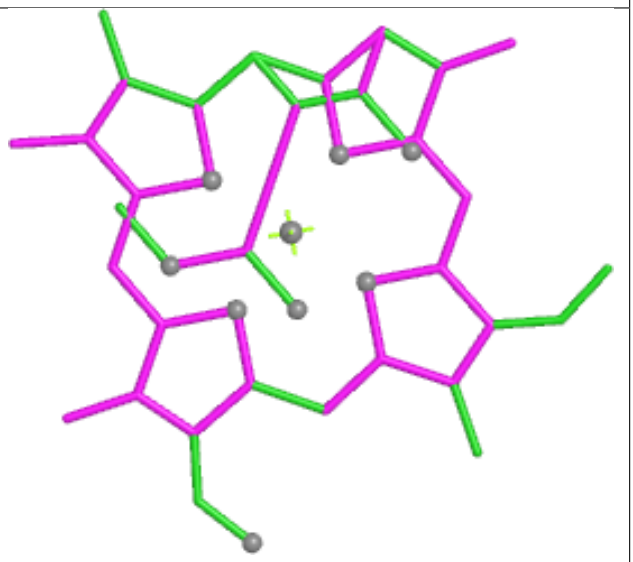


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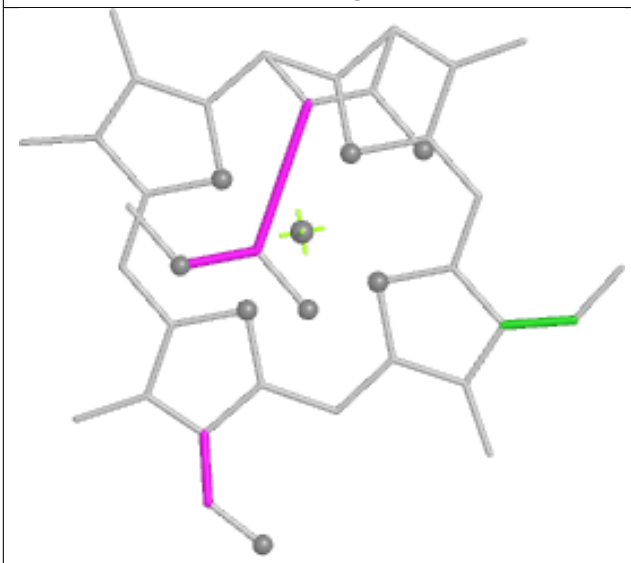
Ligand CL7 C 518



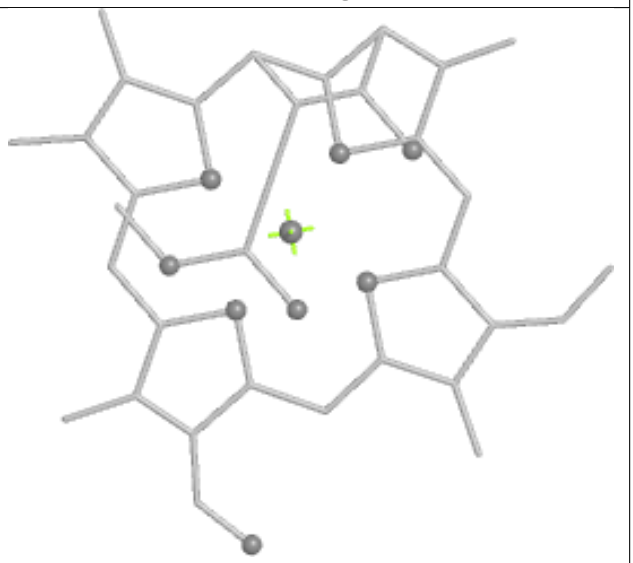
Bond lengths



Bond angles

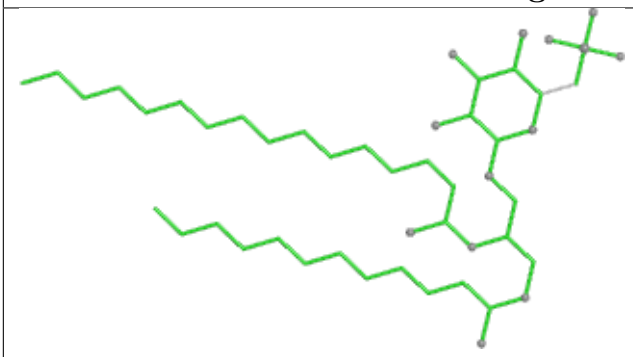


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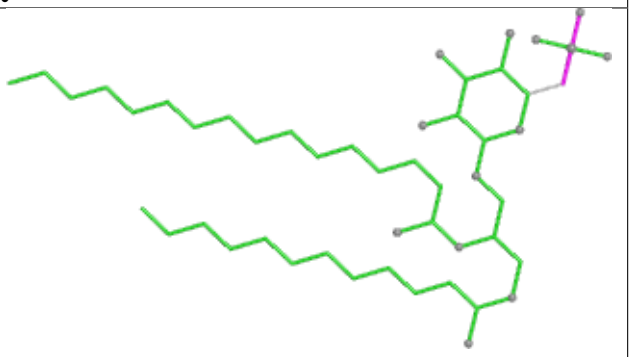


Rings

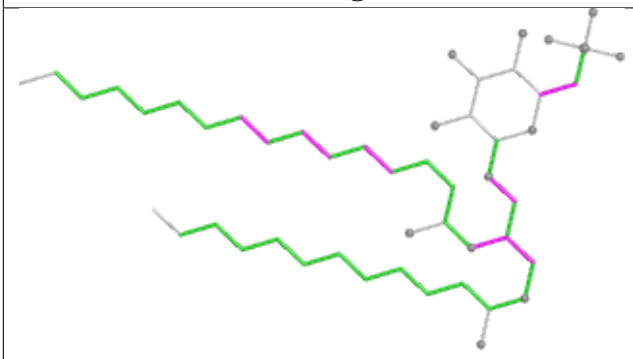
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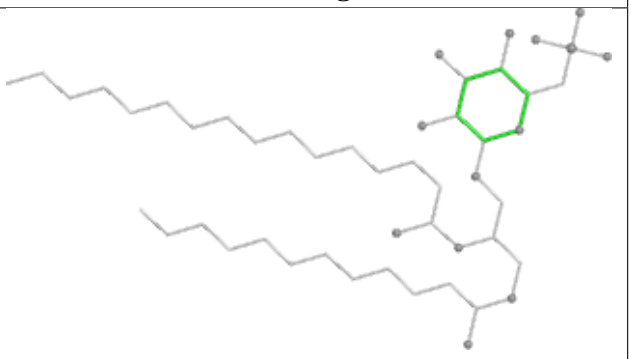
Bond lengths



Bond angles

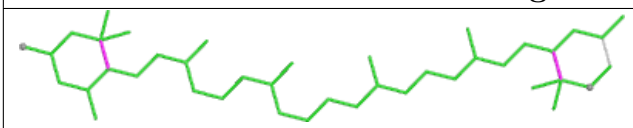


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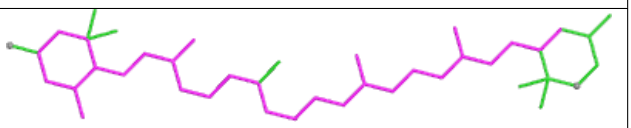


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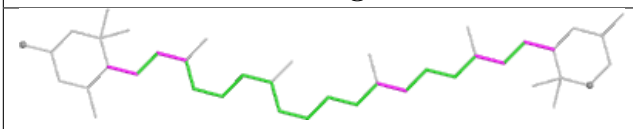
Ligand ZEX 3 520



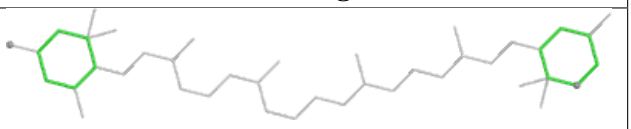
Bond lengths



Bond angles

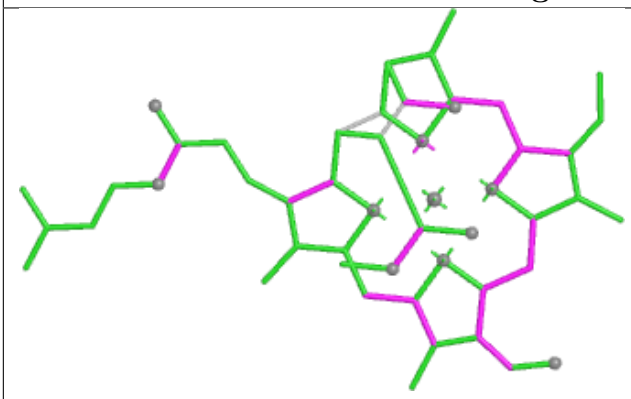


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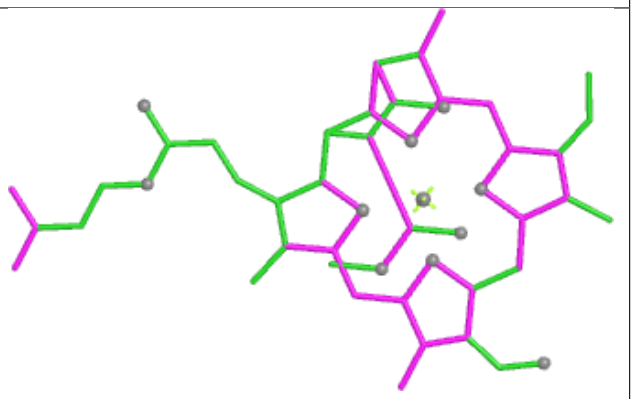


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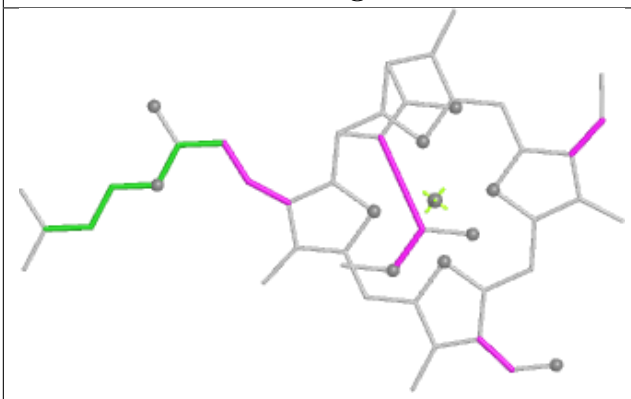
Ligand CL7 d 402



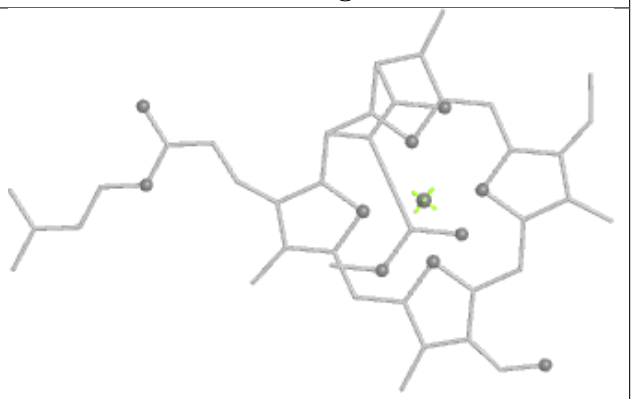
Bond lengths



Bond angles

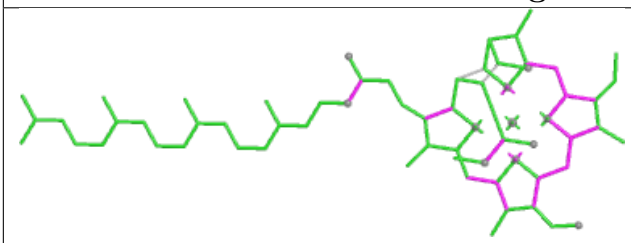


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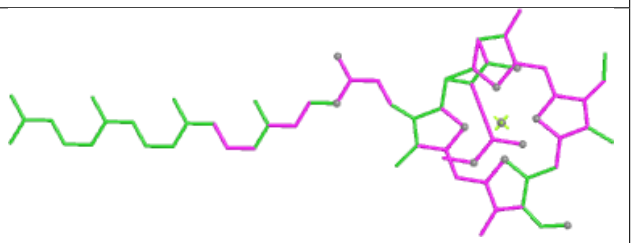


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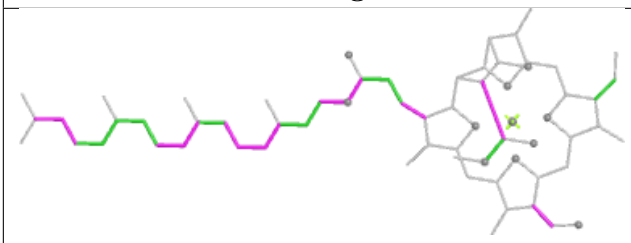
Ligand CL7 C 509



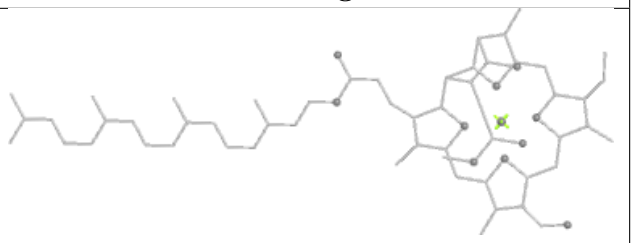
Bond lengths



Bond angles

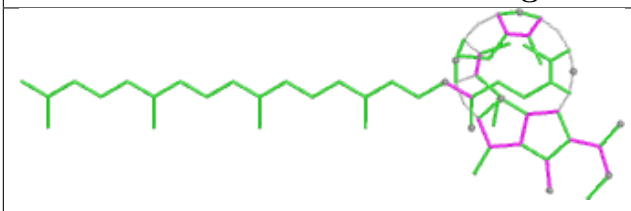


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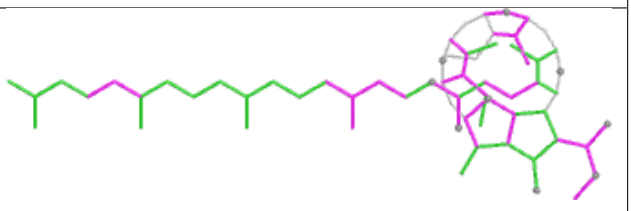


Rings

Ligand PHO D 408



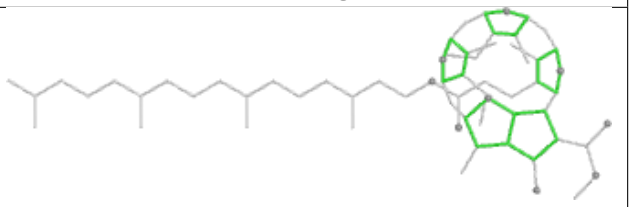
Bond lengths



Bond angles

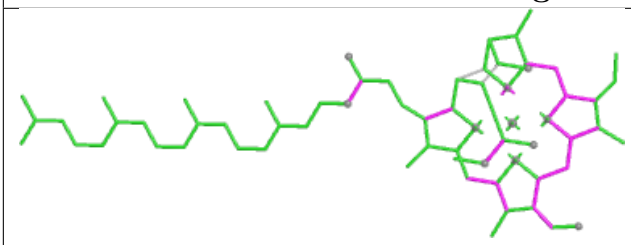


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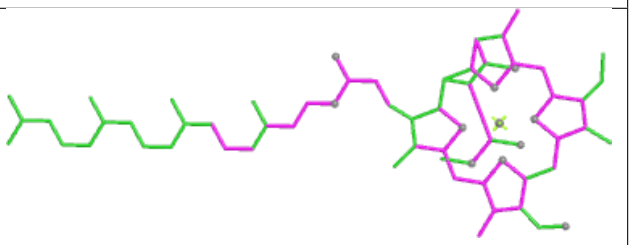


Rings

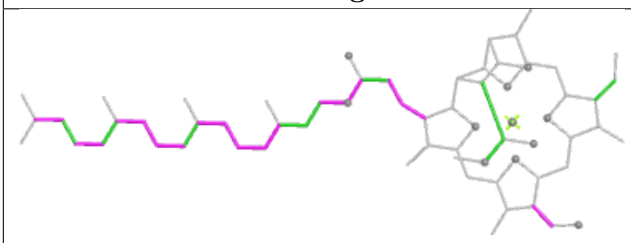
Ligand CL7 4 405



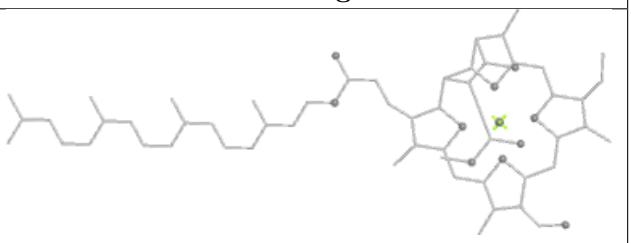
Bond lengths



Bond angles



Torsions

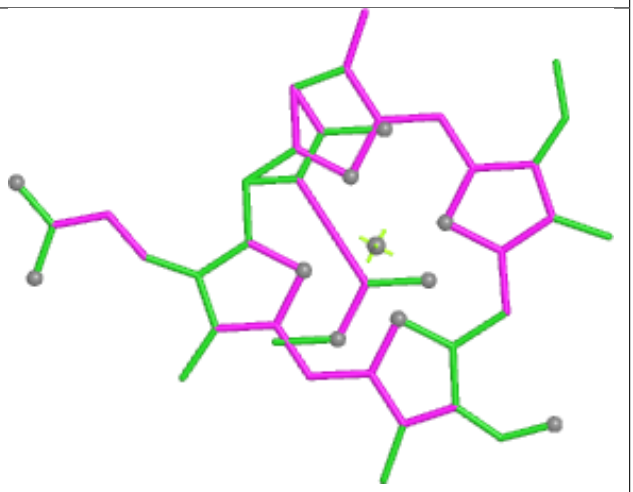


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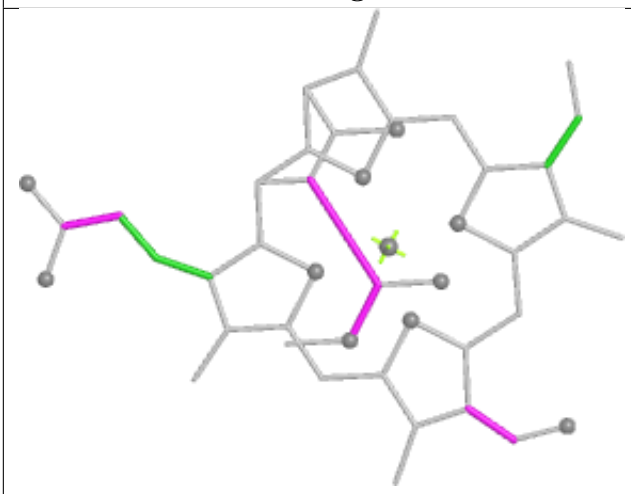
Ligand CL7 5 411



Bond lengths



Bond angles

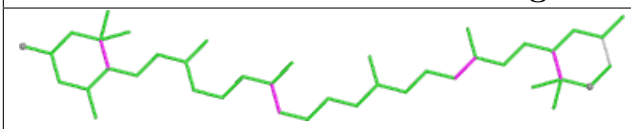


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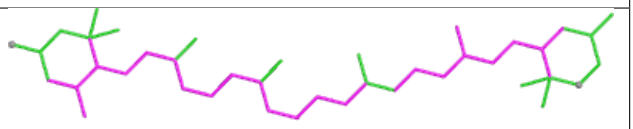


Rings

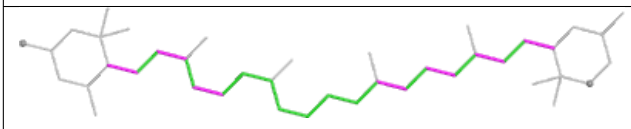
Ligand ZEX 6 524



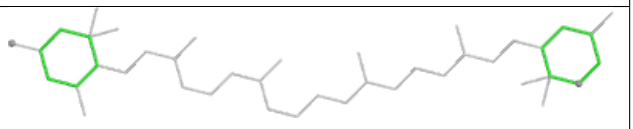
Bond lengths



Bond angles

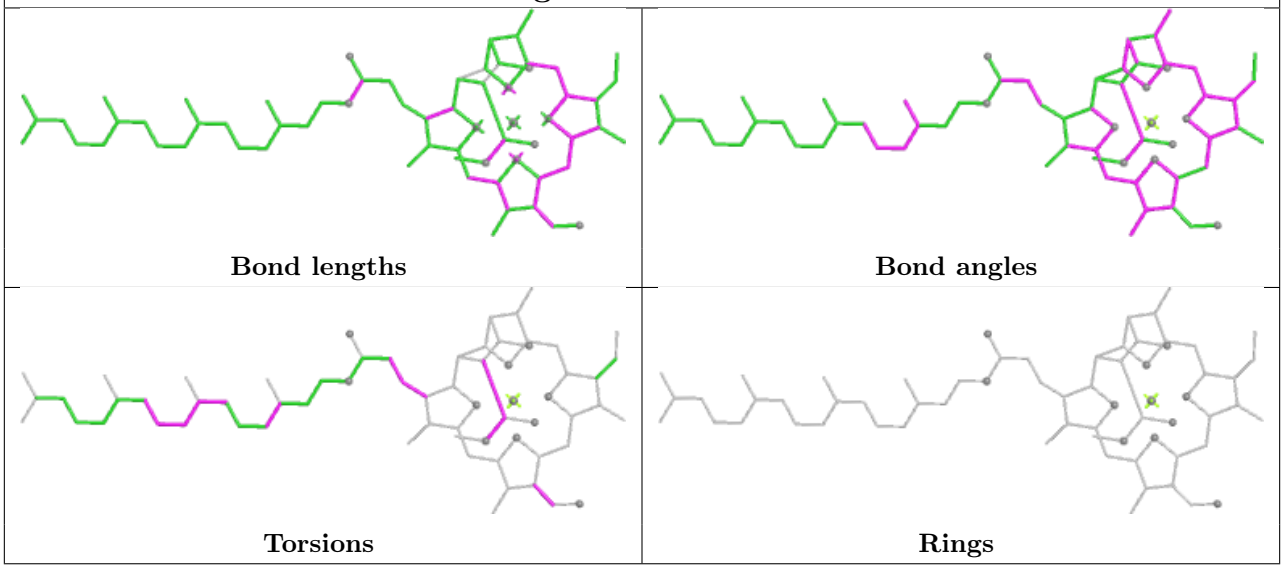


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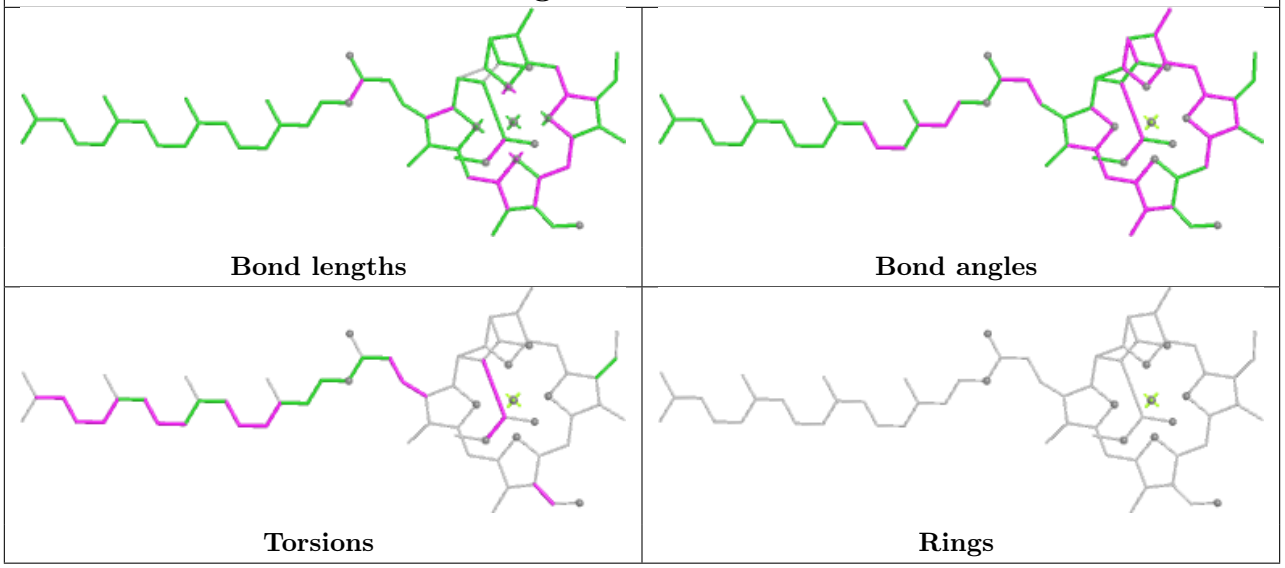


Rings

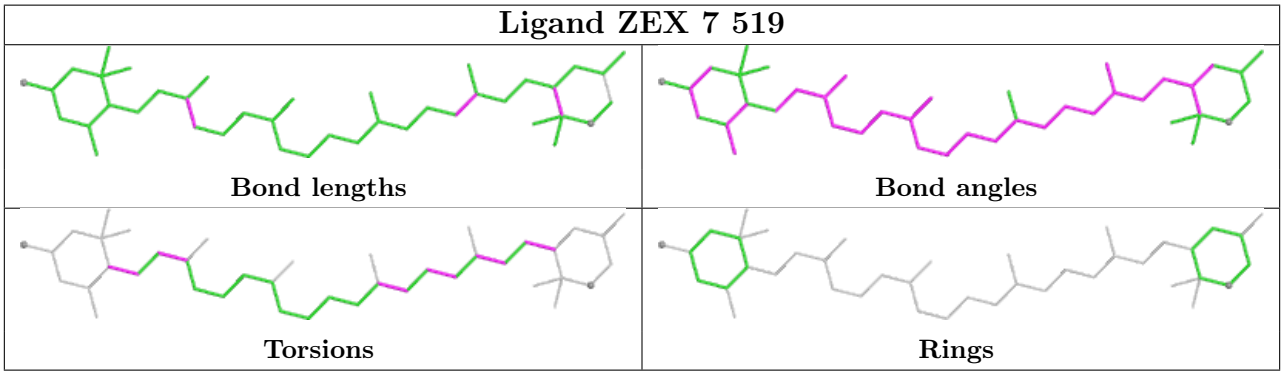
Ligand CL7 2 502



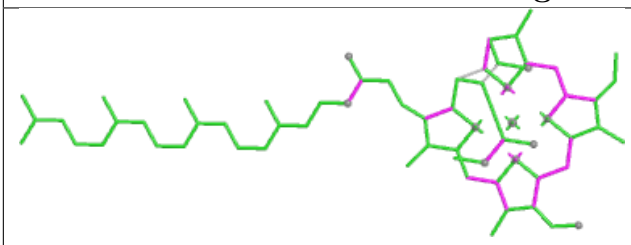
Ligand CL7 6 517



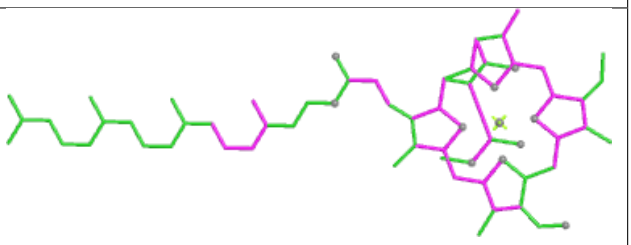
Ligand ZEX 7 519



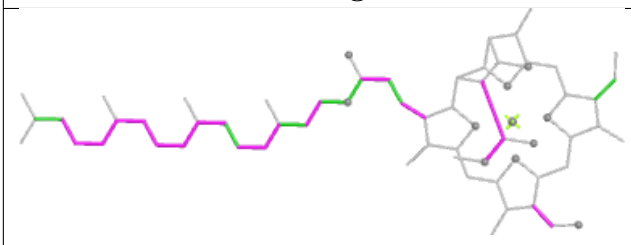
Ligand CL7 c 511



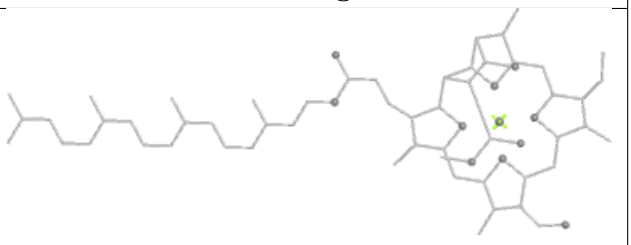
Bond lengths



Bond angles

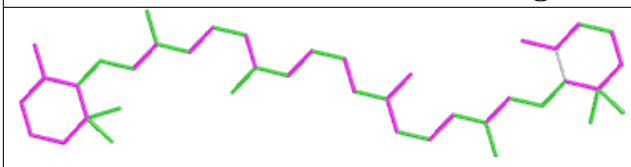


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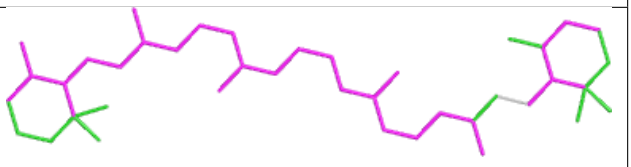


Rings

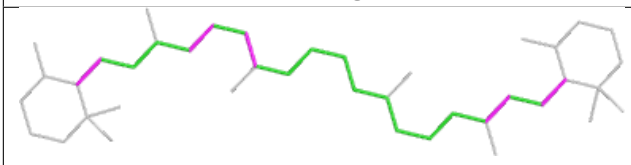
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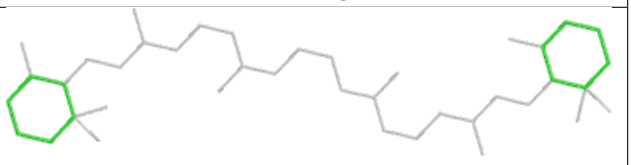
Bond lengths



Bond angles

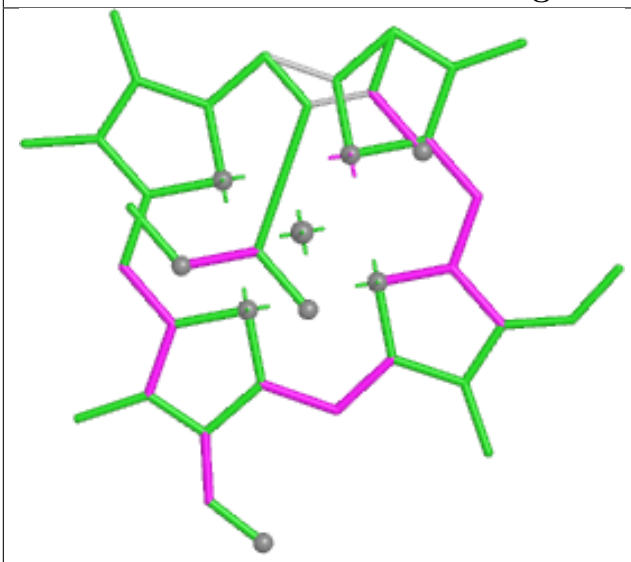


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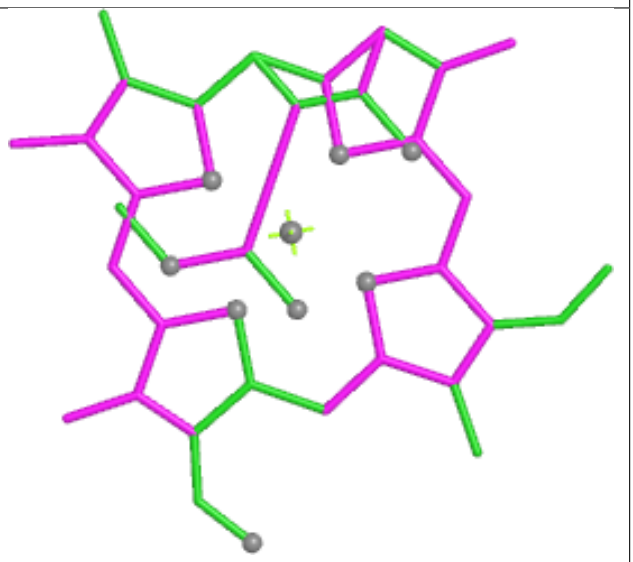


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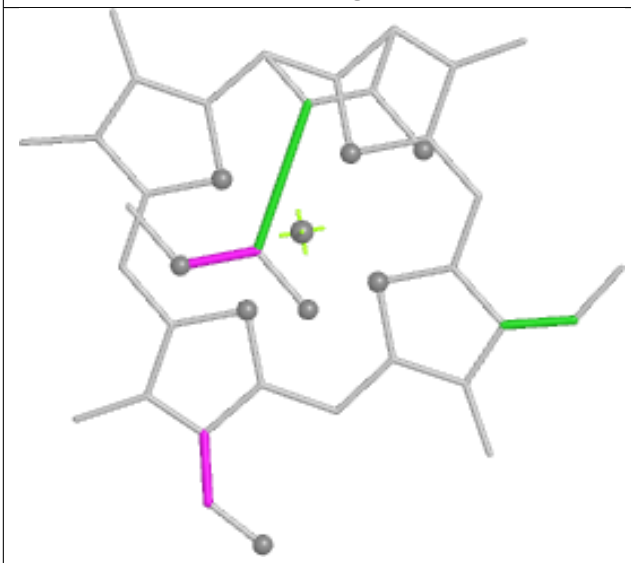
Ligand CL7 1 416



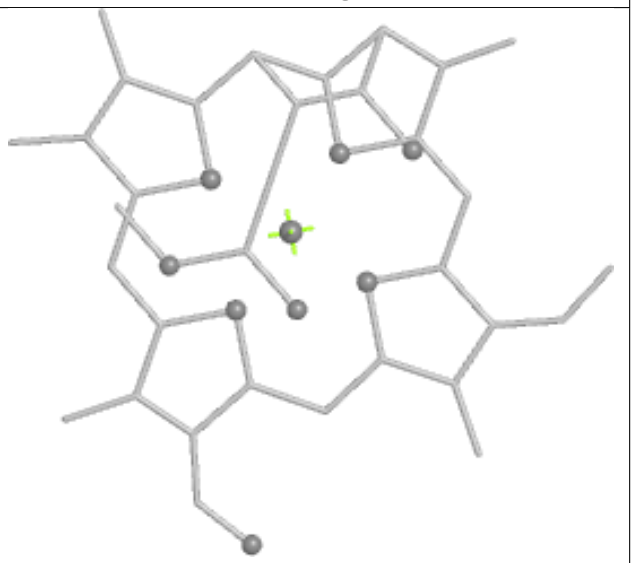
Bond lengths



Bond angles

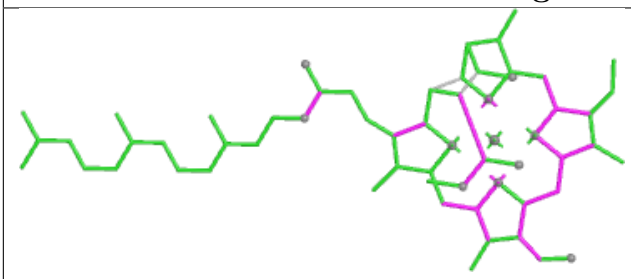


Torsions

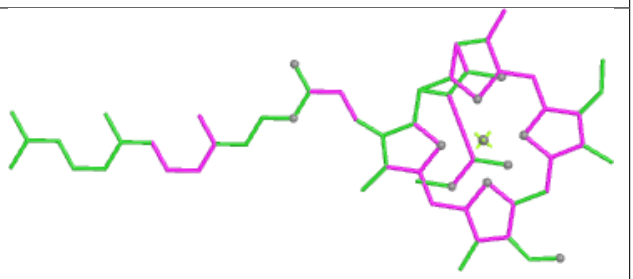


Rings

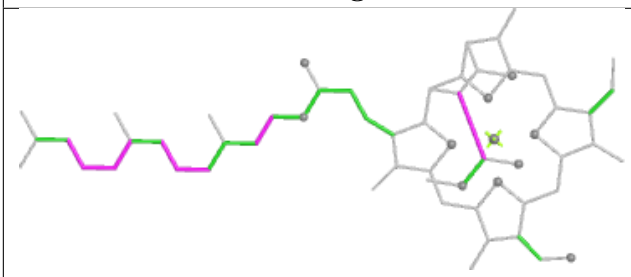
Ligand CL7 4 413



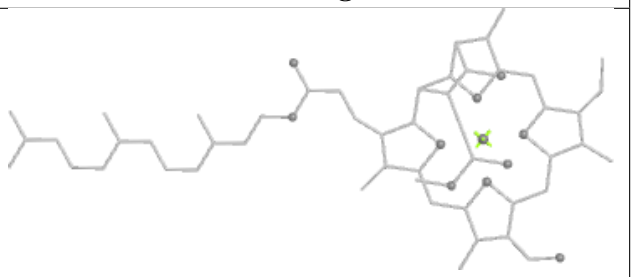
Bond lengths



Bond angles

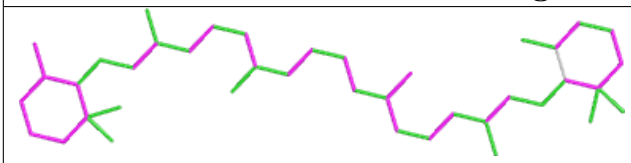


Torsions

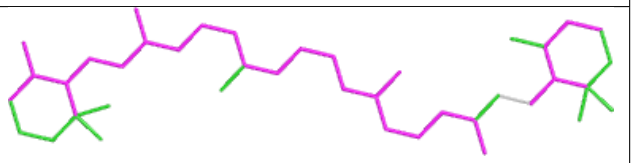


Rings

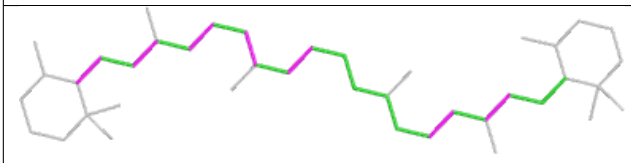
Ligand 8CT c 516



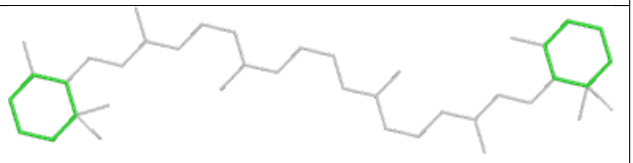
Bond lengths



Bond angles

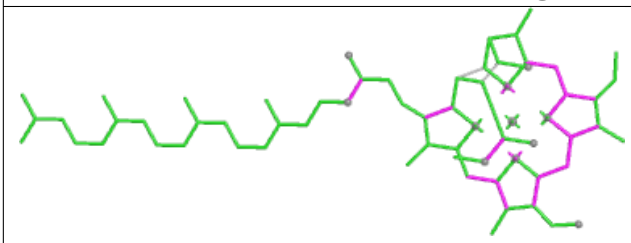


Torsions

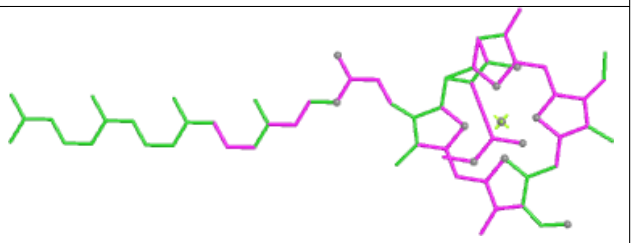


Rings

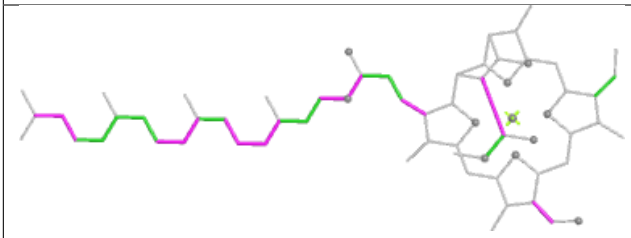
Ligand CL7 c 509



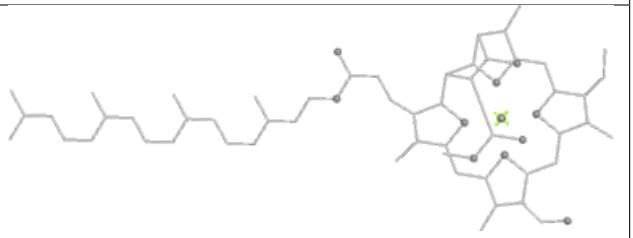
Bond lengths



Bond angles

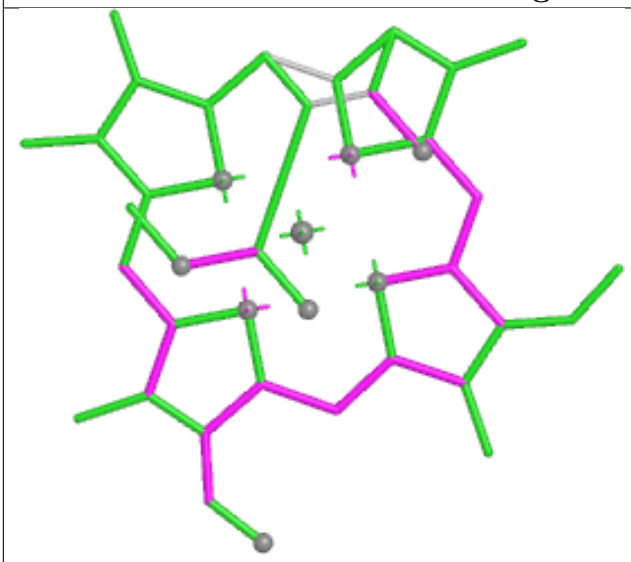


Torsions

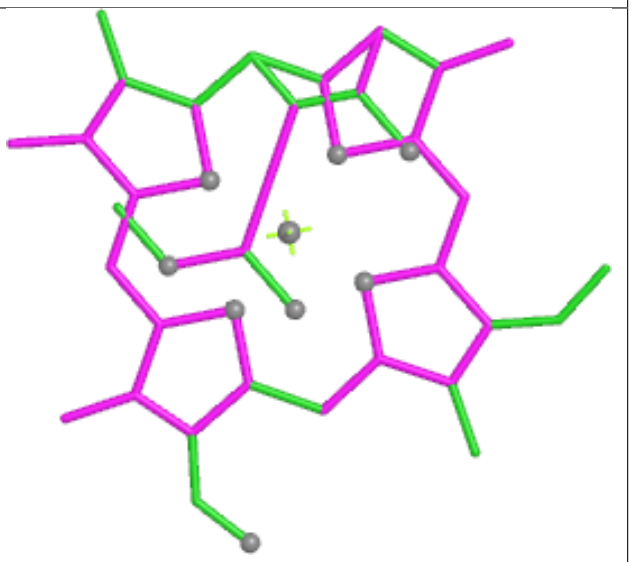


Rings

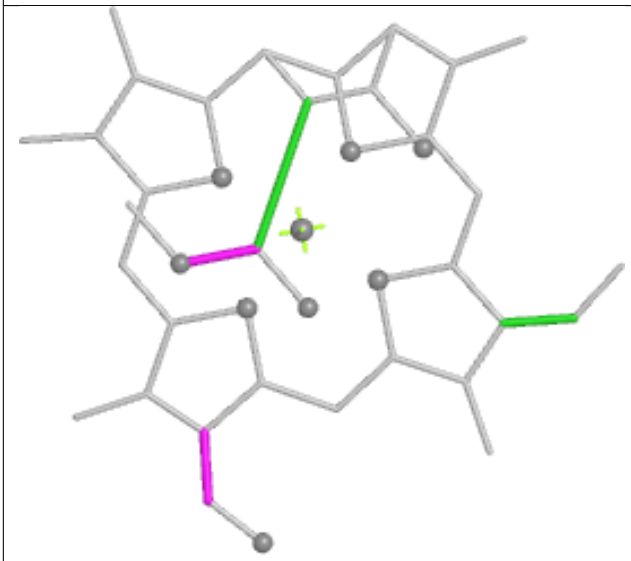
Ligand CL7 1 407



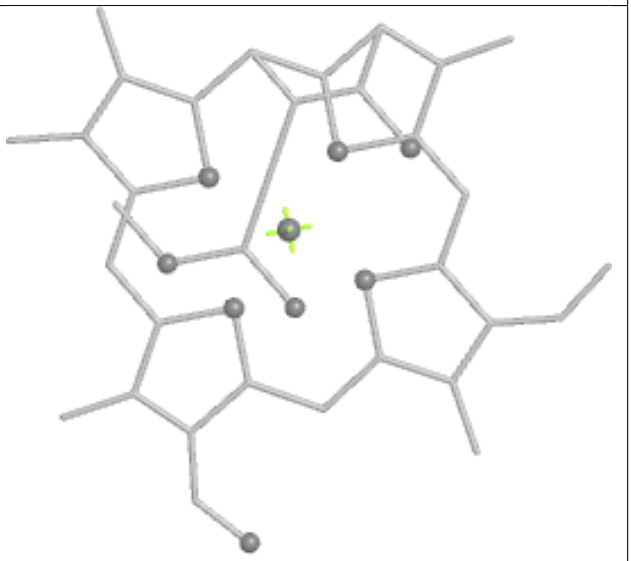
Bond lengths



Bond angles

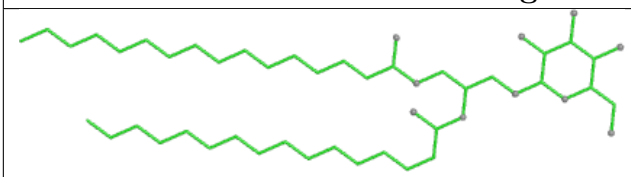


Torsions

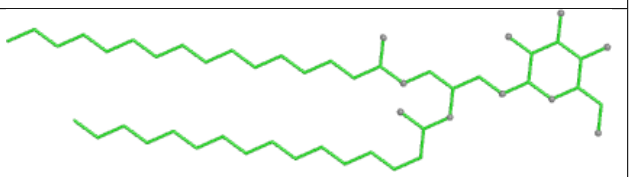


Rings

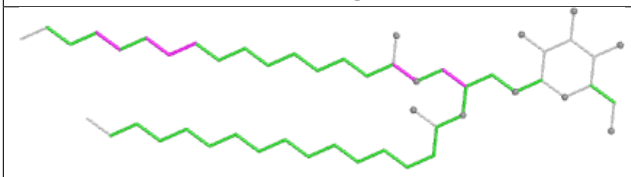
Ligand LMG B 621



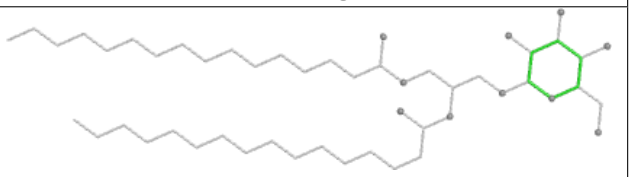
Bond lengths



Bond angles

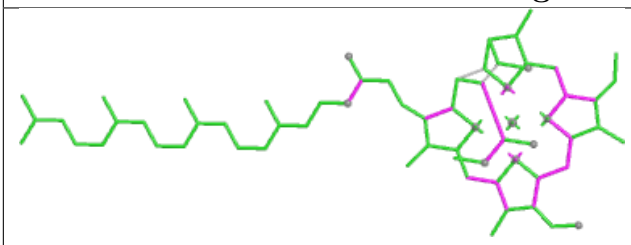


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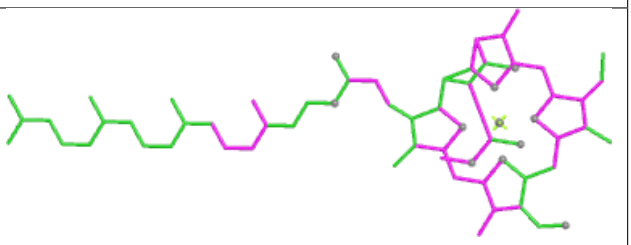


Rings

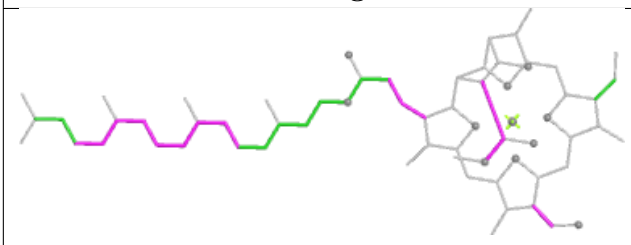
Ligand CL7 7 503



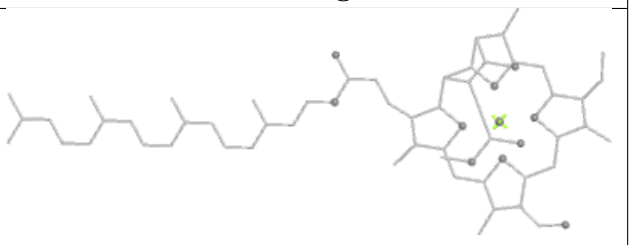
Bond lengths



Bond angles

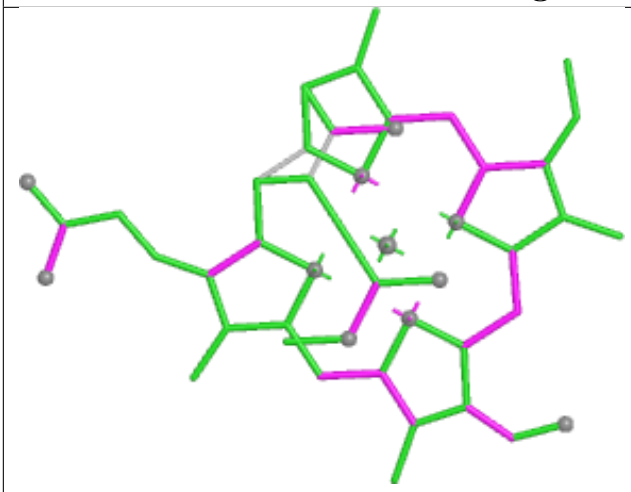


Torsions

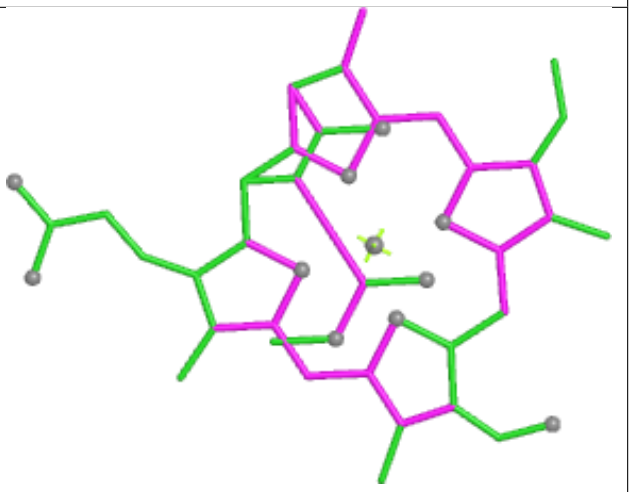


Rings

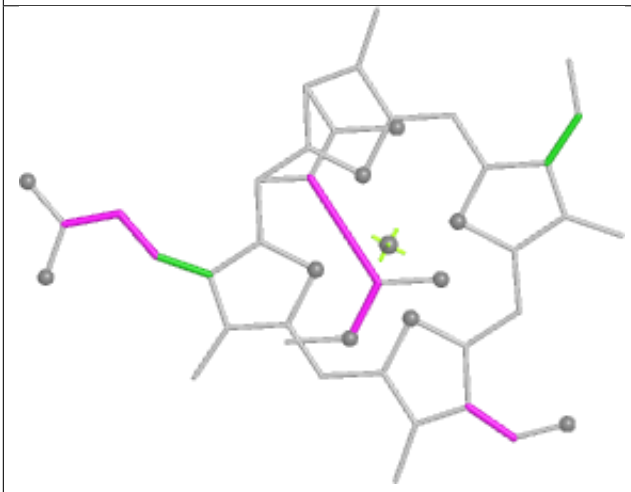
Ligand CL7 b 623



Bond lengths



Bond angles

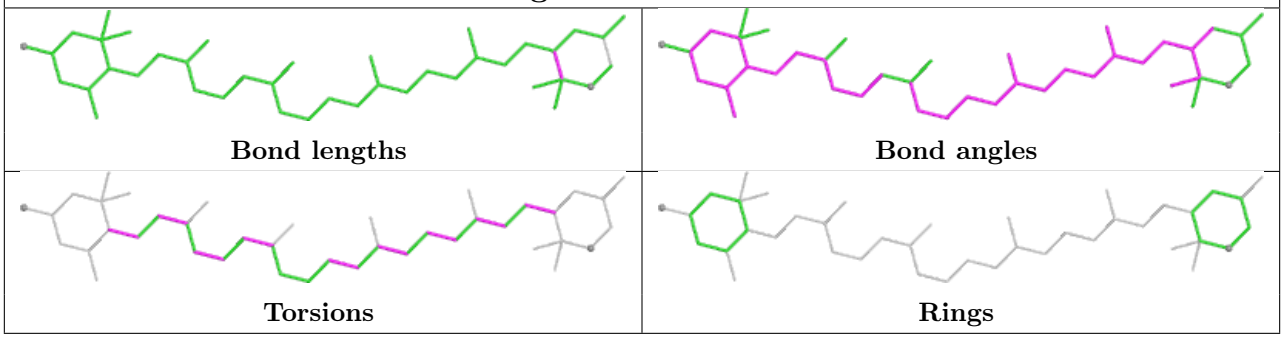


Torsions

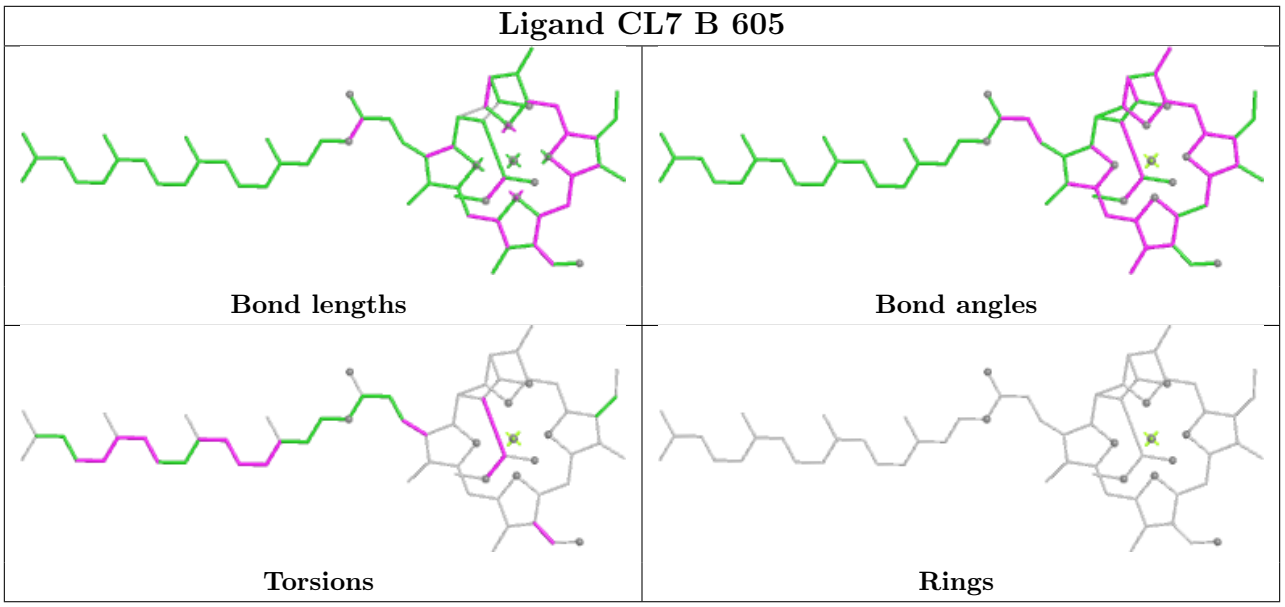


Rings

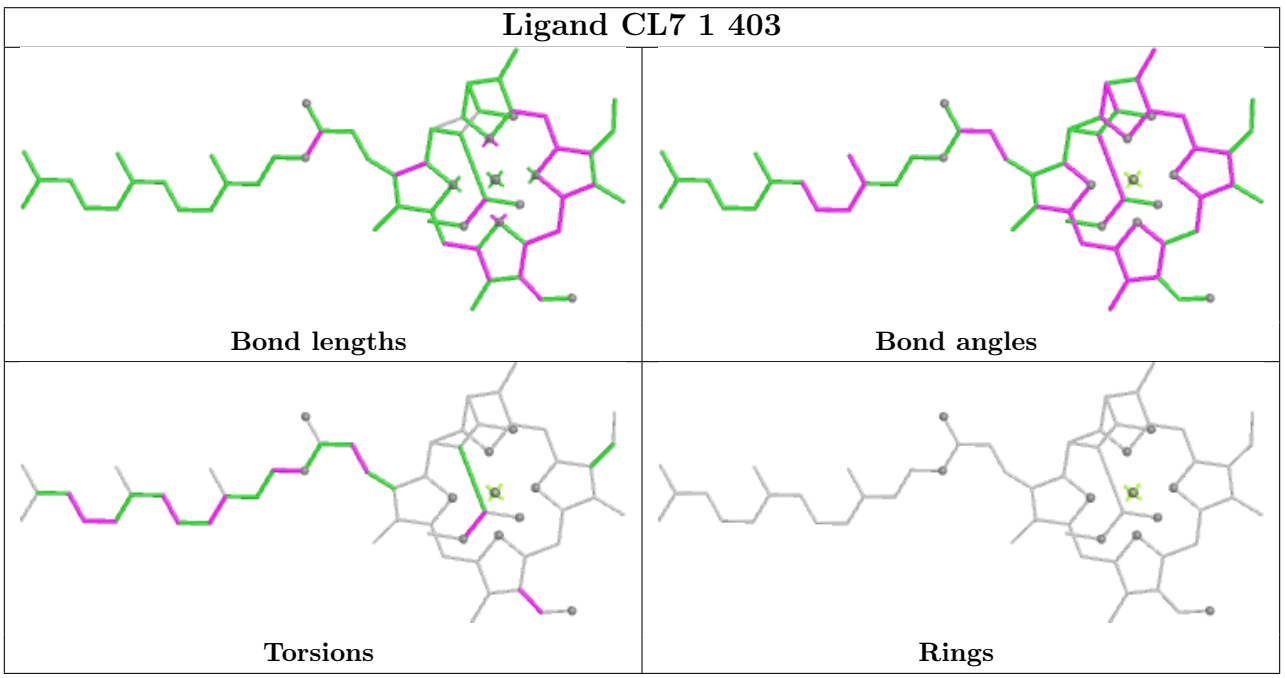
Ligand ZEX 5 421



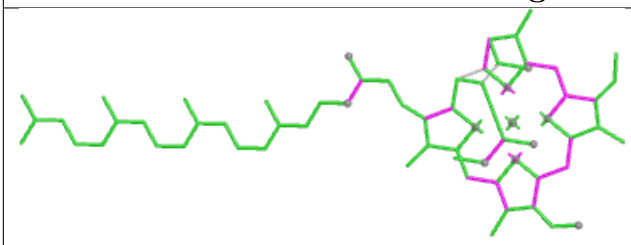
Ligand CL7 B 605



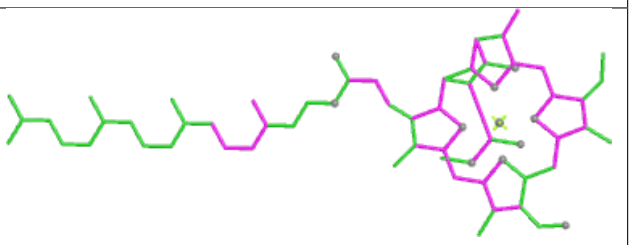
Ligand CL7 1 403



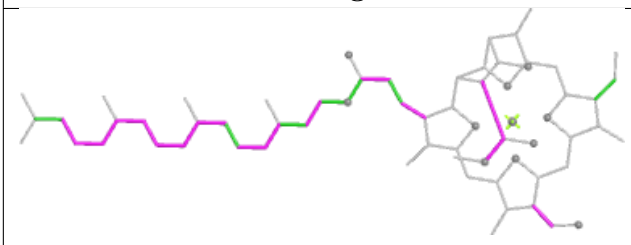
Ligand CL7 C 511



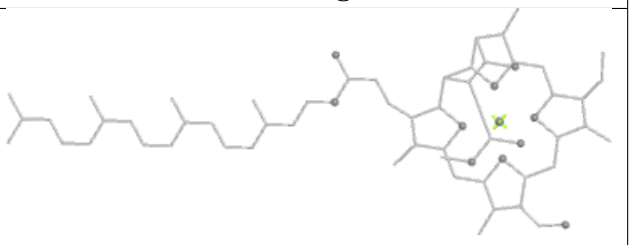
Bond lengths



Bond angles

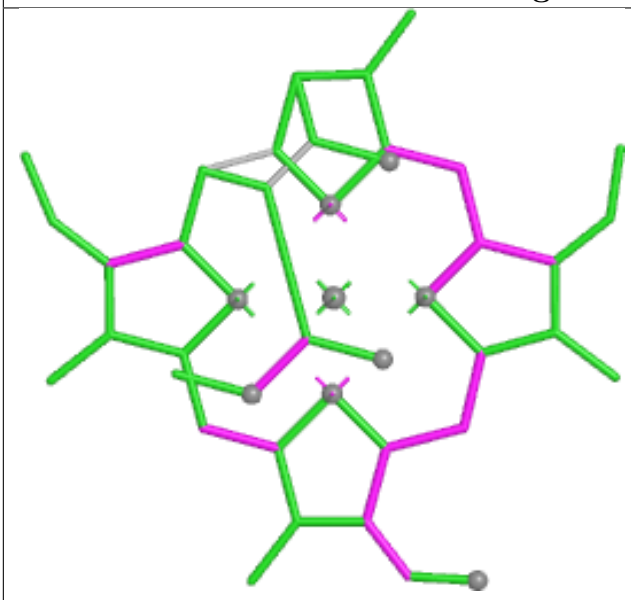


Torsions

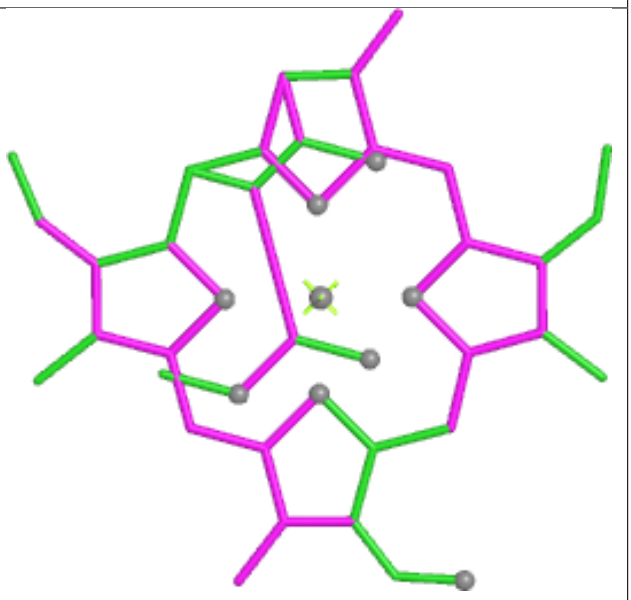


Rings

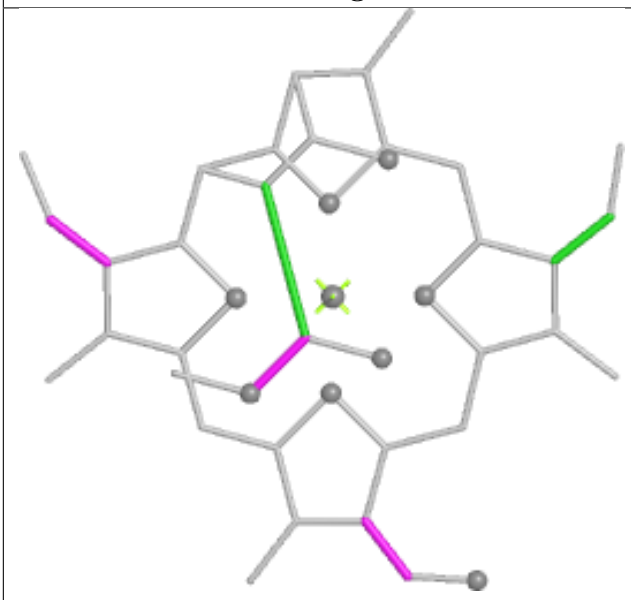
Ligand CL7 4 417



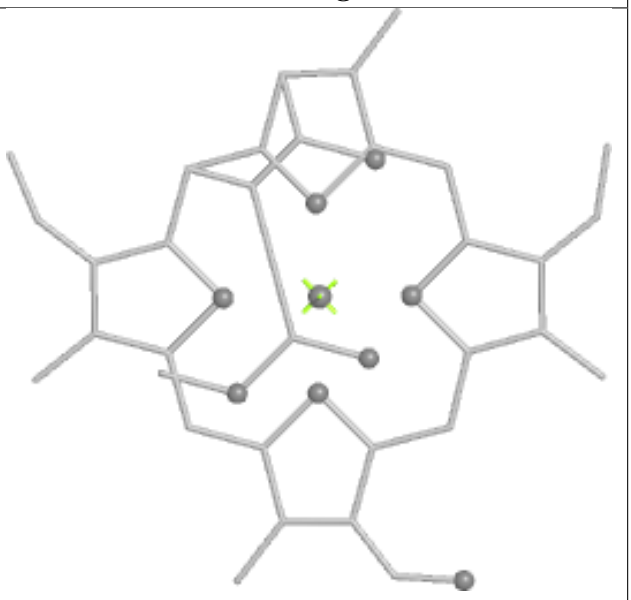
Bond lengths



Bond angles

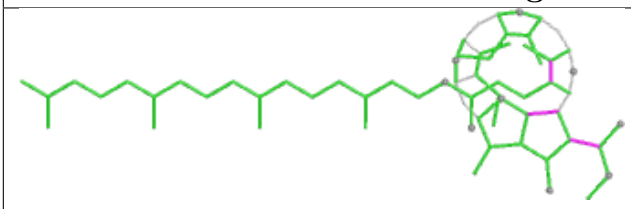


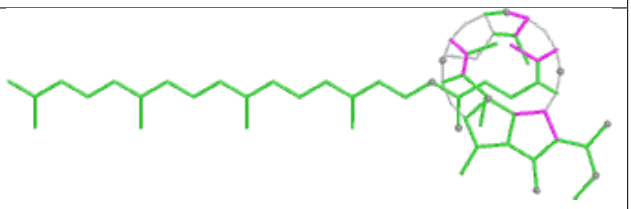
Torsions

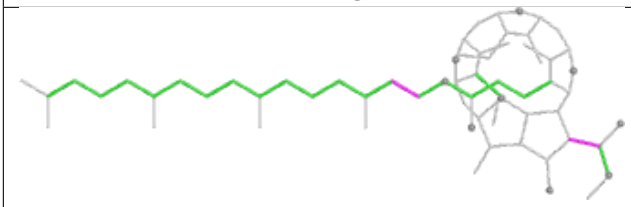


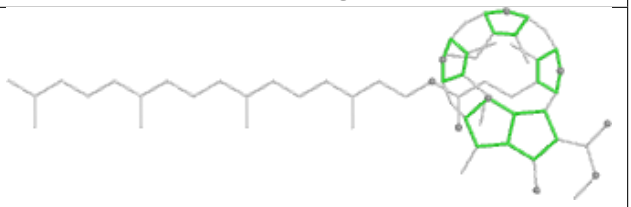
Rings

Ligand PHO a 402

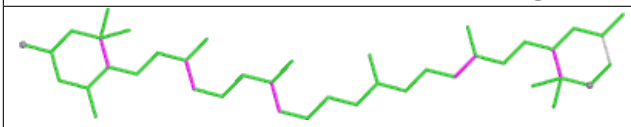

Bond lengths

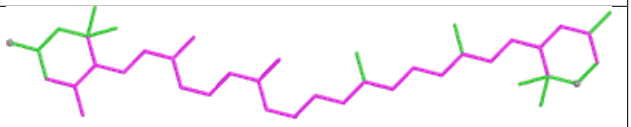

Bond angles

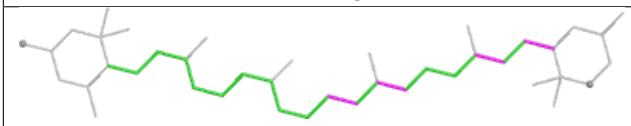

Torsions

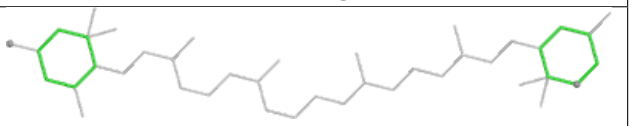

Rings

Ligand ZEX 3 525

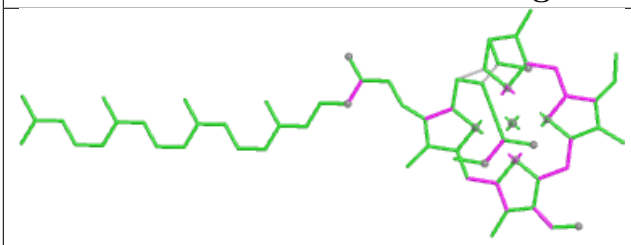

Bond lengths

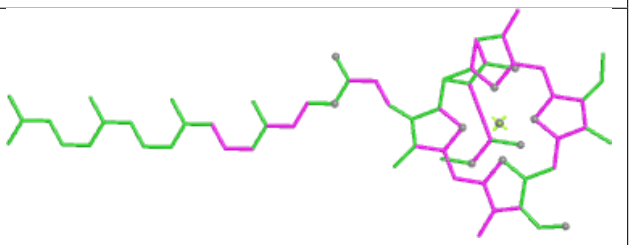

Bond angles

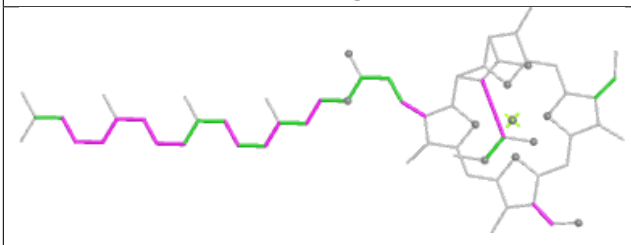

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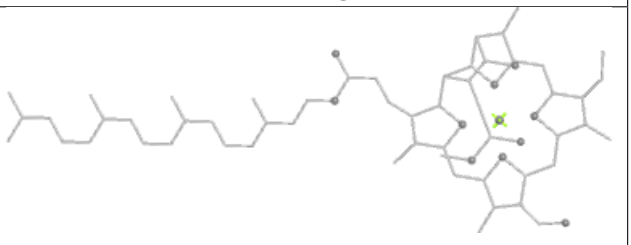

Rings

Ligand CL7 1 404

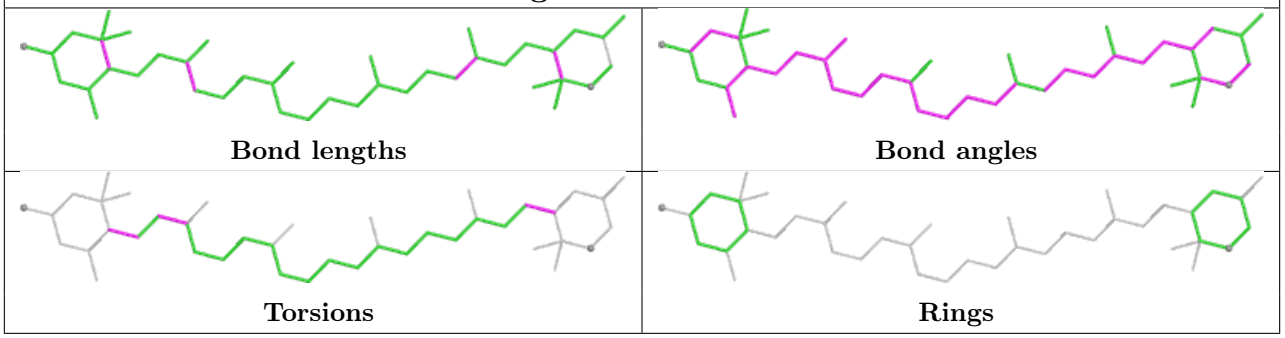

Bond lengths


Bond angles

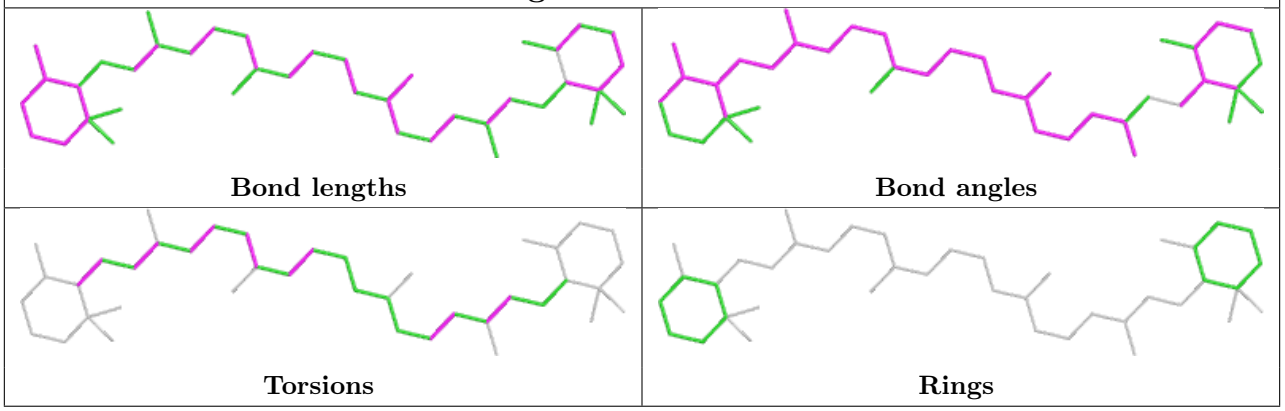

Torsions


Rings

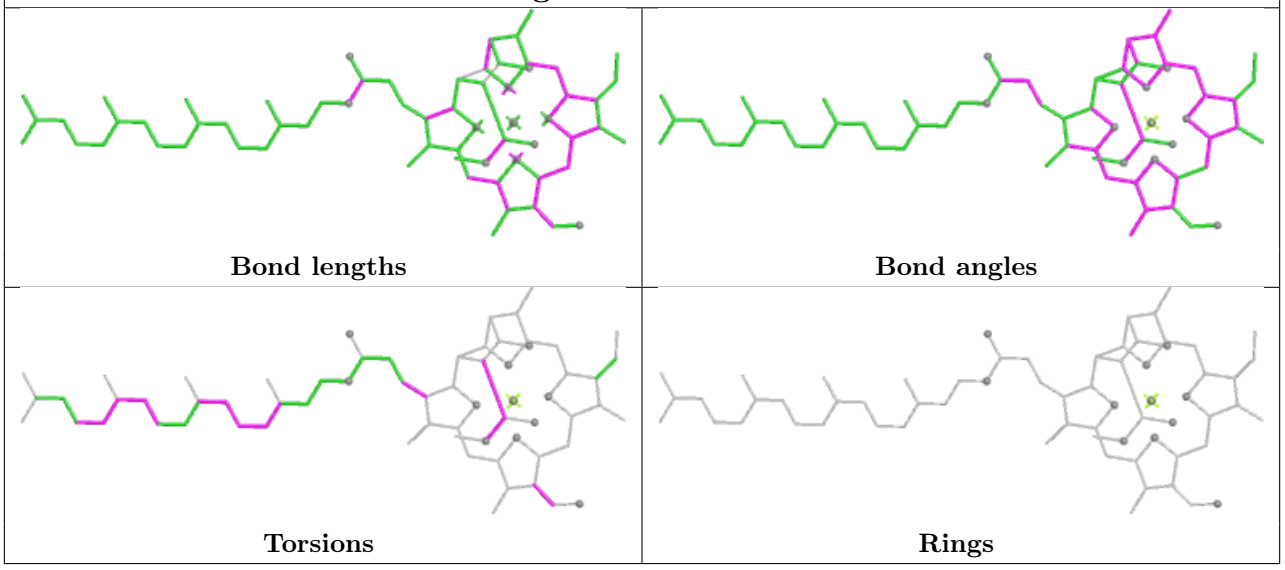
Ligand ZEX 3 522



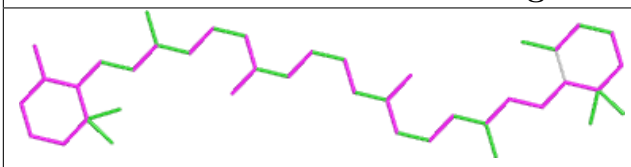
Ligand 8CT C 516

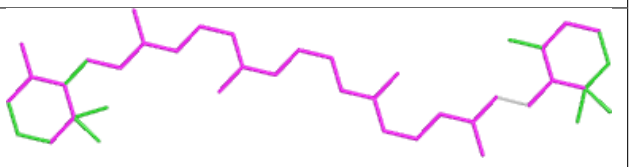


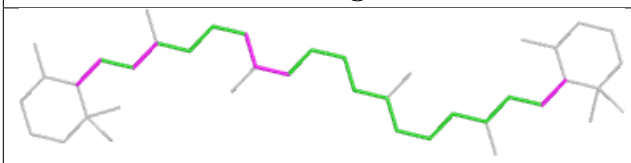
Ligand CL7 b 606

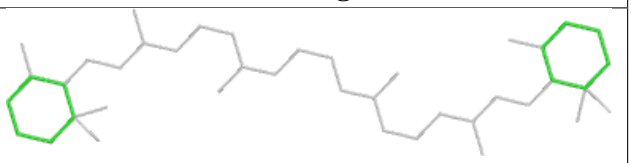


Ligand 8CT B 627

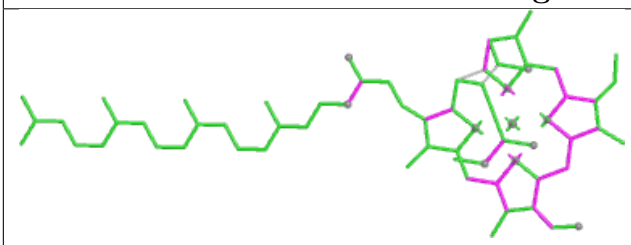

Bond lengths

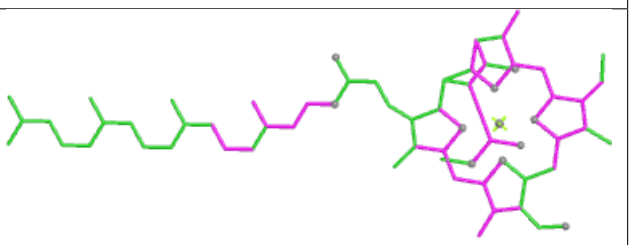

Bond angles

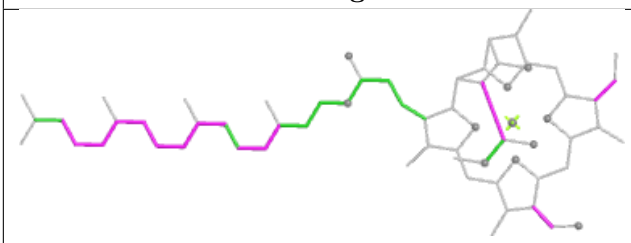

Torsions

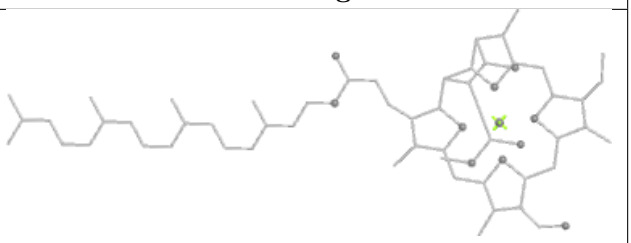

Rings

Ligand CL7 2 505

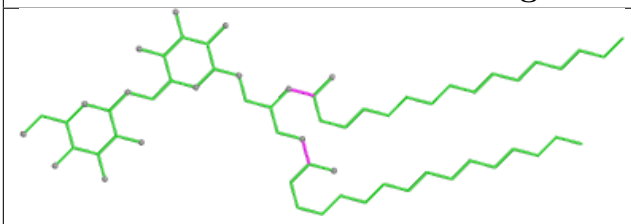

Bond lengths

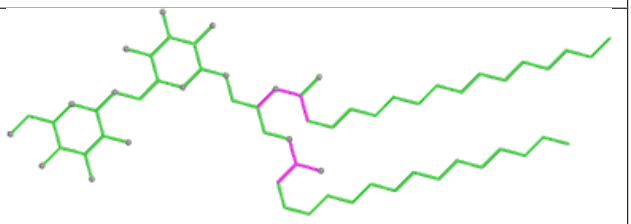

Bond angles

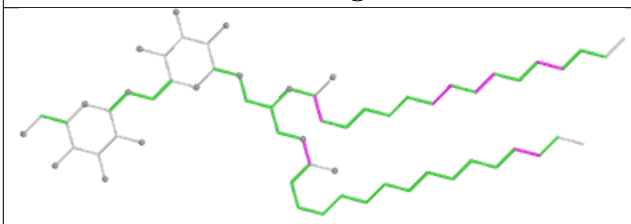

Torsions

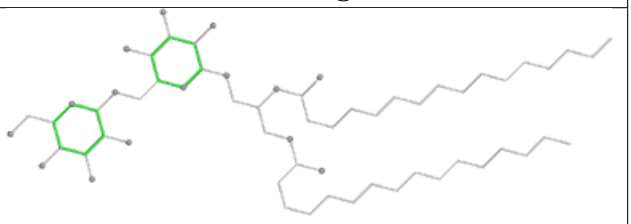

Rings

Ligand DGD B 624

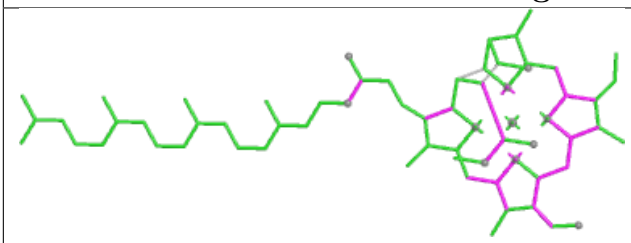

Bond lengths


Bond angles

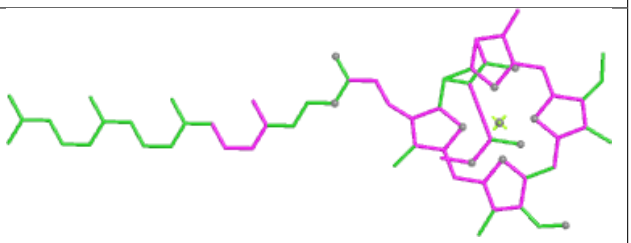

Torsions


Rings

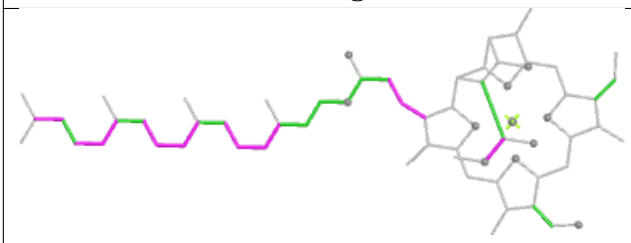
Ligand CL7 2 503



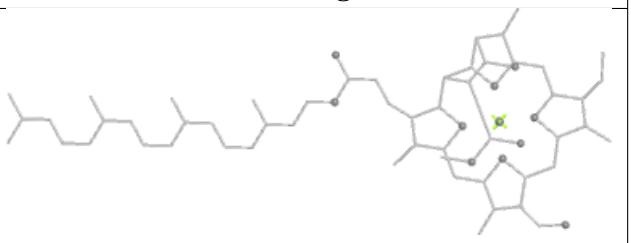
Bond lengths



Bond angles

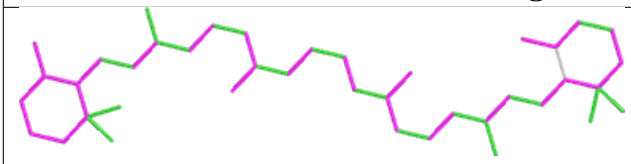


Torsions

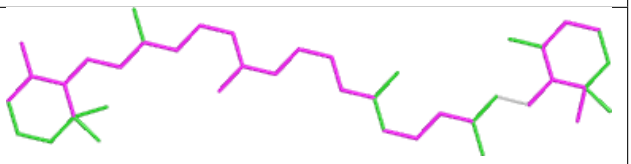


Rings

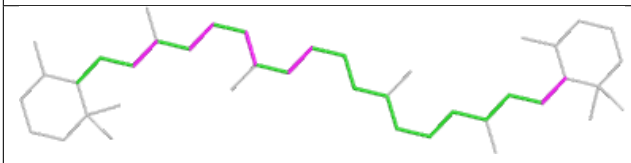
Ligand 8CT B 617



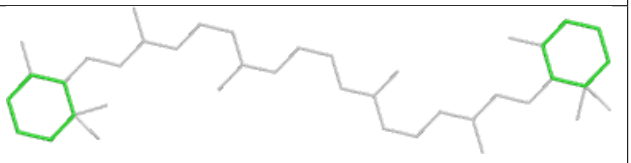
Bond lengths



Bond angles

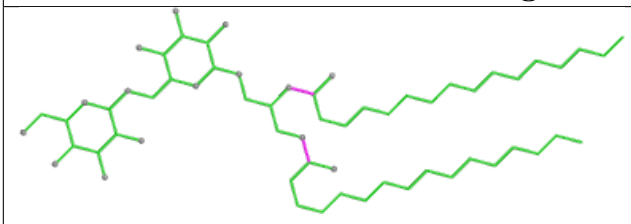


Torsions

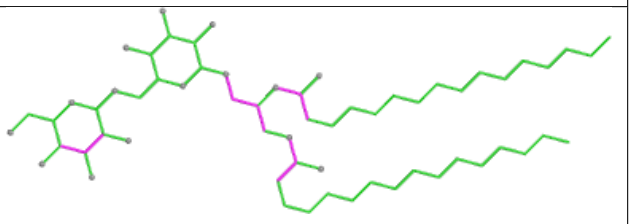


Rings

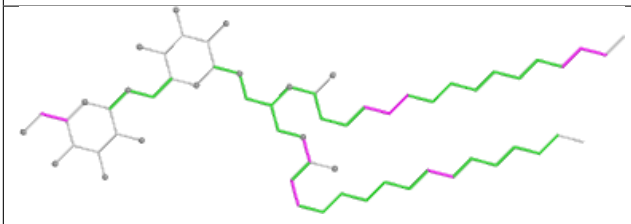
Ligand DGD C 517



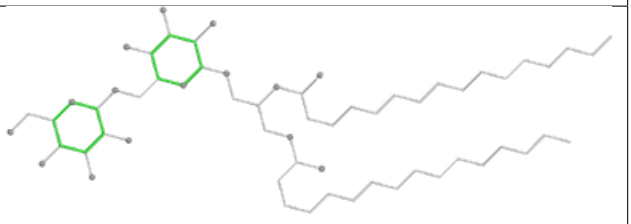
Bond lengths



Bond angles

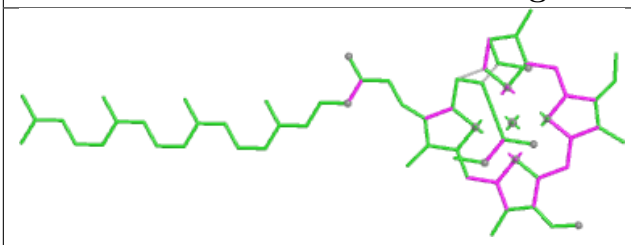


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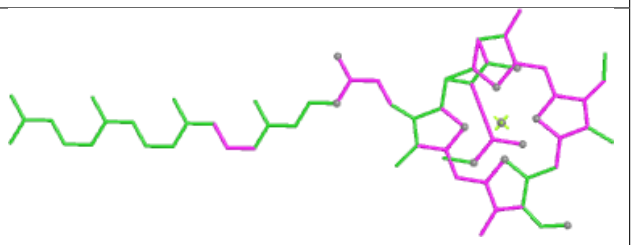


Rings

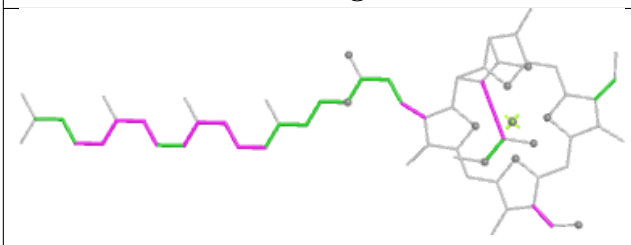
Ligand CL7 B 612



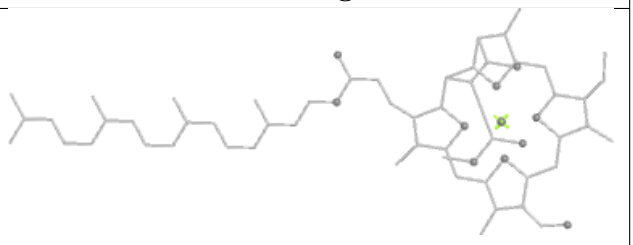
Bond lengths



Bond angles

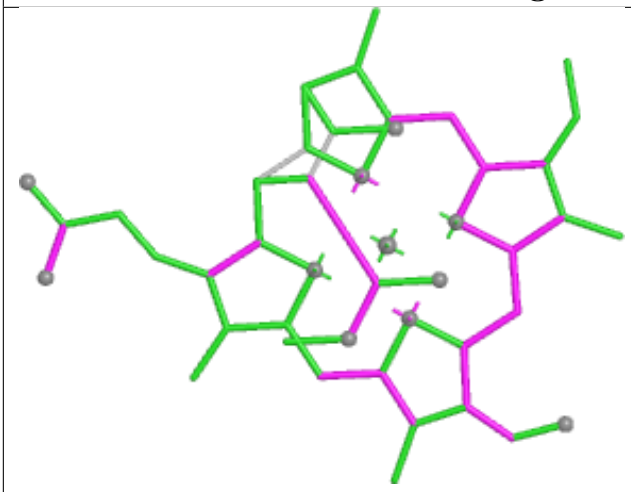


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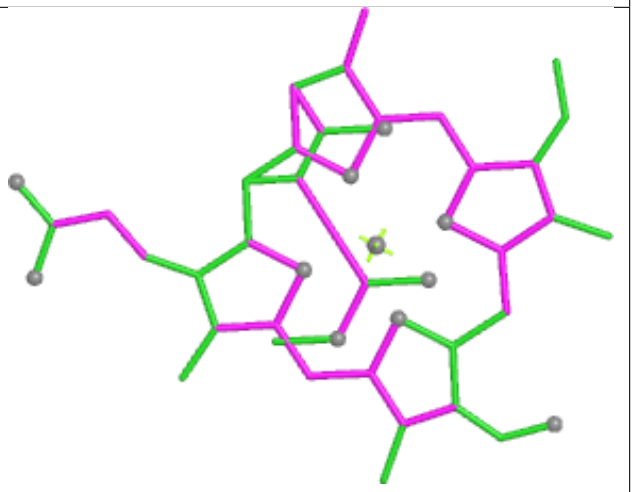


Rings

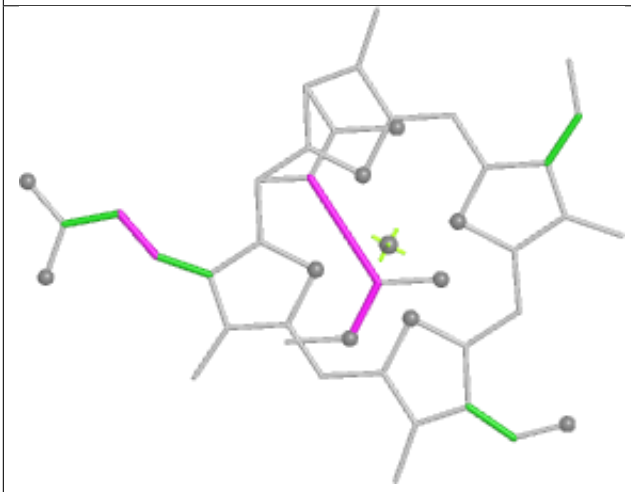
Ligand CL7 B 616



Bond lengths



Bond angles

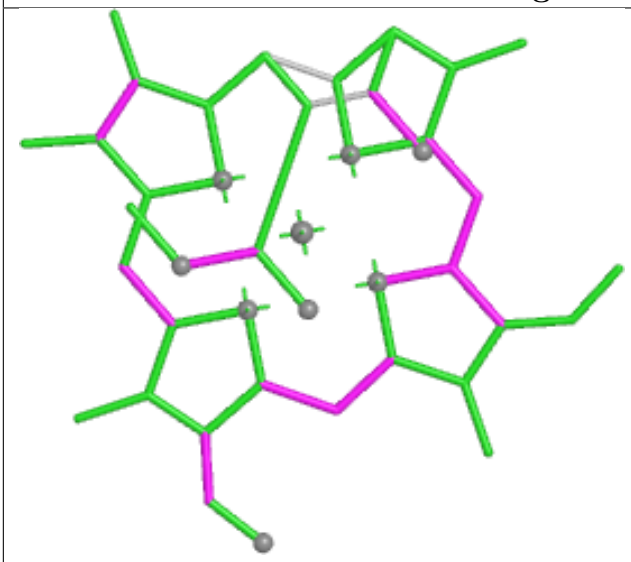


Torsions

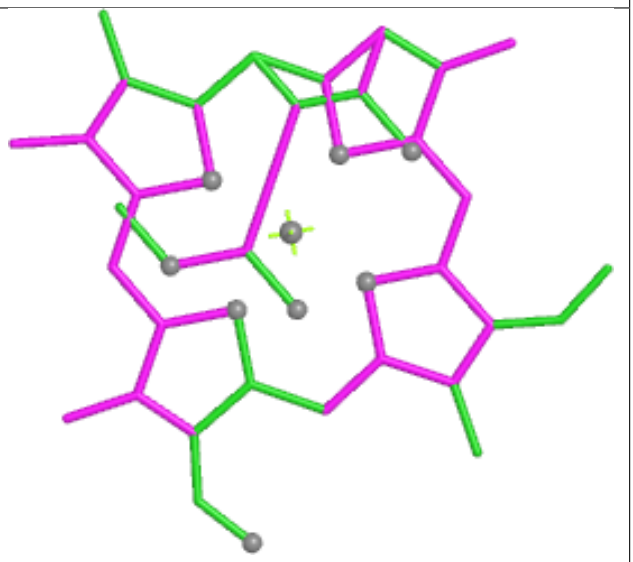


Rings

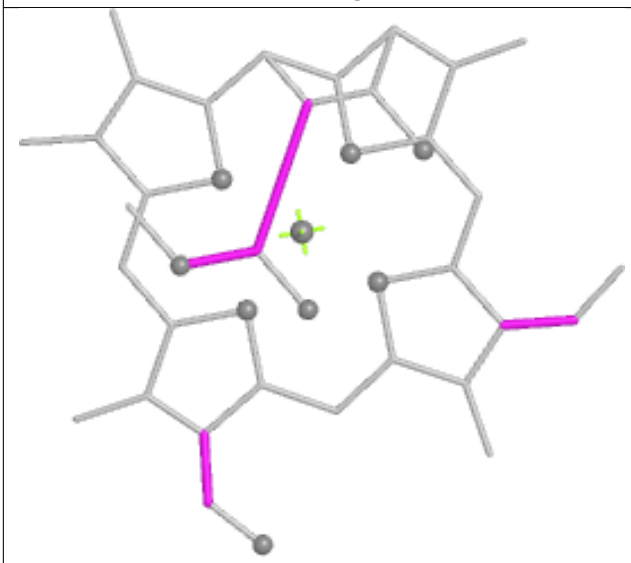
Ligand CL7 1 415



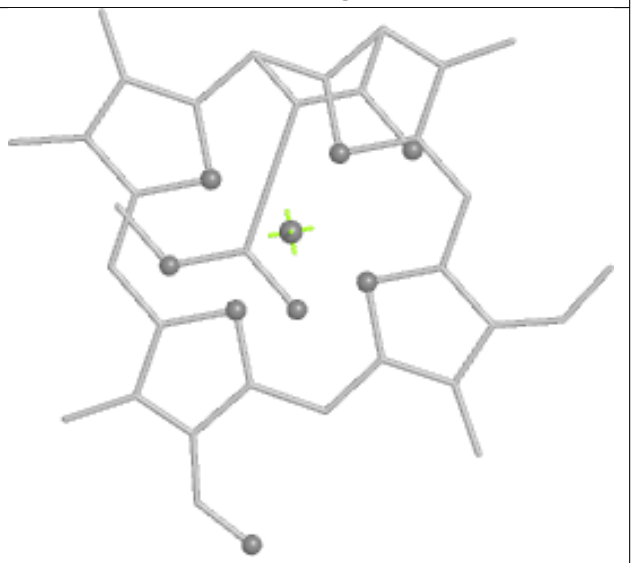
Bond lengths



Bond angles

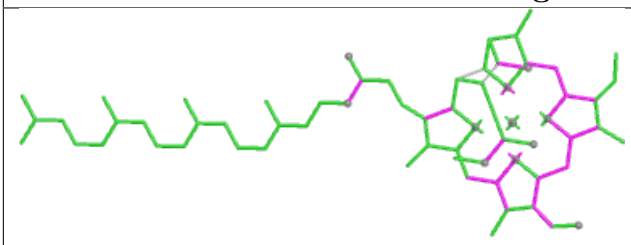


Torsions

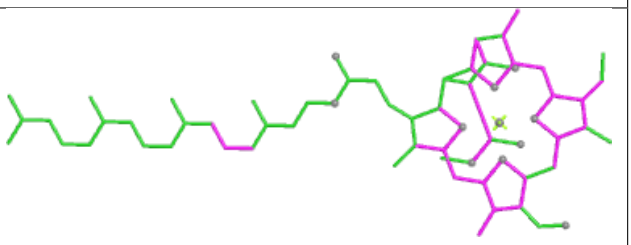


Rings

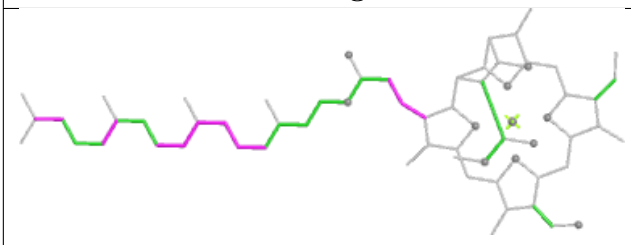
Ligand CL7 4 404



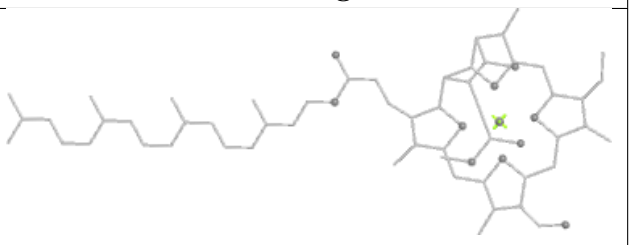
Bond lengths



Bond angles

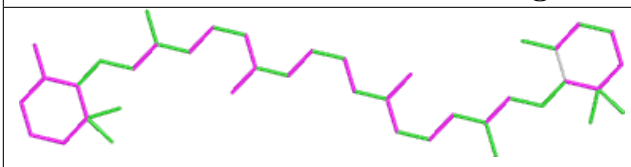


Torsions

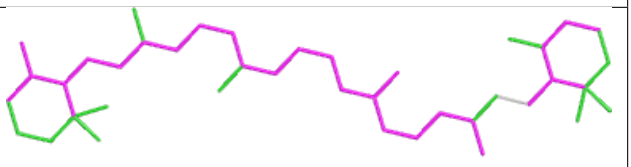


Rings

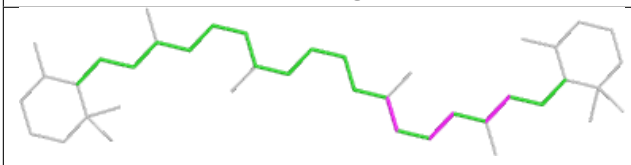
Ligand 8CT a 404



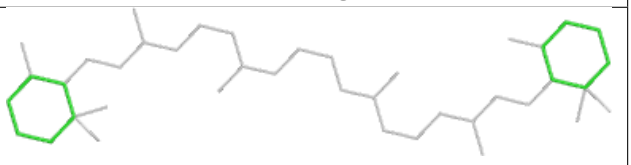
Bond lengths



Bond angles

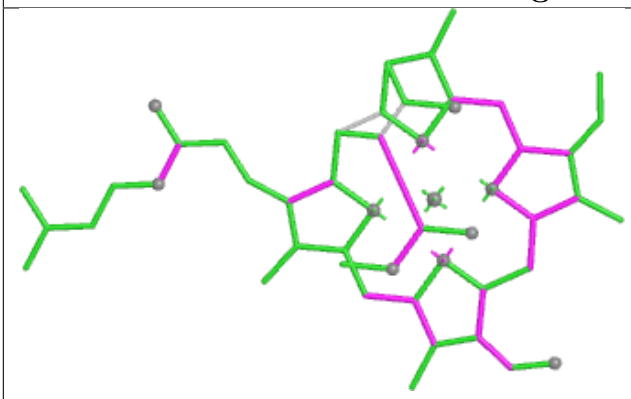


Torsions

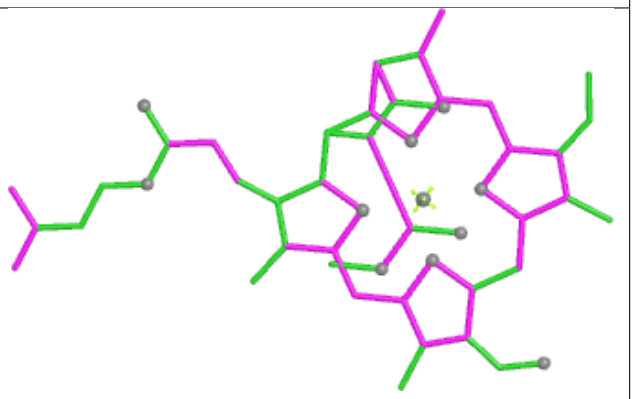


Rings

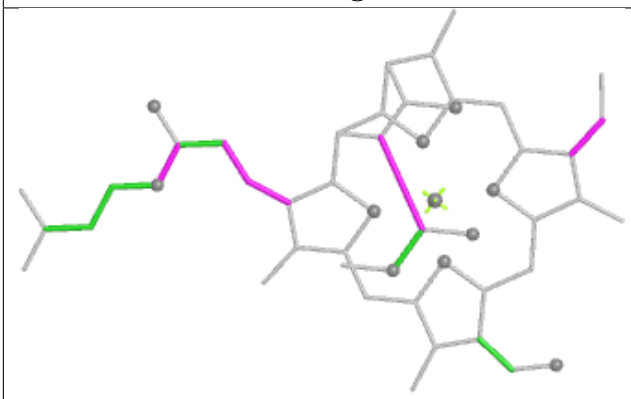
Ligand CL7 b 616



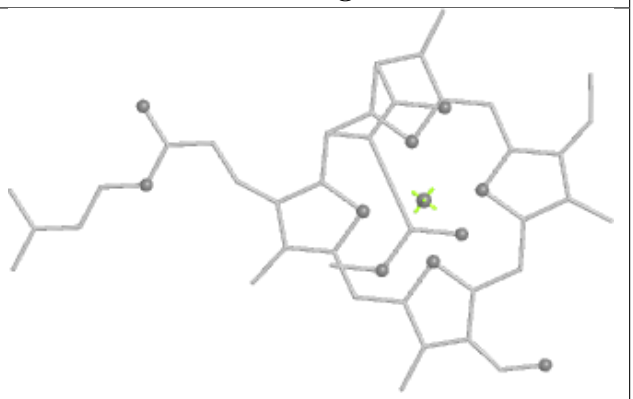
Bond lengths



Bond angles

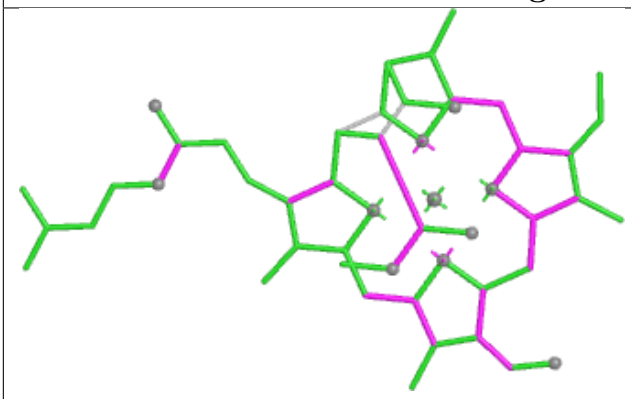


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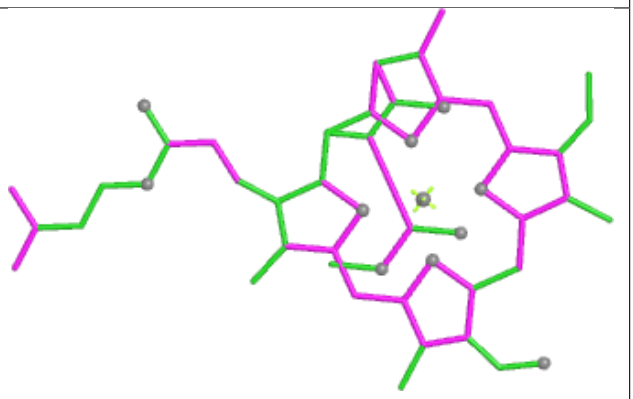


Rings

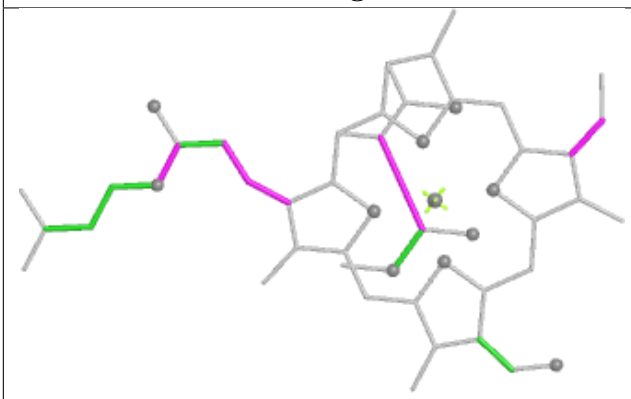
Ligand CL7 B 615



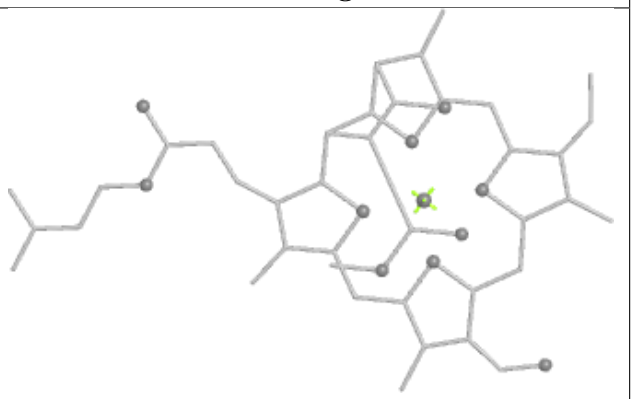
Bond lengths



Bond angles

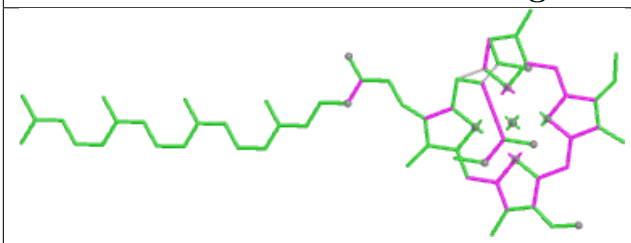


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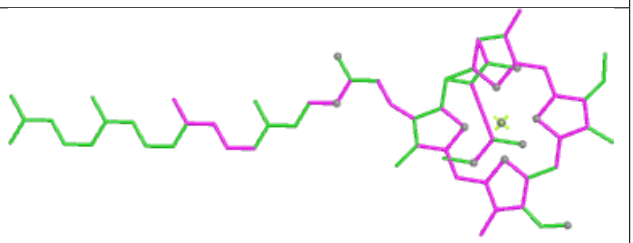


Rings

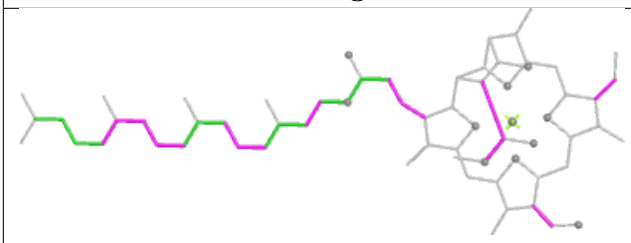
Ligand CL7 C 506



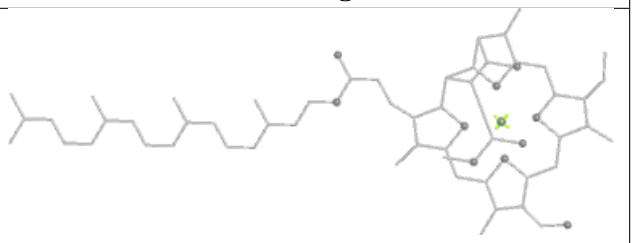
Bond lengths



Bond angles

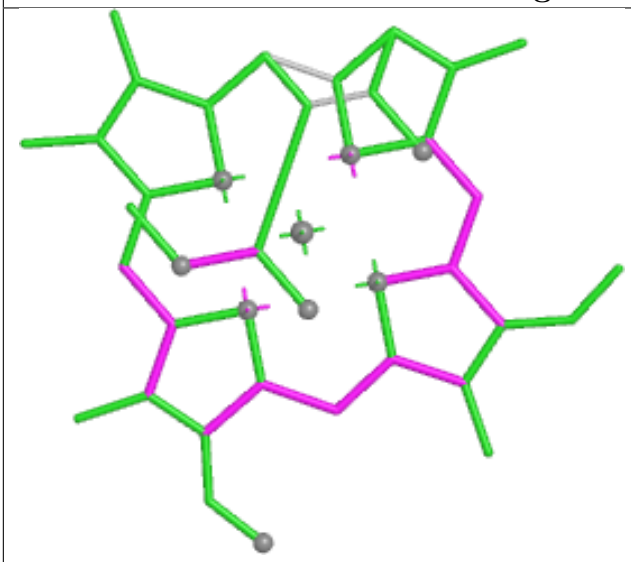


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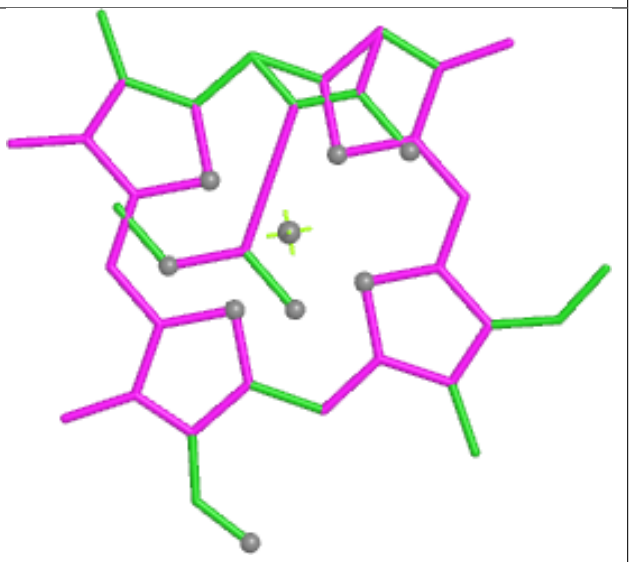


Rings

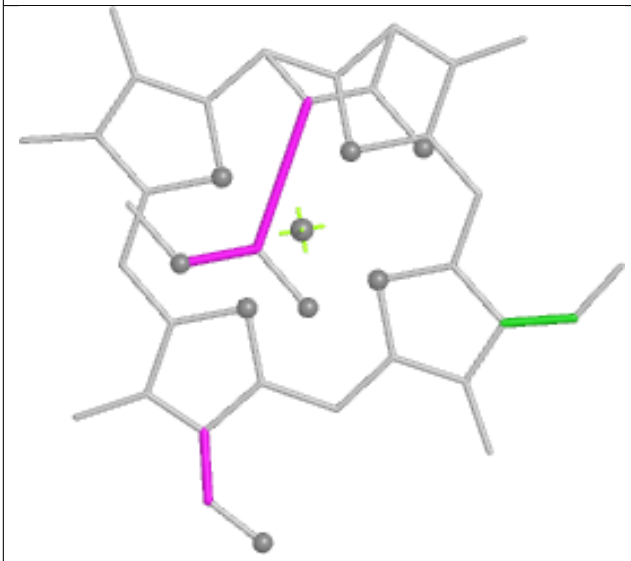
Ligand CL7 c 518



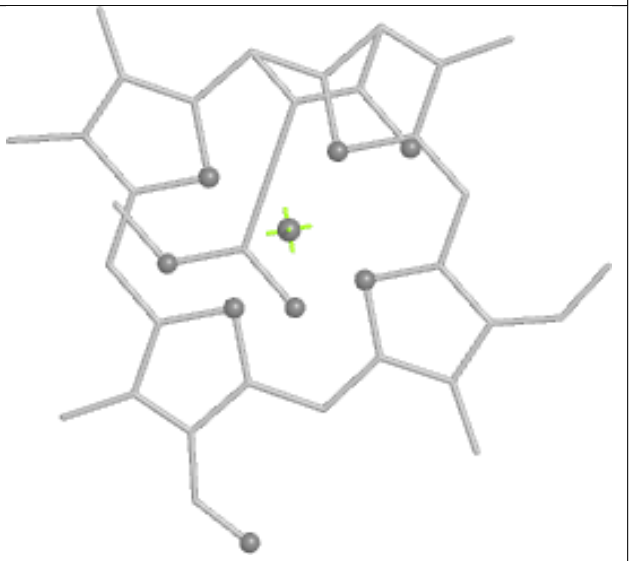
Bond lengths



Bond angles

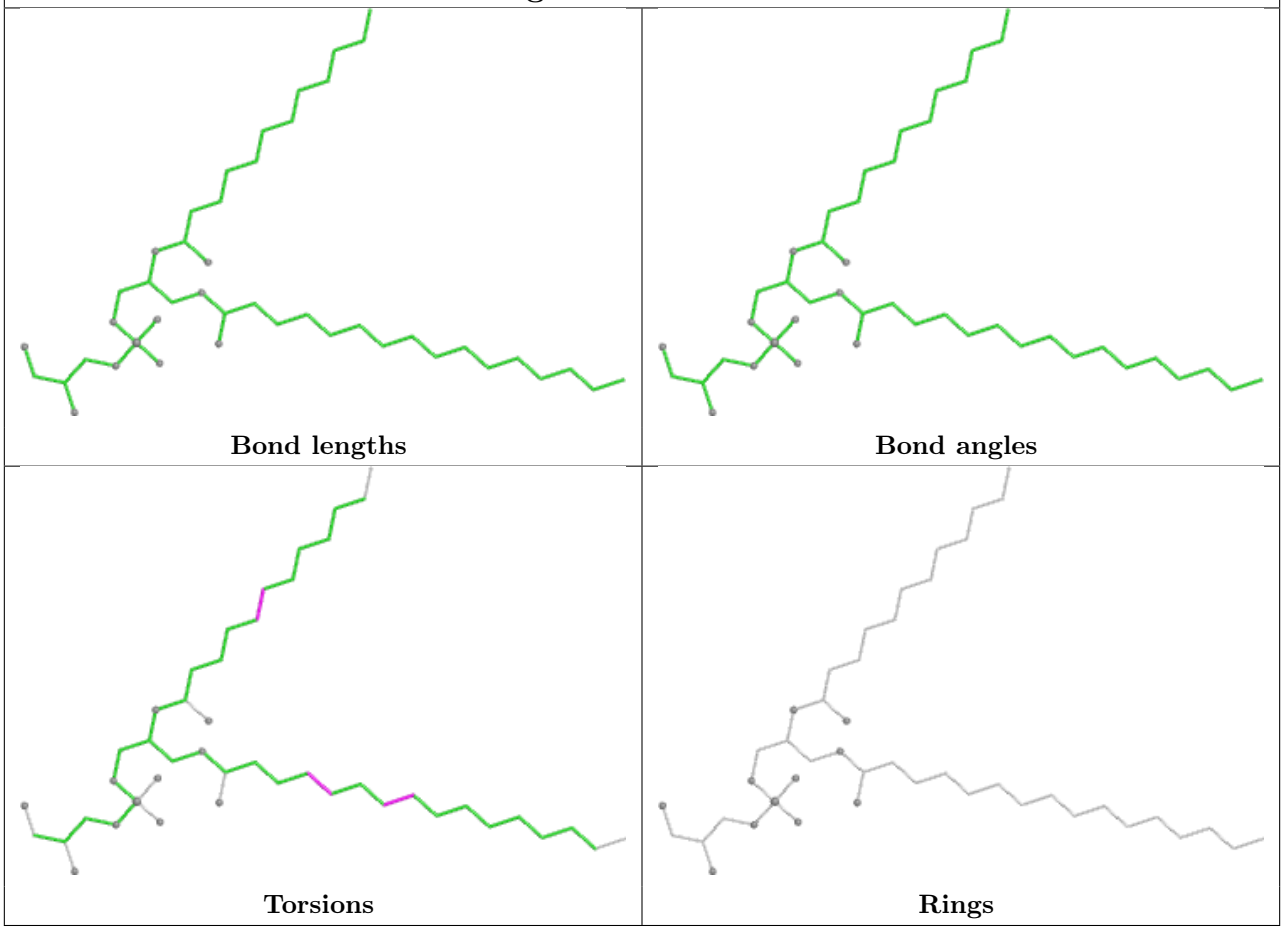


Torsions

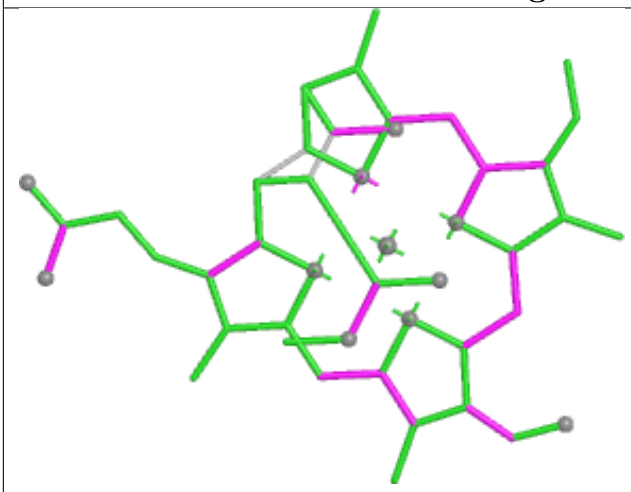


Rings

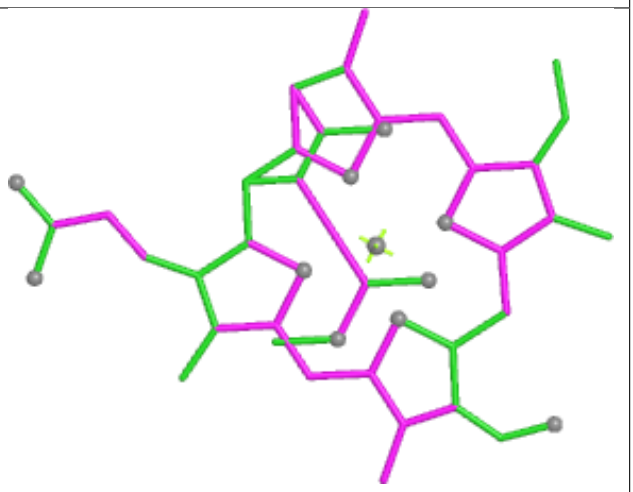
Ligand LHG b 624



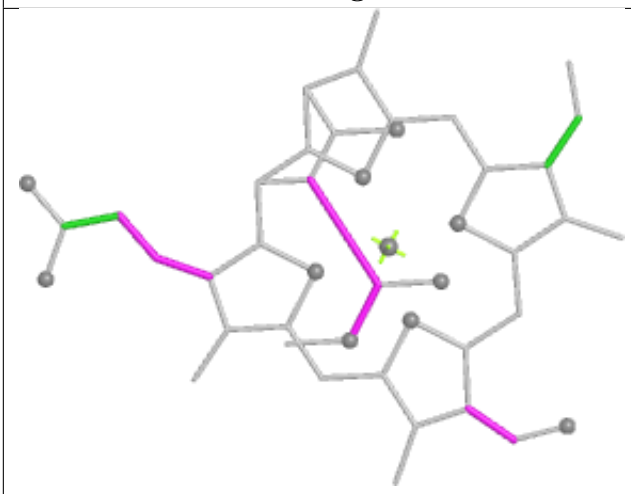
Ligand CL7 C 514



Bond lengths



Bond angles

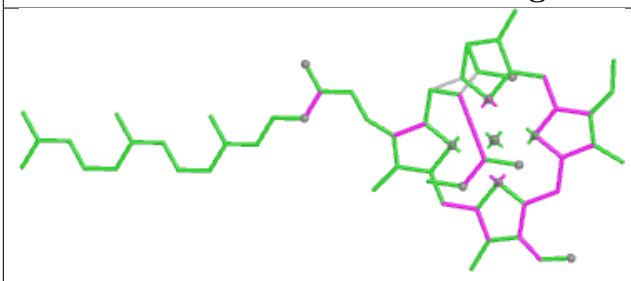


Torsions

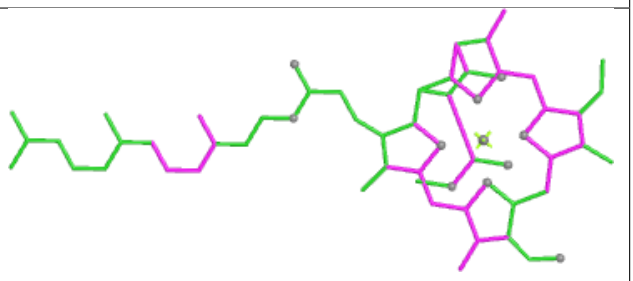


Rings

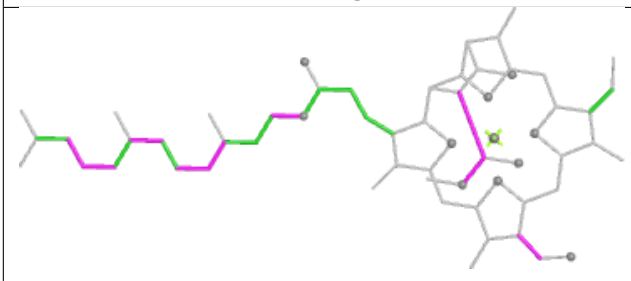
Ligand CL7 C 503



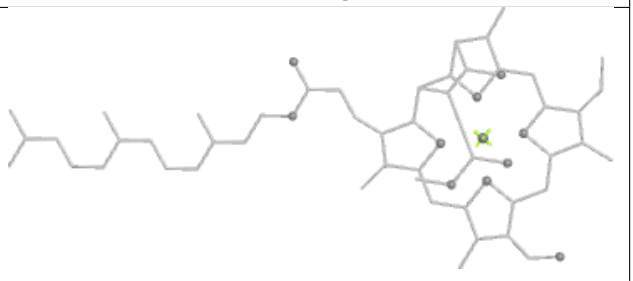
Bond lengths



Bond angles

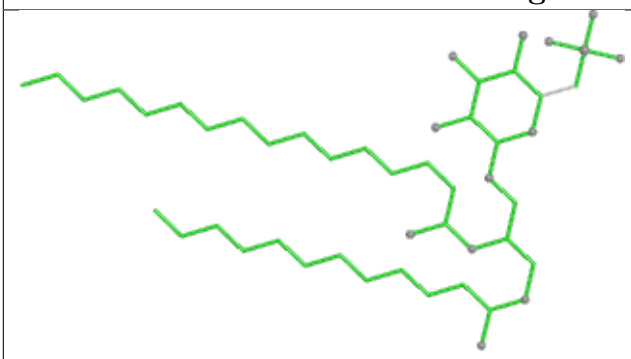


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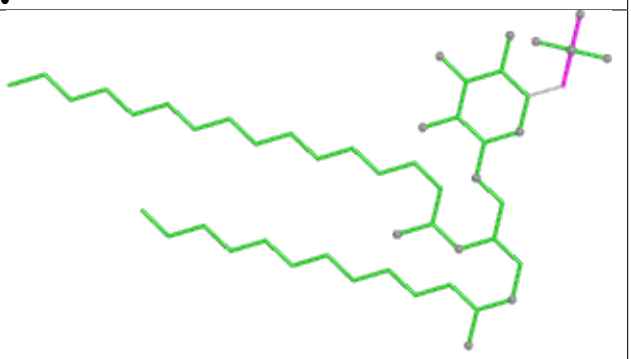


Rings

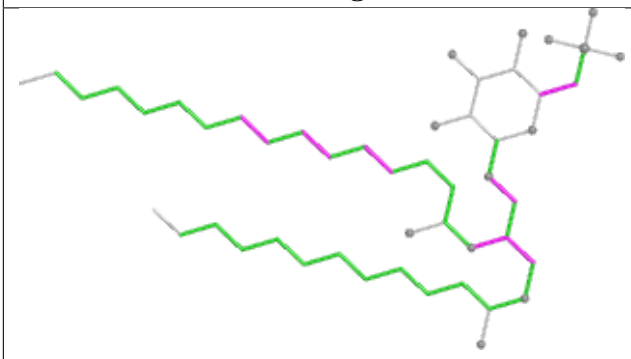
Ligand SQD 7 523



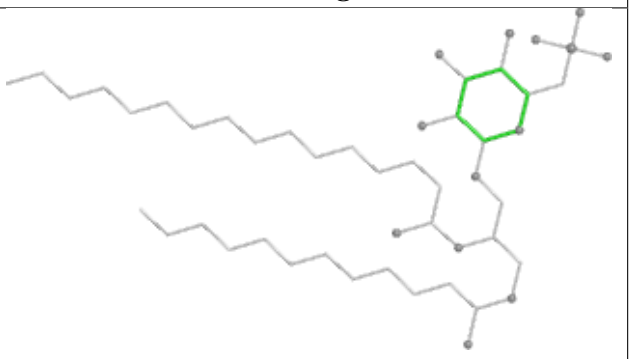
Bond lengths



Bond angles

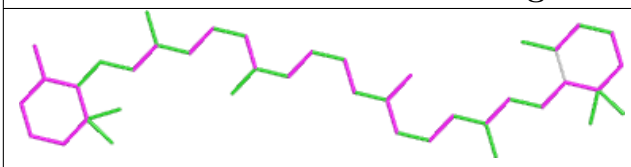


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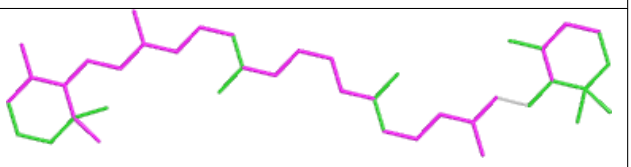


Rings

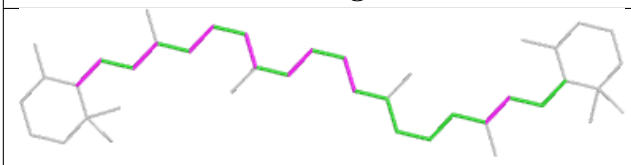
Ligand 8CT B 618



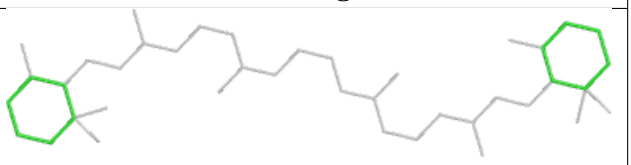
Bond lengths



Bond angles

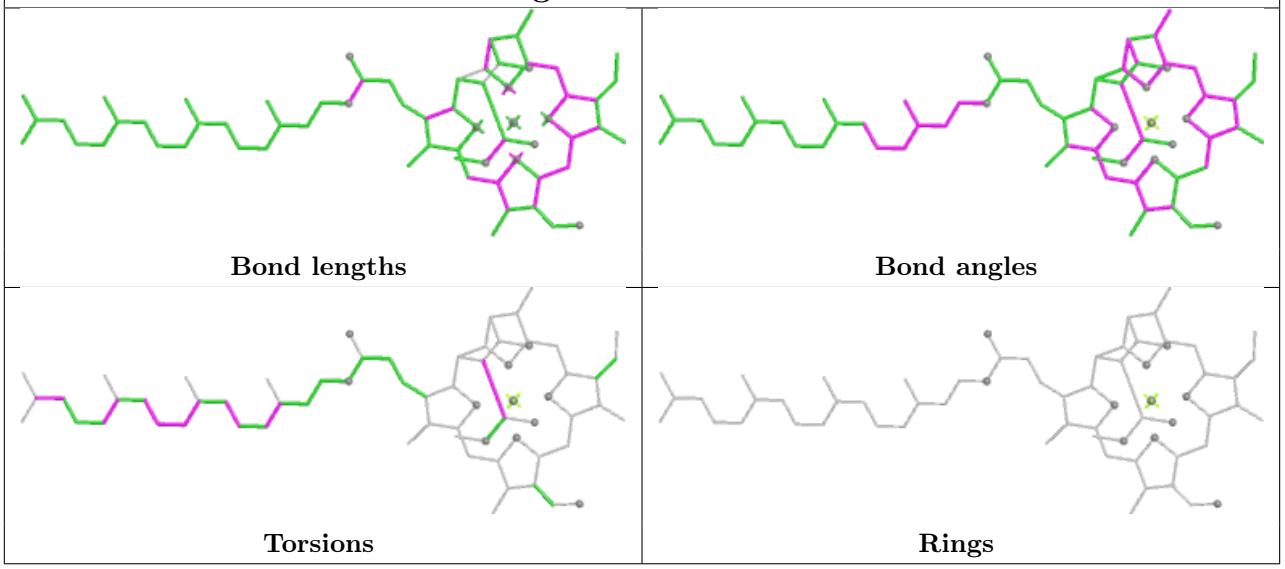


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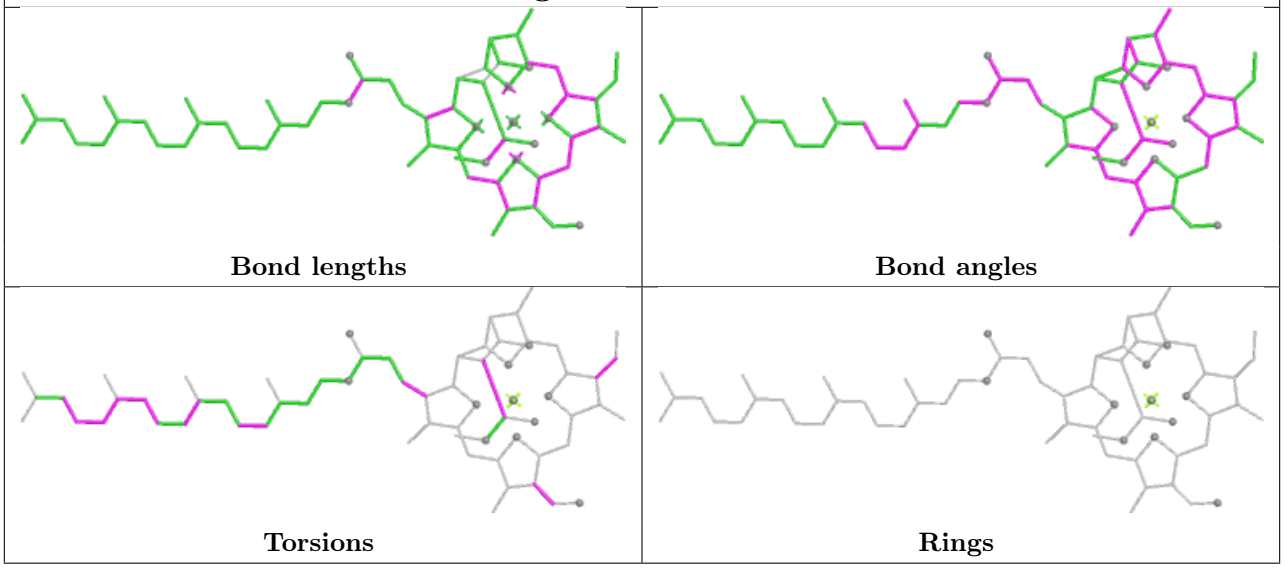


Rings

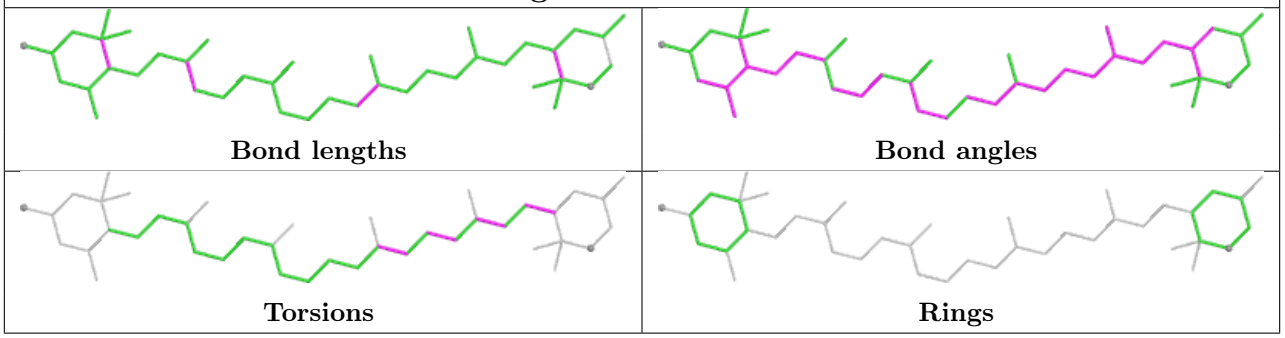
Ligand CL7 b 604



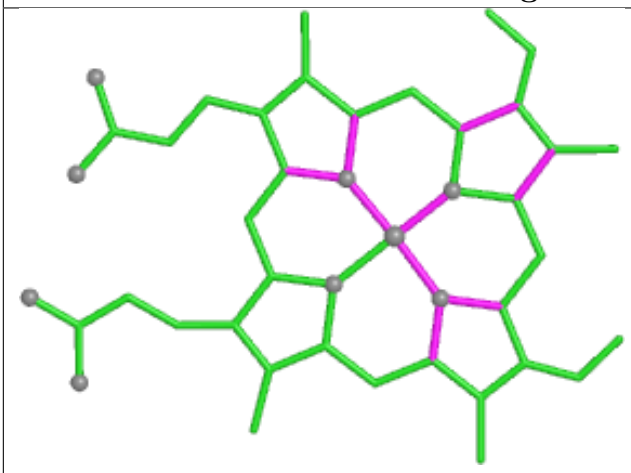
Ligand CL7 1 408



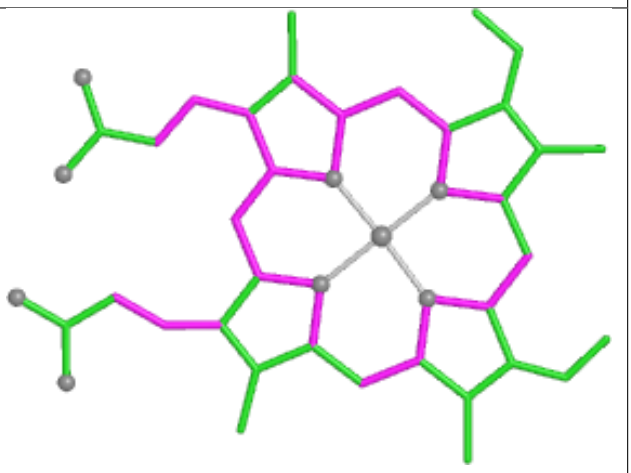
Ligand ZEX 2 523



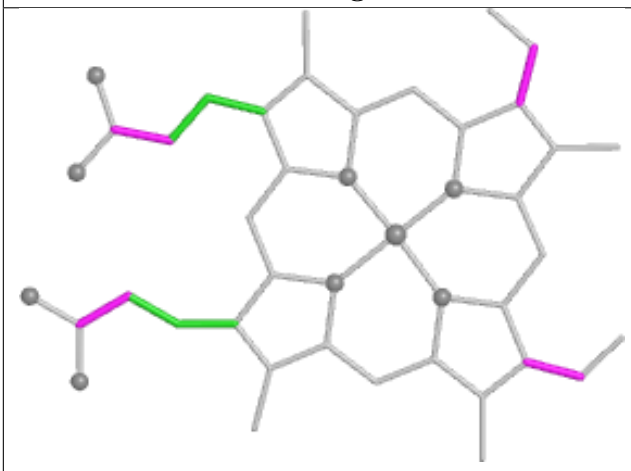
Ligand HEM F 101



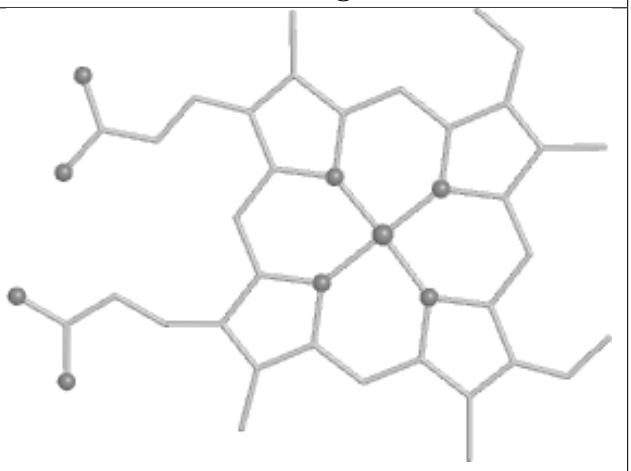
Bond lengths



Bond angles

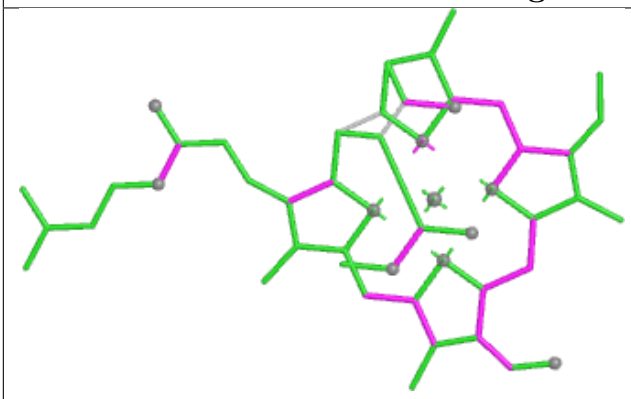


Torsions

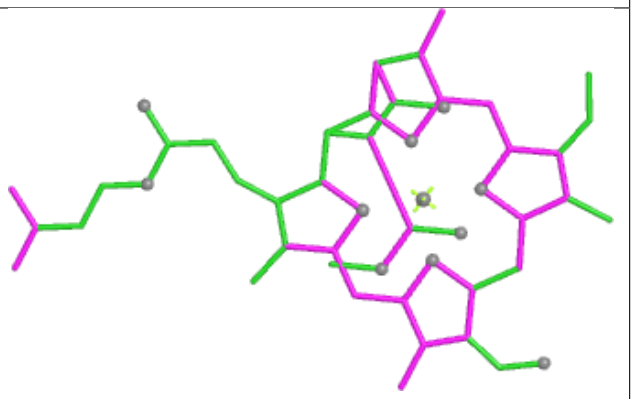


Rings

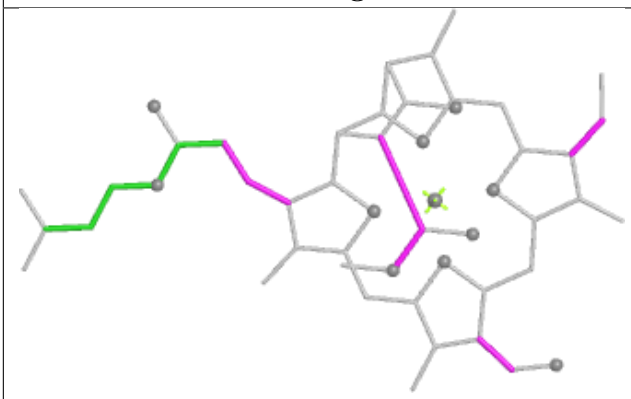
Ligand CL7 D 402



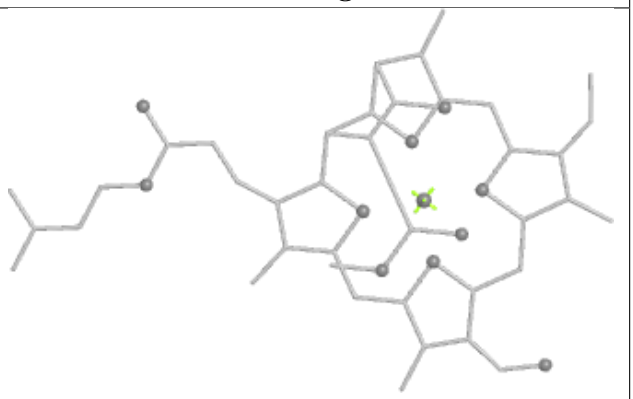
Bond lengths



Bond angles

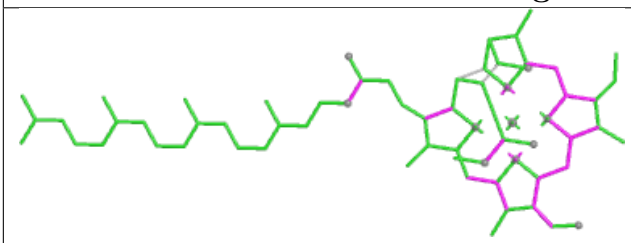


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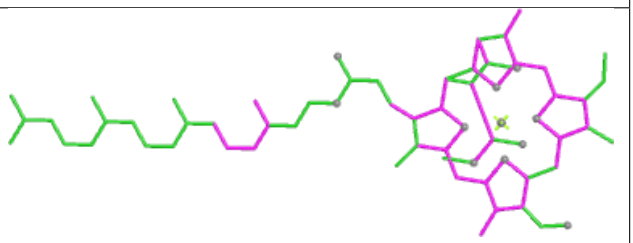


Rings

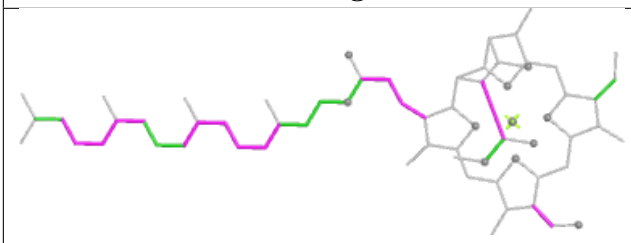
Ligand CL7 7 501



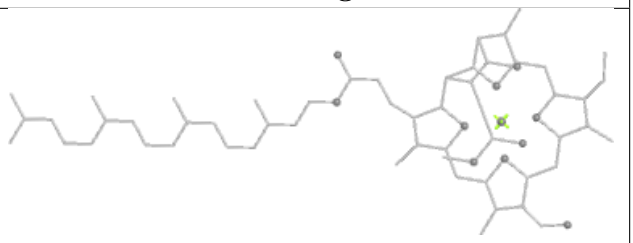
Bond lengths



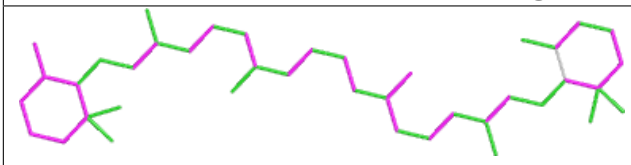
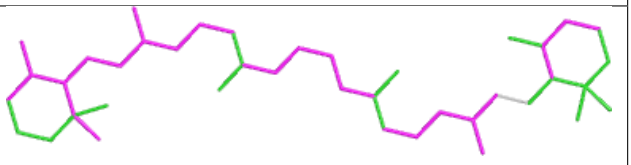
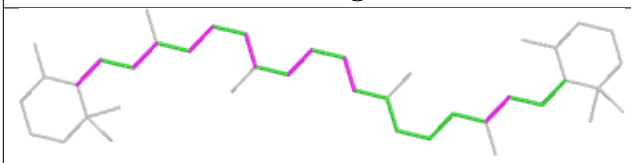
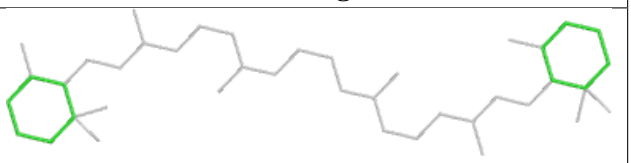
Bond angles

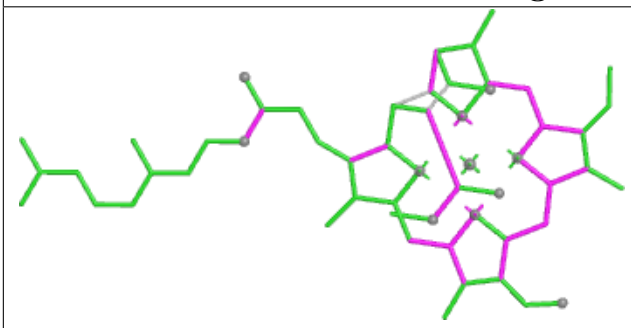
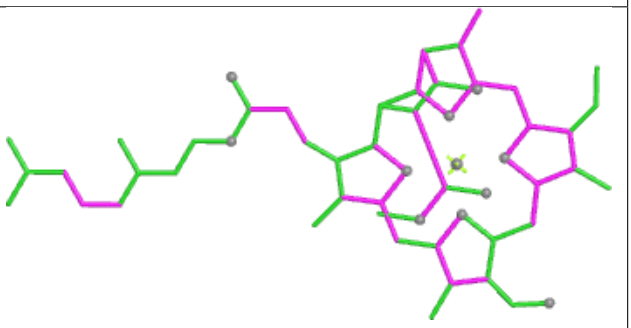
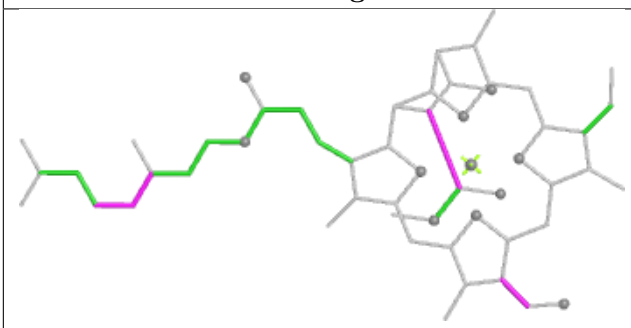
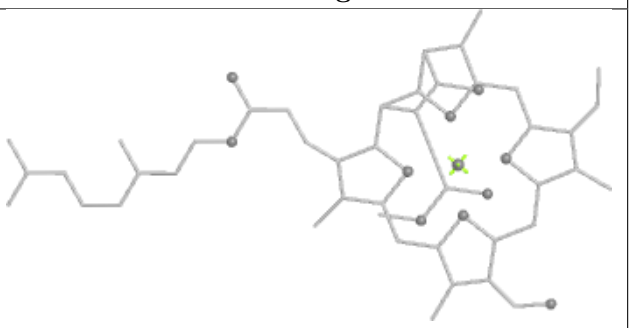


Torsions

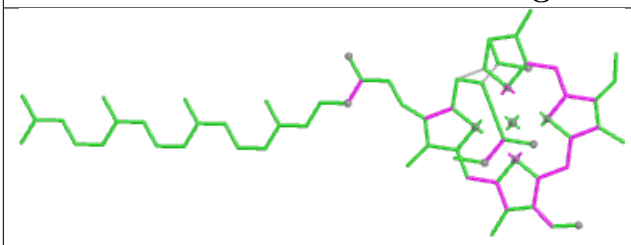


Rings

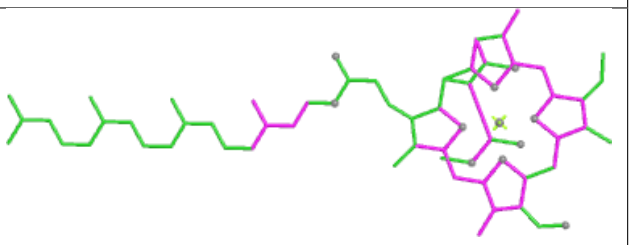
Ligand 8CT b 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CL7 B 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

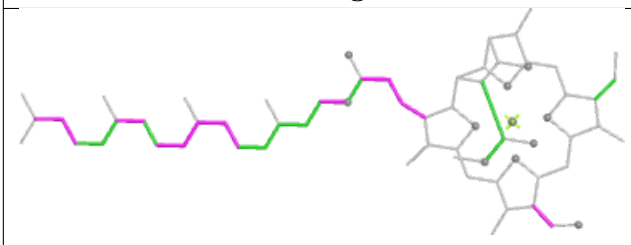
Ligand CL7 2 501



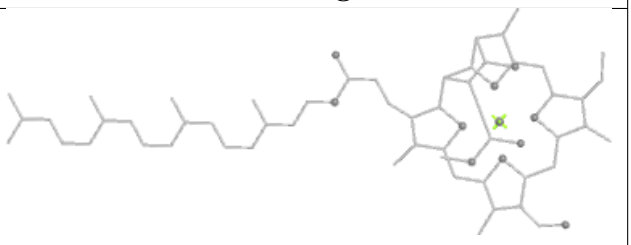
Bond lengths



Bond angles

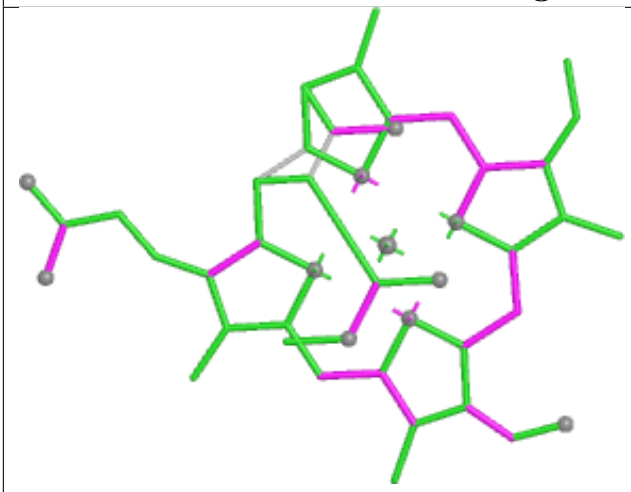


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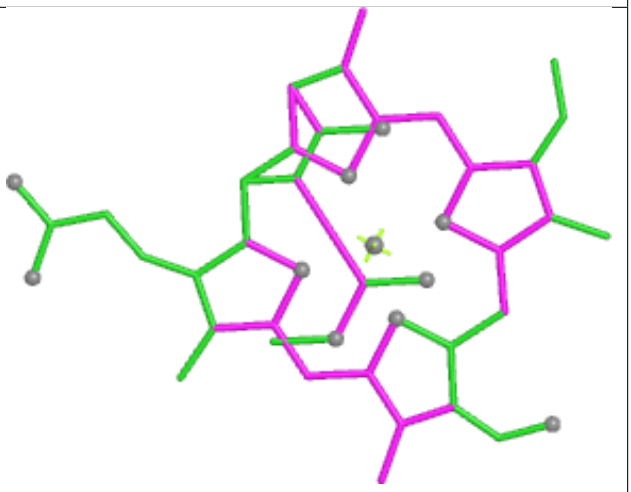


Rings

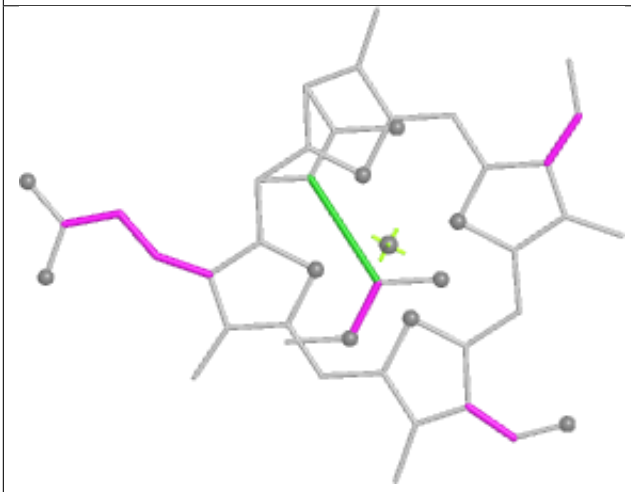
Ligand CL7 1 419



Bond lengths



Bond angles

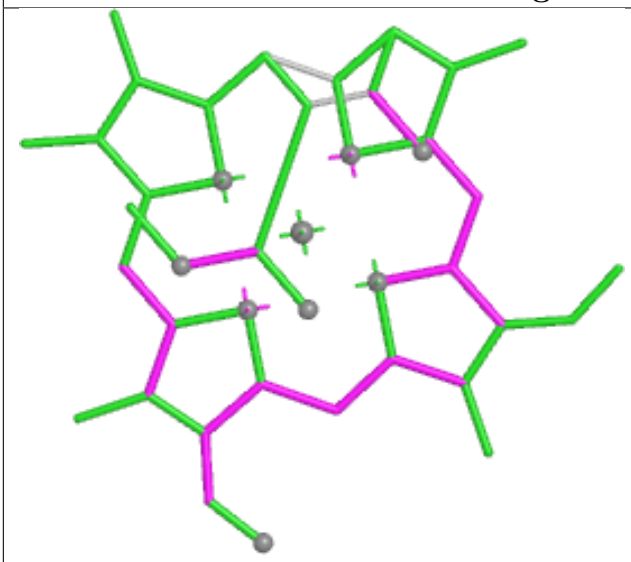


Torsions

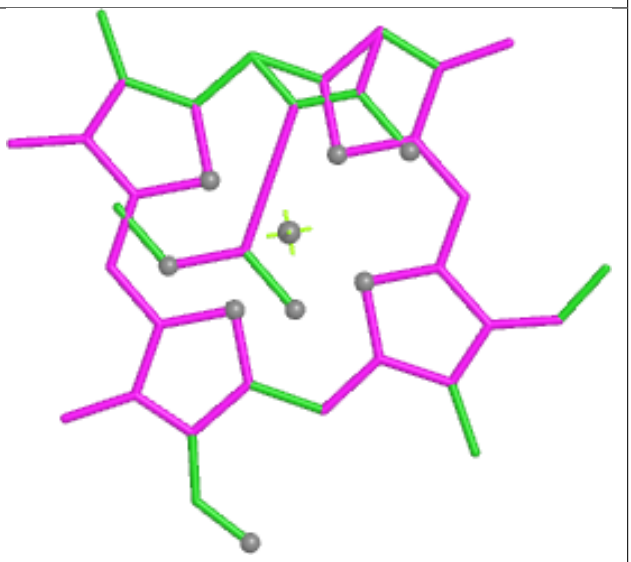


Rings

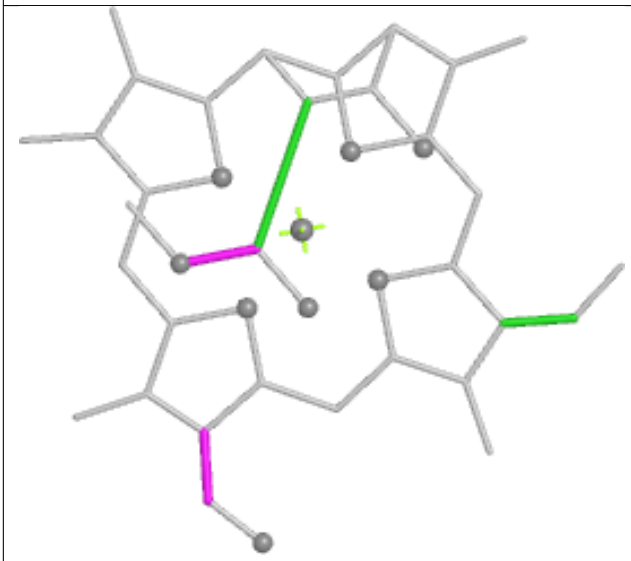
Ligand CL7 5 407



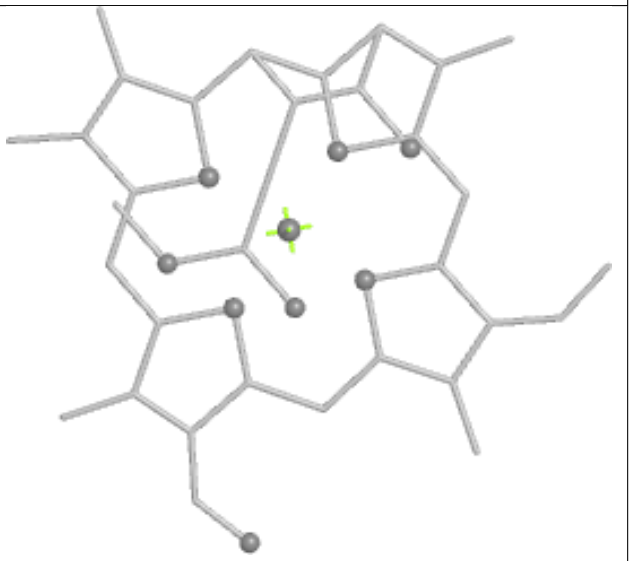
Bond lengths



Bond angles

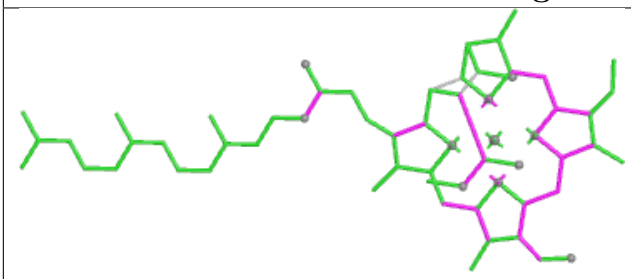


Torsions

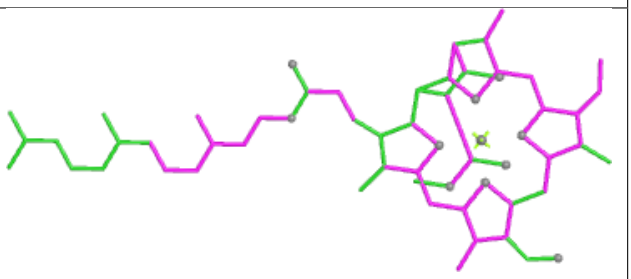


Rings

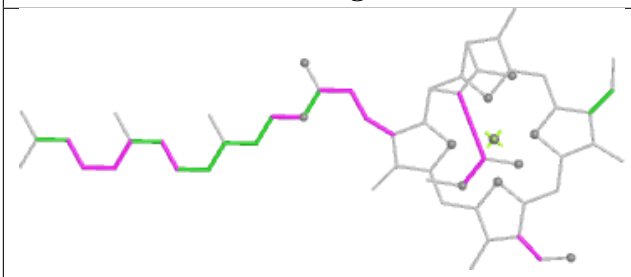
Ligand CL7 8 409



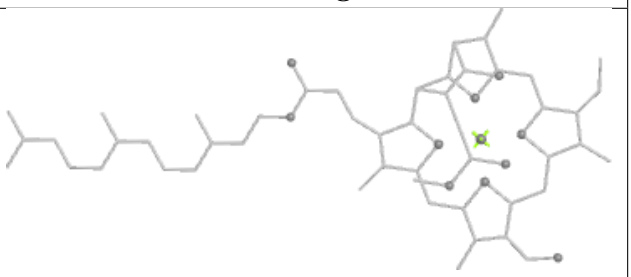
Bond lengths



Bond angles

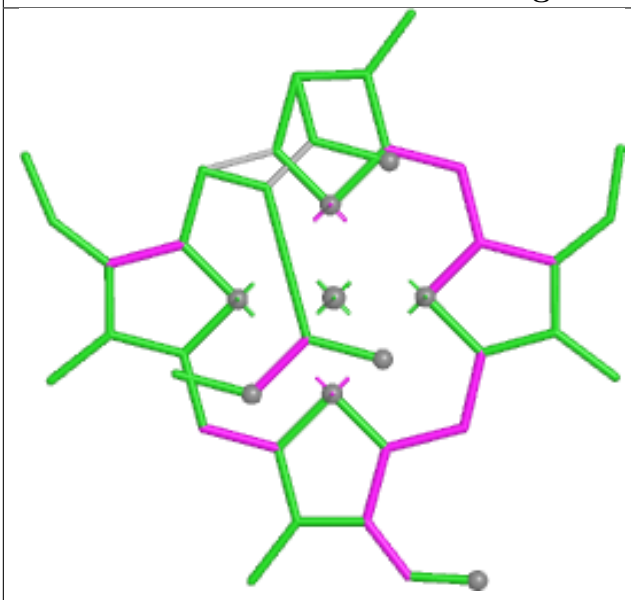


Torsions

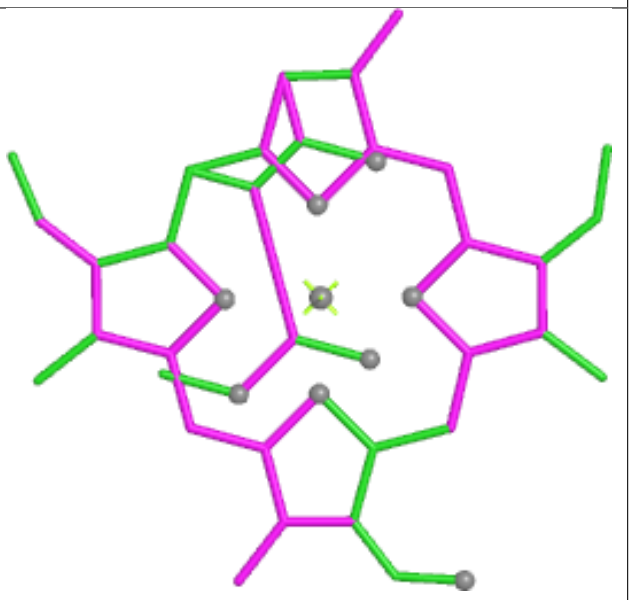


Rings

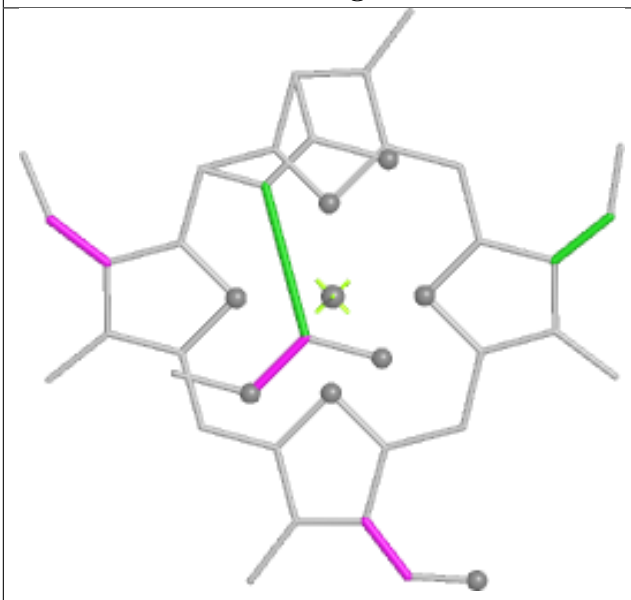
Ligand CL7 8 417



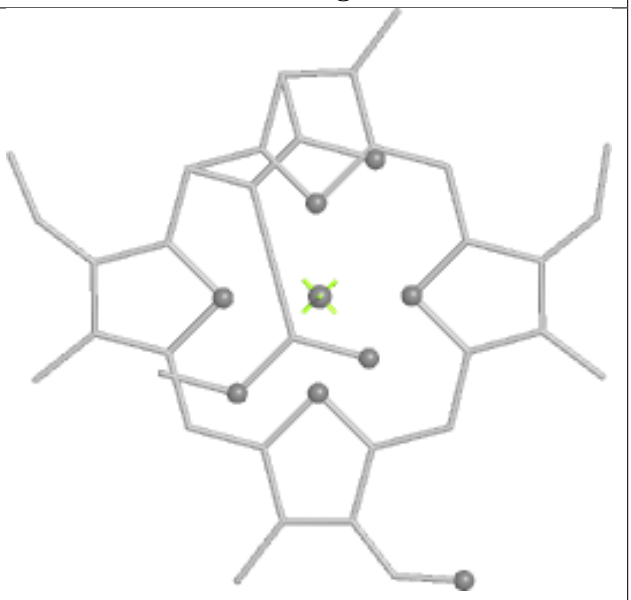
Bond lengths



Bond angles

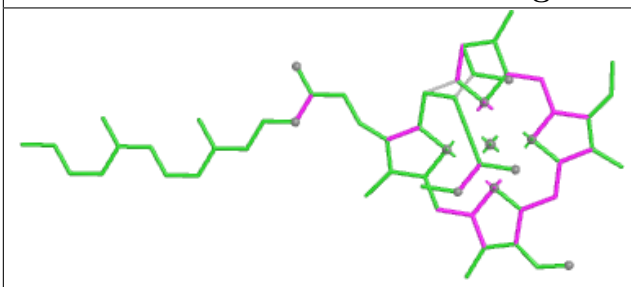


Torsions

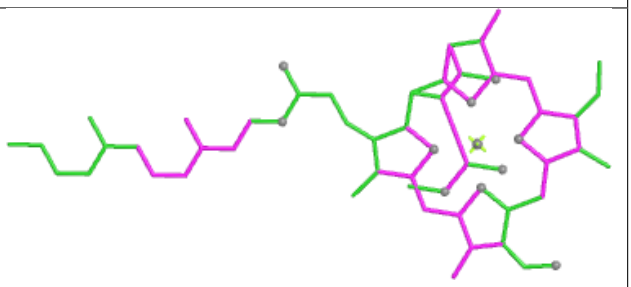


Rings

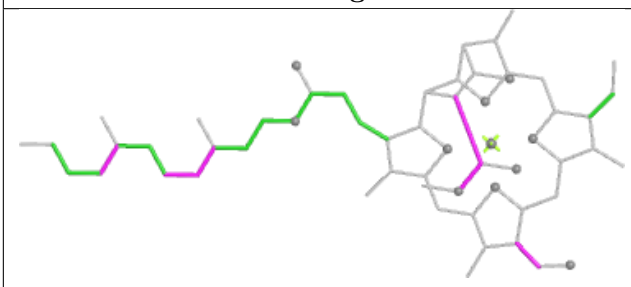
Ligand CL7 7 502



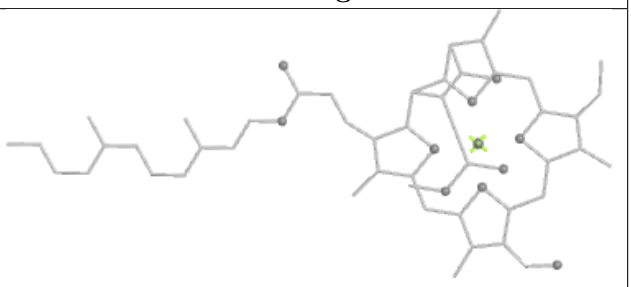
Bond lengths



Bond angles

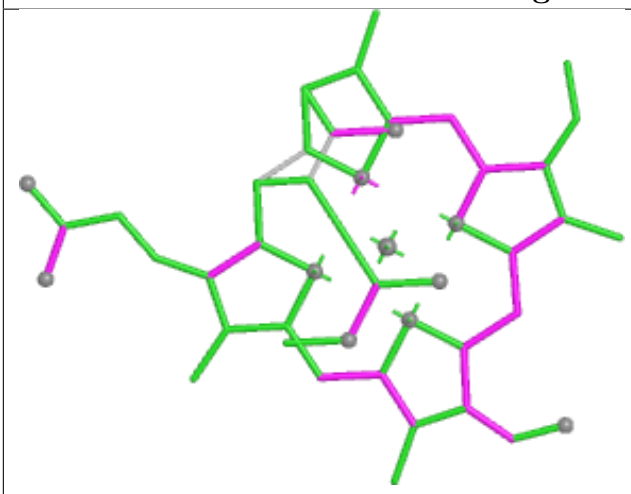


Torsions

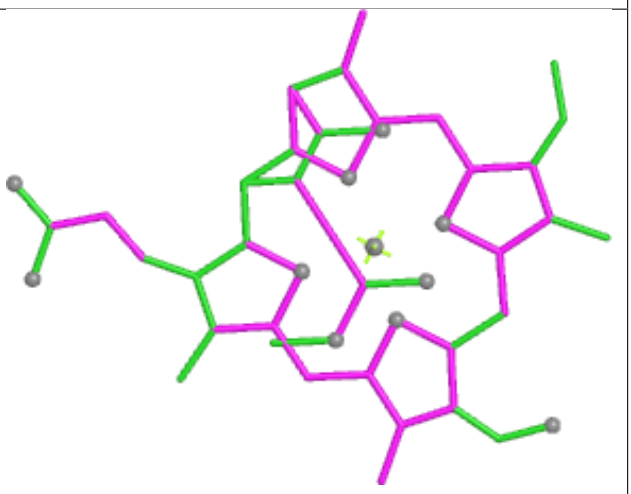


Rings

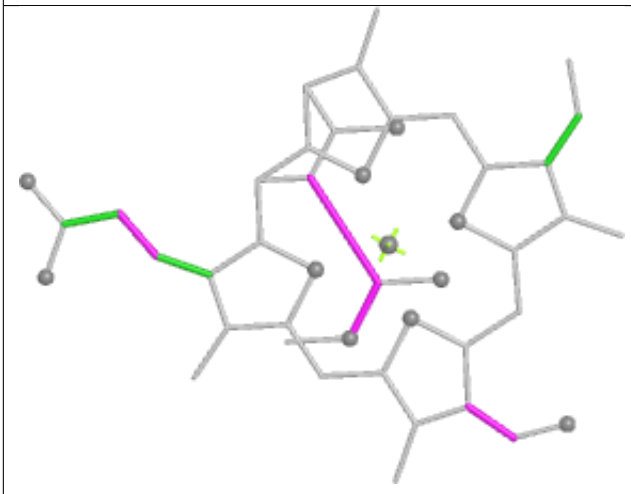
Ligand CL7 1 409



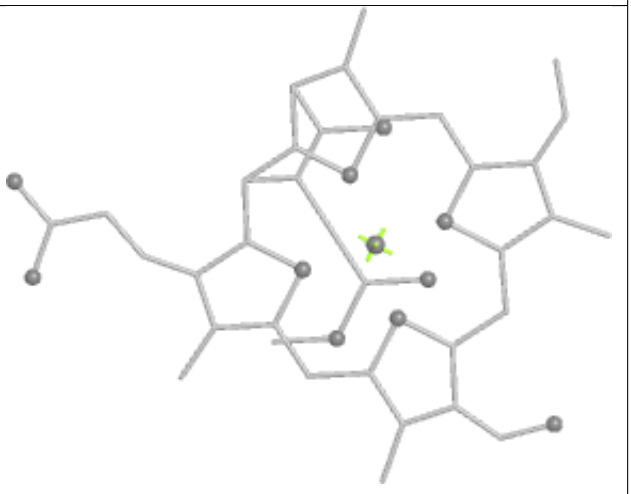
Bond lengths



Bond angles

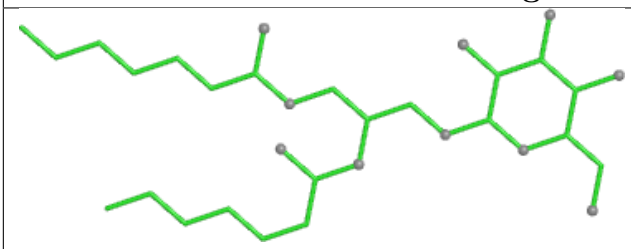


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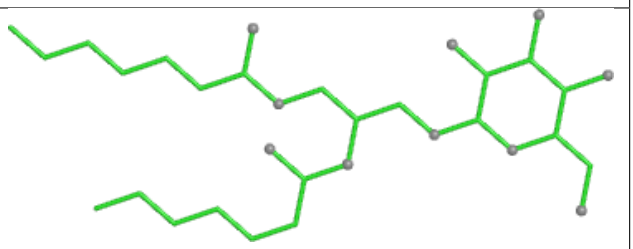


Rings

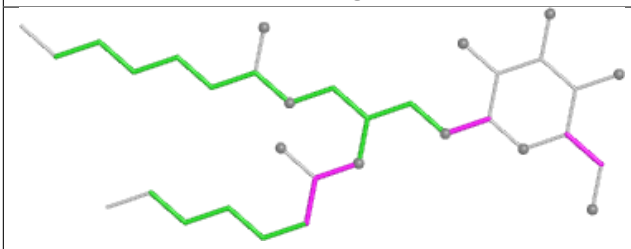
Ligand LMG d 410



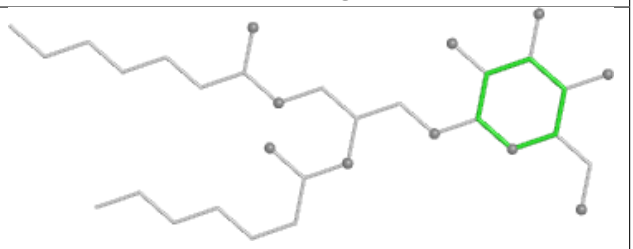
Bond lengths



Bond angles

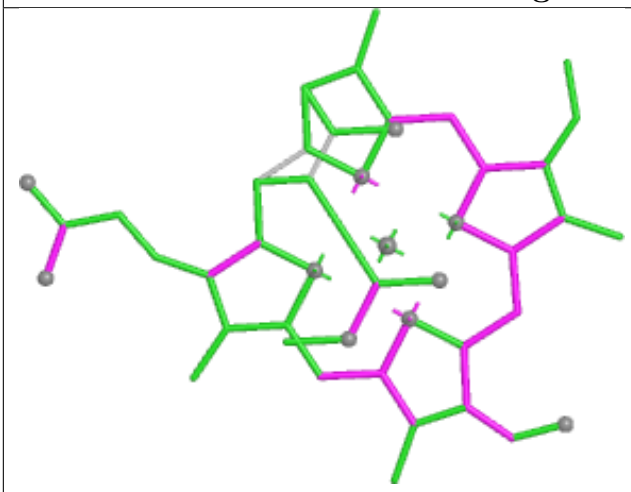


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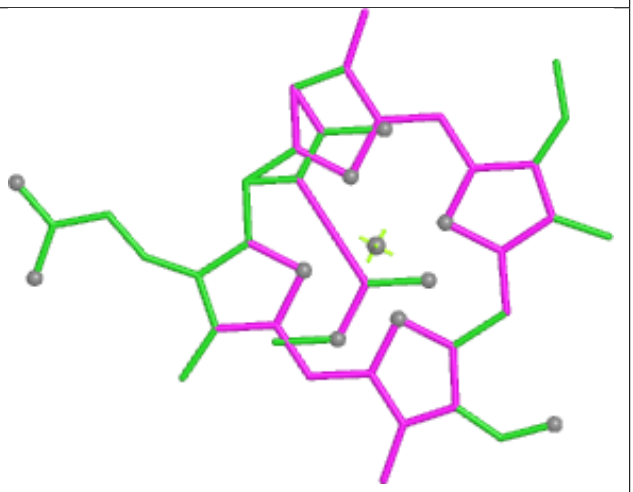


Rings

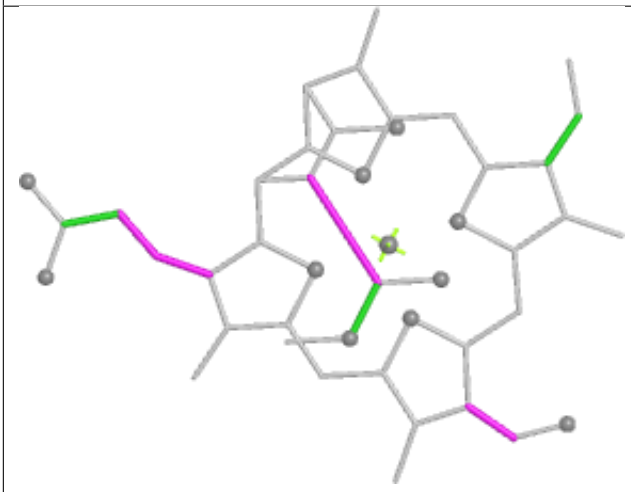
Ligand CL7 2 508



Bond lengths



Bond angles

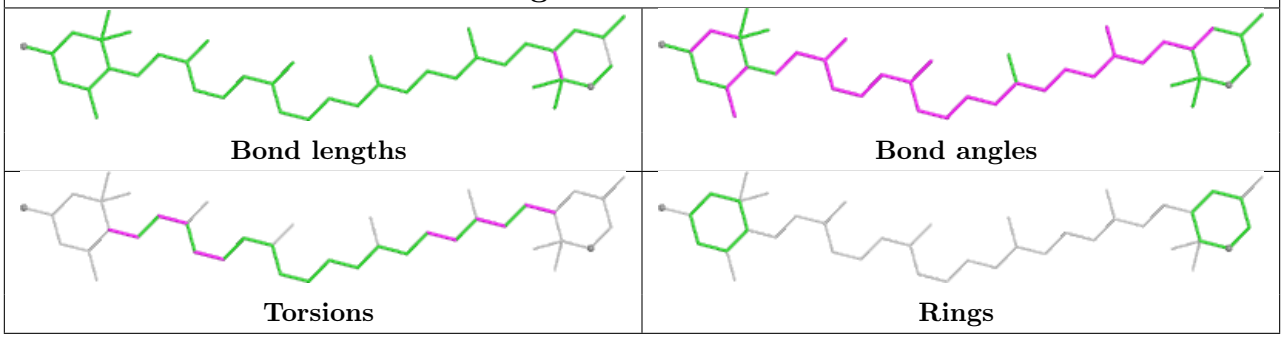


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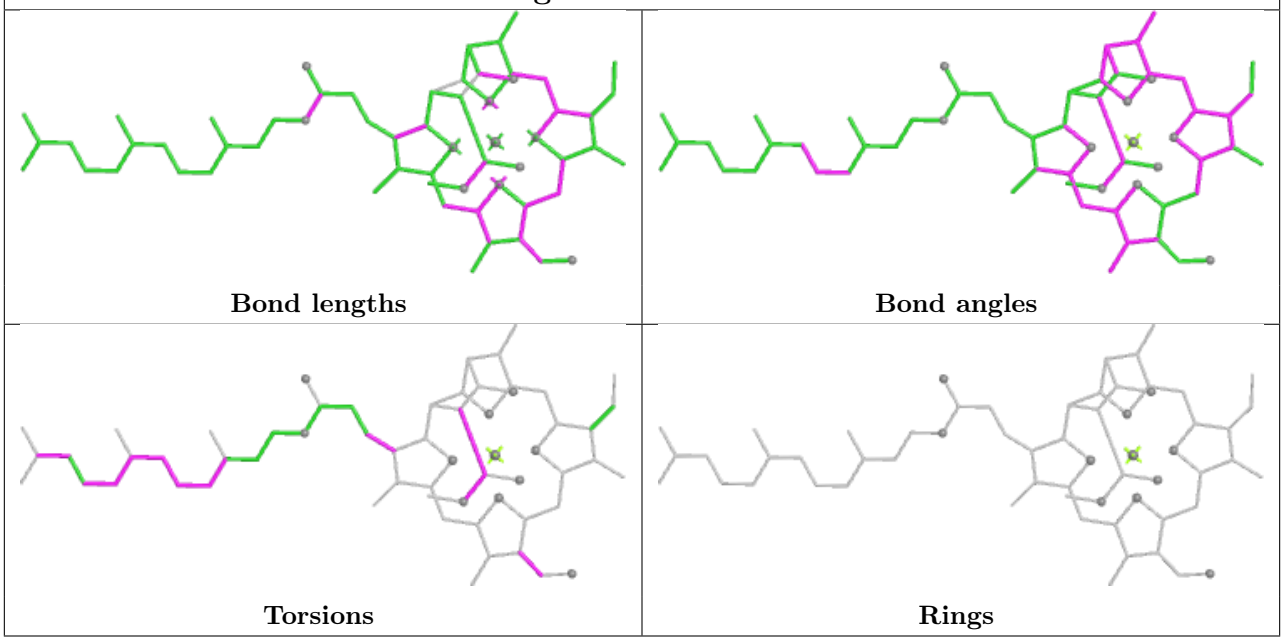


Rings

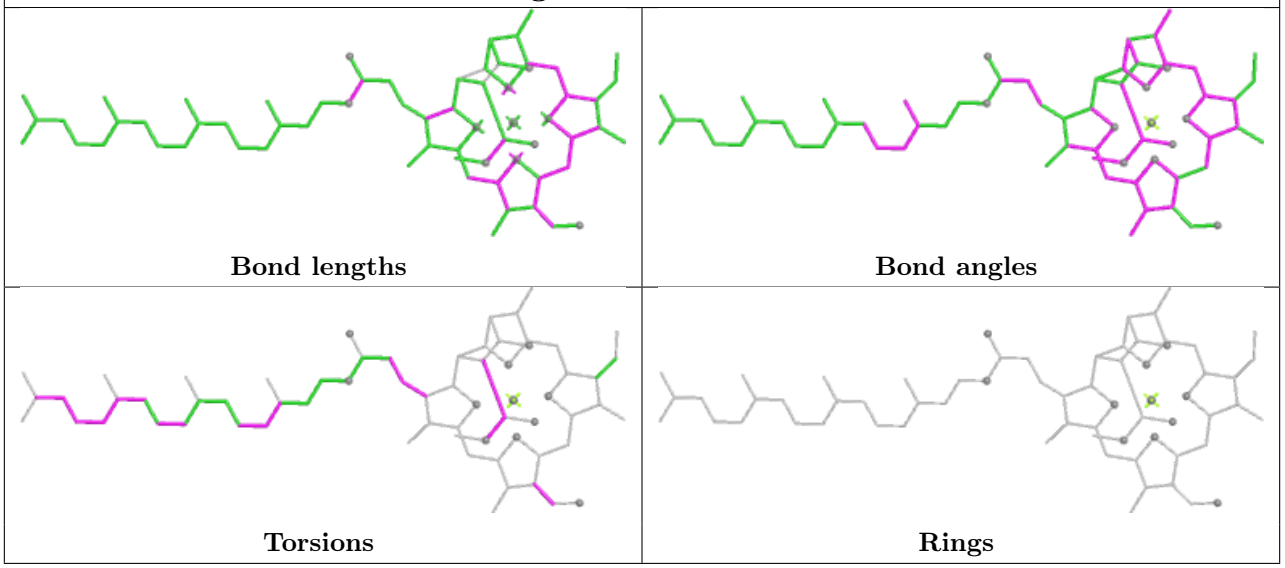
Ligand ZEX 4 418



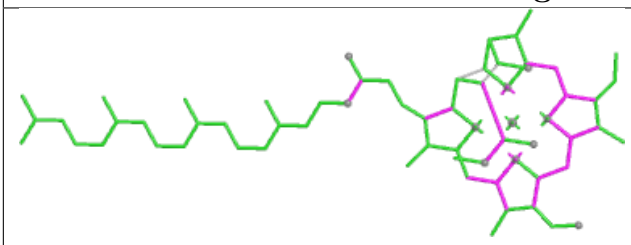
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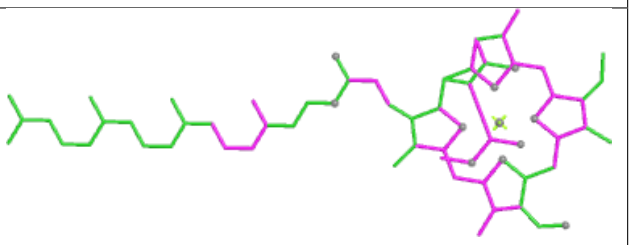
Ligand CL7 B 604



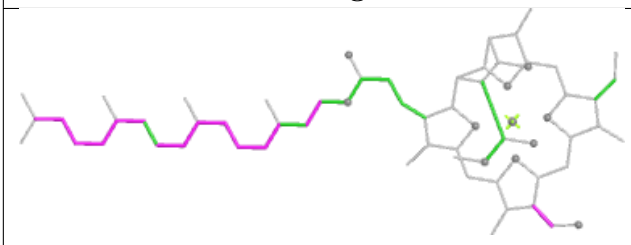
Ligand CL7 c 508



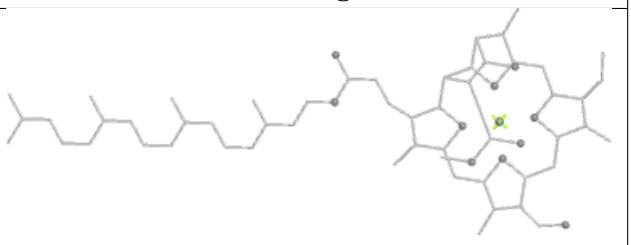
Bond lengths



Bond angles

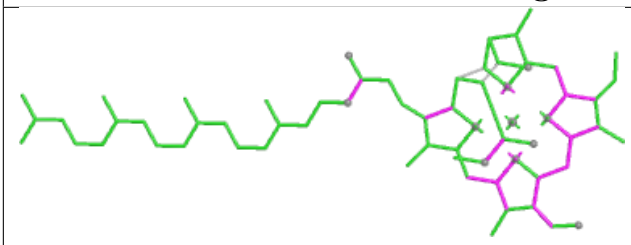


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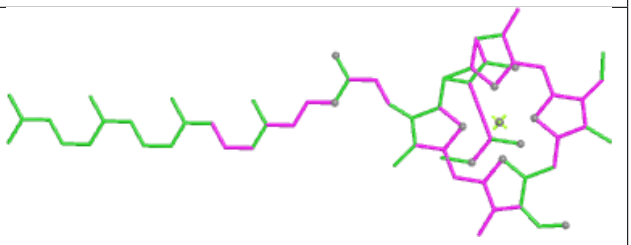


Rings

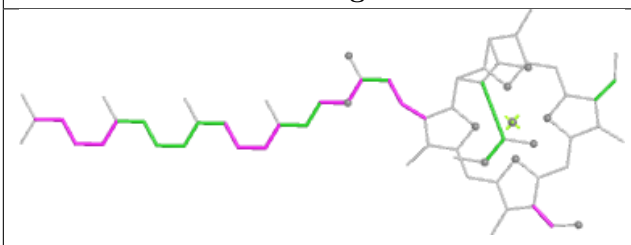
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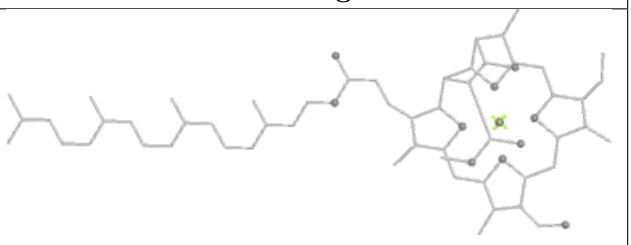
Bond lengths



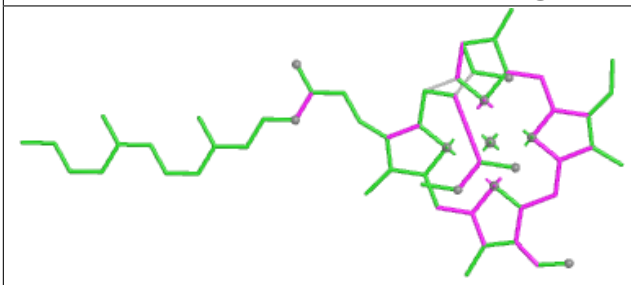
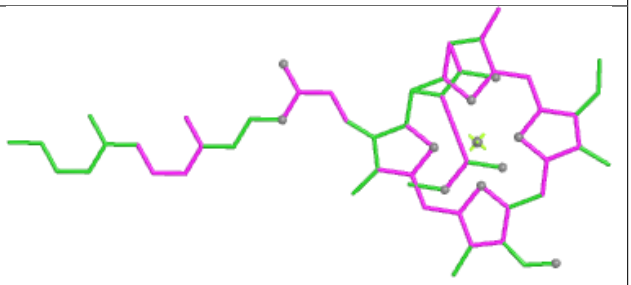
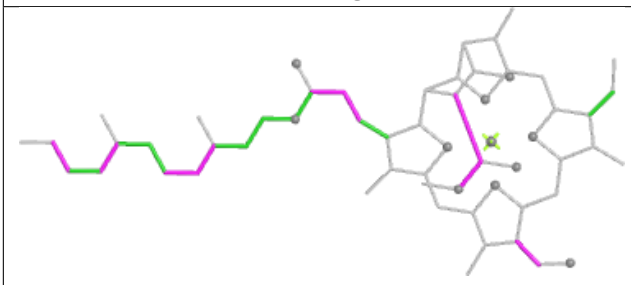
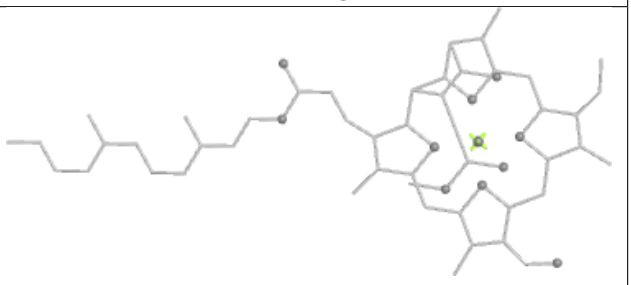
Bond angles

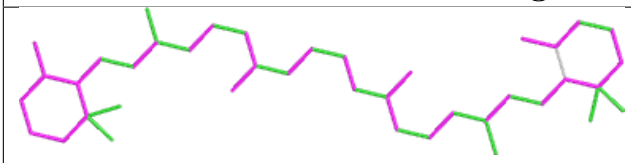
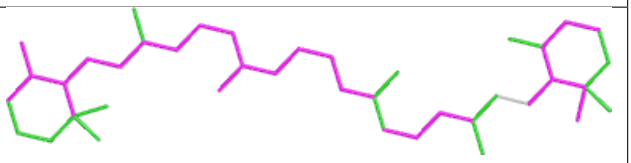
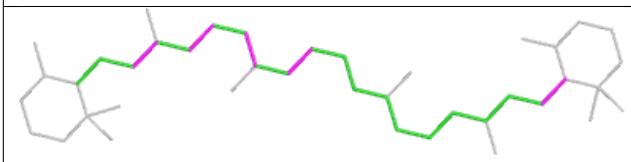
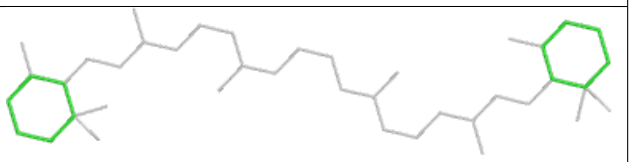


Torsions



Rings

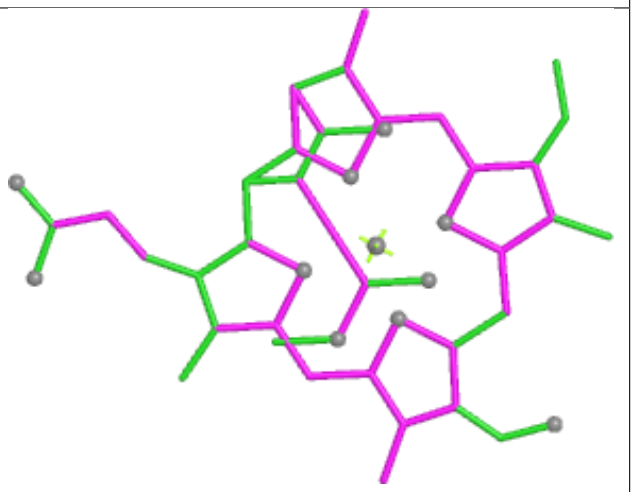
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 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 8CT b 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

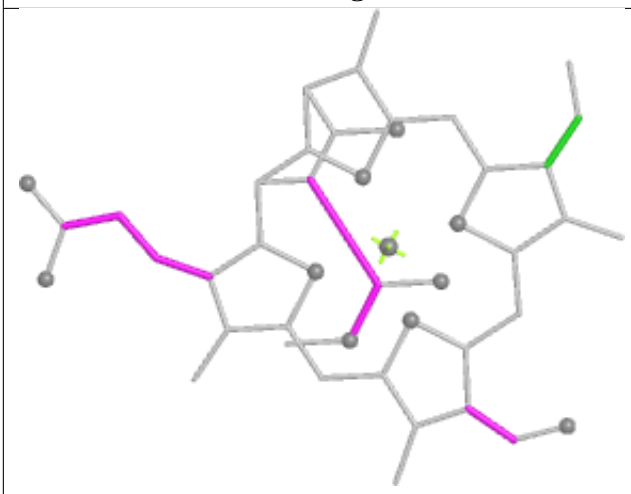
Ligand CL7 1 412



Bond lengths



Bond angles

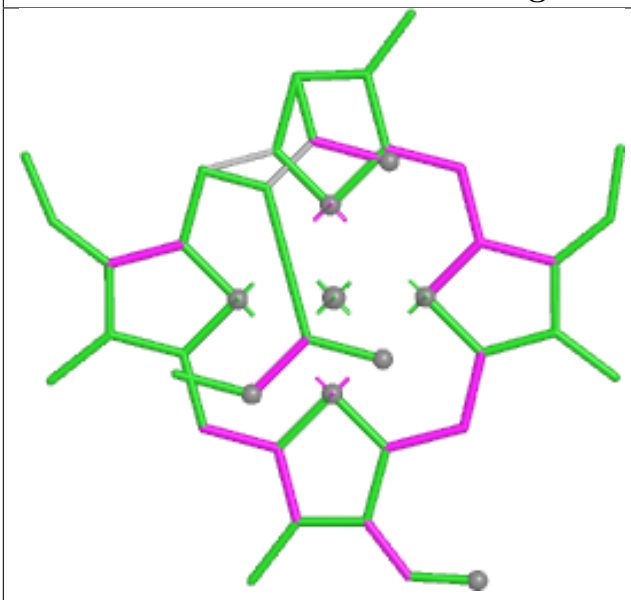


Torsions

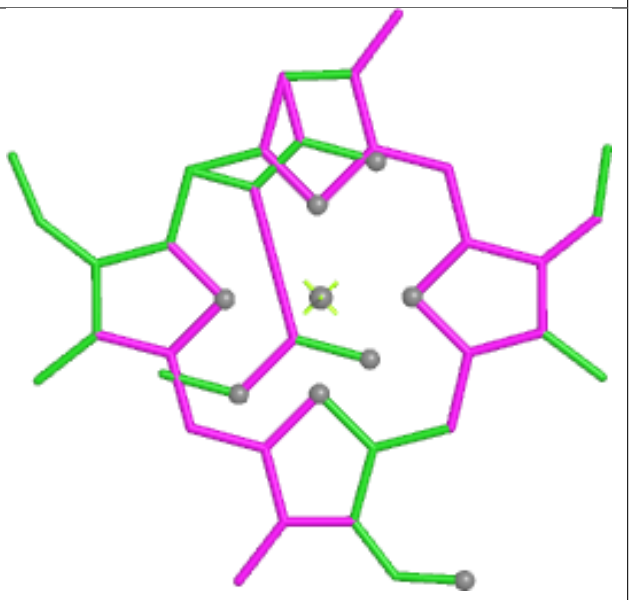


Rings

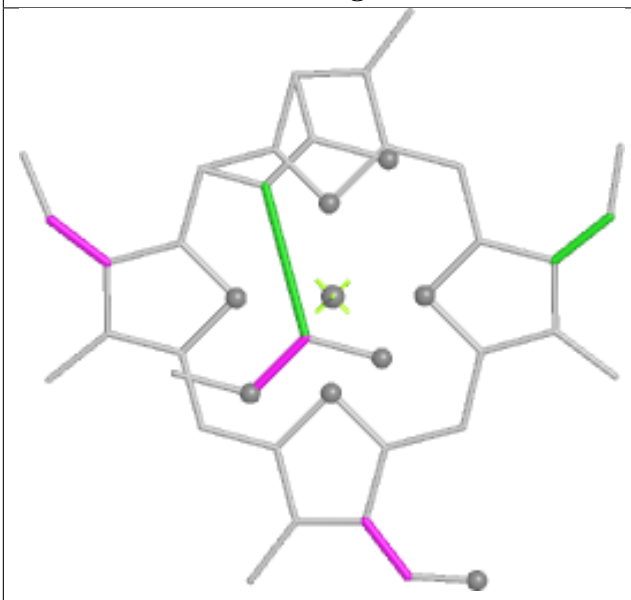
Ligand CL7 C 512



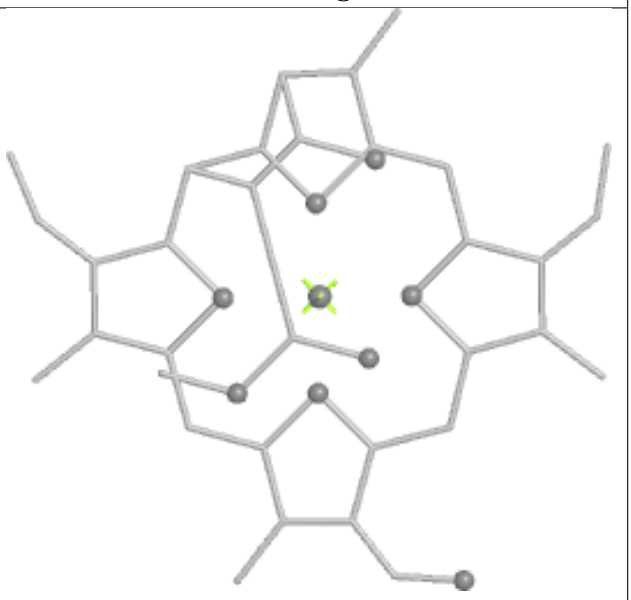
Bond lengths



Bond angles

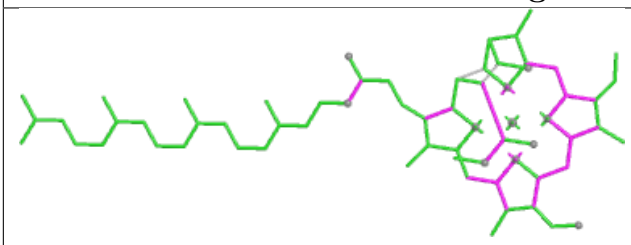


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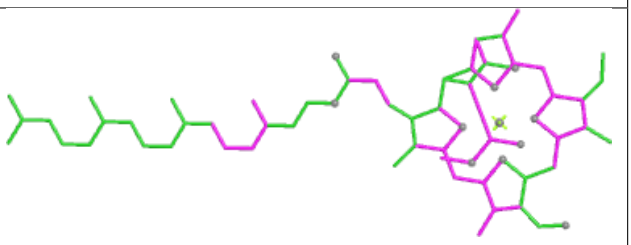


Rings

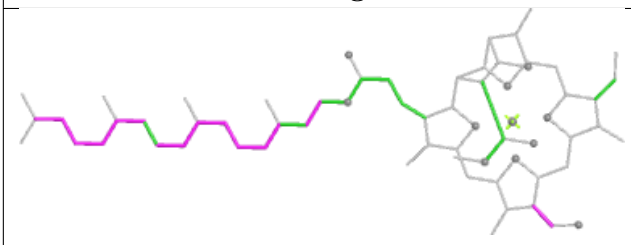
Ligand CL7 C 508



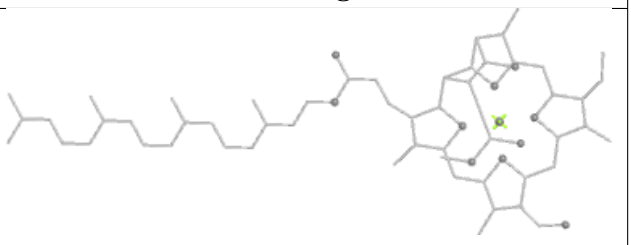
Bond lengths



Bond angles

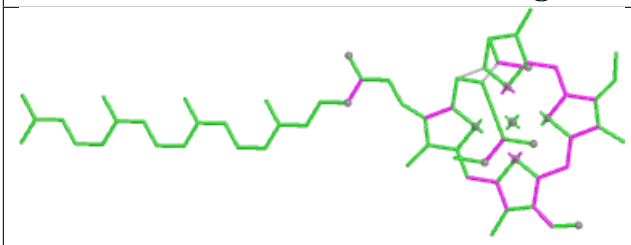


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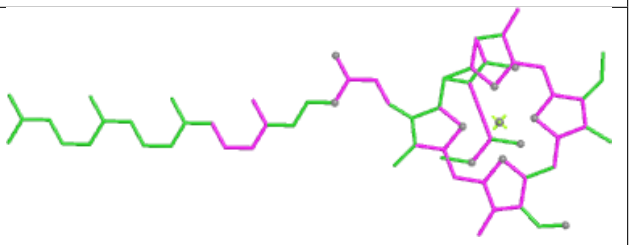


Rings

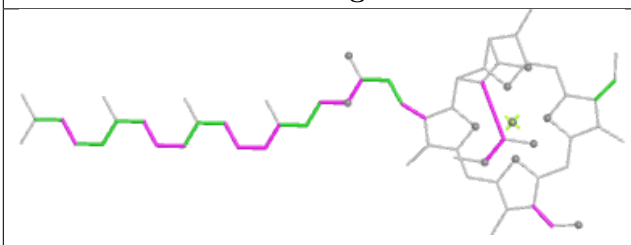
Ligand CL7 1 410



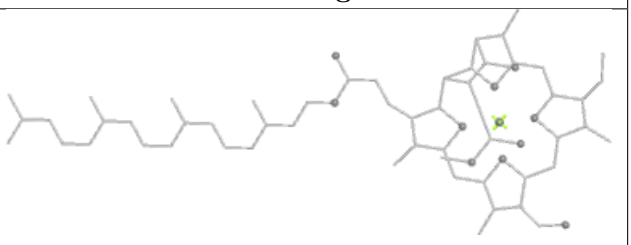
Bond lengths



Bond angles

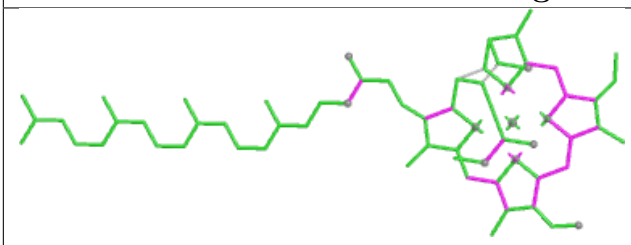


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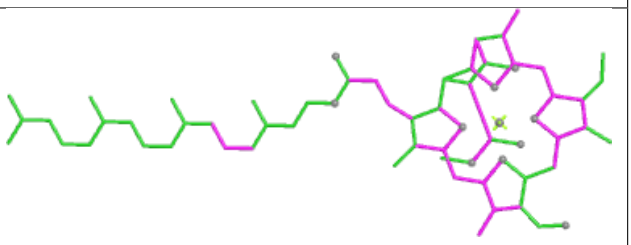


Rings

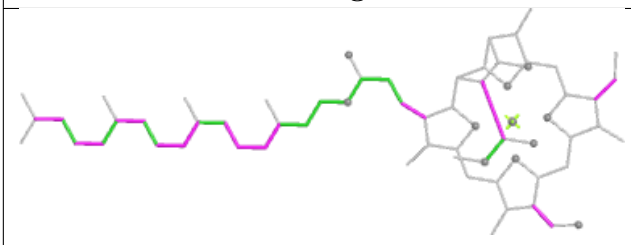
Ligand CL7 7 504



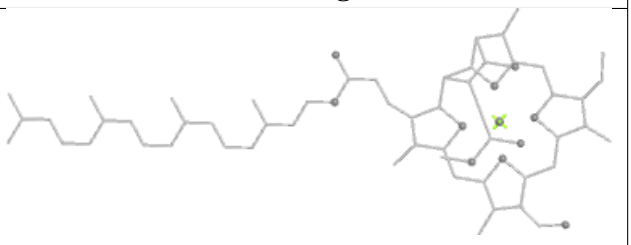
Bond lengths



Bond angles

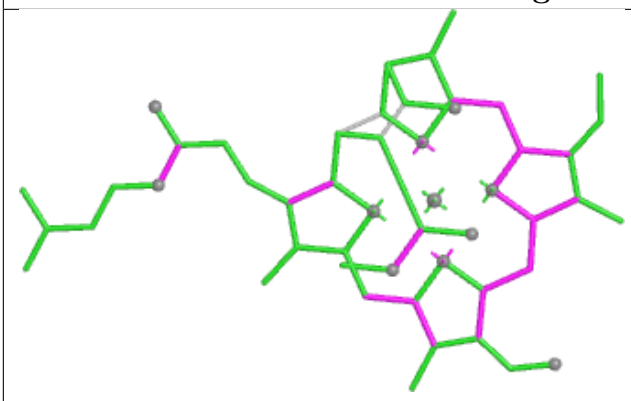


Torsions

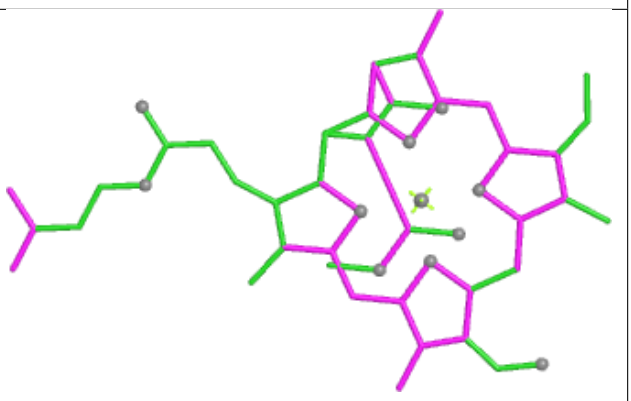


Rings

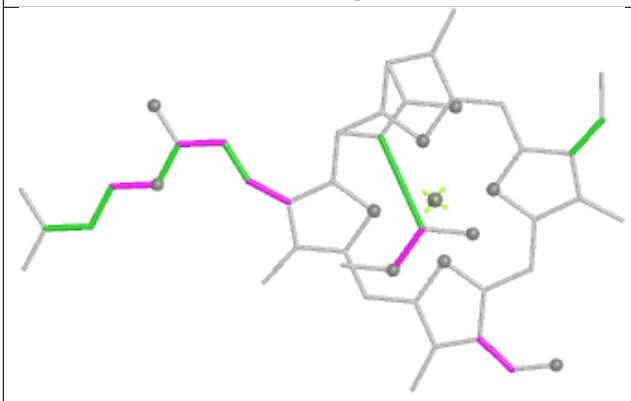
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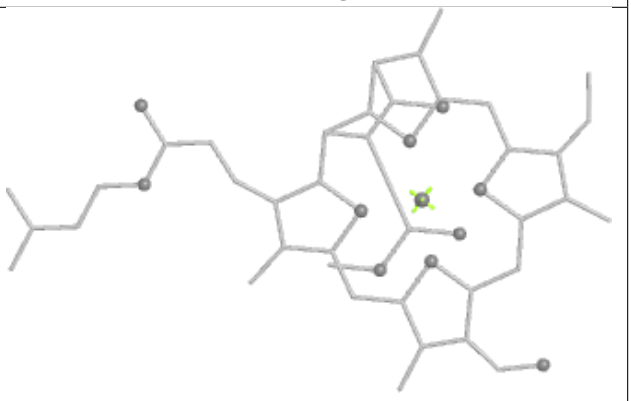
Bond lengths



Bond angles

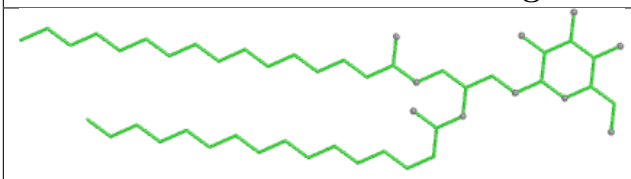


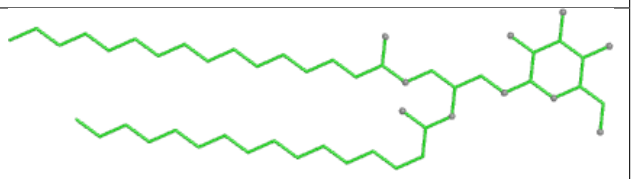
Torsions

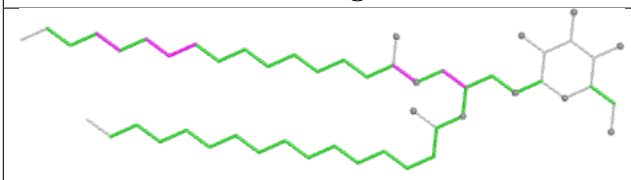


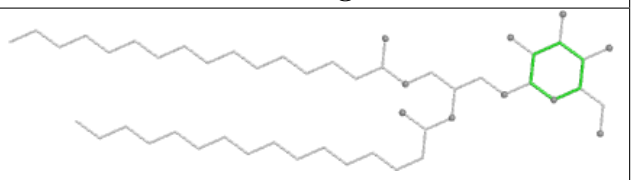
Rings

Ligand LMG b 622

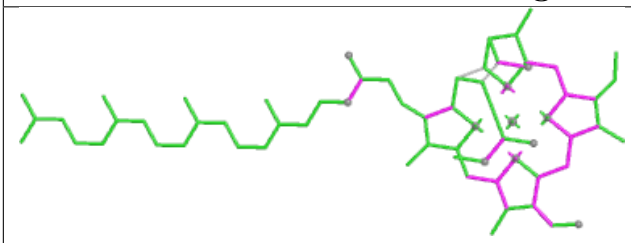

Bond lengths

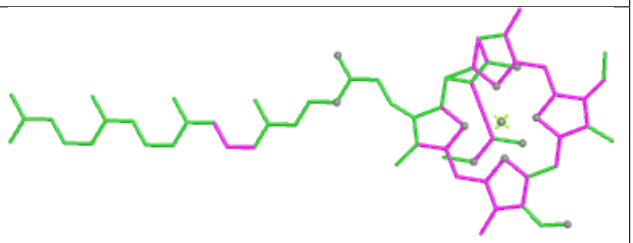

Bond angles

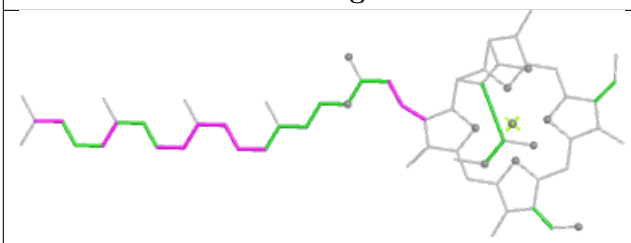

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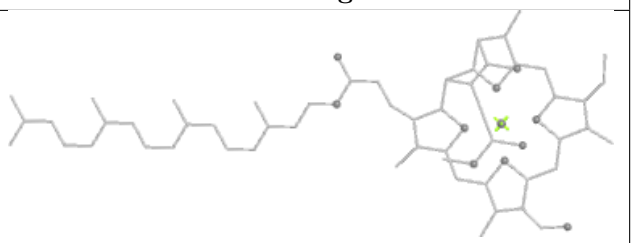

Rings

Ligand CL7 8 404

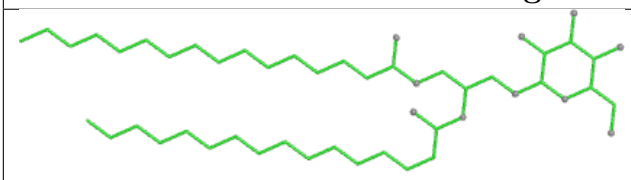

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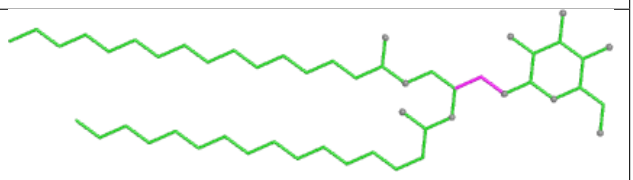

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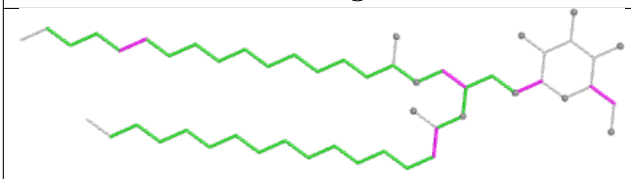

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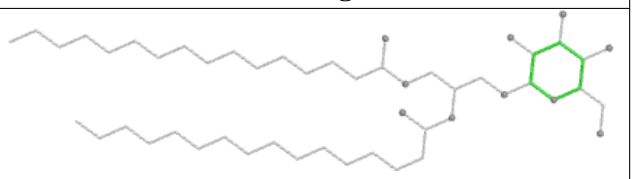

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Ligand LMG 1 401

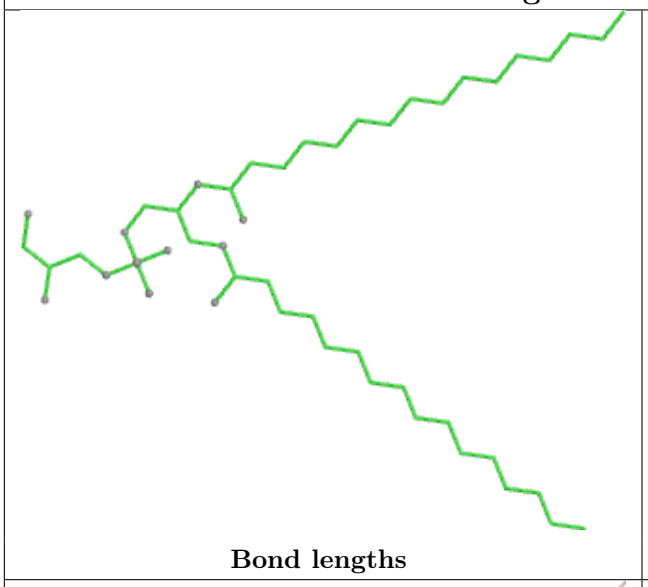

Bond lengths


Bond angles

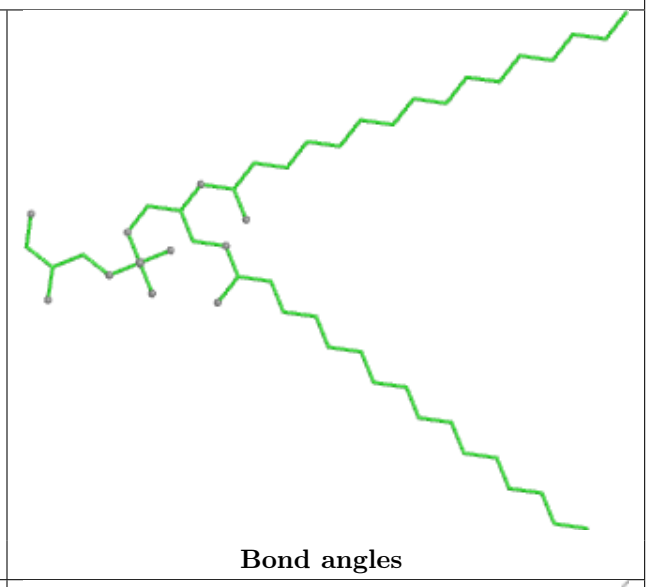

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Rings

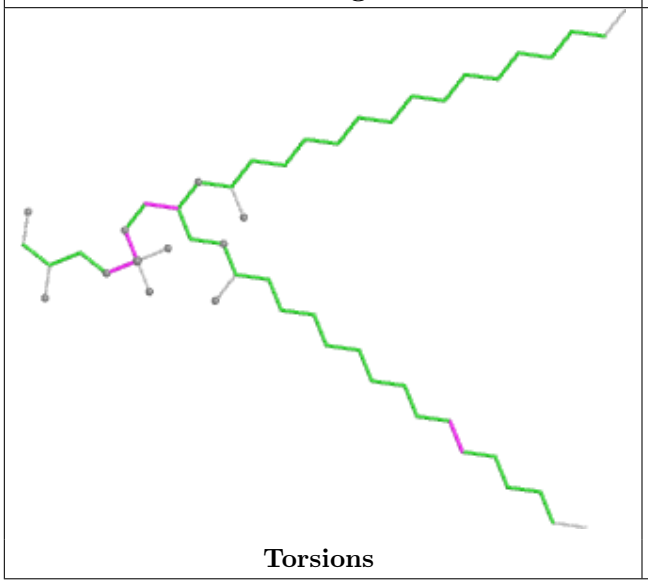
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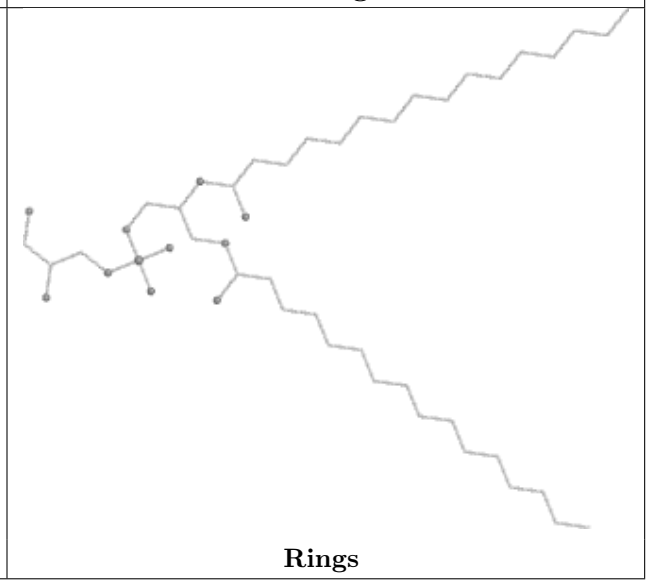
Bond lengths



Bond angles

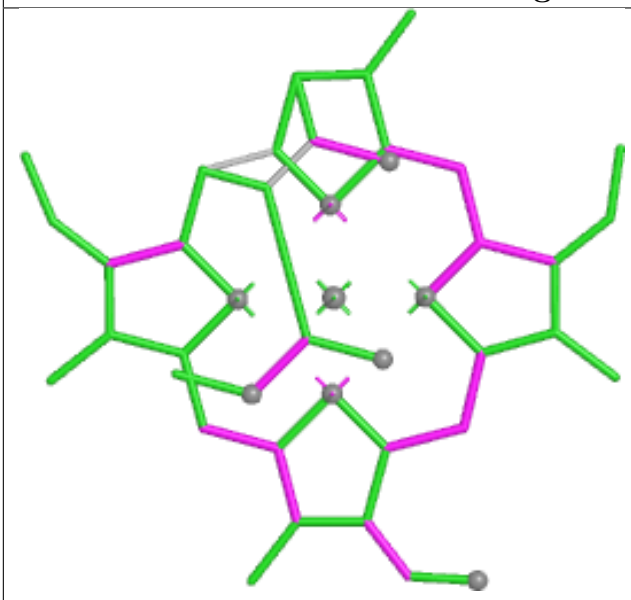


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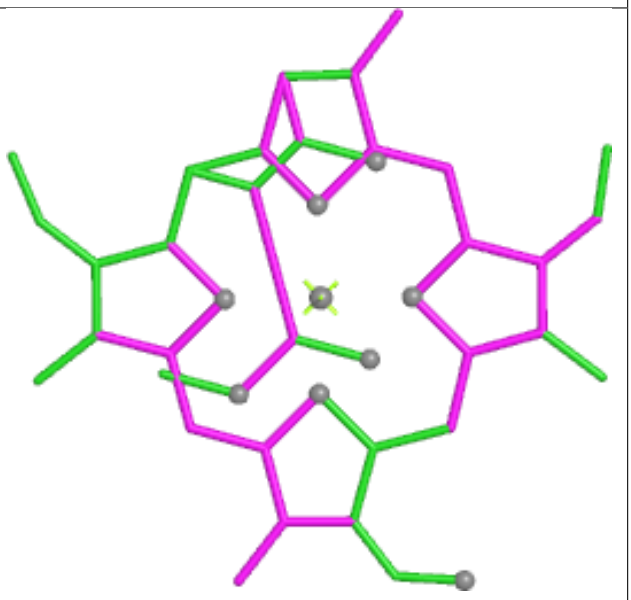


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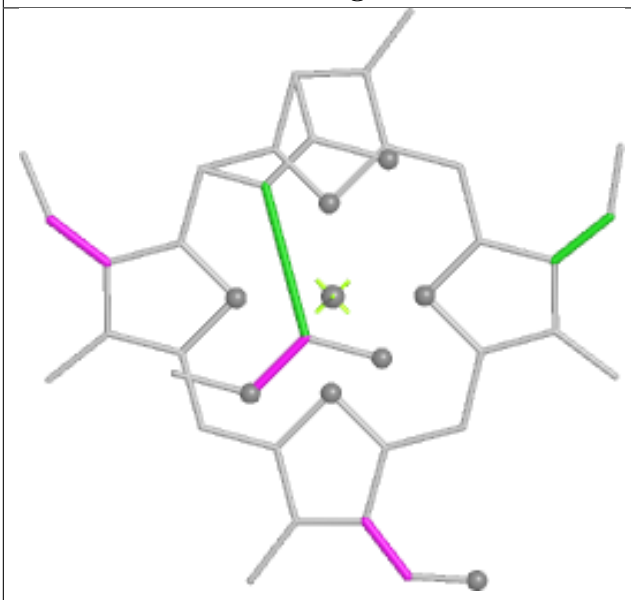
Ligand CL7 c 512



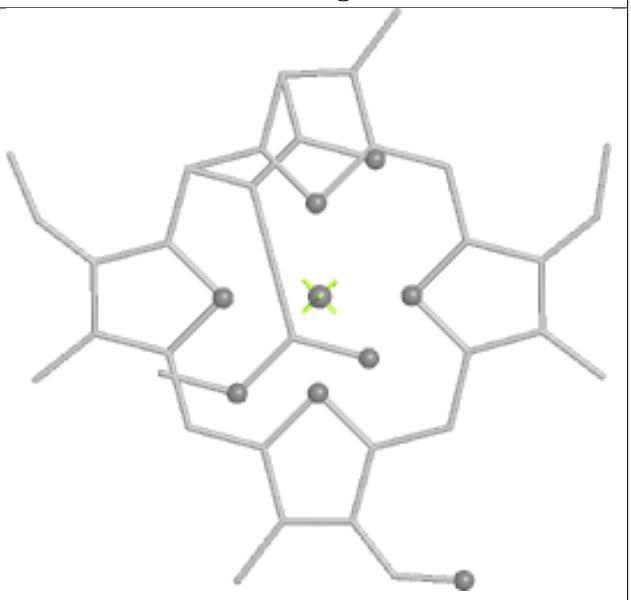
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Bond angles

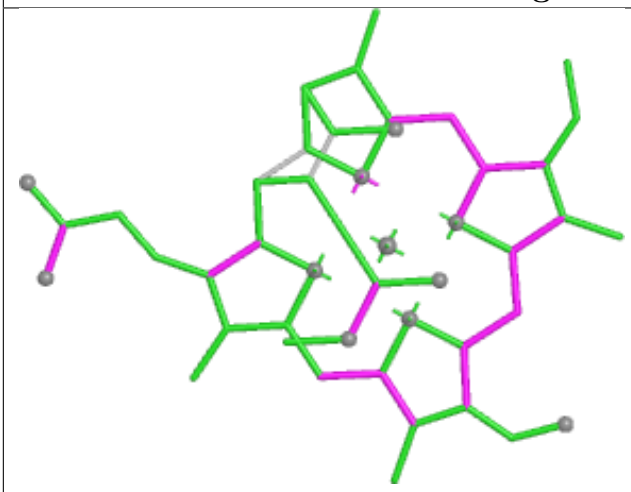


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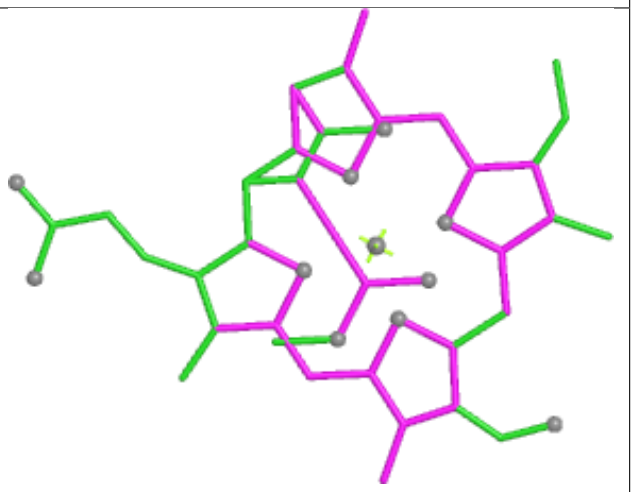


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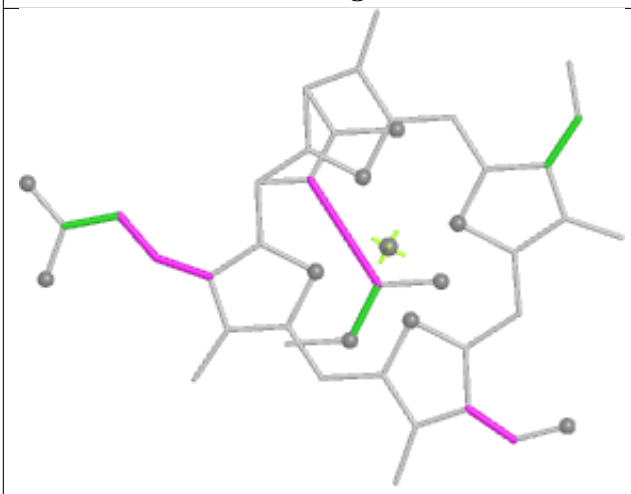
Ligand CL7 2 513



Bond lengths



Bond angles

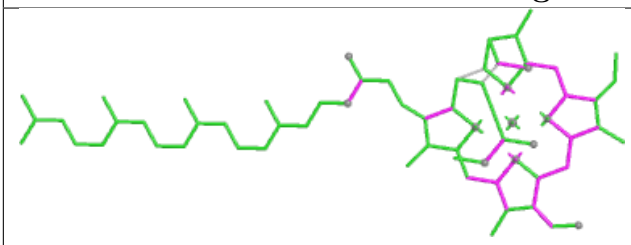


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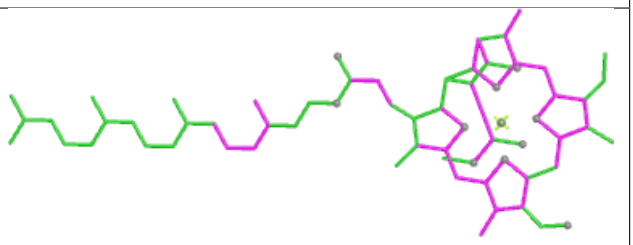


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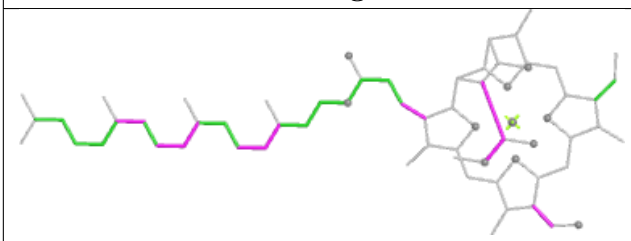
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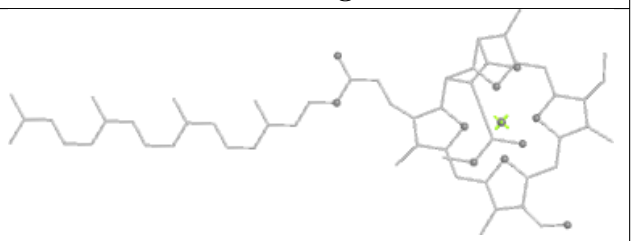
Bond lengths



Bond angles

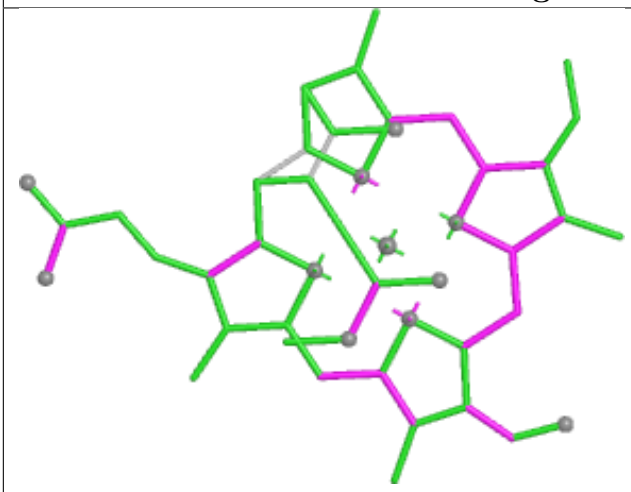


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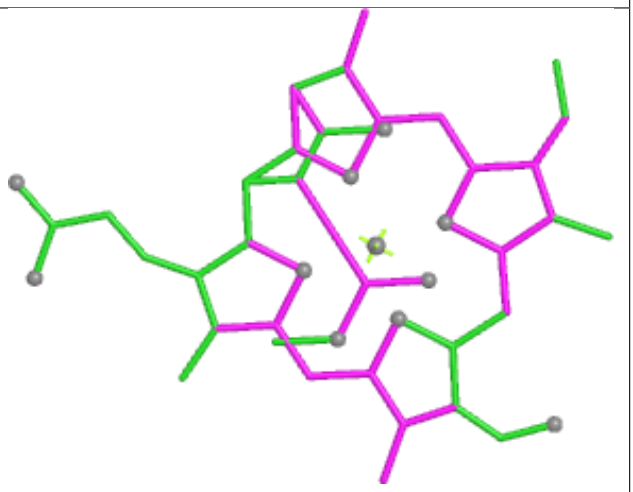


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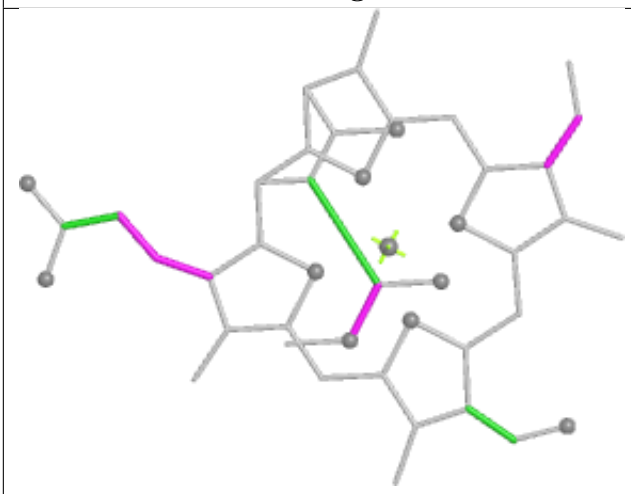
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Bond lengths



Bond angles

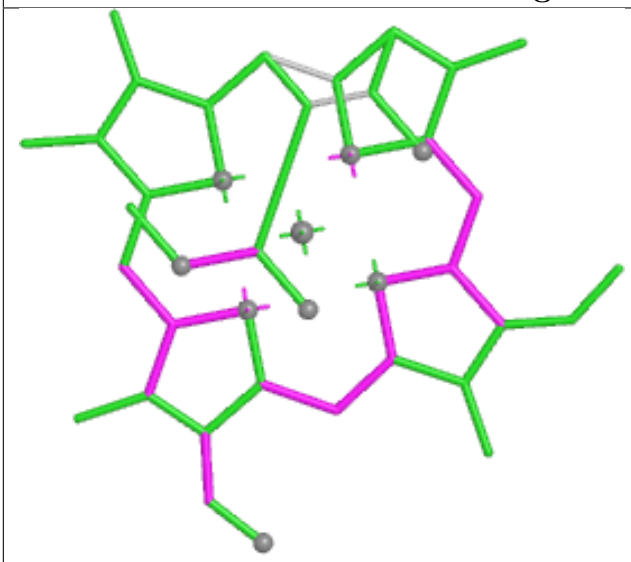


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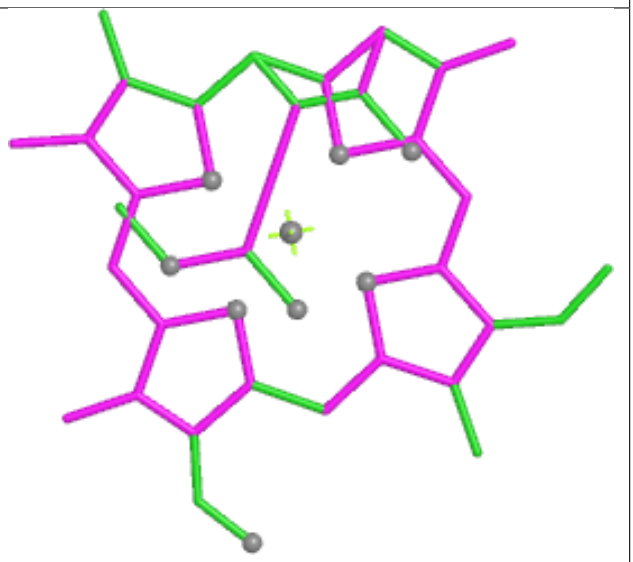


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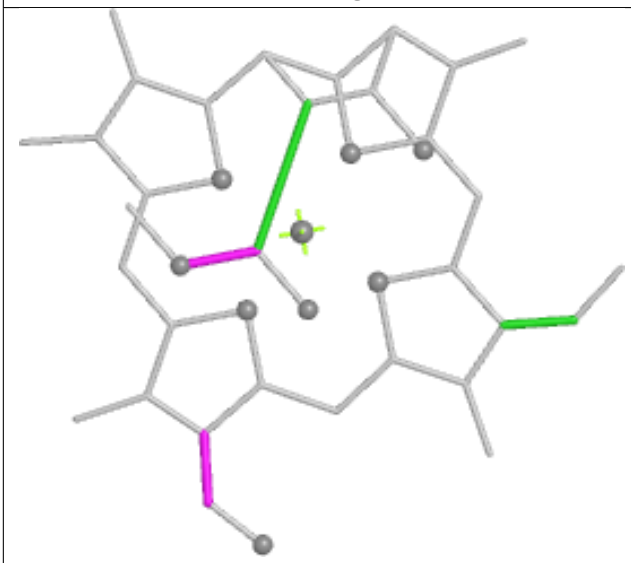
Ligand CL7 c 513



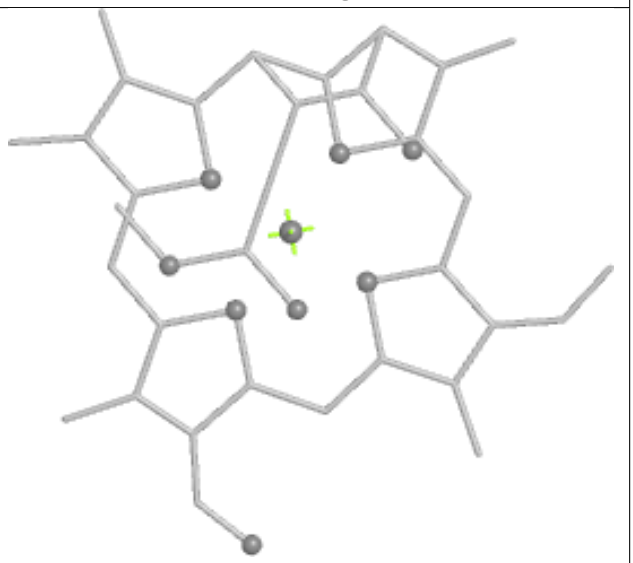
Bond lengths



Bond angles

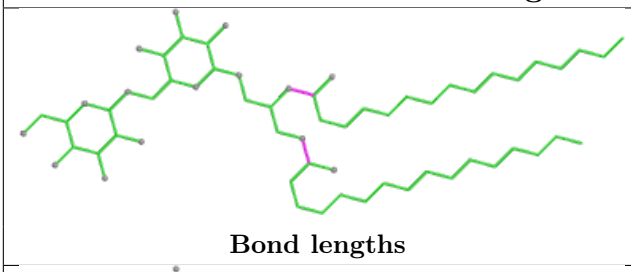


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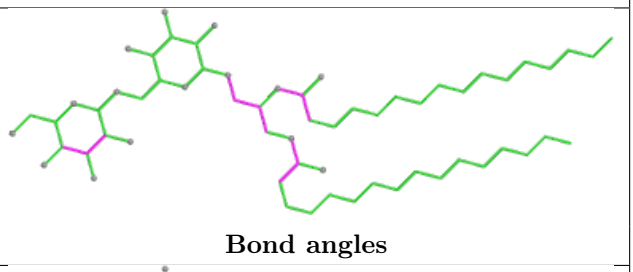


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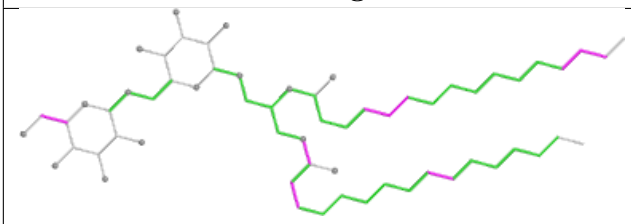
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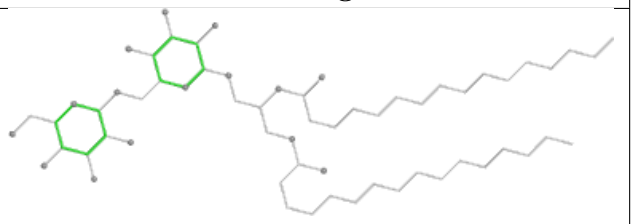
Bond lengths



Bond angles

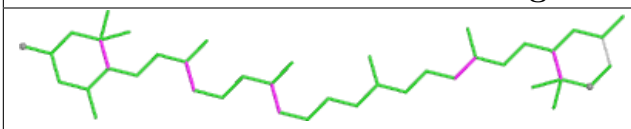


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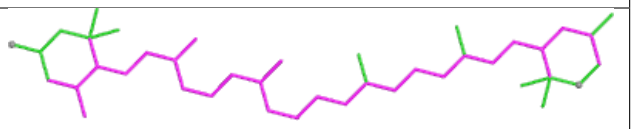


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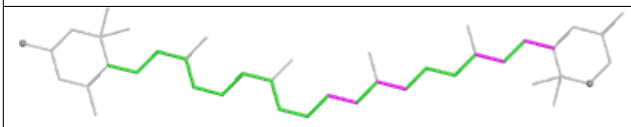
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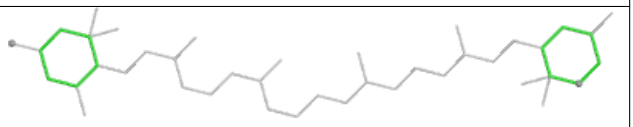
Bond lengths



Bond angles

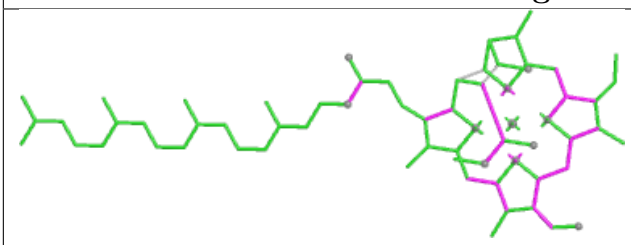


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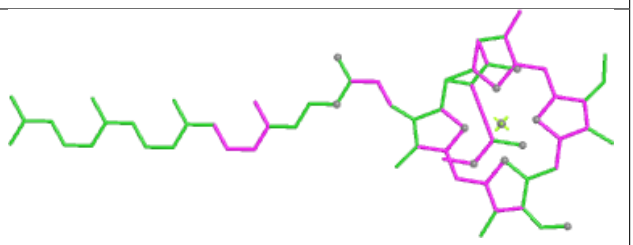


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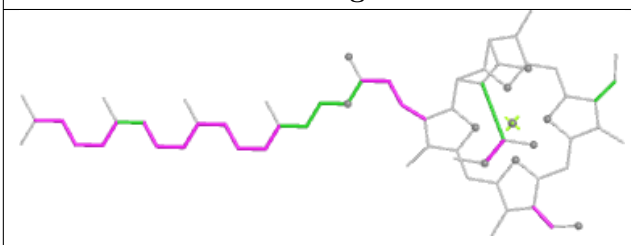
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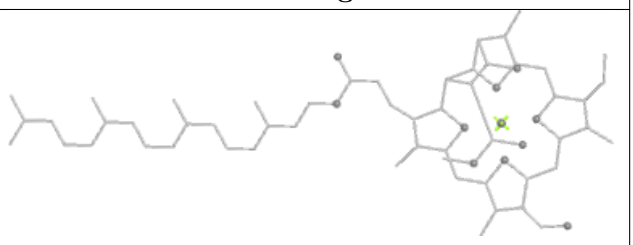
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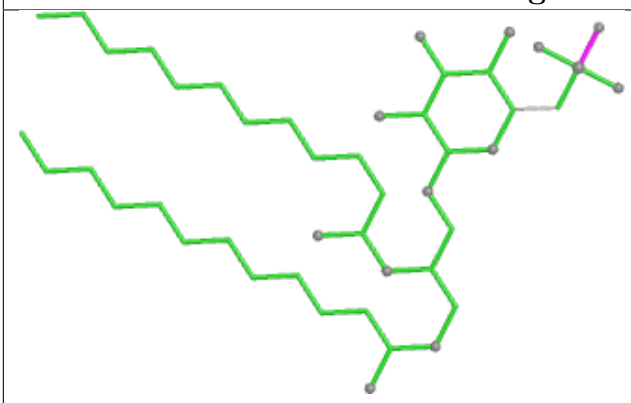


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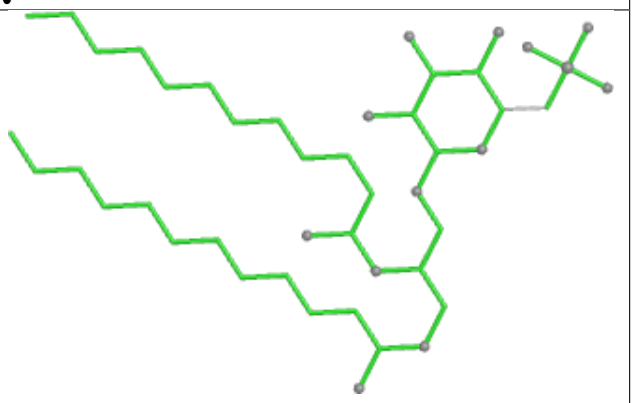


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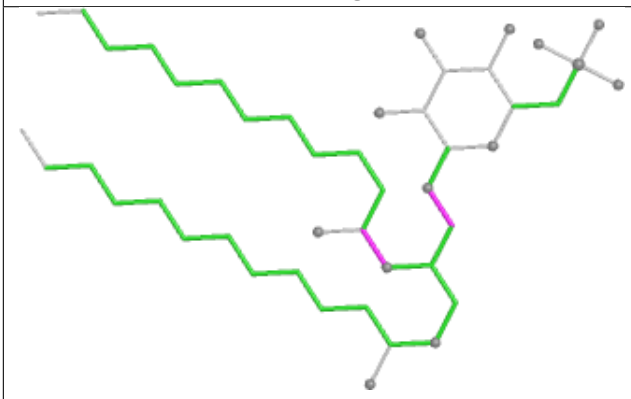
Ligand SQD 3 521



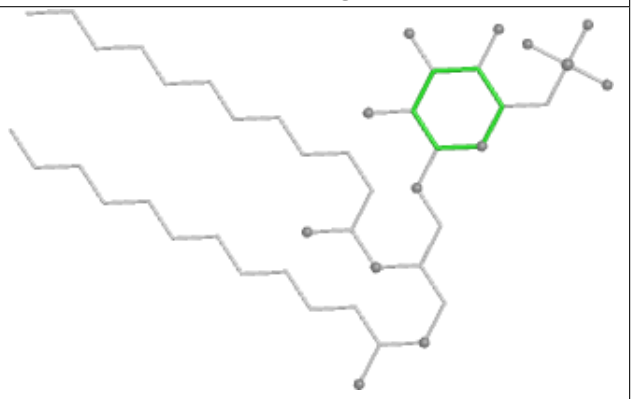
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Bond angles

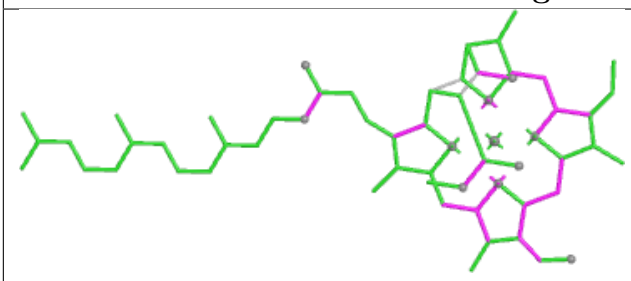


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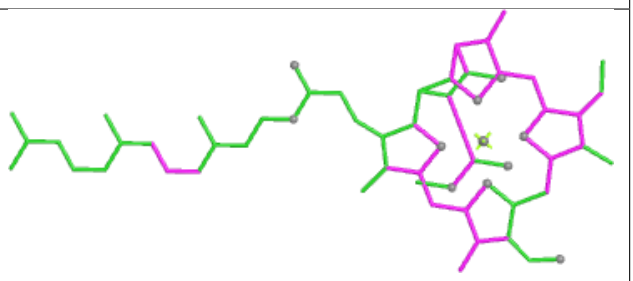


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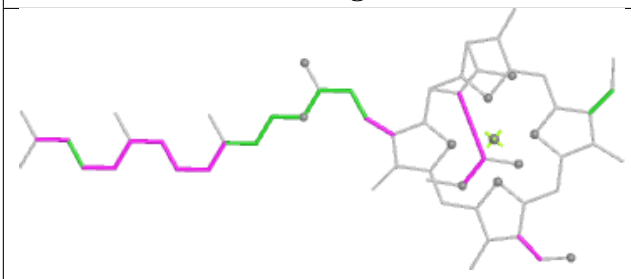
Ligand CL7 2 511



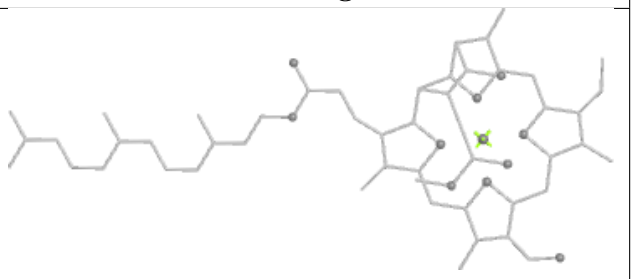
Bond lengths



Bond angles

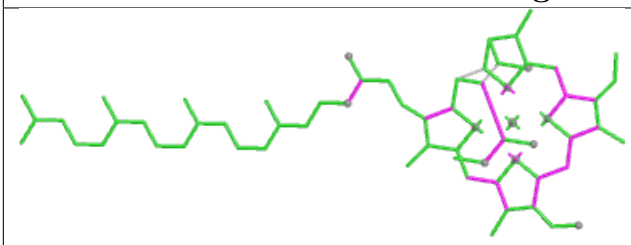


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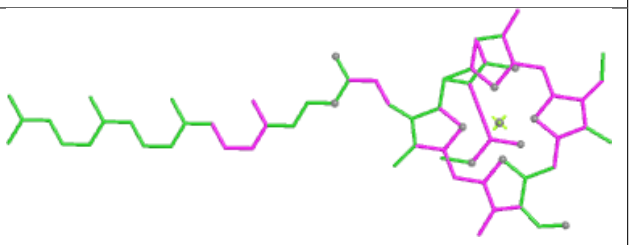


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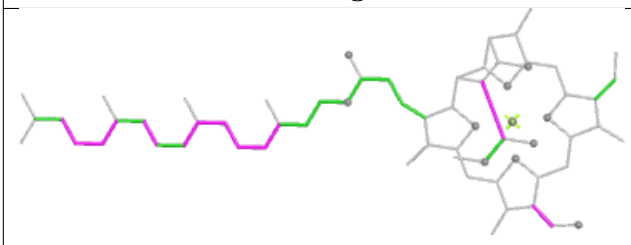
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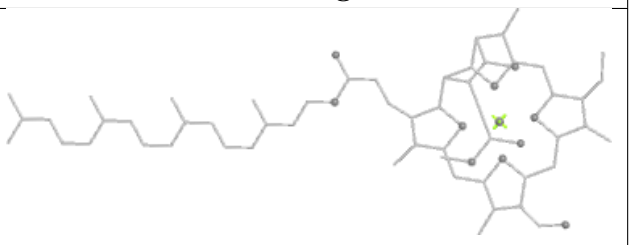
Bond lengths



Bond angles

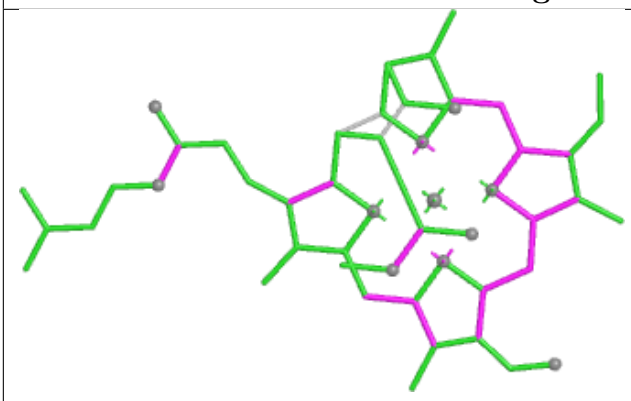


Torsions

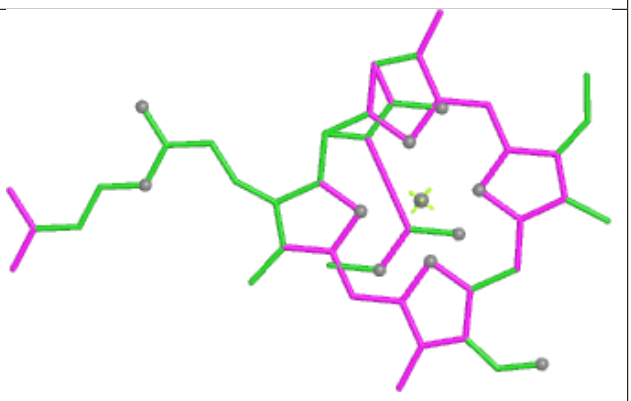


Rings

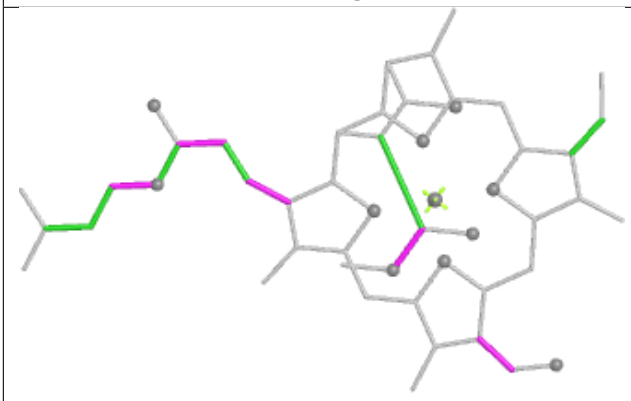
Ligand CL7 3 517



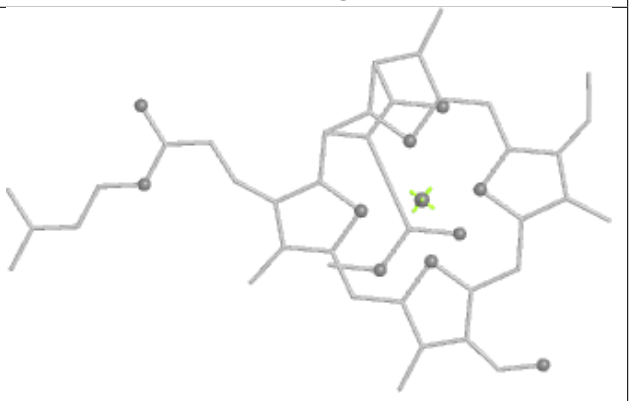
Bond lengths



Bond angles

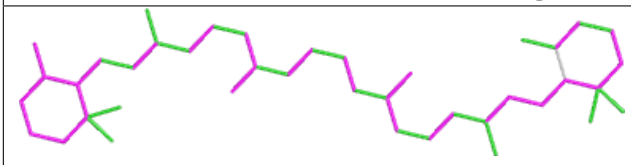


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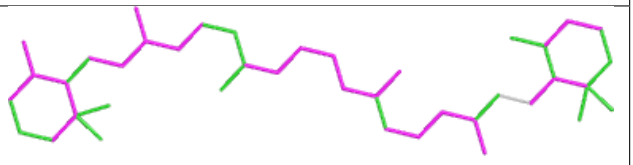


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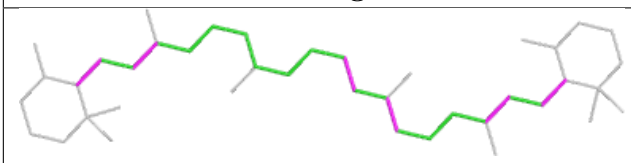
Ligand 8CT k 101



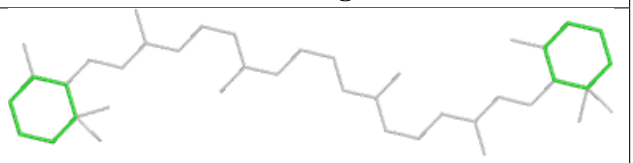
Bond lengths



Bond angles



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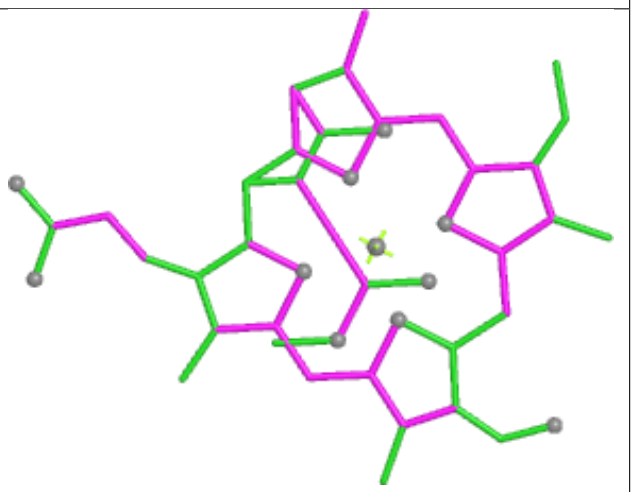


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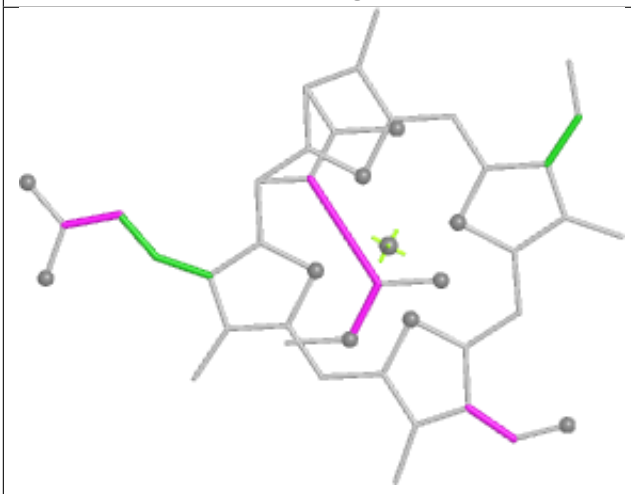
Ligand CL7 1 411



Bond lengths



Bond angles

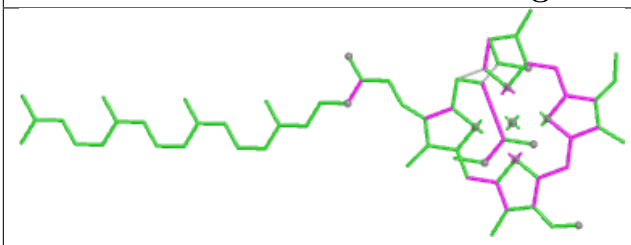


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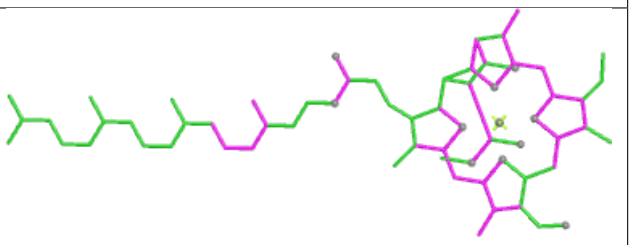


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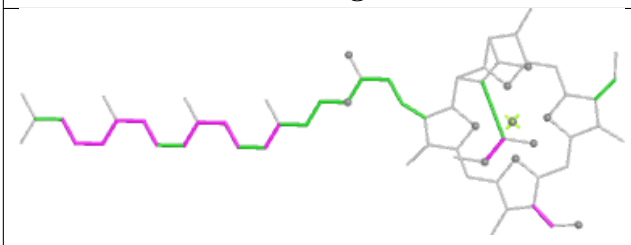
Ligand CL7 b 612



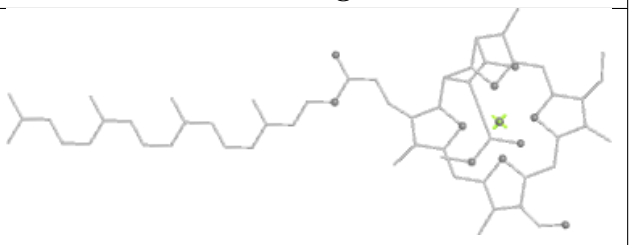
Bond lengths



Bond angles

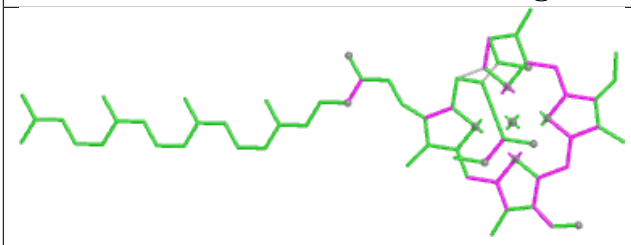


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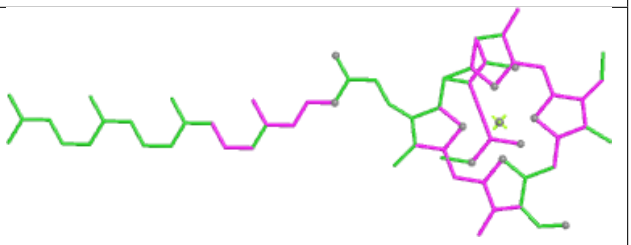


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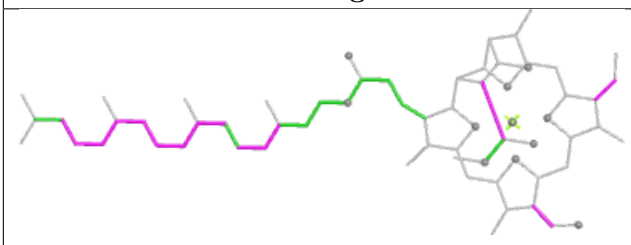
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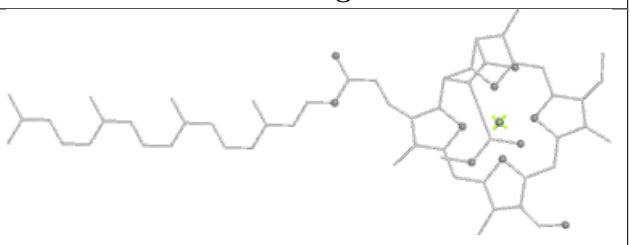
Bond lengths



Bond angles

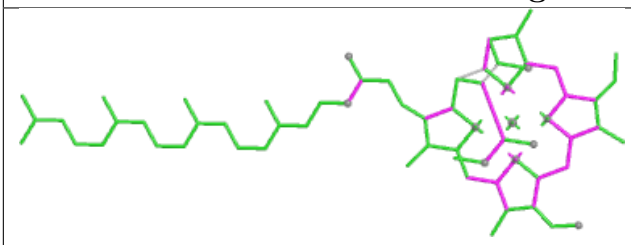


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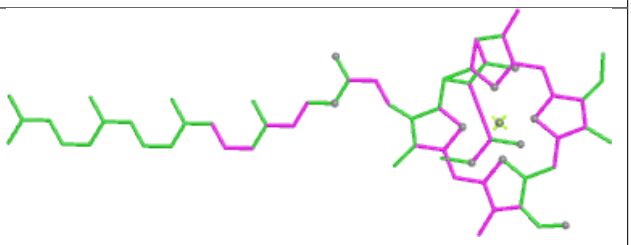


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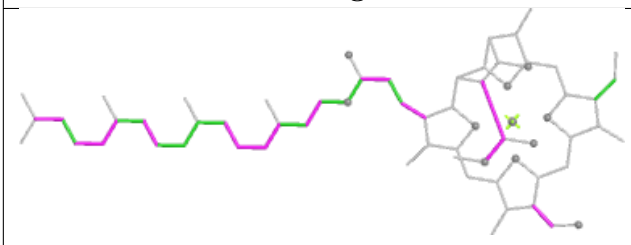
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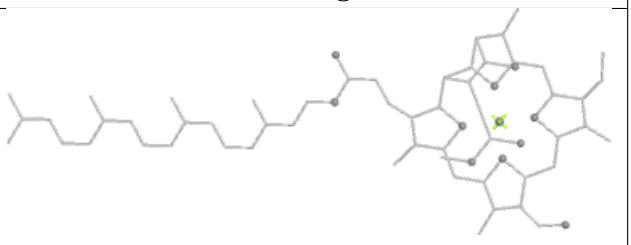
Bond lengths



Bond angles

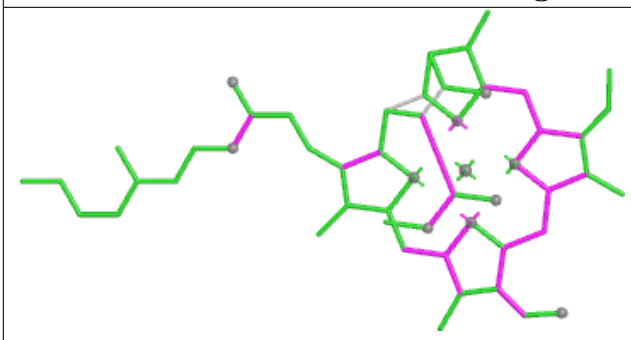


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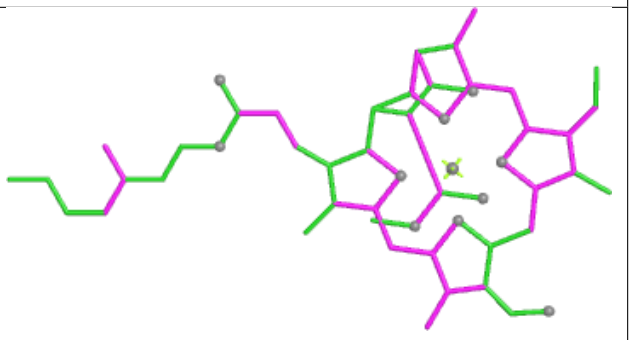


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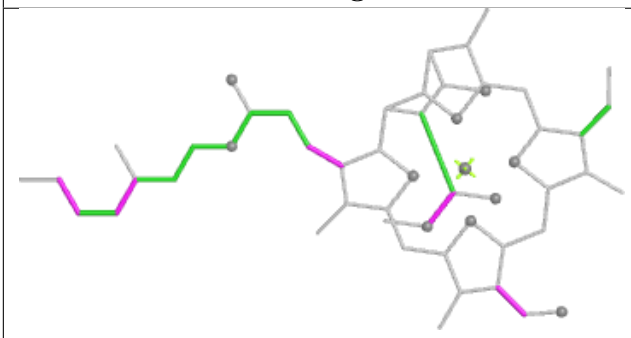
Ligand CL7 8 414



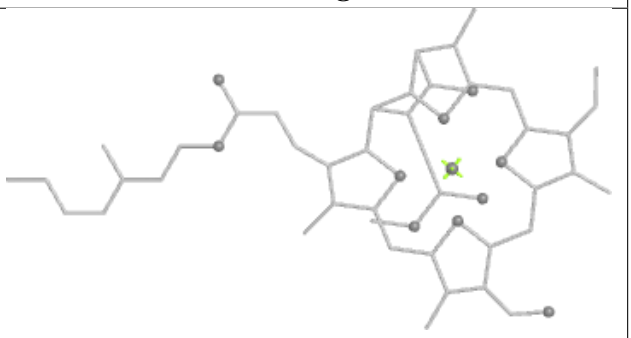
Bond lengths



Bond angles

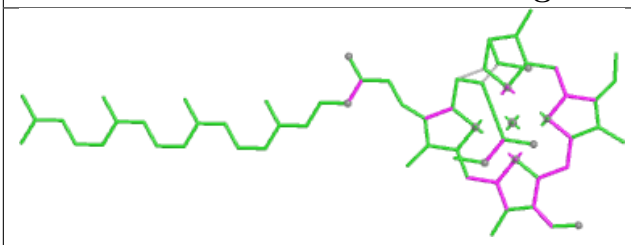


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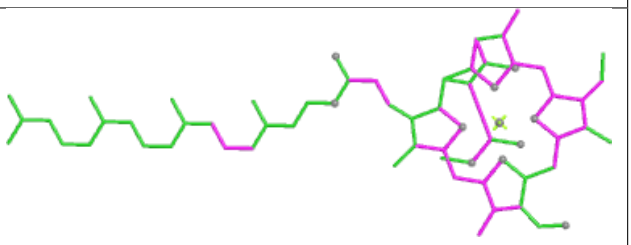


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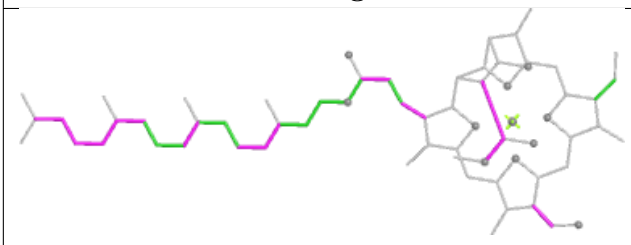
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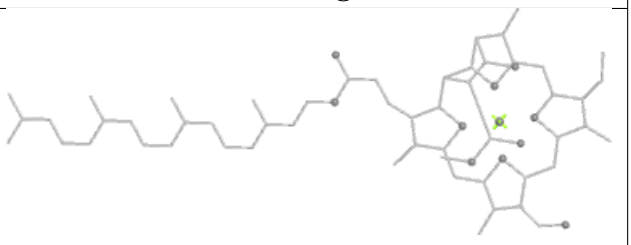
Bond lengths



Bond angles

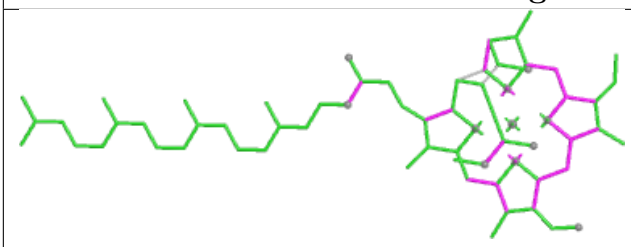


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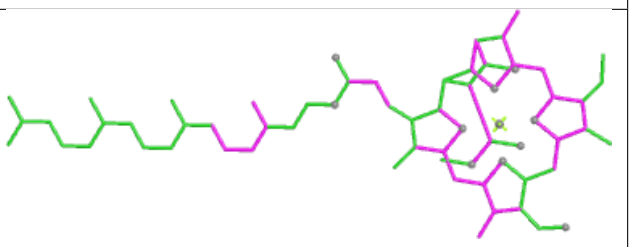


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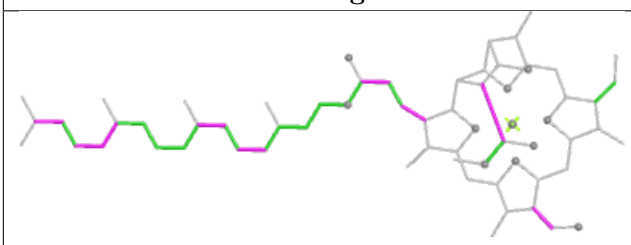
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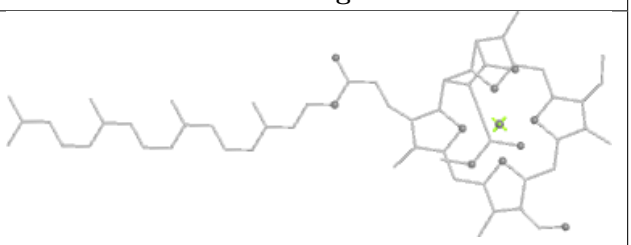
Bond lengths



Bond angles

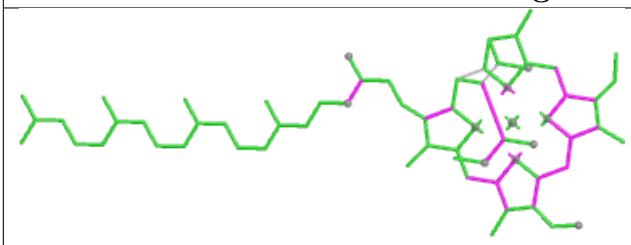


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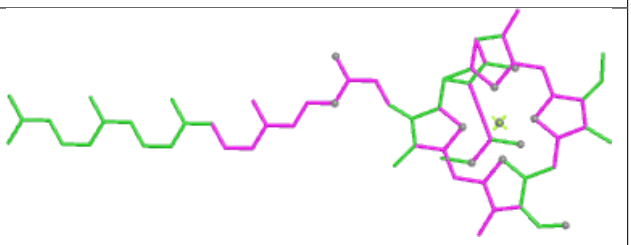


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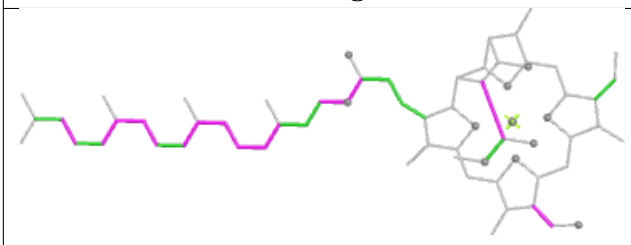
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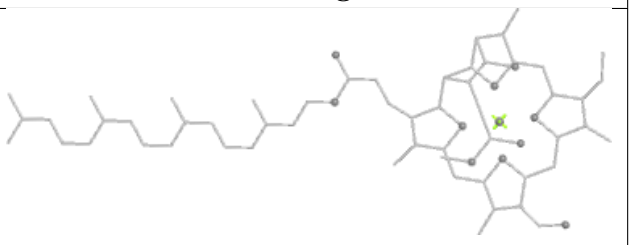
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Bond angles

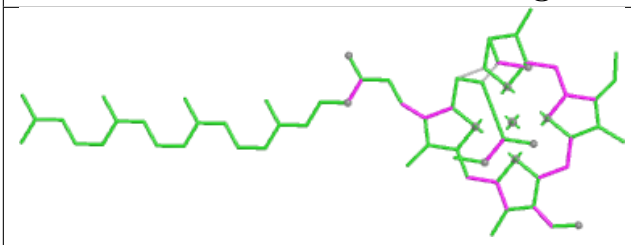


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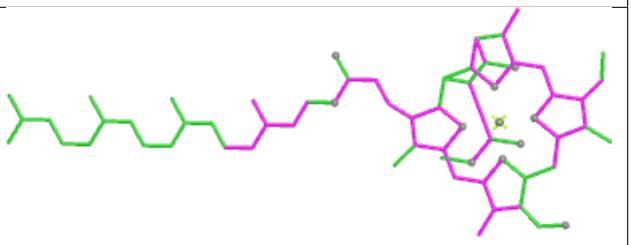


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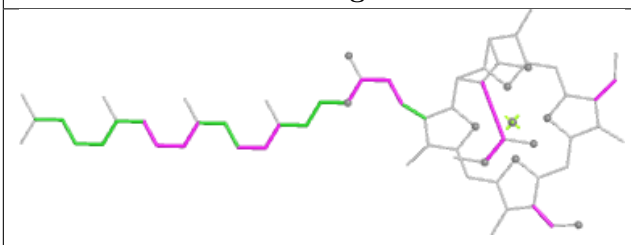
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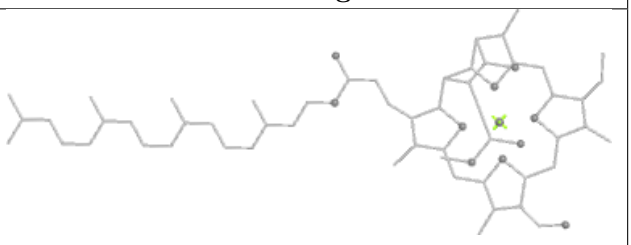
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Bond angles

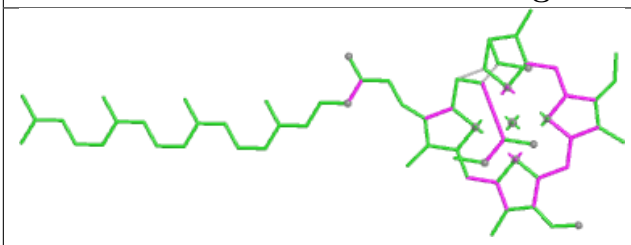


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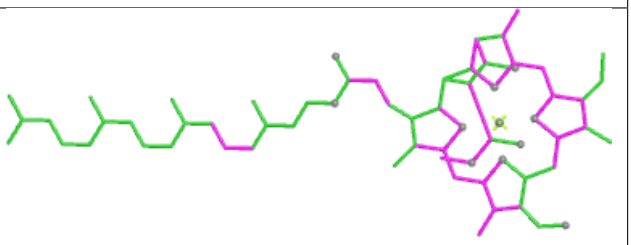


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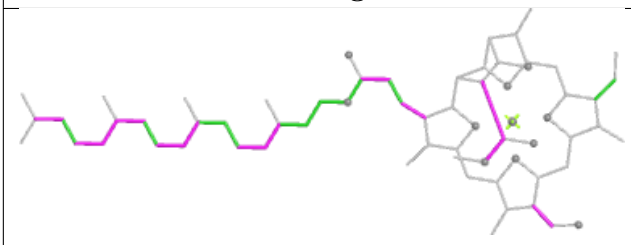
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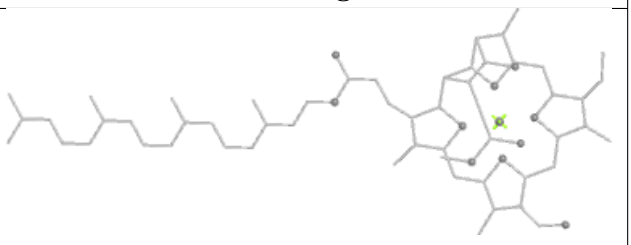
Bond lengths



Bond angles

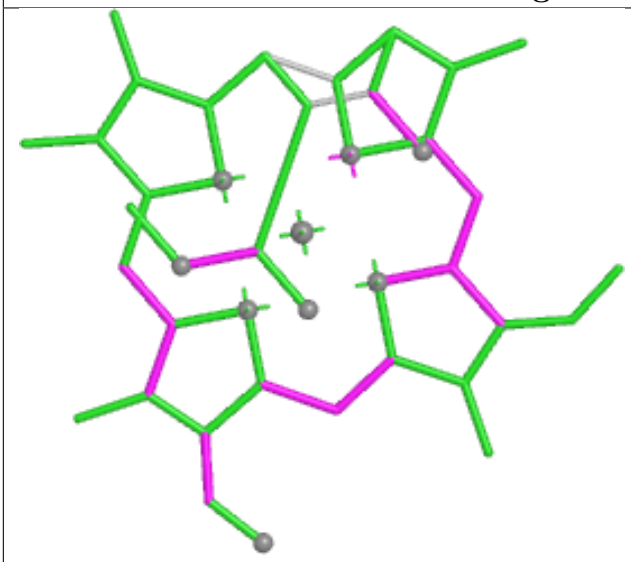


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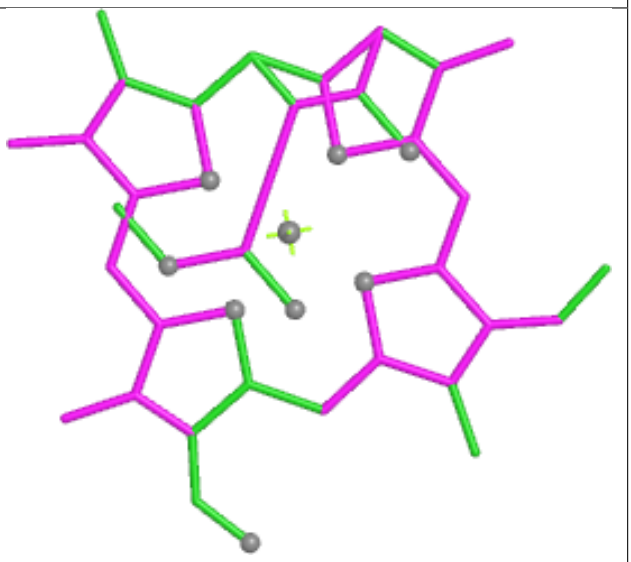


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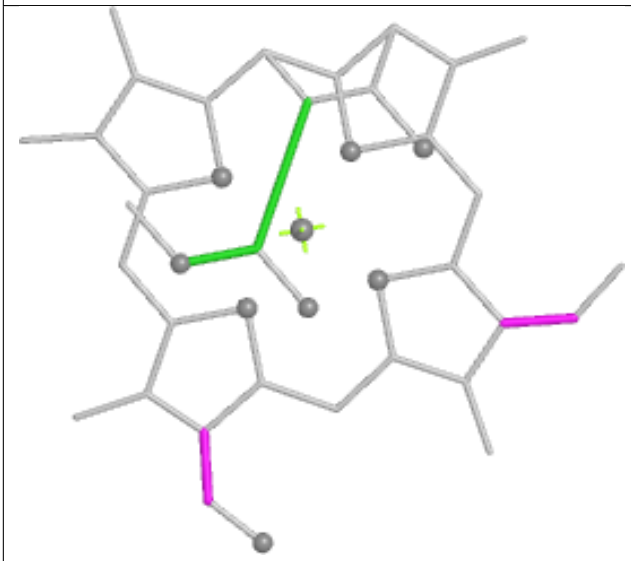
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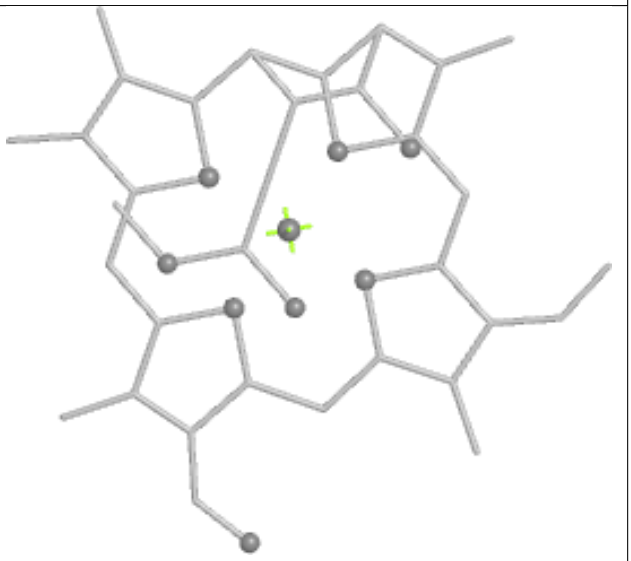
Bond lengths



Bond angles

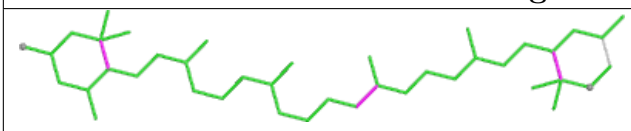


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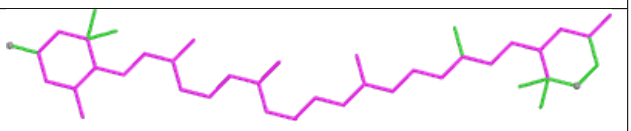


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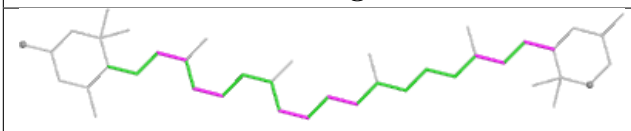
Ligand ZEX 4 419



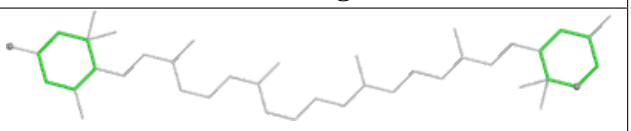
Bond lengths



Bond angles

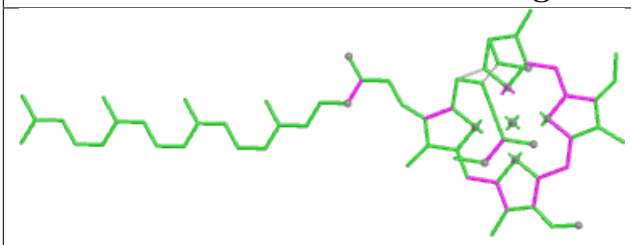


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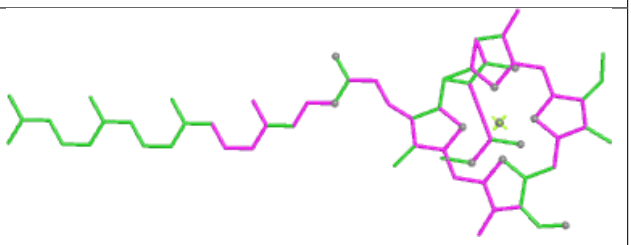


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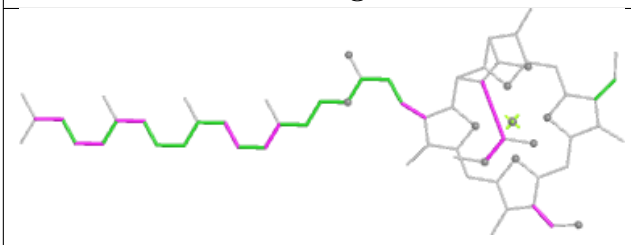
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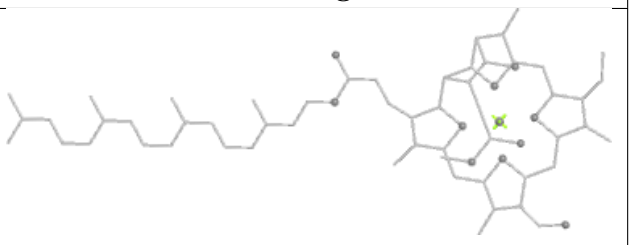
Bond lengths



Bond angles

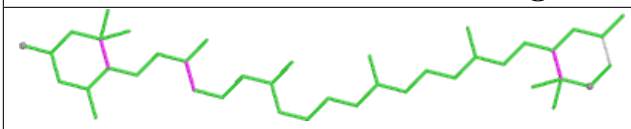


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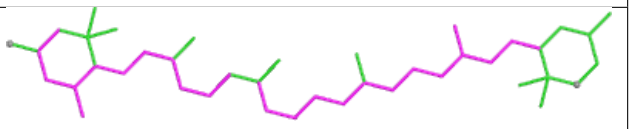


Rings

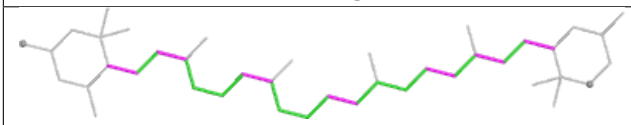
Ligand ZEX 6 519



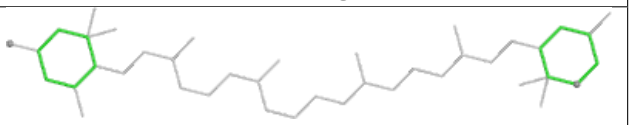
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Bond angles

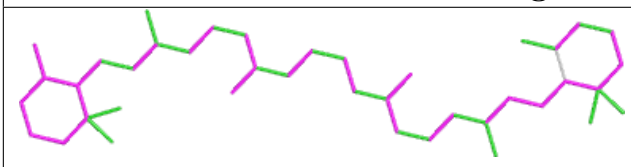


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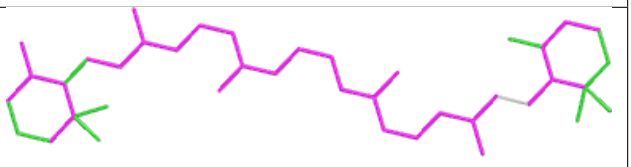


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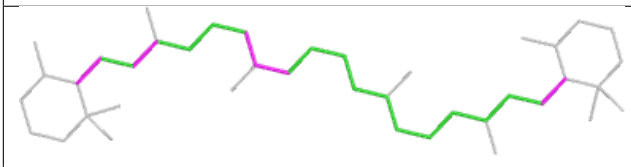
Ligand 8CT b 601



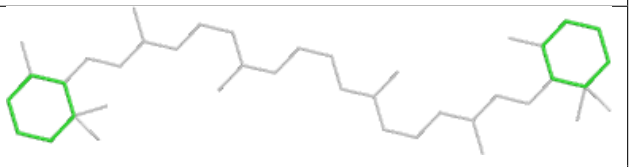
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Bond angles

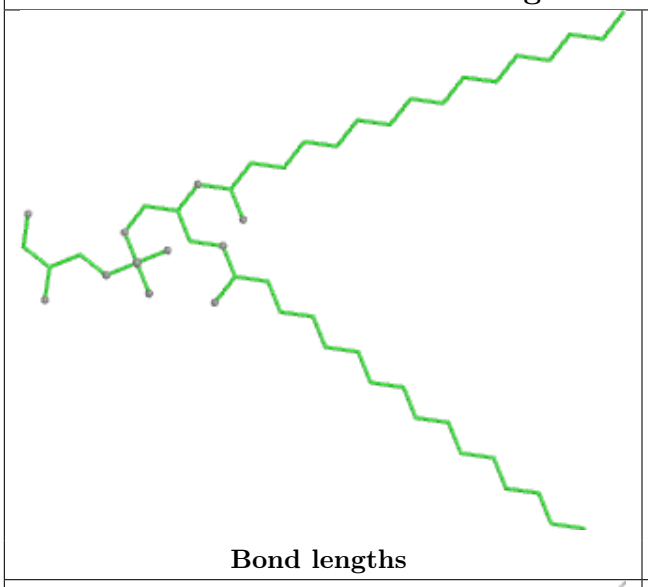


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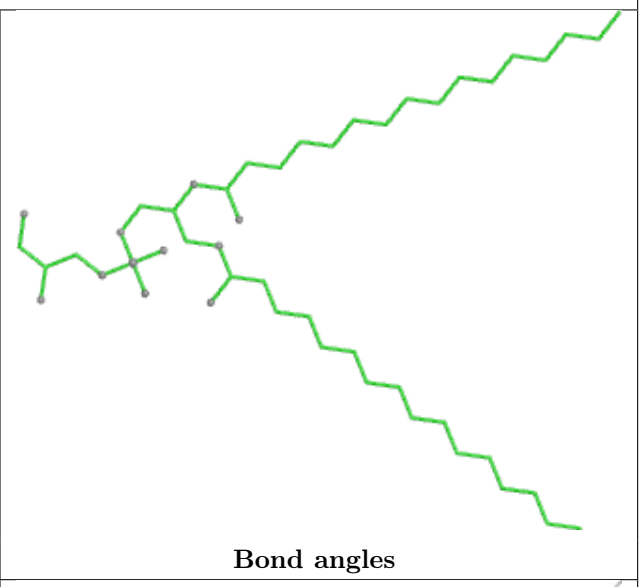


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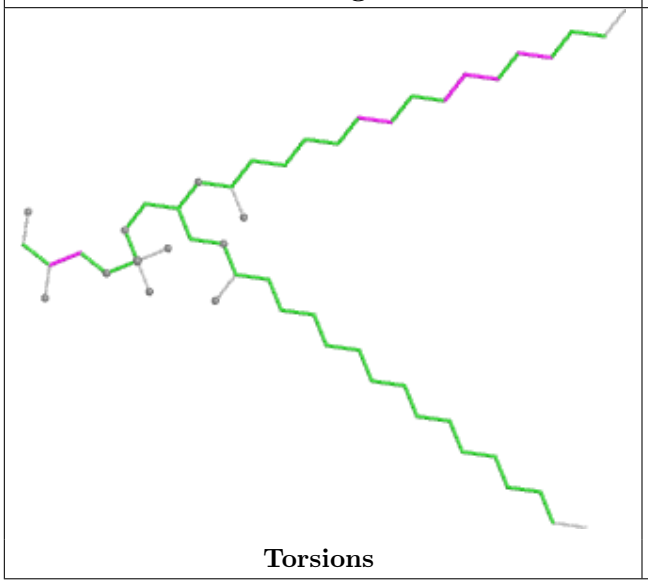
Ligand LHG B 625



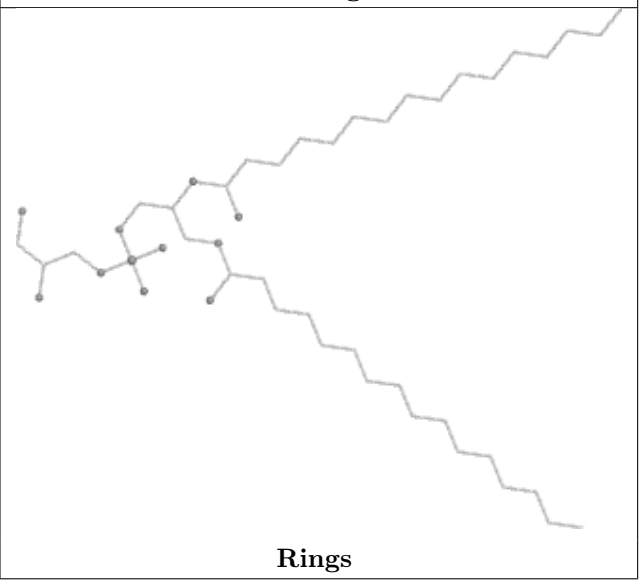
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Bond angles

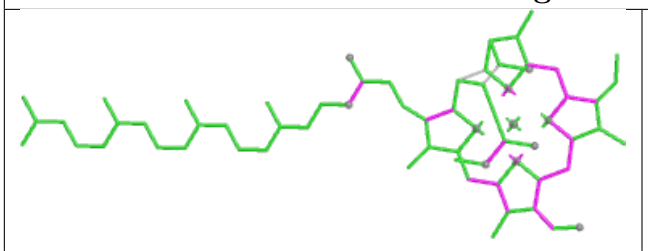


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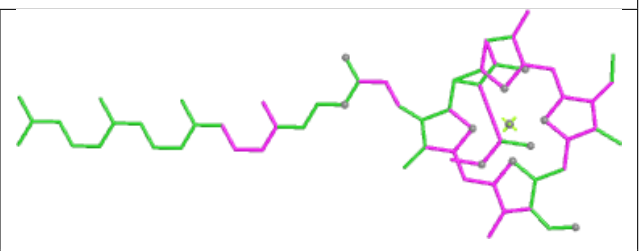


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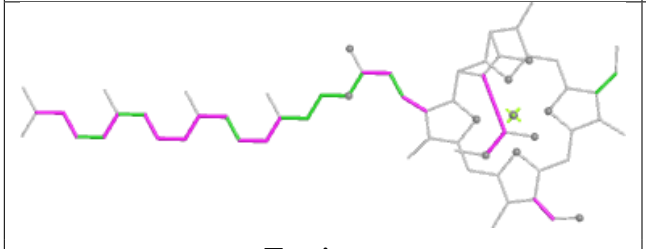
Ligand CL7 5 418



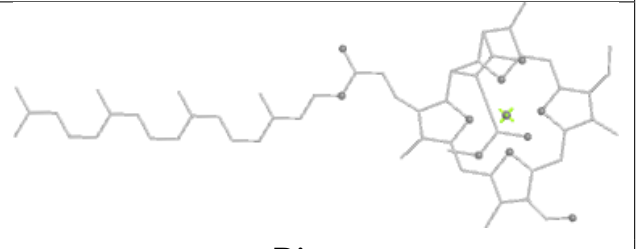
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Bond angles

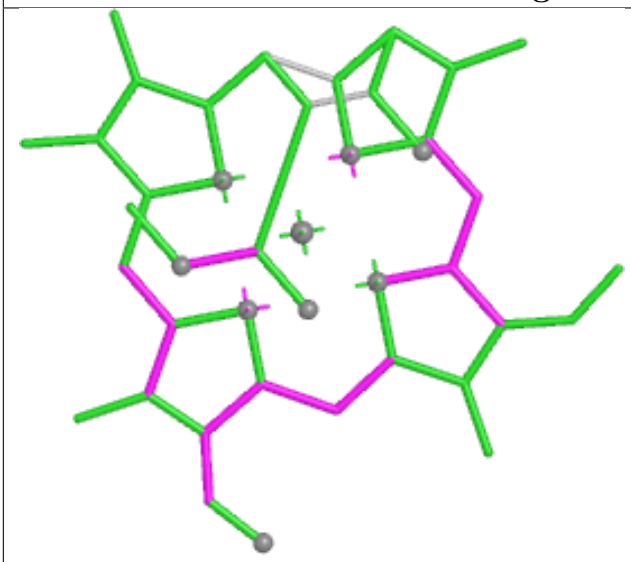


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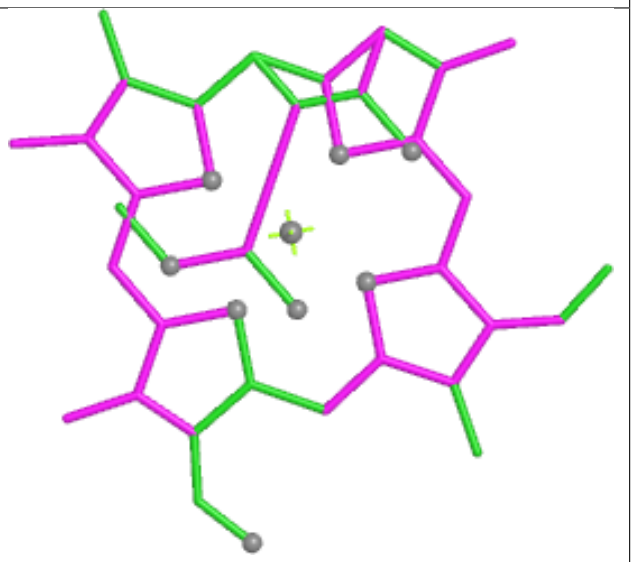


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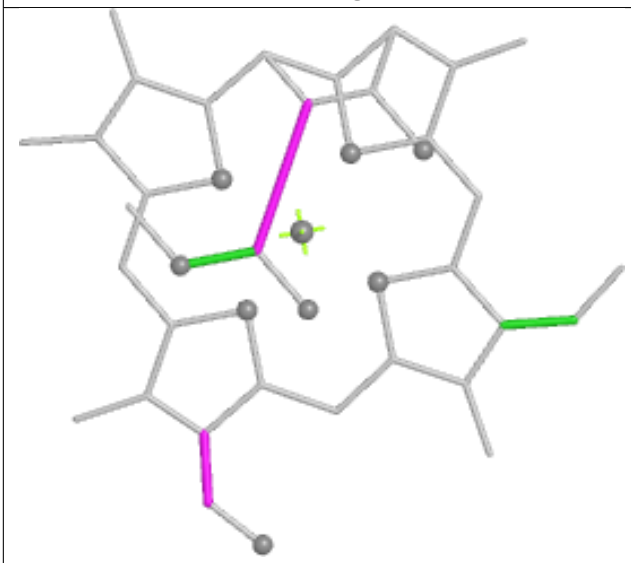
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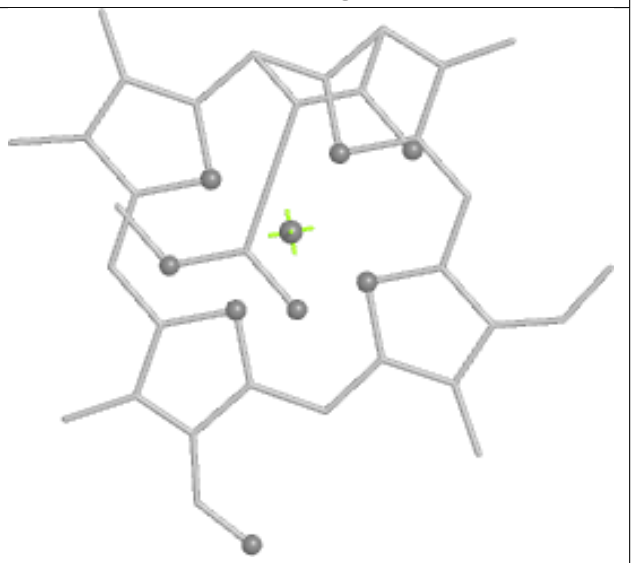
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Bond angles

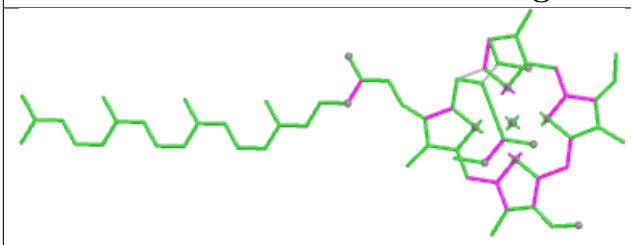


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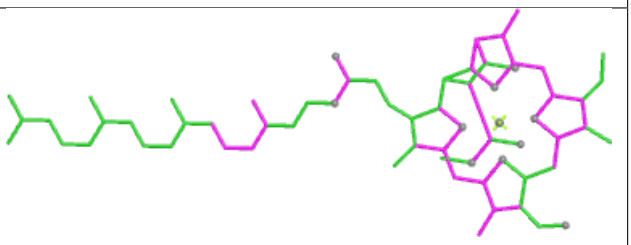


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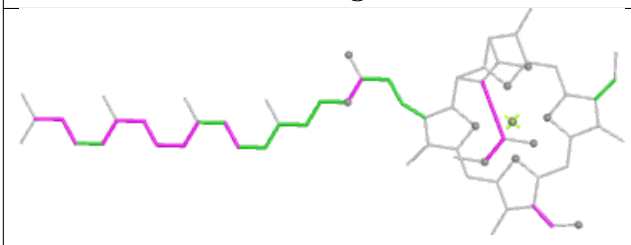
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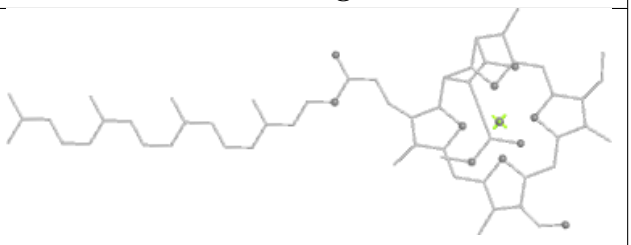
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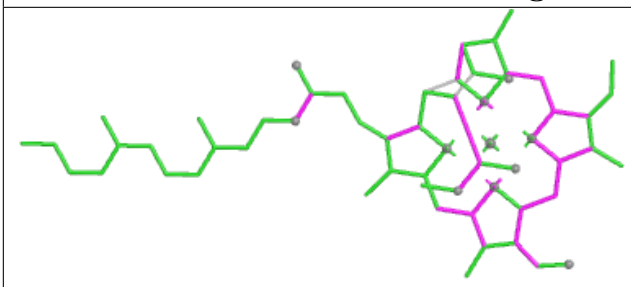


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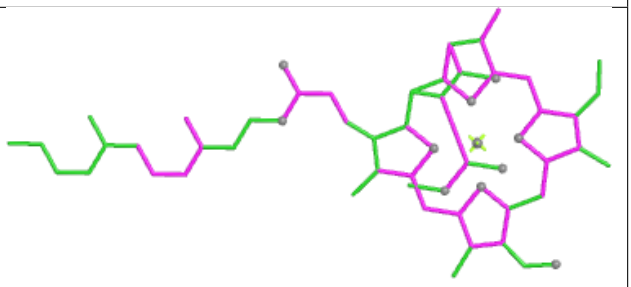


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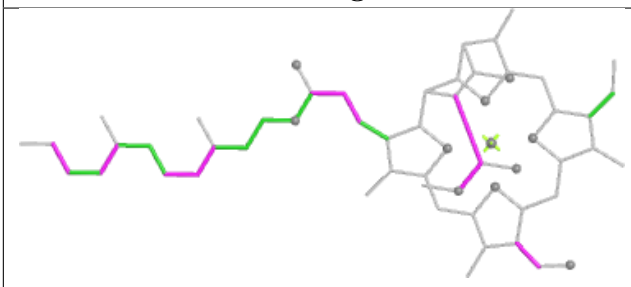
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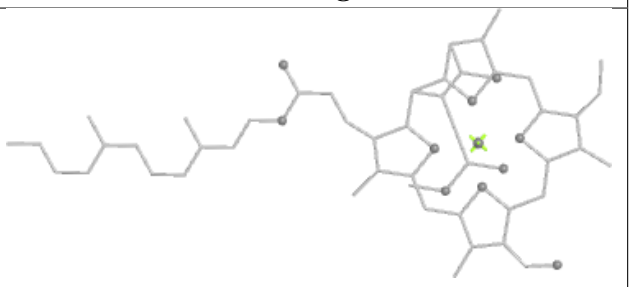
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Bond angles

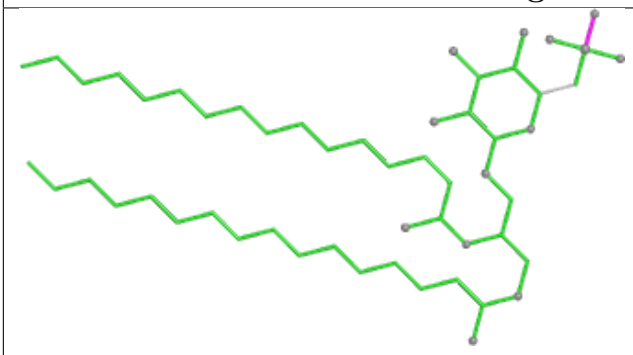


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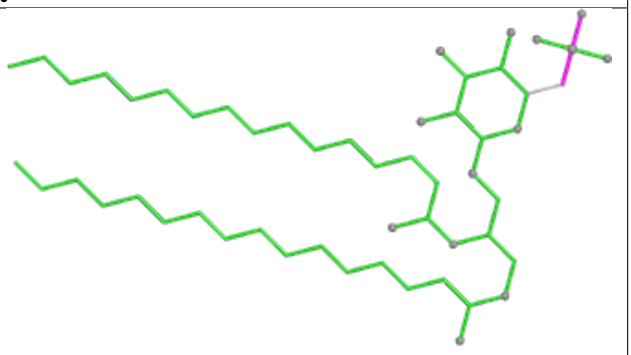


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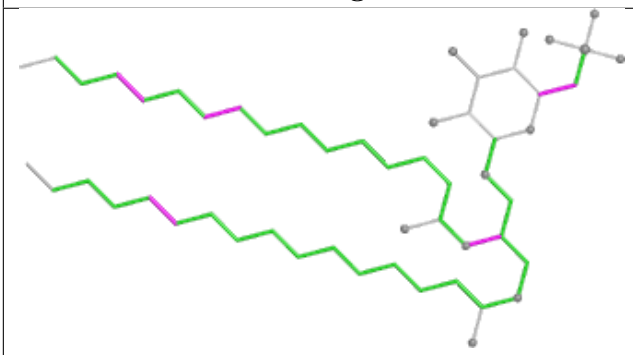
Ligand SQD b 621



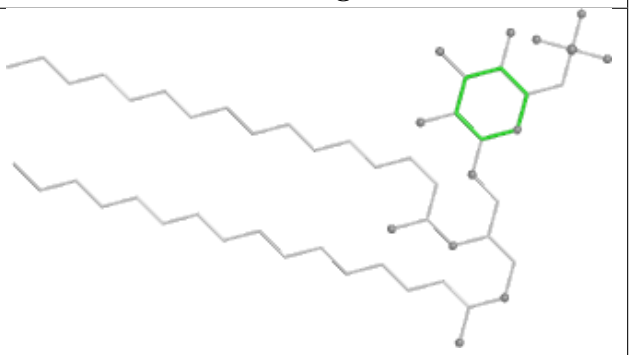
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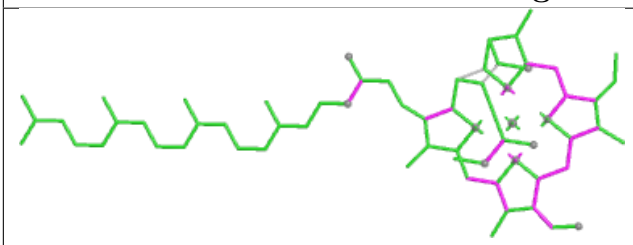


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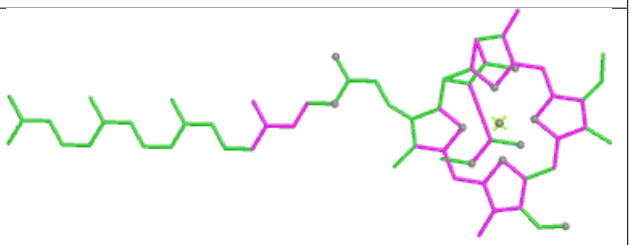


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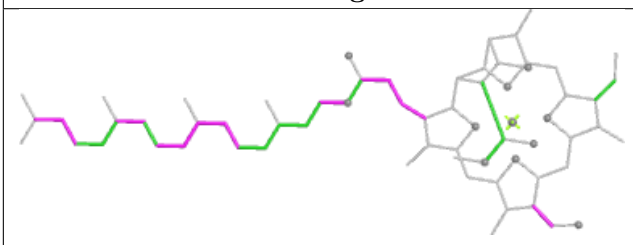
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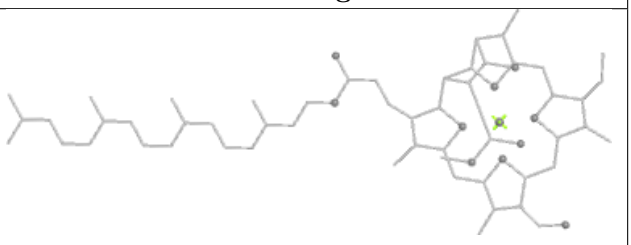
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Bond angles

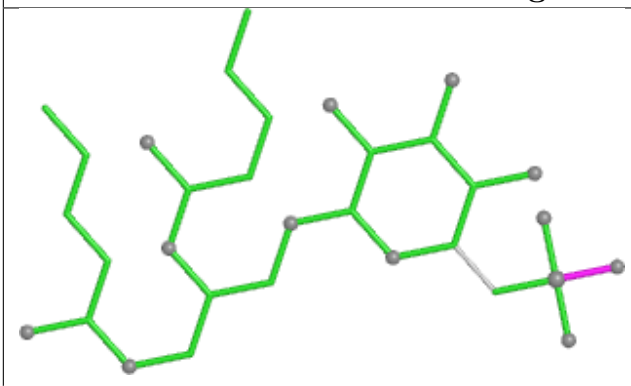


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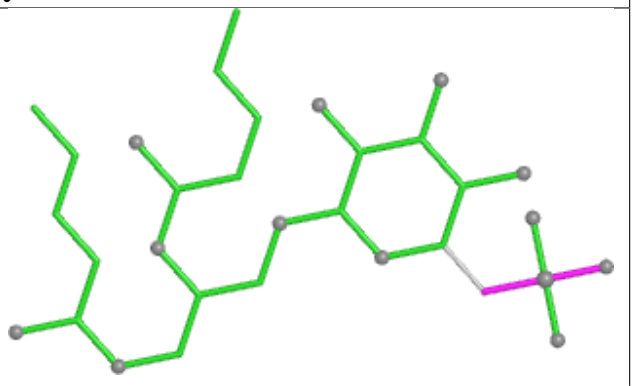


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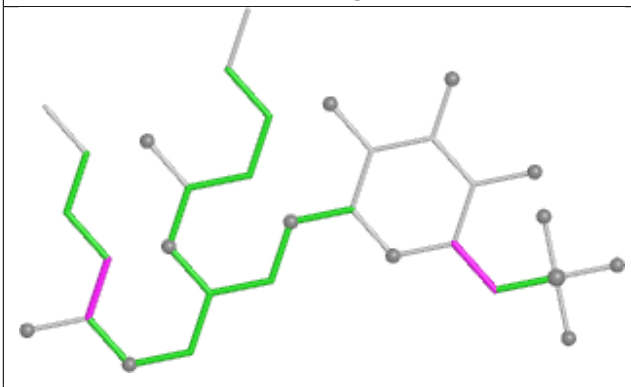
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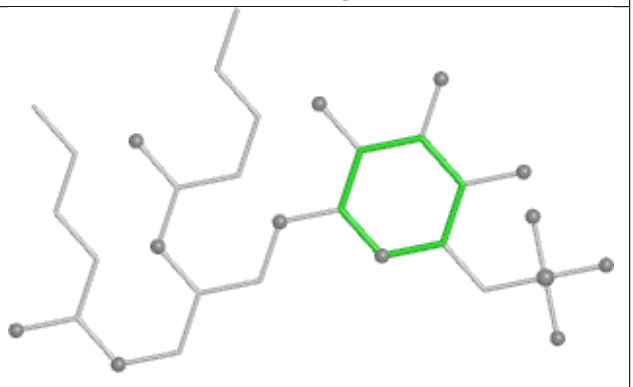
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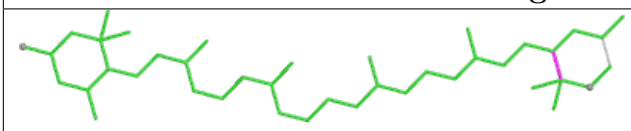


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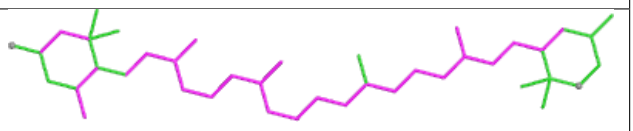


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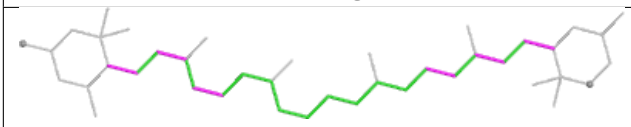
Ligand ZEX 8 418



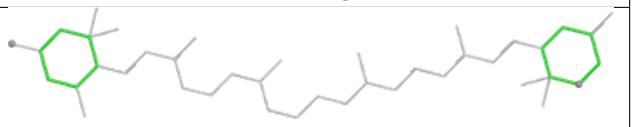
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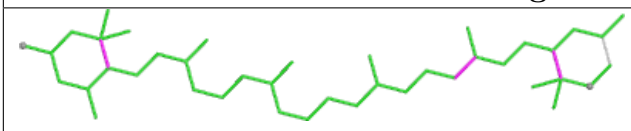


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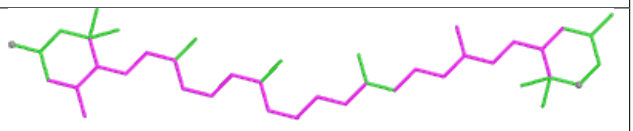


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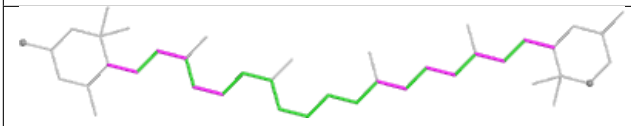
Ligand ZEX 2 525



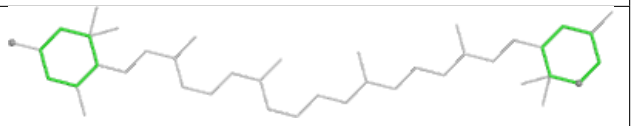
Bond lengths



Bond angles

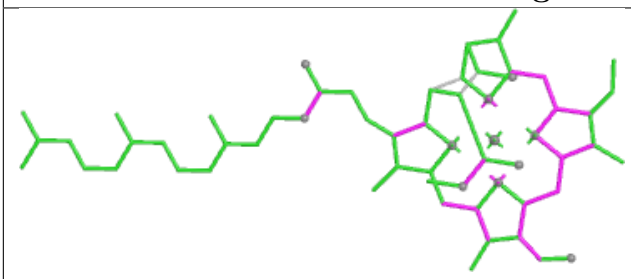


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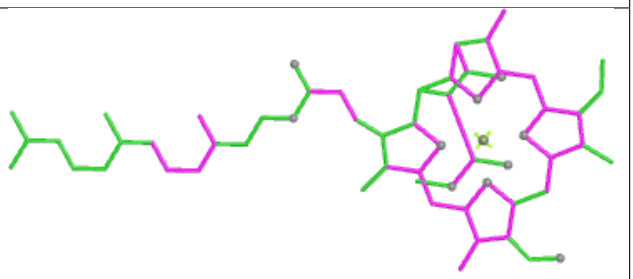


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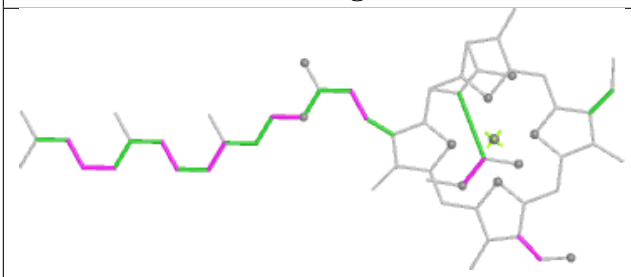
Ligand CL7 5 403



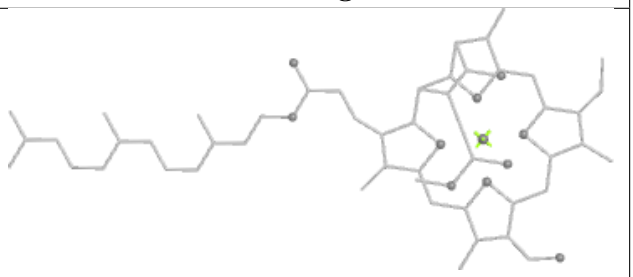
Bond lengths



Bond angles

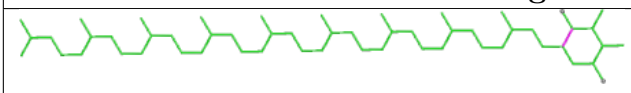


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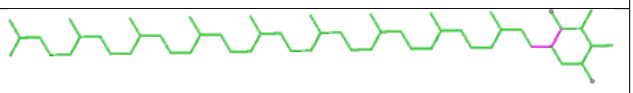


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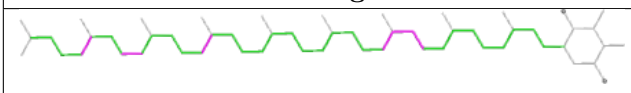
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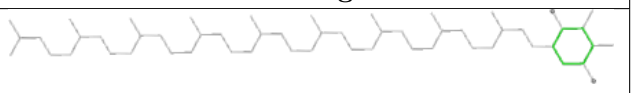
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Bond angles

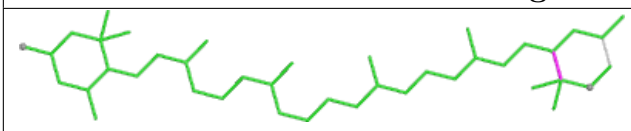


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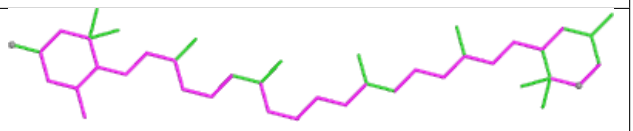


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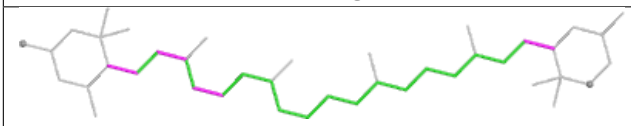
Ligand ZEX 1 422



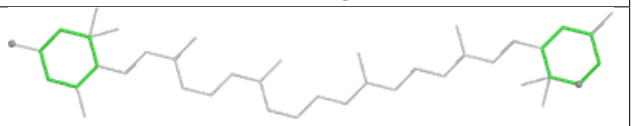
Bond lengths



Bond angles

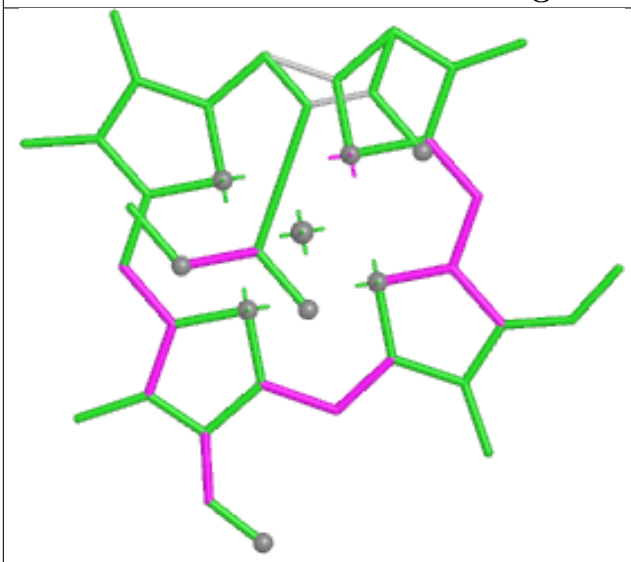


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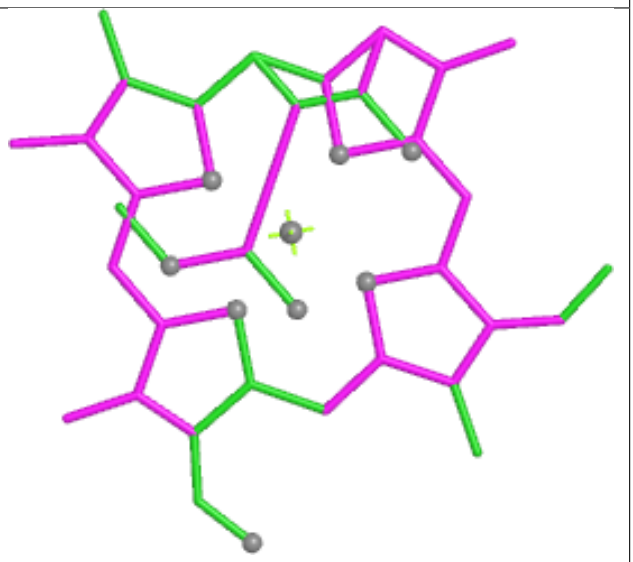


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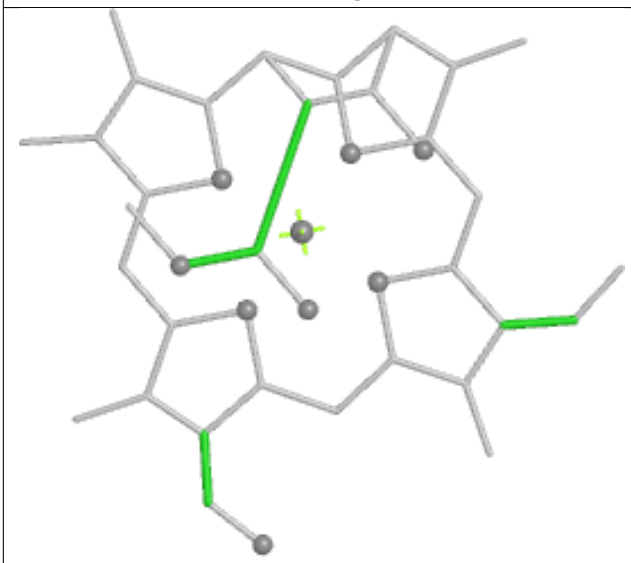
Ligand CL7 3 515



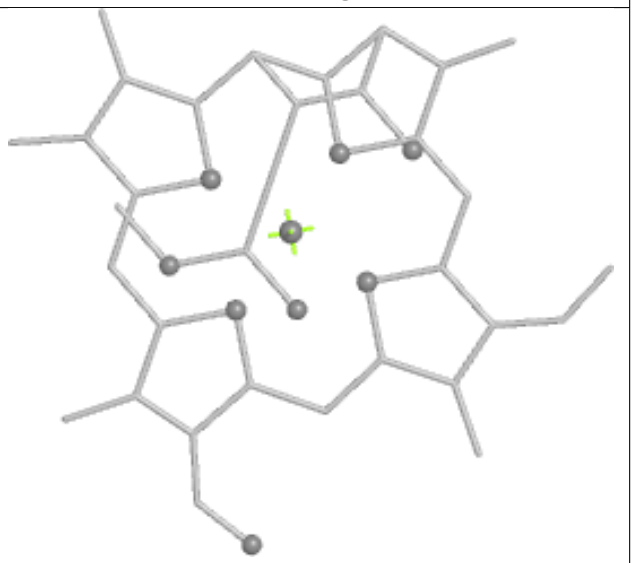
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Bond angles

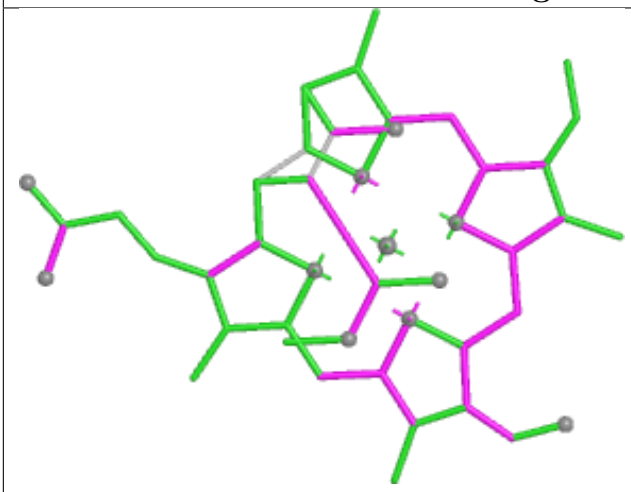


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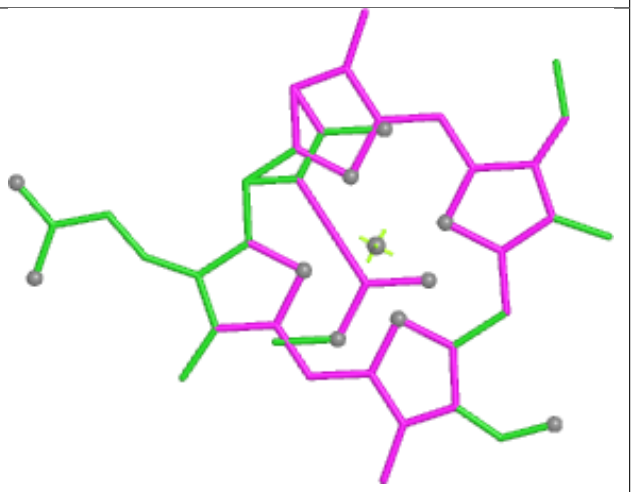


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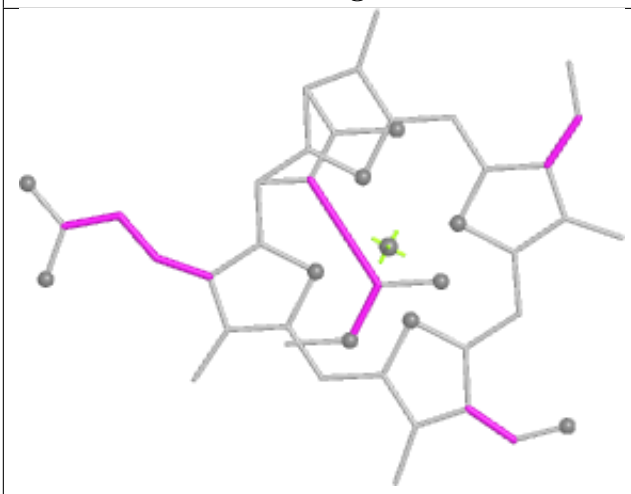
Ligand CL7 8 415



Bond lengths



Bond angles

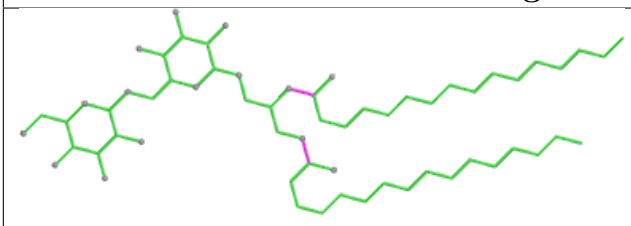


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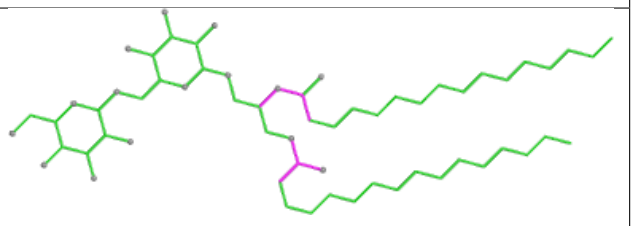


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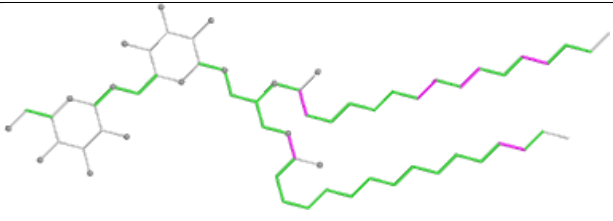
Ligand DGD b 625



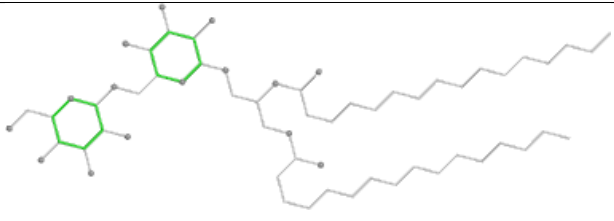
Bond lengths



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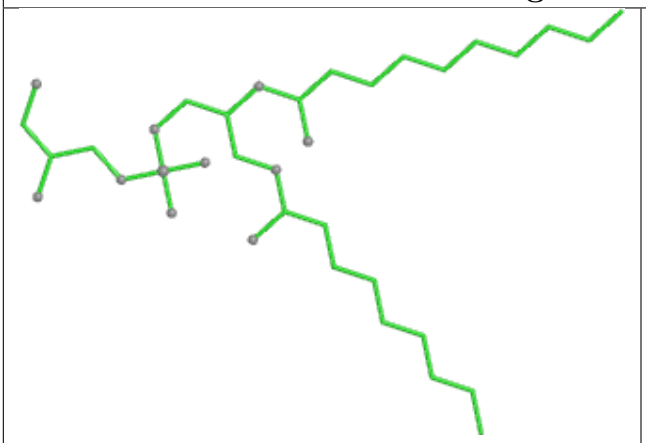


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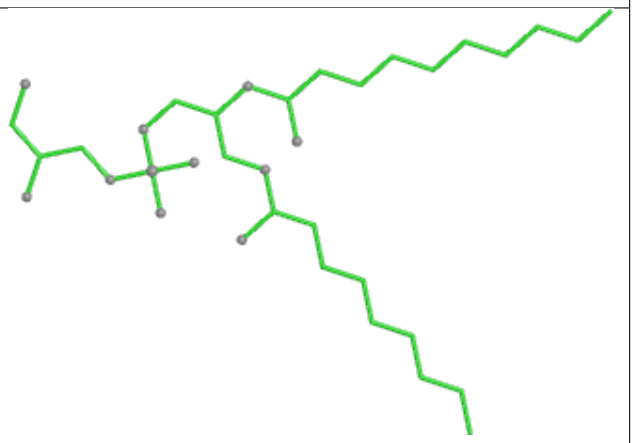


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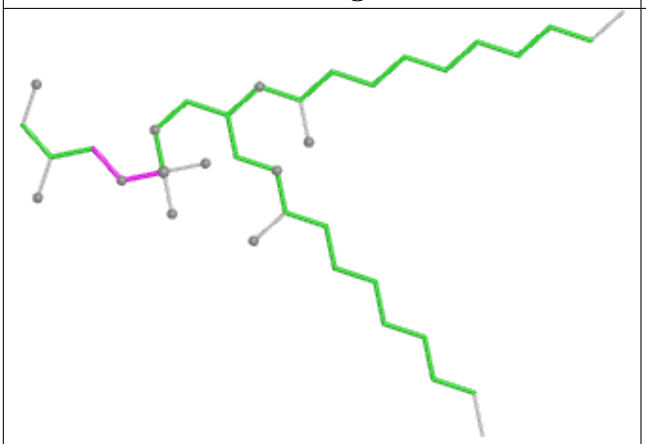
Ligand LHG 3 524



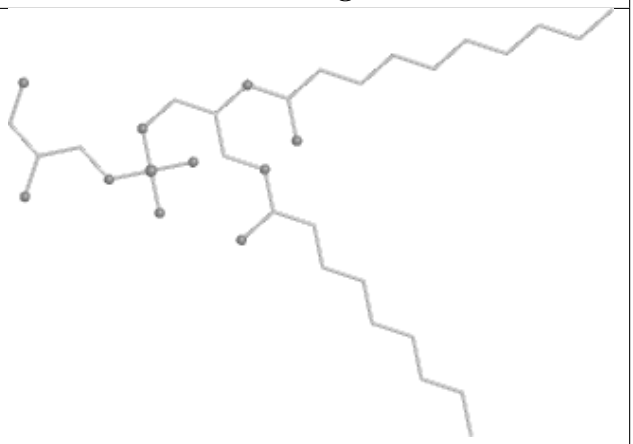
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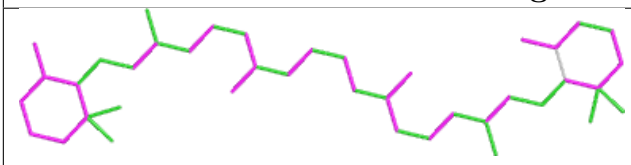


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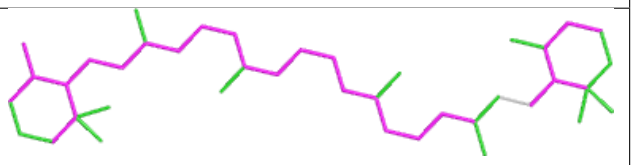


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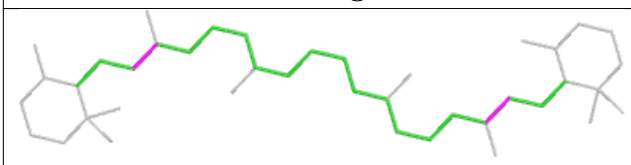
Ligand 8CT b 620



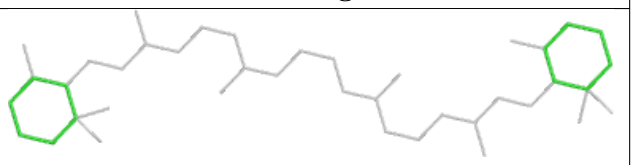
Bond lengths



Bond angles

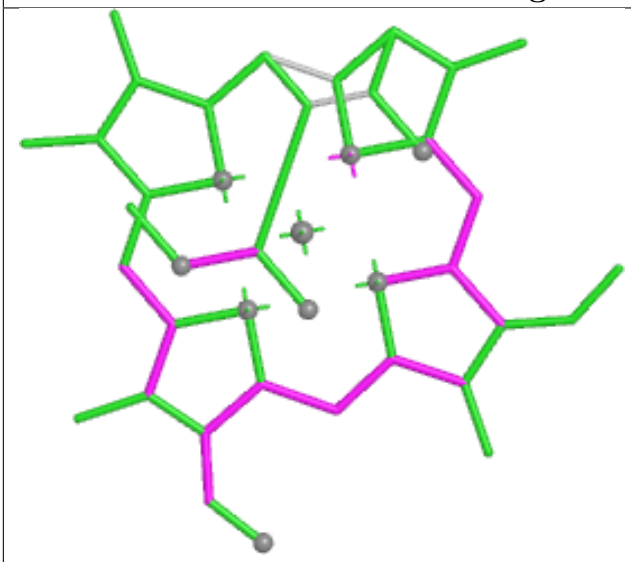


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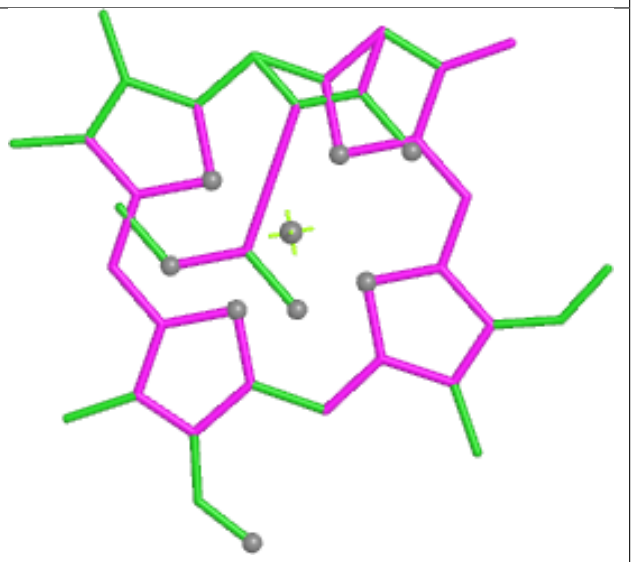


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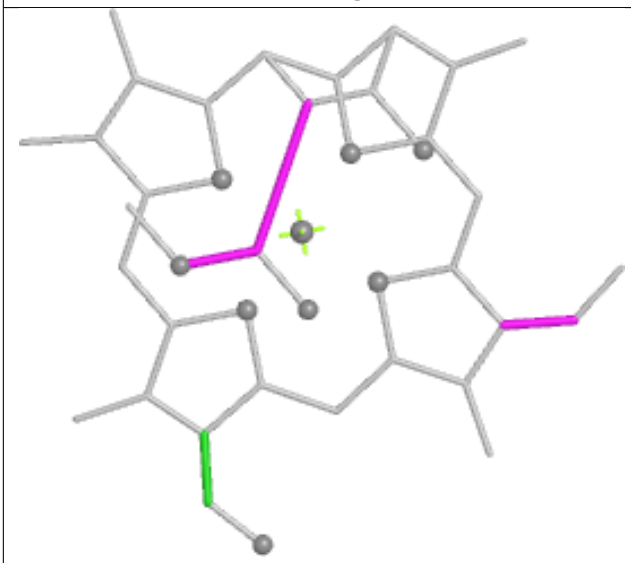
Ligand CL7 B 601



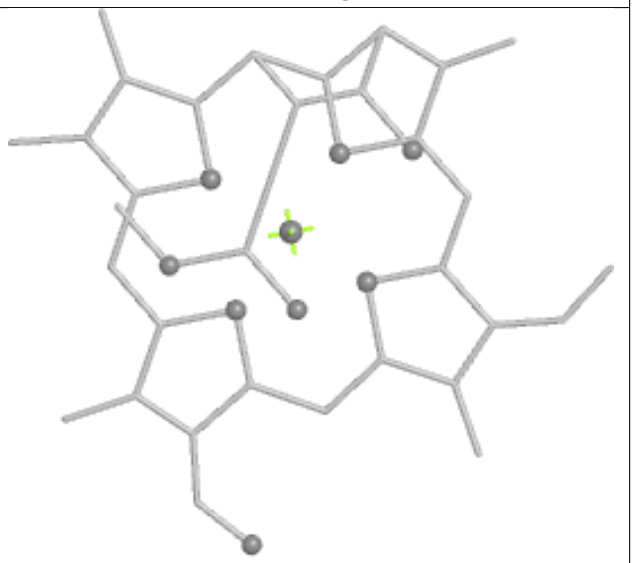
Bond lengths



Bond angles

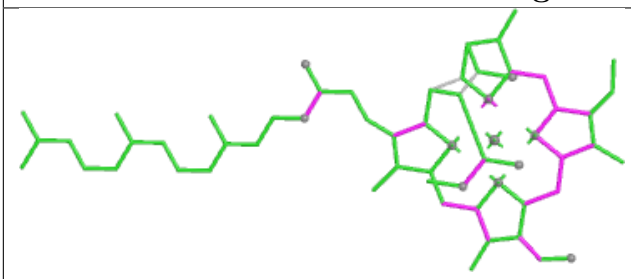


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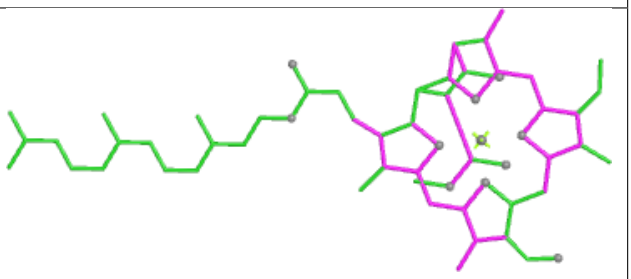


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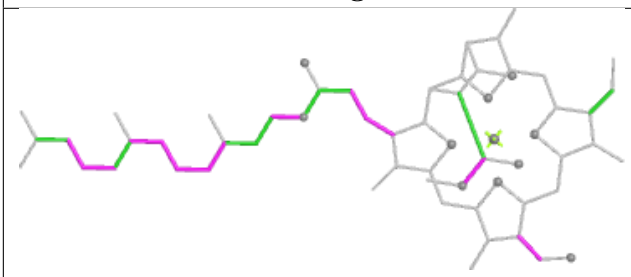
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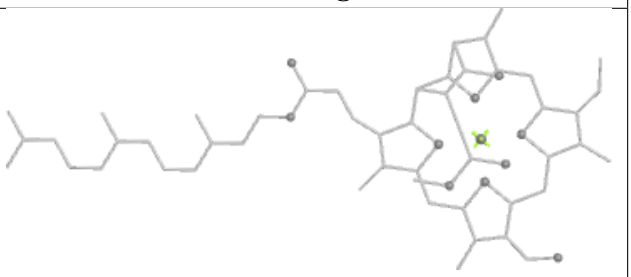
Bond lengths



Bond angles



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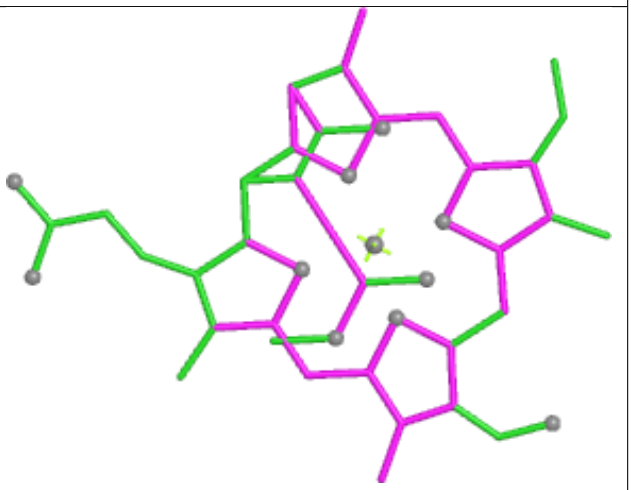


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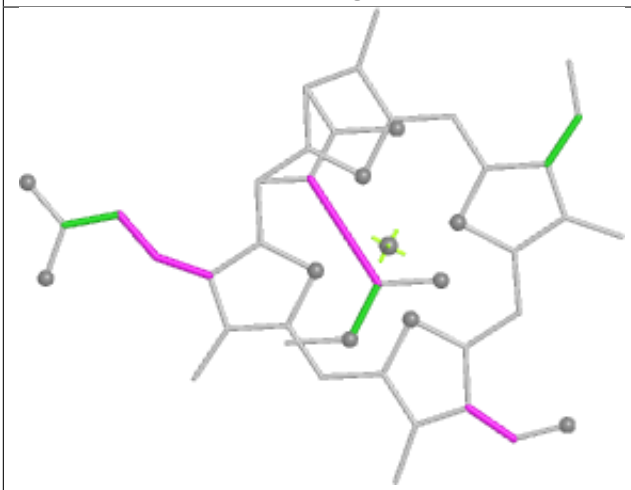
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Bond lengths



Bond angles

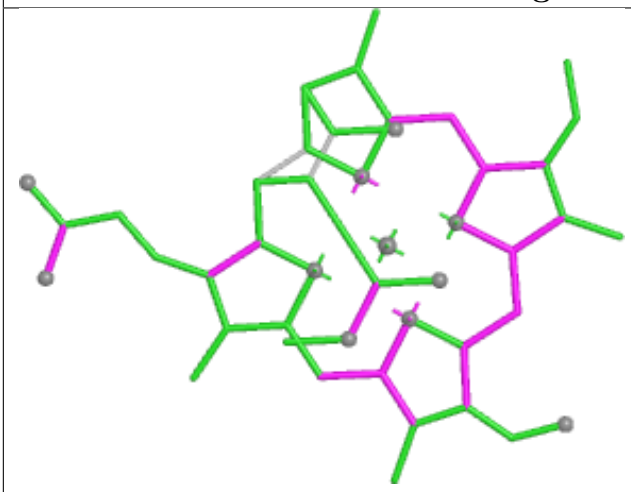


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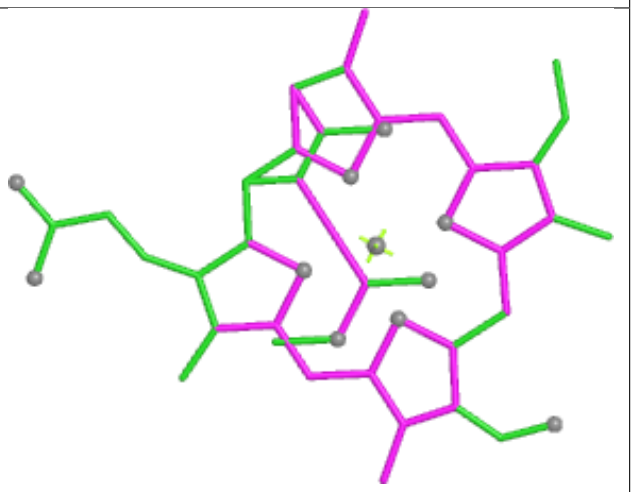


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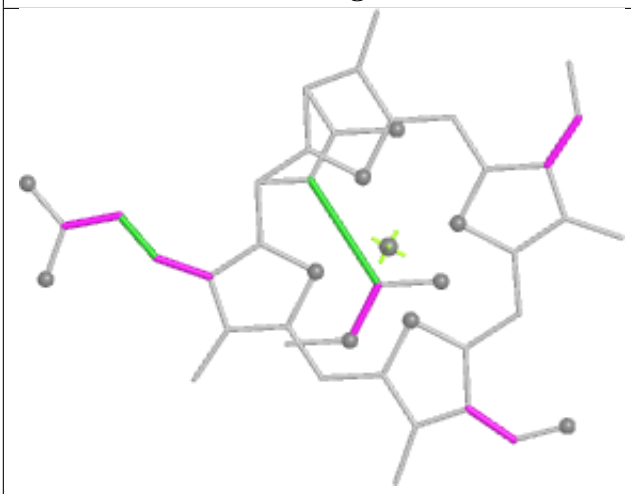
Ligand CL7 6 514



Bond lengths



Bond angles

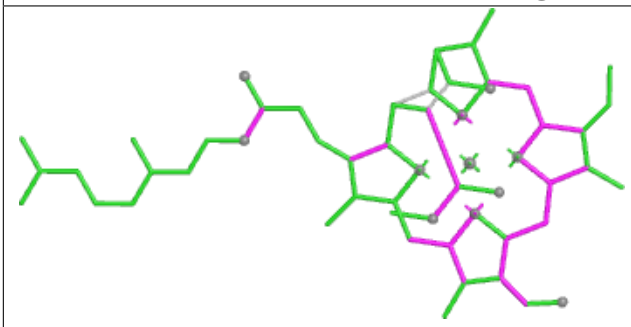


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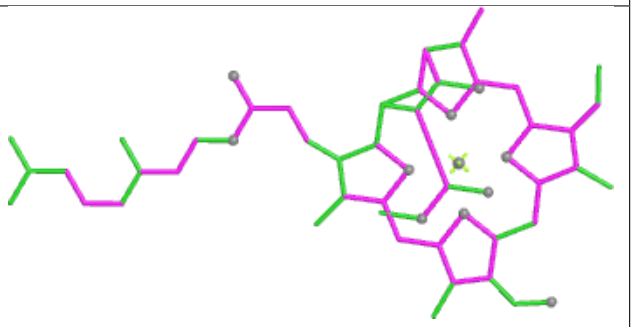


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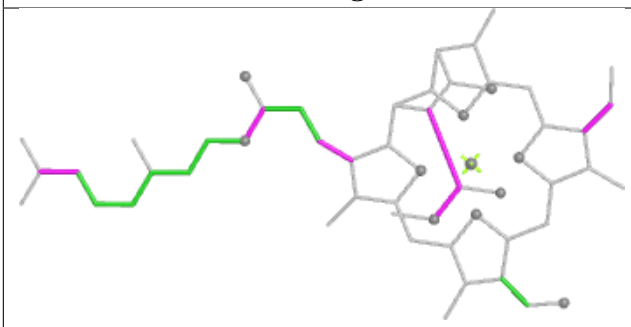
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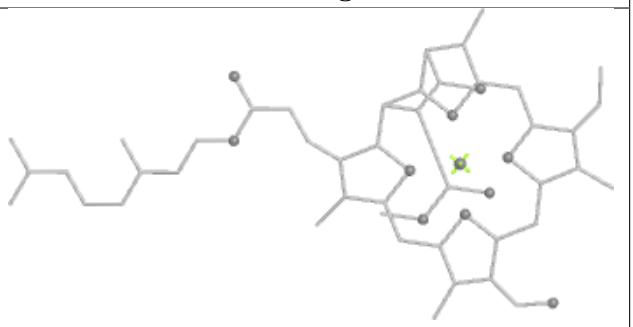
Bond lengths



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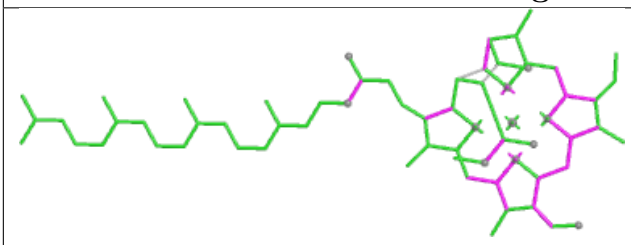


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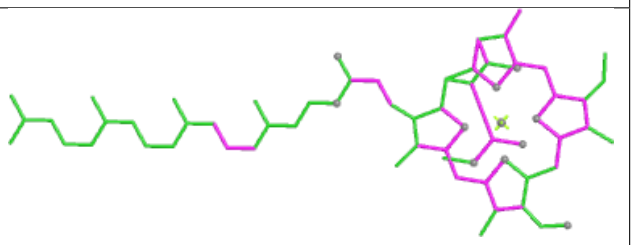


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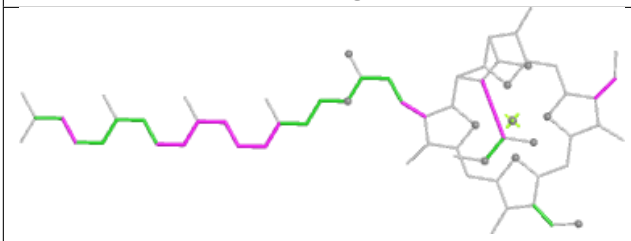
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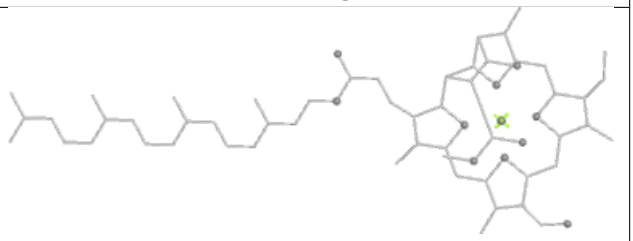
Bond lengths



Bond angles

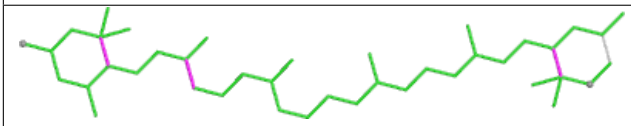


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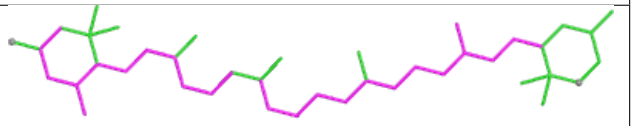


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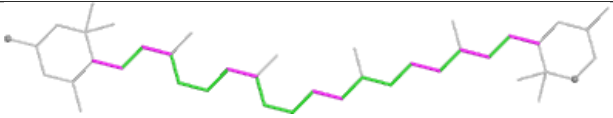
Ligand ZEX 2 519



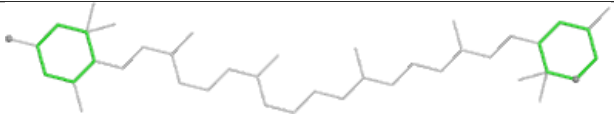
Bond lengths



Bond angles

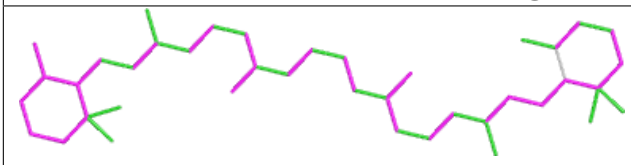


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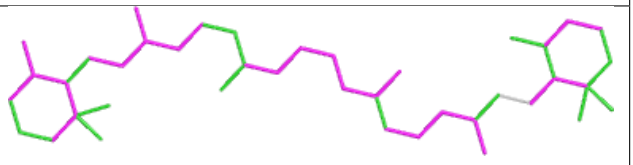


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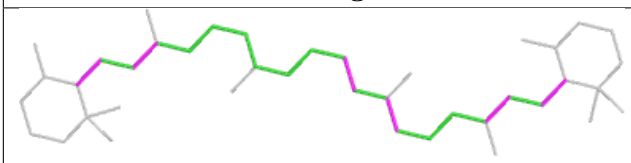
Ligand 8CT K 101



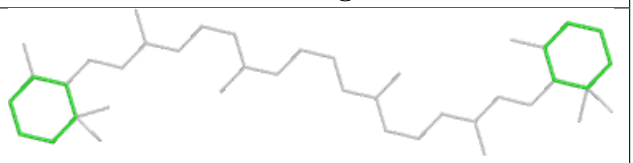
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Bond angles

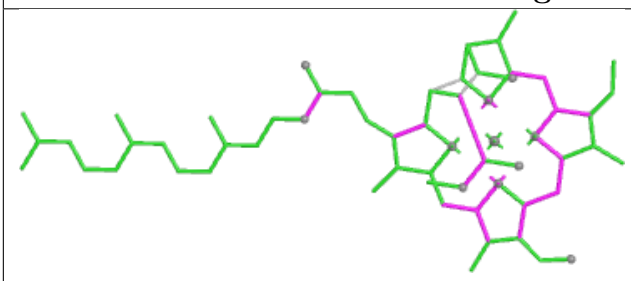


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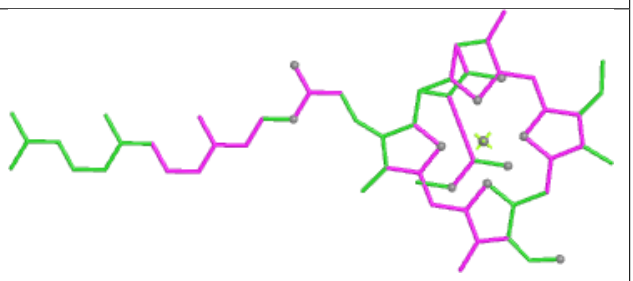


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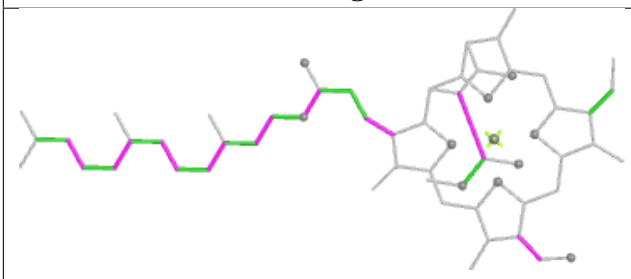
Ligand CL7 c 507



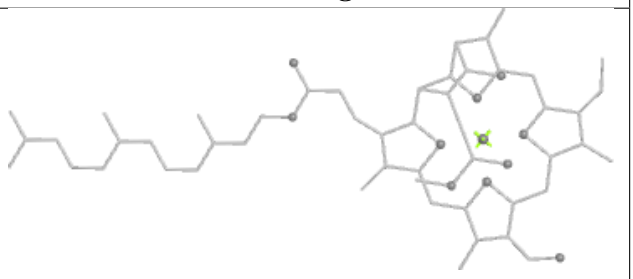
Bond lengths



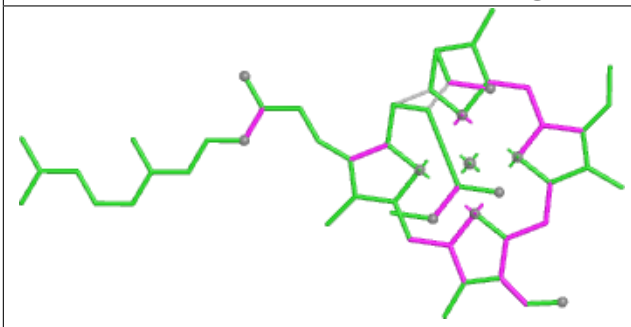
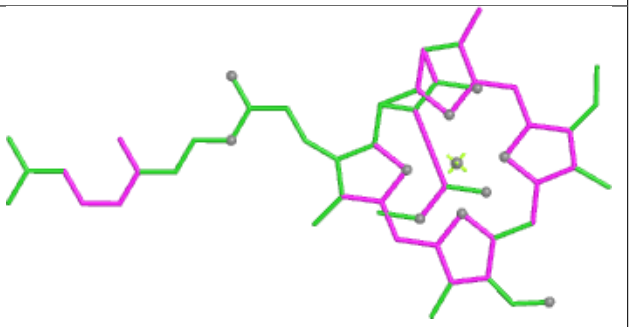
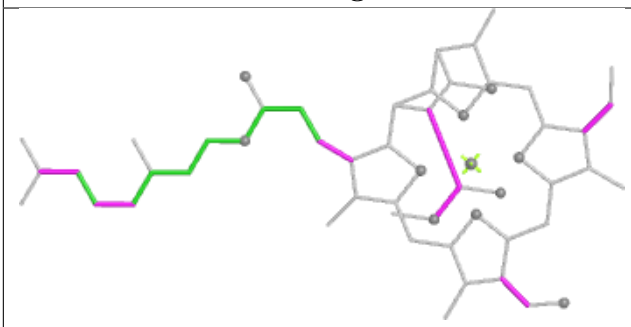
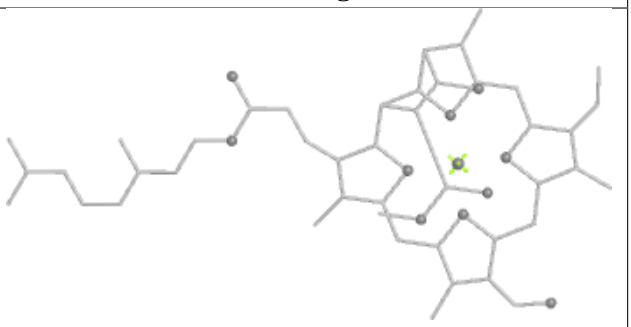
Bond angles

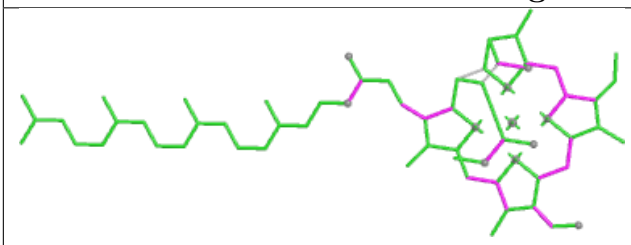
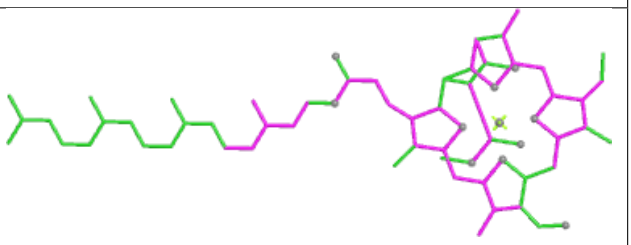
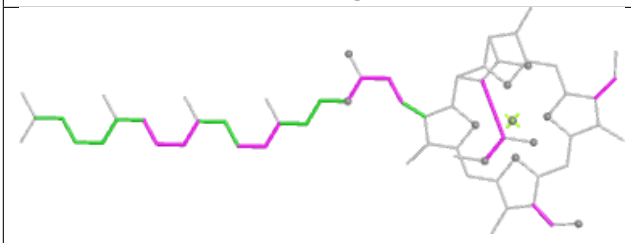
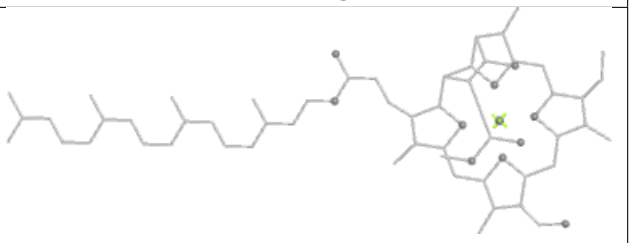


Torsions

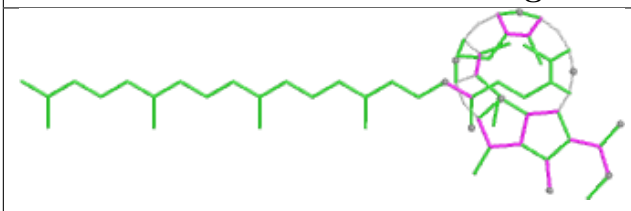


Rings

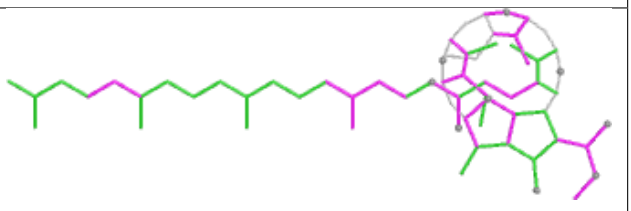
Ligand CL7 C 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CL7 A 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PHO d 408



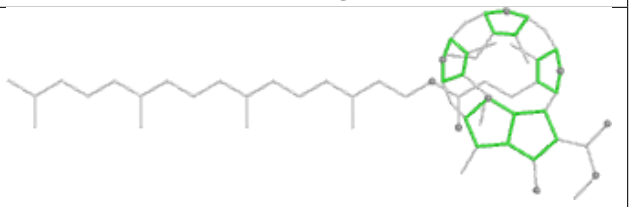
Bond lengths



Bond angles

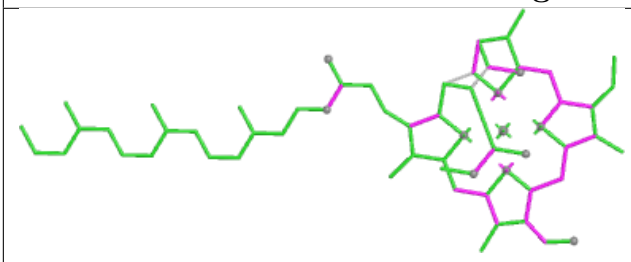


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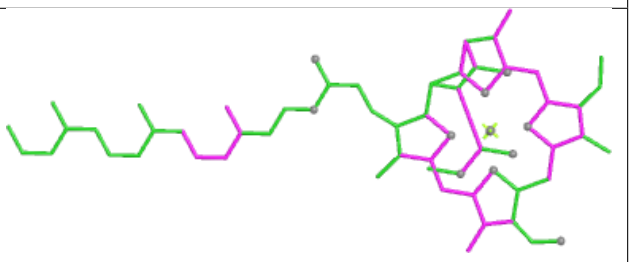


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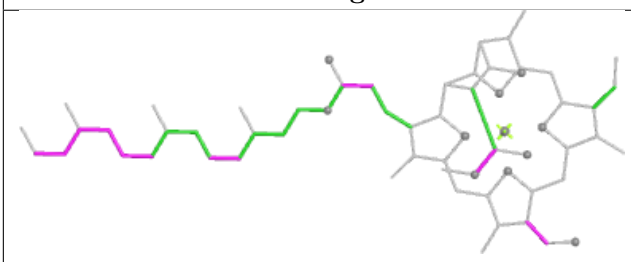
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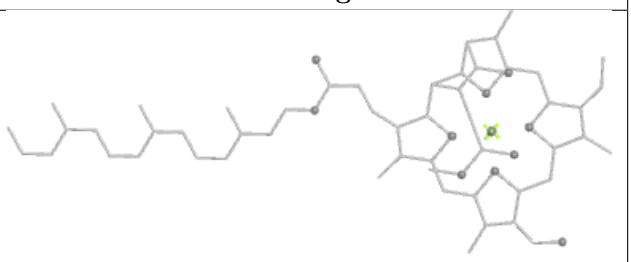
Bond lengths



Bond angles

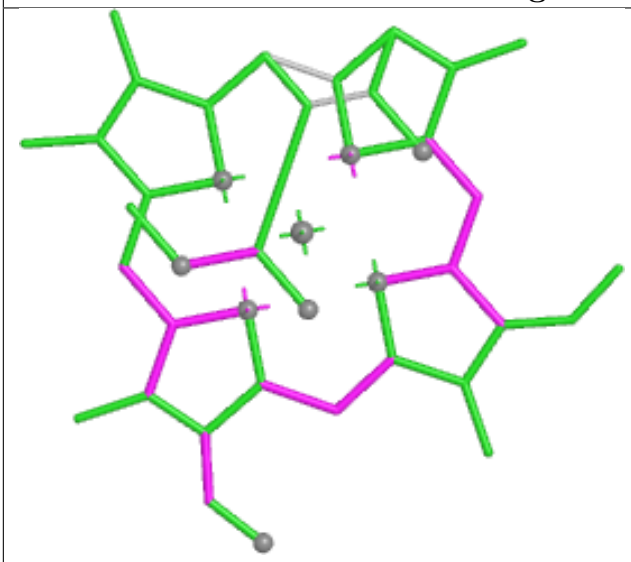


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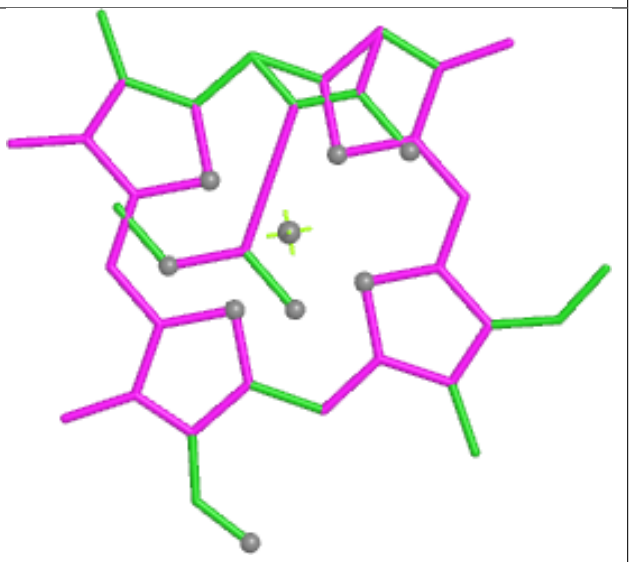


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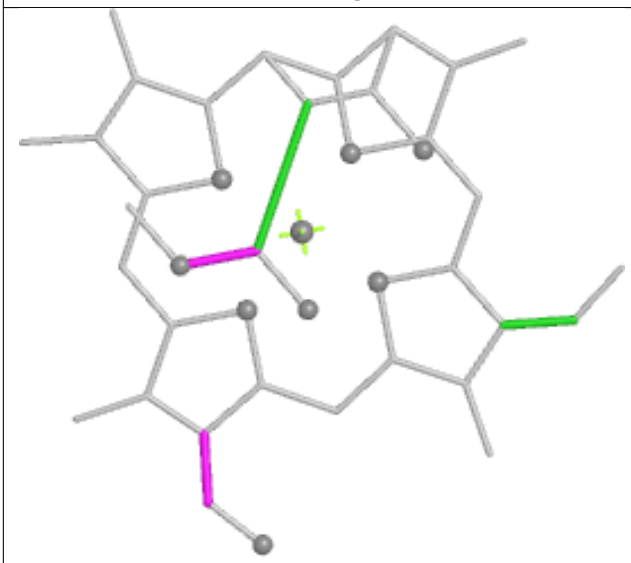
Ligand CL7 C 513



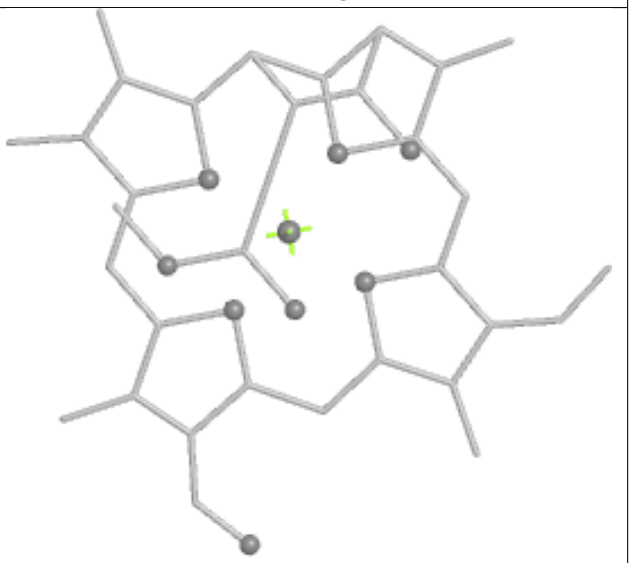
Bond lengths



Bond angles

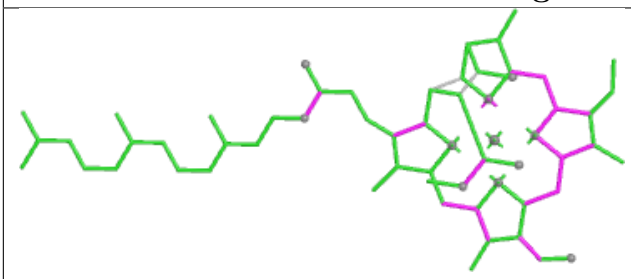


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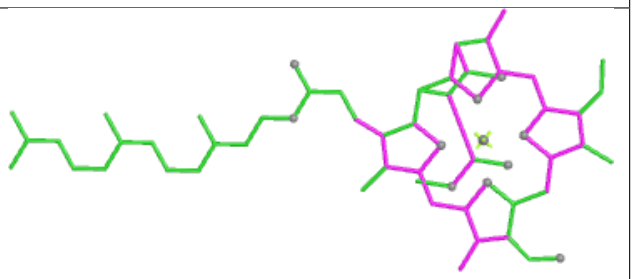


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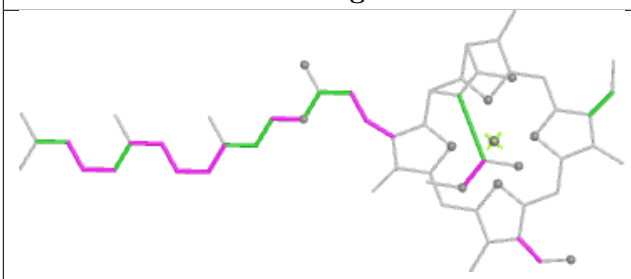
Ligand CL7 1 402



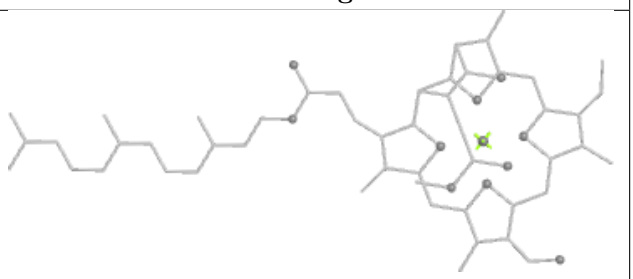
Bond lengths



Bond angles

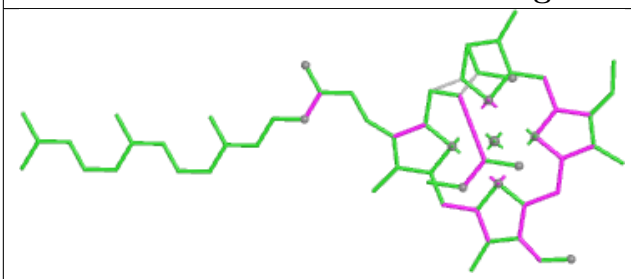


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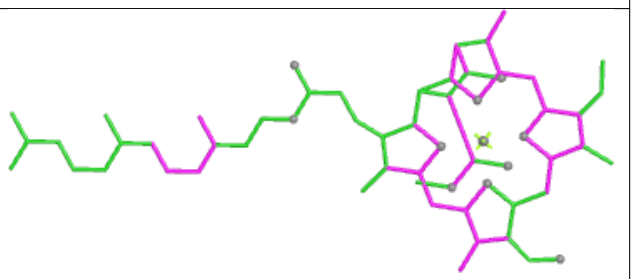


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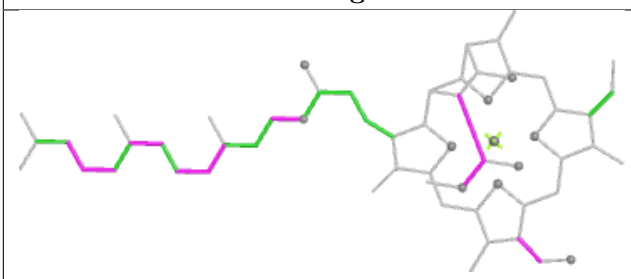
Ligand CL7 c 503



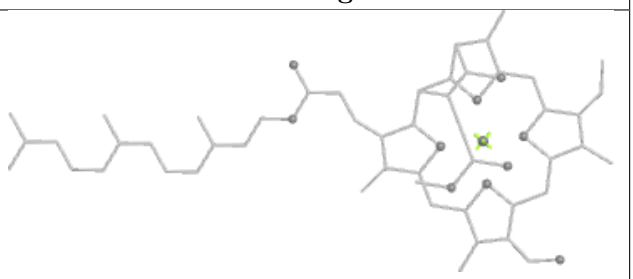
Bond lengths



Bond angles

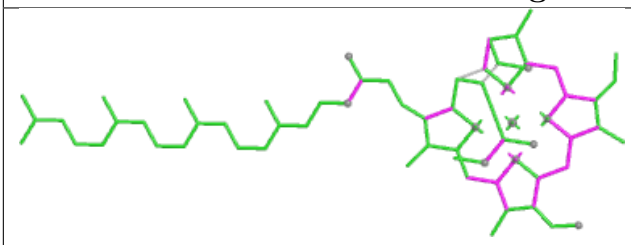


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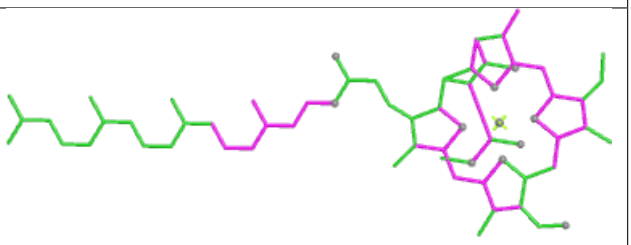


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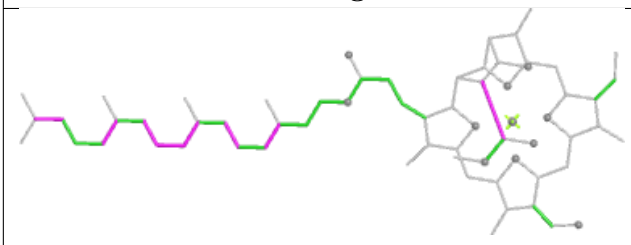
Ligand CL7 B 603



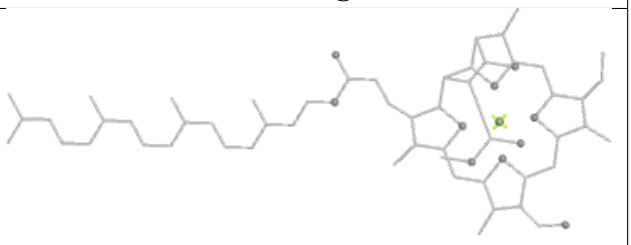
Bond lengths



Bond angles

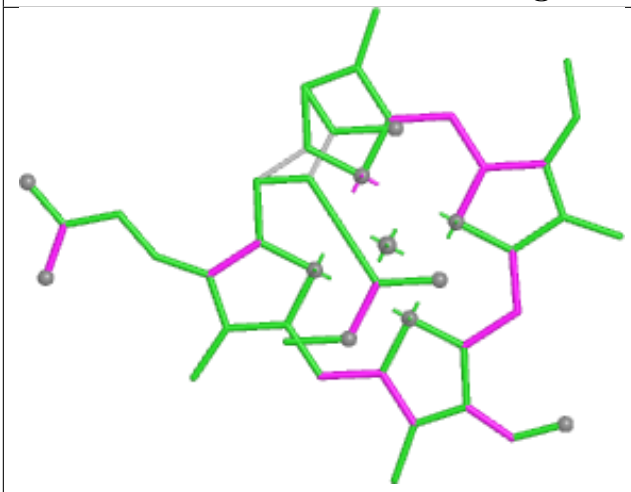


Torsions



Rings

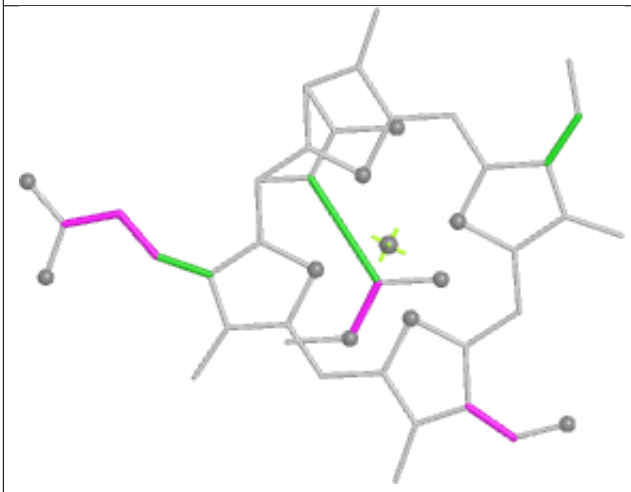
Ligand CL7 3 518



Bond lengths



Bond angles

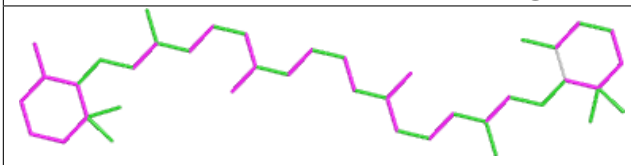


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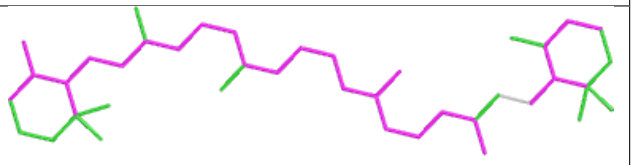


Rings

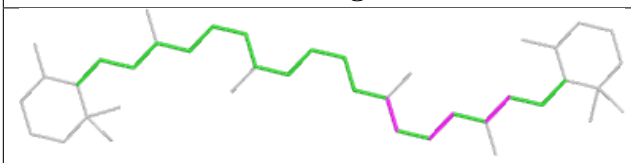
Ligand 8CT A 404



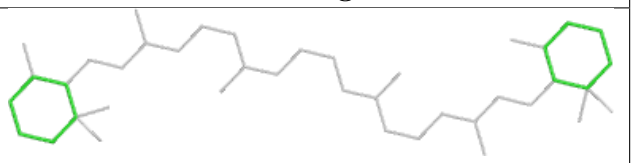
Bond lengths



Bond angles

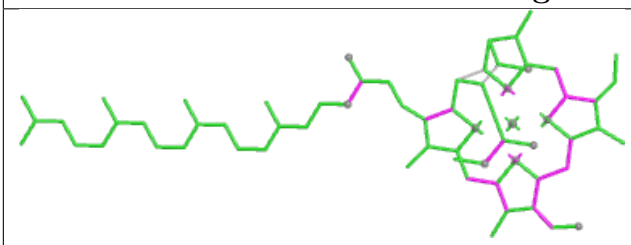


Torsions

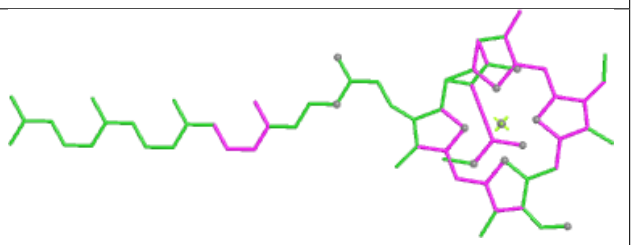


Rings

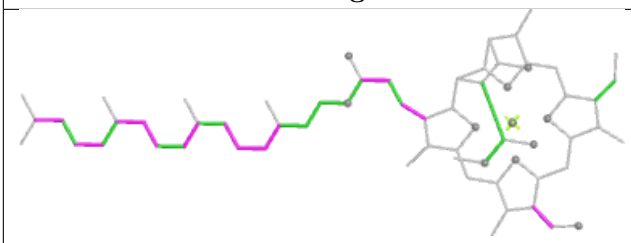
Ligand CL7 6 512



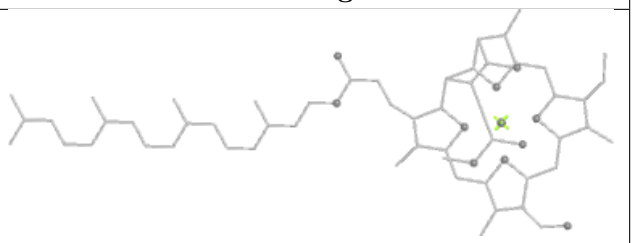
Bond lengths



Bond angles

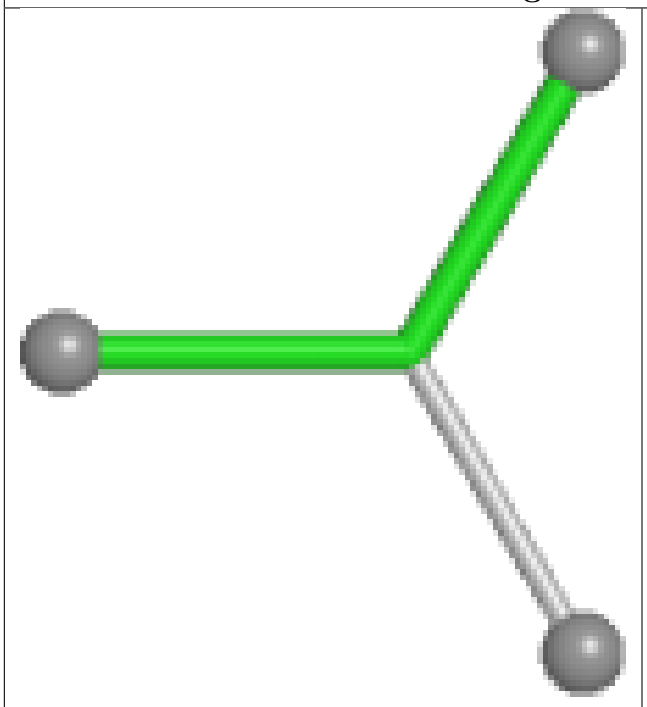


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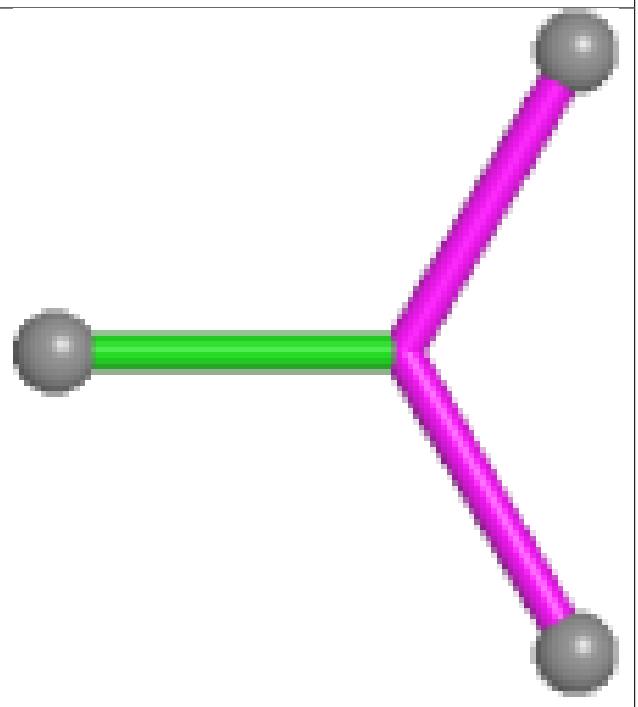


Rings

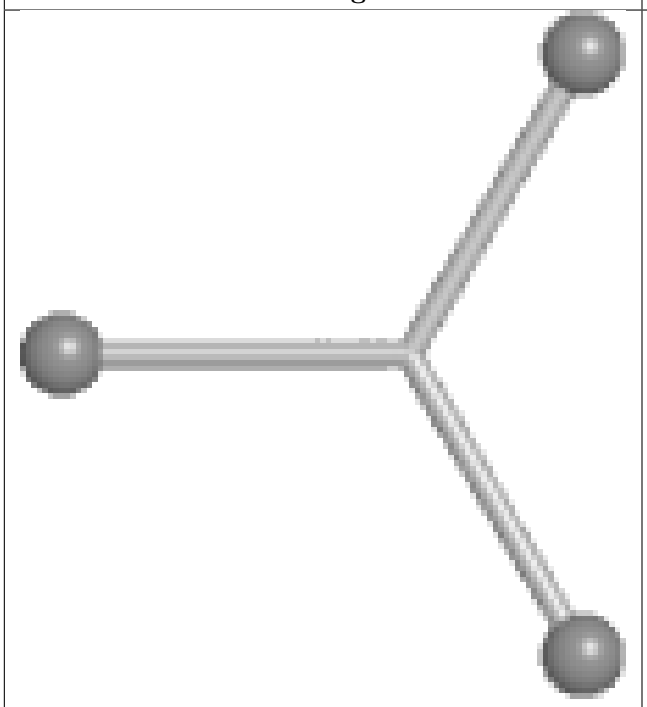
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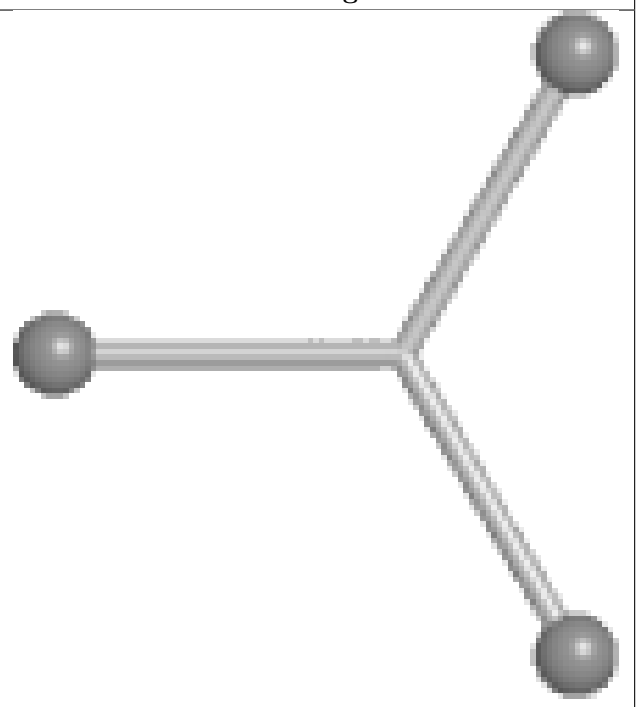
Bond lengths



Bond angles

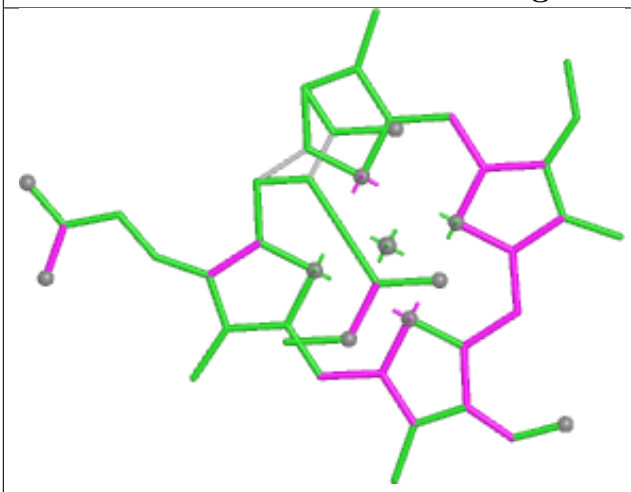


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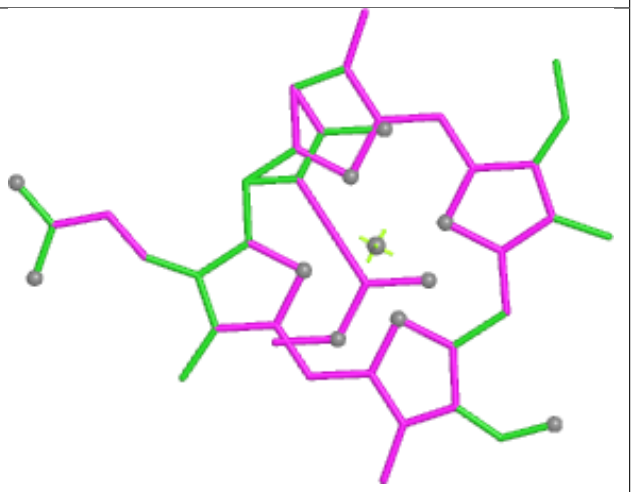


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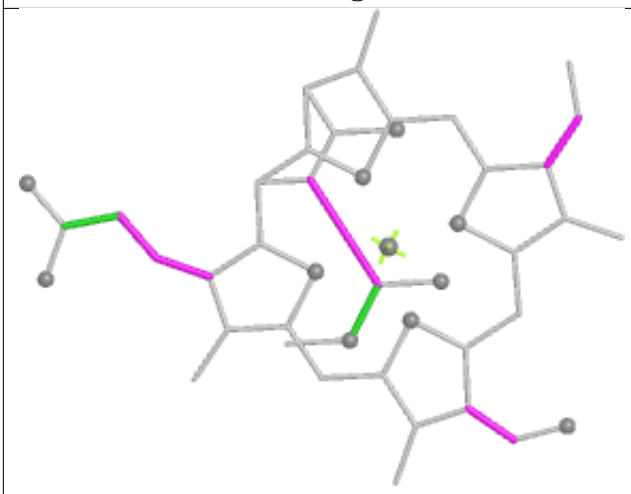
Ligand CL7 d 405



Bond lengths



Bond angles

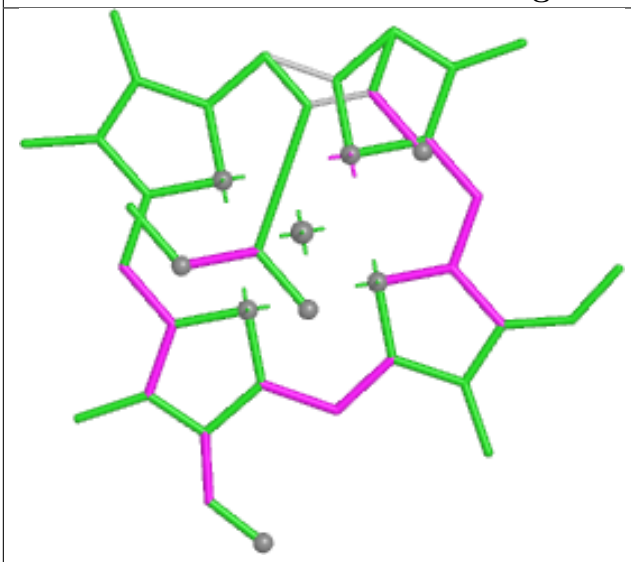


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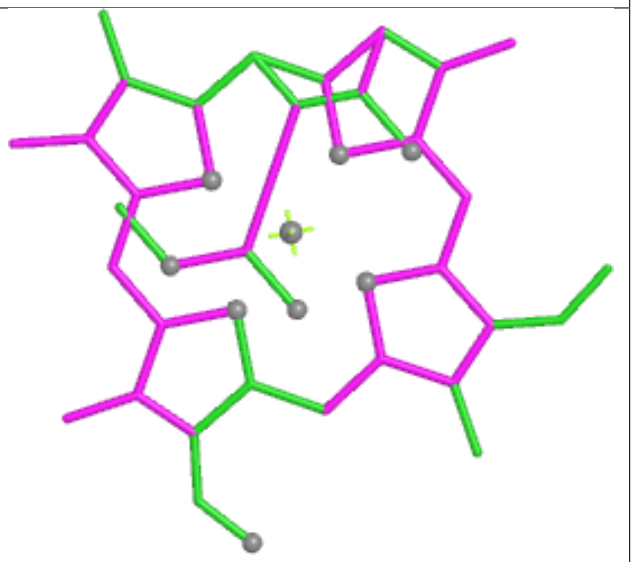


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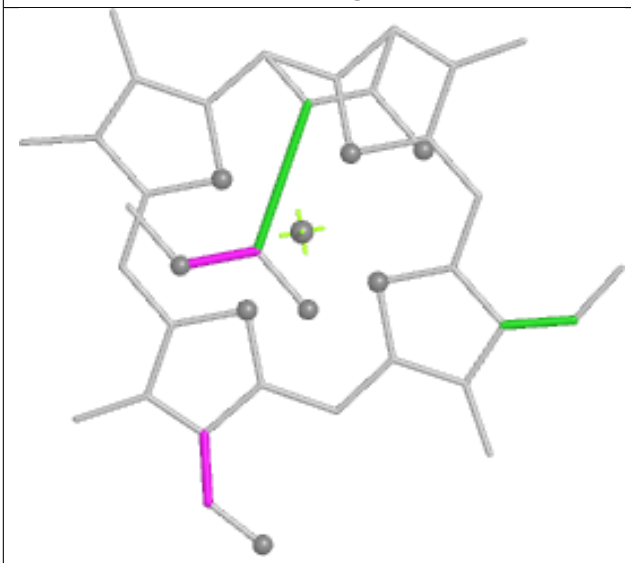
Ligand CL7 5 416



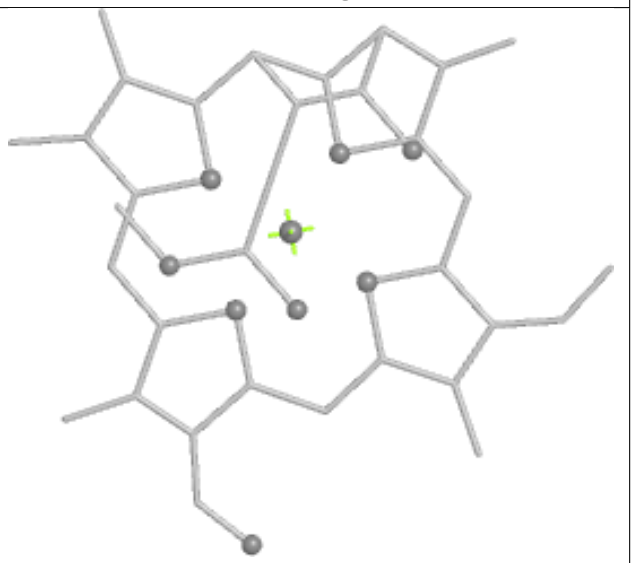
Bond lengths



Bond angles

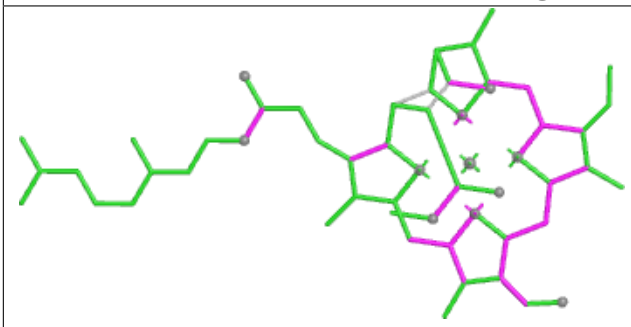


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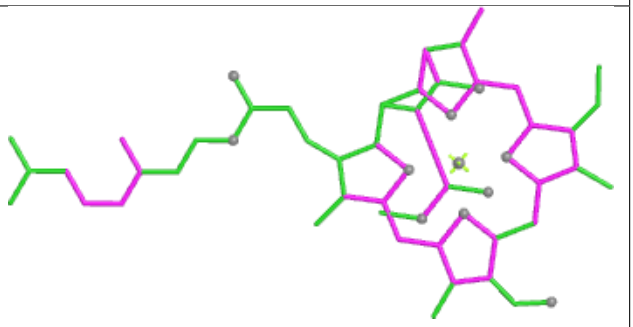


Rings

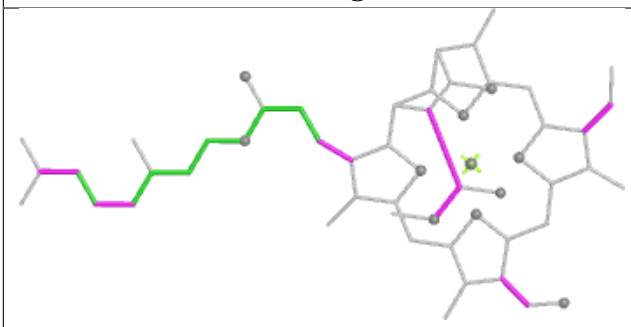
Ligand CL7 c 505



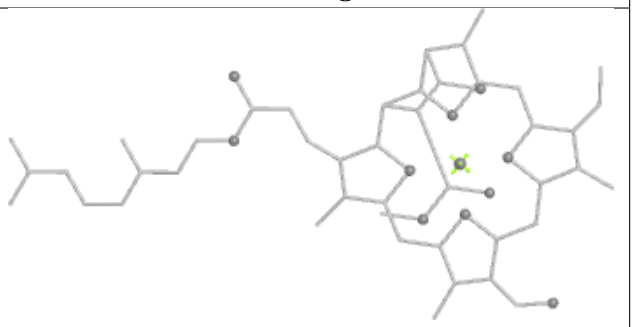
Bond lengths



Bond angles

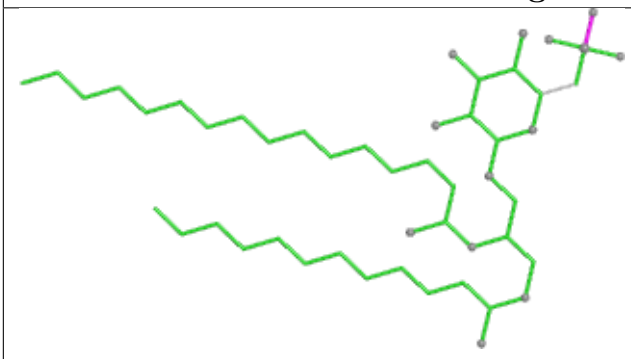


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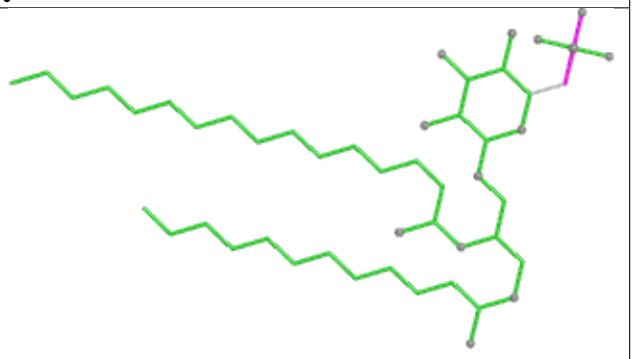


Rings

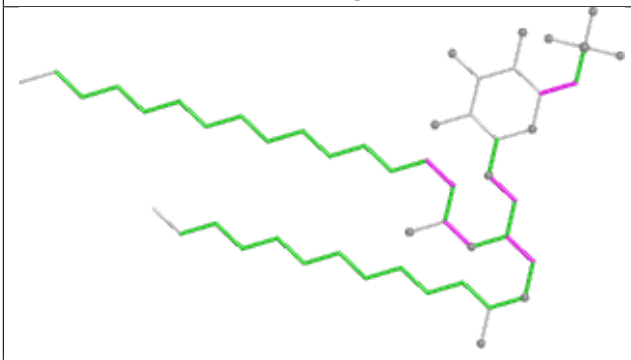
Ligand SQD 6 521



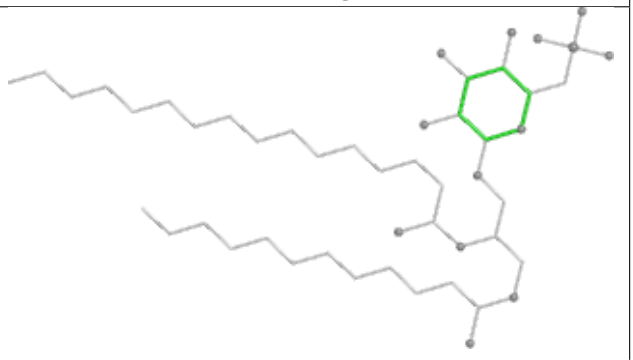
Bond lengths



Bond angles

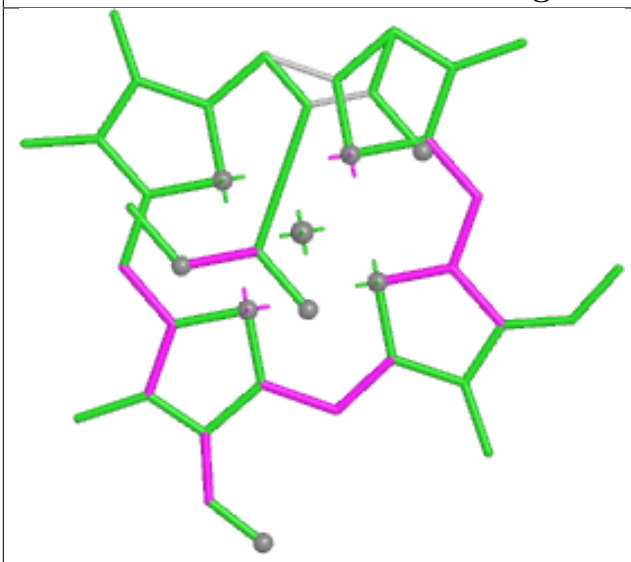


Torsions

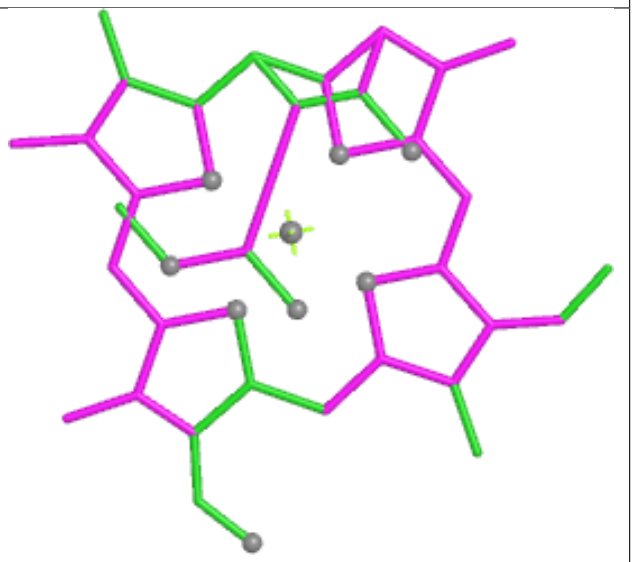


Rings

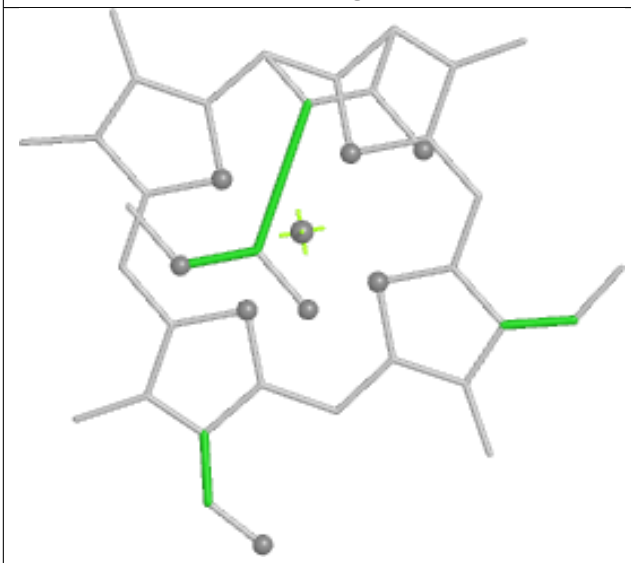
Ligand CL7 7 515



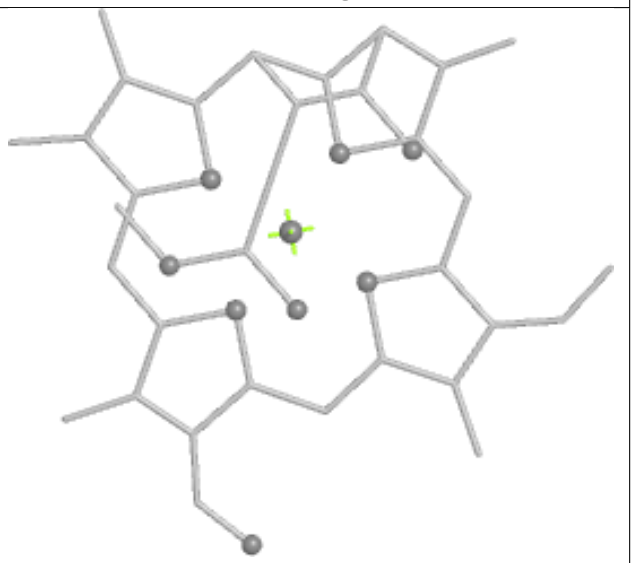
Bond lengths



Bond angles

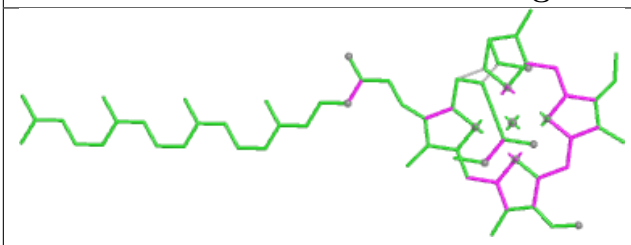


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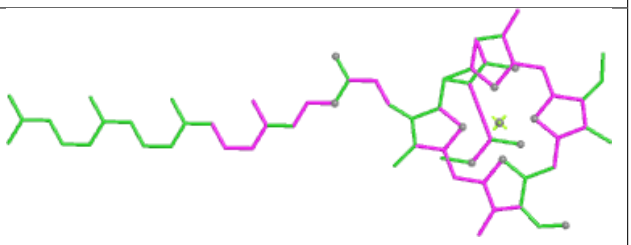


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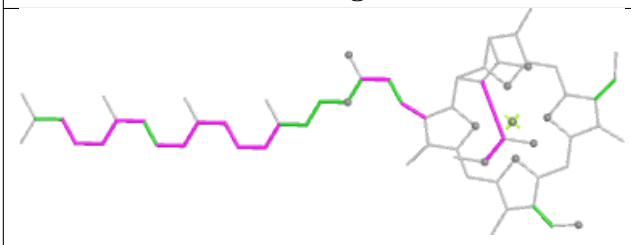
Ligand CL7 6 510



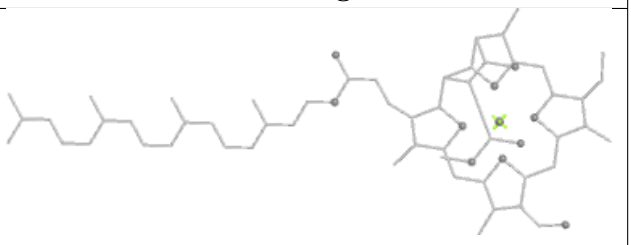
Bond lengths



Bond angles

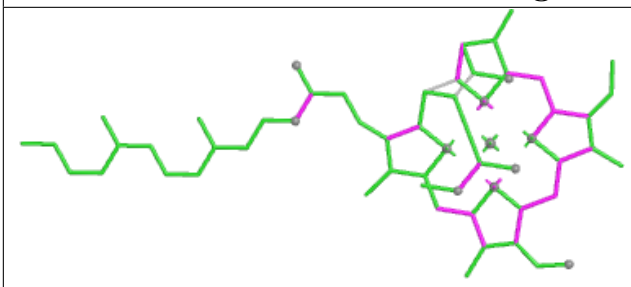


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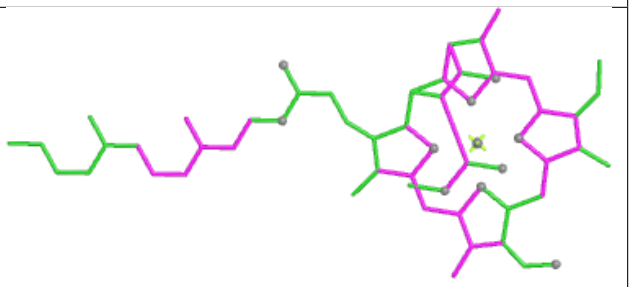


Rings

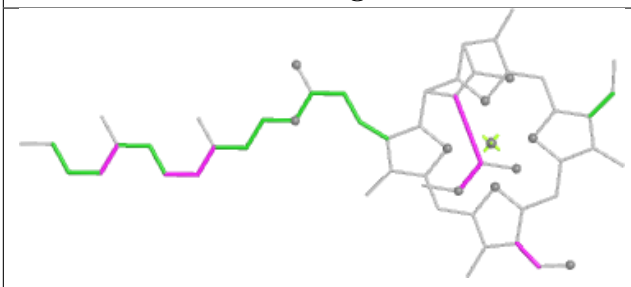
Ligand CL7 3 502



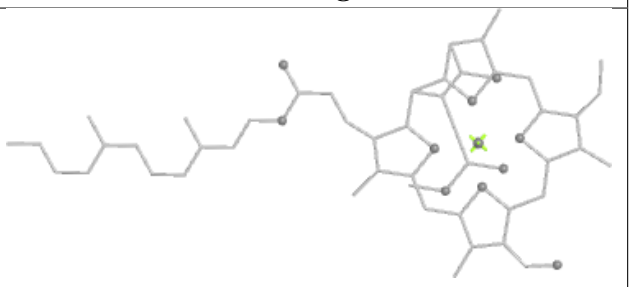
Bond lengths



Bond angles

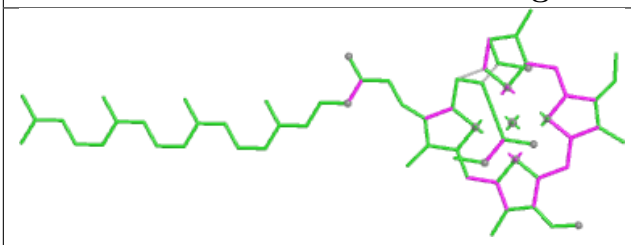


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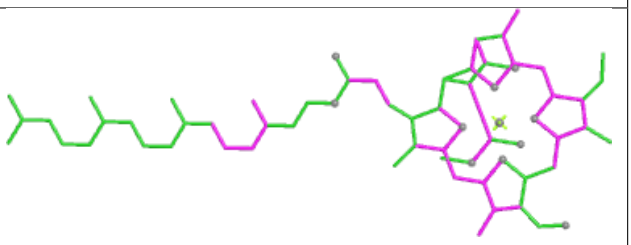


Rings

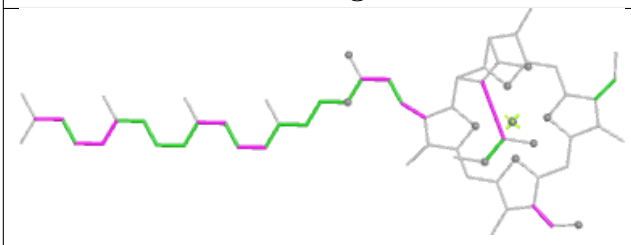
Ligand CL7 b 610



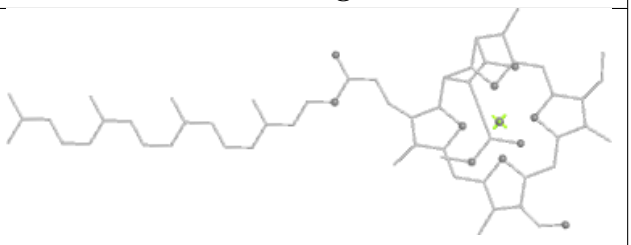
Bond lengths



Bond angles

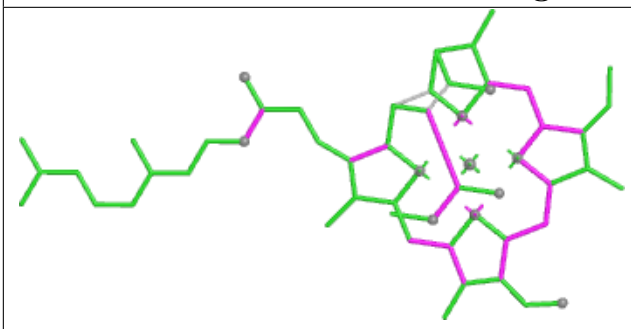


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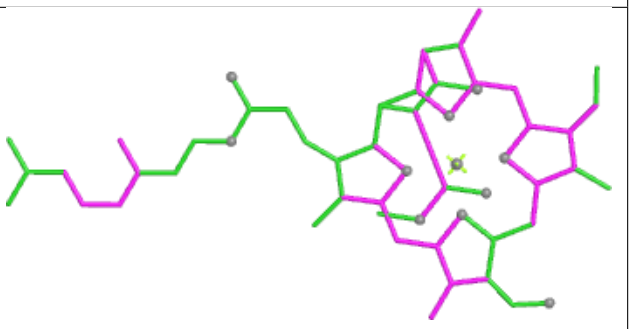


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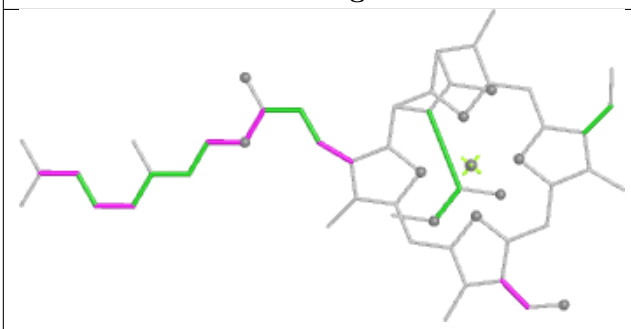
Ligand CL7 1 417



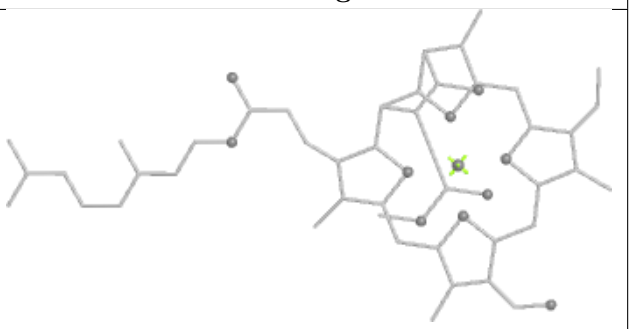
Bond lengths



Bond angles

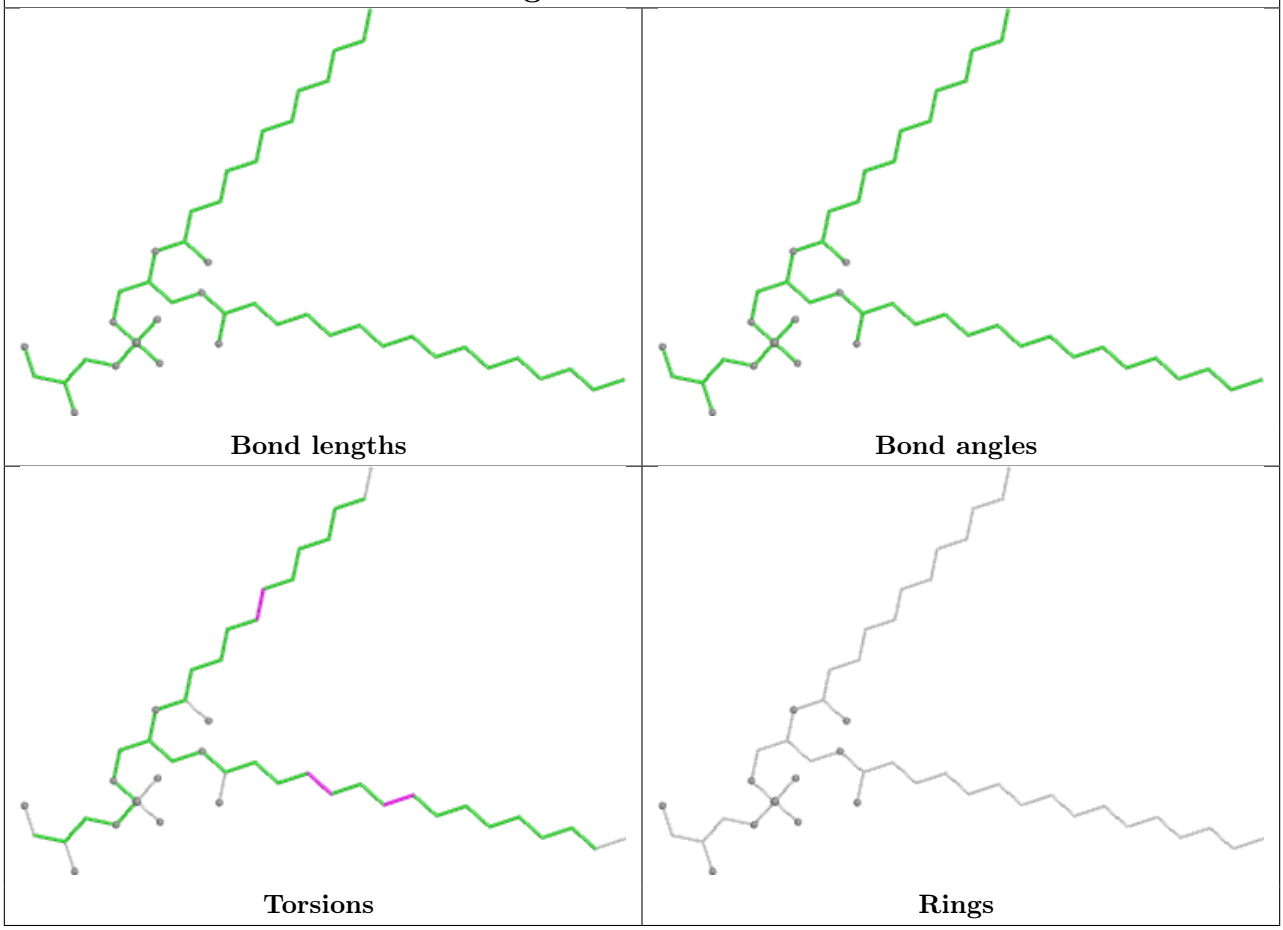


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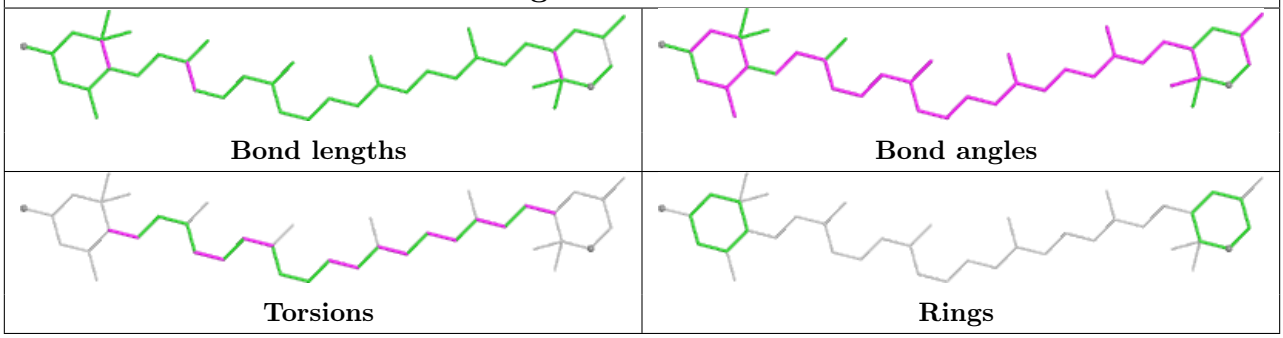


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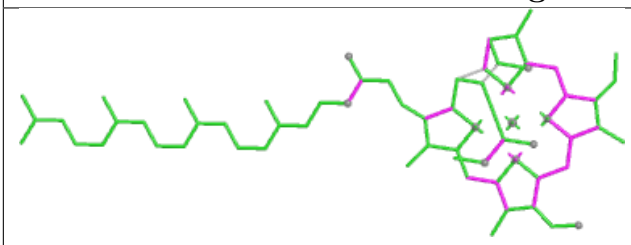
Ligand LHG B 623



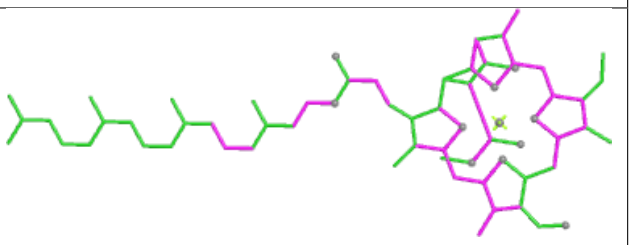
Ligand ZEX 4 420



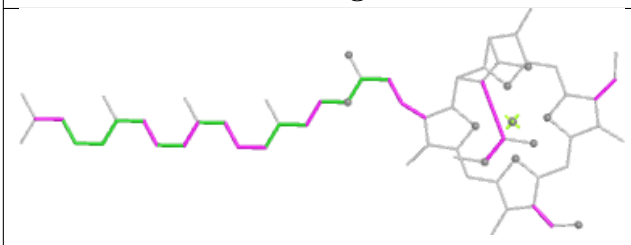
Ligand CL7 A 406



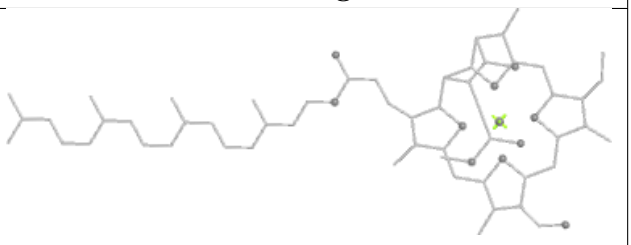
Bond lengths



Bond angles

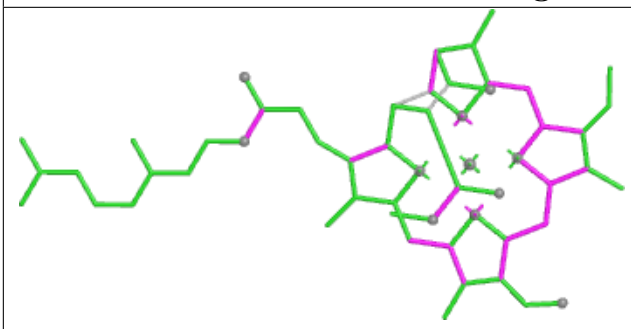


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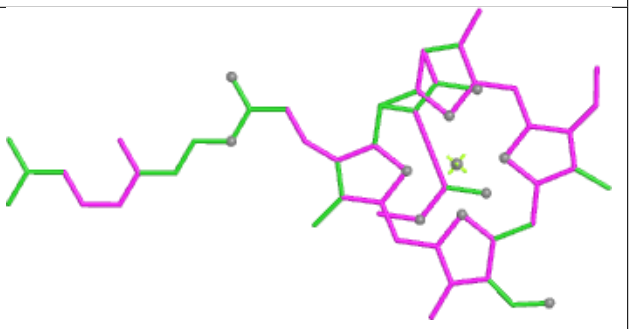


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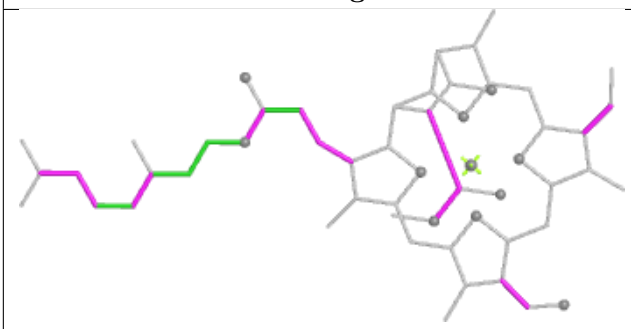
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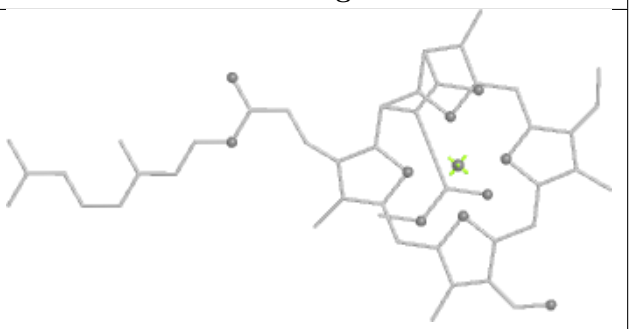
Bond lengths



Bond angles

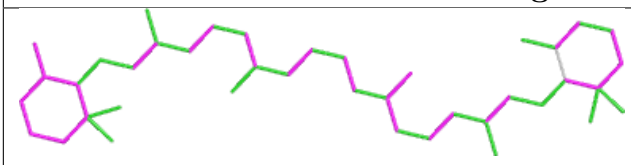


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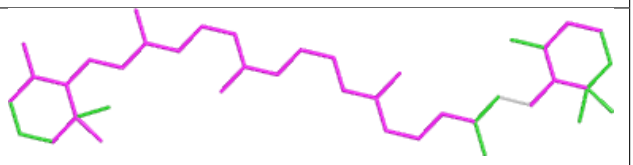


Rings

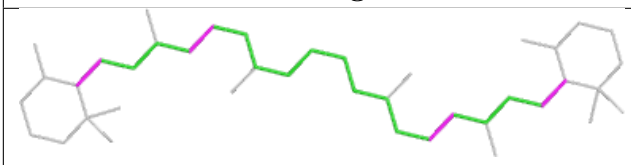
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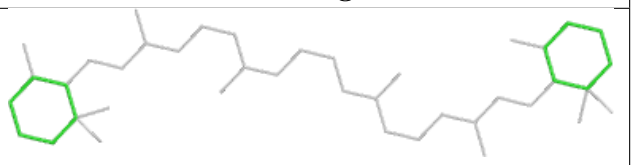
Bond lengths



Bond angles

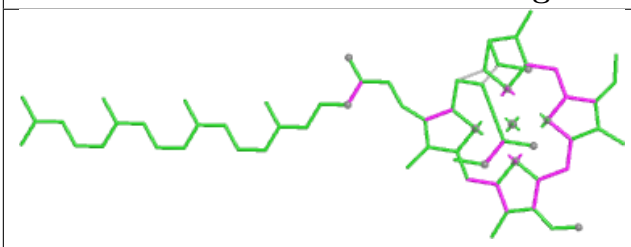


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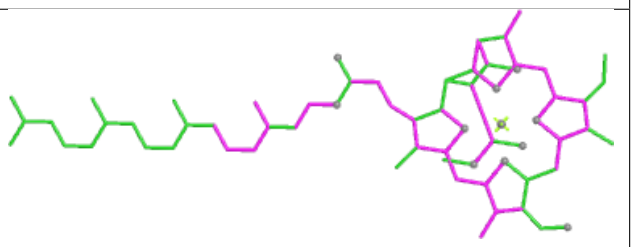


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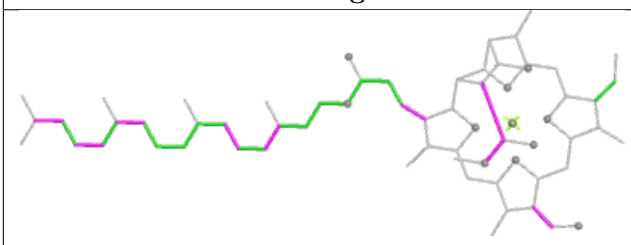
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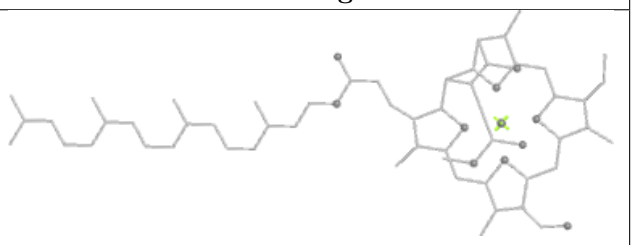
Bond lengths



Bond angles

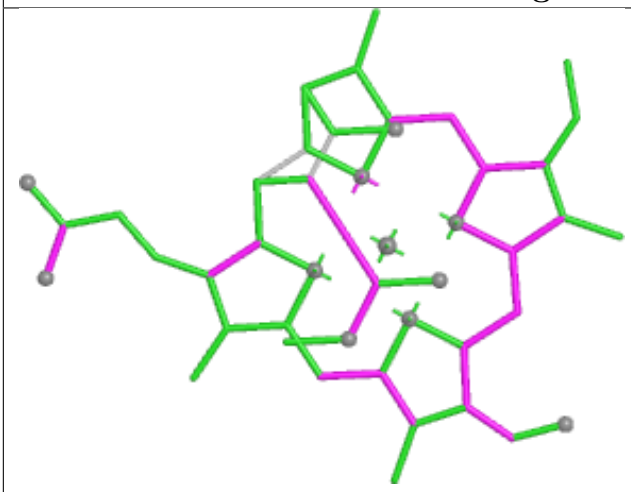


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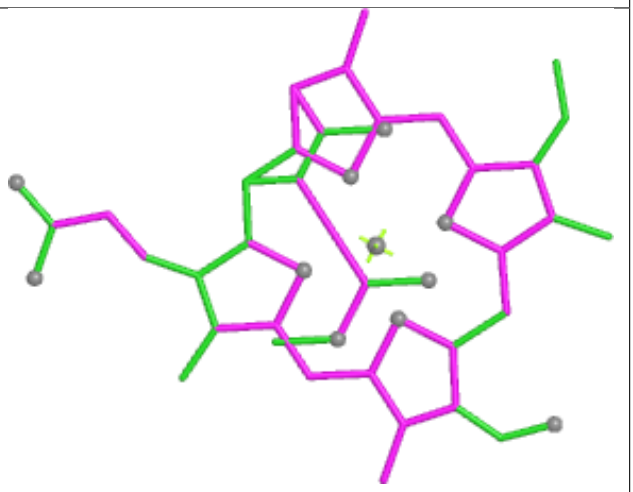


Rings

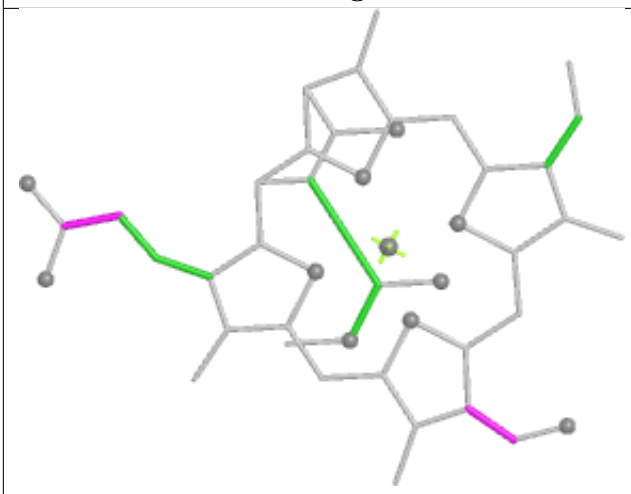
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Bond lengths



Bond angles



Torsions

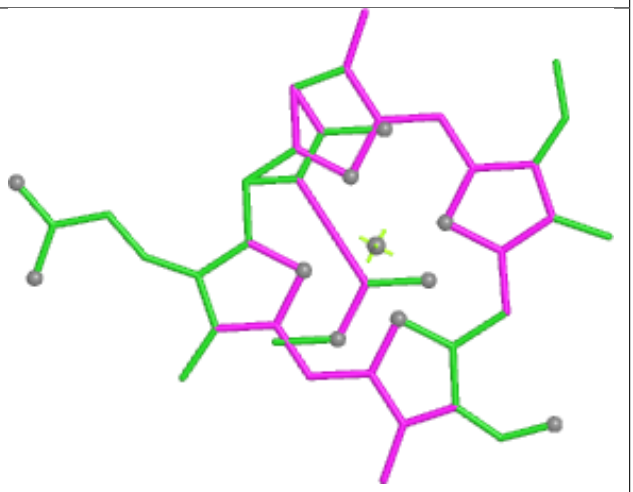


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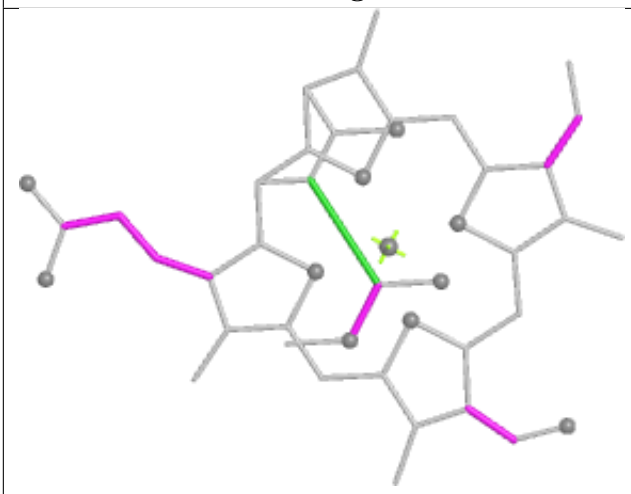
Ligand CL7 5 419



Bond lengths



Bond angles

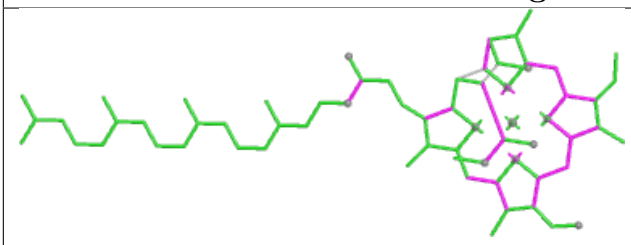


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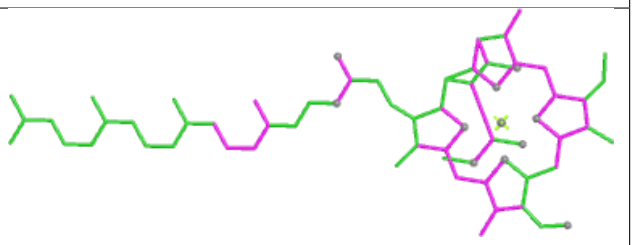


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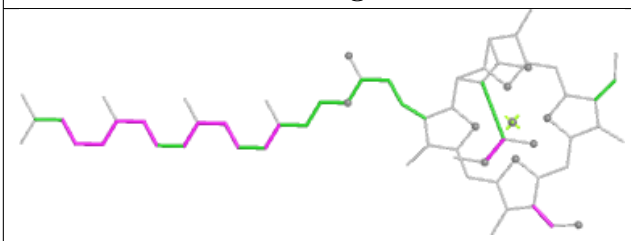
Ligand CL7 B 611



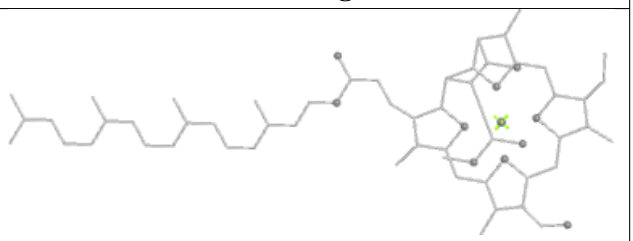
Bond lengths



Bond angles

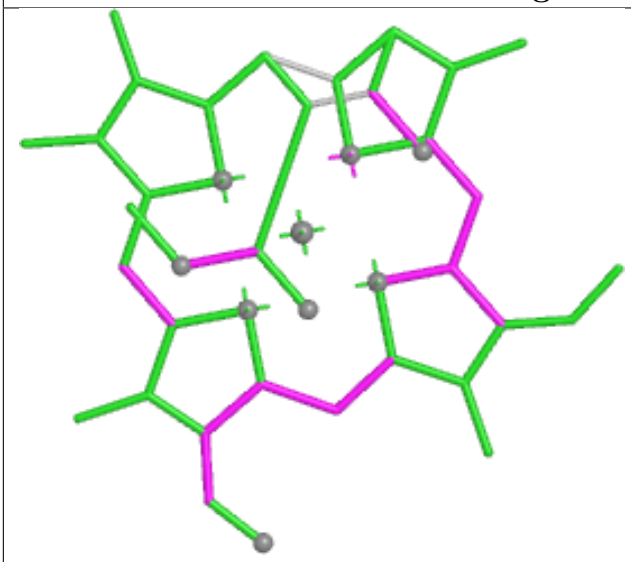


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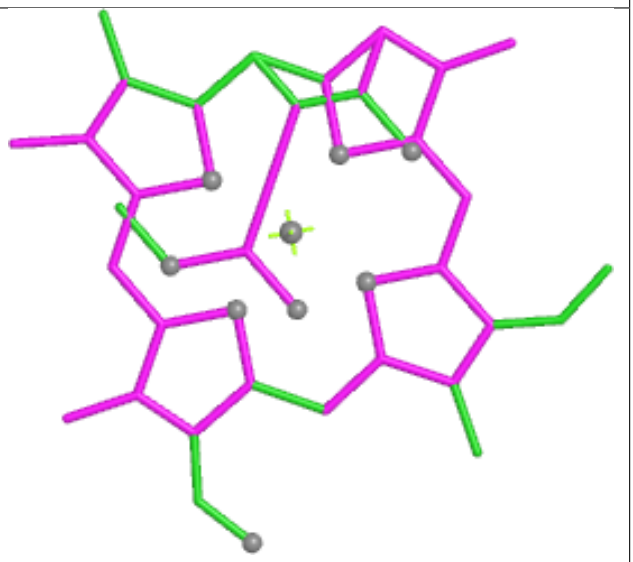


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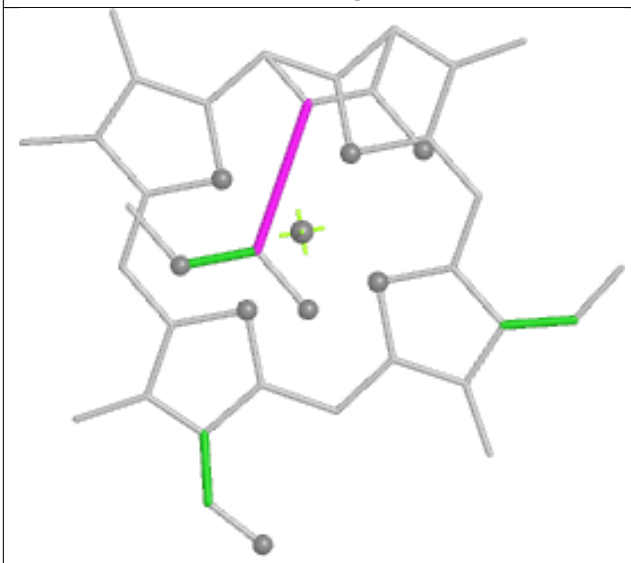
Ligand CL7 1 413



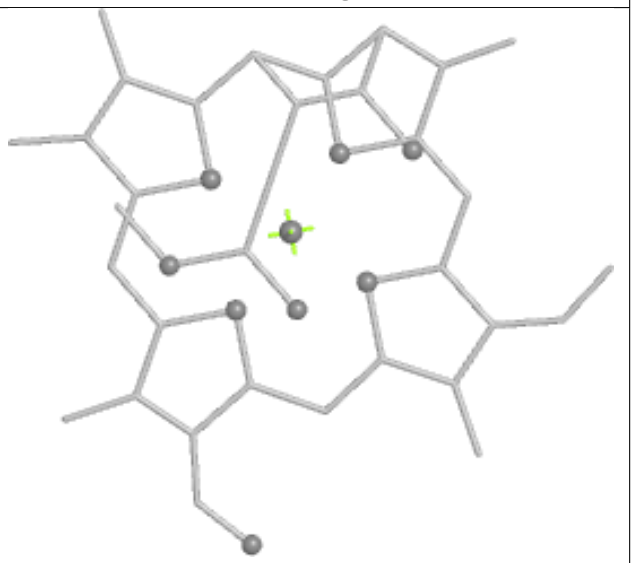
Bond lengths



Bond angles

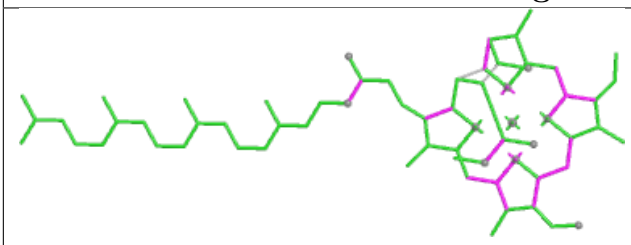


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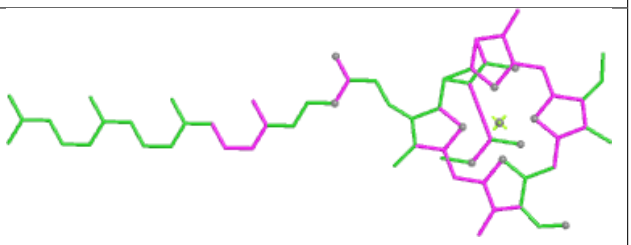


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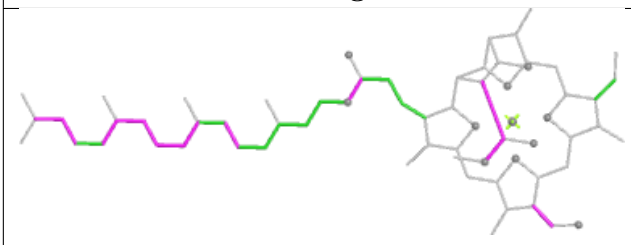
Ligand CL7 7 509



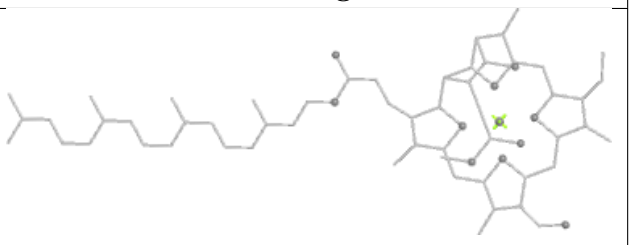
Bond lengths



Bond angles

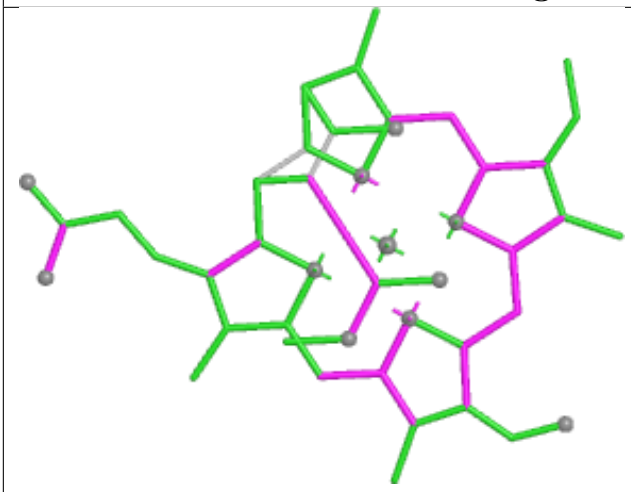


Torsions



Rings

Ligand CL7 7 513



Bond lengths



Bond angles

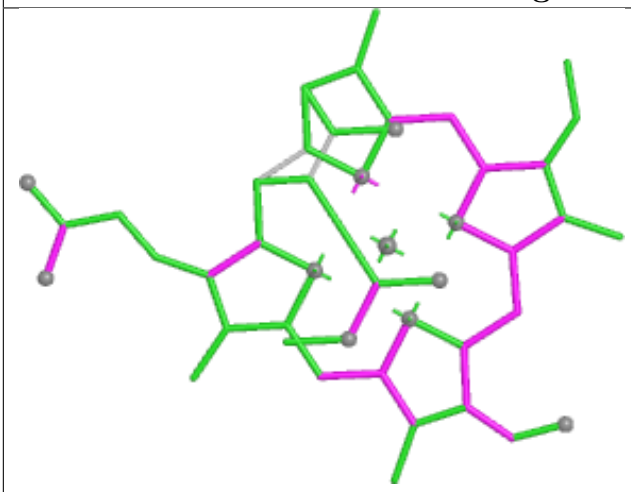


Torsions

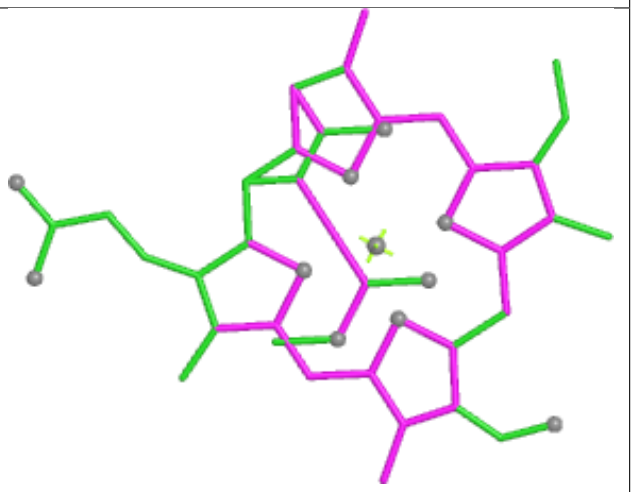


Rings

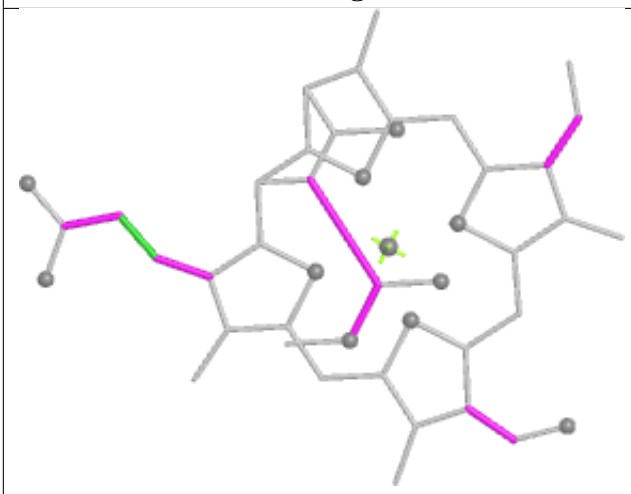
Ligand CL7 7 506



Bond lengths



Bond angles

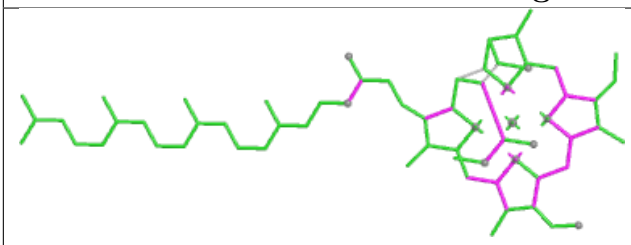


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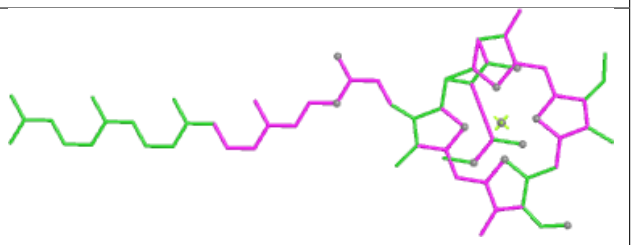


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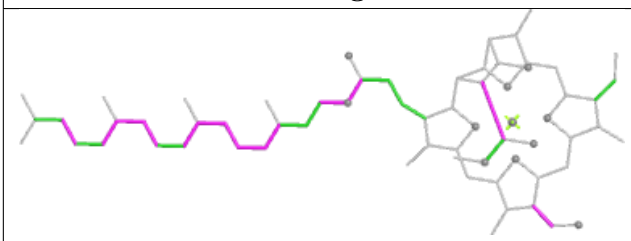
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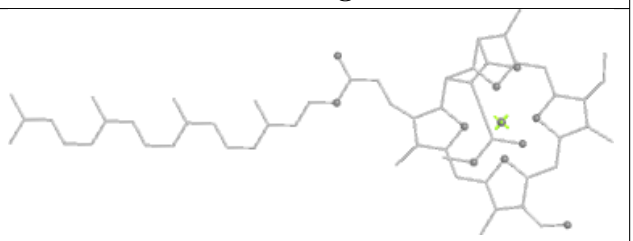
Bond lengths



Bond angles

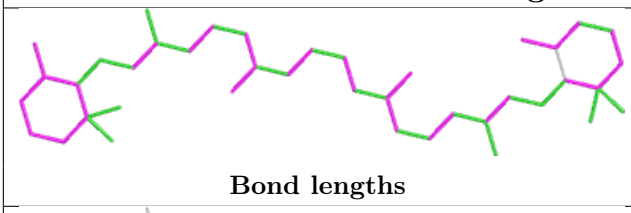


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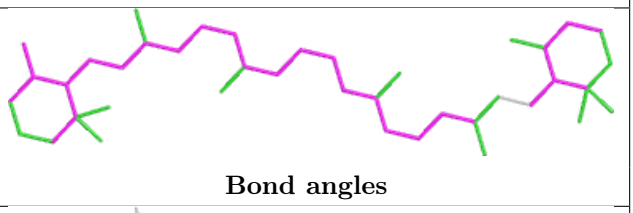


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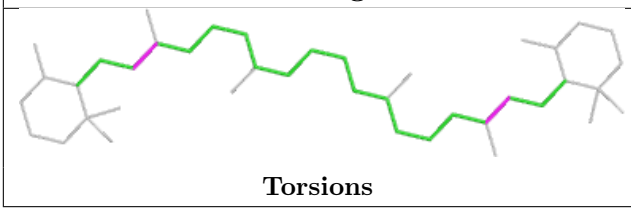
Ligand 8CT B 619



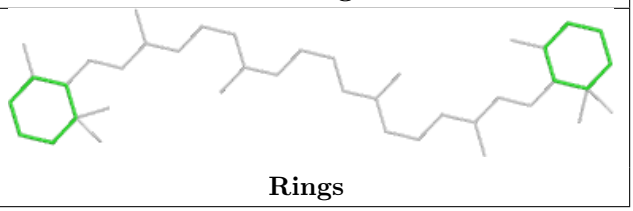
Bond lengths



Bond angles

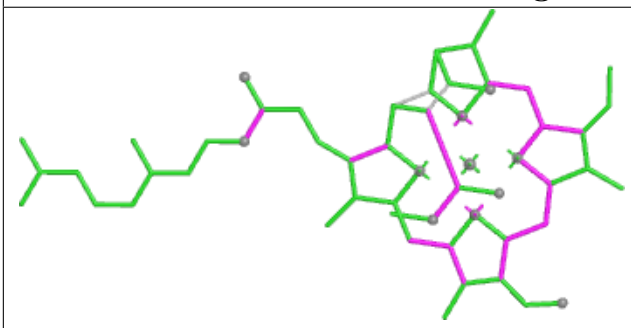


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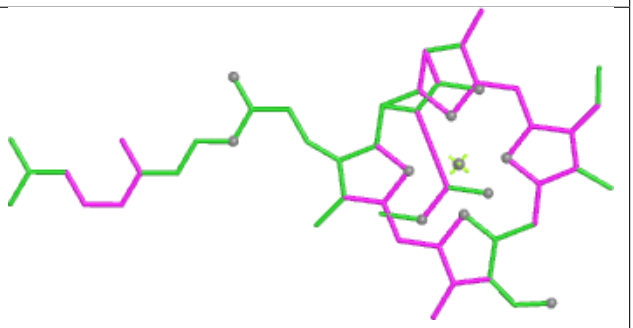


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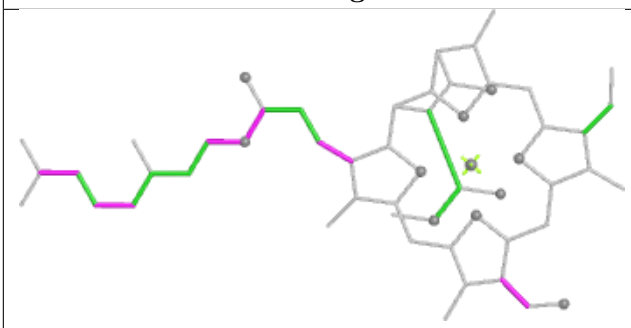
Ligand CL7 5 417



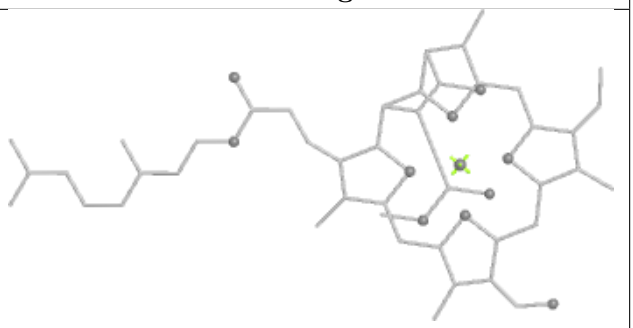
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Bond angles

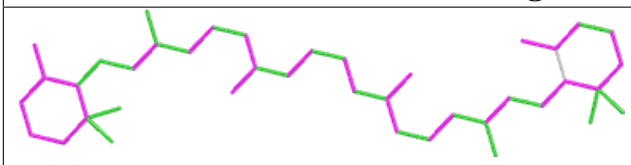


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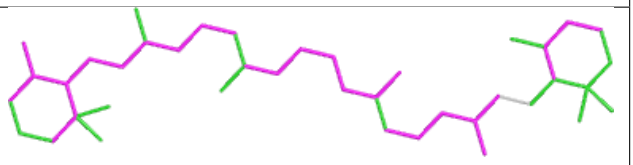


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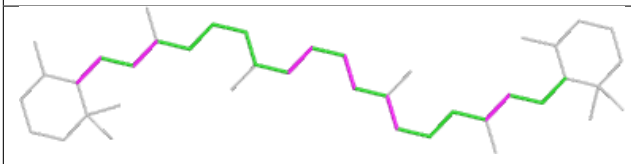
Ligand 8CT D 406



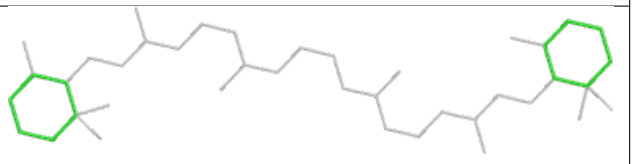
Bond lengths



Bond angles

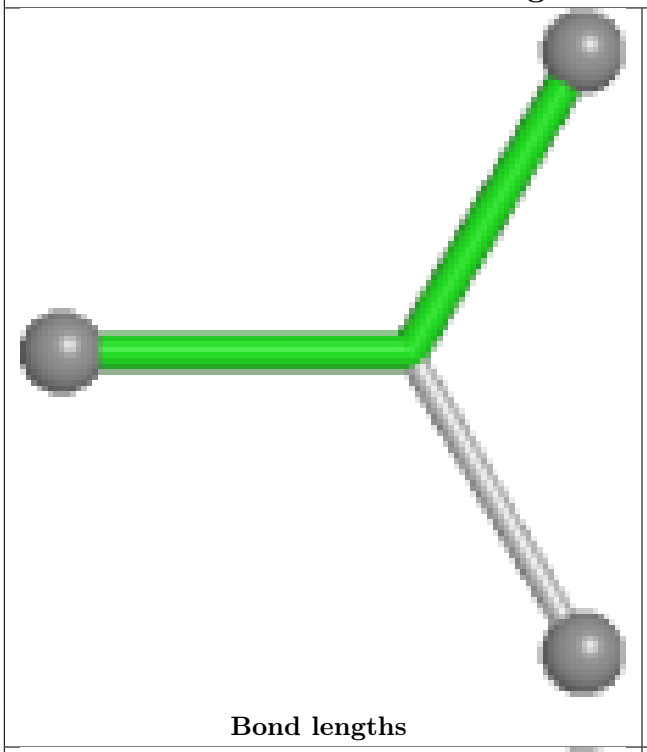


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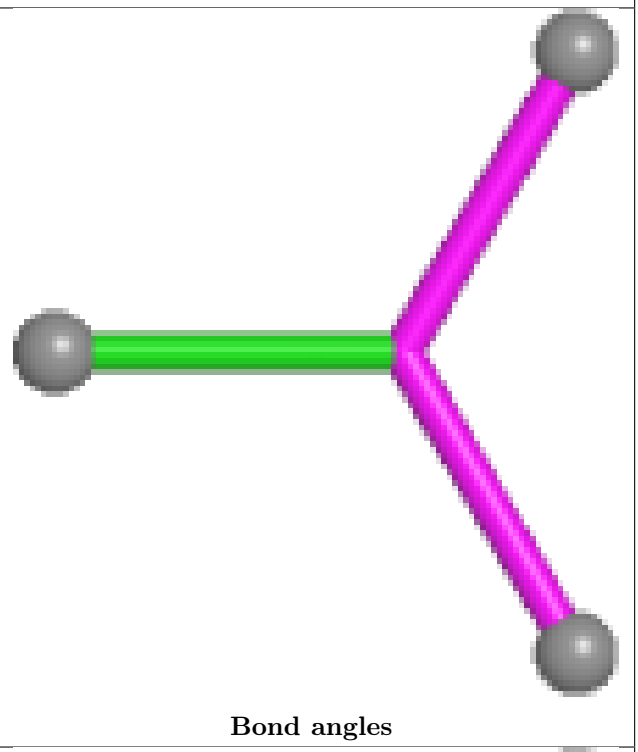


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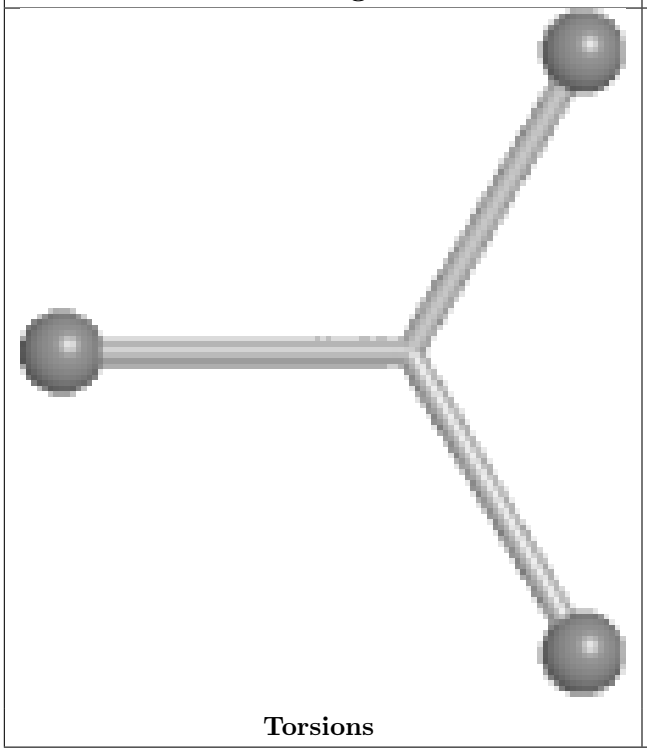
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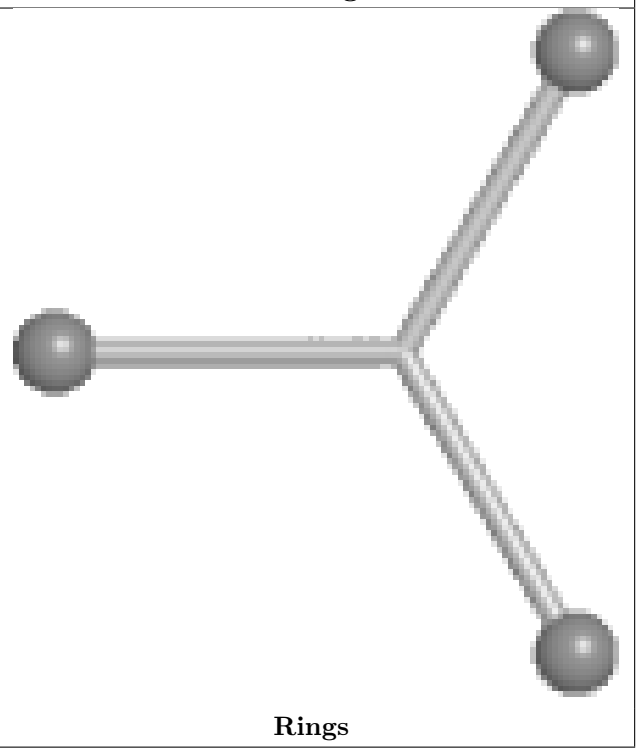
Bond lengths



Bond angles

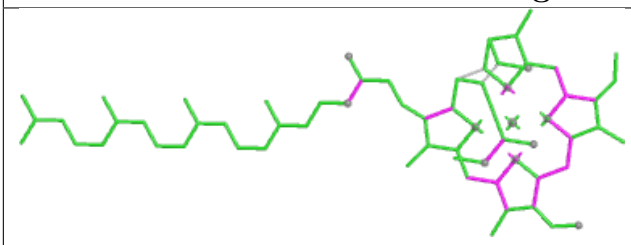


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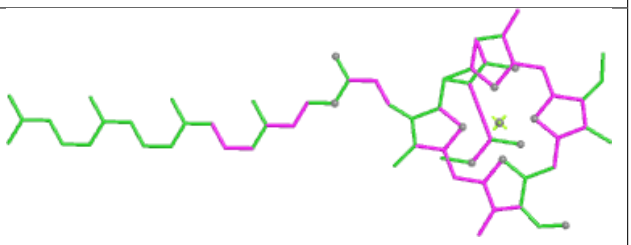


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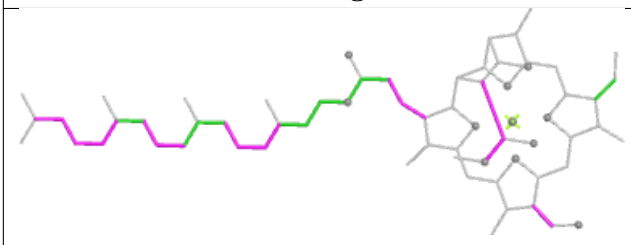
Ligand CL7 2 517



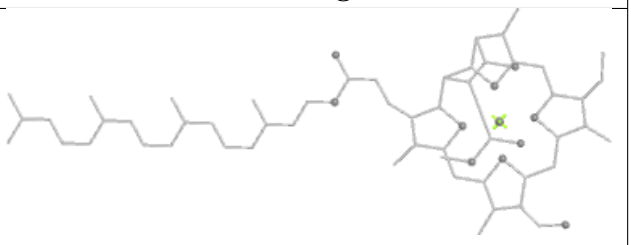
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Bond angles

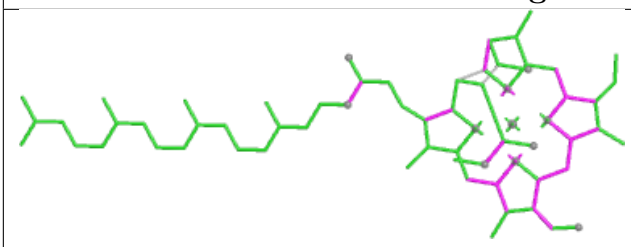


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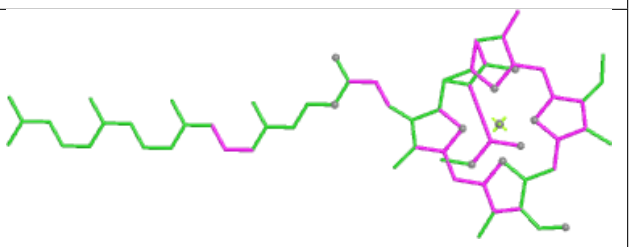


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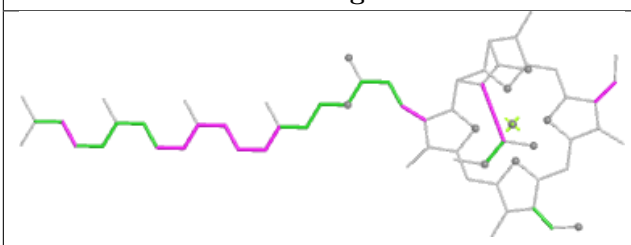
Ligand CL7 B 608



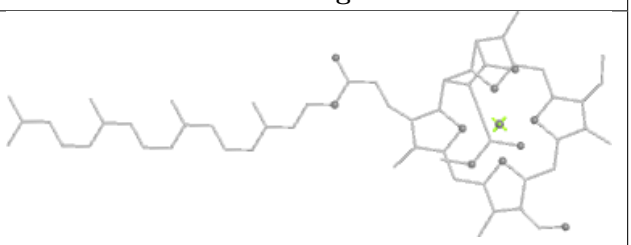
Bond lengths



Bond angles

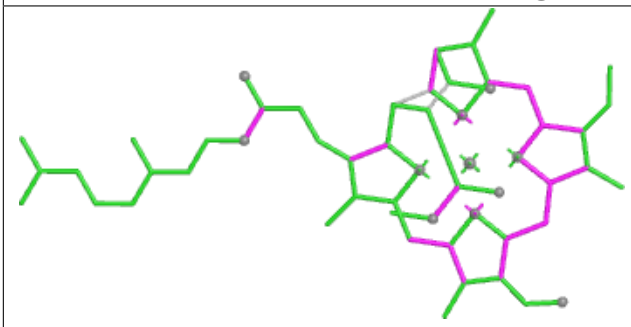


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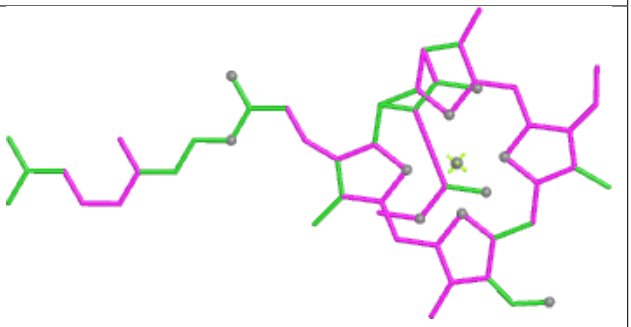


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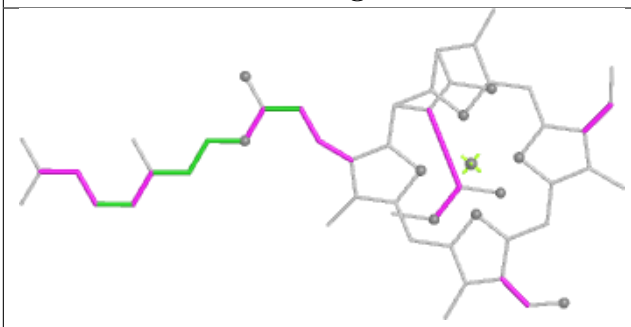
Ligand CL7 7 516



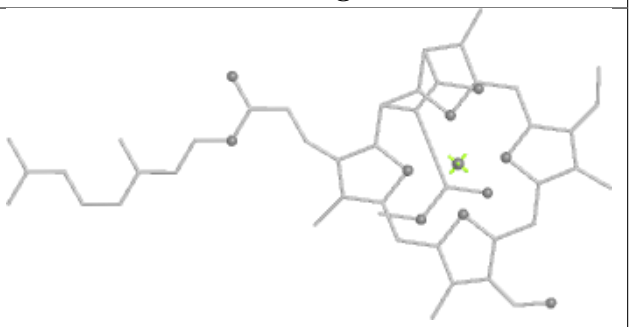
Bond lengths



Bond angles

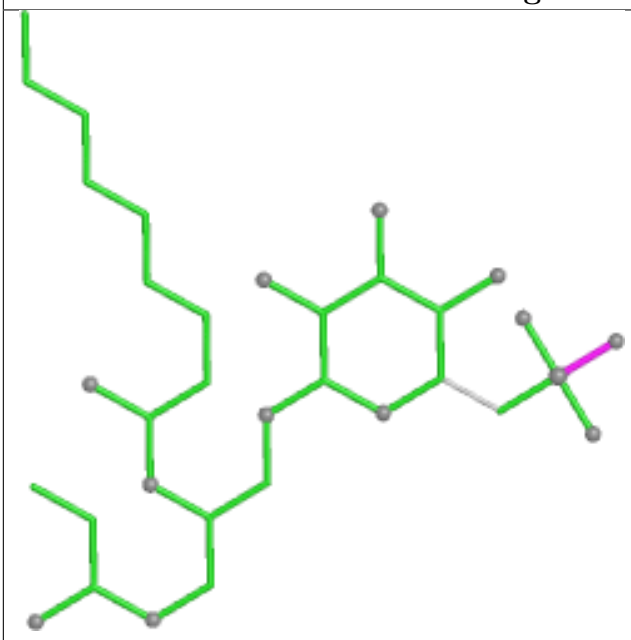


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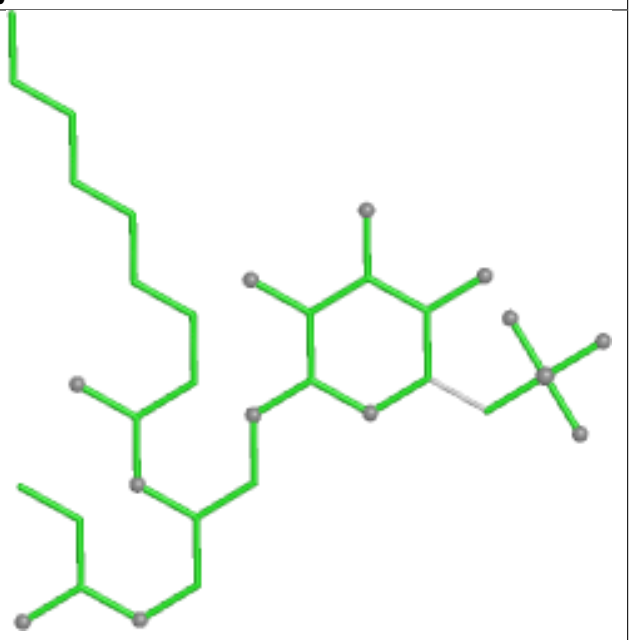


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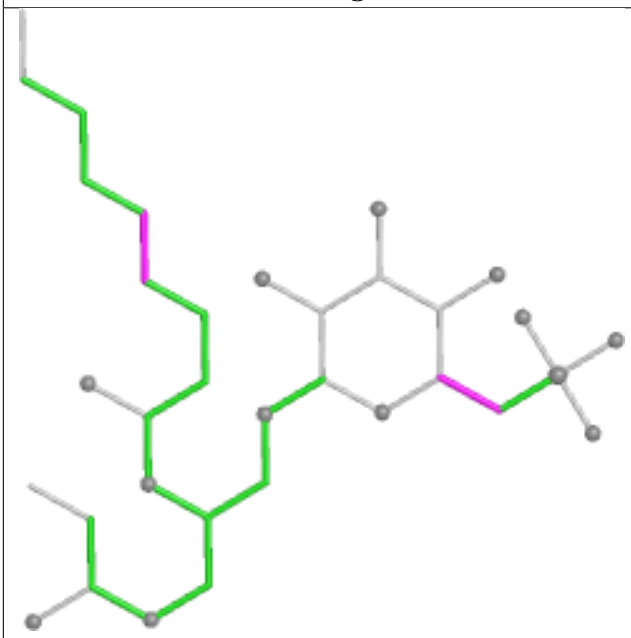
Ligand SQD A 405



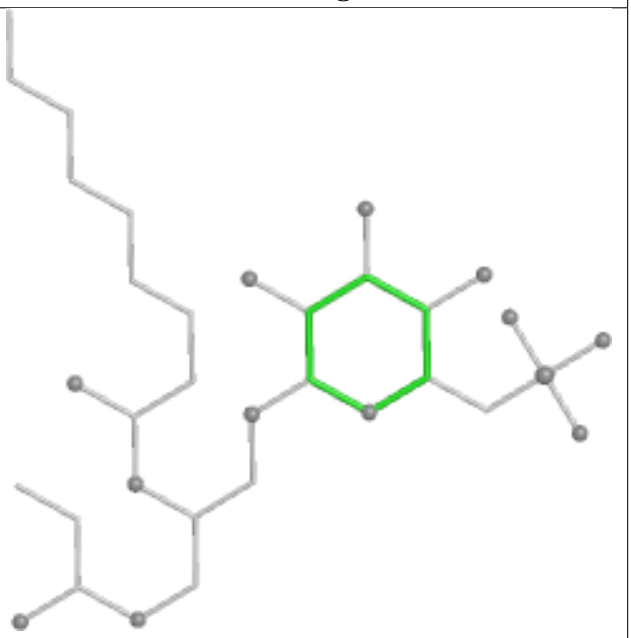
Bond lengths



Bond angles

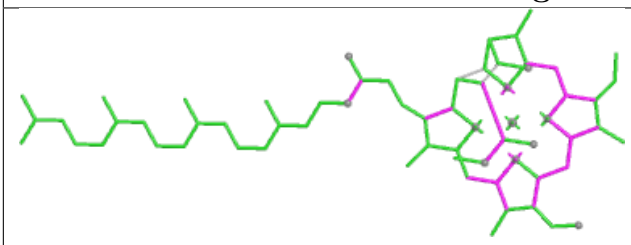


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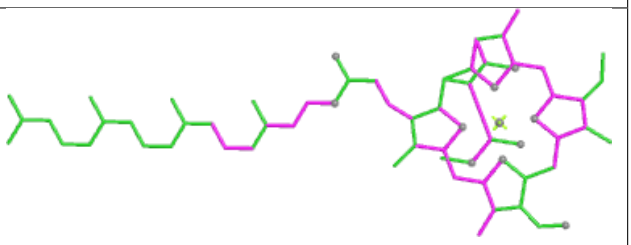


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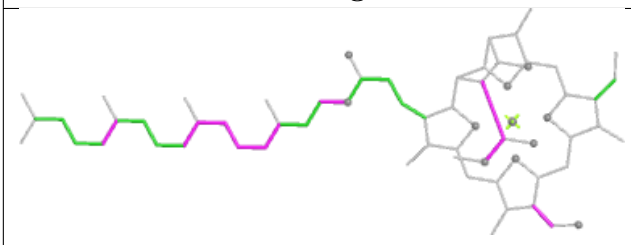
Ligand CL7 3 508



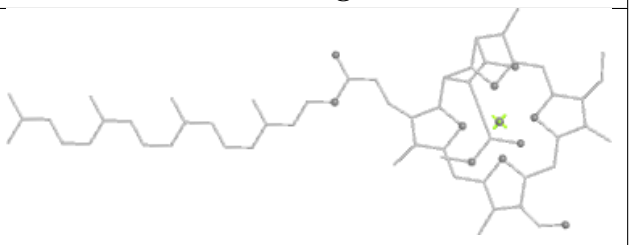
Bond lengths



Bond angles

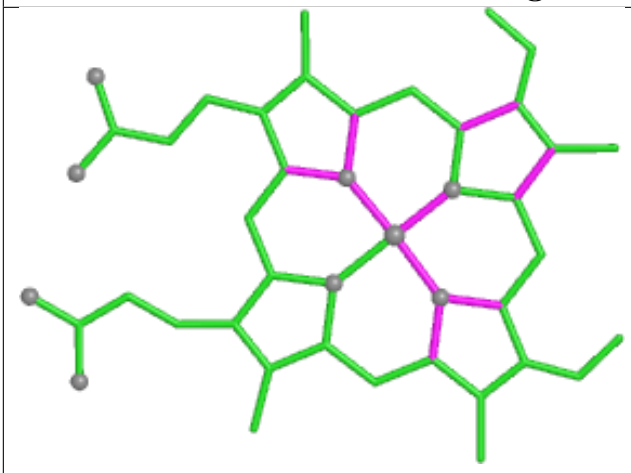


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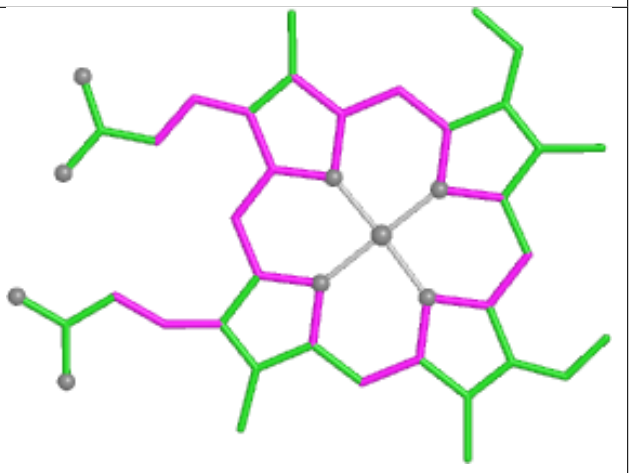


Rings

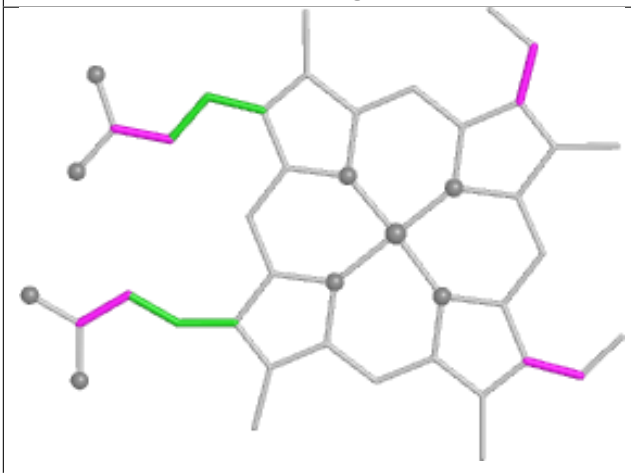
Ligand HEM f 101



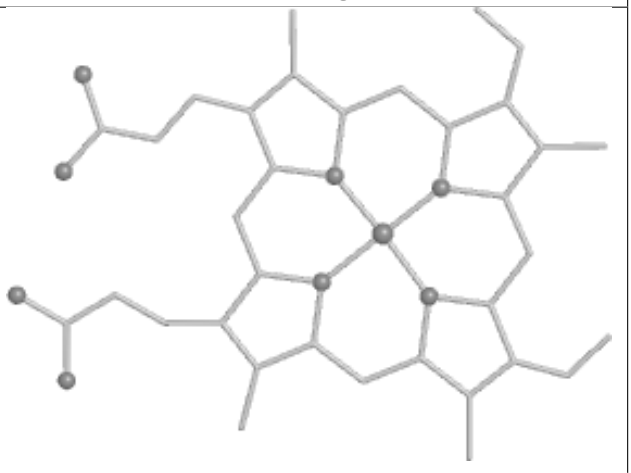
Bond lengths



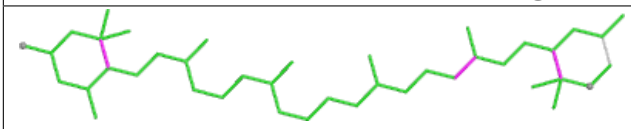
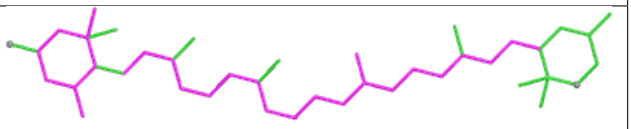
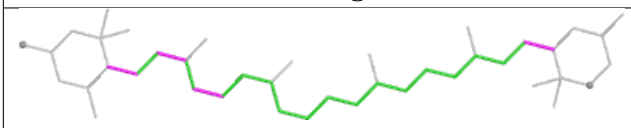
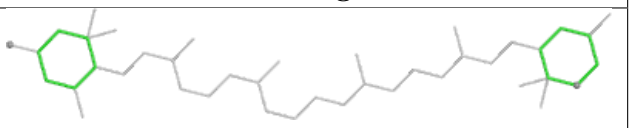
Bond angles

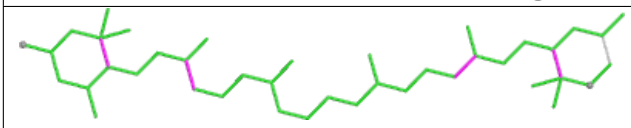
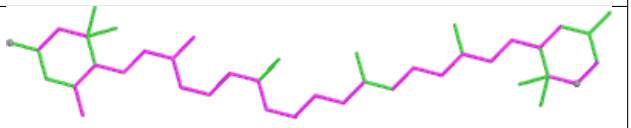
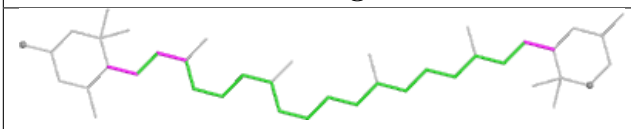
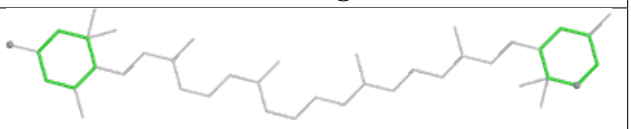


Torsions

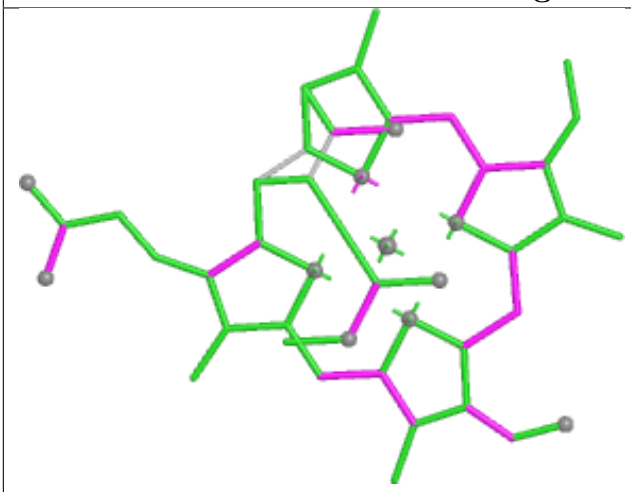


Rings

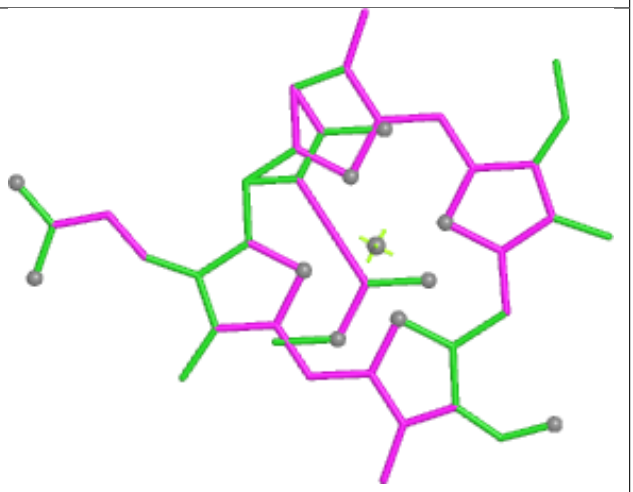
Ligand ZEX 6 520	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ZEX 7 522	
 Bond lengths	 Bond angles
 Torsions	 Rings

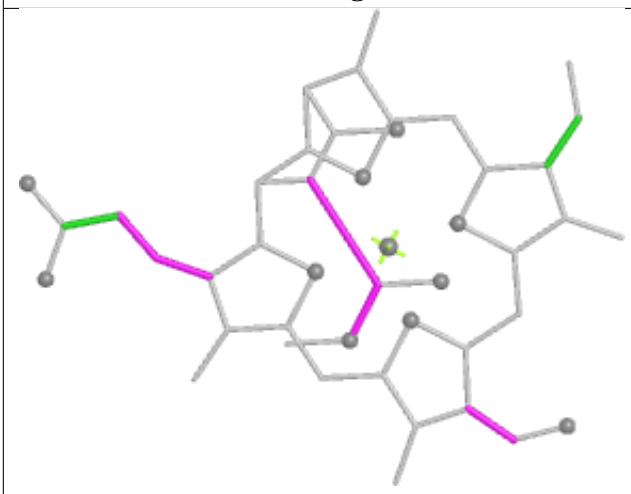
Ligand CL7 c 514



Bond lengths



Bond angles

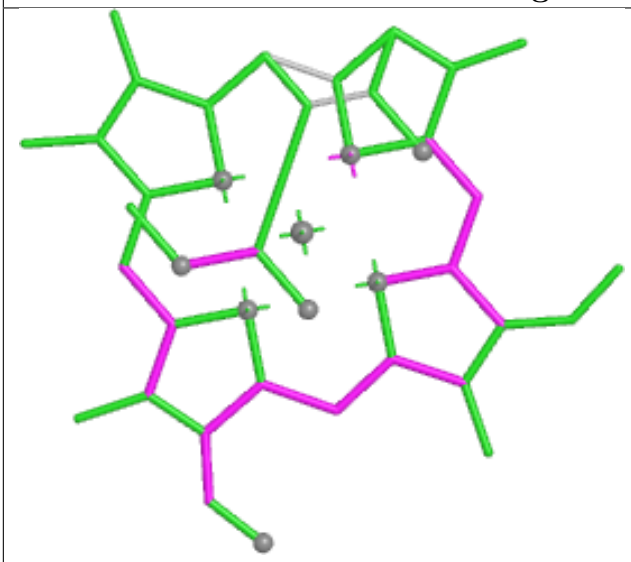


Torsions

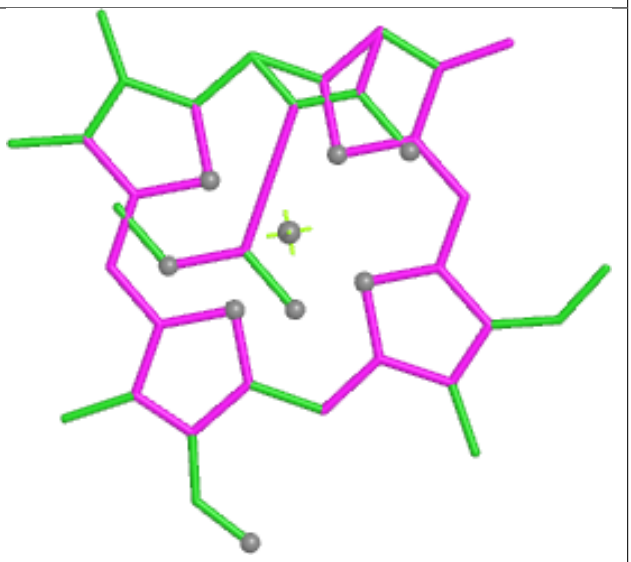


Rings

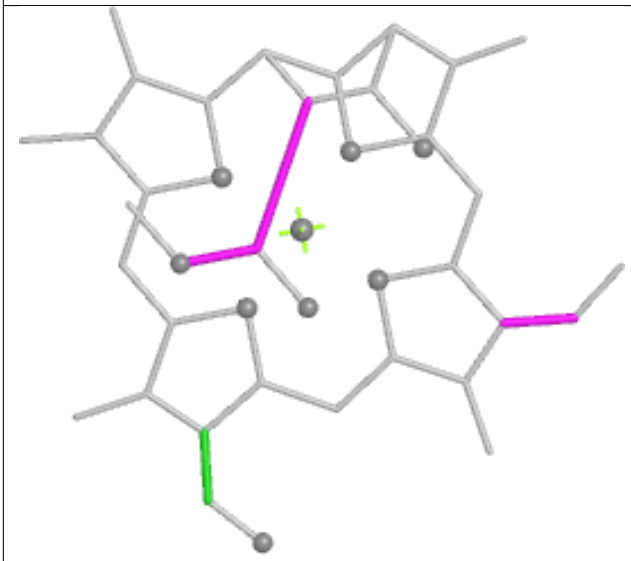
Ligand CL7 b 602



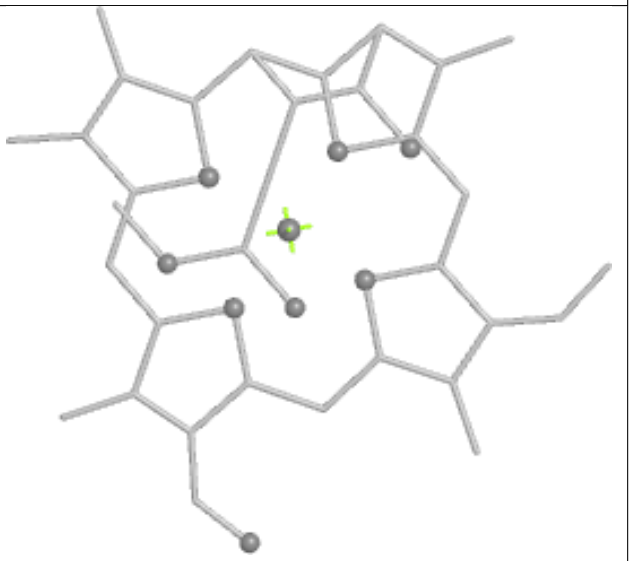
Bond lengths



Bond angles

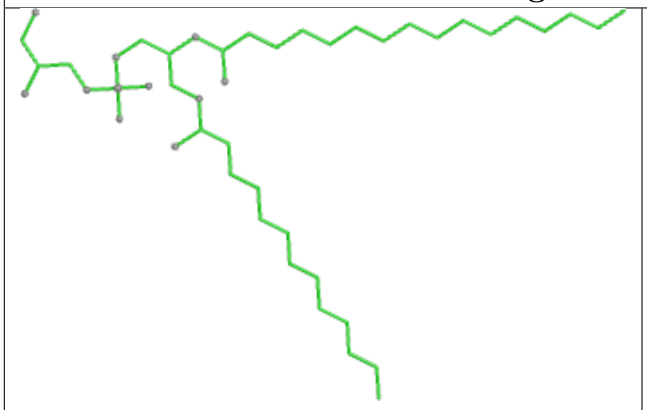


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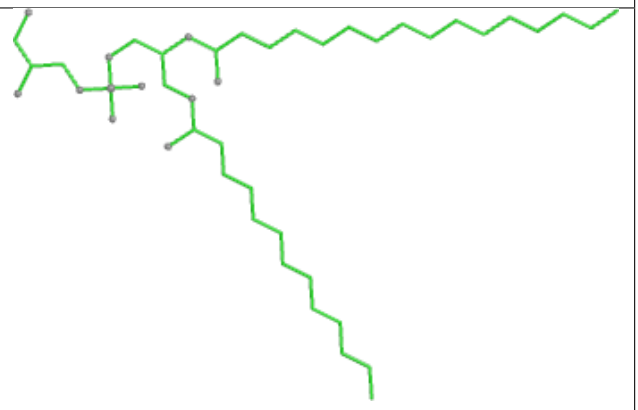


Rings

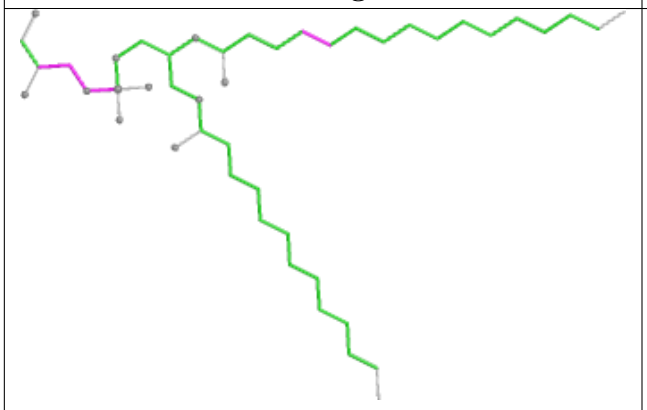
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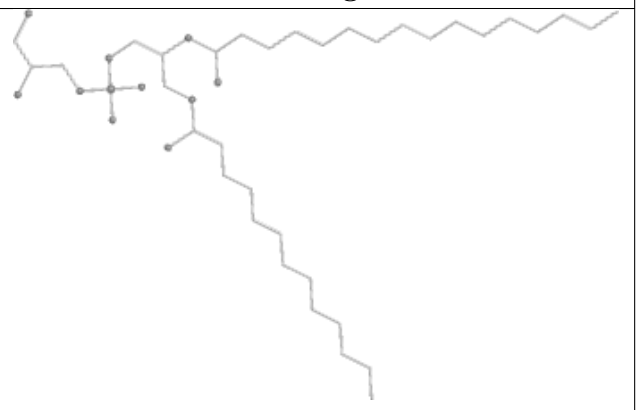
Bond lengths



Bond angles

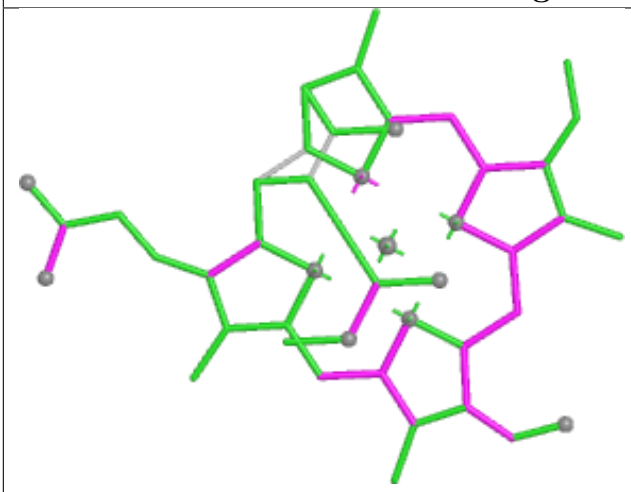


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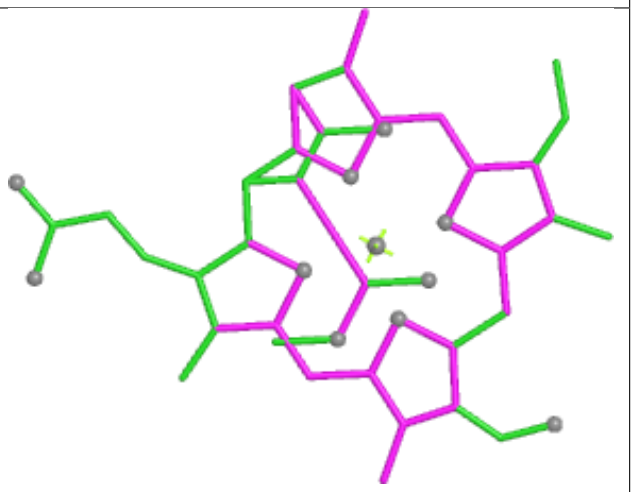


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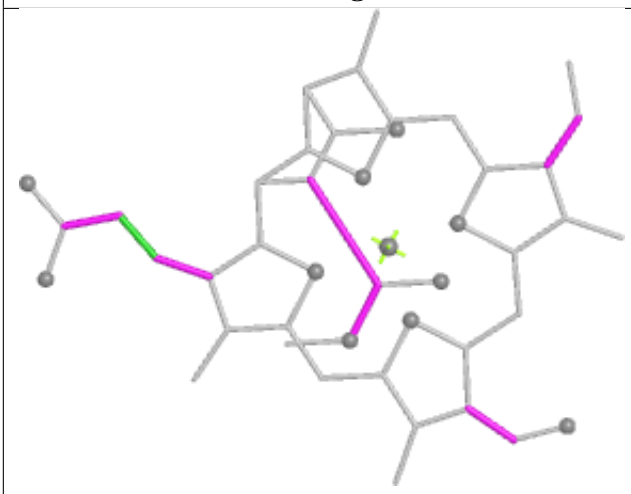
Ligand CL7 3 506



Bond lengths



Bond angles

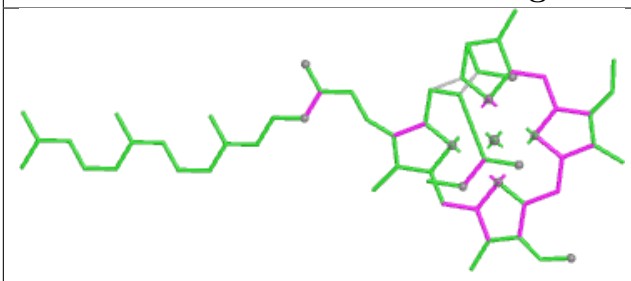


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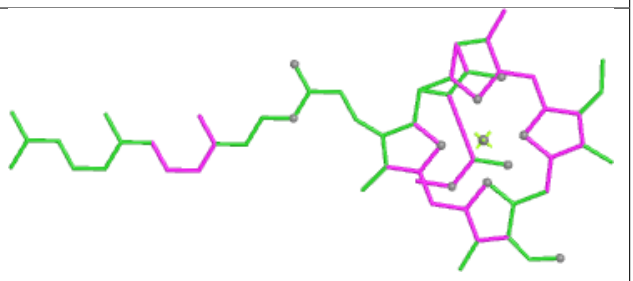


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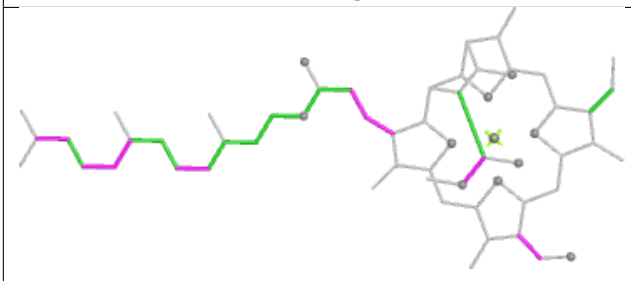
Ligand CL7 B 607



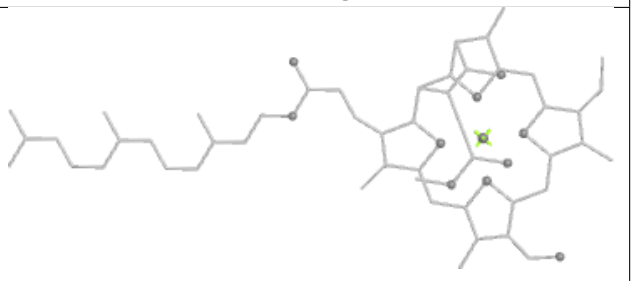
Bond lengths



Bond angles

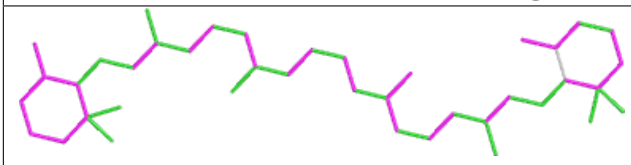


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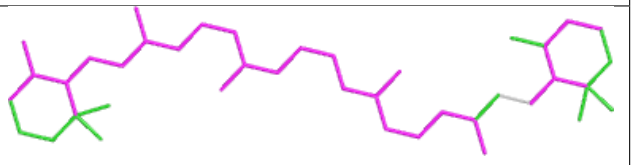


Rings

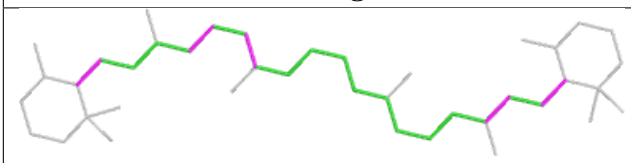
Ligand 8CT C 519



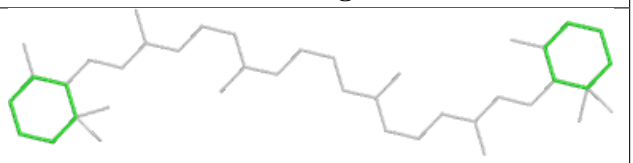
Bond lengths



Bond angles



Torsions

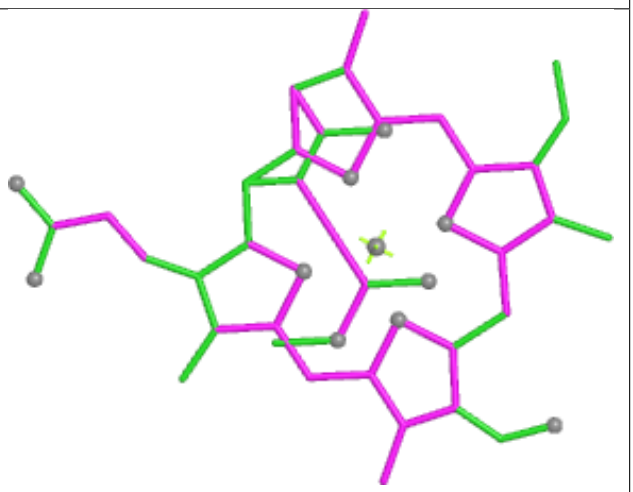


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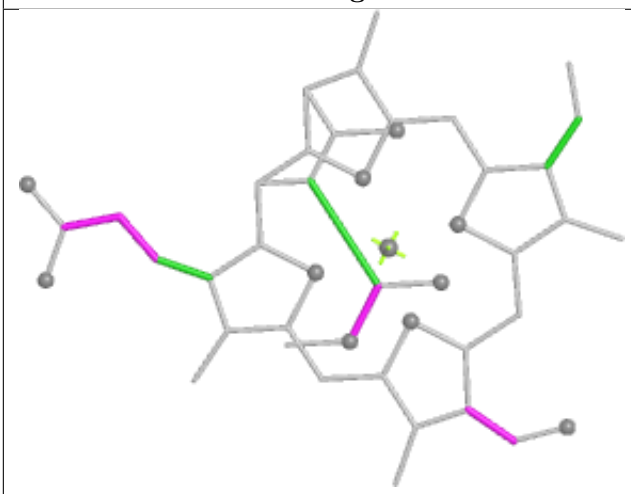
Ligand CL7 7 518



Bond lengths



Bond angles

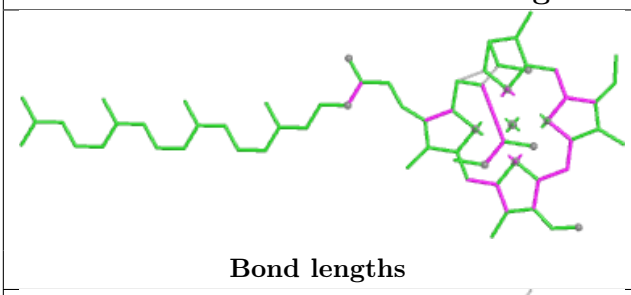


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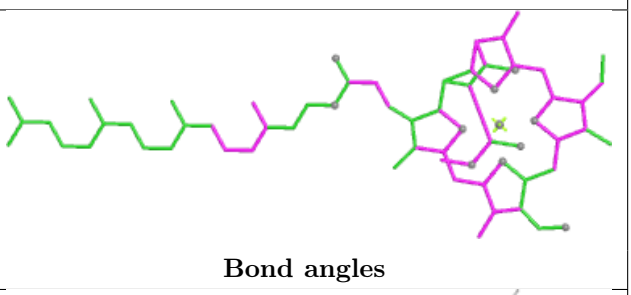


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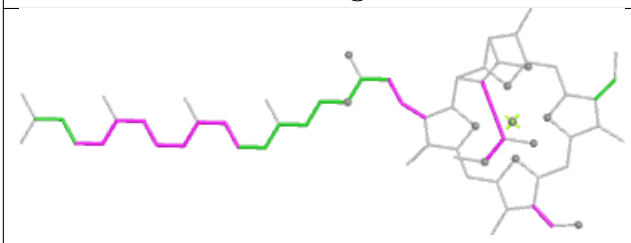
Ligand CL7 3 503



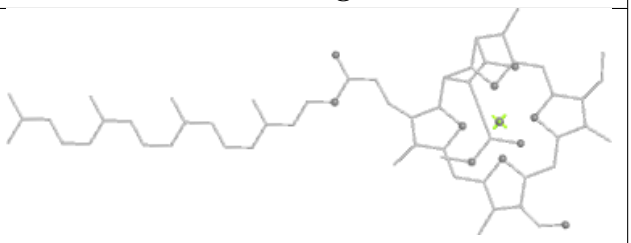
Bond lengths



Bond angles



Torsions



Rings

Ligand PL9 d 407



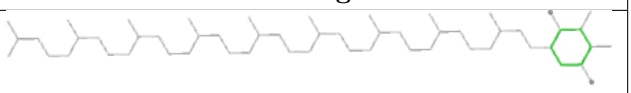
Bond lengths



Bond angles

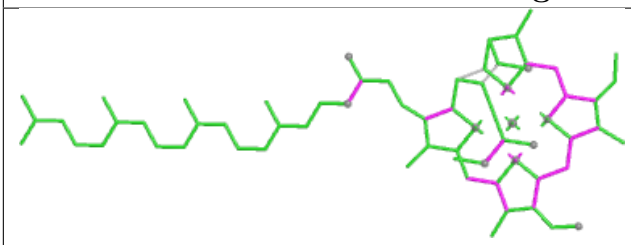


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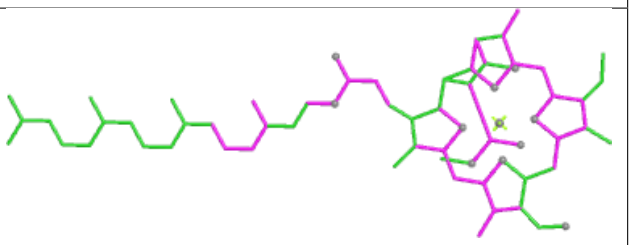


Rings

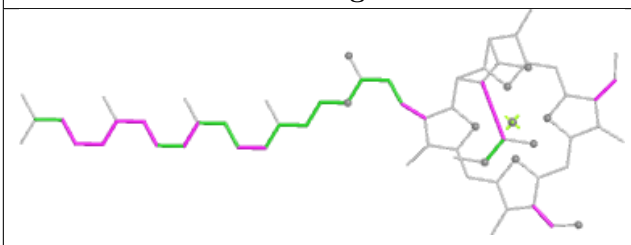
Ligand CL7 5 408



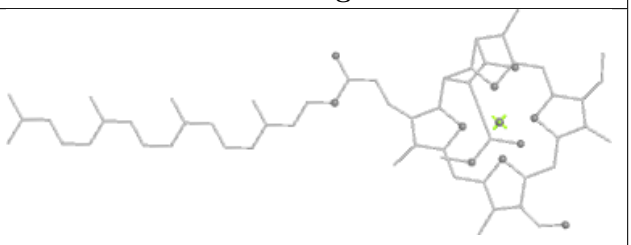
Bond lengths



Bond angles

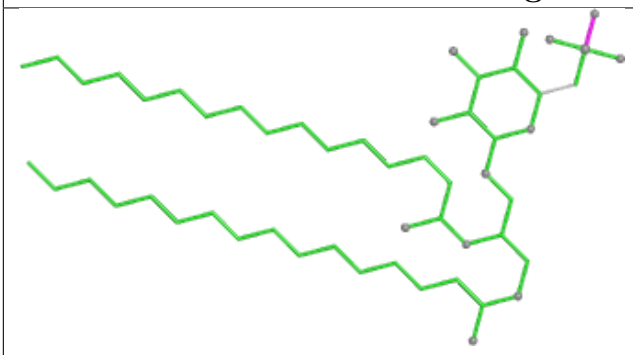


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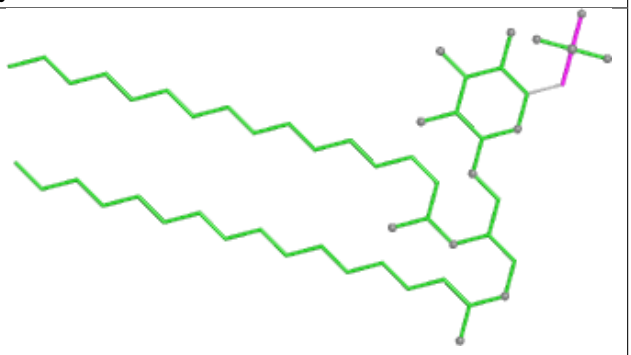


Rings

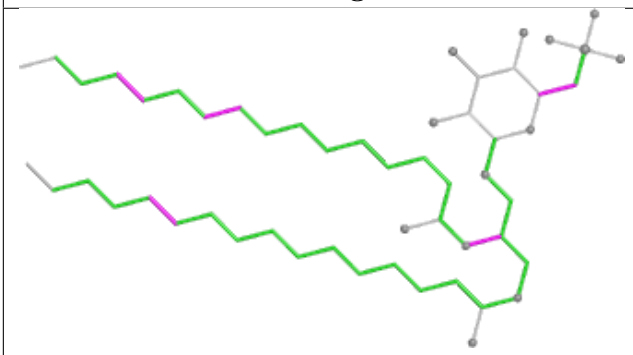
Ligand SQD B 620



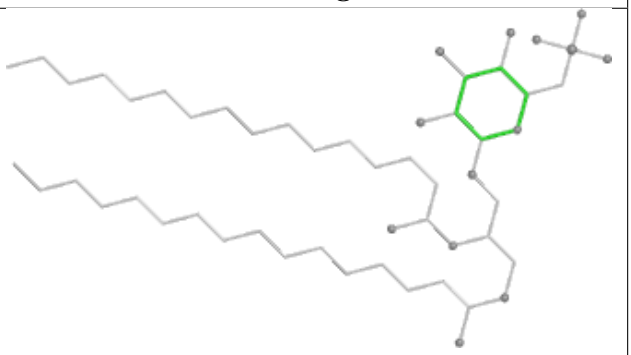
Bond lengths



Bond angles

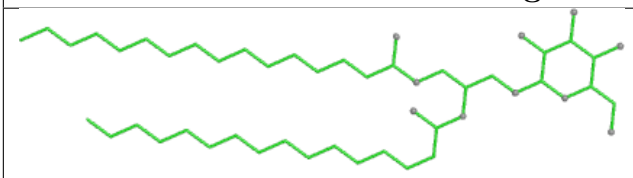


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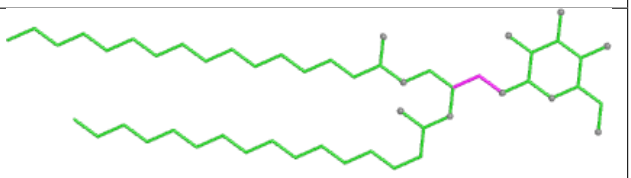


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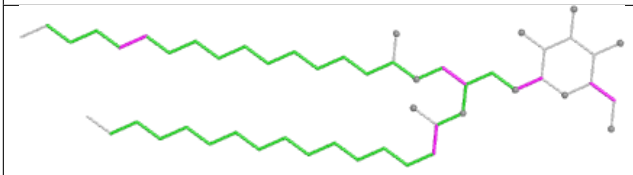
Ligand LMG 5 401



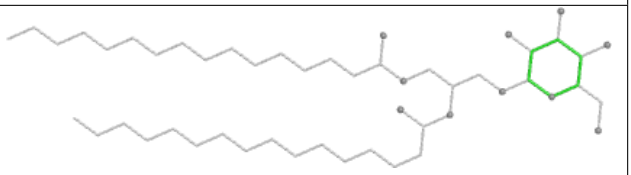
Bond lengths



Bond angles

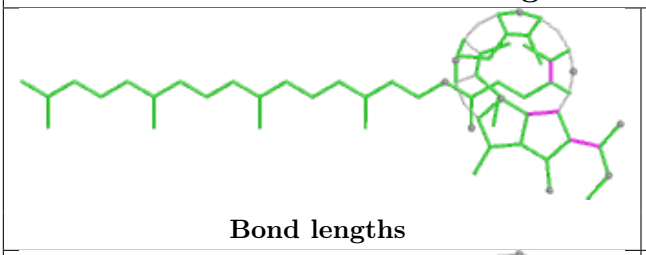


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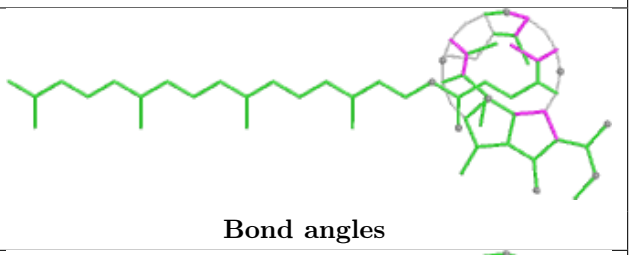


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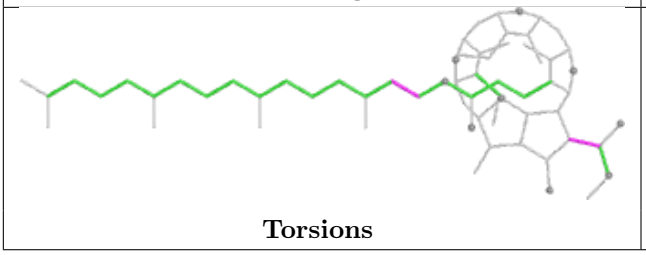
Ligand PHO A 402



Bond lengths



Bond angles

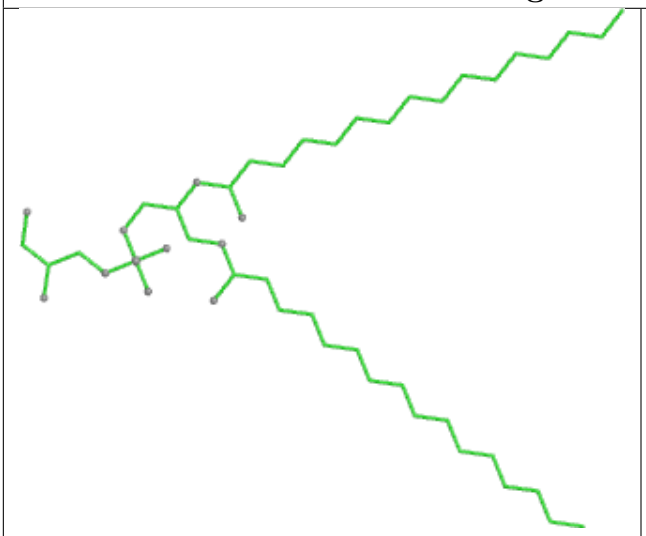


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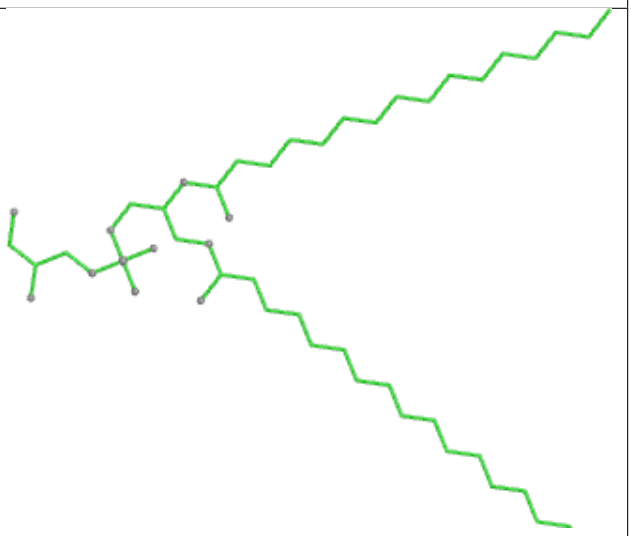


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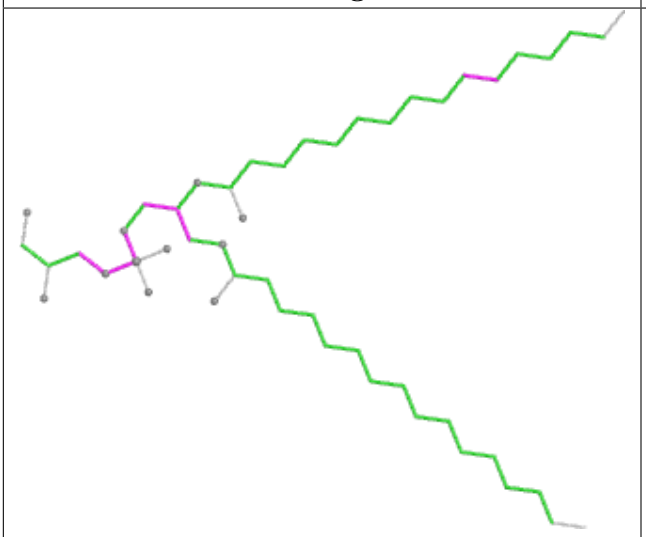
Ligand LHG 4 401



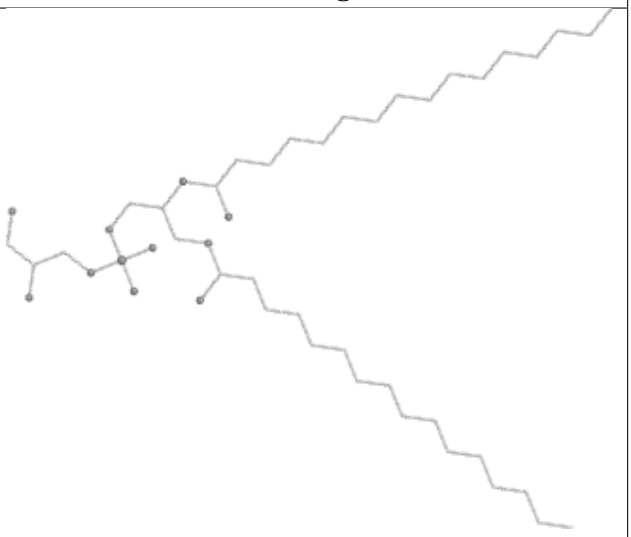
Bond lengths



Bond angles

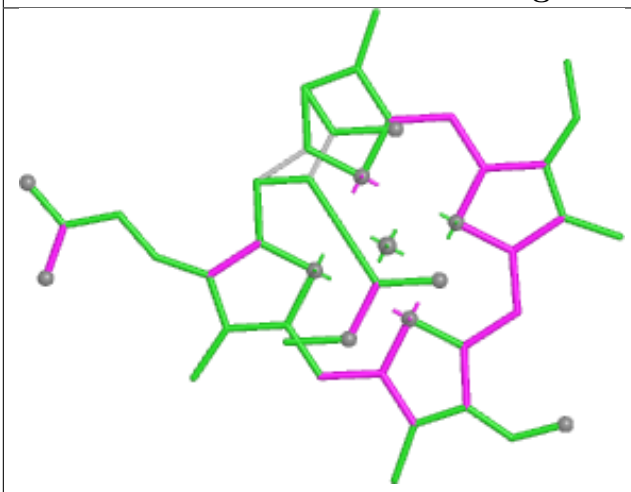


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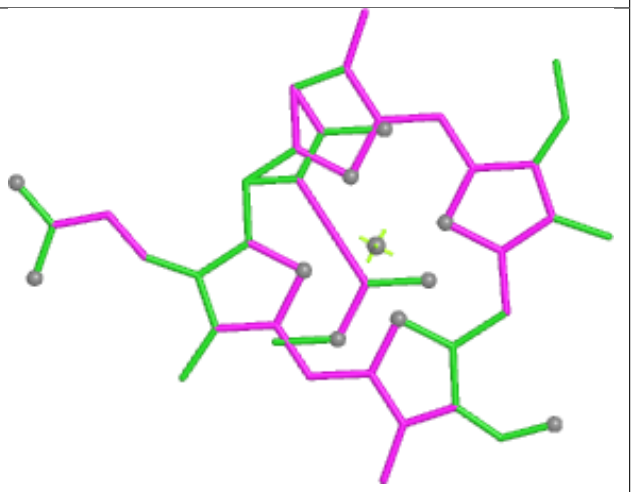


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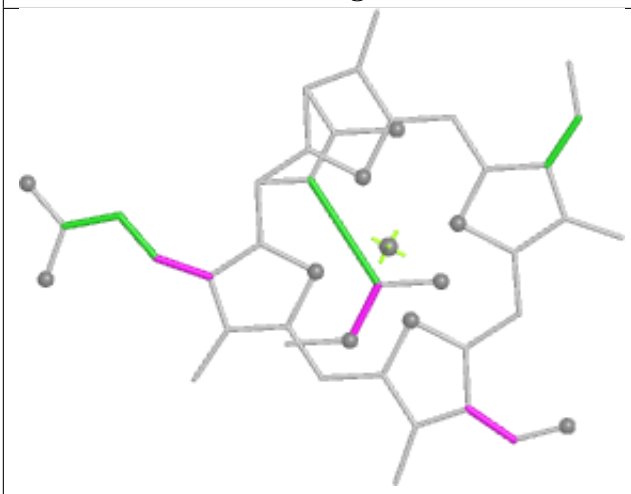
Ligand CL7 6 504



Bond lengths



Bond angles

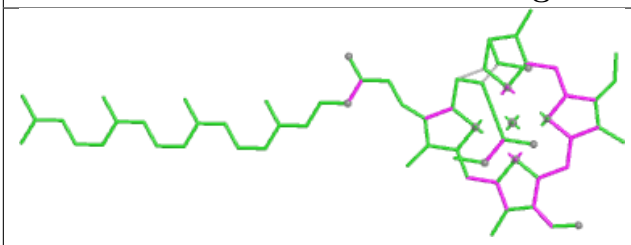


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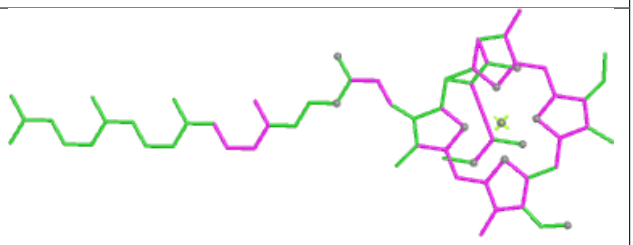


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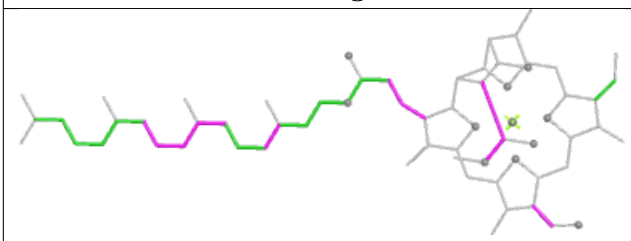
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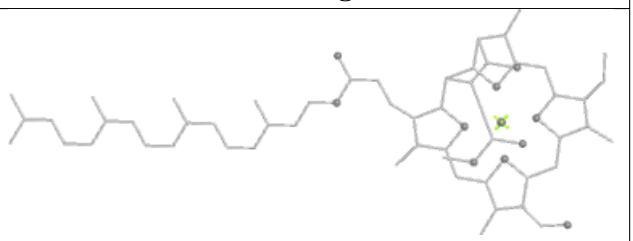
Bond lengths



Bond angles

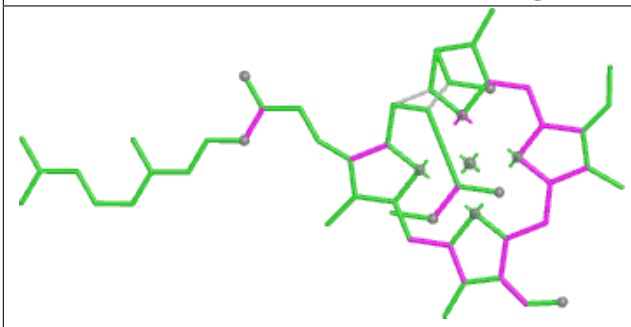


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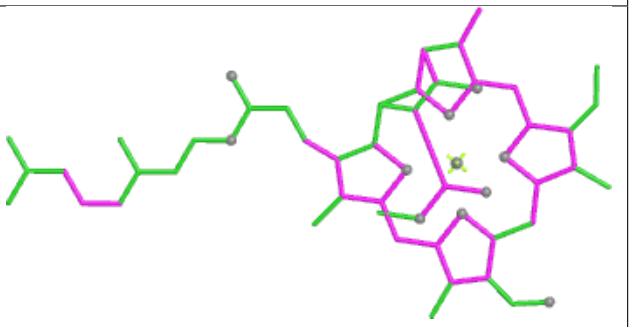


Rings

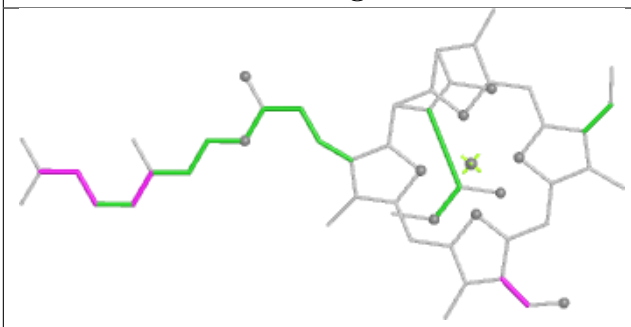
Ligand CL7 B 606



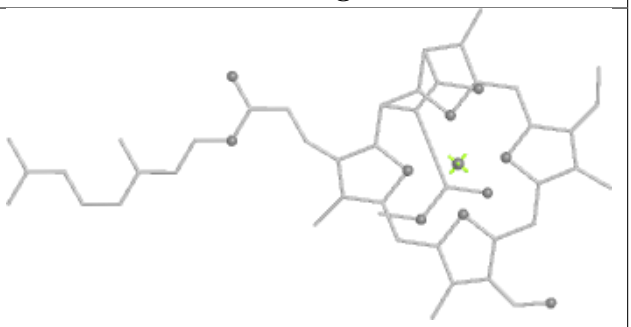
Bond lengths



Bond angles

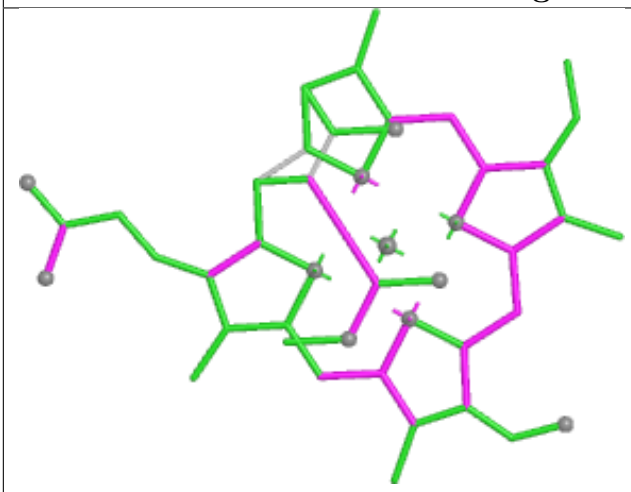


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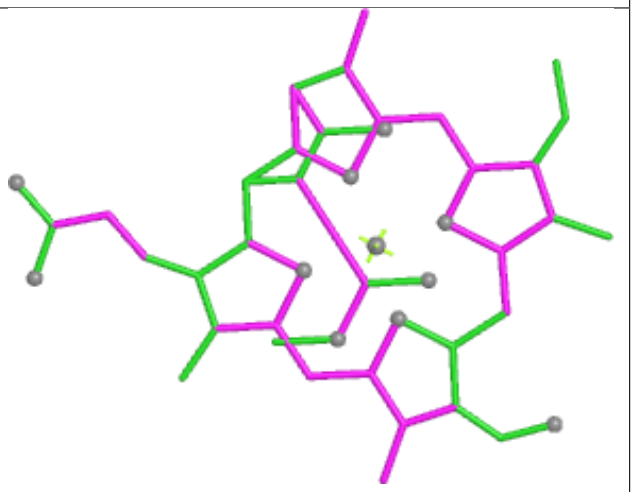


Rings

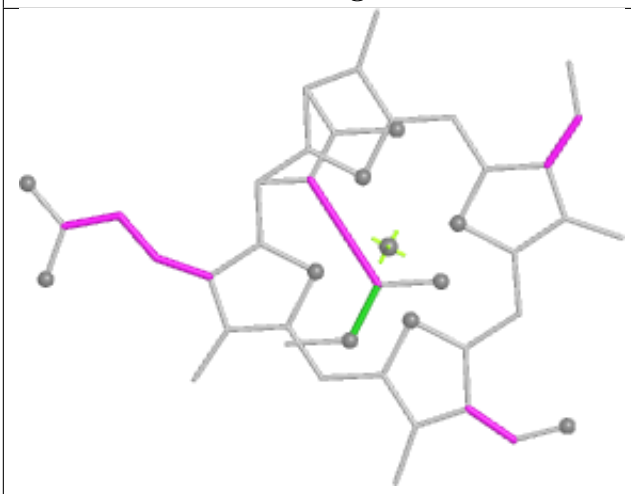
Ligand CL7 3 513



Bond lengths



Bond angles

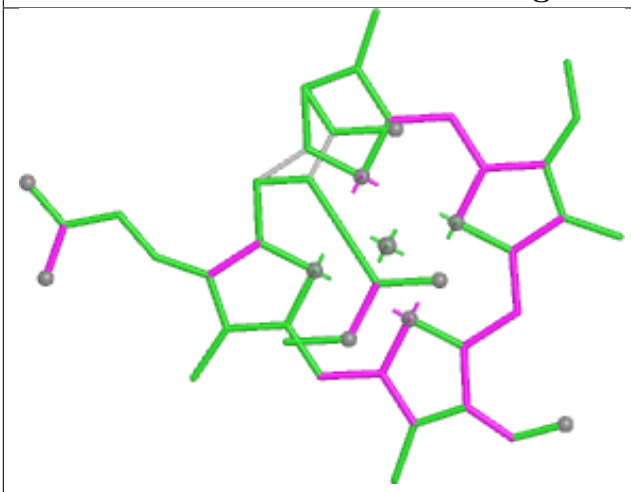


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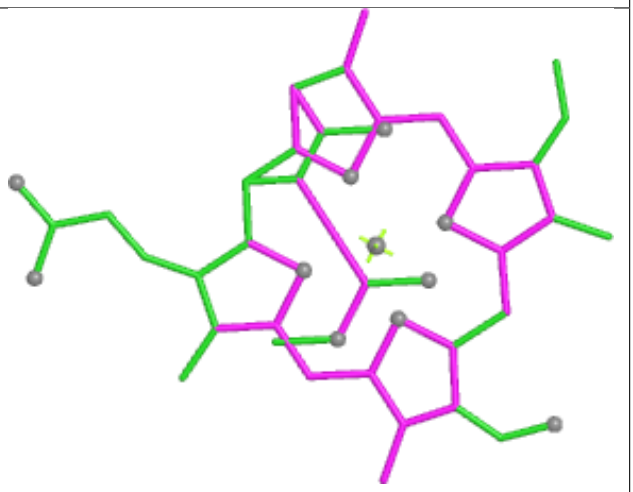


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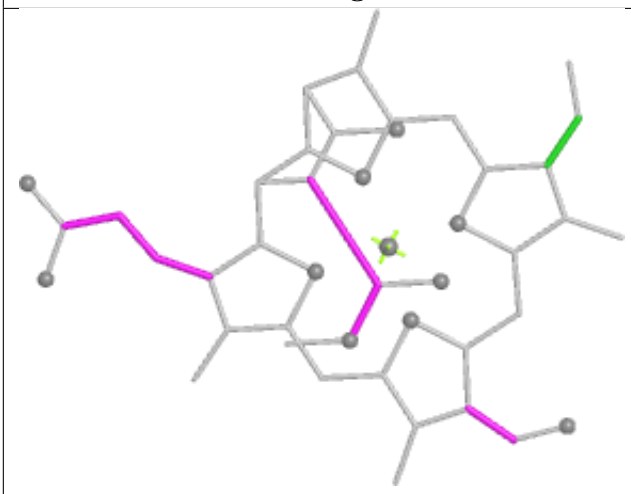
Ligand CL7 8 410



Bond lengths



Bond angles

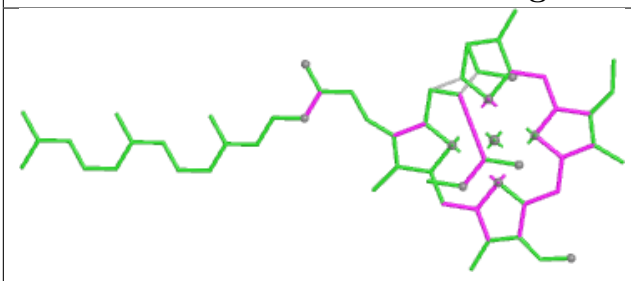


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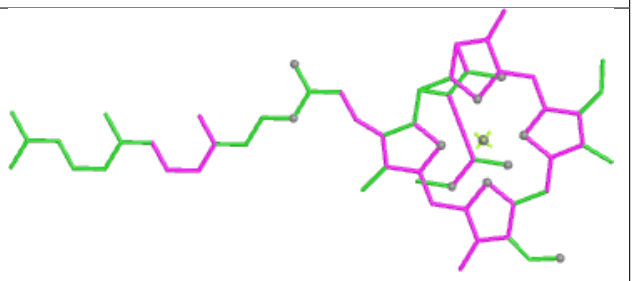


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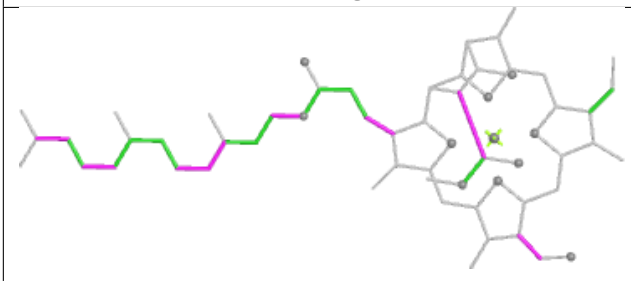
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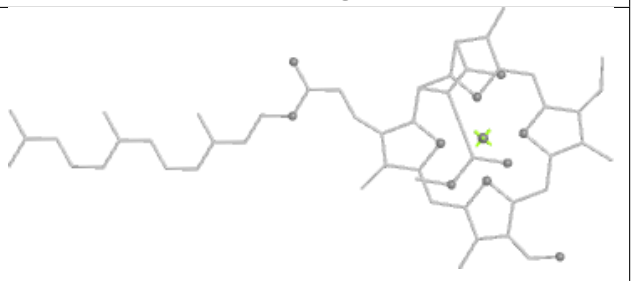
Bond lengths



Bond angles

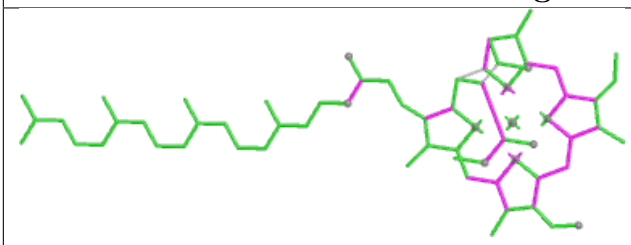


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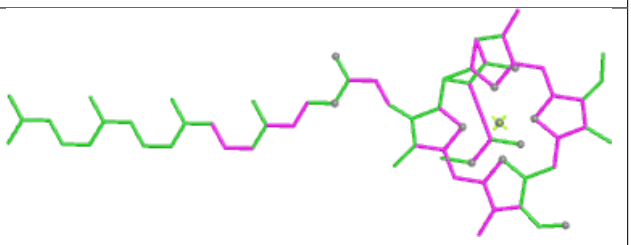


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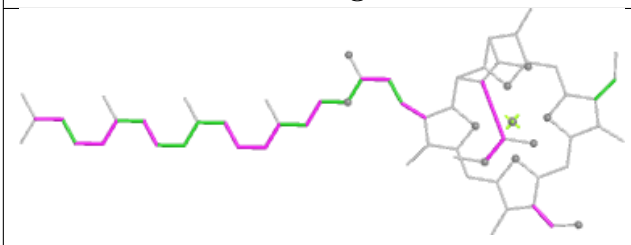
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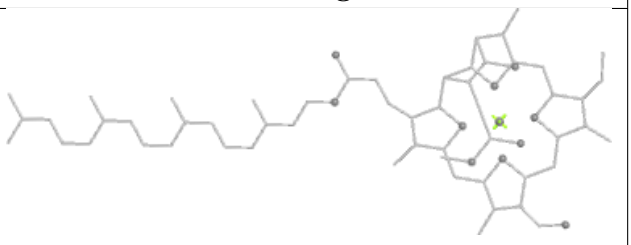
Bond lengths



Bond angles

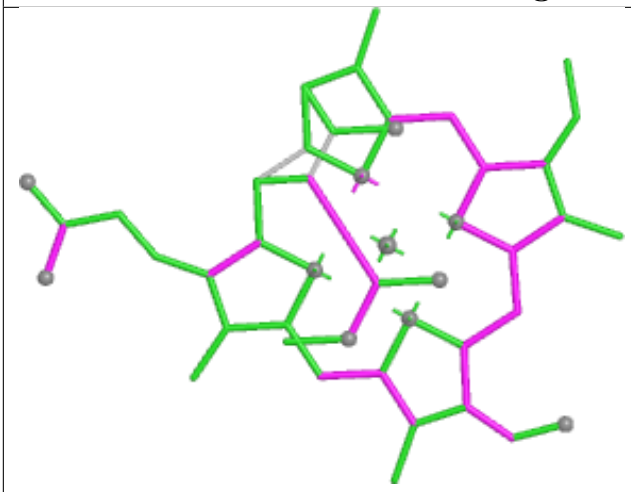


Torsions



Rings

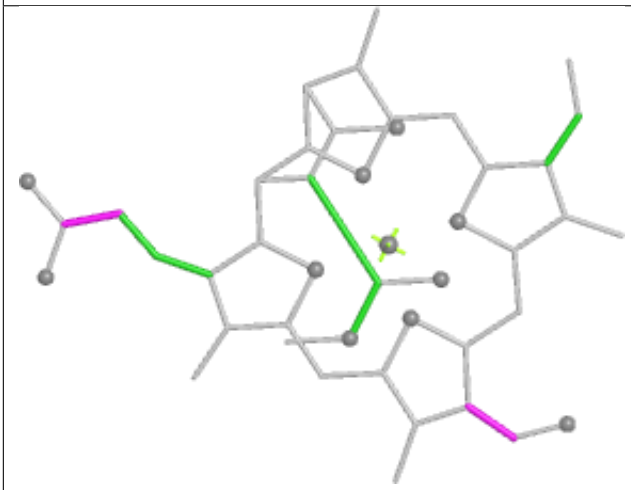
Ligand CL7 4 408



Bond lengths



Bond angles

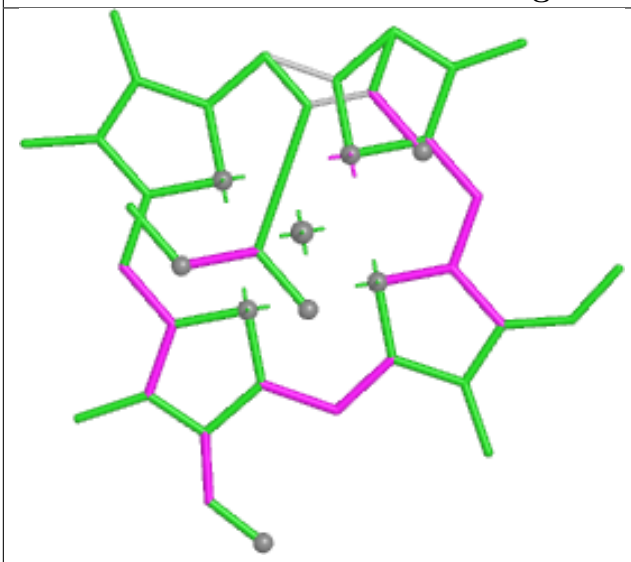


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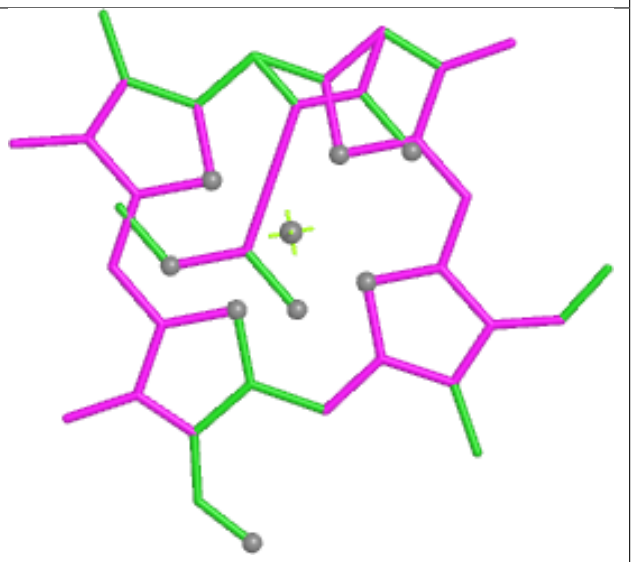


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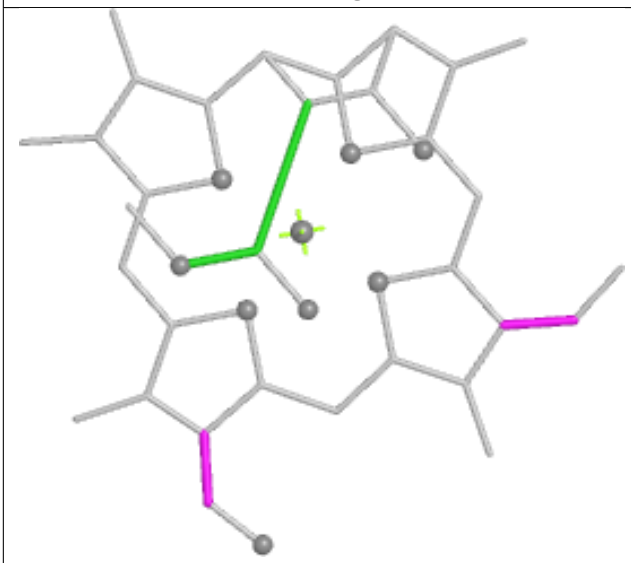
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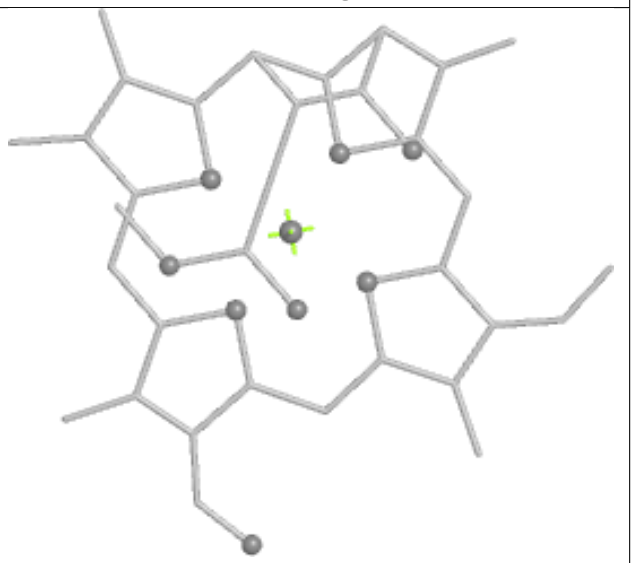
Bond lengths



Bond angles

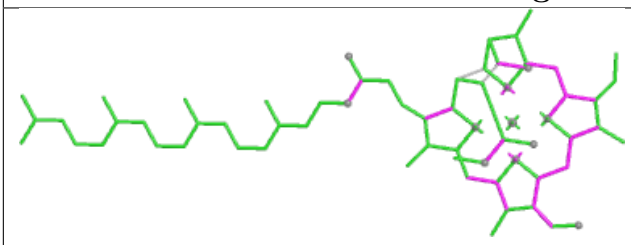


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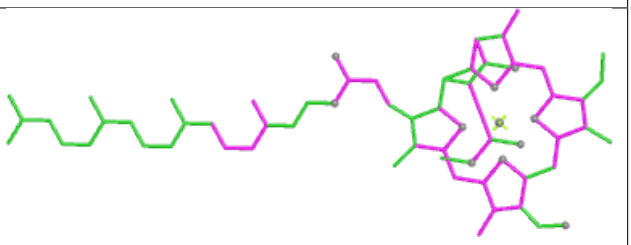


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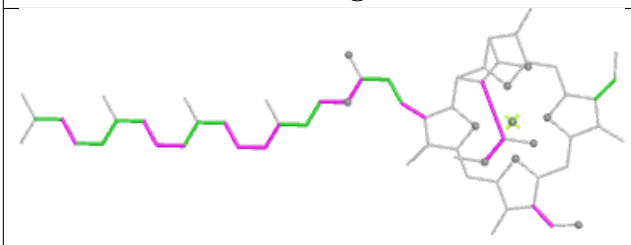
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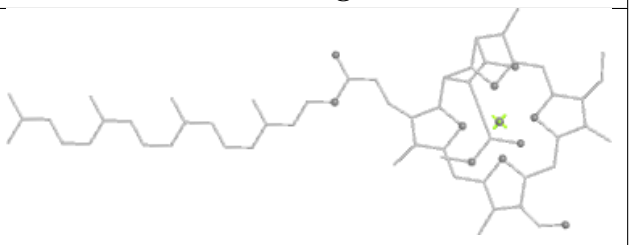
Bond lengths



Bond angles

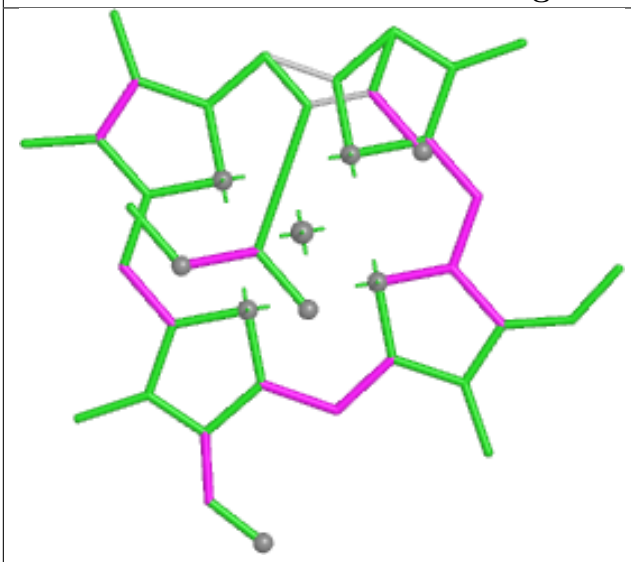


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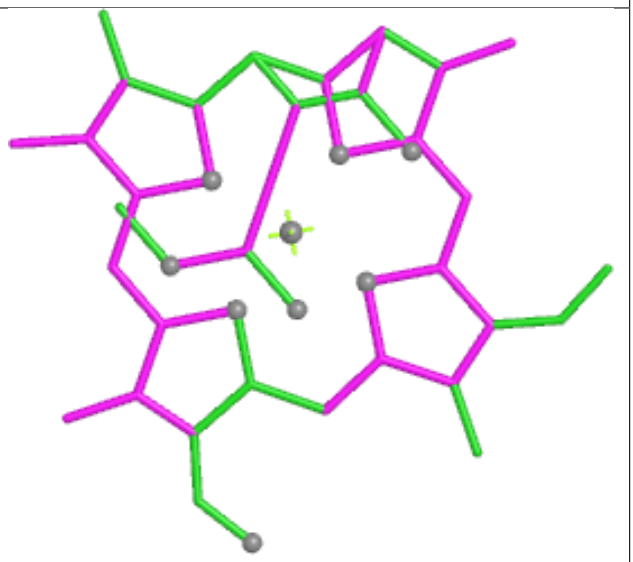


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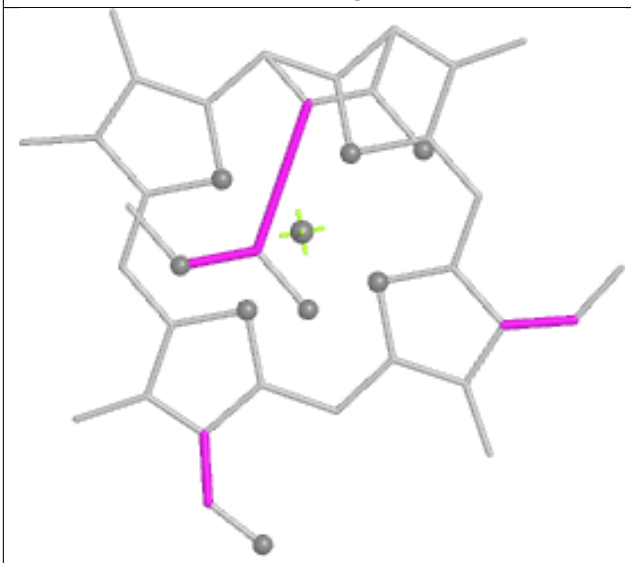
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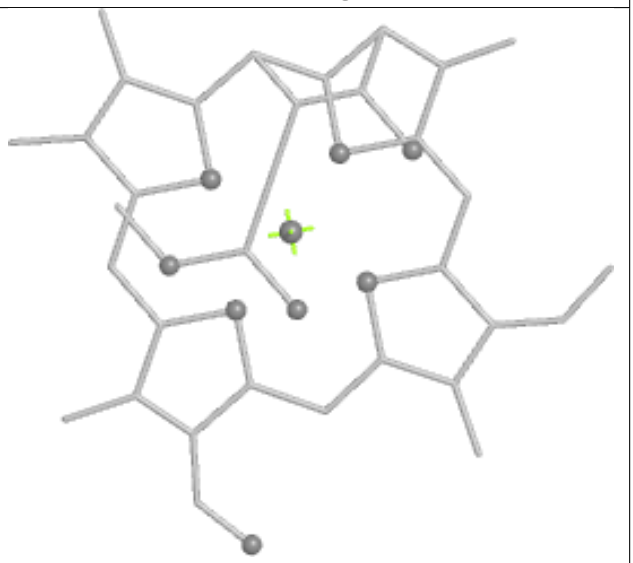
Bond lengths



Bond angles

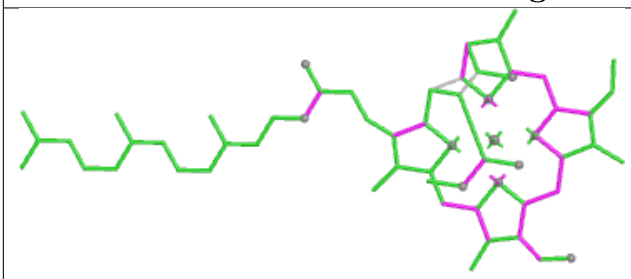


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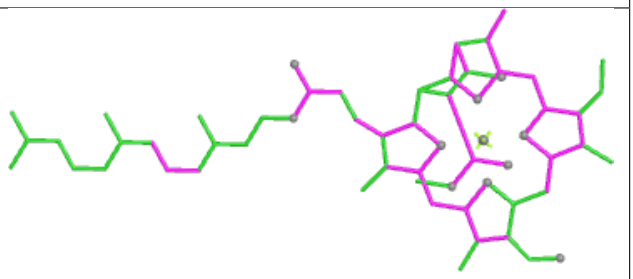


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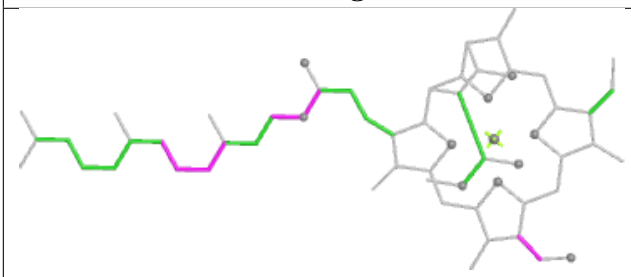
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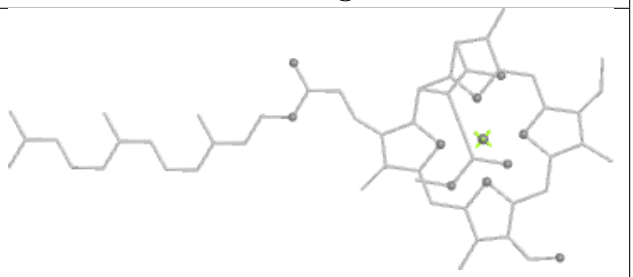
Bond lengths



Bond angles

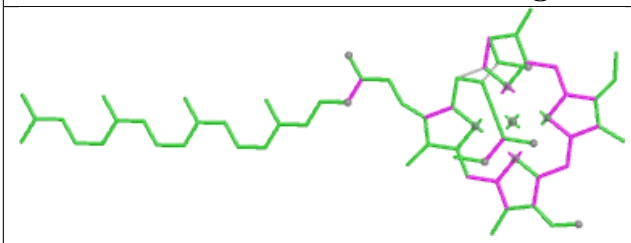


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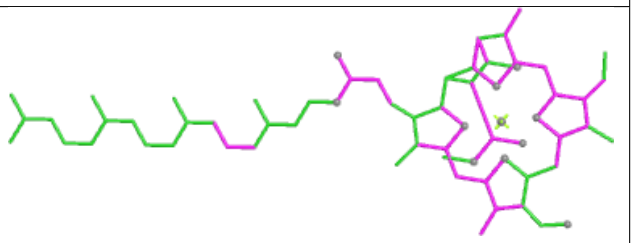


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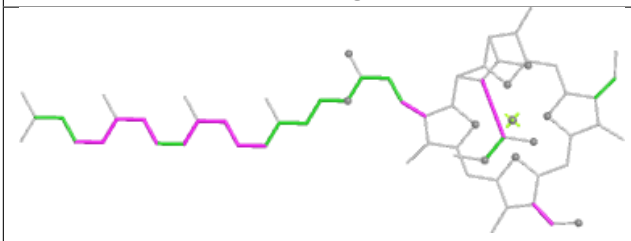
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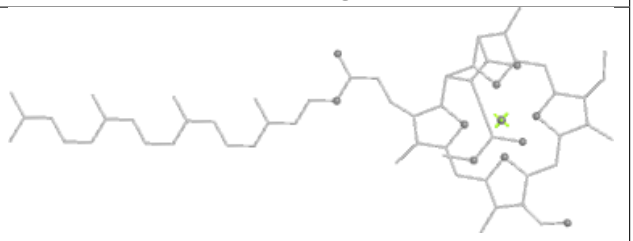
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Bond angles

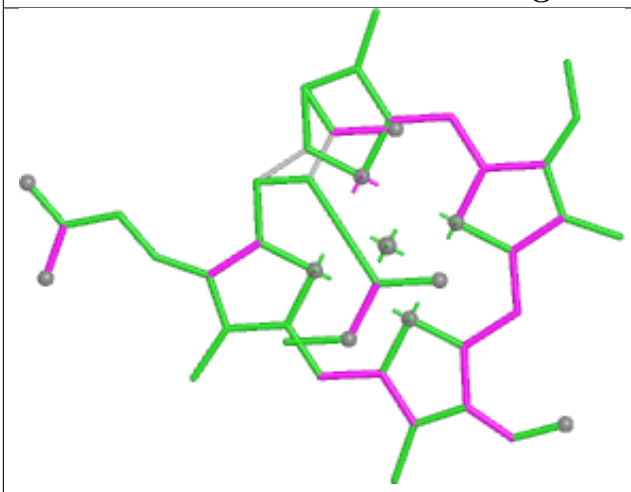


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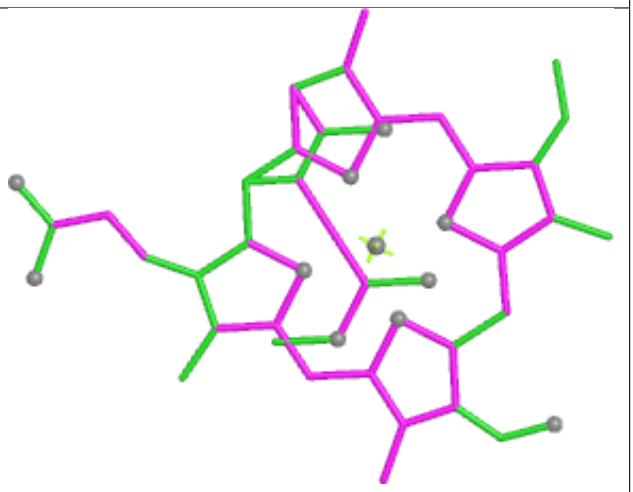


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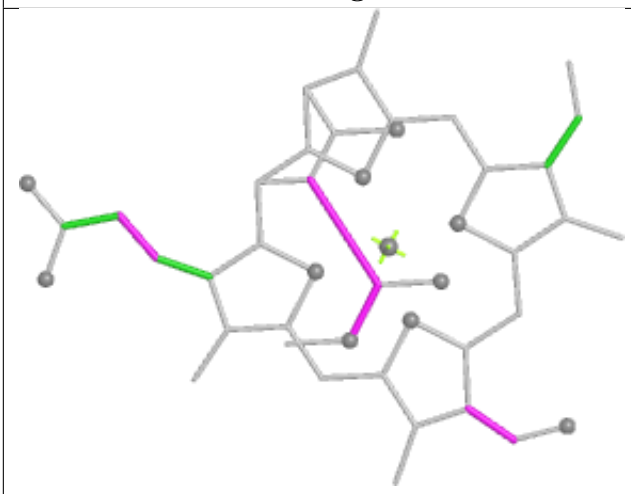
Ligand CL7 5 409



Bond lengths



Bond angles

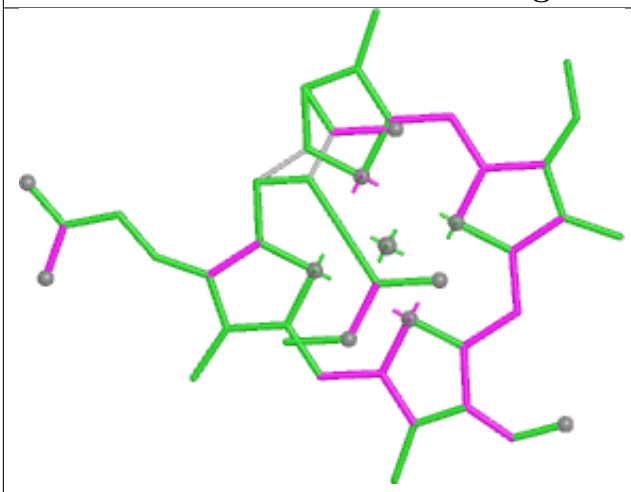


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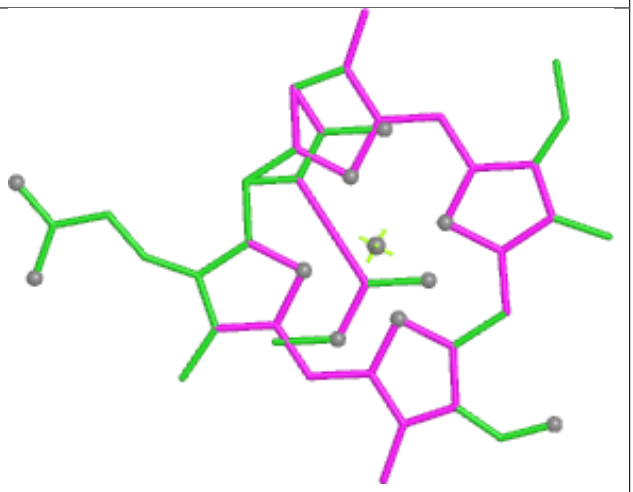


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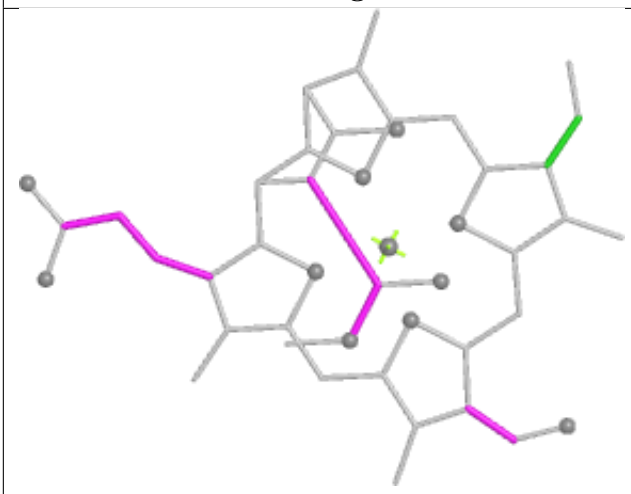
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Bond lengths



Bond angles

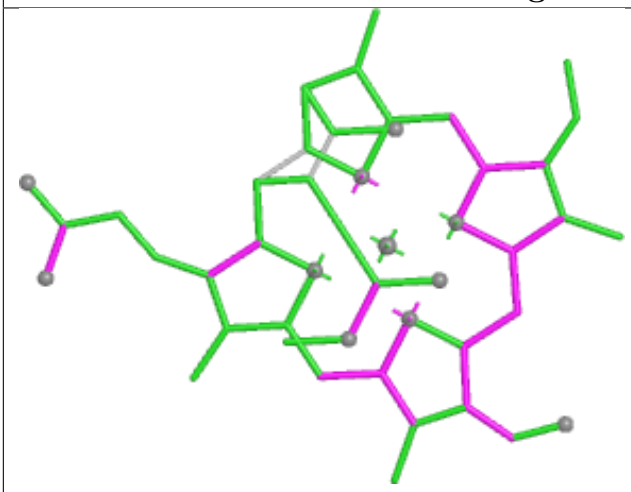


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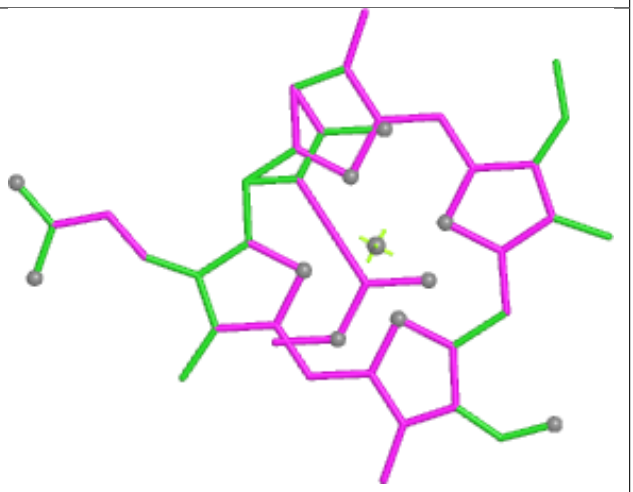


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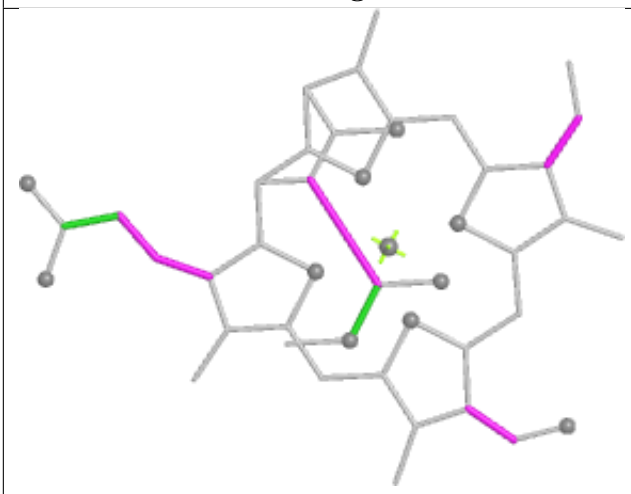
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Bond lengths



Bond angles

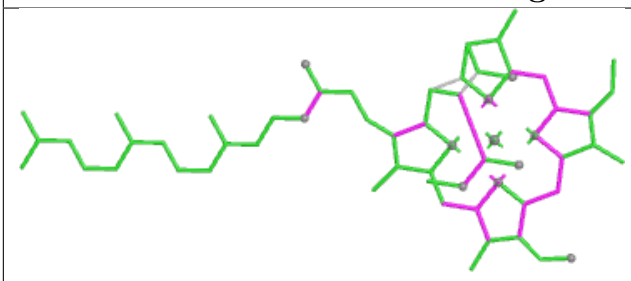


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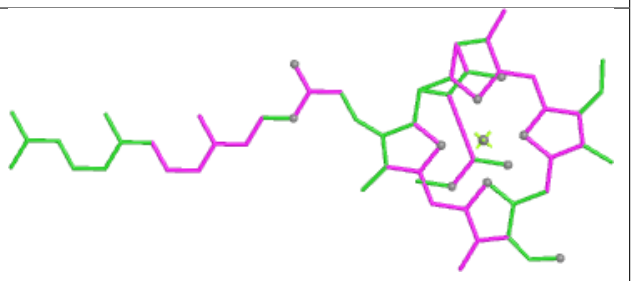


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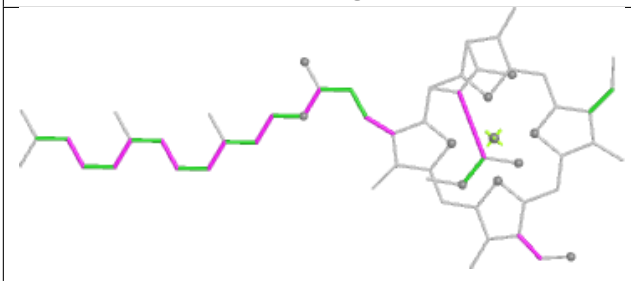
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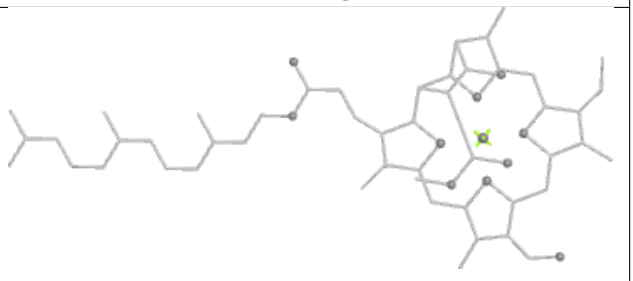
Bond lengths



Bond angles

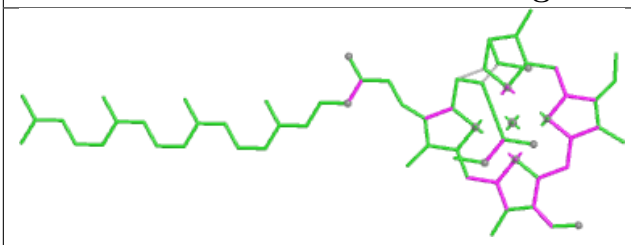


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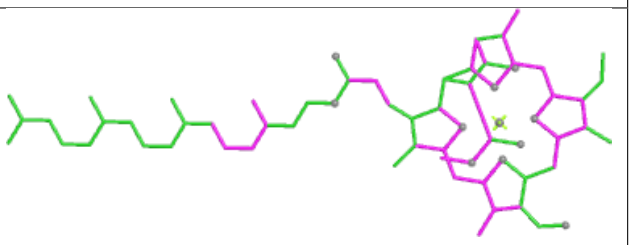


Rings

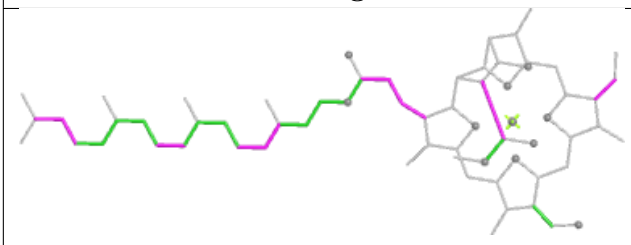
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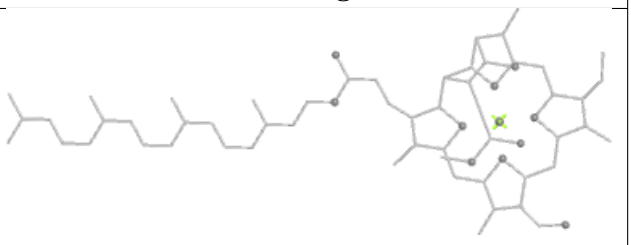
Bond lengths



Bond angles

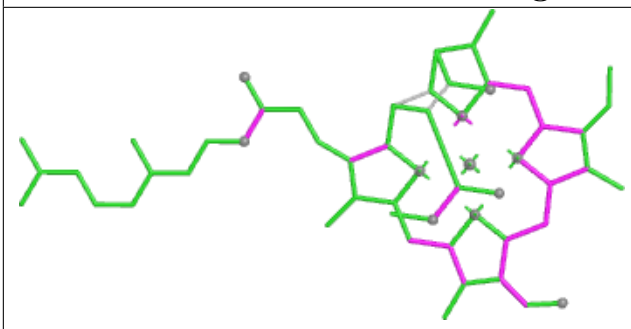


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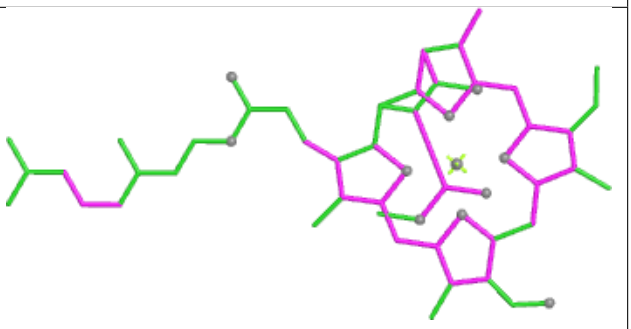


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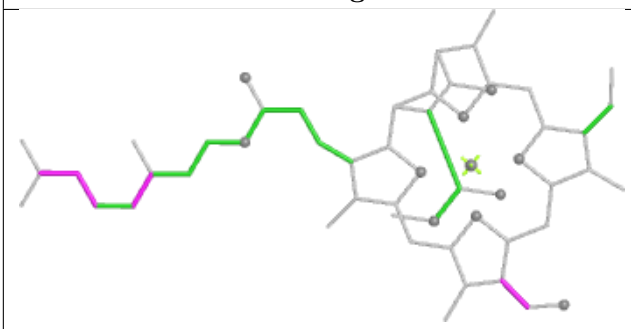
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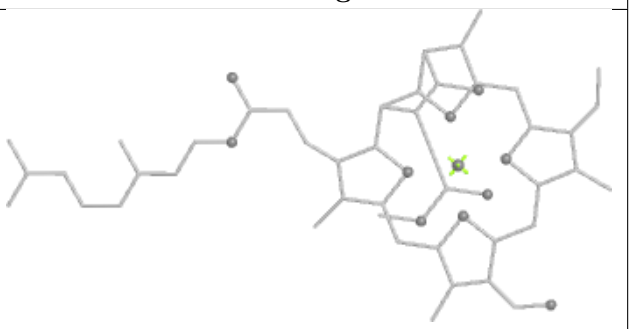
Bond lengths



Bond angles

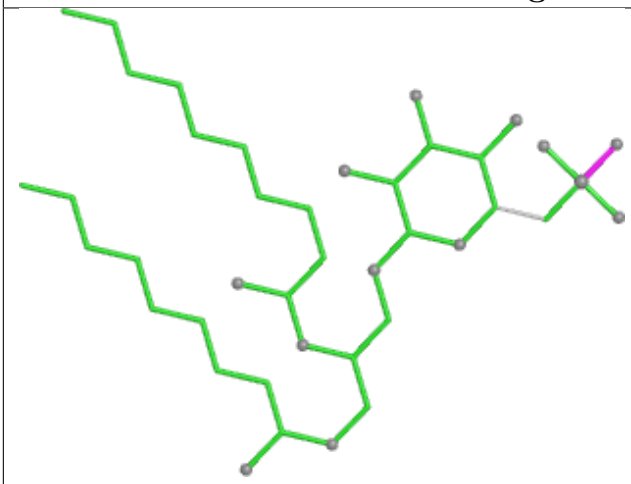


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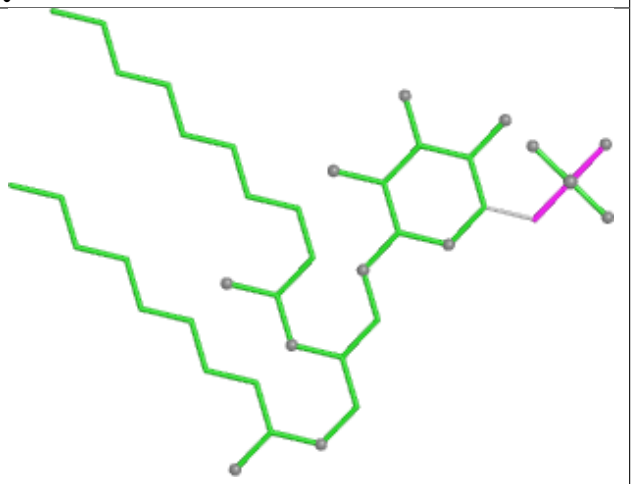


Rings

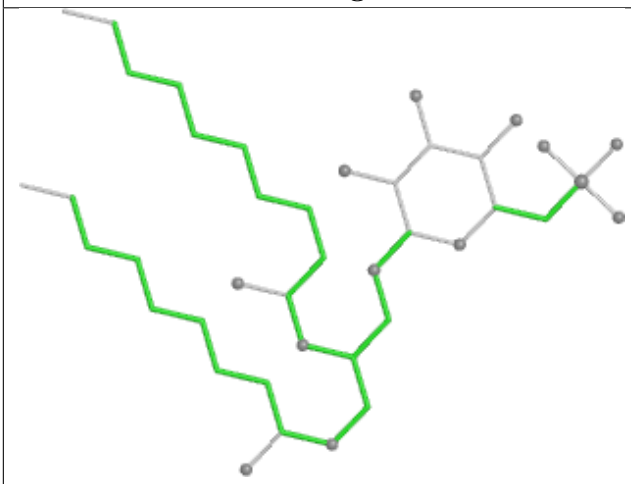
Ligand SQD 2 524



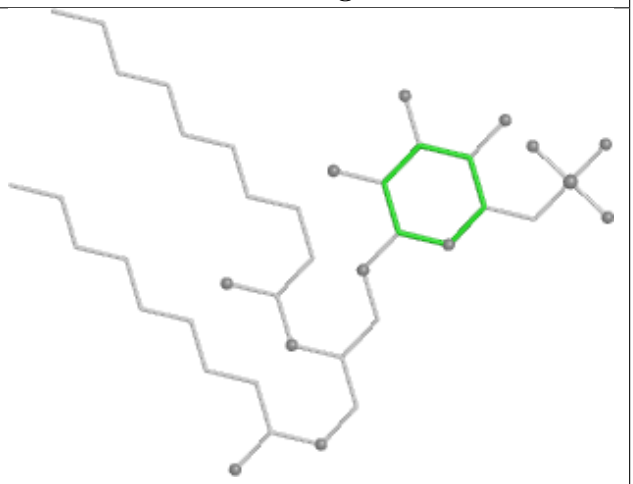
Bond lengths



Bond angles

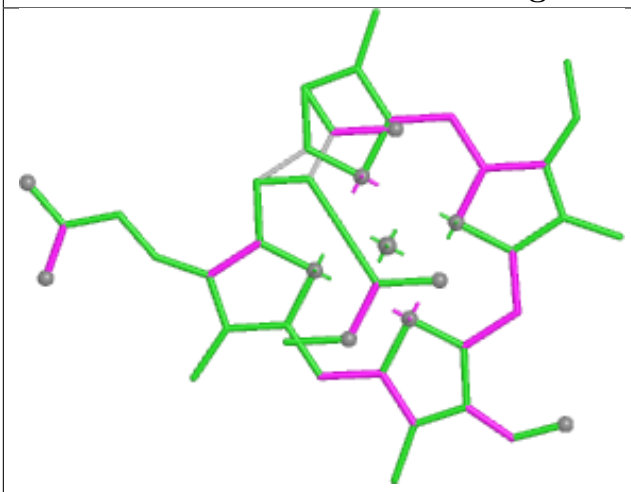


Torsions

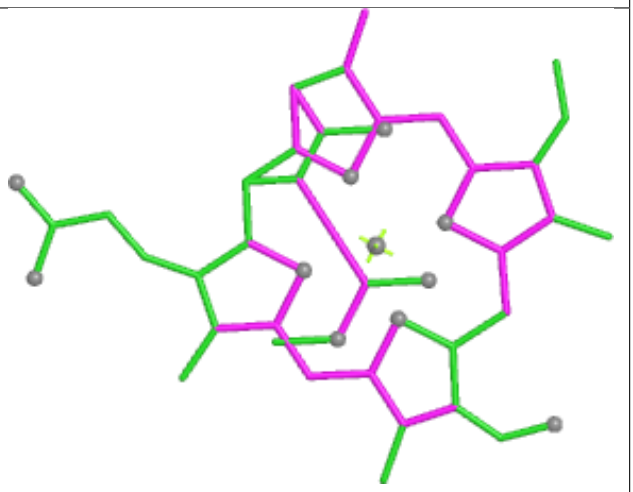


Rings

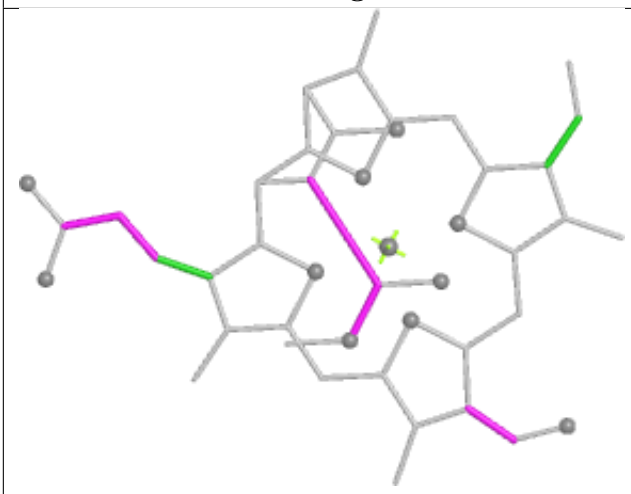
Ligand CL7 B 622



Bond lengths



Bond angles

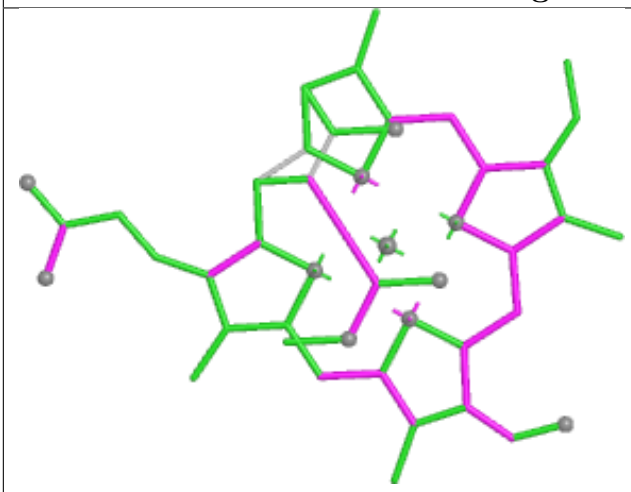


Torsions

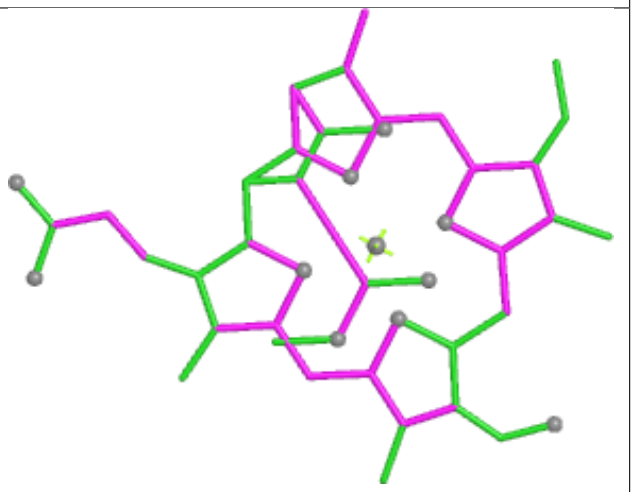


Rings

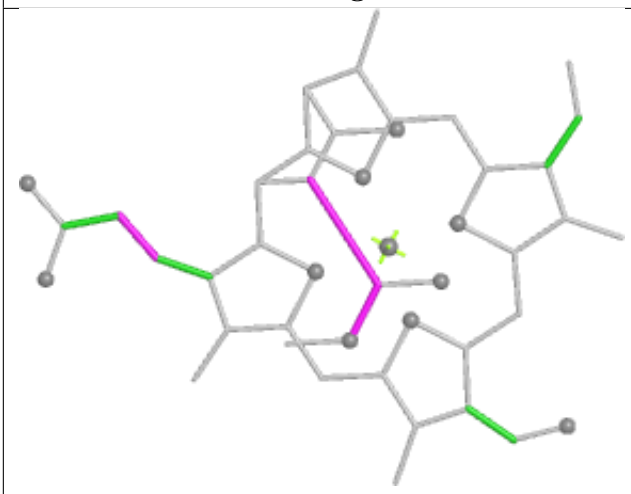
Ligand CL7 b 617



Bond lengths



Bond angles

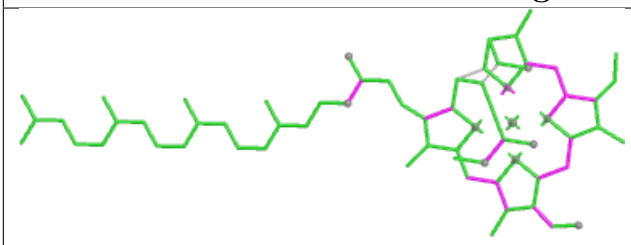


Torsions

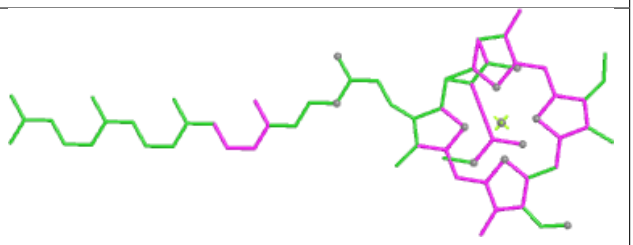


Rings

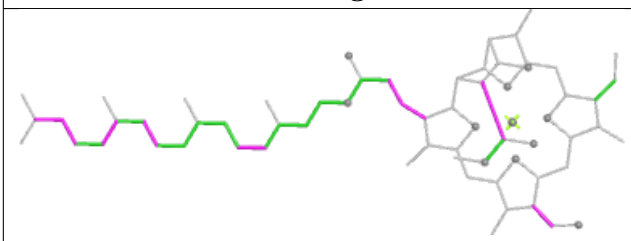
Ligand CL7 6 518



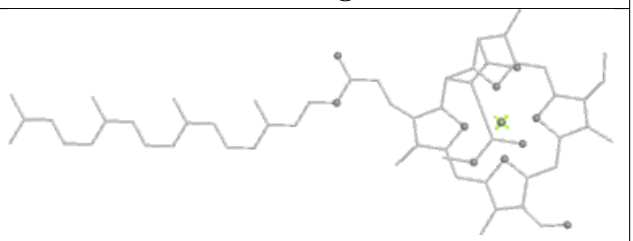
Bond lengths



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.

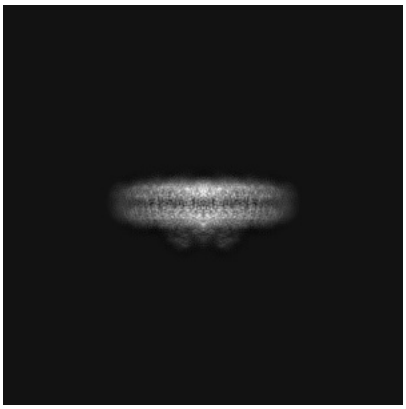
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33929. These allow visual inspection of the internal detail of the map and identification of artifacts.

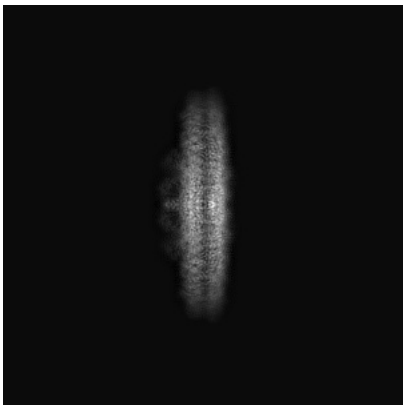
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

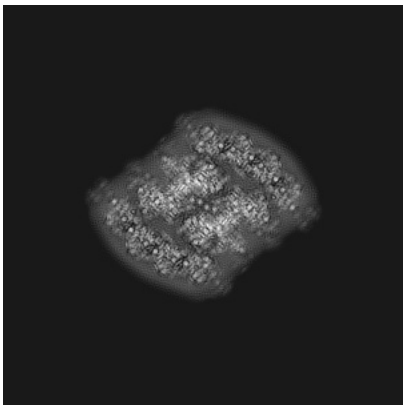
6.1.1 Primary map



X

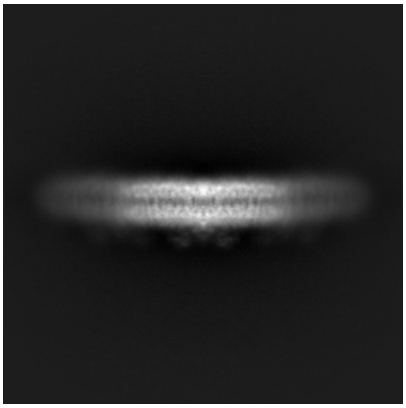


Y

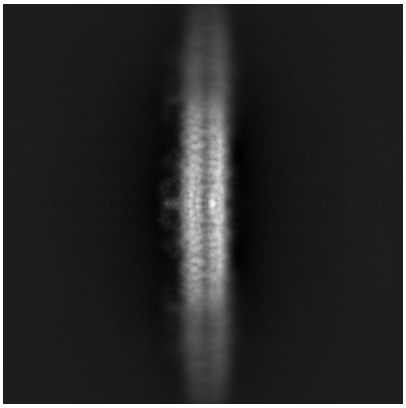


Z

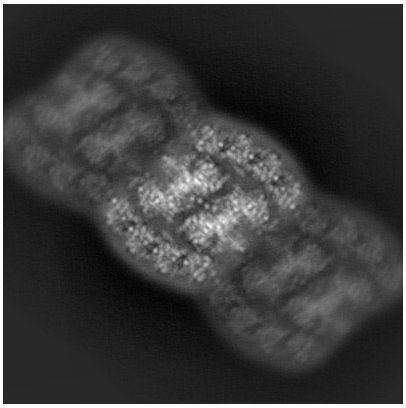
6.1.2 Raw map



X



Y

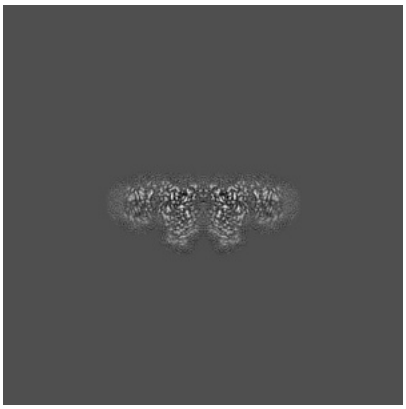


Z

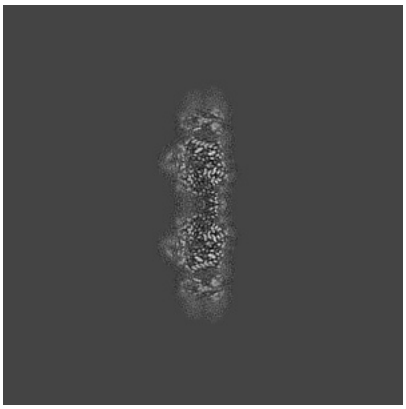
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

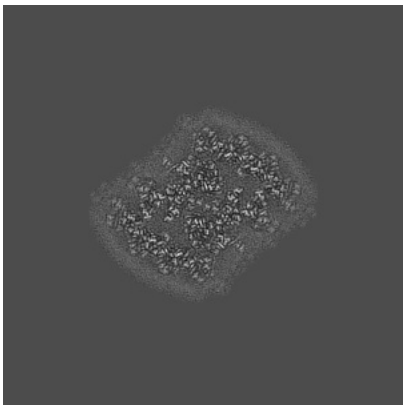
6.2.1 Primary map



X Index: 240

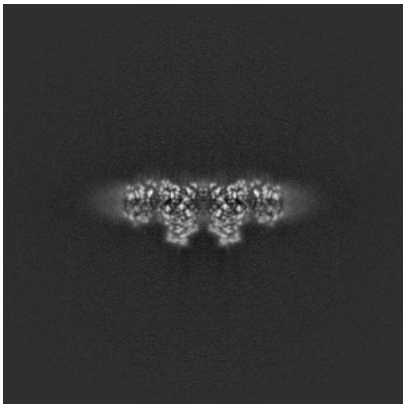


Y Index: 240

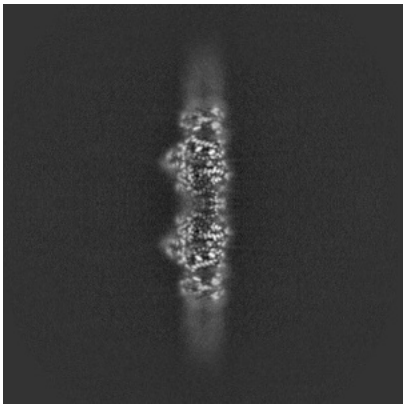


Z Index: 240

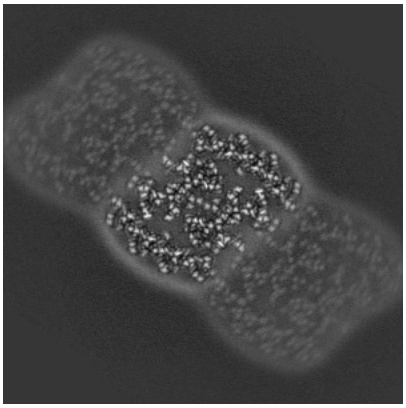
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

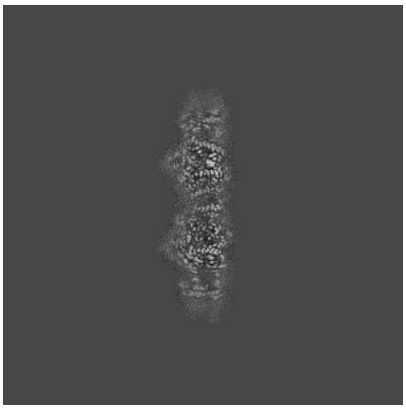
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

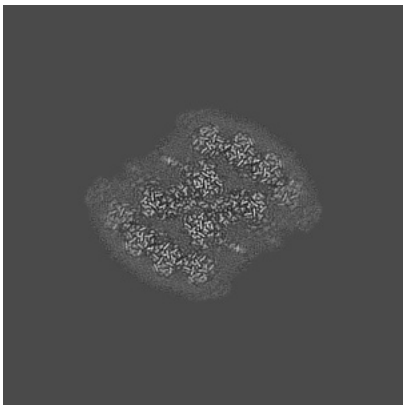
6.3.1 Primary map



X Index: 237



Y Index: 242

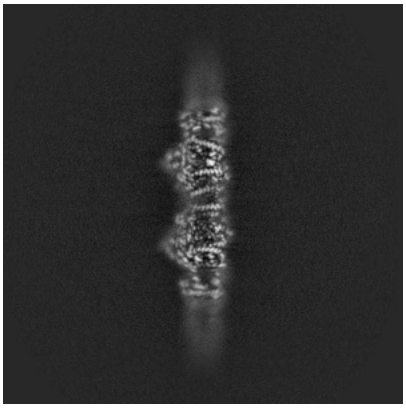


Z Index: 251

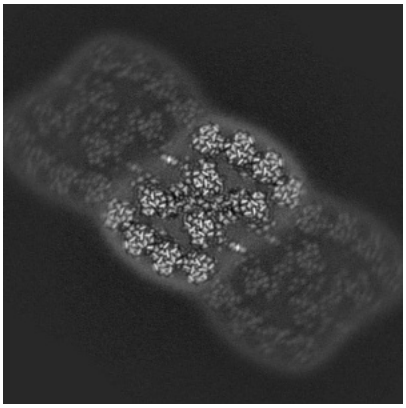
6.3.2 Raw map



X Index: 237



Y Index: 242

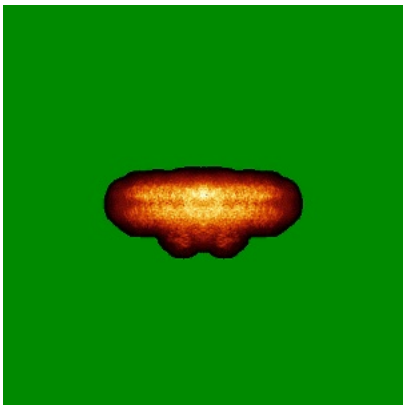


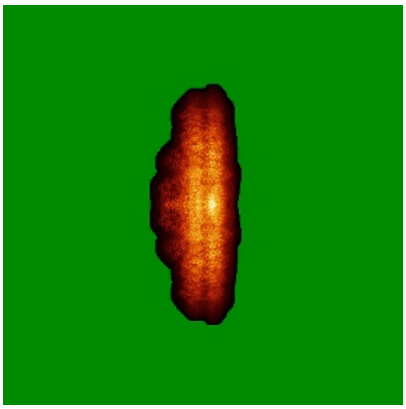
Z Index: 251

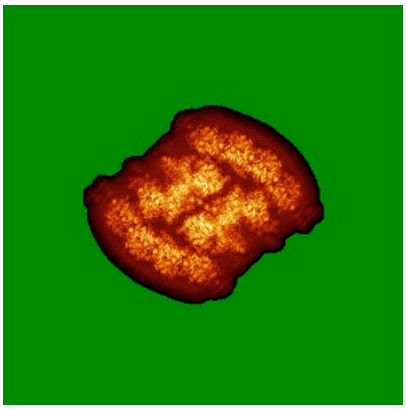
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

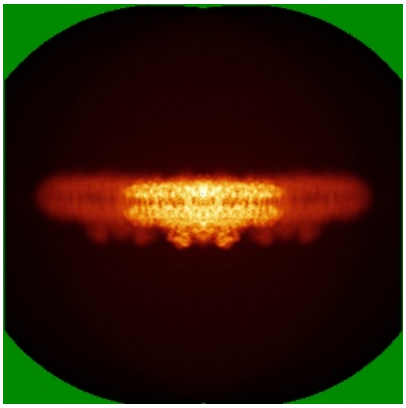
6.4.1 Primary map

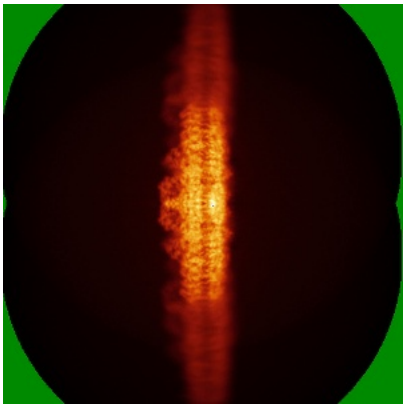

X

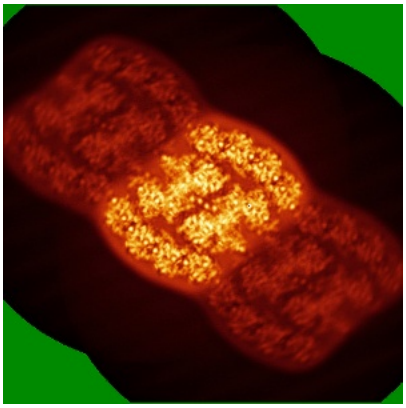

Y


Z

6.4.2 Raw map


X

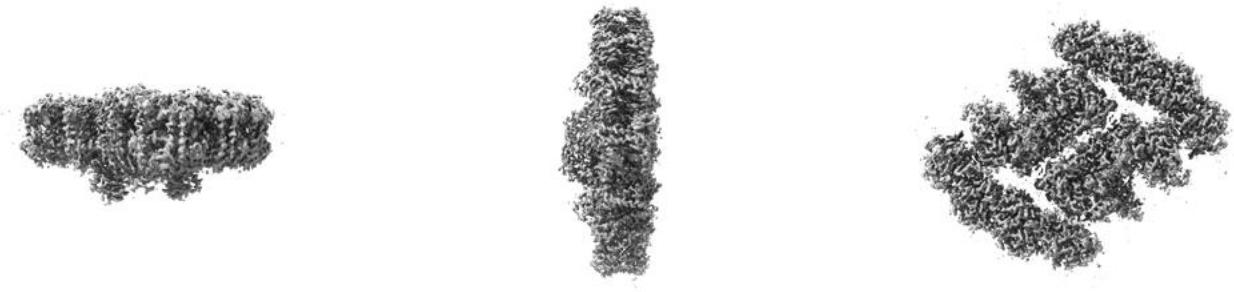

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0188. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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.

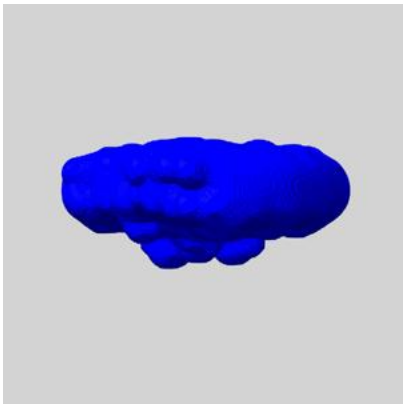
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

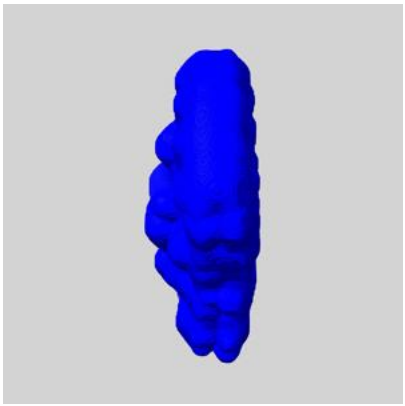
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

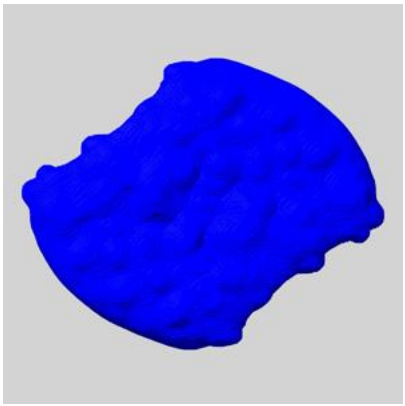
6.6.1 emd_33929_msk_1.map



X



Y

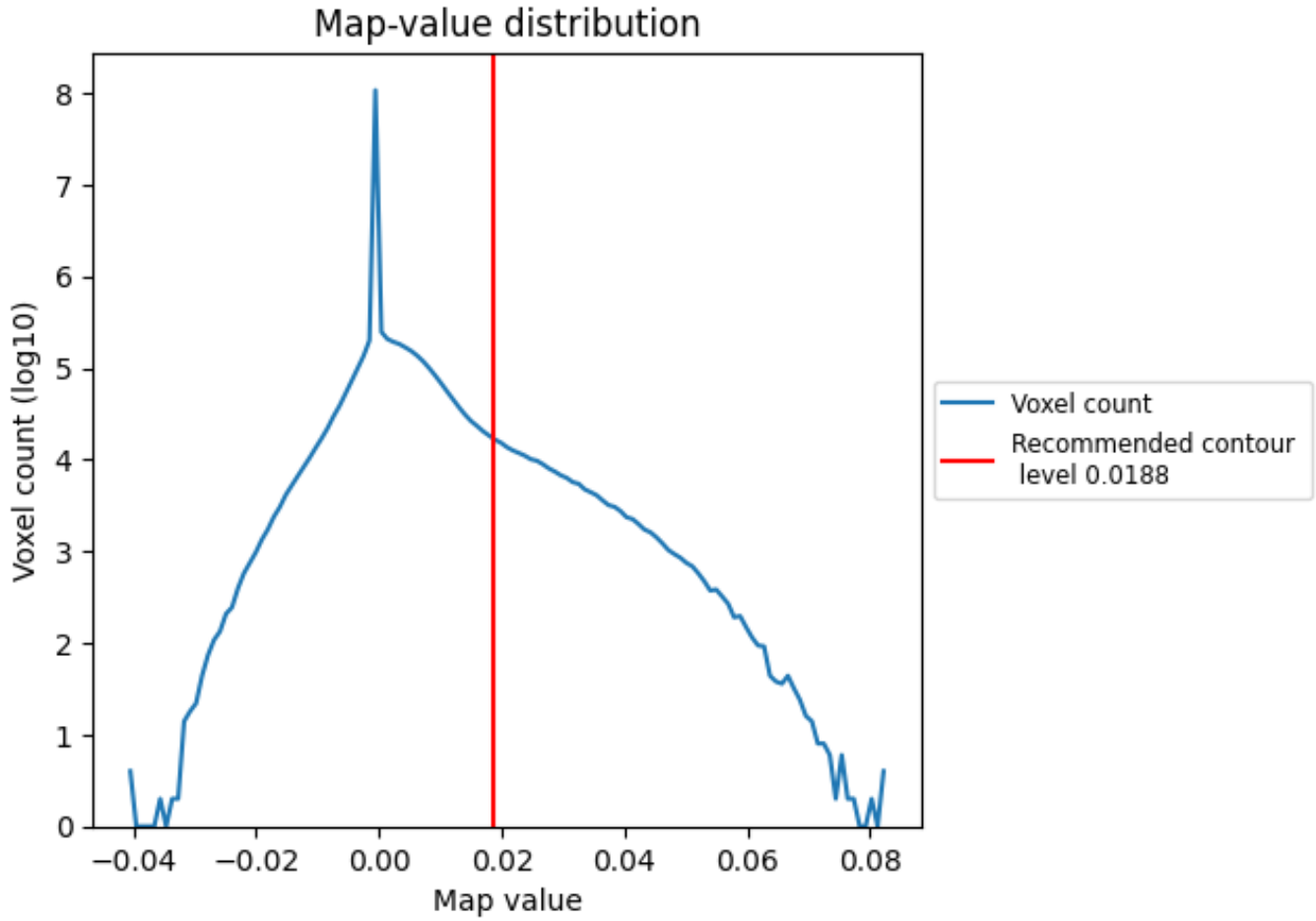


Z

7 Map analysis

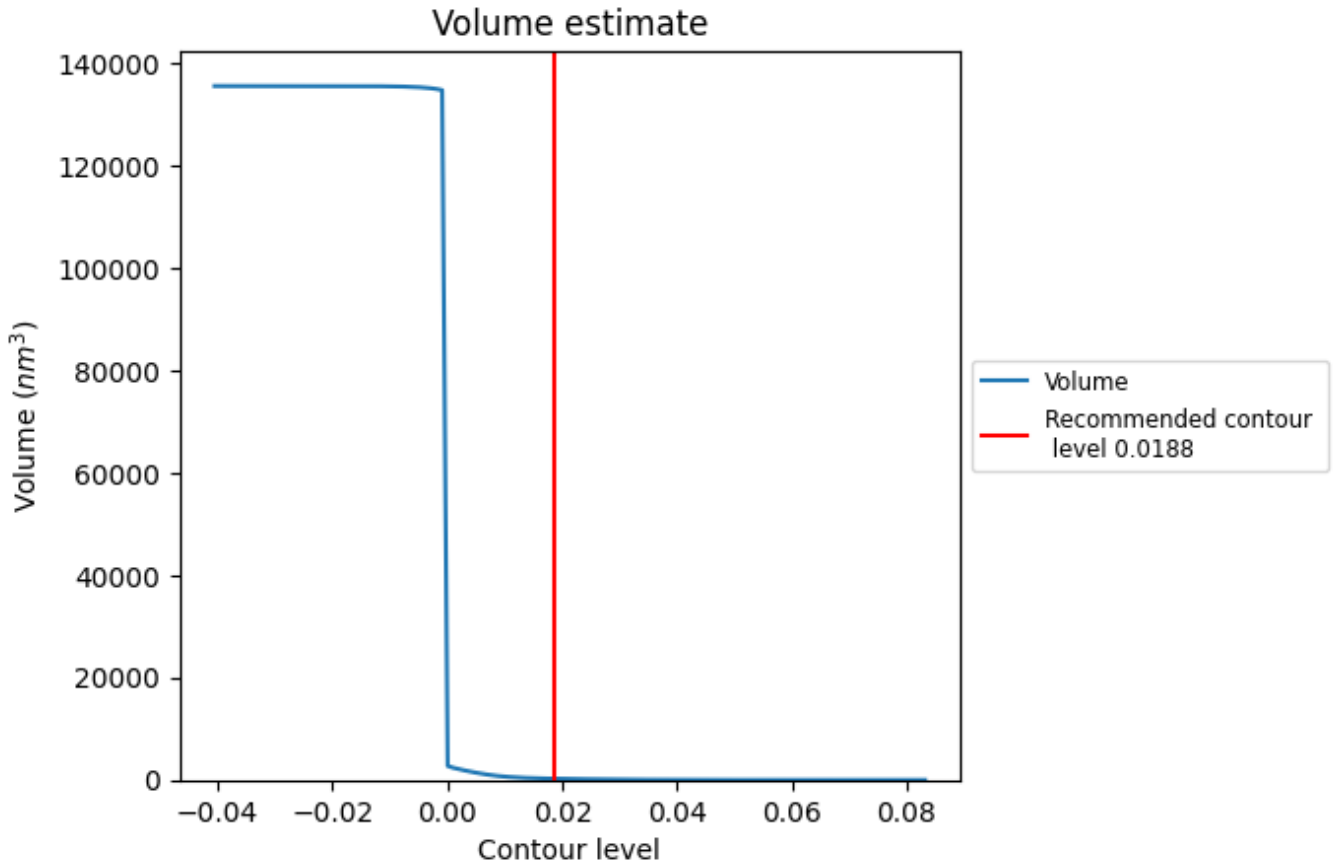
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

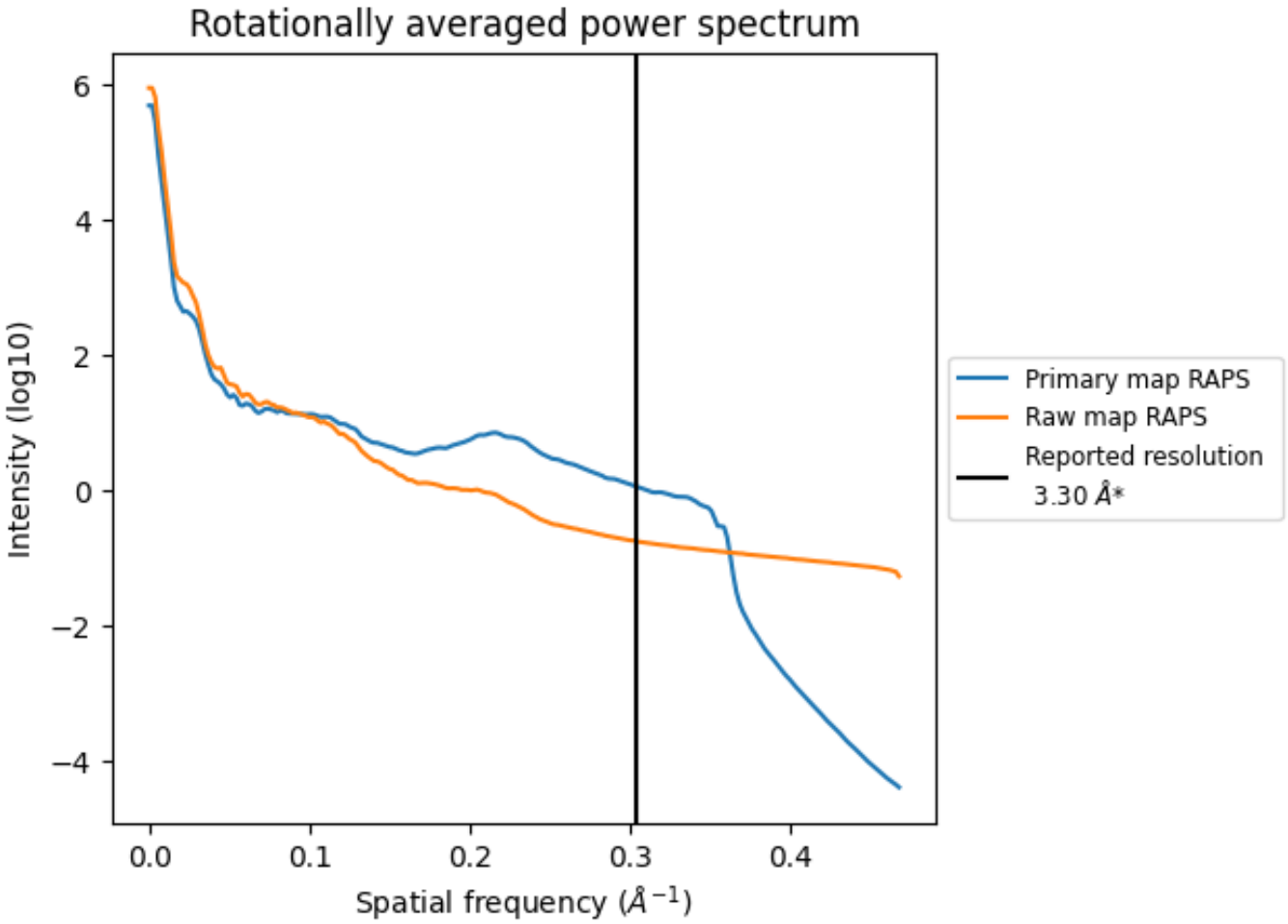
7.2 Volume estimate



The volume at the recommended contour level is 243 nm^3; this corresponds to an approximate mass of 219 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)

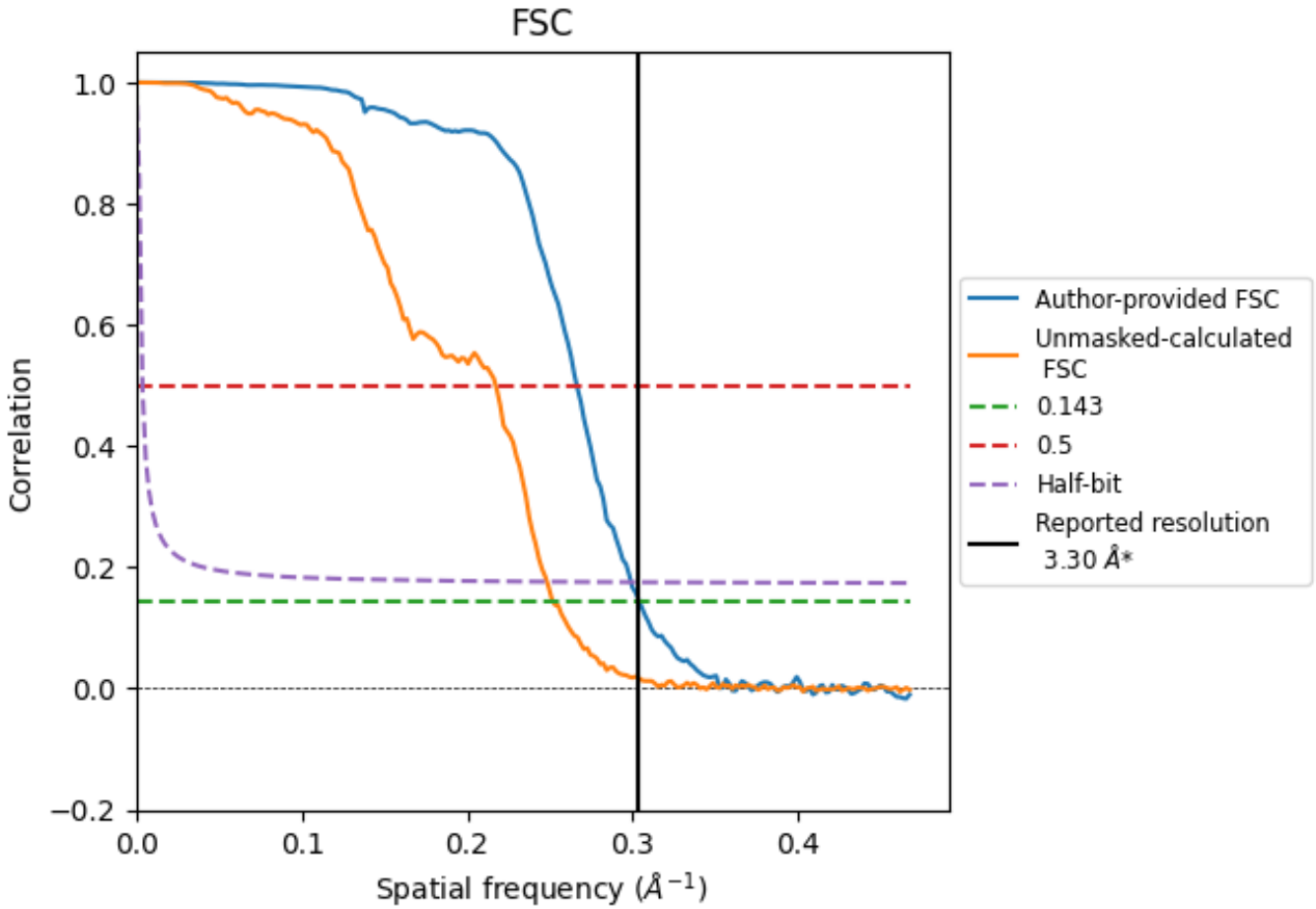


*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

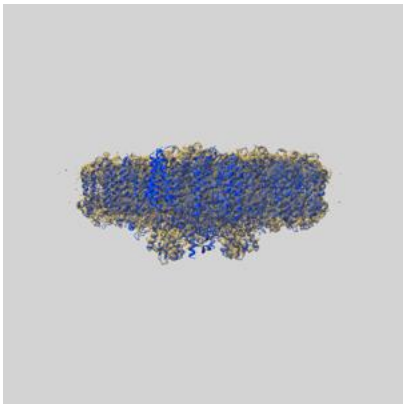
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.76	3.34
Unmasked-calculated*	3.97	4.60	4.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.97 differs from the reported value 3.3 by more than 10 %

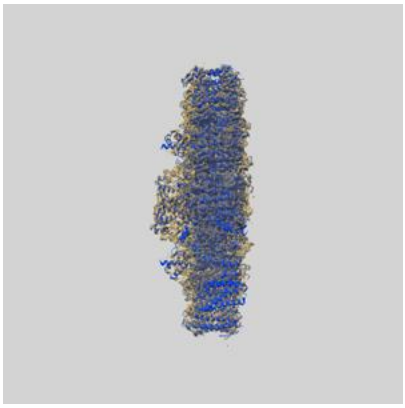
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33929 and PDB model 7YMI. Per-residue inclusion information can be found in section 3 on page 35.

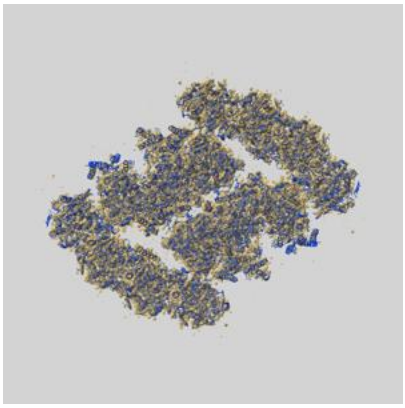
9.1 Map-model overlay



X



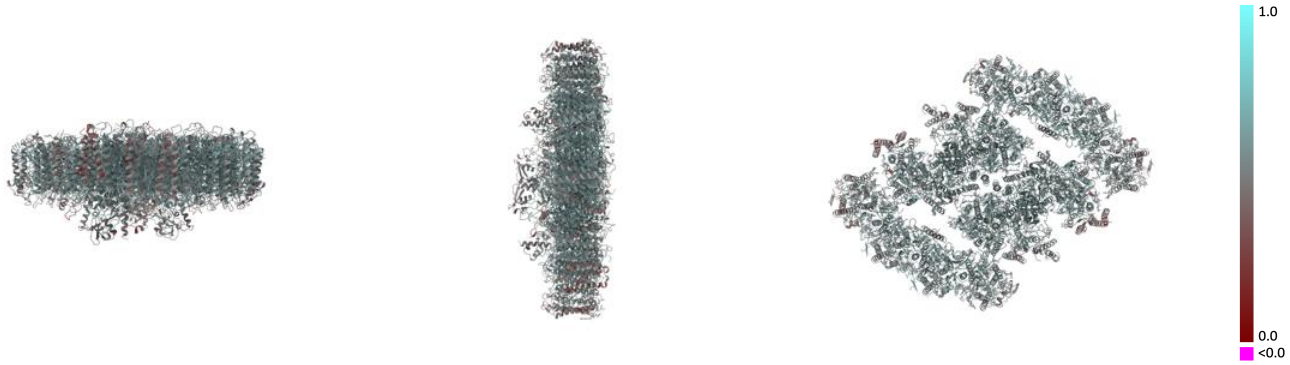
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0188 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.

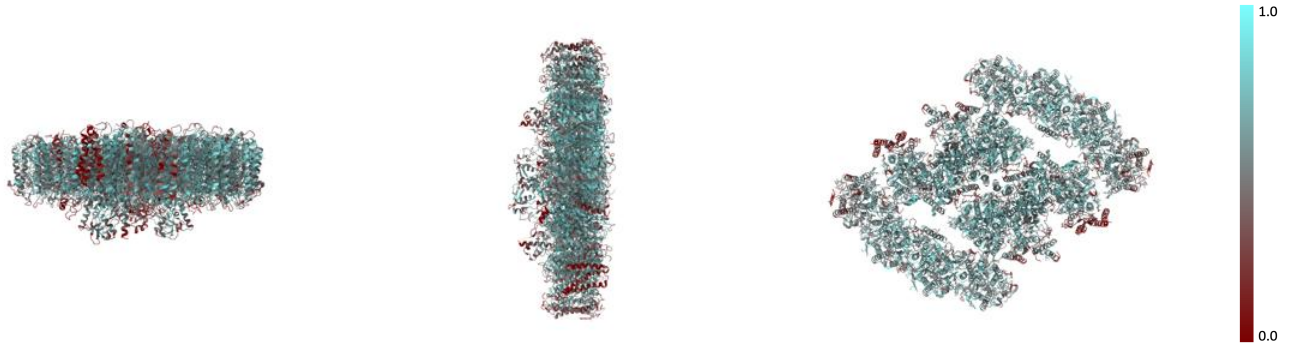
9.2 Q-score mapped to coordinate model (i)



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.

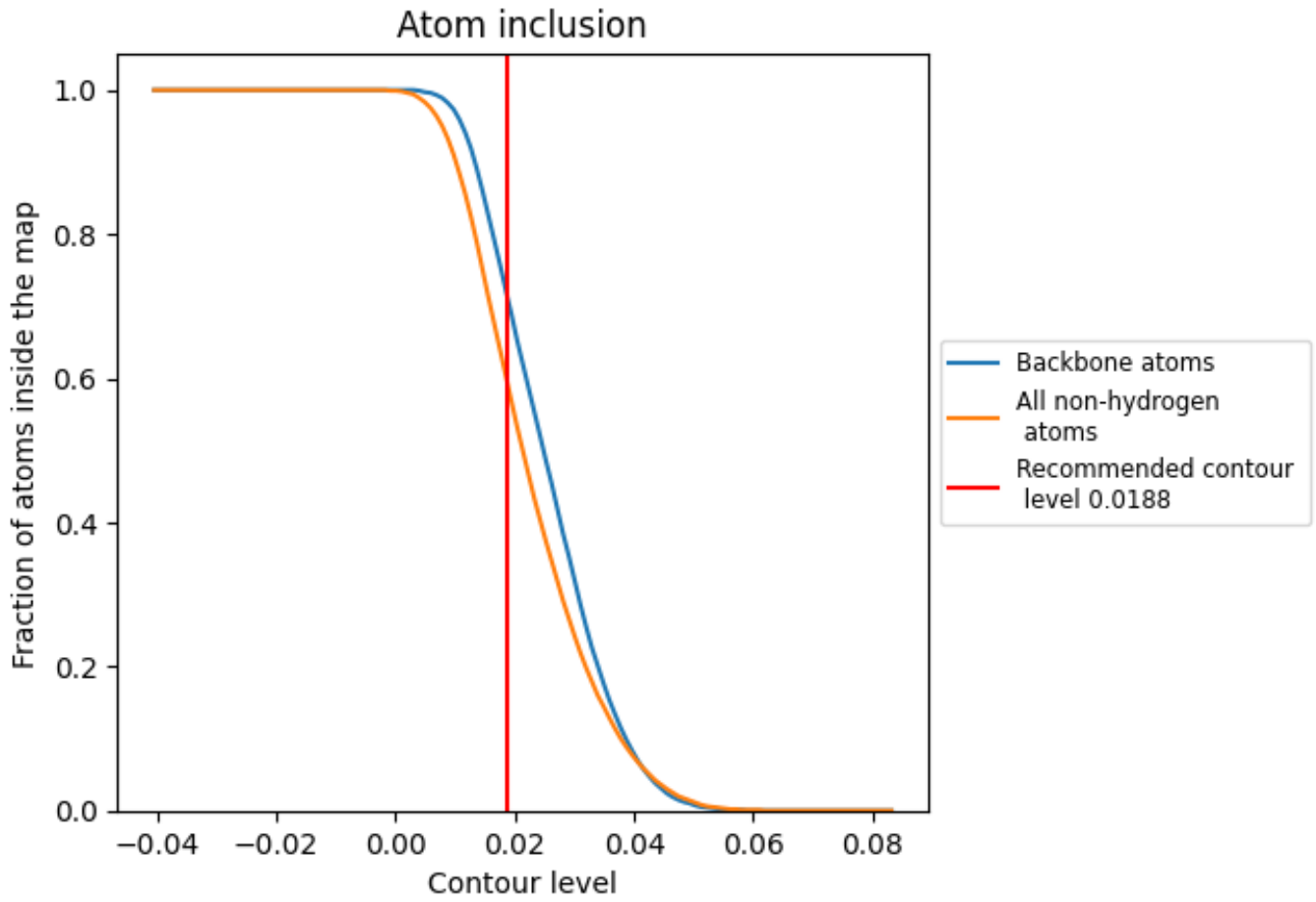
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0188).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0188) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5910	0.5380
1	0.4760	0.5010
2	0.6300	0.5500
3	0.6430	0.5510
4	0.5670	0.5290
5	0.4770	0.5000
6	0.6280	0.5490
7	0.6410	0.5510
8	0.5670	0.5310
A	0.6660	0.5610
B	0.6550	0.5590
C	0.5910	0.5410
D	0.6720	0.5710
E	0.3170	0.4380
F	0.4820	0.4780
G	0.5660	0.4670
H	0.5860	0.5430
I	0.6350	0.5470
K	0.3050	0.4820
L	0.6320	0.5700
M	0.5240	0.5200
T	0.5130	0.5430
X	0.3360	0.4910
Y	0.0560	0.4000
Z	0.1340	0.3830
a	0.6740	0.5610
b	0.6590	0.5590
c	0.5920	0.5410
d	0.6720	0.5700
e	0.3190	0.4380
f	0.4820	0.4720
g	0.5660	0.4590
h	0.5880	0.5420
i	0.6350	0.5490
k	0.3050	0.4810



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Chain	Atom inclusion	Q-score
l	0.6280	0.5630
m	0.5240	0.5180
t	0.5130	0.5400
x	0.3360	0.4860
y	0.0560	0.3990
z	0.1340	0.3810