Full wwPDB EM Validation Report ⓘ

Sep 9, 2026 – 05:52 am BST

PDB ID	:	6SL5 / pdb_00006sl5
EMDB ID	:	EMD-10236
Title	:	Dunaliella Photosystem I Supercomplex
Authors	:	Nelson, N.; Caspy, I.; Malavath, T.; Klaiman, D.; Shkolinsky, Y.
Deposited on	:	2019-08-18
Resolution	:	2.84 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:

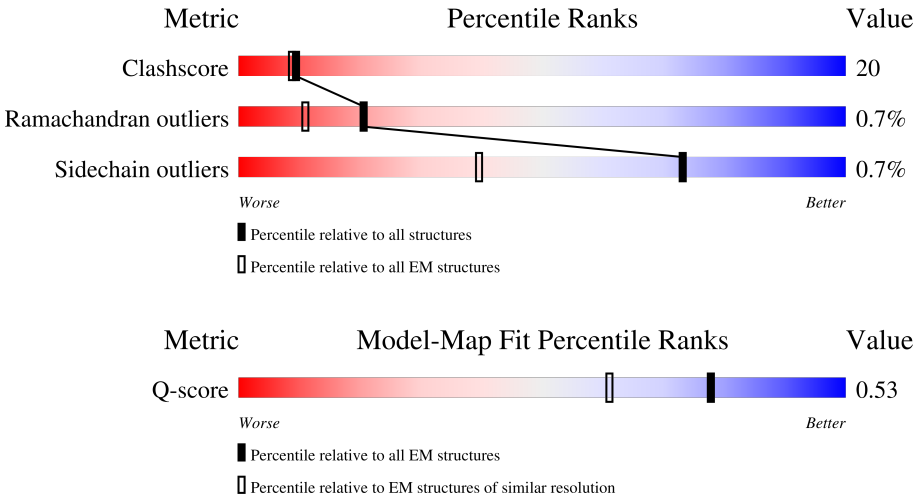
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.84 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	11884 (2.34 - 3.34)

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	740	79% 21%
2	B	733	78% 21%
3	C	80	78% 22%
4	D	144	74% 24%

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Mol	Chain	Length	Quality of chain
5	E	64	75% 25%
6	F	162	80% 20%
7	J	41	5% 66% 27% 7%
8	G	101	73% 59% 36%
9	H	92	63% 53% 43%
10	I	39	8% 49% 44% 8%
11	K	84	37% 50% 44% 6%
12	L	155	20% 58% 37%
13	O	86	62% 64% 36%
14	1	197	6% 81% 19%
15	2	208	81% 19%
16	3	228	76% 23%
17	4	211	5% 77% 23%
18	5	202	25% 71% 23% 6%
19	6	178	14% 58% 35% 6%

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	CLA	1	601	-	-	X	-
21	CLA	5	604	-	-	X	-
21	CLA	5	606	-	-	X	-
21	CLA	6	601	-	-	X	-
21	CLA	A	1121	-	-	X	-
21	CLA	B	1023	-	-	X	-
34	LUT	4	501	X	-	-	-
34	LUT	5	501	X	-	-	-
34	LUT	5	504	X	-	-	-
34	LUT	6	501	X	-	X	-
35	XAT	1	502	X	-	-	-
35	XAT	2	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	XAT	3	502	X	-	-	-
35	XAT	4	502	X	-	-	-
35	XAT	6	502	X	-	-	-
35	XAT	6	504	X	-	-	-
36	CHL	1	609	X	-	-	-
36	CHL	2	609	X	-	-	-
36	CHL	2	610	X	-	-	-
36	CHL	3	604	X	-	-	-
36	CHL	4	613	X	-	-	-
36	CHL	5	609	X	-	X	-
36	CHL	5	610	X	-	-	-

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 43789 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 I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	740	5808	3795	993	1002	18	0	0

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	733	5808	3815	974	1006	13	0	0

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	600	370	104	115	11	0	0

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	143	1134	727	197	204	6	0	0

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	64	515	327	89	99	0	0

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	162	1278	823	217	236	2	0	0

- Molecule 7 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	41	Total	C	N	O	S	0	0
			327	223	47	56	1		

- Molecule 8 is a protein called PsaG.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	101	Total	C	N	O	S	0	0
			773	500	135	136	2		

- Molecule 9 is a protein called PsaH.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	92	Total	C	N	O	S	0	0
			704	445	120	137	2		

- Molecule 10 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	39	Total	C	N	O	S	0	0
			301	208	43	49	1		

- Molecule 11 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	84	Total	C	N	O	S	0	0
			573	354	106	110	3		

- Molecule 12 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	155	Total	C	N	O	S	0	0
			1137	736	191	203	7		

- Molecule 13 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	86	Total	C	N	O	S	0	0
			684	456	108	118	2		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1	197	Total	C	N	O	S	0	0
			1501	963	255	276	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	204	ALA	GLU	conflict	UNP C1K003

- Molecule 15 is a protein called Lhca2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	2	208	Total	C	N	O	S	0	0
			1609	1033	272	297	7		

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3	228	Total	C	N	O	S	0	0
			1740	1134	284	317	5		

- Molecule 17 is a protein called Lhca4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	4	211	Total	C	N	O	S	0	0
			1637	1058	272	303	4		

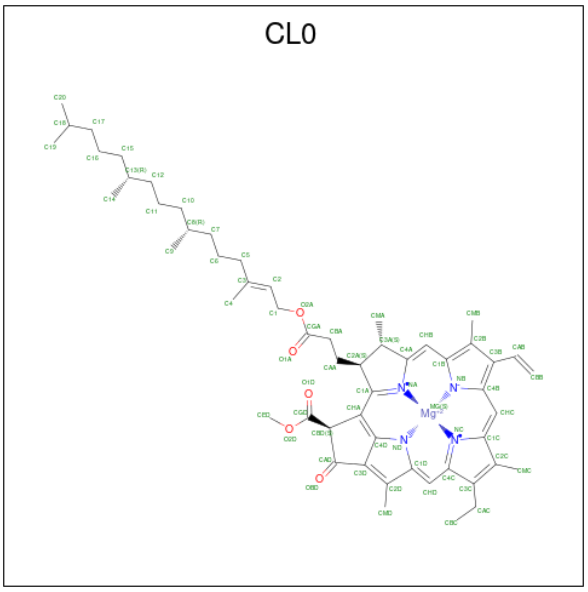
- Molecule 18 is a protein called Lhca5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	5	202	Total	C	N	O	S	0	0
			1525	977	257	284	7		

- Molecule 19 is a protein called Lhca6.

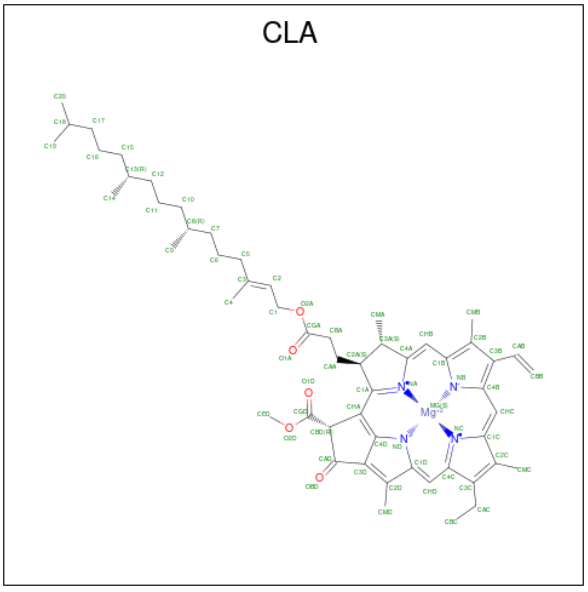
Mol	Chain	Residues	Atoms					AltConf	Trace
19	6	178	Total	C	N	O	S	0	0
			1378	896	230	245	7		

- Molecule 20 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	F	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	F	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	J	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
21	G	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	K	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
21	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	O	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
21	O	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
21	O	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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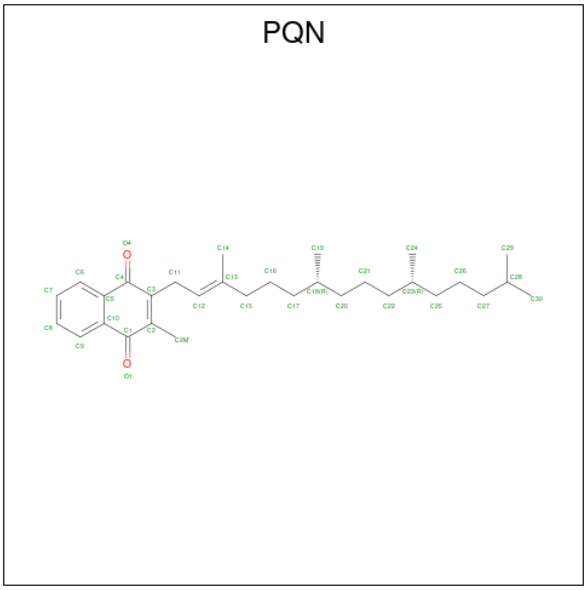
Mol	Chain	Residues	Atoms					AltConf
21	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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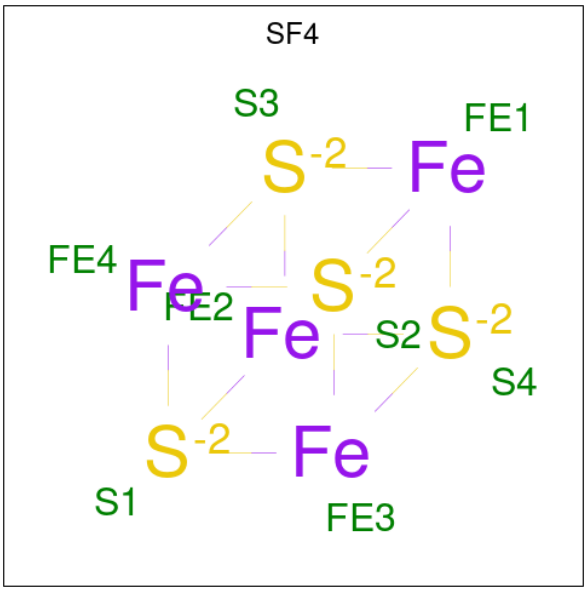
Mol	Chain	Residues	Atoms					AltConf
21	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 22 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



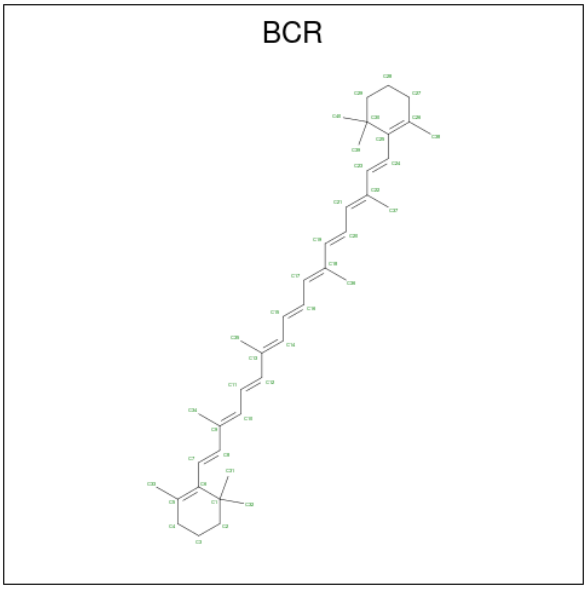
Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total	C	O	0
			33	31	2	
22	B	1	Total	C	O	0
			33	31	2	

- Molecule 23 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	C	0
			40	40	

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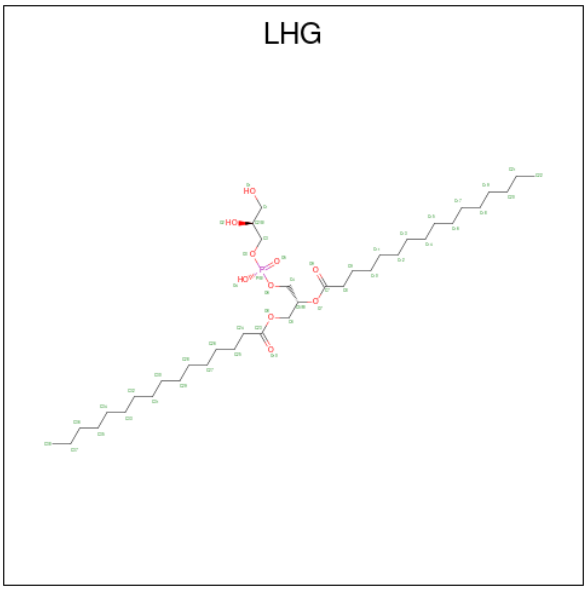
Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	H	1	Total C 40 40	0
24	I	1	Total C 40 40	0
24	I	1	Total C 40 40	0
24	K	1	Total C 40 40	0

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

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



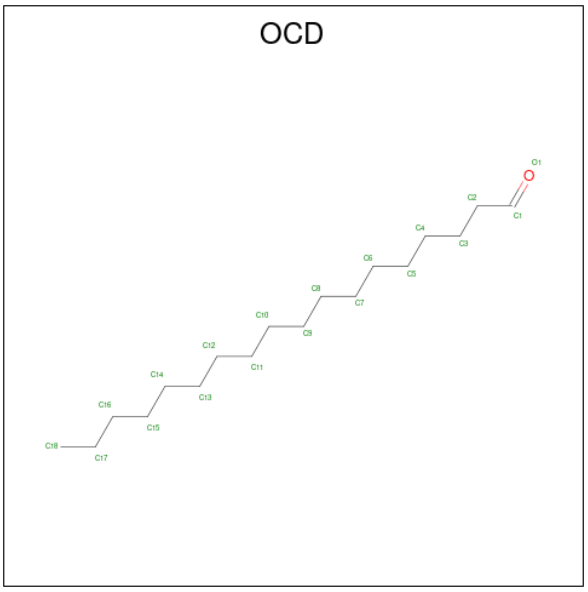
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C O P 49 38 10 1	0
25	A	1	Total C O P 49 38 10 1	0

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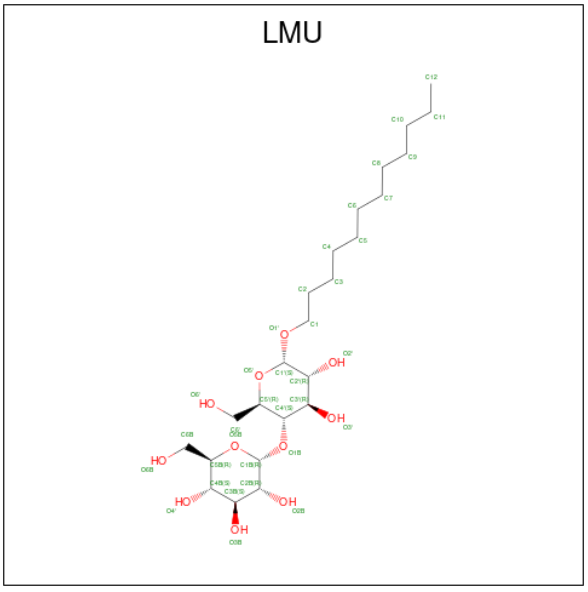
Mol	Chain	Residues	Atoms				AltConf
25	B	1	Total	C	O	P	0
			42	31	10	1	
25	F	1	Total	C	O	P	0
			49	38	10	1	
25	1	1	Total	C	O	P	0
			49	38	10	1	
25	1	1	Total	C	O	P	0
			26	15	10	1	
25	1	1	Total	C	O	P	0
			31	20	10	1	
25	2	1	Total	C	O	P	0
			35	24	10	1	
25	2	1	Total	C	O	P	0
			43	32	10	1	
25	2	1	Total	C	O	P	0
			36	25	10	1	
25	3	1	Total	C	O	P	0
			17	8	8	1	
25	4	1	Total	C	O	P	0
			29	18	10	1	
25	5	1	Total	C	O	P	0
			43	32	10	1	
25	5	1	Total	C	O	P	0
			24	13	10	1	
25	6	1	Total	C	O	P	0
			25	14	10	1	

- Molecule 26 is octadecanal (CCD ID: OCD) (formula: $C_{18}H_{36}O$).



Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			19	18	1	

- Molecule 27 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



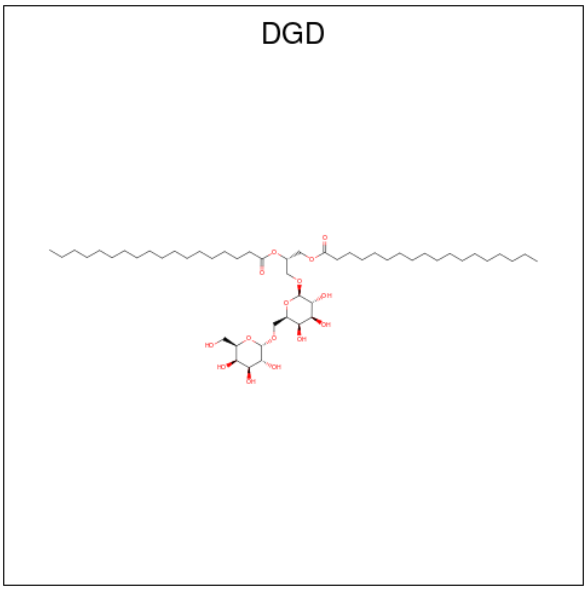
Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			35	24	11	
27	A	1	Total	C	O	0
			35	24	11	
27	B	1	Total	C	O	0
			35	24	11	

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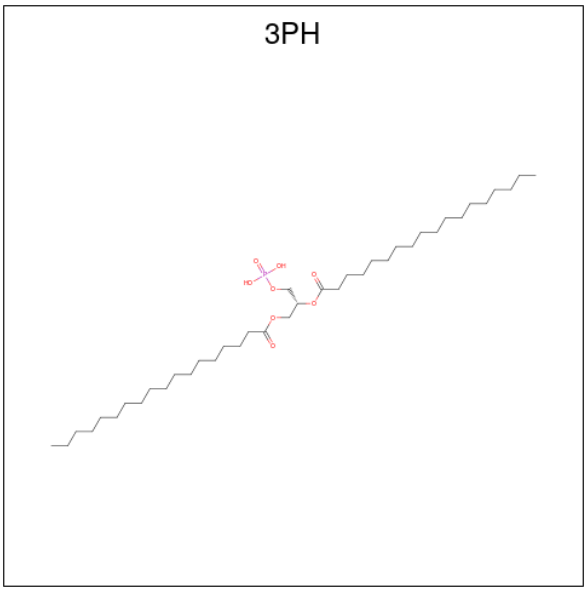
Mol	Chain	Residues	Atoms			AltConf
27	6	1	Total	C	O	0
			35	24	11	

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	C	O	0
			61	46	15	
28	2	1	Total	C	O	0
			39	24	15	
28	3	1	Total	C	O	0
			39	24	15	
28	3	1	Total	C	O	0
			45	30	15	

- Molecule 29 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).

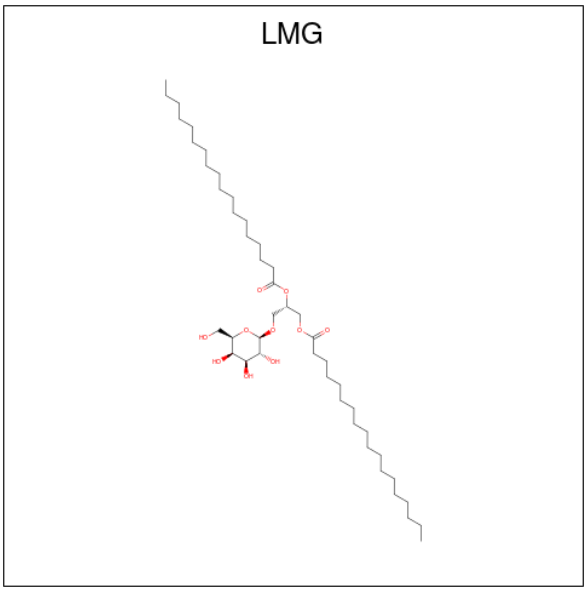


Mol	Chain	Residues	Atoms				AltConf
29	B	1	Total	C	O	P	0
			31	22	8	1	
29	F	1	Total	C	O	P	0
			34	25	8	1	
29	5	1	Total	C	O	P	0
			28	19	8	1	
29	5	1	Total	C	O	P	0
			29	20	8	1	

- Molecule 30 is CALCIUM ION (CCD ID: CA) (formula: Ca).

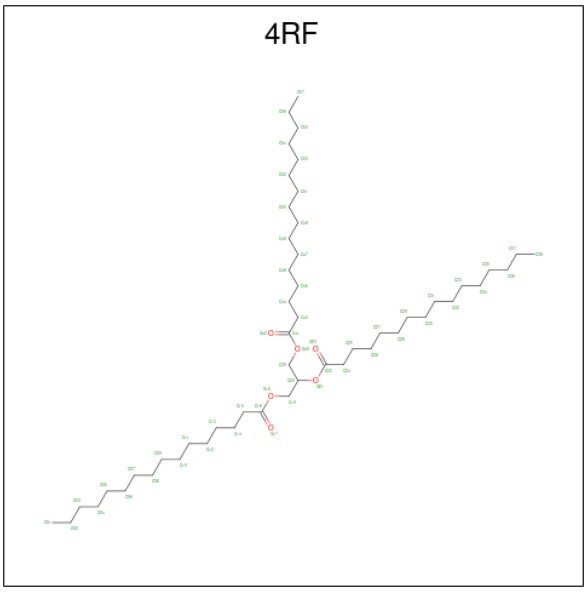
Mol	Chain	Residues	Atoms		AltConf
30	B	1	Total	Ca	0
			1	1	

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



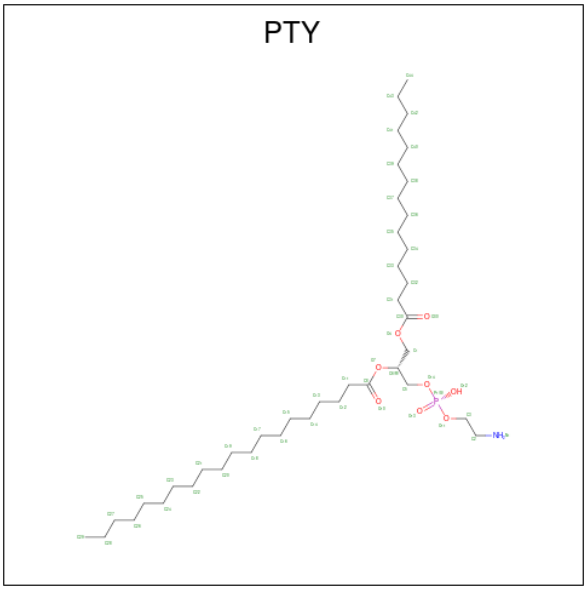
Mol	Chain	Residues	Atoms	AltConf
31	F	1	Total C O 50 40 10	0
31	1	1	Total C O 32 22 10	0
31	2	1	Total C O 50 40 10	0
31	3	1	Total C O 32 22 10	0
31	3	1	Total C O 50 40 10	0
31	4	1	Total C O 46 36 10	0
31	4	1	Total C O 39 29 10	0
31	6	1	Total C O 37 27 10	0

- Molecule 32 is Tripalmitoylglycerol (CCD ID: 4RF) (formula: $C_{51}H_{98}O_6$).



Mol	Chain	Residues	Atoms			AltConf
32	L	1	Total 39	C 33	O 6	0
32	5	1	Total 32	C 26	O 6	0

- Molecule 33 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



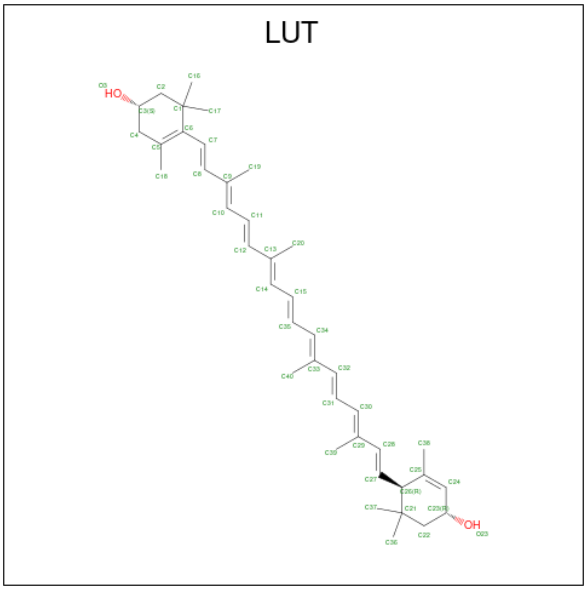
Mol	Chain	Residues	Atoms					AltConf
33	L	1	Total 20	C 10	N 1	O 8	P 1	0
33	O	1	Total 22	C 12	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
33	1	1	Total	C	N	O	P	0
			40	30	1	8	1	
33	1	1	Total	C	N	O	P	0
			18	8	1	8	1	
33	3	1	Total	C	N	O	P	0
			26	16	1	8	1	
33	3	1	Total	C	N	O	P	0
			20	10	1	8	1	
33	4	1	Total	C	N	O	P	0
			35	25	1	8	1	
33	5	1	Total	C	N	O	P	0
			36	26	1	8	1	
33	6	1	Total	C	N	O	P	0
			24	14	1	8	1	

- Molecule 34 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



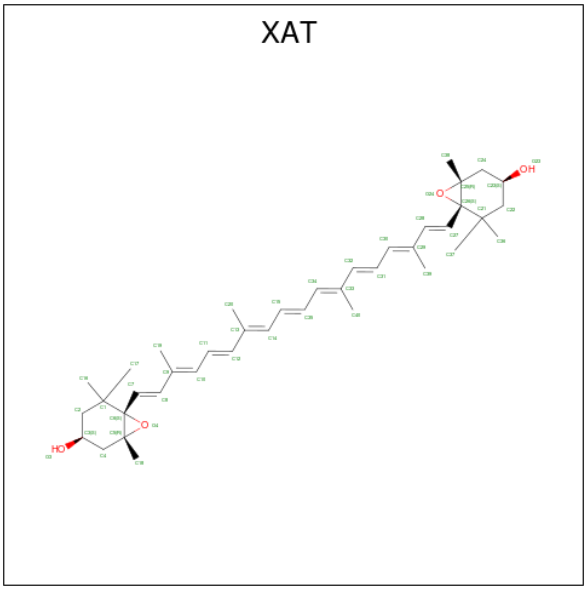
Mol	Chain	Residues	Atoms			AltConf
34	1	1	Total	C	O	0
			42	40	2	
34	2	1	Total	C	O	0
			42	40	2	
34	3	1	Total	C	O	0
			42	40	2	
34	4	1	Total	C	O	0
			42	40	2	

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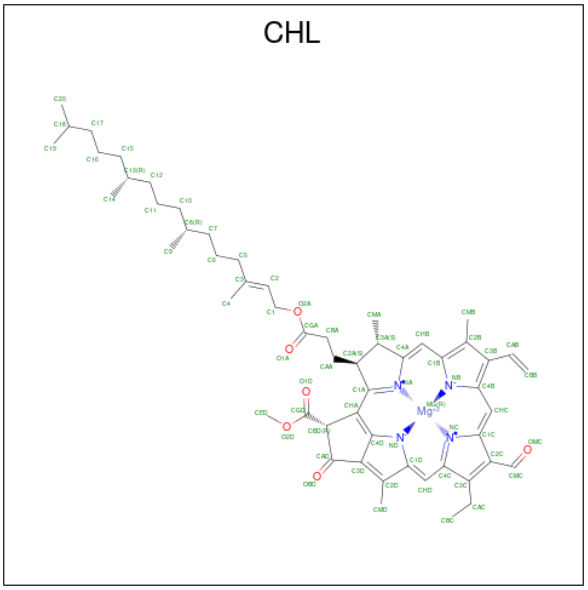
Mol	Chain	Residues	Atoms	AltConf
34	5	1	Total C O 42 40 2	0
34	5	1	Total C O 42 40 2	0
34	5	1	Total C O 42 40 2	0
34	5	1	Total C O 42 40 2	0
34	6	1	Total C O 42 40 2	0

- Molecule 35 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



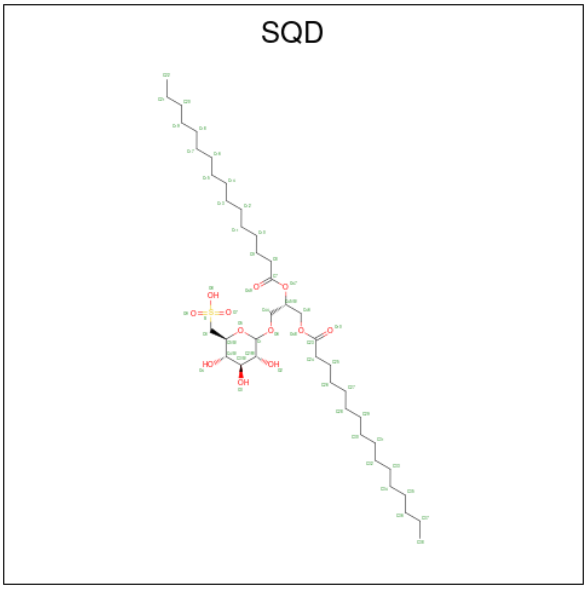
Mol	Chain	Residues	Atoms	AltConf
35	1	1	Total C O 44 40 4	0
35	2	1	Total C O 44 40 4	0
35	3	1	Total C O 44 40 4	0
35	4	1	Total C O 44 40 4	0
35	6	1	Total C O 44 40 4	0
35	6	1	Total C O 44 40 4	0

- Molecule 36 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



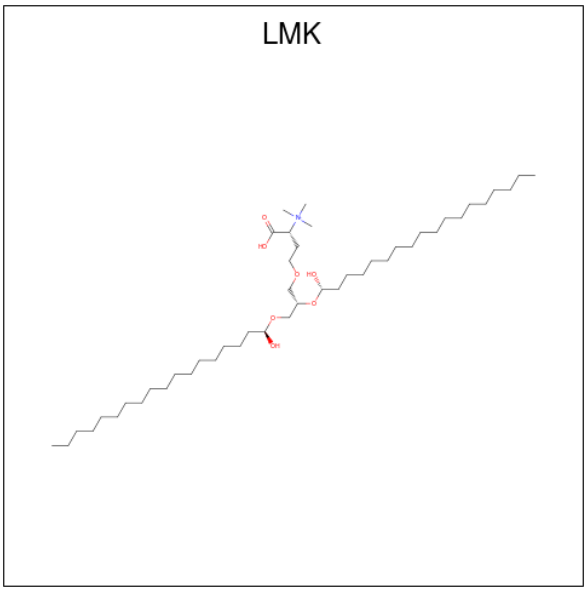
Mol	Chain	Residues	Atoms					AltConf
36	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
36	1	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
36	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
36	2	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
36	2	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
36	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
36	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
36	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
36	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
36	4	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
36	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
36	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
36	6	1	Total	C	Mg	N	O	0
			47	36	1	4	6	

- Molecule 37 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



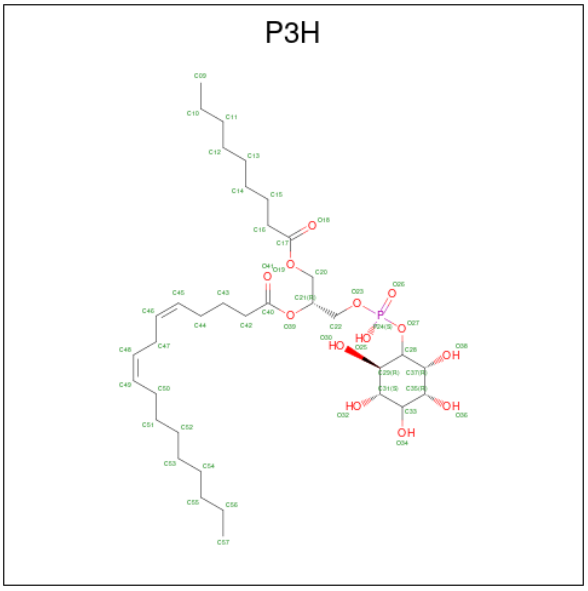
Mol	Chain	Residues	Atoms				AltConf
37	2	1	Total	C	O	S	0
			40	27	12	1	
37	3	1	Total	C	O	S	0
			35	22	12	1	
37	6	1	Total	C	O	S	0
			32	19	12	1	

- Molecule 38 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxidanyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanium (CCD ID: LMK) (formula: $C_{46}H_{94}NO_7$).



Mol	Chain	Residues	Atoms				AltConf
38	2	1	Total	C	N	O	0
			31	23	1	7	
38	4	1	Total	C	N	O	0
			35	27	1	7	

- Molecule 39 is [(2 {R})-1-nonanoyloxy-3-[oxidanyl-[(2 {R},3 {S},5 {R},6 {R})-2,3,4,5,6-pentakis(oxidanyl)cyclohexyl]oxy-phosphoryl]oxy-propan-2-yl] (5 {Z},8 {Z})-heptadeca-5,8-dienoate (CCD ID: P3H) (formula: $C_{35}H_{63}O_{13}P$).



Mol	Chain	Residues	Atoms				AltConf
39	2	1	Total	C	O	P	0
			49	35	13	1	

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Mol	Chain	Residues	Atoms				AltConf
39	5	1	Total	C	O	P	0
			32	18	13	1	

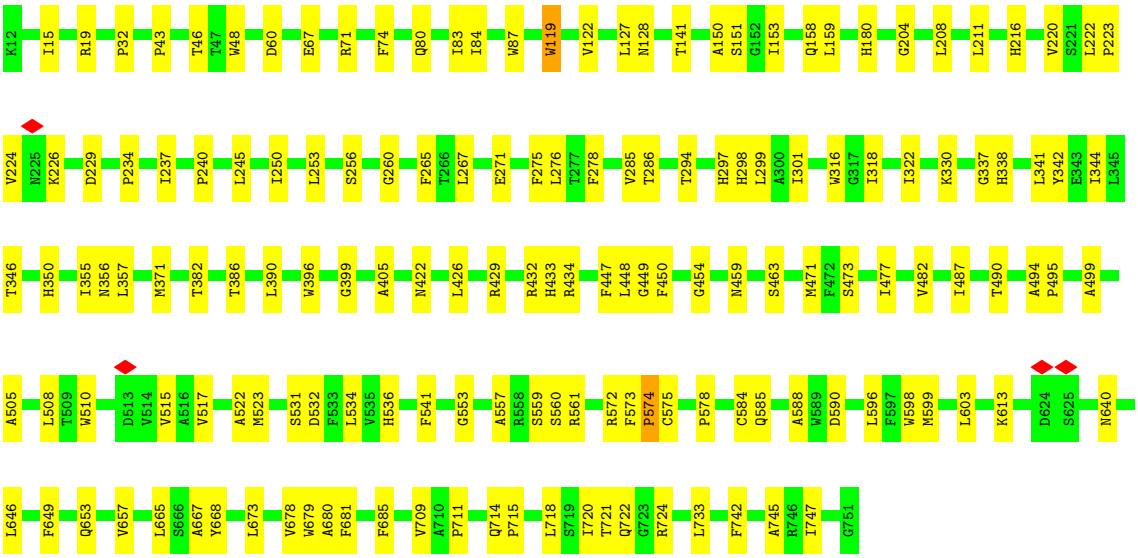
3 Residue-property plots (i)

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 I P700 chlorophyll a apoprotein A1

Chain A:

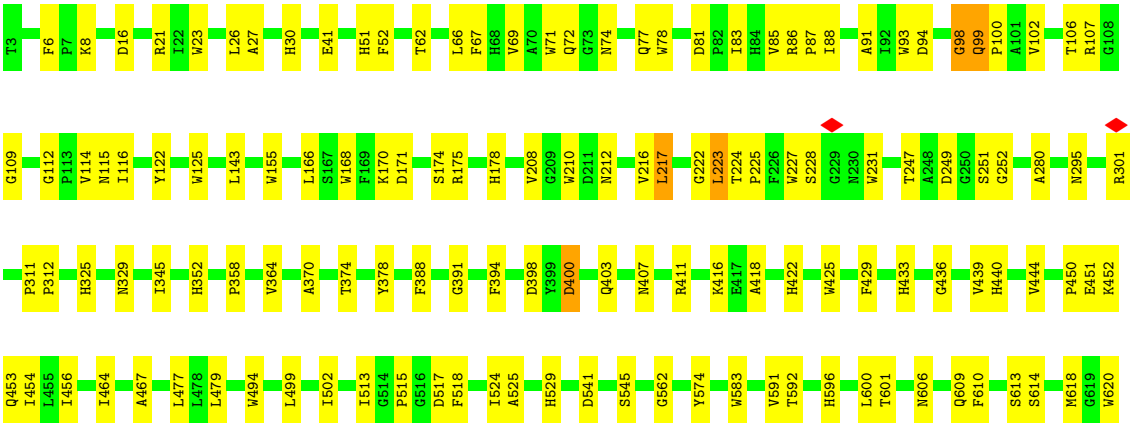




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

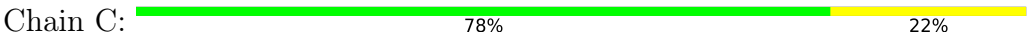
Chain B:

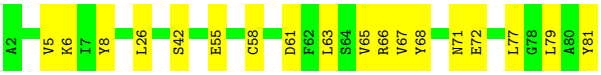






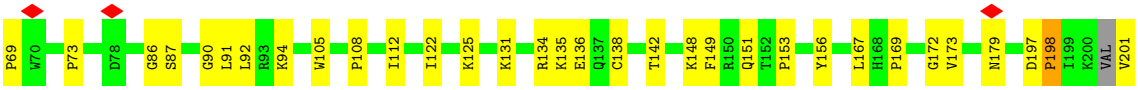
• Molecule 3: Photosystem I iron-sulfur center





• Molecule 4: PsaD

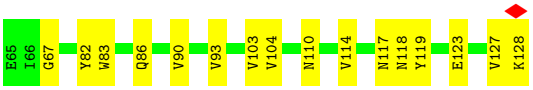




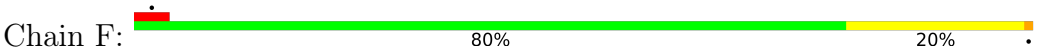


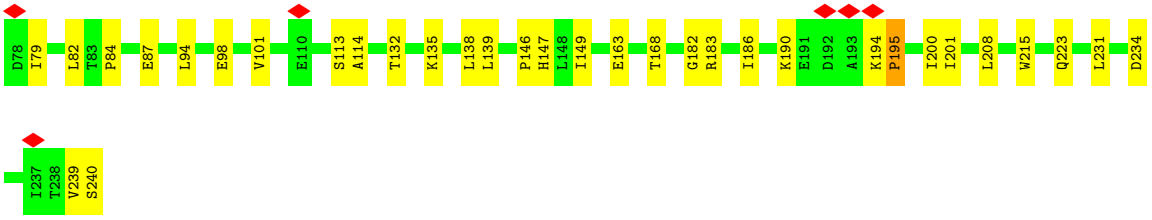
• Molecule 5: PsaE





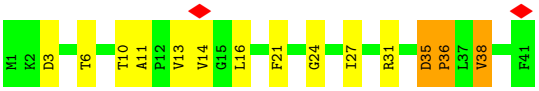
• Molecule 6: PsaF





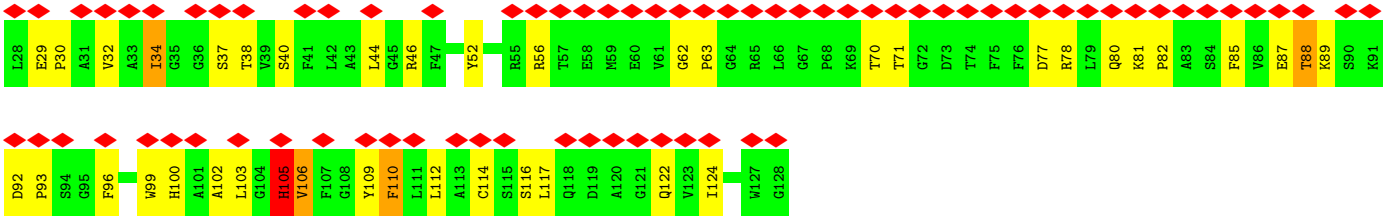
• Molecule 7: Photosystem I reaction center subunit IX





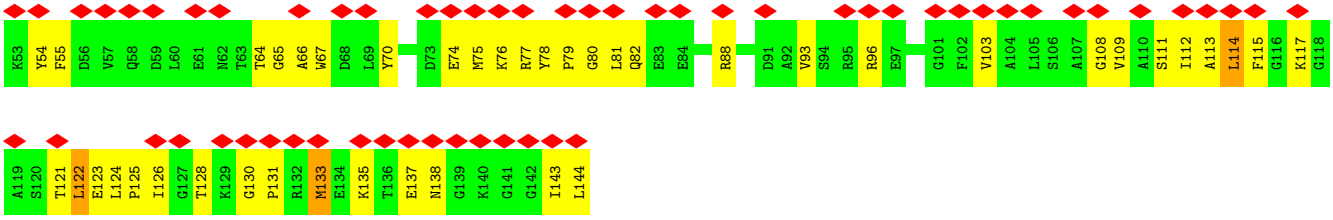
• Molecule 8: PsaG





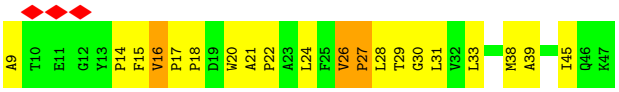
• Molecule 9: PsaH





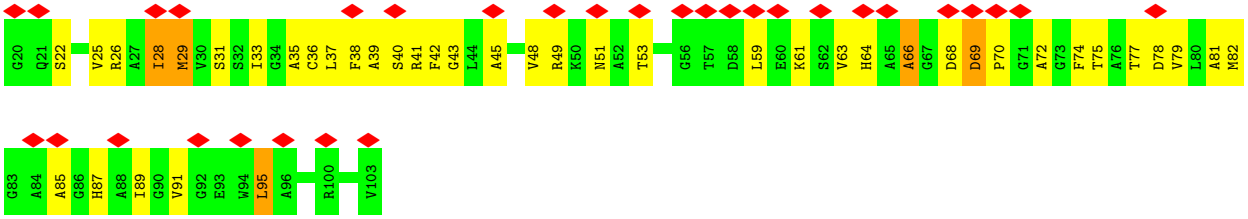
• Molecule 10: PsaI





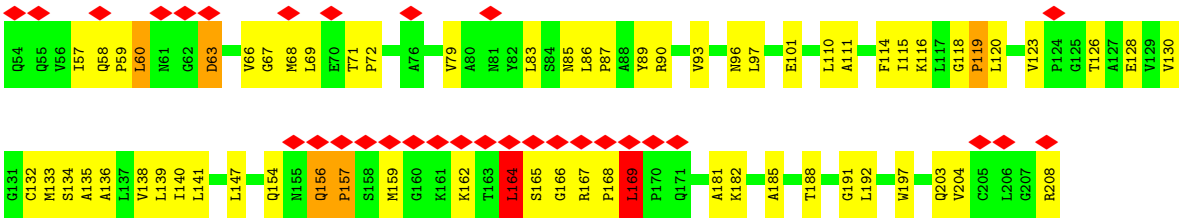
• Molecule 11: PsaK





• Molecule 12: PsaL

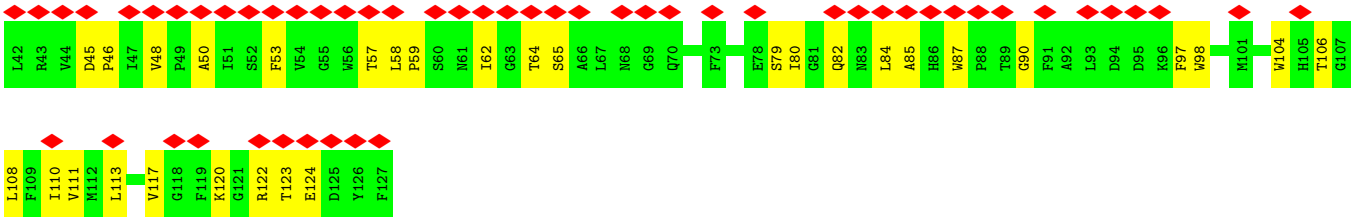




• Molecule 13: PsaO

Chain O:

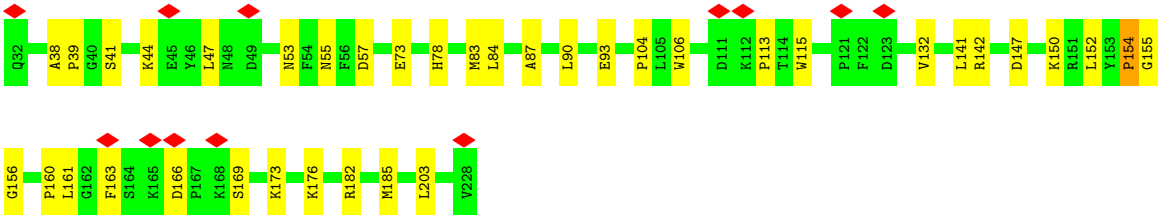




• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 1:

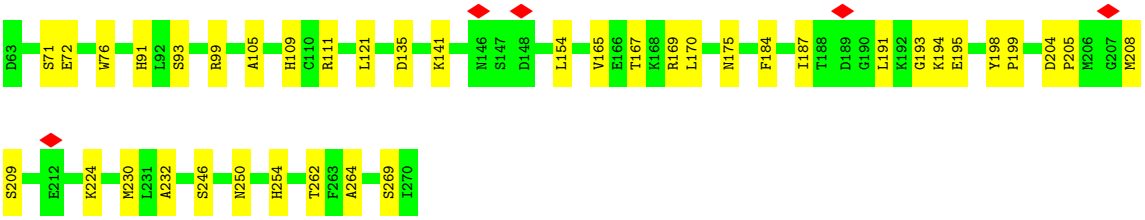




• Molecule 15: Lhca2

Chain 2:

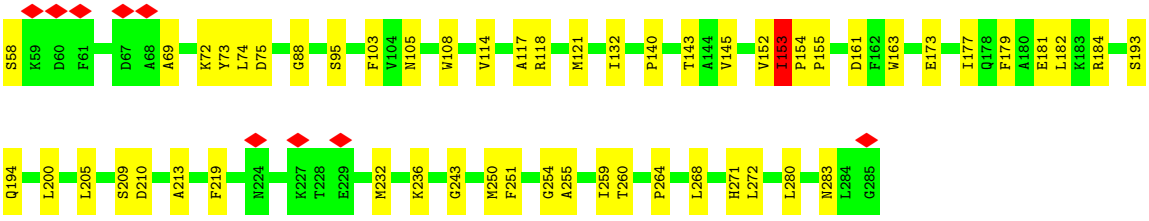




• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 3:

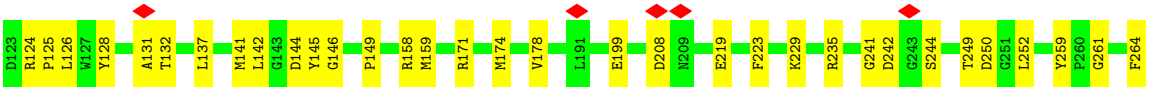


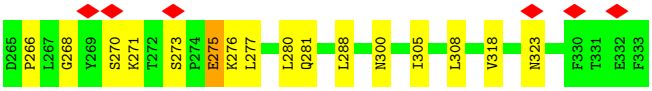


• Molecule 17: Lhca4

Chain 4:



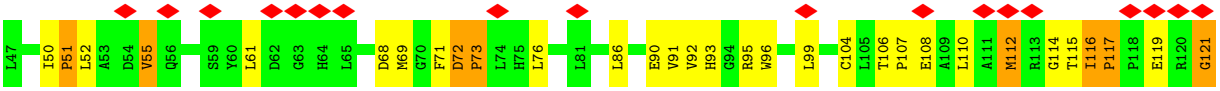


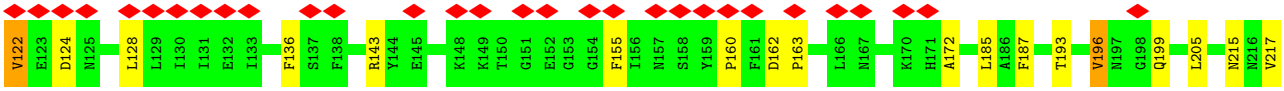


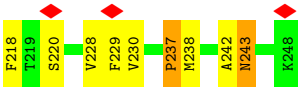
• Molecule 18: Lhca5

Chain 5:





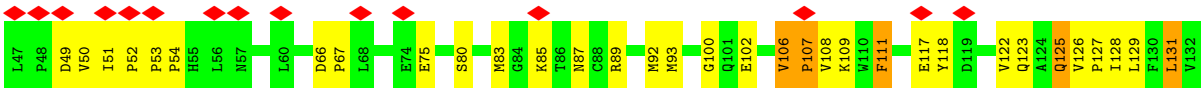


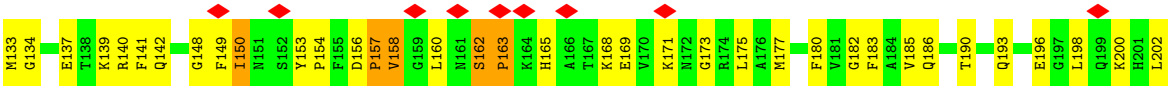


• Molecule 19: Lhca6

Chain 6:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	189006	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42.68	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.155	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0247	Depositor
Map size (Å)	384.12003, 384.12003, 384.12003	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.067, 1.067, 1.067	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 4RF, OCD, PQN, CL0, P3H, BCR, XAT, CLA, LMK, PTY, SQD, DGD, LHG, 3PH, CHL, LMU, LMG, LUT, SF4

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	0.56	4/6004 (0.1%)	0.77	7/8190 (0.1%)
2	B	0.58	3/6021 (0.0%)	0.79	8/8230 (0.1%)
3	C	0.43	0/610	0.67	0/828
4	D	0.77	2/1164 (0.2%)	1.03	3/1570 (0.2%)
5	E	0.50	0/525	0.62	0/712
6	F	0.78	2/1305 (0.2%)	1.02	3/1764 (0.2%)
7	J	1.15	2/338 (0.6%)	1.39	3/461 (0.7%)
8	G	0.76	1/796 (0.1%)	1.14	8/1077 (0.7%)
9	H	0.75	0/716	1.16	2/963 (0.2%)
10	I	1.55	3/315 (1.0%)	1.97	6/437 (1.4%)
11	K	0.96	1/581 (0.2%)	1.47	7/785 (0.9%)
12	L	1.32	8/1164 (0.7%)	1.71	13/1589 (0.8%)
13	O	0.69	0/708	0.93	1/966 (0.1%)
14	1	0.42	0/1540	0.68	0/2088
15	2	0.37	0/1656	0.59	0/2243
16	3	0.46	0/1790	0.67	1/2432 (0.0%)
17	4	0.46	0/1687	0.73	1/2300 (0.0%)
18	5	0.96	3/1561 (0.2%)	1.25	7/2123 (0.3%)
19	6	0.92	2/1417 (0.1%)	1.31	10/1929 (0.5%)
All	All	0.70	31/29898 (0.1%)	0.96	80/40687 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	K	0	2
16	3	0	1
All	All	0	3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	157	PRO	N-CA	22.30	1.70	1.47
18	5	73	PRO	N-CA	19.88	1.70	1.47
7	J	36	PRO	N-CA	18.05	1.70	1.47
6	F	195	PRO	N-CA	18.00	1.70	1.47
1	A	574	PRO	N-CA	17.69	1.70	1.47
19	6	218	PRO	N-CA	17.46	1.70	1.47
4	D	198	PRO	N-CA	17.28	1.70	1.47
12	L	119	PRO	N-CA	17.25	1.70	1.47
10	I	27	PRO	N-CA	16.98	1.70	1.47
12	L	63	ASP	C-N	15.43	1.50	1.34
2	B	400	ASP	C-N	14.53	1.51	1.33
10	I	16	VAL	C-N	14.30	1.50	1.33
12	L	169	LEU	C-N	14.18	1.50	1.33
2	B	99	GLN	C-N	14.17	1.51	1.34
18	5	237	PRO	N-CD	-11.17	1.32	1.47
10	I	26	VAL	C-N	10.32	1.45	1.34
19	6	217	THR	C-N	9.94	1.45	1.33
18	5	72	ASP	C-N	9.65	1.45	1.33
12	L	118	GLY	C-N	9.11	1.45	1.33
4	D	197	ASP	C-N	8.59	1.45	1.34
2	B	311	PRO	CA-C	8.12	1.57	1.52
11	K	69	ASP	C-N	7.11	1.50	1.33
1	A	714	GLN	C-N	7.11	1.50	1.33
12	L	86	LEU	C-N	7.02	1.50	1.33
1	A	119	TRP	C-N	6.94	1.50	1.33
8	G	106	VAL	CB-CG1	-5.82	1.33	1.52
12	L	71	THR	C-N	5.24	1.41	1.33
7	J	35	ASP	C-N	5.11	1.45	1.33
12	L	156	GLN	C-N	5.09	1.45	1.33
1	A	573	PHE	C-N	5.09	1.45	1.33
6	F	194	LYS	C-N	5.08	1.45	1.33

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	5	72	ASP	CA-C-N	19.41	139.70	119.90
18	5	72	ASP	C-N-CA	19.41	139.70	119.90
19	6	217	THR	CA-C-N	19.13	139.07	119.56
19	6	217	THR	C-N-CA	19.13	139.07	119.56
12	L	169	LEU	CA-C-N	18.37	138.31	120.31
12	L	169	LEU	C-N-CA	18.37	138.31	120.31
12	L	118	GLY	CA-C-N	18.24	139.35	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	118	GLY	C-N-CA	18.24	139.35	119.28
10	I	26	VAL	CA-C-N	17.99	138.58	119.87
10	I	26	VAL	C-N-CA	17.99	138.58	119.87
4	D	197	ASP	CA-C-N	17.88	138.89	119.05
4	D	197	ASP	C-N-CA	17.88	138.89	119.05
12	L	63	ASP	CA-C-N	16.51	137.87	120.04
12	L	63	ASP	C-N-CA	16.51	137.87	120.04
7	J	35	ASP	CA-C-N	16.49	140.46	119.84
7	J	35	ASP	C-N-CA	16.49	140.46	119.84
10	I	16	VAL	CA-C-N	16.28	137.15	120.38
10	I	16	VAL	C-N-CA	16.28	137.15	120.38
1	A	573	PHE	CA-C-N	15.70	139.47	119.84
1	A	573	PHE	C-N-CA	15.70	139.47	119.84
6	F	194	LYS	CA-C-N	15.56	139.29	119.84
6	F	194	LYS	C-N-CA	15.56	139.29	119.84
12	L	86	LEU	CA-C-N	14.65	138.16	119.84
12	L	86	LEU	C-N-CA	14.65	138.16	119.84
12	L	156	GLN	CA-C-N	14.58	139.74	120.79
12	L	156	GLN	C-N-CA	14.58	139.74	120.79
1	A	714	GLN	CA-C-N	13.98	137.32	119.84
1	A	714	GLN	C-N-CA	13.98	137.32	119.84
2	B	400	ASP	CA-C-N	13.08	132.90	119.56
2	B	400	ASP	C-N-CA	13.08	132.90	119.56
11	K	69	ASP	CA-C-N	12.69	135.70	119.84
11	K	69	ASP	C-N-CA	12.69	135.70	119.84
2	B	99	GLN	CA-C-N	12.15	132.06	119.19
2	B	99	GLN	C-N-CA	12.15	132.06	119.19
7	J	36	PRO	CA-N-CD	-10.17	97.76	112.00
2	B	311	PRO	O-C-N	9.20	125.47	121.15
1	A	574	PRO	CA-N-CD	-8.91	99.52	112.00
8	G	105	HIS	CA-CB-CG	8.71	122.51	113.80
18	5	73	PRO	CA-N-CD	-8.64	99.90	112.00
2	B	98	GLY	O-C-N	8.36	132.37	123.09
19	6	218	PRO	CA-N-CD	-8.32	100.36	112.00
12	L	119	PRO	CA-N-CD	-8.25	100.45	112.00
4	D	198	PRO	CA-N-CD	-8.21	100.50	112.00
6	F	195	PRO	CA-N-CD	-8.21	100.50	112.00
12	L	157	PRO	CA-N-CD	-8.16	100.58	112.00
10	I	27	PRO	CA-N-CD	-8.14	100.60	112.00
10	I	27	PRO	N-CA-C	-7.65	104.62	114.03
11	K	29	MET	N-CA-C	-7.49	103.20	111.36
11	K	66	ALA	CA-C-N	-6.96	115.84	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	K	66	ALA	C-N-CA	-6.96	115.84	122.66
19	6	51	ILE	N-CA-C	6.90	123.78	108.88
19	6	117	GLU	CA-C-N	6.81	134.55	121.54
19	6	117	GLU	C-N-CA	6.81	134.55	121.54
13	O	64	THR	N-CA-C	6.63	119.11	111.02
8	G	106	VAL	CG1-CB-CG2	-6.42	96.68	110.80
2	B	400	ASP	CA-C-O	-6.21	115.25	119.29
1	A	119	TRP	CA-C-N	6.11	135.92	120.53
1	A	119	TRP	C-N-CA	6.11	135.92	120.53
9	H	80	GLY	CA-C-N	5.91	132.84	121.54
9	H	80	GLY	C-N-CA	5.91	132.84	121.54
18	5	119	GLU	CA-CB-CG	5.84	125.78	114.10
11	K	36	CYS	CA-CB-SG	-5.83	100.98	114.40
19	6	131	LEU	CB-CG-CD1	-5.83	93.22	110.70
8	G	109	TYR	CA-CB-CG	5.74	124.24	113.90
19	6	106	VAL	CA-C-N	5.59	126.83	119.84
19	6	106	VAL	C-N-CA	5.59	126.83	119.84
11	K	36	CYS	N-CA-CB	-5.56	101.67	110.28
17	4	275	GLU	N-CA-C	-5.51	99.07	110.80
16	3	153	ILE	O-C-N	-5.40	114.95	121.10
19	6	148	GLY	CA-C-O	-5.39	118.27	122.52
8	G	110	PHE	N-CA-C	-5.36	106.25	112.89
18	5	121	GLY	CA-C-N	5.28	131.47	121.97
18	5	121	GLY	C-N-CA	5.28	131.47	121.97
8	G	37	SER	CA-CB-OG	-5.23	100.64	111.10
8	G	37	SER	CB-CA-C	-5.13	102.18	110.79
2	B	669	ARG	N-CA-C	5.11	116.85	111.28
8	G	88	THR	N-CA-C	-5.09	107.73	114.04
18	5	196	VAL	N-CA-CB	-5.04	97.98	111.75
12	L	164	LEU	CA-CB-CG	5.01	133.84	116.30
8	G	34	ILE	N-CA-C	-5.01	107.97	113.43

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	3	153	ILE	Mainchain
11	K	66	ALA	Mainchain
11	K	68	ASP	Mainchain

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	5808	0	5642	142	0
2	B	5808	0	5560	189	0
3	C	600	0	582	13	0
4	D	1134	0	1142	26	0
5	E	515	0	508	10	0
6	F	1278	0	1299	41	0
7	J	327	0	328	18	0
8	G	773	0	756	45	0
9	H	704	0	693	91	0
10	I	301	0	297	41	0
11	K	573	0	567	55	0
12	L	1137	0	1165	80	0
13	O	684	0	661	33	0
14	1	1501	0	1469	38	0
15	2	1609	0	1556	31	0
16	3	1740	0	1698	54	0
17	4	1637	0	1579	47	0
18	5	1525	0	1517	91	0
19	6	1378	0	1382	96	0
20	A	65	0	72	10	0
21	1	682	0	648	52	0
21	2	602	0	609	13	0
21	3	746	0	722	49	0
21	4	632	0	600	28	0
21	5	602	0	549	100	0
21	6	602	0	542	98	0
21	A	2658	0	2762	220	0
21	B	2619	0	2762	200	0
21	F	96	0	74	2	0
21	G	138	0	99	18	0
21	H	106	0	92	4	0
21	J	49	0	38	3	0
21	K	193	0	148	35	0
21	L	230	0	219	24	0
21	O	136	0	95	3	0
22	A	33	0	46	3	0
22	B	33	0	46	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	A	8	0	0	0	0
23	C	16	0	0	0	0
24	1	40	0	53	5	0
24	2	40	0	53	1	0
24	3	120	0	159	15	0
24	4	40	0	53	1	0
24	A	280	0	367	41	0
24	B	240	0	317	38	0
24	F	80	0	106	24	0
24	G	40	0	53	20	0
24	H	40	0	53	5	0
24	I	80	0	106	16	0
24	J	80	0	105	7	0
24	K	40	0	53	8	0
24	L	80	0	106	5	0
24	O	40	0	52	7	0
25	1	106	0	128	5	0
25	2	114	0	141	8	0
25	3	17	0	12	0	0
25	4	29	0	28	0	0
25	5	67	0	77	11	0
25	6	25	0	20	0	0
25	A	98	0	148	6	0
25	B	42	0	57	3	0
25	F	49	0	74	2	0
26	A	19	0	0	0	0
27	6	35	0	46	1	0
27	A	70	0	92	2	0
27	B	35	0	46	2	0
28	2	39	0	36	2	0
28	3	84	0	84	6	0
28	B	61	0	83	5	0
29	5	57	0	60	5	0
29	B	31	0	35	2	0
29	F	34	0	41	0	0
30	B	1	0	0	0	0
31	1	32	0	34	1	0
31	2	50	0	73	0	0
31	3	82	0	107	19	0
31	4	85	0	113	2	0
31	6	37	0	44	12	0
31	F	50	0	73	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	5	32	0	39	1	0
32	L	39	0	53	2	0
33	1	58	0	64	0	0
33	3	46	0	38	0	0
33	4	35	0	43	0	0
33	5	36	0	48	10	0
33	6	24	0	21	1	0
33	L	20	0	13	0	0
33	O	22	0	17	5	0
34	1	42	0	55	7	0
34	2	42	0	55	6	0
34	3	42	0	55	9	0
34	4	42	0	55	4	0
34	5	168	0	220	41	0
34	6	42	0	55	22	0
35	1	44	0	56	2	0
35	2	44	0	56	3	0
35	3	44	0	56	7	0
35	4	44	0	56	3	0
35	6	88	0	112	14	0
36	1	113	0	100	7	0
36	2	216	0	180	8	0
36	3	66	0	69	3	0
36	4	159	0	124	1	0
36	5	113	0	100	40	0
36	6	47	0	30	7	0
37	2	40	0	46	2	0
37	3	35	0	33	2	0
37	6	32	0	27	1	0
38	2	31	0	0	0	0
38	4	35	0	0	0	0
39	2	49	0	0	0	0
39	5	32	0	0	1	0
All	All	43789	0	43688	1758	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 20.

All (1758) 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)
10:I:27:PRO:N	10:I:27:PRO:CA	1.69	1.49
12:L:157:PRO:N	12:L:157:PRO:CA	1.69	1.47
1:A:574:PRO:N	1:A:574:PRO:CA	1.70	1.45
6:F:195:PRO:N	6:F:195:PRO:CA	1.70	1.42
18:5:73:PRO:N	18:5:73:PRO:CA	1.70	1.42
19:6:218:PRO:N	19:6:218:PRO:CA	1.70	1.40
7:J:36:PRO:N	7:J:36:PRO:CA	1.70	1.38
12:L:119:PRO:N	12:L:119:PRO:CA	1.70	1.37
4:D:198:PRO:N	4:D:198:PRO:CA	1.70	1.36
11:K:40:SER:CB	11:K:82:MET:HG3	1.70	1.21
21:6:608:CLA:HHC	21:6:608:CLA:HBB1	1.25	1.15
34:5:502:LUT:H28	34:5:502:LUT:H361	1.26	1.15
21:A:1012:CLA:H43	2:B:439:VAL:HG22	1.26	1.14
34:6:501:LUT:H363	21:6:601:CLA:O1A	1.47	1.14
36:5:610:CHL:HMA1	33:5:803:PTY:H431	1.17	1.13
2:B:106:THR:HG21	9:H:128:THR:HB	1.31	1.12
2:B:112:GLY:HA2	9:H:128:THR:HG21	1.32	1.11
21:6:602:CLA:HHC	21:6:602:CLA:HBB1	1.29	1.11
1:A:211:LEU:HD21	24:A:4001:BCR:H10C	1.33	1.10
21:6:603:CLA:HHC	21:6:603:CLA:HBB1	1.28	1.09
21:B:1212:CLA:H93	24:B:4001:BCR:H311	1.23	1.09
21:A:1121:CLA:H92	21:K:1403:CLA:HBC2	1.08	1.08
21:A:1121:CLA:HHC	21:A:1121:CLA:HBB1	1.29	1.08
10:I:38:MET:HG2	24:L:4001:BCR:H10C	1.35	1.08
21:6:601:CLA:HED2	21:6:601:CLA:H2A	1.08	1.07
14:1:83:MET:HE1	21:1:601:CLA:HAB	1.26	1.07
21:A:1132:CLA:H143	21:L:1502:CLA:HBB1	1.36	1.07
21:B:1023:CLA:H2	21:B:1023:CLA:HMA2	1.37	1.07
21:B:1239:CLA:HHC	21:B:1239:CLA:HBB1	1.32	1.06
21:B:1208:CLA:HBB1	21:B:1208:CLA:HHC	1.35	1.05
9:H:70:TYR:CE1	12:L:83:LEU:HD12	1.91	1.04
8:G:81:LYS:HA	8:G:81:LYS:HE2	1.40	1.04
21:B:1207:CLA:HBB1	21:B:1207:CLA:HHC	1.34	1.04
16:3:153:ILE:HG22	16:3:155:PRO:HD2	1.40	1.03
21:A:1121:CLA:C9	21:K:1403:CLA:HBC2	1.89	1.02
34:6:501:LUT:H28	34:6:501:LUT:H361	1.39	1.02
2:B:99:GLN:HB3	2:B:100:PRO:HD3	1.41	1.01
2:B:168:TRP:CE2	21:B:1208:CLA:HMA3	1.94	1.01
11:K:40:SER:HB2	11:K:82:MET:HG3	1.03	1.01
34:5:503:LUT:H28	34:5:503:LUT:H371	1.41	1.00
21:A:1121:CLA:H92	21:K:1403:CLA:CBC	1.89	1.00
21:A:1112:CLA:HBB1	21:A:1112:CLA:HMB3	1.42	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1132:CLA:C14	21:L:1502:CLA:HBB1	1.93	0.99
11:K:40:SER:HB2	11:K:82:MET:CG	1.91	0.99
14:1:83:MET:HE1	21:1:601:CLA:CAB	1.92	0.99
21:B:1206:CLA:HBB1	21:B:1206:CLA:HMB1	1.44	0.99
21:1:601:CLA:HBB1	21:1:601:CLA:HMB3	1.46	0.97
21:6:603:CLA:C4D	21:6:603:CLA:H12	1.93	0.97
21:B:1212:CLA:H93	24:B:4001:BCR:C31	1.94	0.97
11:K:69:ASP:OD1	11:K:70:PRO:HD2	1.65	0.96
21:6:601:CLA:HED2	21:6:601:CLA:C2A	1.95	0.96
24:I:4002:BCR:H23C	24:I:4002:BCR:H403	1.48	0.96
21:G:1601:CLA:HBB1	21:G:1601:CLA:HMB3	1.46	0.96
21:6:601:CLA:H41	21:6:601:CLA:H71	1.47	0.95
19:6:153:TYR:HB3	19:6:154:PRO:HD2	1.47	0.95
21:6:601:CLA:HBB1	21:6:601:CLA:HMB1	1.43	0.95
18:5:52:LEU:HD22	18:5:237:PRO:HG3	1.47	0.95
18:5:99:LEU:HD11	34:5:504:LUT:H403	1.48	0.94
1:A:487:ILE:HD11	21:A:1135:CLA:H2	1.47	0.94
35:6:504:XAT:H10	21:6:606:CLA:HBA2	1.46	0.94
21:K:1404:CLA:HBB1	21:K:1404:CLA:HMB1	1.50	0.93
21:5:606:CLA:HBB1	21:5:606:CLA:HMB3	1.52	0.92
18:5:69:MET:HB2	21:5:604:CLA:HMD1	1.53	0.91
6:F:186:ILE:O	6:F:190:LYS:HG3	1.71	0.91
21:3:610:CLA:HBB1	21:3:610:CLA:HMB1	1.53	0.91
21:A:1132:CLA:H91	21:L:1502:CLA:CBB	2.00	0.91
2:B:93:TRP:HH2	9:H:114:LEU:HD13	1.31	0.91
21:A:1012:CLA:HAB	2:B:583:TRP:CH2	2.04	0.91
24:3:504:BCR:H341	21:3:610:CLA:HBC2	1.53	0.91
18:5:99:LEU:CD2	34:5:504:LUT:H391	2.01	0.91
21:6:606:CLA:HBB1	21:6:606:CLA:HMB3	1.54	0.90
34:5:502:LUT:H373	21:5:606:CLA:C2B	2.00	0.90
21:A:1119:CLA:CMD	21:A:1121:CLA:CBB	2.50	0.89
21:A:1114:CLA:HBB1	21:A:1114:CLA:HMB3	1.53	0.89
2:B:659:ALA:HB3	21:B:1023:CLA:HBB2	1.53	0.89
21:A:1120:CLA:H121	21:A:1121:CLA:H122	1.55	0.88
10:I:20:TRP:CH2	33:5:803:PTY:H122	2.09	0.88
19:6:125:GLN:HE21	19:6:125:GLN:HA	1.38	0.88
12:L:188:THR:O	12:L:192:LEU:HD23	1.73	0.87
21:3:610:CLA:HBB1	31:3:803:LMG:H292	1.57	0.86
24:1:504:BCR:H353	21:1:611:CLA:CBB	2.05	0.86
35:6:504:XAT:H10	21:6:606:CLA:CBA	2.05	0.85
19:6:171:LYS:HG2	21:6:607:CLA:HMD1	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:5:503:LUT:H371	34:5:503:LUT:C28	2.05	0.85
21:5:604:CLA:HMB1	21:5:604:CLA:HBB1	1.56	0.85
21:A:1132:CLA:C14	21:L:1502:CLA:CBB	2.54	0.84
17:4:137:LEU:HD13	17:4:146:GLY:HA2	1.59	0.84
18:5:196:VAL:HG12	18:5:199:GLN:HB2	1.57	0.84
9:H:122:LEU:O	9:H:125:PRO:HD2	1.77	0.84
8:G:29:GLU:HB2	8:G:32:VAL:HG22	1.59	0.84
2:B:86:ARG:HG2	9:H:144:LEU:HB2	1.58	0.84
21:B:1205:CLA:HAB	21:B:1206:CLA:O1A	1.77	0.83
9:H:70:TYR:CE1	12:L:83:LEU:CD1	2.60	0.83
14:1:83:MET:CE	21:1:601:CLA:HAB	2.07	0.83
28:3:805:DGD:O5E	28:3:805:DGD:O3E	1.94	0.83
19:6:162:SER:H	19:6:163:PRO:HD2	1.43	0.83
6:F:139:LEU:HD12	6:F:139:LEU:O	1.78	0.83
21:A:1132:CLA:H91	21:L:1502:CLA:HBB2	1.58	0.82
2:B:99:GLN:N	9:H:123:GLU:HG2	1.93	0.82
18:5:99:LEU:HG	21:5:606:CLA:HAB	1.60	0.82
18:5:71:PHE:CZ	18:5:73:PRO:HG3	2.14	0.82
21:A:1120:CLA:H121	21:A:1121:CLA:C12	2.09	0.82
19:6:75:GLU:HG3	31:6:802:LMG:O2	1.80	0.82
19:6:198:LEU:O	19:6:202:LEU:HG	1.79	0.82
19:6:85:LYS:HD2	19:6:149:PHE:CZ	2.14	0.82
1:A:454:GLY:HA3	21:A:1132:CLA:HAB	1.61	0.82
2:B:659:ALA:CB	21:B:1023:CLA:HBB2	2.11	0.81
35:6:504:XAT:H393	21:6:601:CLA:HBC1	1.60	0.81
2:B:168:TRP:NE1	21:B:1208:CLA:HMA3	1.95	0.81
8:G:30:PRO:O	8:G:34:ILE:HG22	1.81	0.81
21:6:602:CLA:HED2	21:6:602:CLA:H2A	1.60	0.81
21:B:1021:CLA:HMB3	21:B:1022:CLA:OBD	1.81	0.81
12:L:154:GLN:HB2	12:L:157:PRO:HG3	1.63	0.81
21:A:1119:CLA:CMD	21:A:1121:CLA:HBB1	2.11	0.80
16:3:152:VAL:HG21	35:3:502:XAT:H172	1.63	0.80
21:6:608:CLA:HHC	21:6:608:CLA:CBB	2.10	0.80
8:G:34:ILE:HD12	8:G:110:PHE:HD1	1.44	0.80
20:A:1011:CL0:CGD	20:A:1011:CL0:H8	2.11	0.80
2:B:93:TRP:CH2	9:H:114:LEU:HD13	2.16	0.80
21:A:1120:CLA:H143	21:A:1121:CLA:H143	1.62	0.80
36:5:609:CHL:HED1	19:6:134:GLY:C	2.06	0.80
2:B:168:TRP:CZ2	21:B:1208:CLA:HMA3	2.17	0.79
1:A:267:LEU:HD11	11:K:29:MET:HE1	1.64	0.79
1:A:598:TRP:CH2	21:B:1022:CLA:HAB	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:3:610:CLA:CBB	31:3:803:LMG:H312	2.12	0.79
16:3:153:ILE:CG2	16:3:155:PRO:HD2	2.12	0.79
18:5:99:LEU:HD22	34:5:504:LUT:H391	1.62	0.79
24:A:4002:BCR:H281	21:K:1401:CLA:HAB	1.64	0.79
21:B:1212:CLA:C6	24:B:4001:BCR:H312	2.12	0.79
6:F:132:THR:HG21	24:F:4001:BCR:HC41	1.63	0.79
18:5:99:LEU:CD1	34:5:504:LUT:H403	2.12	0.79
18:5:110:LEU:HD11	18:5:112:MET:HE2	1.64	0.79
2:B:112:GLY:HA2	9:H:128:THR:CG2	2.10	0.79
36:5:609:CHL:C3C	25:5:801:LHG:HC81	2.12	0.79
21:A:1134:CLA:HED2	21:A:1134:CLA:H2A	1.65	0.79
24:A:4001:BCR:C24	11:K:85:ALA:HB2	2.13	0.79
12:L:154:GLN:HB2	12:L:157:PRO:CG	2.13	0.79
8:G:34:ILE:HD12	8:G:110:PHE:CD1	2.18	0.79
24:I:4002:BCR:H403	24:I:4002:BCR:C23	2.13	0.78
21:B:1212:CLA:H62	24:B:4001:BCR:H312	1.65	0.78
2:B:659:ALA:O	21:B:1023:CLA:HAB	1.83	0.78
21:A:1114:CLA:HED2	21:A:1114:CLA:H2A	1.65	0.78
14:1:163:PHE:HB2	21:1:601:CLA:O2A	1.83	0.78
21:5:605:CLA:HMB3	21:5:605:CLA:HBB1	1.64	0.78
21:A:1115:CLA:C4D	21:A:1115:CLA:H12	2.14	0.78
21:6:602:CLA:HHC	21:6:602:CLA:CBB	2.13	0.77
1:A:396:TRP:CD1	21:A:1126:CLA:HAB	2.19	0.77
21:A:1121:CLA:HHC	21:A:1121:CLA:CBB	2.14	0.77
21:6:601:CLA:H41	21:6:601:CLA:C7	2.05	0.77
21:A:1132:CLA:H143	21:L:1502:CLA:CBB	2.14	0.77
21:6:601:CLA:H2A	21:6:601:CLA:CED	2.03	0.77
21:A:1116:CLA:H12	21:A:1125:CLA:HBB2	1.66	0.77
19:6:171:LYS:HD2	21:6:607:CLA:CGD	2.14	0.77
21:6:603:CLA:H12	21:6:603:CLA:ND	1.98	0.77
2:B:99:GLN:HA	2:B:99:GLN:NE2	1.98	0.77
18:5:106:THR:HB	18:5:107:PRO:HD3	1.67	0.77
24:A:4007:BCR:H363	21:B:1023:CLA:H101	1.66	0.77
21:G:1602:CLA:HMB3	21:G:1602:CLA:HBB1	1.67	0.77
2:B:112:GLY:CA	9:H:128:THR:HG21	2.13	0.77
36:5:609:CHL:HHC	36:5:609:CHL:HBB1	1.67	0.76
9:H:93:VAL:HG23	12:L:185:ALA:HB1	1.67	0.76
19:6:168:LYS:HE2	19:6:168:LYS:H	1.50	0.76
2:B:659:ALA:C	21:B:1023:CLA:HAB	2.10	0.76
19:6:165:HIS:HE1	21:6:602:CLA:HBA2	1.50	0.76
8:G:81:LYS:HE2	8:G:81:LYS:CA	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:108:GLY:O	9:H:112:ILE:HG22	1.86	0.76
2:B:433:HIS:HB3	24:F:4001:BCR:H292	1.67	0.76
4:D:207:ALA:O	4:D:211:ILE:HG12	1.85	0.76
18:5:52:LEU:HD22	18:5:237:PRO:CG	2.15	0.76
21:A:1132:CLA:H142	21:L:1502:CLA:CBB	2.17	0.75
13:O:65:SER:HB3	24:O:4001:BCR:HC32	1.69	0.75
24:3:504:BCR:H341	21:3:610:CLA:CBC	2.15	0.75
17:4:142:LEU:HD21	17:4:276:LYS:HD3	1.68	0.75
36:6:610:CHL:HHC	36:6:610:CHL:HBB1	1.68	0.75
10:I:31:LEU:CD2	24:I:4001:BCR:H351	2.16	0.75
21:B:1208:CLA:HHC	21:B:1208:CLA:CBB	2.17	0.75
21:L:1503:CLA:HBA2	21:L:1504:CLA:HMB3	1.68	0.75
21:A:1012:CLA:H43	2:B:439:VAL:CG2	2.14	0.75
2:B:407:ASN:O	2:B:411:ARG:HB2	1.87	0.75
21:B:1213:CLA:HBD	8:G:117:LEU:HD11	1.69	0.75
19:6:183:PHE:CE1	34:6:501:LUT:H41	2.22	0.75
19:6:185:VAL:HG11	21:6:603:CLA:HAC2	1.69	0.75
34:6:501:LUT:C16	21:6:603:CLA:HMB2	2.16	0.75
2:B:429:PHE:CE2	21:B:1235:CLA:HAB	2.22	0.75
10:I:20:TRP:CZ2	33:5:803:PTY:H122	2.22	0.75
11:K:49:ARG:HD2	11:K:72:ALA:O	1.87	0.75
8:G:46:ARG:O	8:G:46:ARG:HD3	1.85	0.74
11:K:48:VAL:HG23	11:K:78:ASP:OD1	1.87	0.74
21:A:1114:CLA:C3D	31:3:803:LMG:H291	2.17	0.74
21:6:603:CLA:HHC	21:6:603:CLA:CBB	2.12	0.74
6:F:84:PRO:HG2	6:F:87:GLU:HG2	1.69	0.74
24:H:4001:BCR:H19C	24:L:4002:BCR:H341	1.68	0.74
2:B:175:ARG:HG3	21:B:1210:CLA:HBC2	1.68	0.74
34:6:501:LUT:H361	34:6:501:LUT:C28	2.16	0.74
21:B:1207:CLA:H112	12:L:136:ALA:HB2	1.69	0.74
21:B:1239:CLA:H11	22:B:2002:PQN:H302	1.69	0.74
1:A:680:ALA:O	21:A:1013:CLA:HAB	1.87	0.74
24:A:4007:BCR:C36	21:B:1023:CLA:H122	2.18	0.73
21:B:1206:CLA:H43	24:I:4001:BCR:C22	2.18	0.73
21:B:1225:CLA:H51	24:B:4002:BCR:H23C	1.70	0.73
16:3:250:MET:HE2	35:3:502:XAT:H10	1.71	0.73
21:5:606:CLA:HMA2	21:5:613:CLA:HBC3	1.70	0.73
21:5:608:CLA:O2D	19:6:128:ILE:HD11	1.87	0.73
28:3:805:DGD:HO3E	28:3:805:DGD:HO5E	1.16	0.73
21:B:1207:CLA:HHC	21:B:1207:CLA:CBB	2.15	0.73
8:G:63:PRO:O	8:G:78:ARG:NH2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:5:609:CHL:C2C	25:5:801:LHG:HC81	2.18	0.73
2:B:51:HIS:HB3	21:B:1210:CLA:HED3	1.70	0.73
18:5:114:GLY:HA2	18:5:117:PRO:O	1.89	0.73
24:A:4001:BCR:H24C	11:K:85:ALA:HB2	1.69	0.73
21:B:1205:CLA:CAB	21:B:1206:CLA:O1A	2.37	0.73
24:A:4007:BCR:H362	21:B:1023:CLA:H122	1.71	0.72
7:J:31:ARG:NH2	21:J:1901:CLA:O1D	2.21	0.72
12:L:169:LEU:HD23	12:L:169:LEU:O	1.88	0.72
2:B:109:GLY:HA2	9:H:135:LYS:HE2	1.71	0.72
34:5:502:LUT:H28	34:5:502:LUT:C36	2.12	0.72
19:6:183:PHE:HE1	34:6:501:LUT:H41	1.55	0.72
21:A:1115:CLA:H2A	21:A:1115:CLA:CED	2.20	0.72
18:5:52:LEU:HD13	18:5:237:PRO:HB3	1.70	0.72
35:3:502:XAT:H362	36:3:604:CHL:H2	1.72	0.72
2:B:440:HIS:NE2	2:B:454:ILE:HG13	2.04	0.72
10:I:38:MET:HG2	24:L:4001:BCR:C10	2.18	0.72
6:F:163:GLU:HA	7:J:38:VAL:HG12	1.72	0.71
21:K:1402:CLA:HBD	21:K:1402:CLA:HBA1	1.72	0.71
33:O:5002:PTY:C11	33:O:5002:PTY:HC11	2.20	0.71
10:I:31:LEU:HD21	24:I:4001:BCR:H351	1.70	0.71
16:3:259:ILE:HG23	16:3:260:THR:HG23	1.72	0.71
20:A:1011:CL0:H15	20:A:1011:CL0:H13	1.72	0.71
21:5:604:CLA:HBB1	21:5:604:CLA:CMB	2.20	0.71
34:6:501:LUT:H161	21:6:603:CLA:HMB2	1.71	0.71
21:B:1208:CLA:HBC3	21:6:605:CLA:H92	1.73	0.71
24:F:4001:BCR:H331	24:F:4001:BCR:C8	2.19	0.71
18:5:108:GLU:OE1	18:5:115:THR:HA	1.91	0.71
1:A:158:GLN:HG2	21:A:1112:CLA:HED1	1.73	0.70
21:K:1402:CLA:HBB1	21:K:1402:CLA:HMB3	1.73	0.70
21:A:1119:CLA:HMD3	21:A:1121:CLA:CBB	2.21	0.70
21:B:1206:CLA:HBB1	21:B:1206:CLA:CMB	2.21	0.70
10:I:26:VAL:N	10:I:27:PRO:HD2	2.05	0.70
1:A:678:VAL:HG11	1:A:733:LEU:HD23	1.72	0.70
21:K:1404:CLA:HBB1	21:K:1404:CLA:CMB	2.21	0.70
19:6:165:HIS:CE1	21:6:602:CLA:HBA2	2.26	0.70
8:G:103:LEU:HD11	24:G:4001:BCR:H372	1.72	0.70
21:4:604:CLA:H12	21:4:604:CLA:CHB	2.21	0.70
21:A:1115:CLA:H12	21:A:1115:CLA:ND	2.06	0.70
19:6:217:THR:H	19:6:218:PRO:CD	2.05	0.70
21:A:1115:CLA:H2A	21:A:1115:CLA:HED2	1.72	0.69
2:B:295:ASN:ND2	8:G:77:ASP:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:5:72:ASP:OD2	21:5:604:CLA:HAA1	1.92	0.69
2:B:67:PHE:HE1	10:I:15:PHE:HB3	1.57	0.69
2:B:596:HIS:O	2:B:600:LEU:HB2	1.92	0.69
21:A:1012:CLA:H13	21:A:1126:CLA:H192	1.74	0.69
2:B:67:PHE:CE1	10:I:15:PHE:HB3	2.27	0.69
20:A:1011:CL0:H8	20:A:1011:CL0:H30	1.74	0.69
2:B:71:TRP:CE2	10:I:17:PRO:HG2	2.28	0.69
2:B:515:PRO:HG3	6:F:147:HIS:CE1	2.28	0.69
19:6:210:ILE:HD13	21:6:603:CLA:H42	1.74	0.69
21:B:1239:CLA:HHC	21:B:1239:CLA:CBB	2.16	0.69
21:K:1402:CLA:HAA1	33:O:5002:PTY:HC12	1.75	0.69
9:H:77:ARG:HG3	12:L:93:VAL:HG21	1.74	0.69
12:L:156:GLN:HB3	12:L:157:PRO:HD3	1.75	0.69
21:6:601:CLA:H71	21:6:601:CLA:C4	2.22	0.69
21:5:604:CLA:HMD3	36:5:609:CHL:HBB2	1.74	0.69
2:B:106:THR:HG21	9:H:128:THR:CB	2.18	0.68
21:3:610:CLA:HBB1	21:3:610:CLA:CMB	2.21	0.68
24:A:4006:BCR:H292	24:J:4001:BCR:H313	1.75	0.68
9:H:122:LEU:HD12	9:H:123:GLU:OE1	1.93	0.68
2:B:81:ASP:O	2:B:85:VAL:HG22	1.94	0.68
21:B:1206:CLA:H43	24:I:4001:BCR:C21	2.22	0.68
21:5:606:CLA:HMA2	21:5:613:CLA:C3C	2.23	0.68
21:5:612:CLA:HED2	21:5:612:CLA:H2A	1.75	0.68
2:B:295:ASN:HB2	8:G:80:GLN:HA	1.74	0.68
18:5:50:ILE:HG22	18:5:51:PRO:HD2	1.76	0.68
21:A:1114:CLA:HBB1	21:A:1114:CLA:CMB	2.23	0.68
6:F:223:GLN:HB2	17:4:158:ARG:HG3	1.74	0.68
21:G:1601:CLA:CBB	24:G:4001:BCR:H363	2.24	0.68
9:H:121:THR:HA	9:H:126:ILE:HD11	1.76	0.68
1:A:709:VAL:HG12	6:F:183:ARG:HG3	1.74	0.68
24:1:504:BCR:H353	21:1:611:CLA:HBB2	1.74	0.68
21:5:605:CLA:H92	21:5:605:CLA:H51	1.74	0.68
21:B:1207:CLA:H62	12:L:133:MET:SD	2.33	0.68
19:6:169:GLU:HB2	21:6:601:CLA:HMB3	1.75	0.68
1:A:318:ILE:CD1	11:K:81:ALA:HB2	2.24	0.68
2:B:494:TRP:HE1	21:B:1231:CLA:HED1	1.57	0.68
19:6:85:LYS:O	19:6:89:ARG:HG3	1.93	0.68
21:6:601:CLA:HBB1	21:6:601:CLA:CMB	2.21	0.68
1:A:127:LEU:HD21	1:A:667:ALA:HB2	1.74	0.67
1:A:267:LEU:HD11	11:K:29:MET:CE	2.24	0.67
21:A:1119:CLA:HMD1	21:A:1121:CLA:CBB	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1131:CLA:HAB	21:A:1132:CLA:HHB	1.77	0.67
24:B:4001:BCR:C13	24:G:4001:BCR:H392	2.24	0.67
17:4:142:LEU:CD2	17:4:276:LYS:HD3	2.24	0.67
21:5:605:CLA:HBB1	21:5:605:CLA:CMB	2.24	0.67
34:6:501:LUT:H28	34:6:501:LUT:C36	2.20	0.67
21:B:1212:CLA:C9	24:B:4001:BCR:C31	2.70	0.67
21:G:1601:CLA:HMC2	24:G:4001:BCR:H383	1.76	0.67
12:L:58:GLN:HB2	12:L:59:PRO:HD2	1.75	0.67
21:1:601:CLA:HBB1	21:1:601:CLA:CMB	2.22	0.67
18:5:242:ALA:CB	31:6:802:LMG:H152	2.24	0.67
19:6:196:GLU:O	19:6:200:LYS:HG3	1.93	0.67
21:A:1012:CLA:HAB	2:B:583:TRP:HH2	1.58	0.67
24:F:4001:BCR:H392	24:F:4001:BCR:H23C	1.77	0.67
21:B:1235:CLA:HBC3	24:F:4001:BCR:H382	1.75	0.67
18:5:50:ILE:HG21	18:5:55:VAL:H	1.60	0.67
18:5:110:LEU:C	18:5:110:LEU:HD12	2.20	0.67
19:6:80:SER:HA	19:6:83:MET:HG2	1.77	0.67
21:B:1022:CLA:O1A	21:B:1022:CLA:H3A	1.95	0.67
9:H:111:SER:HB2	10:I:24:LEU:CD1	2.24	0.67
13:O:65:SER:CB	24:O:4001:BCR:HC32	2.24	0.67
21:A:1116:CLA:H12	21:A:1125:CLA:CBB	2.24	0.66
21:B:1212:CLA:C9	24:B:4001:BCR:H311	2.14	0.66
34:6:501:LUT:H32	21:6:601:CLA:HAB	1.78	0.66
1:A:204:GLY:O	1:A:208:LEU:HB2	1.95	0.66
19:6:75:GLU:CG	31:6:802:LMG:O2	2.44	0.66
2:B:518:PHE:CZ	24:F:4001:BCR:H381	2.30	0.66
16:3:268:LEU:HB2	34:3:501:LUT:H22	1.77	0.66
16:3:152:VAL:CG2	35:3:502:XAT:H21	2.26	0.66
18:5:52:LEU:HD12	18:5:52:LEU:O	1.95	0.66
21:5:606:CLA:HBB1	21:5:606:CLA:CMB	2.24	0.66
7:J:27:ILE:HD13	24:J:4002:BCR:H10C	1.77	0.66
11:K:22:SER:CB	11:K:26:ARG:HG2	2.26	0.66
21:L:1504:CLA:HBB1	21:L:1504:CLA:HHC	1.78	0.66
15:2:204:ASP:OD1	34:2:501:LUT:O3	2.13	0.66
1:A:204:GLY:HA3	21:A:1111:CLA:HBB1	1.76	0.65
21:B:1212:CLA:HMB1	21:B:1212:CLA:HBB1	1.77	0.65
18:5:104:CYS:O	18:5:108:GLU:HG2	1.96	0.65
9:H:78:TYR:CE2	12:L:97:LEU:HB3	2.31	0.65
34:5:502:LUT:H361	34:5:502:LUT:C28	2.14	0.65
21:G:1602:CLA:HBB1	21:G:1602:CLA:CMB	2.25	0.65
13:O:84:LEU:HD22	21:O:1803:CLA:H52	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:5:242:ALA:HB1	31:6:802:LMG:H152	1.78	0.65
21:5:604:CLA:CMD	36:5:609:CHL:HBB2	2.27	0.65
19:6:171:LYS:HD2	21:6:607:CLA:CAD	2.26	0.65
21:A:1132:CLA:H121	21:L:1502:CLA:HBB1	1.78	0.65
21:A:1132:CLA:H121	21:L:1502:CLA:CBB	2.27	0.65
9:H:124:LEU:CB	9:H:125:PRO:HD3	2.27	0.65
21:5:606:CLA:H43	21:5:613:CLA:CAD	2.25	0.65
21:1:601:CLA:H41	21:1:602:CLA:O1A	1.97	0.65
16:3:173:GLU:OE1	21:3:610:CLA:HED2	1.96	0.65
19:6:171:LYS:HG2	21:6:607:CLA:CMD	2.27	0.65
21:A:1112:CLA:HBB1	21:A:1112:CLA:CMB	2.21	0.65
21:A:1116:CLA:C1	21:A:1125:CLA:HBB2	2.26	0.65
11:K:33:ILE:O	11:K:37:LEU:HG	1.97	0.65
17:4:288:LEU:HD21	21:4:603:CLA:H91	1.78	0.65
1:A:487:ILE:HD12	21:A:1135:CLA:CGA	2.28	0.64
1:A:515:VAL:HG13	1:A:522:ALA:HB3	1.78	0.64
16:3:177:ILE:HG23	21:3:612:CLA:HAB	1.77	0.64
21:5:608:CLA:C4B	36:5:609:CHL:H18	2.27	0.64
1:A:487:ILE:HD11	21:A:1135:CLA:C2	2.23	0.64
34:5:503:LUT:H28	34:5:503:LUT:C37	2.22	0.64
21:B:1204:CLA:O1D	10:I:22:PRO:HB3	1.97	0.64
12:L:60:LEU:HD11	12:L:66:VAL:HG21	1.79	0.64
21:B:1212:CLA:C6	24:B:4001:BCR:C31	2.75	0.64
21:A:1113:CLA:HBB1	24:A:4001:BCR:H323	1.79	0.64
21:A:1119:CLA:H111	24:A:4004:BCR:H10C	1.79	0.64
19:6:125:GLN:OE1	21:6:613:CLA:C2D	2.46	0.64
24:B:4001:BCR:H353	24:G:4001:BCR:C39	2.26	0.64
10:I:27:PRO:N	10:I:27:PRO:C	2.56	0.64
21:1:601:CLA:H71	21:1:602:CLA:HMA2	1.79	0.64
2:B:94:ASP:H	9:H:124:LEU:HD21	1.63	0.64
8:G:106:VAL:HG12	24:G:4001:BCR:H292	1.80	0.64
18:5:229:PHE:HB2	21:5:614:CLA:HAC1	1.80	0.64
2:B:168:TRP:CE2	21:B:1208:CLA:CMA	2.75	0.64
2:B:171:ASP:OD2	2:B:174:SER:OG	2.16	0.64
2:B:388:PHE:HZ	21:B:1222:CLA:HAB	1.63	0.64
9:H:122:LEU:HD12	9:H:123:GLU:H	1.63	0.64
14:1:166:ASP:HB3	14:1:169:SER:HB3	1.79	0.64
8:G:87:GLU:HA	8:G:93:PRO:HG2	1.79	0.64
7:J:16:LEU:HD11	24:J:4002:BCR:H21C	1.80	0.63
9:H:122:LEU:HD12	9:H:123:GLU:N	2.13	0.63
16:3:154:PRO:HG2	21:3:610:CLA:HMB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:479:LEU:HD21	21:B:1231:CLA:HED2	1.80	0.63
17:4:144:ASP:HA	21:4:604:CLA:HED2	1.79	0.63
1:A:158:GLN:HG2	21:A:1112:CLA:CED	2.29	0.63
9:H:114:LEU:O	9:H:117:LYS:HD2	1.99	0.63
36:5:609:CHL:C1D	25:5:801:LHG:H122	2.29	0.63
21:6:606:CLA:HMA3	21:6:613:CLA:C2C	2.29	0.63
36:6:610:CHL:HAA2	36:6:610:CHL:HBD	1.79	0.63
21:K:1402:CLA:HBB1	21:K:1402:CLA:CMB	2.28	0.63
12:L:154:GLN:O	12:L:157:PRO:HG2	1.99	0.63
15:2:205:PRO:HD2	34:2:501:LUT:H3	1.81	0.63
21:5:603:CLA:H43	36:5:609:CHL:H51	1.81	0.63
21:B:1235:CLA:CBC	24:F:4001:BCR:H382	2.28	0.63
6:F:139:LEU:HD12	6:F:139:LEU:C	2.22	0.63
21:5:605:CLA:HBC1	36:5:610:CHL:HAB	1.80	0.63
1:A:119:TRP:NE1	27:A:5004:LMU:O2'	2.30	0.63
21:A:1012:CLA:H41	2:B:439:VAL:HG13	1.79	0.63
36:5:610:CHL:CMA	33:5:803:PTY:H431	2.11	0.63
19:6:125:GLN:HE21	19:6:125:GLN:CA	2.05	0.63
9:H:124:LEU:HB2	9:H:125:PRO:HD3	1.79	0.63
18:5:230:VAL:HG11	19:6:127:PRO:HB3	1.81	0.63
15:2:93:SER:HB2	15:2:99:ARG:HA	1.80	0.63
18:5:52:LEU:HD22	18:5:237:PRO:CB	2.29	0.63
21:A:1121:CLA:H91	11:K:89:ILE:HD11	1.80	0.62
36:6:610:CHL:HMA2	27:6:805:LMU:H42	1.81	0.62
2:B:400:ASP:OD2	2:B:403:GLN:HG2	1.99	0.62
15:2:194:LYS:NZ	15:2:209:SER:O	2.32	0.62
10:I:21:ALA:H	10:I:22:PRO:HD2	1.63	0.62
11:K:69:ASP:CG	11:K:70:PRO:HD2	2.24	0.62
21:5:604:CLA:HMD3	36:5:609:CHL:CBB	2.29	0.62
19:6:165:HIS:HE1	21:6:602:CLA:CBA	2.12	0.62
12:L:139:LEU:C	12:L:139:LEU:HD23	2.24	0.62
12:L:156:GLN:N	12:L:157:PRO:HD2	2.15	0.62
18:5:242:ALA:CB	31:6:802:LMG:H121	2.30	0.62
2:B:107:ARG:NH2	2:B:115:ASN:HA	2.15	0.62
2:B:217:LEU:HD12	2:B:217:LEU:O	1.98	0.62
21:B:1208:CLA:C12	21:6:612:CLA:H143	2.29	0.62
9:H:138:ASN:HD21	9:H:144:LEU:HA	1.64	0.62
11:K:51:ASN:HB3	11:K:61:LYS:HD3	1.80	0.62
29:5:804:3PH:H232	29:5:804:3PH:H331	1.82	0.62
21:6:606:CLA:HBB1	21:6:606:CLA:CMB	2.27	0.62
21:A:1116:CLA:HAC1	21:A:1133:CLA:H42	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:524:ILE:HG12	2:B:591:VAL:HG12	1.81	0.62
8:G:34:ILE:HD11	8:G:106:VAL:HG22	1.80	0.62
21:5:606:CLA:CMA	21:5:613:CLA:HBC3	2.29	0.62
18:5:71:PHE:CE2	18:5:73:PRO:HG3	2.35	0.62
19:6:153:TYR:CB	19:6:154:PRO:HD2	2.25	0.62
1:A:541:PHE:HZ	21:B:1022:CLA:CBB	2.13	0.62
6:F:84:PRO:HG2	6:F:87:GLU:CG	2.30	0.62
24:A:4007:BCR:H343	21:B:1022:CLA:H202	1.82	0.61
21:A:1106:CLA:HAB	21:A:1126:CLA:H152	1.82	0.61
2:B:99:GLN:CB	2:B:100:PRO:HD3	2.26	0.61
16:3:268:LEU:HD22	34:3:501:LUT:H172	1.81	0.61
1:A:119:TRP:CH2	21:A:1105:CLA:HBA2	2.36	0.61
1:A:240:PRO:HG3	21:A:1112:CLA:HED2	1.82	0.61
21:5:604:CLA:CMD	36:5:609:CHL:CBB	2.79	0.61
9:H:114:LEU:O	9:H:117:LYS:CG	2.49	0.61
21:L:1504:CLA:HHC	21:L:1504:CLA:CBB	2.29	0.61
17:4:178:VAL:HG12	21:4:602:CLA:HAB	1.82	0.61
19:6:153:TYR:HB3	19:6:154:PRO:CD	2.28	0.61
19:6:122:VAL:HA	19:6:125:GLN:HB2	1.81	0.61
3:C:8:TYR:HH	3:C:68:TYR:HH	1.48	0.61
19:6:156:ASP:N	19:6:157:PRO:HD3	2.16	0.61
34:6:501:LUT:C36	21:6:601:CLA:O1A	2.38	0.61
21:B:1212:CLA:HBB1	21:B:1212:CLA:CMB	2.31	0.61
21:6:606:CLA:HBA1	21:6:606:CLA:CHA	2.26	0.61
21:A:1113:CLA:H62	24:3:504:BCR:H21C	1.83	0.61
21:G:1601:CLA:HBB1	21:G:1601:CLA:CMB	2.27	0.61
21:B:1229:CLA:HAC2	6:F:168:THR:HB	1.83	0.60
21:G:1603:CLA:HBC1	36:1:610:CHL:C2D	2.32	0.60
17:4:241:GLY:O	17:4:249:THR:OG1	2.19	0.60
11:K:53:THR:HG21	11:K:59:LEU:HD11	1.83	0.60
12:L:85:ASN:HB3	21:L:1501:CLA:HAC1	1.83	0.60
15:2:169:ARG:NH2	21:2:612:CLA:O1D	2.35	0.60
2:B:601:THR:HG21	2:B:610:PHE:HB3	1.83	0.60
1:A:450:PHE:O	21:A:1132:CLA:HBB2	2.01	0.60
2:B:52:PHE:HE1	21:B:1208:CLA:CBB	2.14	0.60
21:B:1208:CLA:H122	21:6:612:CLA:H143	1.83	0.60
21:B:1208:CLA:H2	21:B:1209:CLA:C1	2.31	0.60
1:A:316:TRP:CD1	11:K:77:THR:HG21	2.37	0.60
21:4:604:CLA:CMB	21:4:604:CLA:HBB1	2.32	0.60
21:5:605:CLA:HED1	21:5:612:CLA:C1	2.31	0.60
19:6:125:GLN:HA	19:6:125:GLN:NE2	2.12	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:6:210:ILE:HG13	21:6:603:CLA:OBD	2.01	0.60
21:B:1208:CLA:H111	21:6:605:CLA:H171	1.83	0.60
6:F:201:ILE:HG12	7:J:10:THR:HG22	1.82	0.60
16:3:271:HIS:CG	21:3:603:CLA:HAA2	2.36	0.60
21:4:604:CLA:HBB1	21:4:604:CLA:HMB1	1.83	0.60
1:A:276:LEU:HD11	21:A:1113:CLA:HBC1	1.84	0.60
2:B:16:ASP:HB3	2:B:21:ARG:HB2	1.84	0.60
6:F:82:LEU:HD13	6:F:139:LEU:CD1	2.32	0.60
10:I:24:LEU:HG	10:I:24:LEU:O	2.00	0.60
28:3:805:DGD:O5E	28:3:805:DGD:HE1	2.01	0.60
21:6:605:CLA:C4	31:6:802:LMG:H312	2.32	0.60
1:A:399:GLY:HA3	1:A:603:LEU:HD11	1.84	0.60
21:A:1012:CLA:C4	2:B:439:VAL:HG13	2.32	0.60
9:H:114:LEU:O	9:H:117:LYS:HG2	2.02	0.60
24:H:4001:BCR:C40	12:L:197:TRP:HE1	2.15	0.60
11:K:40:SER:OG	11:K:82:MET:HG3	1.99	0.60
21:A:1112:CLA:HMB3	21:A:1112:CLA:CBB	2.26	0.60
2:B:325:HIS:O	2:B:329:ASN:HB2	2.02	0.60
21:K:1404:CLA:H2A	21:K:1404:CLA:O1D	2.02	0.60
21:3:610:CLA:CBB	31:3:803:LMG:H292	2.32	0.59
36:5:609:CHL:C2D	25:5:801:LHG:H122	2.32	0.59
19:6:123:GLN:OE1	19:6:123:GLN:HA	2.02	0.59
1:A:490:THR:O	1:A:494:ALA:HB2	2.01	0.59
21:A:1133:CLA:HBB1	21:A:1135:CLA:HED2	1.83	0.59
36:5:609:CHL:HED1	19:6:134:GLY:O	2.01	0.59
24:1:504:BCR:H353	21:1:611:CLA:HBB1	1.82	0.59
21:A:1120:CLA:C12	21:A:1121:CLA:H122	2.31	0.59
24:H:4001:BCR:H402	12:L:197:TRP:HE1	1.67	0.59
11:K:22:SER:HB3	11:K:26:ARG:HG2	1.84	0.59
24:1:504:BCR:H362	21:1:611:CLA:HMB3	1.83	0.59
2:B:99:GLN:CA	9:H:123:GLU:HG2	2.31	0.59
21:B:1207:CLA:HBA2	21:B:1207:CLA:HBD	1.83	0.59
24:F:4001:BCR:C23	24:F:4001:BCR:H403	2.32	0.59
17:4:128:TYR:HD2	17:4:132:THR:HG21	1.67	0.59
18:5:50:ILE:CG2	18:5:51:PRO:HD2	2.31	0.59
21:A:1113:CLA:H11	24:3:504:BCR:H393	1.84	0.59
4:D:112:ILE:HG12	4:D:122:ILE:HG22	1.84	0.59
9:H:96:ARG:HD3	12:L:181:ALA:HB2	1.83	0.59
9:H:109:VAL:HA	9:H:112:ILE:CG2	2.32	0.59
21:5:605:CLA:O1D	21:5:605:CLA:H2A	2.03	0.59
1:A:245:LEU:HD22	28:3:805:DGD:HG32	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1114:CLA:C1C	31:3:803:LMG:H352	2.32	0.59
24:A:4004:BCR:H291	13:O:110:ILE:HB	1.84	0.59
24:3:506:BCR:H21C	21:3:606:CLA:HAC1	1.84	0.59
21:3:610:CLA:HMB1	21:3:610:CLA:CBB	2.31	0.59
17:4:219:GLU:O	17:4:223:PHE:HB2	2.02	0.59
21:5:608:CLA:HAA1	19:6:128:ILE:HD13	1.84	0.59
7:J:21:PHE:HA	21:J:1901:CLA:HBB2	1.84	0.59
9:H:93:VAL:HG23	12:L:185:ALA:CB	2.32	0.59
1:A:598:TRP:HH2	21:B:1022:CLA:HAB	1.65	0.59
20:A:1011:CL0:H15	20:A:1011:CL0:CMB	2.32	0.59
21:B:1207:CLA:H121	9:H:109:VAL:CG1	2.33	0.59
12:L:57:ILE:HG12	12:L:72:PRO:HD3	1.84	0.59
13:O:108:LEU:HD21	21:O:1801:CLA:C2B	2.33	0.59
19:6:158:VAL:O	19:6:158:VAL:HG12	2.02	0.59
2:B:93:TRP:CZ2	9:H:117:LYS:NZ	2.71	0.59
21:B:1206:CLA:HMB1	21:B:1206:CLA:CBB	2.27	0.59
16:3:259:ILE:HG21	21:3:603:CLA:HMD2	1.84	0.59
19:6:100:GLY:HA3	21:6:606:CLA:HBC3	1.84	0.59
21:6:602:CLA:HED2	21:6:602:CLA:CGA	2.32	0.59
21:B:1238:CLA:HAB	22:B:2002:PQN:H141	1.84	0.58
14:1:38:ALA:HB3	14:1:41:SER:HB3	1.85	0.58
21:A:1139:CLA:H111	31:F:5002:LMG:H431	1.84	0.58
9:H:133:MET:HE2	9:H:135:LYS:HE3	1.85	0.58
21:K:1404:CLA:HMB1	21:K:1404:CLA:CBB	2.30	0.58
14:1:173:LYS:HB3	21:1:601:CLA:CMA	2.33	0.58
20:A:1011:CL0:H8	20:A:1011:CL0:CED	2.34	0.58
8:G:34:ILE:HG12	8:G:105:HIS:HD2	1.69	0.58
11:K:41:ARG:C	11:K:43:GLY:H	2.12	0.58
24:K:4001:BCR:H331	24:K:4001:BCR:C8	2.33	0.58
16:3:268:LEU:HD13	34:3:501:LUT:H163	1.84	0.58
2:B:102:VAL:HG21	9:H:123:GLU:HB3	1.84	0.58
21:6:601:CLA:HMB1	21:6:601:CLA:CBB	2.27	0.58
12:L:111:ALA:O	12:L:115:ILE:HG23	2.03	0.58
14:1:163:PHE:HB2	21:1:601:CLA:CGA	2.32	0.58
18:5:71:PHE:CZ	18:5:73:PRO:CG	2.85	0.58
19:6:129:LEU:HD13	21:6:613:CLA:CHB	2.33	0.58
2:B:78:TRP:HA	2:B:85:VAL:HG21	1.85	0.58
24:F:4001:BCR:H14C	7:J:36:PRO:HB2	1.85	0.58
24:I:4001:BCR:H341	24:I:4002:BCR:H403	1.86	0.58
1:A:657:VAL:HG22	1:A:745:ALA:HB3	1.86	0.58
21:A:1138:CLA:H162	21:A:1139:CLA:H11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:5002:DGD:O2E	3:C:71:ASN:OD1	2.16	0.58
11:K:39:ALA:HB1	11:K:45:ALA:HB2	1.85	0.58
14:1:87:ALA:HB2	34:1:501:LUT:H15	1.86	0.58
18:5:52:LEU:HD22	18:5:237:PRO:HB3	1.85	0.58
21:A:1101:CLA:HBB2	21:A:1109:CLA:H13	1.86	0.58
21:5:604:CLA:H72	21:5:605:CLA:HMA2	1.85	0.58
12:L:154:GLN:O	12:L:157:PRO:O	2.22	0.57
14:1:141:LEU:HD12	21:1:611:CLA:HAB	1.85	0.57
21:A:1118:CLA:O1A	11:K:77:THR:HG22	2.05	0.57
2:B:86:ARG:HG3	9:H:143:ILE:HG22	1.86	0.57
2:B:98:GLY:O	2:B:102:VAL:HG23	2.04	0.57
21:5:604:CLA:HMB1	21:5:604:CLA:CBB	2.32	0.57
21:A:1132:CLA:H142	21:L:1502:CLA:HBB2	1.86	0.57
4:D:108:PRO:O	4:D:125:LYS:NZ	2.37	0.57
14:1:115:TRP:HD1	21:1:606:CLA:HBA2	1.69	0.57
1:A:665:LEU:HB2	1:A:668:TYR:HD2	1.69	0.57
24:A:4001:BCR:H321	24:A:4001:BCR:C8	2.32	0.57
2:B:143:LEU:HD11	24:B:4003:BCR:H292	1.85	0.57
18:5:50:ILE:CG2	18:5:51:PRO:CD	2.83	0.57
29:5:804:3PH:O22	29:5:804:3PH:H31	2.04	0.57
13:O:53:PHE:O	13:O:57:THR:OG1	2.18	0.57
21:A:1119:CLA:H101	24:A:4005:BCR:H21C	1.86	0.57
24:A:4007:BCR:HC41	2:B:649:TRP:CZ3	2.39	0.57
21:B:1207:CLA:HBB1	21:B:1207:CLA:CHC	2.22	0.57
21:B:1208:CLA:HBC2	21:6:605:CLA:H72	1.85	0.57
4:D:86:GLY:HA3	12:L:69:LEU:HD13	1.87	0.57
9:H:77:ARG:CG	12:L:93:VAL:HG21	2.34	0.57
21:B:1212:CLA:O1A	24:B:4003:BCR:H333	2.04	0.57
6:F:79:ILE:HD11	6:F:149:ILE:HG13	1.87	0.57
21:5:606:CLA:HMA2	21:5:613:CLA:CBC	2.35	0.57
1:A:211:LEU:CD2	24:A:4001:BCR:H10C	2.22	0.57
21:A:1114:CLA:O1A	27:A:5005:LMU:H82	2.05	0.57
2:B:93:TRP:HH2	9:H:114:LEU:CD1	2.12	0.57
2:B:93:TRP:CE2	9:H:124:LEU:HD13	2.40	0.57
21:B:1220:CLA:HAB	21:B:1227:CLA:HMD1	1.87	0.57
4:D:69:PRO:HA	4:D:172:GLY:HA3	1.87	0.57
10:I:20:TRP:CH2	33:5:803:PTY:C12	2.86	0.57
21:5:606:CLA:HBA1	21:5:606:CLA:CHA	2.35	0.57
1:A:158:GLN:CG	21:A:1112:CLA:HED1	2.35	0.57
1:A:337:GLY:HA2	1:A:426:LEU:HG	1.86	0.57
2:B:518:PHE:HZ	24:F:4001:BCR:H381	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:G:1601:CLA:HMB3	21:G:1601:CLA:CBB	2.30	0.57
4:D:135:LYS:HE3	4:D:167:LEU:HD13	1.87	0.56
13:O:59:PRO:HA	13:O:62:ILE:HD12	1.87	0.56
34:1:501:LUT:H30	21:1:601:CLA:H72	1.88	0.56
2:B:227:TRP:CZ2	21:B:1212:CLA:H42	2.40	0.56
21:A:1120:CLA:H121	21:A:1121:CLA:H121	1.87	0.56
21:A:1139:CLA:H142	6:F:208:LEU:HD21	1.87	0.56
2:B:109:GLY:CA	9:H:135:LYS:HE2	2.35	0.56
2:B:301:ARG:NH1	8:G:62:GLY:O	2.37	0.56
12:L:123:VAL:HB	12:L:126:THR:HB	1.86	0.56
12:L:139:LEU:HD23	12:L:139:LEU:O	2.05	0.56
15:2:175:ASN:HB2	17:4:131:ALA:HB2	1.87	0.56
16:3:280:LEU:N	21:3:603:CLA:O1A	2.38	0.56
21:5:604:CLA:HHD	36:5:609:CHL:HBB2	1.87	0.56
19:6:168:LYS:H	19:6:168:LYS:CE	2.18	0.56
21:B:1229:CLA:HMB2	24:B:4006:BCR:H21C	1.87	0.56
18:5:121:GLY:O	18:5:122:VAL:HG22	2.06	0.56
2:B:345:ILE:HG21	21:B:1221:CLA:H42	1.88	0.56
17:4:242:ASP:N	17:4:242:ASP:OD1	2.38	0.56
17:4:300:ASN:ND2	17:4:323:ASN:OD1	2.38	0.56
34:5:502:LUT:H373	21:5:606:CLA:CMB	2.34	0.56
1:A:673:LEU:HD11	2:B:618:MET:HB2	1.86	0.56
21:B:1226:CLA:H102	21:B:1239:CLA:HED1	1.88	0.56
11:K:39:ALA:O	11:K:45:ALA:HB3	2.05	0.56
16:3:181:GLU:OE2	16:3:184:ARG:NH1	2.39	0.56
1:A:60:ASP:OD2	1:A:350:HIS:NE2	2.36	0.56
2:B:312:PRO:HG2	25:B:5001:LHG:HC32	1.88	0.56
2:B:515:PRO:HD3	6:F:147:HIS:CE1	2.40	0.56
21:B:1203:CLA:H91	28:B:5002:DGD:HBN1	1.88	0.56
9:H:67:TRP:HD1	12:L:166:GLY:N	2.03	0.56
21:L:1503:CLA:C1D	21:L:1504:CLA:HAB	2.35	0.56
18:5:61:LEU:HD11	18:5:72:ASP:HB2	1.88	0.56
18:5:99:LEU:HD23	34:5:504:LUT:H391	1.84	0.56
21:B:1212:CLA:HMA3	24:B:4003:BCR:H343	1.87	0.56
9:H:70:TYR:HE1	12:L:83:LEU:HD12	1.61	0.56
17:4:235:ARG:NH1	31:4:802:LMG:O9	2.38	0.56
21:5:606:CLA:HMB3	21:5:606:CLA:CBB	2.32	0.56
2:B:30:HIS:ND1	21:B:1203:CLA:O1A	2.35	0.56
3:C:79:LEU:O	4:D:94:LYS:NZ	2.39	0.56
34:6:501:LUT:H183	21:6:603:CLA:C3B	2.36	0.56
24:B:4001:BCR:H353	24:G:4001:BCR:H392	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:203:GLN:HG3	12:L:204:VAL:HG13	1.88	0.56
1:A:508:LEU:HB2	1:A:523:MET:HG3	1.89	0.55
2:B:212:ASN:O	2:B:216:VAL:HG12	2.06	0.55
8:G:88:THR:H	8:G:93:PRO:HG2	1.71	0.55
17:4:141:MET:HE1	17:4:159:MET:HE3	1.87	0.55
19:6:49:ASP:HB3	21:6:609:CLA:HBC3	1.88	0.55
24:I:4001:BCR:H353	24:I:4002:BCR:H401	1.87	0.55
1:A:265:PHE:HA	21:K:1401:CLA:HAC2	1.88	0.55
21:B:1217:CLA:HBB1	24:B:4001:BCR:H14C	1.86	0.55
21:B:1225:CLA:H112	24:B:4002:BCR:H19C	1.88	0.55
18:5:238:MET:HG2	21:6:612:CLA:HHB	1.87	0.55
21:A:1104:CLA:HMD3	24:J:4001:BCR:H271	1.89	0.55
21:A:1104:CLA:HED3	21:A:1128:CLA:H61	1.87	0.55
21:G:1602:CLA:CHB	24:G:4001:BCR:H323	2.36	0.55
16:3:153:ILE:O	16:3:154:PRO:C	2.49	0.55
1:A:584:CYS:HB2	2:B:668:TRP:HB3	1.88	0.55
21:A:1131:CLA:HAA1	24:I:4002:BCR:C14	2.37	0.55
21:B:1228:CLA:HAA2	6:F:231:LEU:HD21	1.89	0.55
12:L:154:GLN:HB2	12:L:157:PRO:CD	2.37	0.55
14:1:142:ARG:NH1	21:1:612:CLA:O2D	2.39	0.55
2:B:374:THR:HG23	2:B:592:THR:HG21	1.87	0.55
5:E:67:GLY:HA3	5:E:93:VAL:HG11	1.88	0.55
18:5:52:LEU:CD1	18:5:237:PRO:HB3	2.36	0.55
21:5:605:CLA:HMB3	21:5:605:CLA:CBB	2.36	0.55
1:A:19:ARG:HE	16:3:95:SER:HB2	1.72	0.55
1:A:356:ASN:ND2	21:A:1103:CLA:OBD	2.38	0.55
21:A:1141:CLA:O1A	13:O:113:LEU:HA	2.07	0.55
2:B:433:HIS:CB	24:F:4001:BCR:H292	2.36	0.55
2:B:444:VAL:HG13	2:B:452:LYS:HB2	1.87	0.55
8:G:38:THR:HA	8:G:105:HIS:HB2	1.88	0.55
1:A:541:PHE:HZ	21:B:1022:CLA:HBB2	1.72	0.55
21:A:1012:CLA:H61	24:A:4006:BCR:H362	1.87	0.55
2:B:71:TRP:CD2	10:I:17:PRO:HG2	2.41	0.55
21:4:604:CLA:H43	21:4:604:CLA:HMB2	1.89	0.55
2:B:545:SER:HA	6:F:239:VAL:HG11	1.88	0.55
24:I:4001:BCR:C32	24:I:4001:BCR:C8	2.85	0.55
16:3:259:ILE:HG21	21:3:603:CLA:CMD	2.37	0.55
34:5:503:LUT:C24	34:5:503:LUT:H363	2.37	0.55
24:B:4001:BCR:C35	24:G:4001:BCR:H392	2.38	0.54
21:1:601:CLA:HMB3	21:1:601:CLA:CBB	2.29	0.54
21:A:1121:CLA:H62	21:K:1403:CLA:CBC	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:91:VAL:HG21	24:K:4001:BCR:H323	1.89	0.54
1:A:721:THR:OG1	25:A:5002:LHG:O5	2.24	0.54
34:1:501:LUT:H28	21:1:601:CLA:H52	1.90	0.54
24:3:504:BCR:C34	21:3:610:CLA:HBC2	2.31	0.54
21:A:1119:CLA:HMD1	21:A:1121:CLA:HBB1	1.89	0.54
21:A:1132:CLA:HBB1	21:A:1132:CLA:CMB	2.37	0.54
16:3:193:SER:OG	16:3:194:GLN:NE2	2.40	0.54
16:3:264:PRO:O	34:3:501:LUT:O3	2.25	0.54
18:5:242:ALA:HA	31:6:802:LMG:H121	1.90	0.54
21:A:1113:CLA:H122	16:3:254:GLY:HA3	1.89	0.54
2:B:174:SER:O	2:B:178:HIS:ND1	2.29	0.54
9:H:130:GLY:N	9:H:131:PRO:CD	2.71	0.54
11:K:91:VAL:HG11	24:K:4001:BCR:HC21	1.89	0.54
13:O:90:GLY:O	13:O:98:TRP:NE1	2.33	0.54
17:4:142:LEU:HD22	17:4:276:LYS:HB2	1.88	0.54
18:5:187:PHE:CZ	34:5:502:LUT:H30	2.42	0.54
24:F:4001:BCR:C8	24:F:4001:BCR:C33	2.85	0.54
11:K:35:ALA:HB1	21:K:1403:CLA:HAB	1.90	0.54
15:2:141:LYS:NZ	28:2:806:DGD:O3D	2.41	0.54
24:A:4007:BCR:H363	21:B:1023:CLA:H122	1.90	0.54
24:B:4001:BCR:H353	24:G:4001:BCR:H391	1.90	0.54
36:5:609:CHL:NC	25:5:801:LHG:H101	2.23	0.54
34:6:501:LUT:C30	21:6:601:CLA:H102	2.38	0.54
21:A:1115:CLA:C1A	21:A:1115:CLA:CGA	2.86	0.54
1:A:83:ILE:HD12	24:J:4001:BCR:H282	1.89	0.54
1:A:220:VAL:HG13	1:A:240:PRO:HB3	1.90	0.54
1:A:585:GLN:HB3	1:A:590:ASP:HB3	1.89	0.54
2:B:464:ILE:HD11	21:B:1234:CLA:H2	1.90	0.54
3:C:5:VAL:HG12	3:C:67:VAL:HG22	1.90	0.54
8:G:96:PHE:HA	8:G:99:TRP:HD1	1.72	0.54
21:K:1402:CLA:HBA1	21:K:1402:CLA:CBD	2.38	0.54
17:4:125:PRO:HB2	21:4:609:CLA:HBC1	1.90	0.54
17:4:250:ASP:OD2	17:4:250:ASP:N	2.41	0.54
18:5:185:LEU:HD11	21:5:604:CLA:CBC	2.38	0.54
34:5:502:LUT:H373	21:5:606:CLA:HMB2	1.90	0.54
21:6:603:CLA:C1A	21:6:603:CLA:CGA	2.85	0.54
1:A:495:PRO:HA	1:A:499:ALA:HB3	1.89	0.53
2:B:672:TRP:HZ3	21:B:1023:CLA:O1D	1.90	0.53
9:H:78:TYR:HB3	9:H:82:GLN:OE1	2.07	0.53
12:L:157:PRO:N	12:L:157:PRO:C	2.59	0.53
17:4:124:ARG:HE	17:4:277:LEU:HD22	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:6:93:MET:HG2	21:6:601:CLA:HMC1	1.90	0.53
19:6:169:GLU:HB2	21:6:601:CLA:CMB	2.37	0.53
1:A:67:GLU:OE2	1:A:71:ARG:NH2	2.40	0.53
1:A:459:ASN:HD22	1:A:640:ASN:HB2	1.73	0.53
2:B:69:VAL:HG11	2:B:125:TRP:CZ3	2.44	0.53
21:B:1208:CLA:H111	21:6:605:CLA:C17	2.38	0.53
9:H:79:PRO:HG3	21:H:1701:CLA:C4D	2.37	0.53
9:H:122:LEU:CD1	9:H:123:GLU:OE1	2.56	0.53
21:1:604:CLA:HBC1	25:1:801:LHG:H162	1.90	0.53
34:5:501:LUT:H34	21:5:601:CLA:HAB	1.90	0.53
2:B:664:PHE:CZ	21:B:1239:CLA:HBC3	2.43	0.53
12:L:154:GLN:C	12:L:157:PRO:HD2	2.33	0.53
12:L:208:ARG:HG3	12:L:208:ARG:O	2.08	0.53
14:1:173:LYS:HB3	21:1:601:CLA:HMA2	1.90	0.53
14:1:176:LYS:HG3	21:1:607:CLA:HED2	1.89	0.53
16:3:117:ALA:HB1	16:3:243:GLY:HA3	1.91	0.53
2:B:99:GLN:HB3	2:B:100:PRO:CD	2.28	0.53
14:1:161:LEU:HD23	34:1:501:LUT:H222	1.91	0.53
1:A:584:CYS:HB3	2:B:668:TRP:HE3	1.74	0.53
21:A:1114:CLA:C4D	31:3:803:LMG:H311	2.39	0.53
4:D:201:VAL:O	4:D:201:VAL:HG23	2.08	0.53
10:I:16:VAL:HG13	10:I:16:VAL:O	2.08	0.53
16:3:152:VAL:HG21	35:3:502:XAT:H21	1.91	0.53
34:5:502:LUT:H193	21:5:604:CLA:H151	1.90	0.53
29:5:804:3PH:H342	29:5:804:3PH:O32	2.09	0.53
21:B:1207:CLA:H121	9:H:109:VAL:HG11	1.89	0.53
4:D:198:PRO:N	4:D:198:PRO:C	2.61	0.53
36:1:610:CHL:HBB2	21:1:612:CLA:HBC1	1.91	0.53
18:5:50:ILE:HG22	18:5:51:PRO:CD	2.39	0.53
21:A:1115:CLA:CMB	21:A:1115:CLA:HBB1	2.39	0.53
21:B:1219:CLA:O1A	8:G:56:ARG:NH1	2.41	0.53
9:H:77:ARG:NH2	12:L:101:GLU:OE1	2.42	0.53
21:A:1121:CLA:H62	21:K:1403:CLA:HBC3	1.90	0.53
21:B:1227:CLA:H71	25:B:5001:LHG:HC91	1.91	0.53
21:B:1230:CLA:HMA2	24:F:4001:BCR:H363	1.89	0.53
18:5:99:LEU:CD1	21:5:606:CLA:HMC3	2.39	0.53
19:6:217:THR:N	19:6:218:PRO:CD	2.72	0.53
1:A:318:ILE:HD13	11:K:81:ALA:HB2	1.91	0.52
21:A:1121:CLA:HBA1	21:A:1121:CLA:CHA	2.35	0.52
21:B:1227:CLA:HBC1	24:B:4004:BCR:H21C	1.90	0.52
8:G:34:ILE:HG12	8:G:105:HIS:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1120:CLA:H142	21:A:1121:CLA:C15	2.38	0.52
21:A:1129:CLA:HED1	12:L:57:ILE:HG21	1.91	0.52
21:A:1134:CLA:H12	21:K:1402:CLA:H72	1.91	0.52
1:A:477:ILE:HD11	32:L:5002:4RF:H5	1.90	0.52
21:A:1128:CLA:H18	21:A:1140:CLA:H3A	1.91	0.52
4:D:149:PHE:O	4:D:151:GLN:NE2	2.42	0.52
21:2:604:CLA:HHD	36:2:609:CHL:HBB2	1.89	0.52
21:3:608:CLA:H2	21:3:608:CLA:HAA1	1.90	0.52
21:5:605:CLA:HBC1	36:5:610:CHL:CAB	2.40	0.52
19:6:106:VAL:HG22	19:6:106:VAL:O	2.09	0.52
21:A:1132:CLA:HBB1	21:A:1132:CLA:HMB1	1.91	0.52
2:B:735:GLY:O	9:H:144:LEU:HD11	2.09	0.52
7:J:13:VAL:HG13	7:J:14:VAL:HG13	1.90	0.52
21:A:1110:CLA:H8	21:A:1110:CLA:HBB1	1.90	0.52
21:A:1132:CLA:H171	21:L:1502:CLA:HMB2	1.90	0.52
16:3:154:PRO:HD2	21:3:610:CLA:C2B	2.39	0.52
1:A:338:HIS:NE2	25:A:5001:LHG:O1	2.35	0.52
21:B:1231:CLA:H61	21:B:1232:CLA:H12	1.91	0.52
6:F:195:PRO:N	6:F:195:PRO:C	2.63	0.52
9:H:77:ARG:HD2	12:L:90:ARG:HG3	1.91	0.52
11:K:40:SER:CB	11:K:82:MET:CG	2.65	0.52
2:B:358:PRO:HG3	21:B:1215:CLA:HBA1	1.91	0.52
21:B:1023:CLA:H2	21:B:1023:CLA:HBA2	1.91	0.52
11:K:48:VAL:HG21	11:K:77:THR:OG1	2.08	0.52
21:1:601:CLA:H41	21:1:602:CLA:CGA	2.40	0.52
19:6:217:THR:H	19:6:218:PRO:HD3	1.73	0.52
2:B:444:VAL:HG11	2:B:453:GLN:N	2.25	0.52
10:I:18:PRO:O	10:I:21:ALA:HB2	2.10	0.52
36:2:611:CHL:HHC	36:2:611:CHL:HBB1	1.91	0.52
18:5:99:LEU:HD21	34:5:504:LUT:H31	1.90	0.52
2:B:102:VAL:O	2:B:106:THR:HG23	2.10	0.52
9:H:124:LEU:CB	9:H:125:PRO:CD	2.88	0.52
11:K:63:VAL:HG13	11:K:75:THR:HG21	1.91	0.52
1:A:396:TRP:HD1	21:A:1126:CLA:HAB	1.73	0.52
21:A:1108:CLA:H61	21:3:605:CLA:H51	1.91	0.52
8:G:46:ARG:HD3	8:G:46:ARG:C	2.34	0.52
21:A:1115:CLA:HBB1	21:A:1115:CLA:HMB1	1.92	0.51
21:B:1023:CLA:HMA2	21:B:1023:CLA:HBA2	1.92	0.51
12:L:128:GLU:OE1	12:L:128:GLU:HA	2.10	0.51
20:A:1011:CL0:H66	21:B:1022:CLA:CMB	2.40	0.51
21:B:1207:CLA:H151	9:H:109:VAL:HG11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:G:1602:CLA:HMB3	21:G:1602:CLA:CBB	2.37	0.51
24:I:4002:BCR:C23	24:I:4002:BCR:C40	2.85	0.51
21:K:1402:CLA:HMB3	21:K:1402:CLA:CBB	2.40	0.51
17:4:145:TYR:OH	17:4:281:GLN:NE2	2.44	0.51
1:A:256:SER:OG	1:A:271:GLU:O	2.24	0.51
24:A:4001:BCR:H311	24:A:4002:BCR:H383	1.93	0.51
2:B:394:PHE:HD1	2:B:398:ASP:OD1	1.92	0.51
21:B:1207:CLA:HAB	10:I:30:GLY:HA3	1.92	0.51
14:1:141:LEU:CD1	21:1:611:CLA:HAB	2.40	0.51
21:5:608:CLA:CED	19:6:128:ILE:HD11	2.39	0.51
34:6:501:LUT:H162	21:6:603:CLA:HMB2	1.90	0.51
1:A:505:ALA:HB1	1:A:510:TRP:HE1	1.74	0.51
2:B:436:GLY:HA3	21:B:1230:CLA:HAB	1.92	0.51
8:G:117:LEU:HD22	8:G:122:GLN:HB2	1.91	0.51
9:H:67:TRP:HD1	12:L:166:GLY:CA	2.23	0.51
21:5:604:CLA:H91	21:5:605:CLA:HMB1	1.93	0.51
2:B:155:TRP:CZ2	18:5:243:ASN:ND2	2.77	0.51
7:J:10:THR:OG1	7:J:11:ALA:N	2.42	0.51
9:H:122:LEU:O	9:H:126:ILE:HG12	2.11	0.51
13:O:65:SER:H	24:O:4001:BCR:HC42	1.75	0.51
19:6:129:LEU:CD1	21:6:613:CLA:CHB	2.88	0.51
21:A:1138:CLA:H72	24:B:4006:BCR:H14C	1.92	0.51
2:B:66:LEU:HD11	24:B:4003:BCR:H291	1.93	0.51
2:B:416:LYS:NZ	2:B:541:ASP:OD1	2.41	0.51
4:D:204:THR:C	4:D:206:SER:H	2.18	0.51
8:G:102:ALA:O	8:G:105:HIS:HB3	2.10	0.51
21:G:1601:CLA:CBB	24:G:4001:BCR:C36	2.88	0.51
21:K:1402:CLA:HAA1	33:O:5002:PTY:C1	2.38	0.51
12:L:110:LEU:O	12:L:134:SER:OG	2.27	0.51
21:5:603:CLA:H43	36:5:609:CHL:C5	2.41	0.51
21:5:606:CLA:HMA2	21:5:613:CLA:C2C	2.40	0.51
21:5:608:CLA:C3B	36:5:609:CHL:H18	2.41	0.51
19:6:180:PHE:CE1	35:6:502:XAT:H12	2.46	0.51
21:B:1208:CLA:H121	21:6:612:CLA:H143	1.93	0.51
21:L:1501:CLA:H42	21:L:1504:CLA:HBC2	1.92	0.51
18:5:99:LEU:HD11	21:5:606:CLA:CMC	2.41	0.51
1:A:487:ILE:CD1	21:A:1135:CLA:CGA	2.88	0.51
2:B:83:ILE:HG23	2:B:364:VAL:HG11	1.93	0.51
21:G:1601:CLA:HBC2	21:G:1601:CLA:HMC1	1.92	0.51
9:H:66:ALA:HB1	12:L:164:LEU:HA	1.92	0.51
18:5:99:LEU:HD11	34:5:504:LUT:C40	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:5:609:CHL:C4C	25:5:801:LHG:HC81	2.41	0.51
19:6:102:GLU:OE1	19:6:193:GLN:NE2	2.44	0.51
21:6:612:CLA:HED2	21:6:612:CLA:H2A	1.92	0.51
1:A:15:ILE:HD13	21:A:1108:CLA:HBA1	1.93	0.51
21:A:1121:CLA:CED	11:K:51:ASN:OD1	2.59	0.51
2:B:601:THR:OG1	2:B:606:ASN:O	2.29	0.51
11:K:63:VAL:HG12	11:K:64:HIS:N	2.26	0.51
16:3:161:ASP:N	16:3:161:ASP:OD1	2.42	0.51
16:3:280:LEU:HB2	21:3:603:CLA:H2	1.93	0.51
17:4:137:LEU:HD13	17:4:146:GLY:CA	2.37	0.51
21:A:1114:CLA:HMB3	21:A:1114:CLA:CBB	2.33	0.51
2:B:222:GLY:C	2:B:224:THR:H	2.18	0.51
21:B:1208:CLA:HBB1	21:B:1208:CLA:CHC	2.23	0.51
9:H:114:LEU:CD1	10:I:27:PRO:HB3	2.41	0.51
18:5:155:PHE:HA	18:5:162:ASP:HB2	1.93	0.51
1:A:285:VAL:HG13	1:A:286:THR:HG23	1.92	0.50
12:L:138:VAL:HG21	12:L:191:GLY:HA3	1.93	0.50
12:L:156:GLN:HB3	12:L:157:PRO:CD	2.40	0.50
18:5:73:PRO:HG2	34:5:502:LUT:H162	1.93	0.50
1:A:531:SER:HA	1:A:534:LEU:HD12	1.93	0.50
21:A:1114:CLA:HBC2	16:3:155:PRO:HG2	1.92	0.50
2:B:722:TYR:HB2	21:B:1021:CLA:HED3	1.93	0.50
18:5:185:LEU:HD11	21:5:604:CLA:HBC1	1.92	0.50
1:A:32:PRO:HG2	1:A:48:TRP:HH2	1.76	0.50
21:A:1120:CLA:H61	21:A:1121:CLA:C2	2.42	0.50
2:B:52:PHE:CE1	21:B:1208:CLA:CBB	2.93	0.50
6:F:138:LEU:HG	6:F:146:PRO:HB3	1.93	0.50
24:F:4001:BCR:H14C	7:J:36:PRO:CB	2.41	0.50
8:G:112:LEU:HD11	31:1:804:LMG:H292	1.94	0.50
14:1:147:ASP:HB3	14:1:150:LYS:HB2	1.92	0.50
19:6:210:ILE:HD12	21:6:603:CLA:C3D	2.41	0.50
2:B:701:LEU:N	2:B:701:LEU:CD1	2.74	0.50
3:C:72:GLU:HB3	3:C:77:LEU:HG	1.93	0.50
21:6:606:CLA:HMB3	21:6:606:CLA:CBB	2.34	0.50
2:B:168:TRP:CZ2	21:B:1208:CLA:CMA	2.93	0.50
2:B:227:TRP:HZ2	21:B:1212:CLA:H42	1.77	0.50
24:I:4001:BCR:H323	24:I:4001:BCR:HC8	1.94	0.50
21:1:611:CLA:HBB1	21:1:611:CLA:CMB	2.41	0.50
21:6:602:CLA:HED2	21:6:602:CLA:O1A	2.12	0.50
1:A:229:ASP:OD1	1:A:229:ASP:N	2.41	0.50
1:A:482:VAL:HG11	32:L:5002:4RF:H75	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1013:CLA:H203	21:A:1140:CLA:H52	1.94	0.50
2:B:672:TRP:CZ3	21:B:1023:CLA:O1D	2.64	0.50
21:B:1229:CLA:H201	24:F:4002:BCR:H14C	1.92	0.50
14:1:57:ASP:OD1	35:1:502:XAT:O3	2.28	0.50
21:5:603:CLA:HBC1	21:5:614:CLA:H13	1.92	0.50
21:A:1013:CLA:H172	21:A:1140:CLA:H61	1.94	0.50
12:L:132:CYS:O	12:L:135:ALA:HB3	2.11	0.50
34:5:504:LUT:H11	21:5:606:CLA:H12	1.94	0.50
34:5:504:LUT:C11	21:5:606:CLA:H12	2.42	0.50
21:A:1104:CLA:H151	21:A:1127:CLA:HBB2	1.92	0.50
21:A:1114:CLA:HBA2	31:3:803:LMG:H302	1.93	0.50
2:B:27:ALA:HB1	28:B:5002:DGD:HB21	1.93	0.50
4:D:134:ARG:NH2	4:D:136:GLU:OE1	2.40	0.50
10:I:21:ALA:HB3	10:I:22:PRO:HD3	1.94	0.50
11:K:25:VAL:HG23	11:K:26:ARG:HD2	1.92	0.50
15:2:135:ASP:N	15:2:135:ASP:OD1	2.41	0.50
19:6:180:PHE:CZ	35:6:502:XAT:H10	2.47	0.50
1:A:267:LEU:CD1	11:K:29:MET:CE	2.90	0.50
24:A:4007:BCR:H363	21:B:1023:CLA:H72	1.94	0.50
36:5:609:CHL:C3D	25:5:801:LHG:H131	2.42	0.50
1:A:222:LEU:HG	1:A:250:ILE:HD11	1.94	0.49
1:A:449:GLY:HA3	21:B:1023:CLA:C1	2.41	0.49
2:B:525:ALA:O	2:B:529:HIS:ND1	2.41	0.49
7:J:35:ASP:OD1	7:J:35:ASP:N	2.45	0.49
9:H:114:LEU:HD12	10:I:27:PRO:HB3	1.94	0.49
16:3:209:SER:OG	16:3:210:ASP:N	2.43	0.49
21:6:606:CLA:H12	21:6:613:CLA:C3D	2.42	0.49
24:F:4002:BCR:H351	25:F:5001:LHG:H282	1.93	0.49
11:K:74:PHE:CE2	11:K:79:VAL:HG22	2.47	0.49
16:3:163:TRP:HE1	21:3:613:CLA:CAD	2.24	0.49
21:A:1115:CLA:HMD3	21:K:1402:CLA:HED2	1.94	0.49
21:A:1137:CLA:HBD	21:A:1137:CLA:HBA1	1.92	0.49
2:B:391:GLY:HA3	24:B:4005:BCR:H382	1.95	0.49
21:B:1023:CLA:H2	21:B:1023:CLA:CMA	2.25	0.49
21:B:1225:CLA:H172	24:B:4003:BCR:H362	1.94	0.49
21:B:1238:CLA:H171	12:L:140:ILE:HD13	1.94	0.49
24:I:4002:BCR:H381	12:L:136:ALA:HB3	1.94	0.49
35:4:502:XAT:O24	21:4:604:CLA:H52	2.12	0.49
1:A:598:TRP:HE1	21:B:1023:CLA:C1D	2.26	0.49
2:B:394:PHE:CD1	2:B:398:ASP:OD1	2.65	0.49
11:K:53:THR:CG2	11:K:59:LEU:CD1	2.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:6:218:PRO:N	19:6:218:PRO:C	2.63	0.49
1:A:234:PRO:HA	1:A:237:ILE:HD12	1.94	0.49
1:A:574:PRO:N	1:A:574:PRO:C	2.60	0.49
21:A:1121:CLA:HBB1	21:A:1121:CLA:CHC	2.19	0.49
2:B:99:GLN:HA	2:B:99:GLN:HE21	1.74	0.49
21:B:1212:CLA:HMB1	21:B:1212:CLA:CBB	2.43	0.49
15:2:195:GLU:HB2	15:2:198:TYR:HB2	1.95	0.49
21:2:604:CLA:HBC1	25:2:801:LHG:H292	1.94	0.49
19:6:162:SER:H	19:6:163:PRO:CD	2.18	0.49
1:A:316:TRP:HD1	11:K:77:THR:HG21	1.76	0.49
1:A:718:LEU:HB3	1:A:722:GLN:HG2	1.95	0.49
21:A:1114:CLA:CAD	31:3:803:LMG:H291	2.42	0.49
5:E:110:ASN:HD21	5:E:114:VAL:HG22	1.77	0.49
5:E:119:TYR:HB3	5:E:123:GLU:HG3	1.94	0.49
14:1:73:GLU:HB3	14:1:152:LEU:CD2	2.42	0.49
17:4:229:LYS:HZ1	17:4:252:LEU:HD13	1.77	0.49
2:B:388:PHE:CZ	21:B:1222:CLA:HAB	2.46	0.49
21:5:608:CLA:C1B	36:5:609:CHL:H18	2.43	0.49
19:6:150:ILE:CG2	19:6:154:PRO:HA	2.43	0.49
21:A:1122:CLA:HMD2	21:A:1123:CLA:HAB	1.95	0.49
21:B:1216:CLA:HBB1	21:B:1221:CLA:H51	1.95	0.49
21:B:1217:CLA:HMB2	8:G:103:LEU:HD21	1.94	0.49
21:G:1602:CLA:C1A	24:G:4001:BCR:HC21	2.43	0.49
12:L:119:PRO:N	12:L:119:PRO:C	2.62	0.49
15:2:262:THR:HG23	15:2:264:ALA:H	1.77	0.49
19:6:137:GLU:OE1	19:6:140:ARG:NH1	2.46	0.49
21:A:1112:CLA:H13	24:A:4002:BCR:H353	1.95	0.48
2:B:610:PHE:O	2:B:614:SER:HB3	2.12	0.48
21:B:1218:CLA:H18	14:1:132:VAL:HG22	1.94	0.48
21:B:1223:CLA:HBB1	21:B:1231:CLA:HAA2	1.95	0.48
12:L:60:LEU:H	12:L:60:LEU:HD12	1.78	0.48
12:L:60:LEU:HD12	12:L:60:LEU:O	2.12	0.48
34:5:503:LUT:H183	37:6:803:SQD:H242	1.95	0.48
19:6:109:LYS:HD3	19:6:111:PHE:CZ	2.48	0.48
21:6:606:CLA:HED2	21:6:606:CLA:H2A	1.95	0.48
1:A:267:LEU:HD21	21:K:1401:CLA:HBC2	1.95	0.48
1:A:596:LEU:HD21	21:A:1128:CLA:HBC1	1.94	0.48
21:B:1223:CLA:H2	24:B:4005:BCR:H14C	1.95	0.48
21:B:1237:CLA:H161	12:L:141:LEU:HD21	1.94	0.48
10:I:21:ALA:N	10:I:22:PRO:HD2	2.28	0.48
17:4:318:VAL:HB	21:4:603:CLA:HED1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:5:86:LEU:HD13	21:5:604:CLA:C1	2.43	0.48
19:6:85:LYS:HB3	19:6:89:ARG:NH1	2.28	0.48
21:B:1209:CLA:HAA1	8:G:77:ASP:HB3	1.94	0.48
21:1:601:CLA:H92	21:1:601:CLA:H61	1.59	0.48
17:4:141:MET:HE1	17:4:159:MET:CE	2.43	0.48
19:6:118:TYR:HA	35:6:504:XAT:H3	1.93	0.48
1:A:382:THR:HG21	1:A:517:VAL:HB	1.96	0.48
1:A:553:GLY:O	1:A:557:ALA:HB2	2.12	0.48
21:A:1121:CLA:H142	21:K:1402:CLA:HBC1	1.94	0.48
21:4:604:CLA:H12	21:4:604:CLA:HHB	1.93	0.48
18:5:99:LEU:HD12	21:5:606:CLA:HMC3	1.96	0.48
2:B:378:TYR:CD2	21:B:1224:CLA:HAB	2.49	0.48
5:E:110:ASN:ND2	5:E:114:VAL:HG22	2.27	0.48
13:O:122:ARG:HH12	24:O:4001:BCR:H281	1.78	0.48
15:2:111:ARG:NH1	36:2:611:CHL:OBD	2.46	0.48
18:5:92:VAL:HG11	18:5:143:ARG:HH12	1.77	0.48
36:5:609:CHL:HAC2	25:5:801:LHG:HC41	1.95	0.48
1:A:572:ARG:NH1	25:A:5002:LHG:O10	2.46	0.48
2:B:166:LEU:HG	2:B:170:LYS:HD2	1.94	0.48
24:B:4001:BCR:H392	8:G:100:HIS:CD2	2.48	0.48
12:L:159:MET:HA	12:L:159:MET:HE3	1.96	0.48
15:2:193:GLY:HA2	15:2:199:PRO:HA	1.95	0.48
1:A:355:ILE:HD11	24:A:4004:BCR:H311	1.95	0.48
8:G:81:LYS:CA	8:G:81:LYS:CE	2.86	0.48
13:O:80:ILE:HG22	13:O:97:PHE:CD1	2.48	0.48
36:5:609:CHL:HED1	19:6:134:GLY:CA	2.43	0.48
36:5:610:CHL:HBB1	36:5:610:CHL:HHC	1.96	0.48
21:6:612:CLA:HAA2	31:6:802:LMG:H142	1.96	0.48
20:A:1011:CL0:CGD	20:A:1011:CL0:CAA	2.89	0.48
21:A:1116:CLA:O2A	21:A:1125:CLA:HBB2	2.14	0.48
2:B:86:ARG:HH12	2:B:107:ARG:HD2	1.79	0.48
2:B:93:TRP:CH2	9:H:114:LEU:CD1	2.91	0.48
15:2:232:ALA:HA	21:2:603:CLA:HBB1	1.96	0.48
21:4:604:CLA:CGA	21:4:604:CLA:C3A	2.92	0.48
1:A:680:ALA:HB3	21:A:1013:CLA:HBB2	1.96	0.48
21:A:1139:CLA:H43	21:F:1301:CLA:HBC3	1.95	0.48
21:B:1023:CLA:HBA2	21:B:1023:CLA:CMA	2.39	0.48
5:E:83:TRP:HA	5:E:86:GLN:HG3	1.96	0.48
9:H:114:LEU:O	9:H:117:LYS:CD	2.61	0.48
11:K:53:THR:CG2	11:K:59:LEU:HD11	2.43	0.48
17:4:124:ARG:HB3	17:4:125:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:5:108:GLU:HA	18:5:108:GLU:OE2	2.13	0.48
1:A:294:THR:O	1:A:298:HIS:ND1	2.46	0.48
1:A:322:ILE:HB	1:A:342:TYR:HE1	1.78	0.48
1:A:87:TRP:HA	21:A:1105:CLA:HBB2	1.95	0.47
21:A:1102:CLA:HAA1	21:A:1109:CLA:H11	1.96	0.47
21:B:1212:CLA:H61	24:B:4001:BCR:C31	2.44	0.47
21:1:601:CLA:H41	21:1:601:CLA:H62	1.57	0.47
19:6:180:PHE:CD1	35:6:502:XAT:H12	2.48	0.47
2:B:515:PRO:HD3	6:F:147:HIS:HE1	1.77	0.47
4:D:112:ILE:HA	4:D:122:ILE:HA	1.96	0.47
21:4:604:CLA:HMB1	21:4:604:CLA:CBB	2.44	0.47
21:B:1210:CLA:H51	21:B:1215:CLA:HBC3	1.96	0.47
21:B:1215:CLA:H3A	21:B:1215:CLA:HBA2	1.47	0.47
8:G:40:SER:O	8:G:44:LEU:HB2	2.15	0.47
8:G:81:LYS:HD3	19:6:67:PRO:O	2.14	0.47
8:G:103:LEU:HD11	24:G:4001:BCR:C37	2.41	0.47
14:1:93:GLU:OE2	14:1:203:LEU:N	2.40	0.47
21:1:608:CLA:H52	21:1:608:CLA:H11	1.69	0.47
18:5:99:LEU:HD11	21:5:606:CLA:HMC2	1.97	0.47
21:6:606:CLA:HMA3	21:6:613:CLA:C3C	2.43	0.47
1:A:585:GLN:HG2	1:A:724:ARG:CZ	2.45	0.47
24:A:4003:BCR:H311	21:3:612:CLA:H192	1.95	0.47
2:B:225:PRO:O	2:B:228:SER:O	2.33	0.47
12:L:111:ALA:HA	12:L:134:SER:OG	2.14	0.47
21:2:612:CLA:H41	21:2:612:CLA:H62	1.72	0.47
1:A:449:GLY:HA3	21:B:1023:CLA:O2A	2.14	0.47
1:A:532:ASP:O	1:A:536:HIS:ND1	2.37	0.47
21:A:1134:CLA:H8	21:K:1402:CLA:H71	1.97	0.47
2:B:91:ALA:HA	2:B:114:VAL:HG12	1.96	0.47
2:B:208:VAL:HG22	2:B:216:VAL:HG11	1.97	0.47
2:B:280:ALA:CB	21:B:1214:CLA:HAB	2.45	0.47
21:B:1239:CLA:HBC1	22:B:2002:PQN:H2M2	1.96	0.47
6:F:139:LEU:C	6:F:139:LEU:CD1	2.87	0.47
8:G:106:VAL:HA	8:G:110:PHE:HB2	1.97	0.47
10:I:39:ALA:HA	12:L:147:LEU:HD21	1.95	0.47
18:5:116:ILE:HG23	33:5:803:PTY:H391	1.95	0.47
3:C:81:TYR:HB3	4:D:92:LEU:HD12	1.96	0.47
8:G:89:LYS:HB3	8:G:89:LYS:HE2	1.72	0.47
15:2:184:PHE:CE2	36:2:611:CHL:HBB2	2.49	0.47
24:3:506:BCR:H21C	21:3:606:CLA:HMC3	1.97	0.47
31:4:802:LMG:H291	31:4:802:LMG:H321	1.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:5:242:ALA:HB2	31:6:802:LMG:H152	1.94	0.47
19:6:177:MET:SD	21:6:604:CLA:HAB	2.55	0.47
21:6:604:CLA:H112	21:6:605:CLA:HMA3	1.96	0.47
20:A:1011:CL0:H30	20:A:1011:CL0:CAA	2.41	0.47
2:B:513:ILE:HG22	2:B:517:ASP:OD2	2.15	0.47
9:H:54:TYR:CD2	12:L:63:ASP:OD1	2.68	0.47
9:H:103:VAL:HB	12:L:139:LEU:HD21	1.96	0.47
9:H:137:GLU:O	9:H:138:ASN:CG	2.57	0.47
21:1:601:CLA:H71	21:1:602:CLA:CMA	2.44	0.47
21:5:608:CLA:NB	36:5:609:CHL:H18	2.30	0.47
35:6:504:XAT:H27	21:6:601:CLA:HBC1	1.97	0.47
1:A:434:ARG:NH1	1:A:559:SER:O	2.43	0.47
20:A:1011:CL0:H21	2:B:626:TRP:HD1	1.78	0.47
2:B:251:SER:OG	2:B:252:GLY:N	2.46	0.47
13:O:62:ILE:HD13	13:O:104:TRP:NE1	2.29	0.47
36:5:609:CHL:C4C	25:5:801:LHG:H101	2.44	0.47
19:6:169:GLU:HA	21:6:601:CLA:HMB1	1.97	0.47
2:B:440:HIS:CD2	2:B:454:ILE:HG13	2.49	0.47
2:B:456:ILE:HG13	24:F:4001:BCR:H383	1.97	0.47
4:D:90:GLY:O	12:L:67:GLY:N	2.48	0.47
21:5:604:CLA:CMB	21:5:604:CLA:CBB	2.92	0.47
21:6:601:CLA:HBA2	21:6:601:CLA:H3A	1.40	0.47
21:6:605:CLA:H42	31:6:802:LMG:H312	1.96	0.47
21:B:1228:CLA:H52	24:F:4002:BCR:H372	1.97	0.47
21:B:1237:CLA:H152	24:I:4002:BCR:C35	2.45	0.47
9:H:109:VAL:O	9:H:113:ALA:HB2	2.15	0.47
14:1:104:PRO:HB2	36:1:610:CHL:C2D	2.45	0.47
14:1:154:PRO:HB2	14:1:155:GLY:H	1.55	0.47
24:1:504:BCR:C35	21:1:611:CLA:HBB1	2.45	0.47
15:2:76:TRP:HB2	15:2:99:ARG:NH1	2.30	0.47
18:5:90:GLU:HB2	21:5:604:CLA:CHB	2.44	0.47
19:6:217:THR:H	19:6:218:PRO:HD2	1.80	0.47
21:B:1230:CLA:H41	21:B:1230:CLA:H62	1.56	0.46
4:D:173:VAL:HG11	4:D:179:ASN:HB2	1.97	0.46
6:F:113:SER:OG	6:F:114:ALA:N	2.48	0.46
9:H:70:TYR:CE1	12:L:83:LEU:HD13	2.49	0.46
11:K:70:PRO:HD3	21:K:1404:CLA:C1D	2.45	0.46
16:3:105:ASN:ND2	16:3:108:TRP:H	2.13	0.46
18:5:99:LEU:CD1	21:5:606:CLA:CMC	2.93	0.46
21:A:1134:CLA:HHC	21:A:1134:CLA:CBB	2.45	0.46
2:B:515:PRO:CG	6:F:147:HIS:CE1	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:1206:CLA:H192	21:B:1206:CLA:H162	1.58	0.46
3:C:55:GLU:OE1	3:C:66:ARG:NH1	2.49	0.46
10:I:27:PRO:N	10:I:28:LEU:N	2.63	0.46
14:1:57:ASP:HB2	21:1:604:CLA:HBA2	1.96	0.46
25:2:802:LHG:H201	37:2:805:SQD:H302	1.96	0.46
18:5:96:TRP:CD2	21:5:612:CLA:HAC2	2.49	0.46
19:6:50:VAL:HG13	19:6:52:PRO:HD2	1.97	0.46
19:6:85:LYS:HD2	19:6:149:PHE:HZ	1.73	0.46
21:A:1112:CLA:HBB1	24:A:4003:BCR:H362	1.97	0.46
21:A:1138:CLA:HED2	2:B:425:TRP:HB2	1.98	0.46
21:B:1021:CLA:CMB	21:B:1022:CLA:OBD	2.56	0.46
3:C:58:CYS:HB3	3:C:63:LEU:HD22	1.97	0.46
9:H:115:PHE:CE2	10:I:24:LEU:HD13	2.50	0.46
16:3:114:VAL:HG21	16:3:213:ALA:HB1	1.97	0.46
16:3:118:ARG:HA	16:3:121:MET:HE3	1.98	0.46
18:5:242:ALA:CA	31:6:802:LMG:H121	2.45	0.46
19:6:92:MET:HG3	19:6:173:GLY:HA2	1.98	0.46
36:6:610:CHL:HAA2	36:6:610:CHL:CBD	2.44	0.46
21:A:1139:CLA:H61	21:A:1139:CLA:H41	1.55	0.46
21:B:1203:CLA:HED1	21:B:1226:CLA:H43	1.98	0.46
21:K:1402:CLA:HBA1	21:K:1402:CLA:O2D	2.16	0.46
21:K:1402:CLA:H2	21:K:1402:CLA:H61	1.72	0.46
18:5:68:ASP:HA	21:5:604:CLA:HED2	1.98	0.46
18:5:99:LEU:CG	21:5:606:CLA:HAB	2.37	0.46
21:5:605:CLA:H51	21:5:605:CLA:C9	2.44	0.46
19:6:210:ILE:HD12	21:6:603:CLA:C2D	2.46	0.46
21:6:602:CLA:HBB1	21:6:602:CLA:CHC	2.18	0.46
1:A:450:PHE:C	21:A:1132:CLA:HBB2	2.41	0.46
21:B:1222:CLA:H92	21:B:1240:CLA:H193	1.98	0.46
29:B:5003:3PH:H222	29:B:5003:3PH:H2	1.83	0.46
10:I:9:ALA:HB3	10:I:16:VAL:HG11	1.97	0.46
21:K:1401:CLA:CMC	24:K:4001:BCR:H332	2.45	0.46
36:1:609:CHL:HHC	36:1:609:CHL:HBB1	1.97	0.46
1:A:122:VAL:O	1:A:122:VAL:HG23	2.15	0.46
1:A:153:ILE:HG21	1:A:159:LEU:HD21	1.97	0.46
2:B:352:HIS:ND1	21:B:1214:CLA:OBD	2.43	0.46
21:B:1212:CLA:H61	21:B:1212:CLA:H92	1.63	0.46
14:1:39:PRO:HB3	17:4:244:SER:HB2	1.97	0.46
21:1:601:CLA:C2	21:1:601:CLA:HBA1	2.44	0.46
35:2:502:XAT:H8	21:2:604:CLA:H52	1.98	0.46
18:5:136:PHE:HE2	21:5:613:CLA:HMA3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:5:185:LEU:HG	21:5:604:CLA:HMC3	1.97	0.46
18:5:205:LEU:HD12	34:5:501:LUT:H22	1.96	0.46
34:5:501:LUT:H32	21:5:601:CLA:CAB	2.45	0.46
34:5:503:LUT:H15	34:5:503:LUT:H201	1.72	0.46
1:A:473:SER:HB2	1:A:640:ASN:HD22	1.80	0.46
2:B:23:TRP:HZ3	22:B:2002:PQN:H293	1.81	0.46
2:B:107:ARG:HH21	2:B:116:ILE:H	1.64	0.46
2:B:223:LEU:HD13	2:B:227:TRP:CH2	2.51	0.46
21:B:1214:CLA:HBC2	21:B:1215:CLA:H203	1.98	0.46
8:G:38:THR:OG1	8:G:105:HIS:HB2	2.15	0.46
8:G:70:THR:OG1	8:G:71:THR:N	2.48	0.46
18:5:93:HIS:CG	21:5:604:CLA:CBB	2.99	0.46
18:5:242:ALA:HA	31:6:802:LMG:C12	2.45	0.46
34:5:503:LUT:H11	34:5:503:LUT:H191	1.73	0.46
1:A:680:ALA:CB	21:A:1013:CLA:HBB2	2.46	0.46
21:A:1013:CLA:H143	22:A:2001:PQN:H261	1.98	0.46
2:B:231:TRP:CH2	21:B:1213:CLA:HBB1	2.51	0.46
9:H:78:TYR:HE2	12:L:97:LEU:HB3	1.75	0.46
12:L:60:LEU:HD21	12:L:68:MET:HB3	1.97	0.46
12:L:120:LEU:HB2	12:L:130:VAL:CG2	2.46	0.46
21:3:603:CLA:H11	21:3:603:CLA:H51	1.70	0.46
18:5:193:THR:OG1	18:5:199:GLN:O	2.34	0.46
2:B:99:GLN:HA	9:H:123:GLU:HG2	1.97	0.46
9:H:70:TYR:HB2	12:L:89:TYR:CE1	2.51	0.46
10:I:29:THR:HA	10:I:33:LEU:HB3	1.97	0.46
13:O:58:LEU:HD13	13:O:111:VAL:HG21	1.97	0.46
15:2:121:LEU:HD21	34:2:501:LUT:H373	1.97	0.46
16:3:283:ASN:HD21	21:3:603:CLA:HED2	1.80	0.46
21:A:1113:CLA:H172	21:3:605:CLA:HMC2	1.98	0.46
21:A:1130:CLA:H52	21:L:1502:CLA:H102	1.98	0.46
21:A:1136:CLA:H142	21:A:1136:CLA:H112	1.83	0.46
24:A:4001:BCR:H392	24:A:4001:BCR:H282	1.33	0.46
22:B:2002:PQN:H242	22:B:2002:PQN:H211	1.83	0.46
17:4:281:GLN:NE2	21:4:607:CLA:O1D	2.49	0.46
18:5:110:LEU:HD11	18:5:112:MET:CE	2.43	0.46
21:A:1102:CLA:H191	21:A:1107:CLA:H93	1.97	0.45
24:A:4004:BCR:H373	25:A:5001:LHG:H172	1.98	0.45
2:B:6:PHE:CG	10:I:45:ILE:HD13	2.52	0.45
2:B:574:TYR:CE1	2:B:704:VAL:HG13	2.51	0.45
5:E:103:VAL:HG22	5:E:118:ASN:HB3	1.98	0.45
34:1:501:LUT:H31	34:1:501:LUT:H391	1.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:5:51:PRO:HG3	18:5:71:PHE:HB2	1.98	0.45
18:5:218:PHE:CZ	21:5:603:CLA:H42	2.50	0.45
21:A:1113:CLA:H42	24:3:504:BCR:H23C	1.97	0.45
21:A:1128:CLA:H201	21:A:1140:CLA:H2	1.98	0.45
2:B:411:ARG:NH1	21:B:1227:CLA:O1D	2.49	0.45
25:B:5001:LHG:H292	25:B:5001:LHG:H262	1.74	0.45
15:2:269:SER:O	15:2:269:SER:OG	2.29	0.45
18:5:52:LEU:CD2	18:5:237:PRO:HB3	2.47	0.45
1:A:43:PRO:HG3	6:F:200:ILE:HD13	1.97	0.45
2:B:72:GLN:HG2	2:B:91:ALA:HB2	1.99	0.45
2:B:518:PHE:CE1	24:F:4001:BCR:H381	2.51	0.45
21:B:1217:CLA:H8	21:B:1217:CLA:H52	1.79	0.45
21:B:1225:CLA:HBA2	21:B:1225:CLA:H3A	1.58	0.45
21:B:1239:CLA:HBB1	21:B:1239:CLA:CHC	2.22	0.45
21:K:1404:CLA:HMA1	24:K:4001:BCR:H21C	1.98	0.45
14:1:73:GLU:HB3	14:1:152:LEU:HD23	1.98	0.45
15:2:170:LEU:HD13	21:2:612:CLA:HMA1	1.97	0.45
17:4:142:LEU:HD22	17:4:276:LYS:CB	2.47	0.45
18:5:110:LEU:C	18:5:110:LEU:CD1	2.89	0.45
21:6:603:CLA:H12	21:6:603:CLA:CHA	2.41	0.45
1:A:318:ILE:HD12	11:K:81:ALA:HB2	1.98	0.45
1:A:557:ALA:CB	1:A:588:ALA:HB2	2.47	0.45
21:A:1116:CLA:H41	21:A:1134:CLA:HMA1	1.98	0.45
2:B:701:LEU:N	2:B:701:LEU:HD12	2.30	0.45
21:B:1239:CLA:H111	21:B:1239:CLA:H152	1.71	0.45
24:B:4002:BCR:H15C	24:B:4002:BCR:H351	1.76	0.45
4:D:91:LEU:HB2	12:L:66:VAL:HA	1.98	0.45
34:2:501:LUT:H11	34:2:501:LUT:H191	1.83	0.45
18:5:99:LEU:CD2	34:5:504:LUT:H31	2.46	0.45
34:5:504:LUT:C40	21:5:606:CLA:HMC2	2.47	0.45
36:5:609:CHL:HHC	36:5:609:CHL:CBB	2.43	0.45
21:A:1116:CLA:H61	21:A:1116:CLA:H92	1.67	0.45
21:A:1126:CLA:H41	21:A:1126:CLA:H92	1.97	0.45
21:A:1138:CLA:HBB2	6:F:182:GLY:HA3	1.98	0.45
6:F:200:ILE:HG13	6:F:201:ILE:HG13	1.99	0.45
24:F:4002:BCR:H351	24:F:4002:BCR:H15C	1.81	0.45
9:H:65:GLY:HA2	9:H:67:TRP:CZ3	2.51	0.45
24:I:4002:BCR:H351	24:I:4002:BCR:H15C	1.58	0.45
12:L:96:ASN:H	12:L:182:LYS:HZ2	1.64	0.45
13:O:58:LEU:CD2	13:O:62:ILE:HD11	2.47	0.45
13:O:123:THR:OG1	13:O:124:GLU:OE1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:4:501:LUT:H35	34:4:501:LUT:H401	1.82	0.45
18:5:228:VAL:HG12	29:5:807:3PH:H351	1.98	0.45
18:5:238:MET:HE1	19:6:141:PHE:CD1	2.50	0.45
21:5:605:CLA:CMB	21:5:605:CLA:CBB	2.94	0.45
19:6:190:THR:HG22	19:6:213:TYR:CD1	2.51	0.45
36:6:610:CHL:HBC3	36:6:610:CHL:HHD	1.98	0.45
21:A:1101:CLA:C4B	24:J:4002:BCR:H393	2.46	0.45
2:B:109:GLY:HA2	9:H:135:LYS:CE	2.43	0.45
8:G:38:THR:HG21	24:G:4001:BCR:H14C	1.98	0.45
13:O:58:LEU:HD22	13:O:108:LEU:HA	1.98	0.45
36:1:610:CHL:HHC	36:1:610:CHL:HBB1	1.99	0.45
15:2:167:THR:HG22	21:4:609:CLA:HED3	1.98	0.45
24:3:504:BCR:H342	31:3:803:LMG:H222	1.98	0.45
21:4:607:CLA:H62	21:4:607:CLA:H102	1.58	0.45
21:A:1109:CLA:HAB	31:3:802:LMG:H142	1.98	0.45
21:A:1114:CLA:C1D	21:3:610:CLA:HBB2	2.46	0.45
2:B:659:ALA:HB1	21:B:1023:CLA:HBB2	1.95	0.45
21:B:1207:CLA:H61	21:B:1207:CLA:H41	1.72	0.45
9:H:79:PRO:HG3	21:H:1701:CLA:C3D	2.47	0.45
21:1:603:CLA:H62	21:1:603:CLA:H41	1.63	0.45
16:3:58:SER:N	16:3:75:ASP:OD2	2.49	0.45
21:6:604:CLA:H62	21:6:604:CLA:H2	1.68	0.45
21:B:1217:CLA:H41	21:B:1217:CLA:H61	1.81	0.45
4:D:73:PRO:O	4:D:156:TYR:OH	2.18	0.45
10:I:20:TRP:CZ3	33:5:803:PTY:H141	2.51	0.45
17:4:171:ARG:NH1	36:4:611:CHL:OBD	2.50	0.45
21:4:602:CLA:HBC3	21:4:607:CLA:H101	1.98	0.45
18:5:96:TRP:CE2	21:5:612:CLA:HAC2	2.52	0.45
18:5:172:ALA:HB1	21:5:601:CLA:H3A	1.98	0.45
21:5:604:CLA:HMD2	36:5:609:CHL:CBB	2.46	0.45
19:6:182:GLY:O	19:6:186:GLN:HB2	2.16	0.45
1:A:429:ARG:O	1:A:433:HIS:ND1	2.48	0.45
1:A:685:PHE:HZ	21:A:1140:CLA:HBC3	1.81	0.45
21:1:611:CLA:HBB1	21:1:611:CLA:HMB1	1.99	0.45
21:5:607:CLA:HBB1	21:5:607:CLA:HHC	1.98	0.45
21:A:1124:CLA:H62	21:A:1124:CLA:H41	1.78	0.45
2:B:370:ALA:HB1	2:B:726:LEU:HD11	1.99	0.45
2:B:660:THR:HG22	21:B:1023:CLA:HMB1	1.99	0.45
24:B:4006:BCR:H351	24:B:4006:BCR:H15C	1.74	0.45
8:G:38:THR:CA	8:G:105:HIS:HB2	2.46	0.45
11:K:38:PHE:CD1	21:K:1404:CLA:HBB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:L:1504:CLA:HBB1	21:L:1504:CLA:CHC	2.47	0.45
13:O:62:ILE:HG21	13:O:104:TRP:CD1	2.52	0.45
33:O:5002:PTY:C11	33:O:5002:PTY:C1	2.86	0.45
17:4:280:LEU:HD12	17:4:280:LEU:HA	1.86	0.45
21:A:1121:CLA:HBC2	21:A:1121:CLA:HHD	1.98	0.44
21:A:1126:CLA:H72	21:A:1126:CLA:H111	1.75	0.44
2:B:62:THR:HG23	2:B:143:LEU:HD13	1.98	0.44
21:B:1219:CLA:H41	21:B:1219:CLA:H62	1.53	0.44
8:G:103:LEU:CD1	24:G:4001:BCR:H372	2.44	0.44
9:H:67:TRP:CD1	12:L:166:GLY:CA	3.00	0.44
10:I:20:TRP:O	10:I:20:TRP:CE3	2.70	0.44
13:O:58:LEU:HD13	13:O:111:VAL:HG11	1.99	0.44
21:1:601:CLA:H141	21:1:601:CLA:H162	1.81	0.44
21:3:602:CLA:H11	21:3:602:CLA:H52	1.75	0.44
34:5:502:LUT:H31	34:5:502:LUT:H391	1.87	0.44
34:6:501:LUT:H15	34:6:501:LUT:H201	1.83	0.44
21:6:602:CLA:H2A	21:6:602:CLA:CED	2.39	0.44
1:A:151:SER:HB2	1:A:216:HIS:NE2	2.32	0.44
2:B:223:LEU:HB3	2:B:227:TRP:CZ3	2.52	0.44
5:E:82:TYR:O	5:E:82:TYR:CD1	2.70	0.44
9:H:81:LEU:HD13	24:H:4001:BCR:H313	1.99	0.44
12:L:87:PRO:HG3	21:L:1502:CLA:HED2	1.99	0.44
12:L:157:PRO:HG2	12:L:157:PRO:O	2.17	0.44
24:L:4002:BCR:H351	24:L:4002:BCR:H15C	1.83	0.44
13:O:85:ALA:HB3	13:O:87:TRP:HE1	1.81	0.44
14:1:83:MET:HE1	21:1:601:CLA:CBB	2.44	0.44
21:1:612:CLA:HAA2	25:1:803:LHG:H101	1.99	0.44
15:2:187:ILE:HG21	15:2:191:LEU:HD13	1.99	0.44
34:5:504:LUT:H401	21:5:606:CLA:HMC2	1.99	0.44
36:6:610:CHL:HHC	36:6:610:CHL:CBB	2.44	0.44
1:A:220:VAL:C	1:A:222:LEU:H	2.26	0.44
21:A:1103:CLA:H8	24:A:4003:BCR:H402	1.99	0.44
21:A:1137:CLA:H92	21:A:1137:CLA:H62	1.88	0.44
2:B:168:TRP:NE1	21:B:1208:CLA:CMA	2.75	0.44
13:O:80:ILE:HG21	21:O:1801:CLA:HMD2	1.99	0.44
31:3:803:LMG:H322	31:3:803:LMG:H351	1.87	0.44
17:4:149:PRO:HD2	35:4:502:XAT:H222	1.98	0.44
21:5:614:CLA:H162	21:5:614:CLA:H141	1.74	0.44
19:6:162:SER:N	19:6:163:PRO:HD2	2.22	0.44
1:A:532:ASP:OD1	1:A:613:LYS:NZ	2.49	0.44
21:A:1113:CLA:H143	16:3:251:PHE:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:PHE:CE1	10:I:15:PHE:O	2.71	0.44
15:2:165:VAL:HG21	24:2:503:BCR:H362	2.00	0.44
21:5:614:CLA:HHC	21:5:614:CLA:HBB1	1.99	0.44
2:B:27:ALA:HB2	28:B:5002:DGD:HA32	2.00	0.44
2:B:41:GLU:HA	2:B:166:LEU:HD13	2.00	0.44
2:B:451:GLU:OE1	2:B:451:GLU:N	2.36	0.44
2:B:499:LEU:HA	2:B:502:ILE:HG22	1.99	0.44
21:5:605:CLA:H111	21:5:605:CLA:H72	1.72	0.44
1:A:599:MET:HE3	1:A:599:MET:HB3	1.93	0.44
4:D:105:TRP:HB3	4:D:153:PRO:HB3	2.00	0.44
4:D:131:LYS:HE3	9:H:55:PHE:HB2	1.99	0.44
18:5:91:VAL:O	18:5:95:ARG:HG3	2.17	0.44
19:6:210:ILE:HD12	21:6:603:CLA:C2	2.47	0.44
21:A:1013:CLA:H62	21:A:1013:CLA:H41	1.71	0.44
21:A:1120:CLA:H8	21:A:1121:CLA:H61	2.00	0.44
24:A:4001:BCR:H15C	24:A:4001:BCR:H351	1.69	0.44
2:B:210:TRP:CZ2	21:B:1211:CLA:H2	2.53	0.44
21:B:1205:CLA:HAB	21:B:1206:CLA:HAA2	2.00	0.44
21:B:1207:CLA:C11	12:L:136:ALA:HB2	2.45	0.44
21:G:1601:CLA:HBB1	24:G:4001:BCR:H363	1.99	0.44
14:1:78:HIS:HB3	14:1:185:MET:HE3	1.98	0.44
21:4:601:CLA:H41	21:4:601:CLA:H62	1.78	0.44
36:5:610:CHL:HMA3	36:5:610:CHL:HAA1	1.84	0.44
1:A:448:LEU:HB3	1:A:541:PHE:HB2	1.99	0.44
21:A:1106:CLA:H143	21:A:1106:CLA:H111	1.80	0.44
25:A:5001:LHG:H211	25:A:5001:LHG:H182	1.76	0.44
2:B:71:TRP:HH2	10:I:21:ALA:HB3	1.83	0.44
2:B:609:GLN:O	2:B:613:SER:HB3	2.17	0.44
2:B:696:ASP:OD1	2:B:696:ASP:N	2.47	0.44
21:B:1235:CLA:CGA	21:B:1235:CLA:C1A	2.96	0.44
3:C:26:LEU:HD23	3:C:42:SER:HB3	2.00	0.44
3:C:61:ASP:O	5:E:117:ASN:ND2	2.49	0.44
14:1:44:LYS:H	14:1:55:ASN:HD21	1.66	0.44
14:1:173:LYS:HD3	21:1:601:CLA:C1	2.48	0.44
15:2:224:LYS:NZ	25:2:801:LHG:O5	2.37	0.44
16:3:259:ILE:HG23	16:3:260:THR:N	2.33	0.44
34:3:501:LUT:H35	34:3:501:LUT:H401	1.84	0.44
21:3:610:CLA:CAB	31:3:803:LMG:H341	2.48	0.44
21:4:602:CLA:HMD2	21:4:607:CLA:H61	2.00	0.44
19:6:126:VAL:N	19:6:127:PRO:HD2	2.33	0.44
19:6:165:HIS:CD2	19:6:165:HIS:O	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1112:CLA:HBB2	24:A:4003:BCR:H16C	2.00	0.44
2:B:69:VAL:HG11	2:B:125:TRP:HZ3	1.82	0.44
2:B:71:TRP:CH2	10:I:21:ALA:HB3	2.53	0.44
2:B:88:ILE:O	2:B:122:TYR:OH	2.27	0.44
21:B:1202:CLA:HBA1	21:B:1202:CLA:H3A	1.63	0.44
21:B:1207:CLA:HBA2	21:B:1207:CLA:CBD	2.48	0.44
21:B:1235:CLA:H3A	21:B:1235:CLA:HBA2	1.77	0.44
21:B:1240:CLA:H162	21:B:1240:CLA:H202	1.85	0.44
10:I:20:TRP:CD1	10:I:20:TRP:H	2.34	0.44
21:1:604:CLA:H122	21:1:605:CLA:H172	2.00	0.44
17:4:264:PHE:CE1	17:4:268:GLY:HA3	2.53	0.44
17:4:318:VAL:HA	17:4:323:ASN:HB2	2.00	0.44
18:5:217:VAL:HB	21:5:603:CLA:C3D	2.47	0.44
34:5:504:LUT:H201	34:5:504:LUT:H15	1.62	0.44
21:5:601:CLA:HBB1	21:5:602:CLA:HAA1	1.99	0.44
19:6:213:TYR:CE2	21:6:603:CLA:HED2	2.53	0.44
1:A:250:ILE:HA	1:A:250:ILE:HD12	1.73	0.43
1:A:711:PRO:HG2	1:A:715:PRO:HD3	1.99	0.43
21:A:1112:CLA:HBA1	24:A:4002:BCR:HC7	2.00	0.43
21:A:1114:CLA:H51	31:3:803:LMG:H181	1.99	0.43
24:B:4001:BCR:H24C	24:B:4001:BCR:H371	1.91	0.43
6:F:183:ARG:HD2	24:F:4002:BCR:H282	2.00	0.43
21:K:1404:CLA:NB	24:K:4001:BCR:H271	2.33	0.43
21:L:1501:CLA:H203	21:L:1501:CLA:H161	1.83	0.43
17:4:261:GLY:HA2	17:4:264:PHE:CE2	2.53	0.43
18:5:73:PRO:N	18:5:73:PRO:C	2.62	0.43
21:5:614:CLA:H142	21:5:614:CLA:H112	1.79	0.43
36:6:610:CHL:CBB	21:6:613:CLA:HBB2	2.48	0.43
1:A:447:PHE:HE2	21:A:1136:CLA:HAB	1.83	0.43
1:A:657:VAL:HG21	1:A:742:PHE:HA	2.00	0.43
21:A:1107:CLA:H202	21:A:1107:CLA:H162	1.80	0.43
21:A:1116:CLA:H41	21:A:1116:CLA:H62	1.70	0.43
21:A:1121:CLA:HED1	11:K:51:ASN:HA	2.00	0.43
21:A:1132:CLA:HMB1	21:A:1132:CLA:CBB	2.48	0.43
21:A:1134:CLA:HHC	21:A:1134:CLA:HBB1	1.99	0.43
21:A:1136:CLA:H202	21:A:1136:CLA:H162	1.73	0.43
4:D:138:CYS:O	4:D:142:THR:OG1	2.29	0.43
6:F:215:TRP:NE1	25:2:802:LHG:H191	2.33	0.43
7:J:24:GLY:HA2	24:J:4002:BCR:H341	2.00	0.43
8:G:114:CYS:O	8:G:116:SER:N	2.51	0.43
25:2:801:LHG:H131	16:3:179:PHE:HZ	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:3:501:LUT:H11	34:3:501:LUT:H191	1.87	0.43
28:3:804:DGD:O5D	28:3:804:DGD:O4D	2.34	0.43
17:4:266:PRO:O	34:4:501:LUT:O23	2.34	0.43
34:5:502:LUT:H15	34:5:502:LUT:H201	1.75	0.43
1:A:649:PHE:O	1:A:653:GLN:HB2	2.18	0.43
21:A:1133:CLA:H71	21:A:1133:CLA:H112	1.85	0.43
24:A:4003:BCR:H351	24:A:4003:BCR:H15C	1.81	0.43
21:B:1209:CLA:HBC2	24:B:4002:BCR:H10C	2.00	0.43
21:B:1215:CLA:H91	21:B:1215:CLA:HAB	2.00	0.43
9:H:109:VAL:O	9:H:113:ALA:CB	2.66	0.43
21:1:601:CLA:H142	21:1:601:CLA:H112	1.77	0.43
15:2:154:LEU:HG	36:2:610:CHL:HBC1	2.00	0.43
15:2:246:SER:O	15:2:250:ASN:ND2	2.50	0.43
15:2:254:HIS:CG	21:2:603:CLA:HAA2	2.54	0.43
17:4:273:SER:O	17:4:275:GLU:N	2.49	0.43
19:6:139:LYS:O	19:6:142:GLN:HB3	2.18	0.43
35:6:504:XAT:H12	21:6:606:CLA:HBA1	1.99	0.43
1:A:150:ALA:O	1:A:224:VAL:HG11	2.19	0.43
21:A:1115:CLA:H91	21:A:1115:CLA:H111	1.69	0.43
21:A:1121:CLA:H112	11:K:89:ILE:CG1	2.49	0.43
21:B:1206:CLA:CMB	21:B:1206:CLA:CBB	2.93	0.43
10:I:20:TRP:CZ2	33:5:803:PTY:C12	2.99	0.43
15:2:91:HIS:CG	25:2:803:LHG:HC62	2.53	0.43
16:3:74:LEU:HD13	36:3:604:CHL:HED1	2.00	0.43
16:3:232:MET:HG3	16:3:236:LYS:HE2	2.00	0.43
19:6:83:MET:HG3	21:6:605:CLA:HBA1	2.00	0.43
1:A:43:PRO:HB3	1:A:48:TRP:CE3	2.54	0.43
1:A:83:ILE:HG13	21:A:1102:CLA:HBB1	2.00	0.43
1:A:681:PHE:HZ	21:A:1140:CLA:HBC2	1.83	0.43
2:B:444:VAL:CG1	2:B:452:LYS:HB2	2.47	0.43
21:B:1212:CLA:C7	24:B:4001:BCR:H312	2.47	0.43
21:B:1213:CLA:H141	21:B:1219:CLA:H202	2.00	0.43
21:B:1223:CLA:H61	21:B:1223:CLA:H102	1.84	0.43
16:3:182:LEU:HA	16:3:182:LEU:HD23	1.86	0.43
24:3:503:BCR:H351	24:3:503:BCR:H15C	1.63	0.43
36:5:609:CHL:NB	25:5:801:LHG:H301	2.33	0.43
33:5:803:PTY:H381	33:5:803:PTY:H352	1.38	0.43
19:6:160:LEU:HD12	34:6:501:LUT:H23	2.00	0.43
34:6:501:LUT:H183	21:6:603:CLA:C4B	2.48	0.43
35:6:502:XAT:H201	35:6:502:XAT:H15	1.77	0.43
1:A:301:ILE:HD13	1:A:301:ILE:HA	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1124:CLA:H51	21:A:1135:CLA:H11	2.01	0.43
21:K:1402:CLA:CMB	21:K:1402:CLA:CBB	2.97	0.43
24:O:4001:BCR:H24C	24:O:4001:BCR:H371	1.90	0.43
16:3:69:ALA:HA	16:3:72:LYS:HD3	2.00	0.43
18:5:99:LEU:HD22	34:5:504:LUT:C39	2.43	0.43
34:5:501:LUT:H31	34:5:501:LUT:H391	1.73	0.43
34:6:501:LUT:H32	21:6:601:CLA:CAB	2.46	0.43
35:6:504:XAT:H393	21:6:601:CLA:CBC	2.41	0.43
35:6:504:XAT:H31	35:6:504:XAT:H391	1.61	0.43
1:A:463:SER:HB2	1:A:471:MET:HE1	2.01	0.43
21:A:1111:CLA:H191	21:3:605:CLA:H52	2.01	0.43
21:A:1124:CLA:HED2	21:A:1124:CLA:H2A	2.01	0.43
21:B:1023:CLA:HBA2	21:B:1023:CLA:C2	2.48	0.43
6:F:82:LEU:HB3	6:F:139:LEU:HD13	2.00	0.43
7:J:3:ASP:HA	7:J:6:THR:HG22	2.01	0.43
35:2:502:XAT:H12	21:2:604:CLA:CBB	2.48	0.43
16:3:132:ILE:HG21	24:3:506:BCR:H282	2.01	0.43
21:5:604:CLA:H3A	21:5:604:CLA:HBA1	1.54	0.43
21:A:1102:CLA:H11	21:A:1102:CLA:H52	1.69	0.43
21:A:1113:CLA:HMA2	28:3:805:DGD:HB61	2.01	0.43
21:A:1114:CLA:ND	31:3:803:LMG:H311	2.34	0.43
21:A:1121:CLA:HED1	11:K:51:ASN:OD1	2.19	0.43
24:A:4003:BCR:H321	21:3:612:CLA:H203	2.01	0.43
21:B:1210:CLA:H143	21:B:1210:CLA:H111	1.88	0.43
9:H:130:GLY:N	9:H:131:PRO:HD2	2.34	0.43
11:K:53:THR:HG21	11:K:59:LEU:CD1	2.48	0.43
12:L:139:LEU:C	12:L:139:LEU:CD2	2.91	0.43
21:L:1503:CLA:C1D	21:L:1504:CLA:CAB	2.97	0.43
14:1:173:LYS:HD3	21:1:601:CLA:H12	1.99	0.43
25:1:801:LHG:H252	24:4:503:BCR:HC31	2.00	0.43
35:3:502:XAT:H31	35:3:502:XAT:H391	1.85	0.43
17:4:208:ASP:N	17:4:208:ASP:OD1	2.49	0.43
18:5:124:ASP:HB3	18:5:128:LEU:HB2	2.01	0.43
21:5:608:CLA:HBB1	21:5:608:CLA:HHC	2.01	0.43
34:6:501:LUT:H363	21:6:601:CLA:CGA	2.37	0.43
21:6:604:CLA:H142	21:6:604:CLA:H111	1.85	0.43
21:A:1105:CLA:H62	21:A:1105:CLA:H2	1.68	0.43
21:A:1115:CLA:H62	21:A:1115:CLA:H41	1.39	0.43
2:B:479:LEU:HD12	2:B:479:LEU:HA	1.87	0.43
21:B:1216:CLA:H111	21:B:1216:CLA:H142	1.82	0.43
24:B:4001:BCR:H15C	24:B:4001:BCR:H351	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:5004:LMU:H31	39:5:806:P3H:O18	2.19	0.43
21:F:1301:CLA:H3A	21:F:1301:CLA:HBA1	1.68	0.43
11:K:22:SER:HA	11:K:26:ARG:HD3	2.01	0.43
13:O:48:VAL:HG22	13:O:50:ALA:H	1.84	0.43
25:1:801:LHG:HC5	25:1:801:LHG:HC81	1.77	0.43
34:2:501:LUT:H35	34:2:501:LUT:H401	1.92	0.43
32:5:805:4RF:H36	32:5:805:4RF:H6	1.71	0.43
19:6:210:ILE:HB	21:6:603:CLA:O1A	2.19	0.43
1:A:297:HIS:HB2	21:A:1116:CLA:CHB	2.49	0.43
21:A:1141:CLA:H3A	21:A:1141:CLA:HBA2	1.75	0.43
24:A:4002:BCR:H402	24:3:504:BCR:H24C	2.01	0.43
21:B:1203:CLA:H2	21:B:1203:CLA:H62	1.72	0.43
7:J:35:ASP:HA	7:J:36:PRO:HD3	1.76	0.43
11:K:41:ARG:C	11:K:43:GLY:N	2.77	0.43
12:L:116:LYS:HD2	12:L:116:LYS:HA	1.81	0.43
13:O:79:SER:O	13:O:82:GLN:NE2	2.49	0.43
17:4:261:GLY:HA2	17:4:264:PHE:HE2	1.83	0.43
21:4:604:CLA:HBC2	21:4:609:CLA:HBB2	2.00	0.43
34:5:501:LUT:H401	34:5:501:LUT:H35	1.75	0.43
34:5:502:LUT:H8	21:5:604:CLA:H61	2.01	0.43
21:5:608:CLA:C4D	36:5:609:CHL:H122	2.49	0.43
21:A:1104:CLA:H72	21:A:1104:CLA:H111	1.88	0.42
21:A:1114:CLA:CMB	21:A:1114:CLA:CBB	2.95	0.42
2:B:107:ARG:HH22	2:B:115:ASN:HA	1.81	0.42
8:G:52:TYR:OH	8:G:56:ARG:NH1	2.52	0.42
9:H:88:ARG:NH1	24:H:4001:BCR:HC41	2.33	0.42
14:1:106:TRP:CD2	14:1:113:PRO:HB3	2.54	0.42
16:3:154:PRO:HD2	21:3:610:CLA:C1B	2.49	0.42
21:3:605:CLA:H193	21:3:605:CLA:H162	1.84	0.42
34:6:501:LUT:H35	34:6:501:LUT:H401	1.71	0.42
35:6:502:XAT:H31	35:6:502:XAT:H391	1.75	0.42
1:A:371:MET:HE1	1:A:390:LEU:HD13	1.99	0.42
21:A:1108:CLA:H41	21:A:1108:CLA:H62	1.74	0.42
21:A:1141:CLA:C4D	13:O:117:VAL:HG22	2.49	0.42
2:B:26:LEU:HD21	24:L:4001:BCR:HC41	2.01	0.42
2:B:650:THR:HA	2:B:653:PHE:HB3	2.01	0.42
2:B:661:GLY:O	2:B:665:LEU:HG	2.19	0.42
2:B:701:LEU:HD13	22:B:2002:PQN:O4	2.19	0.42
14:1:154:PRO:HG3	21:1:611:CLA:HMD1	2.00	0.42
17:4:142:LEU:HD13	17:4:259:TYR:OH	2.19	0.42
35:4:502:XAT:H15	35:4:502:XAT:H201	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:5:218:PHE:O	19:6:123:GLN:HG3	2.19	0.42
21:6:606:CLA:HMA1	21:6:613:CLA:HAC2	2.02	0.42
1:A:709:VAL:CG1	6:F:183:ARG:HG3	2.46	0.42
24:A:4007:BCR:H401	21:B:1023:CLA:O2D	2.19	0.42
2:B:620:TRP:O	2:B:624:TYR:HB3	2.19	0.42
5:E:127:VAL:HG12	5:E:128:LYS:HG2	2.01	0.42
6:F:82:LEU:HD13	6:F:139:LEU:HD13	2.00	0.42
6:F:163:GLU:HG2	7:J:38:VAL:CG1	2.49	0.42
21:1:611:CLA:H111	21:1:611:CLA:H93	1.67	0.42
36:2:610:CHL:HED1	28:2:806:DGD:HE62	2.01	0.42
21:5:614:CLA:C1	33:5:803:PTY:H142	2.50	0.42
34:6:501:LUT:H362	21:6:601:CLA:C2	2.49	0.42
1:A:46:THR:CG2	1:A:715:PRO:HA	2.49	0.42
1:A:344:ILE:HD11	1:A:422:ASN:HD21	1.84	0.42
1:A:578:PRO:HD3	2:B:562:GLY:HA2	2.00	0.42
21:A:1101:CLA:H112	21:A:1101:CLA:H142	1.76	0.42
21:A:1115:CLA:HMB1	21:A:1115:CLA:CBB	2.49	0.42
2:B:515:PRO:HG3	6:F:147:HIS:NE2	2.33	0.42
8:G:38:THR:OG1	8:G:105:HIS:CD2	2.73	0.42
9:H:70:TYR:CZ	12:L:83:LEU:CD1	3.01	0.42
9:H:124:LEU:HB2	9:H:125:PRO:CD	2.49	0.42
13:O:45:ASP:HA	13:O:46:PRO:HD3	1.92	0.42
13:O:120:LYS:HD3	13:O:120:LYS:HA	1.84	0.42
21:1:604:CLA:HHD	36:1:609:CHL:HBB2	2.01	0.42
16:3:272:LEU:HD21	21:3:608:CLA:HMC2	2.02	0.42
21:4:604:CLA:H62	21:4:604:CLA:H41	1.51	0.42
36:5:609:CHL:H62	19:6:131:LEU:HD11	2.01	0.42
1:A:679:TRP:CD2	20:A:1011:CL0:H5	2.54	0.42
21:A:1106:CLA:H3A	21:A:1106:CLA:HBA2	1.43	0.42
21:A:1113:CLA:H202	21:3:610:CLA:HAC2	2.01	0.42
21:A:1128:CLA:H122	21:A:1128:CLA:H161	1.86	0.42
2:B:515:PRO:CD	6:F:147:HIS:CE1	3.02	0.42
21:B:1217:CLA:H41	21:B:1217:CLA:H92	2.01	0.42
21:B:1218:CLA:H62	21:B:1218:CLA:H41	1.51	0.42
21:B:1219:CLA:H192	21:B:1219:CLA:H162	1.89	0.42
21:B:1236:CLA:H62	21:B:1236:CLA:H41	1.57	0.42
24:B:4004:BCR:H15C	24:B:4004:BCR:H351	1.80	0.42
11:K:91:VAL:HG12	11:K:95:LEU:HD11	2.01	0.42
16:3:280:LEU:HD22	21:3:603:CLA:H43	2.02	0.42
21:3:608:CLA:H2	21:3:608:CLA:H62	1.65	0.42
21:3:612:CLA:H162	21:3:612:CLA:H141	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:6:85:LYS:CD	19:6:149:PHE:CZ	2.96	0.42
1:A:80:GLN:HE21	1:A:84:ILE:HG13	1.84	0.42
1:A:220:VAL:O	1:A:223:PRO:HD2	2.20	0.42
1:A:341:LEU:HA	1:A:341:LEU:HD23	1.81	0.42
1:A:560:SER:OG	1:A:561:ARG:N	2.53	0.42
2:B:450:PRO:HG2	6:F:94:LEU:HD21	2.02	0.42
21:B:1223:CLA:H141	21:B:1223:CLA:H161	1.77	0.42
28:B:5002:DGD:HA42	28:B:5002:DGD:HA71	1.88	0.42
24:F:4001:BCR:C14	7:J:36:PRO:HB2	2.48	0.42
31:F:5002:LMG:H332	31:F:5002:LMG:H361	1.98	0.42
9:H:75:MET:N	9:H:75:MET:SD	2.93	0.42
16:3:140:PRO:HG2	16:3:143:THR:HG22	2.02	0.42
17:4:159:MET:HE1	21:4:604:CLA:HAA2	2.01	0.42
19:6:53:PRO:HA	19:6:54:PRO:HD3	1.91	0.42
1:A:330:LYS:HB3	1:A:330:LYS:HE2	1.74	0.42
1:A:432:ARG:HG2	4:D:87:SER:HA	2.02	0.42
21:A:1132:CLA:H62	21:A:1132:CLA:H41	1.80	0.42
2:B:247:THR:HG23	2:B:249:ASP:H	1.85	0.42
21:B:1220:CLA:O1A	24:B:4004:BCR:H14C	2.19	0.42
14:1:90:LEU:HD21	34:1:501:LUT:H173	2.01	0.42
34:3:501:LUT:H15	34:3:501:LUT:H201	1.84	0.42
36:3:604:CHL:H61	36:3:604:CHL:H41	1.68	0.42
21:5:604:CLA:H13	21:5:604:CLA:H101	1.66	0.42
1:A:680:ALA:C	21:A:1013:CLA:HAB	2.43	0.42
21:A:1113:CLA:H112	24:3:504:BCR:H15C	2.01	0.42
21:A:1126:CLA:H3A	21:A:1126:CLA:HBA2	1.69	0.42
2:B:416:LYS:HE3	6:F:240:SER:HA	2.02	0.42
21:B:1238:CLA:HAB	22:B:2002:PQN:H161	2.01	0.42
24:B:4003:BCR:H24C	24:B:4003:BCR:H21C	1.89	0.42
4:D:169:PRO:HG2	4:D:172:GLY:HA2	2.01	0.42
21:G:1602:CLA:C1B	24:G:4001:BCR:H323	2.50	0.42
9:H:82:GLN:HG3	21:H:1701:CLA:C1C	2.50	0.42
12:L:58:GLN:HB2	12:L:59:PRO:CD	2.47	0.42
21:2:601:CLA:HBA2	21:2:601:CLA:H3A	1.70	0.42
37:3:806:SQD:H282	37:3:806:SQD:H92	2.00	0.42
21:4:604:CLA:H12	21:4:604:CLA:C4A	2.50	0.42
34:5:504:LUT:H11	34:5:504:LUT:H191	1.78	0.42
21:5:607:CLA:H72	21:5:607:CLA:H112	1.56	0.42
19:6:156:ASP:N	19:6:157:PRO:CD	2.83	0.42
1:A:574:PRO:HB3	1:A:720:ILE:HB	2.01	0.42
21:B:1207:CLA:H121	9:H:109:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:69:PRO:HD2	4:D:73:PRO:HD3	2.01	0.42
6:F:234:ASP:N	6:F:234:ASP:OD1	2.53	0.42
24:K:4001:BCR:H351	24:K:4001:BCR:H15C	1.84	0.42
12:L:79:VAL:O	12:L:83:LEU:HG	2.20	0.42
21:1:604:CLA:H151	21:1:605:CLA:H203	2.01	0.42
16:3:153:ILE:HG22	16:3:155:PRO:CD	2.30	0.42
16:3:205:LEU:HD22	16:3:219:PHE:HB2	2.01	0.42
19:6:165:HIS:O	19:6:165:HIS:CG	2.71	0.42
1:A:747:ILE:HD12	1:A:747:ILE:HA	1.96	0.42
21:A:1138:CLA:H93	21:A:1138:CLA:H62	1.95	0.42
21:B:1227:CLA:HMC1	21:B:1236:CLA:HBB1	2.01	0.42
21:B:1230:CLA:HMA2	24:F:4001:BCR:C36	2.50	0.42
4:D:148:LYS:HE3	4:D:148:LYS:HB2	1.83	0.42
31:F:5002:LMG:H162	31:F:5002:LMG:H131	1.81	0.42
9:H:74:GLU:HG2	9:H:76:LYS:H	1.85	0.42
9:H:111:SER:HB2	10:I:24:LEU:HD11	2.00	0.42
10:I:16:VAL:HA	10:I:17:PRO:HD3	1.74	0.42
11:K:63:VAL:CG1	11:K:75:THR:HG21	2.49	0.42
35:3:502:XAT:H28	35:3:502:XAT:H371	2.02	0.42
21:3:610:CLA:C1B	31:3:803:LMG:H152	2.50	0.42
21:3:610:CLA:CHC	31:3:803:LMG:H192	2.50	0.42
17:4:199:GLU:OE1	17:4:199:GLU:N	2.52	0.42
19:6:66:ASP:OD1	19:6:66:ASP:N	2.53	0.42
1:A:226:LYS:HB3	1:A:253:LEU:HD22	2.02	0.41
21:A:1101:CLA:H93	22:A:2001:PQN:H271	2.02	0.41
21:A:1112:CLA:H142	21:A:1112:CLA:H111	1.70	0.41
24:A:4002:BCR:H282	24:3:504:BCR:H402	2.01	0.41
6:F:82:LEU:HD13	6:F:139:LEU:HD11	2.01	0.41
21:G:1602:CLA:C4A	24:G:4001:BCR:H323	2.50	0.41
13:O:58:LEU:HD22	13:O:111:VAL:HG11	2.01	0.41
14:1:160:PRO:HB3	21:1:611:CLA:H93	2.02	0.41
36:5:609:CHL:C1C	25:5:801:LHG:HC81	2.49	0.41
1:A:275:PHE:HE2	21:A:1113:CLA:HBC3	1.85	0.41
21:A:1112:CLA:CMB	21:A:1112:CLA:CBB	2.93	0.41
2:B:67:PHE:HE1	10:I:15:PHE:O	2.03	0.41
2:B:87:PRO:HB3	2:B:122:TYR:CD1	2.56	0.41
2:B:467:ALA:HB2	2:B:477:LEU:HD23	2.00	0.41
2:B:735:GLY:HA2	9:H:144:LEU:HD12	2.00	0.41
21:B:1226:CLA:H143	21:B:1226:CLA:H111	1.86	0.41
35:1:502:XAT:H35	35:1:502:XAT:H401	1.95	0.41
36:2:609:CHL:HBB1	36:2:609:CHL:HHC	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:3:803:LMG:H342	31:3:803:LMG:H372	1.80	0.41
34:4:501:LUT:H15	34:4:501:LUT:H201	1.91	0.41
18:5:215:ASN:HA	18:5:220:SER:HB3	2.02	0.41
21:5:605:CLA:CBC	36:5:610:CHL:HAB	2.49	0.41
21:5:608:CLA:C2B	36:5:609:CHL:H18	2.51	0.41
1:A:299:LEU:HD21	21:A:1115:CLA:HMB1	2.01	0.41
21:A:1105:CLA:H92	21:A:1105:CLA:H61	1.89	0.41
21:A:1107:CLA:HBC2	21:A:1126:CLA:H141	2.01	0.41
2:B:659:ALA:CB	21:B:1023:CLA:CBB	2.92	0.41
21:B:1223:CLA:H152	21:B:1223:CLA:H112	1.89	0.41
21:B:1226:CLA:H61	21:B:1226:CLA:H41	1.84	0.41
9:H:137:GLU:HA	9:H:137:GLU:OE2	2.20	0.41
21:K:1404:CLA:CMB	21:K:1404:CLA:CBB	2.93	0.41
21:L:1503:CLA:C2D	21:L:1504:CLA:CAB	2.98	0.41
13:O:65:SER:HB2	24:O:4001:BCR:HC32	2.00	0.41
33:O:5002:PTY:O30	33:O:5002:PTY:H331	2.19	0.41
25:2:802:LHG:H161	37:2:805:SQD:H331	2.02	0.41
16:3:145:VAL:HG22	21:3:606:CLA:HED3	2.02	0.41
21:3:612:CLA:H161	21:3:612:CLA:H202	1.81	0.41
21:5:603:CLA:H43	36:5:609:CHL:C3	2.50	0.41
19:6:210:ILE:CD1	21:6:603:CLA:C2	2.99	0.41
22:A:2001:PQN:H142	24:B:4006:BCR:H312	2.01	0.41
2:B:637:ASN:OD1	2:B:637:ASN:N	2.52	0.41
7:J:21:PHE:CD2	21:J:1901:CLA:HBB2	2.55	0.41
9:H:77:ARG:HD3	12:L:93:VAL:HG11	2.01	0.41
34:4:501:LUT:H391	34:4:501:LUT:H31	1.81	0.41
21:A:1103:CLA:H72	24:A:4003:BCR:H373	2.01	0.41
21:B:1204:CLA:HBA2	21:B:1204:CLA:H3A	1.84	0.41
21:B:1224:CLA:HBA2	21:B:1224:CLA:H3A	1.84	0.41
21:G:1601:CLA:CBB	21:G:1601:CLA:CMB	2.97	0.41
24:G:4001:BCR:H383	24:G:4001:BCR:H23C	2.01	0.41
13:O:53:PHE:O	13:O:57:THR:CB	2.68	0.41
25:1:801:LHG:H122	25:1:801:LHG:HC91	1.91	0.41
17:4:305:ILE:HA	17:4:308:LEU:HB3	2.01	0.41
18:5:61:LEU:HB3	18:5:68:ASP:OD2	2.20	0.41
21:5:604:CLA:H61	21:5:604:CLA:H93	1.68	0.41
21:5:608:CLA:HAA1	19:6:128:ILE:CD1	2.48	0.41
21:A:1119:CLA:HMD2	21:A:1121:CLA:HBB1	1.98	0.41
21:A:1130:CLA:H41	21:A:1130:CLA:H61	1.73	0.41
21:A:1140:CLA:H41	21:A:1140:CLA:H62	1.80	0.41
21:B:1023:CLA:H62	21:B:1023:CLA:H41	1.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:1203:CLA:H193	21:B:1203:CLA:H161	1.88	0.41
21:B:1240:CLA:H162	21:B:1240:CLA:H141	1.83	0.41
27:B:5004:LMU:O6'	33:6:804:PTY:N1	2.53	0.41
21:H:1701:CLA:H52	21:H:1701:CLA:H8	1.87	0.41
13:O:65:SER:N	24:O:4001:BCR:HC42	2.35	0.41
15:2:208:MET:HE2	15:2:208:MET:HB3	1.82	0.41
21:2:604:CLA:HBA2	21:2:604:CLA:H3A	1.64	0.41
36:2:609:CHL:HMD1	24:3:503:BCR:HC42	2.01	0.41
21:3:608:CLA:H122	21:3:608:CLA:H161	1.89	0.41
21:3:612:CLA:H93	21:3:612:CLA:H61	1.86	0.41
17:4:126:LEU:HG	17:4:128:TYR:H	1.84	0.41
21:A:1012:CLA:CAB	2:B:583:TRP:HH2	2.27	0.41
24:A:4004:BCR:H16C	24:A:4004:BCR:H19C	1.88	0.41
24:A:4004:BCR:H282	13:O:106:THR:HA	2.02	0.41
21:B:1207:CLA:C12	9:H:109:VAL:HG11	2.51	0.41
21:B:1217:CLA:CBB	24:B:4001:BCR:H14C	2.51	0.41
21:B:1223:CLA:H191	21:B:1240:CLA:H143	2.02	0.41
21:B:1225:CLA:H142	21:B:1225:CLA:H111	1.84	0.41
3:C:66:ARG:HA	3:C:66:ARG:HD2	1.89	0.41
8:G:117:LEU:HD13	8:G:124:ILE:HD11	2.03	0.41
12:L:120:LEU:HD13	12:L:126:THR:CG2	2.50	0.41
13:O:80:ILE:HG22	13:O:97:PHE:HD1	1.85	0.41
21:4:603:CLA:H11	21:4:603:CLA:H51	1.85	0.41
21:4:615:CLA:H3A	21:4:615:CLA:HBA1	1.65	0.41
19:6:175:LEU:HD21	34:6:501:LUT:H191	2.03	0.41
21:A:1112:CLA:HMC1	21:A:1112:CLA:HBC2	2.02	0.41
24:A:4004:BCR:H372	24:A:4004:BCR:H361	2.02	0.41
21:G:1601:CLA:HAC2	24:G:4001:BCR:H381	2.01	0.41
11:K:33:ILE:HD11	11:K:87:HIS:ND1	2.36	0.41
11:K:41:ARG:O	11:K:43:GLY:N	2.52	0.41
16:3:73:TYR:OH	16:3:88:GLY:HA2	2.21	0.41
21:3:610:CLA:CBB	21:3:610:CLA:CMB	2.94	0.41
18:5:51:PRO:CG	18:5:71:PHE:HB2	2.50	0.41
34:5:504:LUT:H401	34:5:504:LUT:H35	1.87	0.41
21:5:608:CLA:H61	21:5:608:CLA:H41	1.81	0.41
34:6:501:LUT:H362	21:6:601:CLA:C3	2.50	0.41
21:6:605:CLA:H43	21:6:605:CLA:HED3	2.03	0.41
1:A:74:PHE:HE2	1:A:180:HIS:CD2	2.39	0.41
1:A:357:LEU:HD23	1:A:357:LEU:HA	1.90	0.41
21:B:1209:CLA:HBB2	21:B:1217:CLA:H8	2.03	0.41
21:B:1215:CLA:H111	21:B:1215:CLA:H72	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:LEU:HD12	3:C:66:ARG:HH11	1.86	0.41
5:E:90:VAL:HG22	5:E:104:VAL:HG12	2.03	0.41
8:G:34:ILE:CD1	8:G:110:PHE:HD1	2.23	0.41
11:K:28:ILE:HB	11:K:31:SER:OG	2.20	0.41
21:K:1401:CLA:HBB1	24:K:4001:BCR:C11	2.51	0.41
14:1:182:ARG:NH2	21:1:604:CLA:O2D	2.54	0.41
21:1:601:CLA:H162	21:1:601:CLA:H202	1.89	0.41
36:1:609:CHL:H61	36:1:609:CHL:H41	1.84	0.41
15:2:105:ALA:O	15:2:109:HIS:ND1	2.34	0.41
15:2:175:ASN:HD22	17:4:131:ALA:H	1.68	0.41
16:3:103:PHE:CE2	37:3:806:SQD:H241	2.56	0.41
16:3:200:LEU:HD23	16:3:200:LEU:HA	1.93	0.41
18:5:86:LEU:HD13	21:5:604:CLA:H11	2.03	0.41
1:A:141:THR:HA	1:A:386:THR:HG22	2.02	0.41
2:B:8:LYS:NZ	29:B:5003:3PH:O21	2.54	0.41
2:B:166:LEU:HA	2:B:166:LEU:HD12	1.86	0.41
21:B:1231:CLA:CHD	21:B:1232:CLA:HAB	2.51	0.41
11:K:53:THR:HG23	11:K:59:LEU:CD1	2.51	0.41
15:2:230:MET:HB2	35:2:502:XAT:C15	2.51	0.41
34:2:501:LUT:H21	21:2:601:CLA:H12	2.03	0.41
21:3:605:CLA:H112	21:3:605:CLA:H91	1.88	0.41
17:4:270:SER:OG	17:4:271:LYS:N	2.54	0.41
19:6:133:MET:HG3	21:6:612:CLA:HMC2	2.01	0.41
1:A:278:PHE:CE1	21:A:1116:CLA:HBB1	2.56	0.40
1:A:355:ILE:HD11	24:A:4004:BCR:HC7	2.04	0.40
21:A:1122:CLA:HMB3	21:A:1141:CLA:HAB	2.03	0.40
2:B:418:ALA:O	2:B:422:HIS:ND1	2.48	0.40
21:B:1230:CLA:CMA	24:F:4001:BCR:H363	2.51	0.40
6:F:98:GLU:HA	6:F:101:VAL:HG12	2.03	0.40
9:H:64:THR:OG1	12:L:162:LYS:NZ	2.54	0.40
21:4:605:CLA:H51	21:4:605:CLA:H11	1.84	0.40
18:5:76:LEU:HD23	21:5:604:CLA:H62	2.03	0.40
21:5:614:CLA:H93	21:5:614:CLA:H61	1.80	0.40
1:A:342:TYR:O	1:A:346:THR:OG1	2.29	0.40
21:A:1114:CLA:NC	31:3:803:LMG:H352	2.36	0.40
21:A:1132:CLA:H143	21:A:1132:CLA:H162	1.60	0.40
2:B:86:ARG:NH1	2:B:107:ARG:HD2	2.35	0.40
21:B:1207:CLA:HED3	12:L:133:MET:HG2	2.03	0.40
21:B:1226:CLA:H141	21:B:1226:CLA:H161	1.74	0.40
13:O:58:LEU:O	13:O:62:ILE:HG13	2.21	0.40
21:2:605:CLA:H192	21:2:605:CLA:H162	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:4:174:MET:SD	21:4:601:CLA:HAB	2.62	0.40
18:5:187:PHE:CE2	34:5:502:LUT:H30	2.56	0.40
21:5:614:CLA:HAB	29:5:807:3PH:H221	2.03	0.40
1:A:260:GLY:HA2	21:A:1113:CLA:OBD	2.22	0.40
1:A:646:LEU:HD22	2:B:652:LEU:HD21	2.03	0.40
21:A:1102:CLA:H202	21:A:1102:CLA:H162	1.89	0.40
21:A:1113:CLA:H72	16:3:255:ALA:HA	2.04	0.40
21:A:1120:CLA:H61	21:A:1120:CLA:H41	1.82	0.40
25:A:5002:LHG:H311	25:A:5002:LHG:H282	1.77	0.40
2:B:8:LYS:HE2	2:B:8:LYS:HB3	1.81	0.40
2:B:78:TRP:CD1	2:B:85:VAL:HG23	2.57	0.40
3:C:6:LYS:O	3:C:65:VAL:HA	2.21	0.40
14:1:47:LEU:O	14:1:53:ASN:ND2	2.54	0.40
14:1:84:LEU:HD13	21:1:606:CLA:HBB2	2.04	0.40
21:1:611:CLA:CBB	21:1:611:CLA:HMB1	2.52	0.40
15:2:71:SER:OG	15:2:72:GLU:N	2.54	0.40
34:3:501:LUT:H373	21:3:601:CLA:H12	2.03	0.40
21:5:605:CLA:C6	21:5:605:CLA:C1	2.99	0.40
19:6:89:ARG:HD3	35:6:504:XAT:H363	2.03	0.40
1:A:253:LEU:HD23	1:A:253:LEU:HA	1.88	0.40
1:A:405:ALA:HB1	24:A:4005:BCR:H383	2.01	0.40
21:A:1131:CLA:HMC1	21:L:1503:CLA:HBB2	2.04	0.40
2:B:74:ASN:HB2	2:B:77:GLN:HB2	2.04	0.40
21:B:1022:CLA:H201	21:B:1206:CLA:H2	2.03	0.40
21:B:1219:CLA:H112	21:B:1219:CLA:H91	1.86	0.40
25:2:803:LHG:H111	31:3:802:LMG:H132	2.04	0.40
34:3:501:LUT:H30	21:3:601:CLA:H72	2.04	0.40
17:4:277:LEU:HD11	17:4:281:GLN:HE21	1.86	0.40
21:4:601:CLA:H93	21:4:601:CLA:H111	1.86	0.40
21:A:1120:CLA:H143	21:A:1121:CLA:C14	2.44	0.40
25:F:5001:LHG:H112	25:F:5001:LHG:HC81	1.93	0.40
24:I:4001:BCR:C35	24:I:4002:BCR:H401	2.50	0.40
11:K:29:MET:HG2	21:K:1401:CLA:CAD	2.51	0.40
34:1:501:LUT:H31	34:1:501:LUT:H403	1.90	0.40
36:5:609:CHL:HAA1	36:5:609:CHL:HBD	2.04	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	738/740 (100%)	693 (94%)	43 (6%)	2 (0%)	36 55
2	B	731/733 (100%)	693 (95%)	37 (5%)	1 (0%)	48 69
3	C	78/80 (98%)	71 (91%)	7 (9%)	0	100 100
4	D	141/144 (98%)	125 (89%)	16 (11%)	0	100 100
5	E	62/64 (97%)	60 (97%)	2 (3%)	0	100 100
6	F	160/162 (99%)	143 (89%)	16 (10%)	1 (1%)	21 39
7	J	39/41 (95%)	33 (85%)	6 (15%)	0	100 100
8	G	99/101 (98%)	86 (87%)	11 (11%)	2 (2%)	6 12
9	H	90/92 (98%)	81 (90%)	9 (10%)	0	100 100
10	I	37/39 (95%)	32 (86%)	4 (11%)	1 (3%)	4 8
11	K	82/84 (98%)	75 (92%)	6 (7%)	1 (1%)	10 22
12	L	153/155 (99%)	143 (94%)	6 (4%)	4 (3%)	4 9
13	O	84/86 (98%)	74 (88%)	10 (12%)	0	100 100
14	1	195/197 (99%)	177 (91%)	16 (8%)	2 (1%)	12 24
15	2	206/208 (99%)	193 (94%)	13 (6%)	0	100 100
16	3	226/228 (99%)	213 (94%)	13 (6%)	0	100 100
17	4	209/211 (99%)	188 (90%)	21 (10%)	0	100 100
18	5	200/202 (99%)	177 (88%)	17 (8%)	6 (3%)	3 7
19	6	176/178 (99%)	152 (86%)	17 (10%)	7 (4%)	2 3
All	All	3706/3745 (99%)	3409 (92%)	270 (7%)	27 (1%)	20 35

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	5	122	VAL
18	5	160	PRO

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Mol	Chain	Res	Type
19	6	107	PRO
6	F	135	LYS
8	G	82	PRO
10	I	14	PRO
14	1	154	PRO
14	1	156	GLY
19	6	163	PRO
2	B	223	LEU
12	L	168	PRO
18	5	51	PRO
18	5	163	PRO
19	6	162	SER
19	6	205	PRO
11	K	42	PHE
19	6	158	VAL
1	A	575	CYS
8	G	92	ASP
12	L	164	LEU
12	L	165	SER
12	L	167	ARG
18	5	117	PRO
19	6	157	PRO
19	6	217	THR
1	A	128	ASN
18	5	116	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	599/599 (100%)	599 (100%)	0	100 100
2	B	593/593 (100%)	591 (100%)	2 (0%)	86 94
3	C	68/68 (100%)	68 (100%)	0	100 100
4	D	122/123 (99%)	122 (100%)	0	100 100
5	E	57/57 (100%)	57 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	135/135 (100%)	135 (100%)	0	100	100
7	J	36/36 (100%)	35 (97%)	1 (3%)	38	62
8	G	78/78 (100%)	76 (97%)	2 (3%)	40	65
9	H	71/71 (100%)	68 (96%)	3 (4%)	26	51
10	I	30/30 (100%)	30 (100%)	0	100	100
11	K	53/53 (100%)	51 (96%)	2 (4%)	29	54
12	L	119/119 (100%)	116 (98%)	3 (2%)	42	66
13	O	71/71 (100%)	71 (100%)	0	100	100
14	1	152/152 (100%)	152 (100%)	0	100	100
15	2	167/167 (100%)	167 (100%)	0	100	100
16	3	173/173 (100%)	173 (100%)	0	100	100
17	4	169/169 (100%)	169 (100%)	0	100	100
18	5	163/163 (100%)	160 (98%)	3 (2%)	51	74
19	6	147/147 (100%)	141 (96%)	6 (4%)	27	52
All	All	3003/3004 (100%)	2981 (99%)	22 (1%)	73	88

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	217	LEU
2	B	646	VAL
7	J	38	VAL
8	G	85	PHE
8	G	105	HIS
9	H	114	LEU
9	H	122	LEU
9	H	133	MET
11	K	28	ILE
11	K	95	LEU
12	L	60	LEU
12	L	114	PHE
12	L	169	LEU
18	5	55	VAL
18	5	112	MET
18	5	243	ASN
19	6	87	ASN
19	6	107	PRO

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Mol	Chain	Res	Type
19	6	108	VAL
19	6	111	PHE
19	6	125	GLN
19	6	150	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	217	GLN
2	B	99	GLN
2	B	206	GLN
2	B	219	HIS
2	B	236	GLN
2	B	325	HIS
2	B	506	GLN
2	B	586	ASN
3	C	16	GLN
4	D	96	GLN
4	D	137	GLN
4	D	187	GLN
6	F	159	ASN
7	J	30	ASN
8	G	53	GLN
8	G	80	GLN
8	G	105	HIS
13	O	61	ASN
13	O	116	GLN
14	1	143	ASN
14	1	221	ASN
15	2	179	GLN
15	2	254	HIS
16	3	116	HIS
16	3	267	ASN
17	4	169	ASN
17	4	281	GLN
17	4	309	GLN
17	4	311	HIS
19	6	73	ASN
19	6	165	HIS

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 292 ligands modelled in this entry, 1 is monoatomic - leaving 291 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	$\#\|Z\| > 2$
21	CLA	5	603	-	64,68,73	1.46	7 (10%)	77,107,113	2.17	23 (29%)
24	BCR	B	4005	-	41,41,41	1.81	5 (12%)	56,56,56	4.27	11 (19%)
21	CLA	B	1206	2	69,73,73	1.34	5 (7%)	83,113,113	1.94	18 (21%)
21	CLA	5	612	18	50,54,73	1.85	10 (20%)	60,90,113	2.28	22 (36%)
24	BCR	F	4002	-	41,41,41	1.82	4 (9%)	56,56,56	4.38	19 (33%)
21	CLA	B	1209	-	50,54,73	1.61	7 (14%)	60,90,113	2.11	18 (30%)
24	BCR	L	4002	-	41,41,41	1.98	7 (17%)	56,56,56	4.33	16 (28%)
25	LHG	1	802	-	25,25,48	0.49	0	28,31,54	1.29	3 (10%)
27	LMU	B	5004	-	36,36,36	0.44	0	47,47,47	0.90	2 (4%)
36	CHL	5	609	-	70,74,74	0.75	1 (1%)	80,114,114	1.29	12 (15%)
36	CHL	5	610	-	51,55,74	0.95	2 (3%)	57,91,114	1.47	10 (17%)
37	SQD	2	805	-	39,40,54	0.89	0	48,51,65	0.99	2 (4%)
25	LHG	F	5001	-	48,48,48	0.40	0	51,54,54	0.95	3 (5%)
24	BCR	3	503	-	41,41,41	1.83	4 (9%)	56,56,56	4.19	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	B	1218	-	69,73,73	1.45	8 (11%)	83,113,113	2.05	19 (22%)
21	CLA	1	601	-	69,73,73	1.36	6 (8%)	83,113,113	1.97	20 (24%)
21	CLA	3	610	16	54,58,73	1.53	7 (12%)	65,95,113	2.19	17 (26%)
21	CLA	5	613	-	49,53,73	1.72	9 (18%)	59,89,113	2.27	17 (28%)
24	BCR	B	4006	-	41,41,41	1.89	5 (12%)	56,56,56	4.24	14 (25%)
31	LMG	1	804	-	32,32,55	0.60	0	40,40,63	1.50	7 (17%)
35	XAT	4	502	-	39,47,47	0.74	1 (2%)	54,74,74	1.70	13 (24%)
21	CLA	A	1122	-	69,73,73	1.37	7 (10%)	83,113,113	1.99	20 (24%)
21	CLA	3	611	-	69,73,73	1.42	7 (10%)	83,113,113	1.94	18 (21%)
21	CLA	A	1138	-	69,73,73	1.38	8 (11%)	83,113,113	2.04	18 (21%)
21	CLA	B	1216	-	69,73,73	1.37	7 (10%)	83,113,113	1.86	17 (20%)
21	CLA	1	613	-	49,53,73	1.63	7 (14%)	59,89,113	2.04	18 (30%)
21	CLA	A	1116	-	60,64,73	1.46	7 (11%)	72,102,113	2.13	19 (26%)
21	CLA	2	605	15	69,73,73	1.39	6 (8%)	83,113,113	1.96	22 (26%)
36	CHL	2	609	15	70,74,74	0.93	3 (4%)	80,114,114	1.33	13 (16%)
24	BCR	A	4006	-	41,41,41	1.84	4 (9%)	56,56,56	4.15	15 (26%)
21	CLA	B	1239	-	69,73,73	1.35	7 (10%)	83,113,113	1.94	19 (22%)
21	CLA	A	1106	-	69,73,73	1.40	7 (10%)	83,113,113	1.97	18 (21%)
21	CLA	A	1129	-	59,63,73	1.49	7 (11%)	71,101,113	2.30	17 (23%)
21	CLA	5	604	18	69,73,73	1.37	6 (8%)	83,113,113	2.00	19 (22%)
35	XAT	2	502	-	39,47,47	0.76	1 (2%)	54,74,74	1.66	12 (22%)
24	BCR	B	4004	-	41,41,41	1.84	4 (9%)	56,56,56	4.23	15 (26%)
21	CLA	3	607	-	64,68,73	1.43	8 (12%)	77,107,113	2.01	20 (25%)
21	CLA	A	1013	-	69,73,73	1.41	9 (13%)	83,113,113	1.92	21 (25%)
21	CLA	6	604	-	64,68,73	1.46	8 (12%)	77,107,113	2.00	22 (28%)
21	CLA	2	607	25	64,68,73	1.43	7 (10%)	77,107,113	2.16	21 (27%)
29	3PH	B	5003	-	30,30,47	1.07	4 (13%)	34,35,52	1.28	2 (5%)
21	CLA	B	1234	-	59,63,73	1.50	7 (11%)	71,101,113	2.14	20 (28%)
20	CL0	A	1011	-	69,73,73	2.37	22 (31%)	83,113,113	2.56	22 (26%)
21	CLA	A	1105	-	64,68,73	1.48	8 (12%)	77,107,113	2.14	22 (28%)
21	CLA	G	1602	-	50,54,73	1.59	6 (12%)	60,90,113	2.10	16 (26%)
21	CLA	4	608	-	50,54,73	1.60	7 (14%)	60,90,113	2.12	16 (26%)
21	CLA	H	1701	9	64,68,73	1.45	7 (10%)	77,107,113	2.29	24 (31%)
21	CLA	A	1114	-	59,63,73	1.46	7 (11%)	71,101,113	2.09	18 (25%)
33	PTY	4	804	-	34,34,49	1.02	3 (8%)	37,39,54	1.13	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	1	611	-	69,73,73	1.36	6 (8%)	83,113,113	1.93	18 (21%)
21	CLA	4	615	17	55,59,73	1.56	7 (12%)	66,96,113	2.08	18 (27%)
21	CLA	B	1210	-	69,73,73	1.41	7 (10%)	83,113,113	2.00	17 (20%)
21	CLA	6	613	-	49,53,73	1.60	6 (12%)	59,89,113	2.19	14 (23%)
21	CLA	A	1140	-	65,69,73	1.42	7 (10%)	78,108,113	2.01	20 (25%)
21	CLA	A	1120	-	64,68,73	1.45	7 (10%)	77,107,113	2.08	22 (28%)
21	CLA	L	1504	-	54,58,73	1.53	7 (12%)	65,95,113	2.16	19 (29%)
29	3PH	5	804	-	27,27,47	1.11	4 (14%)	31,32,52	1.19	2 (6%)
21	CLA	A	1104	-	69,73,73	1.42	7 (10%)	83,113,113	2.12	19 (22%)
21	CLA	2	602	-	56,60,73	1.53	8 (14%)	67,97,113	2.08	20 (29%)
21	CLA	3	605	-	69,73,73	1.39	7 (10%)	83,113,113	1.92	15 (18%)
24	BCR	L	4001	-	41,41,41	1.84	6 (14%)	56,56,56	4.29	16 (28%)
21	CLA	K	1401	-	49,53,73	1.66	7 (14%)	59,89,113	2.69	19 (32%)
21	CLA	B	1215	-	69,73,73	1.38	7 (10%)	83,113,113	1.97	17 (20%)
21	CLA	2	612	-	69,73,73	1.37	7 (10%)	83,113,113	2.02	20 (24%)
21	CLA	A	1115	1	64,68,73	1.41	7 (10%)	77,107,113	1.99	20 (25%)
21	CLA	A	1103	-	69,73,73	1.33	7 (10%)	83,113,113	2.11	19 (22%)
21	CLA	B	1229	2	69,73,73	1.41	8 (11%)	83,113,113	2.08	25 (30%)
24	BCR	A	4007	-	41,41,41	1.88	4 (9%)	56,56,56	4.63	16 (28%)
25	LHG	5	801	-	42,42,48	0.44	0	45,48,54	1.17	5 (11%)
33	PTY	L	5003	-	19,19,49	1.37	4 (21%)	22,24,54	1.46	2 (9%)
21	CLA	6	601	-	64,68,73	1.40	6 (9%)	77,107,113	1.99	19 (24%)
24	BCR	I	4002	-	41,41,41	1.85	4 (9%)	56,56,56	4.39	19 (33%)
25	LHG	A	5002	-	48,48,48	0.39	0	51,54,54	1.01	2 (3%)
36	CHL	2	610	-	60,64,74	1.12	4 (6%)	68,102,114	1.45	14 (20%)
33	PTY	6	804	-	23,23,49	1.12	2 (8%)	26,28,54	1.24	2 (7%)
25	LHG	3	801	-	16,16,48	0.82	1 (6%)	17,20,54	0.72	0
21	CLA	5	606	-	54,58,73	1.54	7 (12%)	65,95,113	2.13	19 (29%)
21	CLA	A	1126	-	69,73,73	1.41	7 (10%)	83,113,113	1.96	21 (25%)
21	CLA	A	1109	-	69,73,73	1.37	7 (10%)	83,113,113	2.03	19 (22%)
21	CLA	B	1213	-	64,68,73	1.44	7 (10%)	77,107,113	2.04	21 (27%)
21	CLA	B	1219	-	69,73,73	1.36	7 (10%)	83,113,113	1.90	17 (20%)
28	DGD	3	804	-	40,40,67	0.89	1 (2%)	54,54,81	1.21	4 (7%)
21	CLA	6	606	-	54,58,73	1.52	6 (11%)	65,95,113	2.16	19 (29%)
21	CLA	B	1205	-	69,73,73	1.37	7 (10%)	83,113,113	2.03	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	LUT	5	501	-	42,43,43	2.53	1 (2%)	51,60,60	4.53	20 (39%)
27	LMU	A	5004	-	36,36,36	0.44	0	47,47,47	1.08	2 (4%)
21	CLA	L	1502	-	69,73,73	1.43	8 (11%)	83,113,113	2.33	27 (32%)
21	CLA	B	1022	-	69,73,73	1.35	7 (10%)	83,113,113	1.97	19 (22%)
24	BCR	G	4001	-	41,41,41	1.93	4 (9%)	56,56,56	4.15	22 (39%)
25	LHG	B	5001	-	41,41,48	0.44	0	44,47,54	1.12	3 (6%)
36	CHL	2	613	-	50,54,74	1.08	3 (6%)	56,90,114	1.64	11 (19%)
21	CLA	1	605	-	69,73,73	1.36	7 (10%)	83,113,113	1.99	22 (26%)
21	CLA	A	1133	-	69,73,73	1.46	8 (11%)	83,113,113	1.80	16 (19%)
21	CLA	B	1214	-	69,73,73	1.37	7 (10%)	83,113,113	1.99	20 (24%)
25	LHG	4	801	-	28,28,48	0.54	0	31,34,54	1.28	4 (12%)
28	DGD	2	806	-	40,40,67	0.89	2 (5%)	54,54,81	1.10	2 (3%)
21	CLA	A	1130	1	59,63,73	1.58	8 (13%)	71,101,113	2.15	23 (32%)
21	CLA	A	1139	-	69,73,73	1.42	8 (11%)	83,113,113	2.05	20 (24%)
21	CLA	G	1603	-	49,53,73	1.55	7 (14%)	59,89,113	2.76	20 (33%)
34	LUT	5	503	-	42,43,43	2.41	1 (2%)	51,60,60	4.39	21 (41%)
39	P3H	2	808	-	49,49,49	1.42	8 (16%)	59,61,61	1.01	3 (5%)
24	BCR	A	4004	-	41,41,41	1.86	5 (12%)	56,56,56	4.53	18 (32%)
21	CLA	B	1240	-	69,73,73	1.38	7 (10%)	83,113,113	1.91	17 (20%)
31	LMG	3	802	-	32,32,55	0.69	1 (3%)	40,40,63	0.98	1 (2%)
21	CLA	2	603	-	69,73,73	1.35	7 (10%)	83,113,113	1.92	18 (21%)
31	LMG	4	802	-	46,46,55	0.95	3 (6%)	54,54,63	1.44	4 (7%)
31	LMG	4	803	-	39,39,55	0.74	2 (5%)	47,47,63	0.99	2 (4%)
24	BCR	4	503	-	41,41,41	1.85	4 (9%)	56,56,56	4.36	16 (28%)
21	CLA	A	1107	1	69,73,73	1.35	5 (7%)	83,113,113	1.98	19 (22%)
21	CLA	3	608	-	69,73,73	1.38	8 (11%)	83,113,113	1.87	21 (25%)
21	CLA	A	1118	-	54,58,73	1.66	9 (16%)	65,95,113	2.29	21 (32%)
21	CLA	A	1119	-	69,73,73	1.40	7 (10%)	83,113,113	1.91	20 (24%)
21	CLA	2	606	-	54,58,73	1.55	7 (12%)	65,95,113	2.21	20 (30%)
21	CLA	3	612	-	69,73,73	1.38	7 (10%)	83,113,113	1.95	19 (22%)
21	CLA	4	604	-	64,68,73	1.40	7 (10%)	77,107,113	2.00	18 (23%)
31	LMG	F	5002	-	50,50,55	1.02	5 (10%)	58,58,63	1.08	2 (3%)
21	CLA	B	1232	-	59,63,73	1.52	7 (11%)	71,101,113	2.09	19 (26%)
24	BCR	K	4001	-	41,41,41	1.85	4 (9%)	56,56,56	4.33	17 (30%)
21	CLA	K	1402	-	59,63,73	1.47	6 (10%)	71,101,113	2.09	20 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	1	615	-	64,68,73	1.45	8 (12%)	77,107,113	2.01	20 (25%)
39	P3H	5	806	-	32,32,49	1.44	6 (18%)	42,44,61	1.03	2 (4%)
21	CLA	3	615	-	60,64,73	1.48	8 (13%)	72,102,113	2.12	21 (29%)
21	CLA	B	1222	-	69,73,73	1.40	7 (10%)	83,113,113	2.00	22 (26%)
21	CLA	A	1125	-	69,73,73	1.42	7 (10%)	83,113,113	1.96	17 (20%)
21	CLA	A	1134	1	59,63,73	1.46	6 (10%)	71,101,113	2.07	18 (25%)
21	CLA	6	602	-	54,58,73	1.53	6 (11%)	65,95,113	2.18	19 (29%)
21	CLA	6	607	-	64,68,73	1.42	7 (10%)	77,107,113	2.01	18 (23%)
25	LHG	6	801	-	24,24,48	0.54	0	27,30,54	1.28	3 (11%)
24	BCR	B	4001	-	41,41,41	1.95	4 (9%)	56,56,56	4.44	16 (28%)
21	CLA	1	603	-	64,68,73	1.41	8 (12%)	77,107,113	2.18	21 (27%)
21	CLA	6	608	19	50,54,73	1.58	6 (12%)	60,90,113	2.12	16 (26%)
21	CLA	6	612	-	69,73,73	1.37	6 (8%)	83,113,113	2.05	21 (25%)
25	LHG	A	5001	21	48,48,48	0.45	0	51,54,54	1.10	3 (5%)
21	CLA	4	601	-	64,68,73	1.45	7 (10%)	77,107,113	2.25	23 (29%)
21	CLA	B	1212	-	59,63,73	1.46	6 (10%)	71,101,113	2.09	18 (25%)
21	CLA	6	609	-	50,54,73	1.60	7 (14%)	60,90,113	2.04	16 (26%)
36	CHL	6	610	-	51,55,74	0.88	1 (1%)	57,91,114	1.46	11 (19%)
27	LMU	6	805	-	36,36,36	0.47	0	47,47,47	0.93	4 (8%)
21	CLA	4	612	-	69,73,73	1.37	7 (10%)	83,113,113	1.90	18 (21%)
33	PTY	5	803	-	35,35,49	1.02	4 (11%)	38,40,54	1.13	2 (5%)
21	CLA	1	608	-	59,63,73	1.50	8 (13%)	71,101,113	2.10	20 (28%)
21	CLA	1	612	-	64,68,73	1.41	7 (10%)	77,107,113	2.08	17 (22%)
36	CHL	4	610	-	51,55,74	0.95	2 (3%)	57,91,114	1.37	12 (21%)
21	CLA	5	601	-	49,53,73	1.88	12 (24%)	59,89,113	2.88	22 (37%)
21	CLA	B	1235	-	64,68,73	1.40	7 (10%)	77,107,113	2.04	19 (24%)
36	CHL	4	611	-	55,59,74	1.02	4 (7%)	62,96,114	1.51	11 (17%)
21	CLA	B	1228	-	64,68,73	1.41	7 (10%)	77,107,113	1.99	17 (22%)
37	SQD	6	803	-	31,32,54	0.99	0	40,43,65	1.07	2 (5%)
21	CLA	5	607	-	64,68,73	1.46	6 (9%)	77,107,113	2.18	18 (23%)
21	CLA	A	1111	-	69,73,73	1.41	7 (10%)	83,113,113	2.01	19 (22%)
21	CLA	A	1131	1	69,73,73	1.40	6 (8%)	83,113,113	2.11	17 (20%)
21	CLA	B	1224	-	69,73,73	1.38	7 (10%)	83,113,113	1.91	17 (20%)
24	BCR	H	4001	-	41,41,41	1.96	4 (9%)	56,56,56	4.45	20 (35%)
35	XAT	3	502	-	39,47,47	0.84	1 (2%)	54,74,74	2.10	16 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	B	1237	-	69,73,73	1.39	6 (8%)	83,113,113	2.01	21 (25%)
24	BCR	B	4003	-	41,41,41	1.86	5 (12%)	56,56,56	4.37	23 (41%)
21	CLA	3	602	-	56,60,73	1.54	6 (10%)	67,97,113	2.15	20 (29%)
24	BCR	I	4001	-	41,41,41	1.86	4 (9%)	56,56,56	4.17	17 (30%)
21	CLA	A	1123	-	69,73,73	1.43	8 (11%)	83,113,113	1.92	17 (20%)
21	CLA	4	609	17	64,68,73	1.40	6 (9%)	77,107,113	2.24	22 (28%)
21	CLA	B	1202	-	69,73,73	1.35	8 (11%)	83,113,113	1.92	21 (25%)
25	LHG	2	801	21	34,34,48	0.47	0	37,40,54	1.18	4 (10%)
21	CLA	A	1113	-	69,73,73	1.39	6 (8%)	83,113,113	1.84	18 (21%)
21	CLA	5	605	18	69,73,73	1.35	6 (8%)	83,113,113	1.96	18 (21%)
25	LHG	5	802	-	23,23,48	0.54	0	26,29,54	1.49	3 (11%)
21	CLA	4	607	-	64,68,73	1.43	7 (10%)	77,107,113	2.02	18 (23%)
22	PQN	A	2001	-	34,34,34	0.34	0	42,45,45	1.13	2 (4%)
21	CLA	H	1702	-	50,54,73	1.73	9 (18%)	60,90,113	2.25	21 (35%)
21	CLA	A	1012	-	69,73,73	1.36	7 (10%)	83,113,113	1.92	19 (22%)
21	CLA	L	1501	-	69,73,73	1.35	9 (13%)	83,113,113	2.15	20 (24%)
21	CLA	A	1128	-	69,73,73	1.41	7 (10%)	83,113,113	1.91	16 (19%)
24	BCR	3	506	-	41,41,41	1.96	4 (9%)	56,56,56	3.96	23 (41%)
21	CLA	B	1227	-	69,73,73	1.36	7 (10%)	83,113,113	2.00	21 (25%)
21	CLA	B	1231	-	64,68,73	1.45	7 (10%)	77,107,113	2.04	18 (23%)
21	CLA	1	607	-	50,54,73	1.63	7 (14%)	60,90,113	2.04	15 (25%)
29	3PH	5	807	-	28,28,47	1.09	3 (10%)	32,33,52	1.39	3 (9%)
24	BCR	A	4002	-	41,41,41	1.84	4 (9%)	56,56,56	4.40	21 (37%)
24	BCR	1	504	-	41,41,41	1.86	4 (9%)	56,56,56	4.11	20 (35%)
32	4RF	5	805	-	31,31,56	1.20	5 (16%)	34,34,59	1.27	4 (11%)
21	CLA	B	1203	-	69,73,73	1.38	7 (10%)	83,113,113	1.92	19 (22%)
21	CLA	A	1110	-	59,63,73	1.50	7 (11%)	71,101,113	2.18	22 (30%)
21	CLA	K	1403	-	52,56,73	1.54	8 (15%)	62,92,113	2.44	18 (29%)
24	BCR	B	4002	-	41,41,41	1.81	4 (9%)	56,56,56	4.22	11 (19%)
31	LMG	3	803	-	50,50,55	1.05	4 (8%)	58,58,63	1.10	3 (5%)
33	PTY	1	805	-	39,39,49	0.97	3 (7%)	42,44,54	1.14	2 (4%)
21	CLA	2	604	15	69,73,73	1.40	8 (11%)	83,113,113	1.99	19 (22%)
26	OCD	A	5003	-	18,18,18	0.30	0	17,17,17	0.97	0
34	LUT	4	501	-	42,43,43	2.31	2 (4%)	51,60,60	2.23	15 (29%)
35	XAT	1	502	-	39,47,47	0.77	1 (2%)	54,74,74	2.05	13 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	3PH	F	5003	-	33,33,47	1.00	4 (12%)	37,38,52	1.17	2 (5%)
23	SF4	C	3002	3	0,12,12	-	-	-		
33	PTY	3	807	-	25,25,49	1.20	3 (12%)	28,30,54	1.28	2 (7%)
21	CLA	4	602	-	54,58,73	1.56	7 (12%)	65,95,113	2.19	17 (26%)
21	CLA	A	1102	-	69,73,73	1.37	7 (10%)	83,113,113	2.03	20 (24%)
21	CLA	B	1236	-	59,63,73	1.50	7 (11%)	71,101,113	2.13	18 (25%)
21	CLA	5	608	-	59,63,73	1.53	8 (13%)	71,101,113	2.15	19 (26%)
21	CLA	1	602	-	50,54,73	1.60	7 (14%)	60,90,113	2.05	15 (25%)
21	CLA	6	603	-	59,63,73	1.46	7 (11%)	71,101,113	2.05	17 (23%)
21	CLA	A	1141	25	64,68,73	1.44	7 (10%)	77,107,113	2.08	19 (24%)
21	CLA	O	1801	-	40,46,73	1.70	7 (17%)	48,80,113	2.95	13 (27%)
24	BCR	A	4005	-	41,41,41	1.79	5 (12%)	56,56,56	4.20	8 (14%)
21	CLA	A	1112	-	69,73,73	1.35	6 (8%)	83,113,113	1.98	20 (24%)
21	CLA	A	1117	-	69,73,73	1.36	6 (8%)	83,113,113	1.96	17 (20%)
21	CLA	2	608	-	54,58,73	1.56	7 (12%)	65,95,113	2.24	20 (30%)
21	CLA	O	1803	-	64,68,73	1.49	8 (12%)	77,107,113	2.03	20 (25%)
21	CLA	A	1108	-	59,63,73	1.49	7 (11%)	71,101,113	2.09	18 (25%)
21	CLA	3	603	-	69,73,73	1.45	7 (10%)	83,113,113	2.07	22 (26%)
33	PTY	3	808	-	19,19,49	1.35	3 (15%)	22,24,54	1.51	2 (9%)
21	CLA	B	1223	2	69,73,73	1.39	7 (10%)	83,113,113	2.00	18 (21%)
36	CHL	1	610	-	51,55,74	1.13	3 (5%)	57,91,114	1.56	14 (24%)
21	CLA	5	614	-	69,73,73	1.34	7 (10%)	83,113,113	2.76	22 (26%)
21	CLA	B	1226	-	69,73,73	1.42	7 (10%)	83,113,113	2.02	19 (22%)
21	CLA	3	606	-	59,63,73	1.50	7 (11%)	71,101,113	2.13	21 (29%)
21	CLA	B	1207	2	69,73,73	1.35	6 (8%)	83,113,113	1.96	18 (21%)
21	CLA	B	1208	-	64,68,73	1.41	7 (10%)	77,107,113	2.00	17 (22%)
28	DGD	3	805	-	46,46,67	0.87	2 (4%)	60,60,81	1.02	3 (5%)
34	LUT	6	501	-	42,43,43	2.39	1 (2%)	51,60,60	2.24	16 (31%)
21	CLA	B	1225	-	69,73,73	1.41	7 (10%)	83,113,113	1.90	16 (19%)
21	CLA	2	615	-	69,73,73	1.38	7 (10%)	83,113,113	1.89	18 (21%)
21	CLA	B	1217	-	69,73,73	1.40	8 (11%)	83,113,113	1.92	18 (21%)
28	DGD	B	5002	-	62,62,67	1.11	6 (9%)	76,76,81	1.06	4 (5%)
35	XAT	6	504	-	39,47,47	0.90	1 (2%)	54,74,74	6.81	18 (33%)
21	CLA	B	1021	-	69,73,73	1.40	7 (10%)	83,113,113	2.09	22 (26%)
34	LUT	5	504	-	42,43,43	2.48	1 (2%)	51,60,60	4.74	22 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	CHL	3	604	-	70,74,74	1.31	10 (14%)	80,114,114	1.33	10 (12%)
24	BCR	F	4001	-	41,41,41	1.85	4 (9%)	56,56,56	4.38	17 (30%)
27	LMU	A	5005	-	36,36,36	0.40	0	47,47,47	0.84	1 (2%)
21	CLA	F	1301	-	51,55,73	1.60	7 (13%)	61,91,113	2.11	17 (27%)
25	LHG	2	803	-	35,35,48	0.46	0	38,41,54	1.19	4 (10%)
34	LUT	5	502	-	42,43,43	2.41	1 (2%)	51,60,60	2.20	14 (27%)
21	CLA	B	1023	-	69,73,73	1.35	7 (10%)	83,113,113	1.97	19 (22%)
35	XAT	6	502	-	39,47,47	0.84	1 (2%)	54,74,74	1.71	12 (22%)
24	BCR	J	4001	-	41,41,41	1.89	5 (12%)	56,56,56	4.49	23 (41%)
21	CLA	3	614	-	46,50,73	1.61	6 (13%)	55,85,113	2.16	15 (27%)
21	CLA	1	604	-	69,73,73	1.40	8 (11%)	83,113,113	2.10	23 (27%)
36	CHL	4	613	-	65,69,74	0.90	2 (3%)	74,108,114	1.22	11 (14%)
21	CLA	L	1503	-	54,58,73	1.56	7 (12%)	65,95,113	2.16	18 (27%)
21	CLA	A	1121	1	64,68,73	1.40	6 (9%)	77,107,113	1.99	19 (24%)
21	CLA	A	1136	-	69,73,73	1.40	8 (11%)	83,113,113	1.92	23 (27%)
23	SF4	C	3003	3	0,12,12	-	-	-		
24	BCR	J	4002	-	41,41,41	1.98	6 (14%)	56,56,56	4.44	18 (32%)
25	LHG	2	802	-	42,42,48	0.44	0	45,48,54	1.18	4 (8%)
32	4RF	L	5002	-	38,38,56	1.05	6 (15%)	41,41,59	0.97	3 (7%)
21	CLA	4	603	-	69,73,73	1.37	8 (11%)	83,113,113	1.91	18 (21%)
24	BCR	O	4001	-	41,41,41	1.92	6 (14%)	56,56,56	5.09	21 (37%)
21	CLA	1	606	-	54,58,73	1.55	6 (11%)	65,95,113	2.06	17 (26%)
37	SQD	3	806	-	34,35,54	0.92	0	43,46,65	1.18	4 (9%)
36	CHL	1	609	14	70,74,74	0.89	2 (2%)	80,114,114	1.28	11 (13%)
21	CLA	4	606	-	54,58,73	1.55	7 (12%)	65,95,113	2.10	16 (24%)
25	LHG	1	803	-	30,30,48	0.44	0	33,36,54	1.19	4 (12%)
21	CLA	A	1124	-	64,68,73	1.45	7 (10%)	77,107,113	2.01	21 (27%)
21	CLA	O	1802	-	41,46,73	1.62	5 (12%)	52,81,113	2.13	15 (28%)
21	CLA	A	1137	-	64,68,73	1.45	6 (9%)	77,107,113	2.07	23 (29%)
34	LUT	3	501	-	42,43,43	2.30	2 (4%)	51,60,60	1.96	12 (23%)
23	SF4	A	3001	2,1	0,12,12	-	-	-		
21	CLA	B	1211	-	69,73,73	1.42	6 (8%)	83,113,113	2.00	18 (21%)
22	PQN	B	2002	-	34,34,34	0.35	0	42,45,45	1.24	2 (4%)
24	BCR	A	4001	-	41,41,41	1.87	4 (9%)	56,56,56	5.02	22 (39%)
21	CLA	6	605	-	69,73,73	1.38	7 (10%)	83,113,113	2.16	22 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	PTY	1	806	-	17,17,49	1.26	2 (11%)	18,21,54	1.21	2 (11%)
21	CLA	K	1404	-	49,53,73	1.60	7 (14%)	59,89,113	2.08	15 (25%)
24	BCR	3	504	-	41,41,41	1.85	5 (12%)	56,56,56	4.33	19 (33%)
21	CLA	F	1302	-	53,57,73	1.57	7 (13%)	62,93,113	2.26	18 (29%)
24	BCR	2	503	-	41,41,41	1.78	4 (9%)	56,56,56	4.27	15 (26%)
21	CLA	B	1238	-	69,73,73	1.39	7 (10%)	83,113,113	2.01	18 (21%)
21	CLA	B	1230	-	69,73,73	1.38	7 (10%)	83,113,113	2.08	22 (26%)
38	LMK	4	805	-	33,34,53	1.66	3 (9%)	36,41,60	1.45	2 (5%)
21	CLA	A	1101	1	69,73,73	1.40	8 (11%)	83,113,113	1.92	20 (24%)
21	CLA	J	1901	-	53,57,73	1.67	7 (13%)	62,93,113	2.55	21 (33%)
25	LHG	1	801	-	48,48,48	0.39	0	51,54,54	1.21	3 (5%)
33	PTY	O	5002	-	21,21,49	1.30	4 (19%)	24,26,54	1.43	2 (8%)
34	LUT	2	501	-	42,43,43	2.31	1 (2%)	51,60,60	2.20	17 (33%)
21	CLA	3	601	-	64,68,73	1.45	7 (10%)	77,107,113	2.13	17 (22%)
31	LMG	6	802	-	37,37,55	0.59	1 (2%)	45,45,63	1.06	3 (6%)
21	CLA	A	1132	-	69,73,73	1.36	7 (10%)	83,113,113	1.97	19 (22%)
21	CLA	A	1135	-	55,59,73	1.61	7 (12%)	66,96,113	2.19	18 (27%)
36	CHL	2	611	-	52,56,74	1.11	3 (5%)	58,92,114	1.57	11 (18%)
21	CLA	B	1204	-	69,73,73	1.38	7 (10%)	83,113,113	2.06	18 (21%)
21	CLA	B	1201	-	52,56,73	1.55	7 (13%)	62,92,113	2.33	20 (32%)
21	CLA	3	613	-	50,54,73	1.58	7 (14%)	60,90,113	2.28	14 (23%)
21	CLA	5	602	-	50,54,73	1.68	9 (18%)	60,90,113	2.06	17 (28%)
24	BCR	A	4003	-	41,41,41	1.87	4 (9%)	56,56,56	4.23	19 (33%)
21	CLA	A	1127	-	69,73,73	1.40	7 (10%)	83,113,113	1.93	19 (22%)
21	CLA	B	1221	-	69,73,73	1.36	7 (10%)	83,113,113	2.07	21 (25%)
21	CLA	2	601	-	69,73,73	1.45	7 (10%)	83,113,113	1.99	17 (20%)
38	LMK	2	807	-	29,30,53	1.74	2 (6%)	32,37,60	1.68	5 (15%)
31	LMG	2	804	-	50,50,55	1.04	5 (10%)	58,58,63	1.19	2 (3%)
21	CLA	G	1601	-	51,55,73	1.57	6 (11%)	61,91,113	2.10	17 (27%)
34	LUT	1	501	-	42,43,43	2.41	2 (4%)	51,60,60	4.98	23 (45%)
21	CLA	B	1220	-	59,63,73	1.52	7 (11%)	71,101,113	2.10	22 (30%)
21	CLA	4	605	-	69,73,73	1.37	7 (10%)	83,113,113	2.03	21 (25%)

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
21	CLA	5	603	-	-	15/33/109/115	-
24	BCR	B	4005	-	-	13/29/63/63	0/2/2/2
21	CLA	B	1206	2	-	17/39/115/115	-
21	CLA	5	612	18	-	11/17/93/115	-
24	BCR	F	4002	-	-	14/29/63/63	0/2/2/2
21	CLA	B	1209	-	-	6/17/93/115	-
24	BCR	L	4002	-	-	8/29/63/63	0/2/2/2
36	CHL	5	609	-	1/1/15/21	7/41/117/117	-
25	LHG	1	802	-	-	18/30/30/53	-
27	LMU	B	5004	-	-	16/21/61/61	0/2/2/2
36	CHL	5	610	-	1/1/11/21	4/19/95/117	-
37	SQD	2	805	-	-	17/34/54/69	0/1/1/1
25	LHG	F	5001	-	-	32/53/53/53	-
24	BCR	3	503	-	-	13/29/63/63	0/2/2/2
21	CLA	B	1218	-	-	24/39/115/115	-
21	CLA	1	601	-	-	14/39/115/115	-
21	CLA	3	610	16	-	10/21/97/115	-
21	CLA	5	613	-	-	8/15/91/115	-
24	BCR	B	4006	-	-	8/29/63/63	0/2/2/2
31	LMG	1	804	-	-	9/27/47/70	0/1/1/1
35	XAT	4	502	-	2/2/12/26	0/31/93/93	0/4/4/4
21	CLA	A	1122	-	-	15/39/115/115	-
21	CLA	3	611	-	-	14/39/115/115	-
21	CLA	A	1138	-	-	17/39/115/115	-
36	CHL	2	609	15	1/1/15/21	3/41/117/117	-
21	CLA	B	1216	-	-	13/39/115/115	-
21	CLA	A	1116	-	-	15/29/105/115	-
21	CLA	1	613	-	-	8/15/91/115	-
21	CLA	2	605	15	-	18/39/115/115	-
24	BCR	A	4006	-	-	20/29/63/63	0/2/2/2
21	CLA	B	1239	-	-	14/39/115/115	-
21	CLA	A	1106	-	-	13/39/115/115	-
21	CLA	A	1129	-	-	14/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	5	604	18	-	16/39/115/115	-
24	BCR	B	4004	-	-	9/29/63/63	0/2/2/2
21	CLA	3	607	-	-	13/33/109/115	-
21	CLA	A	1013	-	-	15/39/115/115	-
21	CLA	6	604	-	-	17/33/109/115	-
21	CLA	2	607	25	-	12/33/109/115	-
29	3PH	B	5003	-	-	24/32/32/49	-
21	CLA	B	1234	-	-	10/27/103/115	-
20	CL0	A	1011	-	-	12/39/115/115	-
21	CLA	A	1105	-	-	13/33/109/115	-
21	CLA	G	1602	-	-	10/17/93/115	-
21	CLA	4	608	-	-	12/17/93/115	-
21	CLA	H	1701	9	-	15/33/109/115	-
21	CLA	A	1114	-	-	8/27/103/115	-
33	PTY	4	804	-	-	23/38/38/53	-
21	CLA	1	611	-	-	19/39/115/115	-
21	CLA	4	615	17	-	13/23/99/115	-
21	CLA	B	1210	-	-	24/39/115/115	-
21	CLA	6	613	-	-	9/15/91/115	-
21	CLA	A	1140	-	-	16/35/111/115	-
21	CLA	A	1120	-	-	18/33/109/115	-
21	CLA	L	1504	-	-	10/21/97/115	-
29	3PH	5	804	-	-	12/29/29/49	-
21	CLA	A	1104	-	-	16/39/115/115	-
21	CLA	2	602	-	-	9/24/100/115	-
21	CLA	3	605	-	-	19/39/115/115	-
24	BCR	L	4001	-	-	11/29/63/63	0/2/2/2
21	CLA	K	1401	-	-	12/15/91/115	-
21	CLA	B	1215	-	-	14/39/115/115	-
21	CLA	2	612	-	-	18/39/115/115	-
21	CLA	A	1115	1	-	14/33/109/115	-
21	CLA	A	1103	-	-	15/39/115/115	-
21	CLA	B	1229	2	-	15/39/115/115	-
24	BCR	A	4007	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LHG	5	801	-	-	23/47/47/53	-
33	PTY	L	5003	-	-	7/22/22/53	-
36	CHL	2	610	-	1/1/13/21	2/29/105/117	-
21	CLA	6	601	-	-	18/33/109/115	-
24	BCR	I	4002	-	-	12/29/63/63	0/2/2/2
25	LHG	A	5002	-	-	37/53/53/53	-
33	PTY	6	804	-	-	8/26/26/53	-
25	LHG	3	801	-	-	14/19/19/53	-
21	CLA	5	606	-	-	9/21/97/115	-
21	CLA	A	1126	-	-	20/39/115/115	-
21	CLA	A	1109	-	-	18/39/115/115	-
21	CLA	B	1213	-	-	17/33/109/115	-
21	CLA	B	1219	-	-	18/39/115/115	-
28	DGD	3	804	-	-	11/28/68/95	0/2/2/2
21	CLA	6	606	-	-	10/21/97/115	-
34	LUT	5	501	-	1/1/12/27	4/29/67/67	0/2/2/2
21	CLA	B	1205	-	-	13/39/115/115	-
27	LMU	A	5004	-	-	10/21/61/61	0/2/2/2
21	CLA	L	1502	-	-	16/39/115/115	-
21	CLA	B	1022	-	-	11/39/115/115	-
24	BCR	G	4001	-	-	12/29/63/63	0/2/2/2
25	LHG	B	5001	-	-	34/46/46/53	-
36	CHL	2	613	-	-	3/17/93/117	-
21	CLA	1	605	-	-	15/39/115/115	-
21	CLA	A	1133	-	-	18/39/115/115	-
21	CLA	B	1214	-	-	20/39/115/115	-
25	LHG	4	801	-	-	20/33/33/53	-
28	DGD	2	806	-	-	14/28/68/95	0/2/2/2
21	CLA	A	1130	1	-	5/27/103/115	-
21	CLA	A	1139	-	-	16/39/115/115	-
21	CLA	G	1603	-	-	7/15/91/115	-
34	LUT	5	503	-	-	8/29/67/67	0/2/2/2
39	P3H	2	808	-	-	20/44/68/68	0/1/1/1
24	BCR	A	4004	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	1240	-	-	15/39/115/115	-
31	LMG	3	802	-	-	7/26/46/70	0/1/1/1
21	CLA	2	603	-	-	18/39/115/115	-
31	LMG	4	802	-	-	16/41/61/70	0/1/1/1
31	LMG	4	803	-	-	12/34/54/70	0/1/1/1
24	BCR	4	503	-	-	11/29/63/63	0/2/2/2
21	CLA	A	1107	1	-	16/39/115/115	-
21	CLA	3	608	-	-	16/39/115/115	-
21	CLA	A	1118	-	-	9/21/97/115	-
21	CLA	A	1119	-	-	18/39/115/115	-
21	CLA	2	606	-	-	7/21/97/115	-
21	CLA	3	612	-	-	17/39/115/115	-
21	CLA	4	604	-	-	12/33/109/115	-
31	LMG	F	5002	-	-	17/45/65/70	0/1/1/1
21	CLA	B	1232	-	-	14/27/103/115	-
24	BCR	K	4001	-	-	13/29/63/63	0/2/2/2
21	CLA	K	1402	-	-	15/27/103/115	-
21	CLA	1	615	-	-	16/33/109/115	-
39	P3H	5	806	-	-	9/27/51/68	0/1/1/1
21	CLA	3	615	-	-	10/29/105/115	-
21	CLA	B	1222	-	-	11/39/115/115	-
21	CLA	A	1125	-	-	19/39/115/115	-
21	CLA	A	1134	1	-	13/27/103/115	-
21	CLA	6	602	-	-	8/21/97/115	-
21	CLA	6	607	-	-	18/33/109/115	-
25	LHG	6	801	-	-	17/29/29/53	-
24	BCR	B	4001	-	-	9/29/63/63	0/2/2/2
21	CLA	1	603	-	-	20/33/109/115	-
21	CLA	6	608	19	-	10/17/93/115	-
21	CLA	6	612	-	-	15/39/115/115	-
25	LHG	A	5001	21	-	24/53/53/53	-
21	CLA	4	601	-	-	19/33/109/115	-
21	CLA	B	1212	-	-	13/27/103/115	-
21	CLA	6	609	-	-	10/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CHL	6	610	-	-	4/19/95/117	-
27	LMU	6	805	-	-	12/21/61/61	0/2/2/2
21	CLA	4	612	-	-	14/39/115/115	-
33	PTY	5	803	-	-	25/39/39/53	-
21	CLA	1	608	-	-	13/27/103/115	-
21	CLA	1	612	-	-	13/33/109/115	-
36	CHL	4	610	-	-	3/19/95/117	-
21	CLA	5	601	-	-	7/15/91/115	-
21	CLA	B	1235	-	-	10/33/109/115	-
36	CHL	4	611	-	-	1/23/99/117	-
21	CLA	B	1228	-	-	15/33/109/115	-
37	SQD	6	803	-	-	3/27/47/69	0/1/1/1
35	XAT	3	502	-	2/2/12/26	4/31/93/93	0/4/4/4
21	CLA	A	1111	-	-	13/39/115/115	-
21	CLA	A	1131	1	-	14/39/115/115	-
21	CLA	B	1224	-	-	19/39/115/115	-
21	CLA	5	607	-	-	16/33/109/115	-
24	BCR	H	4001	-	-	19/29/63/63	0/2/2/2
21	CLA	B	1237	-	-	20/39/115/115	-
24	BCR	B	4003	-	-	15/29/63/63	0/2/2/2
21	CLA	3	602	-	-	10/24/100/115	-
24	BCR	I	4001	-	-	13/29/63/63	0/2/2/2
21	CLA	A	1123	-	-	15/39/115/115	-
21	CLA	4	609	17	-	22/33/109/115	-
21	CLA	B	1202	-	-	19/39/115/115	-
25	LHG	2	801	21	-	25/39/39/53	-
21	CLA	A	1113	-	-	20/39/115/115	-
21	CLA	5	605	18	-	18/39/115/115	-
25	LHG	5	802	-	-	17/27/27/53	-
21	CLA	4	607	-	-	18/33/109/115	-
22	PQN	A	2001	-	-	6/23/43/43	0/2/2/2
21	CLA	H	1702	-	-	11/17/93/115	-
21	CLA	A	1012	-	-	16/39/115/115	-
21	CLA	L	1501	-	-	21/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	1128	-	-	12/39/115/115	-
24	BCR	3	506	-	-	9/29/63/63	0/2/2/2
21	CLA	B	1227	-	-	20/39/115/115	-
21	CLA	B	1231	-	-	15/33/109/115	-
21	CLA	1	607	-	-	10/17/93/115	-
29	3PH	5	807	-	-	11/30/30/49	-
24	BCR	A	4002	-	-	16/29/63/63	0/2/2/2
24	BCR	1	504	-	-	12/29/63/63	0/2/2/2
32	4RF	5	805	-	-	16/34/34/59	-
21	CLA	B	1203	-	-	18/39/115/115	-
21	CLA	A	1110	-	-	9/27/103/115	-
21	CLA	K	1403	-	-	9/19/95/115	-
24	BCR	B	4002	-	-	13/29/63/63	0/2/2/2
31	LMG	3	803	-	-	20/45/65/70	0/1/1/1
33	PTY	1	805	-	-	18/43/43/53	-
35	XAT	1	502	-	2/2/12/26	6/31/93/93	0/4/4/4
34	LUT	4	501	-	1/1/12/27	5/29/67/67	0/2/2/2
21	CLA	2	604	15	-	19/39/115/115	-
26	OCD	A	5003	-	-	2/15/16/16	-
29	3PH	F	5003	-	-	22/35/35/49	-
23	SF4	C	3002	3	-	-	0/6/5/5
33	PTY	3	807	-	-	8/29/29/53	-
21	CLA	4	602	-	-	10/21/97/115	-
21	CLA	A	1102	-	-	17/39/115/115	-
21	CLA	B	1236	-	-	12/27/103/115	-
21	CLA	5	608	-	-	12/27/103/115	-
21	CLA	1	602	-	-	9/17/93/115	-
21	CLA	6	603	-	-	10/27/103/115	-
21	CLA	A	1141	25	-	15/33/109/115	-
21	CLA	O	1801	-	-	4/6/78/115	-
24	BCR	A	4005	-	-	7/29/63/63	0/2/2/2
21	CLA	A	1112	-	-	17/39/115/115	-
21	CLA	A	1117	-	-	21/39/115/115	-
21	CLA	2	608	-	-	13/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	O	1803	-	-	15/33/109/115	-
21	CLA	A	1108	-	-	18/27/103/115	-
21	CLA	3	603	-	-	17/39/115/115	-
33	PTY	3	808	-	-	13/22/22/53	-
21	CLA	B	1223	2	-	13/39/115/115	-
36	CHL	1	610	-	-	1/19/95/117	-
21	CLA	5	614	-	-	21/39/115/115	-
21	CLA	B	1226	-	-	14/39/115/115	-
34	LUT	6	501	-	1/1/12/27	4/29/67/67	0/2/2/2
21	CLA	B	1207	2	-	18/39/115/115	-
21	CLA	B	1208	-	-	12/33/109/115	-
21	CLA	3	606	-	-	10/27/103/115	-
28	DGD	3	805	-	-	12/34/74/95	0/2/2/2
36	CHL	3	604	-	1/1/15/21	9/41/117/117	-
35	XAT	6	504	-	1/1/12/26	6/31/93/93	0/4/4/4
21	CLA	B	1217	-	-	14/39/115/115	-
21	CLA	B	1225	-	-	19/39/115/115	-
21	CLA	2	615	-	-	21/39/115/115	-
21	CLA	B	1021	-	-	15/39/115/115	-
28	DGD	B	5002	-	-	17/50/90/95	0/2/2/2
24	BCR	F	4001	-	-	9/29/63/63	0/2/2/2
27	LMU	A	5005	-	-	11/21/61/61	0/2/2/2
21	CLA	F	1301	-	-	11/18/94/115	-
25	LHG	2	803	-	-	24/40/40/53	-
21	CLA	G	1601	-	-	11/18/94/115	-
34	LUT	5	502	-	-	5/29/67/67	0/2/2/2
21	CLA	B	1023	-	-	22/39/115/115	-
35	XAT	6	502	-	2/2/12/26	0/31/93/93	0/4/4/4
24	BCR	J	4001	-	-	11/29/63/63	0/2/2/2
21	CLA	3	614	-	-	6/12/88/115	-
36	CHL	4	613	-	1/1/14/21	7/35/111/117	-
21	CLA	1	604	-	-	18/39/115/115	-
21	CLA	L	1503	-	-	4/21/97/115	-
21	CLA	A	1121	1	-	17/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	1136	-	-	15/39/115/115	-
25	LHG	2	802	-	-	26/47/47/53	-
24	BCR	J	4002	-	-	14/29/63/63	0/2/2/2
23	SF4	C	3003	3	-	-	0/6/5/5
32	4RF	L	5002	-	-	17/41/41/59	-
21	CLA	4	603	-	-	11/39/115/115	-
24	BCR	O	4001	-	-	13/29/63/63	0/2/2/2
21	CLA	1	606	-	-	10/21/97/115	-
37	SQD	3	806	-	-	12/30/50/69	0/1/1/1
36	CHL	1	609	14	1/1/15/21	6/41/117/117	-
21	CLA	4	606	-	-	12/21/97/115	-
25	LHG	1	803	-	-	15/35/35/53	-
21	CLA	A	1124	-	-	15/33/109/115	-
21	CLA	O	1802	-	-	1/4/80/115	-
21	CLA	A	1137	-	-	12/33/109/115	-
34	LUT	3	501	-	-	4/29/67/67	0/2/2/2
23	SF4	A	3001	2,1	-	-	0/6/5/5
21	CLA	B	1211	-	-	15/39/115/115	-
22	PQN	B	2002	-	-	11/23/43/43	0/2/2/2
24	BCR	A	4001	-	-	14/29/63/63	0/2/2/2
21	CLA	6	605	-	-	20/39/115/115	-
33	PTY	1	806	-	-	7/19/19/53	-
21	CLA	K	1404	-	-	6/15/91/115	-
24	BCR	3	504	-	-	12/29/63/63	0/2/2/2
21	CLA	F	1302	-	-	8/20/96/115	-
24	BCR	2	503	-	-	15/29/63/63	0/2/2/2
21	CLA	B	1238	-	-	14/39/115/115	-
21	CLA	B	1230	-	-	17/39/115/115	-
38	LMK	4	805	-	-	6/41/41/60	-
21	CLA	A	1101	1	-	22/39/115/115	-
21	CLA	J	1901	-	-	10/20/96/115	-
25	LHG	1	801	-	-	32/53/53/53	-
33	PTY	O	5002	-	-	10/24/24/53	-
34	LUT	2	501	-	-	2/29/67/67	0/2/2/2
21	CLA	3	601	-	-	18/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	6	802	-	-	11/32/52/70	0/1/1/1
21	CLA	A	1132	-	-	18/39/115/115	-
21	CLA	A	1135	-	-	9/23/99/115	-
36	CHL	2	611	-	-	0/20/96/117	-
21	CLA	B	1204	-	-	17/39/115/115	-
21	CLA	B	1201	-	-	13/19/95/115	-
21	CLA	3	613	-	-	11/17/93/115	-
21	CLA	5	602	-	-	10/17/93/115	-
24	BCR	A	4003	-	-	6/29/63/63	0/2/2/2
21	CLA	A	1127	-	-	16/39/115/115	-
21	CLA	B	1221	-	-	14/39/115/115	-
21	CLA	2	601	-	-	22/39/115/115	-
38	LMK	2	807	-	-	5/37/37/60	-
31	LMG	2	804	-	-	16/45/65/70	0/1/1/1
35	XAT	2	502	-	2/2/12/26	2/31/93/93	0/4/4/4
34	LUT	5	504	-	1/1/12/27	7/29/67/67	0/2/2/2
34	LUT	1	501	-	-	5/29/67/67	0/2/2/2
21	CLA	B	1220	-	-	17/27/103/115	-
21	CLA	4	605	-	-	15/39/115/115	-

All (1541) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	5	501	LUT	C24-C25	15.69	1.52	1.33
34	5	504	LUT	C24-C25	15.24	1.52	1.33
34	5	503	LUT	C24-C25	14.74	1.51	1.33
34	5	502	LUT	C24-C25	14.67	1.51	1.33
34	6	501	LUT	C24-C25	14.53	1.51	1.33
34	1	501	LUT	C24-C25	14.46	1.51	1.33
34	4	501	LUT	C24-C25	14.11	1.50	1.33
34	2	501	LUT	C24-C25	13.94	1.50	1.33
34	3	501	LUT	C24-C25	13.94	1.50	1.33
20	A	1011	CL0	MG-NA	9.09	2.27	2.06
24	G	4001	BCR	C10-C9	7.95	1.46	1.35
24	3	506	BCR	C10-C9	7.92	1.46	1.35
24	H	4001	BCR	C10-C9	7.83	1.46	1.35
24	1	504	BCR	C10-C9	7.52	1.45	1.35
24	B	4001	BCR	C10-C9	7.46	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	4001	BCR	C10-C9	7.41	1.45	1.35
24	I	4001	BCR	C10-C9	7.23	1.45	1.35
24	L	4002	BCR	C10-C9	7.21	1.45	1.35
38	2	807	LMK	O3-C4	7.21	1.44	1.22
24	F	4001	BCR	C10-C9	7.20	1.45	1.35
38	4	805	LMK	O3-C4	7.20	1.44	1.22
24	K	4001	BCR	C10-C9	7.16	1.45	1.35
24	I	4002	BCR	C10-C9	7.15	1.45	1.35
24	A	4007	BCR	C10-C9	7.13	1.45	1.35
24	A	4002	BCR	C10-C9	7.00	1.45	1.35
24	B	4006	BCR	C10-C9	6.82	1.44	1.35
24	3	503	BCR	C10-C9	6.82	1.44	1.35
24	J	4001	BCR	C10-C9	6.75	1.44	1.35
24	B	4004	BCR	C10-C9	6.72	1.44	1.35
24	3	504	BCR	C10-C9	6.70	1.44	1.35
24	O	4001	BCR	C10-C9	6.69	1.44	1.35
24	4	503	BCR	C10-C9	6.61	1.44	1.35
24	F	4002	BCR	C10-C9	6.59	1.44	1.35
24	J	4002	BCR	C10-C9	6.58	1.44	1.35
24	B	4002	BCR	C10-C9	6.57	1.44	1.35
21	A	1101	CLA	MG-NA	6.54	2.21	2.06
21	O	1803	CLA	MG-NA	6.53	2.21	2.06
21	5	613	CLA	MG-NA	6.53	2.21	2.06
21	3	602	CLA	MG-NA	6.42	2.21	2.06
24	A	4004	BCR	C10-C9	6.41	1.44	1.35
21	5	607	CLA	MG-NA	6.41	2.21	2.06
21	G	1602	CLA	MG-NA	6.40	2.21	2.06
21	4	615	CLA	MG-NA	6.40	2.21	2.06
21	A	1116	CLA	MG-NA	6.40	2.21	2.06
21	K	1402	CLA	MG-NA	6.40	2.21	2.06
21	5	606	CLA	MG-NA	6.39	2.21	2.06
21	4	602	CLA	MG-NA	6.38	2.21	2.06
21	A	1123	CLA	MG-NA	6.38	2.21	2.06
24	B	4005	BCR	C10-C9	6.37	1.44	1.35
21	5	603	CLA	MG-NA	6.37	2.21	2.06
21	1	613	CLA	MG-NA	6.37	2.21	2.06
21	1	611	CLA	MG-NA	6.37	2.21	2.06
21	3	615	CLA	MG-NA	6.37	2.21	2.06
21	1	615	CLA	MG-NA	6.37	2.21	2.06
24	A	4003	BCR	C10-C9	6.36	1.44	1.35
21	B	1232	CLA	MG-NA	6.36	2.21	2.06
21	G	1601	CLA	MG-NA	6.35	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	602	CLA	MG-NA	6.35	2.21	2.06
21	6	602	CLA	MG-NA	6.35	2.21	2.06
21	1	608	CLA	MG-NA	6.34	2.21	2.06
21	A	1121	CLA	MG-NA	6.33	2.21	2.06
21	A	1012	CLA	MG-NA	6.33	2.21	2.06
21	B	1217	CLA	MG-NA	6.33	2.21	2.06
21	6	603	CLA	MG-NA	6.33	2.21	2.06
21	3	611	CLA	MG-NA	6.33	2.21	2.06
21	3	608	CLA	MG-NA	6.32	2.21	2.06
21	B	1207	CLA	MG-NA	6.32	2.21	2.06
21	A	1136	CLA	MG-NA	6.32	2.21	2.06
21	A	1114	CLA	MG-NA	6.32	2.21	2.06
21	B	1229	CLA	MG-NA	6.32	2.21	2.06
21	1	601	CLA	MG-NA	6.32	2.21	2.06
21	A	1115	CLA	MG-NA	6.32	2.21	2.06
21	A	1130	CLA	MG-NA	6.31	2.21	2.06
21	6	601	CLA	MG-NA	6.31	2.21	2.06
21	6	609	CLA	MG-NA	6.30	2.21	2.06
21	A	1107	CLA	MG-NA	6.30	2.21	2.06
21	6	607	CLA	MG-NA	6.30	2.21	2.06
24	A	4006	BCR	C10-C9	6.30	1.44	1.35
21	A	1110	CLA	MG-NA	6.30	2.21	2.06
21	2	605	CLA	MG-NA	6.30	2.21	2.06
21	2	615	CLA	MG-NA	6.30	2.21	2.06
21	K	1404	CLA	MG-NA	6.30	2.21	2.06
21	5	605	CLA	MG-NA	6.30	2.21	2.06
21	A	1112	CLA	MG-NA	6.30	2.21	2.06
21	6	608	CLA	MG-NA	6.30	2.21	2.06
21	A	1132	CLA	MG-NA	6.30	2.21	2.06
21	B	1208	CLA	MG-NA	6.29	2.21	2.06
21	L	1503	CLA	MG-NA	6.28	2.21	2.06
21	3	610	CLA	MG-NA	6.28	2.21	2.06
21	1	607	CLA	MG-NA	6.28	2.21	2.06
21	B	1206	CLA	MG-NA	6.28	2.21	2.06
21	A	1135	CLA	MG-NA	6.27	2.21	2.06
21	3	614	CLA	MG-NA	6.27	2.21	2.06
21	B	1022	CLA	MG-NA	6.27	2.21	2.06
21	A	1134	CLA	MG-NA	6.26	2.21	2.06
21	1	602	CLA	MG-NA	6.26	2.21	2.06
21	3	607	CLA	MG-NA	6.26	2.21	2.06
24	A	4005	BCR	C10-C9	6.26	1.44	1.35
21	5	604	CLA	MG-NA	6.26	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	603	CLA	MG-NA	6.26	2.21	2.06
21	B	1239	CLA	MG-NA	6.25	2.21	2.06
21	B	1023	CLA	MG-NA	6.25	2.21	2.06
21	B	1212	CLA	MG-NA	6.25	2.21	2.06
21	4	604	CLA	MG-NA	6.25	2.21	2.06
21	5	608	CLA	MG-NA	6.24	2.21	2.06
21	A	1113	CLA	MG-NA	6.23	2.21	2.06
21	B	1235	CLA	MG-NA	6.23	2.21	2.06
21	B	1223	CLA	MG-NA	6.23	2.21	2.06
21	B	1204	CLA	MG-NA	6.22	2.21	2.06
21	A	1141	CLA	MG-NA	6.22	2.21	2.06
24	A	4003	BCR	C24-C23	6.21	1.51	1.33
21	6	606	CLA	MG-NA	6.21	2.21	2.06
21	A	1140	CLA	MG-NA	6.20	2.21	2.06
21	B	1214	CLA	MG-NA	6.19	2.21	2.06
21	B	1240	CLA	MG-NA	6.19	2.21	2.06
21	2	606	CLA	MG-NA	6.19	2.21	2.06
21	4	605	CLA	MG-NA	6.18	2.21	2.06
21	L	1504	CLA	MG-NA	6.18	2.21	2.06
21	4	607	CLA	MG-NA	6.18	2.20	2.06
21	F	1301	CLA	MG-NA	6.16	2.20	2.06
21	2	608	CLA	MG-NA	6.15	2.20	2.06
21	A	1109	CLA	MG-NA	6.15	2.20	2.06
24	2	503	BCR	C10-C9	6.15	1.43	1.35
21	B	1225	CLA	MG-NA	6.15	2.20	2.06
21	O	1802	CLA	MG-NA	6.14	2.20	2.06
21	3	612	CLA	MG-NA	6.14	2.20	2.06
21	2	607	CLA	MG-NA	6.13	2.20	2.06
21	4	609	CLA	MG-NA	6.13	2.20	2.06
21	1	606	CLA	MG-NA	6.13	2.20	2.06
21	1	603	CLA	MG-NA	6.13	2.20	2.06
21	1	605	CLA	MG-NA	6.12	2.20	2.06
21	A	1122	CLA	MG-NA	6.11	2.20	2.06
21	A	1137	CLA	MG-NA	6.11	2.20	2.06
21	B	1227	CLA	MG-NA	6.11	2.20	2.06
21	4	608	CLA	MG-NA	6.11	2.20	2.06
21	3	606	CLA	MG-NA	6.11	2.20	2.06
21	A	1104	CLA	MG-NA	6.10	2.20	2.06
21	B	1201	CLA	MG-NA	6.09	2.20	2.06
21	B	1234	CLA	MG-NA	6.09	2.20	2.06
21	B	1236	CLA	MG-NA	6.09	2.20	2.06
21	4	606	CLA	MG-NA	6.09	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	H	1702	CLA	MG-NA	6.09	2.20	2.06
21	2	601	CLA	MG-NA	6.09	2.20	2.06
21	5	602	CLA	MG-NA	6.08	2.20	2.06
21	A	1105	CLA	MG-NA	6.08	2.20	2.06
21	A	1120	CLA	MG-NA	6.08	2.20	2.06
21	A	1117	CLA	MG-NA	6.08	2.20	2.06
21	B	1213	CLA	MG-NA	6.08	2.20	2.06
21	2	603	CLA	MG-NA	6.08	2.20	2.06
21	B	1218	CLA	MG-NA	6.06	2.20	2.06
21	B	1203	CLA	MG-NA	6.06	2.20	2.06
21	K	1403	CLA	MG-NA	6.05	2.20	2.06
21	B	1211	CLA	MG-NA	6.05	2.20	2.06
24	B	4001	BCR	C24-C23	6.05	1.51	1.33
21	B	1224	CLA	MG-NA	6.05	2.20	2.06
21	A	1139	CLA	MG-NA	6.04	2.20	2.06
21	6	604	CLA	MG-NA	6.04	2.20	2.06
21	3	605	CLA	MG-NA	6.04	2.20	2.06
21	F	1302	CLA	MG-NA	6.04	2.20	2.06
21	4	601	CLA	MG-NA	6.02	2.20	2.06
21	A	1127	CLA	MG-NA	6.02	2.20	2.06
21	A	1108	CLA	MG-NA	6.02	2.20	2.06
21	B	1210	CLA	MG-NA	6.01	2.20	2.06
21	A	1106	CLA	MG-NA	6.01	2.20	2.06
21	A	1111	CLA	MG-NA	6.00	2.20	2.06
21	K	1401	CLA	MG-NA	5.99	2.20	2.06
21	B	1202	CLA	MG-NA	5.98	2.20	2.06
21	A	1124	CLA	MG-NA	5.98	2.20	2.06
21	A	1128	CLA	MG-NA	5.98	2.20	2.06
21	4	612	CLA	MG-NA	5.98	2.20	2.06
21	B	1238	CLA	MG-NA	5.98	2.20	2.06
21	L	1502	CLA	MG-NA	5.97	2.20	2.06
21	3	603	CLA	MG-NA	5.95	2.20	2.06
21	B	1226	CLA	MG-NA	5.95	2.20	2.06
21	A	1013	CLA	MG-NA	5.95	2.20	2.06
21	A	1138	CLA	MG-NA	5.95	2.20	2.06
21	B	1216	CLA	MG-NA	5.94	2.20	2.06
21	B	1215	CLA	MG-NA	5.94	2.20	2.06
21	A	1133	CLA	MG-NA	5.94	2.20	2.06
21	6	612	CLA	MG-NA	5.94	2.20	2.06
21	B	1228	CLA	MG-NA	5.92	2.20	2.06
21	B	1219	CLA	MG-NA	5.92	2.20	2.06
21	J	1901	CLA	MG-NA	5.92	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1209	CLA	MG-NA	5.92	2.20	2.06
21	6	613	CLA	MG-NA	5.91	2.20	2.06
21	B	1231	CLA	MG-NA	5.91	2.20	2.06
21	6	605	CLA	MG-NA	5.91	2.20	2.06
21	H	1701	CLA	MG-NA	5.90	2.20	2.06
21	1	612	CLA	MG-NA	5.89	2.20	2.06
21	B	1220	CLA	MG-NA	5.88	2.20	2.06
21	B	1222	CLA	MG-NA	5.88	2.20	2.06
21	A	1119	CLA	MG-NA	5.87	2.20	2.06
21	A	1102	CLA	MG-NA	5.86	2.20	2.06
24	J	4002	BCR	C11-C12	-5.86	1.19	1.34
24	1	504	BCR	C24-C23	5.86	1.50	1.33
21	5	612	CLA	MG-ND	-5.85	1.94	2.05
24	G	4001	BCR	C24-C23	5.85	1.50	1.33
24	L	4001	BCR	C10-C9	5.84	1.43	1.35
24	3	506	BCR	C24-C23	5.83	1.50	1.33
21	B	1230	CLA	MG-NA	5.81	2.20	2.06
21	B	1221	CLA	MG-NA	5.80	2.20	2.06
24	A	4001	BCR	C24-C23	5.78	1.50	1.33
21	A	1118	CLA	MG-NA	5.78	2.20	2.06
24	H	4001	BCR	C24-C23	5.78	1.50	1.33
21	A	1125	CLA	MG-NA	5.78	2.20	2.06
24	B	4003	BCR	C11-C12	-5.77	1.19	1.34
21	A	1126	CLA	MG-NA	5.76	2.19	2.06
21	2	604	CLA	MG-NA	5.75	2.19	2.06
21	B	1205	CLA	MG-NA	5.75	2.19	2.06
24	K	4001	BCR	C24-C23	5.75	1.50	1.33
24	4	503	BCR	C24-C23	5.73	1.50	1.33
24	O	4001	BCR	C24-C23	5.71	1.50	1.33
24	J	4001	BCR	C24-C23	5.71	1.50	1.33
24	B	4006	BCR	C24-C23	5.71	1.50	1.33
24	I	4001	BCR	C24-C23	5.69	1.50	1.33
21	1	604	CLA	MG-NA	5.69	2.19	2.06
24	B	4003	BCR	C10-C9	5.69	1.43	1.35
21	B	1237	CLA	MG-NA	5.69	2.19	2.06
24	A	4004	BCR	C24-C23	5.68	1.50	1.33
21	5	612	CLA	MG-NA	5.68	2.19	2.06
24	F	4001	BCR	C24-C23	5.68	1.50	1.33
21	O	1801	CLA	MG-NA	5.67	2.19	2.06
24	B	4003	BCR	C24-C23	5.66	1.50	1.33
24	L	4002	BCR	C24-C23	5.66	1.50	1.33
21	3	601	CLA	MG-NA	5.65	2.19	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1021	CLA	MG-NA	5.64	2.19	2.06
21	A	1103	CLA	MG-NA	5.62	2.19	2.06
21	2	612	CLA	MG-NA	5.62	2.19	2.06
24	I	4002	BCR	C24-C23	5.61	1.50	1.33
21	A	1129	CLA	MG-NA	5.59	2.19	2.06
24	A	4007	BCR	C24-C23	5.58	1.49	1.33
21	L	1501	CLA	MG-NA	5.57	2.19	2.06
24	2	503	BCR	C24-C23	5.57	1.49	1.33
24	F	4002	BCR	C24-C23	5.57	1.49	1.33
24	J	4002	BCR	C24-C23	5.53	1.49	1.33
24	3	504	BCR	C24-C23	5.51	1.49	1.33
24	A	4005	BCR	C24-C23	5.49	1.49	1.33
24	A	4006	BCR	C24-C23	5.49	1.49	1.33
36	3	604	CHL	C1D-ND	-5.49	1.31	1.37
24	B	4002	BCR	C24-C23	5.47	1.49	1.33
24	B	4005	BCR	C11-C12	-5.46	1.20	1.34
24	A	4006	BCR	C11-C12	-5.46	1.20	1.34
24	L	4001	BCR	C11-C12	-5.44	1.20	1.34
24	3	503	BCR	C24-C23	5.43	1.49	1.33
24	O	4001	BCR	C11-C12	-5.42	1.20	1.34
24	A	4004	BCR	C11-C12	-5.42	1.20	1.34
24	B	4005	BCR	C24-C23	5.41	1.49	1.33
21	A	1131	CLA	MG-NA	5.40	2.19	2.06
24	A	4005	BCR	C11-C12	-5.39	1.20	1.34
24	A	4002	BCR	C24-C23	5.39	1.49	1.33
21	G	1603	CLA	MG-NA	5.39	2.19	2.06
24	A	4003	BCR	C11-C12	-5.38	1.20	1.34
21	3	613	CLA	MG-NA	5.37	2.19	2.06
24	B	4002	BCR	C11-C12	-5.36	1.20	1.34
24	B	4004	BCR	C11-C12	-5.35	1.20	1.34
24	B	4004	BCR	C24-C23	5.35	1.49	1.33
24	2	503	BCR	C11-C12	-5.34	1.20	1.34
24	J	4001	BCR	C11-C12	-5.34	1.20	1.34
24	4	503	BCR	C11-C12	-5.31	1.20	1.34
24	3	504	BCR	C11-C12	-5.31	1.20	1.34
24	3	503	BCR	C11-C12	-5.30	1.20	1.34
24	L	4002	BCR	C11-C12	-5.29	1.20	1.34
24	F	4002	BCR	C11-C12	-5.29	1.20	1.34
24	A	4002	BCR	C11-C12	-5.27	1.21	1.34
24	L	4001	BCR	C24-C23	5.20	1.48	1.33
24	B	4006	BCR	C11-C12	-5.16	1.21	1.34
21	5	614	CLA	MG-NA	5.15	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	F	4001	BCR	C11-C12	-5.13	1.21	1.34
24	I	4002	BCR	C11-C12	-5.11	1.21	1.34
20	A	1011	CL0	O2A-C1	5.11	1.60	1.46
21	5	601	CLA	MG-NA	5.10	2.18	2.06
24	I	4001	BCR	C11-C12	-5.09	1.21	1.34
24	K	4001	BCR	C11-C12	-5.08	1.21	1.34
20	A	1011	CL0	O2D-CGD	5.07	1.45	1.33
24	A	4007	BCR	C11-C12	-5.07	1.21	1.34
24	3	506	BCR	C11-C12	-5.05	1.21	1.34
24	A	4001	BCR	C11-C12	-5.03	1.21	1.34
21	J	1901	CLA	C1C-NC	-5.02	1.30	1.37
24	H	4001	BCR	C11-C12	-4.96	1.21	1.34
24	B	4001	BCR	C11-C12	-4.96	1.21	1.34
24	1	504	BCR	C11-C12	-4.88	1.22	1.34
21	5	601	CLA	MG-ND	-4.86	1.96	2.05
24	G	4001	BCR	C11-C12	-4.83	1.22	1.34
20	A	1011	CL0	CHC-C1C	4.82	1.48	1.38
21	5	601	CLA	C4B-NB	-4.80	1.31	1.37
21	A	1133	CLA	MG-ND	-4.80	1.96	2.05
20	A	1011	CL0	CHD-C1D	4.77	1.47	1.38
20	A	1011	CL0	C3C-C2C	4.70	1.46	1.36
21	H	1702	CLA	CBB-CAB	4.70	1.53	1.30
21	A	1125	CLA	C1C-NC	-4.68	1.30	1.37
21	5	601	CLA	C1C-NC	-4.67	1.30	1.37
21	B	1218	CLA	MG-ND	-4.65	1.96	2.05
21	A	1130	CLA	MG-ND	-4.63	1.96	2.05
21	3	603	CLA	MG-ND	-4.59	1.96	2.05
24	3	506	BCR	C16-C17	-4.57	1.29	1.43
24	A	4004	BCR	C16-C17	-4.57	1.29	1.43
24	B	4004	BCR	C16-C17	-4.57	1.29	1.43
36	3	604	CHL	C1B-NB	-4.56	1.32	1.37
21	A	1126	CLA	MG-ND	-4.54	1.96	2.05
21	2	601	CLA	MG-ND	-4.54	1.96	2.05
21	A	1135	CLA	MG-ND	-4.53	1.96	2.05
24	B	4005	BCR	C16-C17	-4.53	1.29	1.43
24	F	4002	BCR	C16-C17	-4.53	1.29	1.43
24	4	503	BCR	C16-C17	-4.52	1.29	1.43
21	A	1118	CLA	MG-ND	-4.51	1.96	2.05
21	J	1901	CLA	C4B-NB	-4.50	1.32	1.37
24	J	4002	BCR	C16-C17	-4.50	1.29	1.43
24	3	503	BCR	C16-C17	-4.49	1.29	1.43
21	H	1702	CLA	MG-ND	-4.48	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	4006	BCR	C16-C17	-4.48	1.29	1.43
24	A	4006	BCR	C16-C17	-4.48	1.29	1.43
21	B	1226	CLA	MG-ND	-4.48	1.96	2.05
21	A	1123	CLA	MG-ND	-4.47	1.96	2.05
24	2	503	BCR	C16-C17	-4.47	1.29	1.43
21	A	1128	CLA	MG-ND	-4.47	1.96	2.05
21	5	613	CLA	CBB-CAB	4.46	1.52	1.30
21	5	614	CLA	CBB-CAB	4.46	1.52	1.30
21	5	608	CLA	CBB-CAB	4.46	1.52	1.30
24	L	4001	BCR	C16-C17	-4.46	1.29	1.43
21	6	609	CLA	CBB-CAB	4.44	1.52	1.30
21	5	607	CLA	CBB-CAB	4.43	1.52	1.30
24	A	4005	BCR	C16-C17	-4.43	1.29	1.43
21	H	1701	CLA	CBB-CAB	4.42	1.52	1.30
24	B	4003	BCR	C16-C17	-4.41	1.29	1.43
24	3	504	BCR	C16-C17	-4.41	1.29	1.43
24	A	4003	BCR	C16-C17	-4.40	1.29	1.43
21	G	1603	CLA	MG-ND	-4.40	1.97	2.05
21	L	1504	CLA	CBB-CAB	4.40	1.52	1.30
21	A	1013	CLA	MG-ND	-4.40	1.97	2.05
21	L	1501	CLA	CBB-CAB	4.39	1.52	1.30
21	3	611	CLA	MG-ND	-4.38	1.97	2.05
24	A	4007	BCR	C16-C17	-4.38	1.29	1.43
21	O	1803	CLA	MG-ND	-4.38	1.97	2.05
21	1	615	CLA	CBB-CAB	4.37	1.51	1.30
28	2	806	DGD	O1G-C1A	4.36	1.46	1.33
21	A	1127	CLA	MG-ND	-4.36	1.97	2.05
21	3	601	CLA	C1C-NC	-4.36	1.31	1.37
24	B	4002	BCR	C16-C17	-4.36	1.29	1.43
20	A	1011	CL0	C3D-C4D	-4.36	1.34	1.44
21	2	608	CLA	CBB-CAB	4.34	1.51	1.30
21	K	1403	CLA	CBB-CAB	4.34	1.51	1.30
21	6	605	CLA	CBB-CAB	4.33	1.51	1.30
21	A	1131	CLA	C1C-NC	-4.33	1.31	1.37
21	6	613	CLA	CBB-CAB	4.33	1.51	1.30
21	5	603	CLA	CBB-CAB	4.33	1.51	1.30
36	3	604	CHL	CBB-CAB	4.33	1.51	1.30
21	H	1701	CLA	C1C-NC	-4.33	1.31	1.37
21	5	613	CLA	MG-ND	-4.33	1.97	2.05
24	H	4001	BCR	C16-C17	-4.32	1.30	1.43
21	4	607	CLA	MG-ND	-4.31	1.97	2.05
21	J	1901	CLA	MG-ND	-4.31	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	O	1803	CLA	CBB-CAB	4.31	1.51	1.30
21	A	1105	CLA	MG-ND	-4.31	1.97	2.05
21	A	1117	CLA	CBB-CAB	4.31	1.51	1.30
21	B	1230	CLA	C1C-NC	-4.31	1.31	1.37
21	3	603	CLA	CBB-CAB	4.31	1.51	1.30
21	L	1502	CLA	MG-ND	-4.30	1.97	2.05
21	1	606	CLA	CBB-CAB	4.30	1.51	1.30
21	3	613	CLA	CBB-CAB	4.30	1.51	1.30
24	L	4002	BCR	C16-C17	-4.30	1.30	1.43
21	A	1136	CLA	CBB-CAB	4.30	1.51	1.30
24	F	4001	BCR	C16-C17	-4.30	1.30	1.43
21	A	1113	CLA	MG-ND	-4.30	1.97	2.05
21	B	1229	CLA	CBB-CAB	4.29	1.51	1.30
21	5	612	CLA	CBB-CAB	4.29	1.51	1.30
21	L	1503	CLA	CBB-CAB	4.29	1.51	1.30
21	G	1603	CLA	CBB-CAB	4.29	1.51	1.30
21	B	1223	CLA	MG-ND	-4.28	1.97	2.05
21	B	1211	CLA	CBB-CAB	4.28	1.51	1.30
28	3	805	DGD	O1G-C1A	4.28	1.45	1.33
21	3	607	CLA	CBB-CAB	4.28	1.51	1.30
21	A	1119	CLA	C1C-NC	-4.28	1.31	1.37
21	K	1402	CLA	CBB-CAB	4.28	1.51	1.30
21	B	1206	CLA	CBB-CAB	4.28	1.51	1.30
21	B	1221	CLA	CBB-CAB	4.28	1.51	1.30
24	B	4001	BCR	C16-C17	-4.28	1.30	1.43
21	1	602	CLA	CBB-CAB	4.28	1.51	1.30
21	F	1302	CLA	CBB-CAB	4.28	1.51	1.30
21	B	1212	CLA	CBB-CAB	4.27	1.51	1.30
21	O	1801	CLA	CBB-CAB	4.27	1.51	1.30
21	B	1226	CLA	CBB-CAB	4.27	1.51	1.30
21	4	612	CLA	CBB-CAB	4.27	1.51	1.30
21	A	1120	CLA	CBB-CAB	4.27	1.51	1.30
21	B	1232	CLA	CBB-CAB	4.27	1.51	1.30
21	1	611	CLA	CBB-CAB	4.27	1.51	1.30
21	2	606	CLA	CBB-CAB	4.27	1.51	1.30
21	A	1106	CLA	CBB-CAB	4.27	1.51	1.30
21	1	603	CLA	CBB-CAB	4.27	1.51	1.30
21	1	601	CLA	CBB-CAB	4.27	1.51	1.30
21	B	1239	CLA	CBB-CAB	4.27	1.51	1.30
21	K	1404	CLA	CBB-CAB	4.26	1.51	1.30
21	A	1103	CLA	CBB-CAB	4.26	1.51	1.30
21	G	1602	CLA	CBB-CAB	4.26	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1115	CLA	CBB-CAB	4.26	1.51	1.30
21	B	1217	CLA	MG-ND	-4.26	1.97	2.05
21	6	602	CLA	CBB-CAB	4.26	1.51	1.30
21	3	615	CLA	CBB-CAB	4.26	1.51	1.30
21	B	1222	CLA	CBB-CAB	4.26	1.51	1.30
21	6	603	CLA	CBB-CAB	4.26	1.51	1.30
21	A	1119	CLA	MG-ND	-4.26	1.97	2.05
21	5	602	CLA	MG-ND	-4.26	1.97	2.05
21	B	1231	CLA	CBB-CAB	4.26	1.51	1.30
21	3	610	CLA	CBB-CAB	4.26	1.51	1.30
21	A	1129	CLA	CBB-CAB	4.26	1.51	1.30
21	5	604	CLA	CBB-CAB	4.26	1.51	1.30
21	6	608	CLA	CBB-CAB	4.26	1.51	1.30
21	6	601	CLA	CBB-CAB	4.26	1.51	1.30
21	B	1240	CLA	CBB-CAB	4.26	1.51	1.30
21	5	606	CLA	CBB-CAB	4.26	1.51	1.30
21	B	1219	CLA	MG-ND	-4.26	1.97	2.05
21	3	602	CLA	CBB-CAB	4.26	1.51	1.30
21	A	1135	CLA	CBB-CAB	4.25	1.51	1.30
21	4	615	CLA	CBB-CAB	4.25	1.51	1.30
21	1	607	CLA	CBB-CAB	4.25	1.51	1.30
21	B	1225	CLA	CBB-CAB	4.25	1.51	1.30
21	3	603	CLA	C1C-NC	-4.25	1.31	1.37
21	B	1023	CLA	CBB-CAB	4.25	1.51	1.30
21	A	1012	CLA	CBB-CAB	4.25	1.51	1.30
21	2	601	CLA	CBB-CAB	4.25	1.51	1.30
21	A	1137	CLA	CBB-CAB	4.25	1.51	1.30
21	B	1228	CLA	CBB-CAB	4.25	1.51	1.30
21	3	611	CLA	CBB-CAB	4.25	1.51	1.30
21	6	604	CLA	CBB-CAB	4.25	1.51	1.30
21	6	607	CLA	CBB-CAB	4.25	1.51	1.30
21	B	1021	CLA	MG-ND	-4.25	1.97	2.05
21	A	1114	CLA	CBB-CAB	4.25	1.51	1.30
21	4	603	CLA	CBB-CAB	4.25	1.51	1.30
21	B	1214	CLA	MG-ND	-4.25	1.97	2.05
21	5	602	CLA	CBB-CAB	4.25	1.51	1.30
36	6	610	CHL	CBB-CAB	4.25	1.51	1.30
21	B	1208	CLA	CBB-CAB	4.25	1.51	1.30
21	A	1141	CLA	CBB-CAB	4.24	1.51	1.30
21	G	1601	CLA	CBB-CAB	4.24	1.51	1.30
21	1	613	CLA	CBB-CAB	4.24	1.51	1.30
21	A	1134	CLA	CBB-CAB	4.24	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1106	CLA	MG-ND	-4.24	1.97	2.05
21	B	1203	CLA	CBB-CAB	4.24	1.51	1.30
21	3	606	CLA	CBB-CAB	4.24	1.51	1.30
21	A	1105	CLA	CBB-CAB	4.24	1.51	1.30
21	A	1132	CLA	CBB-CAB	4.24	1.51	1.30
21	B	1207	CLA	CBB-CAB	4.24	1.51	1.30
24	J	4001	BCR	C16-C17	-4.24	1.30	1.43
21	B	1235	CLA	CBB-CAB	4.24	1.51	1.30
21	B	1217	CLA	CBB-CAB	4.24	1.51	1.30
21	A	1112	CLA	CBB-CAB	4.24	1.51	1.30
21	A	1109	CLA	CBB-CAB	4.24	1.51	1.30
21	A	1107	CLA	CBB-CAB	4.24	1.51	1.30
21	4	604	CLA	CBB-CAB	4.24	1.51	1.30
21	5	605	CLA	CBB-CAB	4.24	1.51	1.30
21	4	606	CLA	CBB-CAB	4.24	1.51	1.30
21	A	1127	CLA	CBB-CAB	4.23	1.51	1.30
21	B	1225	CLA	MG-ND	-4.23	1.97	2.05
21	B	1022	CLA	CBB-CAB	4.23	1.51	1.30
21	2	615	CLA	CBB-CAB	4.23	1.51	1.30
21	6	606	CLA	CBB-CAB	4.23	1.51	1.30
21	A	1124	CLA	CBB-CAB	4.23	1.51	1.30
21	A	1104	CLA	MG-ND	-4.23	1.97	2.05
21	B	1205	CLA	MG-ND	-4.23	1.97	2.05
21	A	1128	CLA	C1C-NC	-4.23	1.31	1.37
28	B	5002	DGD	O1G-C1A	4.23	1.45	1.33
21	B	1223	CLA	CBB-CAB	4.23	1.51	1.30
21	A	1130	CLA	CBB-CAB	4.23	1.51	1.30
36	5	609	CHL	CBB-CAB	4.23	1.51	1.30
21	B	1232	CLA	MG-ND	-4.23	1.97	2.05
24	I	4001	BCR	C16-C17	-4.23	1.30	1.43
21	A	1128	CLA	CBB-CAB	4.22	1.51	1.30
21	A	1120	CLA	MG-ND	-4.22	1.97	2.05
21	B	1021	CLA	CBB-CAB	4.22	1.51	1.30
21	B	1209	CLA	CBB-CAB	4.22	1.51	1.30
21	2	607	CLA	CBB-CAB	4.22	1.51	1.30
28	3	804	DGD	O1G-C1A	4.22	1.45	1.33
21	B	1204	CLA	CBB-CAB	4.22	1.51	1.30
21	2	612	CLA	CBB-CAB	4.22	1.51	1.30
21	3	612	CLA	CBB-CAB	4.22	1.51	1.30
21	2	602	CLA	CBB-CAB	4.22	1.51	1.30
24	G	4001	BCR	C16-C17	-4.22	1.30	1.43
21	4	602	CLA	CBB-CAB	4.22	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	608	CLA	CBB-CAB	4.22	1.51	1.30
21	A	1138	CLA	CBB-CAB	4.22	1.51	1.30
21	4	607	CLA	CBB-CAB	4.22	1.51	1.30
24	I	4002	BCR	C16-C17	-4.22	1.30	1.43
21	4	608	CLA	CBB-CAB	4.22	1.51	1.30
21	A	1124	CLA	MG-ND	-4.22	1.97	2.05
21	A	1125	CLA	MG-ND	-4.22	1.97	2.05
21	A	1121	CLA	CBB-CAB	4.22	1.51	1.30
21	2	604	CLA	MG-ND	-4.21	1.97	2.05
21	A	1116	CLA	CBB-CAB	4.21	1.51	1.30
21	B	1224	CLA	CBB-CAB	4.21	1.51	1.30
24	A	4002	BCR	C16-C17	-4.21	1.30	1.43
21	3	608	CLA	CBB-CAB	4.21	1.51	1.30
21	B	1221	CLA	MG-ND	-4.21	1.97	2.05
21	5	608	CLA	C1C-NC	-4.21	1.31	1.37
21	B	1211	CLA	MG-ND	-4.21	1.97	2.05
21	A	1126	CLA	CBB-CAB	4.21	1.51	1.30
21	B	1228	CLA	MG-ND	-4.20	1.97	2.05
21	B	1237	CLA	CBB-CAB	4.20	1.51	1.30
24	K	4001	BCR	C16-C17	-4.20	1.30	1.43
21	B	1234	CLA	CBB-CAB	4.20	1.51	1.30
21	4	602	CLA	MG-ND	-4.20	1.97	2.05
21	A	1122	CLA	CBB-CAB	4.20	1.51	1.30
21	A	1123	CLA	CBB-CAB	4.20	1.51	1.30
21	1	607	CLA	MG-ND	-4.19	1.97	2.05
21	6	612	CLA	MG-ND	-4.19	1.97	2.05
21	A	1133	CLA	CBB-CAB	4.18	1.51	1.30
21	3	601	CLA	CBB-CAB	4.18	1.51	1.30
38	4	805	LMK	O2-C4	4.18	1.44	1.30
21	A	1101	CLA	CBB-CAB	4.18	1.51	1.30
21	B	1238	CLA	CBB-CAB	4.18	1.51	1.30
21	A	1138	CLA	MG-ND	-4.17	1.97	2.05
21	1	612	CLA	MG-ND	-4.17	1.97	2.05
21	1	605	CLA	CBB-CAB	4.17	1.51	1.30
36	1	609	CHL	CBB-CAB	4.17	1.51	1.30
21	B	1237	CLA	MG-ND	-4.17	1.97	2.05
21	A	1102	CLA	MG-ND	-4.17	1.97	2.05
21	B	1219	CLA	CBB-CAB	4.17	1.51	1.30
21	4	601	CLA	CBB-CAB	4.17	1.51	1.30
21	2	602	CLA	MG-ND	-4.17	1.97	2.05
21	B	1220	CLA	CBB-CAB	4.17	1.50	1.30
21	4	609	CLA	CBB-CAB	4.17	1.50	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1227	CLA	CBB-CAB	4.16	1.50	1.30
21	B	1210	CLA	CBB-CAB	4.16	1.50	1.30
21	A	1111	CLA	C1C-NC	-4.16	1.31	1.37
21	B	1220	CLA	MG-ND	-4.16	1.97	2.05
21	B	1218	CLA	CBB-CAB	4.16	1.50	1.30
21	A	1110	CLA	CBB-CAB	4.16	1.50	1.30
21	A	1131	CLA	CBB-CAB	4.16	1.50	1.30
21	A	1118	CLA	CBB-CAB	4.16	1.50	1.30
21	4	605	CLA	CBB-CAB	4.16	1.50	1.30
21	1	612	CLA	CBB-CAB	4.15	1.50	1.30
21	B	1205	CLA	CBB-CAB	4.15	1.50	1.30
21	2	604	CLA	CBB-CAB	4.15	1.50	1.30
21	A	1140	CLA	CBB-CAB	4.15	1.50	1.30
21	A	1119	CLA	CBB-CAB	4.15	1.50	1.30
21	B	1216	CLA	CBB-CAB	4.15	1.50	1.30
21	B	1230	CLA	CBB-CAB	4.15	1.50	1.30
21	A	1013	CLA	CBB-CAB	4.14	1.50	1.30
21	H	1702	CLA	C1C-NC	-4.14	1.31	1.37
36	4	610	CHL	CBB-CAB	4.14	1.50	1.30
21	3	605	CLA	CBB-CAB	4.14	1.50	1.30
21	K	1401	CLA	CBB-CAB	4.14	1.50	1.30
21	3	614	CLA	CBB-CAB	4.14	1.50	1.30
21	J	1901	CLA	CBB-CAB	4.13	1.50	1.30
21	B	1213	CLA	CBB-CAB	4.13	1.50	1.30
21	B	1222	CLA	MG-ND	-4.13	1.97	2.05
21	B	1201	CLA	CBB-CAB	4.13	1.50	1.30
21	A	1113	CLA	CBB-CAB	4.13	1.50	1.30
21	F	1301	CLA	CBB-CAB	4.12	1.50	1.30
21	A	1108	CLA	MG-ND	-4.12	1.97	2.05
38	2	807	LMK	O2-C4	4.12	1.44	1.30
20	A	1011	CL0	CHD-C4C	4.12	1.48	1.39
21	F	1302	CLA	MG-ND	-4.12	1.97	2.05
21	4	615	CLA	MG-ND	-4.12	1.97	2.05
21	5	607	CLA	C1C-NC	-4.11	1.31	1.37
21	2	607	CLA	MG-ND	-4.11	1.97	2.05
21	3	612	CLA	MG-ND	-4.11	1.97	2.05
21	1	606	CLA	MG-ND	-4.11	1.97	2.05
21	2	615	CLA	MG-ND	-4.11	1.97	2.05
21	A	1108	CLA	CBB-CAB	4.10	1.50	1.30
21	A	1125	CLA	CBB-CAB	4.10	1.50	1.30
24	A	4001	BCR	C16-C17	-4.10	1.30	1.43
21	2	612	CLA	MG-ND	-4.10	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1104	CLA	CBB-CAB	4.09	1.50	1.30
21	2	605	CLA	CBB-CAB	4.09	1.50	1.30
36	2	611	CHL	CBB-CAB	4.09	1.50	1.30
21	A	1139	CLA	MG-ND	-4.09	1.97	2.05
21	5	614	CLA	C1C-NC	-4.09	1.31	1.37
21	B	1215	CLA	CBB-CAB	4.09	1.50	1.30
21	A	1140	CLA	MG-ND	-4.08	1.97	2.05
21	B	1213	CLA	MG-ND	-4.08	1.97	2.05
21	B	1236	CLA	CBB-CAB	4.08	1.50	1.30
36	2	610	CHL	CBB-CAB	4.07	1.50	1.30
24	O	4001	BCR	C16-C17	-4.07	1.30	1.43
21	B	1209	CLA	MG-ND	-4.07	1.97	2.05
21	A	1139	CLA	CBB-CAB	4.07	1.50	1.30
21	3	605	CLA	C1C-NC	-4.07	1.31	1.37
21	B	1231	CLA	MG-ND	-4.07	1.97	2.05
24	1	504	BCR	C16-C17	-4.06	1.30	1.43
21	3	608	CLA	MG-ND	-4.06	1.97	2.05
21	L	1502	CLA	C4B-NB	-4.06	1.32	1.37
21	B	1238	CLA	MG-ND	-4.06	1.97	2.05
21	1	604	CLA	CBB-CAB	4.06	1.50	1.30
21	6	607	CLA	MG-ND	-4.05	1.97	2.05
36	1	610	CHL	CBB-CAB	4.05	1.50	1.30
21	F	1301	CLA	MG-ND	-4.05	1.97	2.05
21	B	1215	CLA	MG-ND	-4.05	1.97	2.05
21	B	1214	CLA	CBB-CAB	4.04	1.50	1.30
21	A	1102	CLA	CBB-CAB	4.04	1.50	1.30
21	B	1224	CLA	MG-ND	-4.04	1.97	2.05
20	A	1011	CL0	CHB-C1B	4.04	1.48	1.39
21	1	604	CLA	MG-ND	-4.04	1.97	2.05
21	B	1236	CLA	MG-ND	-4.04	1.97	2.05
21	1	613	CLA	MG-ND	-4.03	1.97	2.05
21	B	1210	CLA	MG-ND	-4.03	1.97	2.05
36	2	610	CHL	C1B-NB	-4.03	1.32	1.37
21	1	602	CLA	MG-ND	-4.03	1.97	2.05
21	A	1111	CLA	CBB-CAB	4.03	1.50	1.30
21	6	609	CLA	MG-ND	-4.02	1.97	2.05
36	5	610	CHL	CBB-CAB	4.02	1.50	1.30
21	4	605	CLA	MG-ND	-4.02	1.97	2.05
21	6	612	CLA	CBB-CAB	4.02	1.50	1.30
21	B	1204	CLA	MG-ND	-4.02	1.97	2.05
21	B	1203	CLA	MG-ND	-4.01	1.97	2.05
21	4	608	CLA	MG-ND	-4.01	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1141	CLA	MG-ND	-4.01	1.97	2.05
21	5	601	CLA	CBB-CAB	4.01	1.50	1.30
21	B	1202	CLA	MG-ND	-4.01	1.97	2.05
21	5	607	CLA	MG-ND	-4.01	1.97	2.05
21	B	1230	CLA	MG-ND	-4.01	1.97	2.05
21	A	1111	CLA	C4B-NB	-4.00	1.32	1.37
21	A	1109	CLA	MG-ND	-4.00	1.97	2.05
20	A	1011	CL0	CHC-C4B	4.00	1.48	1.39
21	1	608	CLA	MG-ND	-4.00	1.97	2.05
21	3	606	CLA	MG-ND	-4.00	1.97	2.05
21	2	603	CLA	CBB-CAB	3.99	1.50	1.30
21	K	1401	CLA	MG-ND	-3.99	1.97	2.05
21	A	1137	CLA	MG-ND	-3.99	1.97	2.05
21	4	612	CLA	MG-ND	-3.99	1.97	2.05
21	4	601	CLA	MG-ND	-3.97	1.97	2.05
21	5	603	CLA	MG-ND	-3.97	1.97	2.05
21	A	1136	CLA	MG-ND	-3.97	1.97	2.05
36	2	613	CHL	CBB-CAB	3.97	1.50	1.30
21	O	1802	CLA	MG-ND	-3.97	1.97	2.05
21	4	603	CLA	MG-ND	-3.97	1.97	2.05
21	B	1216	CLA	MG-ND	-3.96	1.97	2.05
21	A	1129	CLA	MG-ND	-3.95	1.98	2.05
21	B	1210	CLA	C1C-NC	-3.95	1.31	1.37
21	2	606	CLA	MG-ND	-3.95	1.98	2.05
21	B	1240	CLA	MG-ND	-3.95	1.98	2.05
21	2	603	CLA	MG-ND	-3.94	1.98	2.05
21	K	1401	CLA	C4B-NB	-3.94	1.32	1.37
21	6	605	CLA	MG-ND	-3.93	1.98	2.05
21	6	604	CLA	MG-ND	-3.93	1.98	2.05
21	3	613	CLA	MG-ND	-3.93	1.98	2.05
21	3	601	CLA	MG-ND	-3.92	1.98	2.05
21	B	1021	CLA	C1C-NC	-3.92	1.31	1.37
21	B	1201	CLA	MG-ND	-3.92	1.98	2.05
21	B	1227	CLA	MG-ND	-3.92	1.98	2.05
21	A	1105	CLA	C1C-NC	-3.92	1.32	1.37
21	A	1101	CLA	MG-ND	-3.92	1.98	2.05
21	1	615	CLA	MG-ND	-3.92	1.98	2.05
21	B	1234	CLA	MG-ND	-3.91	1.98	2.05
21	L	1502	CLA	CBB-CAB	3.91	1.49	1.30
21	3	615	CLA	MG-ND	-3.91	1.98	2.05
21	B	1215	CLA	C1C-NC	-3.91	1.32	1.37
21	B	1202	CLA	CBB-CAB	3.90	1.49	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1229	CLA	MG-ND	-3.89	1.98	2.05
21	3	613	CLA	C1C-NC	-3.89	1.32	1.37
21	4	601	CLA	C1C-NC	-3.89	1.32	1.37
21	A	1122	CLA	MG-ND	-3.89	1.98	2.05
21	2	608	CLA	MG-ND	-3.88	1.98	2.05
21	B	1220	CLA	C1C-NC	-3.88	1.32	1.37
21	3	605	CLA	MG-ND	-3.88	1.98	2.05
21	A	1111	CLA	MG-ND	-3.88	1.98	2.05
21	1	603	CLA	MG-ND	-3.87	1.98	2.05
21	A	1131	CLA	MG-ND	-3.87	1.98	2.05
21	2	605	CLA	MG-ND	-3.87	1.98	2.05
21	4	606	CLA	MG-ND	-3.87	1.98	2.05
21	A	1110	CLA	MG-ND	-3.86	1.98	2.05
21	3	602	CLA	MG-ND	-3.86	1.98	2.05
21	3	607	CLA	MG-ND	-3.86	1.98	2.05
21	5	608	CLA	MG-ND	-3.86	1.98	2.05
21	B	1210	CLA	C4B-NB	-3.85	1.33	1.37
36	4	613	CHL	CBB-CAB	3.85	1.49	1.30
36	2	609	CHL	CBB-CAB	3.85	1.49	1.30
21	3	614	CLA	MG-ND	-3.84	1.98	2.05
21	B	1211	CLA	C1C-NC	-3.84	1.32	1.37
21	B	1205	CLA	C1C-NC	-3.83	1.32	1.37
21	5	612	CLA	C1C-NC	-3.83	1.32	1.37
21	A	1139	CLA	C1C-NC	-3.82	1.32	1.37
21	L	1503	CLA	MG-ND	-3.81	1.98	2.05
21	A	1133	CLA	C1C-NC	-3.80	1.32	1.37
21	B	1234	CLA	C1C-NC	-3.79	1.32	1.37
21	B	1216	CLA	C1C-NC	-3.79	1.32	1.37
39	2	808	P3H	O39-C40	3.79	1.45	1.34
21	A	1130	CLA	C1C-NC	-3.78	1.32	1.37
21	A	1139	CLA	C4B-NB	-3.77	1.33	1.37
21	1	605	CLA	MG-ND	-3.77	1.98	2.05
21	A	1117	CLA	MG-ND	-3.76	1.98	2.05
21	6	612	CLA	C4B-NB	-3.76	1.33	1.37
21	O	1802	CLA	C1C-NC	-3.75	1.32	1.37
21	6	613	CLA	MG-ND	-3.75	1.98	2.05
21	1	615	CLA	C1C-NC	-3.75	1.32	1.37
21	F	1301	CLA	C1C-NC	-3.75	1.32	1.37
21	4	609	CLA	C1C-NC	-3.75	1.32	1.37
21	2	601	CLA	C1C-NC	-3.74	1.32	1.37
21	B	1238	CLA	C1C-NC	-3.74	1.32	1.37
21	O	1801	CLA	MG-ND	-3.73	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	604	CLA	C4B-NB	-3.72	1.33	1.37
21	A	1106	CLA	C1C-NC	-3.70	1.32	1.37
21	A	1103	CLA	MG-ND	-3.70	1.98	2.05
21	5	612	CLA	C4B-NB	-3.70	1.33	1.37
39	5	806	P3H	O39-C40	3.70	1.44	1.34
21	2	612	CLA	C1C-NC	-3.70	1.32	1.37
21	A	1109	CLA	C1C-NC	-3.69	1.32	1.37
21	A	1125	CLA	C4B-NB	-3.69	1.33	1.37
20	A	1011	CL0	OBD-CAD	3.69	1.28	1.22
21	K	1401	CLA	C1C-NC	-3.69	1.32	1.37
21	B	1228	CLA	C1C-NC	-3.68	1.32	1.37
21	B	1237	CLA	C1C-NC	-3.67	1.32	1.37
21	B	1215	CLA	C4B-NB	-3.67	1.33	1.37
21	A	1105	CLA	C4B-NB	-3.67	1.33	1.37
21	B	1229	CLA	C1C-NC	-3.67	1.32	1.37
21	A	1129	CLA	C1C-NC	-3.66	1.32	1.37
21	4	609	CLA	MG-ND	-3.66	1.98	2.05
21	2	608	CLA	C1C-NC	-3.65	1.32	1.37
21	2	605	CLA	C1C-NC	-3.65	1.32	1.37
21	B	1209	CLA	C1C-NC	-3.65	1.32	1.37
21	3	612	CLA	C1C-NC	-3.65	1.32	1.37
21	A	1110	CLA	C1C-NC	-3.64	1.32	1.37
21	L	1502	CLA	C1C-NC	-3.64	1.32	1.37
21	B	1223	CLA	C1C-NC	-3.63	1.32	1.37
21	B	1226	CLA	C1C-NC	-3.63	1.32	1.37
21	6	612	CLA	C1C-NC	-3.63	1.32	1.37
21	B	1204	CLA	C1C-NC	-3.62	1.32	1.37
21	B	1218	CLA	C1C-NC	-3.62	1.32	1.37
21	A	1126	CLA	C1C-NC	-3.61	1.32	1.37
21	1	612	CLA	C1C-NC	-3.61	1.32	1.37
21	5	602	CLA	C1C-NC	-3.61	1.32	1.37
21	4	601	CLA	C4B-NB	-3.60	1.33	1.37
21	B	1225	CLA	C1C-NC	-3.60	1.32	1.37
21	2	606	CLA	C1C-NC	-3.60	1.32	1.37
21	A	1013	CLA	C1C-NC	-3.60	1.32	1.37
21	A	1122	CLA	C1C-NC	-3.60	1.32	1.37
21	4	608	CLA	C1C-NC	-3.59	1.32	1.37
21	B	1219	CLA	C1C-NC	-3.59	1.32	1.37
21	A	1129	CLA	C4B-NB	-3.59	1.33	1.37
21	B	1222	CLA	C1C-NC	-3.58	1.32	1.37
21	A	1115	CLA	MG-ND	-3.58	1.98	2.05
21	1	604	CLA	C1C-NC	-3.58	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1231	CLA	C1C-NC	-3.58	1.32	1.37
21	4	606	CLA	C1C-NC	-3.58	1.32	1.37
21	A	1140	CLA	C1C-NC	-3.57	1.32	1.37
21	B	1236	CLA	C1C-NC	-3.57	1.32	1.37
21	A	1124	CLA	C1C-NC	-3.57	1.32	1.37
21	A	1120	CLA	C1C-NC	-3.56	1.32	1.37
21	A	1127	CLA	C1C-NC	-3.56	1.32	1.37
21	A	1103	CLA	C1C-NC	-3.56	1.32	1.37
21	B	1240	CLA	C1C-NC	-3.56	1.32	1.37
21	K	1403	CLA	MG-ND	-3.55	1.98	2.05
21	4	607	CLA	C1C-NC	-3.55	1.32	1.37
21	A	1137	CLA	C1C-NC	-3.55	1.32	1.37
21	B	1224	CLA	C1C-NC	-3.54	1.32	1.37
21	A	1101	CLA	C1C-NC	-3.53	1.32	1.37
21	A	1108	CLA	C1C-NC	-3.53	1.32	1.37
21	4	612	CLA	C1C-NC	-3.53	1.32	1.37
21	F	1302	CLA	C1C-NC	-3.53	1.32	1.37
21	B	1022	CLA	MG-ND	-3.52	1.98	2.05
21	L	1501	CLA	C1C-NC	-3.52	1.32	1.37
21	B	1238	CLA	C4B-NB	-3.52	1.33	1.37
21	5	604	CLA	MG-ND	-3.51	1.98	2.05
21	6	606	CLA	MG-ND	-3.51	1.98	2.05
21	1	607	CLA	C1C-NC	-3.51	1.32	1.37
21	A	1116	CLA	MG-ND	-3.51	1.98	2.05
21	A	1130	CLA	C4B-NB	-3.51	1.33	1.37
21	B	1213	CLA	C1C-NC	-3.51	1.32	1.37
21	A	1013	CLA	C4B-NB	-3.50	1.33	1.37
21	A	1138	CLA	C1C-NC	-3.50	1.32	1.37
21	B	1227	CLA	C1C-NC	-3.50	1.32	1.37
21	A	1012	CLA	MG-ND	-3.50	1.98	2.05
21	A	1102	CLA	C1C-NC	-3.50	1.32	1.37
21	A	1113	CLA	C1C-NC	-3.50	1.32	1.37
21	B	1023	CLA	MG-ND	-3.50	1.98	2.05
21	B	1221	CLA	C1C-NC	-3.50	1.32	1.37
21	A	1112	CLA	MG-ND	-3.50	1.98	2.05
21	2	603	CLA	C1C-NC	-3.49	1.32	1.37
21	B	1217	CLA	C1C-NC	-3.49	1.32	1.37
21	A	1106	CLA	C4B-NB	-3.49	1.33	1.37
21	A	1114	CLA	MG-ND	-3.49	1.98	2.05
21	A	1123	CLA	C1C-NC	-3.49	1.32	1.37
21	1	608	CLA	C1C-NC	-3.49	1.32	1.37
21	3	607	CLA	C1C-NC	-3.49	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1222	CLA	C4B-NB	-3.49	1.33	1.37
21	6	608	CLA	MG-ND	-3.48	1.98	2.05
21	4	602	CLA	C1C-NC	-3.48	1.32	1.37
21	A	1107	CLA	MG-ND	-3.48	1.98	2.05
21	B	1232	CLA	C1C-NC	-3.48	1.32	1.37
21	2	604	CLA	C1C-NC	-3.47	1.32	1.37
21	A	1126	CLA	C4B-NB	-3.47	1.33	1.37
21	6	602	CLA	MG-ND	-3.47	1.98	2.05
21	4	604	CLA	MG-ND	-3.46	1.98	2.05
21	B	1235	CLA	MG-ND	-3.46	1.98	2.05
21	B	1208	CLA	MG-ND	-3.46	1.98	2.05
21	1	605	CLA	C1C-NC	-3.46	1.32	1.37
21	2	612	CLA	C4B-NB	-3.46	1.33	1.37
21	4	605	CLA	C1C-NC	-3.46	1.32	1.37
21	A	1132	CLA	MG-ND	-3.46	1.98	2.05
21	B	1230	CLA	C4B-NB	-3.46	1.33	1.37
21	B	1236	CLA	C4B-NB	-3.45	1.33	1.37
21	A	1131	CLA	C4B-NB	-3.45	1.33	1.37
21	B	1202	CLA	C1C-NC	-3.45	1.32	1.37
21	B	1214	CLA	C1C-NC	-3.45	1.32	1.37
21	O	1803	CLA	C1C-NC	-3.45	1.32	1.37
21	5	605	CLA	MG-ND	-3.45	1.99	2.05
21	A	1118	CLA	C1C-NC	-3.45	1.32	1.37
21	5	603	CLA	C1C-NC	-3.44	1.32	1.37
21	5	606	CLA	MG-ND	-3.44	1.99	2.05
21	6	604	CLA	C4B-NB	-3.44	1.33	1.37
21	A	1134	CLA	MG-ND	-3.44	1.99	2.05
21	1	601	CLA	MG-ND	-3.43	1.99	2.05
36	4	611	CHL	CBB-CAB	3.43	1.47	1.30
21	6	603	CLA	MG-ND	-3.43	1.99	2.05
21	B	1239	CLA	MG-ND	-3.43	1.99	2.05
21	B	1218	CLA	C4B-NB	-3.43	1.33	1.37
21	6	601	CLA	MG-ND	-3.43	1.99	2.05
21	A	1121	CLA	MG-ND	-3.43	1.99	2.05
21	1	611	CLA	MG-ND	-3.43	1.99	2.05
21	3	601	CLA	C4B-NB	-3.43	1.33	1.37
21	6	605	CLA	C1C-NC	-3.43	1.32	1.37
21	3	610	CLA	MG-ND	-3.43	1.99	2.05
20	A	1011	CL0	MG-NC	3.42	2.14	2.06
21	3	602	CLA	C1C-NC	-3.42	1.32	1.37
21	5	602	CLA	C4B-NB	-3.42	1.33	1.37
21	G	1601	CLA	MG-ND	-3.41	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1135	CLA	C1C-NC	-3.41	1.32	1.37
21	B	1212	CLA	MG-ND	-3.41	1.99	2.05
21	B	1203	CLA	C1C-NC	-3.41	1.32	1.37
21	B	1207	CLA	MG-ND	-3.40	1.99	2.05
21	A	1119	CLA	C4B-NB	-3.40	1.33	1.37
21	A	1141	CLA	C1C-NC	-3.40	1.32	1.37
21	3	605	CLA	C4B-NB	-3.40	1.33	1.37
21	A	1104	CLA	C1C-NC	-3.40	1.32	1.37
21	2	615	CLA	C1C-NC	-3.39	1.32	1.37
21	B	1237	CLA	C4B-NB	-3.39	1.33	1.37
21	L	1503	CLA	C1C-NC	-3.39	1.32	1.37
21	1	602	CLA	C1C-NC	-3.39	1.32	1.37
21	K	1402	CLA	MG-ND	-3.39	1.99	2.05
21	B	1223	CLA	C4B-NB	-3.39	1.33	1.37
21	B	1229	CLA	C4B-NB	-3.38	1.33	1.37
21	G	1602	CLA	MG-ND	-3.38	1.99	2.05
21	6	604	CLA	C1C-NC	-3.38	1.32	1.37
21	3	606	CLA	C1C-NC	-3.37	1.32	1.37
21	A	1136	CLA	C1C-NC	-3.37	1.32	1.37
21	B	1206	CLA	MG-ND	-3.37	1.99	2.05
21	B	1205	CLA	C4B-NB	-3.37	1.33	1.37
21	K	1404	CLA	MG-ND	-3.37	1.99	2.05
21	4	615	CLA	C1C-NC	-3.36	1.32	1.37
21	3	611	CLA	C1C-NC	-3.36	1.32	1.37
21	F	1301	CLA	C4B-NB	-3.36	1.33	1.37
21	B	1211	CLA	C4B-NB	-3.35	1.33	1.37
21	A	1117	CLA	C1C-NC	-3.35	1.32	1.37
21	1	613	CLA	C1C-NC	-3.35	1.32	1.37
21	6	609	CLA	C1C-NC	-3.35	1.32	1.37
21	A	1104	CLA	C4B-NB	-3.34	1.33	1.37
21	2	607	CLA	C1C-NC	-3.34	1.32	1.37
21	B	1201	CLA	C1C-NC	-3.34	1.32	1.37
21	A	1102	CLA	C4B-NB	-3.34	1.33	1.37
21	3	615	CLA	C1C-NC	-3.33	1.32	1.37
21	B	1225	CLA	C4B-NB	-3.33	1.33	1.37
21	3	606	CLA	C4B-NB	-3.33	1.33	1.37
31	3	803	LMG	C37-C36	-3.32	1.32	1.51
21	6	607	CLA	C1C-NC	-3.32	1.32	1.37
21	A	1123	CLA	C4B-NB	-3.32	1.33	1.37
21	B	1234	CLA	C4B-NB	-3.32	1.33	1.37
21	1	612	CLA	C4B-NB	-3.31	1.33	1.37
36	1	610	CHL	C1B-NB	-3.31	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	5002	DGD	CDB-CCB	-3.31	1.33	1.51
21	B	1213	CLA	C4B-NB	-3.31	1.33	1.37
21	A	1127	CLA	C4B-NB	-3.30	1.33	1.37
21	2	601	CLA	C4B-NB	-3.30	1.33	1.37
28	B	5002	DGD	CAB-C9B	-3.29	1.33	1.51
21	B	1224	CLA	C4B-NB	-3.29	1.33	1.37
21	B	1021	CLA	C4B-NB	-3.28	1.33	1.37
28	B	5002	DGD	CGB-CFB	-3.28	1.33	1.51
31	F	5002	LMG	C19-C18	-3.28	1.33	1.51
21	K	1403	CLA	C1C-NC	-3.28	1.32	1.37
31	2	804	LMG	C19-C18	-3.27	1.33	1.51
21	1	606	CLA	C1C-NC	-3.27	1.32	1.37
36	2	611	CHL	C1B-NB	-3.26	1.33	1.37
31	4	803	LMG	C37-C36	-3.26	1.33	1.51
21	B	1220	CLA	C4B-NB	-3.26	1.33	1.37
21	2	605	CLA	C4B-NB	-3.26	1.33	1.37
21	A	1108	CLA	C4B-NB	-3.25	1.33	1.37
21	L	1504	CLA	MG-ND	-3.25	1.99	2.05
21	2	602	CLA	C1C-NC	-3.25	1.33	1.37
28	B	5002	DGD	CAA-C9A	-3.24	1.33	1.51
21	A	1117	CLA	C4B-NB	-3.24	1.33	1.37
21	5	614	CLA	MG-ND	-3.24	1.99	2.05
21	A	1137	CLA	C4B-NB	-3.24	1.33	1.37
21	4	603	CLA	C1C-NC	-3.24	1.33	1.37
21	1	603	CLA	C1C-NC	-3.23	1.33	1.37
31	2	804	LMG	C37-C36	-3.22	1.33	1.51
21	B	1204	CLA	C4B-NB	-3.21	1.33	1.37
21	B	1216	CLA	C4B-NB	-3.21	1.33	1.37
21	H	1702	CLA	C1B-NB	-3.21	1.33	1.37
20	A	1011	CL0	C1D-ND	-3.21	1.33	1.37
31	4	802	LMG	C25-C24	-3.21	1.33	1.51
21	6	606	CLA	C1C-NC	-3.20	1.33	1.37
31	3	803	LMG	C19-C18	-3.20	1.33	1.51
31	3	803	LMG	C25-C24	-3.20	1.33	1.51
21	4	612	CLA	C4B-NB	-3.19	1.33	1.37
21	B	1203	CLA	C4B-NB	-3.19	1.33	1.37
31	3	803	LMG	C22-C21	-3.19	1.33	1.51
21	A	1112	CLA	C1C-NC	-3.19	1.33	1.37
21	A	1133	CLA	C4B-NB	-3.19	1.33	1.37
21	5	603	CLA	C4B-NB	-3.19	1.33	1.37
31	4	802	LMG	C22-C21	-3.18	1.33	1.51
21	A	1141	CLA	C4B-NB	-3.18	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	613	CLA	C4B-NB	-3.18	1.33	1.37
21	A	1138	CLA	C4B-NB	-3.18	1.33	1.37
31	F	5002	LMG	C40-C39	-3.18	1.33	1.51
21	L	1504	CLA	C1C-NC	-3.18	1.33	1.37
31	4	802	LMG	C19-C18	-3.18	1.33	1.51
21	B	1232	CLA	C4B-NB	-3.17	1.33	1.37
21	4	606	CLA	C4B-NB	-3.17	1.33	1.37
36	2	613	CHL	C1B-NB	-3.17	1.33	1.37
21	B	1239	CLA	C1C-NC	-3.17	1.33	1.37
31	2	804	LMG	C43-C42	-3.17	1.33	1.51
21	B	1023	CLA	C1C-NC	-3.17	1.33	1.37
21	F	1302	CLA	C4B-NB	-3.16	1.33	1.37
21	L	1501	CLA	MG-ND	-3.16	1.99	2.05
21	3	603	CLA	C4B-NB	-3.16	1.33	1.37
21	A	1115	CLA	C1C-NC	-3.16	1.33	1.37
21	B	1226	CLA	C4B-NB	-3.16	1.33	1.37
31	2	804	LMG	C40-C39	-3.16	1.33	1.51
21	A	1124	CLA	C4B-NB	-3.15	1.33	1.37
35	6	502	XAT	O24-C25	-3.15	1.41	1.46
21	6	605	CLA	C4B-NB	-3.15	1.33	1.37
21	2	608	CLA	C4B-NB	-3.14	1.33	1.37
21	5	606	CLA	C1C-NC	-3.14	1.33	1.37
21	A	1107	CLA	C1C-NC	-3.14	1.33	1.37
21	B	1208	CLA	C1C-NC	-3.14	1.33	1.37
21	A	1128	CLA	C4B-NB	-3.13	1.33	1.37
21	2	604	CLA	C4B-NB	-3.13	1.33	1.37
21	3	608	CLA	C1C-NC	-3.12	1.33	1.37
21	1	601	CLA	C1C-NC	-3.12	1.33	1.37
21	A	1120	CLA	C4B-NB	-3.12	1.33	1.37
21	H	1702	CLA	C4B-NB	-3.12	1.33	1.37
31	F	5002	LMG	C43-C42	-3.12	1.34	1.51
21	4	608	CLA	C4B-NB	-3.12	1.34	1.37
21	B	1235	CLA	C1C-NC	-3.12	1.33	1.37
21	4	604	CLA	C1C-NC	-3.12	1.33	1.37
21	A	1132	CLA	C1C-NC	-3.11	1.33	1.37
21	3	611	CLA	C4B-NB	-3.11	1.34	1.37
21	6	613	CLA	C1C-NC	-3.11	1.33	1.37
21	1	605	CLA	C4B-NB	-3.11	1.34	1.37
21	1	611	CLA	C1C-NC	-3.10	1.33	1.37
31	F	5002	LMG	C37-C36	-3.10	1.34	1.51
21	B	1221	CLA	C4B-NB	-3.10	1.34	1.37
21	A	1135	CLA	C4B-NB	-3.10	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1101	CLA	C4B-NB	-3.09	1.34	1.37
21	A	1107	CLA	C4B-NB	-3.09	1.34	1.37
21	5	604	CLA	C1C-NC	-3.09	1.33	1.37
21	A	1114	CLA	C1C-NC	-3.08	1.33	1.37
21	A	1116	CLA	C1C-NC	-3.08	1.33	1.37
21	K	1402	CLA	C1C-NC	-3.08	1.33	1.37
21	B	1212	CLA	C1C-NC	-3.08	1.33	1.37
21	4	603	CLA	C4B-NB	-3.07	1.34	1.37
39	5	806	P3H	O19-C17	3.07	1.42	1.33
21	3	610	CLA	C1C-NC	-3.07	1.33	1.37
21	1	608	CLA	C4B-NB	-3.07	1.34	1.37
21	6	608	CLA	C1C-NC	-3.06	1.33	1.37
21	B	1240	CLA	C4B-NB	-3.06	1.34	1.37
21	1	613	CLA	C4B-NB	-3.06	1.34	1.37
21	A	1103	CLA	C4B-NB	-3.06	1.34	1.37
21	A	1134	CLA	C1C-NC	-3.06	1.33	1.37
21	6	603	CLA	C1C-NC	-3.06	1.33	1.37
32	5	805	4RF	O40-C41	3.06	1.42	1.33
21	B	1207	CLA	C1C-NC	-3.06	1.33	1.37
21	A	1012	CLA	C1C-NC	-3.05	1.33	1.37
21	6	602	CLA	C1C-NC	-3.05	1.33	1.37
21	A	1122	CLA	C4B-NB	-3.05	1.34	1.37
21	B	1022	CLA	C1C-NC	-3.04	1.33	1.37
20	A	1011	CL0	C3D-C2D	3.04	1.47	1.39
21	6	601	CLA	C1C-NC	-3.04	1.33	1.37
21	A	1109	CLA	C4B-NB	-3.04	1.34	1.37
21	A	1132	CLA	C4B-NB	-3.04	1.34	1.37
21	B	1228	CLA	C4B-NB	-3.03	1.34	1.37
21	3	613	CLA	C4B-NB	-3.03	1.34	1.37
21	4	602	CLA	C4B-NB	-3.03	1.34	1.37
21	G	1601	CLA	C1C-NC	-3.03	1.33	1.37
21	G	1602	CLA	C1C-NC	-3.03	1.33	1.37
21	O	1801	CLA	C1C-NC	-3.03	1.33	1.37
21	G	1603	CLA	C4B-NB	-3.03	1.34	1.37
21	B	1201	CLA	C4B-NB	-3.02	1.34	1.37
21	5	605	CLA	C1C-NC	-3.02	1.33	1.37
36	1	610	CHL	C3A-C2A	-3.02	1.46	1.54
39	2	808	P3H	O19-C17	3.02	1.42	1.33
21	B	1209	CLA	C4B-NB	-3.02	1.34	1.37
21	B	1206	CLA	C1C-NC	-3.02	1.33	1.37
21	4	615	CLA	C4B-NB	-3.01	1.34	1.37
21	6	606	CLA	C4B-NB	-3.01	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	O	1802	CLA	C4B-NB	-3.01	1.34	1.37
21	5	613	CLA	C1C-NC	-3.01	1.33	1.37
21	A	1121	CLA	C1C-NC	-3.00	1.33	1.37
21	5	608	CLA	C4B-NB	-3.00	1.34	1.37
21	L	1504	CLA	C4B-NB	-3.00	1.34	1.37
21	B	1214	CLA	C4B-NB	-3.00	1.34	1.37
21	3	610	CLA	C4B-NB	-3.00	1.34	1.37
34	1	501	LUT	C22-C21	-2.99	1.51	1.54
21	3	602	CLA	C4B-NB	-2.99	1.34	1.37
21	4	604	CLA	C4B-NB	-2.99	1.34	1.37
36	1	609	CHL	C1B-NB	-2.98	1.34	1.37
21	K	1404	CLA	C1C-NC	-2.98	1.33	1.37
21	B	1207	CLA	C4B-NB	-2.98	1.34	1.37
21	3	612	CLA	C4B-NB	-2.98	1.34	1.37
21	A	1112	CLA	C4B-NB	-2.97	1.34	1.37
21	5	606	CLA	C4B-NB	-2.97	1.34	1.37
21	B	1023	CLA	C4B-NB	-2.97	1.34	1.37
21	A	1114	CLA	C4B-NB	-2.97	1.34	1.37
21	2	607	CLA	C4B-NB	-2.97	1.34	1.37
21	O	1803	CLA	C4B-NB	-2.96	1.34	1.37
21	1	606	CLA	C4B-NB	-2.96	1.34	1.37
21	A	1012	CLA	C4B-NB	-2.96	1.34	1.37
21	A	1116	CLA	C4B-NB	-2.96	1.34	1.37
21	1	602	CLA	C4B-NB	-2.96	1.34	1.37
21	A	1140	CLA	C4B-NB	-2.96	1.34	1.37
21	3	615	CLA	C4B-NB	-2.95	1.34	1.37
21	A	1115	CLA	C4B-NB	-2.95	1.34	1.37
21	B	1022	CLA	C4B-NB	-2.95	1.34	1.37
21	5	604	CLA	C4B-NB	-2.95	1.34	1.37
21	A	1113	CLA	C4B-NB	-2.94	1.34	1.37
21	A	1134	CLA	C4B-NB	-2.94	1.34	1.37
21	B	1235	CLA	C4B-NB	-2.94	1.34	1.37
21	L	1503	CLA	C4B-NB	-2.94	1.34	1.37
21	4	607	CLA	C4B-NB	-2.93	1.34	1.37
35	2	502	XAT	O24-C25	-2.93	1.42	1.46
21	5	601	CLA	C3D-C4D	-2.93	1.37	1.44
21	1	601	CLA	C4B-NB	-2.92	1.34	1.37
21	4	605	CLA	C4B-NB	-2.92	1.34	1.37
21	K	1404	CLA	C4B-NB	-2.91	1.34	1.37
21	2	603	CLA	C4B-NB	-2.91	1.34	1.37
21	3	614	CLA	C4B-NB	-2.91	1.34	1.37
21	5	605	CLA	C4B-NB	-2.91	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1212	CLA	C4B-NB	-2.91	1.34	1.37
21	A	1136	CLA	C4B-NB	-2.90	1.34	1.37
21	H	1701	CLA	C4-C3	-2.90	1.43	1.50
21	K	1402	CLA	C4B-NB	-2.90	1.34	1.37
36	2	609	CHL	C1B-NB	-2.89	1.34	1.37
21	G	1603	CLA	C1C-NC	-2.89	1.33	1.37
21	2	602	CLA	C4B-NB	-2.89	1.34	1.37
21	2	615	CLA	C4B-NB	-2.88	1.34	1.37
39	2	808	P3H	C55-C54	-2.88	1.35	1.51
21	6	607	CLA	C4B-NB	-2.88	1.34	1.37
21	B	1239	CLA	C4B-NB	-2.87	1.34	1.37
21	1	611	CLA	C4B-NB	-2.87	1.34	1.37
21	3	607	CLA	C4B-NB	-2.87	1.34	1.37
21	B	1206	CLA	C4B-NB	-2.86	1.34	1.37
21	3	608	CLA	C4B-NB	-2.86	1.34	1.37
21	4	609	CLA	C4B-NB	-2.86	1.34	1.37
21	A	1121	CLA	C4B-NB	-2.86	1.34	1.37
21	6	608	CLA	C4B-NB	-2.86	1.34	1.37
21	1	607	CLA	C4B-NB	-2.86	1.34	1.37
36	2	613	CHL	C3B-C2B	-2.86	1.31	1.41
21	1	615	CLA	C4B-NB	-2.86	1.34	1.37
21	B	1227	CLA	C4B-NB	-2.85	1.34	1.37
21	G	1601	CLA	C4B-NB	-2.85	1.34	1.37
21	A	1133	CLA	C1D-ND	-2.85	1.34	1.37
21	H	1701	CLA	MG-ND	-2.85	2.00	2.05
21	B	1208	CLA	C4B-NB	-2.84	1.34	1.37
21	6	609	CLA	C4B-NB	-2.84	1.34	1.37
21	1	603	CLA	C4B-NB	-2.84	1.34	1.37
21	6	602	CLA	C4B-NB	-2.84	1.34	1.37
21	6	603	CLA	C4B-NB	-2.83	1.34	1.37
20	A	1011	CL0	C1B-C2B	2.82	1.49	1.43
21	O	1801	CLA	CAC-C3C	-2.82	1.44	1.50
21	3	614	CLA	C1C-NC	-2.82	1.33	1.37
21	2	606	CLA	C4B-NB	-2.82	1.34	1.37
21	6	601	CLA	C4B-NB	-2.82	1.34	1.37
21	B	1231	CLA	C4B-NB	-2.81	1.34	1.37
21	G	1602	CLA	C4B-NB	-2.81	1.34	1.37
21	A	1110	CLA	C4B-NB	-2.79	1.34	1.37
21	5	607	CLA	C4B-NB	-2.79	1.34	1.37
21	K	1403	CLA	C4B-NB	-2.78	1.34	1.37
21	H	1701	CLA	C4B-NB	-2.77	1.34	1.37
21	L	1501	CLA	C4B-NB	-2.77	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	612	CLA	C3D-C4D	-2.77	1.37	1.44
21	5	601	CLA	CMA-C3A	-2.76	1.47	1.53
39	2	808	P3H	P24-O27	2.74	1.67	1.60
20	A	1011	CL0	C1B-NB	-2.74	1.34	1.37
20	A	1011	CL0	C4D-CHA	2.73	1.48	1.38
21	B	1219	CLA	C4B-NB	-2.73	1.34	1.37
35	1	502	XAT	O24-C25	-2.71	1.42	1.46
21	A	1118	CLA	C3D-C4D	-2.70	1.38	1.44
21	A	1118	CLA	C4B-NB	-2.68	1.34	1.37
24	L	4002	BCR	C35-C13	-2.68	1.45	1.50
21	B	1202	CLA	C4B-NB	-2.68	1.34	1.37
24	J	4002	BCR	C12-C13	-2.67	1.40	1.45
21	5	601	CLA	C1B-NB	-2.67	1.34	1.37
21	A	1104	CLA	C3D-C4D	-2.66	1.38	1.44
21	O	1801	CLA	C4B-NB	-2.66	1.34	1.37
21	A	1135	CLA	C3D-C4D	-2.66	1.38	1.44
33	1	806	PTY	O7-C6	-2.66	1.39	1.46
21	5	612	CLA	C1D-ND	-2.65	1.34	1.37
21	5	612	CLA	OBD-CAD	-2.65	1.17	1.22
21	5	614	CLA	C4B-NB	-2.62	1.34	1.37
21	5	613	CLA	C4B-NB	-2.60	1.34	1.37
36	4	611	CHL	C1B-NB	-2.60	1.34	1.37
35	6	504	XAT	C24-C23	-2.60	1.48	1.52
36	3	604	CHL	C3A-C2A	-2.59	1.47	1.54
24	B	4003	BCR	C12-C13	-2.59	1.40	1.45
36	2	610	CHL	C1C-NC	-2.58	1.33	1.37
21	B	1226	CLA	C3D-C4D	-2.58	1.38	1.44
33	3	807	PTY	O7-C6	-2.58	1.40	1.46
39	5	806	P3H	P24-O27	2.58	1.67	1.60
39	2	808	P3H	C52-C51	-2.57	1.37	1.51
36	2	611	CHL	C1C-NC	-2.57	1.34	1.37
20	A	1011	CL0	C1C-NC	-2.57	1.34	1.37
31	3	802	LMG	C19-C18	-2.57	1.33	1.51
32	L	5002	4RF	O18-C16	2.56	1.40	1.33
29	5	807	3PH	O21-C21	2.56	1.41	1.34
21	A	1118	CLA	C3A-C2A	-2.56	1.47	1.54
29	5	807	3PH	O31-C31	2.55	1.40	1.33
24	B	4006	BCR	C40-C30	-2.55	1.48	1.53
21	B	1217	CLA	C4B-NB	-2.54	1.34	1.37
20	A	1011	CL0	C4B-NB	-2.54	1.34	1.37
21	3	608	CLA	C1C-C2C	2.53	1.49	1.44
36	4	613	CHL	C1B-NB	-2.53	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1118	CLA	C1B-NB	-2.52	1.34	1.37
21	1	604	CLA	CMA-C3A	-2.51	1.47	1.53
21	3	603	CLA	C3D-C4D	-2.50	1.38	1.44
33	O	5002	PTY	O7-C6	-2.49	1.40	1.46
20	A	1011	CL0	C1D-C2D	2.49	1.50	1.45
33	3	807	PTY	O4-C30	2.49	1.40	1.33
33	5	803	PTY	O7-C6	-2.49	1.40	1.46
21	O	1803	CLA	OBD-CAD	-2.49	1.18	1.22
21	3	611	CLA	C3D-C4D	-2.49	1.38	1.44
33	L	5003	PTY	O4-C30	2.47	1.40	1.33
32	5	805	4RF	O18-C19	-2.47	1.39	1.45
33	L	5003	PTY	O7-C6	-2.47	1.40	1.46
33	3	808	PTY	O4-C30	2.47	1.40	1.33
33	3	808	PTY	O7-C6	-2.46	1.40	1.46
33	1	805	PTY	O7-C6	-2.45	1.40	1.46
39	2	808	P3H	C16-C17	2.45	1.57	1.50
36	5	610	CHL	C1B-NB	-2.45	1.34	1.37
35	4	502	XAT	O24-C25	-2.44	1.42	1.46
33	1	805	PTY	O4-C30	2.44	1.40	1.33
29	B	5003	3PH	O21-C2	-2.44	1.40	1.46
32	L	5002	4RF	O40-C41	2.43	1.40	1.33
29	F	5003	3PH	O21-C2	-2.43	1.40	1.46
29	5	804	3PH	O31-C31	2.42	1.40	1.33
29	5	804	3PH	O21-C2	-2.42	1.40	1.46
20	A	1011	CL0	C3B-C4B	2.42	1.48	1.42
33	5	803	PTY	O4-C30	2.42	1.40	1.33
33	O	5002	PTY	O4-C30	2.41	1.40	1.33
33	4	804	PTY	O7-C6	-2.41	1.40	1.46
21	B	1232	CLA	C1A-CHA	2.40	1.53	1.43
21	A	1129	CLA	C3D-C4D	-2.40	1.38	1.44
21	B	1211	CLA	C3D-C4D	-2.40	1.38	1.44
32	L	5002	4RF	O21-C20	-2.40	1.40	1.46
21	B	1231	CLA	C3D-C4D	-2.40	1.38	1.44
33	4	804	PTY	O4-C30	2.39	1.40	1.33
21	A	1109	CLA	C3D-C4D	-2.39	1.38	1.44
33	6	804	PTY	O7-C8	2.39	1.41	1.34
36	4	610	CHL	C1B-NB	-2.39	1.34	1.37
21	K	1401	CLA	C3D-C4D	-2.39	1.38	1.44
21	4	609	CLA	C1A-CHA	2.39	1.53	1.43
36	2	610	CHL	C3A-C2A	-2.39	1.47	1.54
29	F	5003	3PH	O31-C31	2.38	1.40	1.33
21	A	1131	CLA	C3D-C4D	-2.38	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	603	CLA	C1C-C2C	2.38	1.49	1.44
33	L	5003	PTY	O7-C8	2.37	1.40	1.35
21	2	601	CLA	C3D-C4D	-2.37	1.38	1.44
21	A	1113	CLA	C3D-C4D	-2.37	1.38	1.44
21	3	606	CLA	C1A-CHA	2.37	1.52	1.43
21	3	607	CLA	C1A-CHA	2.36	1.52	1.43
21	5	614	CLA	C1A-CHA	2.36	1.52	1.43
39	5	806	P3H	C16-C17	2.36	1.57	1.50
21	B	1222	CLA	C3D-C4D	-2.36	1.38	1.44
21	B	1237	CLA	C3D-C4D	-2.35	1.38	1.44
29	B	5003	3PH	O31-C31	2.35	1.40	1.33
21	1	604	CLA	C3D-C4D	-2.35	1.38	1.44
39	2	808	P3H	P24-O23	2.34	1.68	1.59
21	A	1101	CLA	C1C-C2C	2.33	1.49	1.44
32	5	805	4RF	O21-C22	2.33	1.40	1.34
39	5	806	P3H	P24-O23	2.32	1.68	1.59
39	2	808	P3H	C42-C40	2.32	1.57	1.50
21	A	1122	CLA	C1A-CHA	2.32	1.52	1.43
36	3	604	CHL	C1C-NC	-2.31	1.34	1.37
21	6	609	CLA	C1A-CHA	2.31	1.52	1.43
21	4	605	CLA	C3D-C4D	-2.31	1.39	1.44
39	5	806	P3H	C42-C40	2.31	1.57	1.50
36	3	604	CHL	C3D-C2D	-2.30	1.32	1.39
21	A	1139	CLA	C1A-CHA	2.30	1.52	1.43
33	O	5002	PTY	O7-C8	2.30	1.40	1.35
32	5	805	4RF	O21-C20	-2.30	1.40	1.46
21	A	1124	CLA	C1A-CHA	2.30	1.52	1.43
21	L	1502	CLA	C1C-C2C	2.30	1.49	1.44
21	B	1214	CLA	C3D-C4D	-2.29	1.39	1.44
33	3	808	PTY	O7-C8	2.29	1.40	1.35
24	J	4002	BCR	C33-C5	-2.29	1.47	1.50
21	A	1127	CLA	C1A-CHA	2.29	1.52	1.43
21	2	604	CLA	C3D-C4D	-2.29	1.39	1.44
21	4	615	CLA	C1A-CHA	2.29	1.52	1.43
21	A	1119	CLA	C3D-C4D	-2.28	1.39	1.44
21	A	1138	CLA	C1A-CHA	2.28	1.52	1.43
35	3	502	XAT	O24-C25	-2.28	1.42	1.46
21	1	603	CLA	C1A-CHA	2.28	1.52	1.43
32	L	5002	4RF	O21-C22	2.28	1.40	1.34
21	2	603	CLA	C1A-CHA	2.28	1.52	1.43
24	A	4004	BCR	C12-C13	-2.28	1.41	1.45
21	3	614	CLA	C1A-CHA	2.28	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1013	CLA	C1A-CHA	2.28	1.52	1.43
29	B	5003	3PH	O21-C21	2.27	1.40	1.34
21	B	1021	CLA	C3D-C4D	-2.27	1.39	1.44
21	1	604	CLA	C1C-C2C	2.27	1.49	1.44
21	6	604	CLA	C1C-C2C	2.27	1.49	1.44
33	4	804	PTY	O7-C8	2.27	1.40	1.34
21	B	1213	CLA	C1C-C2C	2.27	1.49	1.44
21	3	615	CLA	C1A-CHA	2.26	1.52	1.43
21	1	607	CLA	C1A-CHA	2.26	1.52	1.43
21	A	1123	CLA	C1A-CHA	2.26	1.52	1.43
21	B	1215	CLA	C1A-CHA	2.26	1.52	1.43
21	A	1127	CLA	C3D-C4D	-2.26	1.39	1.44
21	A	1128	CLA	C3D-C4D	-2.26	1.39	1.44
21	A	1111	CLA	C3D-C4D	-2.26	1.39	1.44
21	L	1501	CLA	C1A-CHA	2.26	1.52	1.43
21	A	1137	CLA	C1A-CHA	2.26	1.52	1.43
21	5	601	CLA	C2A-C1A	-2.26	1.47	1.52
21	L	1502	CLA	C1A-CHA	2.25	1.52	1.43
21	A	1105	CLA	C3D-C4D	-2.25	1.39	1.44
21	B	1238	CLA	C3D-C4D	-2.25	1.39	1.44
21	B	1225	CLA	C1A-CHA	2.25	1.52	1.43
21	3	605	CLA	C1A-CHA	2.25	1.52	1.43
21	4	603	CLA	C1A-CHA	2.25	1.52	1.43
21	B	1201	CLA	C1A-CHA	2.25	1.52	1.43
21	B	1240	CLA	C1A-CHA	2.25	1.52	1.43
21	A	1140	CLA	C3D-C4D	-2.24	1.39	1.44
21	B	1224	CLA	C1A-CHA	2.24	1.52	1.43
21	3	602	CLA	C1A-CHA	2.24	1.52	1.43
21	1	613	CLA	C1A-CHA	2.24	1.52	1.43
21	5	608	CLA	C1A-CHA	2.24	1.52	1.43
21	5	603	CLA	C1A-CHA	2.24	1.52	1.43
21	B	1218	CLA	C1D-ND	-2.24	1.35	1.37
32	5	805	4RF	O18-C16	2.24	1.39	1.33
21	B	1219	CLA	C1A-CHA	2.24	1.52	1.43
36	3	604	CHL	C3D-C4D	-2.24	1.39	1.44
21	2	602	CLA	C1A-CHA	2.24	1.52	1.43
21	A	1105	CLA	C1A-CHA	2.24	1.52	1.43
21	O	1803	CLA	C1C-C2C	2.24	1.48	1.44
21	A	1123	CLA	C3D-C4D	-2.23	1.39	1.44
21	5	614	CLA	C1D-ND	-2.23	1.35	1.37
21	1	615	CLA	C1A-CHA	2.23	1.52	1.43
21	A	1120	CLA	C3D-C4D	-2.23	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	602	CLA	C1A-CHA	2.23	1.52	1.43
21	B	1230	CLA	C1A-CHA	2.23	1.52	1.43
21	A	1103	CLA	C3D-C4D	-2.23	1.39	1.44
21	B	1221	CLA	C3D-C4D	-2.22	1.39	1.44
21	B	1217	CLA	C3D-C4D	-2.22	1.39	1.44
21	G	1602	CLA	C1C-C2C	2.22	1.48	1.44
21	1	602	CLA	C1A-CHA	2.22	1.52	1.43
21	B	1218	CLA	C3D-C4D	-2.22	1.39	1.44
21	A	1128	CLA	C1A-CHA	2.22	1.52	1.43
21	K	1404	CLA	C1C-C2C	2.21	1.48	1.44
21	B	1209	CLA	C3D-C4D	-2.21	1.39	1.44
21	A	1108	CLA	C3D-C4D	-2.21	1.39	1.44
21	4	601	CLA	C1A-CHA	2.21	1.52	1.43
21	B	1229	CLA	C1A-CHA	2.21	1.52	1.43
21	J	1901	CLA	C1A-CHA	2.21	1.52	1.43
21	6	605	CLA	C3D-C4D	-2.21	1.39	1.44
21	A	1125	CLA	C3D-C4D	-2.21	1.39	1.44
21	H	1701	CLA	C1A-CHA	2.21	1.52	1.43
21	4	612	CLA	C1A-CHA	2.21	1.52	1.43
21	A	1125	CLA	C1A-CHA	2.21	1.52	1.43
21	A	1102	CLA	C1A-CHA	2.21	1.52	1.43
21	B	1214	CLA	C1A-CHA	2.21	1.52	1.43
21	A	1141	CLA	C3D-C4D	-2.20	1.39	1.44
21	A	1133	CLA	C1A-CHA	2.20	1.52	1.43
21	4	608	CLA	C1A-CHA	2.20	1.52	1.43
21	6	601	CLA	C1C-C2C	2.20	1.48	1.44
21	A	1102	CLA	C3D-C4D	-2.20	1.39	1.44
21	5	607	CLA	C1A-CHA	2.20	1.52	1.43
36	4	611	CHL	C1D-ND	-2.20	1.35	1.37
21	5	606	CLA	C1C-C2C	2.20	1.48	1.44
21	2	607	CLA	C1A-CHA	2.20	1.52	1.43
21	A	1126	CLA	C1A-CHA	2.20	1.52	1.43
21	B	1234	CLA	C3D-C4D	-2.20	1.39	1.44
21	3	612	CLA	C1A-CHA	2.19	1.52	1.43
21	B	1228	CLA	C1A-CHA	2.19	1.52	1.43
29	5	804	3PH	O21-C21	2.19	1.40	1.34
21	5	613	CLA	C3D-C4D	-2.19	1.39	1.44
29	F	5003	3PH	O21-C21	2.19	1.40	1.34
21	A	1121	CLA	C1C-C2C	2.19	1.48	1.44
21	L	1501	CLA	C1C-C2C	2.19	1.48	1.44
21	3	605	CLA	C3D-C4D	-2.19	1.39	1.44
21	2	604	CLA	CMA-C3A	-2.19	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1227	CLA	C3D-C4D	-2.19	1.39	1.44
21	B	1216	CLA	C3D-C4D	-2.19	1.39	1.44
21	B	1205	CLA	C3D-C4D	-2.19	1.39	1.44
21	B	1204	CLA	C1A-CHA	2.19	1.52	1.43
21	4	601	CLA	C3D-C4D	-2.19	1.39	1.44
21	4	603	CLA	C1C-C2C	2.19	1.48	1.44
33	1	805	PTY	O7-C8	2.18	1.40	1.34
21	4	605	CLA	C1A-CHA	2.18	1.52	1.43
21	A	1136	CLA	C1A-CHA	2.18	1.52	1.43
21	6	607	CLA	C1A-CHA	2.18	1.52	1.43
21	A	1117	CLA	C1A-CHA	2.18	1.52	1.43
21	B	1234	CLA	C1A-CHA	2.18	1.52	1.43
21	A	1109	CLA	C1A-CHA	2.18	1.52	1.43
21	1	615	CLA	C1C-C2C	2.18	1.48	1.44
21	A	1138	CLA	C3D-C4D	-2.18	1.39	1.44
21	6	602	CLA	C1C-C2C	2.18	1.48	1.44
21	A	1130	CLA	C3D-C4D	-2.17	1.39	1.44
21	5	602	CLA	C1A-CHA	2.17	1.52	1.43
21	4	607	CLA	C1A-CHA	2.17	1.52	1.43
21	B	1221	CLA	C1A-CHA	2.17	1.52	1.43
21	B	1229	CLA	C1C-C2C	2.17	1.48	1.44
33	3	807	PTY	O7-C8	2.17	1.40	1.34
21	F	1302	CLA	C1A-CHA	2.17	1.52	1.43
21	A	1106	CLA	C3D-C4D	-2.17	1.39	1.44
21	K	1402	CLA	C1C-C2C	2.17	1.48	1.44
21	B	1220	CLA	C1A-CHA	2.17	1.52	1.43
21	B	1210	CLA	C3D-C4D	-2.17	1.39	1.44
21	3	612	CLA	C3D-C4D	-2.17	1.39	1.44
21	2	615	CLA	C1A-CHA	2.17	1.52	1.43
21	O	1801	CLA	C3D-C4D	-2.17	1.39	1.44
21	B	1236	CLA	C3D-C4D	-2.17	1.39	1.44
21	5	612	CLA	C1D-C2D	-2.17	1.41	1.45
21	6	605	CLA	C1A-CHA	2.17	1.52	1.43
21	A	1118	CLA	C1D-ND	-2.17	1.35	1.37
21	2	605	CLA	C3D-C4D	-2.17	1.39	1.44
21	6	608	CLA	C1C-C2C	2.16	1.48	1.44
21	B	1202	CLA	C1A-CHA	2.16	1.52	1.43
21	A	1116	CLA	C1C-C2C	2.16	1.48	1.44
33	L	5003	PTY	O4-C1	-2.16	1.40	1.45
21	A	1126	CLA	C3D-C4D	-2.16	1.39	1.44
21	A	1111	CLA	C1A-CHA	2.16	1.52	1.43
21	G	1601	CLA	C1C-C2C	2.16	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	605	CLA	C3D-C4D	-2.16	1.39	1.44
21	6	603	CLA	C1C-C2C	2.16	1.48	1.44
21	A	1115	CLA	C1C-C2C	2.15	1.48	1.44
21	2	604	CLA	C1C-C2C	2.15	1.48	1.44
21	B	1224	CLA	C3D-C4D	-2.15	1.39	1.44
21	B	1205	CLA	C1A-CHA	2.15	1.52	1.43
36	4	611	CHL	C3B-C2B	-2.15	1.33	1.41
21	B	1203	CLA	C3D-C4D	-2.15	1.39	1.44
21	1	612	CLA	C1A-CHA	2.15	1.52	1.43
21	B	1216	CLA	C1A-CHA	2.15	1.52	1.43
21	6	613	CLA	C3D-C4D	-2.15	1.39	1.44
25	3	801	LHG	O7-C7	-2.15	1.34	1.42
21	B	1203	CLA	C1A-CHA	2.15	1.52	1.43
21	3	603	CLA	C1A-CHA	2.15	1.52	1.43
21	B	1215	CLA	C3D-C4D	-2.15	1.39	1.44
21	3	608	CLA	C1A-CHA	2.15	1.52	1.43
21	A	1012	CLA	C1C-C2C	2.15	1.48	1.44
21	2	601	CLA	C1A-CHA	2.15	1.52	1.43
21	B	1239	CLA	C1C-C2C	2.14	1.48	1.44
33	1	806	PTY	O7-C8	2.14	1.40	1.35
21	B	1238	CLA	C1A-CHA	2.14	1.52	1.43
21	B	1223	CLA	C3D-C4D	-2.14	1.39	1.44
21	A	1141	CLA	C1A-CHA	2.14	1.52	1.43
21	B	1217	CLA	C3B-C4B	2.14	1.47	1.42
21	H	1702	CLA	C3B-C4B	2.14	1.47	1.42
21	2	615	CLA	C3D-C4D	-2.14	1.39	1.44
21	A	1106	CLA	C1A-CHA	2.14	1.52	1.43
21	A	1140	CLA	C1A-CHA	2.14	1.52	1.43
21	B	1202	CLA	C3D-C4D	-2.14	1.39	1.44
21	B	1210	CLA	C1A-CHA	2.14	1.52	1.43
21	B	1218	CLA	C1A-CHA	2.14	1.52	1.43
21	B	1232	CLA	C3D-C4D	-2.14	1.39	1.44
32	L	5002	4RF	O40-C39	-2.13	1.40	1.45
21	A	1122	CLA	C3D-C4D	-2.13	1.39	1.44
21	1	607	CLA	C3D-C4D	-2.13	1.39	1.44
21	B	1021	CLA	C1A-CHA	2.13	1.52	1.43
21	B	1209	CLA	C1A-CHA	2.13	1.51	1.43
21	B	1223	CLA	C1A-CHA	2.13	1.51	1.43
21	B	1217	CLA	C1A-CHA	2.13	1.51	1.43
21	4	606	CLA	C3D-C4D	-2.13	1.39	1.44
21	B	1208	CLA	C1C-C2C	2.13	1.48	1.44
21	5	604	CLA	C1C-C2C	2.13	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	611	CLA	C1C-C2C	2.13	1.48	1.44
21	A	1108	CLA	C1A-CHA	2.13	1.51	1.43
24	L	4001	BCR	C12-C13	-2.13	1.41	1.45
21	O	1802	CLA	C1A-CHA	2.13	1.51	1.43
21	F	1301	CLA	C1A-CHA	2.12	1.51	1.43
21	2	608	CLA	C3D-C4D	-2.12	1.39	1.44
21	F	1302	CLA	C3D-C4D	-2.12	1.39	1.44
21	B	1207	CLA	C1C-C2C	2.12	1.48	1.44
21	B	1235	CLA	C1C-C2C	2.12	1.48	1.44
29	5	807	3PH	O21-C2	-2.12	1.41	1.46
21	5	605	CLA	C1C-C2C	2.12	1.48	1.44
21	1	608	CLA	C1A-CHA	2.12	1.51	1.43
21	1	601	CLA	C1C-C2C	2.12	1.48	1.44
21	A	1133	CLA	C3D-C4D	-2.12	1.39	1.44
21	5	613	CLA	C3B-C4B	2.12	1.47	1.42
21	4	606	CLA	C1A-CHA	2.12	1.51	1.43
21	3	606	CLA	C3D-C4D	-2.12	1.39	1.44
21	B	1220	CLA	C3D-C4D	-2.12	1.39	1.44
21	2	607	CLA	C3D-C4D	-2.11	1.39	1.44
21	6	607	CLA	C1C-C2C	2.11	1.48	1.44
21	A	1105	CLA	C1D-ND	-2.11	1.35	1.37
29	5	804	3PH	O31-C3	-2.11	1.40	1.45
21	B	1228	CLA	C3D-C4D	-2.11	1.39	1.44
21	A	1112	CLA	C1C-C2C	2.11	1.48	1.44
21	B	1240	CLA	C3D-C4D	-2.11	1.39	1.44
21	A	1135	CLA	C1A-CHA	2.11	1.51	1.43
21	A	1136	CLA	C1C-C2C	2.11	1.48	1.44
21	B	1225	CLA	C3D-C4D	-2.11	1.39	1.44
21	O	1803	CLA	C3D-C4D	-2.11	1.39	1.44
21	L	1501	CLA	MG-NC	2.11	2.11	2.06
21	5	601	CLA	MG-NB	-2.11	2.01	2.05
24	O	4001	BCR	C4-C5	-2.11	1.46	1.51
21	1	603	CLA	C3D-C4D	-2.10	1.39	1.44
21	2	612	CLA	C1A-CHA	2.10	1.51	1.43
21	1	605	CLA	C1A-CHA	2.10	1.51	1.43
21	1	608	CLA	C3D-C4D	-2.10	1.39	1.44
21	A	1110	CLA	C1A-CHA	2.10	1.51	1.43
21	3	611	CLA	C1A-CHA	2.10	1.51	1.43
21	2	608	CLA	C1A-CHA	2.10	1.51	1.43
21	3	615	CLA	C1C-C2C	2.10	1.48	1.44
21	5	603	CLA	C3D-C4D	-2.10	1.39	1.44
21	4	602	CLA	C3D-C4D	-2.10	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	607	CLA	C3D-C4D	-2.10	1.39	1.44
20	A	1011	CL0	C4C-C3C	2.10	1.48	1.45
21	A	1110	CLA	C3D-C4D	-2.10	1.39	1.44
33	O	5002	PTY	O4-C1	-2.10	1.40	1.45
21	A	1130	CLA	C1A-CHA	2.10	1.51	1.43
36	3	604	CHL	MG-ND	-2.10	2.01	2.05
21	B	1213	CLA	C3D-C4D	-2.10	1.39	1.44
21	1	606	CLA	C1A-CHA	2.09	1.51	1.43
24	L	4002	BCR	C12-C13	-2.09	1.41	1.45
21	B	1236	CLA	C1A-CHA	2.09	1.51	1.43
33	6	804	PTY	O4-C1	-2.09	1.40	1.45
21	A	1124	CLA	C3D-C4D	-2.09	1.39	1.44
21	4	615	CLA	C3D-C4D	-2.09	1.39	1.44
21	3	601	CLA	C1A-CHA	2.09	1.51	1.43
21	B	1222	CLA	C1A-CHA	2.09	1.51	1.43
21	B	1212	CLA	C1C-C2C	2.09	1.48	1.44
21	A	1115	CLA	C3D-C4D	-2.08	1.39	1.44
21	2	606	CLA	C1A-CHA	2.08	1.51	1.43
21	5	613	CLA	C1C-C2C	2.08	1.48	1.44
21	5	613	CLA	C1B-NB	-2.08	1.35	1.37
21	A	1139	CLA	C3D-C4D	-2.08	1.39	1.44
21	B	1023	CLA	C1C-C2C	2.08	1.48	1.44
21	A	1119	CLA	C1A-CHA	2.08	1.51	1.43
21	A	1104	CLA	CHD-C1D	2.08	1.42	1.38
21	A	1134	CLA	C1C-C2C	2.08	1.48	1.44
21	L	1502	CLA	C3D-C4D	-2.08	1.39	1.44
21	6	604	CLA	C3D-C4D	-2.08	1.39	1.44
21	A	1129	CLA	C1A-CHA	2.08	1.51	1.43
24	L	4001	BCR	C29-C30	-2.07	1.49	1.54
21	B	1022	CLA	C1C-C2C	2.07	1.48	1.44
21	2	606	CLA	C3D-C4D	-2.07	1.39	1.44
21	B	1227	CLA	C1A-CHA	2.07	1.51	1.43
29	F	5003	3PH	O31-C3	-2.07	1.40	1.45
21	A	1136	CLA	C3D-C4D	-2.07	1.39	1.44
21	5	601	CLA	C1D-ND	-2.07	1.35	1.37
21	3	607	CLA	C1C-C2C	2.07	1.48	1.44
33	5	803	PTY	O7-C8	2.07	1.40	1.34
21	B	1204	CLA	C3D-C4D	-2.07	1.39	1.44
24	A	4005	BCR	C12-C13	-2.07	1.41	1.45
21	3	601	CLA	C3D-C4D	-2.07	1.39	1.44
21	5	602	CLA	CAA-C2A	-2.06	1.50	1.54
38	4	805	LMK	O8-C28	2.06	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	G	1603	CLA	C3D-C4D	-2.06	1.39	1.44
24	3	504	BCR	C12-C13	-2.06	1.41	1.45
21	A	1130	CLA	C1B-NB	-2.06	1.35	1.37
21	6	612	CLA	C3D-C4D	-2.06	1.39	1.44
21	4	612	CLA	C3D-C4D	-2.06	1.39	1.44
21	A	1132	CLA	C1C-C2C	2.06	1.48	1.44
34	4	501	LUT	C22-C21	-2.05	1.52	1.54
21	5	608	CLA	C3B-C4B	2.05	1.47	1.42
21	1	608	CLA	C1C-C2C	2.05	1.48	1.44
21	B	1201	CLA	C3D-C4D	-2.05	1.39	1.44
32	L	5002	4RF	O18-C19	-2.05	1.40	1.45
21	K	1401	CLA	C1A-CHA	2.05	1.51	1.43
21	1	612	CLA	C3D-C4D	-2.05	1.39	1.44
21	3	610	CLA	C1C-C2C	2.05	1.48	1.44
21	1	615	CLA	MG-NC	2.05	2.11	2.06
31	4	803	LMG	O1-C1	2.05	1.43	1.40
36	3	604	CHL	C1A-CHA	-2.05	1.34	1.43
21	3	615	CLA	C3D-C4D	-2.05	1.39	1.44
21	A	1101	CLA	C3D-C4D	-2.05	1.39	1.44
21	B	1226	CLA	C1A-CHA	2.05	1.51	1.43
21	3	613	CLA	C1A-CHA	2.05	1.51	1.43
21	B	1235	CLA	C3D-C4D	-2.04	1.39	1.44
21	B	1239	CLA	C3D-C4D	-2.04	1.39	1.44
24	O	4001	BCR	C12-C13	-2.04	1.41	1.45
21	L	1504	CLA	C1C-C2C	2.04	1.48	1.44
21	1	602	CLA	C3D-C4D	-2.04	1.39	1.44
21	B	1230	CLA	C3D-C4D	-2.04	1.39	1.44
21	6	604	CLA	C1A-CHA	2.04	1.51	1.43
24	B	4005	BCR	C12-C13	-2.04	1.41	1.45
21	H	1702	CLA	MG-NB	-2.04	2.01	2.05
21	A	1114	CLA	C1C-C2C	2.04	1.48	1.44
36	2	609	CHL	C1D-ND	-2.04	1.35	1.37
21	2	602	CLA	C3D-C4D	-2.04	1.39	1.44
21	3	613	CLA	C3D-C4D	-2.04	1.39	1.44
21	4	603	CLA	C3D-C4D	-2.04	1.39	1.44
21	A	1116	CLA	MG-NC	2.04	2.11	2.06
21	A	1120	CLA	C1A-CHA	2.04	1.51	1.43
21	L	1503	CLA	C1C-C2C	2.04	1.48	1.44
21	A	1012	CLA	C3D-C4D	-2.04	1.39	1.44
21	A	1103	CLA	C1A-CHA	2.04	1.51	1.43
21	2	603	CLA	C3D-C4D	-2.04	1.39	1.44
21	K	1403	CLA	C3D-C4D	-2.04	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	J	4001	BCR	C12-C13	-2.04	1.41	1.45
33	5	803	PTY	O4-C1	-2.03	1.40	1.45
21	A	1123	CLA	MG-NC	2.03	2.11	2.06
21	A	1101	CLA	C1A-CHA	2.03	1.51	1.43
21	5	601	CLA	C3A-C2A	-2.03	1.48	1.54
21	A	1114	CLA	C3D-C4D	-2.03	1.39	1.44
21	3	607	CLA	MG-NC	2.03	2.11	2.06
21	2	602	CLA	C1C-C2C	2.03	1.48	1.44
21	5	612	CLA	C1A-CHA	2.03	1.51	1.43
21	B	1231	CLA	C1A-CHA	2.03	1.51	1.43
21	B	1229	CLA	C3D-C4D	-2.03	1.39	1.44
21	B	1219	CLA	C3D-C4D	-2.03	1.39	1.44
21	5	602	CLA	C1D-ND	-2.02	1.35	1.37
21	4	604	CLA	C1C-C2C	2.02	1.48	1.44
21	K	1403	CLA	C1A-CHA	2.02	1.51	1.43
21	4	604	CLA	C3D-C4D	-2.02	1.39	1.44
21	6	606	CLA	C1C-C2C	2.02	1.48	1.44
21	5	602	CLA	C3D-C4D	-2.02	1.39	1.44
21	1	613	CLA	MG-NC	2.02	2.11	2.06
31	F	5002	LMG	C22-C21	-2.02	1.33	1.49
21	L	1504	CLA	MG-NC	2.02	2.11	2.06
28	B	5002	DGD	CDA-CCA	-2.02	1.33	1.49
21	4	608	CLA	C3D-C4D	-2.02	1.39	1.44
21	K	1403	CLA	CHD-C1D	2.02	1.42	1.38
21	H	1702	CLA	C3D-C4D	-2.02	1.39	1.44
21	A	1013	CLA	C1D-ND	-2.01	1.35	1.37
34	3	501	LUT	C1-C6	-2.01	1.51	1.53
21	B	1022	CLA	C3D-C4D	-2.01	1.39	1.44
21	K	1404	CLA	C3D-C4D	-2.01	1.39	1.44
21	3	610	CLA	C3D-C4D	-2.01	1.39	1.44
21	3	608	CLA	MG-NC	2.01	2.11	2.06
28	2	806	DGD	O5D-C1E	2.01	1.43	1.40
21	A	1013	CLA	C1B-NB	-2.01	1.35	1.37
21	G	1603	CLA	C1A-CHA	2.01	1.51	1.43
21	L	1501	CLA	C3D-C4D	-2.01	1.39	1.44
21	5	608	CLA	C3D-C4D	-2.01	1.39	1.44
21	B	1202	CLA	C3B-C4B	2.01	1.47	1.42
21	J	1901	CLA	C3D-C4D	-2.01	1.39	1.44
21	2	612	CLA	C3D-C4D	-2.01	1.39	1.44
21	A	1139	CLA	C1C-C2C	2.01	1.48	1.44
21	A	1132	CLA	C3D-C4D	-2.01	1.39	1.44
21	A	1138	CLA	C1C-C2C	2.01	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	5003	3PH	O31-C3	-2.01	1.40	1.45
21	6	609	CLA	C1C-C2C	2.01	1.48	1.44
36	3	604	CHL	MG-NB	-2.01	2.01	2.05
21	5	606	CLA	MG-NC	2.01	2.11	2.06
21	6	603	CLA	C3D-C4D	-2.01	1.39	1.44
21	B	1208	CLA	MG-NC	2.01	2.11	2.06
31	2	804	LMG	C22-C21	-2.01	1.33	1.49
21	A	1013	CLA	C3D-C4D	-2.00	1.39	1.44
28	3	805	DGD	CAB-C9B	-2.00	1.33	1.49
21	L	1503	CLA	C1A-CHA	2.00	1.51	1.43
31	6	802	LMG	C19-C18	-2.00	1.33	1.49
21	F	1301	CLA	C1C-C2C	2.00	1.48	1.44
24	L	4002	BCR	C32-C1	-2.00	1.49	1.53
21	B	1023	CLA	MG-NC	2.00	2.11	2.06

All (4383) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	6	504	XAT	C20-C13-C14	-31.64	78.60	122.92
35	6	504	XAT	C12-C13-C14	25.27	157.72	118.94
35	6	504	XAT	C20-C13-C12	-24.73	79.12	118.08
34	5	501	LUT	C37-C21-C36	-19.58	79.03	107.89
34	5	504	LUT	C37-C21-C36	-19.44	79.24	107.89
24	O	4001	BCR	C16-C15-C14	19.36	163.14	123.47
24	F	4001	BCR	C10-C11-C12	18.05	179.55	123.22
24	L	4002	BCR	C10-C11-C12	17.99	179.36	123.22
24	I	4002	BCR	C10-C11-C12	17.90	179.07	123.22
24	K	4001	BCR	C10-C11-C12	17.66	178.31	123.22
24	A	4001	BCR	C10-C11-C12	17.65	178.31	123.22
24	L	4001	BCR	C10-C11-C12	17.61	178.17	123.22
24	4	503	BCR	C10-C11-C12	17.46	177.70	123.22
24	B	4003	BCR	C10-C11-C12	17.34	177.34	123.22
24	A	4002	BCR	C10-C11-C12	17.31	177.24	123.22
24	B	4001	BCR	C10-C11-C12	17.26	177.08	123.22
24	B	4006	BCR	C10-C11-C12	17.23	176.99	123.22
34	1	501	LUT	C37-C21-C36	-17.22	82.50	107.89
24	3	503	BCR	C10-C11-C12	17.17	176.80	123.22
24	F	4002	BCR	C10-C11-C12	17.15	176.75	123.22
24	B	4005	BCR	C10-C11-C12	17.11	176.60	123.22
24	J	4001	BCR	C10-C11-C12	17.09	176.56	123.22
24	A	4007	BCR	C10-C11-C12	16.99	176.23	123.22
24	B	4002	BCR	C10-C11-C12	16.95	176.10	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	503	BCR	C10-C11-C12	16.95	176.10	123.22
24	B	4004	BCR	C10-C11-C12	16.90	175.96	123.22
34	5	503	LUT	C36-C21-C26	-16.83	84.05	109.55
24	A	4005	BCR	C10-C11-C12	16.76	175.53	123.22
24	3	504	BCR	C10-C11-C12	16.75	175.48	123.22
24	O	4001	BCR	C10-C11-C12	16.70	175.34	123.22
24	J	4002	BCR	C10-C11-C12	16.64	175.14	123.22
24	I	4001	BCR	C10-C11-C12	16.63	175.12	123.22
24	A	4004	BCR	C10-C11-C12	16.58	174.95	123.22
24	A	4003	BCR	C10-C11-C12	16.53	174.81	123.22
24	H	4001	BCR	C10-C11-C12	16.43	174.48	123.22
24	G	4001	BCR	C10-C11-C12	16.39	174.36	123.22
24	A	4007	BCR	C16-C15-C14	16.21	156.68	123.47
24	J	4002	BCR	C11-C10-C9	16.17	150.39	127.31
24	1	504	BCR	C10-C11-C12	16.09	173.44	123.22
24	A	4006	BCR	C10-C11-C12	15.87	172.74	123.22
24	A	4004	BCR	C16-C15-C14	15.64	155.51	123.47
34	5	504	LUT	C36-C21-C26	-15.60	85.92	109.55
24	3	506	BCR	C10-C11-C12	15.57	171.80	123.22
24	L	4002	BCR	C11-C10-C9	15.29	149.14	127.31
24	H	4001	BCR	C16-C15-C14	14.95	154.09	123.47
24	A	4005	BCR	C16-C15-C14	14.91	154.01	123.47
34	5	503	LUT	C37-C21-C36	-14.81	86.07	107.89
24	H	4001	BCR	C11-C10-C9	14.69	148.28	127.31
34	1	501	LUT	C36-C21-C22	-14.69	81.62	109.44
24	4	503	BCR	C16-C15-C14	14.63	153.45	123.47
24	O	4001	BCR	C11-C10-C9	14.50	148.00	127.31
24	B	4002	BCR	C11-C10-C9	14.39	147.85	127.31
24	A	4007	BCR	C11-C10-C9	14.35	147.79	127.31
24	J	4001	BCR	C21-C20-C19	14.31	167.87	123.22
24	A	4006	BCR	C11-C10-C9	14.22	147.60	127.31
24	I	4002	BCR	C16-C15-C14	13.96	152.08	123.47
24	B	4004	BCR	C11-C10-C9	13.60	146.73	127.31
24	B	4001	BCR	C21-C20-C19	13.52	165.42	123.22
24	A	4001	BCR	C29-C30-C25	-13.49	89.71	110.48
24	A	4002	BCR	C21-C20-C19	13.46	165.22	123.22
24	3	504	BCR	C11-C10-C9	13.45	146.51	127.31
24	I	4001	BCR	C16-C15-C14	13.37	150.86	123.47
24	B	4005	BCR	C16-C15-C14	13.34	150.81	123.47
21	5	614	CLA	C4A-NA-C1A	13.31	112.69	106.71
24	A	4004	BCR	C11-C10-C9	13.26	146.24	127.31
24	F	4001	BCR	C16-C15-C14	13.22	150.55	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	4001	BCR	C16-C15-C14	13.15	150.40	123.47
24	2	503	BCR	C11-C10-C9	13.08	145.98	127.31
24	B	4001	BCR	C11-C10-C9	13.03	145.91	127.31
24	2	503	BCR	C16-C15-C14	12.98	150.06	123.47
24	F	4002	BCR	C11-C10-C9	12.97	145.83	127.31
24	F	4001	BCR	C21-C20-C19	12.94	163.61	123.22
24	F	4002	BCR	C21-C20-C19	12.93	163.57	123.22
24	B	4003	BCR	C21-C20-C19	12.86	163.34	123.22
24	B	4006	BCR	C11-C10-C9	12.85	145.65	127.31
24	1	504	BCR	C21-C20-C19	12.78	163.11	123.22
24	B	4003	BCR	C11-C10-C9	12.77	145.54	127.31
24	1	504	BCR	C16-C15-C14	12.75	149.60	123.47
24	A	4001	BCR	C21-C20-C19	12.75	162.99	123.22
24	K	4001	BCR	C21-C20-C19	12.64	162.67	123.22
24	B	4005	BCR	C11-C10-C9	12.63	145.33	127.31
34	5	501	LUT	C36-C21-C26	-12.62	90.43	109.55
24	A	4003	BCR	C11-C10-C9	12.58	145.26	127.31
24	A	4004	BCR	C21-C20-C19	12.57	162.43	123.22
24	A	4002	BCR	C16-C15-C14	12.50	149.08	123.47
24	3	506	BCR	C21-C20-C19	12.31	161.63	123.22
34	5	503	LUT	C36-C21-C22	-12.31	86.13	109.44
24	A	4001	BCR	C11-C10-C9	12.29	144.85	127.31
24	L	4001	BCR	C11-C10-C9	12.29	144.85	127.31
34	5	501	LUT	C36-C21-C22	-12.11	86.49	109.44
24	L	4001	BCR	C16-C15-C14	12.05	148.16	123.47
24	I	4002	BCR	C21-C20-C19	12.04	160.78	123.22
24	3	504	BCR	C16-C15-C14	12.03	148.12	123.47
24	3	503	BCR	C11-C10-C9	12.00	144.43	127.31
24	K	4001	BCR	C16-C15-C14	11.98	148.01	123.47
24	J	4001	BCR	C16-C15-C14	11.95	147.96	123.47
24	K	4001	BCR	C11-C10-C9	11.94	144.36	127.31
24	3	503	BCR	C16-C15-C14	11.94	147.93	123.47
24	F	4002	BCR	C16-C15-C14	11.86	147.77	123.47
24	L	4002	BCR	C21-C20-C19	11.86	160.23	123.22
24	G	4001	BCR	C21-C20-C19	11.83	160.15	123.22
24	J	4001	BCR	C11-C12-C13	11.82	159.62	126.42
24	A	4007	BCR	C21-C20-C19	11.81	160.07	123.22
24	B	4003	BCR	C16-C15-C14	11.78	147.60	123.47
24	B	4002	BCR	C16-C15-C14	11.72	147.48	123.47
24	B	4006	BCR	C16-C15-C14	11.65	147.34	123.47
24	G	4001	BCR	C16-C15-C14	11.59	147.21	123.47
24	A	4003	BCR	C11-C12-C13	11.56	158.89	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	4005	BCR	C21-C20-C19	11.54	159.23	123.22
24	O	4001	BCR	C21-C20-C19	11.46	158.98	123.22
24	B	4004	BCR	C16-C15-C14	11.43	146.89	123.47
24	B	4006	BCR	C21-C20-C19	11.43	158.89	123.22
24	J	4002	BCR	C16-C15-C14	11.39	146.81	123.47
24	4	503	BCR	C11-C10-C9	11.26	143.38	127.31
24	A	4006	BCR	C11-C12-C13	11.26	158.05	126.42
21	O	1801	CLA	C4A-NA-C1A	11.24	111.76	106.71
24	B	4001	BCR	C16-C15-C14	11.22	146.46	123.47
24	3	506	BCR	C16-C15-C14	11.16	146.34	123.47
24	3	504	BCR	C21-C20-C19	11.16	158.05	123.22
24	A	4005	BCR	C11-C10-C9	11.16	143.24	127.31
24	L	4001	BCR	C21-C20-C19	11.16	158.03	123.22
24	I	4001	BCR	C21-C20-C19	11.12	157.91	123.22
24	J	4001	BCR	C11-C10-C9	11.11	143.16	127.31
24	4	503	BCR	C21-C20-C19	11.09	157.84	123.22
24	F	4001	BCR	C11-C10-C9	11.09	143.13	127.31
24	B	4001	BCR	C11-C12-C13	11.08	157.53	126.42
24	A	4003	BCR	C21-C20-C19	11.08	157.78	123.22
24	A	4006	BCR	C21-C20-C19	11.02	157.61	123.22
24	A	4002	BCR	C11-C12-C13	11.00	157.31	126.42
24	B	4004	BCR	C11-C12-C13	10.98	157.25	126.42
21	B	1205	CLA	C4A-NA-C1A	10.96	111.63	106.71
24	F	4002	BCR	C11-C12-C13	10.91	157.07	126.42
24	3	504	BCR	C11-C12-C13	10.84	156.88	126.42
24	B	4006	BCR	C11-C12-C13	10.82	156.81	126.42
21	B	1021	CLA	C4A-NA-C1A	10.78	111.55	106.71
21	3	613	CLA	C4A-NA-C1A	10.71	111.52	106.71
24	B	4002	BCR	C21-C20-C19	10.65	156.46	123.22
24	3	503	BCR	C21-C20-C19	10.55	156.14	123.22
24	4	503	BCR	C11-C12-C13	10.54	156.02	126.42
21	L	1501	CLA	C4A-NA-C1A	10.52	111.44	106.71
24	A	4003	BCR	C16-C15-C14	10.45	144.87	123.47
21	4	609	CLA	C4A-NA-C1A	10.44	111.40	106.71
24	A	4006	BCR	C16-C15-C14	10.43	144.84	123.47
24	L	4002	BCR	C16-C15-C14	10.41	144.79	123.47
21	A	1103	CLA	C4A-NA-C1A	10.40	111.38	106.71
24	L	4001	BCR	C11-C12-C13	10.39	155.59	126.42
24	B	4005	BCR	C11-C12-C13	10.38	155.57	126.42
21	A	1125	CLA	C4A-NA-C1A	10.37	111.37	106.71
21	2	612	CLA	C4A-NA-C1A	10.37	111.37	106.71
34	5	504	LUT	C36-C21-C22	-10.34	89.85	109.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	I	4002	BCR	C11-C10-C9	10.34	142.07	127.31
24	B	4004	BCR	C21-C20-C19	10.32	155.44	123.22
21	B	1219	CLA	C4A-NA-C1A	10.29	111.33	106.71
24	I	4001	BCR	C11-C10-C9	10.28	141.98	127.31
24	2	503	BCR	C11-C12-C13	10.24	155.18	126.42
21	1	603	CLA	C4A-NA-C1A	10.22	111.30	106.71
24	A	4005	BCR	C21-C20-C19	10.21	155.07	123.22
24	J	4002	BCR	C21-C20-C19	10.21	155.07	123.22
21	G	1603	CLA	C4A-NA-C1A	10.19	111.29	106.71
24	2	503	BCR	C21-C20-C19	10.18	155.00	123.22
24	K	4001	BCR	C11-C12-C13	10.16	154.96	126.42
21	1	612	CLA	C4A-NA-C1A	10.14	111.26	106.71
21	H	1701	CLA	C4A-NA-C1A	10.12	111.26	106.71
21	3	601	CLA	C4A-NA-C1A	10.10	111.25	106.71
24	A	4002	BCR	C11-C10-C9	10.08	141.70	127.31
24	I	4002	BCR	C11-C12-C13	10.07	154.70	126.42
21	J	1901	CLA	C4A-NA-C1A	10.06	111.23	106.71
24	A	4005	BCR	C11-C12-C13	10.03	154.59	126.42
24	J	4002	BCR	C11-C12-C13	10.01	154.55	126.42
21	B	1215	CLA	C4A-NA-C1A	9.98	111.19	106.71
21	L	1502	CLA	C4A-NA-C1A	9.97	111.19	106.71
21	3	605	CLA	C4A-NA-C1A	9.97	111.19	106.71
24	G	4001	BCR	C11-C10-C9	9.92	141.47	127.31
21	4	612	CLA	C4A-NA-C1A	9.91	111.16	106.71
24	A	4001	BCR	C11-C12-C13	9.90	154.22	126.42
21	5	608	CLA	C4A-NA-C1A	9.89	111.15	106.71
24	F	4001	BCR	C11-C12-C13	9.89	154.19	126.42
21	F	1302	CLA	C4A-NA-C1A	9.88	111.15	106.71
24	3	503	BCR	C11-C12-C13	9.88	154.18	126.42
24	1	504	BCR	C11-C10-C9	9.88	141.41	127.31
21	A	1131	CLA	C4A-NA-C1A	9.86	111.14	106.71
21	B	1204	CLA	C4A-NA-C1A	9.80	111.11	106.71
21	A	1013	CLA	C4A-NA-C1A	9.79	111.11	106.71
21	A	1122	CLA	C4A-NA-C1A	9.76	111.09	106.71
21	A	1139	CLA	C4A-NA-C1A	9.73	111.08	106.71
21	6	605	CLA	C4A-NA-C1A	9.72	111.08	106.71
21	B	1232	CLA	C4A-NA-C1A	9.70	111.07	106.71
24	J	4002	BCR	C20-C19-C18	9.69	153.65	126.42
24	B	4002	BCR	C11-C12-C13	9.69	153.64	126.42
21	B	1230	CLA	C4A-NA-C1A	9.69	111.06	106.71
21	B	1238	CLA	C4A-NA-C1A	9.65	111.04	106.71
21	B	1228	CLA	C4A-NA-C1A	9.62	111.03	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1234	CLA	C4A-NA-C1A	9.62	111.03	106.71
21	B	1201	CLA	C4A-NA-C1A	9.60	111.02	106.71
21	A	1111	CLA	C4A-NA-C1A	9.58	111.01	106.71
24	H	4001	BCR	C21-C20-C19	9.57	153.08	123.22
21	2	607	CLA	C4A-NA-C1A	9.56	111.00	106.71
21	A	1106	CLA	C4A-NA-C1A	9.56	111.00	106.71
21	B	1237	CLA	C4A-NA-C1A	9.54	111.00	106.71
21	B	1223	CLA	C4A-NA-C1A	9.52	110.99	106.71
24	A	4007	BCR	C11-C12-C13	9.51	153.13	126.42
21	4	602	CLA	C4A-NA-C1A	9.51	110.98	106.71
21	A	1138	CLA	C4A-NA-C1A	9.50	110.97	106.71
24	A	4005	BCR	C20-C19-C18	9.49	153.09	126.42
21	5	602	CLA	C4A-NA-C1A	9.49	110.97	106.71
21	B	1209	CLA	C4A-NA-C1A	9.48	110.97	106.71
21	3	603	CLA	C4A-NA-C1A	9.48	110.97	106.71
21	3	615	CLA	C4A-NA-C1A	9.48	110.97	106.71
21	3	612	CLA	C4A-NA-C1A	9.43	110.94	106.71
21	B	1210	CLA	C4A-NA-C1A	9.41	110.94	106.71
21	B	1225	CLA	C4A-NA-C1A	9.40	110.93	106.71
21	B	1227	CLA	C4A-NA-C1A	9.40	110.93	106.71
21	2	606	CLA	C4A-NA-C1A	9.39	110.93	106.71
21	A	1102	CLA	C4A-NA-C1A	9.37	110.92	106.71
21	B	1221	CLA	C4A-NA-C1A	9.35	110.91	106.71
21	A	1109	CLA	C4A-NA-C1A	9.34	110.90	106.71
21	A	1127	CLA	C4A-NA-C1A	9.31	110.89	106.71
21	4	606	CLA	C4A-NA-C1A	9.30	110.89	106.71
21	4	607	CLA	C4A-NA-C1A	9.29	110.88	106.71
21	5	607	CLA	C4A-NA-C1A	9.25	110.86	106.71
21	A	1126	CLA	C4A-NA-C1A	9.24	110.86	106.71
21	A	1140	CLA	C4A-NA-C1A	9.22	110.85	106.71
21	B	1231	CLA	C4A-NA-C1A	9.21	110.85	106.71
21	2	602	CLA	C4A-NA-C1A	9.20	110.84	106.71
21	4	608	CLA	C4A-NA-C1A	9.18	110.83	106.71
21	B	1236	CLA	C4A-NA-C1A	9.18	110.83	106.71
21	B	1224	CLA	C4A-NA-C1A	9.17	110.83	106.71
21	2	603	CLA	C4A-NA-C1A	9.16	110.83	106.71
21	B	1226	CLA	C4A-NA-C1A	9.14	110.81	106.71
21	A	1129	CLA	C4A-NA-C1A	9.14	110.81	106.71
21	1	602	CLA	C4A-NA-C1A	9.13	110.81	106.71
21	3	607	CLA	C4A-NA-C1A	9.13	110.81	106.71
34	1	501	LUT	C15-C35-C34	-9.13	104.78	123.47
24	I	4001	BCR	C20-C19-C18	9.12	152.04	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1108	CLA	C4A-NA-C1A	9.12	110.81	106.71
21	A	1133	CLA	C4A-NA-C1A	9.10	110.80	106.71
21	3	606	CLA	C4A-NA-C1A	9.09	110.79	106.71
21	A	1105	CLA	C4A-NA-C1A	9.08	110.79	106.71
21	K	1403	CLA	C4A-NA-C1A	9.08	110.79	106.71
21	1	607	CLA	C4A-NA-C1A	9.07	110.78	106.71
21	2	608	CLA	C4A-NA-C1A	9.06	110.78	106.71
21	A	1123	CLA	C4A-NA-C1A	9.06	110.78	106.71
34	1	501	LUT	C36-C21-C26	-9.04	95.85	109.55
21	2	604	CLA	C4A-NA-C1A	9.03	110.77	106.71
24	O	4001	BCR	C20-C19-C18	9.03	151.78	126.42
21	5	601	CLA	CMA-C3A-C2A	-9.01	77.48	113.83
21	O	1802	CLA	C4A-NA-C1A	9.01	110.76	106.71
24	B	4004	BCR	C20-C19-C18	9.01	151.71	126.42
21	4	615	CLA	C4A-NA-C1A	8.98	110.74	106.71
21	B	1240	CLA	C4A-NA-C1A	8.97	110.74	106.71
21	A	1116	CLA	C4A-NA-C1A	8.97	110.74	106.71
21	6	608	CLA	C4A-NA-C1A	8.95	110.73	106.71
21	B	1206	CLA	C4A-NA-C1A	8.95	110.73	106.71
21	4	601	CLA	C4A-NA-C1A	8.95	110.73	106.71
21	2	601	CLA	C4A-NA-C1A	8.94	110.72	106.71
21	B	1218	CLA	C4A-NA-C1A	8.93	110.72	106.71
21	2	615	CLA	C4A-NA-C1A	8.85	110.69	106.71
21	5	603	CLA	C4A-NA-C1A	8.85	110.68	106.71
24	1	504	BCR	C11-C12-C13	8.84	151.26	126.42
21	B	1023	CLA	C4A-NA-C1A	8.84	110.68	106.71
21	B	1220	CLA	C4A-NA-C1A	8.84	110.68	106.71
21	L	1504	CLA	C4A-NA-C1A	8.82	110.67	106.71
21	A	1141	CLA	C4A-NA-C1A	8.82	110.67	106.71
21	A	1110	CLA	C4A-NA-C1A	8.82	110.67	106.71
21	3	602	CLA	C4A-NA-C1A	8.82	110.67	106.71
24	A	4004	BCR	C11-C12-C13	8.82	151.18	126.42
21	1	615	CLA	C4A-NA-C1A	8.80	110.66	106.71
21	A	1107	CLA	C4A-NA-C1A	8.79	110.66	106.71
21	B	1214	CLA	C4A-NA-C1A	8.79	110.66	106.71
21	A	1114	CLA	C4A-NA-C1A	8.78	110.65	106.71
21	G	1602	CLA	C4A-NA-C1A	8.77	110.65	106.71
21	5	601	CLA	CMA-C3A-C4A	8.74	135.27	111.77
21	A	1124	CLA	C4A-NA-C1A	8.74	110.64	106.71
21	L	1503	CLA	C4A-NA-C1A	8.73	110.63	106.71
21	A	1128	CLA	C4A-NA-C1A	8.72	110.62	106.71
21	B	1235	CLA	C4A-NA-C1A	8.72	110.62	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	613	CLA	C4A-NA-C1A	8.72	110.62	106.71
21	6	602	CLA	C4A-NA-C1A	8.70	110.62	106.71
21	4	603	CLA	C4A-NA-C1A	8.69	110.61	106.71
34	5	504	LUT	C37-C21-C26	8.69	122.70	109.55
21	B	1211	CLA	C4A-NA-C1A	8.68	110.61	106.71
21	A	1137	CLA	C4A-NA-C1A	8.68	110.61	106.71
21	B	1022	CLA	C4A-NA-C1A	8.67	110.61	106.71
21	1	605	CLA	C4A-NA-C1A	8.67	110.60	106.71
21	A	1112	CLA	C4A-NA-C1A	8.67	110.60	106.71
21	B	1222	CLA	C4A-NA-C1A	8.66	110.60	106.71
21	B	1216	CLA	C4A-NA-C1A	8.66	110.60	106.71
21	A	1132	CLA	C4A-NA-C1A	8.64	110.59	106.71
21	4	605	CLA	C4A-NA-C1A	8.63	110.58	106.71
21	K	1402	CLA	C4A-NA-C1A	8.62	110.58	106.71
21	3	614	CLA	C4A-NA-C1A	8.61	110.58	106.71
21	A	1119	CLA	C4A-NA-C1A	8.61	110.58	106.71
21	3	610	CLA	C4A-NA-C1A	8.60	110.57	106.71
21	A	1121	CLA	C4A-NA-C1A	8.59	110.57	106.71
21	A	1120	CLA	C4A-NA-C1A	8.58	110.56	106.71
21	6	607	CLA	C4A-NA-C1A	8.58	110.56	106.71
21	1	613	CLA	C4A-NA-C1A	8.57	110.56	106.71
21	5	605	CLA	C4A-NA-C1A	8.57	110.56	106.71
21	B	1213	CLA	C4A-NA-C1A	8.56	110.56	106.71
21	1	601	CLA	C4A-NA-C1A	8.56	110.55	106.71
34	1	501	LUT	C37-C21-C22	8.54	125.61	109.44
21	B	1239	CLA	C4A-NA-C1A	8.54	110.55	106.71
21	6	601	CLA	C4A-NA-C1A	8.53	110.54	106.71
24	B	4001	BCR	C20-C19-C18	8.53	150.37	126.42
21	6	606	CLA	C4A-NA-C1A	8.53	110.54	106.71
21	1	604	CLA	C4A-NA-C1A	8.52	110.54	106.71
21	B	1202	CLA	C4A-NA-C1A	8.51	110.53	106.71
21	B	1203	CLA	C4A-NA-C1A	8.50	110.53	106.71
21	A	1136	CLA	C4A-NA-C1A	8.50	110.53	106.71
21	5	606	CLA	C4A-NA-C1A	8.50	110.53	106.71
21	6	609	CLA	C4A-NA-C1A	8.49	110.52	106.71
21	G	1601	CLA	C4A-NA-C1A	8.48	110.52	106.71
21	L	1502	CLA	O2A-C1-C2	8.48	130.92	108.64
21	3	611	CLA	C4A-NA-C1A	8.47	110.51	106.71
21	F	1301	CLA	C4A-NA-C1A	8.45	110.50	106.71
24	G	4001	BCR	C20-C19-C18	8.44	150.12	126.42
21	1	611	CLA	C4A-NA-C1A	8.43	110.50	106.71
21	B	1208	CLA	C4A-NA-C1A	8.43	110.49	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	606	CLA	C4A-NA-C1A	8.42	110.49	106.71
24	4	503	BCR	C20-C19-C18	8.42	150.06	126.42
24	3	503	BCR	C20-C19-C18	8.41	150.06	126.42
24	2	503	BCR	C20-C19-C18	8.41	150.04	126.42
24	A	4004	BCR	C20-C19-C18	8.40	150.03	126.42
24	O	4001	BCR	C11-C12-C13	8.40	150.03	126.42
24	3	504	BCR	C20-C19-C18	8.40	150.02	126.42
21	B	1207	CLA	C4A-NA-C1A	8.40	110.48	106.71
21	B	1212	CLA	C4A-NA-C1A	8.38	110.47	106.71
24	H	4001	BCR	C11-C12-C13	8.37	149.94	126.42
21	A	1134	CLA	C4A-NA-C1A	8.34	110.46	106.71
21	A	1115	CLA	C4A-NA-C1A	8.33	110.45	106.71
21	A	1135	CLA	C4A-NA-C1A	8.32	110.45	106.71
21	K	1404	CLA	C4A-NA-C1A	8.31	110.44	106.71
24	B	4002	BCR	C20-C19-C18	8.30	149.72	126.42
21	A	1012	CLA	C4A-NA-C1A	8.29	110.43	106.71
21	5	614	CLA	C2D-C1D-ND	8.27	116.20	110.10
21	1	608	CLA	C4A-NA-C1A	8.27	110.42	106.71
21	6	612	CLA	C4A-NA-C1A	8.27	110.42	106.71
21	4	604	CLA	C4A-NA-C1A	8.26	110.42	106.71
21	6	603	CLA	C4A-NA-C1A	8.26	110.42	106.71
21	5	604	CLA	C4A-NA-C1A	8.25	110.41	106.71
21	A	1117	CLA	C4A-NA-C1A	8.23	110.41	106.71
21	B	1229	CLA	C4A-NA-C1A	8.23	110.41	106.71
34	5	501	LUT	C37-C21-C26	8.20	121.97	109.55
21	K	1403	CLA	CMD-C2D-C1D	8.20	139.16	124.71
21	2	605	CLA	C4A-NA-C1A	8.19	110.39	106.71
24	A	4006	BCR	C20-C19-C18	8.19	149.41	126.42
21	3	608	CLA	C4A-NA-C1A	8.16	110.38	106.71
21	K	1401	CLA	C4A-NA-C1A	8.15	110.37	106.71
21	A	1104	CLA	CMD-C2D-C1D	8.12	139.02	124.71
24	B	4003	BCR	C11-C12-C13	8.10	149.18	126.42
24	B	4005	BCR	C20-C19-C18	8.08	149.13	126.42
24	I	4001	BCR	C11-C12-C13	8.08	149.11	126.42
21	B	1217	CLA	C4A-NA-C1A	8.07	110.33	106.71
24	B	4006	BCR	C20-C19-C18	8.05	149.04	126.42
21	5	613	CLA	O2D-CGD-CBD	8.02	125.51	111.27
21	4	601	CLA	O2D-CGD-CBD	7.98	125.45	111.27
21	5	612	CLA	C4A-NA-C1A	7.96	110.28	106.71
20	A	1011	CL0	CMD-C2D-C1D	7.95	138.72	124.71
24	I	4002	BCR	C20-C19-C18	7.89	148.57	126.42
24	H	4001	BCR	C20-C19-C18	7.88	148.56	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	O	1801	CLA	CMD-C2D-C1D	7.74	138.36	124.71
24	L	4002	BCR	C20-C19-C18	7.74	148.16	126.42
24	F	4002	BCR	C20-C19-C18	7.66	147.93	126.42
24	O	4001	BCR	C4-C5-C6	-7.63	111.66	122.73
21	6	604	CLA	C4A-NA-C1A	7.56	110.10	106.71
21	6	612	CLA	O2D-CGD-CBD	7.54	124.67	111.27
21	5	601	CLA	C4A-NA-C1A	7.51	110.08	106.71
21	K	1401	CLA	CMD-C2D-C1D	7.47	137.87	124.71
21	A	1117	CLA	O2D-CGD-CBD	7.46	124.52	111.27
21	A	1113	CLA	C4A-NA-C1A	7.46	110.06	106.71
34	1	501	LUT	C37-C21-C26	7.46	120.84	109.55
21	4	609	CLA	O2D-CGD-CBD	7.42	124.45	111.27
24	A	4001	BCR	C40-C30-C29	-7.35	79.50	108.91
21	G	1603	CLA	CMD-C2D-C1D	7.35	137.66	124.71
34	1	501	LUT	C40-C33-C34	-7.34	112.64	122.92
24	G	4001	BCR	C11-C12-C13	7.32	146.97	126.42
24	J	4001	BCR	C20-C19-C18	7.31	146.95	126.42
34	1	501	LUT	C31-C30-C29	-7.31	116.88	127.31
24	L	4001	BCR	C28-C27-C26	-7.29	101.07	114.08
34	4	501	LUT	C21-C26-C27	7.28	121.90	112.70
21	O	1803	CLA	C4A-NA-C1A	7.23	109.95	106.71
21	A	1101	CLA	C4A-NA-C1A	7.21	109.95	106.71
24	A	4001	BCR	C20-C19-C18	7.21	146.67	126.42
21	O	1801	CLA	C1C-C2C-C3C	-7.21	100.46	107.07
21	B	1201	CLA	O2D-CGD-CBD	7.19	124.05	111.27
24	1	504	BCR	C20-C19-C18	7.07	146.29	126.42
24	3	506	BCR	C11-C10-C9	7.07	137.40	127.31
24	A	4003	BCR	C20-C19-C18	7.06	146.25	126.42
24	K	4001	BCR	C20-C19-C18	7.04	146.20	126.42
21	A	1130	CLA	C4A-NA-C1A	7.03	109.86	106.71
34	1	501	LUT	C35-C15-C14	7.01	137.84	123.47
21	5	601	CLA	CMD-C2D-C1D	6.96	136.97	124.71
35	6	504	XAT	C31-C30-C29	-6.93	117.42	127.31
21	B	1204	CLA	O2D-CGD-CBD	6.89	123.51	111.27
34	5	501	LUT	C37-C21-C22	6.89	122.48	109.44
34	5	503	LUT	C37-C21-C26	6.82	119.88	109.55
21	A	1118	CLA	C4A-NA-C1A	6.79	109.76	106.71
24	F	4001	BCR	C20-C19-C18	6.76	145.41	126.42
21	A	1104	CLA	C4A-NA-C1A	6.73	109.73	106.71
21	B	1211	CLA	O2A-C1-C2	6.73	126.33	108.64
21	2	601	CLA	O2D-CGD-CBD	6.72	123.21	111.27
24	3	506	BCR	C20-C19-C18	6.70	145.24	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	J	1901	CLA	O2D-CGD-CBD	6.69	123.16	111.27
21	2	604	CLA	O2D-CGD-CBD	6.65	123.08	111.27
24	L	4001	BCR	C20-C19-C18	6.64	145.07	126.42
21	A	1109	CLA	CMD-C2D-C1D	6.63	136.40	124.71
24	O	4001	BCR	C15-C14-C13	-6.59	117.91	127.31
21	A	1108	CLA	O2D-CGD-CBD	6.57	122.94	111.27
21	5	601	CLA	O2D-CGD-CBD	6.52	122.85	111.27
38	2	807	LMK	O2-C4-O3	-6.51	109.31	124.09
21	1	603	CLA	CMD-C2D-C1D	6.49	136.15	124.71
34	5	504	LUT	C37-C21-C22	6.46	121.68	109.44
21	B	1218	CLA	O2A-C1-C2	6.44	125.57	108.64
21	A	1138	CLA	O2D-CGD-CBD	6.42	122.67	111.27
36	2	613	CHL	C2B-C1B-NB	-6.41	105.94	110.23
21	5	614	CLA	CHD-C1D-ND	-6.40	118.57	124.45
21	B	1221	CLA	O2D-CGD-CBD	6.38	122.60	111.27
20	A	1011	CL0	C4A-NA-C1A	6.37	109.57	106.71
21	3	601	CLA	O2A-C1-C2	6.36	125.34	108.64
21	A	1129	CLA	O2A-C1-C2	6.32	125.24	108.64
34	5	504	LUT	C15-C14-C13	-6.31	118.31	127.31
21	2	608	CLA	CMD-C2D-C1D	6.30	135.82	124.71
38	4	805	LMK	O2-C4-O3	-6.30	109.78	124.09
34	1	501	LUT	C21-C26-C27	6.27	120.63	112.70
21	B	1221	CLA	CMD-C2D-C1D	6.27	135.76	124.71
21	G	1603	CLA	C2D-C1D-ND	6.26	114.71	110.10
21	H	1702	CLA	O2D-CGD-CBD	6.25	122.38	111.27
21	G	1603	CLA	CHD-C1D-ND	-6.25	118.71	124.45
21	6	613	CLA	CMD-C2D-C1D	6.24	135.72	124.71
34	5	504	LUT	C21-C26-C25	6.22	122.56	111.42
21	5	614	CLA	C1D-ND-C4D	-6.19	101.94	106.33
21	1	604	CLA	O2D-CGD-CBD	6.18	122.25	111.27
21	6	607	CLA	O2D-CGD-CBD	6.18	122.25	111.27
34	1	501	LUT	C32-C33-C34	6.16	128.40	118.94
21	F	1302	CLA	O2A-C1-C2	6.13	123.30	108.97
21	2	607	CLA	O2D-CGD-CBD	6.12	122.15	111.27
20	A	1011	CL0	C2D-C1D-ND	6.12	114.62	110.10
21	5	614	CLA	O2A-C1-C2	6.10	124.68	108.64
21	B	1213	CLA	CMD-C2D-C1D	6.08	135.42	124.71
21	B	1227	CLA	O2D-CGD-CBD	6.06	122.04	111.27
21	A	1110	CLA	O2A-C1-C2	6.04	124.52	108.64
21	A	1118	CLA	O2D-CGD-CBD	6.03	121.98	111.27
24	A	4007	BCR	C15-C14-C13	-6.03	118.71	127.31
24	A	4002	BCR	C20-C19-C18	6.02	143.34	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1131	CLA	O2D-CGD-CBD	6.02	121.97	111.27
21	B	1238	CLA	O2D-CGD-CBD	6.02	121.97	111.27
21	1	612	CLA	O2D-CGD-CBD	6.02	121.97	111.27
21	A	1102	CLA	O2D-CGD-CBD	6.01	121.96	111.27
21	5	613	CLA	C4A-NA-C1A	6.00	109.40	106.71
20	A	1011	CL0	C2C-C1C-NC	6.00	115.59	109.97
21	4	605	CLA	CMD-C2D-C1D	6.00	135.28	124.71
24	A	4004	BCR	C15-C14-C13	-6.00	118.75	127.31
24	O	4001	BCR	C36-C18-C17	-5.98	114.55	122.92
24	3	506	BCR	C12-C13-C14	5.96	128.09	118.94
21	B	1222	CLA	O2D-CGD-CBD	5.96	121.85	111.27
21	A	1106	CLA	O2D-CGD-CBD	5.95	121.85	111.27
24	L	4002	BCR	C12-C13-C14	5.94	128.06	118.94
21	G	1603	CLA	C1D-ND-C4D	-5.93	102.12	106.33
31	4	802	LMG	O7-C10-C11	5.93	124.28	111.50
34	6	501	LUT	C21-C26-C25	5.93	122.03	111.42
34	5	502	LUT	C21-C26-C25	5.92	122.03	111.42
21	5	612	CLA	O2D-CGD-CBD	5.92	121.79	111.27
24	L	4002	BCR	C11-C12-C13	5.91	143.01	126.42
21	B	1231	CLA	CMD-C2D-C1D	5.90	135.12	124.71
21	B	1234	CLA	O2A-C1-C2	5.90	124.14	108.64
21	A	1105	CLA	O2A-C1-C2	5.89	124.13	108.64
24	A	4001	BCR	C40-C30-C25	5.89	119.85	110.30
21	B	1229	CLA	O2D-CGD-CBD	5.88	121.72	111.27
21	B	1203	CLA	CMD-C2D-C1D	5.88	135.08	124.71
21	A	1138	CLA	O2A-C1-C2	5.85	124.02	108.64
21	3	603	CLA	O2A-C1-C2	5.84	123.99	108.64
21	B	1214	CLA	CMD-C2D-C1D	5.84	135.01	124.71
21	L	1501	CLA	CMD-C2D-C1D	5.83	135.00	124.71
21	B	1230	CLA	O2D-CGD-CBD	5.83	121.63	111.27
21	1	604	CLA	CMD-C2D-C1D	5.82	134.97	124.71
21	A	1131	CLA	CMD-C2D-C1D	5.82	134.97	124.71
21	1	608	CLA	CMD-C2D-C1D	5.82	134.96	124.71
21	6	605	CLA	CMD-C2D-C1D	5.80	134.94	124.71
21	A	1110	CLA	CMD-C2D-C1D	5.79	134.92	124.71
34	1	501	LUT	C15-C14-C13	5.79	135.57	127.31
21	5	614	CLA	CMD-C2D-C1D	5.78	134.91	124.71
21	A	1135	CLA	O2A-C1-C2	5.78	123.83	108.64
21	A	1135	CLA	O2D-CGD-CBD	5.77	121.52	111.27
21	O	1803	CLA	CMD-C2D-C1D	5.76	134.87	124.71
21	A	1133	CLA	O2D-CGD-CBD	5.76	121.50	111.27
21	J	1901	CLA	CMD-C2D-C1D	5.75	134.85	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	603	CLA	O2D-CGD-CBD	5.74	121.47	111.27
21	A	1129	CLA	CMD-C2D-C1D	5.74	134.83	124.71
21	A	1128	CLA	O2D-CGD-CBD	5.74	121.47	111.27
21	A	1111	CLA	O2D-CGD-CBD	5.74	121.46	111.27
21	A	1112	CLA	O2D-CGD-CBD	5.73	121.45	111.27
21	A	1119	CLA	CMD-C2D-C1D	5.73	134.81	124.71
21	5	603	CLA	CMD-C2D-C1D	5.73	134.81	124.71
21	L	1501	CLA	O2D-CGD-CBD	5.72	121.44	111.27
25	1	801	LHG	O7-C7-C8	5.72	123.84	111.50
21	3	605	CLA	CMD-C2D-C1D	5.71	134.78	124.71
21	B	1202	CLA	CMD-C2D-C1D	5.71	134.78	124.71
21	2	607	CLA	O2A-C1-C2	5.70	123.61	108.64
21	B	1236	CLA	O2A-C1-C2	5.70	123.60	108.64
21	4	607	CLA	O2D-CGD-CBD	5.69	121.38	111.27
21	2	601	CLA	O2A-C1-C2	5.68	123.57	108.64
21	B	1211	CLA	CMD-C2D-C1D	5.68	134.73	124.71
21	A	1101	CLA	CMD-C2D-C1D	5.68	134.72	124.71
34	4	501	LUT	C22-C23-C24	-5.67	105.29	111.74
21	4	602	CLA	O2D-CGD-CBD	5.66	121.33	111.27
21	4	606	CLA	CMD-C2D-C1D	5.66	134.69	124.71
21	A	1127	CLA	O2A-C1-C2	5.66	123.52	108.64
21	2	612	CLA	O2A-C1-C2	5.66	123.50	108.64
21	A	1101	CLA	O2D-CGD-CBD	5.65	121.30	111.27
21	L	1504	CLA	CMD-C2D-C1D	5.65	134.66	124.71
35	1	502	XAT	O4-C5-C18	-5.64	108.30	115.06
21	A	1103	CLA	O2D-CGD-CBD	5.63	121.28	111.27
21	B	1210	CLA	O2D-CGD-CBD	5.63	121.27	111.27
21	4	609	CLA	CMD-C2D-C1D	5.62	134.63	124.71
21	A	1119	CLA	O2A-C1-C2	5.62	123.42	108.64
24	3	506	BCR	C11-C12-C13	5.62	142.21	126.42
21	3	614	CLA	CMD-C2D-C1D	5.62	134.62	124.71
21	A	1114	CLA	CMD-C2D-C1D	5.62	134.62	124.71
21	4	603	CLA	CMD-C2D-C1D	5.62	134.61	124.71
21	1	604	CLA	O2A-C1-C2	5.61	123.39	108.64
21	A	1104	CLA	O2A-C1-C2	5.61	123.39	108.64
21	2	606	CLA	CMD-C2D-C1D	5.61	134.60	124.71
21	4	605	CLA	O2D-CGD-CBD	5.61	121.23	111.27
21	A	1102	CLA	CMD-C2D-C1D	5.60	134.59	124.71
21	3	615	CLA	O2A-C1-C2	5.60	123.36	108.64
21	B	1238	CLA	CMD-C2D-C1D	5.60	134.58	124.71
21	5	613	CLA	CMD-C2D-C1D	5.59	134.56	124.71
21	B	1214	CLA	O2D-CGD-CBD	5.59	121.19	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	K	1401	CLA	O2D-CGD-CBD	5.59	121.19	111.27
21	A	1136	CLA	O2D-CGD-CBD	5.59	121.19	111.27
21	3	610	CLA	CMD-C2D-C1D	5.58	134.55	124.71
21	B	1202	CLA	O2D-CGD-CBD	5.58	121.19	111.27
21	5	607	CLA	O2D-CGD-CBD	5.58	121.18	111.27
21	B	1021	CLA	O2A-C1-C2	5.58	123.30	108.64
21	A	1130	CLA	O2A-C1-C2	5.57	123.29	108.64
21	2	603	CLA	CMD-C2D-C1D	5.57	134.53	124.71
21	A	1137	CLA	CAA-C2A-C3A	-5.57	97.53	112.78
21	F	1301	CLA	CMD-C2D-C1D	5.57	134.52	124.71
21	6	601	CLA	CMD-C2D-C1D	5.57	134.52	124.71
21	A	1141	CLA	CMD-C2D-C1D	5.57	134.52	124.71
21	4	608	CLA	O2D-CGD-CBD	5.56	121.16	111.27
21	A	1130	CLA	CMD-C2D-C1D	5.56	134.51	124.71
21	A	1132	CLA	CMD-C2D-C1D	5.56	134.51	124.71
21	3	615	CLA	CMD-C2D-C1D	5.55	134.50	124.71
21	A	1102	CLA	O2A-C1-C2	5.55	123.22	108.64
21	A	1129	CLA	O2D-CGD-CBD	5.55	121.13	111.27
21	3	612	CLA	O2D-CGD-CBD	5.55	121.12	111.27
21	B	1230	CLA	O2A-C1-C2	5.55	123.21	108.64
21	3	601	CLA	CMD-C2D-C1D	5.55	134.49	124.71
21	A	1113	CLA	O2A-C1-C2	5.54	123.21	108.64
21	A	1111	CLA	CMD-C2D-C1D	5.54	134.48	124.71
21	1	608	CLA	O2D-CGD-CBD	5.54	121.11	111.27
21	A	1112	CLA	CMD-C2D-C1D	5.53	134.46	124.71
21	3	611	CLA	O2A-C1-C2	5.53	123.17	108.64
21	1	606	CLA	CMD-C2D-C1D	5.53	134.45	124.71
21	5	602	CLA	O2D-CGD-CBD	5.52	121.07	111.27
21	A	1120	CLA	CAA-C2A-C3A	-5.51	97.69	112.78
21	B	1222	CLA	CMD-C2D-C1D	5.51	134.42	124.71
21	1	615	CLA	CMD-C2D-C1D	5.50	134.41	124.71
21	K	1404	CLA	CMD-C2D-C1D	5.50	134.41	124.71
21	O	1801	CLA	C4C-C3C-C2C	5.50	112.11	107.07
21	5	614	CLA	C1C-C2C-C3C	-5.50	101.18	106.96
21	6	602	CLA	CMD-C2D-C1D	5.49	134.40	124.71
34	2	501	LUT	C7-C8-C9	-5.49	117.93	126.23
21	B	1236	CLA	CMD-C2D-C1D	5.49	134.39	124.71
21	K	1402	CLA	CMD-C2D-C1D	5.49	134.39	124.71
21	1	601	CLA	CMD-C2D-C1D	5.49	134.39	124.71
24	A	4007	BCR	C20-C19-C18	5.49	141.84	126.42
24	G	4001	BCR	C12-C13-C14	5.49	127.36	118.94
24	B	4001	BCR	C23-C22-C21	5.49	127.36	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	611	CLA	CMD-C2D-C1D	5.48	134.38	124.71
21	A	1121	CLA	CMD-C2D-C1D	5.48	134.38	124.71
21	6	604	CLA	CMD-C2D-C1D	5.48	134.37	124.71
21	6	609	CLA	CMD-C2D-C1D	5.48	134.37	124.71
21	B	1201	CLA	CMD-C2D-C1D	5.48	134.37	124.71
21	A	1115	CLA	O2D-CGD-CBD	5.48	121.00	111.27
24	L	4002	BCR	C35-C13-C12	-5.47	109.45	118.08
21	A	1140	CLA	O2D-CGD-CBD	5.47	120.99	111.27
21	B	1206	CLA	CMD-C2D-C1D	5.47	134.35	124.71
21	B	1226	CLA	CMD-C2D-C1D	5.47	134.35	124.71
34	3	501	LUT	C21-C26-C27	5.47	119.62	112.70
21	B	1207	CLA	CMD-C2D-C1D	5.47	134.35	124.71
20	A	1011	CL0	O2D-CGD-CBD	5.46	120.97	111.27
21	A	1134	CLA	O2D-CGD-CBD	5.46	120.97	111.27
21	G	1602	CLA	CMD-C2D-C1D	5.46	134.34	124.71
21	A	1139	CLA	CMD-C2D-C1D	5.46	134.33	124.71
21	1	613	CLA	CMD-C2D-C1D	5.46	134.33	124.71
21	6	608	CLA	CMD-C2D-C1D	5.46	134.33	124.71
21	B	1208	CLA	CMD-C2D-C1D	5.46	134.33	124.71
21	5	606	CLA	CMD-C2D-C1D	5.46	134.33	124.71
21	A	1122	CLA	CMD-C2D-C1D	5.46	134.33	124.71
21	B	1212	CLA	O2D-CGD-CBD	5.45	120.96	111.27
21	A	1137	CLA	CMD-C2D-C1D	5.45	134.32	124.71
21	2	615	CLA	CMD-C2D-C1D	5.45	134.31	124.71
21	G	1601	CLA	CMD-C2D-C1D	5.44	134.31	124.71
21	2	605	CLA	CMD-C2D-C1D	5.44	134.30	124.71
21	5	605	CLA	CMD-C2D-C1D	5.44	134.30	124.71
21	3	603	CLA	O2D-CGD-CBD	5.44	120.94	111.27
21	B	1236	CLA	O2D-CGD-CBD	5.44	120.94	111.27
21	F	1302	CLA	O2D-CGD-CBD	5.44	120.94	111.27
21	5	614	CLA	O2D-CGD-CBD	5.44	120.93	111.27
34	1	501	LUT	C35-C34-C33	5.44	135.07	127.31
21	A	1103	CLA	CMD-C2D-C1D	5.43	134.29	124.71
21	3	607	CLA	O2D-CGD-CBD	5.43	120.92	111.27
21	B	1212	CLA	CMD-C2D-C1D	5.43	134.28	124.71
21	3	602	CLA	CMD-C2D-C1D	5.43	134.28	124.71
21	A	1105	CLA	CMD-C2D-C1D	5.43	134.28	124.71
21	O	1803	CLA	O2A-C1-C2	5.43	122.89	108.64
21	B	1209	CLA	CMD-C2D-C1D	5.42	134.27	124.71
21	6	603	CLA	CMD-C2D-C1D	5.42	134.26	124.71
21	H	1701	CLA	O2D-CGD-CBD	5.42	120.89	111.27
21	1	605	CLA	CMD-C2D-C1D	5.42	134.26	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1140	CLA	O2A-C1-C2	5.41	122.87	108.64
21	5	604	CLA	CMD-C2D-C1D	5.41	134.25	124.71
21	4	615	CLA	CMD-C2D-C1D	5.41	134.25	124.71
21	3	611	CLA	CMD-C2D-C1D	5.41	134.25	124.71
21	A	1132	CLA	O2D-CGD-CBD	5.41	120.88	111.27
21	6	606	CLA	O2D-CGD-CBD	5.41	120.87	111.27
21	2	605	CLA	O2A-C1-C2	5.40	122.83	108.64
21	3	607	CLA	CMD-C2D-C1D	5.40	134.23	124.71
21	B	1228	CLA	CMD-C2D-C1D	5.40	134.22	124.71
21	B	1225	CLA	O2A-C1-C2	5.40	122.81	108.64
21	B	1234	CLA	CMD-C2D-C1D	5.39	134.22	124.71
21	A	1118	CLA	O2A-C1-C2	5.39	122.80	108.64
21	B	1021	CLA	O2D-CGD-CBD	5.39	120.84	111.27
21	B	1210	CLA	CMD-C2D-C1D	5.39	134.21	124.71
21	A	1126	CLA	CMD-C2D-C1D	5.39	134.21	124.71
21	A	1134	CLA	CMD-C2D-C1D	5.39	134.21	124.71
21	A	1104	CLA	O2D-CGD-CBD	5.39	120.84	111.27
21	4	604	CLA	CMD-C2D-C1D	5.39	134.20	124.71
21	1	605	CLA	O2A-C1-C2	5.39	122.79	108.64
21	A	1128	CLA	CMD-C2D-C1D	5.38	134.20	124.71
21	6	607	CLA	CMD-C2D-C1D	5.38	134.20	124.71
21	B	1239	CLA	CMD-C2D-C1D	5.38	134.20	124.71
21	A	1107	CLA	CMD-C2D-C1D	5.38	134.20	124.71
21	J	1901	CLA	O2A-C1-C2	5.38	121.55	108.97
21	L	1502	CLA	CMD-C2D-C1D	5.38	134.19	124.71
21	B	1022	CLA	CMD-C2D-C1D	5.38	134.19	124.71
21	B	1235	CLA	CMD-C2D-C1D	5.38	134.19	124.71
20	A	1011	CL0	C1C-C2C-C3C	-5.38	101.30	106.96
21	A	1116	CLA	CMD-C2D-C1D	5.37	134.18	124.71
34	5	501	LUT	C15-C14-C13	-5.37	119.65	127.31
21	A	1110	CLA	O2D-CGD-CBD	5.37	120.81	111.27
21	A	1116	CLA	O2A-C1-C2	5.37	122.74	108.64
21	6	606	CLA	CMD-C2D-C1D	5.37	134.17	124.71
34	5	503	LUT	C21-C26-C27	5.36	119.48	112.70
20	A	1011	CL0	CHD-C1D-ND	-5.36	119.53	124.45
21	A	1115	CLA	CMD-C2D-C1D	5.36	134.16	124.71
21	B	1230	CLA	CMD-C2D-C1D	5.36	134.16	124.71
21	B	1209	CLA	O2D-CGD-CBD	5.36	120.79	111.27
21	1	608	CLA	O2A-C1-C2	5.36	122.71	108.64
35	3	502	XAT	O24-C25-C24	5.36	117.41	113.38
21	2	607	CLA	CMD-C2D-C1D	5.35	134.14	124.71
21	O	1802	CLA	CMD-C2D-C1D	5.34	134.12	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	L	1503	CLA	O2D-CGD-CBD	5.33	120.75	111.27
21	B	1217	CLA	CMD-C2D-C1D	5.33	134.11	124.71
35	6	502	XAT	C31-C30-C29	-5.33	119.70	127.31
21	L	1503	CLA	CMD-C2D-C1D	5.33	134.10	124.71
21	2	605	CLA	O2D-CGD-CBD	5.33	120.73	111.27
21	B	1239	CLA	O2D-CGD-CBD	5.32	120.73	111.27
21	K	1403	CLA	CHD-C1D-ND	-5.32	119.56	124.45
21	O	1801	CLA	CHD-C1D-ND	-5.32	119.56	124.45
21	K	1401	CLA	CAC-C3C-C4C	5.32	131.71	124.81
21	A	1107	CLA	O2A-C1-C2	5.32	122.61	108.64
21	B	1224	CLA	CMD-C2D-C1D	5.32	134.08	124.71
24	B	4003	BCR	C20-C19-C18	5.31	141.34	126.42
21	A	1125	CLA	CMD-C2D-C1D	5.31	134.06	124.71
21	B	1220	CLA	O2A-C1-C2	5.30	122.57	108.64
21	B	1023	CLA	CMD-C2D-C1D	5.30	134.06	124.71
21	B	1216	CLA	O2A-C1-C2	5.30	122.56	108.64
31	2	804	LMG	O7-C10-C11	5.30	122.91	111.50
24	A	4007	BCR	C19-C18-C17	5.29	127.06	118.94
34	5	504	LUT	C7-C8-C9	-5.29	118.24	126.23
21	B	1215	CLA	CMD-C2D-C1D	5.29	134.03	124.71
21	B	1217	CLA	O2A-C1-C2	5.29	122.53	108.64
21	K	1403	CLA	O2D-CGD-CBD	5.29	120.66	111.27
21	A	1113	CLA	CMD-C2D-C1D	5.28	134.02	124.71
21	4	607	CLA	O2A-C1-C2	5.27	122.49	108.64
34	6	501	LUT	C31-C30-C29	-5.27	119.79	127.31
21	B	1223	CLA	O2D-CGD-CBD	5.27	120.62	111.27
21	A	1131	CLA	O2A-C1-C2	5.25	122.44	108.64
21	6	602	CLA	O2D-CGD-CBD	5.25	120.60	111.27
21	4	609	CLA	O2A-C1-C2	5.25	122.44	108.64
21	B	1224	CLA	O2D-CGD-CBD	5.25	120.60	111.27
21	A	1120	CLA	O2D-CGD-CBD	5.25	120.59	111.27
21	H	1702	CLA	CMD-C2D-C1D	5.24	133.95	124.71
21	L	1503	CLA	O2A-C1-C2	5.24	122.41	108.64
34	5	501	LUT	C21-C26-C25	5.24	120.81	111.42
21	B	1227	CLA	O2A-C1-C2	5.24	122.41	108.64
34	6	501	LUT	C35-C34-C33	-5.24	119.83	127.31
21	3	606	CLA	CMD-C2D-C1D	5.24	133.94	124.71
21	B	1235	CLA	O2D-CGD-CBD	5.23	120.57	111.27
21	B	1229	CLA	O2A-C1-C2	5.23	122.39	108.64
21	2	612	CLA	O2D-CGD-CBD	5.23	120.56	111.27
21	K	1404	CLA	O2D-CGD-CBD	5.22	120.55	111.27
21	A	1012	CLA	CMD-C2D-C1D	5.21	133.90	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1213	CLA	O2D-CGD-CBD	5.21	120.53	111.27
21	5	605	CLA	O2D-CGD-CBD	5.21	120.53	111.27
21	1	605	CLA	O2D-CGD-CBD	5.21	120.52	111.27
21	2	608	CLA	O2D-CGD-CBD	5.21	120.52	111.27
21	A	1118	CLA	C2A-C3A-C4A	5.20	110.28	101.87
21	B	1208	CLA	O2D-CGD-CBD	5.20	120.51	111.27
21	3	610	CLA	O2D-CGD-CBD	5.20	120.51	111.27
21	4	612	CLA	CMD-C2D-C1D	5.20	133.87	124.71
21	B	1217	CLA	O2D-CGD-CBD	5.19	120.50	111.27
21	A	1101	CLA	O2A-C1-C2	5.19	122.28	108.64
21	B	1223	CLA	O2A-C1-C2	5.18	122.26	108.64
21	B	1218	CLA	O2D-CGD-CBD	5.18	120.47	111.27
21	B	1227	CLA	CMD-C2D-C1D	5.17	133.83	124.71
21	F	1302	CLA	CMD-C2D-C1D	5.17	133.83	124.71
21	B	1237	CLA	CMD-C2D-C1D	5.17	133.83	124.71
21	4	602	CLA	O2A-C1-C2	5.16	122.20	108.64
21	2	602	CLA	CMD-C2D-C1D	5.16	133.81	124.71
21	A	1130	CLA	O2D-CGD-CBD	5.16	120.44	111.27
21	A	1107	CLA	O2D-CGD-CBD	5.16	120.44	111.27
21	4	608	CLA	CMD-C2D-C1D	5.16	133.81	124.71
21	6	603	CLA	O2D-CGD-CBD	5.15	120.42	111.27
21	6	608	CLA	O2D-CGD-CBD	5.15	120.42	111.27
21	1	603	CLA	O2A-C1-C2	5.15	122.16	108.64
21	1	602	CLA	CMD-C2D-C1D	5.15	133.78	124.71
21	B	1231	CLA	O2A-C1-C2	5.15	122.16	108.64
21	B	1226	CLA	O2A-C1-C2	5.14	122.15	108.64
35	6	504	XAT	O23-C23-C24	-5.14	99.58	109.80
21	B	1231	CLA	O2D-CGD-CBD	5.14	120.40	111.27
35	1	502	XAT	C7-C8-C9	-5.14	117.56	125.53
21	1	612	CLA	CMD-C2D-C1D	5.13	133.75	124.71
21	B	1229	CLA	CMD-C2D-C1D	5.13	133.75	124.71
21	6	613	CLA	O2D-CGD-CBD	5.12	120.37	111.27
34	5	503	LUT	C37-C21-C22	5.12	119.14	109.44
21	B	1023	CLA	O2A-C1-C2	5.12	122.09	108.64
21	A	1118	CLA	CMD-C2D-C1D	5.12	133.74	124.71
21	B	1240	CLA	CMD-C2D-C1D	5.12	133.74	124.71
21	4	604	CLA	O2A-C1-C2	5.12	122.08	108.64
21	B	1232	CLA	O2A-C1-C2	5.12	122.08	108.64
21	A	1135	CLA	CMD-C2D-C1D	5.11	133.72	124.71
21	A	1114	CLA	O2D-CGD-CBD	5.11	120.35	111.27
21	B	1022	CLA	O2D-CGD-CBD	5.11	120.35	111.27
21	5	604	CLA	O2A-C1-C2	5.10	122.05	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	2	501	LUT	C21-C26-C27	5.10	119.15	112.70
21	1	601	CLA	O2A-C1-C2	5.09	122.02	108.64
21	5	604	CLA	O2D-CGD-CBD	5.09	120.32	111.27
21	B	1223	CLA	CMD-C2D-C1D	5.09	133.68	124.71
21	5	607	CLA	CMD-C2D-C1D	5.09	133.68	124.71
21	1	611	CLA	O2D-CGD-CBD	5.09	120.31	111.27
21	1	601	CLA	O2D-CGD-CBD	5.08	120.29	111.27
34	4	501	LUT	C21-C26-C25	5.08	120.51	111.42
21	B	1234	CLA	O2D-CGD-CBD	5.08	120.29	111.27
21	B	1232	CLA	CMD-C2D-C1D	5.08	133.66	124.71
21	K	1402	CLA	O2D-CGD-CBD	5.08	120.29	111.27
21	5	607	CLA	C2C-C1C-NC	5.07	114.73	109.97
21	4	601	CLA	O2A-C1-C2	5.07	121.96	108.64
20	A	1011	CL0	O2A-C1-C2	5.07	121.96	108.64
34	5	501	LUT	C35-C34-C33	-5.07	120.08	127.31
34	5	503	LUT	C15-C14-C13	-5.06	120.08	127.31
21	4	612	CLA	O2A-C1-C2	5.06	121.93	108.64
21	3	610	CLA	O2A-C1-C2	5.05	121.90	108.64
21	2	604	CLA	O2A-C1-C2	5.04	121.87	108.64
21	B	1207	CLA	O2D-CGD-CBD	5.04	120.22	111.27
34	1	501	LUT	C12-C13-C14	-5.03	111.22	118.94
21	B	1218	CLA	CAA-C2A-C3A	-5.03	98.99	112.78
21	6	601	CLA	O2D-CGD-CBD	5.03	120.21	111.27
21	A	1124	CLA	O2A-C1-C2	5.03	121.86	108.64
21	A	1104	CLA	CMD-C2D-C3D	-5.03	116.05	127.61
21	1	612	CLA	O2A-C1-C2	5.03	121.85	108.64
21	B	1205	CLA	O2D-CGD-CBD	5.03	120.20	111.27
21	4	601	CLA	CMD-C2D-C1D	5.02	133.57	124.71
21	A	1116	CLA	O2D-CGD-CBD	5.02	120.19	111.27
21	A	1140	CLA	CMD-C2D-C1D	5.02	133.56	124.71
21	B	1211	CLA	O2D-CGD-CBD	5.02	120.19	111.27
20	A	1011	CL0	O2A-CGA-O1A	-5.02	110.93	123.59
21	4	615	CLA	O2D-CGD-CBD	5.02	120.18	111.27
21	3	608	CLA	O2A-C1-C2	5.01	121.81	108.64
21	B	1204	CLA	CMD-C2D-C1D	5.01	133.55	124.71
21	A	1124	CLA	O2D-CGD-CBD	5.00	120.16	111.27
21	A	1106	CLA	O2A-C1-C2	5.00	121.77	108.64
21	G	1601	CLA	O2D-CGD-CBD	5.00	120.15	111.27
21	B	1208	CLA	O2A-C1-C2	5.00	121.77	108.64
34	5	503	LUT	C31-C30-C29	-5.00	120.18	127.31
21	2	615	CLA	O2D-CGD-CBD	4.99	120.14	111.27
21	B	1022	CLA	O2A-C1-C2	4.99	121.75	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1120	CLA	CMD-C2D-C1D	4.98	133.49	124.71
21	6	609	CLA	O2D-CGD-CBD	4.98	120.12	111.27
21	B	1220	CLA	CMD-C2D-C1D	4.98	133.48	124.71
21	A	1132	CLA	O2A-C1-C2	4.97	121.70	108.64
21	3	613	CLA	O2D-CGD-CBD	4.97	120.10	111.27
25	5	802	LHG	O7-C7-C8	4.97	120.23	111.09
21	A	1133	CLA	O2A-C1-C2	4.97	121.69	108.64
21	6	603	CLA	O2A-C1-C2	4.97	121.69	108.64
21	A	1111	CLA	O2A-C1-C2	4.97	121.69	108.64
33	O	5002	PTY	O7-C8-C11	4.97	120.23	111.09
21	3	602	CLA	O2D-CGD-CBD	4.97	120.09	111.27
21	B	1212	CLA	O2A-C1-C2	4.96	121.68	108.64
21	B	1216	CLA	CMD-C2D-C1D	4.96	133.45	124.71
21	B	1235	CLA	O2A-C1-C2	4.95	121.63	108.64
21	4	601	CLA	O1D-CGD-CBD	-4.94	114.37	124.48
21	H	1701	CLA	CMD-C2D-C1D	4.94	133.42	124.71
34	5	503	LUT	C11-C10-C9	-4.94	120.27	127.31
21	A	1012	CLA	O2D-CGD-CBD	4.93	120.03	111.27
21	1	602	CLA	O2D-CGD-CBD	4.93	120.03	111.27
21	3	612	CLA	CMD-C2D-C1D	4.93	133.40	124.71
24	A	4001	BCR	C39-C30-C25	4.93	118.29	110.30
21	A	1125	CLA	O2D-CGD-CBD	4.93	120.02	111.27
21	A	1124	CLA	CMD-C2D-C1D	4.92	133.38	124.71
21	3	602	CLA	O2A-C1-C2	4.92	121.56	108.64
21	B	1021	CLA	CMD-C2D-C1D	4.92	133.38	124.71
24	B	4003	BCR	C15-C14-C13	-4.92	120.29	127.31
21	B	1205	CLA	CMD-C2D-C1D	4.92	133.38	124.71
24	3	506	BCR	C35-C13-C14	-4.92	116.04	122.92
21	B	1207	CLA	O2A-C1-C2	4.91	121.55	108.64
21	2	606	CLA	O2A-C1-C2	4.91	121.55	108.64
21	G	1602	CLA	O2D-CGD-CBD	4.91	120.00	111.27
21	2	606	CLA	O2D-CGD-CBD	4.91	119.99	111.27
20	A	1011	CL0	C3D-C2D-C1D	-4.90	99.14	105.83
21	3	606	CLA	O2A-C1-C2	4.90	121.51	108.64
21	6	606	CLA	O2A-C1-C2	4.90	121.51	108.64
21	1	615	CLA	O2A-C1-C2	4.89	121.49	108.64
34	5	501	LUT	C31-C30-C29	-4.89	120.33	127.31
21	3	615	CLA	O2D-CGD-CBD	4.89	119.96	111.27
21	A	1109	CLA	O2D-CGD-CBD	4.89	119.95	111.27
35	2	502	XAT	C18-C5-C4	4.88	119.77	114.28
21	4	603	CLA	O2A-C1-C2	4.88	121.46	108.64
21	5	612	CLA	CAC-C3C-C4C	4.88	131.14	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	605	CLA	O2A-C1-C2	4.88	121.45	108.64
21	B	1216	CLA	O2D-CGD-CBD	4.87	119.92	111.27
21	B	1215	CLA	O2D-CGD-CBD	4.87	119.92	111.27
21	L	1504	CLA	O2D-CGD-CBD	4.87	119.92	111.27
21	2	608	CLA	O2A-C1-C2	4.87	121.42	108.64
21	A	1121	CLA	O2A-C1-C2	4.86	121.42	108.64
21	H	1702	CLA	CMB-C2B-C1B	-4.86	117.97	125.37
21	F	1301	CLA	O2D-CGD-CBD	4.85	119.89	111.27
20	A	1011	CL0	C3B-C2B-C1B	-4.85	101.31	107.16
21	4	602	CLA	CMD-C2D-C1D	4.85	133.25	124.71
24	I	4002	BCR	C33-C5-C6	-4.84	119.09	124.53
33	L	5003	PTY	O7-C8-C11	4.84	120.00	111.09
35	3	502	XAT	O3-C3-C4	-4.84	100.19	109.80
21	5	606	CLA	O2D-CGD-CBD	4.84	119.86	111.27
21	A	1108	CLA	O2A-C1-C2	4.84	121.34	108.64
35	1	502	XAT	C38-C25-C24	4.83	119.72	114.28
21	A	1115	CLA	O2A-C1-C2	4.83	121.33	108.64
21	B	1225	CLA	CMD-C2D-C1D	4.83	133.22	124.71
21	3	605	CLA	O2A-C1-C2	4.82	121.31	108.64
21	3	601	CLA	O2D-CGD-CBD	4.82	119.83	111.27
21	A	1105	CLA	O2D-CGD-CBD	4.82	119.83	111.27
21	B	1206	CLA	O2D-CGD-CBD	4.82	119.83	111.27
21	3	612	CLA	O2A-C1-C2	4.82	121.30	108.64
21	6	604	CLA	O2A-C1-C2	4.81	121.28	108.64
21	4	604	CLA	O2D-CGD-CBD	4.81	119.82	111.27
21	A	1120	CLA	O2A-C1-C2	4.81	121.26	108.64
21	B	1239	CLA	O2A-C1-C2	4.80	121.26	108.64
21	B	1228	CLA	O2A-C1-C2	4.80	121.25	108.64
33	3	808	PTY	O7-C8-C11	4.80	119.92	111.09
21	L	1504	CLA	O2A-C1-C2	4.80	121.24	108.64
21	A	1126	CLA	O2D-CGD-CBD	4.80	119.79	111.27
21	6	607	CLA	O2A-C1-C2	4.80	121.24	108.64
21	6	602	CLA	O2A-C1-C2	4.79	121.23	108.64
21	A	1123	CLA	CMD-C2D-C1D	4.79	133.16	124.71
21	1	606	CLA	O2A-C1-C2	4.79	121.23	108.64
21	G	1603	CLA	CBC-CAC-C3C	-4.79	99.22	112.43
24	A	4003	BCR	C37-C22-C23	4.78	125.62	118.08
21	B	1237	CLA	O2D-CGD-CBD	4.78	119.77	111.27
21	1	607	CLA	O2D-CGD-CBD	4.78	119.76	111.27
21	5	608	CLA	O2A-C1-C2	4.78	121.19	108.64
21	5	608	CLA	CMD-C2D-C1D	4.78	133.13	124.71
21	4	603	CLA	O2D-CGD-CBD	4.78	119.76	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1225	CLA	O2D-CGD-CBD	4.77	119.75	111.27
21	3	613	CLA	CMD-C2D-C1D	4.77	133.12	124.71
21	1	611	CLA	O2A-C1-C2	4.77	121.17	108.64
21	6	612	CLA	O2D-CGD-O1D	-4.77	114.51	123.84
21	A	1138	CLA	CMD-C2D-C1D	4.77	133.12	124.71
21	B	1228	CLA	O2D-CGD-CBD	4.76	119.73	111.27
21	3	611	CLA	O2D-CGD-CBD	4.76	119.72	111.27
21	A	1114	CLA	O2A-C1-C2	4.74	121.10	108.64
21	B	1237	CLA	O2A-C1-C2	4.73	121.07	108.64
21	A	1106	CLA	CMD-C2D-C1D	4.73	133.05	124.71
21	3	608	CLA	O2D-CGD-CBD	4.73	119.67	111.27
21	4	615	CLA	O2A-C1-C2	4.72	121.05	108.64
21	A	1122	CLA	O2D-CGD-CBD	4.72	119.65	111.27
21	3	606	CLA	CAC-C3C-C4C	4.72	130.93	124.81
21	A	1121	CLA	O2D-CGD-CBD	4.72	119.65	111.27
21	B	1206	CLA	O2A-C1-C2	4.71	121.02	108.64
34	6	501	LUT	C18-C5-C6	-4.71	119.24	124.53
21	A	1139	CLA	CAA-CBA-CGA	-4.71	99.49	113.25
21	2	603	CLA	O2D-CGD-CBD	4.71	119.64	111.27
21	A	1141	CLA	O2D-CGD-CBD	4.71	119.63	111.27
21	6	605	CLA	O2A-C1-C2	4.70	120.99	108.64
21	5	613	CLA	O2D-CGD-O1D	-4.70	114.65	123.84
21	A	1137	CLA	O2D-CGD-CBD	4.70	119.61	111.27
21	L	1502	CLA	C1-C2-C3	-4.69	117.92	126.04
34	5	503	LUT	C18-C5-C6	-4.69	119.26	124.53
21	B	1219	CLA	O2D-CGD-CBD	4.69	119.61	111.27
21	2	612	CLA	CMD-C2D-C1D	4.69	132.97	124.71
21	A	1116	CLA	C1-C2-C3	-4.69	117.94	126.04
21	6	601	CLA	O2A-C1-C2	4.68	120.94	108.64
21	O	1803	CLA	O2D-CGD-CBD	4.68	119.58	111.27
21	1	607	CLA	CMD-C2D-C1D	4.68	132.96	124.71
21	A	1112	CLA	O2A-C1-C2	4.68	120.93	108.64
21	B	1222	CLA	O2A-C1-C2	4.68	120.92	108.64
34	5	502	LUT	C18-C5-C6	-4.67	119.28	124.53
24	A	4002	BCR	C34-C9-C10	-4.67	116.38	122.92
21	B	1205	CLA	O2A-C1-C2	4.67	120.90	108.64
34	5	502	LUT	C15-C14-C13	-4.66	120.66	127.31
21	5	608	CLA	O2D-CGD-CBD	4.66	119.54	111.27
21	A	1103	CLA	O2A-C1-C2	4.66	120.87	108.64
21	A	1134	CLA	O2A-C1-C2	4.66	120.87	108.64
21	5	614	CLA	CAC-C3C-C4C	-4.65	118.77	124.81
21	B	1240	CLA	O2D-CGD-CBD	4.65	119.53	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	1	501	LUT	C31-C32-C33	-4.65	113.35	126.42
21	B	1203	CLA	O2A-C1-C2	4.65	120.85	108.64
21	A	1130	CLA	CMB-C2B-C1B	-4.65	118.29	125.37
21	B	1203	CLA	O2D-CGD-CBD	4.64	119.52	111.27
21	3	613	CLA	C2D-C1D-ND	4.64	113.52	110.10
21	A	1123	CLA	O2A-C1-C2	4.63	120.80	108.64
21	2	603	CLA	O2A-C1-C2	4.62	120.79	108.64
21	A	1137	CLA	O2A-C1-C2	4.62	120.79	108.64
21	3	607	CLA	O2A-C1-C2	4.62	120.79	108.64
21	5	607	CLA	O2A-C1-C2	4.61	120.76	108.64
36	3	604	CHL	CMA-C3A-C4A	4.61	124.17	111.77
34	3	501	LUT	C7-C8-C9	-4.61	119.28	126.23
21	A	1113	CLA	O2D-CGD-CBD	4.60	119.45	111.27
24	I	4002	BCR	C15-C14-C13	-4.60	120.74	127.31
34	5	504	LUT	C11-C10-C9	-4.60	120.75	127.31
21	A	1122	CLA	O2A-C1-C2	4.60	120.72	108.64
21	4	606	CLA	O2A-C1-C2	4.59	120.70	108.64
21	2	602	CLA	O2D-CGD-CBD	4.59	119.43	111.27
21	5	613	CLA	CMB-C2B-C1B	-4.59	118.38	125.37
21	K	1402	CLA	O2A-C1-C2	4.58	120.67	108.64
21	A	1125	CLA	O2A-C1-C2	4.58	120.67	108.64
21	5	606	CLA	O2A-C1-C2	4.58	120.66	108.64
29	5	807	3PH	O21-C21-C22	4.58	121.36	111.50
21	6	612	CLA	O2A-C1-C2	4.57	120.65	108.64
34	5	501	LUT	C7-C8-C9	-4.57	119.33	126.23
21	4	606	CLA	O2D-CGD-CBD	4.55	119.36	111.27
21	1	615	CLA	O2D-CGD-CBD	4.55	119.35	111.27
21	B	1023	CLA	O2D-CGD-CBD	4.55	119.35	111.27
21	1	606	CLA	O2D-CGD-CBD	4.55	119.35	111.27
21	2	604	CLA	CMD-C2D-C1D	4.54	132.72	124.71
21	A	1136	CLA	CMD-C2D-C1D	4.54	132.71	124.71
24	G	4001	BCR	C35-C13-C14	-4.54	116.57	122.92
21	6	604	CLA	O2D-CGD-CBD	4.54	119.33	111.27
24	K	4001	BCR	C33-C5-C6	-4.53	119.44	124.53
21	A	1119	CLA	O2D-CGD-CBD	4.52	119.30	111.27
21	B	1204	CLA	O2A-C1-C2	4.52	120.52	108.64
21	K	1401	CLA	CHD-C1D-ND	-4.52	120.30	124.45
21	A	1108	CLA	CMD-C2D-C1D	4.52	132.68	124.71
34	5	504	LUT	C22-C23-C24	4.52	116.89	111.74
21	A	1118	CLA	C2B-C1B-NB	-4.52	107.20	110.23
21	6	612	CLA	CMD-C2D-C1D	4.50	132.65	124.71
21	K	1401	CLA	CAC-C3C-C2C	-4.50	119.84	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	H	1702	CLA	C2C-C1C-NC	4.49	114.18	109.97
24	H	4001	BCR	C23-C22-C21	4.48	125.81	118.94
21	3	605	CLA	O2D-CGD-CBD	4.47	119.22	111.27
22	B	2002	PQN	C14-C13-C15	4.47	122.78	115.27
35	6	504	XAT	C15-C14-C13	-4.46	120.94	127.31
24	I	4001	BCR	C33-C5-C6	-4.46	119.52	124.53
21	5	603	CLA	O2A-C1-C2	4.46	120.35	108.64
21	4	607	CLA	CMD-C2D-C1D	4.46	132.57	124.71
21	A	1139	CLA	O2D-CGD-CBD	4.45	119.18	111.27
34	2	501	LUT	C22-C23-C24	-4.45	106.67	111.74
21	3	608	CLA	CMD-C2D-C1D	4.45	132.55	124.71
34	5	502	LUT	C21-C26-C27	4.44	118.32	112.70
21	A	1123	CLA	O2D-CGD-CBD	4.44	119.16	111.27
36	2	611	CHL	C4A-NA-C1A	4.44	108.70	106.71
21	1	603	CLA	O2D-CGD-CBD	4.44	119.16	111.27
35	1	502	XAT	C15-C14-C13	-4.43	120.98	127.31
21	A	1141	CLA	O2A-CGA-CBA	4.43	125.81	111.91
24	F	4001	BCR	C33-C5-C6	-4.43	119.55	124.53
21	3	603	CLA	CMD-C2D-C1D	4.43	132.52	124.71
21	A	1141	CLA	O2A-C1-C2	4.43	120.27	108.64
21	K	1403	CLA	CMD-C2D-C3D	-4.42	117.44	127.61
36	3	604	CHL	C1-O2A-CGA	4.42	128.03	116.44
21	4	605	CLA	O2A-C1-C2	4.41	120.22	108.64
21	3	614	CLA	O2D-CGD-CBD	4.40	119.09	111.27
21	2	602	CLA	O2A-C1-C2	4.40	120.20	108.64
34	5	503	LUT	C21-C26-C25	4.39	119.29	111.42
36	6	610	CHL	CHD-C1D-ND	-4.38	120.43	124.45
24	B	4003	BCR	C27-C26-C25	-4.38	116.37	122.73
25	B	5001	LHG	O7-C7-C8	4.38	120.93	111.50
35	3	502	XAT	O4-C5-C4	-4.37	110.10	113.38
21	B	1214	CLA	O2A-C1-C2	4.37	120.12	108.64
34	2	501	LUT	C21-C26-C25	4.36	119.23	111.42
21	H	1701	CLA	O2A-C1-C2	4.36	120.09	108.64
35	6	504	XAT	O24-C25-C38	-4.36	109.84	115.06
24	J	4001	BCR	C33-C5-C6	-4.35	119.64	124.53
21	B	1219	CLA	O2A-C1-C2	4.35	120.07	108.64
35	6	502	XAT	C15-C14-C13	-4.35	121.10	127.31
24	A	4001	BCR	C33-C5-C6	-4.35	119.64	124.53
21	B	1215	CLA	O2A-C1-C2	4.34	120.05	108.64
24	A	4001	BCR	C39-C30-C29	-4.34	91.55	108.91
21	5	601	CLA	CMB-C2B-C1B	-4.34	118.76	125.37
21	G	1603	CLA	O2D-CGD-CBD	4.34	118.97	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1012	CLA	O2A-C1-C2	4.33	120.02	108.64
24	A	4002	BCR	C34-C9-C8	4.33	124.90	118.08
36	4	611	CHL	CHD-C1D-ND	-4.33	120.48	124.45
21	A	1127	CLA	O2D-CGD-CBD	4.32	118.95	111.27
35	1	502	XAT	O4-C5-C4	-4.32	110.14	113.38
25	2	801	LHG	O7-C7-C8	4.32	120.81	111.50
21	B	1221	CLA	O2A-C1-C2	4.32	119.98	108.64
34	5	504	LUT	C35-C34-C33	-4.32	121.15	127.31
34	5	503	LUT	C7-C8-C9	-4.31	119.72	126.23
21	6	605	CLA	O2D-CGD-CBD	4.31	118.92	111.27
21	1	613	CLA	O2D-CGD-CBD	4.30	118.91	111.27
35	6	504	XAT	C38-C25-C26	4.30	129.46	122.26
34	5	501	LUT	C38-C25-C24	-4.29	114.38	123.56
21	B	1210	CLA	O2A-C1-C2	4.29	119.90	108.64
20	A	1011	CL0	C1D-ND-C4D	-4.28	103.29	106.33
21	H	1701	CLA	C2C-C1C-NC	4.28	113.99	109.97
21	H	1702	CLA	C4A-NA-C1A	4.28	108.63	106.71
28	3	805	DGD	O2G-C1B-C2B	4.28	120.72	111.50
29	B	5003	3PH	O21-C21-C22	4.27	120.70	111.50
33	1	805	PTY	O7-C8-C11	4.27	120.70	111.50
24	A	4002	BCR	C19-C18-C17	4.27	125.49	118.94
21	1	604	CLA	CMA-C3A-C4A	4.26	123.23	111.77
33	3	807	PTY	O7-C8-C11	4.26	120.68	111.50
21	6	605	CLA	C1-C2-C3	-4.25	118.68	126.04
21	A	1103	CLA	CAA-C2A-C3A	-4.25	101.14	112.78
21	O	1801	CLA	C2C-C1C-NC	4.25	113.95	109.97
21	5	601	CLA	CHD-C1D-ND	-4.24	120.55	124.45
34	6	501	LUT	C21-C26-C27	4.24	118.06	112.70
20	A	1011	CL0	C2B-C1B-NB	4.20	113.05	110.23
21	L	1502	CLA	C2D-C1D-ND	4.19	113.19	110.10
21	B	1226	CLA	O2D-CGD-CBD	4.18	118.69	111.27
21	J	1901	CLA	C2C-C1C-NC	4.18	113.88	109.97
34	3	501	LUT	C21-C26-C25	4.17	118.89	111.42
21	6	605	CLA	C4-C3-C2	-4.17	112.97	123.68
21	O	1801	CLA	CMD-C2D-C3D	-4.17	118.02	127.61
34	5	501	LUT	C21-C26-C27	4.17	117.97	112.70
24	A	4002	BCR	C28-C27-C26	-4.17	106.63	114.08
28	2	806	DGD	O2G-C1B-C2B	4.17	120.49	111.50
34	5	502	LUT	C11-C10-C9	-4.17	121.36	127.31
21	B	1207	CLA	C1-C2-C3	-4.16	118.85	126.04
34	5	502	LUT	C35-C34-C33	-4.16	121.37	127.31
25	2	802	LHG	O7-C7-C8	4.16	120.46	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	613	CLA	CHD-C1D-ND	-4.16	120.63	124.45
25	A	5001	LHG	O7-C7-C8	4.16	120.46	111.50
35	3	502	XAT	C7-C8-C9	-4.15	119.09	125.53
21	B	1204	CLA	O2D-CGD-O1D	-4.14	115.74	123.84
21	K	1401	CLA	C3B-C4B-NB	-4.14	106.68	110.52
34	5	504	LUT	C38-C25-C24	-4.13	114.72	123.56
24	3	506	BCR	C19-C18-C17	4.13	125.27	118.94
21	J	1901	CLA	C4B-CHC-C1C	4.13	136.12	126.34
34	4	501	LUT	C31-C30-C29	-4.12	121.43	127.31
31	3	803	LMG	O7-C10-C11	4.12	120.38	111.50
39	5	806	P3H	O39-C40-C42	4.11	120.37	111.50
24	H	4001	BCR	C37-C22-C21	-4.11	117.17	122.92
21	A	1013	CLA	O2D-CGD-CBD	4.11	118.57	111.27
21	K	1403	CLA	C1C-C2C-C3C	-4.11	102.64	106.96
21	G	1603	CLA	C1C-C2C-C3C	-4.11	102.64	106.96
36	5	609	CHL	CHD-C1D-ND	-4.10	120.69	124.45
21	5	604	CLA	CAA-C2A-C3A	-4.10	101.55	112.78
24	B	4003	BCR	C30-C25-C26	-4.10	116.84	122.61
24	O	4001	BCR	C8-C9-C10	4.09	125.22	118.94
25	1	802	LHG	O7-C7-C8	4.08	120.30	111.50
35	4	502	XAT	C38-C25-C24	4.08	118.87	114.28
21	2	615	CLA	O2A-C1-C2	4.08	119.36	108.64
21	4	612	CLA	O2D-CGD-CBD	4.07	118.51	111.27
21	A	1127	CLA	C1-C2-C3	-4.07	119.00	126.04
28	3	804	DGD	O2G-C1B-C2B	4.07	120.28	111.50
36	4	611	CHL	C3B-C4B-NB	-4.07	106.74	110.52
21	B	1210	CLA	C2C-C1C-NC	4.07	113.78	109.97
33	1	806	PTY	O7-C8-C11	4.05	118.55	111.09
24	A	4001	BCR	C40-C30-C39	4.05	120.97	108.53
21	A	1128	CLA	O2A-C1-C2	4.05	119.28	108.64
35	4	502	XAT	C15-C14-C13	-4.04	121.54	127.31
21	A	1126	CLA	O2A-C1-C2	4.04	119.26	108.64
33	6	804	PTY	O7-C8-C11	4.04	120.21	111.50
24	J	4002	BCR	C36-C18-C17	-4.04	117.27	122.92
35	3	502	XAT	C37-C21-C36	-4.04	101.41	107.37
21	L	1501	CLA	CMA-C3A-C4A	4.04	122.62	111.77
21	B	1201	CLA	O2A-C1-C2	4.03	123.12	109.49
21	B	1218	CLA	C1-C2-C3	-4.03	119.07	126.04
35	6	504	XAT	C38-C25-C24	-4.02	109.75	114.28
21	H	1701	CLA	CAC-C3C-C4C	4.02	130.02	124.81
21	A	1109	CLA	CHD-C1D-ND	-4.01	120.77	124.45
21	B	1213	CLA	O2A-C1-C2	4.01	119.18	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1135	CLA	OBD-CAD-C3D	-4.01	118.87	128.52
33	4	804	PTY	O7-C8-C11	4.00	120.13	111.50
21	6	605	CLA	C4-C3-C5	4.00	122.00	115.27
21	K	1401	CLA	C2C-C1C-NC	4.00	113.72	109.97
21	5	614	CLA	C2C-C1C-NC	4.00	113.72	109.97
35	3	502	XAT	C15-C14-C13	-3.99	121.61	127.31
24	3	506	BCR	C27-C26-C25	-3.99	116.94	122.73
21	B	1210	CLA	O2D-CGD-O1D	-3.99	116.05	123.84
20	A	1011	CL0	O2A-CGA-CBA	3.98	124.39	111.91
24	H	4001	BCR	C30-C25-C26	-3.98	117.01	122.61
21	5	607	CLA	C1-O2A-CGA	3.97	126.87	116.44
24	A	4003	BCR	C37-C22-C21	-3.97	117.36	122.92
36	2	613	CHL	C3B-C2B-C1B	3.97	111.96	107.16
21	A	1130	CLA	CMB-C2B-C3B	3.97	136.19	126.59
34	6	501	LUT	C11-C10-C9	-3.96	121.65	127.31
36	1	610	CHL	C4B-CHC-C1C	3.96	135.73	126.34
21	3	610	CLA	C1-C2-C3	-3.96	120.35	126.75
24	O	4001	BCR	C2-C1-C6	3.96	116.57	110.48
25	A	5002	LHG	O7-C7-C8	3.95	120.02	111.50
21	5	614	CLA	C1-C2-C3	-3.95	119.21	126.04
24	J	4001	BCR	C29-C28-C27	-3.95	102.56	111.38
21	5	608	CLA	C2C-C1C-NC	3.95	113.67	109.97
21	A	1105	CLA	CAA-C2A-C3A	-3.95	101.97	112.78
21	L	1501	CLA	O2A-C1-C2	3.94	118.99	108.64
21	5	614	CLA	C3D-C2D-C1D	-3.94	100.45	105.83
34	5	502	LUT	C7-C8-C9	-3.94	120.28	126.23
33	5	803	PTY	O7-C8-C11	3.94	119.99	111.50
35	4	502	XAT	C31-C30-C29	-3.93	121.70	127.31
21	O	1803	CLA	O2A-CGA-CBA	3.92	124.22	111.91
29	F	5003	3PH	O21-C21-C22	3.92	119.94	111.50
21	B	1220	CLA	CAA-C2A-C3A	-3.92	102.06	112.78
21	A	1127	CLA	CMD-C2D-C1D	3.91	131.61	124.71
34	1	501	LUT	C10-C11-C12	-3.91	111.03	123.22
21	B	1240	CLA	O2A-C1-C2	3.91	118.90	108.64
21	3	603	CLA	C2D-C1D-ND	3.91	112.98	110.10
24	J	4001	BCR	C32-C1-C6	-3.91	103.97	110.30
24	F	4002	BCR	C23-C22-C21	3.90	124.93	118.94
21	A	1117	CLA	CMD-C2D-C1D	3.90	131.58	124.71
29	5	804	3PH	O21-C21-C22	3.90	119.90	111.50
24	B	4003	BCR	C38-C26-C27	3.89	121.10	113.62
21	K	1401	CLA	CAA-C2A-C3A	-3.89	102.12	112.78
24	H	4001	BCR	C3-C4-C5	-3.89	107.13	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	801	LHG	O7-C7-C8	3.89	119.89	111.50
21	A	1013	CLA	CMD-C2D-C1D	3.89	131.57	124.71
35	6	504	XAT	O24-C25-C24	3.89	116.30	113.38
21	A	1117	CLA	O2D-CGD-O1D	-3.88	116.25	123.84
21	H	1701	CLA	CMA-C3A-C4A	3.88	122.20	111.77
21	3	608	CLA	CMC-C2C-C1C	3.88	130.94	125.04
21	L	1502	CLA	CHD-C1D-ND	-3.88	120.89	124.45
21	2	601	CLA	O1D-CGD-CBD	-3.87	116.56	124.48
34	4	501	LUT	C35-C34-C33	-3.87	121.78	127.31
21	6	602	CLA	C1-C2-C3	-3.87	120.48	126.75
31	6	802	LMG	O7-C10-C11	3.87	119.85	111.50
21	A	1123	CLA	C2C-C1C-NC	3.87	113.60	109.97
35	1	502	XAT	C31-C30-C29	-3.86	121.79	127.31
34	2	501	LUT	C38-C25-C24	-3.86	115.29	123.56
36	1	609	CHL	CHD-C1D-ND	-3.86	120.91	124.45
24	H	4001	BCR	C27-C26-C25	-3.85	117.14	122.73
24	A	4007	BCR	C34-C9-C10	-3.85	117.53	122.92
39	2	808	P3H	O39-C40-C42	3.84	119.78	111.50
35	6	504	XAT	C7-C8-C9	-3.84	119.58	125.53
35	3	502	XAT	C31-C30-C29	-3.84	121.83	127.31
21	A	1117	CLA	O2A-C1-C2	3.83	118.70	108.64
34	5	503	LUT	C35-C34-C33	-3.82	121.85	127.31
21	B	1229	CLA	C2D-C1D-ND	3.82	112.92	110.10
34	6	501	LUT	C15-C14-C13	-3.82	121.86	127.31
36	2	610	CHL	C4B-CHC-C1C	3.82	135.40	126.34
24	L	4001	BCR	C29-C28-C27	3.82	119.91	111.38
21	5	607	CLA	O2A-CGA-CBA	3.81	123.88	111.91
21	K	1401	CLA	CMD-C2D-C3D	-3.81	118.84	127.61
36	5	610	CHL	C4D-CHA-C1A	3.80	125.88	121.25
21	A	1125	CLA	C2D-C1D-ND	3.80	112.91	110.10
21	B	1226	CLA	C2C-C1C-NC	3.80	113.53	109.97
36	2	609	CHL	C3C-C4C-NC	-3.80	106.31	110.57
21	B	1023	CLA	C1-C2-C3	-3.80	119.47	126.04
21	B	1202	CLA	O2A-C1-C2	3.80	118.62	108.64
34	6	501	LUT	C7-C8-C9	-3.80	120.50	126.23
21	A	1139	CLA	O2A-C1-C2	3.80	118.62	108.64
21	5	601	CLA	CAA-C2A-C3A	-3.80	102.38	112.78
21	5	612	CLA	O2D-CGD-O1D	-3.80	116.42	123.84
21	5	606	CLA	C1-C2-C3	-3.80	120.61	126.75
35	6	504	XAT	C39-C29-C30	-3.79	117.61	122.92
34	5	502	LUT	C31-C30-C29	-3.79	121.90	127.31
34	1	501	LUT	C7-C8-C9	-3.79	120.51	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	4003	BCR	C34-C9-C10	-3.79	117.61	122.92
21	F	1301	CLA	O2A-C1-C2	3.79	122.33	108.42
34	2	501	LUT	C18-C5-C4	3.78	121.36	114.36
21	B	1232	CLA	O2D-CGD-CBD	3.77	117.97	111.27
21	B	1219	CLA	CMD-C2D-C1D	3.77	131.36	124.71
31	F	5002	LMG	O7-C10-C11	3.76	119.61	111.50
31	4	803	LMG	O7-C10-C11	3.75	119.58	111.50
24	B	4005	BCR	C23-C24-C25	-3.74	116.69	127.20
35	2	502	XAT	C31-C30-C29	-3.74	121.97	127.31
25	2	803	LHG	O7-C7-C8	3.74	119.56	111.50
34	1	501	LUT	C20-C13-C12	3.74	123.96	118.08
21	A	1129	CLA	CBC-CAC-C3C	-3.74	102.13	112.43
21	B	1238	CLA	O2A-C1-C2	3.73	118.44	108.64
24	O	4001	BCR	C37-C22-C23	-3.73	112.20	118.08
24	3	506	BCR	C15-C14-C13	3.73	132.63	127.31
36	4	613	CHL	C3B-C4B-NB	-3.73	107.06	110.52
21	A	1104	CLA	C1-C2-C3	-3.73	119.60	126.04
36	3	604	CHL	C4B-CHC-C1C	3.73	135.17	126.34
24	G	4001	BCR	C27-C26-C25	-3.72	117.33	122.73
35	3	502	XAT	C38-C25-C24	3.72	118.46	114.28
21	A	1103	CLA	C2D-C1D-ND	3.70	112.83	110.10
31	1	804	LMG	C7-O1-C1	3.70	120.97	113.74
32	5	805	4RF	O21-C22-C24	3.70	119.47	111.50
34	5	504	LUT	C11-C12-C13	-3.70	116.03	126.42
21	B	1223	CLA	C2C-C1C-NC	3.70	113.44	109.97
31	3	802	LMG	O7-C10-C11	3.69	119.45	111.50
21	H	1702	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
21	B	1222	CLA	CAA-C2A-C3A	-3.69	102.68	112.78
21	B	1238	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
21	1	603	CLA	CHD-C1D-ND	-3.68	121.07	124.45
21	K	1403	CLA	O2A-C1-C2	3.68	121.92	109.49
21	O	1803	CLA	C1-O2A-CGA	3.67	126.07	116.44
34	5	504	LUT	C21-C26-C27	3.67	117.34	112.70
36	2	610	CHL	C3C-C4C-NC	-3.67	106.46	110.57
24	A	4007	BCR	C8-C9-C10	3.66	124.56	118.94
21	6	603	CLA	C1-C2-C3	-3.66	119.71	126.04
21	A	1105	CLA	CHD-C1D-ND	-3.66	121.09	124.45
21	H	1701	CLA	C4-C3-C5	-3.66	109.11	115.27
21	A	1138	CLA	O2D-CGD-O1D	-3.66	116.68	123.84
24	3	503	BCR	C15-C14-C13	-3.66	122.09	127.31
21	A	1013	CLA	C2D-C1D-ND	3.66	112.80	110.10
21	B	1213	CLA	C2D-C1D-ND	3.66	112.80	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	601	CLA	C2D-C1D-ND	3.66	112.80	110.10
21	L	1503	CLA	C1-C2-C3	-3.66	120.83	126.75
34	5	502	LUT	C22-C23-C24	-3.66	107.58	111.74
21	K	1403	CLA	C2C-C1C-NC	3.65	113.39	109.97
21	A	1141	CLA	CHD-C1D-ND	-3.65	121.10	124.45
24	B	4003	BCR	C33-C5-C6	-3.65	120.43	124.53
21	B	1211	CLA	C1-C2-C3	-3.65	119.74	126.04
36	2	611	CHL	CHD-C1D-ND	-3.65	121.10	124.45
21	3	601	CLA	C1-O2A-CGA	3.64	126.00	116.44
21	B	1208	CLA	C1-C2-C3	-3.64	119.74	126.04
21	A	1104	CLA	CHD-C1D-ND	-3.64	121.11	124.45
21	A	1013	CLA	O2A-C1-C2	3.64	118.20	108.64
21	A	1113	CLA	CHD-C1D-ND	-3.63	121.11	124.45
21	1	601	CLA	C1-C2-C3	-3.63	119.76	126.04
21	4	601	CLA	CAA-C2A-C3A	-3.63	102.83	112.78
24	F	4001	BCR	C15-C14-C13	-3.63	122.13	127.31
35	1	502	XAT	C18-C5-C4	3.63	118.36	114.28
34	4	501	LUT	C7-C8-C9	-3.63	120.75	126.23
21	5	608	CLA	C4B-CHC-C1C	3.62	134.93	126.34
21	5	607	CLA	C4B-CHC-C1C	3.62	134.93	126.34
24	2	503	BCR	C34-C9-C10	-3.62	117.86	122.92
21	1	607	CLA	C2C-C1C-NC	3.62	113.36	109.97
24	3	504	BCR	C37-C22-C23	3.61	123.77	118.08
21	3	614	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
21	3	613	CLA	CHD-C1D-ND	-3.61	121.14	124.45
24	G	4001	BCR	C33-C5-C6	-3.61	120.48	124.53
21	6	606	CLA	C1-C2-C3	-3.61	120.92	126.75
21	5	604	CLA	CMA-C3A-C4A	3.60	121.46	111.77
37	6	803	SQD	O7-S-C6	-3.60	102.66	106.94
21	5	607	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
34	4	501	LUT	C38-C25-C24	-3.59	115.88	123.56
21	H	1701	CLA	C4B-CHC-C1C	3.58	134.84	126.34
36	2	609	CHL	CHD-C1D-ND	-3.58	121.17	124.45
21	A	1129	CLA	CAA-C2A-C3A	-3.58	102.98	112.78
21	B	1219	CLA	C2C-C1C-NC	3.58	113.32	109.97
21	G	1603	CLA	C3D-C2D-C1D	-3.58	100.95	105.83
34	2	501	LUT	C11-C10-C9	-3.58	122.21	127.31
21	2	601	CLA	CMD-C2D-C1D	3.57	131.01	124.71
21	B	1236	CLA	C2D-C1D-ND	3.57	112.74	110.10
21	4	602	CLA	C2C-C1C-NC	3.57	113.31	109.97
37	2	805	SQD	O7-S-C6	-3.57	102.70	106.94
25	6	801	LHG	O7-C7-C8	3.57	120.75	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	803	LHG	O7-C7-C8	3.57	119.19	111.50
21	6	612	CLA	C2D-C1D-ND	3.56	112.73	110.10
21	A	1136	CLA	O2A-C1-C2	3.56	118.00	108.64
21	L	1501	CLA	CHD-C1D-ND	-3.56	121.18	124.45
21	L	1502	CLA	C1-O2A-CGA	3.56	125.79	116.44
21	B	1226	CLA	CBA-CAA-C2A	3.56	124.37	113.86
27	A	5004	LMU	C1B-O1B-C4'	-3.56	109.16	117.96
28	B	5002	DGD	O2G-C1B-C2B	3.56	119.17	111.50
21	A	1103	CLA	CHD-C1D-ND	-3.56	121.19	124.45
21	B	1203	CLA	C1-C2-C3	-3.55	119.89	126.04
21	B	1224	CLA	O2A-C1-C2	3.55	117.97	108.64
24	4	503	BCR	C37-C22-C21	-3.55	117.96	122.92
24	3	504	BCR	C23-C24-C25	-3.54	117.25	127.20
21	4	604	CLA	C1-C2-C3	-3.54	119.92	126.04
34	3	501	LUT	C15-C14-C13	-3.54	122.26	127.31
33	3	808	PTY	O4-C30-C31	3.54	120.66	111.38
24	3	506	BCR	C33-C5-C4	3.54	120.42	113.62
21	B	1021	CLA	C2D-C1D-ND	3.54	112.71	110.10
21	5	605	CLA	C1-C2-C3	-3.53	119.93	126.04
34	5	504	LUT	C18-C5-C6	-3.53	120.56	124.53
21	A	1129	CLA	CHD-C1D-ND	-3.53	121.21	124.45
21	3	603	CLA	C2C-C1C-NC	3.53	113.28	109.97
25	F	5001	LHG	O7-C7-C8	3.53	119.10	111.50
24	B	4001	BCR	C37-C22-C21	-3.53	117.98	122.92
24	A	4002	BCR	C8-C7-C6	3.52	137.10	127.20
21	K	1401	CLA	CAA-CBA-CGA	-3.52	103.16	112.51
21	5	608	CLA	C2D-C1D-ND	3.52	112.70	110.10
21	A	1122	CLA	C2C-C1C-NC	3.52	113.27	109.97
31	1	804	LMG	O7-C10-C11	3.51	119.08	111.50
21	A	1132	CLA	C1-C2-C3	-3.51	119.97	126.04
21	3	602	CLA	C2C-C1C-NC	3.51	113.26	109.97
21	L	1502	CLA	O2D-CGD-CBD	3.51	117.50	111.27
37	3	806	SQD	O7-S-C6	-3.51	102.77	106.94
24	J	4002	BCR	C23-C24-C25	-3.50	117.38	127.20
32	L	5002	4RF	O21-C22-C24	3.50	119.03	111.50
21	4	603	CLA	C1-C2-C3	-3.49	120.00	126.04
36	5	610	CHL	C4B-CHC-C1C	3.49	134.62	126.34
21	5	613	CLA	CMA-C3A-C4A	3.49	121.16	111.77
21	B	1235	CLA	C1-C2-C3	-3.49	120.01	126.04
21	L	1503	CLA	C2C-C1C-NC	3.49	113.24	109.97
34	3	501	LUT	C35-C34-C33	-3.49	122.33	127.31
36	1	609	CHL	C3B-C4B-NB	-3.49	107.28	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	O	4001	BCR	C33-C5-C4	3.48	120.31	113.62
21	5	603	CLA	C5-C3-C2	3.48	128.17	121.12
21	A	1120	CLA	CAA-CBA-CGA	-3.48	103.08	113.25
21	B	1220	CLA	O2D-CGD-CBD	3.48	117.45	111.27
21	H	1702	CLA	CMB-C2B-C3B	3.48	135.01	126.59
21	4	607	CLA	C2C-C1C-NC	3.48	113.23	109.97
24	G	4001	BCR	C33-C5-C4	3.47	120.28	113.62
21	B	1220	CLA	CAA-CBA-CGA	-3.47	103.12	113.25
21	B	1202	CLA	C3B-C4B-NB	-3.47	107.30	110.52
21	B	1232	CLA	C2C-C1C-NC	3.47	113.22	109.97
35	2	502	XAT	C7-C8-C9	-3.46	120.16	125.53
36	5	609	CHL	C4D-CHA-C1A	3.46	125.46	121.25
24	A	4001	BCR	C28-C27-C26	-3.46	107.90	114.08
36	3	604	CHL	C3B-C4B-NB	-3.46	107.31	110.52
21	3	614	CLA	C2C-C1C-NC	3.46	113.21	109.97
21	B	1022	CLA	C1-C2-C3	-3.46	120.06	126.04
21	B	1221	CLA	CHD-C1D-ND	-3.46	121.28	124.45
21	1	604	CLA	CHD-C1D-ND	-3.46	121.28	124.45
21	B	1214	CLA	C2C-C1C-NC	3.46	113.21	109.97
21	A	1126	CLA	C6-C5-C3	-3.46	104.39	113.45
21	A	1119	CLA	C3B-C4B-NB	-3.46	107.31	110.52
21	4	609	CLA	C2C-C1C-NC	3.45	113.21	109.97
36	1	609	CHL	C4B-CHC-C1C	3.45	134.53	126.34
34	3	501	LUT	C22-C23-C24	-3.45	107.81	111.74
24	3	503	BCR	C32-C1-C6	-3.45	104.71	110.30
21	A	1135	CLA	C2C-C1C-NC	3.45	113.20	109.97
21	B	1231	CLA	C1-C2-C3	-3.44	120.09	126.04
21	A	1107	CLA	C1-C2-C3	-3.44	120.09	126.04
21	A	1129	CLA	C1-C2-C3	-3.44	120.09	126.04
24	A	4004	BCR	C28-C27-C26	-3.44	107.93	114.08
21	2	608	CLA	C1-C2-C3	-3.44	121.19	126.75
21	A	1120	CLA	C2C-C1C-NC	3.44	113.19	109.97
21	A	1131	CLA	C2C-C1C-NC	3.44	113.19	109.97
21	5	603	CLA	C2C-C1C-NC	3.44	113.19	109.97
21	2	601	CLA	C2D-C1D-ND	3.44	112.64	110.10
21	A	1108	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
21	H	1701	CLA	C1-C2-C3	-3.44	120.10	126.04
21	5	601	CLA	CMD-C2D-C3D	-3.43	119.71	127.61
24	A	4003	BCR	C23-C24-C25	3.43	136.84	127.20
21	A	1126	CLA	C3B-C4B-NB	-3.43	107.33	110.52
21	O	1802	CLA	CAA-C2A-C3A	-3.43	108.10	116.10
36	2	611	CHL	CHC-C1C-NC	3.43	129.40	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1215	CLA	C2C-C1C-NC	3.42	113.18	109.97
36	2	613	CHL	C4A-NA-C1A	3.42	108.24	106.71
21	A	1109	CLA	CAA-C2A-C3A	-3.42	103.42	112.78
34	5	504	LUT	C40-C33-C34	-3.42	118.14	122.92
21	A	1137	CLA	C2D-C1D-ND	3.42	112.62	110.10
21	6	605	CLA	C2D-C1D-ND	3.41	112.62	110.10
21	J	1901	CLA	CBB-CAB-C3B	-3.40	110.68	127.62
35	2	502	XAT	C15-C14-C13	-3.40	122.45	127.31
24	3	506	BCR	C36-C18-C17	-3.40	118.16	122.92
21	K	1401	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
21	A	1136	CLA	C1-O2A-CGA	3.40	125.37	116.44
21	A	1131	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
21	6	609	CLA	C2C-C1C-NC	3.40	113.16	109.97
21	A	1103	CLA	C1-C2-C3	-3.40	120.17	126.04
21	A	1131	CLA	C4B-CHC-C1C	3.40	134.40	126.34
24	F	4001	BCR	C28-C27-C26	-3.39	108.03	114.08
24	3	506	BCR	C33-C5-C6	-3.39	120.72	124.53
36	2	613	CHL	CHB-C4A-NA	3.39	129.20	124.51
24	A	4007	BCR	C36-C18-C19	-3.39	112.74	118.08
21	B	1236	CLA	CHD-C1D-ND	-3.38	121.35	124.45
21	B	1213	CLA	O2A-CGA-CBA	3.38	122.52	111.91
21	2	606	CLA	C1-C2-C3	-3.38	121.28	126.75
21	O	1803	CLA	C2C-C1C-NC	3.38	113.14	109.97
21	6	607	CLA	C2C-C1C-NC	3.38	113.14	109.97
21	A	1124	CLA	C2D-C1D-ND	3.38	112.59	110.10
21	5	604	CLA	C1-C2-C3	-3.38	120.20	126.04
21	6	612	CLA	CHD-C1D-ND	-3.37	121.35	124.45
21	4	609	CLA	C2D-C1D-ND	3.37	112.59	110.10
21	5	602	CLA	CMA-C3A-C4A	3.37	120.84	111.77
35	6	502	XAT	C18-C5-C4	3.37	118.07	114.28
21	3	606	CLA	CED-O2D-CGD	3.37	123.56	115.94
21	G	1601	CLA	O2A-C1-C2	3.37	120.80	108.42
36	4	613	CHL	C2B-C1B-NB	-3.37	107.97	110.23
21	B	1218	CLA	C1-O2A-CGA	3.37	125.28	116.44
21	B	1201	CLA	C2D-C1D-ND	3.37	112.58	110.10
21	6	604	CLA	CHD-C1D-ND	-3.37	121.36	124.45
21	L	1504	CLA	C1-C2-C3	-3.36	121.31	126.75
21	A	1105	CLA	C2D-C1D-ND	3.36	112.58	110.10
21	2	601	CLA	C1-C2-C3	-3.36	120.23	126.04
21	A	1102	CLA	C1-C2-C3	-3.36	120.23	126.04
21	A	1139	CLA	C1-C2-C3	-3.36	120.23	126.04
35	3	502	XAT	O4-C5-C18	-3.36	111.03	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1224	CLA	CHD-C1D-ND	-3.35	121.37	124.45
21	4	607	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
21	B	1212	CLA	C1-C2-C3	-3.35	120.25	126.04
21	A	1118	CLA	C2C-C1C-NC	3.35	113.11	109.97
24	O	4001	BCR	C37-C22-C21	3.35	127.61	122.92
21	2	608	CLA	CHD-C1D-ND	-3.34	121.38	124.45
21	A	1109	CLA	O2A-C1-C2	3.34	117.42	108.64
21	B	1214	CLA	CHD-C1D-ND	-3.34	121.38	124.45
24	K	4001	BCR	C36-C18-C17	-3.34	118.24	122.92
34	1	501	LUT	C18-C5-C6	-3.34	120.78	124.53
36	6	610	CHL	C4D-CHA-C1A	3.34	125.31	121.25
21	A	1138	CLA	C1-C2-C3	-3.34	120.27	126.04
21	B	1223	CLA	OBD-CAD-C3D	-3.34	120.49	128.52
21	B	1229	CLA	CAA-CBA-CGA	-3.34	103.51	113.25
34	2	501	LUT	C15-C14-C13	-3.34	122.55	127.31
24	J	4001	BCR	C2-C1-C6	3.33	115.61	110.48
34	1	501	LUT	C21-C26-C25	3.33	117.38	111.42
36	5	610	CHL	CHD-C1D-ND	-3.33	121.39	124.45
21	2	608	CLA	C2C-C1C-NC	3.33	113.09	109.97
21	B	1230	CLA	CAA-CBA-CGA	-3.33	103.52	113.25
21	B	1202	CLA	C2D-C1D-ND	3.33	112.56	110.10
35	6	502	XAT	C7-C8-C9	-3.33	120.37	125.53
21	2	604	CLA	CMC-C2C-C1C	3.33	130.10	125.04
24	G	4001	BCR	C28-C27-C26	-3.32	108.14	114.08
21	O	1801	CLA	CMC-C2C-C1C	3.32	130.10	125.04
21	6	606	CLA	C2C-C1C-NC	3.32	113.08	109.97
21	4	609	CLA	O1D-CGD-CBD	-3.32	117.69	124.48
21	3	606	CLA	O2D-CGD-CBD	3.32	117.17	111.27
27	A	5005	LMU	C1B-O1B-C4'	-3.32	109.75	117.96
21	A	1126	CLA	C1-C2-C3	-3.32	120.30	126.04
24	B	4003	BCR	C19-C18-C17	3.32	124.03	118.94
24	A	4006	BCR	C23-C24-C25	-3.31	117.89	127.20
21	A	1104	CLA	C2C-C1C-NC	3.31	113.08	109.97
21	B	1228	CLA	C1-C2-C3	-3.31	120.31	126.04
21	A	1116	CLA	C2D-C1D-ND	3.31	112.55	110.10
21	L	1504	CLA	C2D-C1D-ND	3.31	112.55	110.10
21	4	602	CLA	C1-C2-C3	-3.31	121.39	126.75
21	A	1136	CLA	CMA-C3A-C4A	3.31	120.67	111.77
21	3	614	CLA	CHD-C1D-ND	-3.31	121.41	124.45
21	B	1238	CLA	C2C-C1C-NC	3.31	113.07	109.97
21	B	1204	CLA	C2D-C1D-ND	3.31	112.54	110.10
38	4	805	LMK	O3-C4-C3	-3.31	111.63	122.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1011	CL0	C1-C2-C3	-3.30	120.33	126.04
21	1	605	CLA	C2C-C1C-NC	3.30	113.06	109.97
36	5	609	CHL	C3C-C4C-NC	-3.30	106.87	110.57
21	H	1702	CLA	CHD-C1D-ND	-3.30	121.42	124.45
21	H	1702	CLA	CAA-C2A-C3A	-3.30	103.75	112.78
21	A	1106	CLA	C2C-C1C-NC	3.29	113.06	109.97
21	3	608	CLA	C2D-C1D-ND	3.29	112.53	110.10
21	A	1128	CLA	C2C-C1C-NC	3.29	113.06	109.97
21	A	1109	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
21	5	603	CLA	C1-O2A-CGA	3.29	125.07	116.44
21	B	1206	CLA	C2D-C1D-ND	3.29	112.53	110.10
36	1	610	CHL	C4D-CHA-C1A	3.28	125.24	121.25
21	A	1131	CLA	C1D-ND-C4D	-3.28	104.00	106.33
24	J	4002	BCR	C2-C1-C6	3.28	115.53	110.48
21	L	1501	CLA	C2D-C1D-ND	3.28	112.52	110.10
21	A	1124	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
24	K	4001	BCR	C27-C26-C25	-3.28	117.97	122.73
21	B	1222	CLA	CHD-C1D-ND	-3.28	121.44	124.45
21	A	1121	CLA	C2D-C1D-ND	3.28	112.52	110.10
21	B	1239	CLA	C1-C2-C3	-3.27	120.38	126.04
21	1	606	CLA	C1-C2-C3	-3.27	121.46	126.75
21	1	615	CLA	C2D-C1D-ND	3.27	112.52	110.10
24	A	4001	BCR	C33-C5-C4	3.27	119.90	113.62
21	6	604	CLA	C2D-C1D-ND	3.27	112.51	110.10
21	B	1228	CLA	CHD-C1D-ND	-3.27	121.45	124.45
21	A	1113	CLA	C2C-C1C-NC	3.27	113.03	109.97
21	A	1129	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
21	A	1136	CLA	C2D-C1D-ND	3.26	112.51	110.10
21	2	607	CLA	C2C-C1C-NC	3.26	113.03	109.97
21	3	602	CLA	C1-C2-C3	-3.26	120.40	126.04
24	F	4002	BCR	C23-C24-C25	-3.26	118.04	127.20
21	1	608	CLA	CHD-C1D-ND	-3.26	121.45	124.45
24	I	4001	BCR	C35-C13-C14	-3.26	118.35	122.92
21	A	1127	CLA	C2C-C1C-NC	3.26	113.03	109.97
21	1	615	CLA	C2C-C1C-NC	3.26	113.03	109.97
34	6	501	LUT	C22-C23-C24	-3.26	108.03	111.74
21	B	1215	CLA	CHD-C1D-ND	-3.26	121.46	124.45
21	3	601	CLA	CAA-C2A-C3A	-3.26	103.85	112.78
21	3	611	CLA	OBD-CAD-C3D	-3.26	120.68	128.52
21	B	1234	CLA	C2D-C1D-ND	3.26	112.50	110.10
21	1	604	CLA	CMC-C2C-C1C	3.25	129.99	125.04
21	B	1229	CLA	CMA-C3A-C4A	3.25	120.51	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	504	BCR	C1-C6-C5	-3.25	118.04	122.61
24	1	504	BCR	C4-C5-C6	-3.25	118.02	122.73
21	L	1504	CLA	C1D-ND-C4D	-3.25	104.03	106.33
31	1	804	LMG	O1-C1-C2	3.25	113.37	108.30
21	A	1105	CLA	C1-C2-C3	-3.25	120.43	126.04
21	6	608	CLA	C2D-C1D-ND	3.25	112.50	110.10
21	A	1129	CLA	CAA-CBA-CGA	-3.25	103.77	113.25
21	B	1235	CLA	C2D-C1D-ND	3.24	112.50	110.10
21	5	603	CLA	C1-C2-C3	-3.24	120.43	126.04
21	6	601	CLA	C2D-C1D-ND	3.24	112.49	110.10
21	2	606	CLA	CHD-C1D-ND	-3.24	121.47	124.45
21	A	1115	CLA	C1-C2-C3	-3.24	120.44	126.04
21	A	1111	CLA	C1-O2A-CGA	3.24	124.95	116.44
21	B	1211	CLA	C2C-C1C-NC	3.24	113.01	109.97
21	A	1112	CLA	C1-C2-C3	-3.24	120.44	126.04
21	A	1101	CLA	C2D-C1D-ND	3.24	112.49	110.10
34	1	501	LUT	C38-C25-C24	-3.24	116.63	123.56
21	A	1104	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
21	2	605	CLA	C2D-C1D-ND	3.24	112.49	110.10
21	B	1236	CLA	C2C-C1C-NC	3.24	113.00	109.97
21	F	1301	CLA	C2C-C1C-NC	3.24	113.00	109.97
21	B	1022	CLA	C2D-C1D-ND	3.23	112.49	110.10
21	2	606	CLA	C2C-C1C-NC	3.23	113.00	109.97
21	A	1110	CLA	CAA-C2A-C3A	-3.23	103.93	112.78
25	5	801	LHG	C6-C5-C4	-3.23	104.15	111.79
34	3	501	LUT	C11-C10-C9	-3.23	122.70	127.31
24	G	4001	BCR	C34-C9-C10	-3.23	118.41	122.92
22	A	2001	PQN	C14-C13-C15	3.22	120.69	115.27
21	A	1104	CLA	CHA-C4D-ND	3.22	139.24	132.50
21	B	1204	CLA	C2C-C1C-NC	3.22	112.99	109.97
21	A	1112	CLA	C2D-C1D-ND	3.22	112.47	110.10
36	3	604	CHL	CHD-C4C-C3C	3.22	129.57	124.84
24	3	506	BCR	C30-C25-C26	-3.21	118.09	122.61
21	A	1129	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
28	B	5002	DGD	O1G-C1A-C2A	3.21	121.99	111.91
21	B	1213	CLA	CHD-C1D-ND	-3.21	121.50	124.45
21	A	1139	CLA	CAA-C2A-C3A	-3.21	103.98	112.78
21	O	1803	CLA	CMA-C3A-C4A	3.21	120.40	111.77
21	B	1234	CLA	C2C-C1C-NC	3.21	112.98	109.97
33	L	5003	PTY	O4-C30-C31	3.21	119.79	111.38
21	A	1110	CLA	CBA-CAA-C2A	3.21	123.33	113.86
21	4	606	CLA	C1-C2-C3	-3.21	121.56	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	504	BCR	C37-C22-C21	-3.21	118.43	122.92
21	A	1118	CLA	C1C-C2C-C3C	-3.21	103.59	106.96
36	6	610	CHL	C3C-C4C-NC	-3.21	106.98	110.57
21	6	602	CLA	C2D-C1D-ND	3.21	112.47	110.10
24	A	4002	BCR	C36-C18-C17	-3.20	118.44	122.92
21	4	601	CLA	CHD-C1D-ND	-3.20	121.51	124.45
21	A	1121	CLA	C1-C2-C3	-3.20	120.50	126.04
21	3	603	CLA	C4B-CHC-C1C	3.20	133.93	126.34
36	4	611	CHL	C4A-NA-C1A	3.20	108.14	106.71
36	4	613	CHL	CHB-C4A-NA	3.20	128.94	124.51
21	O	1802	CLA	C2D-C1D-ND	3.20	112.46	110.10
21	A	1118	CLA	CAA-C2A-C3A	-3.20	104.02	112.78
36	1	610	CHL	C1-O2A-CGA	3.20	126.64	116.11
36	2	610	CHL	CHC-C1C-NC	3.20	129.05	124.20
24	J	4001	BCR	C32-C1-C31	3.20	118.34	108.53
25	1	803	LHG	O8-C23-C24	3.20	121.94	111.91
21	B	1231	CLA	CHD-C1D-ND	-3.20	121.52	124.45
21	5	603	CLA	CMA-C3A-C4A	3.20	120.36	111.77
21	3	611	CLA	C2C-C1C-NC	3.19	112.97	109.97
21	A	1128	CLA	CHD-C1D-ND	-3.19	121.52	124.45
24	O	4001	BCR	C19-C18-C17	3.19	123.84	118.94
21	4	601	CLA	OBD-CAD-C3D	-3.19	120.84	128.52
21	A	1107	CLA	C2C-C1C-NC	3.19	112.96	109.97
21	F	1302	CLA	C2C-C1C-NC	3.19	112.96	109.97
21	1	613	CLA	C2C-C1C-NC	3.19	112.96	109.97
25	2	802	LHG	C5-O7-C7	-3.19	109.95	117.79
24	B	4002	BCR	C23-C24-C25	-3.18	118.26	127.20
21	5	612	CLA	CGD-CBD-CAD	3.18	121.04	110.73
21	B	1220	CLA	CHD-C1D-ND	-3.18	121.53	124.45
21	3	615	CLA	C1-C2-C3	-3.18	120.54	126.04
21	B	1224	CLA	C2D-C1D-ND	3.18	112.45	110.10
21	A	1133	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
21	B	1209	CLA	C2C-C1C-NC	3.18	112.95	109.97
21	5	602	CLA	C2D-C1D-ND	3.18	112.44	110.10
21	A	1130	CLA	C2D-C1D-ND	3.18	112.44	110.10
21	5	605	CLA	C2D-C1D-ND	3.18	112.44	110.10
21	2	604	CLA	O1D-CGD-CBD	-3.18	117.99	124.48
24	F	4002	BCR	C34-C9-C10	-3.17	118.48	122.92
24	A	4002	BCR	C23-C22-C21	3.17	123.81	118.94
21	K	1402	CLA	C1-C2-C3	-3.17	120.56	126.04
21	B	1239	CLA	C2D-C1D-ND	3.17	112.44	110.10
24	2	503	BCR	C28-C27-C26	-3.17	108.42	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	6	502	XAT	C11-C10-C9	3.17	131.83	127.31
21	J	1901	CLA	C2D-C1D-ND	3.17	112.44	110.10
21	A	1134	CLA	C1-C2-C3	-3.17	120.57	126.04
21	3	603	CLA	C1-C2-C3	-3.16	120.57	126.04
21	5	601	CLA	CMB-C2B-C3B	3.16	134.25	126.59
21	1	605	CLA	C1-C2-C3	-3.16	120.58	126.04
21	6	605	CLA	CHD-C1D-ND	-3.16	121.55	124.45
34	5	504	LUT	C39-C29-C30	3.16	127.35	122.92
21	B	1223	CLA	C2D-C1D-ND	3.16	112.43	110.10
21	5	608	CLA	CMA-C3A-C4A	3.16	120.27	111.77
21	4	604	CLA	CHD-C1D-ND	-3.16	121.55	124.45
21	2	607	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
21	A	1134	CLA	C2D-C1D-ND	3.16	112.43	110.10
21	5	603	CLA	C7-C6-C5	3.16	121.93	113.36
21	K	1401	CLA	CMA-C3A-C4A	3.16	120.26	111.77
25	5	802	LHG	C5-O7-C7	-3.16	112.01	117.90
31	4	802	LMG	C1-O6-C5	3.16	119.88	113.69
21	J	1901	CLA	C3B-C4B-NB	-3.16	107.59	110.52
21	6	601	CLA	C1-C2-C3	-3.15	120.59	126.04
21	A	1109	CLA	C4-C3-C2	-3.15	115.59	123.68
36	4	610	CHL	C2C-C3C-C4C	3.15	108.74	106.49
21	B	1022	CLA	C2C-C1C-NC	3.15	112.93	109.97
38	2	807	LMK	O3-C4-C3	-3.15	112.16	122.98
21	A	1140	CLA	CMA-C3A-C4A	3.15	120.25	111.77
21	1	608	CLA	C2C-C1C-NC	3.15	112.92	109.97
36	1	610	CHL	CHB-C4A-NA	3.15	128.87	124.51
21	4	608	CLA	C2C-C1C-NC	3.15	112.92	109.97
21	B	1237	CLA	CMA-C3A-C4A	3.15	120.23	111.77
21	B	1224	CLA	C2C-C1C-NC	3.15	112.92	109.97
35	1	502	XAT	C26-C27-C28	-3.15	119.34	125.99
24	B	4003	BCR	C30-C25-C24	3.15	124.68	115.78
21	A	1109	CLA	CMD-C2D-C3D	-3.14	120.38	127.61
21	A	1101	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
21	G	1602	CLA	CMA-C3A-C4A	3.14	120.22	111.77
21	A	1114	CLA	C2C-C1C-NC	3.14	112.92	109.97
21	A	1118	CLA	CHD-C1D-ND	-3.14	121.57	124.45
24	J	4001	BCR	C23-C22-C21	-3.14	114.12	118.94
36	2	611	CHL	C4B-CHC-C1C	3.14	133.78	126.34
21	A	1012	CLA	C3B-C4B-NB	-3.14	107.61	110.52
21	K	1401	CLA	CHD-C4C-C3C	3.13	129.45	124.84
24	K	4001	BCR	C34-C9-C10	-3.13	118.53	122.92
21	A	1131	CLA	C2D-C1D-ND	3.13	112.41	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	4003	BCR	C23-C22-C21	-3.13	114.13	118.94
21	3	606	CLA	CHD-C1D-ND	-3.13	121.57	124.45
21	B	1240	CLA	C1-C2-C3	-3.13	120.63	126.04
24	A	4001	BCR	C34-C9-C10	-3.13	118.54	122.92
21	6	601	CLA	CHD-C1D-ND	-3.13	121.58	124.45
21	2	602	CLA	C2D-C1D-ND	3.13	112.41	110.10
21	1	615	CLA	C4B-CHC-C1C	3.13	133.76	126.34
21	6	607	CLA	CMA-C3A-C4A	3.13	120.18	111.77
21	A	1137	CLA	CHD-C1D-ND	-3.13	121.58	124.45
21	1	611	CLA	C2D-C1D-ND	3.13	112.41	110.10
36	2	609	CHL	C3B-C4B-NB	-3.13	107.61	110.52
21	A	1118	CLA	C3A-C2A-C1A	-3.12	96.66	101.34
24	G	4001	BCR	C30-C25-C26	-3.12	118.21	122.61
24	A	4007	BCR	C12-C13-C14	3.12	123.73	118.94
29	B	5003	3PH	O31-C31-C32	3.12	121.71	111.91
21	1	604	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
21	A	1131	CLA	C3B-C4B-NB	-3.12	107.62	110.52
24	I	4001	BCR	C23-C24-C25	-3.12	118.43	127.20
36	4	610	CHL	C3C-C4C-NC	-3.12	107.07	110.57
21	B	1212	CLA	C2D-C1D-ND	3.12	112.40	110.10
21	A	1122	CLA	CHD-C1D-ND	-3.12	121.59	124.45
21	B	1225	CLA	C2C-C1C-NC	3.12	112.89	109.97
21	1	602	CLA	C2C-C1C-NC	3.12	112.89	109.97
24	I	4001	BCR	C27-C26-C25	-3.12	118.20	122.73
21	A	1139	CLA	C4-C3-C2	-3.12	115.68	123.68
24	A	4006	BCR	C12-C13-C14	-3.12	114.16	118.94
21	B	1201	CLA	O1D-CGD-CBD	-3.12	118.11	124.48
21	2	603	CLA	CMA-C3A-C4A	3.12	120.15	111.77
21	A	1116	CLA	C2C-C1C-NC	3.11	112.89	109.97
24	F	4002	BCR	C37-C22-C21	-3.11	118.56	122.92
21	3	607	CLA	C2C-C1C-NC	3.11	112.89	109.97
34	5	503	LUT	C31-C32-C33	-3.11	117.68	126.42
21	6	613	CLA	C1C-C2C-C3C	-3.11	103.69	106.96
21	A	1114	CLA	C1-C2-C3	-3.11	120.67	126.04
21	B	1230	CLA	C2D-C1D-ND	3.11	112.39	110.10
24	J	4002	BCR	C27-C26-C25	-3.10	118.22	122.73
21	A	1139	CLA	CMA-C3A-C4A	3.10	120.11	111.77
21	A	1012	CLA	C1-C2-C3	-3.10	120.68	126.04
21	2	602	CLA	C2C-C1C-NC	3.10	112.88	109.97
21	B	1226	CLA	CAC-C3C-C4C	3.10	128.84	124.81
21	5	606	CLA	C2D-C1D-ND	3.10	112.39	110.10
21	B	1217	CLA	C2C-C1C-NC	3.10	112.88	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1235	CLA	C1D-ND-C4D	-3.10	104.13	106.33
21	B	1023	CLA	C2D-C1D-ND	3.10	112.39	110.10
21	5	612	CLA	CHA-C4D-ND	3.10	138.98	132.50
24	O	4001	BCR	C33-C5-C6	3.10	128.01	124.53
21	A	1136	CLA	CHD-C1D-ND	-3.09	121.61	124.45
21	3	615	CLA	CHD-C1D-ND	-3.09	121.61	124.45
24	3	503	BCR	C36-C18-C17	-3.09	118.59	122.92
21	3	612	CLA	C3B-C4B-NB	-3.09	107.65	110.52
21	6	601	CLA	C1D-ND-C4D	-3.09	104.14	106.33
34	5	501	LUT	C35-C15-C14	-3.09	117.14	123.47
21	G	1603	CLA	CMA-C3A-C4A	3.09	120.08	111.77
21	A	1130	CLA	C3B-C4B-NB	-3.09	107.65	110.52
21	6	603	CLA	CHD-C1D-ND	-3.09	121.61	124.45
24	I	4001	BCR	C34-C9-C10	-3.09	118.60	122.92
21	B	1240	CLA	C3B-C4B-NB	-3.09	107.65	110.52
21	A	1123	CLA	C1-C2-C3	-3.09	120.70	126.04
21	A	1128	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
24	3	504	BCR	C27-C26-C25	-3.09	118.25	122.73
36	5	610	CHL	C4A-NA-C1A	3.09	108.09	106.71
21	A	1121	CLA	C3B-C4B-NB	-3.09	107.65	110.52
21	1	601	CLA	C2D-C1D-ND	3.08	112.38	110.10
21	H	1702	CLA	CHC-C4B-NB	-3.08	120.99	124.26
21	5	606	CLA	C2C-C1C-NC	3.08	112.86	109.97
35	6	502	XAT	O4-C5-C18	-3.08	111.36	115.06
21	2	615	CLA	C2C-C1C-NC	3.08	112.86	109.97
24	A	4007	BCR	C23-C24-C25	-3.08	118.55	127.20
21	B	1021	CLA	C1-C2-C3	-3.08	120.72	126.04
24	I	4001	BCR	C33-C5-C4	3.08	119.53	113.62
36	6	610	CHL	CMA-C3A-C4A	3.08	120.05	111.77
21	B	1222	CLA	C2D-C1D-ND	3.08	112.37	110.10
21	2	612	CLA	C2D-C1D-ND	3.08	112.37	110.10
21	3	610	CLA	CHD-C1D-ND	-3.08	121.63	124.45
21	A	1108	CLA	C2C-C1C-NC	3.08	112.85	109.97
36	2	610	CHL	C4A-NA-C1A	3.08	108.09	106.71
24	1	504	BCR	C19-C18-C17	3.08	123.66	118.94
21	2	605	CLA	C3B-C4B-NB	-3.08	107.66	110.52
36	5	610	CHL	C3B-C4B-NB	-3.08	107.66	110.52
21	4	601	CLA	C2D-C1D-ND	3.07	112.37	110.10
21	5	606	CLA	CMA-C3A-C4A	3.07	120.04	111.77
21	B	1229	CLA	C3B-C4B-NB	-3.07	107.66	110.52
21	A	1117	CLA	C2C-C1C-NC	3.07	112.85	109.97
21	A	1132	CLA	C2C-C1C-NC	3.07	112.85	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	606	CLA	CHD-C1D-ND	-3.07	121.63	124.45
35	3	502	XAT	C32-C33-C34	3.07	123.66	118.94
24	B	4001	BCR	C33-C5-C6	-3.07	121.08	124.53
21	B	1230	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
21	A	1104	CLA	CAA-C2A-C3A	-3.07	104.37	112.78
21	B	1201	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
21	B	1210	CLA	CHD-C1D-ND	-3.07	121.63	124.45
24	J	4002	BCR	C39-C30-C25	-3.07	105.32	110.30
21	B	1202	CLA	CHD-C1D-ND	-3.07	121.64	124.45
24	I	4002	BCR	C38-C26-C27	3.07	119.50	113.62
21	G	1602	CLA	C2D-C1D-ND	3.07	112.36	110.10
21	4	609	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
24	B	4003	BCR	C28-C27-C26	-3.06	108.61	114.08
21	L	1502	CLA	CMA-C3A-C4A	3.06	120.01	111.77
24	A	4001	BCR	C36-C18-C17	-3.06	118.63	122.92
21	2	608	CLA	CMA-C3A-C4A	3.06	120.01	111.77
21	2	607	CLA	C1-C2-C3	-3.06	120.75	126.04
21	A	1117	CLA	CMA-C3A-C4A	3.06	120.00	111.77
21	B	1208	CLA	C2D-C1D-ND	3.06	112.36	110.10
21	G	1602	CLA	C2C-C1C-NC	3.06	112.84	109.97
21	6	603	CLA	C2D-C1D-ND	3.06	112.36	110.10
21	5	604	CLA	C2D-C1D-ND	3.06	112.36	110.10
36	2	609	CHL	C4A-NA-C1A	3.06	108.08	106.71
21	6	613	CLA	C2C-C1C-NC	3.06	112.84	109.97
21	4	606	CLA	C2C-C1C-NC	3.06	112.84	109.97
36	5	609	CHL	CMA-C3A-C4A	3.06	119.99	111.77
27	B	5004	LMU	C1-O1'-C1'	-3.06	108.77	113.84
36	2	609	CHL	CHB-C4A-NA	3.05	128.74	124.51
21	A	1134	CLA	CHD-C1D-ND	-3.05	121.65	124.45
24	G	4001	BCR	C15-C14-C13	3.05	131.66	127.31
21	4	615	CLA	C2C-C1C-NC	3.05	112.83	109.97
21	O	1803	CLA	CHA-C4D-ND	3.05	138.88	132.50
36	4	613	CHL	C1-O2A-CGA	3.05	124.44	116.44
21	4	605	CLA	C2C-C1C-NC	3.05	112.83	109.97
21	B	1227	CLA	C2D-C1D-ND	3.05	112.35	110.10
21	B	1208	CLA	C3B-C4B-NB	-3.05	107.69	110.52
21	B	1206	CLA	C1D-ND-C4D	-3.04	104.17	106.33
21	A	1109	CLA	CMA-C3A-C4A	3.04	119.95	111.77
21	A	1132	CLA	C2D-C1D-ND	3.04	112.35	110.10
21	3	601	CLA	CHD-C1D-ND	-3.04	121.66	124.45
21	A	1141	CLA	C2C-C1C-NC	3.04	112.82	109.97
21	3	606	CLA	C1-C2-C3	-3.04	120.78	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	503	BCR	C2-C1-C6	3.04	115.16	110.48
21	L	1503	CLA	CHD-C1D-ND	-3.04	121.66	124.45
36	2	610	CHL	C1C-C2C-C3C	3.04	109.53	107.11
21	A	1115	CLA	C2D-C1D-ND	3.04	112.34	110.10
21	G	1601	CLA	C2C-C1C-NC	3.04	112.82	109.97
24	3	504	BCR	C35-C13-C12	3.04	122.86	118.08
21	A	1110	CLA	CHD-C1D-ND	-3.03	121.67	124.45
21	A	1101	CLA	C1-C2-C3	-3.03	120.80	126.04
21	A	1111	CLA	O2A-CGA-CBA	3.03	121.43	111.91
21	K	1401	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
21	4	604	CLA	C2D-C1D-ND	3.03	112.34	110.10
21	A	1134	CLA	C3B-C4B-NB	-3.03	107.70	110.52
21	1	611	CLA	CHD-C1D-ND	-3.03	121.67	124.45
21	5	613	CLA	CHD-C1D-ND	-3.03	121.67	124.45
21	6	604	CLA	CMA-C3A-C4A	3.02	119.90	111.77
21	2	603	CLA	C2D-C1D-ND	3.02	112.33	110.10
21	A	1118	CLA	CHA-C4D-ND	3.02	138.83	132.50
21	B	1207	CLA	CHD-C1D-ND	-3.02	121.67	124.45
21	5	601	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
36	1	609	CHL	CMA-C3A-C4A	3.02	119.89	111.77
21	2	612	CLA	C2C-C1C-NC	3.02	112.80	109.97
21	6	608	CLA	C2C-C1C-NC	3.02	112.80	109.97
21	B	1203	CLA	C2D-C1D-ND	3.02	112.33	110.10
21	6	606	CLA	C3B-C4B-NB	-3.02	107.72	110.52
21	A	1112	CLA	CHD-C1D-ND	-3.02	121.68	124.45
21	6	603	CLA	C1D-ND-C4D	-3.02	104.19	106.33
35	2	502	XAT	C38-C25-C24	3.02	117.67	114.28
36	1	610	CHL	CHC-C4B-NB	-3.02	121.06	124.26
21	5	608	CLA	CAA-C2A-C3A	-3.01	104.52	112.78
21	G	1601	CLA	C2D-C1D-ND	3.01	112.33	110.10
21	A	1012	CLA	CHD-C1D-ND	-3.01	121.69	124.45
36	1	609	CHL	C3C-C4C-NC	-3.01	107.19	110.57
21	5	603	CLA	C1C-C2C-C3C	-3.01	103.79	106.96
21	B	1213	CLA	C4D-CHA-C1A	3.01	124.91	121.25
21	A	1121	CLA	C1D-ND-C4D	-3.01	104.20	106.33
21	1	603	CLA	CMD-C2D-C3D	-3.01	120.69	127.61
36	4	611	CHL	CHB-C4A-NA	3.01	128.67	124.51
35	4	502	XAT	C18-C5-C4	3.01	117.67	114.28
21	L	1502	CLA	C1D-ND-C4D	-3.01	104.20	106.33
21	A	1129	CLA	C2C-C1C-NC	3.01	112.79	109.97
21	K	1402	CLA	C2C-C1C-NC	3.01	112.79	109.97
21	A	1127	CLA	C2D-C1D-ND	3.01	112.32	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	602	CLA	C6-C5-C3	-3.01	109.70	114.62
21	6	605	CLA	C1-O2A-CGA	3.01	124.33	116.44
21	H	1702	CLA	CHB-C1B-NB	3.01	127.44	124.26
21	B	1223	CLA	C1-C2-C3	-3.01	120.84	126.04
36	4	610	CHL	C3B-C4B-NB	-3.01	107.73	110.52
24	G	4001	BCR	C8-C9-C10	3.01	123.55	118.94
21	3	614	CLA	CAA-C2A-C3A	-3.01	106.75	114.26
21	A	1109	CLA	C2C-C1C-NC	3.00	112.79	109.97
21	A	1133	CLA	C2C-C1C-NC	3.00	112.79	109.97
21	A	1114	CLA	CHD-C1D-ND	-3.00	121.69	124.45
21	2	603	CLA	CHD-C1D-ND	-3.00	121.69	124.45
21	A	1103	CLA	C1D-ND-C4D	-3.00	104.20	106.33
21	L	1502	CLA	CAA-C2A-C3A	-3.00	104.56	112.78
21	B	1203	CLA	CHD-C1D-ND	-3.00	121.69	124.45
32	5	805	4RF	O40-C41-C43	3.00	121.33	111.91
21	B	1235	CLA	C2C-C1C-NC	3.00	112.78	109.97
21	K	1402	CLA	C2D-C1D-ND	3.00	112.31	110.10
21	B	1216	CLA	CHD-C1D-ND	-3.00	121.70	124.45
21	L	1501	CLA	CMB-C2B-C1B	-3.00	120.80	125.37
21	A	1141	CLA	C2D-C1D-ND	3.00	112.31	110.10
21	4	604	CLA	C1D-ND-C4D	-3.00	104.20	106.33
24	B	4004	BCR	C23-C24-C25	-3.00	118.78	127.20
21	3	606	CLA	CAC-C3C-C2C	-3.00	122.40	127.53
21	K	1404	CLA	CHD-C1D-ND	-3.00	121.70	124.45
21	A	1115	CLA	C2C-C1C-NC	3.00	112.78	109.97
37	3	806	SQD	O3-C3-C2	-3.00	103.42	110.35
24	K	4001	BCR	C19-C18-C17	3.00	123.54	118.94
21	3	603	CLA	C3D-C2D-C1D	-3.00	101.74	105.83
21	A	1113	CLA	C1-C2-C3	-2.99	120.86	126.04
21	A	1112	CLA	C2C-C1C-NC	2.99	112.78	109.97
21	6	602	CLA	C2C-C1C-NC	2.99	112.78	109.97
21	K	1404	CLA	CMA-C3A-C4A	2.99	119.82	111.77
21	1	601	CLA	C2C-C1C-NC	2.99	112.78	109.97
24	B	4003	BCR	C37-C22-C23	2.99	122.79	118.08
21	A	1123	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
21	3	613	CLA	C1D-ND-C4D	-2.99	104.21	106.33
21	B	1228	CLA	C2C-C1C-NC	2.99	112.77	109.97
21	L	1501	CLA	CAA-CBA-CGA	2.99	121.99	113.25
21	6	607	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
34	3	501	LUT	C2-C3-C4	-2.99	106.21	110.30
21	A	1128	CLA	C1-C2-C3	-2.99	120.87	126.04
21	5	605	CLA	CHD-C1D-ND	-2.99	121.71	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	602	CLA	CMA-C3A-C4A	2.99	119.80	111.77
21	A	1140	CLA	C2D-C1D-ND	2.99	112.31	110.10
21	A	1101	CLA	CAA-C2A-C3A	-2.99	104.60	112.78
25	A	5001	LHG	O8-C23-C24	2.99	121.28	111.91
21	A	1102	CLA	CHD-C1D-ND	-2.99	121.71	124.45
21	4	602	CLA	C2D-C1D-ND	2.99	112.31	110.10
21	A	1101	CLA	CHD-C1D-ND	-2.98	121.71	124.45
21	6	601	CLA	C3B-C4B-NB	-2.98	107.75	110.52
21	4	604	CLA	C2C-C1C-NC	2.98	112.77	109.97
21	B	1232	CLA	OBD-CAD-C3D	-2.98	121.34	128.52
21	3	610	CLA	C2D-C1D-ND	2.98	112.30	110.10
21	A	1139	CLA	C2C-C1C-NC	2.98	112.77	109.97
21	3	610	CLA	C2C-C1C-NC	2.98	112.77	109.97
21	A	1123	CLA	C2D-C1D-ND	2.98	112.30	110.10
21	1	606	CLA	C2D-C1D-ND	2.98	112.30	110.10
21	4	603	CLA	CHD-C1D-ND	-2.98	121.71	124.45
21	4	604	CLA	C3B-C4B-NB	-2.98	107.75	110.52
25	2	802	LHG	O8-C23-C24	2.98	121.26	111.91
21	A	1120	CLA	CMA-C3A-C4A	2.98	119.78	111.77
21	B	1238	CLA	CMA-C3A-C4A	2.98	119.78	111.77
21	3	603	CLA	CAC-C3C-C4C	2.98	128.68	124.81
24	2	503	BCR	C34-C9-C8	2.98	122.77	118.08
21	3	611	CLA	C2D-C1D-ND	2.98	112.30	110.10
21	5	601	CLA	C4B-CHC-C1C	2.98	133.40	126.34
21	A	1110	CLA	O2A-CGA-CBA	2.98	121.25	111.91
21	4	605	CLA	C1-C2-C3	-2.98	120.89	126.04
21	O	1801	CLA	C3C-C4C-NC	-2.98	107.32	110.57
21	5	612	CLA	OBD-CAD-C3D	-2.98	121.36	128.52
21	A	1012	CLA	C2D-C1D-ND	2.98	112.30	110.10
21	A	1134	CLA	C1D-ND-C4D	-2.97	104.22	106.33
21	B	1213	CLA	CMC-C2C-C1C	2.97	129.57	125.04
21	B	1023	CLA	CHD-C1D-ND	-2.97	121.72	124.45
21	B	1229	CLA	CHD-C1D-ND	-2.97	121.72	124.45
21	6	604	CLA	C1-C2-C3	-2.97	120.90	126.04
36	2	609	CHL	C4B-CHC-C1C	2.97	133.39	126.34
21	B	1220	CLA	C2D-C1D-ND	2.97	112.30	110.10
21	6	608	CLA	CMA-C3A-C4A	2.97	119.76	111.77
21	A	1108	CLA	C2D-C1D-ND	2.97	112.29	110.10
21	1	611	CLA	CMA-C3A-C4A	2.97	119.76	111.77
21	6	608	CLA	C1D-ND-C4D	-2.97	104.22	106.33
21	5	604	CLA	CHD-C1D-ND	-2.97	121.72	124.45
21	B	1201	CLA	CHD-C1D-ND	-2.97	121.72	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1107	CLA	C2D-C1D-ND	2.97	112.29	110.10
21	5	605	CLA	C1D-ND-C4D	-2.97	104.23	106.33
20	A	1011	CL0	CMB-C2B-C1B	2.97	129.89	125.37
24	A	4003	BCR	C33-C5-C6	-2.97	121.19	124.53
21	A	1118	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
21	1	608	CLA	CMA-C3A-C4A	2.97	119.75	111.77
36	1	610	CHL	CMA-C3A-C4A	2.97	119.75	111.77
21	2	603	CLA	C1-O2A-CGA	2.97	124.23	116.44
24	B	4006	BCR	C29-C30-C25	2.97	115.05	110.48
24	B	4006	BCR	C30-C25-C26	-2.97	118.44	122.61
21	B	1207	CLA	C3B-C4B-NB	-2.97	107.76	110.52
21	L	1504	CLA	C2C-C1C-NC	2.97	112.75	109.97
24	1	504	BCR	C23-C22-C21	2.97	123.49	118.94
21	1	605	CLA	C1C-C2C-C3C	-2.97	103.84	106.96
21	A	1114	CLA	C2D-C1D-ND	2.96	112.29	110.10
36	2	610	CHL	CHB-C4A-NA	2.96	128.61	124.51
21	B	1218	CLA	CAA-CBA-CGA	-2.96	104.59	113.25
21	B	1239	CLA	C3B-C4B-NB	-2.96	107.77	110.52
21	1	603	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
36	5	609	CHL	C4B-CHC-C1C	2.96	133.36	126.34
21	B	1239	CLA	C1D-ND-C4D	-2.96	104.23	106.33
24	L	4002	BCR	C8-C9-C10	2.96	123.48	118.94
21	B	1216	CLA	C2C-C1C-NC	2.96	112.75	109.97
21	3	611	CLA	CHA-C4D-ND	2.96	138.69	132.50
21	B	1226	CLA	CMD-C2D-C3D	-2.96	120.81	127.61
21	B	1240	CLA	C2C-C1C-NC	2.96	112.74	109.97
21	3	615	CLA	C2C-C1C-NC	2.96	112.74	109.97
21	1	611	CLA	C1D-ND-C4D	-2.96	104.23	106.33
21	A	1107	CLA	CMA-C3A-C4A	2.96	119.72	111.77
21	A	1104	CLA	C3B-C4B-NB	-2.96	107.77	110.52
21	A	1115	CLA	C3B-C4B-NB	-2.96	107.77	110.52
21	O	1803	CLA	C3D-C2D-C1D	-2.96	101.80	105.83
21	L	1501	CLA	O1D-CGD-CBD	-2.95	118.44	124.48
21	B	1239	CLA	C2C-C1C-NC	2.95	112.74	109.97
21	K	1402	CLA	CMA-C3A-C4A	2.95	119.71	111.77
21	B	1217	CLA	C3B-C4B-NB	-2.95	107.78	110.52
21	J	1901	CLA	O1D-CGD-CBD	-2.95	118.44	124.48
21	F	1301	CLA	CHD-C1D-ND	-2.95	121.74	124.45
21	6	603	CLA	CMA-C3A-C4A	2.95	119.71	111.77
21	B	1207	CLA	C2D-C1D-ND	2.95	112.28	110.10
27	A	5004	LMU	C2'-C3'-C4'	2.95	116.42	109.68
21	B	1236	CLA	O2D-CGD-O1D	-2.95	118.07	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	J	4002	BCR	C3-C4-C5	-2.95	108.81	114.08
21	4	608	CLA	C2D-C1D-ND	2.95	112.28	110.10
24	B	4001	BCR	C36-C18-C17	-2.95	118.79	122.92
21	B	1235	CLA	CHD-C1D-ND	-2.95	121.75	124.45
21	B	1208	CLA	C2C-C1C-NC	2.95	112.73	109.97
21	4	605	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
24	G	4001	BCR	C38-C26-C27	2.95	119.28	113.62
21	B	1023	CLA	C3B-C4B-NB	-2.94	107.78	110.52
21	5	607	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
21	A	1128	CLA	CAA-C2A-C3A	-2.94	104.72	112.78
21	4	605	CLA	C2D-C1D-ND	2.94	112.27	110.10
21	B	1227	CLA	OBD-CAD-C3D	-2.94	121.44	128.52
21	5	605	CLA	CMA-C3A-C4A	2.94	119.68	111.77
21	2	612	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
21	1	605	CLA	CHD-C1D-ND	-2.94	121.75	124.45
21	1	612	CLA	C2C-C1C-NC	2.94	112.73	109.97
24	A	4007	BCR	C35-C13-C14	-2.94	118.81	122.92
21	3	610	CLA	C1D-ND-C4D	-2.94	104.25	106.33
24	I	4002	BCR	C8-C7-C6	-2.94	118.95	127.20
21	4	605	CLA	O2A-CGA-CBA	2.94	121.13	111.91
21	A	1127	CLA	C1-O2A-CGA	2.94	124.15	116.44
21	G	1601	CLA	CMA-C3A-C4A	2.94	119.67	111.77
21	A	1113	CLA	C1C-C2C-C3C	-2.94	103.87	106.96
24	J	4001	BCR	C37-C22-C23	2.94	122.70	118.08
21	A	1123	CLA	C1C-C2C-C3C	-2.94	103.87	106.96
21	A	1133	CLA	C2D-C1D-ND	2.94	112.27	110.10
21	3	613	CLA	CAA-C2A-C3A	-2.94	104.74	112.78
21	6	602	CLA	C1D-ND-C4D	-2.94	104.25	106.33
21	H	1702	CLA	CHA-C1A-NA	-2.94	119.67	126.40
24	A	4005	BCR	C23-C24-C25	-2.94	118.96	127.20
21	4	605	CLA	C1-O2A-CGA	2.94	124.15	116.44
21	O	1802	CLA	C3B-C4B-NB	-2.94	108.26	110.23
21	2	605	CLA	C2C-C1C-NC	2.94	112.72	109.97
21	3	606	CLA	C2C-C1C-NC	2.94	112.72	109.97
21	A	1115	CLA	CMA-C3A-C4A	2.93	119.66	111.77
21	1	615	CLA	C3B-C4B-NB	-2.93	107.79	110.52
21	5	603	CLA	CHD-C1D-ND	-2.93	121.76	124.45
21	B	1212	CLA	CHD-C1D-ND	-2.93	121.76	124.45
21	5	604	CLA	C3B-C4B-NB	-2.93	107.80	110.52
21	A	1122	CLA	C1-C2-C3	-2.93	120.97	126.04
34	3	501	LUT	C38-C25-C24	-2.93	117.29	123.56
22	A	2001	PQN	C12-C11-C3	-2.93	104.14	112.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1126	CLA	CHD-C1D-ND	-2.93	121.76	124.45
21	2	612	CLA	C1C-C2C-C3C	-2.93	103.88	106.96
21	B	1239	CLA	CHD-C1D-ND	-2.93	121.76	124.45
24	3	506	BCR	C1-C6-C5	-2.93	118.49	122.61
24	O	4001	BCR	C39-C30-C25	2.93	115.05	110.30
24	A	4006	BCR	C35-C13-C12	2.93	122.69	118.08
21	2	605	CLA	C1C-C2C-C3C	-2.93	103.88	106.96
21	B	1205	CLA	O2A-CGA-CBA	2.93	121.09	111.91
21	3	610	CLA	CMA-C3A-C4A	2.93	119.64	111.77
21	2	612	CLA	CAA-C2A-C3A	-2.93	104.77	112.78
21	O	1803	CLA	CHA-C1A-NA	-2.93	119.70	126.40
21	1	611	CLA	C2C-C1C-NC	2.92	112.71	109.97
21	A	1112	CLA	C1D-ND-C4D	-2.92	104.26	106.33
21	B	1206	CLA	C2C-C1C-NC	2.92	112.71	109.97
36	2	611	CHL	CHB-C4A-NA	2.92	128.56	124.51
21	G	1602	CLA	C3B-C4B-NB	-2.92	107.80	110.52
21	6	602	CLA	C3B-C4B-NB	-2.92	107.80	110.52
21	1	607	CLA	CMA-C3A-C4A	2.92	119.63	111.77
21	B	1216	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
21	A	1122	CLA	C1C-C2C-C3C	-2.92	103.89	106.96
36	2	610	CHL	CHD-C4C-C3C	2.92	129.13	124.84
21	1	611	CLA	C3B-C4B-NB	-2.92	107.81	110.52
21	A	1117	CLA	CAA-C2A-C3A	-2.92	104.78	112.78
21	A	1132	CLA	CMA-C3A-C4A	2.92	119.62	111.77
24	A	4007	BCR	C31-C1-C6	-2.92	105.56	110.30
21	B	1214	CLA	C1C-C2C-C3C	-2.92	103.89	106.96
24	A	4002	BCR	C29-C28-C27	2.92	117.90	111.38
21	L	1503	CLA	CMA-C3A-C4A	2.92	119.62	111.77
24	1	504	BCR	C15-C14-C13	-2.92	123.14	127.31
21	2	606	CLA	C2D-C1D-ND	2.92	112.25	110.10
24	I	4002	BCR	C33-C5-C4	2.92	119.22	113.62
21	1	608	CLA	C1-C2-C3	-2.92	121.00	126.04
21	L	1501	CLA	C1D-ND-C4D	-2.92	104.26	106.33
24	4	503	BCR	C33-C5-C4	2.92	119.22	113.62
21	4	607	CLA	C2D-C1D-ND	2.91	112.25	110.10
21	K	1402	CLA	C3B-C4B-NB	-2.91	107.81	110.52
21	A	1121	CLA	CMA-C3A-C4A	2.91	119.61	111.77
35	6	502	XAT	O4-C5-C4	-2.91	111.19	113.38
21	A	1012	CLA	C1D-ND-C4D	-2.91	104.27	106.33
21	4	604	CLA	CMA-C3A-C4A	2.91	119.60	111.77
21	4	601	CLA	CMA-C3A-C4A	2.91	119.60	111.77
21	5	605	CLA	C2C-C1C-NC	2.91	112.70	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	607	CLA	CHD-C1D-ND	-2.91	121.78	124.45
21	5	612	CLA	CMB-C2B-C3B	2.91	133.64	126.59
21	1	601	CLA	C3B-C4B-NB	-2.91	107.81	110.52
21	B	1212	CLA	C2C-C1C-NC	2.91	112.70	109.97
21	A	1107	CLA	CHD-C1D-ND	-2.91	121.78	124.45
21	B	1213	CLA	O1D-CGD-CBD	-2.91	118.53	124.48
21	A	1012	CLA	C2C-C1C-NC	2.91	112.70	109.97
21	B	1215	CLA	O2A-CGA-CBA	2.91	121.04	111.91
21	4	607	CLA	C1-C2-C3	-2.91	121.01	126.04
21	6	603	CLA	C2C-C1C-NC	2.91	112.70	109.97
21	B	1221	CLA	O2A-CGA-CBA	2.91	121.03	111.91
21	K	1404	CLA	C3B-C4B-NB	-2.91	107.82	110.52
21	A	1117	CLA	C1C-C2C-C3C	-2.91	103.90	106.96
21	B	1217	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
24	I	4001	BCR	C30-C25-C26	-2.91	118.52	122.61
21	A	1131	CLA	C1-C2-C3	-2.91	121.02	126.04
21	A	1121	CLA	CHD-C1D-ND	-2.90	121.78	124.45
21	6	613	CLA	CMD-C2D-C3D	-2.90	120.93	127.61
21	A	1112	CLA	C3B-C4B-NB	-2.90	107.82	110.52
21	1	613	CLA	C2D-C1D-ND	2.90	112.24	110.10
21	A	1119	CLA	CHD-C1D-ND	-2.90	121.79	124.45
34	2	501	LUT	C18-C5-C6	-2.90	121.27	124.53
21	K	1404	CLA	C1D-ND-C4D	-2.90	104.27	106.33
21	H	1702	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
21	B	1232	CLA	C2D-C1D-ND	2.90	112.24	110.10
21	6	604	CLA	C3B-C4B-NB	-2.90	107.82	110.52
21	B	1212	CLA	CMA-C3A-C4A	2.90	119.57	111.77
21	K	1404	CLA	C2D-C1D-ND	2.90	112.24	110.10
21	5	604	CLA	C2C-C1C-NC	2.90	112.69	109.97
21	B	1022	CLA	C3B-C4B-NB	-2.90	107.83	110.52
21	6	609	CLA	C1C-C2C-C3C	-2.90	103.91	106.96
21	A	1141	CLA	CHA-C1A-NA	-2.90	119.76	126.40
21	B	1023	CLA	C2C-C1C-NC	2.90	112.69	109.97
21	1	603	CLA	C2D-C1D-ND	2.90	112.24	110.10
21	G	1602	CLA	CHD-C1D-ND	-2.90	121.79	124.45
24	F	4001	BCR	C37-C22-C21	-2.90	118.87	122.92
21	5	613	CLA	CMB-C2B-C3B	2.90	133.60	126.59
21	A	1116	CLA	CMA-C3A-C4A	2.89	119.55	111.77
21	A	1111	CLA	C2D-C1D-ND	2.89	112.24	110.10
21	6	606	CLA	C2D-C1D-ND	2.89	112.24	110.10
21	5	605	CLA	C3B-C4B-NB	-2.89	107.83	110.52
24	F	4001	BCR	C8-C7-C6	-2.89	119.08	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	F	1302	CLA	C2D-C1D-ND	2.89	112.24	110.10
21	A	1114	CLA	CMA-C3A-C4A	2.89	119.55	111.77
21	1	604	CLA	C2D-C1D-ND	2.89	112.23	110.10
21	B	1237	CLA	C11-C10-C8	-2.89	106.58	115.92
25	5	801	LHG	O8-C23-C24	2.89	120.98	111.91
21	6	607	CLA	C1C-C2C-C3C	-2.89	103.92	106.96
36	4	610	CHL	CHB-C4A-NA	2.89	128.51	124.51
21	B	1221	CLA	CMD-C2D-C3D	-2.89	120.97	127.61
21	B	1226	CLA	C1C-C2C-C3C	-2.89	103.92	106.96
24	3	504	BCR	C38-C26-C27	2.89	119.16	113.62
21	A	1132	CLA	CHD-C1D-ND	-2.89	121.80	124.45
21	3	610	CLA	C3B-C4B-NB	-2.89	107.84	110.52
21	6	603	CLA	C3B-C4B-NB	-2.89	107.84	110.52
21	2	607	CLA	C2D-C1D-ND	2.89	112.23	110.10
21	2	601	CLA	C2C-C1C-NC	2.88	112.67	109.97
21	3	612	CLA	C2C-C1C-NC	2.88	112.67	109.97
21	B	1230	CLA	CMA-C3A-C4A	2.88	119.52	111.77
21	6	602	CLA	CHD-C1D-ND	-2.88	121.80	124.45
21	O	1803	CLA	C2D-C1D-ND	2.88	112.23	110.10
21	B	1215	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
21	A	1134	CLA	C2C-C1C-NC	2.88	112.67	109.97
21	B	1226	CLA	C1-C2-C3	-2.88	121.06	126.04
21	B	1206	CLA	CHD-C1D-ND	-2.88	121.81	124.45
21	5	606	CLA	C3B-C4B-NB	-2.88	107.84	110.52
21	1	601	CLA	CMA-C3A-C4A	2.88	119.51	111.77
24	A	4004	BCR	C8-C9-C10	2.88	123.36	118.94
21	A	1131	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
21	B	1206	CLA	CMA-C3A-C4A	2.88	119.51	111.77
21	B	1207	CLA	CMA-C3A-C4A	2.88	119.51	111.77
21	6	601	CLA	C2C-C1C-NC	2.88	112.67	109.97
21	A	1116	CLA	C1D-ND-C4D	-2.88	104.29	106.33
21	B	1022	CLA	CHD-C1D-ND	-2.88	121.81	124.45
33	3	807	PTY	O4-C30-C31	2.88	120.94	111.91
24	B	4005	BCR	C33-C5-C6	-2.88	121.30	124.53
21	6	604	CLA	O1D-CGD-CBD	-2.88	118.60	124.48
21	B	1212	CLA	C1D-ND-C4D	-2.87	104.29	106.33
21	B	1216	CLA	CAA-C2A-C3A	-2.87	104.91	112.78
21	3	608	CLA	C3B-C4B-NB	-2.87	107.85	110.52
21	1	612	CLA	CHD-C1D-ND	-2.87	121.81	124.45
36	6	610	CHL	C2C-C3C-C4C	2.87	108.54	106.49
21	B	1212	CLA	C3B-C4B-NB	-2.87	107.85	110.52
21	B	1208	CLA	CHD-C1D-ND	-2.87	121.82	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	611	CLA	C1-C2-C3	-2.87	121.08	126.04
21	B	1210	CLA	CAA-C2A-C3A	-2.87	104.92	112.78
21	A	1111	CLA	C4B-CHC-C1C	2.87	133.14	126.34
21	A	1139	CLA	C4-C3-C5	2.87	120.09	115.27
21	B	1222	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
24	I	4001	BCR	C12-C13-C14	2.87	123.34	118.94
21	B	1227	CLA	CHD-C1D-ND	-2.87	121.82	124.45
21	5	604	CLA	C1D-ND-C4D	-2.86	104.30	106.33
21	2	601	CLA	CHA-C4D-ND	2.86	138.49	132.50
21	2	612	CLA	CHD-C1D-ND	-2.86	121.82	124.45
21	G	1601	CLA	C1D-ND-C4D	-2.86	104.30	106.33
21	5	612	CLA	CAC-C3C-C2C	-2.86	122.63	127.53
21	L	1504	CLA	CHD-C1D-ND	-2.86	121.83	124.45
21	B	1218	CLA	C2C-C1C-NC	2.86	112.65	109.97
21	A	1121	CLA	C2C-C1C-NC	2.86	112.65	109.97
21	B	1207	CLA	C2C-C1C-NC	2.86	112.65	109.97
21	5	612	CLA	C2C-C1C-NC	2.86	112.65	109.97
21	1	602	CLA	CMA-C3A-C4A	2.86	119.45	111.77
21	O	1801	CLA	C1D-ND-C4D	-2.86	104.31	106.33
21	A	1140	CLA	C2C-C1C-NC	2.86	112.65	109.97
21	G	1601	CLA	CHD-C1D-ND	-2.86	121.83	124.45
24	B	4004	BCR	C37-C22-C23	2.86	122.58	118.08
21	1	606	CLA	CHD-C1D-ND	-2.86	121.83	124.45
24	A	4002	BCR	C37-C22-C21	-2.86	118.92	122.92
21	B	1218	CLA	CMD-C2D-C1D	2.86	129.75	124.71
21	K	1404	CLA	C2C-C1C-NC	2.86	112.65	109.97
21	1	605	CLA	C2D-C1D-ND	2.86	112.21	110.10
36	6	610	CHL	C4B-CHC-C1C	2.85	133.11	126.34
21	B	1235	CLA	CMA-C3A-C4A	2.85	119.44	111.77
21	3	611	CLA	O2A-CGA-CBA	2.85	120.86	111.91
21	A	1105	CLA	C2C-C1C-NC	2.85	112.64	109.97
21	A	1110	CLA	C2C-C1C-NC	2.85	112.64	109.97
21	4	607	CLA	CMA-C3A-C4A	2.85	119.44	111.77
21	6	601	CLA	CMA-C3A-C4A	2.85	119.44	111.77
21	1	602	CLA	C2D-C1D-ND	2.85	112.20	110.10
21	A	1141	CLA	C1-C2-C3	-2.85	121.11	126.04
21	5	613	CLA	CHB-C1B-NB	2.85	127.27	124.26
21	H	1702	CLA	C2A-C1A-CHA	2.85	128.84	123.86
21	B	1023	CLA	C1D-ND-C4D	-2.85	104.31	106.33
21	K	1402	CLA	CHD-C1D-ND	-2.85	121.84	124.45
21	J	1901	CLA	CMA-C3A-C4A	2.85	119.42	111.77
25	1	801	LHG	O7-C7-O9	-2.85	116.83	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	4003	BCR	C31-C1-C6	-2.84	105.69	110.30
21	B	1236	CLA	C1-C2-C3	-2.84	121.12	126.04
21	B	1215	CLA	C2D-C1D-ND	2.84	112.20	110.10
21	3	605	CLA	C1-C2-C3	-2.84	121.13	126.04
21	B	1202	CLA	O2A-CGA-CBA	2.84	120.82	111.91
21	B	1235	CLA	C3B-C4B-NB	-2.84	107.88	110.52
34	5	504	LUT	C32-C33-C34	2.84	123.30	118.94
21	B	1203	CLA	C2C-C1C-NC	2.84	112.63	109.97
21	K	1401	CLA	C3B-C2B-C1B	-2.84	103.74	107.16
21	1	615	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
21	A	1127	CLA	CMA-C3A-C4A	2.84	119.40	111.77
21	B	1238	CLA	CHD-C1D-ND	-2.84	121.85	124.45
21	1	606	CLA	C2C-C1C-NC	2.83	112.63	109.97
24	H	4001	BCR	C38-C26-C27	2.83	119.06	113.62
21	3	613	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
21	1	601	CLA	CHD-C1D-ND	-2.83	121.85	124.45
24	H	4001	BCR	C40-C30-C29	-2.83	97.57	108.91
21	1	612	CLA	C1-C2-C3	-2.83	121.15	126.04
21	B	1208	CLA	CMA-C3A-C4A	2.83	119.38	111.77
21	B	1229	CLA	O2A-CGA-CBA	2.83	120.79	111.91
21	5	607	CLA	C2D-C1D-ND	2.83	112.19	110.10
24	I	4002	BCR	C30-C25-C26	-2.83	118.63	122.61
21	A	1110	CLA	C2D-C1D-ND	2.83	112.19	110.10
24	L	4002	BCR	C33-C5-C6	-2.83	121.36	124.53
21	B	1215	CLA	C1C-C2C-C3C	-2.83	103.99	106.96
21	B	1228	CLA	C2D-C1D-ND	2.83	112.19	110.10
21	A	1119	CLA	CMA-C3A-C4A	2.82	119.36	111.77
21	F	1301	CLA	C3B-C4B-NB	-2.82	107.90	110.52
36	6	610	CHL	C3B-C4B-NB	-2.82	107.90	110.52
21	A	1112	CLA	CMA-C3A-C4A	2.82	119.36	111.77
21	G	1602	CLA	C1D-ND-C4D	-2.82	104.33	106.33
21	B	1021	CLA	CAA-C2A-C3A	-2.82	105.05	112.78
21	6	608	CLA	CHD-C1D-ND	-2.82	121.86	124.45
21	4	608	CLA	CHD-C1D-ND	-2.82	121.86	124.45
24	1	504	BCR	C33-C5-C4	2.82	119.03	113.62
21	B	1231	CLA	C2C-C1C-NC	2.82	112.61	109.97
21	3	611	CLA	CMA-C3A-C4A	2.82	119.35	111.77
21	5	613	CLA	CHA-C4D-ND	2.82	138.39	132.50
21	A	1135	CLA	CMA-C3A-C4A	2.82	119.34	111.77
21	A	1102	CLA	C2D-C1D-ND	2.82	112.18	110.10
31	4	802	LMG	O7-C10-O9	-2.82	116.89	123.70
24	F	4001	BCR	C36-C18-C17	-2.82	118.98	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	605	CLA	CHD-C1D-ND	-2.82	121.87	124.45
36	5	609	CHL	C2C-C3C-C4C	2.82	108.50	106.49
36	2	611	CHL	C4D-CHA-C1A	2.82	124.67	121.25
36	4	611	CHL	C3C-C4C-NC	-2.82	107.41	110.57
21	F	1302	CLA	O2A-CGA-CBA	2.81	120.74	111.91
21	5	612	CLA	CMA-C3A-C4A	2.81	119.34	111.77
35	3	502	XAT	C38-C25-C26	-2.81	117.55	122.26
31	4	802	LMG	O8-C28-C29	2.81	120.73	111.91
25	5	801	LHG	O7-C7-C8	2.81	117.56	111.50
36	2	609	CHL	CMA-C3A-C4A	2.81	119.33	111.77
21	A	1101	CLA	C3B-C4B-NB	-2.81	107.91	110.52
21	5	612	CLA	CHD-C4C-NC	-2.81	119.78	124.20
21	B	1210	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
21	6	604	CLA	CMB-C2B-C3B	2.81	133.40	126.59
36	5	609	CHL	C3B-C4B-NB	-2.81	107.91	110.52
21	3	607	CLA	CMA-C3A-C4A	2.81	119.33	111.77
21	A	1102	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
21	3	615	CLA	CMA-C3A-C4A	2.81	119.32	111.77
21	2	607	CLA	CMA-C3A-C4A	2.81	119.32	111.77
36	3	604	CHL	C3C-C4C-NC	-2.81	107.42	110.57
21	L	1503	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
21	1	612	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
21	A	1132	CLA	C3B-C4B-NB	-2.81	107.91	110.52
21	5	606	CLA	CHD-C1D-ND	-2.81	121.88	124.45
21	B	1209	CLA	C1C-C2C-C3C	-2.81	104.01	106.96
21	O	1802	CLA	CHD-C1D-ND	-2.81	121.88	124.45
21	A	1130	CLA	CHA-C4D-ND	2.81	138.37	132.50
21	B	1201	CLA	C2C-C1C-NC	2.80	112.60	109.97
24	B	4003	BCR	C34-C9-C8	2.80	122.50	118.08
21	5	603	CLA	O1D-CGD-CBD	-2.80	118.75	124.48
21	4	601	CLA	C2A-C1A-CHA	2.80	128.76	123.86
21	2	604	CLA	C2D-C1D-ND	2.80	112.17	110.10
21	2	608	CLA	CMD-C2D-C3D	-2.80	121.17	127.61
21	1	603	CLA	CAA-C2A-C3A	-2.80	105.11	112.78
21	5	606	CLA	C1D-ND-C4D	-2.80	104.35	106.33
20	A	1011	CL0	O2D-CGD-O1D	-2.80	118.37	123.84
21	J	1901	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
21	A	1106	CLA	C2D-C1D-ND	2.80	112.17	110.10
21	2	615	CLA	C2D-C1D-ND	2.80	112.17	110.10
21	6	606	CLA	CHD-C1D-ND	-2.80	121.88	124.45
21	A	1131	CLA	CHA-C4D-ND	2.80	138.35	132.50
21	4	612	CLA	C2D-C1D-ND	2.80	112.16	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1236	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
36	2	610	CHL	CHD-C1D-ND	-2.79	121.89	124.45
21	3	602	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
24	K	4001	BCR	C38-C26-C27	2.79	118.98	113.62
24	1	504	BCR	C36-C18-C17	-2.79	119.01	122.92
21	B	1023	CLA	CMA-C3A-C4A	2.79	119.28	111.77
21	4	609	CLA	CMA-C3A-C4A	2.79	119.28	111.77
21	A	1124	CLA	CHD-C1D-ND	-2.79	121.89	124.45
36	1	610	CHL	C3C-C4C-NC	-2.79	107.44	110.57
34	4	501	LUT	C15-C14-C13	-2.79	123.33	127.31
21	1	604	CLA	C6-C7-C8	-2.79	106.90	115.92
21	A	1117	CLA	C1-O2A-CGA	2.79	123.76	116.44
21	B	1217	CLA	C2D-C1D-ND	2.79	112.16	110.10
21	B	1022	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
21	3	608	CLA	CMA-C3A-C4A	2.79	119.27	111.77
24	4	503	BCR	C15-C14-C13	-2.79	123.33	127.31
21	B	1204	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
21	6	612	CLA	C2C-C1C-NC	2.79	112.58	109.97
21	B	1211	CLA	CHA-C4D-ND	2.79	138.33	132.50
21	B	1022	CLA	C1D-ND-C4D	-2.79	104.36	106.33
21	3	612	CLA	CAA-C2A-C3A	-2.79	105.15	112.78
24	B	4006	BCR	C35-C13-C12	2.78	122.47	118.08
21	5	613	CLA	C2C-C1C-NC	2.78	112.58	109.97
25	1	801	LHG	O8-C23-C24	2.78	120.65	111.91
21	4	612	CLA	CHD-C1D-ND	-2.78	121.89	124.45
34	5	504	LUT	C12-C13-C14	2.78	123.21	118.94
36	1	610	CHL	CHC-C1C-NC	2.78	128.43	124.20
24	K	4001	BCR	C30-C25-C26	-2.78	118.69	122.61
21	B	1237	CLA	C2D-C1D-ND	2.78	112.16	110.10
21	1	601	CLA	C1D-ND-C4D	-2.78	104.36	106.33
21	5	612	CLA	C3B-C4B-NB	-2.78	107.93	110.52
21	A	1133	CLA	C1-C2-C3	-2.78	121.23	126.04
21	6	606	CLA	CMA-C3A-C4A	2.78	119.25	111.77
21	4	605	CLA	CHA-C4D-ND	2.78	138.32	132.50
21	A	1134	CLA	CMA-C3A-C4A	2.78	119.25	111.77
21	3	613	CLA	C3D-C2D-C1D	-2.78	102.04	105.83
21	A	1116	CLA	C3B-C4B-NB	-2.78	107.94	110.52
21	A	1135	CLA	CHA-C4D-ND	2.78	138.31	132.50
21	B	1221	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
21	A	1122	CLA	C2D-C1D-ND	2.78	112.15	110.10
21	B	1221	CLA	C1-C2-C3	-2.78	121.24	126.04
21	B	1213	CLA	C3B-C4B-NB	-2.78	107.94	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1135	CLA	C1C-C2C-C3C	-2.78	104.04	106.96
21	K	1402	CLA	C1D-ND-C4D	-2.78	104.36	106.33
21	G	1601	CLA	C3B-C4B-NB	-2.78	107.94	110.52
21	B	1220	CLA	CAA-C2A-C1A	-2.78	102.88	111.97
21	B	1203	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
25	5	801	LHG	C25-C24-C23	-2.78	103.53	113.62
21	4	602	CLA	CMA-C3A-C4A	2.77	119.23	111.77
21	B	1214	CLA	C1-C2-C3	-2.77	121.25	126.04
24	L	4001	BCR	C24-C25-C26	-2.77	114.75	121.46
21	A	1123	CLA	CHA-C4D-ND	2.77	138.29	132.50
21	A	1106	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
24	J	4002	BCR	C37-C22-C23	2.77	122.44	118.08
21	2	605	CLA	CHA-C4D-ND	2.77	138.29	132.50
21	6	608	CLA	C3B-C4B-NB	-2.77	107.95	110.52
20	A	1011	CL0	C4-C3-C5	2.77	119.93	115.27
21	3	602	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
21	1	603	CLA	CMA-C3A-C4A	2.77	119.21	111.77
21	A	1106	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
21	B	1229	CLA	C1D-ND-C4D	-2.77	104.37	106.33
21	A	1111	CLA	CHD-C1D-ND	-2.77	121.91	124.45
21	F	1302	CLA	CHD-C1D-ND	-2.77	121.91	124.45
21	6	604	CLA	C1D-ND-C4D	-2.77	104.37	106.33
21	B	1232	CLA	C2A-C1A-CHA	2.77	128.69	123.86
21	A	1130	CLA	CHD-C1D-ND	-2.77	121.91	124.45
21	B	1229	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
21	2	605	CLA	CHD-C1D-ND	-2.76	121.91	124.45
21	B	1205	CLA	C2D-C1D-ND	2.76	112.14	110.10
21	6	604	CLA	C4B-CHC-C1C	2.76	132.89	126.34
24	1	504	BCR	C34-C9-C10	-2.76	119.06	122.92
21	5	608	CLA	C1D-ND-C4D	-2.76	104.37	106.33
21	A	1132	CLA	C1D-ND-C4D	-2.76	104.38	106.33
21	B	1227	CLA	C3B-C4B-NB	-2.76	107.96	110.52
21	L	1501	CLA	C11-C12-C13	-2.76	107.00	115.92
21	A	1105	CLA	CMA-C3A-C4A	2.76	119.18	111.77
24	A	4004	BCR	C38-C26-C27	2.76	118.91	113.62
21	B	1226	CLA	CHA-C4D-ND	2.76	138.26	132.50
21	4	605	CLA	C3B-C4B-NB	-2.76	107.96	110.52
21	B	1208	CLA	C1D-ND-C4D	-2.76	104.38	106.33
21	3	606	CLA	C2D-C1D-ND	2.76	112.14	110.10
21	B	1240	CLA	CHD-C1D-ND	-2.76	121.92	124.45
21	6	612	CLA	C3B-C4B-NB	-2.76	107.96	110.52
21	L	1504	CLA	CMA-C3A-C4A	2.76	119.18	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	F	1301	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
21	3	607	CLA	C2D-C1D-ND	2.75	112.13	110.10
21	4	603	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
21	B	1214	CLA	CMA-C3A-C4A	2.75	119.17	111.77
21	4	608	CLA	CMA-C3A-C4A	2.75	119.17	111.77
24	B	4002	BCR	C19-C18-C17	2.75	123.17	118.94
21	3	611	CLA	C1-C2-C3	-2.75	121.28	126.04
21	A	1102	CLA	C3B-C4B-NB	-2.75	107.96	110.52
24	O	4001	BCR	C32-C1-C2	-2.75	97.90	108.91
21	5	614	CLA	CAC-C3C-C2C	2.75	132.23	127.53
21	F	1301	CLA	C2D-C1D-ND	2.75	112.13	110.10
21	A	1013	CLA	CMB-C2B-C3B	2.75	133.25	126.59
21	A	1114	CLA	C3B-C4B-NB	-2.75	107.97	110.52
21	2	603	CLA	C3B-C4B-NB	-2.75	107.97	110.52
21	1	604	CLA	C1D-ND-C4D	-2.75	104.38	106.33
25	4	801	LHG	O8-C23-C24	2.75	120.53	111.91
24	A	4001	BCR	C19-C18-C17	2.75	123.16	118.94
21	B	1230	CLA	O2A-CGA-CBA	2.74	120.52	111.91
21	B	1239	CLA	CMA-C3A-C4A	2.74	119.15	111.77
21	K	1403	CLA	CMA-C3A-C4A	2.74	119.15	111.77
24	B	4001	BCR	C34-C9-C10	-2.74	119.08	122.92
21	3	611	CLA	C3D-C2D-C1D	-2.74	102.09	105.83
21	B	1021	CLA	O2A-CGA-CBA	2.74	120.52	111.91
34	5	503	LUT	C40-C33-C34	-2.74	119.08	122.92
21	A	1131	CLA	C2A-C3A-C4A	2.74	106.30	101.87
21	5	614	CLA	CMA-C3A-C4A	2.74	119.14	111.77
21	A	1138	CLA	C2D-C1D-ND	2.74	112.12	110.10
21	A	1012	CLA	CMA-C3A-C4A	2.74	119.14	111.77
21	B	1231	CLA	C3B-C4B-NB	-2.74	107.97	110.52
21	5	612	CLA	C2A-C1A-CHA	2.74	128.65	123.86
21	3	605	CLA	CHA-C4D-ND	2.74	138.23	132.50
21	B	1231	CLA	CMD-C2D-C3D	-2.74	121.32	127.61
21	1	608	CLA	C2D-C1D-ND	2.74	112.12	110.10
21	B	1021	CLA	CHD-C1D-ND	-2.74	121.94	124.45
21	B	1212	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
21	B	1205	CLA	C2C-C1C-NC	2.73	112.53	109.97
21	A	1013	CLA	C3B-C4B-NB	-2.73	107.98	110.52
21	B	1216	CLA	C2D-C1D-ND	2.73	112.12	110.10
21	3	612	CLA	C1-C2-C3	-2.73	121.31	126.04
28	3	804	DGD	C1D-O6D-C5D	2.73	119.05	113.69
21	3	615	CLA	C2D-C1D-ND	2.73	112.12	110.10
21	B	1237	CLA	CMB-C2B-C1B	-2.73	121.21	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	4001	BCR	C15-C14-C13	-2.73	123.41	127.31
21	5	602	CLA	C2C-C1C-NC	2.73	112.53	109.97
21	A	1126	CLA	C2D-C1D-ND	2.73	112.12	110.10
21	B	1240	CLA	CMA-C3A-C4A	2.73	119.11	111.77
21	3	612	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
24	3	504	BCR	C12-C13-C14	-2.73	114.76	118.94
36	4	610	CHL	CMA-C3A-C4A	2.73	119.10	111.77
21	A	1130	CLA	C4-C3-C5	-2.73	110.69	115.27
21	A	1141	CLA	C2A-C1A-CHA	2.73	128.62	123.86
21	1	612	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
21	A	1139	CLA	CHD-C1D-ND	-2.72	121.95	124.45
21	O	1803	CLA	CHD-C1D-ND	-2.72	121.95	124.45
21	B	1201	CLA	CMA-C3A-C4A	2.72	119.09	111.77
21	B	1225	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
21	5	601	CLA	OBD-CAD-C3D	-2.72	121.97	128.52
20	A	1011	CL0	C3D-C4D-ND	2.72	114.64	110.24
21	B	1217	CLA	CHA-C4D-ND	2.72	138.19	132.50
21	4	601	CLA	C2C-C1C-NC	2.72	112.52	109.97
25	2	803	LHG	O8-C23-C24	2.72	120.44	111.91
36	4	611	CHL	C2B-C1B-NB	-2.72	108.41	110.23
21	2	608	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
31	F	5002	LMG	O8-C28-C29	2.72	120.44	111.91
31	1	804	LMG	C4-C3-C2	2.72	115.57	110.82
21	A	1114	CLA	C1D-ND-C4D	-2.72	104.41	106.33
21	6	612	CLA	CMA-C3A-C4A	2.72	119.07	111.77
21	B	1220	CLA	C2C-C1C-NC	2.72	112.52	109.97
21	B	1206	CLA	C1-C2-C3	-2.71	121.35	126.04
21	H	1701	CLA	O1D-CGD-CBD	-2.71	118.93	124.48
21	1	605	CLA	CAA-C2A-C3A	-2.71	105.35	112.78
24	K	4001	BCR	C33-C5-C4	2.71	118.83	113.62
21	3	606	CLA	C2A-C1A-CHA	2.71	128.60	123.86
21	A	1109	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
21	B	1203	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
21	B	1203	CLA	CHA-C4D-ND	2.71	138.17	132.50
24	G	4001	BCR	C36-C18-C17	-2.71	119.12	122.92
36	5	609	CHL	C1-C2-C3	-2.71	121.35	126.04
21	6	606	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
21	B	1213	CLA	CHA-C1A-NA	-2.71	120.19	126.40
21	B	1207	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
21	B	1202	CLA	C11-C12-C13	-2.71	107.16	115.92
21	6	609	CLA	CHD-C1D-ND	-2.71	121.96	124.45
24	O	4001	BCR	C34-C9-C10	-2.71	119.13	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	615	CLA	C3B-C4B-NB	-2.71	108.00	110.52
21	1	607	CLA	CHA-C4D-ND	2.71	138.17	132.50
21	1	604	CLA	CAA-C2A-C3A	-2.71	105.36	112.78
36	2	611	CHL	CHC-C4B-NB	-2.71	121.39	124.26
21	G	1603	CLA	CMD-C2D-C3D	-2.71	121.39	127.61
24	H	4001	BCR	C29-C30-C25	2.71	114.65	110.48
24	L	4001	BCR	C33-C5-C6	-2.71	121.49	124.53
21	1	603	CLA	O2A-CGA-CBA	2.71	120.40	111.91
21	3	605	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
21	1	613	CLA	CHA-C4D-ND	2.71	138.16	132.50
24	I	4002	BCR	C38-C26-C25	-2.70	121.49	124.53
31	3	803	LMG	O8-C28-C29	2.70	120.39	111.91
21	6	606	CLA	C1D-ND-C4D	-2.70	104.41	106.33
25	6	801	LHG	O8-C23-C24	2.70	120.39	111.91
36	3	604	CHL	C1-C2-C3	-2.70	121.37	126.04
21	1	615	CLA	C1-C2-C3	-2.70	121.37	126.04
35	4	502	XAT	O24-C25-C38	-2.70	111.82	115.06
21	3	603	CLA	C3B-C4B-NB	-2.70	108.01	110.52
21	4	601	CLA	C4D-CHA-C1A	2.70	124.53	121.25
24	1	504	BCR	C28-C27-C26	-2.70	109.26	114.08
21	A	1102	CLA	C2C-C1C-NC	2.70	112.50	109.97
21	2	602	CLA	CHA-C4D-ND	2.70	138.15	132.50
21	A	1104	CLA	C4D-C3D-CAD	2.70	111.28	108.10
21	J	1901	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
21	A	1107	CLA	C1D-ND-C4D	-2.70	104.42	106.33
21	1	603	CLA	C1D-ND-C4D	-2.70	104.42	106.33
35	2	502	XAT	C6-C7-C8	-2.70	120.29	125.99
21	A	1140	CLA	C1-C2-C3	-2.70	121.38	126.04
21	B	1217	CLA	CMA-C3A-C4A	2.70	119.02	111.77
24	3	506	BCR	C34-C9-C10	-2.69	119.15	122.92
21	A	1107	CLA	C1C-C2C-C3C	-2.69	104.12	106.96
21	A	1134	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
28	3	805	DGD	O1G-C1A-C2A	2.69	120.36	111.91
21	O	1803	CLA	C3B-C4B-NB	-2.69	108.02	110.52
21	B	1232	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
21	A	1124	CLA	C3B-C4B-NB	-2.69	108.02	110.52
24	A	4003	BCR	C35-C13-C12	2.69	122.32	118.08
34	2	501	LUT	C3-C4-C5	-2.69	106.50	111.85
21	3	602	CLA	CHD-C1D-ND	-2.69	121.98	124.45
36	2	613	CHL	CHD-C1D-ND	-2.69	121.98	124.45
21	2	607	CLA	CHD-C1D-ND	-2.69	121.98	124.45
21	B	1218	CLA	CAA-C2A-C1A	-2.69	103.17	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1232	CLA	CHA-C4D-ND	2.69	138.12	132.50
21	A	1013	CLA	C4-C3-C5	2.69	119.79	115.27
21	B	1217	CLA	CHD-C1D-ND	-2.69	121.98	124.45
21	B	1206	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
21	A	1138	CLA	O2A-CGA-CBA	2.69	120.34	111.91
21	1	615	CLA	CMA-C3A-C4A	2.69	118.99	111.77
21	B	1240	CLA	C2D-C1D-ND	2.69	112.08	110.10
21	L	1503	CLA	C2D-C1D-ND	2.69	112.08	110.10
21	2	606	CLA	O2A-CGA-CBA	2.69	120.33	111.91
21	L	1502	CLA	C3B-C2B-C1B	-2.69	103.92	107.16
21	B	1218	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
21	B	1237	CLA	CMB-C2B-C3B	2.68	133.09	126.59
21	A	1122	CLA	CMA-C3A-C4A	2.68	118.99	111.77
28	3	804	DGD	O1G-C1A-C2A	2.68	120.33	111.91
21	B	1223	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
21	B	1209	CLA	CHA-C4D-ND	2.68	138.11	132.50
21	B	1221	CLA	O1D-CGD-CBD	-2.68	118.99	124.48
21	5	602	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
25	4	801	LHG	C5-O7-C7	-2.68	111.19	117.79
21	A	1114	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
21	B	1227	CLA	C2C-C1C-NC	2.68	112.48	109.97
21	2	615	CLA	CHD-C1D-ND	-2.68	121.99	124.45
21	H	1702	CLA	C4B-CHC-C1C	2.68	132.70	126.34
21	B	1022	CLA	CMA-C3A-C4A	2.68	118.98	111.77
21	4	615	CLA	CHA-C4D-ND	2.68	138.11	132.50
35	6	502	XAT	C26-C27-C28	-2.68	120.33	125.99
21	3	603	CLA	CHA-C4D-ND	2.68	138.10	132.50
21	2	605	CLA	CMA-C3A-C4A	2.68	118.97	111.77
36	5	609	CHL	C1-O2A-CGA	2.68	123.47	116.44
21	A	1115	CLA	C1D-ND-C4D	-2.68	104.43	106.33
21	B	1235	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
21	6	612	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
21	B	1220	CLA	O2A-CGA-CBA	2.68	120.31	111.91
36	1	610	CHL	CHD-C4C-C3C	2.68	128.78	124.84
21	3	607	CLA	C1-C2-C3	-2.68	121.41	126.04
21	A	1138	CLA	CHD-C1D-ND	-2.68	121.99	124.45
21	3	608	CLA	O2A-CGA-CBA	2.68	120.31	111.91
21	A	1136	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
21	2	607	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
21	B	1221	CLA	CHA-C4D-ND	2.68	138.10	132.50
21	3	603	CLA	CMA-C3A-C4A	2.67	118.96	111.77
21	5	607	CLA	C2B-C1B-NB	-2.67	108.44	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	2	801	LHG	O8-C23-C24	2.67	120.30	111.91
21	A	1119	CLA	C2D-C1D-ND	2.67	112.07	110.10
27	6	805	LMU	O5'-C5'-C6'	2.67	113.08	106.44
21	A	1105	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
21	B	1215	CLA	CMA-C3A-C4A	2.67	118.95	111.77
21	B	1214	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
21	B	1230	CLA	C2C-C1C-NC	2.67	112.47	109.97
21	B	1223	CLA	CMA-C3A-C4A	2.67	118.95	111.77
21	3	608	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
21	1	615	CLA	CMC-C2C-C1C	2.67	129.10	125.04
21	6	608	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
24	H	4001	BCR	C1-C6-C5	-2.67	118.85	122.61
21	A	1127	CLA	C6-C5-C3	-2.67	106.46	113.45
21	5	612	CLA	CAA-CBA-CGA	-2.67	105.46	113.25
21	A	1117	CLA	C2D-C1D-ND	2.67	112.07	110.10
21	5	606	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
21	A	1116	CLA	CHD-C1D-ND	-2.67	122.00	124.45
24	3	506	BCR	C4-C5-C6	-2.67	118.86	122.73
21	B	1204	CLA	CHD-C1D-ND	-2.67	122.00	124.45
34	5	501	LUT	C22-C23-C24	2.67	114.78	111.74
21	6	605	CLA	C10-C8-C7	-2.67	98.11	112.13
21	1	606	CLA	CHA-C1A-NA	-2.66	120.30	126.40
24	L	4002	BCR	C36-C18-C17	-2.66	119.19	122.92
21	B	1224	CLA	C3B-C4B-NB	-2.66	108.04	110.52
21	B	1234	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
21	B	1202	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
21	A	1108	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
21	B	1223	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
21	B	1231	CLA	CHA-C4D-ND	2.66	138.07	132.50
21	A	1012	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
21	A	1013	CLA	CAA-C2A-C3A	-2.66	105.49	112.78
21	4	608	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
35	4	502	XAT	C24-C23-C22	-2.66	105.63	110.77
21	K	1404	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
24	I	4001	BCR	C38-C26-C27	2.66	118.73	113.62
21	B	1217	CLA	C4B-CHC-C1C	2.66	132.65	126.34
31	4	803	LMG	O8-C28-C29	2.66	120.25	111.91
25	5	802	LHG	O8-C23-C24	2.66	120.25	111.91
21	B	1223	CLA	CHA-C4D-ND	2.66	138.06	132.50
36	2	611	CHL	CMA-C3A-C4A	2.66	118.92	111.77
21	A	1107	CLA	C3B-C4B-NB	-2.66	108.05	110.52
34	4	501	LUT	C10-C11-C12	-2.66	114.92	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	607	CLA	C3B-C4B-NB	-2.66	108.05	110.52
21	F	1301	CLA	C4B-CHC-C1C	2.66	132.64	126.34
33	O	5002	PTY	O4-C30-C31	2.66	120.24	111.91
21	3	607	CLA	CHD-C1D-ND	-2.66	122.01	124.45
21	A	1130	CLA	CMA-C3A-C4A	2.66	118.91	111.77
21	A	1112	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
21	H	1701	CLA	CHD-C1D-ND	-2.65	122.02	124.45
21	B	1205	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
21	2	607	CLA	O2A-CGA-CBA	2.65	120.23	111.91
21	1	604	CLA	C4B-CHC-C1C	2.65	132.63	126.34
21	B	1214	CLA	C3B-C4B-NB	-2.65	108.05	110.52
21	B	1211	CLA	CMD-C2D-C3D	-2.65	121.51	127.61
21	B	1237	CLA	O2A-CGA-CBA	2.65	120.22	111.91
24	A	4001	BCR	C38-C26-C25	-2.65	121.55	124.53
21	5	603	CLA	CHA-C4D-ND	2.65	138.04	132.50
21	A	1132	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
21	5	608	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
21	B	1224	CLA	O2A-CGA-CBA	2.65	120.22	111.91
21	2	607	CLA	CHA-C4D-ND	2.65	138.04	132.50
21	B	1218	CLA	C3B-C4B-NB	-2.65	108.06	110.52
21	B	1207	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
24	A	4004	BCR	C36-C18-C17	-2.65	119.22	122.92
21	2	604	CLA	C3B-C4B-NB	-2.65	108.06	110.52
21	B	1225	CLA	C2D-C1D-ND	2.65	112.05	110.10
36	1	609	CHL	C2C-C3C-C4C	2.65	108.38	106.49
21	A	1127	CLA	CAA-C2A-C3A	-2.65	105.53	112.78
36	2	609	CHL	C1-O2A-CGA	2.65	123.39	116.44
24	A	4003	BCR	C33-C5-C4	2.64	118.70	113.62
24	J	4001	BCR	C36-C18-C17	-2.64	119.22	122.92
21	A	1103	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
35	4	502	XAT	C11-C10-C9	2.64	131.08	127.31
24	J	4002	BCR	C32-C1-C6	-2.64	106.01	110.30
21	3	614	CLA	C2D-C1D-ND	2.64	112.05	110.10
39	2	808	P3H	O19-C17-C16	2.64	120.20	111.91
21	4	612	CLA	CHA-C4D-ND	2.64	138.03	132.50
21	A	1110	CLA	CMA-C3A-C4A	2.64	118.88	111.77
21	B	1226	CLA	O2A-CGA-CBA	2.64	120.20	111.91
21	5	614	CLA	C4B-CHC-C1C	2.64	132.60	126.34
21	A	1109	CLA	C4-C3-C5	2.64	119.71	115.27
35	4	502	XAT	C6-C7-C8	-2.64	120.41	125.99
21	G	1601	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
21	3	610	CLA	C1C-C2C-C3C	-2.64	104.18	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	602	CLA	CMB-C2B-C3B	2.64	132.98	126.59
24	B	4005	BCR	C27-C26-C25	-2.64	118.90	122.73
21	B	1225	CLA	CHD-C1D-ND	-2.64	122.03	124.45
36	4	611	CHL	CMA-C3A-C4A	2.64	118.87	111.77
21	1	608	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
24	A	4004	BCR	C27-C26-C25	-2.64	118.90	122.73
34	5	503	LUT	C18-C5-C4	2.64	119.24	114.36
21	4	605	CLA	CMA-C3A-C4A	2.64	118.86	111.77
21	A	1102	CLA	CHA-C4D-ND	2.64	138.02	132.50
21	B	1234	CLA	CHD-C1D-ND	-2.64	122.03	124.45
24	2	503	BCR	C35-C13-C12	2.64	122.23	118.08
21	2	606	CLA	C1C-C2C-C3C	-2.64	104.19	106.96
21	3	615	CLA	C1C-C2C-C3C	-2.64	104.19	106.96
21	B	1227	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
21	2	603	CLA	C2C-C1C-NC	2.63	112.44	109.97
21	K	1402	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
21	A	1141	CLA	C3D-C2D-C1D	-2.63	102.24	105.83
21	A	1132	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
21	4	607	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
21	6	601	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
21	A	1013	CLA	C2A-C1A-CHA	2.63	128.46	123.86
24	B	4004	BCR	C31-C1-C6	-2.63	106.03	110.30
21	4	603	CLA	C2D-C1D-ND	2.63	112.04	110.10
24	A	4003	BCR	C36-C18-C17	-2.63	119.24	122.92
24	3	503	BCR	C23-C24-C25	-2.63	119.82	127.20
21	4	603	CLA	C2C-C1C-NC	2.63	112.43	109.97
21	A	1141	CLA	C1C-C2C-C3C	-2.63	104.20	106.96
21	B	1205	CLA	C1C-C2C-C3C	-2.63	104.20	106.96
21	J	1901	CLA	CHA-C4D-ND	2.63	137.99	132.50
21	B	1239	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
34	2	501	LUT	C30-C31-C32	-2.62	115.03	123.22
21	1	606	CLA	CHA-C4D-ND	2.62	137.99	132.50
21	6	605	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
21	J	1901	CLA	C3B-C2B-C1B	-2.62	104.00	107.16
21	B	1217	CLA	CHA-C1A-NA	-2.62	120.39	126.40
21	4	605	CLA	OBD-CAD-C3D	-2.62	122.21	128.52
21	K	1404	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
34	5	501	LUT	C10-C11-C12	-2.62	115.04	123.22
21	A	1105	CLA	C4B-CHC-C1C	2.62	132.56	126.34
21	B	1227	CLA	CMA-C3A-C4A	2.62	118.81	111.77
21	1	607	CLA	C2D-C1D-ND	2.62	112.03	110.10
24	4	503	BCR	C3-C4-C5	-2.62	109.40	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	G	1602	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
21	B	1240	CLA	C4B-CHC-C1C	2.62	132.55	126.34
31	6	802	LMG	O8-C28-C29	2.62	120.12	111.91
35	3	502	XAT	C19-C9-C10	-2.62	119.26	122.92
21	1	602	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
21	B	1237	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
21	A	1113	CLA	C3B-C4B-NB	-2.62	108.09	110.52
21	4	605	CLA	C1C-C2C-C3C	-2.62	104.21	106.96
21	3	612	CLA	C1C-C2C-C3C	-2.62	104.21	106.96
21	2	605	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
21	4	606	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
34	4	501	LUT	C36-C21-C26	2.61	113.50	109.55
21	B	1226	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
21	A	1102	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
21	6	602	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
21	1	605	CLA	C3B-C4B-NB	-2.61	108.09	110.52
21	A	1125	CLA	C3D-C2D-C1D	-2.61	102.27	105.83
36	1	609	CHL	C1-O2A-CGA	2.61	123.30	116.44
21	1	615	CLA	CHA-C4D-ND	2.61	137.96	132.50
21	6	609	CLA	C2D-C1D-ND	2.61	112.03	110.10
21	K	1402	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
24	F	4002	BCR	C27-C26-C25	-2.61	118.94	122.73
38	2	807	LMK	C12-C11-C10	-2.61	107.34	113.38
21	A	1121	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
21	2	605	CLA	O2A-CGA-CBA	2.61	120.10	111.91
21	6	605	CLA	CHA-C4D-ND	2.61	137.96	132.50
21	B	1228	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
21	B	1232	CLA	CMA-C3A-C4A	2.61	118.78	111.77
21	L	1504	CLA	C3B-C4B-NB	-2.61	108.09	110.52
28	B	5002	DGD	C2G-O2G-C1B	-2.61	111.37	117.79
21	1	607	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
33	4	804	PTY	O4-C30-C31	2.61	120.09	111.91
21	2	605	CLA	C1-C2-C3	-2.61	121.53	126.04
21	1	612	CLA	CHA-C4D-ND	2.61	137.96	132.50
21	A	1116	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
21	5	601	CLA	C1D-ND-C4D	-2.61	104.48	106.33
21	A	1124	CLA	C2C-C1C-NC	2.61	112.41	109.97
21	B	1239	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
25	A	5002	LHG	O8-C23-C24	2.61	120.08	111.91
21	F	1302	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
21	A	1120	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
21	B	1237	CLA	CHA-C4D-ND	2.61	137.95	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1208	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
21	B	1221	CLA	CBC-CAC-C3C	-2.60	105.25	112.43
21	B	1213	CLA	C1D-ND-C4D	-2.60	104.49	106.33
21	3	602	CLA	CHA-C4D-ND	2.60	137.94	132.50
21	5	601	CLA	CHA-C4D-ND	2.60	137.94	132.50
21	A	1013	CLA	C1-C2-C3	-2.60	121.54	126.04
21	1	606	CLA	C1-O2A-CGA	2.60	123.27	116.44
21	B	1214	CLA	CHA-C4D-ND	2.60	137.94	132.50
21	3	601	CLA	C1-C2-C3	-2.60	121.55	126.04
21	O	1803	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
21	B	1231	CLA	CAA-C2A-C3A	-2.60	105.66	112.78
24	3	506	BCR	C3-C4-C5	-2.60	109.44	114.08
21	1	613	CLA	CHD-C1D-ND	-2.60	122.07	124.45
21	A	1131	CLA	CMD-C2D-C3D	-2.60	121.64	127.61
34	5	502	LUT	C18-C5-C4	2.60	119.17	114.36
21	3	615	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
21	L	1504	CLA	C1C-C2C-C3C	-2.60	104.23	106.96
24	J	4001	BCR	C12-C13-C14	-2.60	114.96	118.94
21	5	601	CLA	CAC-C3C-C4C	2.60	128.18	124.81
24	F	4001	BCR	C19-C18-C17	2.60	122.92	118.94
21	B	1226	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
21	4	602	CLA	C1C-C2C-C3C	-2.60	104.23	106.96
21	B	1202	CLA	CHA-C1A-NA	-2.60	120.45	126.40
21	4	612	CLA	C2C-C1C-NC	2.59	112.40	109.97
21	B	1021	CLA	CAA-CBA-CGA	-2.59	105.67	113.25
21	A	1114	CLA	O2A-CGA-CBA	2.59	120.05	111.91
24	B	4004	BCR	C35-C13-C12	2.59	122.17	118.08
21	B	1238	CLA	C1-C2-C3	-2.59	121.56	126.04
21	L	1504	CLA	C4B-CHC-C1C	2.59	132.49	126.34
21	1	601	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
36	2	611	CHL	C1-O2A-CGA	2.59	124.27	116.73
21	B	1222	CLA	C1-C2-C3	-2.59	121.56	126.04
21	A	1140	CLA	C1-O2A-CGA	2.59	123.25	116.44
21	2	601	CLA	C3B-C4B-NB	-2.59	108.11	110.52
21	A	1122	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
21	B	1235	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
21	A	1115	CLA	CHD-C1D-ND	-2.59	122.07	124.45
21	A	1101	CLA	CHA-C4D-ND	2.59	137.92	132.50
21	A	1117	CLA	CHD-C1D-ND	-2.59	122.07	124.45
21	A	1125	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
21	B	1209	CLA	CHD-C1D-ND	-2.59	122.07	124.45
21	A	1136	CLA	C1-C2-C3	-2.59	121.56	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	503	BCR	C33-C5-C6	-2.59	121.62	124.53
21	B	1237	CLA	C4-C3-C5	2.59	119.63	115.27
21	6	605	CLA	C1D-ND-C4D	-2.59	104.50	106.33
21	A	1138	CLA	C2C-C1C-NC	2.59	112.40	109.97
21	A	1111	CLA	O1D-CGD-CBD	-2.59	119.19	124.48
21	6	603	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
32	L	5002	4RF	O18-C16-C15	2.59	120.03	111.91
35	6	504	XAT	C6-C7-C8	-2.59	120.52	125.99
21	A	1135	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
21	3	612	CLA	CHA-C4D-ND	2.59	137.91	132.50
34	6	501	LUT	C18-C5-C4	2.59	119.15	114.36
21	A	1012	CLA	OBD-CAD-C3D	-2.59	122.30	128.52
21	1	611	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
21	A	1103	CLA	CAA-C2A-C1A	-2.59	103.50	111.97
21	B	1202	CLA	CHA-C4D-ND	2.59	137.91	132.50
24	A	4006	BCR	C37-C22-C23	2.59	122.15	118.08
29	5	804	3PH	O31-C31-C32	2.58	120.02	111.91
21	6	613	CLA	CHA-C4D-ND	2.58	137.91	132.50
21	A	1117	CLA	O1D-CGD-CBD	-2.58	119.20	124.48
24	B	4006	BCR	C37-C22-C23	2.58	122.15	118.08
21	A	1140	CLA	CHD-C1D-ND	-2.58	122.08	124.45
21	4	609	CLA	O2A-CGA-CBA	2.58	120.01	111.91
21	5	601	CLA	O1D-CGD-CBD	-2.58	119.20	124.48
36	5	610	CHL	C2B-C1B-NB	-2.58	108.50	110.23
21	A	1134	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
21	B	1023	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
39	5	806	P3H	O19-C17-C16	2.58	120.00	111.91
21	B	1213	CLA	C3D-C2D-C1D	-2.58	102.31	105.83
21	A	1012	CLA	O2A-CGA-CBA	2.58	120.00	111.91
35	6	504	XAT	C39-C29-C28	2.58	122.14	118.08
21	B	1224	CLA	O1D-CGD-CBD	-2.58	119.21	124.48
36	2	611	CHL	C3C-C4C-NC	-2.58	107.68	110.57
24	I	4002	BCR	C36-C18-C17	-2.58	119.31	122.92
21	1	603	CLA	CHA-C4D-ND	2.58	137.89	132.50
21	G	1603	CLA	CAC-C3C-C2C	-2.58	123.12	127.53
21	K	1402	CLA	O2A-CGA-CBA	2.57	119.99	111.91
21	4	606	CLA	C2D-C1D-ND	2.57	112.00	110.10
21	1	603	CLA	CMC-C2C-C1C	2.57	128.96	125.04
21	B	1225	CLA	CHA-C4D-ND	2.57	137.88	132.50
21	A	1101	CLA	CMA-C3A-C4A	2.57	118.69	111.77
34	5	502	LUT	C8-C7-C6	-2.57	119.98	127.20
21	B	1022	CLA	O2D-CGD-O1D	-2.57	118.81	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	O	1803	CLA	C4B-CHC-C1C	2.57	132.44	126.34
21	5	605	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
24	B	4002	BCR	C15-C14-C13	-2.57	123.64	127.31
34	1	501	LUT	C22-C23-C24	-2.57	108.82	111.74
21	5	604	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
21	A	1140	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
21	2	601	CLA	C3D-C2D-C1D	-2.57	102.33	105.83
24	I	4002	BCR	C27-C26-C25	-2.57	119.00	122.73
35	3	502	XAT	C18-C5-C4	2.57	117.17	114.28
21	4	615	CLA	C1-C2-C3	-2.57	121.60	126.04
36	4	611	CHL	C1-O2A-CGA	2.57	123.18	116.44
21	B	1217	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
21	3	602	CLA	O2A-CGA-CBA	2.57	119.97	111.91
21	4	615	CLA	CHD-C1D-ND	-2.57	122.09	124.45
21	B	1207	CLA	C1D-ND-C4D	-2.57	104.51	106.33
21	A	1115	CLA	CHA-C4D-ND	2.57	137.87	132.50
21	A	1120	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
21	B	1205	CLA	CMA-C3A-C4A	2.57	118.67	111.77
21	6	605	CLA	C2C-C1C-NC	2.57	112.38	109.97
21	A	1115	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
21	A	1131	CLA	CHD-C1D-ND	-2.57	122.09	124.45
21	B	1234	CLA	CHA-C4D-ND	2.57	137.87	132.50
21	B	1208	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
21	5	608	CLA	C1-C2-C3	-2.56	121.61	126.04
21	B	1222	CLA	CHA-C4D-ND	2.56	137.86	132.50
21	B	1229	CLA	CMB-C2B-C3B	2.56	132.80	126.59
21	3	608	CLA	CHA-C4D-ND	2.56	137.86	132.50
21	6	607	CLA	CHA-C4D-ND	2.56	137.86	132.50
24	F	4002	BCR	C35-C13-C12	2.56	122.11	118.08
36	5	610	CHL	CMA-C3A-C4A	2.56	118.66	111.77
21	B	1219	CLA	C2D-C1D-ND	2.56	111.99	110.10
21	A	1138	CLA	C3B-C4B-NB	-2.56	108.14	110.52
21	A	1103	CLA	C2C-C1C-NC	2.56	112.37	109.97
21	H	1701	CLA	CMB-C2B-C1B	2.56	129.27	125.37
33	5	803	PTY	O4-C30-C31	2.56	119.94	111.91
21	A	1140	CLA	CHA-C4D-ND	2.56	137.85	132.50
28	2	806	DGD	O1G-C1A-C2A	2.56	119.94	111.91
21	K	1401	CLA	CHA-C4D-ND	2.56	137.85	132.50
21	3	611	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
20	A	1011	CL0	CMC-C2C-C1C	2.56	128.93	125.04
21	B	1211	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
21	2	602	CLA	C3B-C4B-NB	-2.56	108.14	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1021	CLA	C2C-C1C-NC	2.56	112.37	109.97
21	L	1501	CLA	C2C-C1C-NC	2.56	112.37	109.97
21	4	604	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
21	A	1110	CLA	C3B-C4B-NB	-2.55	108.14	110.52
21	H	1701	CLA	C2D-C1D-ND	2.55	111.99	110.10
21	A	1139	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
36	2	609	CHL	C2C-C3C-C4C	2.55	108.31	106.49
21	1	605	CLA	CHA-C4D-ND	2.55	137.84	132.50
24	A	4004	BCR	C34-C9-C10	-2.55	119.35	122.92
21	3	612	CLA	CHD-C1D-ND	-2.55	122.11	124.45
21	A	1119	CLA	CHA-C4D-ND	2.55	137.84	132.50
21	B	1022	CLA	CHA-C4D-ND	2.55	137.84	132.50
21	B	1210	CLA	C6-C5-C3	-2.55	106.77	113.45
29	F	5003	3PH	O31-C31-C32	2.55	119.91	111.91
21	A	1115	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
21	4	602	CLA	CHA-C4D-ND	2.55	137.83	132.50
21	A	1105	CLA	CMC-C2C-C1C	2.55	128.92	125.04
21	B	1227	CLA	O1D-CGD-CBD	-2.55	119.27	124.48
21	3	605	CLA	C2C-C1C-NC	2.55	112.36	109.97
21	G	1603	CLA	C4D-C3D-CAD	2.55	111.10	108.10
21	B	1229	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
24	J	4002	BCR	C1-C6-C5	-2.55	119.02	122.61
21	A	1138	CLA	CHA-C4D-ND	2.55	137.83	132.50
21	H	1702	CLA	CHA-C4D-ND	2.55	137.83	132.50
21	3	601	CLA	C1D-ND-C4D	-2.55	104.53	106.33
21	2	608	CLA	CHA-C4D-ND	2.55	137.83	132.50
21	6	609	CLA	CHA-C4D-ND	2.55	137.83	132.50
36	2	610	CHL	CMA-C3A-C4A	2.55	118.61	111.77
21	2	615	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
21	6	602	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
34	5	501	LUT	C39-C29-C30	-2.54	119.36	122.92
24	L	4001	BCR	C19-C18-C17	2.54	122.85	118.94
21	B	1021	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
36	4	610	CHL	CHD-C1D-ND	-2.54	122.12	124.45
21	A	1133	CLA	C3B-C4B-NB	-2.54	108.16	110.52
21	B	1238	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
21	B	1218	CLA	CHA-C4D-ND	2.54	137.82	132.50
21	A	1107	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
36	2	610	CHL	C4D-CHA-C1A	2.54	124.34	121.25
21	6	603	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
21	B	1216	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
21	A	1126	CLA	CHA-C4D-ND	2.54	137.81	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	604	CLA	CAC-C3C-C4C	2.54	128.11	124.81
21	K	1403	CLA	CHA-C4D-ND	2.54	137.81	132.50
21	3	607	CLA	CHA-C4D-ND	2.54	137.81	132.50
21	2	615	CLA	CHA-C4D-ND	2.54	137.81	132.50
21	5	607	CLA	CMA-C3A-C4A	2.54	118.60	111.77
21	A	1109	CLA	CHA-C4D-ND	2.54	137.81	132.50
21	A	1112	CLA	O1D-CGD-CBD	-2.54	119.29	124.48
21	A	1126	CLA	CMC-C2C-C1C	2.54	128.90	125.04
21	3	603	CLA	OBD-CAD-C3D	-2.54	122.41	128.52
21	2	602	CLA	C6-C5-C3	-2.54	110.47	114.62
21	A	1108	CLA	CHD-C1D-ND	-2.54	122.12	124.45
21	A	1130	CLA	C2C-C1C-NC	2.54	112.35	109.97
21	A	1101	CLA	C4B-CHC-C1C	2.53	132.35	126.34
35	1	502	XAT	C38-C25-C26	-2.53	118.01	122.26
21	O	1802	CLA	CHA-C1A-NA	-2.53	120.60	126.40
21	B	1212	CLA	C1C-C2C-C3C	-2.53	104.29	106.96
21	2	602	CLA	C1C-C2C-C3C	-2.53	104.29	106.96
24	J	4002	BCR	C29-C30-C25	2.53	114.38	110.48
21	A	1101	CLA	CHA-C1A-NA	-2.53	120.60	126.40
21	A	1134	CLA	C4B-CHC-C1C	2.53	132.34	126.34
21	B	1206	CLA	C3B-C4B-NB	-2.53	108.17	110.52
21	1	603	CLA	C3B-C4B-NB	-2.53	108.17	110.52
21	2	603	CLA	CHA-C4D-ND	2.53	137.79	132.50
21	L	1503	CLA	O1D-CGD-CBD	-2.53	119.31	124.48
21	A	1101	CLA	C1D-ND-C4D	-2.53	104.54	106.33
21	3	612	CLA	CMA-C3A-C4A	2.53	118.57	111.77
21	A	1140	CLA	C3B-C4B-NB	-2.53	108.17	110.52
21	1	608	CLA	C3B-C4B-NB	-2.53	108.17	110.52
21	4	603	CLA	CHA-C4D-ND	2.53	137.79	132.50
21	F	1302	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
24	K	4001	BCR	C8-C9-C10	2.53	122.82	118.94
21	3	602	CLA	CMA-C3A-C4A	2.53	118.57	111.77
21	4	607	CLA	CHA-C4D-ND	2.53	137.78	132.50
21	6	606	CLA	C4B-CHC-C1C	2.53	132.33	126.34
21	1	604	CLA	O2A-CGA-CBA	2.52	119.83	111.91
21	A	1106	CLA	CHA-C4D-ND	2.52	137.78	132.50
31	2	804	LMG	O8-C28-C29	2.52	119.83	111.91
36	3	604	CHL	C1D-CHD-C4C	-2.52	120.61	126.06
21	B	1219	CLA	C1C-C2C-C3C	-2.52	104.30	106.96
21	6	606	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
21	A	1112	CLA	C4B-CHC-C1C	2.52	132.32	126.34
21	A	1110	CLA	CMD-C2D-C3D	-2.52	121.81	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1104	CLA	O2A-CGA-CBA	2.52	119.82	111.91
21	1	613	CLA	C3B-C4B-NB	-2.52	108.17	110.52
21	B	1240	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
21	G	1603	CLA	CHA-C4D-ND	2.52	137.77	132.50
21	A	1127	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
21	6	605	CLA	CBA-CAA-C2A	-2.52	106.42	113.86
21	A	1128	CLA	CHA-C4D-ND	2.52	137.77	132.50
21	3	607	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
21	1	602	CLA	CHA-C4D-ND	2.52	137.77	132.50
21	O	1802	CLA	CMA-C3A-C4A	2.52	118.54	111.77
36	4	611	CHL	C1-C2-C3	-2.52	122.68	126.75
21	A	1114	CLA	CHA-C4D-ND	2.52	137.76	132.50
24	I	4001	BCR	C8-C9-C10	2.52	122.80	118.94
21	A	1116	CLA	C1-O2A-CGA	2.52	123.04	116.44
21	4	615	CLA	C1C-C2C-C3C	-2.51	104.31	106.96
21	2	604	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
21	H	1702	CLA	C2D-C1D-ND	2.51	111.96	110.10
21	6	603	CLA	C4B-CHC-C1C	2.51	132.30	126.34
21	A	1137	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
21	B	1231	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
24	F	4001	BCR	C33-C5-C4	2.51	118.44	113.62
21	B	1219	CLA	CMA-C3A-C4A	2.51	118.52	111.77
24	H	4001	BCR	C30-C25-C24	2.51	122.88	115.78
24	3	506	BCR	C8-C9-C10	2.51	122.79	118.94
24	A	4003	BCR	C28-C27-C26	-2.51	109.59	114.08
21	B	1227	CLA	C1-C2-C3	-2.51	121.70	126.04
21	B	1232	CLA	CHA-C1A-NA	-2.51	120.65	126.40
21	A	1113	CLA	CHA-C4D-ND	2.51	137.75	132.50
21	K	1402	CLA	C4B-CHC-C1C	2.51	132.28	126.34
21	B	1227	CLA	CHA-C4D-ND	2.51	137.74	132.50
21	1	607	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
21	1	608	CLA	CHA-C4D-ND	2.50	137.74	132.50
21	5	612	CLA	C2D-C1D-ND	2.50	111.95	110.10
21	6	601	CLA	C4B-CHC-C1C	2.50	132.28	126.34
21	A	1119	CLA	C1-C2-C3	-2.50	121.72	126.04
24	A	4001	BCR	C8-C9-C10	2.50	122.78	118.94
21	3	607	CLA	C3B-C4B-NB	-2.50	108.19	110.52
21	B	1219	CLA	CAA-C2A-C3A	-2.50	105.93	112.78
21	B	1239	CLA	C4B-CHC-C1C	2.50	132.27	126.34
21	3	612	CLA	C2D-C1D-ND	2.50	111.95	110.10
21	A	1114	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
21	B	1221	CLA	C2A-C1A-CHA	2.50	128.23	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1212	CLA	C4B-CHC-C1C	2.50	132.27	126.34
21	3	610	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
21	B	1220	CLA	C1-C2-C3	-2.50	121.72	126.04
24	4	503	BCR	C34-C9-C10	-2.50	119.42	122.92
21	2	608	CLA	C2D-C1D-ND	2.50	111.94	110.10
21	K	1404	CLA	CHA-C4D-ND	2.50	137.72	132.50
21	5	606	CLA	C4B-CHC-C1C	2.50	132.26	126.34
21	A	1121	CLA	C4B-CHC-C1C	2.50	132.26	126.34
21	B	1216	CLA	C1-C2-C3	-2.50	121.72	126.04
21	G	1602	CLA	CHA-C4D-ND	2.50	137.72	132.50
21	3	611	CLA	CHA-C1A-NA	-2.50	120.68	126.40
21	4	608	CLA	CHA-C4D-ND	2.50	137.72	132.50
21	A	1105	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
21	5	608	CLA	CHD-C1D-ND	-2.50	122.16	124.45
21	A	1012	CLA	C4B-CHC-C1C	2.49	132.25	126.34
21	A	1110	CLA	C4B-CHC-C1C	2.49	132.25	126.34
21	B	1221	CLA	C1-O2A-CGA	2.49	122.98	116.44
21	A	1113	CLA	CAA-C2A-C3A	-2.49	105.95	112.78
21	F	1301	CLA	CHA-C1A-NA	-2.49	120.69	126.40
21	B	1216	CLA	C3B-C4B-NB	-2.49	108.20	110.52
21	3	605	CLA	CHD-C1D-ND	-2.49	122.16	124.45
21	3	613	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
21	B	1208	CLA	C4B-CHC-C1C	2.49	132.25	126.34
25	4	801	LHG	C9-C8-C7	-2.49	104.56	113.62
21	6	613	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
21	F	1302	CLA	CHA-C4D-ND	2.49	137.71	132.50
21	1	604	CLA	CHA-C4D-ND	2.49	137.71	132.50
21	6	613	CLA	CMB-C2B-C3B	2.49	132.62	126.59
21	A	1130	CLA	C4B-CHC-C1C	2.49	132.24	126.34
21	3	603	CLA	O1D-CGD-CBD	-2.49	119.39	124.48
21	B	1223	CLA	CHA-C1A-NA	-2.49	120.70	126.40
24	3	503	BCR	C19-C18-C17	2.49	122.76	118.94
21	A	1116	CLA	CHA-C4D-ND	2.49	137.70	132.50
24	A	4005	BCR	C15-C14-C13	-2.49	123.76	127.31
21	5	604	CLA	C4B-CHC-C1C	2.49	132.24	126.34
24	F	4002	BCR	C30-C25-C26	-2.49	119.11	122.61
21	B	1221	CLA	CHA-C1A-NA	-2.49	120.70	126.40
21	A	1139	CLA	CHA-C4D-ND	2.49	137.70	132.50
21	4	606	CLA	CHA-C4D-ND	2.49	137.70	132.50
21	G	1603	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
21	B	1201	CLA	C3B-C4B-NB	-2.49	108.21	110.52
21	B	1218	CLA	C1C-C2C-C3C	-2.49	104.34	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	615	CLA	CHD-C1D-ND	-2.49	122.17	124.45
21	3	608	CLA	CHA-C1A-NA	-2.49	120.71	126.40
21	5	605	CLA	C4B-CHC-C1C	2.48	132.23	126.34
21	L	1501	CLA	CMB-C2B-C3B	2.48	132.61	126.59
21	B	1207	CLA	CHA-C4D-ND	2.48	137.69	132.50
21	A	1111	CLA	C1D-ND-C4D	-2.48	104.57	106.33
21	B	1238	CLA	CHA-C4D-ND	2.48	137.69	132.50
21	B	1204	CLA	C1-C2-C3	-2.48	121.75	126.04
36	1	609	CHL	C4D-CHA-C1A	2.48	124.27	121.25
25	1	802	LHG	O8-C23-C24	2.48	119.70	111.91
21	1	611	CLA	C4B-CHC-C1C	2.48	132.22	126.34
21	B	1021	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
21	B	1224	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
21	A	1113	CLA	CMA-C3A-C4A	2.48	118.44	111.77
21	G	1601	CLA	C4B-CHC-C1C	2.48	132.22	126.34
21	A	1108	CLA	CHA-C4D-ND	2.48	137.69	132.50
21	A	1125	CLA	CHA-C4D-ND	2.48	137.69	132.50
34	2	501	LUT	C35-C34-C33	-2.48	123.77	127.31
21	5	605	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
21	2	604	CLA	CHA-C4D-ND	2.48	137.69	132.50
21	4	604	CLA	C4B-CHC-C1C	2.48	132.22	126.34
21	B	1237	CLA	CHD-C1D-ND	-2.48	122.18	124.45
21	4	608	CLA	CAA-C2A-C3A	-2.48	105.99	112.78
21	B	1208	CLA	CHA-C4D-ND	2.48	137.68	132.50
21	O	1801	CLA	CHA-C4D-ND	2.48	137.68	132.50
25	2	801	LHG	C5-O7-C7	-2.48	111.69	117.79
21	6	604	CLA	CHA-C1A-NA	-2.48	120.72	126.40
21	B	1206	CLA	C4B-CHC-C1C	2.48	132.21	126.34
24	I	4002	BCR	C30-C25-C24	2.48	122.78	115.78
21	A	1132	CLA	C4B-CHC-C1C	2.48	132.21	126.34
36	5	609	CHL	CHC-C1C-NC	2.48	127.96	124.20
21	A	1129	CLA	CHA-C4D-ND	2.48	137.68	132.50
21	B	1210	CLA	CHA-C4D-ND	2.48	137.68	132.50
21	5	606	CLA	CHA-C4D-ND	2.48	137.68	132.50
25	F	5001	LHG	O8-C23-C24	2.48	119.67	111.91
21	B	1219	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
21	3	601	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
21	B	1207	CLA	C4B-CHC-C1C	2.47	132.21	126.34
21	H	1701	CLA	C7-C6-C5	-2.47	106.64	113.36
24	K	4001	BCR	C37-C22-C21	-2.47	119.46	122.92
21	1	601	CLA	CHA-C4D-ND	2.47	137.67	132.50
21	A	1137	CLA	C1D-ND-C4D	-2.47	104.58	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1116	CLA	C4B-CHC-C1C	2.47	132.20	126.34
32	L	5002	4RF	O40-C41-C43	2.47	119.67	111.91
21	B	1235	CLA	C4B-CHC-C1C	2.47	132.20	126.34
21	A	1107	CLA	CHA-C4D-ND	2.47	137.67	132.50
21	B	1201	CLA	O2A-CGA-CBA	2.47	119.67	111.91
21	1	604	CLA	CMD-C2D-C3D	-2.47	121.93	127.61
21	1	601	CLA	C4B-CHC-C1C	2.47	132.20	126.34
21	4	609	CLA	CHA-C1A-NA	-2.47	120.74	126.40
21	A	1139	CLA	C2D-C1D-ND	2.47	111.92	110.10
35	2	502	XAT	C24-C23-C22	-2.47	106.00	110.77
24	F	4002	BCR	C36-C18-C17	-2.47	119.46	122.92
21	4	615	CLA	C3B-C4B-NB	-2.47	108.22	110.52
21	1	603	CLA	C1-O2A-CGA	2.47	122.93	116.44
21	B	1210	CLA	C4B-CHC-C1C	2.47	132.20	126.34
21	4	609	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
24	3	504	BCR	C36-C18-C17	-2.47	119.47	122.92
24	B	4006	BCR	C31-C1-C6	-2.47	106.30	110.30
36	2	613	CHL	C4B-CHC-C1C	2.47	132.19	126.34
21	3	610	CLA	C4B-CHC-C1C	2.47	132.19	126.34
21	K	1404	CLA	C4B-CHC-C1C	2.47	132.19	126.34
21	4	603	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
21	6	602	CLA	C4B-CHC-C1C	2.47	132.19	126.34
21	2	606	CLA	CAA-C2A-C3A	-2.47	106.03	112.78
24	4	503	BCR	C4-C5-C6	-2.47	119.15	122.73
24	H	4001	BCR	C15-C14-C13	-2.47	123.79	127.31
21	2	602	CLA	C1-C2-C3	-2.46	121.78	126.04
21	G	1602	CLA	C4B-CHC-C1C	2.46	132.18	126.34
21	A	1132	CLA	CHA-C4D-ND	2.46	137.65	132.50
21	2	604	CLA	CMA-C3A-C4A	2.46	118.40	111.77
21	A	1108	CLA	C3B-C4B-NB	-2.46	108.23	110.52
21	B	1201	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
21	A	1137	CLA	CBA-CAA-C2A	2.46	121.13	113.86
21	4	612	CLA	CHA-C1A-NA	-2.46	120.76	126.40
21	B	1223	CLA	C4B-CHC-C1C	2.46	132.18	126.34
21	B	1231	CLA	C4B-CHC-C1C	2.46	132.18	126.34
21	A	1116	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
24	F	4001	BCR	C38-C26-C27	2.46	118.34	113.62
21	3	614	CLA	CHA-C4D-ND	2.46	137.65	132.50
36	6	610	CHL	C2B-C1B-NB	-2.46	108.58	110.23
21	3	602	CLA	C2D-C1D-ND	2.46	111.92	110.10
21	6	602	CLA	CHA-C4D-ND	2.46	137.65	132.50
21	B	1222	CLA	CAA-C2A-C1A	-2.46	103.91	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	614	CLA	C3B-C4B-NB	-2.46	108.23	110.52
21	A	1107	CLA	O2A-CGA-CBA	2.46	119.63	111.91
21	L	1504	CLA	O1D-CGD-CBD	-2.46	119.45	124.48
21	H	1702	CLA	O1D-CGD-CBD	-2.46	119.45	124.48
21	B	1201	CLA	CHA-C4D-ND	2.46	137.64	132.50
21	2	612	CLA	CHA-C4D-ND	2.46	137.64	132.50
34	4	501	LUT	C18-C5-C6	-2.46	121.77	124.53
21	L	1502	CLA	C3B-C4B-NB	-2.46	108.23	110.52
21	3	614	CLA	C3B-C4B-NB	-2.46	108.23	110.52
36	2	610	CHL	CHB-C1B-NB	-2.46	121.66	124.26
24	2	503	BCR	C23-C24-C25	-2.46	120.31	127.20
21	A	1125	CLA	O2A-CGA-CBA	2.46	119.61	111.91
21	A	1110	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
21	3	615	CLA	CHA-C4D-ND	2.45	137.63	132.50
21	3	602	CLA	C3B-C4B-NB	-2.45	108.24	110.52
24	B	4006	BCR	C23-C24-C25	-2.45	120.31	127.20
21	3	601	CLA	CHA-C4D-ND	2.45	137.63	132.50
21	B	1023	CLA	C4B-CHC-C1C	2.45	132.16	126.34
21	3	611	CLA	CHD-C1D-ND	-2.45	122.20	124.45
21	B	1214	CLA	O2A-CGA-CBA	2.45	119.61	111.91
21	A	1106	CLA	C12-C11-C10	2.45	124.51	113.24
21	5	604	CLA	CHA-C4D-ND	2.45	137.63	132.50
21	5	607	CLA	CHA-C4D-ND	2.45	137.63	132.50
21	4	601	CLA	C3D-C2D-C1D	-2.45	102.48	105.83
21	1	607	CLA	C3B-C4B-NB	-2.45	108.24	110.52
21	B	1225	CLA	O2A-CGA-CBA	2.45	119.60	111.91
21	A	1115	CLA	C4B-CHC-C1C	2.45	132.15	126.34
21	A	1135	CLA	O2A-CGA-CBA	2.45	119.60	111.91
21	B	1223	CLA	O2A-CGA-CBA	2.45	119.60	111.91
21	1	611	CLA	CHA-C4D-ND	2.45	137.63	132.50
21	G	1603	CLA	C2C-C1C-NC	2.45	112.27	109.97
21	A	1114	CLA	C4B-CHC-C1C	2.45	132.15	126.34
21	A	1125	CLA	CMA-C3A-C4A	2.45	118.36	111.77
24	L	4002	BCR	C34-C9-C10	-2.45	119.49	122.92
35	6	502	XAT	C6-C7-C8	-2.45	120.81	125.99
34	6	501	LUT	C8-C7-C6	-2.45	120.32	127.20
21	A	1106	CLA	C4B-CHC-C1C	2.45	132.15	126.34
21	B	1238	CLA	C2D-C1D-ND	2.45	111.91	110.10
21	B	1205	CLA	C1-C2-C3	-2.45	121.81	126.04
21	2	608	CLA	O2A-CGA-CBA	2.45	119.59	111.91
21	B	1232	CLA	C3D-C2D-C1D	-2.45	102.49	105.83
21	1	611	CLA	O2D-CGD-O1D	-2.45	119.05	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	604	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
21	2	602	CLA	CHA-C1A-NA	-2.45	120.79	126.40
21	K	1402	CLA	CHA-C4D-ND	2.45	137.62	132.50
21	B	1230	CLA	C1-O2A-CGA	2.45	122.87	116.44
21	6	608	CLA	CHA-C4D-ND	2.45	137.62	132.50
21	4	602	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
21	5	603	CLA	CMD-C2D-C3D	-2.45	121.98	127.61
21	B	1230	CLA	CHD-C1D-ND	-2.45	122.20	124.45
21	A	1110	CLA	CHA-C4D-ND	2.45	137.62	132.50
21	B	1209	CLA	CAA-C2A-C3A	-2.45	106.08	112.78
21	A	1124	CLA	CHA-C4D-ND	2.45	137.62	132.50
21	O	1802	CLA	CHA-C4D-ND	2.45	137.62	132.50
21	4	601	CLA	CHA-C1A-NA	-2.44	120.80	126.40
21	A	1117	CLA	CMB-C2B-C3B	2.44	132.51	126.59
21	A	1129	CLA	CMD-C2D-C3D	-2.44	121.99	127.61
21	4	609	CLA	C1-O2A-CGA	2.44	122.86	116.44
21	2	606	CLA	CHA-C4D-ND	2.44	137.61	132.50
21	B	1213	CLA	C4B-CHC-C1C	2.44	132.13	126.34
21	A	1104	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
21	B	1203	CLA	C3B-C4B-NB	-2.44	108.25	110.52
36	1	609	CHL	C1-C2-C3	-2.44	121.82	126.04
21	K	1403	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
21	3	605	CLA	CMD-C2D-C3D	-2.44	122.00	127.61
21	A	1013	CLA	CHD-C1D-ND	-2.44	122.21	124.45
21	B	1232	CLA	O2A-CGA-CBA	2.44	119.56	111.91
21	B	1230	CLA	CAA-C2A-C1A	-2.44	103.99	111.97
21	G	1601	CLA	CHA-C4D-ND	2.44	137.60	132.50
21	6	604	CLA	CHA-C4D-ND	2.44	137.60	132.50
21	B	1203	CLA	CMD-C2D-C3D	-2.44	122.01	127.61
21	4	601	CLA	C1-C2-C3	-2.44	121.83	126.04
21	4	609	CLA	CHD-C1D-ND	-2.44	122.22	124.45
24	A	4002	BCR	C23-C24-C25	-2.44	120.36	127.20
34	3	501	LUT	C35-C15-C14	-2.44	118.48	123.47
21	H	1701	CLA	CHA-C4D-ND	2.43	137.59	132.50
21	2	615	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
21	2	601	CLA	C2A-C1A-CHA	2.43	128.12	123.86
21	6	608	CLA	C4B-CHC-C1C	2.43	132.11	126.34
21	A	1130	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
21	3	610	CLA	CHA-C4D-ND	2.43	137.59	132.50
21	A	1128	CLA	CMA-C3A-C4A	2.43	118.31	111.77
21	A	1102	CLA	CHA-C1A-NA	-2.43	120.83	126.40
21	B	1238	CLA	CMD-C2D-C3D	-2.43	122.02	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1220	CLA	CMA-C3A-C4A	2.43	118.31	111.77
25	B	5001	LHG	O8-C23-C24	2.43	119.53	111.91
21	A	1121	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
21	B	1236	CLA	C3D-C2D-C1D	-2.43	102.52	105.83
21	L	1501	CLA	CMD-C2D-C3D	-2.43	122.03	127.61
21	L	1504	CLA	CHA-C4D-ND	2.43	137.58	132.50
21	A	1133	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
36	2	611	CHL	C3B-C4B-NB	-2.43	108.26	110.52
21	A	1117	CLA	CHA-C4D-ND	2.43	137.58	132.50
21	A	1140	CLA	C4B-CHC-C1C	2.43	132.10	126.34
21	3	602	CLA	C4B-CHC-C1C	2.43	132.10	126.34
21	A	1012	CLA	CHA-C4D-ND	2.43	137.58	132.50
21	A	1123	CLA	CHA-C1A-NA	-2.43	120.84	126.40
21	A	1138	CLA	C1C-C2C-C3C	-2.43	104.41	106.96
21	1	602	CLA	O2D-CGD-O1D	-2.43	119.10	123.84
21	B	1021	CLA	CHA-C4D-ND	2.43	137.57	132.50
21	B	1209	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
21	6	609	CLA	CHA-C1A-NA	-2.42	120.84	126.40
21	1	612	CLA	O1D-CGD-CBD	-2.42	119.52	124.48
21	B	1206	CLA	O2A-CGA-CBA	2.42	119.52	111.91
21	L	1502	CLA	CMB-C2B-C3B	2.42	132.46	126.59
21	A	1124	CLA	CAA-C2A-C3A	-2.42	106.14	112.78
21	2	602	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
21	B	1236	CLA	CHA-C4D-ND	2.42	137.56	132.50
24	J	4002	BCR	C23-C22-C21	-2.42	115.22	118.94
21	B	1238	CLA	C1-O2A-CGA	2.42	122.80	116.44
21	B	1216	CLA	CHA-C4D-ND	2.42	137.56	132.50
21	1	608	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
21	B	1230	CLA	CHA-C4D-ND	2.42	137.56	132.50
21	6	601	CLA	CHA-C4D-ND	2.42	137.56	132.50
21	3	601	CLA	C4B-CHC-C1C	2.42	132.08	126.34
21	B	1204	CLA	CHA-C4D-ND	2.42	137.56	132.50
21	1	612	CLA	C2D-C1D-ND	2.42	111.89	110.10
21	B	1229	CLA	CHA-C4D-ND	2.42	137.56	132.50
21	2	608	CLA	CAA-C2A-C3A	-2.42	106.16	112.78
21	4	603	CLA	CMA-C3A-C4A	2.42	118.27	111.77
24	F	4001	BCR	C27-C26-C25	-2.42	119.22	122.73
21	5	605	CLA	CHA-C4D-ND	2.42	137.56	132.50
21	B	1235	CLA	O2A-CGA-CBA	2.42	119.49	111.91
21	G	1601	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
21	2	603	CLA	C4B-CHC-C1C	2.42	132.07	126.34
21	B	1023	CLA	CHA-C4D-ND	2.42	137.56	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	4006	BCR	C27-C26-C25	-2.42	119.22	122.73
21	A	1120	CLA	C3B-C4B-NB	-2.42	108.27	110.52
21	2	603	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
21	A	1112	CLA	CHA-C4D-ND	2.41	137.55	132.50
21	B	1239	CLA	CHA-C4D-ND	2.41	137.55	132.50
24	G	4001	BCR	C1-C6-C5	-2.41	119.21	122.61
21	5	613	CLA	C1C-C2C-C3C	-2.41	104.42	106.96
21	B	1234	CLA	C1-C2-C3	-2.41	121.87	126.04
21	A	1110	CLA	C1D-ND-C4D	-2.41	104.62	106.33
25	6	801	LHG	C5-O7-C7	-2.41	111.85	117.79
21	B	1212	CLA	CHA-C4D-ND	2.41	137.54	132.50
21	B	1239	CLA	O2A-CGA-CBA	2.41	119.47	111.91
21	B	1219	CLA	C1-C2-C3	-2.41	121.87	126.04
21	A	1134	CLA	O2A-CGA-CBA	2.41	119.47	111.91
21	A	1130	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
21	B	1211	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
21	5	603	CLA	CMC-C2C-C3C	2.41	132.66	126.12
21	A	1125	CLA	C1-C2-C3	-2.41	121.88	126.04
21	A	1107	CLA	C4B-CHC-C1C	2.41	132.05	126.34
21	1	605	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
21	1	611	CLA	O2A-CGA-CBA	2.41	119.46	111.91
21	B	1224	CLA	CHA-C1A-NA	-2.41	120.88	126.40
21	1	615	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
21	L	1502	CLA	C2C-C1C-NC	2.41	112.23	109.97
21	2	608	CLA	C4B-CHC-C1C	2.41	132.05	126.34
35	2	502	XAT	O4-C5-C18	-2.41	112.17	115.06
21	B	1237	CLA	C6-C7-C8	-2.41	108.14	115.92
35	1	502	XAT	C19-C9-C10	-2.41	119.55	122.92
21	6	606	CLA	CHA-C4D-ND	2.41	137.53	132.50
21	4	601	CLA	C3B-C4B-NB	-2.41	108.28	110.52
21	O	1803	CLA	O1A-CGA-CBA	-2.41	114.35	123.73
21	A	1118	CLA	C1-O2A-CGA	2.41	122.75	116.44
21	A	1121	CLA	CHA-C4D-ND	2.40	137.53	132.50
24	G	4001	BCR	C4-C5-C6	-2.40	119.24	122.73
36	5	609	CHL	CHD-C4C-C3C	2.40	128.37	124.84
21	L	1502	CLA	C6-C5-C3	-2.40	107.15	113.45
21	A	1106	CLA	C1-C2-C3	-2.40	121.89	126.04
21	1	606	CLA	C3B-C4B-NB	-2.40	108.29	110.52
24	A	4002	BCR	C39-C30-C25	2.40	114.19	110.30
21	2	606	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
21	L	1502	CLA	C9-C8-C7	-2.40	102.60	111.29
21	3	607	CLA	CHA-C1A-NA	-2.40	120.90	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	613	CLA	CMA-C3A-C4A	2.40	118.23	111.77
21	5	603	CLA	C2D-C1D-ND	2.40	111.87	110.10
21	6	608	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
21	B	1237	CLA	C1D-ND-C4D	-2.40	104.63	106.33
21	A	1013	CLA	O2A-CGA-CBA	2.40	119.44	111.91
21	A	1137	CLA	CHA-C1A-NA	-2.40	120.90	126.40
21	A	1137	CLA	C2C-C1C-NC	2.40	112.22	109.97
21	A	1102	CLA	C1-O2A-CGA	2.40	122.73	116.44
21	4	605	CLA	CMD-C2D-C3D	-2.40	122.10	127.61
21	2	612	CLA	C3B-C2B-C1B	-2.40	104.27	107.16
21	2	603	CLA	C1-C2-C3	-2.40	121.90	126.04
21	A	1130	CLA	C1D-ND-C4D	-2.40	104.63	106.33
21	J	1901	CLA	O2A-CGA-CBA	2.40	119.43	111.91
21	A	1012	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
21	B	1217	CLA	C3D-C2D-C1D	-2.40	102.56	105.83
21	A	1124	CLA	CED-O2D-CGD	-2.39	110.52	115.94
21	B	1236	CLA	C1D-ND-C4D	-2.39	104.63	106.33
21	2	601	CLA	C1C-C2C-C3C	-2.39	104.44	106.96
21	A	1104	CLA	C4B-CHC-C1C	2.39	132.02	126.34
21	5	602	CLA	C4B-CHC-C1C	2.39	132.02	126.34
24	A	4001	BCR	C37-C22-C21	-2.39	119.57	122.92
21	B	1211	CLA	CHD-C1D-ND	-2.39	122.25	124.45
21	B	1206	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
31	3	803	LMG	C8-O7-C10	-2.39	111.90	117.79
21	A	1120	CLA	C2D-C1D-ND	2.39	111.87	110.10
21	B	1235	CLA	CHA-C4D-ND	2.39	137.50	132.50
21	4	603	CLA	C3B-C4B-NB	-2.39	108.30	110.52
29	5	807	3PH	O31-C31-C32	2.39	119.41	111.91
21	G	1602	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
21	L	1502	CLA	C2A-C1A-CHA	2.39	128.04	123.86
21	B	1205	CLA	CAA-C2A-C3A	-2.39	106.23	112.78
21	2	606	CLA	CMA-C3A-C4A	2.39	118.20	111.77
21	2	608	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
21	5	602	CLA	CMD-C2D-C1D	2.39	128.93	124.71
31	1	804	LMG	C14-C13-C12	-2.39	102.29	114.42
24	B	4001	BCR	C30-C25-C26	-2.39	119.25	122.61
34	5	504	LUT	C20-C13-C14	-2.39	119.58	122.92
21	B	1230	CLA	C3B-C4B-NB	-2.39	108.30	110.52
21	4	615	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
21	A	1013	CLA	CHA-C4D-ND	2.39	137.49	132.50
35	6	504	XAT	C40-C33-C34	-2.39	119.58	122.92
35	2	502	XAT	C37-C21-C36	2.39	110.89	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1111	CLA	CHA-C4D-ND	2.39	137.49	132.50
21	4	615	CLA	O2A-CGA-CBA	2.39	119.39	111.91
21	B	1222	CLA	C4B-CHC-C1C	2.39	132.00	126.34
24	A	4003	BCR	C34-C9-C10	-2.39	119.58	122.92
21	F	1301	CLA	O2A-CGA-CBA	2.38	119.39	111.91
21	A	1119	CLA	C1-O2A-CGA	2.38	122.70	116.44
21	A	1124	CLA	C1C-C2C-C3C	-2.38	104.45	106.96
21	B	1203	CLA	O2A-CGA-CBA	2.38	119.39	111.91
21	A	1139	CLA	C4B-CHC-C1C	2.38	131.99	126.34
24	B	4005	BCR	C35-C13-C12	2.38	121.83	118.08
21	L	1502	CLA	CHC-C4B-NB	2.38	126.78	124.26
21	J	1901	CLA	CHA-C1A-NA	-2.38	120.94	126.40
21	B	1240	CLA	C2A-C1A-CHA	2.38	128.02	123.86
21	B	1214	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
21	4	602	CLA	O1D-CGD-CBD	-2.38	119.61	124.48
20	A	1011	CL0	CMD-C2D-C3D	-2.38	122.14	127.61
21	1	608	CLA	C4B-CHC-C1C	2.38	131.99	126.34
21	3	614	CLA	CMA-C3A-C4A	2.38	118.17	111.77
21	L	1503	CLA	CHA-C4D-ND	2.38	137.48	132.50
21	4	608	CLA	O1D-CGD-CBD	-2.38	119.61	124.48
21	4	609	CLA	C3B-C4B-NB	-2.38	108.31	110.52
21	6	609	CLA	C3B-C4B-NB	-2.38	108.31	110.52
21	3	601	CLA	C3D-C2D-C1D	-2.38	102.58	105.83
24	3	504	BCR	C29-C28-C27	2.38	116.69	111.38
21	A	1137	CLA	CHA-C4D-ND	2.38	137.48	132.50
21	6	603	CLA	CHA-C4D-ND	2.38	137.48	132.50
21	A	1013	CLA	CMB-C2B-C1B	-2.38	121.75	125.37
21	A	1013	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
21	A	1134	CLA	CHA-C4D-ND	2.38	137.47	132.50
21	B	1215	CLA	CHA-C4D-ND	2.38	137.47	132.50
21	6	607	CLA	C2D-C1D-ND	2.38	111.86	110.10
21	1	608	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
21	O	1802	CLA	CMB-C2B-C3B	2.38	129.75	123.59
24	I	4001	BCR	C15-C14-C13	-2.38	123.92	127.31
21	A	1111	CLA	CAC-C3C-C4C	2.38	127.89	124.81
21	3	611	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
25	1	802	LHG	C5-O7-C7	-2.38	111.94	117.79
21	6	612	CLA	CAA-C2A-C3A	-2.38	106.27	112.78
21	B	1221	CLA	C2C-C1C-NC	2.38	112.20	109.97
21	B	1219	CLA	CHA-C4D-ND	2.37	137.47	132.50
21	B	1222	CLA	C1D-ND-C4D	-2.37	104.65	106.33
21	2	603	CLA	C1C-C2C-C3C	-2.37	104.46	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	F	1301	CLA	CHA-C4D-ND	2.37	137.47	132.50
21	B	1022	CLA	C4B-CHC-C1C	2.37	131.97	126.34
21	6	609	CLA	CMA-C3A-C4A	2.37	118.15	111.77
34	5	501	LUT	O23-C23-C24	2.37	115.89	110.53
21	J	1901	CLA	C3D-C2D-C1D	-2.37	102.59	105.83
21	A	1112	CLA	O2A-CGA-CBA	2.37	119.35	111.91
37	3	806	SQD	O8-S-C6	-2.37	101.96	105.74
21	4	615	CLA	C2D-C1D-ND	2.37	111.85	110.10
21	B	1224	CLA	CHA-C4D-ND	2.37	137.46	132.50
36	4	610	CHL	C4B-CHC-C1C	2.37	131.96	126.34
21	4	615	CLA	CHA-C1A-NA	-2.37	120.97	126.40
21	B	1219	CLA	C3B-C4B-NB	-2.37	108.32	110.52
21	B	1240	CLA	CHA-C4D-ND	2.37	137.45	132.50
36	2	610	CHL	C1-O2A-CGA	2.37	122.66	116.44
21	L	1502	CLA	C3D-C2D-C1D	-2.37	102.60	105.83
21	A	1110	CLA	C1C-C2C-C3C	-2.37	104.47	106.96
24	L	4001	BCR	C28-C29-C30	-2.37	106.14	114.60
21	2	615	CLA	CMA-C3A-C4A	2.37	118.13	111.77
21	B	1204	CLA	C4B-CHC-C1C	2.37	131.95	126.34
36	2	613	CHL	C3B-C4B-NB	-2.36	108.32	110.52
21	2	601	CLA	CHA-C1A-NA	-2.36	120.98	126.40
21	B	1216	CLA	O2A-CGA-CBA	2.36	119.32	111.91
21	B	1228	CLA	CMA-C3A-C4A	2.36	118.12	111.77
21	2	608	CLA	C3B-C4B-NB	-2.36	108.32	110.52
21	2	602	CLA	C2A-C1A-CHA	2.36	127.99	123.86
21	B	1206	CLA	CHA-C4D-ND	2.36	137.44	132.50
21	1	615	CLA	C3D-C2D-C1D	-2.36	102.61	105.83
25	1	803	LHG	O8-C23-O10	-2.36	117.63	123.59
24	J	4002	BCR	C19-C18-C17	2.36	122.56	118.94
33	1	805	PTY	O4-C30-C31	2.36	119.31	111.91
21	A	1105	CLA	CHA-C4D-ND	2.36	137.43	132.50
21	B	1210	CLA	C1-C2-C3	-2.36	121.97	126.04
21	4	608	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
21	4	609	CLA	CHA-C4D-ND	2.36	137.43	132.50
21	A	1135	CLA	CHA-C1A-NA	-2.36	121.00	126.40
24	A	4002	BCR	C31-C1-C6	-2.36	106.48	110.30
21	3	606	CLA	CHA-C4D-ND	2.35	137.43	132.50
21	B	1213	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
21	A	1136	CLA	C2C-C1C-NC	2.35	112.18	109.97
21	5	612	CLA	CMB-C2B-C1B	-2.35	121.78	125.37
21	4	605	CLA	C3D-C2D-C1D	-2.35	102.62	105.83
21	L	1503	CLA	C4B-CHC-C1C	2.35	131.92	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1123	CLA	C3D-C2D-C1D	-2.35	102.62	105.83
21	4	606	CLA	CMD-C2D-C3D	-2.35	122.20	127.61
21	1	613	CLA	CHA-C1A-NA	-2.35	121.01	126.40
21	A	1120	CLA	CHD-C1D-ND	-2.35	122.29	124.45
21	A	1130	CLA	O2A-CGA-CBA	2.35	119.29	111.91
24	J	4001	BCR	C28-C29-C30	-2.35	106.19	114.60
21	5	603	CLA	CMB-C2B-C3B	2.35	132.28	126.59
21	B	1216	CLA	C4B-CHC-C1C	2.35	131.91	126.34
21	A	1120	CLA	CHA-C4D-ND	2.35	137.41	132.50
21	3	605	CLA	C4B-CHC-C1C	2.35	131.91	126.34
21	B	1225	CLA	CMA-C3A-C4A	2.35	118.09	111.77
21	A	1126	CLA	C3B-C2B-C1B	-2.35	104.33	107.16
24	J	4001	BCR	C33-C5-C4	2.35	118.13	113.62
24	A	4002	BCR	C33-C5-C6	-2.35	121.89	124.53
21	1	602	CLA	CHD-C1D-ND	-2.35	122.30	124.45
21	2	606	CLA	C3B-C4B-NB	-2.35	108.34	110.52
21	4	607	CLA	C4B-CHC-C1C	2.35	131.90	126.34
21	B	1205	CLA	CHA-C4D-ND	2.35	137.41	132.50
36	2	609	CHL	CHD-C4C-C3C	2.35	128.29	124.84
21	B	1234	CLA	C3D-C2D-C1D	-2.35	102.63	105.83
21	2	605	CLA	C4B-CHC-C1C	2.35	131.90	126.34
21	A	1112	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
21	A	1103	CLA	C3D-C2D-C1D	-2.34	102.63	105.83
36	4	613	CHL	CMA-C3A-C4A	2.34	118.08	111.77
34	3	501	LUT	C18-C5-C6	-2.34	121.90	124.53
21	B	1203	CLA	CHA-C1A-NA	-2.34	121.03	126.40
21	4	604	CLA	CHA-C4D-ND	2.34	137.40	132.50
21	1	613	CLA	C1C-C2C-C3C	-2.34	104.49	106.96
21	B	1211	CLA	O2A-CGA-CBA	2.34	119.26	111.91
21	A	1135	CLA	O1D-CGD-CBD	-2.34	119.69	124.48
21	1	607	CLA	C4B-CHC-C1C	2.34	131.89	126.34
24	1	504	BCR	C8-C9-C10	2.34	122.53	118.94
21	A	1122	CLA	CHA-C4D-ND	2.34	137.40	132.50
21	A	1140	CLA	CAA-C2A-C3A	-2.34	106.37	112.78
21	3	615	CLA	CHA-C1A-NA	-2.34	121.04	126.40
24	F	4002	BCR	C3-C4-C5	-2.34	109.90	114.08
21	B	1229	CLA	C1-O2A-CGA	2.34	122.58	116.44
21	5	614	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
21	4	609	CLA	C4B-CHC-C1C	2.34	131.89	126.34
21	A	1102	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
21	2	604	CLA	C1-C2-C3	-2.34	122.00	126.04
21	A	1130	CLA	CAA-C2A-C3A	-2.34	106.38	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1201	CLA	C3D-C2D-C1D	-2.34	102.64	105.83
24	A	4003	BCR	C19-C18-C17	2.34	122.53	118.94
21	B	1220	CLA	C1C-C2C-C3C	-2.34	104.50	106.96
21	A	1141	CLA	CHA-C4D-ND	2.33	137.38	132.50
21	B	1237	CLA	C1-C2-C3	-2.33	122.01	126.04
34	4	501	LUT	C35-C15-C14	-2.33	118.69	123.47
21	B	1224	CLA	C2A-C1A-CHA	2.33	127.94	123.86
35	4	502	XAT	C40-C33-C34	-2.33	119.65	122.92
21	6	609	CLA	C4B-CHC-C1C	2.33	131.87	126.34
21	O	1802	CLA	C3D-C2D-C1D	-2.33	102.65	105.83
21	A	1140	CLA	O2A-CGA-CBA	2.33	119.23	111.91
21	B	1238	CLA	C4B-CHC-C1C	2.33	131.87	126.34
21	1	606	CLA	C1C-C2C-C3C	-2.33	104.50	106.96
21	B	1211	CLA	C4B-CHC-C1C	2.33	131.87	126.34
21	B	1226	CLA	CMA-C3A-C4A	2.33	118.04	111.77
21	3	607	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
21	4	603	CLA	CMD-C2D-C3D	-2.33	122.25	127.61
24	B	4003	BCR	C36-C18-C17	-2.33	119.66	122.92
21	4	601	CLA	C4B-CHC-C1C	2.33	131.87	126.34
21	B	1202	CLA	C3D-C2D-C1D	-2.33	102.65	105.83
24	B	4003	BCR	C23-C24-C25	-2.33	120.66	127.20
21	B	1217	CLA	C2A-C1A-CHA	2.33	127.93	123.86
21	B	1228	CLA	CHA-C4D-ND	2.33	137.37	132.50
21	2	605	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
21	5	612	CLA	C4B-CHC-C1C	2.33	131.86	126.34
32	5	805	4RF	O18-C16-C15	2.33	119.22	111.91
21	3	614	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
24	B	4001	BCR	C27-C26-C25	-2.33	119.35	122.73
21	A	1013	CLA	C3D-C2D-C1D	-2.33	102.66	105.83
21	H	1701	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
34	5	503	LUT	C8-C7-C6	-2.33	120.67	127.20
21	6	601	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
21	2	607	CLA	C3B-C4B-NB	-2.33	108.36	110.52
21	3	610	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
21	6	612	CLA	C1-C2-C3	-2.33	122.02	126.04
21	A	1128	CLA	C1C-C2C-C3C	-2.33	104.51	106.96
21	B	1213	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
21	B	1236	CLA	C3B-C4B-NB	-2.33	108.36	110.52
21	B	1217	CLA	O2A-CGA-CBA	2.32	119.20	111.91
21	6	612	CLA	C3B-C2B-C1B	-2.32	104.36	107.16
21	A	1106	CLA	O1D-CGD-CBD	-2.32	119.73	124.48
21	A	1104	CLA	CHA-C1A-NA	-2.32	121.08	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1113	CLA	CHA-C1A-NA	-2.32	121.08	126.40
21	2	615	CLA	CHA-C1A-NA	-2.32	121.08	126.40
21	3	615	CLA	C1-O2A-CGA	2.32	122.54	116.44
21	B	1205	CLA	CHD-C1D-ND	-2.32	122.32	124.45
21	5	613	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
35	6	504	XAT	C40-C33-C32	2.32	121.74	118.08
21	B	1220	CLA	C3A-C2A-C1A	2.32	104.82	101.34
21	5	614	CLA	CBA-CAA-C2A	2.32	120.72	113.86
21	A	1114	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
21	3	605	CLA	O2A-CGA-CBA	2.32	119.19	111.91
21	4	606	CLA	O2A-CGA-CBA	2.32	119.19	111.91
21	4	604	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
21	4	601	CLA	C1-O2A-CGA	2.32	122.53	116.44
21	A	1129	CLA	C2D-C1D-ND	2.32	111.81	110.10
21	3	610	CLA	O2A-CGA-CBA	2.32	119.19	111.91
21	3	612	CLA	C4B-CHC-C1C	2.32	131.84	126.34
21	A	1102	CLA	C2A-C1A-CHA	2.32	127.91	123.86
21	A	1133	CLA	CHA-C4D-ND	2.32	137.35	132.50
24	A	4006	BCR	C2-C3-C4	-2.32	106.20	111.38
21	3	607	CLA	O2A-CGA-CBA	2.32	119.18	111.91
21	5	605	CLA	O2A-CGA-CBA	2.32	119.18	111.91
21	A	1103	CLA	CAA-CBA-CGA	-2.32	106.49	113.25
21	A	1125	CLA	C1D-ND-C4D	-2.32	104.69	106.33
21	B	1225	CLA	C2A-C1A-CHA	2.32	127.91	123.86
21	1	608	CLA	CHA-C1A-NA	-2.32	121.09	126.40
21	1	602	CLA	C3B-C4B-NB	-2.32	108.37	110.52
35	1	502	XAT	C40-C33-C34	-2.31	119.68	122.92
21	1	615	CLA	O2A-CGA-CBA	2.31	119.17	111.91
21	A	1124	CLA	CMA-C3A-C4A	2.31	117.99	111.77
21	A	1101	CLA	C1C-C2C-C3C	-2.31	104.52	106.96
21	B	1232	CLA	C3B-C4B-NB	-2.31	108.37	110.52
21	A	1120	CLA	C4B-CHC-C1C	2.31	131.82	126.34
21	A	1126	CLA	O2A-CGA-CBA	2.31	119.16	111.91
21	6	607	CLA	CHA-C1A-NA	-2.31	121.10	126.40
21	B	1023	CLA	O2A-CGA-CBA	2.31	119.16	111.91
21	A	1113	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
21	1	603	CLA	C4B-CHC-C1C	2.31	131.82	126.34
21	A	1136	CLA	CHA-C1A-NA	-2.31	121.11	126.40
21	1	601	CLA	O2A-CGA-CBA	2.31	119.16	111.91
21	3	607	CLA	C4B-CHC-C1C	2.31	131.82	126.34
21	A	1133	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
21	6	607	CLA	O1D-CGD-CBD	-2.31	119.76	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1220	CLA	CHA-C4D-ND	2.31	137.33	132.50
21	4	602	CLA	CHA-C1A-NA	-2.31	121.11	126.40
35	6	502	XAT	C38-C25-C24	2.31	116.88	114.28
21	6	607	CLA	C4B-CHC-C1C	2.31	131.82	126.34
21	O	1803	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
21	4	606	CLA	C4B-CHC-C1C	2.31	131.81	126.34
21	1	608	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
21	A	1105	CLA	C2A-C1A-CHA	2.31	127.89	123.86
21	B	1212	CLA	O2A-CGA-CBA	2.31	119.15	111.91
24	A	4006	BCR	C34-C9-C10	-2.31	119.69	122.92
35	4	502	XAT	C26-C27-C28	-2.31	121.11	125.99
21	A	1137	CLA	C4B-CHC-C1C	2.31	131.81	126.34
21	1	615	CLA	CHA-C1A-NA	-2.31	121.11	126.40
21	1	606	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
21	L	1504	CLA	CMD-C2D-C3D	-2.31	122.31	127.61
21	5	601	CLA	CAA-CBA-CGA	2.31	118.63	112.51
21	4	609	CLA	C3D-C2D-C1D	-2.31	102.69	105.83
24	3	503	BCR	C38-C26-C25	-2.30	121.94	124.53
21	K	1403	CLA	C1D-ND-C4D	-2.30	104.70	106.33
21	5	606	CLA	O2A-CGA-CBA	2.30	119.13	111.91
36	2	610	CHL	C1-C2-C3	-2.30	122.06	126.04
21	2	605	CLA	CHA-C1A-NA	-2.30	121.13	126.40
21	2	604	CLA	C4B-CHC-C1C	2.30	131.80	126.34
21	B	1230	CLA	C1D-ND-C4D	-2.30	104.70	106.33
21	1	602	CLA	C4B-CHC-C1C	2.30	131.80	126.34
24	B	4001	BCR	C19-C18-C17	2.30	122.47	118.94
21	B	1218	CLA	C6-C7-C8	-2.30	108.48	115.92
21	5	613	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
21	6	612	CLA	CMB-C2B-C3B	2.30	132.16	126.59
21	3	615	CLA	CAA-C2A-C3A	-2.30	106.48	112.78
21	B	1231	CLA	O2A-CGA-CBA	2.30	119.12	111.91
21	A	1124	CLA	O2A-CGA-CBA	2.30	119.12	111.91
21	6	607	CLA	O2A-CGA-CBA	2.30	119.12	111.91
21	2	615	CLA	C2A-C1A-CHA	2.30	127.88	123.86
21	A	1107	CLA	CAA-CBA-CGA	-2.30	106.54	113.25
21	5	606	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
21	2	601	CLA	OBD-CAD-C3D	-2.30	122.99	128.52
21	A	1124	CLA	C1-C2-C3	-2.30	122.07	126.04
21	5	602	CLA	CAA-C2A-C3A	-2.30	106.49	112.78
21	3	611	CLA	C1-O2A-CGA	2.30	122.47	116.44
36	5	610	CHL	CHB-C4A-NA	2.30	127.69	124.51
21	2	605	CLA	C1D-ND-C4D	-2.30	104.70	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	L	1501	CLA	CAA-C2A-C1A	-2.30	104.45	111.97
21	3	614	CLA	CHA-C1A-NA	-2.30	121.14	126.40
21	B	1223	CLA	C3D-C2D-C1D	-2.30	102.70	105.83
21	L	1502	CLA	CMC-C2C-C1C	2.29	128.53	125.04
21	B	1222	CLA	C1C-C2C-C3C	-2.29	104.54	106.96
21	A	1111	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
21	4	615	CLA	C4B-CHC-C1C	2.29	131.78	126.34
21	4	601	CLA	C1C-C2C-C3C	-2.29	104.55	106.96
21	6	605	CLA	CMD-C2D-C3D	-2.29	122.34	127.61
21	B	1229	CLA	C6-C5-C3	-2.29	107.44	113.45
36	4	610	CHL	C2B-C1B-NB	-2.29	108.69	110.23
21	A	1137	CLA	C1-C2-C3	-2.29	122.08	126.04
21	A	1118	CLA	C1-C2-C3	-2.29	123.04	126.75
21	B	1222	CLA	O2A-CGA-CBA	2.29	119.10	111.91
21	5	612	CLA	C3A-C2A-C1A	2.29	104.77	101.34
21	1	601	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
21	A	1129	CLA	C4B-CHC-C1C	2.29	131.77	126.34
21	3	607	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
21	6	605	CLA	C3D-C2D-C1D	-2.29	102.71	105.83
21	B	1209	CLA	C3B-C4B-NB	-2.29	108.39	110.52
21	A	1105	CLA	CHA-C1A-NA	-2.29	121.16	126.40
36	2	609	CHL	CHC-C1C-NC	2.29	127.67	124.20
21	A	1141	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
21	5	614	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
21	A	1128	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
21	4	602	CLA	C3B-C4B-NB	-2.29	108.39	110.52
21	B	1220	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
21	A	1123	CLA	CMA-C3A-C4A	2.29	117.92	111.77
34	5	501	LUT	C11-C10-C9	-2.29	124.05	127.31
21	A	1132	CLA	O2A-CGA-CBA	2.29	119.08	111.91
21	A	1138	CLA	C4B-CHC-C1C	2.29	131.76	126.34
21	1	604	CLA	C2A-C3A-C4A	2.29	105.56	101.87
21	5	608	CLA	CAC-C3C-C4C	2.29	127.78	124.81
21	B	1211	CLA	CHA-C1A-NA	-2.29	121.16	126.40
21	3	602	CLA	CHA-C1A-NA	-2.29	121.16	126.40
21	5	604	CLA	CHA-C1A-NA	-2.29	121.16	126.40
21	B	1229	CLA	C2C-C1C-NC	2.29	112.11	109.97
21	3	601	CLA	CMA-C3A-C2A	-2.29	104.61	113.83
21	5	608	CLA	CHA-C4D-ND	2.29	137.28	132.50
24	G	4001	BCR	C23-C24-C25	-2.28	120.78	127.20
21	B	1230	CLA	C4B-CHC-C1C	2.28	131.76	126.34
21	B	1232	CLA	C4B-CHC-C1C	2.28	131.76	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	612	CLA	C1D-ND-C4D	-2.28	104.71	106.33
35	2	502	XAT	O4-C5-C4	-2.28	111.67	113.38
21	6	607	CLA	C1-C2-C3	-2.28	122.09	126.04
21	K	1404	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
21	2	606	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
24	L	4002	BCR	C23-C24-C25	-2.28	120.79	127.20
34	5	504	LUT	C31-C32-C33	-2.28	120.00	126.42
24	K	4001	BCR	C23-C24-C25	-2.28	120.79	127.20
21	1	606	CLA	C2A-C1A-CHA	2.28	127.85	123.86
21	A	1136	CLA	C3B-C4B-NB	-2.28	108.40	110.52
21	L	1503	CLA	CHA-C1A-NA	-2.28	121.17	126.40
21	6	604	CLA	C1C-C2C-C3C	-2.28	104.56	106.96
21	4	605	CLA	C4B-CHC-C1C	2.28	131.75	126.34
27	6	805	LMU	C1B-O1B-C4'	-2.28	112.32	117.96
21	A	1013	CLA	C1C-C2C-C3C	-2.28	104.56	106.96
34	6	501	LUT	C31-C32-C33	-2.28	120.02	126.42
21	A	1137	CLA	C2A-C1A-CHA	2.28	127.84	123.86
21	H	1701	CLA	C2B-C1B-NB	-2.28	108.70	110.23
21	B	1231	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
21	4	606	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
21	A	1136	CLA	CHA-C4D-ND	2.28	137.26	132.50
21	K	1402	CLA	CAA-C2A-C3A	-2.28	106.54	112.78
24	A	4007	BCR	C33-C5-C6	-2.28	121.97	124.53
21	B	1209	CLA	C4B-CHC-C1C	2.28	131.74	126.34
21	4	602	CLA	C4B-CHC-C1C	2.28	131.73	126.34
21	4	607	CLA	CHA-C1A-NA	-2.27	121.19	126.40
21	4	612	CLA	CAA-C2A-C3A	-2.27	106.55	112.78
21	1	602	CLA	CHA-C1A-NA	-2.27	121.19	126.40
21	B	1202	CLA	C1D-ND-C4D	-2.27	104.72	106.33
21	B	1218	CLA	CAC-C3C-C4C	2.27	127.76	124.81
21	A	1120	CLA	CAA-C2A-C1A	-2.27	104.53	111.97
21	B	1236	CLA	C4B-CHC-C1C	2.27	131.72	126.34
21	3	606	CLA	C4B-CHC-C1C	2.27	131.72	126.34
21	B	1220	CLA	C3B-C4B-NB	-2.27	108.41	110.52
21	G	1601	CLA	O2A-CGA-CBA	2.27	119.03	111.91
21	2	601	CLA	C4B-CHC-C1C	2.27	131.72	126.34
21	B	1207	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
21	B	1225	CLA	CHA-C1A-NA	-2.27	121.20	126.40
21	L	1502	CLA	CHA-C1A-NA	-2.27	121.20	126.40
24	H	4001	BCR	C36-C18-C17	-2.27	119.74	122.92
24	F	4002	BCR	C31-C1-C6	-2.27	106.62	110.30
21	A	1119	CLA	CMD-C2D-C3D	-2.27	122.39	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1108	CLA	C4B-CHC-C1C	2.27	131.72	126.34
24	H	4001	BCR	C34-C9-C10	-2.27	119.75	122.92
21	K	1401	CLA	CHA-C1A-NA	-2.27	121.20	126.40
21	B	1229	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
21	B	1211	CLA	CAA-C2A-C3A	-2.27	106.57	112.78
21	6	612	CLA	C3D-C2D-C1D	-2.27	102.74	105.83
21	3	605	CLA	CHA-C1A-NA	-2.27	121.21	126.40
21	6	613	CLA	C1D-ND-C4D	-2.27	104.72	106.33
21	3	606	CLA	CHD-C4C-C3C	2.26	128.17	124.84
21	G	1603	CLA	CGD-CBD-CAD	-2.26	103.40	110.73
21	5	604	CLA	O2A-CGA-CBA	2.26	119.01	111.91
21	6	601	CLA	O2A-CGA-CBA	2.26	119.01	111.91
21	B	1202	CLA	C4B-CHC-C1C	2.26	131.71	126.34
21	2	612	CLA	C3B-C4B-NB	-2.26	108.42	110.52
21	1	612	CLA	CHA-C1A-NA	-2.26	121.22	126.40
21	4	608	CLA	CHA-C1A-NA	-2.26	121.22	126.40
21	4	612	CLA	C1C-C2C-C3C	-2.26	104.58	106.96
21	6	613	CLA	C2D-C1D-ND	2.26	111.77	110.10
21	A	1101	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
21	A	1132	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
36	4	613	CHL	CHD-C1D-ND	-2.26	122.38	124.45
24	L	4001	BCR	C36-C18-C17	-2.26	119.76	122.92
21	A	1124	CLA	C4B-CHC-C1C	2.26	131.70	126.34
21	B	1203	CLA	C4B-CHC-C1C	2.26	131.70	126.34
37	6	803	SQD	O3-C3-C2	-2.26	105.12	110.35
36	4	611	CHL	C2C-C3C-C4C	2.26	108.10	106.49
21	A	1125	CLA	C4B-CHC-C1C	2.26	131.70	126.34
21	A	1130	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
21	4	612	CLA	O2A-CGA-CBA	2.26	119.00	111.91
21	4	607	CLA	O2A-CGA-CBA	2.26	118.99	111.91
24	F	4002	BCR	C2-C1-C6	2.26	113.95	110.48
21	A	1109	CLA	C2D-C1D-ND	2.26	111.77	110.10
21	4	615	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
21	3	612	CLA	CHA-C1A-NA	-2.25	121.24	126.40
34	4	501	LUT	C31-C32-C33	-2.25	120.08	126.42
21	5	602	CLA	CHA-C4D-ND	2.25	137.21	132.50
21	A	1108	CLA	CHA-C1A-NA	-2.25	121.24	126.40
24	H	4001	BCR	C1-C6-C7	2.25	122.15	115.78
34	6	501	LUT	C39-C29-C30	-2.25	119.77	122.92
21	B	1205	CLA	CBA-CAA-C2A	2.25	120.51	113.86
21	4	608	CLA	C4B-CHC-C1C	2.25	131.68	126.34
21	A	1135	CLA	C3B-C4B-NB	-2.25	108.43	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1119	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
21	4	605	CLA	CHA-C1A-NA	-2.25	121.24	126.40
21	B	1222	CLA	C2C-C1C-NC	2.25	112.08	109.97
21	B	1204	CLA	C3B-C4B-NB	-2.25	108.43	110.52
21	B	1229	CLA	C4B-CHC-C1C	2.25	131.68	126.34
21	1	606	CLA	C4B-CHC-C1C	2.25	131.67	126.34
21	6	613	CLA	CHA-C1A-NA	-2.25	121.25	126.40
21	3	614	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
21	3	615	CLA	C4B-CHC-C1C	2.25	131.67	126.34
27	B	5004	LMU	C1B-O1B-C4'	-2.25	112.40	117.96
21	B	1237	CLA	CAC-C3C-C4C	2.25	127.73	124.81
21	A	1139	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
21	A	1127	CLA	CHA-C4D-ND	2.25	137.20	132.50
21	1	604	CLA	C3B-C2B-C1B	-2.25	104.45	107.16
21	6	604	CLA	C3B-C2B-C1B	-2.25	104.45	107.16
33	1	806	PTY	C6-O7-C8	-2.25	113.71	117.90
21	H	1701	CLA	C6-C7-C8	-2.25	108.66	115.92
21	B	1201	CLA	C2A-C1A-CHA	2.25	127.79	123.86
21	B	1214	CLA	C2D-C1D-ND	2.25	111.76	110.10
21	1	607	CLA	CHA-C1A-NA	-2.25	121.25	126.40
21	5	602	CLA	C3B-C4B-NB	-2.25	108.43	110.52
35	1	502	XAT	C16-C1-C6	-2.25	103.98	110.05
21	4	603	CLA	C4B-CHC-C1C	2.25	131.66	126.34
21	B	1224	CLA	C6-C5-C3	-2.24	107.57	113.45
21	6	601	CLA	CMD-C2D-C3D	-2.24	122.45	127.61
21	2	612	CLA	C4B-CHC-C1C	2.24	131.66	126.34
21	2	607	CLA	CHA-C1A-NA	-2.24	121.26	126.40
34	5	503	LUT	C11-C12-C13	-2.24	120.11	126.42
21	2	602	CLA	O2A-CGA-CBA	2.24	118.95	111.91
21	B	1214	CLA	CHA-C1A-NA	-2.24	121.26	126.40
21	5	607	CLA	CHD-C1D-ND	-2.24	122.39	124.45
21	4	605	CLA	CAA-CBA-CGA	-2.24	106.70	113.25
21	B	1221	CLA	C3B-C4B-NB	-2.24	108.44	110.52
21	B	1022	CLA	O2A-CGA-CBA	2.24	118.94	111.91
21	B	1234	CLA	C2A-C1A-CHA	2.24	127.78	123.86
21	K	1402	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
21	B	1205	CLA	C1D-ND-C4D	-2.24	104.74	106.33
36	1	610	CHL	C2A-C1A-CHA	2.24	127.78	123.86
21	3	608	CLA	C2C-C1C-NC	2.24	112.07	109.97
21	B	1201	CLA	CHA-C1A-NA	-2.24	121.27	126.40
21	A	1105	CLA	O2A-CGA-CBA	2.24	118.93	111.91
21	6	605	CLA	C2A-C1A-CHA	2.24	127.77	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1222	CLA	C3B-C4B-NB	-2.24	108.44	110.52
21	K	1403	CLA	C1-O2A-CGA	2.24	122.32	116.44
21	5	614	CLA	O2A-CGA-CBA	2.24	118.93	111.91
21	5	603	CLA	C4-C3-C2	-2.24	117.94	123.68
21	A	1126	CLA	C2C-C1C-NC	2.24	112.07	109.97
21	1	603	CLA	C1C-C2C-C3C	-2.24	104.60	106.96
34	2	501	LUT	C35-C15-C14	-2.24	118.89	123.47
21	A	1111	CLA	C1-C2-C3	-2.24	122.17	126.04
21	3	612	CLA	O2A-CGA-CBA	2.24	118.93	111.91
24	B	4003	BCR	C33-C5-C4	2.24	117.91	113.62
21	B	1204	CLA	C1D-ND-C4D	-2.24	104.75	106.33
24	A	4004	BCR	C30-C25-C24	2.24	122.11	115.78
21	A	1140	CLA	C1C-C2C-C3C	-2.24	104.61	106.96
21	A	1119	CLA	C4B-CHC-C1C	2.24	131.64	126.34
21	3	615	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
21	B	1202	CLA	C2A-C1A-CHA	2.24	127.77	123.86
21	A	1110	CLA	C5-C3-C2	2.24	125.64	121.12
21	A	1137	CLA	CAC-C3C-C4C	2.24	127.71	124.81
24	3	506	BCR	C1-C6-C7	2.24	122.10	115.78
21	2	602	CLA	C3D-C2D-C1D	-2.24	102.78	105.83
25	2	803	LHG	C6-C5-C4	-2.24	106.50	111.79
21	A	1118	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
24	4	503	BCR	C23-C22-C21	2.24	122.37	118.94
21	B	1229	CLA	CHA-C1A-NA	-2.24	121.28	126.40
21	6	604	CLA	C2C-C1C-NC	2.24	112.07	109.97
21	O	1801	CLA	C2D-C1D-ND	2.23	111.75	110.10
21	B	1234	CLA	CHA-C1A-NA	-2.23	121.28	126.40
21	B	1222	CLA	O1D-CGD-CBD	-2.23	119.91	124.48
21	6	609	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
21	F	1301	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
21	A	1141	CLA	C4B-CHC-C1C	2.23	131.63	126.34
21	A	1111	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
21	A	1119	CLA	CHA-C1A-NA	-2.23	121.28	126.40
21	B	1209	CLA	CHA-C1A-NA	-2.23	121.28	126.40
34	2	501	LUT	C1-C6-C7	2.23	122.09	115.78
21	B	1023	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
21	B	1202	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
21	B	1211	CLA	C6-C5-C3	-2.23	107.60	113.45
21	A	1125	CLA	CHA-C1A-NA	-2.23	121.29	126.40
21	A	1108	CLA	C1-C2-C3	-2.23	122.18	126.04
21	A	1118	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
21	3	602	CLA	CMD-C2D-C3D	-2.23	122.48	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1228	CLA	C1C-C2C-C3C	-2.23	104.61	106.96
21	B	1021	CLA	C2A-C1A-CHA	2.23	127.76	123.86
31	1	804	LMG	O8-C28-C29	2.23	118.90	111.91
36	5	609	CHL	C2B-C1B-NB	-2.23	108.74	110.23
21	B	1229	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
24	B	4002	BCR	C34-C9-C10	-2.23	119.80	122.92
21	A	1103	CLA	C1C-C2C-C3C	-2.23	104.61	106.96
21	2	607	CLA	C4B-CHC-C1C	2.23	131.62	126.34
21	B	1240	CLA	CHA-C1A-NA	-2.23	121.30	126.40
21	2	612	CLA	O2A-CGA-CBA	2.23	118.90	111.91
24	O	4001	BCR	C36-C18-C19	2.23	121.59	118.08
21	2	603	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
21	4	609	CLA	C2A-C1A-CHA	2.23	127.75	123.86
21	L	1501	CLA	C1C-C2C-C3C	-2.23	104.61	106.96
21	B	1234	CLA	O2A-CGA-CBA	2.23	118.90	111.91
21	B	1204	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
21	B	1234	CLA	OBD-CAD-C3D	-2.23	123.16	128.52
21	4	612	CLA	C4B-CHC-C1C	2.23	131.62	126.34
24	2	503	BCR	C37-C22-C23	2.23	121.58	118.08
34	4	501	LUT	C17-C1-C6	2.23	113.91	110.30
21	F	1302	CLA	CHA-C1A-NA	-2.22	121.30	126.40
21	1	613	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
37	2	805	SQD	O3-C3-C2	-2.22	105.21	110.35
21	B	1206	CLA	CHA-C1A-NA	-2.22	121.30	126.40
21	1	605	CLA	CBC-CAC-C3C	-2.22	106.30	112.43
21	A	1119	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
21	A	1119	CLA	C2C-C1C-NC	2.22	112.05	109.97
25	B	5001	LHG	C5-O7-C7	-2.22	112.32	117.79
21	A	1108	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
36	2	610	CHL	C1D-CHD-C4C	-2.22	121.27	126.06
36	1	609	CHL	CHB-C4A-NA	2.22	127.58	124.51
21	1	611	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
21	B	1220	CLA	CAC-C3C-C4C	2.22	127.69	124.81
21	B	1213	CLA	CMA-C3A-C4A	2.22	117.74	111.77
21	1	608	CLA	O2A-CGA-CBA	2.22	118.88	111.91
21	4	604	CLA	O2A-CGA-CBA	2.22	118.88	111.91
21	5	607	CLA	C6-C5-C3	-2.22	107.63	113.45
21	5	613	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
21	5	602	CLA	CBA-CAA-C2A	-2.22	107.31	113.86
21	A	1105	CLA	CAC-C3C-C4C	2.22	127.69	124.81
21	A	1105	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
21	B	1207	CLA	CMD-C2D-C3D	-2.22	122.51	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1234	CLA	CMA-C3A-C4A	2.22	117.73	111.77
21	A	1109	CLA	C3B-C4B-NB	-2.22	108.46	110.52
21	A	1102	CLA	C4B-CHC-C1C	2.22	131.60	126.34
21	B	1203	CLA	C2A-C1A-CHA	2.22	127.74	123.86
21	4	609	CLA	C1D-ND-C4D	-2.22	104.76	106.33
21	B	1210	CLA	O2A-CGA-CBA	2.22	118.86	111.91
21	3	603	CLA	O2A-CGA-CBA	2.22	118.86	111.91
21	2	608	CLA	CHA-C1A-NA	-2.22	121.32	126.40
36	6	610	CHL	CHD-C4C-C3C	2.22	128.10	124.84
21	B	1234	CLA	C1C-C2C-C3C	-2.22	104.63	106.96
21	A	1112	CLA	CMD-C2D-C3D	-2.22	122.52	127.61
21	4	608	CLA	C3B-C4B-NB	-2.22	108.46	110.52
21	A	1106	CLA	CMA-C3A-C4A	2.21	117.73	111.77
21	A	1108	CLA	CMA-C3A-C4A	2.21	117.73	111.77
36	2	613	CHL	CHC-C1C-NC	2.21	127.56	124.20
21	B	1236	CLA	O2A-CGA-CBA	2.21	118.86	111.91
21	3	606	CLA	O2A-CGA-CBA	2.21	118.86	111.91
21	B	1205	CLA	C4B-CHC-C1C	2.21	131.59	126.34
21	L	1502	CLA	CHA-C4D-ND	2.21	137.13	132.50
21	3	606	CLA	O1D-CGD-CBD	-2.21	119.95	124.48
21	1	608	CLA	C1-O2A-CGA	2.21	122.25	116.44
21	6	612	CLA	C4B-CHC-C1C	2.21	131.59	126.34
21	A	1013	CLA	C2C-C1C-NC	2.21	112.05	109.97
35	4	502	XAT	O24-C25-C24	2.21	115.04	113.38
21	6	607	CLA	C3B-C4B-NB	-2.21	108.46	110.52
36	2	609	CHL	CHC-C4B-NB	-2.21	121.92	124.26
21	6	604	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
21	B	1232	CLA	CHD-C1D-ND	-2.21	122.42	124.45
21	5	601	CLA	C2C-C1C-NC	2.21	112.04	109.97
21	5	603	CLA	CHA-C1A-NA	-2.21	121.34	126.40
24	3	504	BCR	C33-C5-C6	-2.21	122.05	124.53
34	2	501	LUT	C1-C6-C5	-2.21	119.50	122.61
21	A	1113	CLA	C4B-CHC-C1C	2.21	131.57	126.34
21	G	1601	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
21	3	605	CLA	C2D-C1D-ND	2.21	111.73	110.10
21	A	1118	CLA	O2A-CGA-CBA	2.21	118.84	111.91
21	B	1209	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
21	6	609	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
21	B	1224	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
21	A	1111	CLA	CHA-C1A-NA	-2.21	121.35	126.40
21	B	1237	CLA	CAA-C2A-C3A	-2.21	106.74	112.78
24	B	4004	BCR	C34-C9-C10	-2.21	119.83	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	604	CLA	C1-C2-C3	-2.21	122.23	126.04
21	A	1133	CLA	C4B-CHC-C1C	2.21	131.57	126.34
21	A	1110	CLA	C1-C2-C3	-2.21	122.23	126.04
21	B	1234	CLA	CBA-CAA-C2A	-2.21	107.35	113.86
21	B	1206	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
21	B	1208	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
21	6	607	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
21	2	605	CLA	O1D-CGD-CBD	-2.20	119.97	124.48
21	J	1901	CLA	CHD-C1D-ND	-2.20	122.43	124.45
21	3	613	CLA	CMC-C2C-C1C	2.20	128.40	125.04
21	3	603	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
21	3	608	CLA	C4B-CHC-C1C	2.20	131.56	126.34
21	A	1126	CLA	C2A-C1A-CHA	2.20	127.71	123.86
21	1	604	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
21	5	601	CLA	CMC-C2C-C1C	2.20	128.39	125.04
36	4	613	CHL	CHC-C4B-NB	-2.20	121.92	124.26
21	5	607	CLA	CHA-C1A-NA	-2.20	121.35	126.40
21	A	1135	CLA	CHD-C1D-ND	-2.20	122.43	124.45
21	3	602	CLA	C2A-C1A-CHA	2.20	127.71	123.86
24	B	4001	BCR	C35-C13-C12	2.20	121.55	118.08
21	B	1021	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
21	B	1227	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
21	2	612	CLA	CHB-C4A-NA	2.20	127.56	124.51
21	B	1222	CLA	CMA-C3A-C4A	2.20	117.68	111.77
21	J	1901	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
21	B	1215	CLA	CHA-C1A-NA	-2.20	121.36	126.40
21	4	603	CLA	CHA-C1A-NA	-2.20	121.36	126.40
21	A	1139	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
21	A	1141	CLA	O1A-CGA-CBA	-2.20	115.16	123.73
21	1	613	CLA	C4B-CHC-C1C	2.20	131.55	126.34
21	6	602	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
21	5	608	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
21	1	613	CLA	C2A-C1A-CHA	2.20	127.70	123.86
21	A	1102	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
21	A	1137	CLA	O2A-CGA-CBA	2.20	118.80	111.91
21	B	1209	CLA	C2D-C1D-ND	2.20	111.72	110.10
21	6	612	CLA	CHA-C1A-NA	-2.20	121.37	126.40
21	G	1602	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
21	A	1124	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
21	1	607	CLA	CAA-C2A-C3A	-2.20	106.77	112.78
21	B	1212	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
21	1	601	CLA	CMD-C2D-C3D	-2.19	122.57	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	605	CLA	C1-O2A-CGA	2.19	122.20	116.44
21	1	613	CLA	CAC-C3C-C4C	2.19	127.66	124.81
21	3	603	CLA	C2A-C1A-CHA	2.19	127.69	123.86
21	1	604	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
21	A	1120	CLA	C1-O2A-CGA	2.19	122.20	116.44
21	B	1202	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
21	4	604	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
34	5	504	LUT	C18-C5-C4	2.19	118.42	114.36
21	2	612	CLA	C1-O2A-CGA	2.19	122.20	116.44
21	A	1127	CLA	O2A-CGA-CBA	2.19	118.79	111.91
24	3	506	BCR	C38-C26-C27	2.19	117.83	113.62
21	A	1102	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
21	5	605	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
21	B	1221	CLA	C2D-C1D-ND	2.19	111.72	110.10
21	2	615	CLA	C4B-CHC-C1C	2.19	131.53	126.34
21	A	1140	CLA	CHA-C1A-NA	-2.19	121.38	126.40
21	5	612	CLA	CHA-C1A-NA	-2.19	121.38	126.40
21	B	1219	CLA	C4-C3-C5	2.19	118.96	115.27
36	6	610	CHL	CHC-C1C-NC	2.19	127.53	124.20
36	2	609	CHL	C2B-C1B-NB	-2.19	108.76	110.23
21	B	1022	CLA	CHA-C1A-NA	-2.19	121.38	126.40
21	B	1209	CLA	CAA-CBA-CGA	-2.19	106.86	113.25
24	L	4001	BCR	C8-C9-C10	2.19	122.30	118.94
21	H	1702	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
21	5	606	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
21	A	1130	CLA	CHA-C1A-NA	-2.19	121.39	126.40
21	2	605	CLA	C3D-C2D-C1D	-2.19	102.85	105.83
21	6	613	CLA	C4B-CHC-C1C	2.19	131.53	126.34
21	A	1013	CLA	CHA-C1A-NA	-2.19	121.39	126.40
21	O	1801	CLA	C2A-C1A-CHA	2.19	126.10	122.71
21	6	603	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
21	2	601	CLA	O2A-CGA-CBA	2.19	118.77	111.91
21	5	602	CLA	C3A-C2A-C1A	2.19	104.61	101.34
21	B	1228	CLA	C3B-C4B-NB	-2.18	108.49	110.52
21	B	1021	CLA	C1D-ND-C4D	-2.18	104.78	106.33
21	3	606	CLA	CHA-C1A-NA	-2.18	121.39	126.40
21	1	613	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
21	F	1301	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
24	A	4002	BCR	C2-C3-C4	-2.18	106.50	111.38
21	A	1105	CLA	C1D-ND-C4D	-2.18	104.78	106.33
21	1	605	CLA	CHA-C1A-NA	-2.18	121.40	126.40
35	6	504	XAT	C10-C11-C12	-2.18	116.41	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	G	1603	CLA	CAC-C3C-C4C	2.18	127.64	124.81
21	B	1214	CLA	C3D-C2D-C1D	-2.18	102.85	105.83
21	A	1115	CLA	O2A-CGA-CBA	2.18	118.75	111.91
21	A	1136	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
21	A	1101	CLA	CMC-C2C-C1C	2.18	128.36	125.04
21	A	1106	CLA	CHD-C1D-ND	-2.18	122.45	124.45
21	B	1231	CLA	C2D-C1D-ND	2.18	111.71	110.10
21	A	1117	CLA	C4B-CHC-C1C	2.18	131.51	126.34
21	5	602	CLA	C1D-ND-C4D	-2.18	104.79	106.33
21	B	1222	CLA	CMB-C2B-C3B	2.18	131.87	126.59
34	5	502	LUT	C38-C25-C24	-2.18	118.90	123.56
21	B	1220	CLA	C4B-CHC-C1C	2.18	131.50	126.34
21	2	607	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
21	2	606	CLA	C4B-CHC-C1C	2.18	131.50	126.34
21	A	1101	CLA	C2C-C1C-NC	2.18	112.01	109.97
21	A	1108	CLA	C1-O2A-CGA	2.18	122.16	116.44
21	A	1125	CLA	CHD-C1D-ND	-2.18	122.45	124.45
21	B	1219	CLA	CAC-C3C-C4C	2.18	127.64	124.81
21	A	1133	CLA	C2A-C1A-CHA	2.18	127.67	123.86
21	B	1223	CLA	C2A-C1A-CHA	2.18	127.67	123.86
21	O	1803	CLA	C2A-C1A-CHA	2.18	127.67	123.86
21	3	613	CLA	CHA-C4D-ND	2.18	137.05	132.50
21	4	603	CLA	O2A-CGA-CBA	2.18	118.74	111.91
21	2	612	CLA	CHA-C1A-NA	-2.18	121.41	126.40
21	B	1222	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
21	5	604	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
34	6	501	LUT	C35-C15-C14	-2.18	119.02	123.47
21	B	1210	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
21	A	1102	CLA	C3B-C2B-C1B	-2.18	104.54	107.16
21	B	1227	CLA	C1D-ND-C4D	-2.17	104.79	106.33
21	B	1224	CLA	C4B-CHC-C1C	2.17	131.50	126.34
21	F	1301	CLA	CMA-C3A-C4A	2.17	117.62	111.77
21	A	1136	CLA	C4B-CHC-C1C	2.17	131.50	126.34
24	B	4001	BCR	C37-C22-C23	-2.17	114.65	118.08
21	5	603	CLA	C2A-C1A-CHA	2.17	127.66	123.86
24	3	504	BCR	C30-C25-C26	-2.17	119.55	122.61
21	A	1101	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
21	A	1107	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
21	3	615	CLA	C2A-C1A-CHA	2.17	127.66	123.86
21	5	601	CLA	C2D-C1D-ND	2.17	111.70	110.10
21	4	612	CLA	C3B-C4B-NB	-2.17	108.50	110.52
24	L	4001	BCR	C34-C9-C10	-2.17	119.88	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1131	CLA	CMA-C3A-C2A	-2.17	105.07	113.83
24	3	506	BCR	C32-C1-C6	-2.17	106.78	110.30
21	A	1121	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
36	5	610	CHL	CHA-C1A-NA	-2.17	121.43	126.40
24	3	504	BCR	C30-C25-C24	2.17	121.91	115.78
21	A	1119	CLA	C11-C12-C13	-2.17	108.91	115.92
34	3	501	LUT	C10-C11-C12	-2.17	116.45	123.22
21	A	1137	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
34	6	501	LUT	C40-C33-C34	-2.17	119.89	122.92
36	3	604	CHL	CHB-C4A-NA	2.17	127.51	124.51
24	B	4003	BCR	C1-C6-C7	2.17	121.91	115.78
24	B	4005	BCR	C34-C9-C10	-2.17	119.89	122.92
21	6	608	CLA	CMD-C2D-C3D	-2.17	122.63	127.61
21	A	1137	CLA	C1C-C2C-C3C	-2.17	104.68	106.96
21	B	1227	CLA	C4B-CHC-C1C	2.17	131.48	126.34
36	1	610	CHL	C3A-C2A-C1A	2.17	104.58	101.34
21	3	608	CLA	C2A-C1A-CHA	2.17	127.65	123.86
21	B	1211	CLA	C6-C7-C8	-2.17	108.92	115.92
21	G	1603	CLA	C3C-C4C-NC	-2.17	108.14	110.57
21	4	606	CLA	CHA-C1A-NA	-2.17	121.44	126.40
21	B	1217	CLA	C1-C2-C3	-2.16	122.30	126.04
21	A	1123	CLA	C4B-CHC-C1C	2.16	131.47	126.34
21	B	1218	CLA	C4B-CHC-C1C	2.16	131.47	126.34
21	A	1117	CLA	CMB-C2B-C1B	-2.16	122.07	125.37
21	A	1116	CLA	CHA-C1A-NA	-2.16	121.44	126.40
21	A	1103	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
21	B	1209	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
21	3	607	CLA	C2A-C1A-CHA	2.16	127.64	123.86
21	6	604	CLA	OBD-CAD-C3D	-2.16	123.31	128.52
21	1	601	CLA	CHA-C1A-NA	-2.16	121.44	126.40
21	A	1112	CLA	CHA-C1A-NA	-2.16	121.44	126.40
21	A	1126	CLA	C4B-CHC-C1C	2.16	131.47	126.34
21	F	1302	CLA	C3B-C4B-NB	-2.16	108.51	110.52
21	A	1127	CLA	C4B-CHC-C1C	2.16	131.47	126.34
22	B	2002	PQN	C15-C13-C12	-2.16	116.74	121.12
21	L	1502	CLA	C6-C7-C8	-2.16	108.93	115.92
21	1	603	CLA	C2C-C1C-NC	2.16	112.00	109.97
21	L	1503	CLA	C1D-ND-C4D	-2.16	104.80	106.33
21	1	604	CLA	C3B-C4B-NB	-2.16	108.51	110.52
21	2	606	CLA	C1D-ND-C4D	-2.16	104.80	106.33
24	1	504	BCR	C1-C6-C7	2.16	121.89	115.78
21	1	605	CLA	C4B-CHC-C1C	2.16	131.46	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	602	CLA	CAA-C2A-C3A	-2.16	106.87	112.78
38	2	807	LMK	C9-O8-C28	-2.16	109.64	113.80
21	5	605	CLA	CHA-C1A-NA	-2.16	121.46	126.40
21	4	601	CLA	CHA-C4D-ND	2.16	137.01	132.50
21	B	1226	CLA	CHD-C1D-ND	-2.16	122.47	124.45
21	5	612	CLA	C3B-C2B-C1B	-2.16	104.56	107.16
21	L	1502	CLA	C1C-C2C-C3C	-2.16	104.69	106.96
21	3	613	CLA	C2A-C1A-CHA	2.16	127.63	123.86
27	6	805	LMU	C2'-C3'-C4'	2.16	114.61	109.68
21	A	1122	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
21	5	613	CLA	CHA-C1A-NA	-2.16	121.46	126.40
21	B	1219	CLA	C4B-CHC-C1C	2.16	131.45	126.34
21	K	1402	CLA	CHA-C1A-NA	-2.16	121.46	126.40
21	B	1220	CLA	C2A-C1A-CHA	2.16	127.63	123.86
21	3	615	CLA	C3B-C4B-NB	-2.15	108.52	110.52
34	1	501	LUT	C1-C6-C5	-2.15	119.58	122.61
21	B	1234	CLA	C4B-CHC-C1C	2.15	131.45	126.34
21	3	603	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
24	1	504	BCR	C30-C25-C24	2.15	121.87	115.78
21	1	608	CLA	C3D-C2D-C1D	-2.15	102.89	105.83
21	B	1207	CLA	CHA-C1A-NA	-2.15	121.47	126.40
21	2	604	CLA	CHD-C1D-ND	-2.15	122.48	124.45
21	4	612	CLA	C2A-C1A-CHA	2.15	127.62	123.86
21	A	1141	CLA	C4D-CHA-C1A	2.15	123.87	121.25
21	4	615	CLA	CMA-C3A-C4A	2.15	117.56	111.77
36	3	604	CHL	CHC-C1C-NC	2.15	127.47	124.20
21	1	603	CLA	C2A-C1A-CHA	2.15	127.62	123.86
24	4	503	BCR	C35-C13-C12	2.15	121.47	118.08
21	A	1124	CLA	CAA-C2A-C1A	-2.15	104.93	111.97
35	3	502	XAT	O23-C23-C24	-2.15	105.53	109.80
35	6	502	XAT	C17-C1-C16	2.15	110.54	107.37
21	A	1134	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
21	6	606	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
21	L	1504	CLA	O2A-CGA-CBA	2.15	118.65	111.91
21	2	605	CLA	C1-O2A-CGA	2.15	122.08	116.44
21	A	1121	CLA	O2A-CGA-CBA	2.15	118.65	111.91
21	2	615	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
34	5	503	LUT	C39-C29-C30	-2.15	119.92	122.92
21	A	1106	CLA	CAA-C2A-C1A	-2.15	104.94	111.97
21	A	1104	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
21	F	1302	CLA	C4B-CHC-C1C	2.15	131.43	126.34
21	6	602	CLA	O2A-CGA-CBA	2.15	118.64	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1012	CLA	CHA-C1A-NA	-2.15	121.48	126.40
21	B	1225	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
21	A	1126	CLA	CHA-C1A-NA	-2.15	121.48	126.40
21	2	607	CLA	C2A-C1A-CHA	2.15	127.61	123.86
21	B	1226	CLA	CHD-C4C-C3C	2.15	127.99	124.84
21	L	1502	CLA	CAC-C3C-C4C	2.14	127.59	124.81
21	2	612	CLA	C2A-C3A-C4A	2.14	105.33	101.87
36	1	609	CHL	C2B-C1B-NB	-2.14	108.80	110.23
34	5	501	LUT	C2-C3-C4	-2.14	107.37	110.30
21	2	604	CLA	O2A-CGA-CBA	2.14	118.63	111.91
21	B	1023	CLA	CMD-C2D-C3D	-2.14	122.68	127.61
34	5	501	LUT	C17-C1-C6	2.14	113.78	110.30
31	6	802	LMG	C8-O7-C10	-2.14	112.52	117.79
27	6	805	LMU	O5'-C1'-C2'	2.14	114.89	110.35
21	B	1211	CLA	CMB-C2B-C3B	2.14	131.78	126.59
21	B	1227	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
21	B	1210	CLA	C2D-C1D-ND	2.14	111.68	110.10
36	4	613	CHL	CHA-C1A-NA	-2.14	121.49	126.40
24	B	4004	BCR	C33-C5-C6	-2.14	122.12	124.53
21	A	1126	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
21	B	1208	CLA	CHA-C1A-NA	-2.14	121.49	126.40
21	4	609	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
24	J	4001	BCR	C1-C6-C7	2.14	121.84	115.78
21	B	1236	CLA	CHA-C1A-NA	-2.14	121.50	126.40
21	B	1203	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
21	B	1238	CLA	C3B-C4B-NB	-2.14	108.53	110.52
21	A	1109	CLA	CHA-C1A-NA	-2.14	121.50	126.40
21	B	1204	CLA	CHA-C1A-NA	-2.14	121.50	126.40
21	B	1023	CLA	CBA-CAA-C2A	-2.14	107.55	113.86
21	B	1237	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
21	B	1228	CLA	O2A-CGA-CBA	2.14	118.62	111.91
21	H	1701	CLA	C9-C8-C10	2.14	119.04	111.29
21	A	1107	CLA	CHA-C1A-NA	-2.14	121.50	126.40
21	B	1210	CLA	CHA-C1A-NA	-2.14	121.50	126.40
21	3	613	CLA	CHA-C1A-NA	-2.14	121.50	126.40
21	2	603	CLA	C1D-ND-C4D	-2.14	104.82	106.33
21	2	602	CLA	CHD-C1D-ND	-2.14	122.49	124.45
21	4	602	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
24	I	4002	BCR	C37-C22-C21	-2.14	119.93	122.92
25	5	801	LHG	C28-C27-C26	-2.14	103.57	114.42
35	2	502	XAT	C4-C3-C2	-2.14	106.64	110.77
21	L	1503	CLA	O2A-CGA-CBA	2.14	118.61	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	5002	DGD	O6D-C5D-C6D	2.14	110.98	106.67
21	A	1103	CLA	CHA-C4D-ND	2.14	136.97	132.50
21	3	608	CLA	CHD-C1D-ND	-2.14	122.49	124.45
21	6	602	CLA	CHA-C1A-NA	-2.14	121.51	126.40
21	B	1023	CLA	CHA-C1A-NA	-2.13	121.51	126.40
21	A	1127	CLA	C1D-ND-C4D	-2.13	104.82	106.33
24	G	4001	BCR	C37-C22-C21	-2.13	119.93	122.92
21	1	612	CLA	C3B-C2B-C1B	-2.13	104.59	107.16
21	B	1228	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
21	G	1602	CLA	CHA-C1A-NA	-2.13	121.51	126.40
21	A	1139	CLA	C2A-C1A-CHA	2.13	127.59	123.86
21	H	1702	CLA	CMA-C3A-C4A	2.13	117.50	111.77
21	B	1209	CLA	C2A-C1A-CHA	2.13	127.59	123.86
21	H	1701	CLA	C1D-ND-C4D	-2.13	104.82	106.33
21	2	604	CLA	C1C-C2C-C3C	-2.13	104.72	106.96
21	2	606	CLA	CHA-C1A-NA	-2.13	121.52	126.40
21	B	1221	CLA	CMA-C3A-C2A	2.13	122.42	113.83
21	3	608	CLA	C1C-C2C-C3C	-2.13	104.72	106.96
21	A	1110	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
24	2	503	BCR	C33-C5-C6	-2.13	122.14	124.53
21	B	1213	CLA	CHA-C4D-ND	2.13	136.94	132.50
21	A	1118	CLA	C2D-C1D-ND	2.13	111.67	110.10
21	B	1225	CLA	CBA-CAA-C2A	2.12	120.13	113.86
21	A	1104	CLA	CBC-CAC-C3C	-2.12	106.58	112.43
21	3	608	CLA	C3D-C2D-C1D	-2.12	102.93	105.83
21	2	602	CLA	C4B-CHC-C1C	2.12	131.37	126.34
21	5	608	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
24	A	4004	BCR	C33-C5-C6	-2.12	122.14	124.53
21	A	1135	CLA	C2A-C1A-CHA	2.12	127.57	123.86
21	B	1238	CLA	O2A-CGA-CBA	2.12	118.56	111.91
21	A	1140	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
21	3	607	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
21	A	1124	CLA	C2A-C1A-CHA	2.12	127.57	123.86
21	A	1136	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
21	4	604	CLA	CHA-C1A-NA	-2.12	121.54	126.40
21	B	1235	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
21	B	1239	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
21	O	1802	CLA	C1D-ND-C4D	-2.12	104.83	106.33
21	B	1215	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
21	L	1503	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
21	B	1240	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
21	A	1113	CLA	C2D-C1D-ND	2.12	111.67	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1021	CLA	CHA-C1A-NA	-2.12	121.55	126.40
21	O	1802	CLA	CMA-C3A-C2A	2.12	121.04	116.10
36	1	610	CHL	CHD-C1D-ND	-2.12	122.51	124.45
21	A	1115	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
21	A	1135	CLA	CMB-C2B-C3B	2.12	131.72	126.59
21	A	1122	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
21	6	606	CLA	CHA-C1A-NA	-2.12	121.55	126.40
21	A	1122	CLA	C3B-C4B-NB	-2.12	108.55	110.52
21	F	1302	CLA	C1-O2A-CGA	2.12	122.00	116.44
36	4	610	CHL	C1-O2A-CGA	2.12	123.08	116.11
21	2	602	CLA	OBD-CAD-C3D	-2.12	123.43	128.52
21	A	1122	CLA	C2A-C1A-CHA	2.11	127.56	123.86
31	1	804	LMG	C3-C4-C5	2.11	114.01	110.24
21	3	608	CLA	CAC-C3C-C4C	2.11	127.55	124.81
36	2	613	CHL	C3C-C4C-NC	-2.11	108.20	110.57
21	1	605	CLA	CMD-C2D-C3D	-2.11	122.75	127.61
36	4	610	CHL	CHA-C1A-NA	-2.11	121.56	126.40
21	2	607	CLA	C1-O2A-CGA	2.11	121.99	116.44
21	6	604	CLA	CMB-C2B-C1B	-2.11	122.15	125.37
21	6	612	CLA	C4D-CHA-C1A	2.11	123.82	121.25
34	2	501	LUT	C39-C29-C28	2.11	121.40	118.08
21	A	1114	CLA	CHA-C1A-NA	-2.11	121.56	126.40
21	F	1302	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
21	A	1122	CLA	CHA-C1A-NA	-2.11	121.56	126.40
21	B	1237	CLA	C4B-CHC-C1C	2.11	131.34	126.34
21	A	1103	CLA	C4B-CHC-C1C	2.11	131.34	126.34
21	B	1229	CLA	C11-C10-C8	-2.11	109.10	115.92
21	A	1132	CLA	CHA-C1A-NA	-2.11	121.57	126.40
21	5	606	CLA	CHA-C1A-NA	-2.11	121.57	126.40
24	4	503	BCR	C1-C6-C5	-2.11	119.64	122.61
21	B	1201	CLA	C1D-ND-C4D	-2.11	104.84	106.33
21	A	1127	CLA	CHD-C1D-ND	-2.11	122.52	124.45
38	2	807	LMK	C9-C8-C7	-2.11	106.81	111.79
21	A	1138	CLA	C3B-C2B-C1B	-2.11	104.62	107.16
21	B	1214	CLA	OBD-CAD-C3D	-2.11	123.45	128.52
21	A	1119	CLA	C2A-C1A-CHA	2.11	127.54	123.86
21	A	1126	CLA	CMD-C2D-C3D	-2.11	122.77	127.61
24	B	4004	BCR	C23-C22-C21	-2.11	115.71	118.94
21	3	602	CLA	C1-O2A-CGA	2.11	121.97	116.44
24	3	504	BCR	C37-C22-C21	-2.11	119.97	122.92
21	A	1118	CLA	C3B-C4B-NB	-2.11	108.56	110.52
21	B	1205	CLA	C3B-C4B-NB	-2.11	108.56	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1202	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
21	3	603	CLA	CHA-C1A-NA	-2.10	121.58	126.40
21	5	608	CLA	CHA-C1A-NA	-2.10	121.58	126.40
21	A	1123	CLA	C2A-C1A-CHA	2.10	127.54	123.86
21	A	1115	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
21	B	1236	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
21	L	1502	CLA	C4B-CHC-C1C	2.10	131.32	126.34
36	4	610	CHL	CHC-C4B-NB	-2.10	122.03	124.26
21	B	1214	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
24	B	4003	BCR	C29-C30-C25	-2.10	107.25	110.48
21	2	607	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
24	A	4002	BCR	C27-C26-C25	-2.10	119.68	122.73
21	1	607	CLA	C2A-C1A-CHA	2.10	127.53	123.86
21	5	602	CLA	C3B-C2B-C1B	-2.10	104.63	107.16
21	3	605	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
21	A	1110	CLA	CHA-C1A-NA	-2.10	121.59	126.40
24	A	4004	BCR	C38-C26-C25	-2.10	122.17	124.53
21	B	1022	CLA	CMD-C2D-C3D	-2.10	122.79	127.61
21	A	1127	CLA	CHA-C1A-NA	-2.10	121.59	126.40
24	J	4001	BCR	C34-C9-C10	-2.10	119.98	122.92
21	3	603	CLA	CAA-CBA-CGA	-2.10	107.12	113.25
21	4	602	CLA	CHD-C1D-ND	-2.10	122.53	124.45
21	3	606	CLA	C1D-ND-C4D	-2.10	104.84	106.33
21	H	1701	CLA	CHA-C1A-NA	-2.10	121.60	126.40
21	A	1140	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
21	A	1136	CLA	C1D-ND-C4D	-2.10	104.85	106.33
21	A	1121	CLA	CHA-C1A-NA	-2.10	121.60	126.40
21	A	1133	CLA	CHA-C1A-NA	-2.10	121.60	126.40
21	A	1116	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
21	J	1901	CLA	C2A-C1A-CHA	2.09	127.52	123.86
21	A	1136	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
21	B	1222	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
21	L	1501	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
21	2	603	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
21	2	604	CLA	C3B-C2B-C1B	-2.09	104.64	107.16
21	4	612	CLA	C1-C2-C3	-2.09	122.42	126.04
36	4	613	CHL	C4A-NA-C1A	2.09	107.65	106.71
21	A	1136	CLA	C6-C5-C3	-2.09	107.97	113.45
21	A	1012	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
21	A	1137	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
21	4	608	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
21	A	1123	CLA	CAA-CBA-CGA	-2.09	107.14	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	6	610	CHL	C1-O2A-CGA	2.09	123.00	116.11
24	A	4003	BCR	C1-C6-C5	-2.09	119.67	122.61
21	3	611	CLA	C2A-C1A-CHA	2.09	127.51	123.86
21	A	1120	CLA	C1-C2-C3	-2.09	122.43	126.04
21	B	1215	CLA	C2A-C1A-CHA	2.09	127.51	123.86
25	2	801	LHG	O7-C7-O9	-2.09	118.66	123.70
21	6	603	CLA	CHA-C1A-NA	-2.09	121.62	126.40
21	B	1231	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
21	B	1203	CLA	C1D-ND-C4D	-2.09	104.85	106.33
21	3	606	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
21	A	1126	CLA	C11-C12-C13	-2.09	109.18	115.92
36	1	610	CHL	CHA-C1A-NA	-2.09	121.62	126.40
21	A	1123	CLA	C3B-C4B-NB	-2.08	108.58	110.52
24	J	4001	BCR	C39-C30-C25	2.08	113.68	110.30
21	1	613	CLA	CAA-C2A-C3A	-2.08	107.07	112.78
21	5	614	CLA	CMC-C2C-C3C	2.08	131.78	126.12
21	6	606	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
21	B	1232	CLA	O2D-CGD-O1D	-2.08	119.76	123.84
21	5	603	CLA	O2D-CGD-O1D	-2.08	119.76	123.84
21	L	1501	CLA	CHA-C4D-ND	2.08	136.86	132.50
24	J	4001	BCR	C23-C24-C25	-2.08	121.35	127.20
21	1	605	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
21	1	607	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
21	B	1231	CLA	CHA-C1A-NA	-2.08	121.63	126.40
21	B	1221	CLA	C1C-C2C-C3C	-2.08	104.77	106.96
21	B	1230	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
21	6	605	CLA	C4B-CHC-C1C	2.08	131.27	126.34
21	4	615	CLA	C2A-C1A-CHA	2.08	127.50	123.86
32	5	805	4RF	C19-O18-C16	-2.08	109.42	117.12
21	4	606	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
28	3	805	DGD	O2G-C1B-O1B	-2.08	118.68	123.70
21	A	1141	CLA	C1-O2A-CGA	2.08	121.90	116.44
34	5	503	LUT	C19-C9-C10	-2.08	120.01	122.92
21	B	1213	CLA	C2A-C1A-CHA	2.08	127.50	123.86
24	F	4002	BCR	C33-C5-C6	-2.08	122.19	124.53
21	3	603	CLA	C3A-C2A-C1A	2.08	104.45	101.34
21	A	1134	CLA	CHA-C1A-NA	-2.08	121.64	126.40
24	A	4003	BCR	C3-C4-C5	-2.08	110.36	114.08
21	A	1138	CLA	C2A-C1A-CHA	2.08	127.49	123.86
21	B	1230	CLA	C4-C3-C5	2.08	118.77	115.27
21	B	1201	CLA	C4B-CHC-C1C	2.08	131.27	126.34
21	6	608	CLA	CHA-C1A-NA	-2.08	121.64	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	K	1403	CLA	O2A-CGA-CBA	2.08	118.43	111.91
21	K	1403	CLA	CHA-C1A-NA	-2.08	121.64	126.40
21	3	607	CLA	CMD-C2D-C3D	-2.08	122.84	127.61
21	A	1115	CLA	CHA-C1A-NA	-2.08	121.64	126.40
24	A	4006	BCR	C29-C28-C27	2.08	116.02	111.38
21	A	1103	CLA	CMA-C3A-C4A	2.08	117.35	111.77
21	F	1302	CLA	C1D-ND-C4D	-2.07	104.86	106.33
21	F	1301	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
21	3	614	CLA	C2A-C1A-CHA	2.07	127.49	123.86
21	G	1601	CLA	CHA-C1A-NA	-2.07	121.65	126.40
24	1	504	BCR	C3-C4-C5	-2.07	110.37	114.08
21	B	1229	CLA	CAA-C2A-C3A	-2.07	107.10	112.78
21	1	602	CLA	C2A-C1A-CHA	2.07	127.48	123.86
24	L	4002	BCR	C37-C22-C21	-2.07	120.02	122.92
21	A	1121	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
21	2	605	CLA	CMD-C2D-C3D	-2.07	122.85	127.61
35	4	502	XAT	C20-C13-C14	-2.07	120.02	122.92
21	A	1122	CLA	C1D-ND-C4D	-2.07	104.86	106.33
21	A	1116	CLA	CMD-C2D-C3D	-2.07	122.85	127.61
35	4	502	XAT	C7-C8-C9	-2.07	122.32	125.53
21	A	1133	CLA	O2A-CGA-CBA	2.07	118.41	111.91
36	4	613	CHL	C2A-C1A-CHA	2.07	127.48	123.86
21	B	1239	CLA	CHA-C1A-NA	-2.07	121.66	126.40
21	1	611	CLA	CHA-C1A-NA	-2.07	121.66	126.40
21	3	601	CLA	C3B-C4B-NB	-2.07	108.59	110.52
21	B	1238	CLA	C11-C12-C13	-2.07	109.23	115.92
21	A	1137	CLA	CMB-C2B-C3B	2.07	131.60	126.59
35	2	502	XAT	O24-C25-C38	-2.07	112.58	115.06
21	A	1120	CLA	CHA-C1A-NA	-2.07	121.66	126.40
21	B	1021	CLA	C11-C10-C8	-2.07	109.23	115.92
25	2	802	LHG	O7-C7-O9	-2.07	118.70	123.70
21	2	615	CLA	CBA-CAA-C2A	-2.07	107.76	113.86
21	B	1225	CLA	C4B-CHC-C1C	2.07	131.24	126.34
24	3	504	BCR	C34-C9-C8	2.07	121.33	118.08
21	A	1124	CLA	C1D-ND-C4D	-2.07	104.87	106.33
24	L	4002	BCR	C19-C18-C17	2.07	122.11	118.94
21	2	608	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
21	B	1227	CLA	CHA-C1A-NA	-2.07	121.67	126.40
21	A	1120	CLA	C4-C3-C5	2.07	118.75	115.27
21	A	1135	CLA	C2D-C1D-ND	2.07	111.63	110.10
21	1	606	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
24	A	4006	BCR	C8-C9-C10	2.07	122.11	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	613	CLA	C4B-CHC-C1C	2.06	131.24	126.34
21	B	1226	CLA	CAC-C3C-C2C	-2.06	124.00	127.53
20	A	1011	CL0	C4D-C3D-CAD	2.06	110.53	108.10
21	2	615	CLA	C3D-C2D-C1D	-2.06	103.01	105.83
21	1	612	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
21	A	1136	CLA	O2A-CGA-CBA	2.06	118.38	111.91
21	6	612	CLA	CHA-C4D-ND	2.06	136.81	132.50
21	B	1230	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
21	B	1235	CLA	CHA-C1A-NA	-2.06	121.67	126.40
21	B	1218	CLA	C2D-C1D-ND	2.06	111.62	110.10
21	5	603	CLA	C4B-CHC-C1C	2.06	131.23	126.34
21	A	1120	CLA	C4-C3-C2	-2.06	118.39	123.68
21	1	613	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
25	A	5001	LHG	O8-C23-O10	-2.06	118.39	123.59
21	6	605	CLA	O2A-CGA-CBA	2.06	118.38	111.91
36	2	613	CHL	C4D-CHA-C1A	2.06	123.76	121.25
21	A	1122	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
21	K	1403	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
21	B	1204	CLA	C2A-C1A-CHA	2.06	127.46	123.86
21	1	605	CLA	CMA-C3A-C4A	2.06	117.31	111.77
24	F	4002	BCR	C8-C9-C10	2.06	122.10	118.94
21	A	1129	CLA	C2A-C1A-CHA	2.06	127.46	123.86
21	B	1213	CLA	CAC-C3C-C4C	2.06	127.48	124.81
21	A	1126	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
21	B	1022	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
21	A	1133	CLA	C6-C5-C3	-2.06	108.06	113.45
21	A	1112	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
21	2	612	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
21	5	608	CLA	C3B-C4B-NB	-2.06	108.61	110.52
21	4	601	CLA	O2A-CGA-CBA	2.06	118.36	111.91
21	O	1802	CLA	C2A-C1A-CHA	2.06	127.44	123.85
21	K	1402	CLA	CAA-CBA-CGA	-2.06	107.25	113.25
21	2	604	CLA	C1D-ND-C4D	-2.06	104.88	106.33
24	J	4001	BCR	C35-C13-C12	2.06	121.31	118.08
37	3	806	SQD	O5-C1-O6	-2.05	105.11	109.97
21	B	1220	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
21	6	601	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
21	5	601	CLA	CHB-C1B-NB	2.05	126.43	124.26
21	B	1223	CLA	CHD-C1D-ND	-2.05	122.57	124.45
21	A	1108	CLA	C2A-C1A-CHA	2.05	127.45	123.86
21	L	1504	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
39	2	808	P3H	C35-C37-C28	2.05	114.37	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	1230	CLA	C1-C2-C3	-2.05	122.49	126.04
21	3	615	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
21	B	1214	CLA	C4B-CHC-C1C	2.05	131.21	126.34
21	B	1204	CLA	O2A-CGA-CBA	2.05	118.35	111.91
21	5	614	CLA	C2A-C1A-CHA	2.05	127.45	123.86
24	B	4006	BCR	C35-C13-C14	-2.05	120.05	122.92
24	A	4004	BCR	C30-C25-C26	-2.05	119.72	122.61
24	L	4002	BCR	C27-C26-C25	-2.05	119.75	122.73
21	B	1234	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
21	A	1109	CLA	C4B-CHC-C1C	2.05	131.20	126.34
21	L	1501	CLA	C3B-C4B-NB	-2.05	108.61	110.52
24	O	4001	BCR	C29-C28-C27	2.05	115.96	111.38
21	B	1021	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
24	3	503	BCR	C33-C5-C6	-2.05	122.23	124.53
21	B	1227	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
36	4	611	CHL	CHA-C1A-NA	-2.05	121.71	126.40
21	B	1218	CLA	CHA-C1A-NA	-2.05	121.71	126.40
28	3	804	DGD	O6E-C5E-C6E	2.05	111.53	106.44
34	5	502	LUT	C15-C35-C34	-2.05	119.28	123.47
21	6	608	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
34	6	501	LUT	C38-C25-C24	-2.05	119.18	123.56
21	B	1240	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
21	2	606	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
24	I	4002	BCR	C23-C24-C25	-2.05	121.46	127.20
36	5	610	CHL	C1-O2A-CGA	2.05	122.85	116.11
21	A	1136	CLA	CMB-C2B-C3B	2.05	131.54	126.59
21	A	1106	CLA	CHA-C1A-NA	-2.05	121.71	126.40
21	B	1212	CLA	CHA-C1A-NA	-2.04	121.72	126.40
21	4	612	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
21	A	1136	CLA	OBD-CAD-C3D	-2.04	123.60	128.52
24	3	503	BCR	C34-C9-C10	-2.04	120.06	122.92
21	1	601	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
21	5	607	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
21	B	1229	CLA	C2A-C1A-CHA	2.04	127.43	123.86
21	A	1122	CLA	CAC-C3C-C4C	2.04	127.46	124.81
35	3	502	XAT	C40-C33-C34	-2.04	120.06	122.92
21	B	1228	CLA	C4B-CHC-C1C	2.04	131.18	126.34
34	5	503	LUT	C20-C13-C14	-2.04	120.06	122.92
21	A	1128	CLA	C4B-CHC-C1C	2.04	131.18	126.34
21	H	1701	CLA	CBA-CAA-C2A	-2.04	107.83	113.86
33	6	804	PTY	O7-C6-C5	2.04	115.80	108.40
21	A	1113	CLA	CMD-C2D-C3D	-2.04	122.92	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1111	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
21	6	602	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
21	A	1105	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
21	H	1701	CLA	CHC-C4B-NB	-2.04	122.10	124.26
21	K	1403	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
21	B	1219	CLA	CHA-C1A-NA	-2.04	121.72	126.40
21	A	1013	CLA	CMC-C2C-C1C	2.04	128.15	125.04
21	K	1404	CLA	CHA-C1A-NA	-2.04	121.73	126.40
21	A	1130	CLA	C1-O2A-CGA	2.04	121.79	116.44
25	1	803	LHG	C9-C8-C7	-2.04	106.20	113.62
21	1	603	CLA	CHA-C1A-NA	-2.04	121.73	126.40
21	3	612	CLA	C11-C10-C8	-2.04	109.33	115.92
24	F	4001	BCR	C23-C24-C25	-2.04	121.48	127.20
21	3	608	CLA	C1-O2A-CGA	2.04	121.79	116.44
36	1	610	CHL	C3B-C4B-NB	-2.04	108.62	110.52
21	2	608	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
21	1	612	CLA	CMC-C2C-C1C	2.04	128.14	125.04
21	5	612	CLA	CMC-C2C-C1C	2.04	128.14	125.04
24	I	4002	BCR	C35-C13-C14	-2.04	120.07	122.92
21	1	612	CLA	C4B-CHC-C1C	2.04	131.17	126.34
21	3	601	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
34	5	502	LUT	C31-C32-C33	-2.04	120.70	126.42
21	A	1138	CLA	CMC-C2C-C1C	2.03	128.14	125.04
21	B	1215	CLA	C4B-CHC-C1C	2.03	131.16	126.34
21	A	1138	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
21	A	1109	CLA	C1D-ND-C4D	-2.03	104.89	106.33
21	1	615	CLA	C2A-C1A-CHA	2.03	127.42	123.86
35	1	502	XAT	C8-C9-C10	2.03	122.06	118.94
24	B	4004	BCR	C33-C5-C4	2.03	117.52	113.62
21	K	1403	CLA	C4B-CHC-C1C	2.03	131.16	126.34
21	4	607	CLA	CHD-C1D-ND	-2.03	122.59	124.45
21	L	1504	CLA	CHA-C1A-NA	-2.03	121.75	126.40
21	A	1125	CLA	C2A-C1A-CHA	2.03	127.41	123.86
24	A	4004	BCR	C33-C5-C4	2.03	117.52	113.62
24	B	4004	BCR	C3-C4-C5	-2.03	110.45	114.08
21	B	1202	CLA	C2C-C1C-NC	2.03	111.87	109.97
21	B	1239	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
21	A	1128	CLA	O2A-CGA-CBA	2.03	118.27	111.91
21	B	1216	CLA	CHA-C1A-NA	-2.03	121.75	126.40
21	A	1113	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
21	4	601	CLA	C3A-C2A-C1A	2.03	104.37	101.34
21	5	602	CLA	O1D-CGD-CBD	-2.03	120.34	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	1106	CLA	C2A-C1A-CHA	2.03	127.40	123.86
24	2	503	BCR	C3-C4-C5	-2.03	110.46	114.08
21	3	606	CLA	CMA-C3A-C4A	2.03	117.22	111.77
35	6	502	XAT	C40-C33-C34	-2.03	120.09	122.92
25	2	803	LHG	O8-C23-O10	-2.02	118.48	123.59
21	4	603	CLA	C2A-C1A-CHA	2.02	127.40	123.86
21	2	602	CLA	CMA-C3A-C4A	2.02	117.21	111.77
36	4	610	CHL	C4A-NA-C1A	2.02	107.62	106.71
21	B	1228	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
21	3	615	CLA	CBA-CAA-C2A	2.02	119.84	113.86
21	A	1111	CLA	CAA-C2A-C3A	-2.02	107.24	112.78
35	6	504	XAT	C24-C23-C22	-2.02	106.86	110.77
21	A	1120	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
21	G	1603	CLA	CAA-C2A-C3A	-2.02	107.24	112.78
21	B	1221	CLA	C4B-CHC-C1C	2.02	131.13	126.34
25	F	5001	LHG	C5-O7-C7	-2.02	112.81	117.79
21	1	601	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
24	2	503	BCR	C33-C5-C4	2.02	117.50	113.62
21	F	1302	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
21	A	1130	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
24	L	4001	BCR	C35-C13-C12	2.02	121.26	118.08
21	A	1125	CLA	C4C-C3C-C2C	-2.02	103.95	106.90
24	A	4006	BCR	C37-C22-C21	-2.02	120.09	122.92
21	B	1235	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
21	1	605	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
21	B	1216	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
21	6	609	CLA	C2A-C1A-CHA	2.02	127.39	123.86
21	A	1128	CLA	CHA-C1A-NA	-2.02	121.78	126.40
29	5	807	3PH	C3-C2-C1	-2.02	107.01	111.79
36	4	613	CHL	C3C-C4C-NC	-2.02	108.31	110.57
21	A	1127	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
36	2	613	CHL	CMA-C3A-C2A	2.02	121.97	113.83
21	4	607	CLA	C2A-C1A-CHA	2.02	127.39	123.86
21	L	1503	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
21	O	1803	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
21	1	615	CLA	CMD-C2D-C3D	-2.02	122.98	127.61
21	A	1137	CLA	CAA-CBA-CGA	-2.02	107.36	113.25
21	A	1132	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
24	J	4001	BCR	C1-C6-C5	-2.01	119.78	122.61
35	3	502	XAT	C20-C13-C14	-2.01	120.10	122.92
21	4	607	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
21	4	612	CLA	C3D-C2D-C1D	-2.01	103.08	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	2	501	LUT	C8-C7-C6	-2.01	121.55	127.20
21	6	605	CLA	CMB-C2B-C3B	2.01	131.46	126.59
21	6	601	CLA	CHA-C1A-NA	-2.01	121.79	126.40
21	3	612	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
21	O	1802	CLA	O2D-CGD-O1D	-2.01	119.53	124.09
21	B	1201	CLA	CMD-C2D-C3D	-2.01	122.99	127.61
21	B	1202	CLA	C6-C5-C3	-2.01	108.19	113.45
21	B	1021	CLA	C4B-CHC-C1C	2.01	131.10	126.34
21	B	1021	CLA	C1-O2A-CGA	2.01	121.71	116.44
21	6	606	CLA	O2A-CGA-CBA	2.01	118.21	111.91
21	1	605	CLA	C1D-ND-C4D	-2.01	104.91	106.33
21	B	1209	CLA	O2A-CGA-CBA	2.01	120.16	112.23
21	5	606	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
21	6	609	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
21	A	1118	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
24	B	4002	BCR	C33-C5-C6	-2.01	122.28	124.53
21	A	1139	CLA	CHA-C1A-NA	-2.01	121.81	126.40
21	K	1401	CLA	C2A-C1A-CHA	2.01	127.36	123.86
21	B	1230	CLA	CAA-C2A-C3A	-2.00	107.29	112.78
21	A	1119	CLA	CMC-C2C-C3C	2.00	131.56	126.12
21	4	609	CLA	C1-C2-C3	-2.00	122.58	126.04
21	2	607	CLA	CMD-C2D-C3D	-2.00	123.00	127.61
21	B	1232	CLA	C1-C2-C3	-2.00	122.58	126.04
21	B	1226	CLA	C1-O2A-CGA	2.00	121.70	116.44
21	A	1115	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
21	1	604	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
21	H	1702	CLA	O2A-CGA-CBA	2.00	120.14	112.23
21	6	604	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
21	3	608	CLA	CAA-C2A-C3A	-2.00	107.30	112.78
21	B	1215	CLA	C1-C2-C3	-2.00	122.58	126.04
21	G	1602	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
34	4	501	LUT	C1-C6-C5	-2.00	119.80	122.61
21	B	1227	CLA	CAC-C3C-C4C	2.00	127.41	124.81

All (22) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
34	4	501	LUT	C26
34	5	501	LUT	C26
34	5	504	LUT	C26
34	6	501	LUT	C26
35	1	502	XAT	C5

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Mol	Chain	Res	Type	Atom
35	1	502	XAT	C26
35	2	502	XAT	C6
35	2	502	XAT	C26
35	3	502	XAT	C5
35	3	502	XAT	C6
35	4	502	XAT	C6
35	4	502	XAT	C26
35	6	502	XAT	C6
35	6	502	XAT	C26
35	6	504	XAT	C25
36	1	609	CHL	C8
36	2	609	CHL	C8
36	2	610	CHL	C8
36	3	604	CHL	C8
36	4	613	CHL	C8
36	5	609	CHL	C8
36	5	610	CHL	C3A

All (3817) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	1011	CL0	C2-C1-O2A-CGA
21	A	1013	CLA	CHA-CBD-CGD-O1D
21	A	1013	CLA	CHA-CBD-CGD-O2D
21	A	1013	CLA	C4-C3-C5-C6
21	A	1101	CLA	C1A-C2A-CAA-CBA
21	A	1101	CLA	CHA-CBD-CGD-O1D
21	A	1101	CLA	CHA-CBD-CGD-O2D
21	A	1102	CLA	C3A-C2A-CAA-CBA
21	A	1102	CLA	CHA-CBD-CGD-O2D
21	A	1105	CLA	C1A-C2A-CAA-CBA
21	A	1106	CLA	C3A-C2A-CAA-CBA
21	A	1106	CLA	CHA-CBD-CGD-O2D
21	A	1108	CLA	C1A-C2A-CAA-CBA
21	A	1108	CLA	C3A-C2A-CAA-CBA
21	A	1108	CLA	CHA-CBD-CGD-O1D
21	A	1108	CLA	CHA-CBD-CGD-O2D
21	A	1109	CLA	C1A-C2A-CAA-CBA
21	A	1109	CLA	CBD-CGD-O2D-CED
21	A	1109	CLA	C4-C3-C5-C6
21	A	1110	CLA	C1A-C2A-CAA-CBA
21	A	1111	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	A	1111	CLA	CHA-CBD-CGD-O2D
21	A	1112	CLA	CBD-CGD-O2D-CED
21	A	1113	CLA	CHA-CBD-CGD-O1D
21	A	1113	CLA	CHA-CBD-CGD-O2D
21	A	1114	CLA	CHA-CBD-CGD-O2D
21	A	1114	CLA	CBD-CGD-O2D-CED
21	A	1115	CLA	CHA-CBD-CGD-O1D
21	A	1115	CLA	CHA-CBD-CGD-O2D
21	A	1115	CLA	CBD-CGD-O2D-CED
21	A	1116	CLA	C3A-C2A-CAA-CBA
21	A	1116	CLA	CBD-CGD-O2D-CED
21	A	1116	CLA	C2-C3-C5-C6
21	A	1116	CLA	C4-C3-C5-C6
21	A	1117	CLA	CBD-CGD-O2D-CED
21	A	1118	CLA	C1A-C2A-CAA-CBA
21	A	1118	CLA	CBD-CGD-O2D-CED
21	A	1119	CLA	C1A-C2A-CAA-CBA
21	A	1119	CLA	C3A-C2A-CAA-CBA
21	A	1119	CLA	CHA-CBD-CGD-O1D
21	A	1119	CLA	CHA-CBD-CGD-O2D
21	A	1120	CLA	C1A-C2A-CAA-CBA
21	A	1120	CLA	CBD-CGD-O2D-CED
21	A	1120	CLA	C2-C3-C5-C6
21	A	1120	CLA	C4-C3-C5-C6
21	A	1121	CLA	C1A-C2A-CAA-CBA
21	A	1122	CLA	CHA-CBD-CGD-O1D
21	A	1122	CLA	CHA-CBD-CGD-O2D
21	A	1122	CLA	CBD-CGD-O2D-CED
21	A	1123	CLA	CHA-CBD-CGD-O1D
21	A	1123	CLA	CHA-CBD-CGD-O2D
21	A	1123	CLA	CAD-CBD-CGD-O1D
21	A	1123	CLA	CBD-CGD-O2D-CED
21	A	1124	CLA	CBD-CGD-O2D-CED
21	A	1125	CLA	CHA-CBD-CGD-O1D
21	A	1125	CLA	CHA-CBD-CGD-O2D
21	A	1125	CLA	C11-C12-C13-C14
21	A	1126	CLA	C1A-C2A-CAA-CBA
21	A	1126	CLA	C3A-C2A-CAA-CBA
21	A	1126	CLA	CHA-CBD-CGD-O1D
21	A	1126	CLA	CHA-CBD-CGD-O2D
21	A	1126	CLA	CBD-CGD-O2D-CED
21	A	1127	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	A	1127	CLA	CHA-CBD-CGD-O2D
21	A	1128	CLA	CHA-CBD-CGD-O1D
21	A	1128	CLA	CHA-CBD-CGD-O2D
21	A	1129	CLA	CHA-CBD-CGD-O1D
21	A	1129	CLA	CHA-CBD-CGD-O2D
21	A	1131	CLA	CBD-CGD-O2D-CED
21	A	1132	CLA	C4-C3-C5-C6
21	A	1134	CLA	C1A-C2A-CAA-CBA
21	A	1134	CLA	C3A-C2A-CAA-CBA
21	A	1135	CLA	C2A-CAA-CBA-CGA
21	A	1137	CLA	C1A-C2A-CAA-CBA
21	A	1138	CLA	C1A-C2A-CAA-CBA
21	A	1138	CLA	C3A-C2A-CAA-CBA
21	A	1138	CLA	CBD-CGD-O2D-CED
21	A	1139	CLA	CHA-CBD-CGD-O1D
21	A	1139	CLA	CHA-CBD-CGD-O2D
21	A	1141	CLA	CBA-CGA-O2A-C1
21	A	1141	CLA	CAD-CBD-CGD-O1D
21	A	1141	CLA	CAD-CBD-CGD-O2D
21	B	1021	CLA	C2A-CAA-CBA-CGA
21	B	1021	CLA	CHA-CBD-CGD-O1D
21	B	1021	CLA	CHA-CBD-CGD-O2D
21	B	1021	CLA	CBD-CGD-O2D-CED
21	B	1022	CLA	CBD-CGD-O2D-CED
21	B	1023	CLA	CHA-CBD-CGD-O1D
21	B	1023	CLA	CHA-CBD-CGD-O2D
21	B	1023	CLA	CBD-CGD-O2D-CED
21	B	1023	CLA	C4-C3-C5-C6
21	B	1023	CLA	C11-C10-C8-C9
21	B	1201	CLA	C1A-C2A-CAA-CBA
21	B	1201	CLA	C3A-C2A-CAA-CBA
21	B	1201	CLA	CHA-CBD-CGD-O1D
21	B	1201	CLA	CHA-CBD-CGD-O2D
21	B	1202	CLA	C1A-C2A-CAA-CBA
21	B	1202	CLA	C3A-C2A-CAA-CBA
21	B	1204	CLA	C2B-C3B-CAB-CBB
21	B	1204	CLA	C4B-C3B-CAB-CBB
21	B	1205	CLA	C2B-C3B-CAB-CBB
21	B	1205	CLA	C4B-C3B-CAB-CBB
21	B	1206	CLA	C2-C1-O2A-CGA
21	B	1207	CLA	C1A-C2A-CAA-CBA
21	B	1207	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	B	1208	CLA	C1A-C2A-CAA-CBA
21	B	1208	CLA	CBD-CGD-O2D-CED
21	B	1209	CLA	C4B-C3B-CAB-CBB
21	B	1210	CLA	CBD-CGD-O2D-CED
21	B	1210	CLA	O1D-CGD-O2D-CED
21	B	1212	CLA	CBD-CGD-O2D-CED
21	B	1213	CLA	CHA-CBD-CGD-O1D
21	B	1213	CLA	CHA-CBD-CGD-O2D
21	B	1213	CLA	C2-C3-C5-C6
21	B	1213	CLA	C4-C3-C5-C6
21	B	1214	CLA	O1A-CGA-O2A-C1
21	B	1214	CLA	CBD-CGD-O2D-CED
21	B	1215	CLA	C3A-C2A-CAA-CBA
21	B	1215	CLA	CBD-CGD-O2D-CED
21	B	1216	CLA	CHA-CBD-CGD-O1D
21	B	1216	CLA	CHA-CBD-CGD-O2D
21	B	1216	CLA	CBD-CGD-O2D-CED
21	B	1217	CLA	C1A-C2A-CAA-CBA
21	B	1217	CLA	C3A-C2A-CAA-CBA
21	B	1217	CLA	C2-C1-O2A-CGA
21	B	1218	CLA	C1A-C2A-CAA-CBA
21	B	1218	CLA	C4-C3-C5-C6
21	B	1219	CLA	CHA-CBD-CGD-O1D
21	B	1219	CLA	CHA-CBD-CGD-O2D
21	B	1219	CLA	CBD-CGD-O2D-CED
21	B	1220	CLA	C1A-C2A-CAA-CBA
21	B	1220	CLA	C3A-C2A-CAA-CBA
21	B	1220	CLA	CHA-CBD-CGD-O1D
21	B	1220	CLA	CHA-CBD-CGD-O2D
21	B	1222	CLA	CHA-CBD-CGD-O2D
21	B	1224	CLA	C1A-C2A-CAA-CBA
21	B	1224	CLA	C3A-C2A-CAA-CBA
21	B	1224	CLA	CHA-CBD-CGD-O1D
21	B	1224	CLA	CHA-CBD-CGD-O2D
21	B	1225	CLA	C1A-C2A-CAA-CBA
21	B	1225	CLA	C3A-C2A-CAA-CBA
21	B	1225	CLA	CHA-CBD-CGD-O1D
21	B	1225	CLA	CHA-CBD-CGD-O2D
21	B	1226	CLA	C1A-C2A-CAA-CBA
21	B	1226	CLA	C3A-C2A-CAA-CBA
21	B	1226	CLA	CBD-CGD-O2D-CED
21	B	1229	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
21	B	1229	CLA	CBD-CGD-O2D-CED
21	B	1230	CLA	C2B-C3B-CAB-CBB
21	B	1230	CLA	C4B-C3B-CAB-CBB
21	B	1230	CLA	C4-C3-C5-C6
21	B	1232	CLA	C1A-C2A-CAA-CBA
21	B	1232	CLA	C3A-C2A-CAA-CBA
21	B	1232	CLA	CHA-CBD-CGD-O1D
21	B	1232	CLA	CAD-CBD-CGD-O1D
21	B	1232	CLA	CAD-CBD-CGD-O2D
21	B	1234	CLA	C1A-C2A-CAA-CBA
21	B	1234	CLA	CBD-CGD-O2D-CED
21	B	1236	CLA	CHA-CBD-CGD-O1D
21	B	1236	CLA	CHA-CBD-CGD-O2D
21	B	1236	CLA	CBD-CGD-O2D-CED
21	B	1236	CLA	C2-C3-C5-C6
21	B	1236	CLA	C4-C3-C5-C6
21	B	1237	CLA	C2-C1-O2A-CGA
21	B	1237	CLA	CHA-CBD-CGD-O1D
21	B	1237	CLA	CHA-CBD-CGD-O2D
21	B	1239	CLA	C3A-C2A-CAA-CBA
21	B	1239	CLA	CBD-CGD-O2D-CED
21	B	1239	CLA	C2-C3-C5-C6
21	B	1239	CLA	C4-C3-C5-C6
21	B	1240	CLA	CHA-CBD-CGD-O1D
21	B	1240	CLA	CHA-CBD-CGD-O2D
21	F	1301	CLA	C1A-C2A-CAA-CBA
21	F	1301	CLA	C3A-C2A-CAA-CBA
21	F	1302	CLA	C2-C1-O2A-CGA
21	F	1302	CLA	CBD-CGD-O2D-CED
21	J	1901	CLA	CHA-CBD-CGD-O1D
21	J	1901	CLA	CHA-CBD-CGD-O2D
21	J	1901	CLA	CBD-CGD-O2D-CED
21	G	1601	CLA	C1A-C2A-CAA-CBA
21	G	1602	CLA	CBA-CGA-O2A-C1
21	G	1602	CLA	CHA-CBD-CGD-O1D
21	G	1602	CLA	CHA-CBD-CGD-O2D
21	G	1602	CLA	CBD-CGD-O2D-CED
21	G	1603	CLA	CBD-CGD-O2D-CED
21	H	1701	CLA	CHA-CBD-CGD-O1D
21	H	1701	CLA	CHA-CBD-CGD-O2D
21	H	1702	CLA	C1A-C2A-CAA-CBA
21	H	1702	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	H	1702	CLA	CHA-CBD-CGD-O2D
21	K	1401	CLA	C1A-C2A-CAA-CBA
21	K	1401	CLA	C3A-C2A-CAA-CBA
21	K	1401	CLA	C2B-C3B-CAB-CBB
21	K	1401	CLA	C4B-C3B-CAB-CBB
21	K	1402	CLA	C1A-C2A-CAA-CBA
21	K	1402	CLA	CHA-CBD-CGD-O1D
21	K	1402	CLA	CHA-CBD-CGD-O2D
21	K	1403	CLA	C1A-C2A-CAA-CBA
21	K	1403	CLA	C3A-C2A-CAA-CBA
21	K	1403	CLA	CBD-CGD-O2D-CED
21	K	1404	CLA	CBD-CGD-O2D-CED
21	L	1501	CLA	C1A-C2A-CAA-CBA
21	L	1501	CLA	C3A-C2A-CAA-CBA
21	L	1501	CLA	C2-C1-O2A-CGA
21	L	1502	CLA	C1A-C2A-CAA-CBA
21	L	1502	CLA	C3A-C2A-CAA-CBA
21	L	1502	CLA	C2-C1-O2A-CGA
21	L	1502	CLA	CHA-CBD-CGD-O1D
21	L	1502	CLA	CHA-CBD-CGD-O2D
21	L	1504	CLA	C1A-C2A-CAA-CBA
21	L	1504	CLA	C3A-C2A-CAA-CBA
21	O	1803	CLA	C2-C1-O2A-CGA
21	1	601	CLA	CBA-CGA-O2A-C1
21	1	601	CLA	O1A-CGA-O2A-C1
21	1	601	CLA	CHA-CBD-CGD-O1D
21	1	601	CLA	CHA-CBD-CGD-O2D
21	1	601	CLA	C2-C3-C5-C6
21	1	601	CLA	C4-C3-C5-C6
21	1	602	CLA	C1A-C2A-CAA-CBA
21	1	602	CLA	C3A-C2A-CAA-CBA
21	1	602	CLA	CBA-CGA-O2A-C1
21	1	602	CLA	CBD-CGD-O2D-CED
21	1	603	CLA	C1A-C2A-CAA-CBA
21	1	603	CLA	CHA-CBD-CGD-O1D
21	1	603	CLA	CHA-CBD-CGD-O2D
21	1	603	CLA	C6-C7-C8-C9
21	1	606	CLA	CHA-CBD-CGD-O1D
21	1	606	CLA	CHA-CBD-CGD-O2D
21	1	606	CLA	CAD-CBD-CGD-O1D
21	1	607	CLA	C4B-C3B-CAB-CBB
21	1	607	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	1	607	CLA	CHA-CBD-CGD-O2D
21	1	607	CLA	CBD-CGD-O2D-CED
21	1	608	CLA	C4B-C3B-CAB-CBB
21	1	608	CLA	CHA-CBD-CGD-O1D
21	1	611	CLA	CBD-CGD-O2D-CED
21	1	612	CLA	CHA-CBD-CGD-O2D
21	1	613	CLA	CBD-CGD-O2D-CED
21	1	615	CLA	CBD-CGD-O2D-CED
21	2	601	CLA	C3A-C2A-CAA-CBA
21	2	601	CLA	CHA-CBD-CGD-O1D
21	2	601	CLA	CHA-CBD-CGD-O2D
21	2	602	CLA	CBD-CGD-O2D-CED
21	2	602	CLA	C3-C5-C6-C7
21	2	603	CLA	CHA-CBD-CGD-O1D
21	2	603	CLA	CHA-CBD-CGD-O2D
21	2	603	CLA	CBD-CGD-O2D-CED
21	2	604	CLA	C1A-C2A-CAA-CBA
21	2	604	CLA	C3A-C2A-CAA-CBA
21	2	604	CLA	CHA-CBD-CGD-O1D
21	2	604	CLA	CHA-CBD-CGD-O2D
21	2	605	CLA	O1A-CGA-O2A-C1
21	2	606	CLA	C4B-C3B-CAB-CBB
21	2	607	CLA	C4B-C3B-CAB-CBB
21	2	608	CLA	C2A-CAA-CBA-CGA
21	2	608	CLA	C4B-C3B-CAB-CBB
21	2	608	CLA	CHA-CBD-CGD-O1D
21	2	608	CLA	CHA-CBD-CGD-O2D
21	2	615	CLA	C1A-C2A-CAA-CBA
21	2	615	CLA	C2-C1-O2A-CGA
21	2	615	CLA	C2B-C3B-CAB-CBB
21	2	615	CLA	C4B-C3B-CAB-CBB
21	2	615	CLA	CHA-CBD-CGD-O1D
21	2	615	CLA	CHA-CBD-CGD-O2D
21	2	615	CLA	CBD-CGD-O2D-CED
21	3	601	CLA	C1A-C2A-CAA-CBA
21	3	601	CLA	CHA-CBD-CGD-O1D
21	3	601	CLA	CHA-CBD-CGD-O2D
21	3	602	CLA	CBD-CGD-O2D-CED
21	3	603	CLA	CHA-CBD-CGD-O1D
21	3	603	CLA	CHA-CBD-CGD-O2D
21	3	606	CLA	CHA-CBD-CGD-O2D
21	3	607	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
21	3	607	CLA	C4B-C3B-CAB-CBB
21	3	608	CLA	C4B-C3B-CAB-CBB
21	3	608	CLA	CBD-CGD-O2D-CED
21	3	610	CLA	C1A-C2A-CAA-CBA
21	3	610	CLA	C3A-C2A-CAA-CBA
21	3	610	CLA	C2A-CAA-CBA-CGA
21	3	610	CLA	CHA-CBD-CGD-O1D
21	3	610	CLA	CHA-CBD-CGD-O2D
21	3	610	CLA	CBD-CGD-O2D-CED
21	3	611	CLA	CHA-CBD-CGD-O1D
21	3	611	CLA	CHA-CBD-CGD-O2D
21	3	611	CLA	CBD-CGD-O2D-CED
21	3	612	CLA	C2B-C3B-CAB-CBB
21	3	612	CLA	C4B-C3B-CAB-CBB
21	3	613	CLA	C3A-C2A-CAA-CBA
21	3	613	CLA	CBA-CGA-O2A-C1
21	3	613	CLA	CBD-CGD-O2D-CED
21	3	614	CLA	CHA-CBD-CGD-O1D
21	3	614	CLA	CHA-CBD-CGD-O2D
21	3	614	CLA	CBD-CGD-O2D-CED
21	3	615	CLA	C1A-C2A-CAA-CBA
21	4	601	CLA	C1A-C2A-CAA-CBA
21	4	601	CLA	CHA-CBD-CGD-O1D
21	4	601	CLA	CHA-CBD-CGD-O2D
21	4	602	CLA	C4B-C3B-CAB-CBB
21	4	602	CLA	CHA-CBD-CGD-O2D
21	4	604	CLA	C3A-C2A-CAA-CBA
21	4	607	CLA	C4B-C3B-CAB-CBB
21	4	607	CLA	CBD-CGD-O2D-CED
21	4	608	CLA	CBD-CGD-O2D-CED
21	4	609	CLA	C1A-C2A-CAA-CBA
21	4	609	CLA	C3A-C2A-CAA-CBA
21	4	615	CLA	C1A-C2A-CAA-CBA
21	4	615	CLA	C3A-C2A-CAA-CBA
21	4	615	CLA	C4B-C3B-CAB-CBB
21	4	615	CLA	C2-C3-C5-C6
21	4	615	CLA	C4-C3-C5-C6
21	5	601	CLA	CHA-CBD-CGD-O1D
21	5	601	CLA	CHA-CBD-CGD-O2D
21	5	603	CLA	CBD-CGD-O2D-CED
21	5	604	CLA	CBA-CGA-O2A-C1
21	5	604	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	5	604	CLA	CBD-CGD-O2D-CED
21	5	605	CLA	CBA-CGA-O2A-C1
21	5	605	CLA	O1A-CGA-O2A-C1
21	5	605	CLA	CAD-CBD-CGD-O1D
21	5	605	CLA	CAD-CBD-CGD-O2D
21	5	605	CLA	CBD-CGD-O2D-CED
21	5	606	CLA	C2-C1-O2A-CGA
21	5	607	CLA	CBA-CGA-O2A-C1
21	5	607	CLA	O1A-CGA-O2A-C1
21	5	608	CLA	CHA-CBD-CGD-O1D
21	5	608	CLA	CHA-CBD-CGD-O2D
21	5	608	CLA	C2-C3-C5-C6
21	5	608	CLA	C4-C3-C5-C6
21	5	613	CLA	CBD-CGD-O2D-CED
21	5	614	CLA	C3A-C2A-CAA-CBA
21	6	601	CLA	C1A-C2A-CAA-CBA
21	6	601	CLA	C3A-C2A-CAA-CBA
21	6	601	CLA	C2-C1-O2A-CGA
21	6	601	CLA	C2-C3-C5-C6
21	6	601	CLA	C4-C3-C5-C6
21	6	602	CLA	CHA-CBD-CGD-O2D
21	6	602	CLA	CBD-CGD-O2D-CED
21	6	603	CLA	CHA-CBD-CGD-O1D
21	6	603	CLA	CHA-CBD-CGD-O2D
21	6	604	CLA	CHA-CBD-CGD-O1D
21	6	604	CLA	CHA-CBD-CGD-O2D
21	6	604	CLA	CBD-CGD-O2D-CED
21	6	605	CLA	C2-C3-C5-C6
21	6	605	CLA	C4-C3-C5-C6
21	6	606	CLA	C1A-C2A-CAA-CBA
21	6	606	CLA	C2-C1-O2A-CGA
21	6	608	CLA	CBD-CGD-O2D-CED
21	6	609	CLA	CBA-CGA-O2A-C1
21	6	609	CLA	CBD-CGD-O2D-CED
21	6	613	CLA	CBD-CGD-O2D-CED
22	B	2002	PQN	C12-C13-C15-C16
22	B	2002	PQN	C14-C13-C15-C16
24	A	4001	BCR	C1-C6-C7-C8
24	A	4001	BCR	C5-C6-C7-C8
24	A	4001	BCR	C11-C10-C9-C8
24	A	4001	BCR	C11-C10-C9-C34
24	A	4001	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	A	4001	BCR	C17-C18-C19-C20
24	A	4001	BCR	C36-C18-C19-C20
24	A	4002	BCR	C1-C6-C7-C8
24	A	4002	BCR	C7-C8-C9-C10
24	A	4002	BCR	C7-C8-C9-C34
24	A	4002	BCR	C11-C10-C9-C8
24	A	4002	BCR	C11-C10-C9-C34
24	A	4002	BCR	C10-C11-C12-C13
24	A	4002	BCR	C23-C24-C25-C26
24	A	4003	BCR	C7-C8-C9-C10
24	A	4003	BCR	C7-C8-C9-C34
24	A	4003	BCR	C11-C10-C9-C8
24	A	4003	BCR	C11-C10-C9-C34
24	A	4004	BCR	C11-C10-C9-C8
24	A	4004	BCR	C11-C10-C9-C34
24	A	4004	BCR	C9-C10-C11-C12
24	A	4004	BCR	C10-C11-C12-C13
24	A	4004	BCR	C21-C22-C23-C24
24	A	4004	BCR	C37-C22-C23-C24
24	A	4004	BCR	C23-C24-C25-C26
24	A	4004	BCR	C23-C24-C25-C30
24	A	4005	BCR	C11-C10-C9-C8
24	A	4005	BCR	C11-C10-C9-C34
24	A	4005	BCR	C10-C11-C12-C13
24	A	4006	BCR	C7-C8-C9-C34
24	A	4006	BCR	C10-C11-C12-C13
24	A	4006	BCR	C11-C12-C13-C14
24	A	4006	BCR	C11-C12-C13-C35
24	A	4006	BCR	C17-C18-C19-C20
24	A	4006	BCR	C36-C18-C19-C20
24	A	4006	BCR	C23-C24-C25-C30
24	A	4007	BCR	C11-C10-C9-C8
24	A	4007	BCR	C11-C10-C9-C34
24	A	4007	BCR	C10-C11-C12-C13
24	B	4001	BCR	C5-C6-C7-C8
24	B	4001	BCR	C7-C8-C9-C34
24	B	4001	BCR	C11-C10-C9-C8
24	B	4001	BCR	C11-C10-C9-C34
24	B	4001	BCR	C17-C18-C19-C20
24	B	4001	BCR	C36-C18-C19-C20
24	B	4002	BCR	C7-C8-C9-C10
24	B	4002	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
24	B	4002	BCR	C11-C10-C9-C8
24	B	4002	BCR	C11-C10-C9-C34
24	B	4002	BCR	C10-C11-C12-C13
24	B	4002	BCR	C17-C18-C19-C20
24	B	4002	BCR	C36-C18-C19-C20
24	B	4002	BCR	C21-C22-C23-C24
24	B	4002	BCR	C37-C22-C23-C24
24	B	4003	BCR	C11-C10-C9-C8
24	B	4003	BCR	C11-C10-C9-C34
24	B	4003	BCR	C9-C10-C11-C12
24	B	4003	BCR	C10-C11-C12-C13
24	B	4003	BCR	C17-C18-C19-C20
24	B	4003	BCR	C36-C18-C19-C20
24	B	4004	BCR	C7-C8-C9-C10
24	B	4004	BCR	C7-C8-C9-C34
24	B	4004	BCR	C11-C10-C9-C8
24	B	4004	BCR	C11-C10-C9-C34
24	B	4004	BCR	C10-C11-C12-C13
24	B	4005	BCR	C11-C10-C9-C8
24	B	4005	BCR	C11-C10-C9-C34
24	B	4005	BCR	C10-C11-C12-C13
24	B	4005	BCR	C36-C18-C19-C20
24	B	4005	BCR	C21-C22-C23-C24
24	B	4005	BCR	C37-C22-C23-C24
24	B	4006	BCR	C11-C10-C9-C8
24	B	4006	BCR	C11-C10-C9-C34
24	B	4006	BCR	C17-C18-C19-C20
24	B	4006	BCR	C36-C18-C19-C20
24	F	4001	BCR	C10-C11-C12-C13
24	F	4002	BCR	C11-C10-C9-C8
24	F	4002	BCR	C11-C10-C9-C34
24	F	4002	BCR	C11-C12-C13-C14
24	F	4002	BCR	C11-C12-C13-C35
24	F	4002	BCR	C17-C18-C19-C20
24	F	4002	BCR	C36-C18-C19-C20
24	F	4002	BCR	C21-C22-C23-C24
24	F	4002	BCR	C37-C22-C23-C24
24	J	4001	BCR	C5-C6-C7-C8
24	J	4001	BCR	C7-C8-C9-C10
24	J	4001	BCR	C7-C8-C9-C34
24	J	4001	BCR	C17-C18-C19-C20
24	J	4001	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
24	J	4001	BCR	C23-C24-C25-C26
24	J	4001	BCR	C23-C24-C25-C30
24	J	4002	BCR	C7-C8-C9-C10
24	J	4002	BCR	C7-C8-C9-C34
24	J	4002	BCR	C11-C10-C9-C8
24	J	4002	BCR	C11-C10-C9-C34
24	J	4002	BCR	C11-C12-C13-C14
24	J	4002	BCR	C11-C12-C13-C35
24	J	4002	BCR	C36-C18-C19-C20
24	G	4001	BCR	C11-C10-C9-C8
24	G	4001	BCR	C11-C10-C9-C34
24	G	4001	BCR	C10-C11-C12-C13
24	H	4001	BCR	C1-C6-C7-C8
24	H	4001	BCR	C5-C6-C7-C8
24	H	4001	BCR	C11-C10-C9-C8
24	H	4001	BCR	C11-C10-C9-C34
24	H	4001	BCR	C10-C11-C12-C13
24	H	4001	BCR	C21-C22-C23-C24
24	H	4001	BCR	C23-C24-C25-C26
24	I	4001	BCR	C1-C6-C7-C8
24	I	4001	BCR	C5-C6-C7-C8
24	I	4001	BCR	C11-C10-C9-C8
24	I	4001	BCR	C11-C10-C9-C34
24	I	4001	BCR	C9-C10-C11-C12
24	I	4001	BCR	C19-C20-C21-C22
24	I	4002	BCR	C11-C12-C13-C14
24	I	4002	BCR	C11-C12-C13-C35
24	I	4002	BCR	C17-C18-C19-C20
24	I	4002	BCR	C36-C18-C19-C20
24	I	4002	BCR	C21-C22-C23-C24
24	I	4002	BCR	C37-C22-C23-C24
24	K	4001	BCR	C11-C10-C9-C8
24	K	4001	BCR	C11-C10-C9-C34
24	K	4001	BCR	C9-C10-C11-C12
24	K	4001	BCR	C10-C11-C12-C13
24	K	4001	BCR	C23-C24-C25-C26
24	L	4001	BCR	C1-C6-C7-C8
24	L	4001	BCR	C11-C10-C9-C8
24	L	4001	BCR	C11-C10-C9-C34
24	L	4001	BCR	C9-C10-C11-C12
24	L	4001	BCR	C10-C11-C12-C13
24	L	4001	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
24	L	4001	BCR	C37-C22-C23-C24
24	L	4001	BCR	C23-C24-C25-C26
24	L	4001	BCR	C23-C24-C25-C30
24	L	4002	BCR	C11-C10-C9-C8
24	L	4002	BCR	C11-C10-C9-C34
24	L	4002	BCR	C10-C11-C12-C13
24	O	4001	BCR	C11-C10-C9-C8
24	O	4001	BCR	C11-C10-C9-C34
24	O	4001	BCR	C10-C11-C12-C13
24	O	4001	BCR	C17-C18-C19-C20
24	O	4001	BCR	C36-C18-C19-C20
24	O	4001	BCR	C23-C24-C25-C26
24	O	4001	BCR	C23-C24-C25-C30
24	1	504	BCR	C11-C10-C9-C8
24	1	504	BCR	C11-C10-C9-C34
24	1	504	BCR	C23-C24-C25-C26
24	1	504	BCR	C23-C24-C25-C30
24	2	503	BCR	C11-C10-C9-C8
24	2	503	BCR	C11-C10-C9-C34
24	2	503	BCR	C10-C11-C12-C13
24	2	503	BCR	C11-C12-C13-C14
24	2	503	BCR	C11-C12-C13-C35
24	2	503	BCR	C36-C18-C19-C20
24	2	503	BCR	C21-C22-C23-C24
24	2	503	BCR	C37-C22-C23-C24
24	2	503	BCR	C23-C24-C25-C26
24	3	503	BCR	C7-C8-C9-C10
24	3	503	BCR	C7-C8-C9-C34
24	3	503	BCR	C11-C10-C9-C8
24	3	503	BCR	C11-C10-C9-C34
24	3	503	BCR	C9-C10-C11-C12
24	3	503	BCR	C10-C11-C12-C13
24	3	504	BCR	C11-C12-C13-C14
24	3	504	BCR	C11-C12-C13-C35
24	3	504	BCR	C17-C18-C19-C20
24	3	504	BCR	C36-C18-C19-C20
24	4	503	BCR	C11-C10-C9-C8
24	4	503	BCR	C11-C10-C9-C34
24	4	503	BCR	C10-C11-C12-C13
24	4	503	BCR	C21-C22-C23-C24
24	4	503	BCR	C37-C22-C23-C24
24	4	503	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
24	4	503	BCR	C23-C24-C25-C30
25	A	5001	LHG	O1-C1-C2-C3
25	A	5001	LHG	C4-O6-P-O4
25	A	5001	LHG	C4-O6-P-O5
25	A	5002	LHG	O1-C1-C2-C3
25	A	5002	LHG	C1-C2-C3-O3
25	A	5002	LHG	C4-O6-P-O3
25	A	5002	LHG	C4-O6-P-O4
25	A	5002	LHG	C4-O6-P-O5
25	B	5001	LHG	O1-C1-C2-O2
25	B	5001	LHG	O1-C1-C2-C3
25	B	5001	LHG	C1-C2-C3-O3
25	B	5001	LHG	O2-C2-C3-O3
25	B	5001	LHG	C3-O3-P-O4
25	B	5001	LHG	C3-O3-P-O5
25	B	5001	LHG	C3-O3-P-O6
25	B	5001	LHG	C4-O6-P-O4
25	F	5001	LHG	O2-C2-C3-O3
25	F	5001	LHG	C3-O3-P-O6
25	F	5001	LHG	C4-O6-P-O4
25	1	801	LHG	O1-C1-C2-C3
25	1	801	LHG	O2-C2-C3-O3
25	1	801	LHG	C3-O3-P-O5
25	1	801	LHG	C4-O6-P-O4
25	1	801	LHG	O9-C7-O7-C5
25	1	801	LHG	C8-C7-O7-C5
25	1	802	LHG	C1-C2-C3-O3
25	1	802	LHG	O6-C4-C5-O7
25	1	802	LHG	C8-C7-O7-C5
25	2	801	LHG	O1-C1-C2-C3
25	2	801	LHG	C3-O3-P-O5
25	2	802	LHG	C4-O6-P-O4
25	2	802	LHG	C8-C7-O7-C5
25	2	803	LHG	O1-C1-C2-C3
25	2	803	LHG	C3-O3-P-O6
25	3	801	LHG	O1-C1-C2-C3
25	3	801	LHG	C4-O6-P-O5
25	3	801	LHG	O7-C5-C6-O8
25	4	801	LHG	O1-C1-C2-O2
25	4	801	LHG	O2-C2-C3-O3
25	4	801	LHG	C3-O3-P-O5
25	4	801	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
25	5	801	LHG	C4-O6-P-O3
25	5	801	LHG	C4-O6-P-O4
25	5	801	LHG	C4-O6-P-O5
25	5	802	LHG	O1-C1-C2-C3
25	5	802	LHG	O2-C2-C3-O3
25	5	802	LHG	C4-O6-P-O3
25	5	802	LHG	C4-O6-P-O5
25	5	802	LHG	C8-C7-O7-C5
25	6	801	LHG	O1-C1-C2-C3
25	6	801	LHG	O2-C2-C3-O3
25	6	801	LHG	O6-C4-C5-O7
25	6	801	LHG	C8-C7-O7-C5
27	6	805	LMU	C2'-C1'-O1'-C1
28	B	5002	DGD	C2B-C1B-O2G-C2G
28	2	806	DGD	C2B-C1B-O2G-C2G
28	2	806	DGD	O6E-C1E-O5D-C6D
28	3	804	DGD	O6E-C1E-O5D-C6D
28	3	805	DGD	C2A-C1A-O1G-C1G
28	3	805	DGD	O1A-C1A-O1G-C1G
28	3	805	DGD	C2B-C1B-O2G-C2G
28	3	805	DGD	O6D-C1D-O3G-C3G
29	B	5003	3PH	C1-O11-P-O13
29	B	5003	3PH	C1-O11-P-O14
29	B	5003	3PH	C1-O11-P-O12
29	B	5003	3PH	O22-C21-O21-C2
29	B	5003	3PH	C22-C21-O21-C2
29	F	5003	3PH	C1-O11-P-O13
29	F	5003	3PH	C1-O11-P-O14
29	F	5003	3PH	C1-O11-P-O12
29	5	807	3PH	C22-C21-O21-C2
31	1	804	LMG	O6-C1-O1-C7
31	2	804	LMG	O6-C1-O1-C7
31	2	804	LMG	O9-C10-O7-C8
31	2	804	LMG	C11-C10-O7-C8
31	3	802	LMG	C11-C10-O7-C8
31	3	803	LMG	O9-C10-O7-C8
31	3	803	LMG	C11-C10-O7-C8
31	4	802	LMG	C2-C1-O1-C7
31	4	802	LMG	O6-C1-O1-C7
31	4	802	LMG	O9-C10-O7-C8
31	4	802	LMG	C11-C10-O7-C8
31	4	803	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
31	4	803	LMG	C11-C10-O7-C8
31	6	802	LMG	O6-C1-O1-C7
31	6	802	LMG	O9-C10-O7-C8
31	6	802	LMG	C11-C10-O7-C8
32	5	805	4RF	O42-C41-O40-C39
32	5	805	4RF	C43-C41-O40-C39
33	O	5002	PTY	C5-O14-P1-O13
33	1	805	PTY	N1-C2-C3-O11
33	1	805	PTY	O10-C8-O7-C6
33	1	805	PTY	C3-O11-P1-O13
33	1	805	PTY	C3-O11-P1-O14
33	1	805	PTY	C5-O14-P1-O11
33	1	805	PTY	C5-O14-P1-O12
33	1	805	PTY	C5-O14-P1-O13
33	1	806	PTY	O10-C8-O7-C6
33	1	806	PTY	C11-C8-O7-C6
33	3	807	PTY	C5-O14-P1-O11
33	3	807	PTY	C5-O14-P1-O13
33	3	808	PTY	N1-C2-C3-O11
33	3	808	PTY	C3-O11-P1-O13
33	3	808	PTY	C5-O14-P1-O11
33	3	808	PTY	C5-O14-P1-O12
33	3	808	PTY	C5-O14-P1-O13
33	4	804	PTY	C3-O11-P1-O12
33	4	804	PTY	C3-O11-P1-O13
33	4	804	PTY	C5-O14-P1-O11
33	4	804	PTY	C5-O14-P1-O12
33	4	804	PTY	C5-O14-P1-O13
33	5	803	PTY	N1-C2-C3-O11
33	5	803	PTY	C11-C8-O7-C6
33	5	803	PTY	C3-O11-P1-O12
33	5	803	PTY	C3-O11-P1-O13
33	6	804	PTY	C11-C8-O7-C6
34	2	501	LUT	C7-C8-C9-C10
34	2	501	LUT	C7-C8-C9-C19
34	3	501	LUT	C25-C26-C27-C28
34	3	501	LUT	C27-C28-C29-C30
34	3	501	LUT	C27-C28-C29-C39
34	4	501	LUT	C27-C28-C29-C30
34	4	501	LUT	C27-C28-C29-C39
34	5	501	LUT	C21-C26-C27-C28
34	5	501	LUT	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
34	5	502	LUT	C21-C26-C27-C28
34	5	502	LUT	C31-C32-C33-C34
34	5	502	LUT	C31-C32-C33-C40
34	5	503	LUT	C21-C26-C27-C28
34	5	503	LUT	C25-C26-C27-C28
34	5	503	LUT	C27-C28-C29-C30
34	5	503	LUT	C27-C28-C29-C39
34	5	503	LUT	C29-C30-C31-C32
34	5	504	LUT	C11-C12-C13-C14
34	5	504	LUT	C11-C12-C13-C20
34	5	504	LUT	C21-C26-C27-C28
34	5	504	LUT	C31-C32-C33-C34
34	5	504	LUT	C31-C32-C33-C40
34	6	501	LUT	C21-C26-C27-C28
35	1	502	XAT	O4-C6-C7-C8
35	2	502	XAT	C27-C28-C29-C30
35	2	502	XAT	C27-C28-C29-C39
35	3	502	XAT	O24-C26-C27-C28
35	3	502	XAT	C27-C28-C29-C30
35	3	502	XAT	C27-C28-C29-C39
35	6	504	XAT	C11-C12-C13-C14
35	6	504	XAT	C11-C12-C13-C20
35	6	504	XAT	C12-C13-C14-C15
35	6	504	XAT	C20-C13-C14-C15
35	6	504	XAT	C26-C27-C28-C29
36	1	609	CHL	CHA-CBD-CGD-O1D
36	1	609	CHL	CHA-CBD-CGD-O2D
36	2	613	CHL	CHA-CBD-CGD-O1D
36	2	613	CHL	CHA-CBD-CGD-O2D
36	3	604	CHL	C1A-C2A-CAA-CBA
36	3	604	CHL	C3A-C2A-CAA-CBA
36	3	604	CHL	C2-C3-C5-C6
36	3	604	CHL	C4-C3-C5-C6
36	5	610	CHL	C1A-C2A-CAA-CBA
36	5	610	CHL	C2A-CAA-CBA-CGA
37	2	805	SQD	C2-C1-O6-C44
37	2	805	SQD	O5-C1-O6-C44
37	2	805	SQD	C8-C7-O47-C45
37	2	805	SQD	O5-C5-C6-S
37	2	805	SQD	C5-C6-S-O7
37	2	805	SQD	C5-C6-S-O9
37	3	806	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
37	3	806	SQD	O5-C5-C6-S
37	6	803	SQD	O5-C5-C6-S
38	2	807	LMK	C1-C2-C3-N4
38	4	805	LMK	O10-C28-C29-C30
39	2	808	P3H	C22-O23-P24-O25
39	2	808	P3H	C22-O23-P24-O26
39	2	808	P3H	C22-O23-P24-O27
39	5	806	P3H	C28-O27-P24-O25
33	L	5003	PTY	C11-C8-O7-C6
21	A	1121	CLA	O1D-CGD-O2D-CED
21	B	1226	CLA	O1D-CGD-O2D-CED
21	1	603	CLA	O1D-CGD-O2D-CED
21	1	608	CLA	O1D-CGD-O2D-CED
21	2	606	CLA	O1D-CGD-O2D-CED
21	3	614	CLA	O1D-CGD-O2D-CED
25	5	802	LHG	O9-C7-O7-C5
37	2	805	SQD	O49-C7-O47-C45
21	A	1126	CLA	O1D-CGD-O2D-CED
21	A	1138	CLA	O1D-CGD-O2D-CED
21	B	1021	CLA	O1D-CGD-O2D-CED
21	B	1023	CLA	O1D-CGD-O2D-CED
21	B	1219	CLA	O1D-CGD-O2D-CED
21	L	1504	CLA	O1D-CGD-O2D-CED
21	O	1803	CLA	O1D-CGD-O2D-CED
21	1	613	CLA	O1D-CGD-O2D-CED
21	1	615	CLA	O1D-CGD-O2D-CED
21	3	605	CLA	O1D-CGD-O2D-CED
21	4	615	CLA	O1D-CGD-O2D-CED
21	5	602	CLA	O1D-CGD-O2D-CED
21	A	1101	CLA	CBD-CGD-O2D-CED
21	A	1103	CLA	CBD-CGD-O2D-CED
21	A	1105	CLA	CBD-CGD-O2D-CED
21	A	1107	CLA	CBD-CGD-O2D-CED
21	A	1108	CLA	CBD-CGD-O2D-CED
21	A	1119	CLA	CBD-CGD-O2D-CED
21	A	1121	CLA	CBD-CGD-O2D-CED
21	A	1132	CLA	CBD-CGD-O2D-CED
21	A	1134	CLA	CBD-CGD-O2D-CED
21	A	1139	CLA	CBD-CGD-O2D-CED
21	A	1140	CLA	CBD-CGD-O2D-CED
21	A	1141	CLA	CBD-CGD-O2D-CED
21	B	1201	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	B	1203	CLA	CBD-CGD-O2D-CED
21	B	1206	CLA	CBD-CGD-O2D-CED
21	B	1213	CLA	CBD-CGD-O2D-CED
21	B	1217	CLA	CBD-CGD-O2D-CED
21	B	1218	CLA	CBD-CGD-O2D-CED
21	B	1221	CLA	CBD-CGD-O2D-CED
21	B	1224	CLA	CBD-CGD-O2D-CED
21	B	1230	CLA	CBD-CGD-O2D-CED
21	B	1235	CLA	CBD-CGD-O2D-CED
21	B	1237	CLA	CBD-CGD-O2D-CED
21	F	1301	CLA	CBD-CGD-O2D-CED
21	G	1601	CLA	CBD-CGD-O2D-CED
21	H	1701	CLA	CBD-CGD-O2D-CED
21	K	1401	CLA	CBD-CGD-O2D-CED
21	L	1501	CLA	CBD-CGD-O2D-CED
21	L	1504	CLA	CBD-CGD-O2D-CED
21	O	1803	CLA	CBD-CGD-O2D-CED
21	1	601	CLA	CBD-CGD-O2D-CED
21	1	603	CLA	CBD-CGD-O2D-CED
21	1	604	CLA	CBD-CGD-O2D-CED
21	1	605	CLA	CBD-CGD-O2D-CED
21	1	608	CLA	CBD-CGD-O2D-CED
21	2	601	CLA	CBD-CGD-O2D-CED
21	2	605	CLA	CBD-CGD-O2D-CED
21	2	606	CLA	CBD-CGD-O2D-CED
21	2	607	CLA	CBD-CGD-O2D-CED
21	2	608	CLA	CBD-CGD-O2D-CED
21	2	612	CLA	CBD-CGD-O2D-CED
21	3	601	CLA	CBD-CGD-O2D-CED
21	3	603	CLA	CBD-CGD-O2D-CED
21	3	605	CLA	CBD-CGD-O2D-CED
21	3	615	CLA	CBD-CGD-O2D-CED
21	4	601	CLA	CBD-CGD-O2D-CED
21	4	603	CLA	CBD-CGD-O2D-CED
21	4	605	CLA	CBD-CGD-O2D-CED
21	4	606	CLA	CBD-CGD-O2D-CED
21	4	609	CLA	CBD-CGD-O2D-CED
21	4	615	CLA	CBD-CGD-O2D-CED
21	5	601	CLA	CBD-CGD-O2D-CED
21	5	602	CLA	CBD-CGD-O2D-CED
21	5	606	CLA	CBD-CGD-O2D-CED
21	5	607	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	5	612	CLA	CBD-CGD-O2D-CED
21	6	601	CLA	CBD-CGD-O2D-CED
21	6	606	CLA	CBD-CGD-O2D-CED
21	6	607	CLA	CBD-CGD-O2D-CED
21	6	612	CLA	CBD-CGD-O2D-CED
21	A	1111	CLA	O1A-CGA-O2A-C1
21	A	1127	CLA	O1A-CGA-O2A-C1
21	A	1141	CLA	O1A-CGA-O2A-C1
21	B	1219	CLA	O1A-CGA-O2A-C1
21	B	1221	CLA	O1A-CGA-O2A-C1
21	O	1803	CLA	O1A-CGA-O2A-C1
21	2	607	CLA	O1A-CGA-O2A-C1
21	3	602	CLA	O1A-CGA-O2A-C1
21	3	611	CLA	O1A-CGA-O2A-C1
31	4	802	LMG	O10-C28-O8-C9
33	O	5002	PTY	O30-C30-O4-C1
33	3	808	PTY	O30-C30-O4-C1
21	B	1209	CLA	O1A-CGA-O2A-C1
21	G	1602	CLA	O1A-CGA-O2A-C1
21	1	602	CLA	O1A-CGA-O2A-C1
21	3	613	CLA	O1A-CGA-O2A-C1
33	L	5003	PTY	O10-C8-O7-C6
21	A	1101	CLA	O1D-CGD-O2D-CED
21	A	1139	CLA	O1D-CGD-O2D-CED
21	B	1203	CLA	O1D-CGD-O2D-CED
21	B	1224	CLA	O1D-CGD-O2D-CED
21	1	601	CLA	O1D-CGD-O2D-CED
21	1	602	CLA	O1D-CGD-O2D-CED
21	2	602	CLA	O1D-CGD-O2D-CED
21	2	605	CLA	O1D-CGD-O2D-CED
21	2	607	CLA	O1D-CGD-O2D-CED
21	2	608	CLA	O1D-CGD-O2D-CED
21	3	611	CLA	O1D-CGD-O2D-CED
21	4	606	CLA	O1D-CGD-O2D-CED
21	4	607	CLA	O1D-CGD-O2D-CED
21	5	606	CLA	O1D-CGD-O2D-CED
21	5	607	CLA	O1D-CGD-O2D-CED
21	6	601	CLA	O1D-CGD-O2D-CED
21	B	1209	CLA	CBA-CGA-O2A-C1
21	A	1109	CLA	O1D-CGD-O2D-CED
21	A	1112	CLA	O1D-CGD-O2D-CED
21	A	1114	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	A	1115	CLA	O1D-CGD-O2D-CED
21	A	1116	CLA	O1D-CGD-O2D-CED
21	A	1122	CLA	O1D-CGD-O2D-CED
21	A	1131	CLA	O1D-CGD-O2D-CED
21	B	1022	CLA	O1D-CGD-O2D-CED
21	B	1206	CLA	O1D-CGD-O2D-CED
21	B	1207	CLA	O1D-CGD-O2D-CED
21	B	1208	CLA	O1D-CGD-O2D-CED
21	B	1215	CLA	O1D-CGD-O2D-CED
21	B	1229	CLA	O1D-CGD-O2D-CED
21	F	1302	CLA	O1D-CGD-O2D-CED
21	G	1601	CLA	O1D-CGD-O2D-CED
21	H	1701	CLA	O1D-CGD-O2D-CED
21	K	1404	CLA	O1D-CGD-O2D-CED
21	2	615	CLA	O1D-CGD-O2D-CED
21	3	602	CLA	O1D-CGD-O2D-CED
21	3	608	CLA	O1D-CGD-O2D-CED
21	3	610	CLA	O1D-CGD-O2D-CED
21	4	608	CLA	O1D-CGD-O2D-CED
21	5	603	CLA	O1D-CGD-O2D-CED
21	5	613	CLA	O1D-CGD-O2D-CED
21	6	602	CLA	O1D-CGD-O2D-CED
21	6	604	CLA	O1D-CGD-O2D-CED
21	6	608	CLA	O1D-CGD-O2D-CED
21	6	609	CLA	O1D-CGD-O2D-CED
21	A	1111	CLA	CBA-CGA-O2A-C1
21	B	1219	CLA	CBA-CGA-O2A-C1
21	2	607	CLA	CBA-CGA-O2A-C1
21	3	602	CLA	CBA-CGA-O2A-C1
21	3	611	CLA	CBA-CGA-O2A-C1
31	4	802	LMG	C29-C28-O8-C9
33	O	5002	PTY	C31-C30-O4-C1
33	3	808	PTY	C31-C30-O4-C1
33	6	804	PTY	O30-C30-O4-C1
21	A	1012	CLA	CBD-CGD-O2D-CED
21	A	1102	CLA	CBD-CGD-O2D-CED
21	A	1104	CLA	CBD-CGD-O2D-CED
21	A	1106	CLA	CBD-CGD-O2D-CED
21	A	1113	CLA	CBD-CGD-O2D-CED
21	A	1133	CLA	CBD-CGD-O2D-CED
21	A	1136	CLA	CBD-CGD-O2D-CED
21	A	1137	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	B	1204	CLA	CBD-CGD-O2D-CED
21	B	1205	CLA	CBD-CGD-O2D-CED
21	B	1211	CLA	CBD-CGD-O2D-CED
21	B	1222	CLA	CBD-CGD-O2D-CED
21	B	1223	CLA	CBD-CGD-O2D-CED
21	B	1227	CLA	CBD-CGD-O2D-CED
21	B	1228	CLA	CBD-CGD-O2D-CED
21	B	1238	CLA	CBD-CGD-O2D-CED
21	H	1702	CLA	CBD-CGD-O2D-CED
21	K	1402	CLA	CBD-CGD-O2D-CED
21	L	1502	CLA	CBD-CGD-O2D-CED
21	1	612	CLA	CBD-CGD-O2D-CED
21	2	604	CLA	CBD-CGD-O2D-CED
21	3	612	CLA	CBD-CGD-O2D-CED
21	4	602	CLA	CBD-CGD-O2D-CED
21	5	614	CLA	CBD-CGD-O2D-CED
21	6	603	CLA	CBD-CGD-O2D-CED
21	6	605	CLA	CBD-CGD-O2D-CED
21	A	1101	CLA	O1A-CGA-O2A-C1
21	A	1112	CLA	O1A-CGA-O2A-C1
21	A	1122	CLA	O1A-CGA-O2A-C1
21	B	1023	CLA	O1A-CGA-O2A-C1
21	B	1201	CLA	O1A-CGA-O2A-C1
21	B	1211	CLA	O1A-CGA-O2A-C1
21	B	1227	CLA	O1A-CGA-O2A-C1
21	F	1301	CLA	O1A-CGA-O2A-C1
21	1	603	CLA	O1A-CGA-O2A-C1
21	1	606	CLA	O1A-CGA-O2A-C1
21	1	608	CLA	O1A-CGA-O2A-C1
21	2	612	CLA	O1A-CGA-O2A-C1
21	3	603	CLA	O1A-CGA-O2A-C1
21	4	603	CLA	O1A-CGA-O2A-C1
21	4	607	CLA	O1A-CGA-O2A-C1
21	4	612	CLA	O1A-CGA-O2A-C1
21	5	606	CLA	O1A-CGA-O2A-C1
21	5	608	CLA	O1A-CGA-O2A-C1
21	5	614	CLA	O1A-CGA-O2A-C1
21	6	607	CLA	O1A-CGA-O2A-C1
21	6	612	CLA	O1A-CGA-O2A-C1
29	5	804	3PH	O32-C31-O31-C3
31	1	804	LMG	O10-C28-O8-C9
31	4	803	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
31	6	802	LMG	O10-C28-O8-C9
32	5	805	4RF	O17-C16-O18-C19
37	3	806	SQD	O10-C23-O48-C46
21	B	1214	CLA	O1D-CGD-O2D-CED
21	B	1216	CLA	O1D-CGD-O2D-CED
21	B	1236	CLA	O1D-CGD-O2D-CED
21	G	1602	CLA	O1D-CGD-O2D-CED
21	G	1603	CLA	O1D-CGD-O2D-CED
21	K	1403	CLA	O1D-CGD-O2D-CED
21	1	607	CLA	O1D-CGD-O2D-CED
21	1	611	CLA	O1D-CGD-O2D-CED
21	2	603	CLA	O1D-CGD-O2D-CED
21	3	613	CLA	O1D-CGD-O2D-CED
21	5	604	CLA	O1D-CGD-O2D-CED
21	6	613	CLA	O1D-CGD-O2D-CED
21	A	1120	CLA	O1D-CGD-O2D-CED
21	A	1123	CLA	O1D-CGD-O2D-CED
21	A	1124	CLA	O1D-CGD-O2D-CED
21	B	1212	CLA	O1D-CGD-O2D-CED
21	B	1234	CLA	O1D-CGD-O2D-CED
21	B	1239	CLA	O1D-CGD-O2D-CED
21	J	1901	CLA	O1D-CGD-O2D-CED
21	2	601	CLA	O1D-CGD-O2D-CED
21	4	605	CLA	O1D-CGD-O2D-CED
33	6	804	PTY	C31-C30-O4-C1
21	A	1013	CLA	CBD-CGD-O2D-CED
21	A	1135	CLA	CBD-CGD-O2D-CED
21	3	607	CLA	CBD-CGD-O2D-CED
21	A	1117	CLA	O1D-CGD-O2D-CED
21	B	1237	CLA	O1D-CGD-O2D-CED
21	1	605	CLA	O1D-CGD-O2D-CED
21	3	601	CLA	O1D-CGD-O2D-CED
21	4	603	CLA	O1D-CGD-O2D-CED
21	5	605	CLA	O1D-CGD-O2D-CED
25	1	802	LHG	O9-C7-O7-C5
25	2	801	LHG	O9-C7-O7-C5
25	2	802	LHG	O9-C7-O7-C5
25	2	803	LHG	O9-C7-O7-C5
25	6	801	LHG	O9-C7-O7-C5
28	B	5002	DGD	O1B-C1B-O2G-C2G
28	2	806	DGD	O1B-C1B-O2G-C2G
28	3	805	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
29	5	807	3PH	O22-C21-O21-C2
31	4	803	LMG	O9-C10-O7-C8
33	5	803	PTY	O10-C8-O7-C6
21	3	612	CLA	O1A-CGA-O2A-C1
21	H	1702	CLA	CBA-CGA-O2A-C1
21	1	607	CLA	CBA-CGA-O2A-C1
21	4	608	CLA	CBA-CGA-O2A-C1
21	1	607	CLA	O1A-CGA-O2A-C1
21	A	1119	CLA	O1D-CGD-O2D-CED
21	6	607	CLA	O1D-CGD-O2D-CED
20	A	1011	CL0	C3-C5-C6-C7
21	A	1012	CLA	C3-C5-C6-C7
21	A	1101	CLA	C3-C5-C6-C7
21	A	1103	CLA	C3-C5-C6-C7
21	A	1111	CLA	C3-C5-C6-C7
21	A	1112	CLA	C3-C5-C6-C7
21	A	1116	CLA	C3-C5-C6-C7
21	A	1129	CLA	C3-C5-C6-C7
21	A	1133	CLA	C3-C5-C6-C7
21	A	1137	CLA	C3-C5-C6-C7
21	A	1140	CLA	C3-C5-C6-C7
21	B	1205	CLA	C3-C5-C6-C7
21	B	1206	CLA	C3-C5-C6-C7
21	B	1214	CLA	C3-C5-C6-C7
21	B	1220	CLA	C3-C5-C6-C7
21	B	1221	CLA	C3-C5-C6-C7
21	B	1229	CLA	C3-C5-C6-C7
21	B	1232	CLA	C3-C5-C6-C7
21	B	1236	CLA	C3-C5-C6-C7
21	B	1237	CLA	C3-C5-C6-C7
21	1	605	CLA	C3-C5-C6-C7
21	1	611	CLA	C3-C5-C6-C7
21	1	615	CLA	C3-C5-C6-C7
21	2	601	CLA	C3-C5-C6-C7
21	3	603	CLA	C3-C5-C6-C7
21	3	615	CLA	C3-C5-C6-C7
21	4	603	CLA	C3-C5-C6-C7
21	4	605	CLA	C3-C5-C6-C7
21	4	609	CLA	C3-C5-C6-C7
21	4	612	CLA	C3-C5-C6-C7
21	5	607	CLA	C3-C5-C6-C7
21	5	608	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	6	603	CLA	C3-C5-C6-C7
21	A	1104	CLA	CBA-CGA-O2A-C1
21	A	1127	CLA	CBA-CGA-O2A-C1
21	B	1201	CLA	CBA-CGA-O2A-C1
21	B	1214	CLA	CBA-CGA-O2A-C1
21	B	1221	CLA	CBA-CGA-O2A-C1
21	B	1222	CLA	CBA-CGA-O2A-C1
21	B	1227	CLA	CBA-CGA-O2A-C1
21	O	1803	CLA	CBA-CGA-O2A-C1
21	1	603	CLA	CBA-CGA-O2A-C1
21	1	608	CLA	CBA-CGA-O2A-C1
21	2	604	CLA	CBA-CGA-O2A-C1
21	2	605	CLA	CBA-CGA-O2A-C1
21	2	612	CLA	CBA-CGA-O2A-C1
21	4	602	CLA	CBA-CGA-O2A-C1
21	4	603	CLA	CBA-CGA-O2A-C1
21	4	607	CLA	CBA-CGA-O2A-C1
21	4	612	CLA	CBA-CGA-O2A-C1
21	5	606	CLA	CBA-CGA-O2A-C1
21	6	607	CLA	CBA-CGA-O2A-C1
21	6	612	CLA	CBA-CGA-O2A-C1
29	5	804	3PH	C32-C31-O31-C3
31	1	804	LMG	C29-C28-O8-C9
31	6	802	LMG	C29-C28-O8-C9
21	G	1601	CLA	C2-C1-O2A-CGA
25	2	801	LHG	C8-C7-O7-C5
25	2	803	LHG	C8-C7-O7-C5
33	1	805	PTY	C11-C8-O7-C6
37	3	806	SQD	C8-C7-O47-C45
21	A	1118	CLA	O1D-CGD-O2D-CED
21	B	1217	CLA	O1D-CGD-O2D-CED
21	3	615	CLA	O1D-CGD-O2D-CED
21	A	1125	CLA	CBD-CGD-O2D-CED
21	5	608	CLA	CBD-CGD-O2D-CED
21	H	1702	CLA	O1A-CGA-O2A-C1
21	4	608	CLA	O1A-CGA-O2A-C1
21	1	603	CLA	C4-C3-C5-C6
21	1	605	CLA	C4-C3-C5-C6
21	4	604	CLA	C4-C3-C5-C6
21	A	1013	CLA	C2-C3-C5-C6
21	A	1109	CLA	C2-C3-C5-C6
21	A	1132	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	B	1023	CLA	C2-C3-C5-C6
21	B	1218	CLA	C2-C3-C5-C6
21	B	1230	CLA	C2-C3-C5-C6
21	1	603	CLA	C2-C3-C5-C6
21	1	605	CLA	C2-C3-C5-C6
21	4	604	CLA	C2-C3-C5-C6
20	A	1011	CL0	CBD-CGD-O2D-CED
21	A	1128	CLA	CBD-CGD-O2D-CED
21	B	1202	CLA	CBD-CGD-O2D-CED
21	A	1105	CLA	C2A-CAA-CBA-CGA
21	A	1106	CLA	C2A-CAA-CBA-CGA
21	A	1123	CLA	C2A-CAA-CBA-CGA
21	A	1133	CLA	C2A-CAA-CBA-CGA
21	F	1301	CLA	C2A-CAA-CBA-CGA
21	J	1901	CLA	C2A-CAA-CBA-CGA
21	3	606	CLA	C2A-CAA-CBA-CGA
21	5	614	CLA	C2A-CAA-CBA-CGA
21	6	606	CLA	C2A-CAA-CBA-CGA
21	6	607	CLA	C2A-CAA-CBA-CGA
36	4	610	CHL	C2A-CAA-CBA-CGA
21	A	1126	CLA	O1A-CGA-O2A-C1
21	4	605	CLA	O1A-CGA-O2A-C1
21	A	1107	CLA	O1D-CGD-O2D-CED
21	2	612	CLA	O1D-CGD-O2D-CED
28	B	5002	DGD	C8A-C9A-CAA-CBA
31	F	5002	LMG	C35-C36-C37-C38
31	F	5002	LMG	C38-C39-C40-C41
31	F	5002	LMG	C41-C42-C43-C44
31	2	804	LMG	C35-C36-C37-C38
31	2	804	LMG	C38-C39-C40-C41
31	2	804	LMG	C41-C42-C43-C44
31	3	803	LMG	C17-C18-C19-C20
31	3	803	LMG	C20-C21-C22-C23
31	3	803	LMG	C23-C24-C25-C26
31	4	802	LMG	C17-C18-C19-C20
31	4	802	LMG	C20-C21-C22-C23
21	6	609	CLA	O1A-CGA-O2A-C1
21	A	1105	CLA	C3-C5-C6-C7
21	A	1106	CLA	C3-C5-C6-C7
21	A	1113	CLA	C3-C5-C6-C7
21	A	1128	CLA	C3-C5-C6-C7
21	A	1136	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	A	1139	CLA	C3-C5-C6-C7
21	B	1219	CLA	C3-C5-C6-C7
21	B	1224	CLA	C3-C5-C6-C7
21	1	612	CLA	C3-C5-C6-C7
21	3	608	CLA	C3-C5-C6-C7
21	6	604	CLA	C3-C5-C6-C7
21	6	612	CLA	C3-C5-C6-C7
21	A	1101	CLA	CBA-CGA-O2A-C1
21	A	1112	CLA	CBA-CGA-O2A-C1
21	A	1122	CLA	CBA-CGA-O2A-C1
21	A	1126	CLA	CBA-CGA-O2A-C1
21	B	1023	CLA	CBA-CGA-O2A-C1
21	B	1208	CLA	CBA-CGA-O2A-C1
21	B	1211	CLA	CBA-CGA-O2A-C1
21	B	1217	CLA	CBA-CGA-O2A-C1
21	B	1231	CLA	CBA-CGA-O2A-C1
21	F	1301	CLA	CBA-CGA-O2A-C1
21	F	1302	CLA	CBA-CGA-O2A-C1
21	L	1501	CLA	CBA-CGA-O2A-C1
21	1	606	CLA	CBA-CGA-O2A-C1
21	1	612	CLA	CBA-CGA-O2A-C1
21	3	603	CLA	CBA-CGA-O2A-C1
21	3	606	CLA	CBA-CGA-O2A-C1
21	3	607	CLA	CBA-CGA-O2A-C1
21	3	612	CLA	CBA-CGA-O2A-C1
21	4	615	CLA	CBA-CGA-O2A-C1
21	5	608	CLA	CBA-CGA-O2A-C1
21	5	614	CLA	CBA-CGA-O2A-C1
21	6	601	CLA	CBA-CGA-O2A-C1
21	6	605	CLA	CBA-CGA-O2A-C1
31	4	803	LMG	C29-C28-O8-C9
32	5	805	4RF	C15-C16-O18-C19
37	3	806	SQD	C24-C23-O48-C46
21	B	1218	CLA	O1D-CGD-O2D-CED
21	B	1235	CLA	O1D-CGD-O2D-CED
21	4	609	CLA	O1D-CGD-O2D-CED
21	4	604	CLA	CBD-CGD-O2D-CED
21	A	1132	CLA	O1D-CGD-O2D-CED
21	A	1134	CLA	O1D-CGD-O2D-CED
21	A	1141	CLA	O1D-CGD-O2D-CED
21	F	1301	CLA	O1D-CGD-O2D-CED
21	K	1401	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	L	1501	CLA	O1D-CGD-O2D-CED
21	1	604	CLA	O1D-CGD-O2D-CED
21	3	603	CLA	O1D-CGD-O2D-CED
21	4	601	CLA	O1D-CGD-O2D-CED
21	6	612	CLA	O1D-CGD-O2D-CED
31	3	802	LMG	O9-C10-O7-C8
33	6	804	PTY	O10-C8-O7-C6
27	A	5004	LMU	C4B-C5B-C6B-O6B
27	A	5005	LMU	C4B-C5B-C6B-O6B
27	B	5004	LMU	C4B-C5B-C6B-O6B
21	A	1013	CLA	O1A-CGA-O2A-C1
21	A	1118	CLA	O1A-CGA-O2A-C1
21	B	1021	CLA	O1A-CGA-O2A-C1
21	B	1208	CLA	O1A-CGA-O2A-C1
21	B	1222	CLA	O1A-CGA-O2A-C1
21	B	1231	CLA	O1A-CGA-O2A-C1
21	1	612	CLA	O1A-CGA-O2A-C1
21	4	602	CLA	O1A-CGA-O2A-C1
21	4	606	CLA	O1A-CGA-O2A-C1
21	4	615	CLA	O1A-CGA-O2A-C1
21	A	1105	CLA	O1D-CGD-O2D-CED
24	A	4005	BCR	C13-C14-C15-C16
24	H	4001	BCR	C9-C10-C11-C12
24	I	4002	BCR	C19-C20-C21-C22
24	L	4002	BCR	C9-C10-C11-C12
24	O	4001	BCR	C9-C10-C11-C12
24	2	503	BCR	C13-C14-C15-C16
24	4	503	BCR	C13-C14-C15-C16
33	O	5002	PTY	C11-C8-O7-C6
21	A	1130	CLA	CBD-CGD-O2D-CED
21	B	1240	CLA	CBD-CGD-O2D-CED
21	4	612	CLA	CBD-CGD-O2D-CED
21	5	612	CLA	O1D-CGD-O2D-CED
25	A	5001	LHG	O2-C2-C3-O3
25	A	5002	LHG	O2-C2-C3-O3
25	1	802	LHG	O2-C2-C3-O3
25	2	803	LHG	O2-C2-C3-O3
21	A	1115	CLA	C3-C5-C6-C7
21	B	1204	CLA	C3-C5-C6-C7
21	B	1228	CLA	C3-C5-C6-C7
21	B	1230	CLA	C3-C5-C6-C7
21	L	1501	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	1	604	CLA	C3-C5-C6-C7
21	3	605	CLA	C3-C5-C6-C7
21	3	607	CLA	C3-C5-C6-C7
21	A	1013	CLA	CBA-CGA-O2A-C1
21	B	1021	CLA	CBA-CGA-O2A-C1
21	B	1229	CLA	CBA-CGA-O2A-C1
21	B	1237	CLA	CBA-CGA-O2A-C1
21	4	605	CLA	CBA-CGA-O2A-C1
28	3	804	DGD	C2A-C1A-O1G-C1G
32	5	805	4RF	C12-C13-C14-C15
33	O	5002	PTY	O10-C8-O7-C6
21	A	1104	CLA	O1A-CGA-O2A-C1
21	B	1215	CLA	O1A-CGA-O2A-C1
21	B	1217	CLA	O1A-CGA-O2A-C1
21	B	1237	CLA	O1A-CGA-O2A-C1
21	2	604	CLA	O1A-CGA-O2A-C1
21	A	1103	CLA	O1D-CGD-O2D-CED
21	A	1140	CLA	O1D-CGD-O2D-CED
21	B	1201	CLA	O1D-CGD-O2D-CED
21	B	1221	CLA	O1D-CGD-O2D-CED
25	B	5001	LHG	C8-C7-O7-C5
21	6	608	CLA	CBA-CGA-O2A-C1
21	B	1220	CLA	CBD-CGD-O2D-CED
21	B	1231	CLA	CBD-CGD-O2D-CED
21	1	606	CLA	CBD-CGD-O2D-CED
21	3	606	CLA	CBD-CGD-O2D-CED
21	5	601	CLA	O1D-CGD-O2D-CED
21	B	1225	CLA	C3-C5-C6-C7
21	L	1502	CLA	C3-C5-C6-C7
21	2	615	CLA	C3-C5-C6-C7
21	A	1118	CLA	CBA-CGA-O2A-C1
21	B	1215	CLA	CBA-CGA-O2A-C1
21	4	606	CLA	CBA-CGA-O2A-C1
25	B	5001	LHG	O9-C7-O7-C5
21	F	1302	CLA	O1A-CGA-O2A-C1
21	L	1501	CLA	O1A-CGA-O2A-C1
21	3	607	CLA	O1A-CGA-O2A-C1
21	6	601	CLA	O1A-CGA-O2A-C1
21	6	605	CLA	O1A-CGA-O2A-C1
21	A	1115	CLA	C4-C3-C5-C6
21	A	1139	CLA	C4-C3-C5-C6
21	B	1219	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	A	1115	CLA	C2-C3-C5-C6
21	A	1139	CLA	C2-C3-C5-C6
21	B	1219	CLA	C2-C3-C5-C6
25	B	5001	LHG	C7-C8-C9-C10
21	A	1013	CLA	C2A-CAA-CBA-CGA
21	A	1109	CLA	C2A-CAA-CBA-CGA
21	B	1201	CLA	C2A-CAA-CBA-CGA
21	B	1215	CLA	C2A-CAA-CBA-CGA
21	B	1237	CLA	C2A-CAA-CBA-CGA
21	3	603	CLA	C2A-CAA-CBA-CGA
36	5	609	CHL	C2A-CAA-CBA-CGA
21	A	1108	CLA	O1D-CGD-O2D-CED
21	A	1137	CLA	O1D-CGD-O2D-CED
21	B	1230	CLA	O1D-CGD-O2D-CED
27	A	5004	LMU	O5B-C5B-C6B-O6B
27	A	5005	LMU	O5B-C5B-C6B-O6B
27	B	5004	LMU	O5B-C5B-C6B-O6B
21	B	1229	CLA	O1A-CGA-O2A-C1
21	3	606	CLA	O1A-CGA-O2A-C1
28	3	804	DGD	O1A-C1A-O1G-C1G
21	B	1211	CLA	O1D-CGD-O2D-CED
21	B	1213	CLA	O1D-CGD-O2D-CED
21	A	1124	CLA	CBA-CGA-O2A-C1
33	4	804	PTY	C31-C30-O4-C1
21	F	1301	CLA	C2-C1-O2A-CGA
21	A	1129	CLA	CBD-CGD-O2D-CED
21	A	1104	CLA	O1D-CGD-O2D-CED
21	A	1133	CLA	O1D-CGD-O2D-CED
21	1	612	CLA	O1D-CGD-O2D-CED
21	4	602	CLA	O1D-CGD-O2D-CED
21	6	605	CLA	O1D-CGD-O2D-CED
21	6	606	CLA	O1D-CGD-O2D-CED
28	3	804	DGD	C2B-C1B-O2G-C2G
33	5	803	PTY	C35-C36-C37-C38
21	A	1102	CLA	O1D-CGD-O2D-CED
21	B	1205	CLA	O1D-CGD-O2D-CED
21	B	1228	CLA	O1D-CGD-O2D-CED
21	H	1702	CLA	O1D-CGD-O2D-CED
25	F	5001	LHG	C1-C2-C3-O3
25	2	803	LHG	C1-C2-C3-O3
25	5	802	LHG	C1-C2-C3-O3
21	A	1124	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	A	1130	CLA	O1A-CGA-O2A-C1
21	B	1230	CLA	O1A-CGA-O2A-C1
21	B	1204	CLA	O1D-CGD-O2D-CED
21	K	1402	CLA	O1D-CGD-O2D-CED
21	A	1109	CLA	CBA-CGA-O2A-C1
21	A	1114	CLA	CBA-CGA-O2A-C1
21	A	1120	CLA	CBA-CGA-O2A-C1
21	A	1130	CLA	CBA-CGA-O2A-C1
21	A	1132	CLA	CBA-CGA-O2A-C1
21	A	1139	CLA	CBA-CGA-O2A-C1
21	A	1140	CLA	CBA-CGA-O2A-C1
21	B	1206	CLA	CBA-CGA-O2A-C1
21	B	1213	CLA	CBA-CGA-O2A-C1
21	B	1226	CLA	CBA-CGA-O2A-C1
21	B	1228	CLA	CBA-CGA-O2A-C1
21	B	1230	CLA	CBA-CGA-O2A-C1
21	B	1232	CLA	CBA-CGA-O2A-C1
21	B	1240	CLA	CBA-CGA-O2A-C1
21	L	1503	CLA	CBA-CGA-O2A-C1
21	1	604	CLA	CBA-CGA-O2A-C1
21	2	606	CLA	CBA-CGA-O2A-C1
21	2	608	CLA	CBA-CGA-O2A-C1
21	2	615	CLA	CBA-CGA-O2A-C1
21	3	608	CLA	CBA-CGA-O2A-C1
21	4	604	CLA	CBA-CGA-O2A-C1
21	4	609	CLA	CBA-CGA-O2A-C1
21	6	604	CLA	CBA-CGA-O2A-C1
28	2	806	DGD	C2A-C1A-O1G-C1G
29	B	5003	3PH	C32-C31-O31-C3
33	L	5003	PTY	C31-C30-O4-C1
25	A	5002	LHG	C26-C27-C28-C29
24	A	4002	BCR	C9-C10-C11-C12
24	1	504	BCR	C13-C14-C15-C16
21	2	612	CLA	C5-C6-C7-C8
27	A	5005	LMU	O5'-C5'-C6'-O6'
21	B	1232	CLA	O1A-CGA-O2A-C1
21	6	608	CLA	O1A-CGA-O2A-C1
21	A	1012	CLA	C5-C6-C7-C8
21	A	1102	CLA	C8-C10-C11-C12
21	A	1103	CLA	C10-C11-C12-C13
21	A	1113	CLA	C15-C16-C17-C18
21	A	1121	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	A	1133	CLA	C13-C15-C16-C17
21	B	1202	CLA	C8-C10-C11-C12
21	B	1211	CLA	C15-C16-C17-C18
21	B	1218	CLA	C5-C6-C7-C8
21	B	1225	CLA	C10-C11-C12-C13
21	B	1237	CLA	C13-C15-C16-C17
21	L	1501	CLA	C13-C15-C16-C17
21	3	603	CLA	C13-C15-C16-C17
21	5	614	CLA	C8-C10-C11-C12
21	A	1125	CLA	C3-C5-C6-C7
21	A	1141	CLA	C3-C5-C6-C7
25	5	802	LHG	C23-C24-C25-C26
32	5	805	4RF	C13-C14-C15-C16
28	3	804	DGD	C2D-C1D-O3G-C3G
28	3	805	DGD	C2D-C1D-O3G-C3G
31	1	804	LMG	C2-C1-O1-C7
31	3	802	LMG	C2-C1-O1-C7
31	6	802	LMG	C2-C1-O1-C7
25	1	802	LHG	O7-C5-C6-O8
21	A	1132	CLA	O1A-CGA-O2A-C1
21	B	1206	CLA	O1A-CGA-O2A-C1
21	3	608	CLA	O1A-CGA-O2A-C1
28	2	806	DGD	O1A-C1A-O1G-C1G
29	B	5003	3PH	O32-C31-O31-C3
21	2	612	CLA	C4-C3-C5-C6
27	B	5004	LMU	C4'-C5'-C6'-O6'
21	A	1112	CLA	C11-C12-C13-C14
21	A	1126	CLA	C14-C13-C15-C16
21	A	1132	CLA	C14-C13-C15-C16
21	A	1137	CLA	C11-C10-C8-C9
21	A	1138	CLA	C6-C7-C8-C9
21	B	1202	CLA	C6-C7-C8-C9
21	B	1207	CLA	C14-C13-C15-C16
21	B	1225	CLA	C11-C12-C13-C14
21	H	1701	CLA	C11-C10-C8-C9
21	L	1501	CLA	C11-C10-C8-C9
21	L	1501	CLA	C14-C13-C15-C16
21	1	601	CLA	C6-C7-C8-C9
21	2	604	CLA	C14-C13-C15-C16
21	2	612	CLA	C11-C12-C13-C14
21	2	615	CLA	C14-C13-C15-C16
21	3	612	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	A	2001	PQN	C21-C22-C23-C24
22	B	2002	PQN	C21-C22-C23-C24
36	3	604	CHL	C11-C12-C13-C14
36	5	609	CHL	C11-C12-C13-C14
21	A	1012	CLA	O1D-CGD-O2D-CED
21	A	1113	CLA	O1D-CGD-O2D-CED
21	B	1222	CLA	O1D-CGD-O2D-CED
21	B	1227	CLA	O1D-CGD-O2D-CED
21	L	1502	CLA	O1D-CGD-O2D-CED
21	5	614	CLA	O1D-CGD-O2D-CED
21	A	1109	CLA	C10-C11-C12-C13
21	L	1502	CLA	C13-C15-C16-C17
21	A	1108	CLA	C2A-CAA-CBA-CGA
21	A	1119	CLA	C2A-CAA-CBA-CGA
21	B	1232	CLA	C2A-CAA-CBA-CGA
21	1	604	CLA	C2A-CAA-CBA-CGA
21	1	613	CLA	C2A-CAA-CBA-CGA
21	5	612	CLA	C2A-CAA-CBA-CGA
24	A	4001	BCR	C11-C12-C13-C35
24	A	4001	BCR	C37-C22-C23-C24
24	A	4006	BCR	C37-C22-C23-C24
24	B	4003	BCR	C7-C8-C9-C34
24	B	4003	BCR	C37-C22-C23-C24
24	B	4006	BCR	C7-C8-C9-C34
24	F	4001	BCR	C11-C12-C13-C35
24	G	4001	BCR	C37-C22-C23-C24
24	H	4001	BCR	C36-C18-C19-C20
24	H	4001	BCR	C37-C22-C23-C24
24	I	4001	BCR	C36-C18-C19-C20
24	1	504	BCR	C11-C12-C13-C35
35	1	502	XAT	C7-C8-C9-C19
24	A	4001	BCR	C21-C22-C23-C24
24	A	4006	BCR	C7-C8-C9-C10
24	A	4006	BCR	C21-C22-C23-C24
24	B	4001	BCR	C7-C8-C9-C10
24	B	4003	BCR	C21-C22-C23-C24
24	B	4005	BCR	C17-C18-C19-C20
24	B	4006	BCR	C7-C8-C9-C10
24	F	4001	BCR	C11-C12-C13-C14
24	G	4001	BCR	C21-C22-C23-C24
24	H	4001	BCR	C17-C18-C19-C20
24	I	4001	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
35	1	502	XAT	C7-C8-C9-C10
27	B	5004	LMU	O5'-C5'-C6'-O6'
25	6	801	LHG	C23-C24-C25-C26
29	B	5003	3PH	C21-C22-C23-C24
21	A	1109	CLA	O1A-CGA-O2A-C1
21	A	1114	CLA	O1A-CGA-O2A-C1
21	1	604	CLA	O1A-CGA-O2A-C1
21	2	608	CLA	O1A-CGA-O2A-C1
21	2	615	CLA	O1A-CGA-O2A-C1
21	6	604	CLA	O1A-CGA-O2A-C1
21	B	1228	CLA	C10-C11-C12-C13
21	1	601	CLA	C10-C11-C12-C13
21	2	612	CLA	C10-C11-C12-C13
21	5	614	CLA	C13-C15-C16-C17
21	2	604	CLA	O1D-CGD-O2D-CED
21	5	602	CLA	CBA-CGA-O2A-C1
21	B	1238	CLA	O1D-CGD-O2D-CED
21	3	612	CLA	O1D-CGD-O2D-CED
21	A	1128	CLA	CBA-CGA-O2A-C1
21	A	1134	CLA	CBA-CGA-O2A-C1
21	A	1106	CLA	C5-C6-C7-C8
21	A	1112	CLA	C15-C16-C17-C18
21	A	1114	CLA	C5-C6-C7-C8
21	A	1119	CLA	C5-C6-C7-C8
21	A	1125	CLA	C5-C6-C7-C8
21	A	1131	CLA	C13-C15-C16-C17
21	A	1138	CLA	C5-C6-C7-C8
21	B	1210	CLA	C8-C10-C11-C12
21	B	1222	CLA	C8-C10-C11-C12
21	B	1225	CLA	C13-C15-C16-C17
21	B	1226	CLA	C10-C11-C12-C13
21	B	1230	CLA	C8-C10-C11-C12
21	B	1238	CLA	C8-C10-C11-C12
21	1	601	CLA	C8-C10-C11-C12
21	1	605	CLA	C13-C15-C16-C17
21	1	615	CLA	C8-C10-C11-C12
21	3	608	CLA	C15-C16-C17-C18
21	3	615	CLA	C5-C6-C7-C8
21	5	603	CLA	C8-C10-C11-C12
21	5	614	CLA	C5-C6-C7-C8
25	A	5002	LHG	C7-C8-C9-C10
25	F	5001	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
25	F	5001	LHG	C23-C24-C25-C26
32	5	805	4RF	C41-C43-C44-C45
21	A	1012	CLA	C13-C15-C16-C17
21	A	1013	CLA	C10-C11-C12-C13
21	A	1107	CLA	C10-C11-C12-C13
21	A	1112	CLA	C8-C10-C11-C12
21	A	1117	CLA	C15-C16-C17-C18
21	A	1119	CLA	C15-C16-C17-C18
21	A	1120	CLA	C5-C6-C7-C8
21	A	1122	CLA	C10-C11-C12-C13
21	A	1125	CLA	C10-C11-C12-C13
21	A	1141	CLA	C5-C6-C7-C8
21	B	1021	CLA	C5-C6-C7-C8
21	B	1207	CLA	C10-C11-C12-C13
21	B	1208	CLA	C5-C6-C7-C8
21	B	1214	CLA	C10-C11-C12-C13
21	B	1221	CLA	C15-C16-C17-C18
21	B	1222	CLA	C13-C15-C16-C17
21	B	1227	CLA	C13-C15-C16-C17
21	B	1234	CLA	C5-C6-C7-C8
21	H	1701	CLA	C8-C10-C11-C12
21	H	1701	CLA	C10-C11-C12-C13
21	L	1501	CLA	C15-C16-C17-C18
21	1	605	CLA	C10-C11-C12-C13
21	1	615	CLA	C10-C11-C12-C13
21	2	604	CLA	C13-C15-C16-C17
21	2	604	CLA	C15-C16-C17-C18
21	3	611	CLA	C10-C11-C12-C13
21	3	612	CLA	C5-C6-C7-C8
21	4	603	CLA	C8-C10-C11-C12
21	4	609	CLA	C5-C6-C7-C8
21	6	601	CLA	C8-C10-C11-C12
21	6	603	CLA	C5-C6-C7-C8
21	6	605	CLA	C15-C16-C17-C18
21	6	607	CLA	C10-C11-C12-C13
22	B	2002	PQN	C25-C26-C27-C28
21	6	603	CLA	O1D-CGD-O2D-CED
21	A	1140	CLA	O1A-CGA-O2A-C1
21	B	1228	CLA	O1A-CGA-O2A-C1
21	B	1240	CLA	O1A-CGA-O2A-C1
25	A	5001	LHG	C23-C24-C25-C26
25	1	802	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
25	2	801	LHG	C23-C24-C25-C26
25	2	802	LHG	C23-C24-C25-C26
25	5	801	LHG	C23-C24-C25-C26
33	3	807	PTY	C8-C11-C12-C13
33	5	803	PTY	C30-C31-C32-C33
21	A	1013	CLA	O1D-CGD-O2D-CED
21	A	1106	CLA	O1D-CGD-O2D-CED
21	A	1136	CLA	O1D-CGD-O2D-CED
21	A	1109	CLA	C15-C16-C17-C18
21	A	1111	CLA	C10-C11-C12-C13
21	A	1116	CLA	C5-C6-C7-C8
21	A	1132	CLA	C13-C15-C16-C17
21	A	1138	CLA	C13-C15-C16-C17
21	A	1139	CLA	C13-C15-C16-C17
21	B	1204	CLA	C15-C16-C17-C18
21	B	1213	CLA	C10-C11-C12-C13
21	B	1226	CLA	C5-C6-C7-C8
21	B	1239	CLA	C5-C6-C7-C8
21	1	604	CLA	C15-C16-C17-C18
21	2	615	CLA	C13-C15-C16-C17
21	B	1223	CLA	O1D-CGD-O2D-CED
28	3	804	DGD	O1B-C1B-O2G-C2G
21	A	1012	CLA	C2-C1-O2A-CGA
21	A	1013	CLA	C2-C1-O2A-CGA
21	A	1112	CLA	C2-C1-O2A-CGA
21	A	1118	CLA	C2-C1-O2A-CGA
21	A	1119	CLA	C2-C1-O2A-CGA
21	A	1129	CLA	C2-C1-O2A-CGA
21	B	1021	CLA	C2-C1-O2A-CGA
21	B	1202	CLA	C2-C1-O2A-CGA
21	B	1211	CLA	C2-C1-O2A-CGA
21	B	1214	CLA	C2-C1-O2A-CGA
21	B	1230	CLA	C2-C1-O2A-CGA
21	B	1232	CLA	C2-C1-O2A-CGA
21	J	1901	CLA	C2-C1-O2A-CGA
21	K	1402	CLA	C2-C1-O2A-CGA
21	L	1503	CLA	C2-C1-O2A-CGA
21	1	611	CLA	C2-C1-O2A-CGA
21	2	602	CLA	C2-C1-O2A-CGA
21	3	610	CLA	C2-C1-O2A-CGA
21	3	612	CLA	C2-C1-O2A-CGA
21	4	606	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
21	5	608	CLA	C2-C1-O2A-CGA
21	6	602	CLA	C2-C1-O2A-CGA
21	6	605	CLA	C2-C1-O2A-CGA
21	6	607	CLA	C2-C1-O2A-CGA
21	A	1140	CLA	C5-C6-C7-C8
21	B	1204	CLA	C13-C15-C16-C17
21	B	1210	CLA	C10-C11-C12-C13
21	B	1218	CLA	C8-C10-C11-C12
21	B	1222	CLA	C5-C6-C7-C8
21	B	1231	CLA	C5-C6-C7-C8
21	B	1238	CLA	C15-C16-C17-C18
21	3	607	CLA	C8-C10-C11-C12
21	4	601	CLA	C8-C10-C11-C12
22	A	2001	PQN	C23-C25-C26-C27
37	6	803	SQD	C8-C7-O47-C45
21	A	1125	CLA	C15-C16-C17-C18
21	2	603	CLA	C10-C11-C12-C13
21	3	608	CLA	C8-C10-C11-C12
21	3	611	CLA	C8-C10-C11-C12
22	B	2002	PQN	C18-C20-C21-C22
22	B	2002	PQN	C20-C21-C22-C23
21	A	1012	CLA	C11-C12-C13-C15
21	1	611	CLA	C11-C12-C13-C15
21	2	604	CLA	C12-C13-C15-C16
21	3	601	CLA	C6-C7-C8-C10
21	5	607	CLA	C11-C10-C8-C7
21	B	1202	CLA	C3-C5-C6-C7
33	4	804	PTY	O30-C30-O4-C1
24	H	4001	BCR	C13-C14-C15-C16
24	1	504	BCR	C9-C10-C11-C12
24	4	503	BCR	C9-C10-C11-C12
21	B	1224	CLA	C2A-CAA-CBA-CGA
21	H	1702	CLA	C2A-CAA-CBA-CGA
21	3	611	CLA	C2A-CAA-CBA-CGA
36	2	613	CHL	C2A-CAA-CBA-CGA
21	A	1135	CLA	O1D-CGD-O2D-CED
21	3	606	CLA	O1D-CGD-O2D-CED
21	3	607	CLA	O1D-CGD-O2D-CED
21	5	608	CLA	O1D-CGD-O2D-CED
21	A	1101	CLA	C8-C10-C11-C12
21	A	1102	CLA	C5-C6-C7-C8
21	A	1105	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	A	1117	CLA	C8-C10-C11-C12
21	A	1123	CLA	C5-C6-C7-C8
21	B	1021	CLA	C13-C15-C16-C17
21	B	1203	CLA	C10-C11-C12-C13
21	B	1219	CLA	C8-C10-C11-C12
21	B	1219	CLA	C13-C15-C16-C17
21	B	1227	CLA	C15-C16-C17-C18
21	B	1235	CLA	C5-C6-C7-C8
21	B	1240	CLA	C15-C16-C17-C18
21	2	603	CLA	C15-C16-C17-C18
21	3	605	CLA	C8-C10-C11-C12
21	6	612	CLA	C8-C10-C11-C12
22	B	2002	PQN	C15-C16-C17-C18
21	A	1120	CLA	O1A-CGA-O2A-C1
21	A	1139	CLA	O1A-CGA-O2A-C1
21	B	1226	CLA	O1A-CGA-O2A-C1
21	L	1503	CLA	O1A-CGA-O2A-C1
21	2	606	CLA	O1A-CGA-O2A-C1
21	4	604	CLA	O1A-CGA-O2A-C1
33	L	5003	PTY	O30-C30-O4-C1
21	B	1205	CLA	C13-C15-C16-C17
21	B	1223	CLA	C5-C6-C7-C8
21	O	1803	CLA	C5-C6-C7-C8
21	1	601	CLA	C5-C6-C7-C8
21	4	605	CLA	C13-C15-C16-C17
21	B	1202	CLA	O1D-CGD-O2D-CED
24	A	4003	BCR	C10-C11-C12-C13
24	B	4001	BCR	C10-C11-C12-C13
24	F	4002	BCR	C10-C11-C12-C13
24	3	504	BCR	C10-C11-C12-C13
35	1	502	XAT	C10-C11-C12-C13
35	3	502	XAT	C30-C31-C32-C33
27	6	805	LMU	O5B-C5B-C6B-O6B
25	2	801	LHG	O2-C2-C3-O3
25	3	801	LHG	O2-C2-C3-O3
21	B	1208	CLA	C3-C5-C6-C7
21	A	1107	CLA	C15-C16-C17-C18
21	A	1113	CLA	C8-C10-C11-C12
21	A	1121	CLA	C5-C6-C7-C8
21	A	1124	CLA	C5-C6-C7-C8
21	A	1124	CLA	C8-C10-C11-C12
21	A	1136	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	B	1206	CLA	C15-C16-C17-C18
21	B	1208	CLA	C10-C11-C12-C13
21	B	1227	CLA	C10-C11-C12-C13
21	L	1502	CLA	C8-C10-C11-C12
21	O	1803	CLA	C10-C11-C12-C13
21	1	605	CLA	C5-C6-C7-C8
21	2	605	CLA	C8-C10-C11-C12
21	3	601	CLA	C8-C10-C11-C12
21	5	605	CLA	C13-C15-C16-C17
21	B	1224	CLA	CBA-CGA-O2A-C1
21	A	1125	CLA	O1D-CGD-O2D-CED
21	B	1213	CLA	O1A-CGA-O2A-C1
21	4	609	CLA	O1A-CGA-O2A-C1
27	A	5005	LMU	O1'-C1-C2-C3
21	A	1109	CLA	C13-C15-C16-C17
21	A	1125	CLA	C8-C10-C11-C12
21	A	1140	CLA	C10-C11-C12-C13
21	B	1212	CLA	C5-C6-C7-C8
21	B	1215	CLA	C10-C11-C12-C13
21	B	1220	CLA	C5-C6-C7-C8
21	B	1231	CLA	C10-C11-C12-C13
21	2	601	CLA	C10-C11-C12-C13
21	3	607	CLA	C5-C6-C7-C8
21	5	607	CLA	C5-C6-C7-C8
21	5	607	CLA	C8-C10-C11-C12
21	6	604	CLA	C8-C10-C11-C12
21	6	605	CLA	C10-C11-C12-C13
21	A	1134	CLA	O1A-CGA-O2A-C1
32	L	5002	4RF	C44-C45-C46-C47
32	5	805	4RF	C24-C25-C26-C27
21	A	1013	CLA	C15-C16-C17-C18
21	A	1113	CLA	C13-C15-C16-C17
21	A	1127	CLA	C15-C16-C17-C18
21	A	1128	CLA	C10-C11-C12-C13
21	A	1131	CLA	C5-C6-C7-C8
21	A	1139	CLA	C8-C10-C11-C12
21	B	1021	CLA	C8-C10-C11-C12
21	B	1204	CLA	C10-C11-C12-C13
21	B	1207	CLA	C15-C16-C17-C18
21	B	1223	CLA	C13-C15-C16-C17
21	B	1227	CLA	C8-C10-C11-C12
21	1	604	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	3	603	CLA	C10-C11-C12-C13
21	4	612	CLA	C15-C16-C17-C18
21	5	604	CLA	C5-C6-C7-C8
36	1	609	CHL	C5-C6-C7-C8
25	A	5001	LHG	C4-O6-P-O3
25	B	5001	LHG	C4-O6-P-O3
25	F	5001	LHG	C4-O6-P-O3
25	1	801	LHG	C4-O6-P-O3
25	2	801	LHG	C4-O6-P-O3
25	2	802	LHG	C3-O3-P-O6
25	2	802	LHG	C4-O6-P-O3
25	2	803	LHG	C4-O6-P-O3
25	4	801	LHG	C4-O6-P-O3
25	6	801	LHG	C3-O3-P-O6
25	6	801	LHG	C4-O6-P-O3
33	L	5003	PTY	C3-O11-P1-O14
33	1	806	PTY	C5-O14-P1-O11
33	4	804	PTY	C3-O11-P1-O14
33	5	803	PTY	C3-O11-P1-O14
33	5	803	PTY	C5-O14-P1-O11
21	A	1120	CLA	C3-C5-C6-C7
21	2	605	CLA	C3-C5-C6-C7
21	A	1106	CLA	CBA-CGA-O2A-C1
21	B	1204	CLA	CBA-CGA-O2A-C1
21	2	602	CLA	CBA-CGA-O2A-C1
21	B	1231	CLA	C8-C10-C11-C12
21	1	612	CLA	C8-C10-C11-C12
27	6	805	LMU	C4B-C5B-C6B-O6B
39	2	808	P3H	C14-C15-C16-C17
25	A	5001	LHG	C1-C2-C3-O3
25	1	801	LHG	C1-C2-C3-O3
25	2	801	LHG	C1-C2-C3-O3
25	3	801	LHG	C1-C2-C3-O3
25	4	801	LHG	C1-C2-C3-O3
25	6	801	LHG	C1-C2-C3-O3
37	6	803	SQD	O49-C7-O47-C45
21	5	604	CLA	C15-C16-C17-C18
20	A	1011	CL0	O1D-CGD-O2D-CED
21	B	1213	CLA	C2A-CAA-CBA-CGA
21	B	1225	CLA	C2A-CAA-CBA-CGA
21	B	1238	CLA	C2A-CAA-CBA-CGA
21	K	1403	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
36	3	604	CHL	C2A-CAA-CBA-CGA
22	A	2001	PQN	C26-C27-C28-C29
21	B	1202	CLA	CBA-CGA-O2A-C1
21	B	1218	CLA	CBA-CGA-O2A-C1
21	A	1102	CLA	C15-C16-C17-C18
21	4	604	CLA	O1D-CGD-O2D-CED
39	5	806	P3H	C28-O27-P24-O23
24	O	4001	BCR	C13-C14-C15-C16
24	4	503	BCR	C19-C20-C21-C22
31	3	803	LMG	C11-C12-C13-C14
25	F	5001	LHG	C8-C7-O7-C5
25	4	801	LHG	C8-C7-O7-C5
21	A	1119	CLA	C10-C11-C12-C13
21	B	1237	CLA	C15-C16-C17-C18
21	3	611	CLA	C5-C6-C7-C8
21	4	604	CLA	C5-C6-C7-C8
24	A	4006	BCR	C11-C10-C9-C34
24	F	4001	BCR	C11-C10-C9-C34
25	A	5001	LHG	C25-C26-C27-C28
25	2	803	LHG	C24-C25-C26-C27
27	A	5004	LMU	C5-C6-C7-C8
21	A	1128	CLA	O1D-CGD-O2D-CED
21	A	1111	CLA	C16-C17-C18-C19
21	B	1208	CLA	C11-C12-C13-C15
21	B	1235	CLA	C11-C12-C13-C15
21	K	1402	CLA	C6-C7-C8-C10
21	2	604	CLA	C16-C17-C18-C19
21	5	603	CLA	C11-C12-C13-C15
21	5	607	CLA	C11-C12-C13-C15
36	4	613	CHL	C11-C12-C13-C14
21	B	1203	CLA	CBA-CGA-O2A-C1
21	G	1601	CLA	CBA-CGA-O2A-C1
25	A	5001	LHG	C11-C12-C13-C14
25	A	5001	LHG	C31-C32-C33-C34
25	F	5001	LHG	C28-C29-C30-C31
25	2	802	LHG	C28-C29-C30-C31
25	2	803	LHG	C11-C12-C13-C14
29	5	807	3PH	C22-C23-C24-C25
29	5	807	3PH	C25-C26-C27-C28
31	3	803	LMG	C30-C31-C32-C33
33	6	804	PTY	C5-C6-O7-C8
25	F	5001	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
25	4	801	LHG	O9-C7-O7-C5
21	B	1221	CLA	C13-C15-C16-C17
25	F	5001	LHG	C34-C35-C36-C37
25	2	801	LHG	C26-C27-C28-C29
25	4	801	LHG	C11-C10-C9-C8
27	B	5004	LMU	C6-C7-C8-C9
29	F	5003	3PH	C22-C23-C24-C25
31	F	5002	LMG	C39-C40-C41-C42
31	2	804	LMG	C36-C37-C38-C39
32	L	5002	4RF	C09-C10-C11-C12
25	5	801	LHG	C13-C14-C15-C16
25	5	801	LHG	C26-C27-C28-C29
21	A	1136	CLA	C15-C16-C17-C18
21	5	608	CLA	C5-C6-C7-C8
25	2	801	LHG	C25-C26-C27-C28
21	B	1218	CLA	C3-C5-C6-C7
21	B	1227	CLA	C3-C5-C6-C7
24	A	4006	BCR	C11-C10-C9-C8
24	F	4001	BCR	C11-C10-C9-C8
25	A	5002	LHG	O7-C5-C6-O8
21	B	1207	CLA	CBA-CGA-O2A-C1
21	2	601	CLA	CBA-CGA-O2A-C1
25	A	5001	LHG	C9-C10-C11-C12
25	2	802	LHG	C13-C14-C15-C16
33	4	804	PTY	C11-C12-C13-C14
21	A	1115	CLA	C8-C10-C11-C12
21	B	1216	CLA	C10-C11-C12-C13
21	K	1402	CLA	C5-C6-C7-C8
21	3	601	CLA	C10-C11-C12-C13
21	4	612	CLA	C13-C15-C16-C17
21	A	1128	CLA	O1A-CGA-O2A-C1
21	B	1202	CLA	O1A-CGA-O2A-C1
20	A	1011	CL0	C16-C17-C18-C19
21	A	1112	CLA	C16-C17-C18-C20
21	A	1117	CLA	C16-C17-C18-C20
21	A	1134	CLA	C6-C7-C8-C9
21	B	1205	CLA	C16-C17-C18-C20
21	B	1225	CLA	C16-C17-C18-C20
21	B	1230	CLA	C16-C17-C18-C20
21	5	614	CLA	C16-C17-C18-C19
21	6	612	CLA	C16-C17-C18-C20
21	A	1130	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	B	1240	CLA	O1D-CGD-O2D-CED
21	A	1117	CLA	C4-C3-C5-C6
21	B	1203	CLA	C4-C3-C5-C6
32	L	5002	4RF	C07-C08-C09-C10
21	A	1117	CLA	C2-C3-C5-C6
21	A	1117	CLA	C11-C10-C8-C9
21	B	1206	CLA	C14-C13-C15-C16
21	B	1214	CLA	C11-C12-C13-C14
21	B	1237	CLA	C11-C10-C8-C9
21	B	1238	CLA	C11-C12-C13-C14
21	1	603	CLA	C11-C10-C8-C9
36	2	609	CHL	C11-C10-C8-C9
36	5	609	CHL	C11-C10-C8-C9
32	L	5002	4RF	C41-C43-C44-C45
39	5	806	P3H	C40-C42-C43-C44
25	A	5001	LHG	C13-C14-C15-C16
25	A	5002	LHG	C30-C31-C32-C33
25	A	5002	LHG	C34-C35-C36-C37
27	A	5005	LMU	C2-C3-C4-C5
21	B	1225	CLA	C15-C16-C17-C18
21	1	611	CLA	C10-C11-C12-C13
21	B	1214	CLA	C2A-CAA-CBA-CGA
21	B	1226	CLA	C2A-CAA-CBA-CGA
21	G	1602	CLA	C2A-CAA-CBA-CGA
24	A	4002	BCR	C11-C12-C13-C35
25	F	5001	LHG	O1-C1-C2-C3
25	1	802	LHG	O1-C1-C2-C3
25	1	803	LHG	O1-C1-C2-C3
25	4	801	LHG	O1-C1-C2-C3
25	5	801	LHG	O1-C1-C2-C3
24	A	4002	BCR	C11-C12-C13-C14
24	B	4003	BCR	C7-C8-C9-C10
24	1	504	BCR	C11-C12-C13-C14
24	2	503	BCR	C17-C18-C19-C20
27	A	5005	LMU	C1-C2-C3-C4
21	2	612	CLA	C3-C5-C6-C7
21	A	1115	CLA	C10-C11-C12-C13
21	1	612	CLA	C5-C6-C7-C8
25	A	5001	LHG	C30-C31-C32-C33
25	B	5001	LHG	C25-C26-C27-C28
25	F	5001	LHG	C25-C26-C27-C28
25	F	5001	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
25	1	801	LHG	C11-C12-C13-C14
29	F	5003	3PH	C36-C37-C38-C39
25	4	801	LHG	C23-C24-C25-C26
25	A	5002	LHG	C17-C18-C19-C20
25	F	5001	LHG	C31-C32-C33-C34
25	1	801	LHG	C32-C33-C34-C35
25	2	802	LHG	C10-C11-C12-C13
29	F	5003	3PH	C38-C39-C3A-C3B
31	4	803	LMG	C29-C30-C31-C32
21	A	1102	CLA	C4B-C3B-CAB-CBB
21	A	1104	CLA	C4B-C3B-CAB-CBB
21	A	1109	CLA	C4B-C3B-CAB-CBB
21	A	1118	CLA	C4B-C3B-CAB-CBB
21	A	1120	CLA	C4B-C3B-CAB-CBB
21	A	1122	CLA	C4B-C3B-CAB-CBB
21	A	1126	CLA	C4B-C3B-CAB-CBB
21	A	1140	CLA	C4B-C3B-CAB-CBB
21	A	1141	CLA	C4B-C3B-CAB-CBB
21	B	1201	CLA	C4B-C3B-CAB-CBB
21	B	1203	CLA	C4B-C3B-CAB-CBB
21	B	1214	CLA	C4B-C3B-CAB-CBB
21	B	1216	CLA	C4B-C3B-CAB-CBB
21	B	1218	CLA	C4B-C3B-CAB-CBB
21	B	1220	CLA	C4B-C3B-CAB-CBB
21	B	1227	CLA	C4B-C3B-CAB-CBB
21	B	1232	CLA	C4B-C3B-CAB-CBB
21	B	1238	CLA	C4B-C3B-CAB-CBB
21	B	1240	CLA	C4B-C3B-CAB-CBB
21	F	1301	CLA	C4B-C3B-CAB-CBB
21	F	1302	CLA	C4B-C3B-CAB-CBB
21	K	1403	CLA	C4B-C3B-CAB-CBB
21	O	1801	CLA	C4B-C3B-CAB-CBB
21	O	1803	CLA	C4B-C3B-CAB-CBB
21	1	602	CLA	C4B-C3B-CAB-CBB
21	1	603	CLA	C4B-C3B-CAB-CBB
21	1	605	CLA	C4B-C3B-CAB-CBB
21	1	613	CLA	C4B-C3B-CAB-CBB
21	2	601	CLA	C4B-C3B-CAB-CBB
21	2	602	CLA	C4B-C3B-CAB-CBB
21	2	605	CLA	C4B-C3B-CAB-CBB
21	3	601	CLA	C4B-C3B-CAB-CBB
21	3	602	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
21	3	614	CLA	C4B-C3B-CAB-CBB
21	3	615	CLA	C4B-C3B-CAB-CBB
21	4	605	CLA	C4B-C3B-CAB-CBB
21	4	608	CLA	C4B-C3B-CAB-CBB
21	4	612	CLA	C4B-C3B-CAB-CBB
21	6	607	CLA	C4B-C3B-CAB-CBB
21	6	609	CLA	C4B-C3B-CAB-CBB
21	A	1139	CLA	C16-C17-C18-C20
21	B	1205	CLA	C16-C17-C18-C19
21	B	1218	CLA	C16-C17-C18-C19
21	B	1239	CLA	C16-C17-C18-C19
21	B	1239	CLA	C16-C17-C18-C20
21	3	603	CLA	C16-C17-C18-C19
21	3	603	CLA	C16-C17-C18-C20
21	5	603	CLA	C11-C12-C13-C14
21	6	612	CLA	C16-C17-C18-C19
27	6	805	LMU	O5'-C1'-O1'-C1
21	A	1123	CLA	C10-C11-C12-C13
21	A	1132	CLA	C8-C10-C11-C12
21	A	1138	CLA	C8-C10-C11-C12
21	B	1226	CLA	C13-C15-C16-C17
21	4	603	CLA	C10-C11-C12-C13
21	6	607	CLA	C5-C6-C7-C8
25	A	5002	LHG	C13-C14-C15-C16
25	1	801	LHG	C28-C29-C30-C31
25	1	801	LHG	C29-C30-C31-C32
29	F	5003	3PH	C37-C38-C39-C3A
32	L	5002	4RF	C10-C11-C12-C13
33	4	804	PTY	C32-C33-C34-C35
33	L	5003	PTY	N1-C2-C3-O11
21	1	606	CLA	O1D-CGD-O2D-CED
25	A	5002	LHG	C11-C12-C13-C14
31	2	804	LMG	C31-C32-C33-C34
39	2	808	P3H	C11-C12-C13-C14
21	A	1111	CLA	C15-C16-C17-C18
21	A	1126	CLA	C13-C15-C16-C17
21	A	1134	CLA	C5-C6-C7-C8
21	L	1501	CLA	C5-C6-C7-C8
21	5	604	CLA	C8-C10-C11-C12
21	B	1218	CLA	O1A-CGA-O2A-C1
25	5	801	LHG	C25-C26-C27-C28
33	3	807	PTY	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	4	612	CLA	O1D-CGD-O2D-CED
21	A	1101	CLA	C3A-C2A-CAA-CBA
21	A	1103	CLA	C3A-C2A-CAA-CBA
21	A	1104	CLA	C3A-C2A-CAA-CBA
21	A	1105	CLA	C3A-C2A-CAA-CBA
21	A	1109	CLA	C3A-C2A-CAA-CBA
21	A	1110	CLA	C3A-C2A-CAA-CBA
21	A	1135	CLA	C3A-C2A-CAA-CBA
21	B	1206	CLA	C3A-C2A-CAA-CBA
21	B	1210	CLA	C3A-C2A-CAA-CBA
21	B	1223	CLA	C3A-C2A-CAA-CBA
21	B	1234	CLA	C3A-C2A-CAA-CBA
21	G	1602	CLA	C3A-C2A-CAA-CBA
21	H	1701	CLA	C3A-C2A-CAA-CBA
21	H	1702	CLA	C3A-C2A-CAA-CBA
21	1	603	CLA	C3A-C2A-CAA-CBA
21	1	615	CLA	C3A-C2A-CAA-CBA
21	2	615	CLA	C3A-C2A-CAA-CBA
21	3	615	CLA	C3A-C2A-CAA-CBA
21	4	605	CLA	C3A-C2A-CAA-CBA
21	5	602	CLA	C3A-C2A-CAA-CBA
21	5	605	CLA	C3A-C2A-CAA-CBA
21	5	607	CLA	C3A-C2A-CAA-CBA
21	5	613	CLA	C3A-C2A-CAA-CBA
21	6	605	CLA	C3A-C2A-CAA-CBA
21	6	606	CLA	C3A-C2A-CAA-CBA
21	6	608	CLA	C3A-C2A-CAA-CBA
21	6	613	CLA	C3A-C2A-CAA-CBA
36	5	610	CHL	C3A-C2A-CAA-CBA
21	A	1136	CLA	C13-C15-C16-C17
21	B	1210	CLA	C15-C16-C17-C18
21	B	1223	CLA	C10-C11-C12-C13
24	A	4004	BCR	C19-C20-C21-C22
24	I	4002	BCR	C9-C10-C11-C12
25	2	802	LHG	C11-C12-C13-C14
27	A	5005	LMU	C7-C8-C9-C10
21	5	612	CLA	CBA-CGA-O2A-C1
21	B	1204	CLA	O1A-CGA-O2A-C1
21	2	602	CLA	O1A-CGA-O2A-C1
20	A	1011	CL0	C16-C17-C18-C20
21	A	1111	CLA	C16-C17-C18-C20
21	A	1121	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	B	1208	CLA	C11-C12-C13-C14
21	B	1217	CLA	C16-C17-C18-C19
21	B	1218	CLA	C16-C17-C18-C20
21	2	604	CLA	C16-C17-C18-C20
21	5	607	CLA	C11-C12-C13-C14
25	A	5002	LHG	C31-C32-C33-C34
29	5	807	3PH	C24-C25-C26-C27
39	2	808	P3H	C13-C14-C15-C16
25	F	5001	LHG	C4-C5-C6-O8
25	2	803	LHG	C4-C5-C6-O8
25	B	5001	LHG	C16-C17-C18-C19
25	5	801	LHG	C11-C12-C13-C14
27	6	805	LMU	C5-C6-C7-C8
27	6	805	LMU	C6-C7-C8-C9
31	3	803	LMG	C18-C19-C20-C21
21	6	605	CLA	C3-C5-C6-C7
21	B	1205	CLA	C4-C3-C5-C6
21	A	1107	CLA	CBA-CGA-O2A-C1
21	B	1205	CLA	C2-C3-C5-C6
21	2	612	CLA	C2-C3-C5-C6
25	A	5001	LHG	C8-C7-O7-C5
33	3	807	PTY	C11-C8-O7-C6
36	1	610	CHL	C2A-CAA-CBA-CGA
25	F	5001	LHG	O1-C1-C2-O2
25	1	801	LHG	O1-C1-C2-O2
25	1	803	LHG	O1-C1-C2-O2
25	2	801	LHG	O1-C1-C2-O2
25	5	802	LHG	O1-C1-C2-O2
38	4	805	LMK	O9-C10-C11-C12
29	B	5003	3PH	C22-C23-C24-C25
25	1	802	LHG	C23-C24-C25-C26
21	A	1106	CLA	O1A-CGA-O2A-C1
21	B	1203	CLA	O1A-CGA-O2A-C1
21	G	1601	CLA	O1A-CGA-O2A-C1
25	B	5001	LHG	C23-C24-C25-C26
21	B	1230	CLA	C16-C17-C18-C19
21	B	1235	CLA	C11-C12-C13-C14
22	A	2001	PQN	C26-C27-C28-C30
29	F	5003	3PH	C25-C26-C27-C28
33	3	808	PTY	C11-C8-O7-C6
21	A	1102	CLA	C2B-C3B-CAB-CBB
21	A	1104	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
21	A	1109	CLA	C2B-C3B-CAB-CBB
21	A	1118	CLA	C2B-C3B-CAB-CBB
21	A	1120	CLA	C2B-C3B-CAB-CBB
21	A	1122	CLA	C2B-C3B-CAB-CBB
21	A	1126	CLA	C2B-C3B-CAB-CBB
21	A	1140	CLA	C2B-C3B-CAB-CBB
21	A	1141	CLA	C2B-C3B-CAB-CBB
21	B	1201	CLA	C2B-C3B-CAB-CBB
21	B	1203	CLA	C2B-C3B-CAB-CBB
21	B	1209	CLA	C2B-C3B-CAB-CBB
21	B	1214	CLA	C2B-C3B-CAB-CBB
21	B	1216	CLA	C2B-C3B-CAB-CBB
21	B	1218	CLA	C2B-C3B-CAB-CBB
21	B	1220	CLA	C2B-C3B-CAB-CBB
21	B	1227	CLA	C2B-C3B-CAB-CBB
21	B	1232	CLA	C2B-C3B-CAB-CBB
21	B	1238	CLA	C2B-C3B-CAB-CBB
21	B	1240	CLA	C2B-C3B-CAB-CBB
21	F	1301	CLA	C2B-C3B-CAB-CBB
21	F	1302	CLA	C2B-C3B-CAB-CBB
21	J	1901	CLA	C2B-C3B-CAB-CBB
21	K	1403	CLA	C2B-C3B-CAB-CBB
21	O	1801	CLA	C2B-C3B-CAB-CBB
21	O	1803	CLA	C2B-C3B-CAB-CBB
21	1	602	CLA	C2B-C3B-CAB-CBB
21	1	603	CLA	C2B-C3B-CAB-CBB
21	1	605	CLA	C2B-C3B-CAB-CBB
21	1	607	CLA	C2B-C3B-CAB-CBB
21	1	608	CLA	C2B-C3B-CAB-CBB
21	1	613	CLA	C2B-C3B-CAB-CBB
21	2	601	CLA	C2B-C3B-CAB-CBB
21	2	602	CLA	C2B-C3B-CAB-CBB
21	2	605	CLA	C2B-C3B-CAB-CBB
21	2	606	CLA	C2B-C3B-CAB-CBB
21	2	607	CLA	C2B-C3B-CAB-CBB
21	2	608	CLA	C2B-C3B-CAB-CBB
21	3	601	CLA	C2B-C3B-CAB-CBB
21	3	602	CLA	C2B-C3B-CAB-CBB
21	3	608	CLA	C2B-C3B-CAB-CBB
21	3	614	CLA	C2B-C3B-CAB-CBB
21	3	615	CLA	C2B-C3B-CAB-CBB
21	4	602	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
21	4	605	CLA	C2B-C3B-CAB-CBB
21	4	607	CLA	C2B-C3B-CAB-CBB
21	4	608	CLA	C2B-C3B-CAB-CBB
21	4	612	CLA	C2B-C3B-CAB-CBB
21	4	615	CLA	C2B-C3B-CAB-CBB
21	6	607	CLA	C2B-C3B-CAB-CBB
21	6	609	CLA	C2B-C3B-CAB-CBB
21	2	605	CLA	C5-C6-C7-C8
29	5	807	3PH	C32-C33-C34-C35
21	5	604	CLA	C3-C5-C6-C7
25	F	5001	LHG	C13-C14-C15-C16
21	B	1224	CLA	O1A-CGA-O2A-C1
28	2	806	DGD	C1A-C2A-C3A-C4A
21	1	608	CLA	C5-C6-C7-C8
25	1	803	LHG	C1-C2-C3-O3
27	A	5004	LMU	C6-C7-C8-C9
25	A	5001	LHG	O9-C7-O7-C5
33	3	807	PTY	O10-C8-O7-C6
21	A	1105	CLA	C2-C1-O2A-CGA
21	A	1113	CLA	C2-C1-O2A-CGA
21	A	1115	CLA	C2-C1-O2A-CGA
21	A	1116	CLA	C2-C1-O2A-CGA
21	A	1123	CLA	C2-C1-O2A-CGA
21	A	1126	CLA	C2-C1-O2A-CGA
21	A	1134	CLA	C2-C1-O2A-CGA
21	B	1022	CLA	C2-C1-O2A-CGA
21	B	1212	CLA	C2-C1-O2A-CGA
21	B	1216	CLA	C2-C1-O2A-CGA
21	B	1218	CLA	C2-C1-O2A-CGA
21	B	1219	CLA	C2-C1-O2A-CGA
21	B	1228	CLA	C2-C1-O2A-CGA
21	H	1701	CLA	C2-C1-O2A-CGA
21	L	1504	CLA	C2-C1-O2A-CGA
21	1	608	CLA	C2-C1-O2A-CGA
21	3	601	CLA	C2-C1-O2A-CGA
21	3	611	CLA	C2-C1-O2A-CGA
21	4	604	CLA	C2-C1-O2A-CGA
21	4	607	CLA	C2-C1-O2A-CGA
21	4	609	CLA	C2-C1-O2A-CGA
21	4	612	CLA	C2-C1-O2A-CGA
21	4	615	CLA	C2-C1-O2A-CGA
21	5	614	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
21	6	603	CLA	C2-C1-O2A-CGA
21	6	604	CLA	C2-C1-O2A-CGA
21	6	612	CLA	C2-C1-O2A-CGA
25	B	5001	LHG	C17-C18-C19-C20
36	6	610	CHL	C2C-C3C-CAC-CBC
38	4	805	LMK	C11-C12-C13-C14
21	A	1113	CLA	C10-C11-C12-C13
21	A	1123	CLA	C15-C16-C17-C18
21	A	1127	CLA	C5-C6-C7-C8
21	B	1208	CLA	C8-C10-C11-C12
21	B	1216	CLA	C15-C16-C17-C18
21	B	1223	CLA	C8-C10-C11-C12
21	2	615	CLA	C10-C11-C12-C13
25	1	801	LHG	C34-C35-C36-C37
25	2	802	LHG	C16-C17-C18-C19
29	5	807	3PH	C34-C35-C36-C37
21	A	1122	CLA	C3-C5-C6-C7
21	B	1234	CLA	C3-C5-C6-C7
24	A	4002	BCR	C5-C6-C7-C8
24	A	4002	BCR	C23-C24-C25-C30
24	A	4005	BCR	C1-C6-C7-C8
24	A	4005	BCR	C5-C6-C7-C8
24	A	4006	BCR	C1-C6-C7-C8
24	A	4006	BCR	C5-C6-C7-C8
24	B	4001	BCR	C1-C6-C7-C8
24	B	4002	BCR	C1-C6-C7-C8
24	B	4002	BCR	C5-C6-C7-C8
24	B	4003	BCR	C1-C6-C7-C8
24	B	4003	BCR	C5-C6-C7-C8
24	B	4004	BCR	C23-C24-C25-C26
24	B	4004	BCR	C23-C24-C25-C30
24	B	4005	BCR	C5-C6-C7-C8
24	F	4001	BCR	C23-C24-C25-C26
24	F	4001	BCR	C23-C24-C25-C30
24	J	4001	BCR	C1-C6-C7-C8
24	J	4002	BCR	C1-C6-C7-C8
24	J	4002	BCR	C5-C6-C7-C8
24	G	4001	BCR	C23-C24-C25-C26
24	G	4001	BCR	C23-C24-C25-C30
24	H	4001	BCR	C23-C24-C25-C30
24	I	4002	BCR	C1-C6-C7-C8
24	I	4002	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	K	4001	BCR	C23-C24-C25-C30
24	L	4001	BCR	C5-C6-C7-C8
24	L	4002	BCR	C1-C6-C7-C8
24	L	4002	BCR	C5-C6-C7-C8
24	1	504	BCR	C1-C6-C7-C8
24	1	504	BCR	C5-C6-C7-C8
24	2	503	BCR	C1-C6-C7-C8
24	2	503	BCR	C5-C6-C7-C8
24	2	503	BCR	C23-C24-C25-C30
24	3	503	BCR	C1-C6-C7-C8
24	3	503	BCR	C5-C6-C7-C8
24	3	504	BCR	C1-C6-C7-C8
24	3	504	BCR	C5-C6-C7-C8
24	3	506	BCR	C23-C24-C25-C26
24	3	506	BCR	C23-C24-C25-C30
34	4	501	LUT	C5-C6-C7-C8
28	B	5002	DGD	C5A-C6A-C7A-C8A
21	A	1012	CLA	CBA-CGA-O2A-C1
21	B	1212	CLA	CBA-CGA-O2A-C1
21	J	1901	CLA	CBA-CGA-O2A-C1
21	3	610	CLA	CBA-CGA-O2A-C1
21	A	1119	CLA	C8-C10-C11-C12
21	A	1127	CLA	C8-C10-C11-C12
21	B	1213	CLA	C5-C6-C7-C8
21	B	1215	CLA	C13-C15-C16-C17
21	B	1228	CLA	C8-C10-C11-C12
21	B	1229	CLA	C15-C16-C17-C18
21	4	612	CLA	C5-C6-C7-C8
31	4	803	LMG	C31-C32-C33-C34
21	B	1207	CLA	O1A-CGA-O2A-C1
21	O	1803	CLA	C8-C10-C11-C12
21	A	1129	CLA	O1D-CGD-O2D-CED
21	A	1124	CLA	C4-C3-C5-C6
21	B	1229	CLA	C4-C3-C5-C6
21	B	1237	CLA	C4-C3-C5-C6
21	A	1117	CLA	C11-C10-C8-C7
21	A	1125	CLA	C2-C3-C5-C6
21	A	1127	CLA	C12-C13-C15-C16
21	A	1132	CLA	C12-C13-C15-C16
21	A	1138	CLA	C6-C7-C8-C10
21	B	1023	CLA	C11-C10-C8-C7
21	B	1203	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	B	1214	CLA	C11-C12-C13-C15
21	B	1229	CLA	C2-C3-C5-C6
21	B	1237	CLA	C11-C10-C8-C7
21	B	1238	CLA	C11-C12-C13-C15
21	B	1240	CLA	C11-C12-C13-C15
21	K	1402	CLA	C2-C3-C5-C6
21	1	603	CLA	C11-C10-C8-C7
21	2	612	CLA	C11-C12-C13-C15
21	2	615	CLA	C6-C7-C8-C10
21	2	615	CLA	C12-C13-C15-C16
21	3	612	CLA	C6-C7-C8-C10
21	6	605	CLA	C11-C10-C8-C7
22	A	2001	PQN	C21-C22-C23-C25
36	3	604	CHL	C11-C12-C13-C15
36	5	609	CHL	C11-C12-C13-C15
21	A	1107	CLA	O1A-CGA-O2A-C1
21	2	601	CLA	O1A-CGA-O2A-C1
24	B	4002	BCR	C9-C10-C11-C12
21	A	1112	CLA	C16-C17-C18-C19
21	A	1117	CLA	C16-C17-C18-C19
21	A	1120	CLA	C11-C12-C13-C15
21	A	1134	CLA	C6-C7-C8-C10
21	B	1225	CLA	C16-C17-C18-C19
21	4	601	CLA	C11-C12-C13-C15
21	5	604	CLA	C16-C17-C18-C19
21	5	602	CLA	O1A-CGA-O2A-C1
21	A	1108	CLA	CBA-CGA-O2A-C1
21	B	1220	CLA	CBA-CGA-O2A-C1
21	B	1235	CLA	CBA-CGA-O2A-C1
33	5	803	PTY	C31-C30-O4-C1
25	B	5001	LHG	C26-C27-C28-C29
25	1	801	LHG	C16-C17-C18-C19
25	5	801	LHG	C19-C20-C21-C22
27	B	5004	LMU	C3-C4-C5-C6
21	A	1121	CLA	C2A-CAA-CBA-CGA
21	2	601	CLA	C2A-CAA-CBA-CGA
21	4	603	CLA	C2A-CAA-CBA-CGA
21	6	604	CLA	C2A-CAA-CBA-CGA
21	A	1107	CLA	C8-C10-C11-C12
21	B	1207	CLA	C8-C10-C11-C12
21	1	604	CLA	C8-C10-C11-C12
33	1	805	PTY	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
21	5	612	CLA	C2C-C3C-CAC-CBC
33	5	803	PTY	C31-C32-C33-C34
37	2	805	SQD	C30-C31-C32-C33
21	B	1231	CLA	O1D-CGD-O2D-CED
21	A	1101	CLA	C10-C11-C12-C13
25	A	5002	LHG	C29-C30-C31-C32
25	B	5001	LHG	C15-C16-C17-C18
21	B	1217	CLA	C3-C5-C6-C7
31	3	802	LMG	O6-C1-O1-C7
37	3	806	SQD	O5-C1-O6-C44
21	A	1139	CLA	C10-C11-C12-C13
21	B	1210	CLA	C5-C6-C7-C8
21	B	1224	CLA	C15-C16-C17-C18
25	2	802	LHG	C11-C10-C9-C8
28	B	5002	DGD	C1B-C2B-C3B-C4B
31	3	802	LMG	C10-C11-C12-C13
32	L	5002	4RF	C22-C24-C25-C26
29	F	5003	3PH	C22-C21-O21-C2
33	4	804	PTY	C11-C8-O7-C6
24	J	4001	BCR	C18-C19-C20-C21
24	I	4001	BCR	C10-C11-C12-C13
29	B	5003	3PH	C27-C28-C29-C2A
31	2	804	LMG	C40-C41-C42-C43
21	3	610	CLA	O1A-CGA-O2A-C1
39	2	808	P3H	C12-C13-C14-C15
29	F	5003	3PH	O22-C21-O21-C2
33	4	804	PTY	O10-C8-O7-C6
25	A	5001	LHG	C29-C30-C31-C32
25	B	5001	LHG	C10-C11-C12-C13
33	5	803	PTY	C38-C39-C40-C41
28	2	806	DGD	C2E-C1E-O5D-C6D
28	3	804	DGD	C2E-C1E-O5D-C6D
31	4	803	LMG	C2-C1-O1-C7
25	B	5001	LHG	O7-C5-C6-O8
25	F	5001	LHG	O7-C5-C6-O8
25	1	803	LHG	O7-C5-C6-O8
25	F	5001	LHG	C11-C12-C13-C14
27	B	5004	LMU	C2-C3-C4-C5
31	4	802	LMG	C19-C20-C21-C22
21	A	1104	CLA	C13-C15-C16-C17
21	B	1219	CLA	C10-C11-C12-C13
39	2	808	P3H	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
21	A	1125	CLA	C4-C3-C5-C6
21	K	1402	CLA	C4-C3-C5-C6
21	A	1124	CLA	C2-C3-C5-C6
21	B	1237	CLA	C2-C3-C5-C6
21	2	607	CLA	C2-C3-C5-C6
25	A	5001	LHG	C33-C34-C35-C36
21	A	1012	CLA	C11-C10-C8-C9
21	A	1127	CLA	C14-C13-C15-C16
21	B	1205	CLA	C11-C12-C13-C14
21	B	1224	CLA	C11-C10-C8-C9
21	B	1238	CLA	C6-C7-C8-C9
21	B	1240	CLA	C11-C12-C13-C14
21	O	1803	CLA	C11-C10-C8-C9
21	1	604	CLA	C11-C12-C13-C14
21	1	611	CLA	C11-C12-C13-C14
21	2	603	CLA	C14-C13-C15-C16
21	2	615	CLA	C6-C7-C8-C9
21	3	601	CLA	C6-C7-C8-C9
21	3	605	CLA	C11-C12-C13-C14
21	4	604	CLA	C11-C10-C8-C9
21	5	604	CLA	C6-C7-C8-C9
21	6	605	CLA	C11-C10-C8-C9
21	A	1131	CLA	C3-C5-C6-C7
21	B	1212	CLA	C3-C5-C6-C7
22	B	2002	PQN	C13-C15-C16-C17
21	B	1220	CLA	C2A-CAA-CBA-CGA
21	L	1502	CLA	C2A-CAA-CBA-CGA
21	3	608	CLA	C2A-CAA-CBA-CGA
21	3	613	CLA	C2A-CAA-CBA-CGA
31	3	803	LMG	C22-C23-C24-C25
24	3	506	BCR	C36-C18-C19-C20
21	B	1220	CLA	O1D-CGD-O2D-CED
21	B	1228	CLA	C5-C6-C7-C8
21	B	1230	CLA	C15-C16-C17-C18
21	A	1012	CLA	O1A-CGA-O2A-C1
21	A	1108	CLA	O1A-CGA-O2A-C1
21	B	1212	CLA	O1A-CGA-O2A-C1
21	B	1235	CLA	O1A-CGA-O2A-C1
21	J	1901	CLA	O1A-CGA-O2A-C1
21	A	1102	CLA	C1A-C2A-CAA-CBA
21	A	1103	CLA	C1A-C2A-CAA-CBA
21	A	1104	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	A	1106	CLA	C1A-C2A-CAA-CBA
21	A	1113	CLA	C1A-C2A-CAA-CBA
21	A	1116	CLA	C1A-C2A-CAA-CBA
21	A	1117	CLA	C1A-C2A-CAA-CBA
21	A	1122	CLA	C1A-C2A-CAA-CBA
21	A	1127	CLA	C1A-C2A-CAA-CBA
21	A	1128	CLA	C1A-C2A-CAA-CBA
21	A	1132	CLA	C1A-C2A-CAA-CBA
21	A	1133	CLA	C1A-C2A-CAA-CBA
21	A	1135	CLA	C1A-C2A-CAA-CBA
21	B	1210	CLA	C1A-C2A-CAA-CBA
21	B	1215	CLA	C1A-C2A-CAA-CBA
21	B	1216	CLA	C1A-C2A-CAA-CBA
21	B	1219	CLA	C1A-C2A-CAA-CBA
21	B	1223	CLA	C1A-C2A-CAA-CBA
21	B	1229	CLA	C1A-C2A-CAA-CBA
21	B	1231	CLA	C1A-C2A-CAA-CBA
21	B	1236	CLA	C1A-C2A-CAA-CBA
21	B	1239	CLA	C1A-C2A-CAA-CBA
21	G	1602	CLA	C1A-C2A-CAA-CBA
21	H	1701	CLA	C1A-C2A-CAA-CBA
21	O	1803	CLA	C1A-C2A-CAA-CBA
21	1	615	CLA	C1A-C2A-CAA-CBA
21	2	601	CLA	C1A-C2A-CAA-CBA
21	2	607	CLA	C1A-C2A-CAA-CBA
21	3	606	CLA	C1A-C2A-CAA-CBA
21	3	613	CLA	C1A-C2A-CAA-CBA
21	4	604	CLA	C1A-C2A-CAA-CBA
21	4	605	CLA	C1A-C2A-CAA-CBA
21	4	607	CLA	C1A-C2A-CAA-CBA
21	4	608	CLA	C1A-C2A-CAA-CBA
21	5	601	CLA	C1A-C2A-CAA-CBA
21	5	602	CLA	C1A-C2A-CAA-CBA
21	5	603	CLA	C1A-C2A-CAA-CBA
21	5	605	CLA	C1A-C2A-CAA-CBA
21	5	606	CLA	C1A-C2A-CAA-CBA
21	5	608	CLA	C1A-C2A-CAA-CBA
21	5	612	CLA	C1A-C2A-CAA-CBA
21	5	613	CLA	C1A-C2A-CAA-CBA
21	5	614	CLA	C1A-C2A-CAA-CBA
21	6	604	CLA	C1A-C2A-CAA-CBA
21	6	605	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	6	608	CLA	C1A-C2A-CAA-CBA
21	6	612	CLA	C1A-C2A-CAA-CBA
21	6	613	CLA	C1A-C2A-CAA-CBA
21	A	1120	CLA	C11-C12-C13-C14
21	A	1121	CLA	C11-C12-C13-C15
21	A	1139	CLA	C16-C17-C18-C19
21	B	1217	CLA	C16-C17-C18-C20
21	4	601	CLA	C11-C12-C13-C14
36	4	613	CHL	C11-C12-C13-C15
31	3	803	LMG	C12-C13-C14-C15
24	B	4005	BCR	C19-C20-C21-C22
24	G	4001	BCR	C9-C10-C11-C12
21	A	1013	CLA	C5-C6-C7-C8
21	A	1101	CLA	C15-C16-C17-C18
21	A	1113	CLA	C5-C6-C7-C8
21	B	1225	CLA	C5-C6-C7-C8
25	3	801	LHG	C4-O6-P-O3
29	B	5003	3PH	C24-C25-C26-C27
21	B	1203	CLA	C3-C5-C6-C7
21	5	603	CLA	C3-C5-C6-C7
31	F	5002	LMG	C37-C38-C39-C40
21	A	1126	CLA	C10-C11-C12-C13
21	A	1141	CLA	C8-C10-C11-C12
21	A	1141	CLA	C10-C11-C12-C13
21	B	1022	CLA	C8-C10-C11-C12
21	2	612	CLA	C8-C10-C11-C12
21	A	1103	CLA	CBA-CGA-O2A-C1
25	1	802	LHG	O6-C4-C5-C6
25	6	801	LHG	O6-C4-C5-C6
29	B	5003	3PH	O11-C1-C2-C3
25	F	5001	LHG	C11-C10-C9-C8
31	F	5002	LMG	C28-C29-C30-C31
33	4	804	PTY	C8-C11-C12-C13
25	A	5002	LHG	C11-C10-C9-C8
21	B	1206	CLA	C16-C17-C18-C20
27	B	5004	LMU	C5-C6-C7-C8
31	2	804	LMG	C37-C38-C39-C40
33	1	805	PTY	C16-C17-C18-C19
27	6	805	LMU	C1-C2-C3-C4
21	2	607	CLA	C4-C3-C5-C6
31	3	803	LMG	C33-C34-C35-C36
31	4	802	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
21	A	1126	CLA	C8-C10-C11-C12
21	B	1023	CLA	C13-C15-C16-C17
21	B	1215	CLA	C8-C10-C11-C12
21	B	1239	CLA	C15-C16-C17-C18
21	6	605	CLA	C5-C6-C7-C8
21	6	607	CLA	C8-C10-C11-C12
25	2	803	LHG	C28-C29-C30-C31
21	B	1220	CLA	O1A-CGA-O2A-C1
33	5	803	PTY	O30-C30-O4-C1
25	2	803	LHG	C25-C26-C27-C28
21	H	1701	CLA	C2A-CAA-CBA-CGA
21	4	608	CLA	C2A-CAA-CBA-CGA
21	K	1402	CLA	C6-C7-C8-C9
21	6	601	CLA	C11-C12-C13-C15
31	3	803	LMG	O6-C5-C6-O5
25	A	5002	LHG	C4-C5-C6-O8
25	B	5001	LHG	C4-C5-C6-O8
25	1	803	LHG	C4-C5-C6-O8
25	3	801	LHG	C4-C5-C6-O8
25	5	801	LHG	C4-C5-C6-O8
25	5	802	LHG	C4-C5-C6-O8
31	F	5002	LMG	C7-C8-C9-O8
32	L	5002	4RF	O18-C19-C20-C39
32	5	805	4RF	O18-C19-C20-C39
38	2	807	LMK	C7-C8-C9-O8
21	B	1217	CLA	C13-C15-C16-C17
28	3	804	DGD	C5D-C6D-O5D-C1E
28	3	805	DGD	C5D-C6D-O5D-C1E
31	F	5002	LMG	C12-C13-C14-C15
31	3	803	LMG	C21-C22-C23-C24
33	1	805	PTY	C17-C18-C19-C20
21	H	1702	CLA	CAA-CBA-CGA-O2A
21	2	603	CLA	O1A-CGA-O2A-C1
21	2	603	CLA	CBA-CGA-O2A-C1
25	2	803	LHG	O1-C1-C2-O2
25	3	801	LHG	O1-C1-C2-O2
25	6	801	LHG	O1-C1-C2-O2
27	6	805	LMU	C7-C8-C9-C10
37	2	805	SQD	C29-C30-C31-C32
39	5	806	P3H	C14-C15-C16-C17
39	2	808	P3H	C49-C50-C51-C52
25	B	5001	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
25	1	801	LHG	C11-C10-C9-C8
31	6	802	LMG	C11-C12-C13-C14
37	3	806	SQD	C11-C10-C9-C8
21	6	612	CLA	C5-C6-C7-C8
21	A	1121	CLA	C4-C3-C5-C6
21	L	1502	CLA	C4-C3-C5-C6
25	B	5001	LHG	C28-C29-C30-C31
27	B	5004	LMU	C9-C10-C11-C12
33	1	805	PTY	C30-C31-C32-C33
21	A	1116	CLA	CBA-CGA-O2A-C1
29	F	5003	3PH	C32-C31-O31-C3
31	F	5002	LMG	C29-C28-O8-C9
21	A	1124	CLA	C10-C11-C12-C13
21	B	1207	CLA	C5-C6-C7-C8
21	B	1214	CLA	C13-C15-C16-C17
28	2	806	DGD	C1G-C2G-O2G-C1B
28	3	805	DGD	C1G-C2G-O2G-C1B
29	5	804	3PH	C3-C2-O21-C21
36	6	610	CHL	C2A-CAA-CBA-CGA
21	A	1129	CLA	C5-C6-C7-C8
21	A	1107	CLA	C2-C1-O2A-CGA
21	A	1121	CLA	C2-C1-O2A-CGA
21	A	1132	CLA	C2-C1-O2A-CGA
21	A	1137	CLA	C2-C1-O2A-CGA
21	B	1213	CLA	C2-C1-O2A-CGA
28	2	806	DGD	O6E-C5E-C6E-O5E
21	B	1223	CLA	C3-C5-C6-C7
25	4	801	LHG	C9-C10-C11-C12
29	B	5003	3PH	C2C-C2D-C2E-C2F
32	L	5002	4RF	C24-C25-C26-C27
32	L	5002	4RF	C47-C48-C49-C50
21	A	1129	CLA	CBA-CGA-O2A-C1
21	3	605	CLA	CBA-CGA-O2A-C1
37	2	805	SQD	C24-C23-O48-C46
25	3	801	LHG	O6-C4-C5-O7
25	4	801	LHG	O6-C4-C5-O7
33	4	804	PTY	O14-C5-C6-O7
21	5	604	CLA	C16-C17-C18-C20
21	A	1103	CLA	O1A-CGA-O2A-C1
27	6	805	LMU	C2-C3-C4-C5
33	5	803	PTY	C33-C34-C35-C36
21	5	605	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	2	803	LHG	O7-C5-C6-O8
31	3	803	LMG	O7-C8-C9-O8
32	L	5002	4RF	O18-C19-C20-O21
38	2	807	LMK	O7-C8-C9-O8
21	5	612	CLA	O1A-CGA-O2A-C1
21	A	1101	CLA	C5-C6-C7-C8
21	B	1203	CLA	C8-C10-C11-C12
21	3	603	CLA	C5-C6-C7-C8
25	1	801	LHG	C25-C26-C27-C28
28	B	5002	DGD	C4B-C5B-C6B-C7B
21	A	1012	CLA	C11-C10-C8-C7
21	A	1101	CLA	C12-C13-C15-C16
21	A	1103	CLA	C11-C12-C13-C15
21	A	1106	CLA	C6-C7-C8-C10
21	A	1115	CLA	C6-C7-C8-C10
21	A	1123	CLA	C11-C12-C13-C15
21	A	1125	CLA	C11-C12-C13-C15
21	A	1126	CLA	C12-C13-C15-C16
21	A	1127	CLA	C11-C12-C13-C15
21	A	1128	CLA	C11-C10-C8-C7
21	A	1131	CLA	C12-C13-C15-C16
21	A	1132	CLA	C11-C12-C13-C15
21	B	1021	CLA	C6-C7-C8-C10
21	B	1203	CLA	C6-C7-C8-C10
21	B	1204	CLA	C11-C12-C13-C15
21	B	1205	CLA	C11-C12-C13-C15
21	B	1210	CLA	C12-C13-C15-C16
21	B	1224	CLA	C11-C10-C8-C7
21	B	1225	CLA	C11-C10-C8-C7
21	B	1238	CLA	C6-C7-C8-C10
21	L	1501	CLA	C12-C13-C15-C16
21	O	1803	CLA	C11-C10-C8-C7
21	1	604	CLA	C11-C12-C13-C15
21	1	615	CLA	C11-C10-C8-C7
21	2	603	CLA	C12-C13-C15-C16
21	2	612	CLA	C12-C13-C15-C16
21	3	605	CLA	C12-C13-C15-C16
21	4	601	CLA	C6-C7-C8-C10
21	4	603	CLA	C6-C7-C8-C10
21	4	604	CLA	C11-C10-C8-C7
21	4	609	CLA	C6-C7-C8-C10
36	4	613	CHL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
21	6	609	CLA	CAA-CBA-CGA-O2A
25	6	801	LHG	O8-C23-C24-C25
21	A	1110	CLA	C3-C5-C6-C7
21	A	1101	CLA	C14-C13-C15-C16
21	A	1113	CLA	C6-C7-C8-C9
21	A	1115	CLA	C6-C7-C8-C9
21	A	1126	CLA	C11-C12-C13-C14
21	A	1127	CLA	C11-C12-C13-C14
21	A	1131	CLA	C14-C13-C15-C16
21	B	1204	CLA	C11-C12-C13-C14
21	B	1210	CLA	C14-C13-C15-C16
21	B	1214	CLA	C11-C10-C8-C9
21	B	1219	CLA	C11-C12-C13-C14
21	B	1224	CLA	C14-C13-C15-C16
21	B	1225	CLA	C11-C10-C8-C9
21	B	1226	CLA	C11-C10-C8-C9
21	B	1226	CLA	C11-C12-C13-C14
21	B	1227	CLA	C14-C13-C15-C16
21	1	611	CLA	C14-C13-C15-C16
21	2	603	CLA	C6-C7-C8-C9
21	2	612	CLA	C14-C13-C15-C16
21	3	603	CLA	C6-C7-C8-C9
21	3	605	CLA	C14-C13-C15-C16
21	4	601	CLA	C6-C7-C8-C9
21	4	603	CLA	C6-C7-C8-C9
21	5	614	CLA	C6-C7-C8-C9
21	5	614	CLA	C11-C10-C8-C9
21	6	604	CLA	C6-C7-C8-C9
21	6	612	CLA	C6-C7-C8-C9
36	4	613	CHL	C11-C10-C8-C9
27	6	805	LMU	C3'-C4'-O1B-C1B
21	2	607	CLA	C5-C6-C7-C8
25	A	5002	LHG	C9-C10-C11-C12
25	1	801	LHG	C13-C14-C15-C16
24	1	504	BCR	C37-C22-C23-C24
21	2	601	CLA	C16-C17-C18-C20
21	6	601	CLA	C11-C12-C13-C14
25	1	801	LHG	C14-C15-C16-C17
31	2	804	LMG	C39-C40-C41-C42
25	4	801	LHG	C7-C8-C9-C10
24	1	504	BCR	C21-C22-C23-C24
29	F	5003	3PH	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
29	5	807	3PH	C26-C27-C28-C29
21	B	1023	CLA	C3-C5-C6-C7
21	B	1211	CLA	C3-C5-C6-C7
21	B	1023	CLA	C15-C16-C17-C18
21	5	604	CLA	C13-C15-C16-C17
25	A	5002	LHG	C8-C7-O7-C5
21	A	1119	CLA	CBA-CGA-O2A-C1
21	A	1105	CLA	C5-C6-C7-C8
21	A	1112	CLA	C10-C11-C12-C13
21	3	602	CLA	C3-C5-C6-C7
21	A	1108	CLA	C4B-C3B-CAB-CBB
21	A	1111	CLA	C4B-C3B-CAB-CBB
21	A	1119	CLA	C4B-C3B-CAB-CBB
21	A	1124	CLA	C4B-C3B-CAB-CBB
21	A	1133	CLA	C4B-C3B-CAB-CBB
21	B	1210	CLA	C4B-C3B-CAB-CBB
21	B	1213	CLA	C4B-C3B-CAB-CBB
21	B	1221	CLA	C4B-C3B-CAB-CBB
21	B	1224	CLA	C4B-C3B-CAB-CBB
21	B	1231	CLA	C4B-C3B-CAB-CBB
21	B	1236	CLA	C4B-C3B-CAB-CBB
21	J	1901	CLA	C4B-C3B-CAB-CBB
21	1	612	CLA	C4B-C3B-CAB-CBB
21	2	604	CLA	C4B-C3B-CAB-CBB
21	2	612	CLA	C4B-C3B-CAB-CBB
21	3	605	CLA	C4B-C3B-CAB-CBB
21	4	609	CLA	C4B-C3B-CAB-CBB
29	F	5003	3PH	O11-C1-C2-C3
29	5	804	3PH	O11-C1-C2-C3
33	4	804	PTY	O14-C5-C6-C1
33	5	803	PTY	C36-C37-C38-C39
33	O	5002	PTY	N1-C2-C3-O11
33	6	804	PTY	N1-C2-C3-O11
21	B	1238	CLA	CBA-CGA-O2A-C1
32	L	5002	4RF	C15-C16-O18-C19
21	A	1140	CLA	C4-C3-C5-C6
21	5	614	CLA	C4-C3-C5-C6
25	1	803	LHG	C7-C8-C9-C10
21	A	1116	CLA	O1A-CGA-O2A-C1
21	A	1129	CLA	O1A-CGA-O2A-C1
21	B	1216	CLA	CBA-CGA-O2A-C1
21	6	602	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
39	2	808	P3H	C16-C17-O19-C20
29	5	807	3PH	C21-C22-C23-C24
31	4	802	LMG	C28-C29-C30-C31
25	A	5001	LHG	C35-C36-C37-C38
25	5	802	LHG	C2-C3-O3-P
33	3	808	PTY	C6-C5-O14-P1
21	A	1120	CLA	C3A-C2A-CAA-CBA
21	B	1207	CLA	C3A-C2A-CAA-CBA
21	G	1601	CLA	C3A-C2A-CAA-CBA
21	5	603	CLA	C3A-C2A-CAA-CBA
21	5	612	CLA	C3A-C2A-CAA-CBA
21	6	604	CLA	C3A-C2A-CAA-CBA
24	A	4006	BCR	C19-C20-C21-C22
24	3	503	BCR	C19-C20-C21-C22
34	1	501	LUT	C13-C14-C15-C35
21	3	612	CLA	C15-C16-C17-C18
21	L	1502	CLA	C16-C17-C18-C20
21	A	1133	CLA	CBA-CGA-O2A-C1
25	B	5001	LHG	C24-C23-O8-C6
21	A	1121	CLA	C2C-C3C-CAC-CBC
29	F	5003	3PH	C3A-C3B-C3C-C3D
31	F	5002	LMG	C36-C37-C38-C39
33	3	808	PTY	O10-C8-O7-C6
21	A	1102	CLA	C13-C15-C16-C17
25	1	802	LHG	C4-C5-C6-O8
25	2	802	LHG	C4-C5-C6-O8
31	2	804	LMG	C7-C8-C9-O8
33	4	804	PTY	O4-C1-C6-C5
33	5	803	PTY	O4-C1-C6-C5
38	2	807	LMK	O1-C7-C8-C9
33	1	805	PTY	C13-C14-C15-C16
21	5	605	CLA	C3-C5-C6-C7
39	2	808	P3H	C28-O27-P24-O26
39	5	806	P3H	C28-O27-P24-O26
31	F	5002	LMG	O10-C28-O8-C9
21	A	1107	CLA	C4-C3-C5-C6
21	1	604	CLA	C4-C3-C5-C6
21	5	614	CLA	C2-C3-C5-C6
21	A	1112	CLA	C5-C6-C7-C8
21	4	609	CLA	C8-C10-C11-C12
21	3	605	CLA	O1A-CGA-O2A-C1
25	A	5001	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
25	A	5002	LHG	O1-C1-C2-O2
25	1	801	LHG	O6-C4-C5-O7
25	1	803	LHG	O6-C4-C5-O7
25	5	802	LHG	O6-C4-C5-O7
21	A	1113	CLA	CBA-CGA-O2A-C1
21	1	611	CLA	CBA-CGA-O2A-C1
29	F	5003	3PH	O32-C31-O31-C3
32	L	5002	4RF	C45-C46-C47-C48
25	F	5001	LHG	O7-C7-C8-C9
25	2	803	LHG	O8-C23-C24-C25
21	A	1108	CLA	C2B-C3B-CAB-CBB
21	A	1111	CLA	C2B-C3B-CAB-CBB
21	A	1119	CLA	C2B-C3B-CAB-CBB
21	B	1210	CLA	C2B-C3B-CAB-CBB
21	B	1213	CLA	C2B-C3B-CAB-CBB
21	B	1224	CLA	C2B-C3B-CAB-CBB
21	B	1231	CLA	C2B-C3B-CAB-CBB
21	B	1236	CLA	C2B-C3B-CAB-CBB
21	3	605	CLA	C2B-C3B-CAB-CBB
37	2	805	SQD	O10-C23-O48-C46
21	A	1108	CLA	C3-C5-C6-C7
31	4	802	LMG	C31-C32-C33-C34
25	5	801	LHG	O7-C5-C6-O8
29	B	5003	3PH	O21-C2-C3-O31
31	1	804	LMG	O1-C7-C8-O7
31	2	804	LMG	O7-C8-C9-O8
32	5	805	4RF	O18-C19-C20-O21
33	3	807	PTY	O4-C1-C6-O7
21	L	1504	CLA	CBA-CGA-O2A-C1
25	2	801	LHG	C28-C29-C30-C31
27	B	5004	LMU	C1-C2-C3-C4
25	5	801	LHG	C1-C2-C3-O3
25	A	5002	LHG	O9-C7-O7-C5
21	4	607	CLA	C3-C5-C6-C7
21	L	1502	CLA	C2-C3-C5-C6
20	A	1011	CL0	C11-C10-C8-C9
21	A	1101	CLA	C11-C12-C13-C14
21	A	1103	CLA	C11-C12-C13-C14
21	A	1104	CLA	C11-C12-C13-C14
21	A	1113	CLA	C11-C12-C13-C14
21	A	1120	CLA	C11-C10-C8-C9
21	A	1132	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	B	1021	CLA	C6-C7-C8-C9
21	B	1203	CLA	C6-C7-C8-C9
21	B	1207	CLA	C6-C7-C8-C9
21	B	1213	CLA	C11-C10-C8-C9
21	B	1227	CLA	C6-C7-C8-C9
21	B	1229	CLA	C14-C13-C15-C16
21	2	605	CLA	C6-C7-C8-C9
21	3	607	CLA	C11-C10-C8-C9
21	4	605	CLA	C11-C10-C8-C9
21	4	609	CLA	C11-C10-C8-C9
21	5	607	CLA	C11-C10-C8-C9
25	F	5001	LHG	C24-C25-C26-C27
21	B	1205	CLA	C15-C16-C17-C18
25	1	803	LHG	C5-C4-O6-P
33	4	804	PTY	C6-C5-O14-P1
39	2	808	P3H	C21-C22-O23-P24
21	B	1238	CLA	O1A-CGA-O2A-C1
33	5	803	PTY	C37-C38-C39-C40
21	A	1117	CLA	C2A-CAA-CBA-CGA
21	L	1504	CLA	C2A-CAA-CBA-CGA
21	B	1206	CLA	C16-C17-C18-C19
21	2	601	CLA	C16-C17-C18-C19
21	5	614	CLA	C16-C17-C18-C20
24	A	4007	BCR	C5-C6-C7-C8
24	B	4005	BCR	C1-C6-C7-C8
24	F	4002	BCR	C5-C6-C7-C8
24	J	4002	BCR	C23-C24-C25-C26
24	L	4002	BCR	C23-C24-C25-C26
24	L	4002	BCR	C23-C24-C25-C30
24	3	503	BCR	C23-C24-C25-C26
24	3	503	BCR	C23-C24-C25-C30
24	3	504	BCR	C23-C24-C25-C26
34	1	501	LUT	C5-C6-C7-C8
34	4	501	LUT	C1-C6-C7-C8
34	6	501	LUT	C1-C6-C7-C8
34	6	501	LUT	C5-C6-C7-C8
21	A	1127	CLA	C10-C11-C12-C13
21	1	611	CLA	C8-C10-C11-C12
25	5	801	LHG	C9-C10-C11-C12
24	J	4002	BCR	C37-C22-C23-C24
24	K	4001	BCR	C36-C18-C19-C20
24	A	4001	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	J	4002	BCR	C17-C18-C19-C20
24	3	506	BCR	C17-C18-C19-C20
21	B	1216	CLA	C13-C15-C16-C17
21	2	615	CLA	C15-C16-C17-C18
21	4	605	CLA	C8-C10-C11-C12
31	F	5002	LMG	C34-C35-C36-C37
31	F	5002	LMG	C40-C41-C42-C43
25	A	5001	LHG	C34-C35-C36-C37
25	1	801	LHG	C33-C34-C35-C36
25	4	801	LHG	C24-C25-C26-C27
31	2	804	LMG	C30-C31-C32-C33
20	A	1011	CL0	C8-C10-C11-C12
21	A	1102	CLA	C10-C11-C12-C13
25	1	803	LHG	O6-C4-C5-C6
25	2	802	LHG	O6-C4-C5-C6
25	3	801	LHG	O6-C4-C5-C6
25	4	801	LHG	O6-C4-C5-C6
25	5	802	LHG	O6-C4-C5-C6
33	O	5002	PTY	O14-C5-C6-C1
25	5	801	LHG	O2-C2-C3-O3
20	A	1011	CL0	C11-C10-C8-C7
21	A	1012	CLA	C12-C13-C15-C16
21	A	1013	CLA	C6-C7-C8-C10
21	A	1103	CLA	C12-C13-C15-C16
21	A	1104	CLA	C12-C13-C15-C16
21	A	1107	CLA	C2-C3-C5-C6
21	A	1113	CLA	C11-C12-C13-C15
21	A	1119	CLA	C11-C12-C13-C15
21	A	1120	CLA	C11-C10-C8-C7
21	A	1126	CLA	C11-C12-C13-C15
21	A	1133	CLA	C11-C12-C13-C15
21	A	1140	CLA	C11-C12-C13-C15
21	B	1023	CLA	C12-C13-C15-C16
21	B	1202	CLA	C6-C7-C8-C10
21	B	1206	CLA	C11-C12-C13-C15
21	B	1207	CLA	C6-C7-C8-C10
21	B	1210	CLA	C6-C7-C8-C10
21	B	1213	CLA	C11-C10-C8-C7
21	B	1214	CLA	C11-C10-C8-C7
21	B	1219	CLA	C11-C12-C13-C15
21	B	1225	CLA	C6-C7-C8-C10
21	B	1226	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
21	B	1226	CLA	C11-C12-C13-C15
21	B	1227	CLA	C6-C7-C8-C10
21	B	1227	CLA	C12-C13-C15-C16
21	B	1229	CLA	C12-C13-C15-C16
21	1	603	CLA	C6-C7-C8-C10
21	1	611	CLA	C12-C13-C15-C16
21	1	612	CLA	C11-C10-C8-C7
21	2	603	CLA	C6-C7-C8-C10
21	2	604	CLA	C11-C10-C8-C7
21	2	605	CLA	C6-C7-C8-C10
21	2	605	CLA	C11-C12-C13-C15
21	3	601	CLA	C11-C10-C8-C7
21	3	603	CLA	C6-C7-C8-C10
21	3	605	CLA	C11-C12-C13-C15
21	3	607	CLA	C11-C10-C8-C7
21	3	608	CLA	C11-C12-C13-C15
21	4	605	CLA	C11-C10-C8-C7
21	4	612	CLA	C11-C10-C8-C7
21	5	603	CLA	C11-C10-C8-C7
21	6	612	CLA	C6-C7-C8-C10
21	B	1203	CLA	C15-C16-C17-C18
21	B	1217	CLA	C15-C16-C17-C18
21	B	1224	CLA	C13-C15-C16-C17
24	A	4002	BCR	C13-C14-C15-C16
24	A	4005	BCR	C19-C20-C21-C22
24	A	4007	BCR	C19-C20-C21-C22
24	B	4003	BCR	C19-C20-C21-C22
24	B	4004	BCR	C9-C10-C11-C12
24	B	4004	BCR	C19-C20-C21-C22
24	B	4005	BCR	C9-C10-C11-C12
24	B	4005	BCR	C13-C14-C15-C16
24	J	4001	BCR	C13-C14-C15-C16
24	2	503	BCR	C9-C10-C11-C12
24	3	504	BCR	C13-C14-C15-C16
24	3	504	BCR	C19-C20-C21-C22
34	3	501	LUT	C29-C30-C31-C32
34	5	504	LUT	C33-C34-C35-C15
33	5	803	PTY	C8-C11-C12-C13
21	3	605	CLA	C10-C11-C12-C13
21	F	1302	CLA	CAA-CBA-CGA-O2A
21	A	1102	CLA	C2A-CAA-CBA-CGA
21	A	1134	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
27	6	805	LMU	C5'-C4'-O1B-C1B
29	B	5003	3PH	C26-C27-C28-C29
37	3	806	SQD	C23-C24-C25-C26
21	A	1108	CLA	C5-C6-C7-C8
21	1	615	CLA	CBA-CGA-O2A-C1
25	1	802	LHG	O8-C23-C24-C25
33	4	804	PTY	C34-C35-C36-C37
21	B	1202	CLA	C5-C6-C7-C8
21	1	601	CLA	C13-C15-C16-C17
21	A	1119	CLA	O1A-CGA-O2A-C1
28	2	806	DGD	O6D-C5D-C6D-O5D
31	3	802	LMG	C15-C16-C17-C18
21	A	1138	CLA	CAD-CBD-CGD-O2D
21	B	1204	CLA	CAD-CBD-CGD-O2D
21	B	1209	CLA	CAD-CBD-CGD-O2D
21	B	1230	CLA	CAD-CBD-CGD-O2D
21	B	1234	CLA	CAD-CBD-CGD-O2D
21	1	606	CLA	CAD-CBD-CGD-O2D
21	2	607	CLA	CAD-CBD-CGD-O2D
36	4	611	CHL	CAD-CBD-CGD-O2D
36	5	609	CHL	CAD-CBD-CGD-O2D
21	5	614	CLA	C3-C5-C6-C7
25	2	803	LHG	C11-C10-C9-C8
21	1	611	CLA	C15-C16-C17-C18
21	1	615	CLA	C5-C6-C7-C8
21	6	604	CLA	C10-C11-C12-C13
25	F	5001	LHG	C33-C34-C35-C36
32	L	5002	4RF	C12-C13-C14-C15
25	2	802	LHG	C24-C23-O8-C6
27	B	5004	LMU	C4-C5-C6-C7
28	3	804	DGD	O6D-C1D-O3G-C3G
21	A	1121	CLA	C2-C3-C5-C6
25	1	801	LHG	C4-C5-C6-O8
25	1	803	LHG	C2-C3-O3-P
25	2	803	LHG	C2-C3-O3-P
29	5	807	3PH	C1-C2-C3-O31
31	3	803	LMG	C7-C8-C9-O8
32	5	805	4RF	C19-C20-C39-O40
33	3	808	PTY	O4-C1-C6-C5
21	L	1504	CLA	O1A-CGA-O2A-C1
25	5	801	LHG	O6-C4-C5-O7
21	B	1206	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
21	B	1240	CLA	CAA-CBA-CGA-O2A
25	A	5001	LHG	C28-C29-C30-C31
21	B	1208	CLA	C2A-CAA-CBA-CGA
21	2	603	CLA	C2A-CAA-CBA-CGA
21	A	1012	CLA	C10-C11-C12-C13
28	B	5002	DGD	C1A-C2A-C3A-C4A
21	A	1105	CLA	C11-C12-C13-C14
21	L	1502	CLA	C16-C17-C18-C19
21	2	605	CLA	C16-C17-C18-C19
21	2	605	CLA	C16-C17-C18-C20
22	B	2002	PQN	C26-C27-C28-C29
27	B	5004	LMU	C11-C10-C9-C8
21	A	1102	CLA	CHA-CBD-CGD-O1D
21	A	1103	CLA	CHA-CBD-CGD-O1D
21	A	1106	CLA	CHA-CBD-CGD-O1D
21	A	1114	CLA	CHA-CBD-CGD-O1D
21	A	1117	CLA	CHA-CBD-CGD-O1D
21	A	1117	CLA	CHA-CBD-CGD-O2D
21	A	1124	CLA	CHA-CBD-CGD-O1D
21	A	1124	CLA	CHA-CBD-CGD-O2D
21	A	1132	CLA	CHA-CBD-CGD-O1D
21	A	1132	CLA	CHA-CBD-CGD-O2D
21	A	1135	CLA	CHA-CBD-CGD-O1D
21	A	1135	CLA	CHA-CBD-CGD-O2D
21	A	1137	CLA	CHA-CBD-CGD-O1D
21	A	1137	CLA	CHA-CBD-CGD-O2D
21	B	1202	CLA	CHA-CBD-CGD-O1D
21	B	1202	CLA	CHA-CBD-CGD-O2D
21	B	1210	CLA	CHA-CBD-CGD-O1D
21	B	1210	CLA	CHA-CBD-CGD-O2D
21	B	1211	CLA	CHA-CBD-CGD-O1D
21	B	1211	CLA	CHA-CBD-CGD-O2D
21	B	1212	CLA	CHA-CBD-CGD-O1D
21	B	1218	CLA	CHA-CBD-CGD-O1D
21	B	1218	CLA	CHA-CBD-CGD-O2D
21	B	1222	CLA	CHA-CBD-CGD-O1D
21	B	1223	CLA	CHA-CBD-CGD-O1D
21	B	1223	CLA	CHA-CBD-CGD-O2D
21	B	1227	CLA	CHA-CBD-CGD-O1D
21	B	1227	CLA	CHA-CBD-CGD-O2D
21	B	1232	CLA	CHA-CBD-CGD-O2D
21	1	608	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	1	611	CLA	CHA-CBD-CGD-O1D
21	1	611	CLA	CHA-CBD-CGD-O2D
21	1	612	CLA	CHA-CBD-CGD-O1D
21	3	612	CLA	CHA-CBD-CGD-O1D
21	3	612	CLA	CHA-CBD-CGD-O2D
21	3	613	CLA	CHA-CBD-CGD-O2D
21	4	602	CLA	CHA-CBD-CGD-O1D
21	4	606	CLA	CHA-CBD-CGD-O1D
21	4	606	CLA	CHA-CBD-CGD-O2D
21	4	607	CLA	CHA-CBD-CGD-O1D
21	4	609	CLA	CHA-CBD-CGD-O1D
21	4	609	CLA	CHA-CBD-CGD-O2D
21	5	606	CLA	CHA-CBD-CGD-O1D
21	5	613	CLA	CHA-CBD-CGD-O1D
21	5	614	CLA	CHA-CBD-CGD-O1D
21	5	614	CLA	CHA-CBD-CGD-O2D
21	6	601	CLA	CHA-CBD-CGD-O1D
21	6	602	CLA	CHA-CBD-CGD-O1D
21	6	607	CLA	CHA-CBD-CGD-O1D
21	6	607	CLA	CHA-CBD-CGD-O2D
21	6	612	CLA	CHA-CBD-CGD-O2D
24	A	4006	BCR	C9-C10-C11-C12
21	A	1133	CLA	O1A-CGA-O2A-C1
21	3	601	CLA	O1A-CGA-O2A-C1
21	6	602	CLA	O1A-CGA-O2A-C1
32	L	5002	4RF	O17-C16-O18-C19
25	2	802	LHG	O7-C5-C6-O8
28	3	804	DGD	O1G-C1G-C2G-O2G
32	5	805	4RF	O21-C20-C39-O40
33	3	808	PTY	O4-C1-C6-O7
38	2	807	LMK	O1-C7-C8-O7
25	2	801	LHG	C9-C10-C11-C12
21	A	1113	CLA	O1A-CGA-O2A-C1
21	B	1216	CLA	O1A-CGA-O2A-C1
21	1	615	CLA	O1A-CGA-O2A-C1
39	2	808	P3H	O18-C17-O19-C20
21	B	1224	CLA	CAA-CBA-CGA-O2A
21	A	1110	CLA	C6-C7-C8-C9
21	B	1220	CLA	C6-C7-C8-C10
27	A	5004	LMU	O1'-C1-C2-C3
21	A	1012	CLA	C11-C12-C13-C14
21	A	1013	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
21	A	1101	CLA	C6-C7-C8-C9
21	A	1104	CLA	C14-C13-C15-C16
21	A	1107	CLA	C11-C10-C8-C9
21	A	1140	CLA	C11-C12-C13-C14
21	B	1203	CLA	C14-C13-C15-C16
21	B	1210	CLA	C6-C7-C8-C9
21	B	1225	CLA	C6-C7-C8-C9
21	B	1227	CLA	C11-C10-C8-C9
21	B	1228	CLA	C11-C10-C8-C9
21	3	608	CLA	C11-C12-C13-C14
21	5	603	CLA	C11-C10-C8-C9
28	B	5002	DGD	C7B-C8B-C9B-CAB
31	3	803	LMG	C36-C37-C38-C39
21	1	611	CLA	O1A-CGA-O2A-C1
25	2	802	LHG	O10-C23-O8-C6
25	A	5001	LHG	C7-C8-C9-C10
25	B	5001	LHG	C14-C15-C16-C17
21	B	1224	CLA	C8-C10-C11-C12
37	2	805	SQD	C5-C6-S-O8
37	3	806	SQD	C4-C5-C6-S
22	B	2002	PQN	C26-C27-C28-C30
24	A	4002	BCR	C37-C22-C23-C24
24	A	4007	BCR	C7-C8-C9-C34
24	K	4001	BCR	C7-C8-C9-C34
34	5	502	LUT	C27-C28-C29-C39
25	2	801	LHG	C12-C13-C14-C15
24	A	4002	BCR	C21-C22-C23-C24
24	A	4007	BCR	C7-C8-C9-C10
24	J	4002	BCR	C21-C22-C23-C24
21	B	1206	CLA	C1A-C2A-CAA-CBA
21	G	1603	CLA	C1A-C2A-CAA-CBA
21	1	607	CLA	C1A-C2A-CAA-CBA
21	1	608	CLA	C1A-C2A-CAA-CBA
21	1	611	CLA	C1A-C2A-CAA-CBA
21	2	606	CLA	C1A-C2A-CAA-CBA
21	2	608	CLA	C1A-C2A-CAA-CBA
21	5	607	CLA	C1A-C2A-CAA-CBA
31	F	5002	LMG	C10-C11-C12-C13
21	A	1138	CLA	C15-C16-C17-C18
39	2	808	P3H	C28-O27-P24-O23
21	A	1108	CLA	C2-C1-O2A-CGA
21	A	1131	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
21	A	1140	CLA	C2-C1-O2A-CGA
21	B	1239	CLA	C2-C1-O2A-CGA
21	3	607	CLA	C2-C1-O2A-CGA
21	4	601	CLA	C2-C1-O2A-CGA
24	A	4007	BCR	C9-C10-C11-C12
24	B	4003	BCR	C13-C14-C15-C16
24	J	4001	BCR	C19-C20-C21-C22
24	H	4001	BCR	C19-C20-C21-C22
25	A	5001	LHG	C3-O3-P-O6
25	1	802	LHG	C4-O6-P-O3
25	2	801	LHG	C3-O3-P-O6
33	3	808	PTY	C3-O11-P1-O14
21	3	605	CLA	C4-C3-C5-C6
21	B	1231	CLA	C3-C5-C6-C7
21	4	601	CLA	C3-C5-C6-C7
25	A	5002	LHG	C2-C3-O3-P
25	B	5001	LHG	C2-C3-O3-P
25	F	5001	LHG	C2-C3-O3-P
25	1	802	LHG	C2-C3-O3-P
39	5	806	P3H	C21-C22-O23-P24
21	G	1601	CLA	C2C-C3C-CAC-CBC
21	A	1110	CLA	C4B-C3B-CAB-CBB
21	A	1113	CLA	C4B-C3B-CAB-CBB
21	B	1219	CLA	C4B-C3B-CAB-CBB
21	2	603	CLA	C4B-C3B-CAB-CBB
25	F	5001	LHG	C3-O3-P-O4
25	F	5001	LHG	C4-O6-P-O5
25	2	801	LHG	C4-O6-P-O5
25	2	802	LHG	C3-O3-P-O5
25	2	803	LHG	C3-O3-P-O4
25	2	803	LHG	C4-O6-P-O4
25	6	801	LHG	C3-O3-P-O5
25	6	801	LHG	C4-O6-P-O5
33	L	5003	PTY	C3-O11-P1-O12
33	1	806	PTY	C5-O14-P1-O12
33	1	806	PTY	C5-O14-P1-O13
33	5	803	PTY	C5-O14-P1-O12
39	5	806	P3H	C22-O23-P24-O25
21	3	608	CLA	C16-C17-C18-C20
21	6	603	CLA	C2C-C3C-CAC-CBC
25	2	803	LHG	C9-C10-C11-C12
21	B	1023	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	B	1214	CLA	C8-C10-C11-C12
21	A	1117	CLA	CBA-CGA-O2A-C1
25	B	5001	LHG	O6-C4-C5-C6
25	1	801	LHG	O6-C4-C5-C6
25	2	801	LHG	O6-C4-C5-C6
25	5	801	LHG	O6-C4-C5-C6
27	A	5005	LMU	C6-C7-C8-C9
25	B	5001	LHG	O10-C23-O8-C6
21	B	1209	CLA	C2A-CAA-CBA-CGA
21	B	1211	CLA	C2A-CAA-CBA-CGA
25	F	5001	LHG	C35-C36-C37-C38
25	2	802	LHG	C18-C19-C20-C21
29	5	804	3PH	C22-C23-C24-C25
21	6	601	CLA	C2C-C3C-CAC-CBC
21	A	1012	CLA	CAD-CBD-CGD-O1D
21	B	1212	CLA	CAD-CBD-CGD-O1D
21	B	1218	CLA	CAD-CBD-CGD-O1D
21	B	1223	CLA	CAD-CBD-CGD-O1D
21	K	1404	CLA	CAD-CBD-CGD-O1D
21	4	606	CLA	CAD-CBD-CGD-O1D
21	4	609	CLA	CAD-CBD-CGD-O1D
25	2	803	LHG	C7-C8-C9-C10
32	L	5002	4RF	O21-C22-C24-C25
21	A	1133	CLA	C5-C6-C7-C8
21	B	1221	CLA	C5-C6-C7-C8
21	5	607	CLA	C10-C11-C12-C13
21	A	1117	CLA	C13-C15-C16-C17
21	2	601	CLA	C5-C6-C7-C8
25	2	801	LHG	C11-C12-C13-C14
21	B	1234	CLA	CBA-CGA-O2A-C1
21	B	1221	CLA	C16-C17-C18-C19
21	B	1231	CLA	C11-C12-C13-C14
21	A	1108	CLA	C4-C3-C5-C6
21	A	1101	CLA	C6-C7-C8-C10
21	A	1104	CLA	C11-C12-C13-C15
21	A	1107	CLA	C11-C10-C8-C7
21	A	1109	CLA	C11-C10-C8-C7
21	A	1112	CLA	C6-C7-C8-C10
21	A	1112	CLA	C12-C13-C15-C16
21	A	1125	CLA	C6-C7-C8-C10
21	A	1138	CLA	C11-C10-C8-C7
21	A	1139	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
21	B	1023	CLA	C6-C7-C8-C10
21	B	1202	CLA	C11-C12-C13-C15
21	B	1203	CLA	C12-C13-C15-C16
21	B	1225	CLA	C11-C12-C13-C15
21	B	1227	CLA	C11-C10-C8-C7
21	B	1228	CLA	C11-C10-C8-C7
21	L	1501	CLA	C11-C10-C8-C7
21	O	1801	CLA	CAD-CBD-CGD-O2D
21	1	604	CLA	C6-C7-C8-C10
21	2	612	CLA	C11-C10-C8-C7
21	2	615	CLA	C11-C12-C13-C15
21	4	607	CLA	C11-C10-C8-C7
21	5	605	CLA	C12-C13-C15-C16
25	B	5001	LHG	O6-C4-C5-O7
25	2	801	LHG	O6-C4-C5-O7
25	2	802	LHG	O6-C4-C5-O7
29	B	5003	3PH	O11-C1-C2-O21
29	F	5003	3PH	O11-C1-C2-O21
29	5	804	3PH	O11-C1-C2-O21
34	4	501	LUT	C25-C26-C27-C28
36	1	609	CHL	C11-C10-C8-C7
39	5	806	P3H	C42-C43-C44-C45
24	A	4002	BCR	C15-C16-C17-C18
32	5	805	4RF	C24-C22-O21-C20
25	1	803	LHG	O2-C2-C3-O3
21	3	612	CLA	C13-C15-C16-C17
21	A	1111	CLA	C2A-CAA-CBA-CGA
21	6	605	CLA	C2A-CAA-CBA-CGA
21	A	1105	CLA	C11-C12-C13-C15
21	L	1501	CLA	C16-C17-C18-C20
25	B	5001	LHG	C11-C12-C13-C14
33	O	5002	PTY	C31-C32-C33-C34
21	6	607	CLA	C3-C5-C6-C7
21	A	1136	CLA	C8-C10-C11-C12
29	B	5003	3PH	C1-C2-C3-O31
31	1	804	LMG	O1-C7-C8-C9
32	5	805	4RF	O23-C22-O21-C20
28	3	805	DGD	O2G-C2G-C3G-O3G
31	F	5002	LMG	O7-C8-C9-O8
33	4	804	PTY	O4-C1-C6-O7
29	F	5003	3PH	C23-C24-C25-C26
21	A	1107	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	2	802	LHG	C15-C16-C17-C18
37	3	806	SQD	C7-C8-C9-C10
29	F	5003	3PH	C39-C3A-C3B-C3C
28	2	806	DGD	C2G-C3G-O3G-C1D
31	4	803	LMG	C8-C7-O1-C1
21	A	1114	CLA	C3-C5-C6-C7
20	A	1011	CL0	CBA-CGA-O2A-C1
31	4	802	LMG	C14-C15-C16-C17
33	4	804	PTY	C16-C17-C18-C19
21	A	1012	CLA	C14-C13-C15-C16
21	A	1103	CLA	C14-C13-C15-C16
21	A	1119	CLA	C11-C12-C13-C14
21	A	1123	CLA	C11-C12-C13-C14
21	A	1124	CLA	C11-C10-C8-C9
21	A	1133	CLA	C11-C12-C13-C14
21	B	1023	CLA	C14-C13-C15-C16
21	B	1204	CLA	C11-C10-C8-C9
21	L	1501	CLA	C11-C12-C13-C14
21	1	612	CLA	C11-C10-C8-C9
21	2	604	CLA	C11-C10-C8-C9
21	2	605	CLA	C11-C12-C13-C14
21	3	601	CLA	C11-C10-C8-C9
21	4	612	CLA	C11-C10-C8-C9
28	B	5002	DGD	O1A-C1A-O1G-C1G
38	4	805	LMK	O8-C28-C29-C30
21	B	1213	CLA	C3-C5-C6-C7
21	B	1239	CLA	C3-C5-C6-C7
21	1	603	CLA	C3-C5-C6-C7
21	B	1231	CLA	C11-C12-C13-C15
36	6	610	CHL	C4C-C3C-CAC-CBC
21	B	1023	CLA	C2A-CAA-CBA-CGA
21	O	1803	CLA	C2A-CAA-CBA-CGA
21	A	1116	CLA	CAA-CBA-CGA-O2A
24	A	4001	BCR	C10-C11-C12-C13
24	A	4003	BCR	C18-C19-C20-C21
24	A	4004	BCR	C18-C19-C20-C21
24	H	4001	BCR	C18-C19-C20-C21
27	A	5004	LMU	C4'-C5'-C6'-O6'
21	B	1220	CLA	C6-C7-C8-C9
21	4	609	CLA	C11-C12-C13-C15
29	B	5003	3PH	C29-C2A-C2B-C2C
27	A	5004	LMU	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
28	B	5002	DGD	C6A-C7A-C8A-C9A
21	A	1110	CLA	C2B-C3B-CAB-CBB
21	A	1124	CLA	C2B-C3B-CAB-CBB
21	A	1133	CLA	C2B-C3B-CAB-CBB
21	A	1138	CLA	C2B-C3B-CAB-CBB
21	B	1219	CLA	C2B-C3B-CAB-CBB
21	B	1221	CLA	C2B-C3B-CAB-CBB
21	B	1228	CLA	C2B-C3B-CAB-CBB
21	1	606	CLA	C2B-C3B-CAB-CBB
21	1	612	CLA	C2B-C3B-CAB-CBB
21	2	603	CLA	C2B-C3B-CAB-CBB
21	2	604	CLA	C2B-C3B-CAB-CBB
21	2	612	CLA	C2B-C3B-CAB-CBB
21	4	606	CLA	C2B-C3B-CAB-CBB
21	4	609	CLA	C2B-C3B-CAB-CBB
27	B	5004	LMU	C7-C8-C9-C10
21	A	1120	CLA	C8-C10-C11-C12
21	B	1210	CLA	C4-C3-C5-C6
21	6	607	CLA	C4-C3-C5-C6
21	A	1138	CLA	CAA-CBA-CGA-O2A
25	2	801	LHG	O8-C23-C24-C25
21	A	1123	CLA	C8-C10-C11-C12
21	4	607	CLA	C5-C6-C7-C8
21	A	1110	CLA	C6-C7-C8-C10
21	6	607	CLA	C11-C12-C13-C15
27	6	805	LMU	C9-C10-C11-C12
21	B	1218	CLA	C10-C11-C12-C13
31	1	804	LMG	C11-C12-C13-C14
31	2	804	LMG	C9-C8-O7-C10
25	A	5002	LHG	O6-C4-C5-C6
20	A	1011	CL0	O1A-CGA-O2A-C1
25	F	5001	LHG	C24-C23-O8-C6
21	A	1102	CLA	C2-C1-O2A-CGA
21	A	1135	CLA	C2-C1-O2A-CGA
21	B	1210	CLA	C2-C1-O2A-CGA
21	B	1234	CLA	C2-C1-O2A-CGA
21	2	601	CLA	C2-C1-O2A-CGA
21	2	608	CLA	C2-C1-O2A-CGA
21	5	603	CLA	C2-C1-O2A-CGA
21	1	608	CLA	C6-C7-C8-C9
33	1	805	PTY	C34-C35-C36-C37
21	O	1803	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	B	1234	CLA	O1A-CGA-O2A-C1
25	A	5001	LHG	C26-C27-C28-C29
29	5	804	3PH	C25-C26-C27-C28
25	2	801	LHG	C2-C3-O3-P
25	6	801	LHG	C2-C3-O3-P
25	A	5002	LHG	C32-C33-C34-C35
25	A	5002	LHG	O6-C4-C5-O7
25	2	803	LHG	O6-C4-C5-O7
21	B	1212	CLA	C6-C7-C8-C9
21	3	612	CLA	C4-C3-C5-C6
24	A	4006	BCR	C23-C24-C25-C26
24	J	4002	BCR	C23-C24-C25-C30
24	I	4001	BCR	C23-C24-C25-C30
24	3	504	BCR	C23-C24-C25-C30
34	5	501	LUT	C1-C6-C7-C8
21	2	604	CLA	C10-C11-C12-C13
25	F	5001	LHG	C30-C31-C32-C33
21	A	1141	CLA	C2A-CAA-CBA-CGA
27	B	5004	LMU	C2'-C1'-O1'-C1
37	3	806	SQD	C2-C1-O6-C44
25	5	802	LHG	O7-C5-C6-O8
31	6	802	LMG	O7-C8-C9-O8
25	B	5001	LHG	C12-C13-C14-C15
33	1	805	PTY	C31-C32-C33-C34
28	B	5002	DGD	C2A-C1A-O1G-C1G
25	A	5002	LHG	C3-O3-P-O6
25	1	801	LHG	C3-O3-P-O6
25	1	802	LHG	C3-O3-P-O6
25	1	803	LHG	C3-O3-P-O6
25	1	803	LHG	C4-O6-P-O3
25	3	801	LHG	C3-O3-P-O6
25	4	801	LHG	C3-O3-P-O6
25	5	801	LHG	C3-O3-P-O6
25	5	802	LHG	C3-O3-P-O6
33	1	806	PTY	C3-O11-P1-O14
25	2	802	LHG	C7-C8-C9-C10
21	A	1127	CLA	C13-C15-C16-C17
28	3	804	DGD	O1G-C1G-C2G-C3G
21	6	608	CLA	C2C-C3C-CAC-CBC
25	A	5002	LHG	C28-C29-C30-C31
21	3	605	CLA	C15-C16-C17-C18
21	B	1206	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	B	5003	3PH	C2A-C2B-C2C-C2D
21	A	1125	CLA	C6-C7-C8-C9
21	A	1128	CLA	C11-C10-C8-C9
21	A	1139	CLA	C14-C13-C15-C16
21	B	1023	CLA	C6-C7-C8-C9
21	B	1202	CLA	C11-C12-C13-C14
21	1	615	CLA	C11-C10-C8-C9
21	4	609	CLA	C6-C7-C8-C9
21	5	605	CLA	C14-C13-C15-C16
36	1	609	CHL	C11-C10-C8-C9
24	B	4006	BCR	C19-C20-C21-C22
21	A	1131	CLA	C16-C17-C18-C19
21	B	1221	CLA	C16-C17-C18-C20
21	L	1501	CLA	C16-C17-C18-C19
21	1	615	CLA	C11-C12-C13-C15
21	5	612	CLA	C4C-C3C-CAC-CBC
29	B	5003	3PH	C2B-C2C-C2D-C2E
21	G	1601	CLA	C2A-CAA-CBA-CGA
24	K	4001	BCR	C11-C12-C13-C35
21	A	1133	CLA	C16-C17-C18-C20
21	6	605	CLA	C16-C17-C18-C19
25	1	801	LHG	C2-C3-O3-P
25	5	801	LHG	C2-C3-O3-P
21	L	1502	CLA	C15-C16-C17-C18
21	5	605	CLA	C5-C6-C7-C8
21	A	1116	CLA	C11-C10-C8-C7
21	B	1204	CLA	C5-C6-C7-C8
31	4	802	LMG	C22-C23-C24-C25
21	B	1207	CLA	C4-C3-C5-C6
25	1	801	LHG	C7-C8-C9-C10
25	1	802	LHG	O1-C1-C2-O2
21	A	1140	CLA	C2-C3-C5-C6
21	4	609	CLA	C11-C12-C13-C14
21	H	1701	CLA	CBA-CGA-O2A-C1
21	3	601	CLA	CBA-CGA-O2A-C1
21	A	1117	CLA	O1A-CGA-O2A-C1
21	H	1701	CLA	CAA-CBA-CGA-O2A
21	A	1132	CLA	C5-C6-C7-C8
21	A	1138	CLA	C4B-C3B-CAB-CBB
21	B	1228	CLA	C4B-C3B-CAB-CBB
21	1	606	CLA	C4B-C3B-CAB-CBB
21	4	601	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
21	4	606	CLA	C4B-C3B-CAB-CBB
21	K	1401	CLA	C2A-CAA-CBA-CGA
21	1	602	CLA	C2A-CAA-CBA-CGA
24	F	4001	BCR	C13-C14-C15-C16
24	O	4001	BCR	C19-C20-C21-C22
24	3	506	BCR	C19-C20-C21-C22
34	6	501	LUT	C29-C30-C31-C32
25	B	5001	LHG	C9-C10-C11-C12
33	O	5002	PTY	O14-C5-C6-O7
29	F	5003	3PH	C21-C22-C23-C24
21	A	1137	CLA	C4-C3-C5-C6
25	A	5002	LHG	C33-C34-C35-C36
21	H	1701	CLA	O1A-CGA-O2A-C1
38	4	805	LMK	C2-C3-C4-O2
21	5	602	CLA	CAA-CBA-CGA-O2A
21	B	1220	CLA	C2-C1-O2A-CGA
21	B	1231	CLA	C2-C1-O2A-CGA
21	1	604	CLA	C2-C1-O2A-CGA
21	5	604	CLA	C2-C1-O2A-CGA
21	6	601	CLA	C10-C11-C12-C13
21	3	608	CLA	C16-C17-C18-C19
25	1	801	LHG	C31-C32-C33-C34
29	5	804	3PH	C33-C34-C35-C36
21	B	1210	CLA	C2A-CAA-CBA-CGA
21	5	602	CLA	C2A-CAA-CBA-CGA
38	4	805	LMK	C8-C7-O1-C1
25	1	803	LHG	C25-C26-C27-C28
25	A	5002	LHG	C25-C26-C27-C28
21	H	1702	CLA	CAA-CBA-CGA-O1A
21	B	1218	CLA	C3A-C2A-CAA-CBA
21	K	1402	CLA	C3A-C2A-CAA-CBA
21	2	605	CLA	C3A-C2A-CAA-CBA
21	1	608	CLA	C6-C7-C8-C10
21	1	607	CLA	CAA-CBA-CGA-O2A
24	F	4002	BCR	C9-C10-C11-C12
32	5	805	4RF	C11-C12-C13-C14
21	3	605	CLA	C2-C3-C5-C6
21	A	1112	CLA	C6-C7-C8-C9
21	A	1116	CLA	C6-C7-C8-C9
21	A	1136	CLA	C11-C12-C13-C14
21	1	611	CLA	C11-C10-C8-C9
21	4	601	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
21	6	601	CLA	C11-C10-C8-C9
24	A	4004	BCR	C16-C17-C18-C36
24	A	4006	BCR	C16-C17-C18-C36
24	A	4007	BCR	C16-C17-C18-C36
24	F	4002	BCR	C16-C17-C18-C36
24	G	4001	BCR	C35-C13-C14-C15
24	G	4001	BCR	C16-C17-C18-C36
24	H	4001	BCR	C20-C21-C22-C37
24	I	4001	BCR	C35-C13-C14-C15
24	I	4002	BCR	C11-C10-C9-C34
24	3	506	BCR	C35-C13-C14-C15
24	3	506	BCR	C16-C17-C18-C36
25	6	801	LHG	C4-C5-C6-O8
28	B	5002	DGD	O1G-C1G-C2G-C3G
29	F	5003	3PH	C1-C2-C3-O31
33	3	807	PTY	O4-C1-C6-C5
34	1	501	LUT	C40-C33-C34-C35
34	5	503	LUT	C40-C33-C34-C35
21	1	601	CLA	C2A-CAA-CBA-CGA
33	1	805	PTY	C12-C13-C14-C15
37	2	805	SQD	C32-C33-C34-C35
21	1	615	CLA	C11-C12-C13-C14
21	6	607	CLA	C11-C12-C13-C14
24	O	4001	BCR	C11-C12-C13-C35
24	O	4001	BCR	C37-C22-C23-C24
24	3	503	BCR	C11-C12-C13-C35
26	A	5003	OCD	C10-C11-C12-C13
28	B	5002	DGD	CCB-CDB-CEB-CFB
39	2	808	P3H	C28-O27-P24-O25
37	3	806	SQD	C46-C45-O47-C7
21	5	605	CLA	C4-C3-C5-C6
21	A	1107	CLA	C1A-C2A-CAA-CBA
21	A	1129	CLA	C1A-C2A-CAA-CBA
21	A	1130	CLA	C1A-C2A-CAA-CBA
21	A	1140	CLA	C1A-C2A-CAA-CBA
21	1	604	CLA	C1A-C2A-CAA-CBA
21	4	606	CLA	C1A-C2A-CAA-CBA
21	A	1117	CLA	C11-C12-C13-C15
21	A	1133	CLA	C12-C13-C15-C16
21	B	1207	CLA	C12-C13-C15-C16
21	B	1211	CLA	C6-C7-C8-C10
21	B	1218	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
21	B	1237	CLA	C6-C7-C8-C10
21	1	605	CLA	C11-C12-C13-C15
21	2	601	CLA	C12-C13-C15-C16
21	5	604	CLA	C6-C7-C8-C10
36	5	609	CHL	C11-C10-C8-C7
39	2	808	P3H	C43-C44-C45-C46
21	B	1023	CLA	C10-C11-C12-C13
21	2	601	CLA	C8-C10-C11-C12
24	A	4006	BCR	C13-C14-C15-C16
24	B	4002	BCR	C15-C16-C17-C18
24	L	4001	BCR	C13-C14-C15-C16
24	4	503	BCR	C15-C16-C17-C18
34	5	504	LUT	C29-C30-C31-C32
27	A	5004	LMU	C9-C10-C11-C12
32	L	5002	4RF	C46-C47-C48-C49
21	B	1239	CLA	CAA-CBA-CGA-O2A
25	F	5001	LHG	O10-C23-O8-C6
33	1	805	PTY	C6-C5-O14-P1
21	3	605	CLA	C5-C6-C7-C8
21	K	1404	CLA	CAA-CBA-CGA-O1A
21	A	1122	CLA	C5-C6-C7-C8
21	A	1136	CLA	C4-C3-C5-C6
21	G	1601	CLA	C4C-C3C-CAC-CBC
21	K	1401	CLA	C2C-C3C-CAC-CBC
21	A	1113	CLA	C2B-C3B-CAB-CBB
21	4	601	CLA	C2B-C3B-CAB-CBB
21	K	1404	CLA	CAA-CBA-CGA-O2A
21	A	1110	CLA	C5-C6-C7-C8
21	B	1232	CLA	C5-C6-C7-C8
29	B	5003	3PH	C23-C24-C25-C26
25	5	801	LHG	C29-C30-C31-C32
24	A	4004	BCR	C16-C17-C18-C19
24	A	4006	BCR	C16-C17-C18-C19
24	A	4007	BCR	C16-C17-C18-C19
24	F	4002	BCR	C16-C17-C18-C19
24	G	4001	BCR	C12-C13-C14-C15
24	G	4001	BCR	C16-C17-C18-C19
24	H	4001	BCR	C20-C21-C22-C23
24	I	4001	BCR	C12-C13-C14-C15
24	I	4002	BCR	C11-C10-C9-C8
24	3	506	BCR	C12-C13-C14-C15
24	3	506	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
34	1	501	LUT	C32-C33-C34-C35
34	5	503	LUT	C32-C33-C34-C35
25	1	801	LHG	O7-C5-C6-O8
28	3	805	DGD	O1G-C1G-C2G-O2G
33	5	803	PTY	O4-C1-C6-O7
21	6	613	CLA	C2A-CAA-CBA-CGA
25	2	803	LHG	C26-C27-C28-C29
24	A	4001	BCR	C19-C20-C21-C22
24	H	4001	BCR	C15-C16-C17-C18
28	B	5002	DGD	C3A-C4A-C5A-C6A
33	4	804	PTY	C14-C15-C16-C17
21	3	603	CLA	C4-C3-C5-C6
25	5	801	LHG	C18-C19-C20-C21
21	B	1238	CLA	C2-C1-O2A-CGA
36	1	609	CHL	C2-C1-O2A-CGA
21	5	605	CLA	C2-C3-C5-C6
21	6	607	CLA	C2-C3-C5-C6
21	A	1123	CLA	O1A-CGA-O2A-C1
21	B	1210	CLA	O1A-CGA-O2A-C1
21	A	1117	CLA	C11-C12-C13-C14
21	A	1117	CLA	C14-C13-C15-C16
21	B	1218	CLA	C11-C12-C13-C14
21	B	1240	CLA	C14-C13-C15-C16
25	A	5002	LHG	C24-C23-O8-C6
25	A	5002	LHG	O10-C23-O8-C6
21	4	612	CLA	C10-C11-C12-C13
21	5	605	CLA	C2A-CAA-CBA-CGA
25	6	801	LHG	O10-C23-C24-C25
24	A	4007	BCR	C1-C6-C7-C8
24	B	4003	BCR	C23-C24-C25-C30
24	F	4002	BCR	C1-C6-C7-C8
24	I	4001	BCR	C23-C24-C25-C26
34	1	501	LUT	C1-C6-C7-C8
34	5	501	LUT	C5-C6-C7-C8
25	B	5001	LHG	C27-C28-C29-C30
21	5	601	CLA	CAA-CBA-CGA-O2A
21	B	1202	CLA	C4-C3-C5-C6
21	1	611	CLA	C4-C3-C5-C6
21	4	607	CLA	C4-C3-C5-C6
24	K	4001	BCR	C17-C18-C19-C20
34	5	502	LUT	C27-C28-C29-C30
21	B	1210	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	3	612	CLA	C2-C3-C5-C6
21	6	604	CLA	C2-C3-C5-C6
21	6	609	CLA	CAA-CBA-CGA-O1A
31	3	803	LMG	O10-C28-O8-C9
28	2	806	DGD	C5D-C6D-O5D-C1E
31	F	5002	LMG	C8-C7-O1-C1
31	3	802	LMG	C8-C7-O1-C1
21	B	1229	CLA	C13-C15-C16-C17
27	A	5005	LMU	C4'-C5'-C6'-O6'
21	A	1126	CLA	C3-C5-C6-C7
25	1	803	LHG	C26-C27-C28-C29
21	2	603	CLA	C8-C10-C11-C12
39	5	806	P3H	O39-C21-C22-O23
21	A	1122	CLA	C2A-CAA-CBA-CGA
21	B	1239	CLA	C2A-CAA-CBA-CGA
21	6	608	CLA	C2A-CAA-CBA-CGA
25	3	801	LHG	C4-C5-O7-C7
25	3	801	LHG	C6-C5-O7-C7
21	A	1129	CLA	C4B-C3B-CAB-CBB
25	B	5001	LHG	C24-C25-C26-C27
21	A	1108	CLA	C2-C3-C5-C6
21	A	1117	CLA	C12-C13-C15-C16
21	A	1124	CLA	C11-C10-C8-C7
21	A	1125	CLA	C12-C13-C15-C16
21	B	1204	CLA	C11-C10-C8-C7
21	3	612	CLA	C11-C10-C8-C7
21	4	607	CLA	C6-C7-C8-C10
21	5	614	CLA	C6-C7-C8-C10
21	6	601	CLA	C11-C10-C8-C7
21	6	613	CLA	CAA-CBA-CGA-O1A
25	2	802	LHG	C26-C27-C28-C29
25	5	801	LHG	O1-C1-C2-O2
33	5	803	PTY	C34-C35-C36-C37
24	F	4001	BCR	C19-C20-C21-C22
24	K	4001	BCR	C13-C14-C15-C16
21	6	613	CLA	CAA-CBA-CGA-O2A
25	4	801	LHG	C5-C4-O6-P
29	5	804	3PH	C24-C25-C26-C27
27	A	5004	LMU	C7-C8-C9-C10
31	3	803	LMG	C15-C16-C17-C18
21	K	1402	CLA	C3-C5-C6-C7
21	A	1125	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	5	603	CLA	CAA-CBA-CGA-O2A
21	B	1230	CLA	C10-C11-C12-C13
21	A	1128	CLA	C16-C17-C18-C20
21	A	1133	CLA	C16-C17-C18-C19
21	6	605	CLA	C16-C17-C18-C20
21	A	1123	CLA	CBA-CGA-O2A-C1
29	5	807	3PH	C1-O11-P-O14
35	1	502	XAT	C20-C13-C14-C15
21	A	1126	CLA	CAA-CBA-CGA-O2A
21	1	615	CLA	CAA-CBA-CGA-O2A
21	B	1212	CLA	C4-C3-C5-C6
21	B	1215	CLA	C4-C3-C5-C6
27	A	5005	LMU	C5-C6-C7-C8
33	6	804	PTY	C3-O11-P1-O14
21	1	604	CLA	C2-C3-C5-C6
25	A	5002	LHG	O7-C7-C8-C9
21	A	1106	CLA	C6-C7-C8-C9
21	A	1109	CLA	C11-C10-C8-C9
21	A	1138	CLA	C11-C10-C8-C9
21	B	1206	CLA	C11-C12-C13-C14
21	B	1211	CLA	C6-C7-C8-C9
21	B	1218	CLA	C6-C7-C8-C9
21	B	1237	CLA	C6-C7-C8-C9
21	2	612	CLA	C11-C10-C8-C9
21	2	615	CLA	C11-C12-C13-C14
21	4	601	CLA	C3A-C2A-CAA-CBA
21	B	1022	CLA	O1A-CGA-O2A-C1
21	A	1127	CLA	CAA-CBA-CGA-O2A
21	A	1136	CLA	CAA-CBA-CGA-O2A
21	4	601	CLA	CAA-CBA-CGA-O2A
37	2	805	SQD	O48-C23-C24-C25
21	A	1140	CLA	CAD-CBD-CGD-O2D
21	G	1603	CLA	CAD-CBD-CGD-O2D
21	4	607	CLA	CAD-CBD-CGD-O2D
21	6	605	CLA	CAD-CBD-CGD-O2D
21	6	609	CLA	CAD-CBD-CGD-O2D
36	5	610	CHL	CAD-CBD-CGD-O2D
25	1	801	LHG	C30-C31-C32-C33
27	A	5005	LMU	C9-C10-C11-C12
21	A	1121	CLA	C10-C11-C12-C13
29	5	804	3PH	O22-C21-O21-C2
21	K	1401	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	A	1121	CLA	CAA-CBA-CGA-O2A
21	3	602	CLA	CAA-CBA-CGA-O2A
21	3	611	CLA	CAA-CBA-CGA-O2A
31	3	803	LMG	C34-C35-C36-C37
36	2	609	CHL	C4-C3-C5-C6
21	A	1136	CLA	C2-C3-C5-C6
21	4	607	CLA	C2-C3-C5-C6
21	B	1210	CLA	CAA-CBA-CGA-O2A
21	B	1235	CLA	CAA-CBA-CGA-O2A
21	1	603	CLA	CAA-CBA-CGA-O2A
24	H	4001	BCR	C11-C12-C13-C14
24	K	4001	BCR	C7-C8-C9-C10
24	K	4001	BCR	C11-C12-C13-C14
24	O	4001	BCR	C11-C12-C13-C14
39	2	808	P3H	C48-C49-C50-C51
33	1	805	PTY	C33-C34-C35-C36
28	3	805	DGD	C1G-C2G-C3G-O3G
31	6	802	LMG	C7-C8-C9-O8
37	2	805	SQD	O6-C44-C45-C46
21	B	1210	CLA	CBA-CGA-O2A-C1
21	4	603	CLA	C5-C6-C7-C8
21	5	604	CLA	C10-C11-C12-C13
21	B	1207	CLA	CAA-CBA-CGA-O2A
21	3	613	CLA	CAA-CBA-CGA-O2A
29	B	5003	3PH	O21-C21-C22-C23
36	3	604	CHL	CAA-CBA-CGA-O2A
21	B	1023	CLA	C16-C17-C18-C20
21	B	1221	CLA	O2A-C1-C2-C3
36	4	613	CHL	O2A-C1-C2-C3
21	A	1136	CLA	C2A-CAA-CBA-CGA
21	B	1222	CLA	C2A-CAA-CBA-CGA
21	A	1120	CLA	C10-C11-C12-C13
31	4	802	LMG	C32-C33-C34-C35
21	2	603	CLA	CAA-CBA-CGA-O2A
21	4	609	CLA	CAA-CBA-CGA-O2A
25	2	803	LHG	O10-C23-C24-C25
25	1	801	LHG	C35-C36-C37-C38
25	F	5001	LHG	O9-C7-C8-C9
21	A	1103	CLA	CHA-CBD-CGD-O2D
21	A	1104	CLA	CHA-CBD-CGD-O1D
21	A	1104	CLA	CHA-CBD-CGD-O2D
21	A	1131	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	A	1133	CLA	CHA-CBD-CGD-O2D
21	A	1134	CLA	CHA-CBD-CGD-O1D
21	A	1134	CLA	CHA-CBD-CGD-O2D
21	A	1136	CLA	CHA-CBD-CGD-O1D
21	A	1136	CLA	CHA-CBD-CGD-O2D
21	A	1141	CLA	CHA-CBD-CGD-O1D
21	B	1203	CLA	CHA-CBD-CGD-O2D
21	B	1212	CLA	CHA-CBD-CGD-O2D
21	B	1214	CLA	CHA-CBD-CGD-O1D
21	B	1214	CLA	CHA-CBD-CGD-O2D
21	B	1228	CLA	CHA-CBD-CGD-O1D
21	B	1228	CLA	CHA-CBD-CGD-O2D
21	K	1401	CLA	CHA-CBD-CGD-O1D
21	K	1401	CLA	CHA-CBD-CGD-O2D
21	K	1403	CLA	CHA-CBD-CGD-O1D
21	K	1403	CLA	CHA-CBD-CGD-O2D
21	L	1501	CLA	CHA-CBD-CGD-O1D
21	L	1501	CLA	CHA-CBD-CGD-O2D
21	1	604	CLA	CHA-CBD-CGD-O2D
21	1	613	CLA	CHA-CBD-CGD-O1D
21	1	613	CLA	CHA-CBD-CGD-O2D
21	3	605	CLA	CHA-CBD-CGD-O1D
21	3	605	CLA	CHA-CBD-CGD-O2D
21	3	606	CLA	CHA-CBD-CGD-O1D
21	3	608	CLA	CHA-CBD-CGD-O2D
21	3	613	CLA	CHA-CBD-CGD-O1D
21	3	615	CLA	CHA-CBD-CGD-O1D
21	3	615	CLA	CHA-CBD-CGD-O2D
21	4	607	CLA	CHA-CBD-CGD-O2D
21	4	608	CLA	CHA-CBD-CGD-O1D
21	4	608	CLA	CHA-CBD-CGD-O2D
21	4	615	CLA	CHA-CBD-CGD-O1D
21	4	615	CLA	CHA-CBD-CGD-O2D
21	5	602	CLA	CHA-CBD-CGD-O1D
21	5	602	CLA	CHA-CBD-CGD-O2D
21	5	606	CLA	CHA-CBD-CGD-O2D
21	5	607	CLA	CHA-CBD-CGD-O1D
21	5	607	CLA	CHA-CBD-CGD-O2D
21	5	612	CLA	CHA-CBD-CGD-O2D
21	5	613	CLA	CHA-CBD-CGD-O2D
21	6	601	CLA	CHA-CBD-CGD-O2D
21	6	605	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	6	606	CLA	CHA-CBD-CGD-O2D
21	6	608	CLA	CHA-CBD-CGD-O1D
21	6	608	CLA	CHA-CBD-CGD-O2D
21	6	612	CLA	CHA-CBD-CGD-O1D
21	6	613	CLA	CHA-CBD-CGD-O1D
21	6	613	CLA	CHA-CBD-CGD-O2D
24	3	504	BCR	C15-C16-C17-C18
36	2	610	CHL	CHA-CBD-CGD-O1D
36	2	610	CHL	CHA-CBD-CGD-O2D
36	4	610	CHL	CHA-CBD-CGD-O1D
36	4	610	CHL	CHA-CBD-CGD-O2D
36	4	613	CHL	CHA-CBD-CGD-O1D
36	4	613	CHL	CHA-CBD-CGD-O2D
21	5	601	CLA	CAA-CBA-CGA-O1A
21	B	1236	CLA	CAA-CBA-CGA-O2A
25	2	801	LHG	C11-C10-C9-C8
21	A	1105	CLA	CAA-CBA-CGA-O2A
21	A	1115	CLA	CAA-CBA-CGA-O2A
21	K	1402	CLA	CAA-CBA-CGA-O2A
21	L	1504	CLA	CAA-CBA-CGA-O2A
25	1	801	LHG	O7-C7-C8-C9
28	B	5002	DGD	O2G-C2G-C3G-O3G
37	2	805	SQD	O47-C45-C46-O48
21	A	1102	CLA	CAA-CBA-CGA-O2A
21	A	1122	CLA	CAA-CBA-CGA-O2A
21	B	1237	CLA	CAA-CBA-CGA-O2A
21	2	601	CLA	CAA-CBA-CGA-O2A
33	5	803	PTY	C12-C11-C8-O7
21	4	605	CLA	CAA-CBA-CGA-O2A
33	4	804	PTY	C12-C11-C8-O7
39	2	808	P3H	C15-C16-C17-O19
28	B	5002	DGD	C3B-C4B-C5B-C6B
21	A	1101	CLA	C11-C10-C8-C7
21	A	1109	CLA	C6-C7-C8-C10
21	B	1207	CLA	C2-C3-C5-C6
21	B	1212	CLA	C2-C3-C5-C6
21	B	1215	CLA	C6-C7-C8-C10
21	H	1701	CLA	C11-C10-C8-C7
36	2	609	CHL	C2-C3-C5-C6
21	A	1129	CLA	C6-C7-C8-C10
21	A	1131	CLA	C16-C17-C18-C20
21	3	606	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	2	802	LHG	C5-C4-O6-P
21	K	1401	CLA	CAA-CBA-CGA-O1A
27	A	5004	LMU	C4-C5-C6-C7
21	A	1101	CLA	C11-C10-C8-C9
21	A	1125	CLA	C14-C13-C15-C16
21	B	1022	CLA	C11-C12-C13-C14
21	B	1022	CLA	C14-C13-C15-C16
21	B	1211	CLA	C11-C10-C8-C9
21	B	1225	CLA	C14-C13-C15-C16
21	1	604	CLA	C6-C7-C8-C9
21	1	605	CLA	C11-C12-C13-C14
21	2	601	CLA	C14-C13-C15-C16
21	4	607	CLA	C11-C10-C8-C9
21	5	603	CLA	CAA-CBA-CGA-O1A
21	A	1129	CLA	C2B-C3B-CAB-CBB
21	5	606	CLA	C2B-C3B-CAB-CBB
21	6	606	CLA	C2B-C3B-CAB-CBB
25	A	5002	LHG	C24-C25-C26-C27
21	G	1603	CLA	CAA-CBA-CGA-O2A
33	5	803	PTY	C11-C12-C13-C14
29	F	5003	3PH	O21-C21-C22-C23
31	1	804	LMG	O8-C28-C29-C30
31	6	802	LMG	O7-C10-C11-C12
36	6	610	CHL	CAA-CBA-CGA-O2A
21	A	1132	CLA	C2A-CAA-CBA-CGA
21	L	1501	CLA	C2A-CAA-CBA-CGA
29	B	5003	3PH	C28-C29-C2A-C2B
31	2	804	LMG	C33-C34-C35-C36
33	5	803	PTY	C39-C40-C41-C42
21	B	1207	CLA	CAA-CBA-CGA-O1A
21	4	601	CLA	CAA-CBA-CGA-O1A
21	B	1240	CLA	C8-C10-C11-C12
25	2	802	LHG	O8-C23-C24-C25
21	B	1236	CLA	CAA-CBA-CGA-O1A
25	A	5002	LHG	O9-C7-C8-C9
21	B	1022	CLA	CBA-CGA-O2A-C1
21	A	1141	CLA	C1A-C2A-CAA-CBA
21	B	1022	CLA	C1A-C2A-CAA-CBA
21	K	1404	CLA	C1A-C2A-CAA-CBA
21	O	1802	CLA	CHA-CBD-CGD-O2D
21	1	613	CLA	C1A-C2A-CAA-CBA
21	2	605	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	3	602	CLA	C1A-C2A-CAA-CBA
21	3	607	CLA	C1A-C2A-CAA-CBA
21	3	608	CLA	C1A-C2A-CAA-CBA
21	6	609	CLA	C1A-C2A-CAA-CBA
21	B	1210	CLA	CAA-CBA-CGA-O1A
21	3	613	CLA	CAA-CBA-CGA-O1A
21	B	1240	CLA	C13-C15-C16-C17
21	1	611	CLA	C5-C6-C7-C8
25	2	801	LHG	C24-C25-C26-C27
21	A	1105	CLA	CAA-CBA-CGA-O1A
21	A	1121	CLA	CAA-CBA-CGA-O1A
21	A	1125	CLA	CAA-CBA-CGA-O1A
21	A	1136	CLA	CAA-CBA-CGA-O1A
21	1	615	CLA	CAA-CBA-CGA-O1A
21	3	601	CLA	CAA-CBA-CGA-O2A
21	B	1204	CLA	C2A-CAA-CBA-CGA
21	B	1217	CLA	C2A-CAA-CBA-CGA
21	6	602	CLA	C2A-CAA-CBA-CGA
25	2	801	LHG	C10-C11-C12-C13
21	B	1237	CLA	CAA-CBA-CGA-O1A
21	3	611	CLA	CAA-CBA-CGA-O1A
21	4	609	CLA	CAA-CBA-CGA-O1A
29	B	5003	3PH	O22-C21-C22-C23
21	B	1235	CLA	C8-C10-C11-C12
31	4	803	LMG	C11-C12-C13-C14
21	5	613	CLA	CAA-CBA-CGA-O1A
31	4	803	LMG	O8-C28-C29-C30
21	A	1137	CLA	C5-C6-C7-C8
21	A	1115	CLA	CAA-CBA-CGA-O1A
21	A	1122	CLA	CAA-CBA-CGA-O1A
21	A	1127	CLA	CAA-CBA-CGA-O1A
21	B	1215	CLA	C2-C3-C5-C6
25	A	5002	LHG	C14-C15-C16-C17
21	A	1121	CLA	C4C-C3C-CAC-CBC
21	G	1603	CLA	C4B-C3B-CAB-CBB
22	A	2001	PQN	C3-C11-C12-C13
25	3	801	LHG	C3-O3-P-O5
25	5	802	LHG	C3-O3-P-O5
33	O	5002	PTY	C3-O11-P1-O13
36	5	609	CHL	C4B-C3B-CAB-CBB
21	2	603	CLA	CAA-CBA-CGA-O1A
25	1	801	LHG	O9-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
36	3	604	CHL	CAA-CBA-CGA-O1A
37	2	805	SQD	O10-C23-C24-C25
33	1	806	PTY	N1-C2-C3-O11
21	K	1402	CLA	CAA-CBA-CGA-O1A
21	L	1504	CLA	CAA-CBA-CGA-O1A
21	1	603	CLA	CAA-CBA-CGA-O1A
29	F	5003	3PH	O22-C21-C22-C23
31	6	802	LMG	O9-C10-C11-C12
39	2	808	P3H	C15-C16-C17-O18
21	5	613	CLA	CAA-CBA-CGA-O2A
21	B	1021	CLA	C16-C17-C18-C19
21	1	603	CLA	C11-C12-C13-C15
21	A	1112	CLA	C2C-C3C-CAC-CBC
35	1	502	XAT	C30-C31-C32-C33
25	2	801	LHG	C7-C8-C9-C10
21	A	1101	CLA	C2A-CAA-CBA-CGA
21	2	605	CLA	C2A-CAA-CBA-CGA
21	4	606	CLA	C2A-CAA-CBA-CGA
21	B	1237	CLA	C5-C6-C7-C8
21	5	603	CLA	C4C-C3C-CAC-CBC
21	G	1602	CLA	CAA-CBA-CGA-O2A
25	A	5002	LHG	O8-C23-C24-C25
21	A	1102	CLA	CAA-CBA-CGA-O1A
21	3	602	CLA	CAA-CBA-CGA-O1A
33	5	803	PTY	C12-C11-C8-O10
21	A	1101	CLA	C4-C3-C5-C6
21	B	1211	CLA	C4-C3-C5-C6
25	5	801	LHG	C14-C15-C16-C17
21	A	1118	CLA	CAD-CBD-CGD-O1D
21	A	1131	CLA	CAD-CBD-CGD-O1D
21	A	1138	CLA	CAD-CBD-CGD-O1D
21	B	1022	CLA	CAD-CBD-CGD-O1D
21	B	1203	CLA	CAD-CBD-CGD-O1D
21	B	1214	CLA	CAD-CBD-CGD-O1D
21	G	1601	CLA	CAD-CBD-CGD-O1D
21	1	605	CLA	CAD-CBD-CGD-O1D
21	2	607	CLA	CAD-CBD-CGD-O1D
33	6	804	PTY	C2-C3-O11-P1
31	4	802	LMG	C10-C11-C12-C13
21	B	1235	CLA	CAA-CBA-CGA-O1A
21	2	601	CLA	CAA-CBA-CGA-O1A
21	6	606	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	4	601	CLA	C10-C11-C12-C13
21	A	1109	CLA	C6-C7-C8-C9
21	A	1111	CLA	C11-C12-C13-C14
21	A	1133	CLA	C14-C13-C15-C16
21	B	1215	CLA	C6-C7-C8-C9
21	B	1229	CLA	C6-C7-C8-C9
21	B	1230	CLA	C11-C10-C8-C9
21	B	1231	CLA	C6-C7-C8-C9
21	6	604	CLA	C11-C10-C8-C9
32	L	5002	4RF	C48-C49-C50-C51
26	A	5003	OCD	C15-C16-C17-C18
21	B	1206	CLA	C8-C10-C11-C12
25	1	802	LHG	O10-C23-C24-C25
25	2	802	LHG	O10-C23-C24-C25
21	B	1202	CLA	CAA-CBA-CGA-O2A
21	B	1220	CLA	CAA-CBA-CGA-O2A
21	L	1503	CLA	CAA-CBA-CGA-O2A
21	1	605	CLA	CAA-CBA-CGA-O2A
21	4	602	CLA	CAA-CBA-CGA-O2A
25	4	801	LHG	O8-C23-C24-C25
28	2	806	DGD	O1G-C1A-C2A-C3A
39	2	808	P3H	O39-C40-C42-C43
21	G	1603	CLA	CAA-CBA-CGA-O1A
32	5	805	4RF	C09-C10-C11-C12
21	A	1116	CLA	C2A-CAA-CBA-CGA
21	A	1131	CLA	CAA-CBA-CGA-O2A
21	F	1301	CLA	CAA-CBA-CGA-O2A
21	2	608	CLA	CAA-CBA-CGA-O2A
21	3	606	CLA	CAA-CBA-CGA-O2A
28	3	805	DGD	O1G-C1A-C2A-C3A
28	B	5002	DGD	CAA-CBA-CCA-CDA
21	A	1131	CLA	CAA-CBA-CGA-O1A
21	B	1217	CLA	C4-C3-C5-C6
21	B	1227	CLA	C4-C3-C5-C6
21	6	604	CLA	C4-C3-C5-C6
21	A	1107	CLA	C12-C13-C15-C16
21	A	1121	CLA	C3A-C2A-CAA-CBA
21	A	1137	CLA	C2-C3-C5-C6
21	A	1137	CLA	C11-C10-C8-C7
21	B	1022	CLA	C11-C12-C13-C15
21	B	1211	CLA	C11-C10-C8-C7
21	B	1218	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
21	B	1222	CLA	C11-C10-C8-C7
21	B	1229	CLA	C6-C7-C8-C10
21	O	1801	CLA	CHA-CBD-CGD-O1D
21	3	603	CLA	C2-C3-C5-C6
21	3	611	CLA	C6-C7-C8-C10
21	5	604	CLA	C12-C13-C15-C16
21	5	605	CLA	C11-C12-C13-C15
22	B	2002	PQN	C21-C22-C23-C25
21	4	605	CLA	CAA-CBA-CGA-O1A
21	6	603	CLA	CAA-CBA-CGA-O1A
31	4	803	LMG	O10-C28-C29-C30
33	4	804	PTY	C12-C11-C8-O10
20	A	1011	CL0	CAA-CBA-CGA-O2A
21	A	1135	CLA	CAA-CBA-CGA-O2A
21	B	1023	CLA	CAA-CBA-CGA-O2A
21	4	608	CLA	CAA-CBA-CGA-O2A
24	A	4001	BCR	C7-C8-C9-C10
24	B	4005	BCR	C11-C12-C13-C14
24	B	4006	BCR	C21-C22-C23-C24
24	3	503	BCR	C11-C12-C13-C14
35	6	504	XAT	C31-C32-C33-C34
21	4	602	CLA	CAA-CBA-CGA-O1A
34	5	503	LUT	C33-C34-C35-C15
29	5	804	3PH	C34-C35-C36-C37
27	B	5004	LMU	C2-C1-O1'-C1'
21	A	1108	CLA	CAA-CBA-CGA-O2A
21	B	1201	CLA	CAA-CBA-CGA-O2A
21	B	1221	CLA	CAA-CBA-CGA-O2A
27	B	5004	LMU	O5'-C1'-O1'-C1
21	A	1103	CLA	C13-C15-C16-C17
21	B	1202	CLA	CAA-CBA-CGA-O1A
21	1	605	CLA	CAA-CBA-CGA-O1A
21	3	601	CLA	CAA-CBA-CGA-O1A
21	6	606	CLA	CAA-CBA-CGA-O1A
31	1	804	LMG	O10-C28-C29-C30
21	A	1110	CLA	CBA-CGA-O2A-C1
31	3	803	LMG	C29-C28-O8-C9
29	5	804	3PH	C22-C21-O21-C2
21	A	1107	CLA	C5-C6-C7-C8
21	5	603	CLA	C2C-C3C-CAC-CBC
21	A	1104	CLA	CAA-CBA-CGA-O2A
21	A	1129	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	B	1223	CLA	CAA-CBA-CGA-O2A
21	6	603	CLA	CAA-CBA-CGA-O2A
25	5	802	LHG	O8-C23-C24-C25
25	1	802	LHG	C11-C10-C9-C8
21	B	1214	CLA	C15-C16-C17-C18
21	B	1201	CLA	CAA-CBA-CGA-O1A
21	4	608	CLA	CAA-CBA-CGA-O1A
21	A	1113	CLA	C16-C17-C18-C20
21	B	1021	CLA	C16-C17-C18-C20
21	A	1108	CLA	CAA-CBA-CGA-O1A
21	2	608	CLA	CAA-CBA-CGA-O1A
25	4	801	LHG	O10-C23-C24-C25
28	2	806	DGD	O1A-C1A-C2A-C3A
21	2	602	CLA	CAA-CBA-CGA-O2A
21	5	612	CLA	CAA-CBA-CGA-O2A
31	F	5002	LMG	C4-C5-C6-O5

There are no ring outliers.

248 monomers are involved in 1116 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	5	603	CLA	6	0
24	B	4005	BCR	2	0
21	B	1206	CLA	11	0
21	5	612	CLA	4	0
24	F	4002	BCR	5	0
21	B	1209	CLA	4	0
24	L	4002	BCR	2	0
27	B	5004	LMU	2	0
36	5	609	CHL	33	0
36	5	610	CHL	7	0
37	2	805	SQD	2	0
25	F	5001	LHG	2	0
24	3	503	BCR	2	0
21	B	1218	CLA	2	0
21	1	601	CLA	25	0
21	3	610	CLA	19	0
21	5	613	CLA	7	0
24	B	4006	BCR	4	0
31	1	804	LMG	1	0
35	4	502	XAT	3	0
21	A	1122	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	1138	CLA	5	0
21	B	1216	CLA	2	0
21	A	1116	CLA	10	0
21	2	605	CLA	1	0
36	2	609	CHL	3	0
24	A	4006	BCR	2	0
21	B	1239	CLA	8	0
21	A	1106	CLA	3	0
21	A	1129	CLA	1	0
21	5	604	CLA	28	0
35	2	502	XAT	3	0
24	B	4004	BCR	3	0
21	A	1013	CLA	8	0
21	6	604	CLA	4	0
29	B	5003	3PH	2	0
21	B	1234	CLA	1	0
20	A	1011	CL0	10	0
21	A	1105	CLA	4	0
21	G	1602	CLA	7	0
21	H	1701	CLA	4	0
21	A	1114	CLA	16	0
21	1	611	CLA	13	0
21	4	615	CLA	1	0
21	B	1210	CLA	4	0
21	6	613	CLA	8	0
21	A	1140	CLA	7	0
21	A	1120	CLA	10	0
21	L	1504	CLA	8	0
29	5	804	3PH	3	0
21	A	1104	CLA	4	0
21	3	605	CLA	5	0
24	L	4001	BCR	3	0
21	K	1401	CLA	6	0
21	B	1215	CLA	6	0
21	2	612	CLA	3	0
21	A	1115	CLA	12	0
21	A	1103	CLA	3	0
21	B	1229	CLA	3	0
24	A	4007	BCR	8	0
25	5	801	LHG	11	0
21	6	601	CLA	25	0
24	I	4002	BCR	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	5002	LHG	3	0
36	2	610	CHL	2	0
33	6	804	PTY	1	0
21	5	606	CLA	24	0
21	A	1126	CLA	8	0
21	A	1109	CLA	3	0
21	B	1213	CLA	3	0
21	B	1219	CLA	5	0
28	3	804	DGD	1	0
21	6	606	CLA	13	0
21	B	1205	CLA	3	0
34	5	501	LUT	5	0
27	A	5004	LMU	1	0
21	L	1502	CLA	13	0
21	B	1022	CLA	10	0
24	G	4001	BCR	20	0
25	B	5001	LHG	3	0
21	1	605	CLA	2	0
21	A	1133	CLA	3	0
21	B	1214	CLA	3	0
28	2	806	DGD	2	0
21	A	1130	CLA	2	0
21	A	1139	CLA	5	0
21	G	1603	CLA	1	0
34	5	503	LUT	7	0
24	A	4004	BCR	8	0
21	B	1240	CLA	4	0
31	3	802	LMG	2	0
21	2	603	CLA	2	0
31	4	802	LMG	2	0
24	4	503	BCR	1	0
21	A	1107	CLA	3	0
21	3	608	CLA	4	0
21	A	1118	CLA	1	0
21	A	1119	CLA	8	0
21	3	612	CLA	6	0
21	4	604	CLA	13	0
31	F	5002	LMG	3	0
21	B	1232	CLA	2	0
24	K	4001	BCR	8	0
21	K	1402	CLA	14	0
39	5	806	P3H	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	1222	CLA	3	0
21	A	1125	CLA	4	0
21	A	1134	CLA	6	0
21	6	602	CLA	10	0
21	6	607	CLA	4	0
24	B	4001	BCR	19	0
21	1	603	CLA	1	0
21	6	608	CLA	2	0
21	6	612	CLA	7	0
25	A	5001	LHG	3	0
21	4	601	CLA	3	0
21	B	1212	CLA	17	0
21	6	609	CLA	1	0
36	6	610	CHL	7	0
27	6	805	LMU	1	0
33	5	803	PTY	10	0
21	1	608	CLA	1	0
21	1	612	CLA	3	0
21	5	601	CLA	4	0
21	B	1235	CLA	5	0
36	4	611	CHL	1	0
21	B	1228	CLA	2	0
37	6	803	SQD	1	0
21	5	607	CLA	2	0
21	A	1111	CLA	2	0
21	A	1131	CLA	3	0
21	B	1224	CLA	2	0
24	H	4001	BCR	5	0
35	3	502	XAT	7	0
21	B	1237	CLA	2	0
24	B	4003	BCR	6	0
21	3	602	CLA	1	0
24	I	4001	BCR	9	0
21	A	1123	CLA	1	0
21	4	609	CLA	3	0
21	B	1202	CLA	1	0
25	2	801	LHG	3	0
21	A	1113	CLA	14	0
21	5	605	CLA	15	0
21	4	607	CLA	4	0
22	A	2001	PQN	3	0
21	A	1012	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	L	1501	CLA	3	0
21	A	1128	CLA	5	0
24	3	506	BCR	3	0
21	B	1227	CLA	5	0
21	B	1231	CLA	5	0
21	1	607	CLA	1	0
29	5	807	3PH	2	0
24	A	4002	BCR	6	0
24	1	504	BCR	5	0
32	5	805	4RF	1	0
21	B	1203	CLA	5	0
21	A	1110	CLA	1	0
21	K	1403	CLA	6	0
24	B	4002	BCR	4	0
31	3	803	LMG	17	0
21	2	604	CLA	5	0
34	4	501	LUT	4	0
35	1	502	XAT	2	0
21	4	602	CLA	3	0
21	A	1102	CLA	5	0
21	B	1236	CLA	2	0
21	5	608	CLA	12	0
21	1	602	CLA	4	0
21	6	603	CLA	20	0
21	A	1141	CLA	4	0
21	O	1801	CLA	2	0
24	A	4005	BCR	2	0
21	A	1112	CLA	14	0
21	O	1803	CLA	1	0
21	A	1108	CLA	3	0
21	3	603	CLA	8	0
21	B	1223	CLA	6	0
36	1	610	CHL	4	0
21	5	614	CLA	8	0
21	B	1226	CLA	5	0
21	3	606	CLA	3	0
21	B	1207	CLA	16	0
21	B	1208	CLA	19	0
28	3	805	DGD	5	0
34	6	501	LUT	22	0
21	B	1225	CLA	5	0
21	B	1217	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	B	5002	DGD	5	0
35	6	504	XAT	9	0
21	B	1021	CLA	3	0
34	5	504	LUT	16	0
36	3	604	CHL	3	0
24	F	4001	BCR	19	0
27	A	5005	LMU	1	0
21	F	1301	CLA	2	0
25	2	803	LHG	2	0
34	5	502	LUT	13	0
21	B	1023	CLA	25	0
35	6	502	XAT	5	0
24	J	4001	BCR	3	0
21	1	604	CLA	6	0
21	L	1503	CLA	5	0
21	A	1121	CLA	31	0
21	A	1136	CLA	3	0
24	J	4002	BCR	4	0
25	2	802	LHG	3	0
32	L	5002	4RF	2	0
21	4	603	CLA	3	0
24	O	4001	BCR	7	0
21	1	606	CLA	2	0
37	3	806	SQD	2	0
36	1	609	CHL	3	0
25	1	803	LHG	1	0
21	A	1124	CLA	3	0
21	A	1137	CLA	2	0
34	3	501	LUT	9	0
21	B	1211	CLA	1	0
22	B	2002	PQN	7	0
24	A	4001	BCR	9	0
21	6	605	CLA	9	0
21	K	1404	CLA	9	0
24	3	504	BCR	10	0
24	2	503	BCR	1	0
21	B	1238	CLA	3	0
21	B	1230	CLA	5	0
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21	J	1901	CLA	3	0
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33	O	5002	PTY	5	0

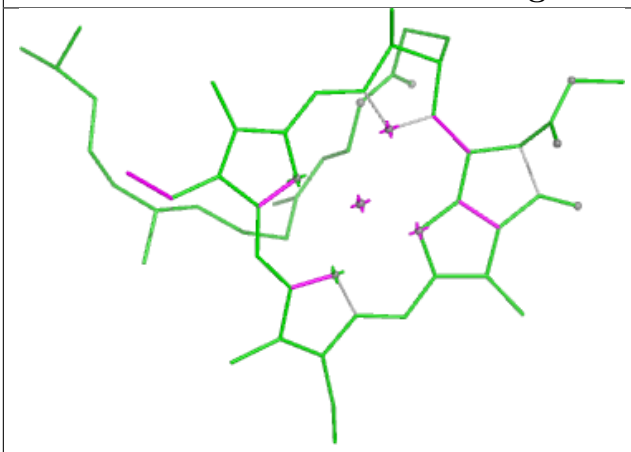
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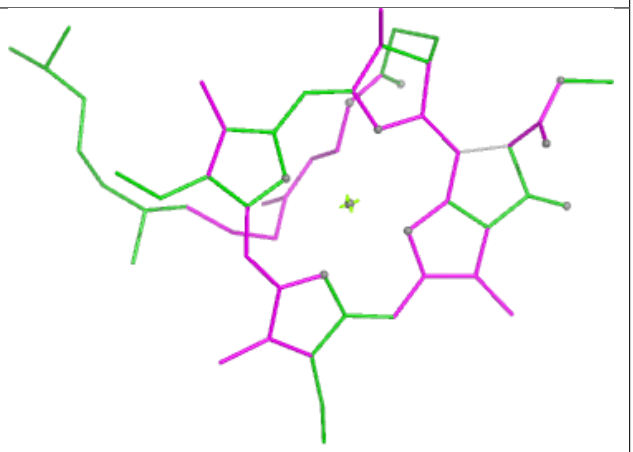
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	2	501	LUT	6	0
21	3	601	CLA	2	0
31	6	802	LMG	12	0
21	A	1132	CLA	20	0
21	A	1135	CLA	6	0
36	2	611	CHL	3	0
21	B	1204	CLA	2	0
21	3	613	CLA	1	0
21	5	602	CLA	1	0
24	A	4003	BCR	7	0
21	A	1127	CLA	1	0
21	B	1221	CLA	2	0
21	2	601	CLA	2	0
21	G	1601	CLA	10	0
34	1	501	LUT	7	0
21	B	1220	CLA	2	0
21	4	605	CLA	1	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.

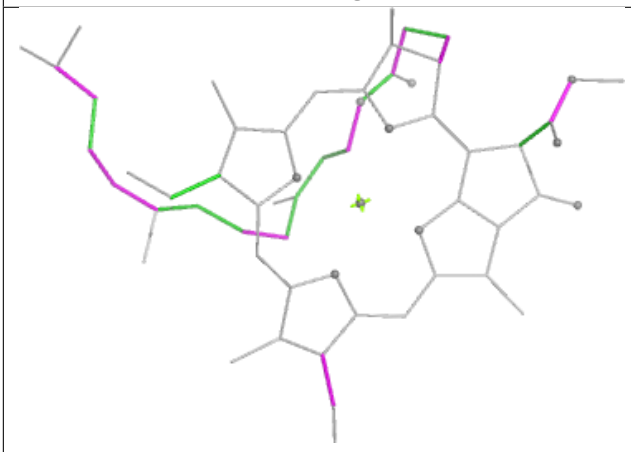
Ligand CLA 5 603



Bond lengths



Bond angles

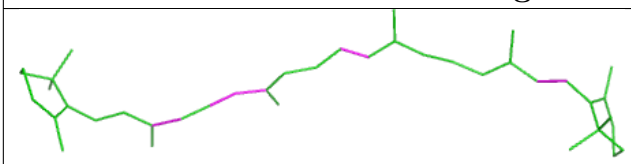


Torsions

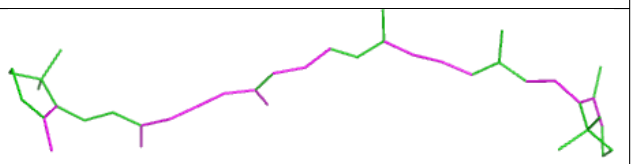


Rings

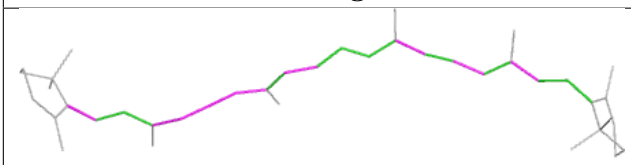
Ligand BCR B 4005



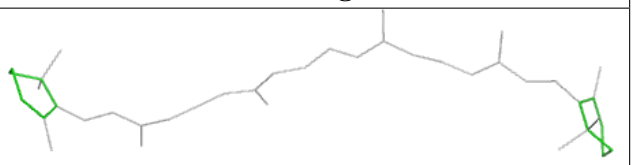
Bond lengths



Bond angles

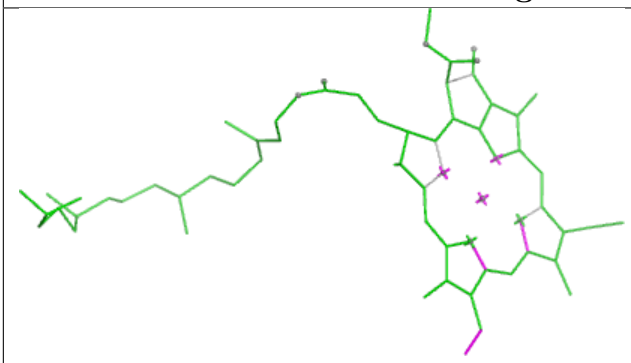


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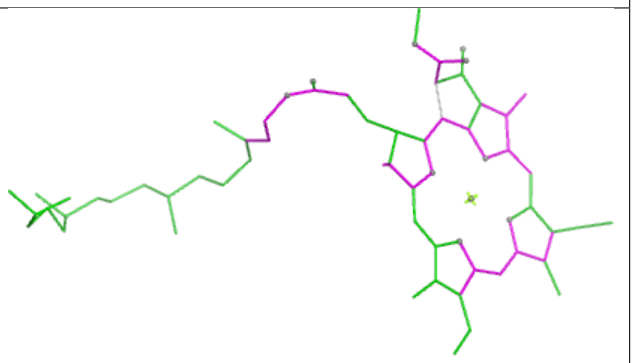


Rings

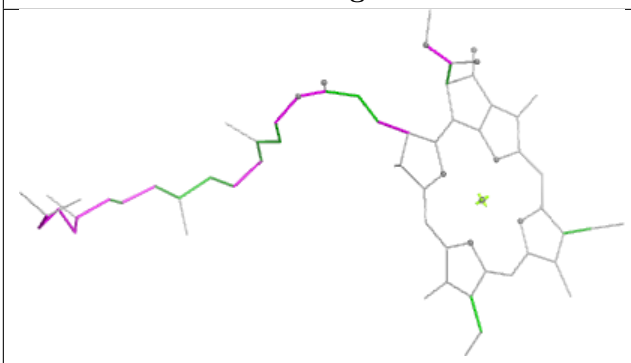
Ligand CLA B 1206



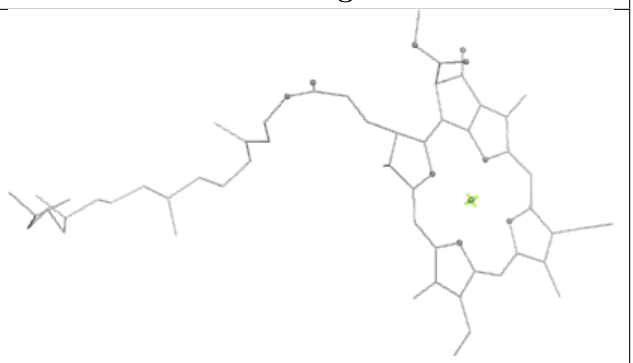
Bond lengths



Bond angles

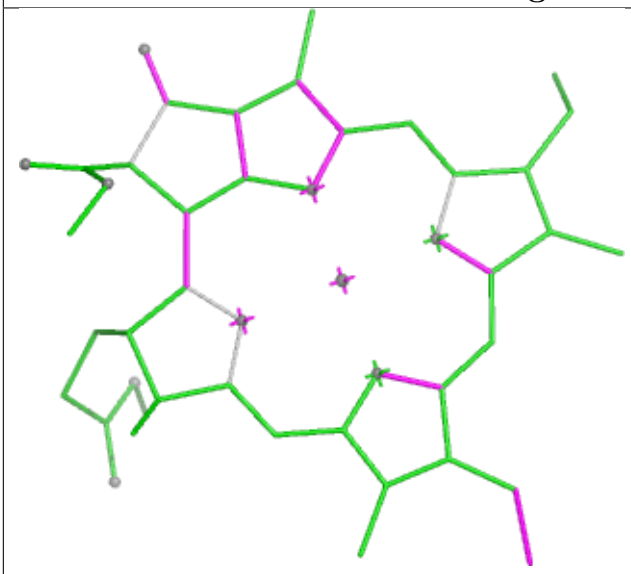


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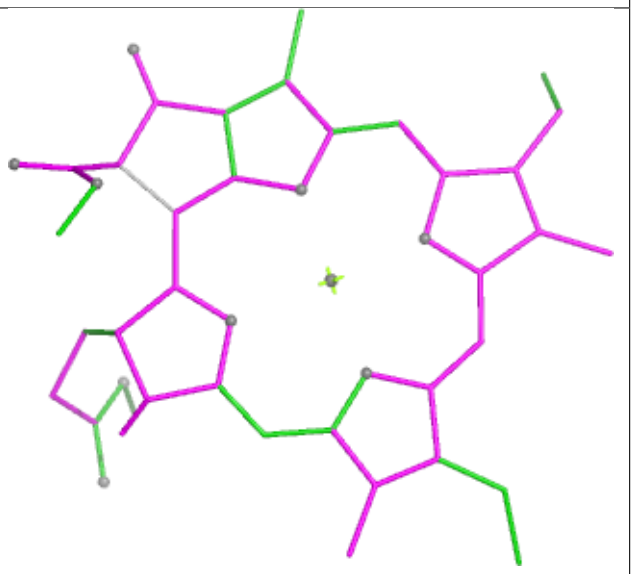


Rings

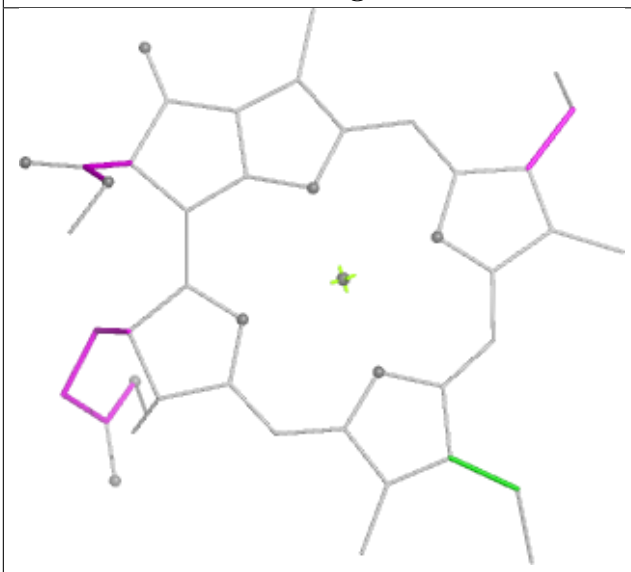
Ligand CLA 5 612



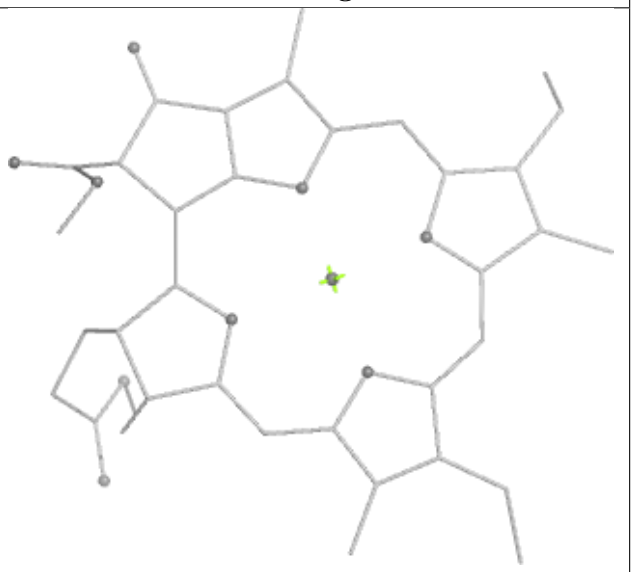
Bond lengths



Bond angles

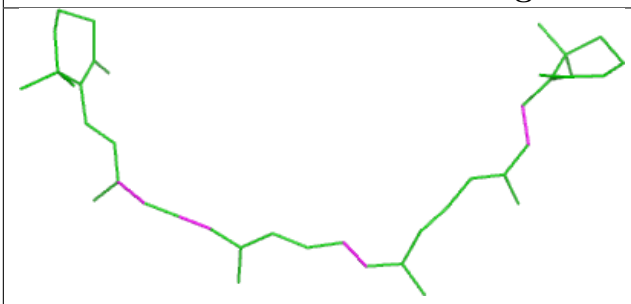


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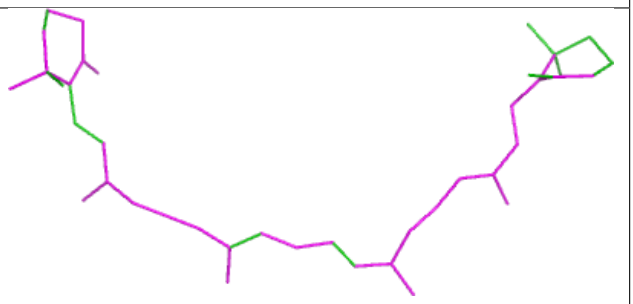


Rings

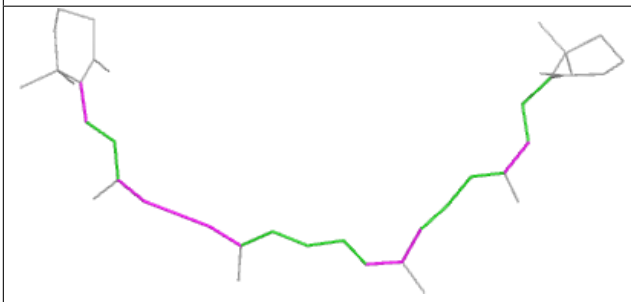
Ligand BCR F 4002



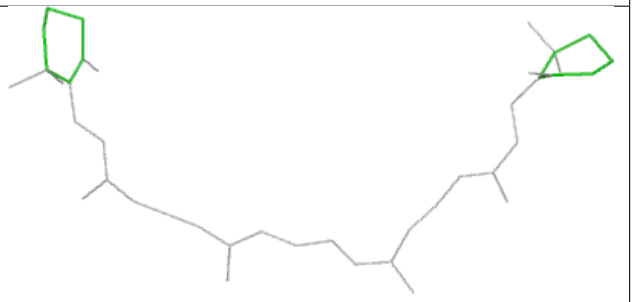
Bond lengths



Bond angles

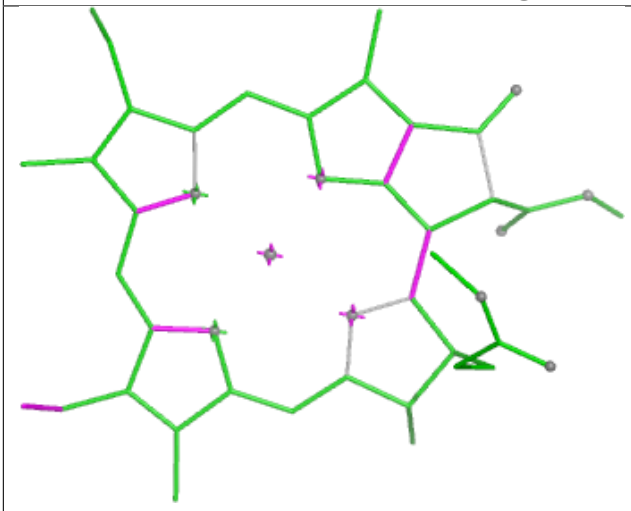


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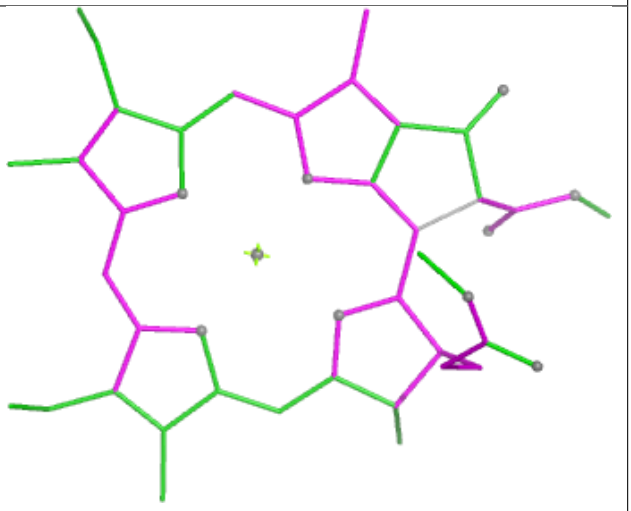


Rings

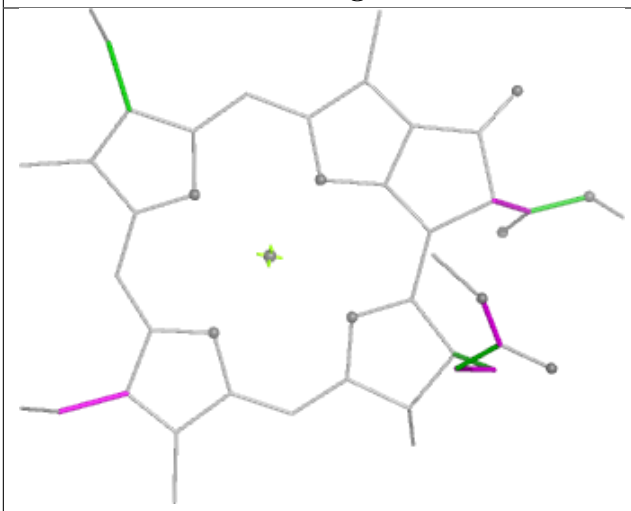
Ligand CLA B 1209



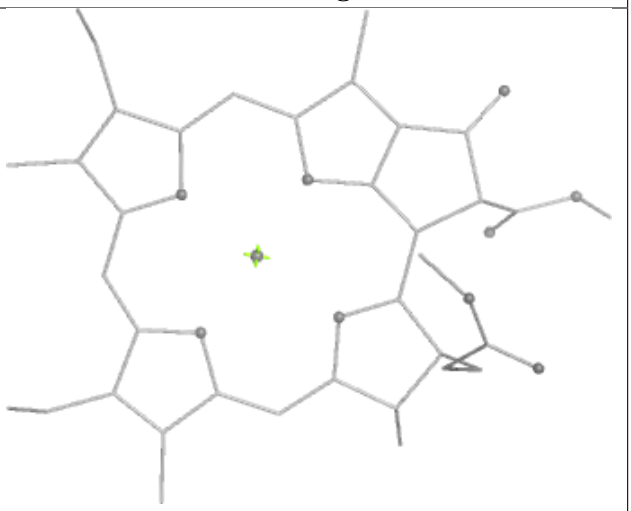
Bond lengths



Bond angles

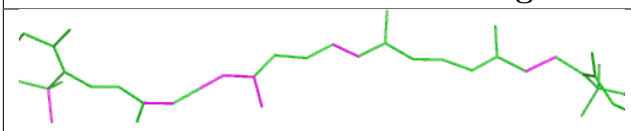


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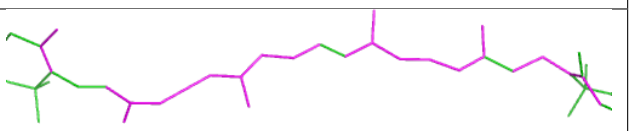


Rings

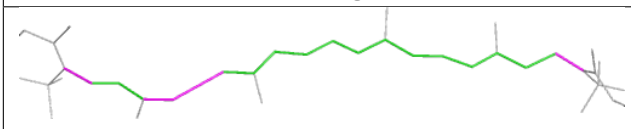
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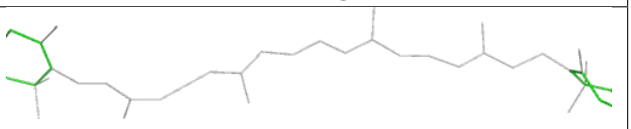
Bond lengths



Bond angles

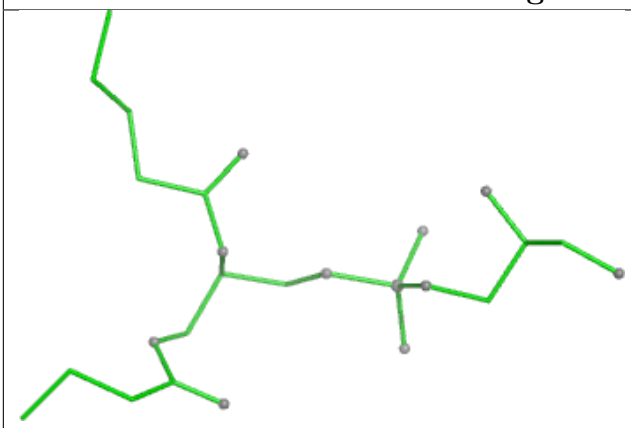


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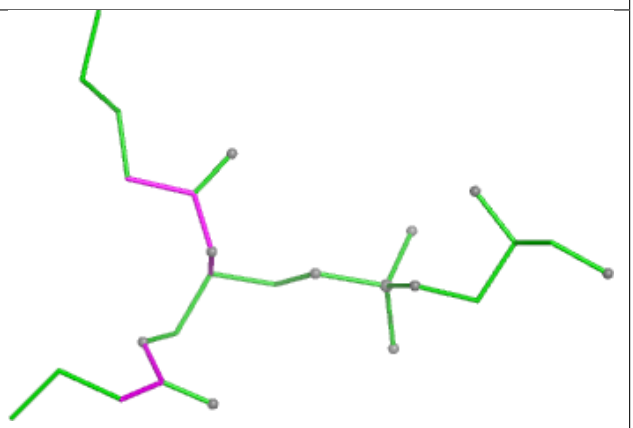


Rings

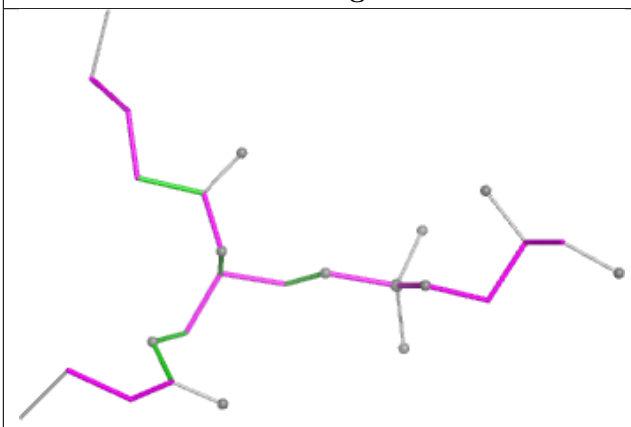
Ligand LHG 1 802



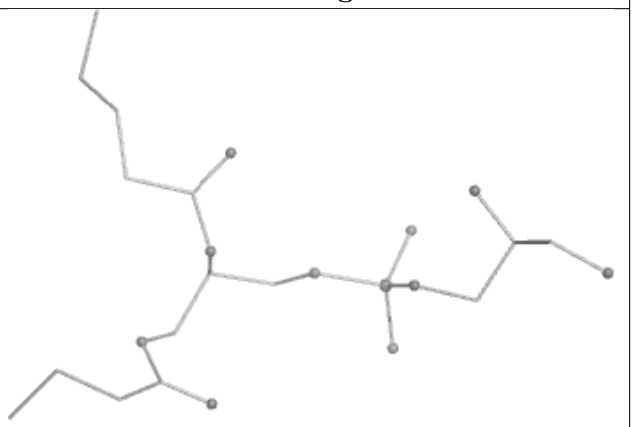
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Bond angles

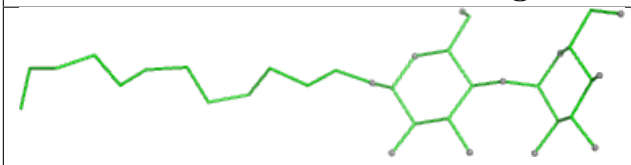


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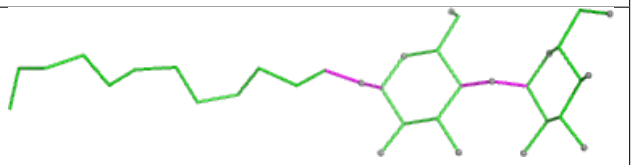


Rings

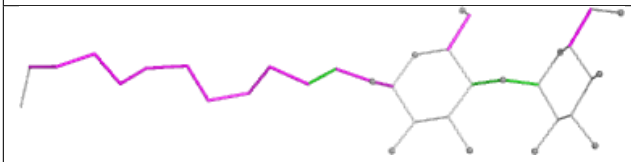
Ligand LMU B 5004



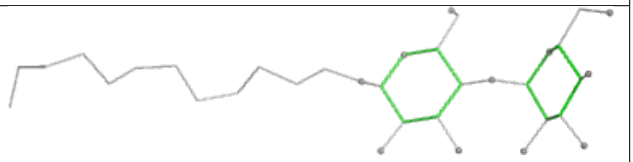
Bond lengths



Bond angles

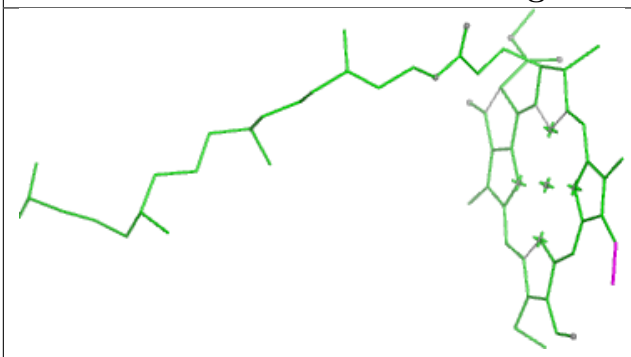


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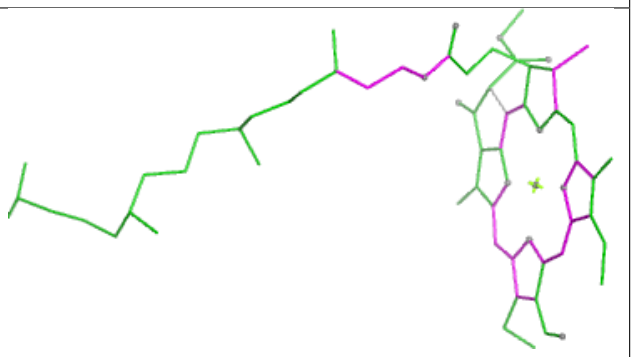


Rings

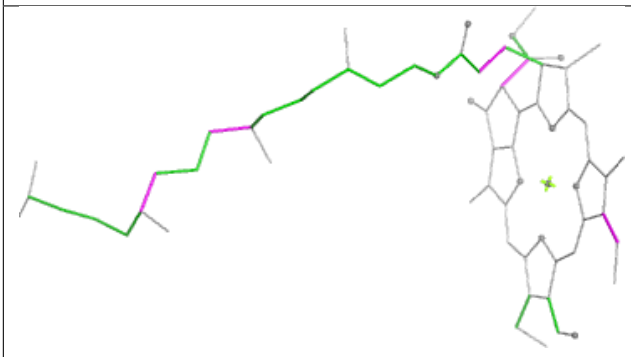
Ligand CHL 5 609



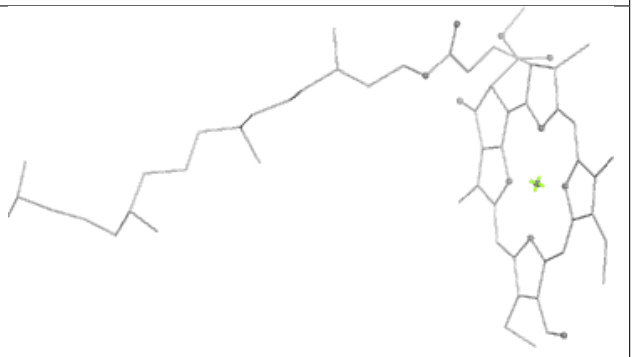
Bond lengths



Bond angles

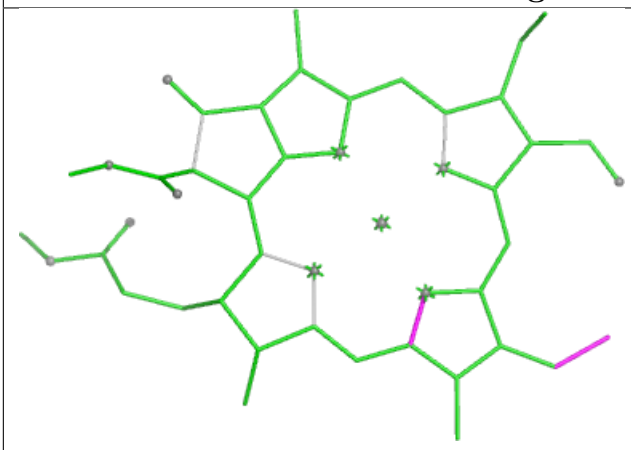


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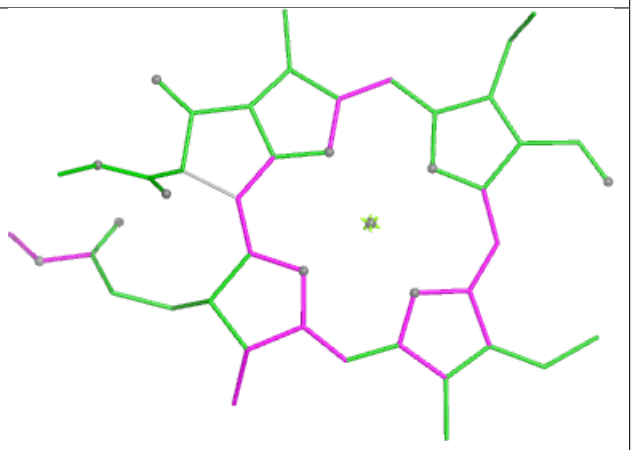


Rings

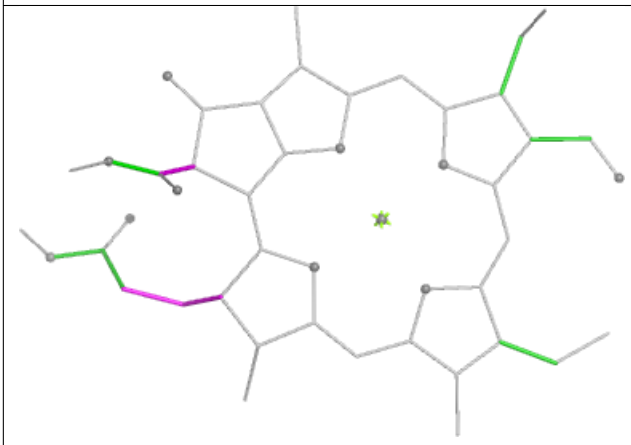
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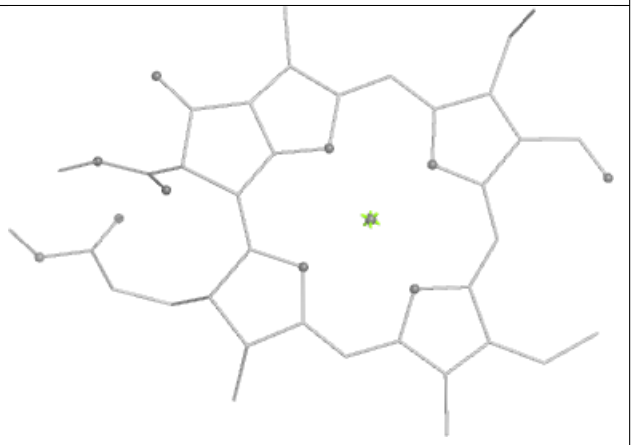
Bond lengths



Bond angles

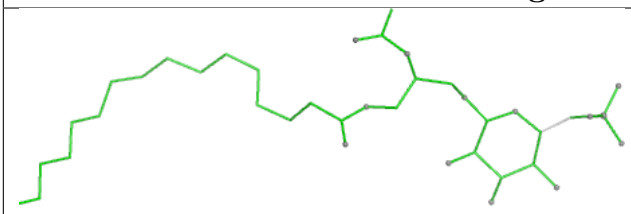


Torsions

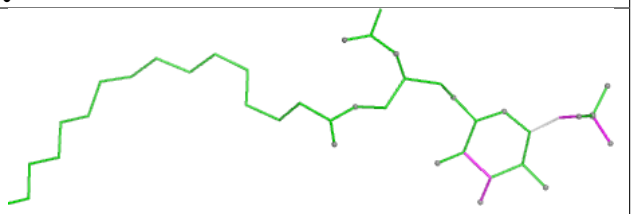


Rings

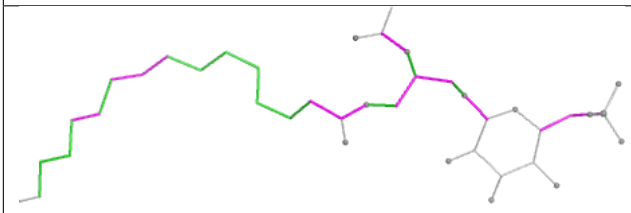
Ligand SQD 2 805



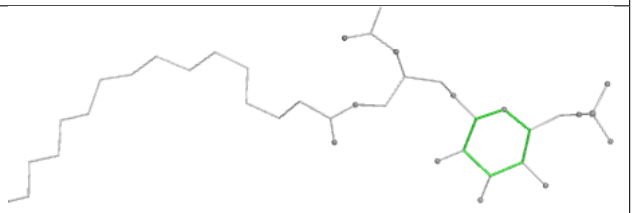
Bond lengths



Bond angles

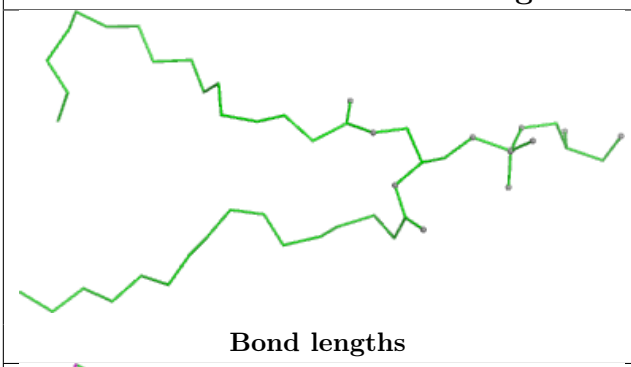


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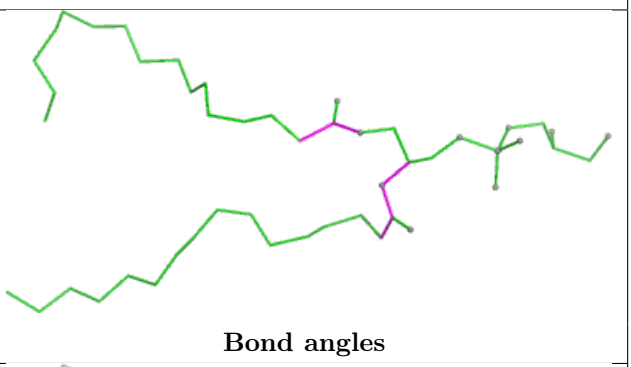


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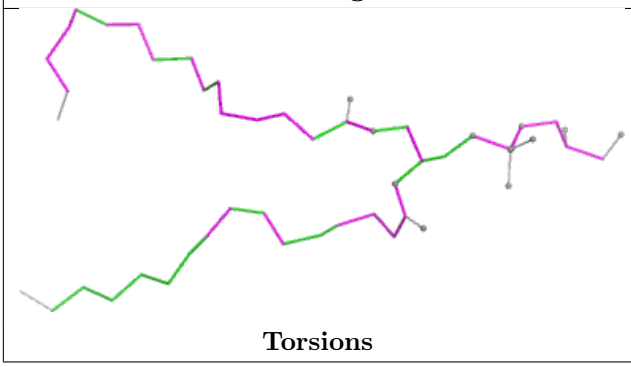
Ligand LHG F 5001



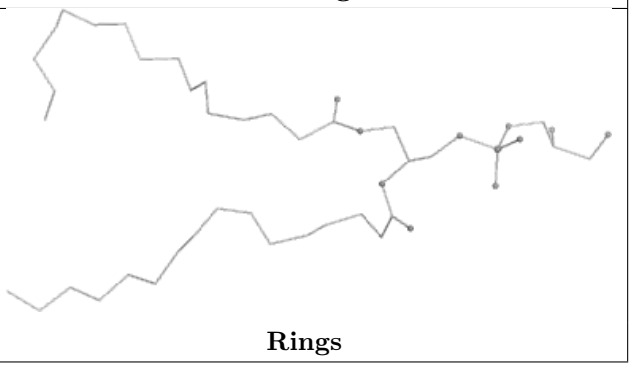
Bond lengths



Bond angles

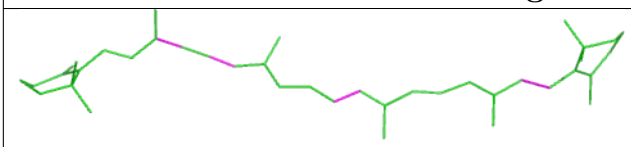


Torsions



Rings

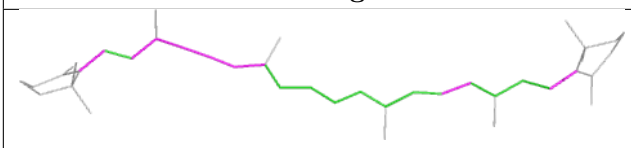
Ligand BCR 3 503



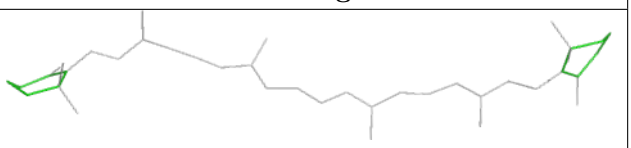
Bond lengths



Bond angles

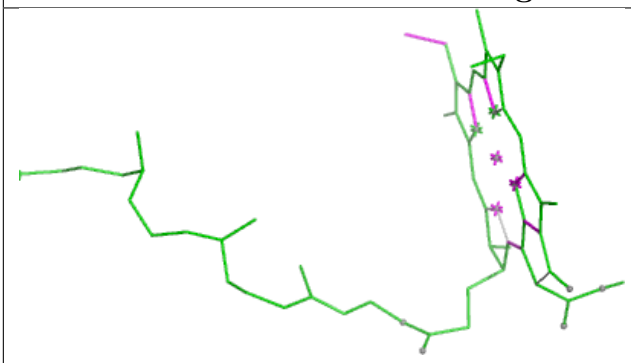


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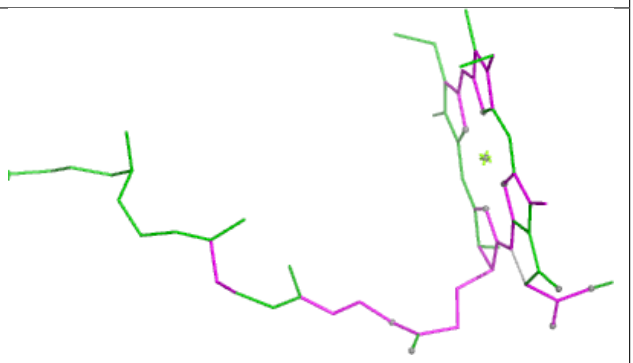


Rings

Ligand CLA B 1218



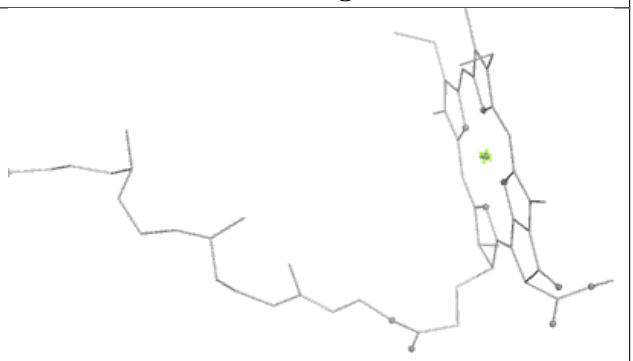
Bond lengths



Bond angles

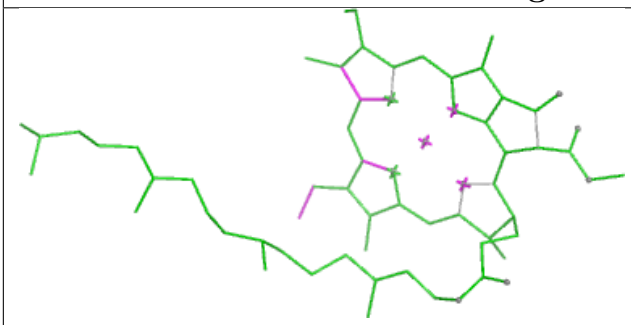


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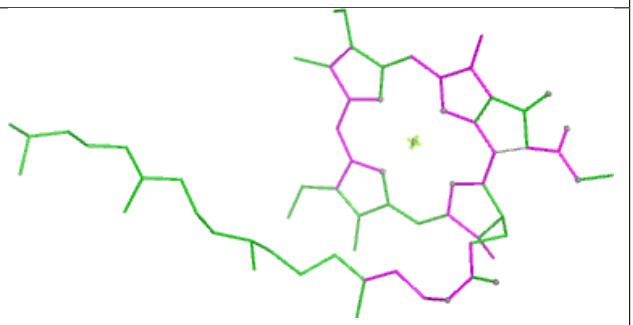


Rings

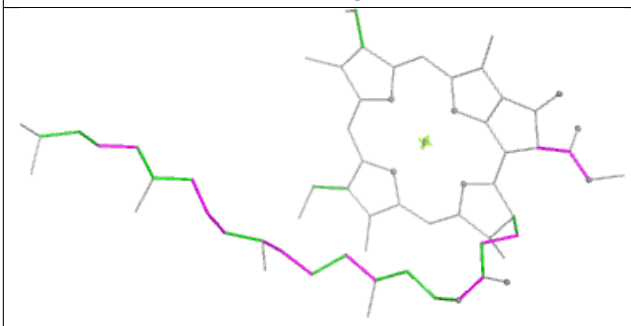
Ligand CLA 1 601



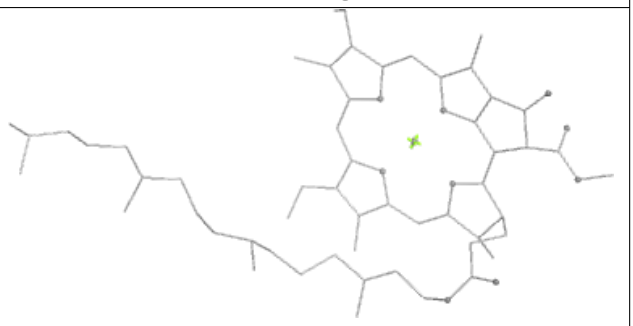
Bond lengths



Bond angles

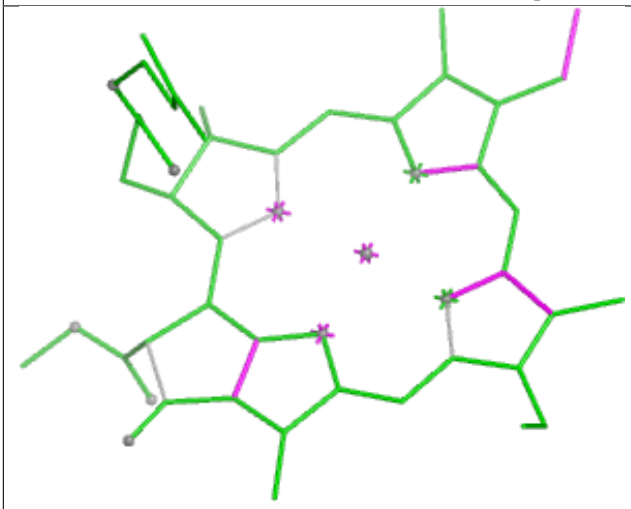


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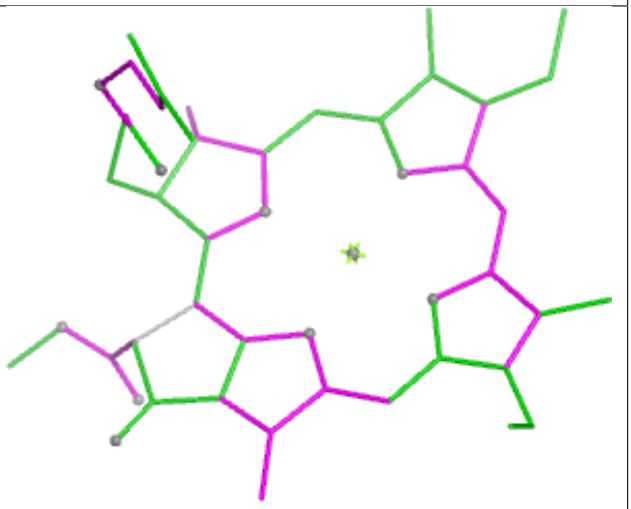


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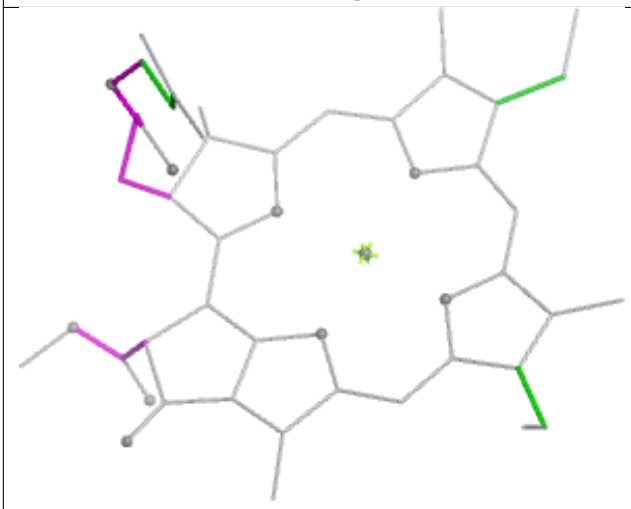
Ligand CLA 3 610



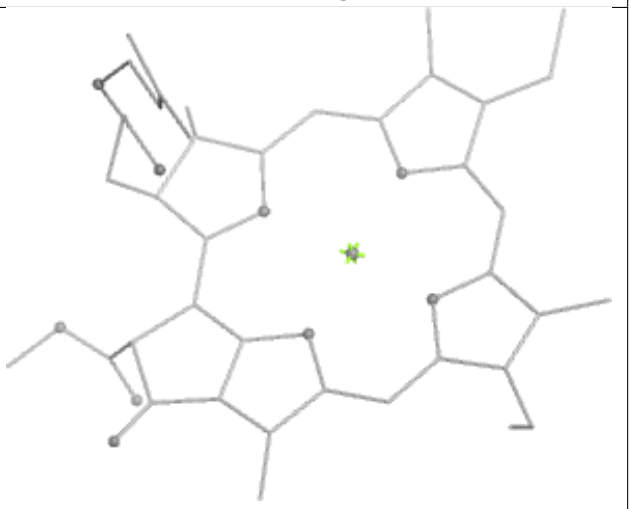
Bond lengths



Bond angles

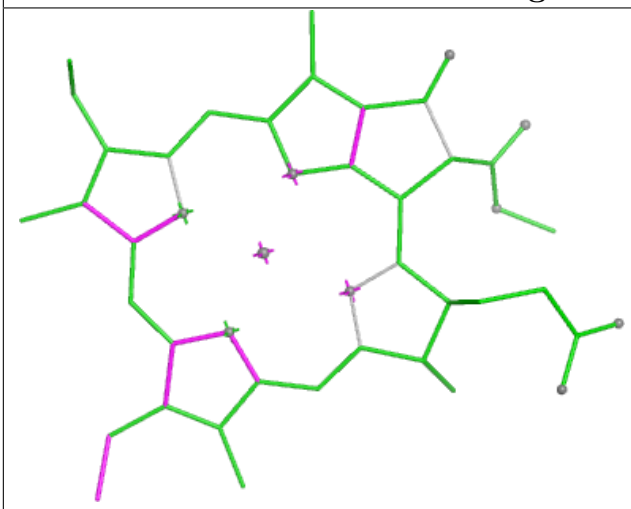


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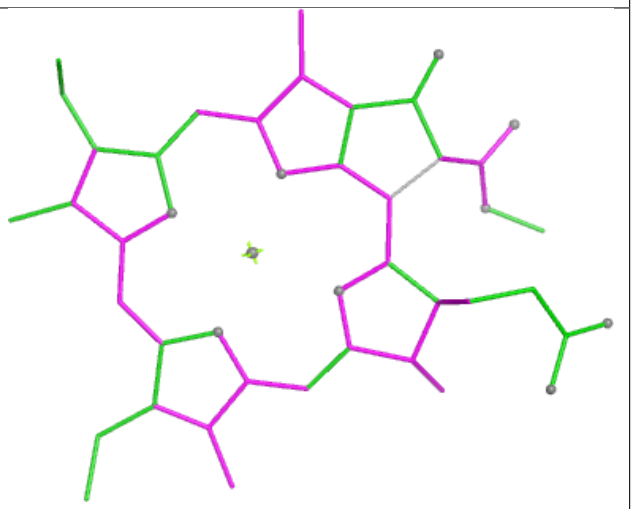


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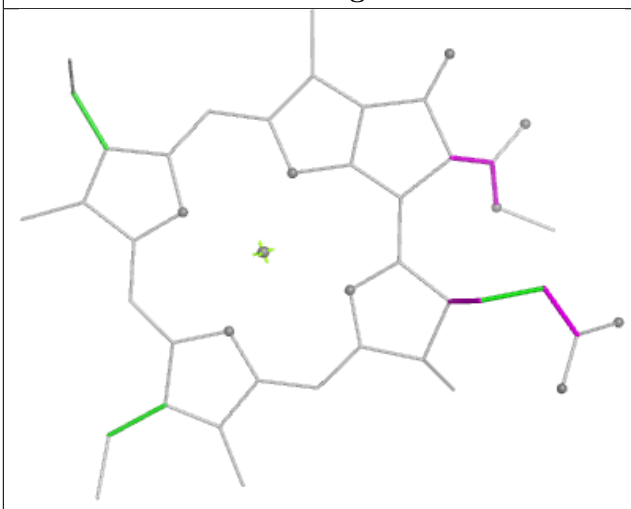
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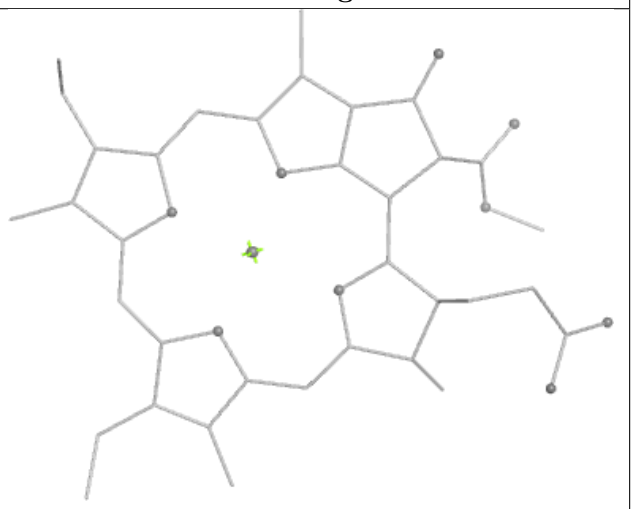
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Bond angles

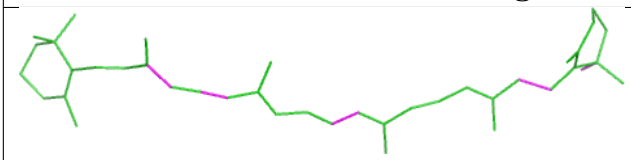


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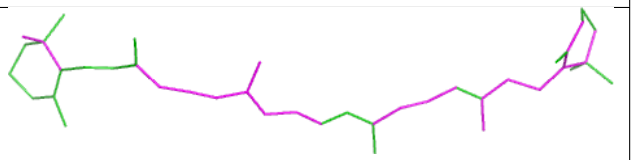


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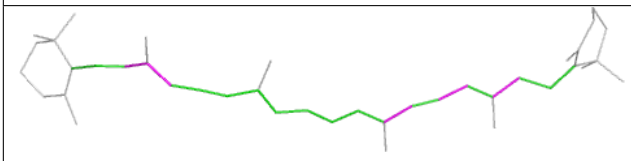
Ligand BCR B 4006



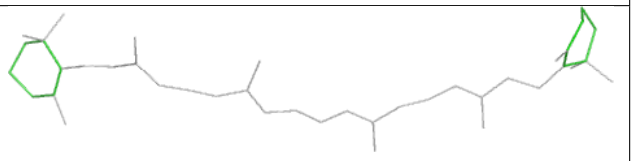
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Bond angles

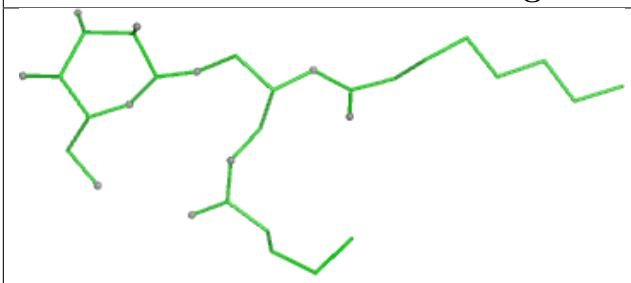


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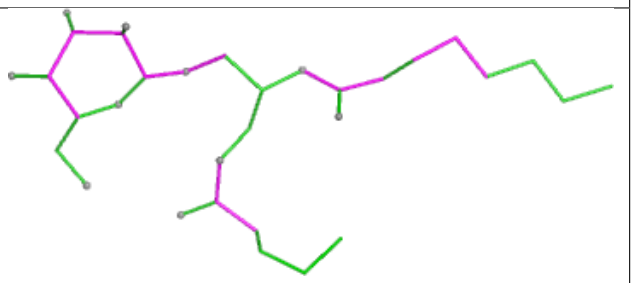


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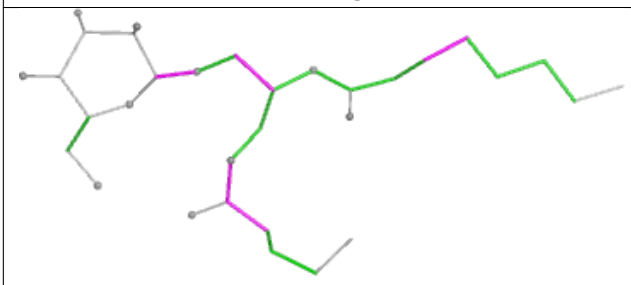
Ligand LMG 1 804



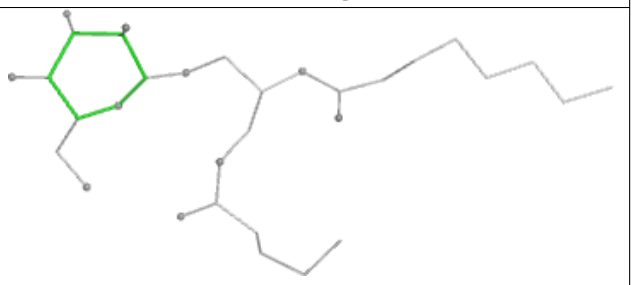
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Bond angles

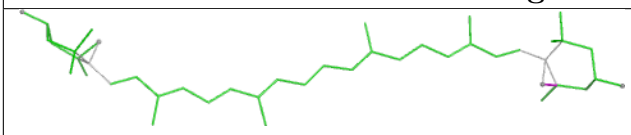


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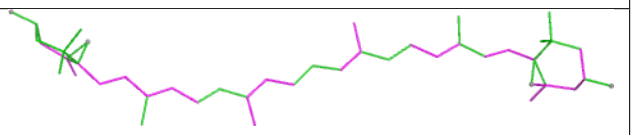


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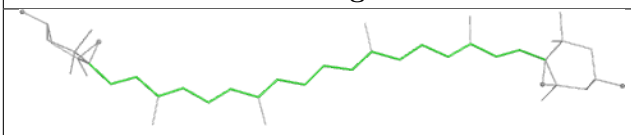
Ligand XAT 4 502



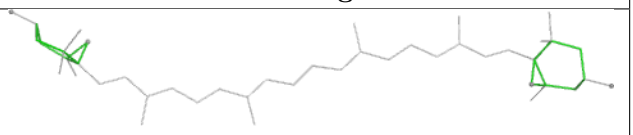
Bond lengths



Bond angles

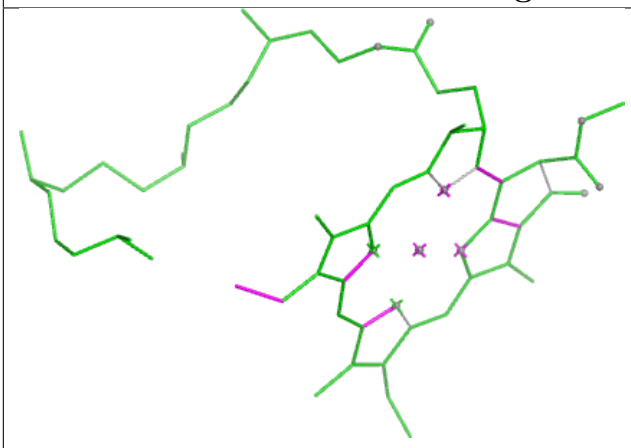


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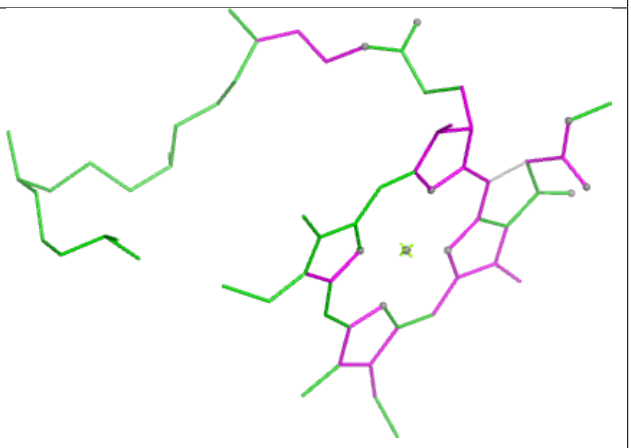


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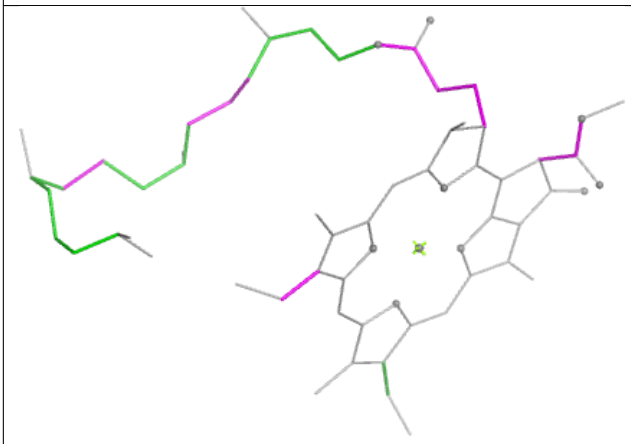
Ligand CLA A 1122



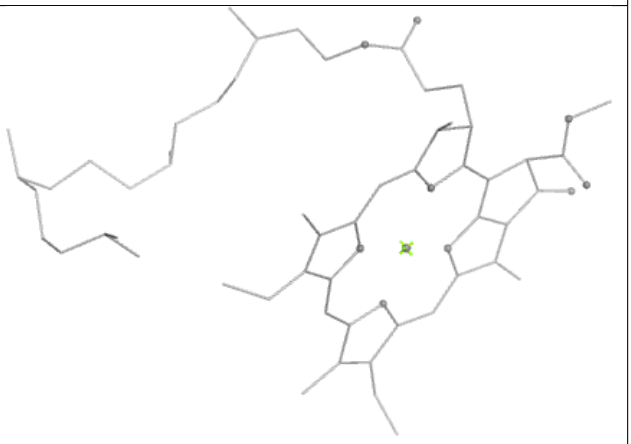
Bond lengths



Bond angles

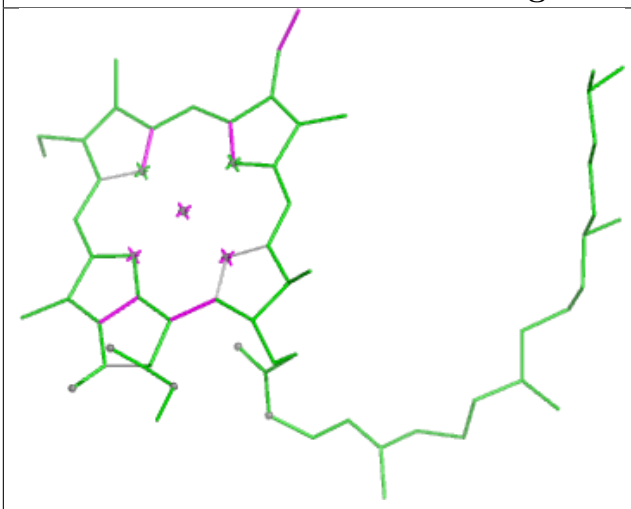


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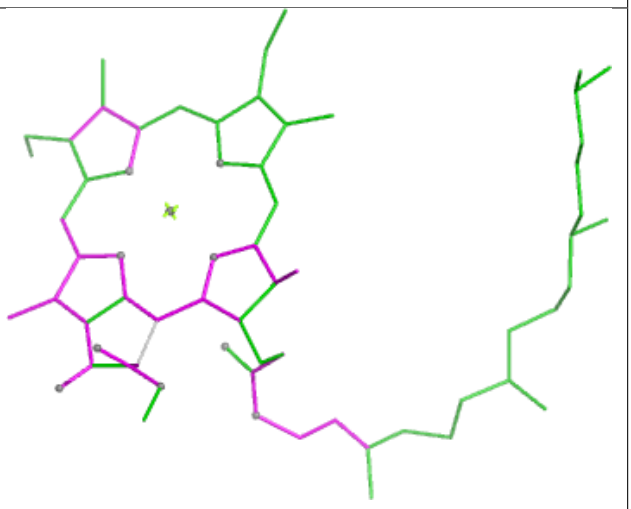


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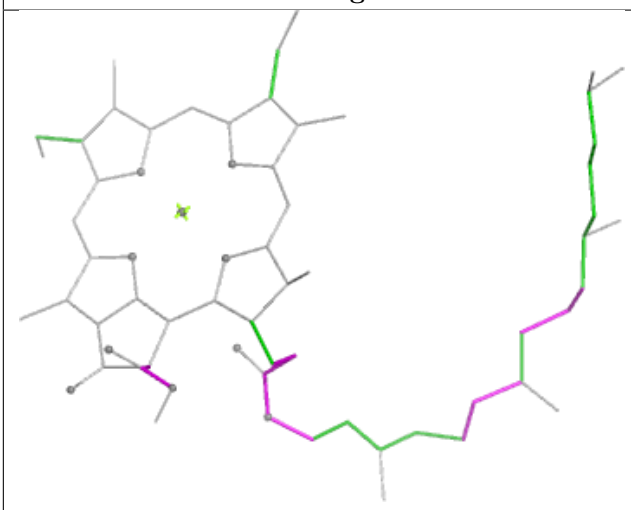
Ligand CLA 3 611



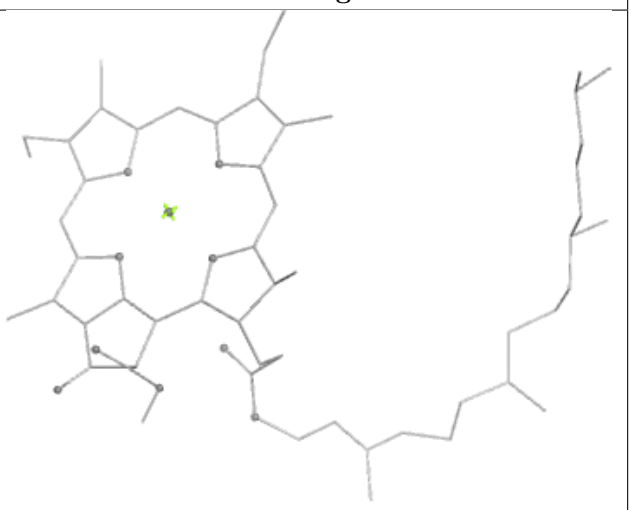
Bond lengths



Bond angles

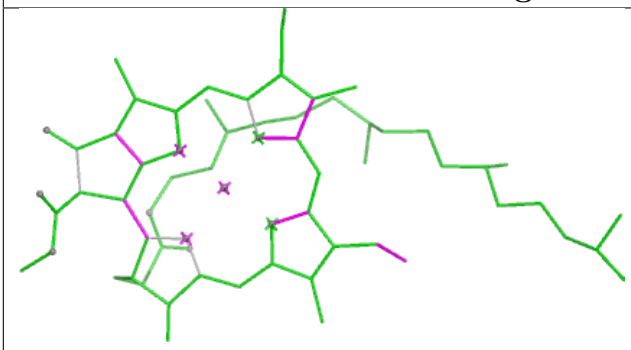


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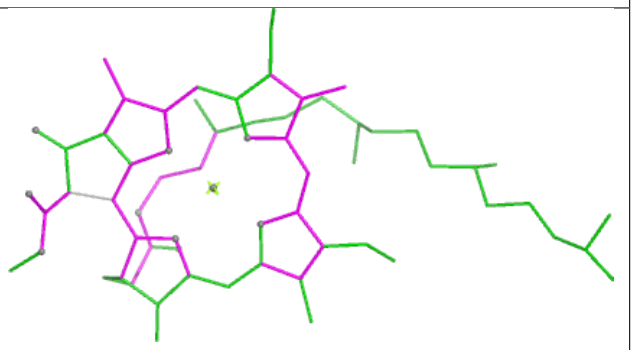


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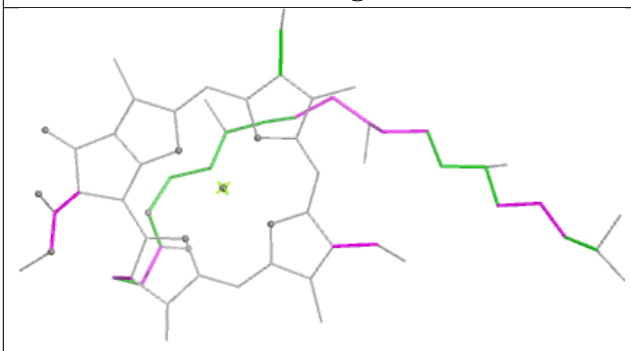
Ligand CLA A 1138



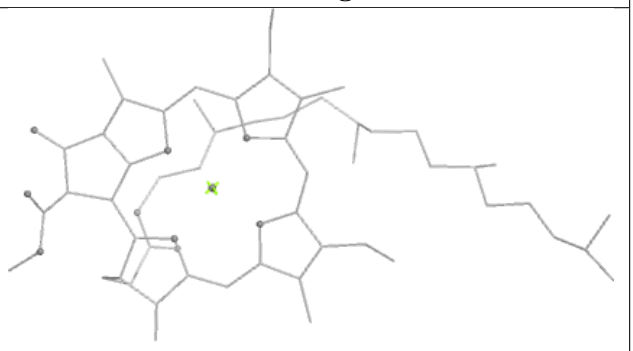
Bond lengths



Bond angles

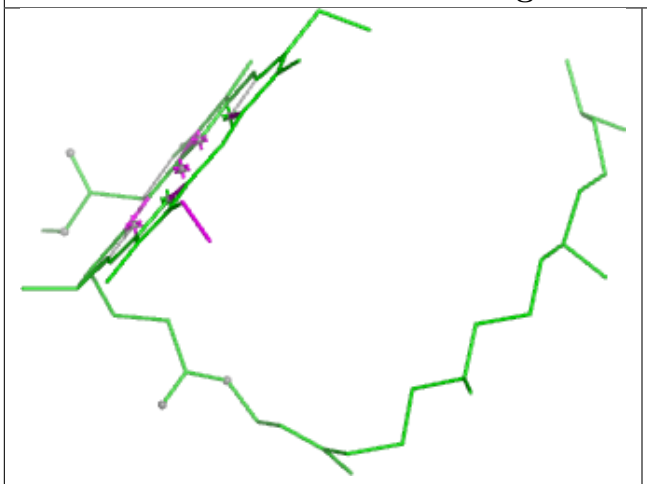


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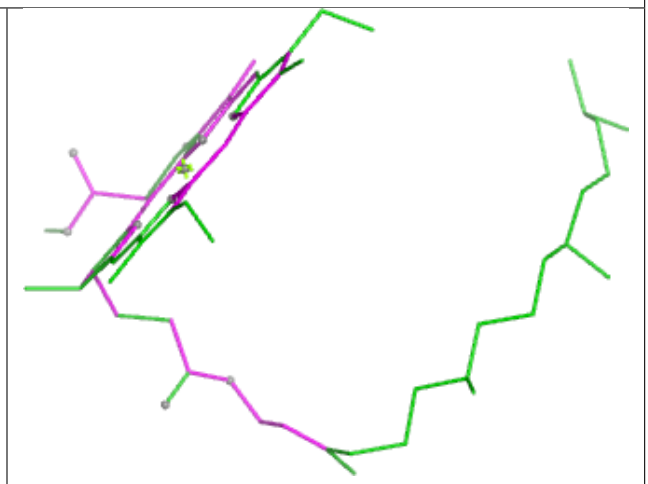


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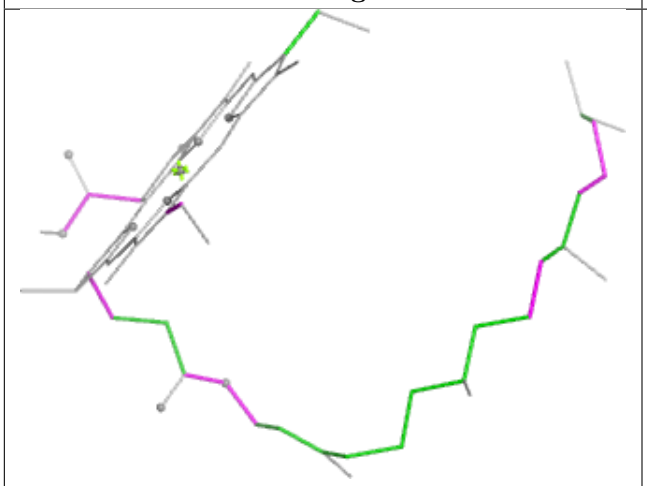
Ligand CLA B 1216



Bond lengths



Bond angles

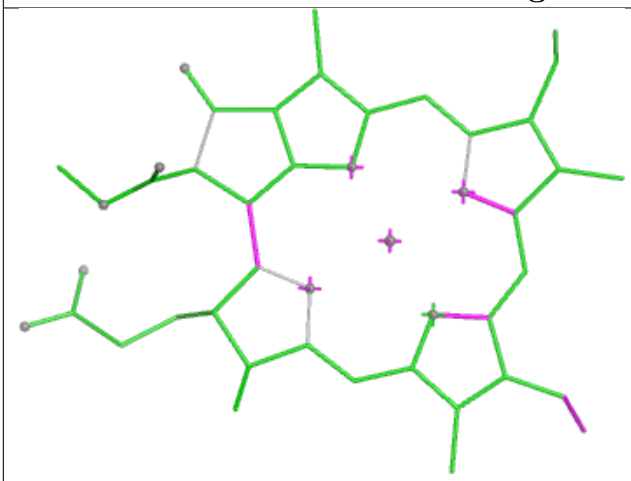


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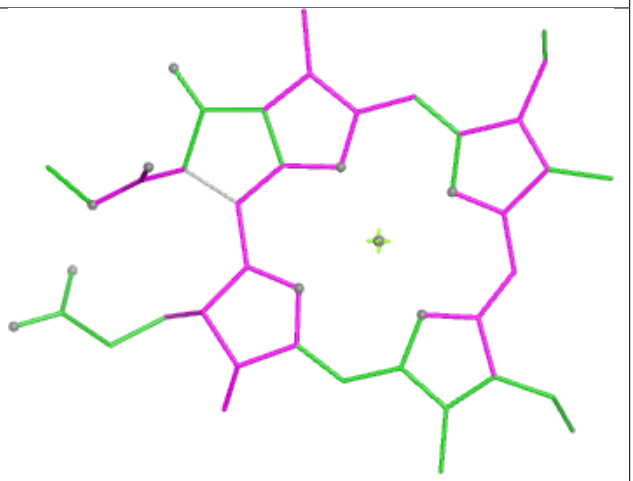


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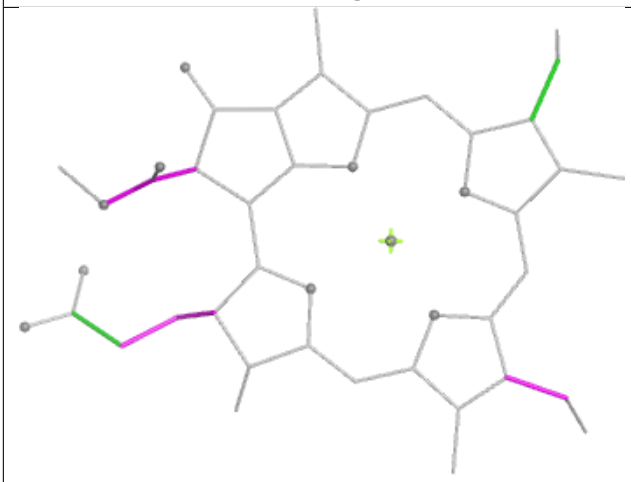
Ligand CLA 1 613



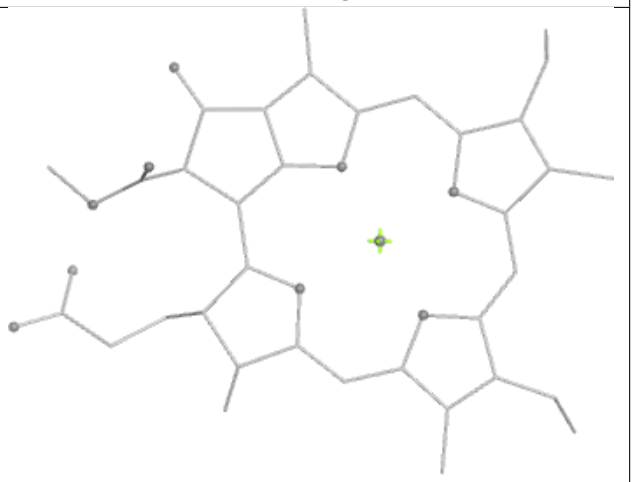
Bond lengths



Bond angles

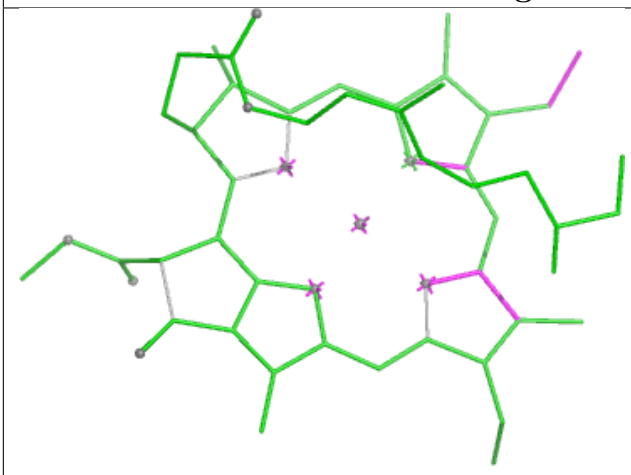


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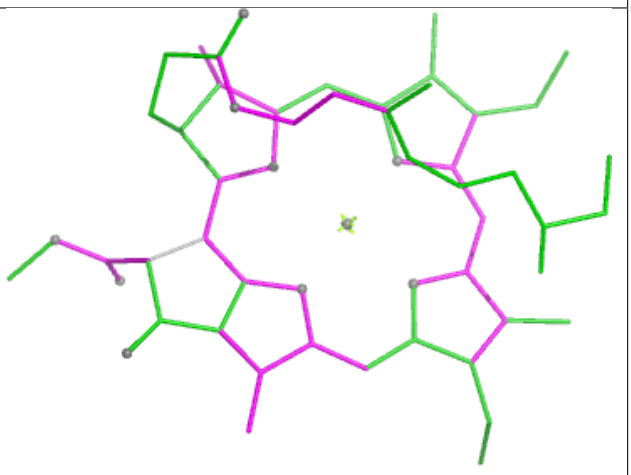


Rings

Ligand CLA A 1116



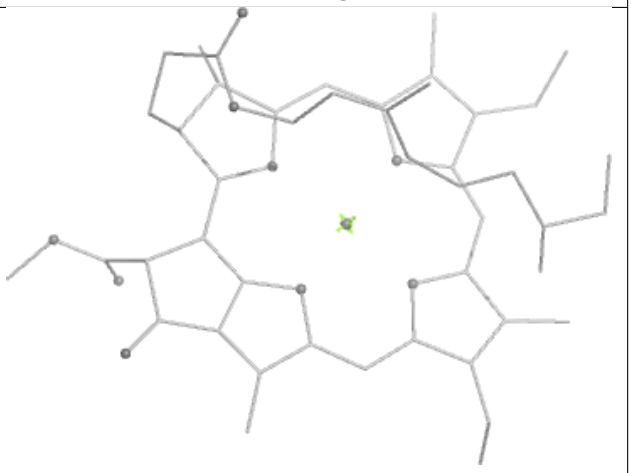
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Bond angles

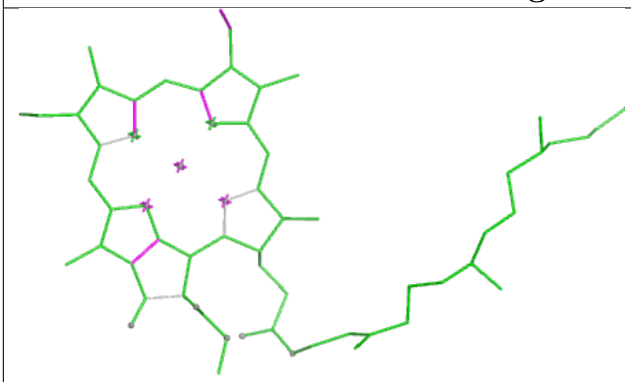


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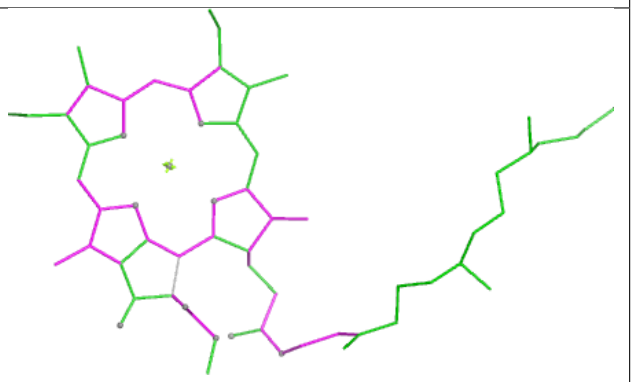


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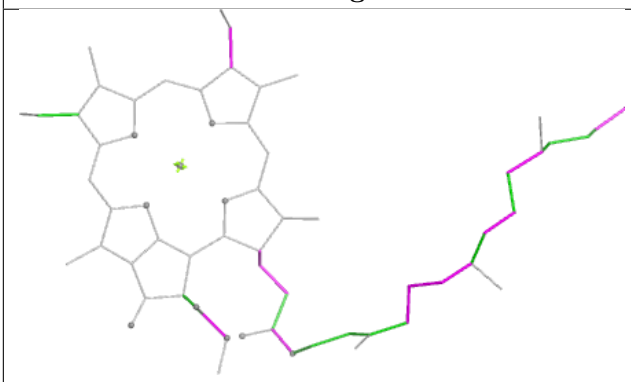
Ligand CLA 2 605



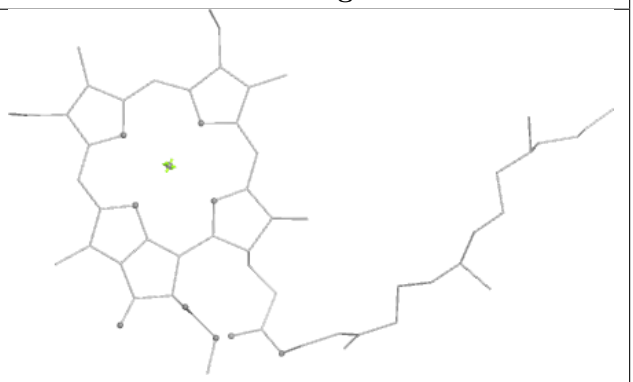
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Bond angles

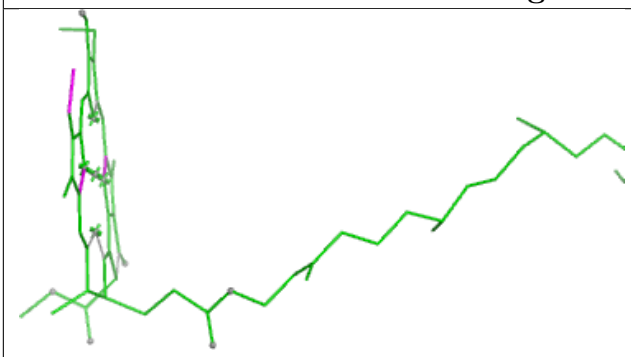


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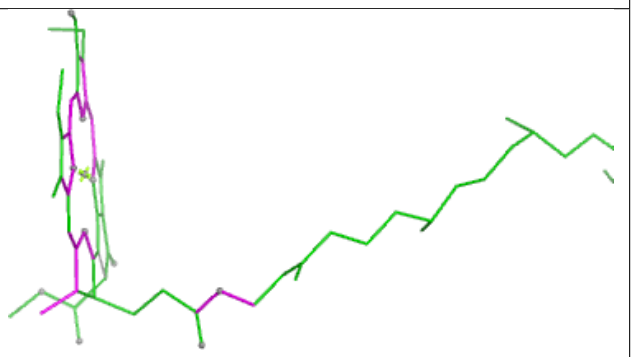


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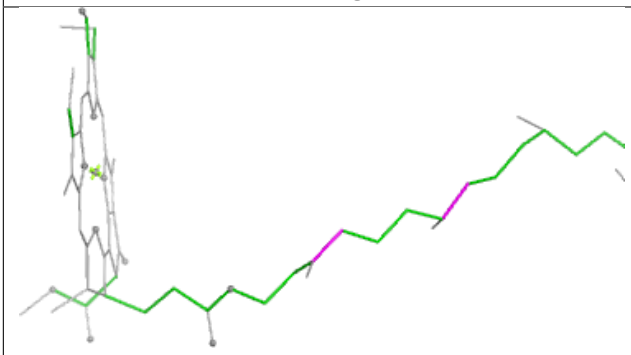
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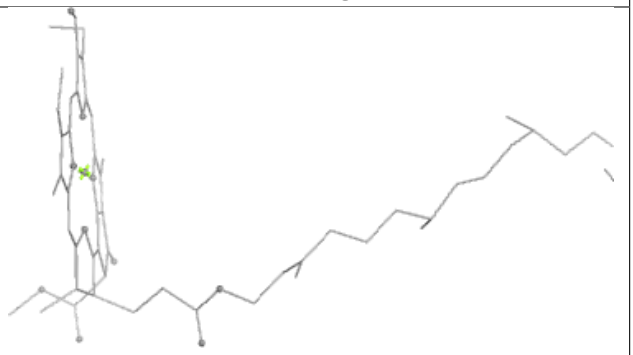
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Bond angles

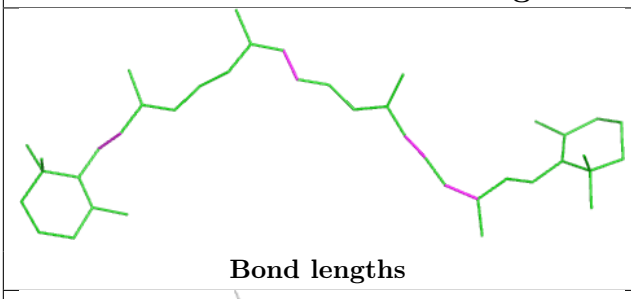


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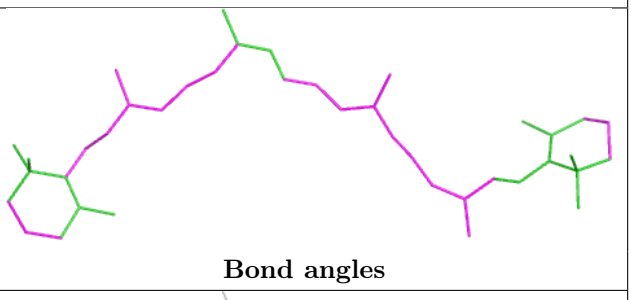


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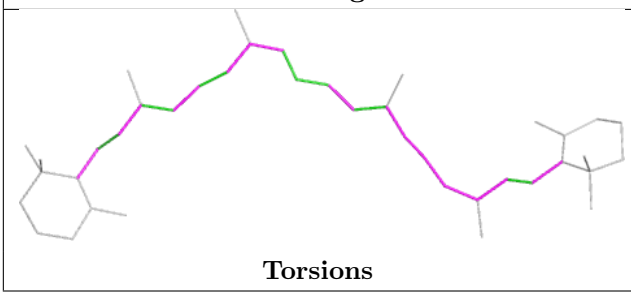
Ligand BCR A 4006



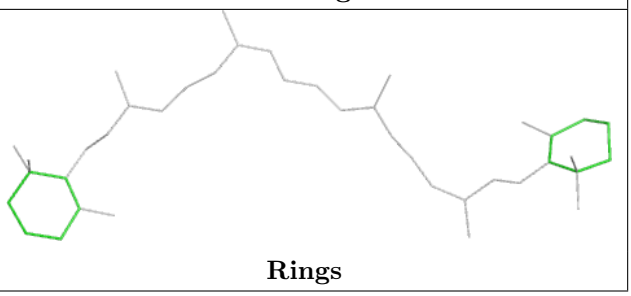
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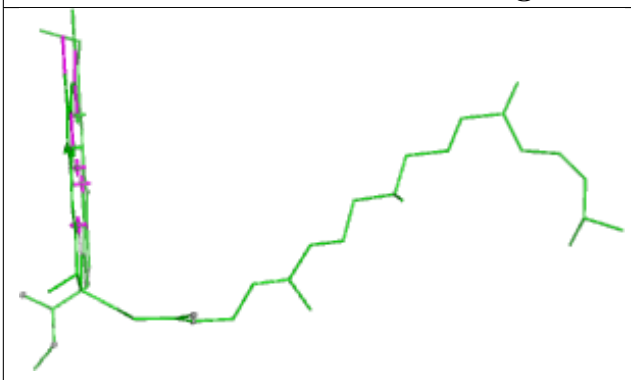


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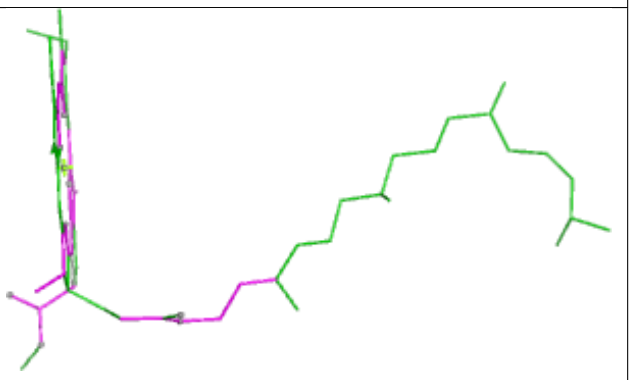


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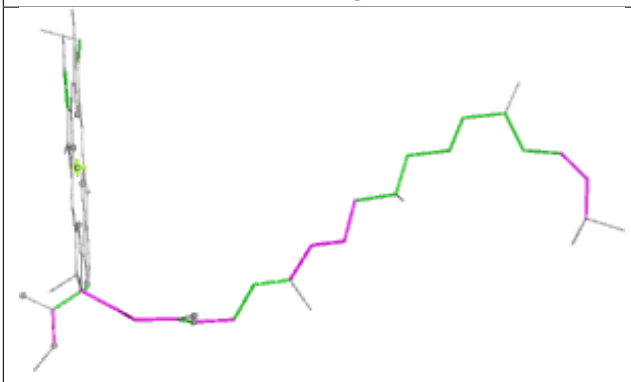
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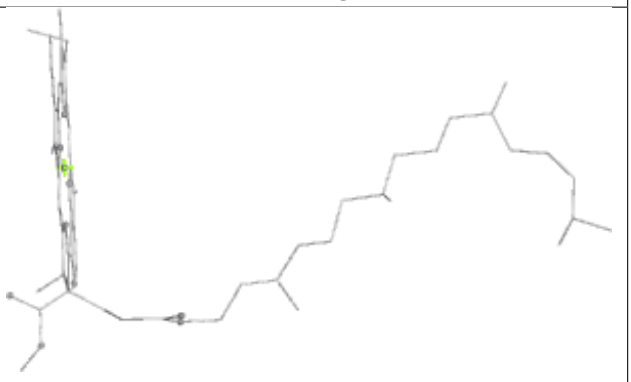
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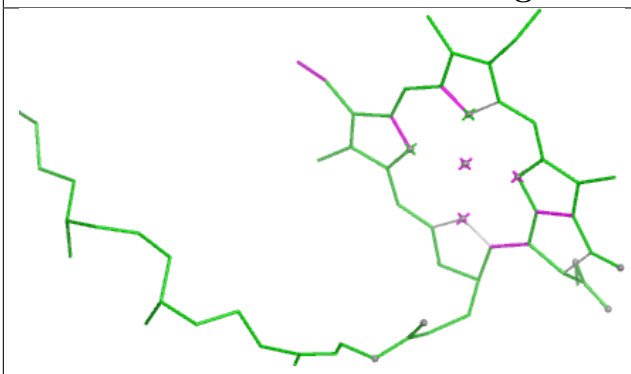


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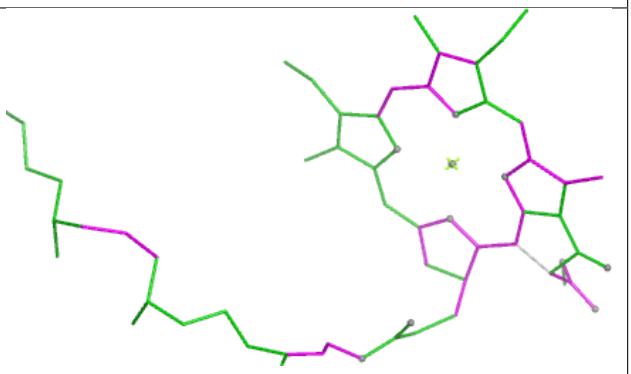


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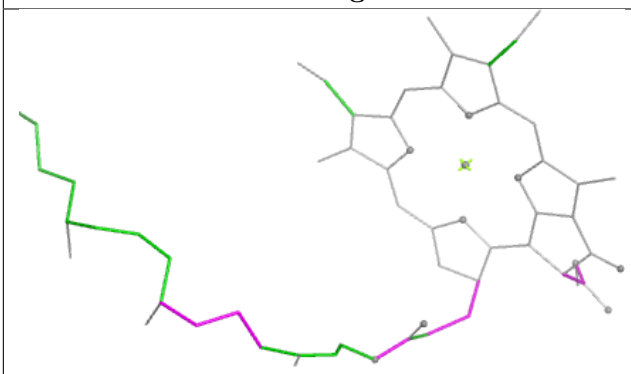
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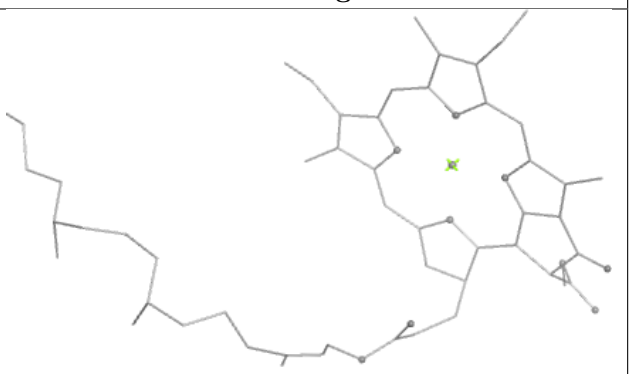
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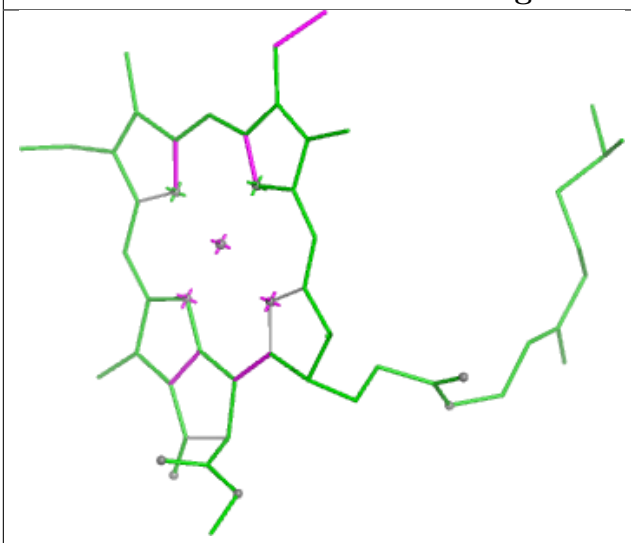


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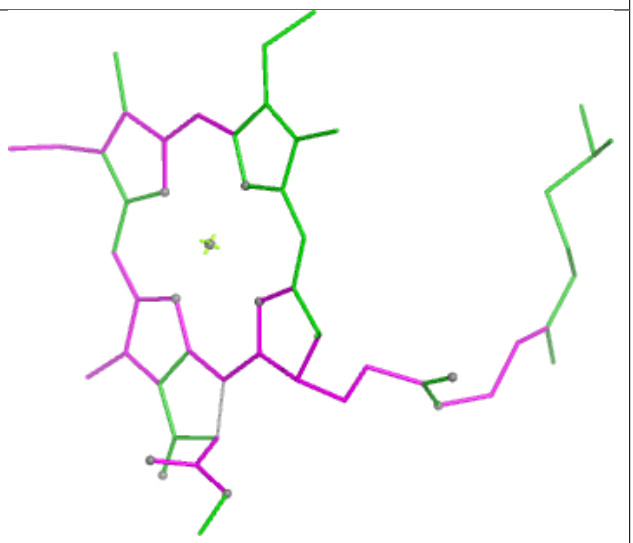


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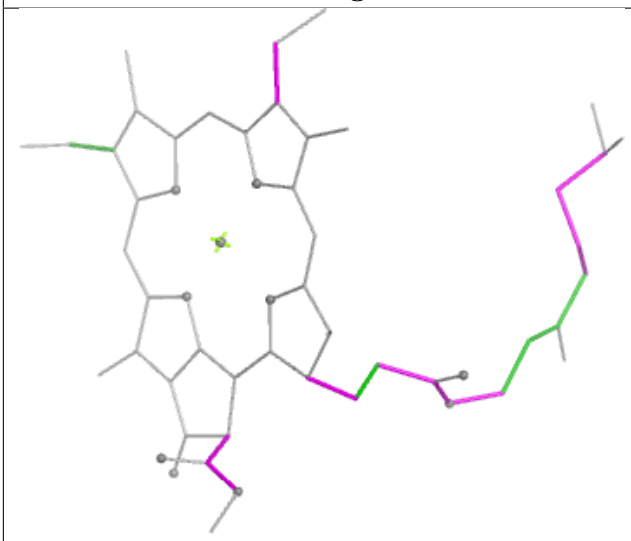
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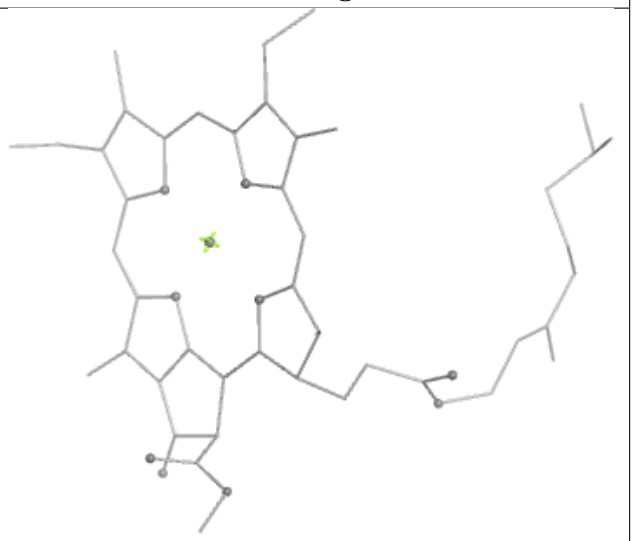
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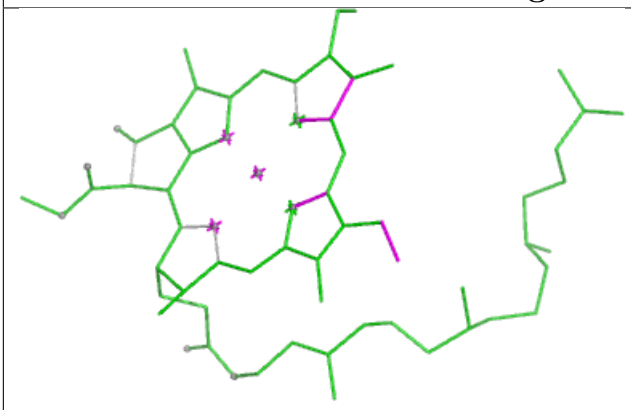


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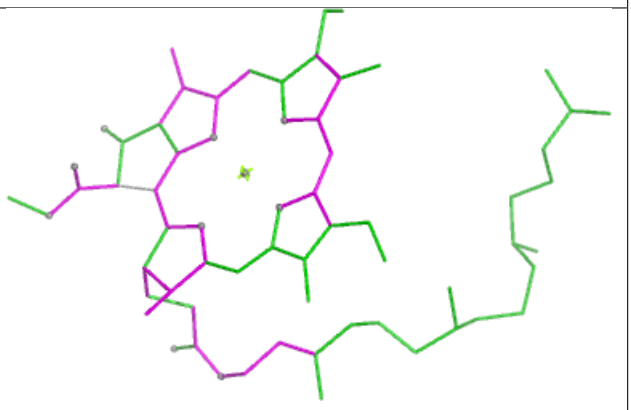


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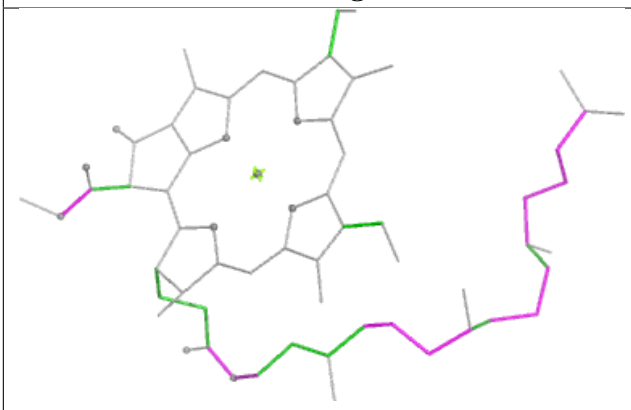
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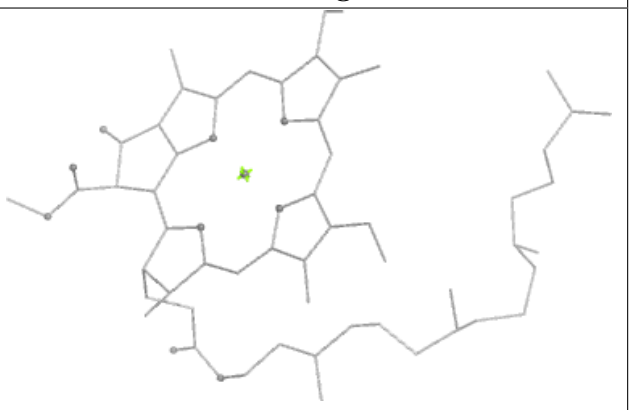
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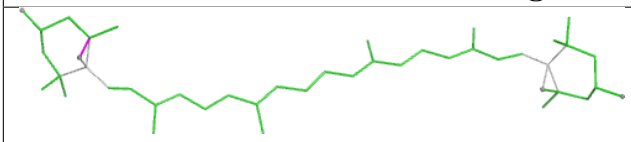


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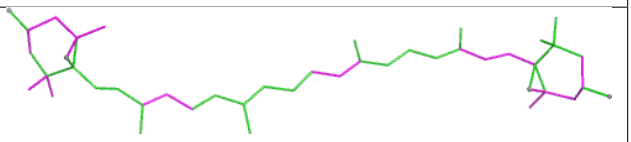


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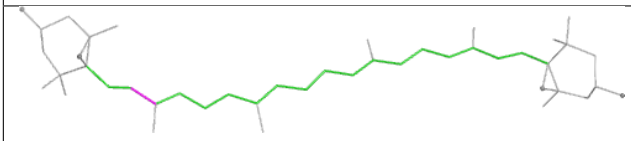
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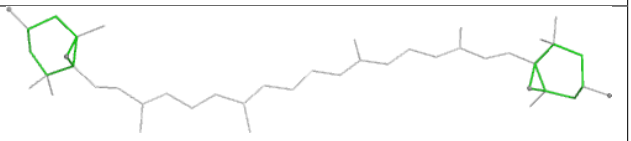
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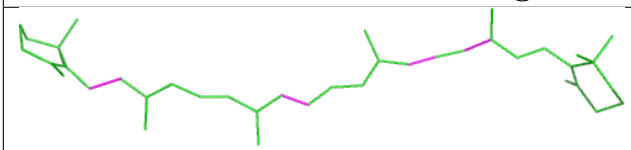


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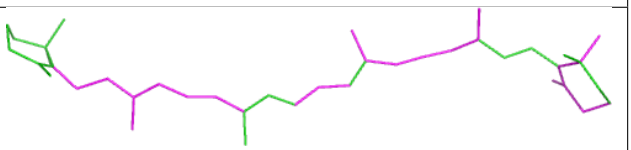


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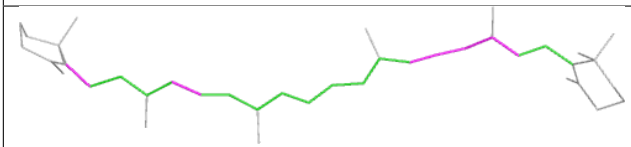
Ligand BCR B 4004



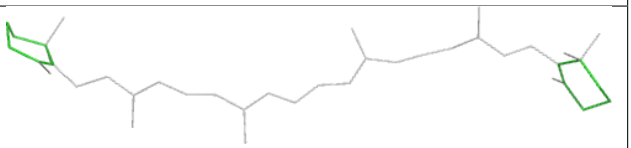
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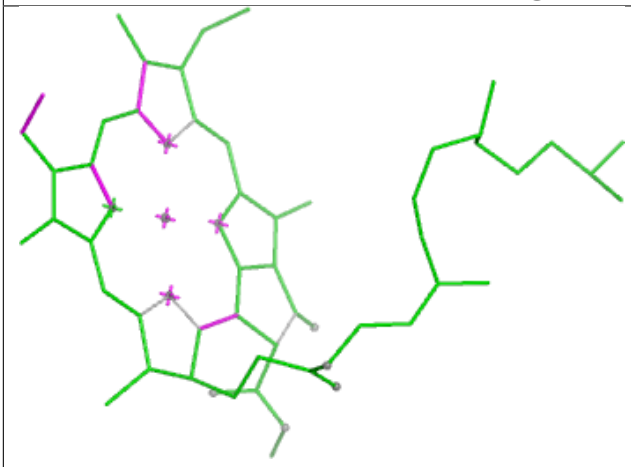


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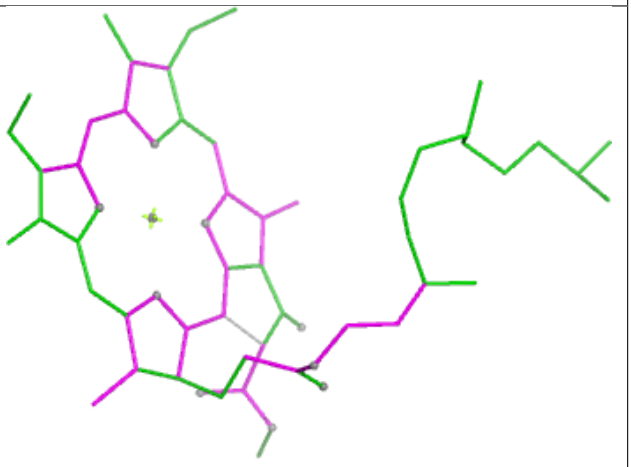


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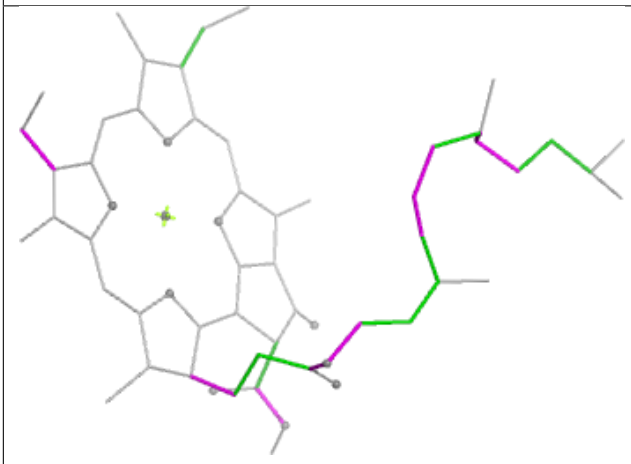
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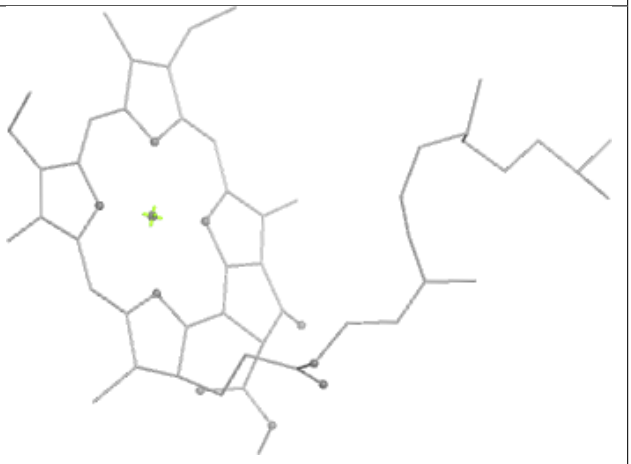
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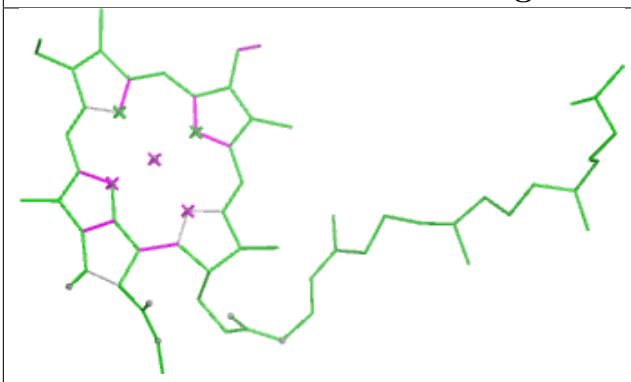


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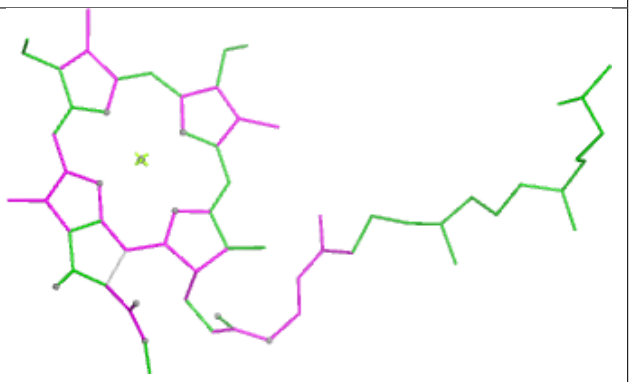


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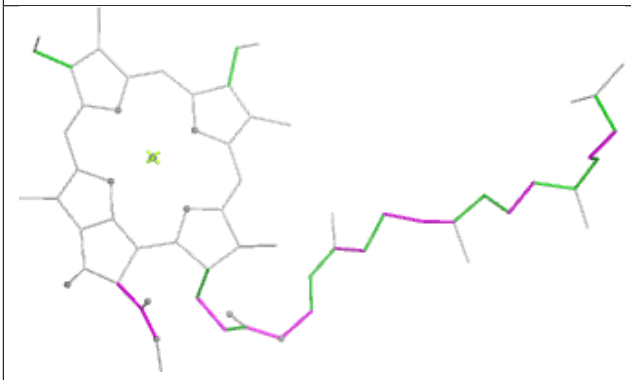
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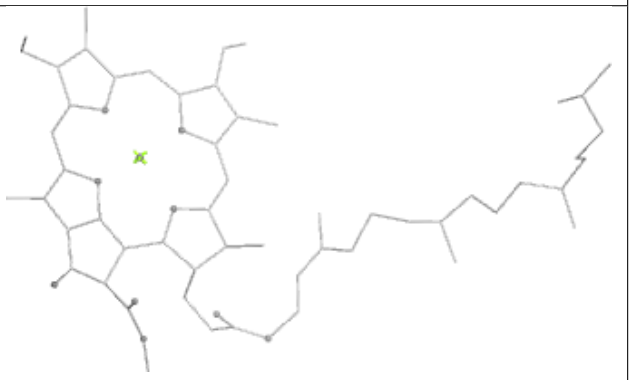
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Bond angles

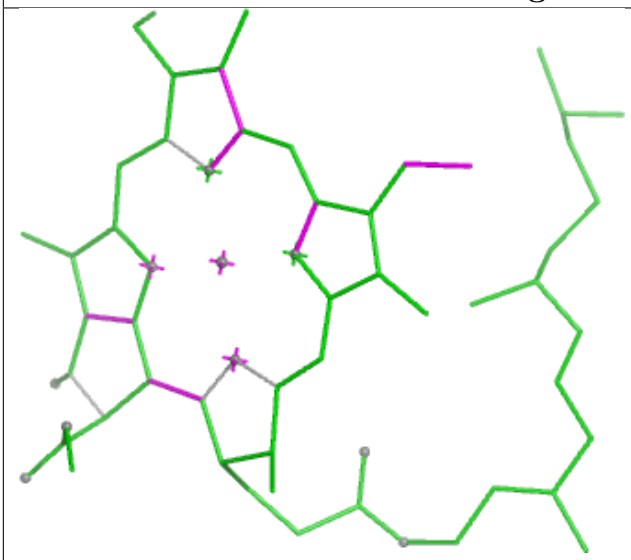


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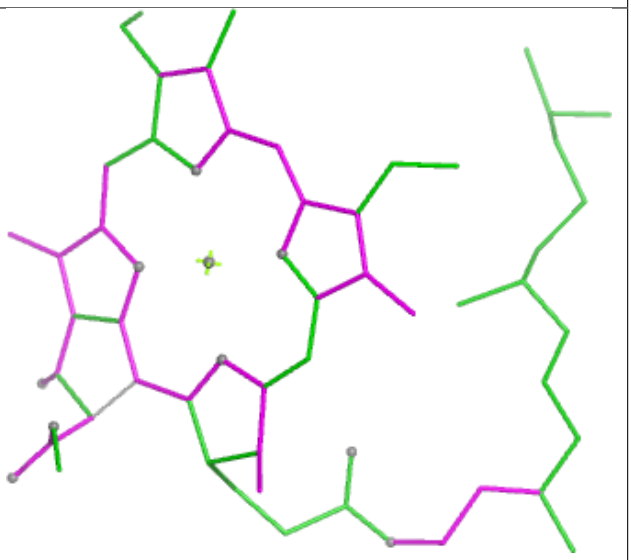


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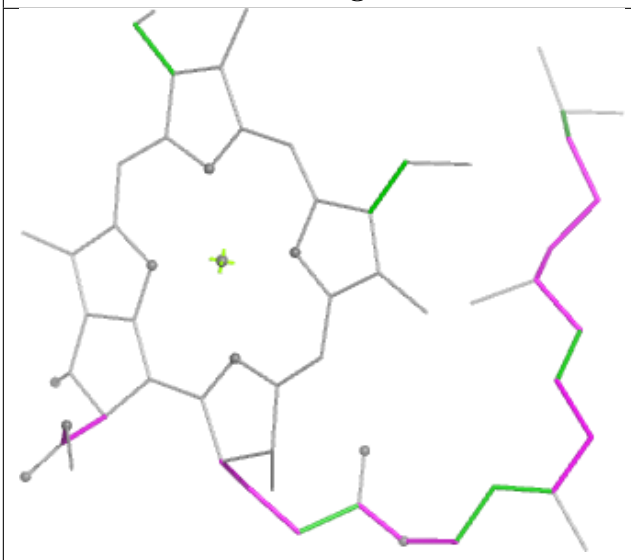
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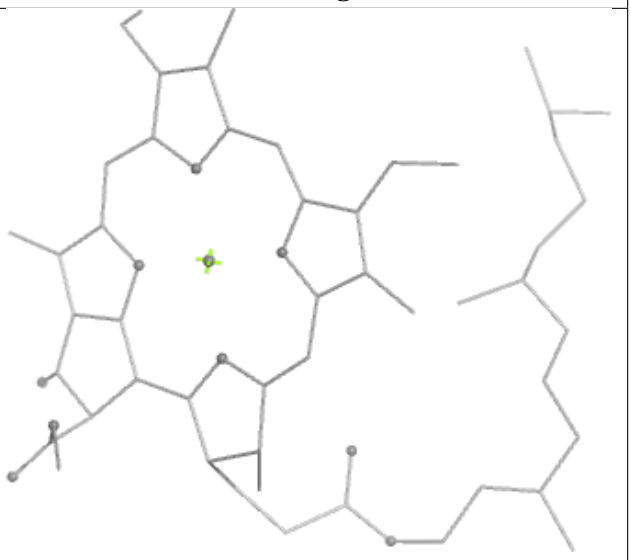
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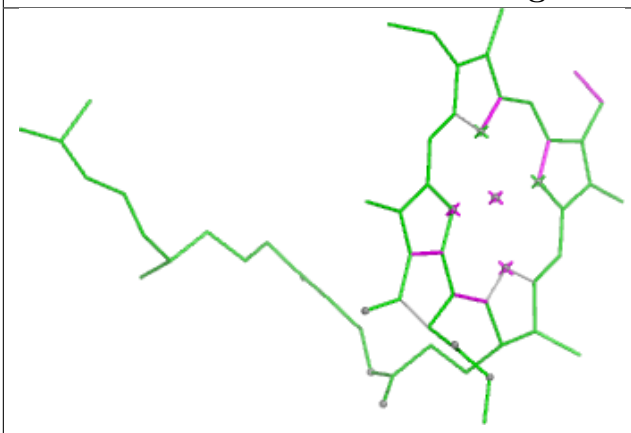


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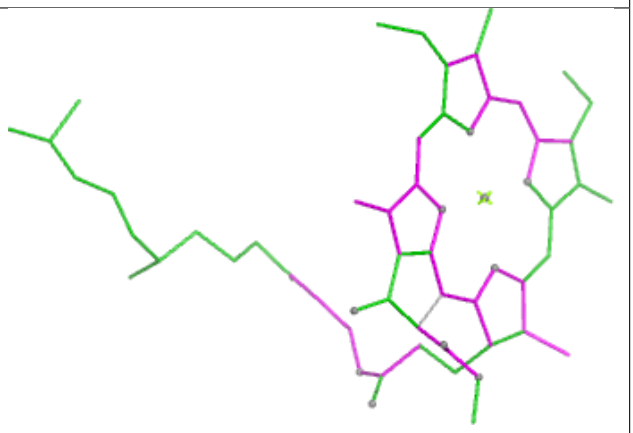


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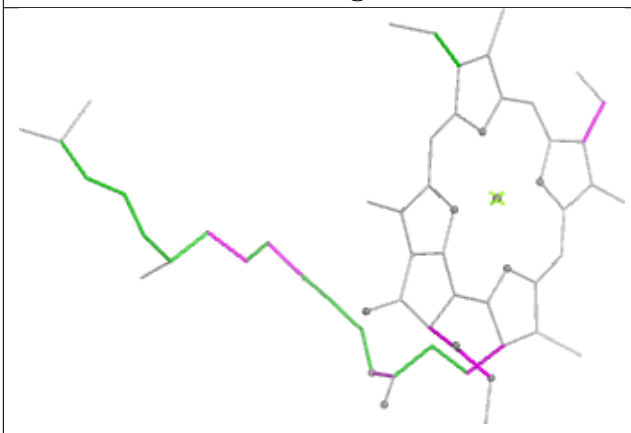
Ligand CLA 2 607



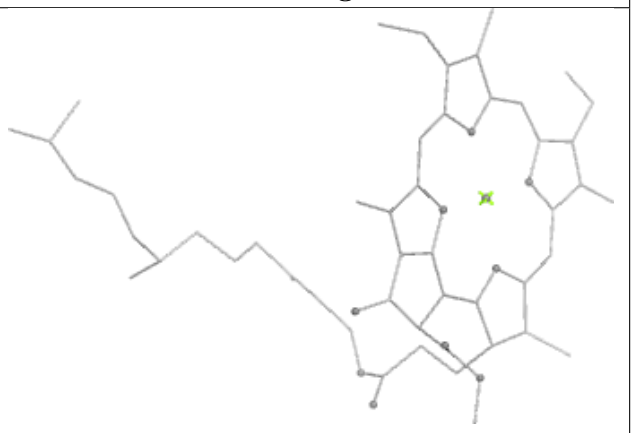
Bond lengths



Bond angles

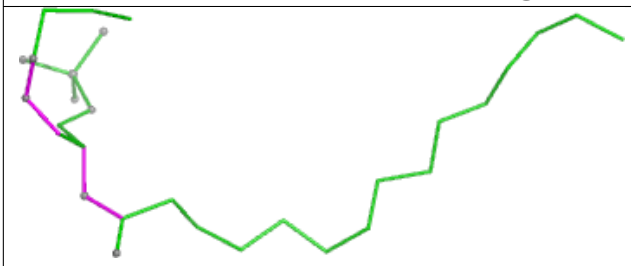


Torsions

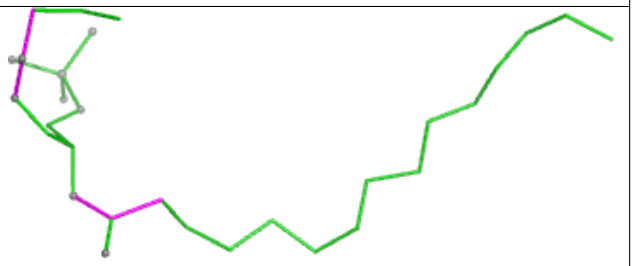


Rings

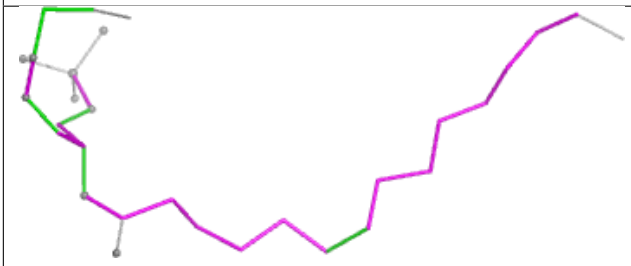
Ligand 3PH B 5003



Bond lengths



Bond angles

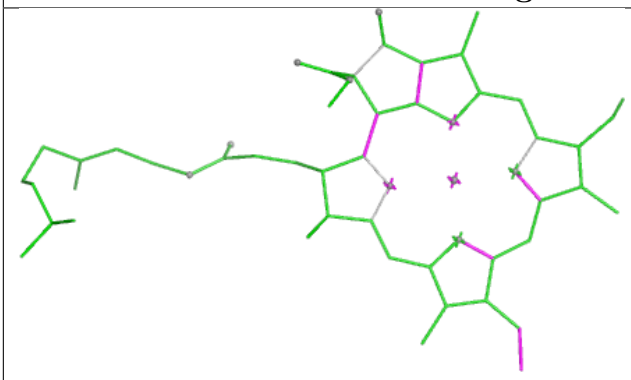


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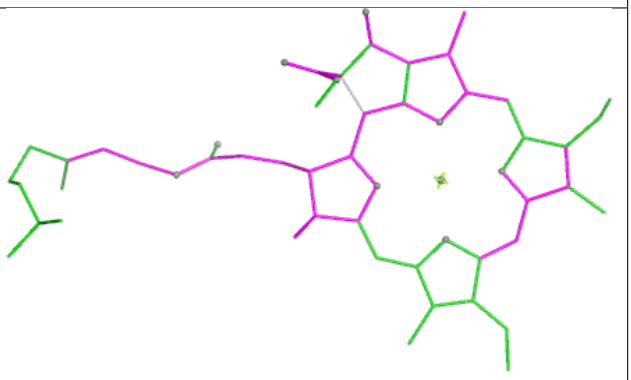


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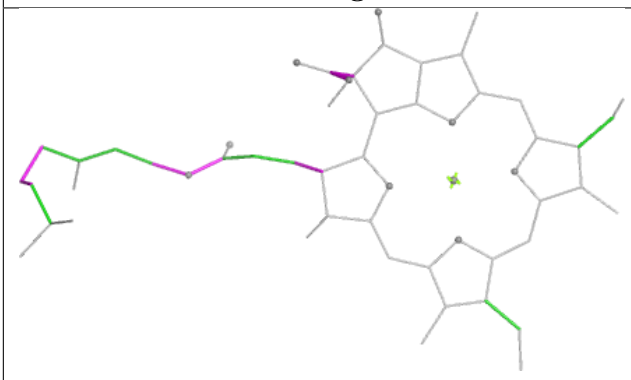
Ligand CLA B 1234



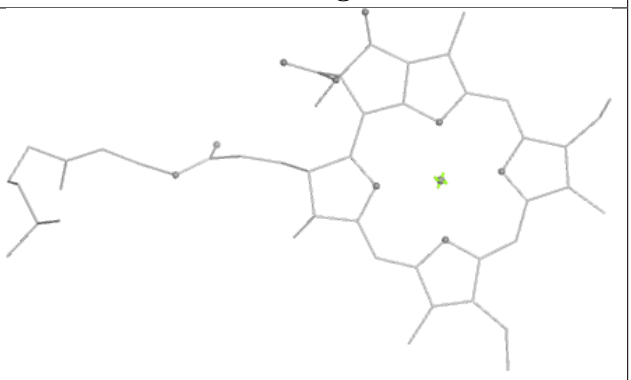
Bond lengths



Bond angles

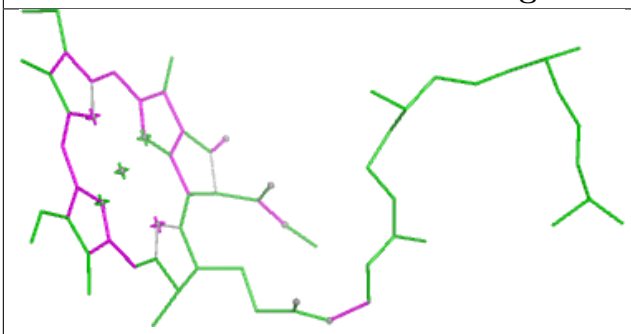


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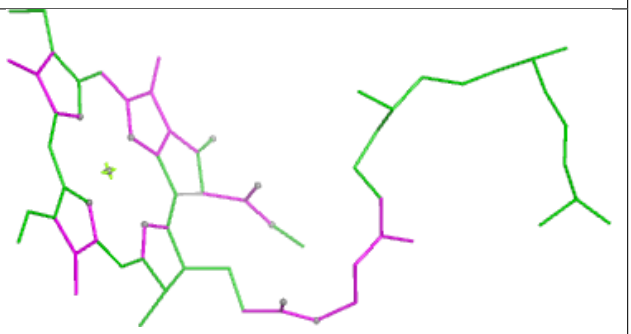


Rings

Ligand CL0 A 1011



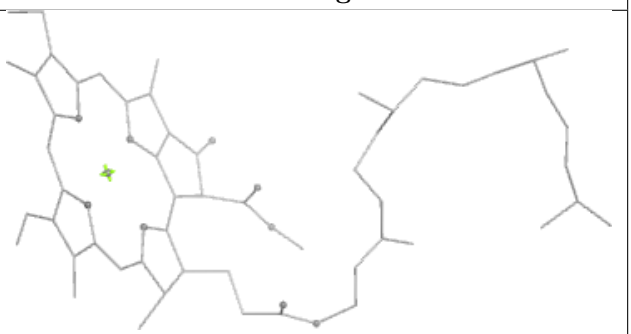
Bond lengths



Bond angles

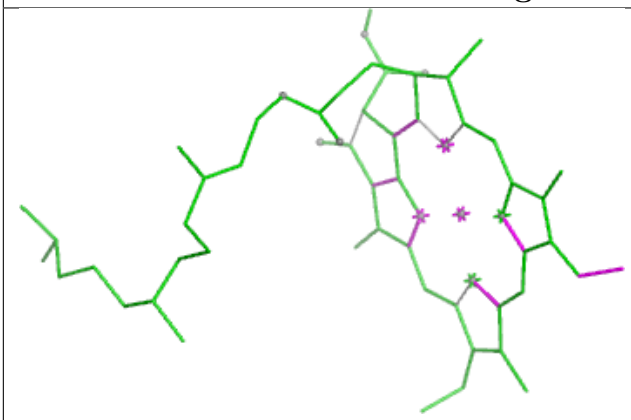


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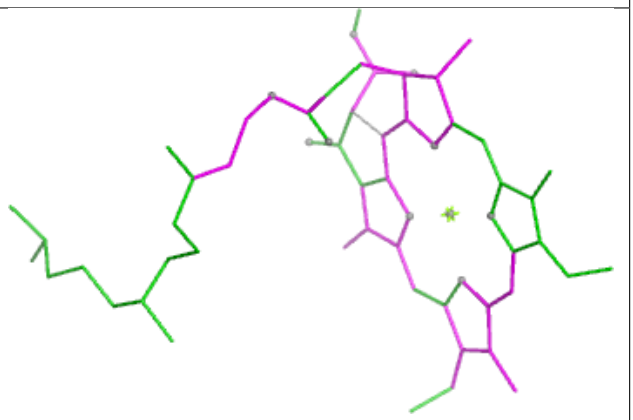


Rings

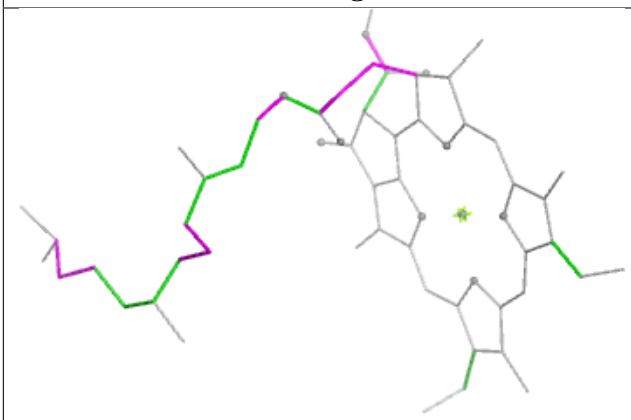
Ligand CLA A 1105



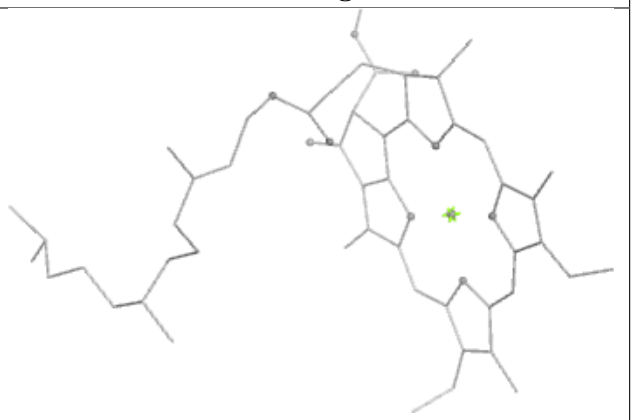
Bond lengths



Bond angles

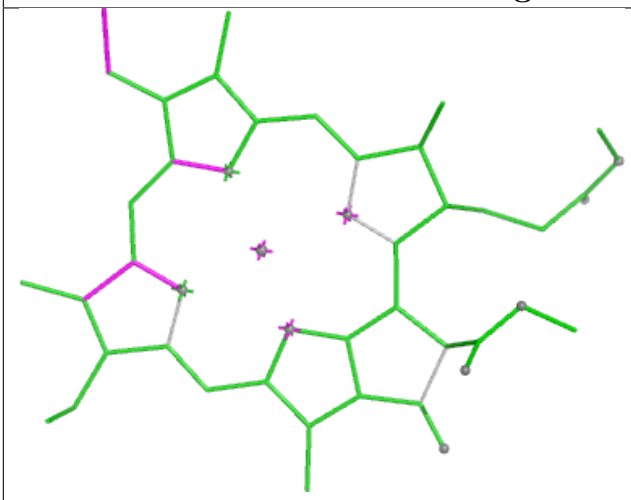


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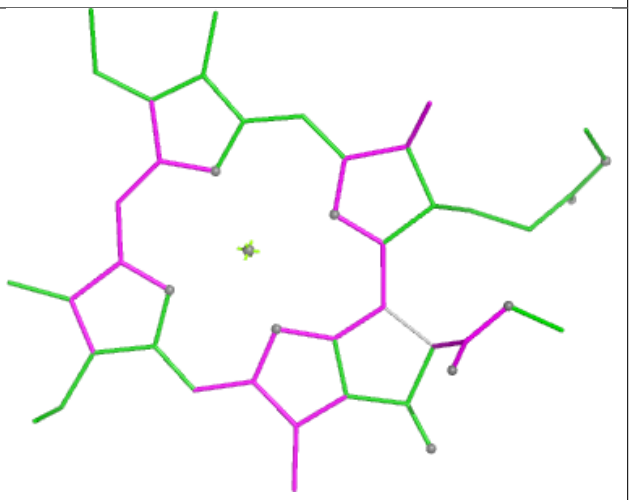


Rings

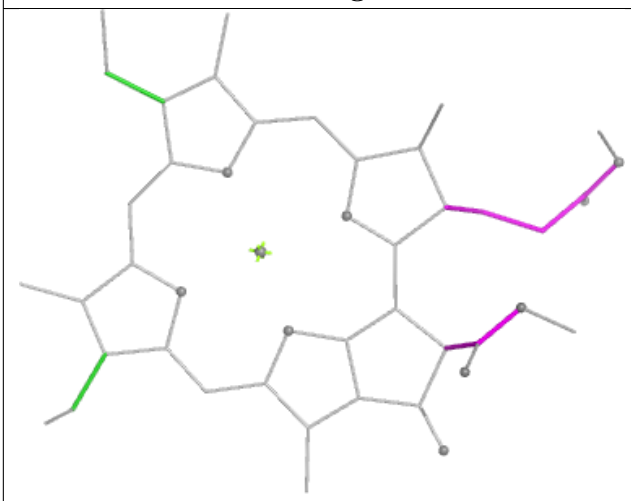
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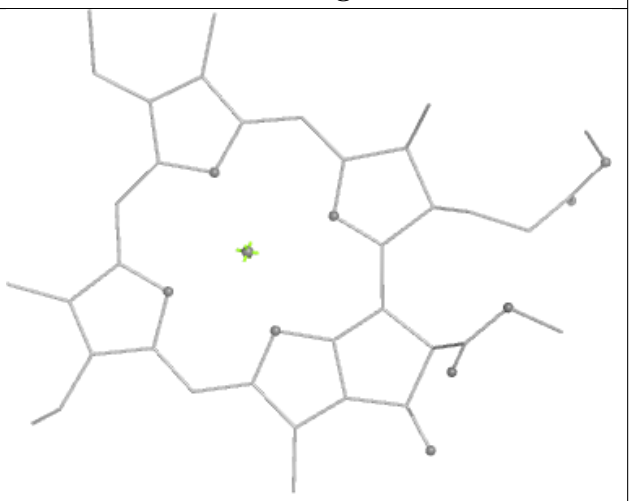
Bond lengths



Bond angles

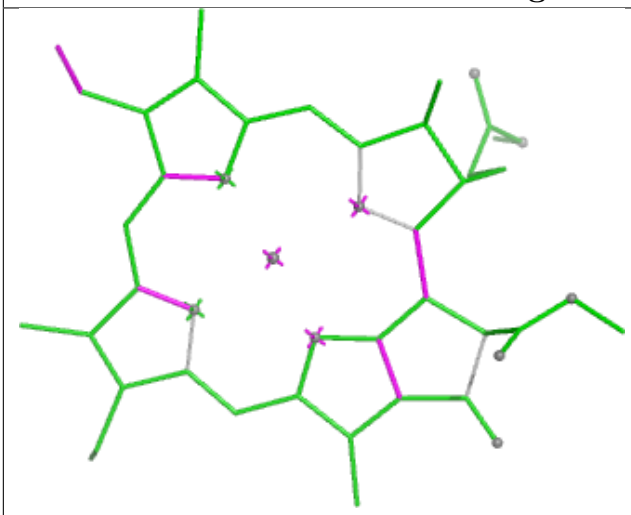


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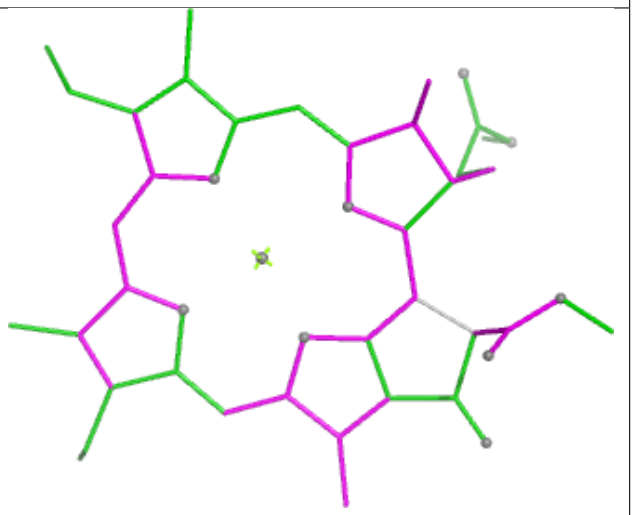


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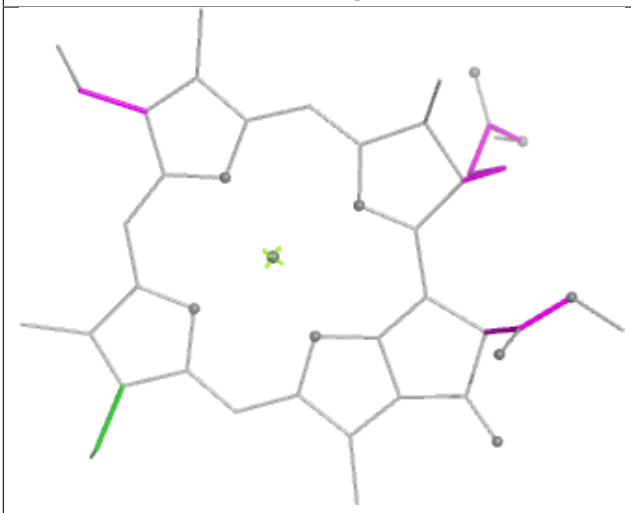
Ligand CLA 4 608



Bond lengths



Bond angles

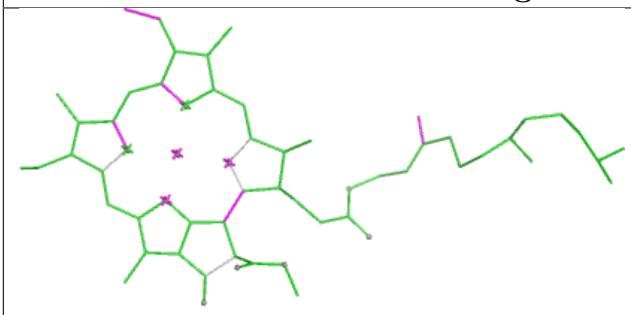


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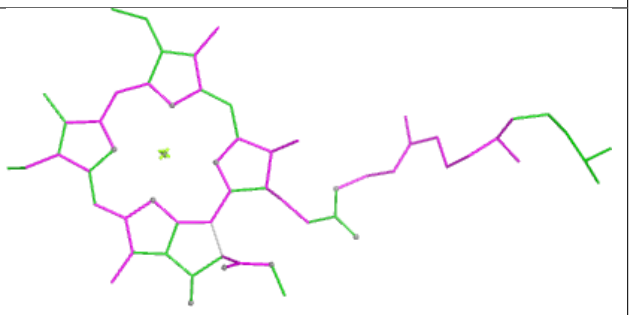


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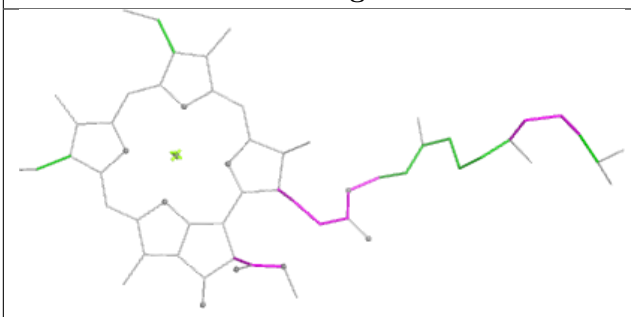
Ligand CLA H 1701



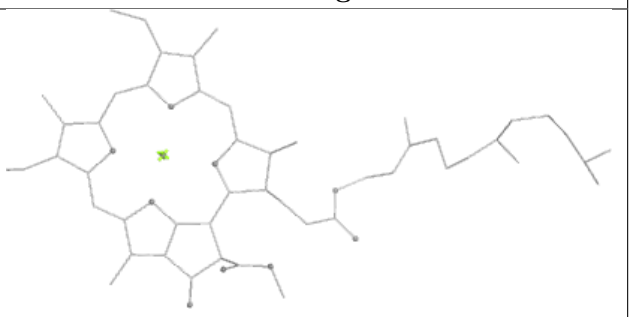
Bond lengths



Bond angles

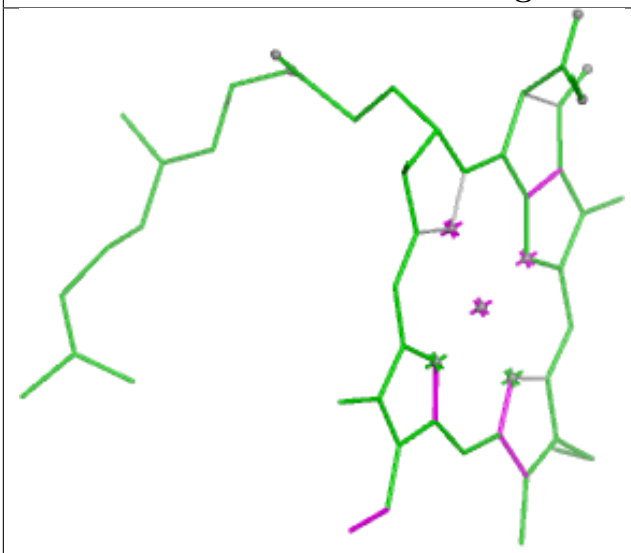


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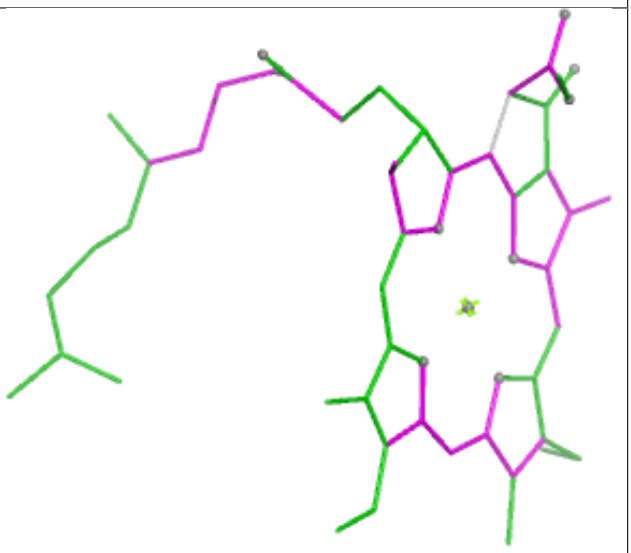


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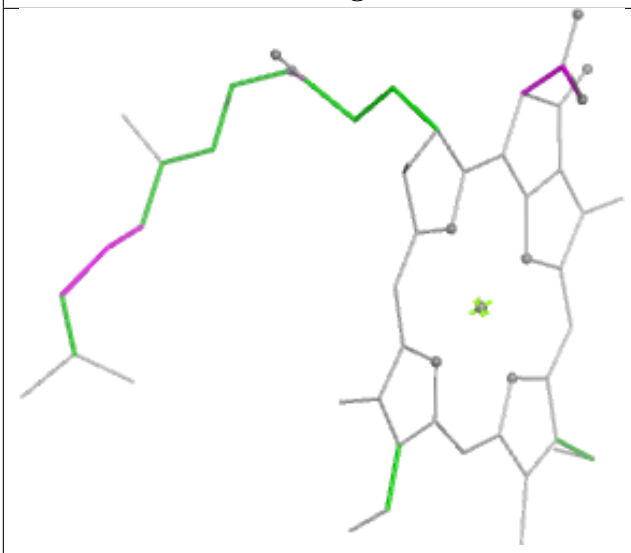
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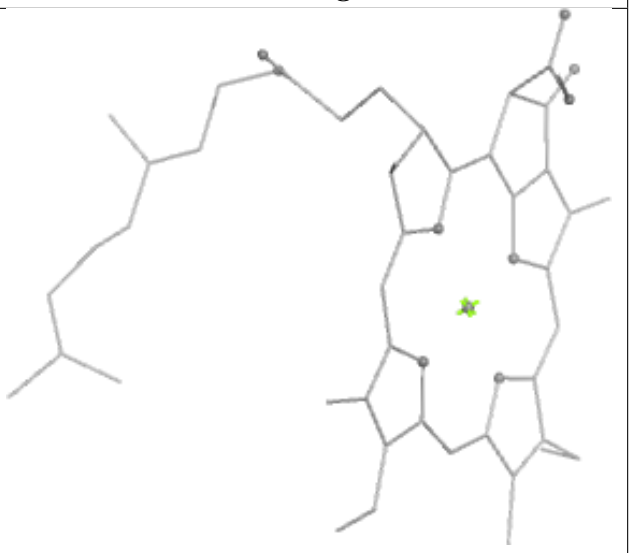
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Bond angles

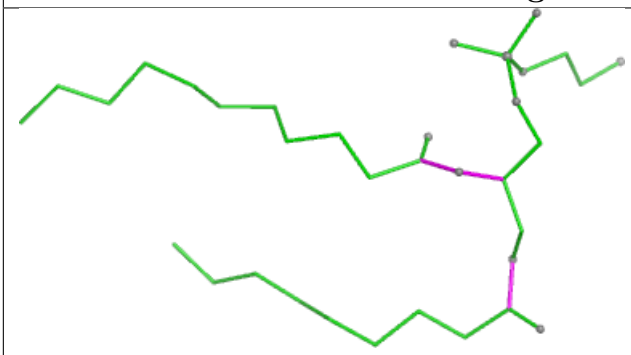


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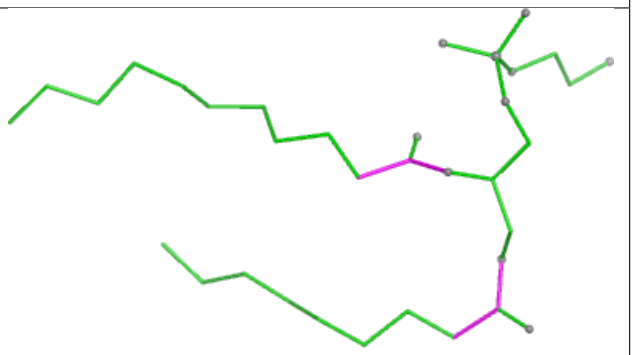


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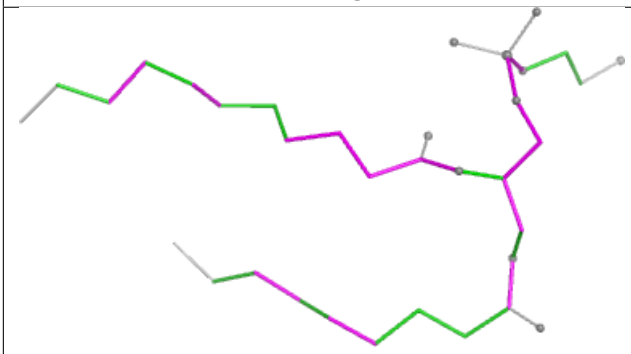
Ligand PTY 4 804



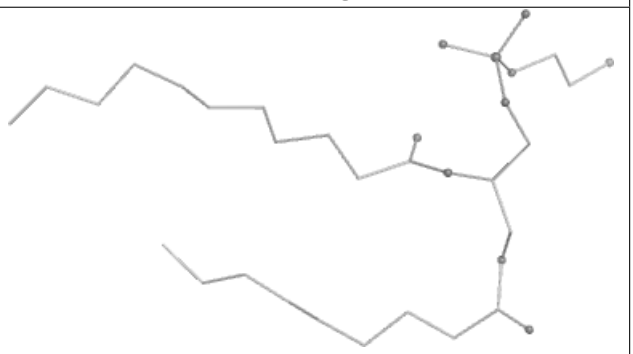
Bond lengths



Bond angles

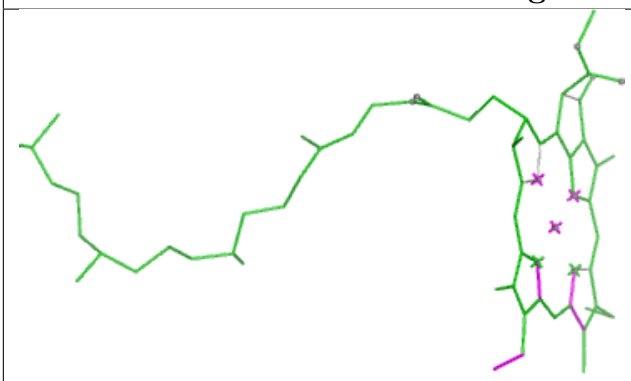


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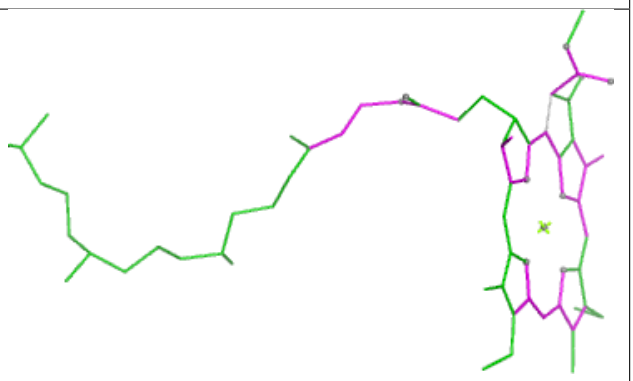


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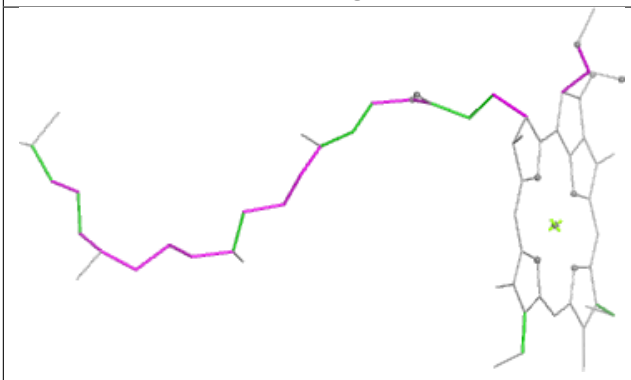
Ligand CLA 1 611



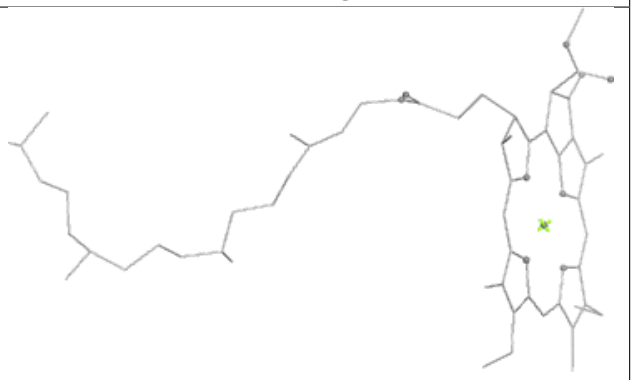
Bond lengths



Bond angles

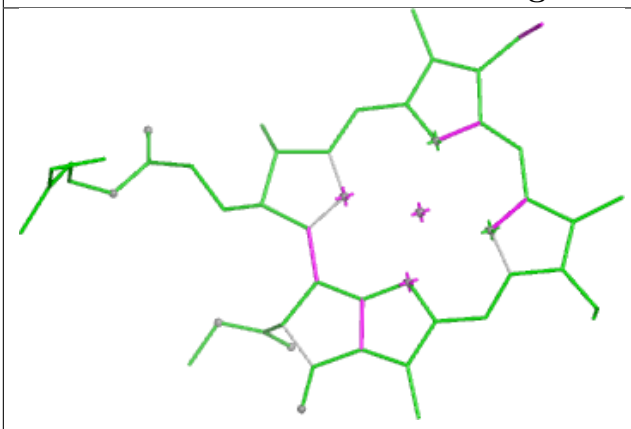


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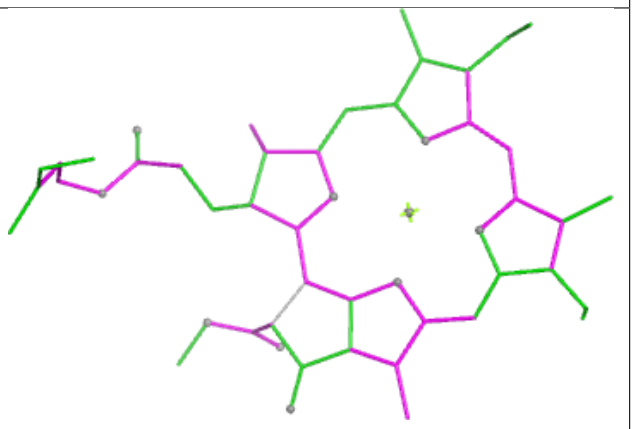


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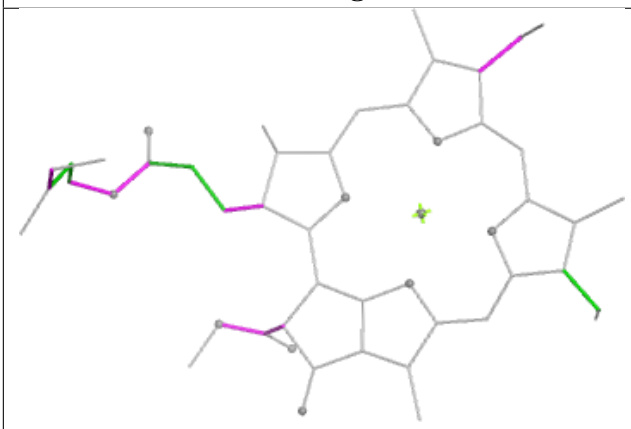
Ligand CLA 4 615



Bond lengths



Bond angles

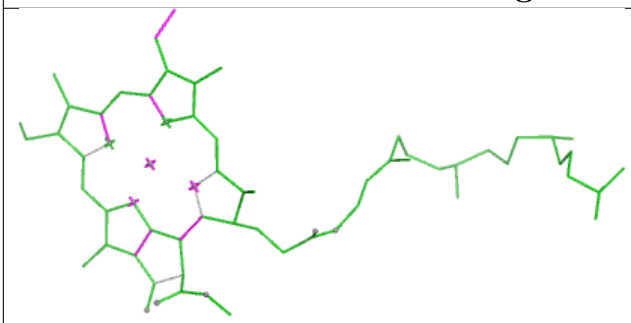


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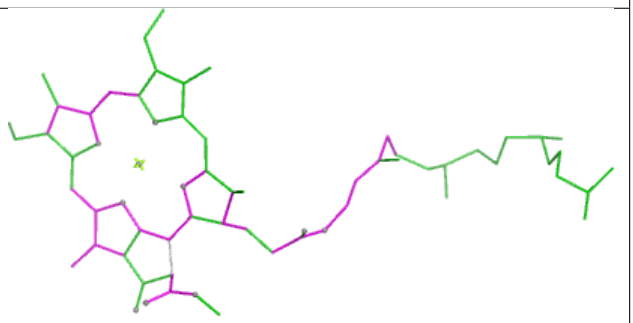


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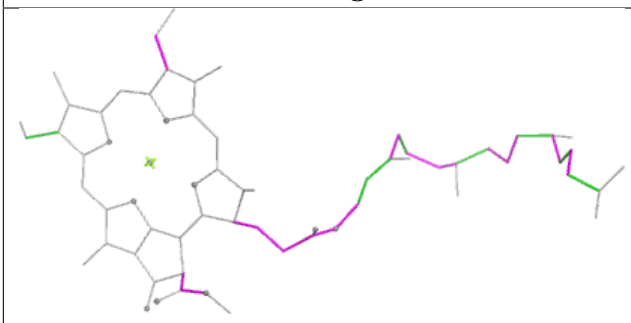
Ligand CLA B 1210



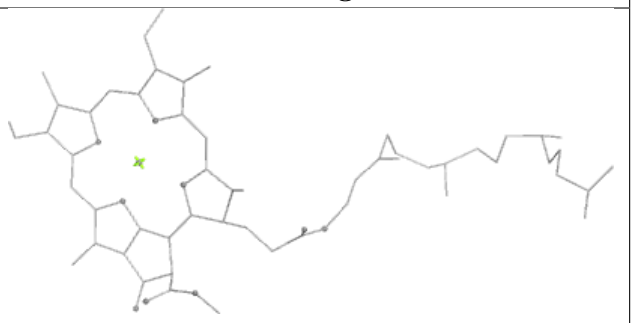
Bond lengths



Bond angles

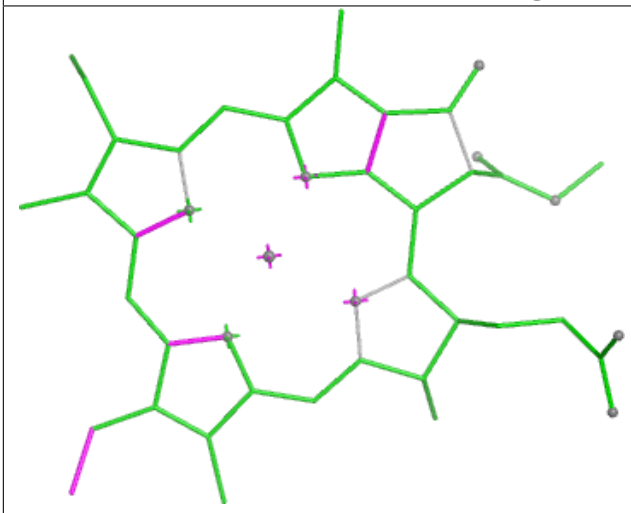


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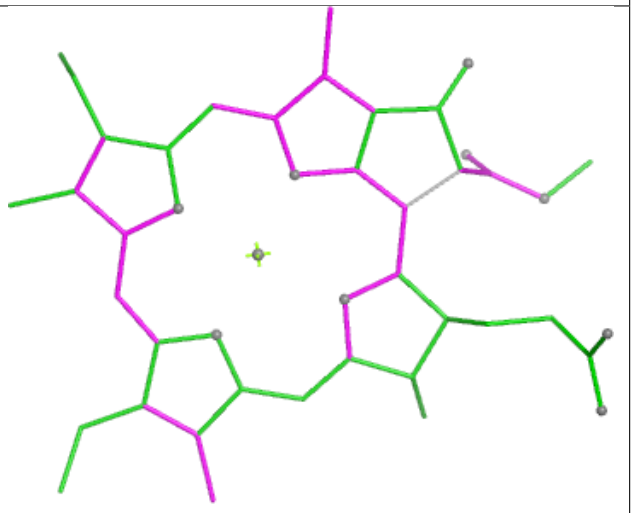


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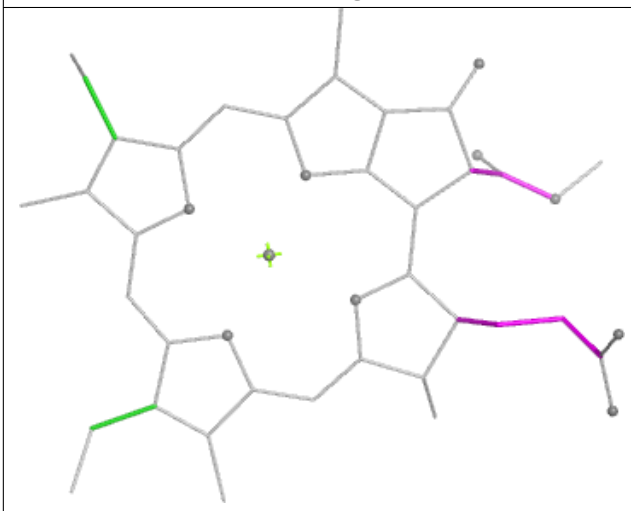
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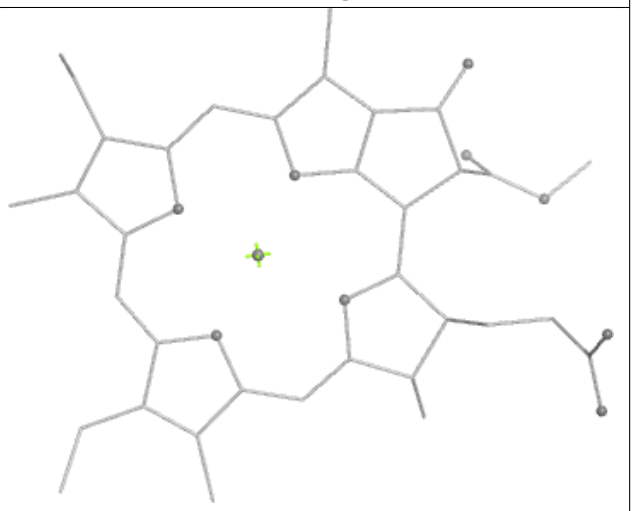
Bond lengths



Bond angles

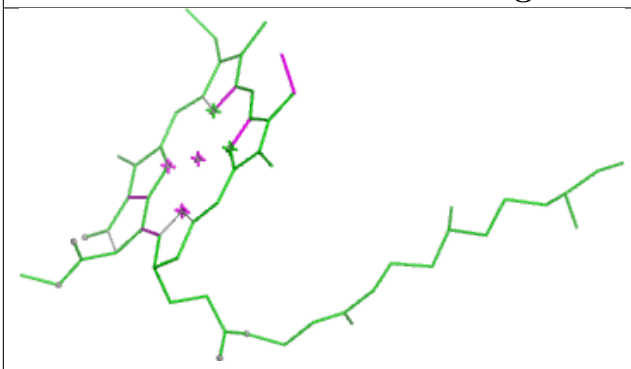


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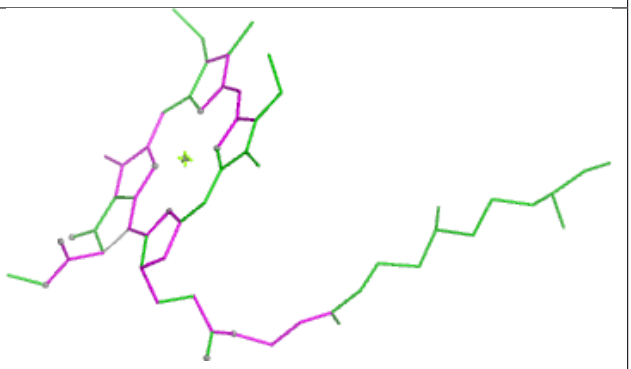


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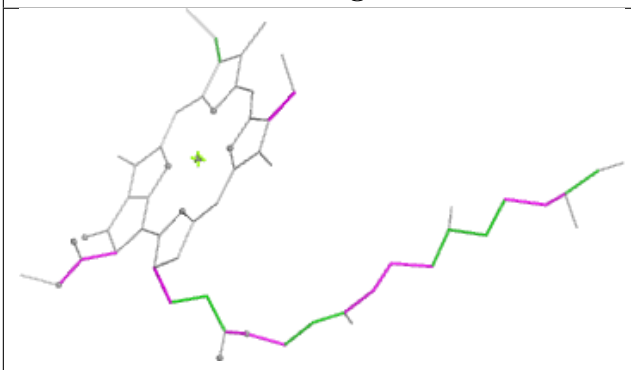
Ligand CLA A 1140



Bond lengths



Bond angles

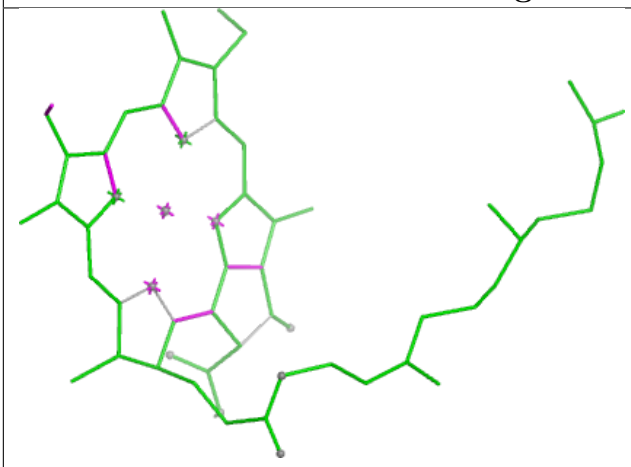


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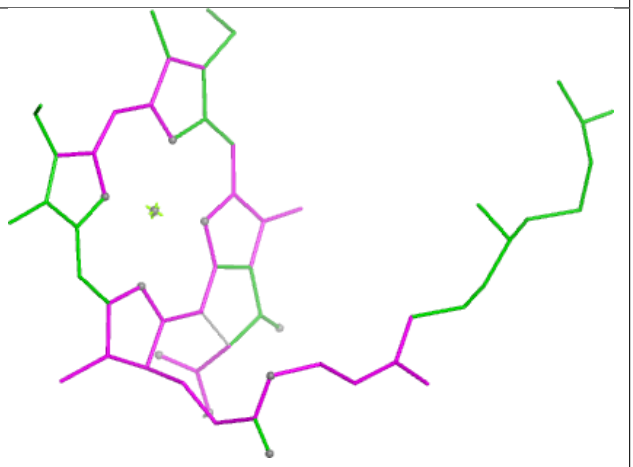


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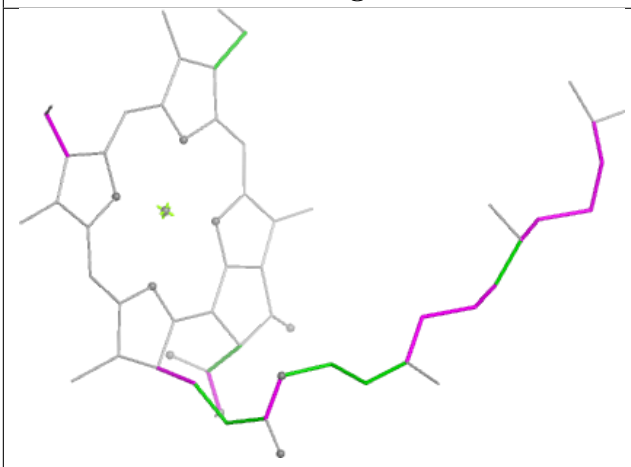
Ligand CLA A 1120



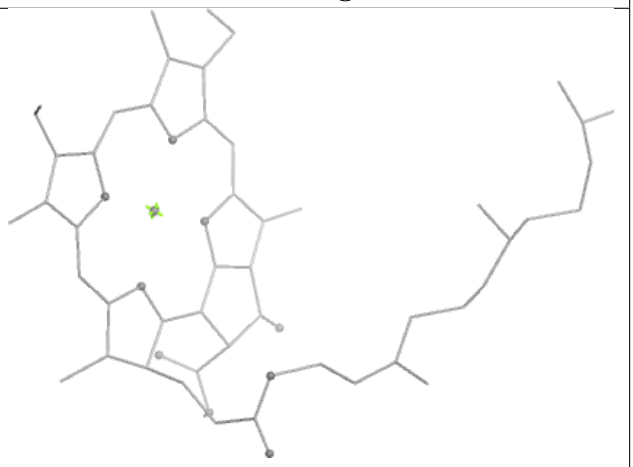
Bond lengths



Bond angles

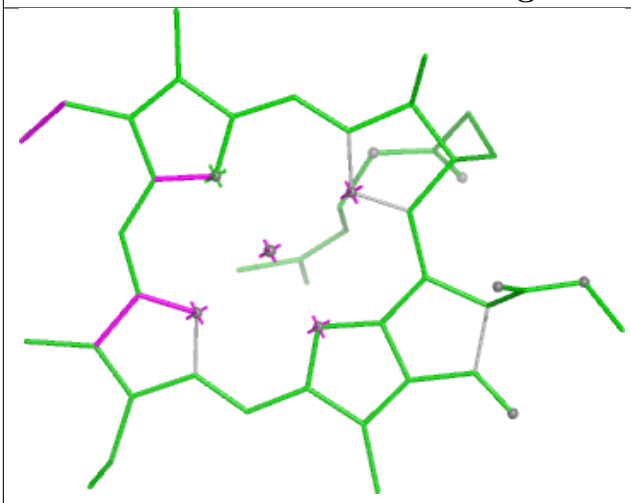


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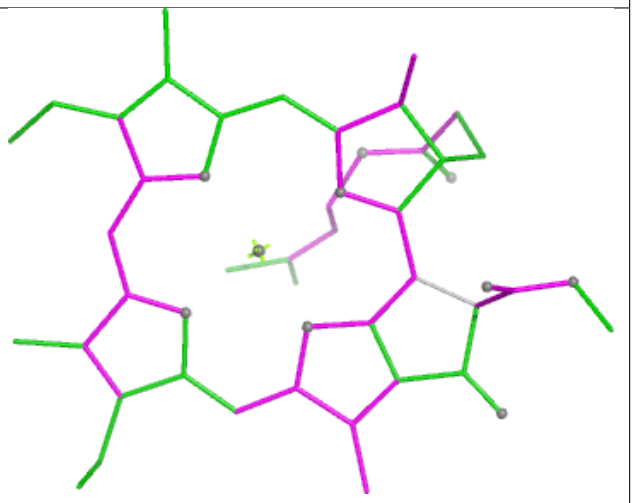


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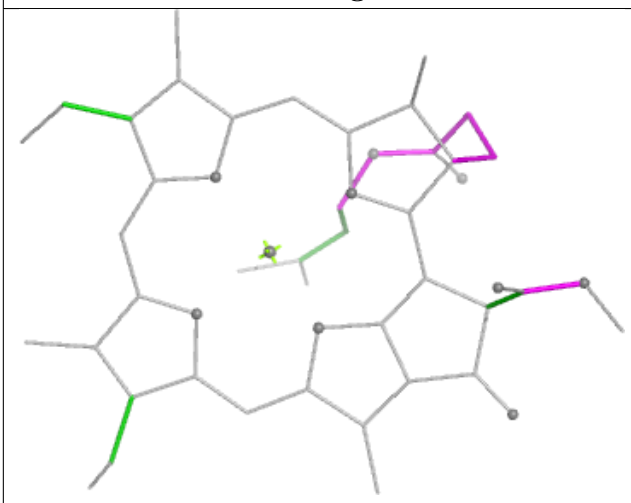
Ligand CLA L 1504



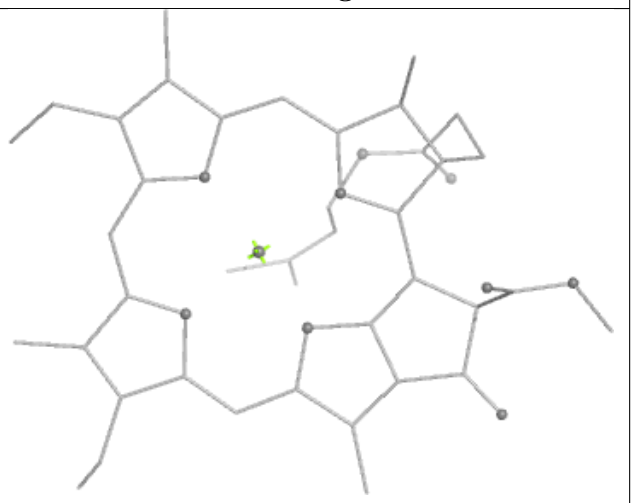
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Bond angles

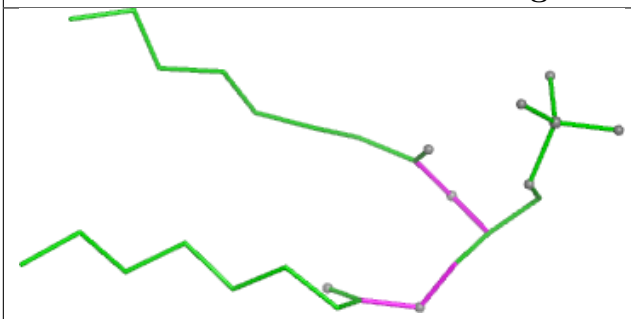


Torsions



Rings

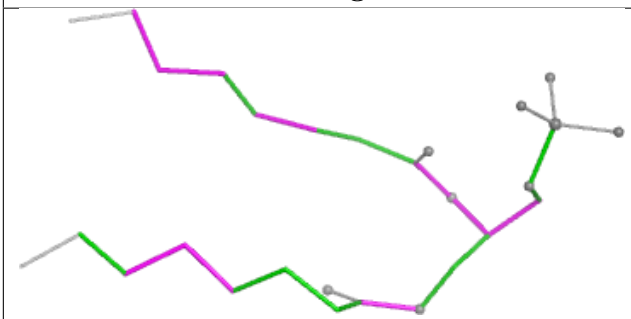
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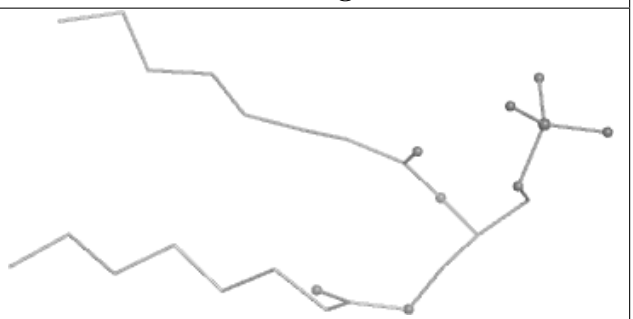
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Bond angles

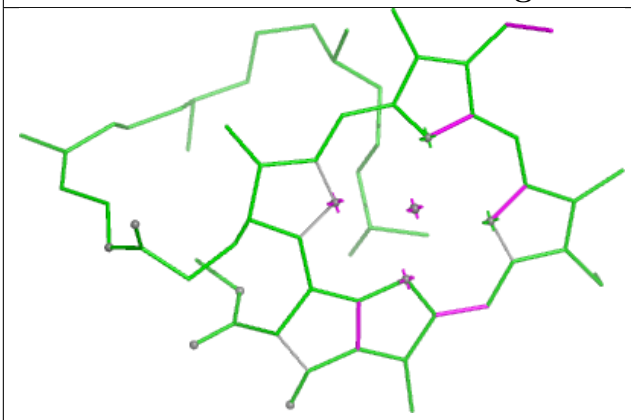


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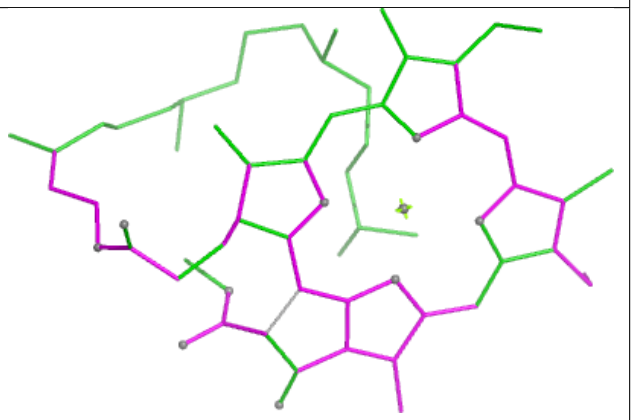


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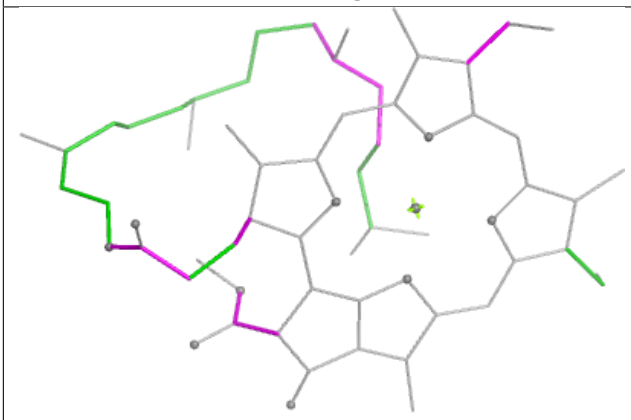
Ligand CLA A 1104



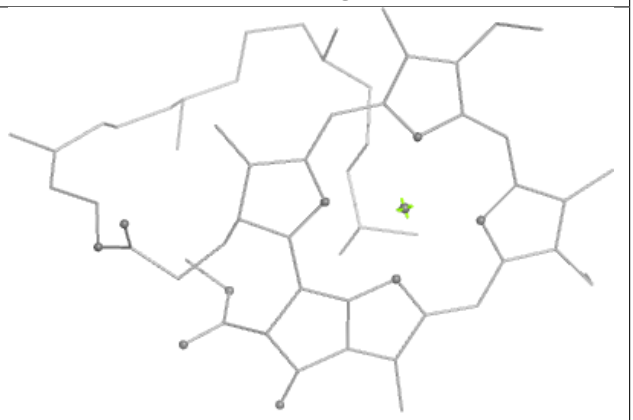
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Bond angles

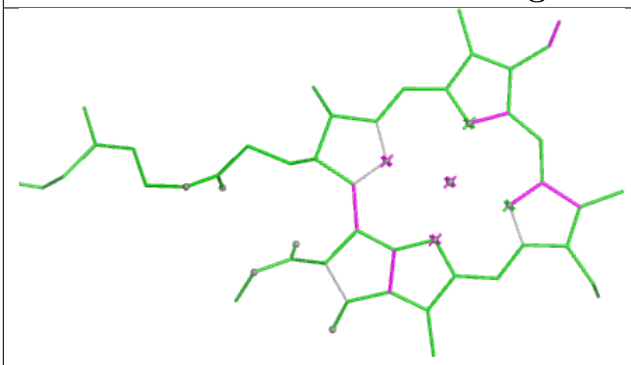


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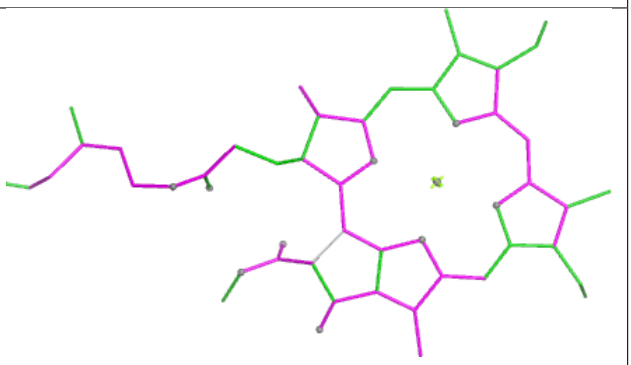


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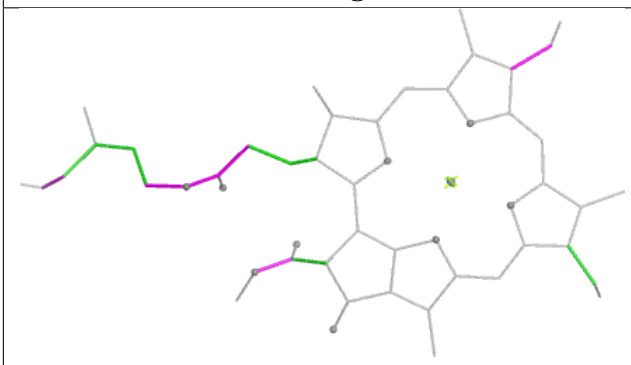
Ligand CLA 2 602



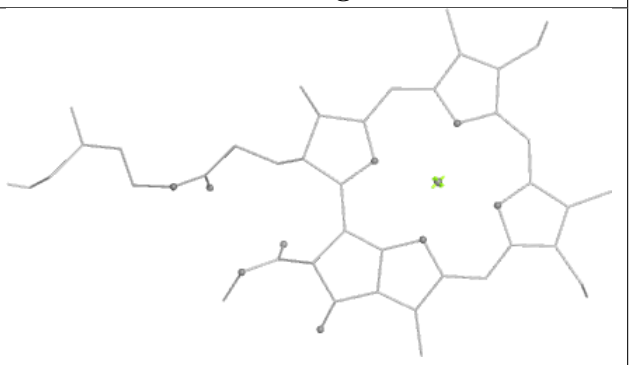
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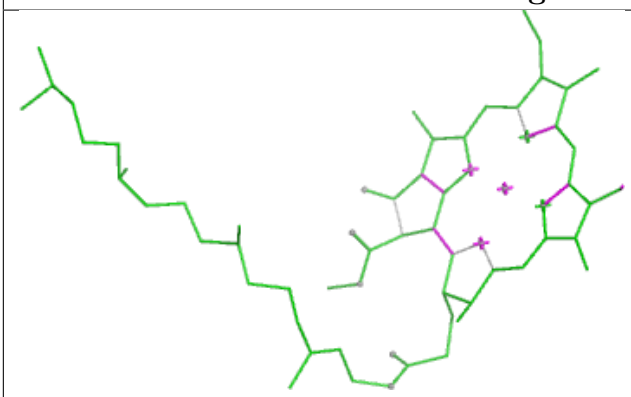


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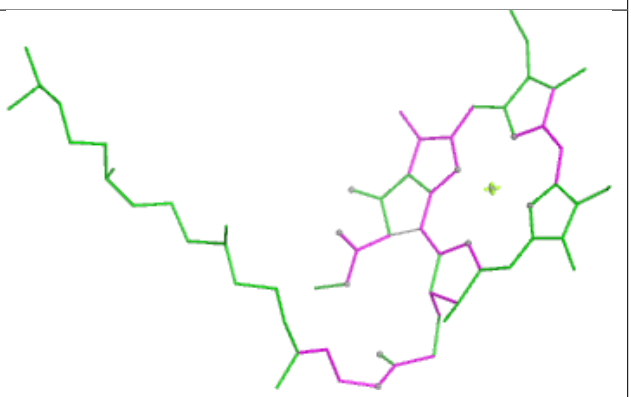


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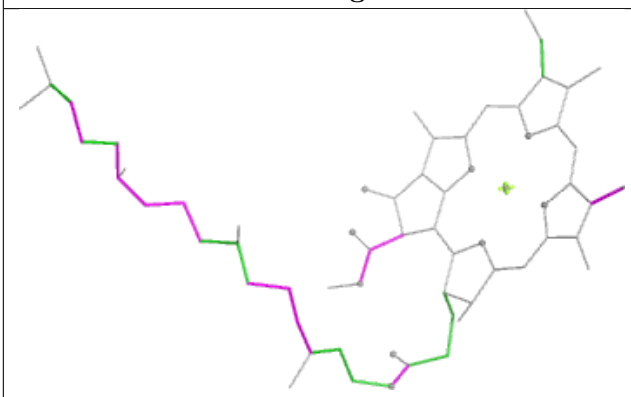
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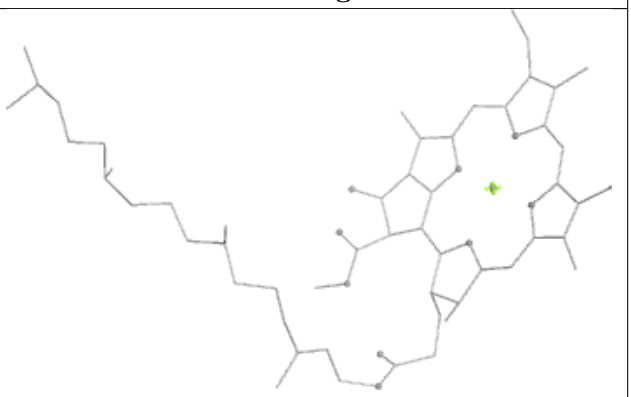
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Bond angles

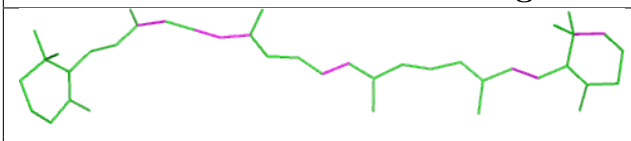


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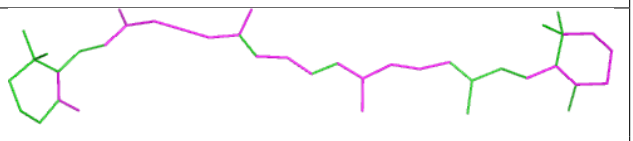


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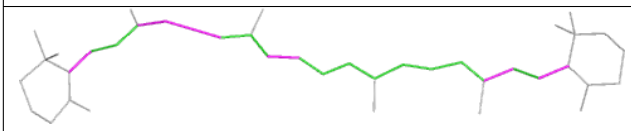
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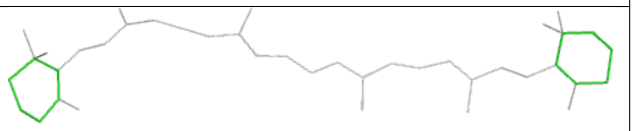
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Bond angles

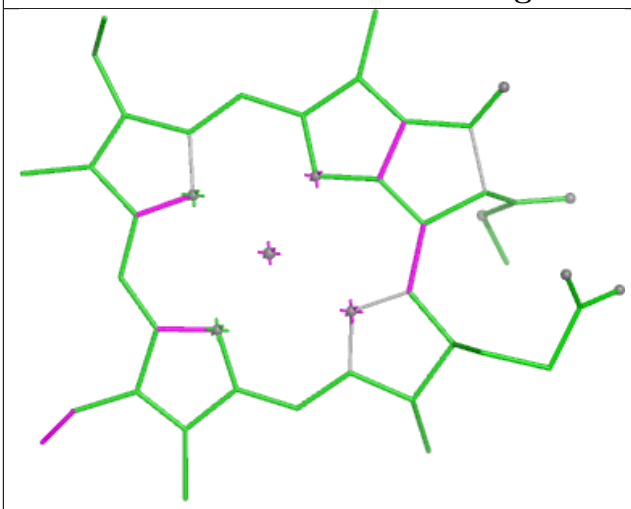


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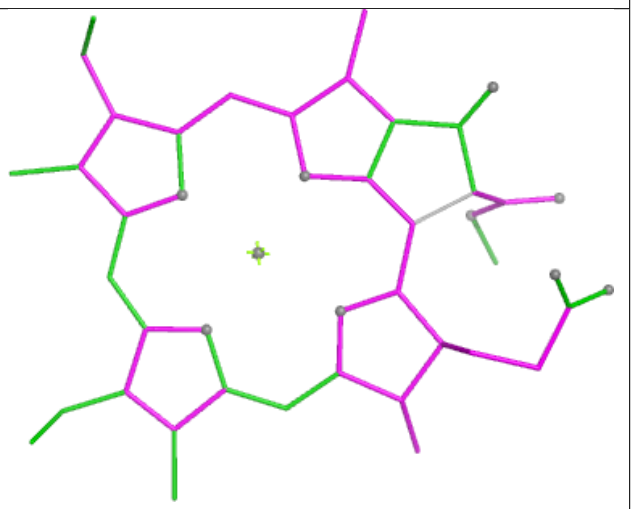


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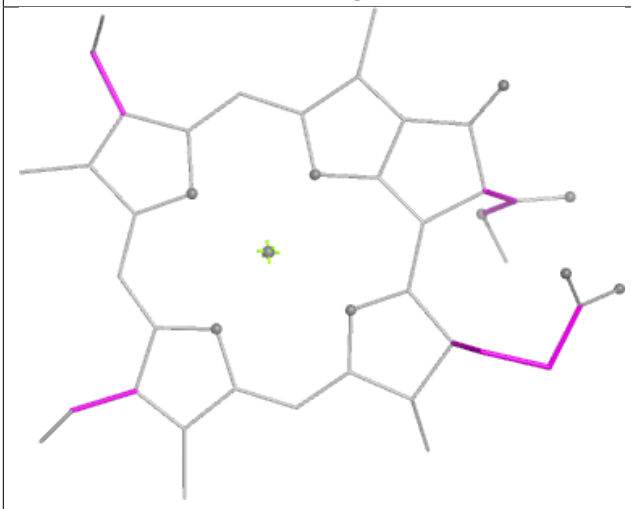
Ligand CLA K 1401



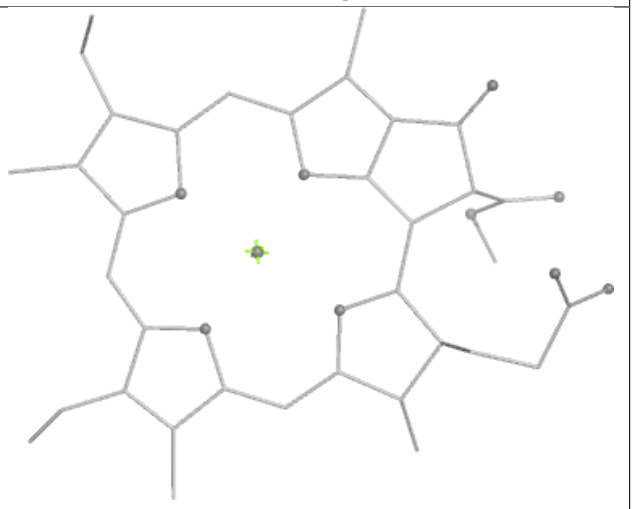
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Bond angles

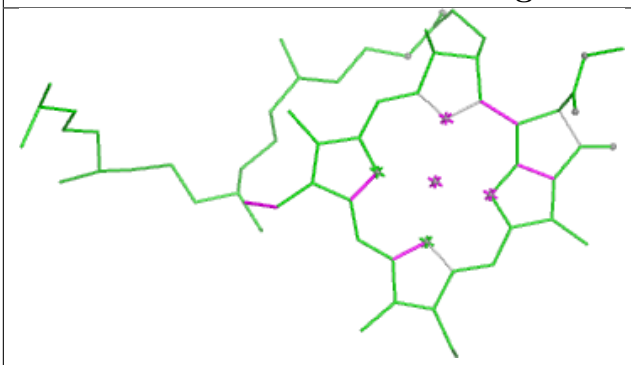


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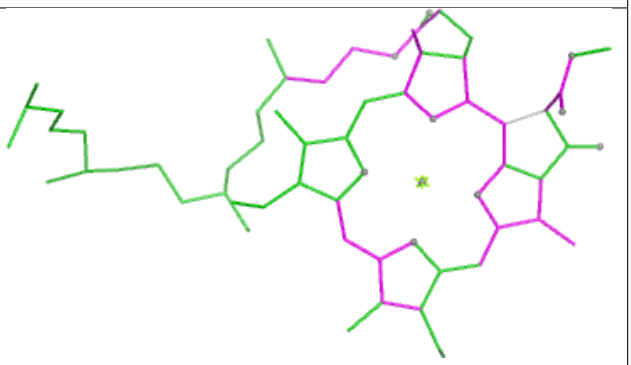


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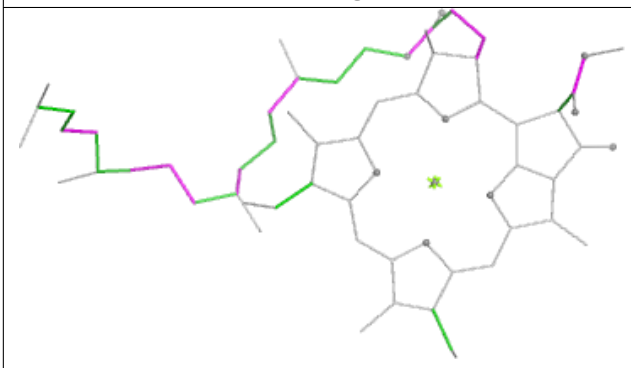
Ligand CLA B 1215



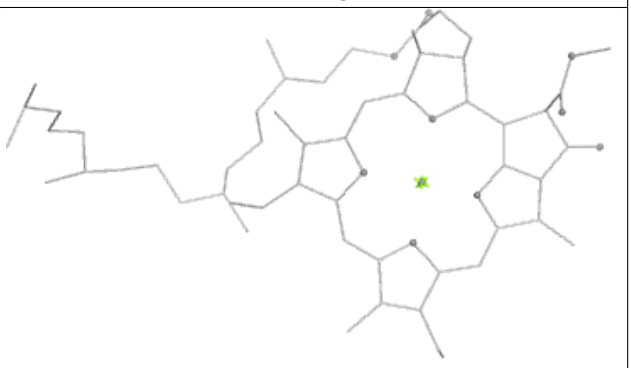
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Bond angles

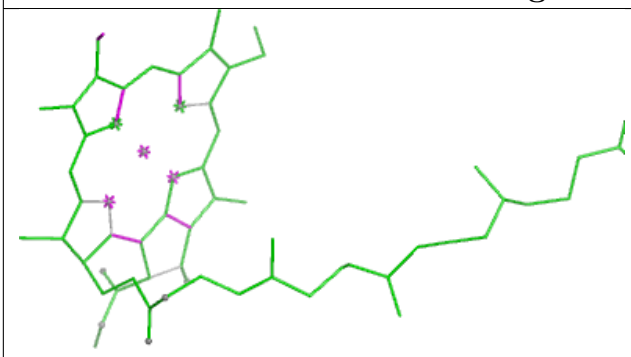


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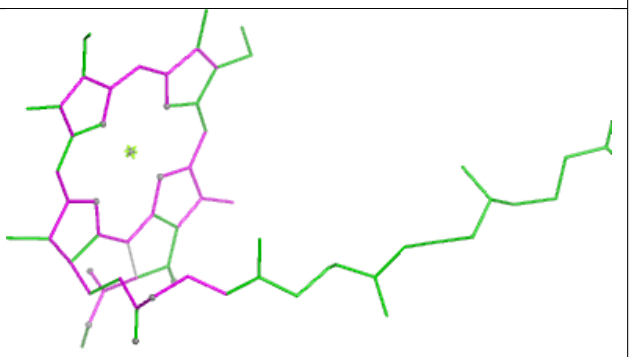


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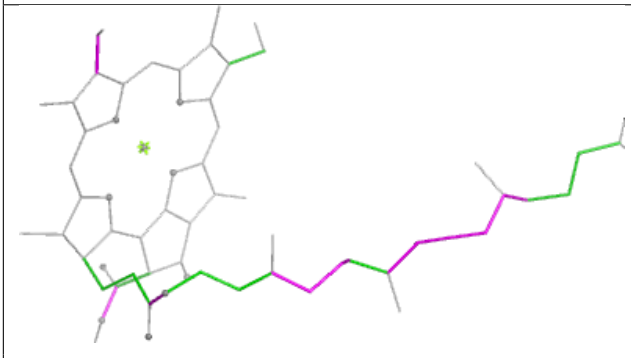
Ligand CLA 2 612



Bond lengths



Bond angles

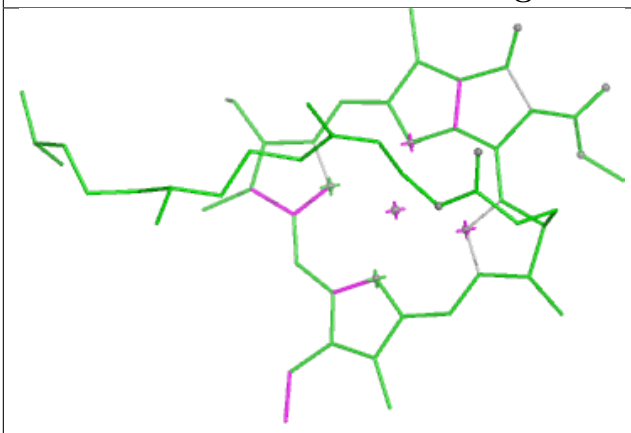


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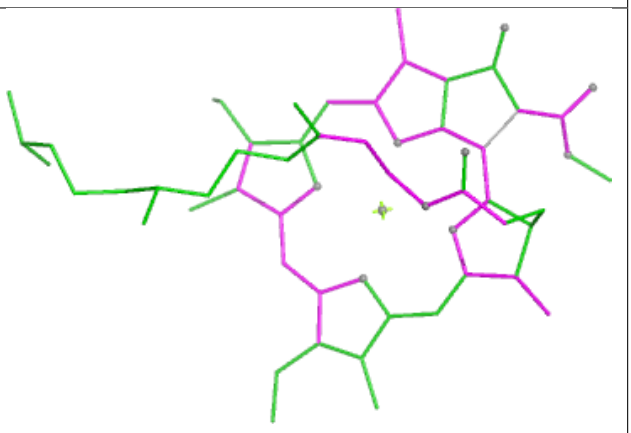


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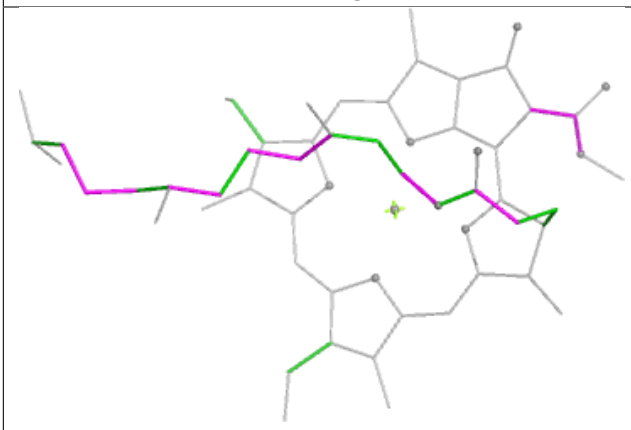
Ligand CLA A 1115



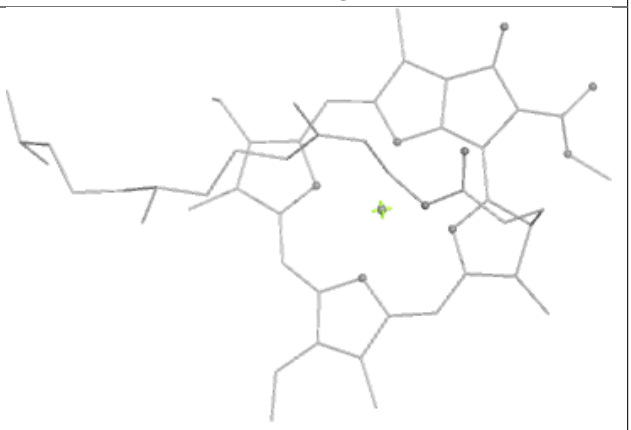
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Bond angles

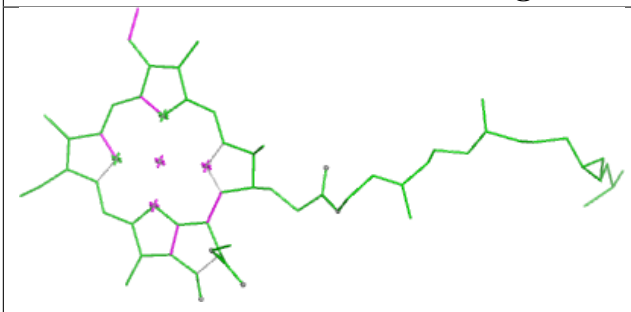


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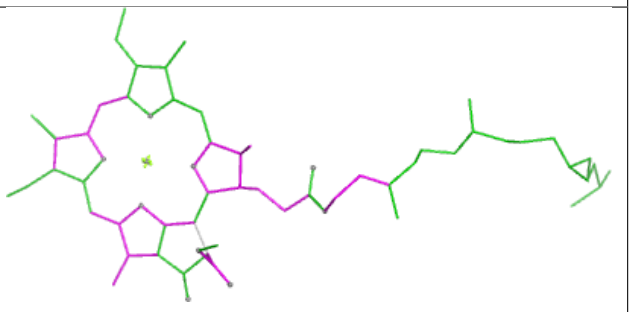


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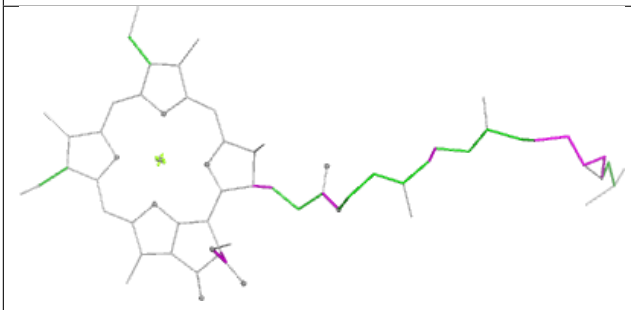
Ligand CLA A 1103



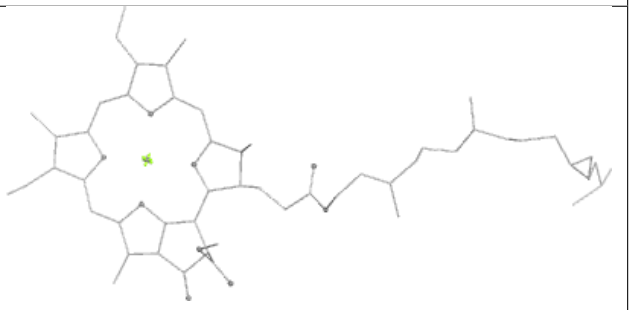
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Bond angles

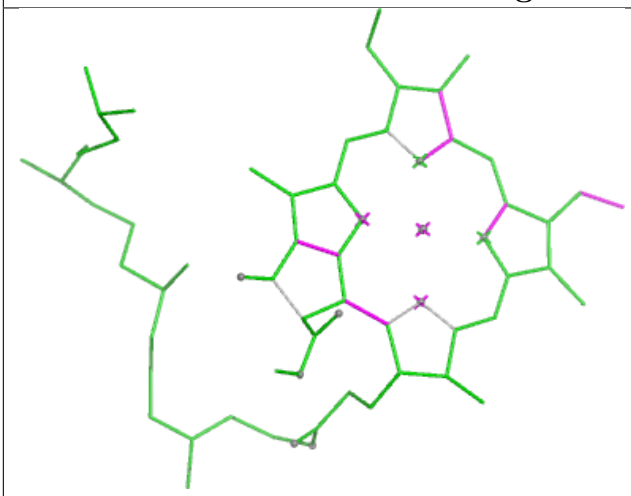


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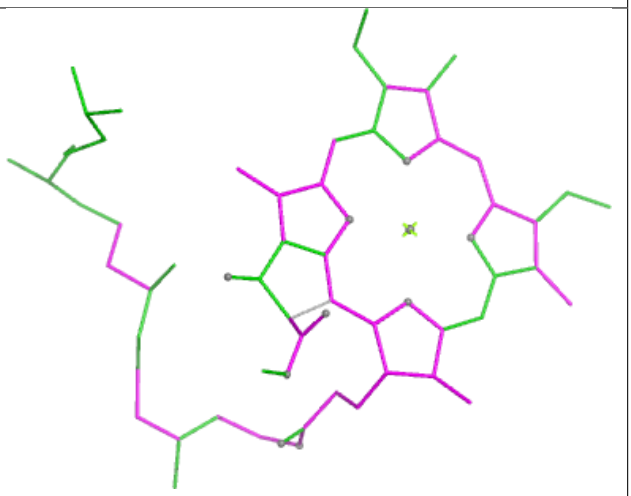


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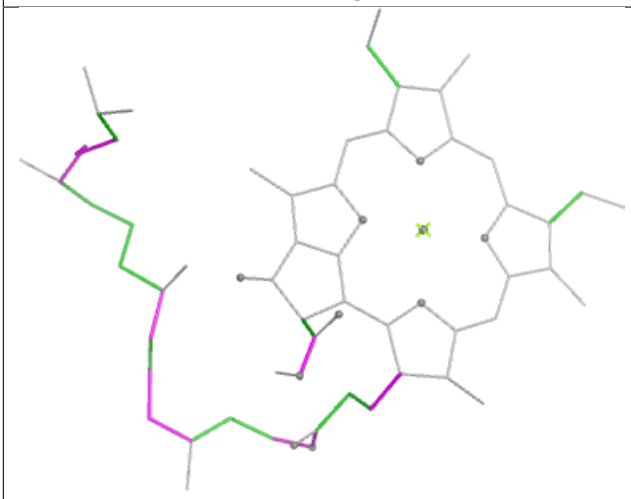
Ligand CLA B 1229



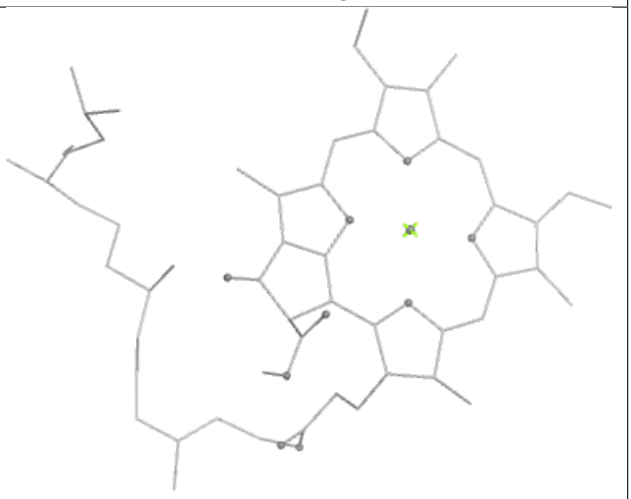
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Bond angles

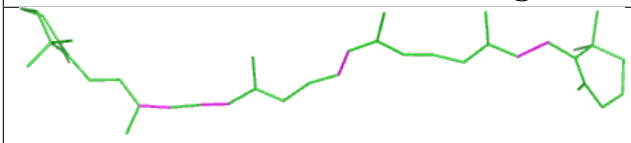


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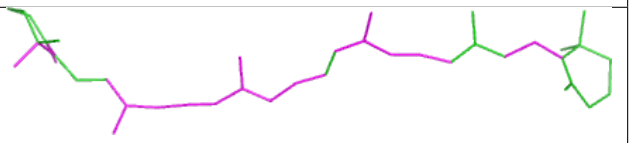


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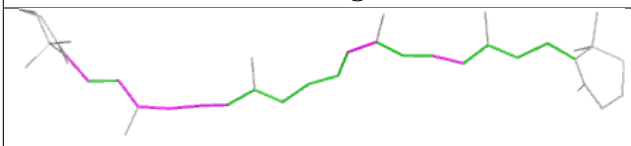
Ligand BCR A 4007



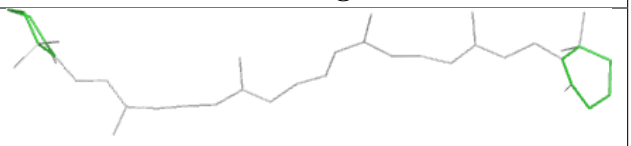
Bond lengths



Bond angles

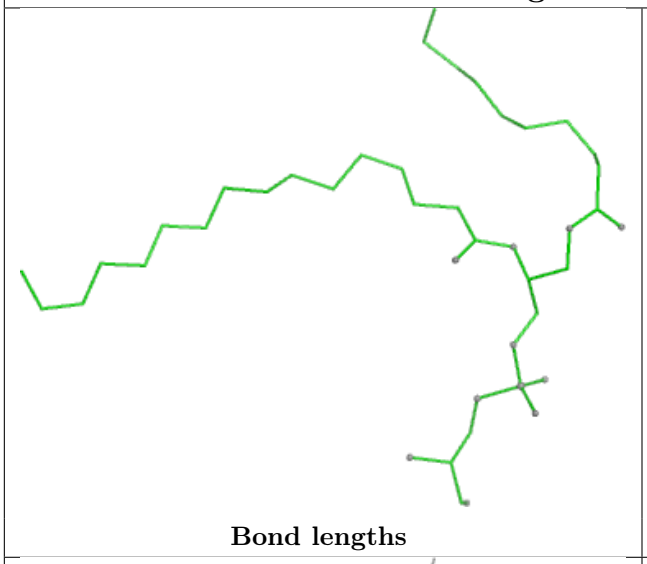


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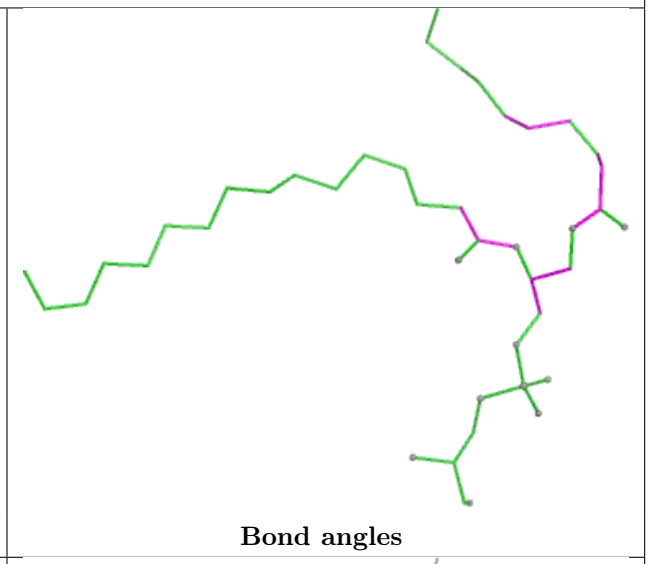


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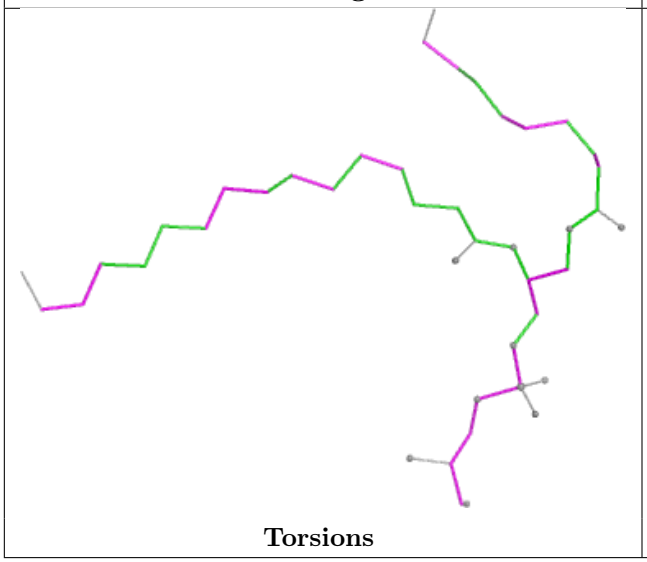
Ligand LHG 5 801



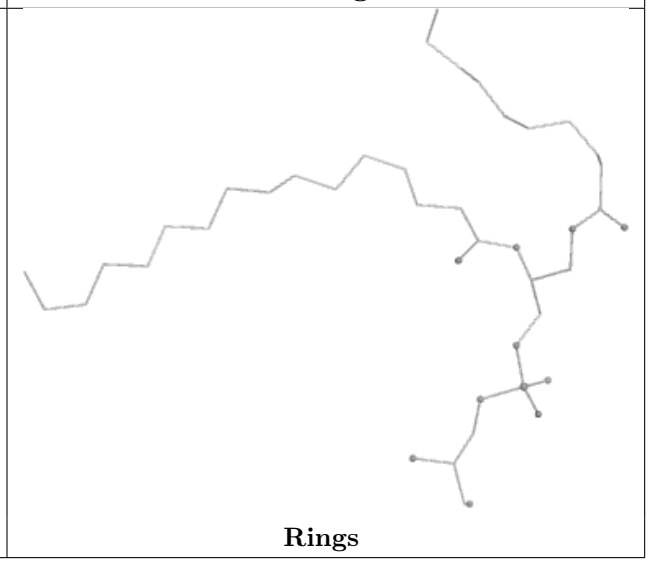
Bond lengths



Bond angles

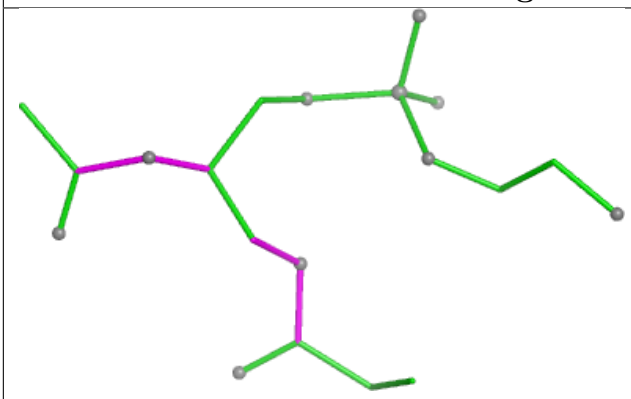


Torsions

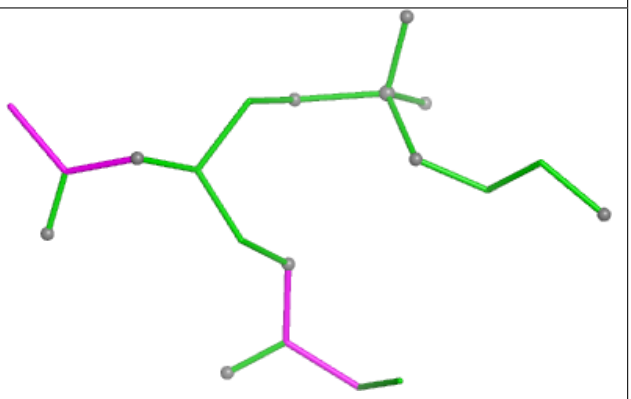


Rings

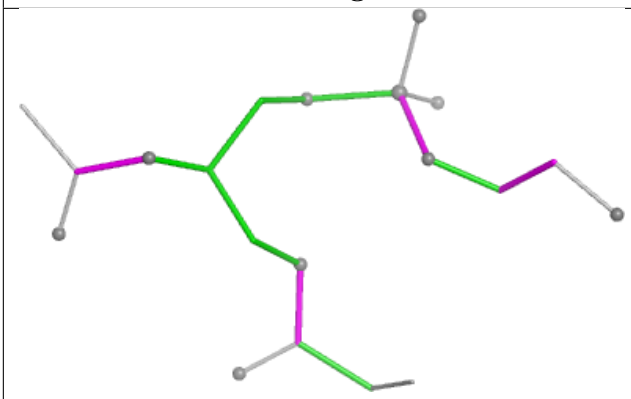
Ligand PTY L 5003



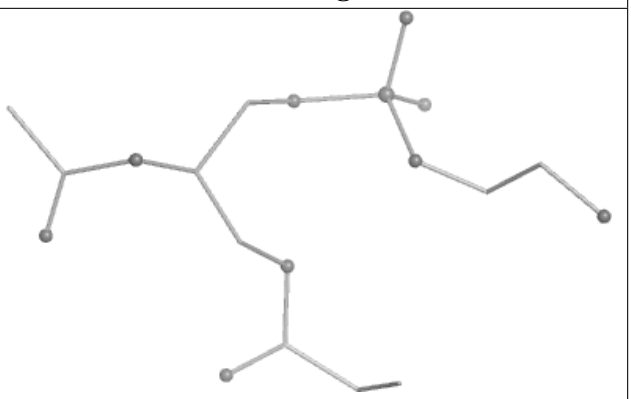
Bond lengths



Bond angles

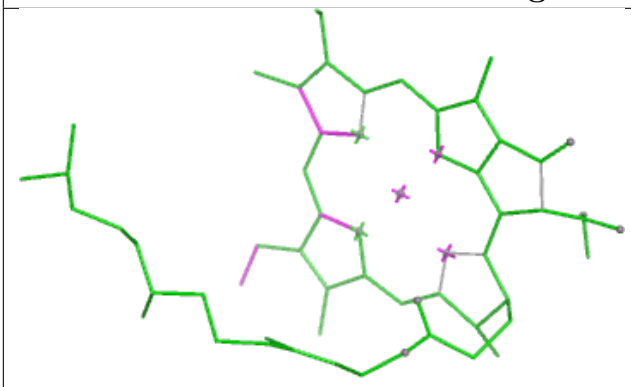


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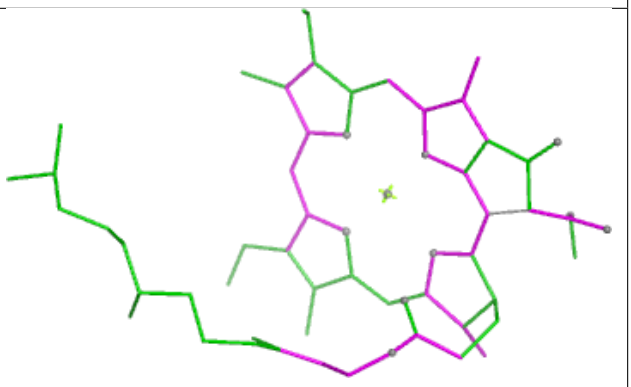


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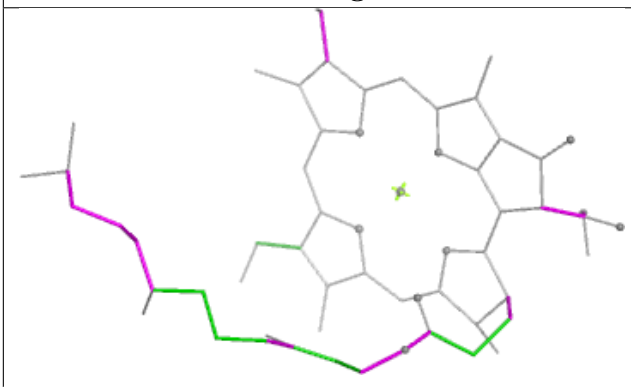
Ligand CLA 6 601



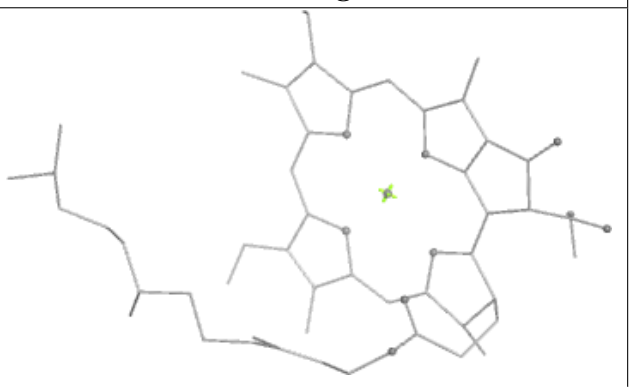
Bond lengths



Bond angles

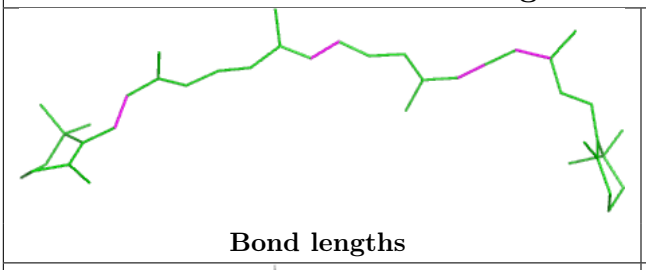


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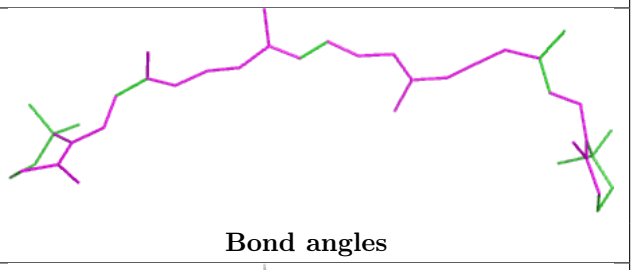


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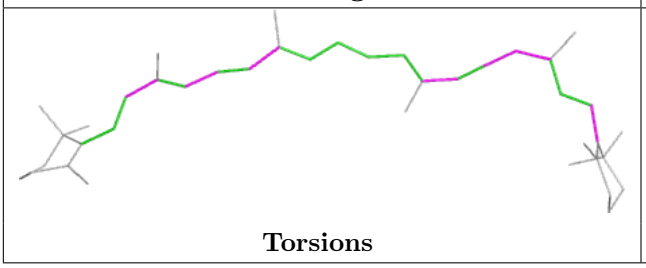
Ligand BCR I 4002



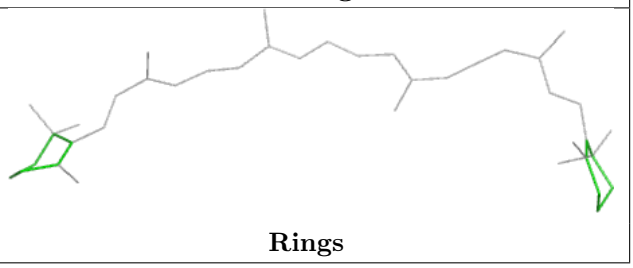
Bond lengths



Bond angles

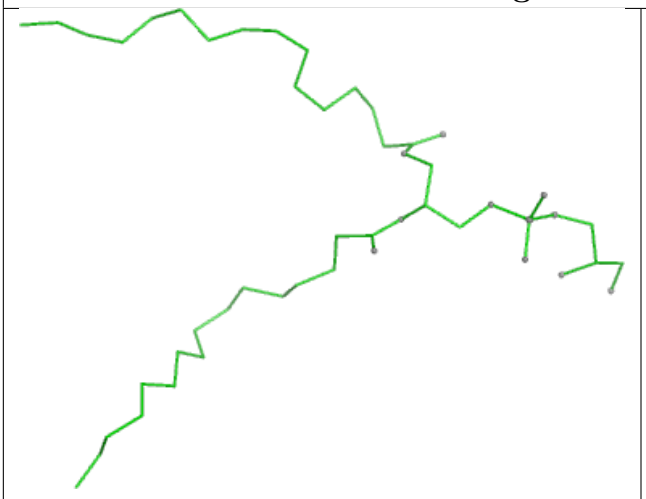


Torsions



Rings

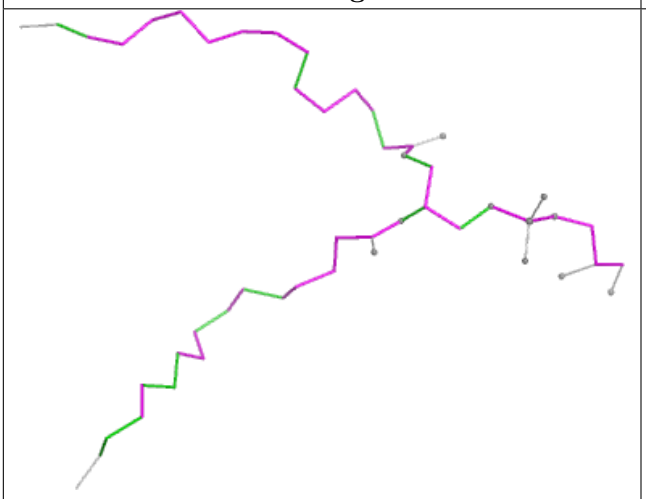
Ligand LHG A 5002



Bond lengths



Bond angles

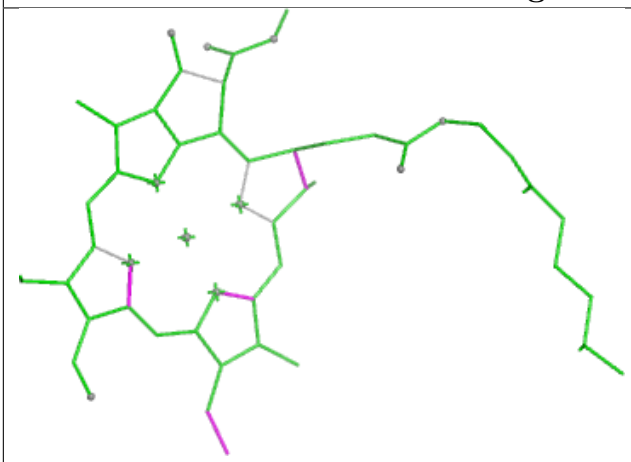


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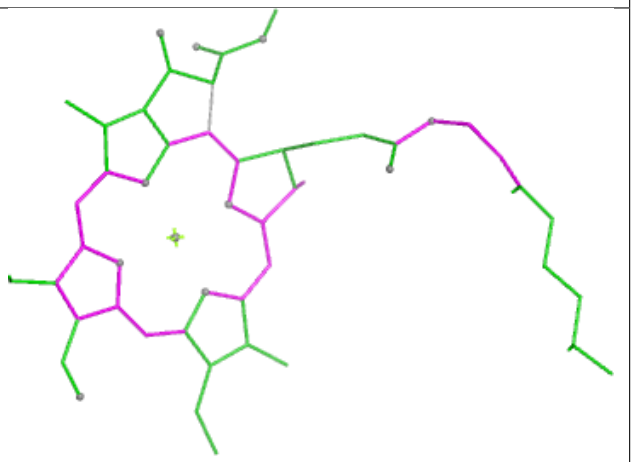


Rings

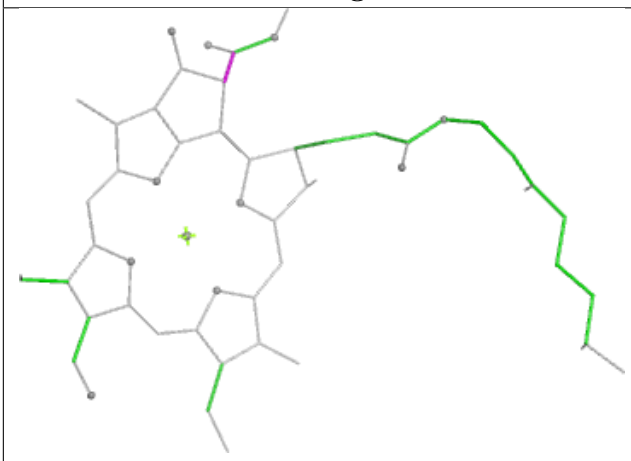
Ligand CHL 2 610



Bond lengths



Bond angles

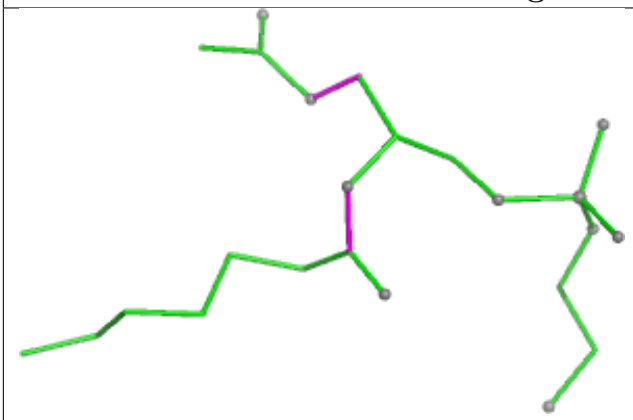


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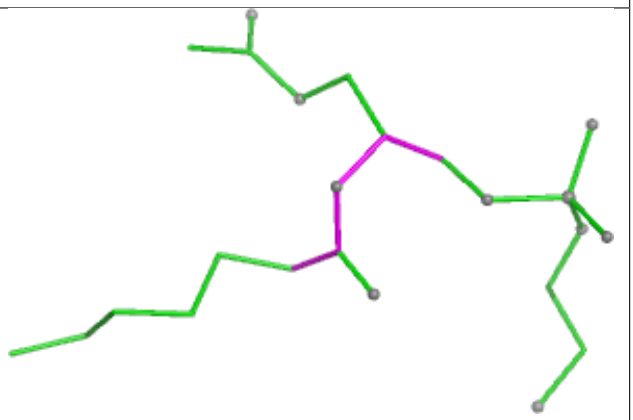


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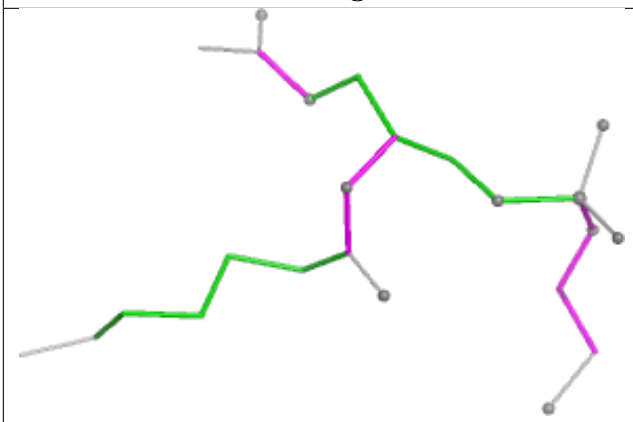
Ligand PTY 6 804



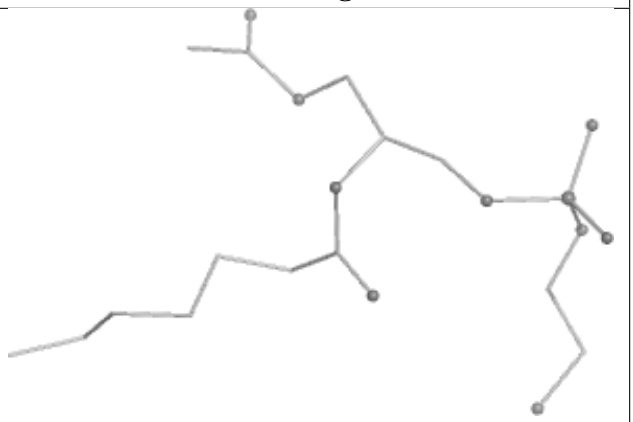
Bond lengths



Bond angles

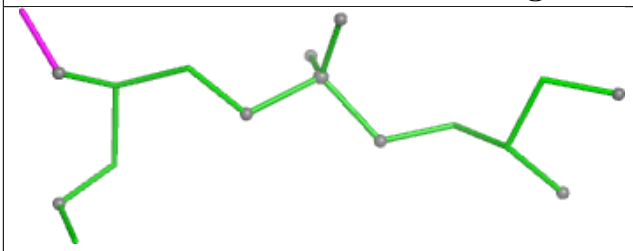


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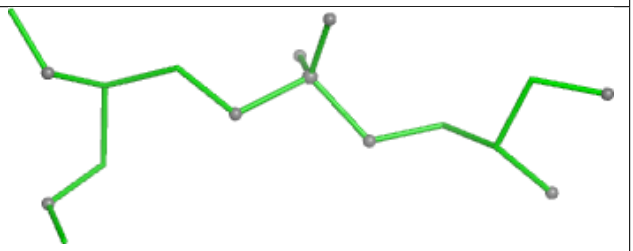


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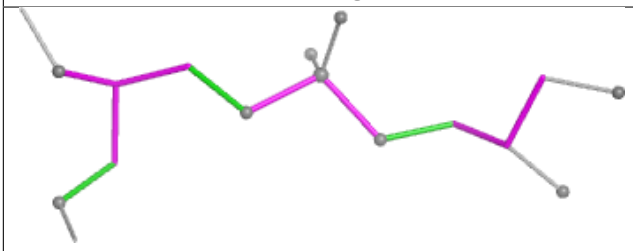
Ligand LHG 3 801



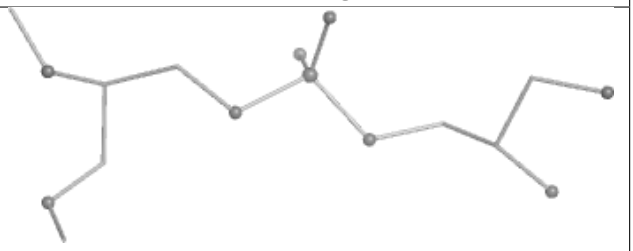
Bond lengths



Bond angles

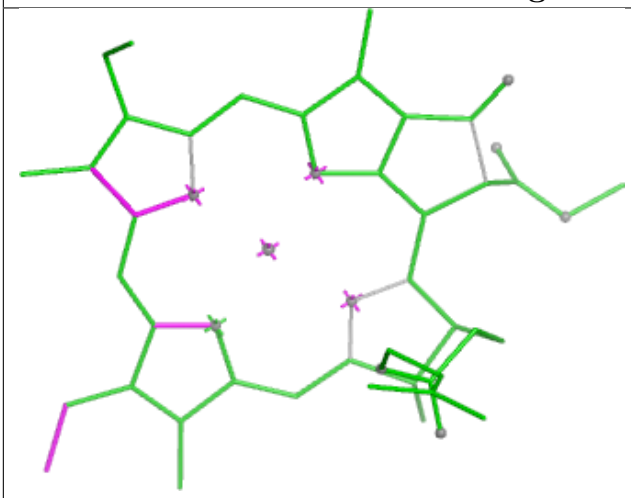


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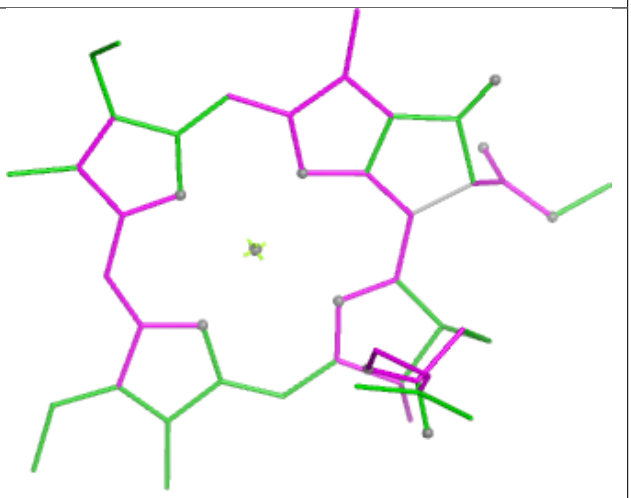


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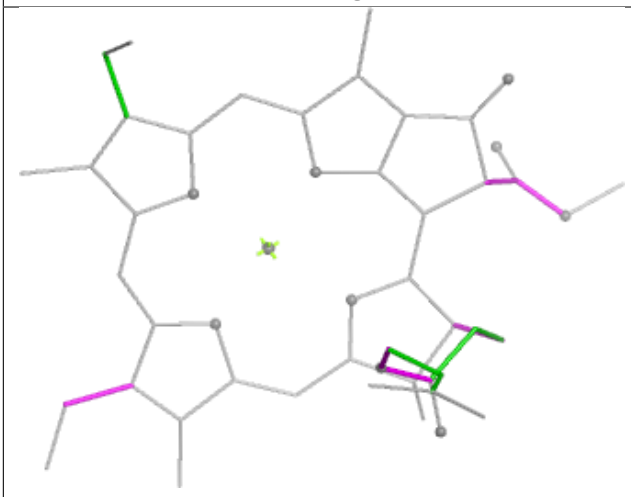
Ligand CLA 5 606



Bond lengths



Bond angles

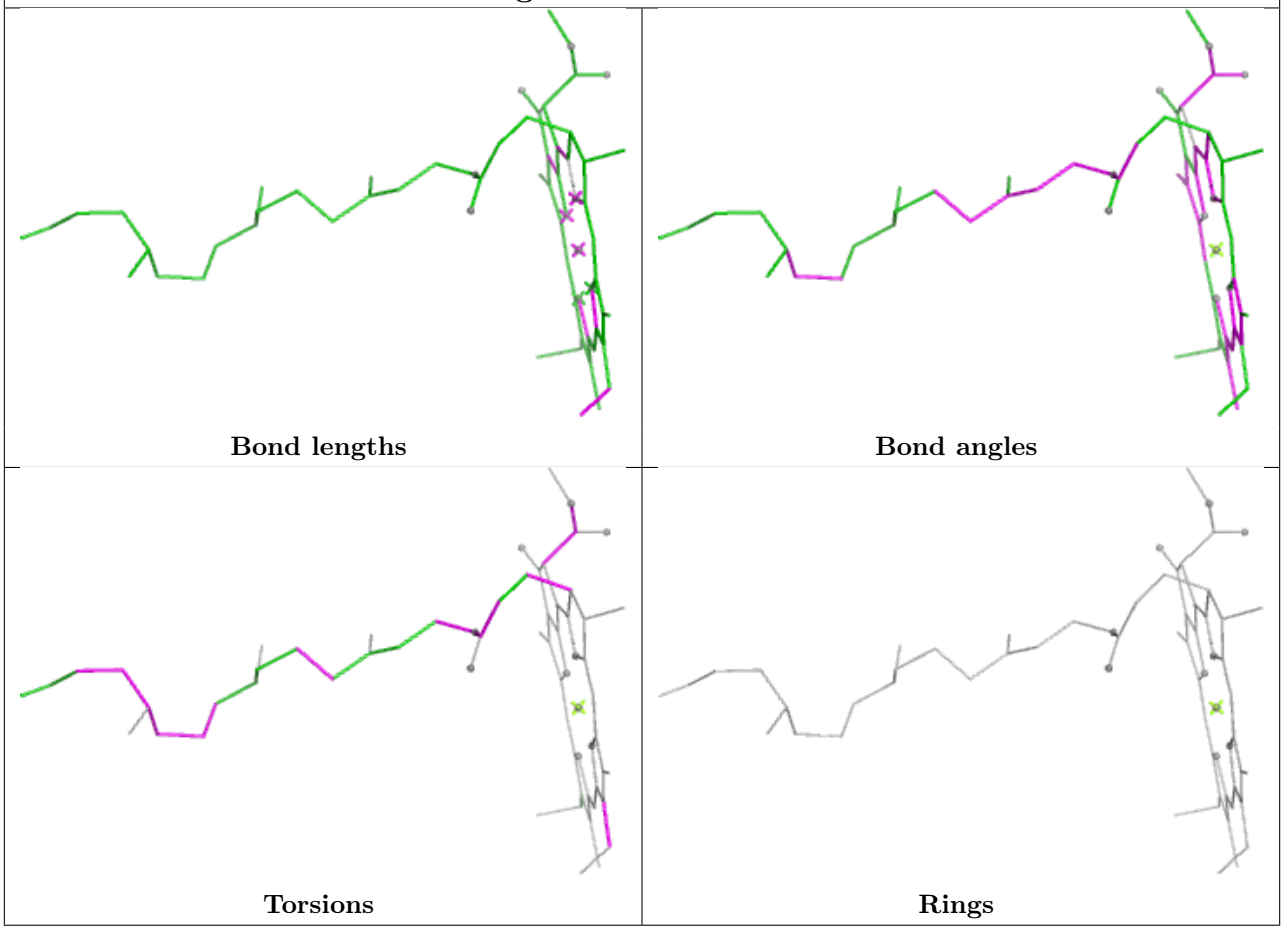


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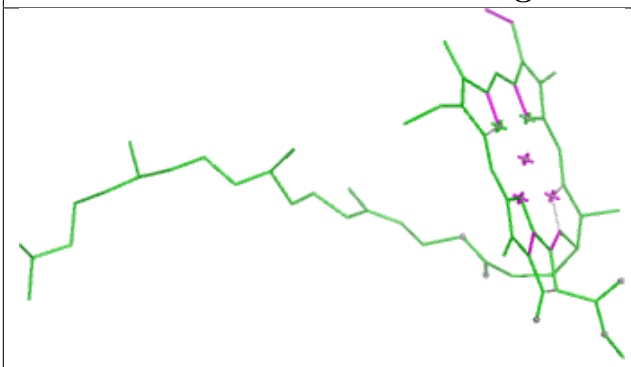


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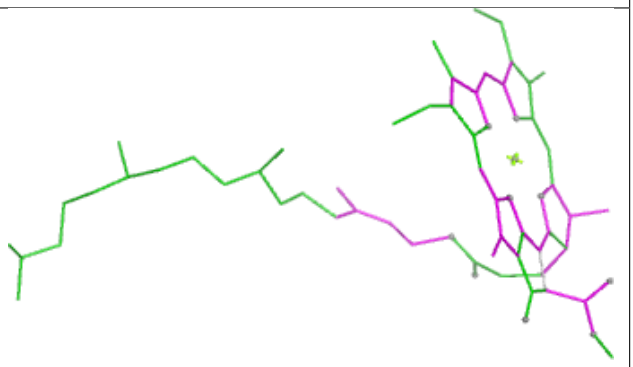
Ligand CLA A 1126



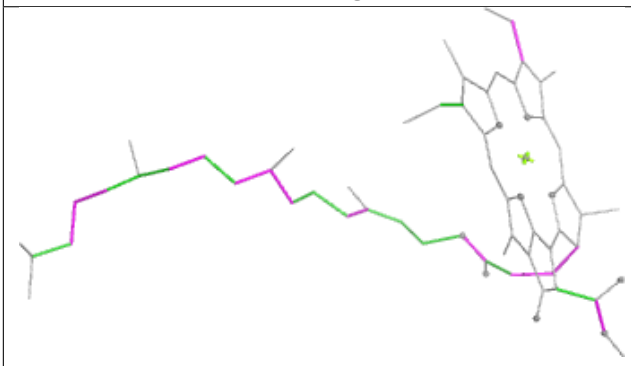
Ligand CLA A 1109



Bond lengths



Bond angles

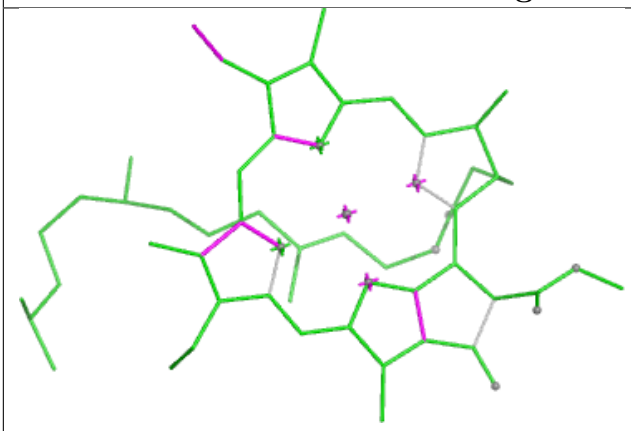


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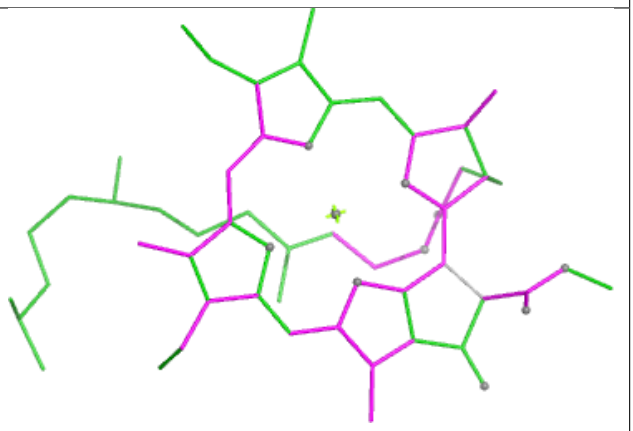


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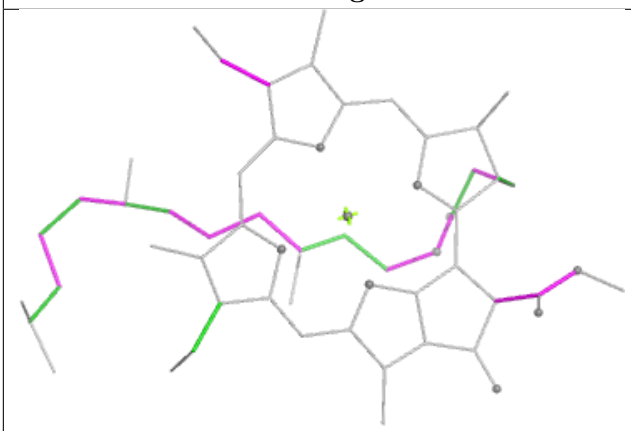
Ligand CLA B 1213



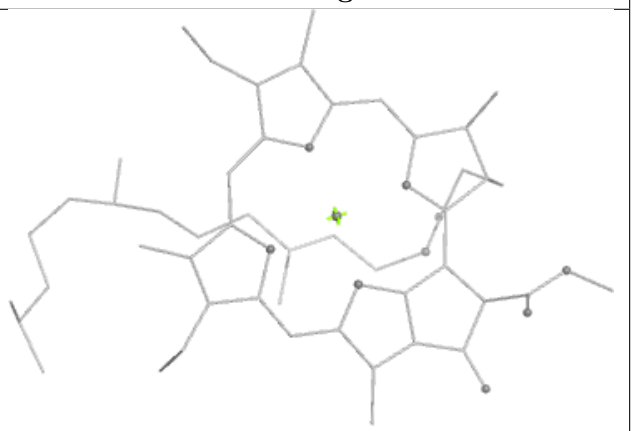
Bond lengths



Bond angles

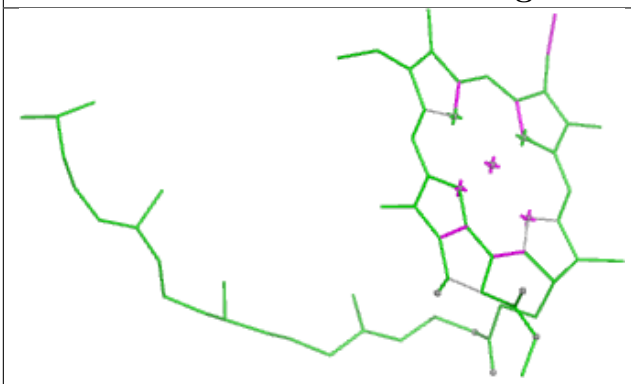


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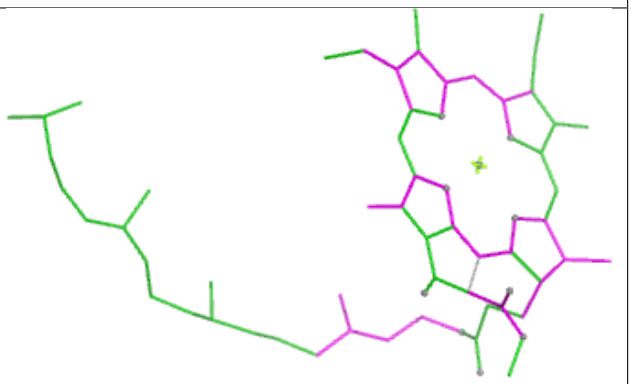


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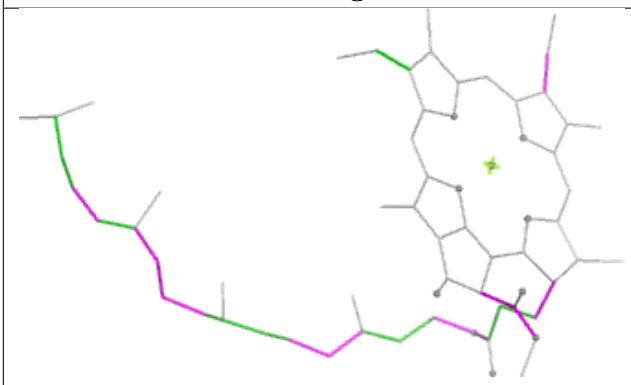
Ligand CLA B 1219



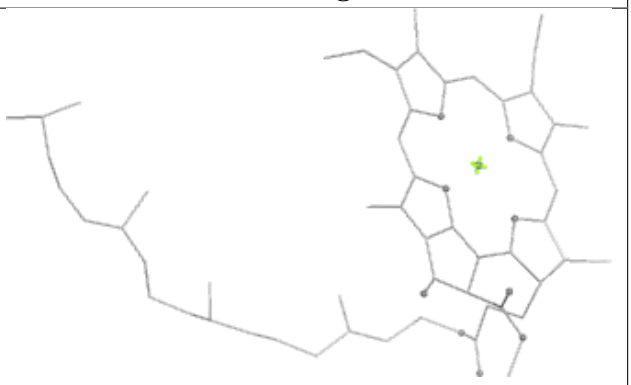
Bond lengths



Bond angles

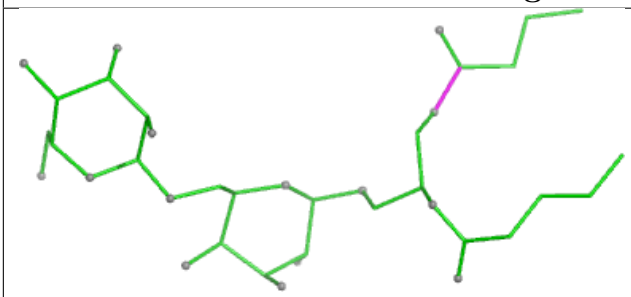


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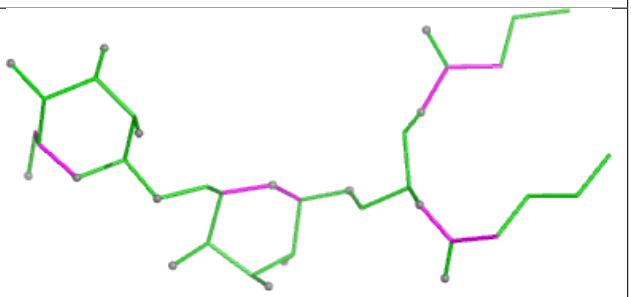


Rings

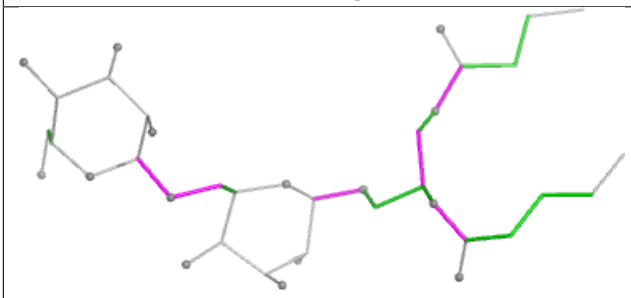
Ligand DGD 3 804



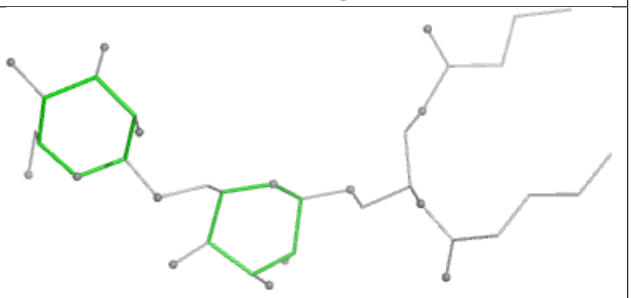
Bond lengths



Bond angles

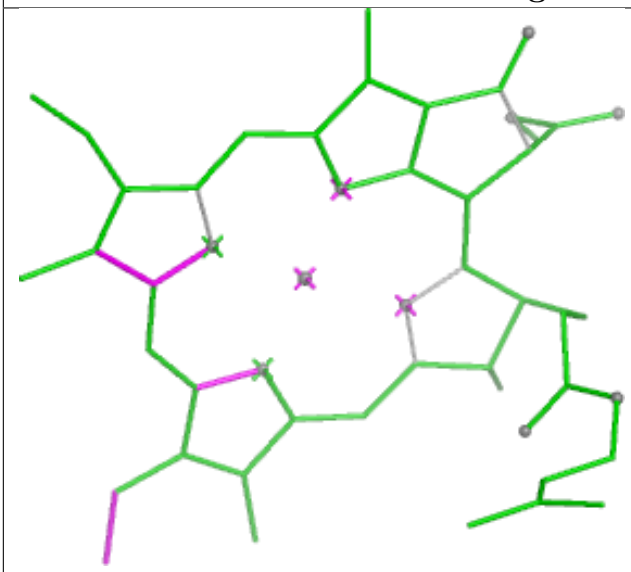


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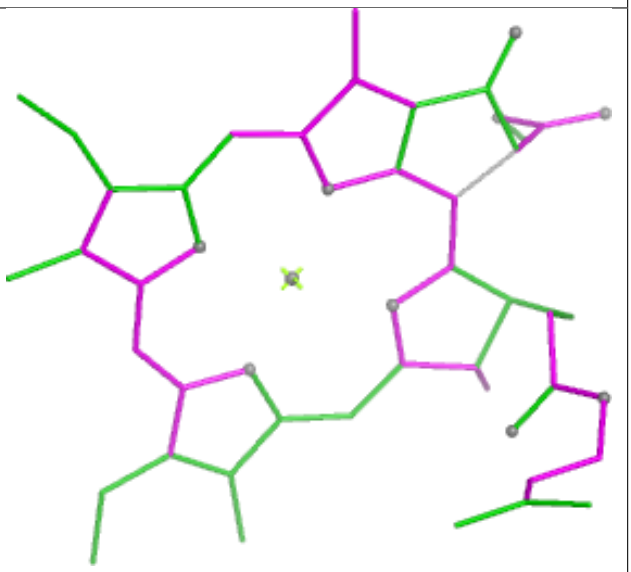


Rings

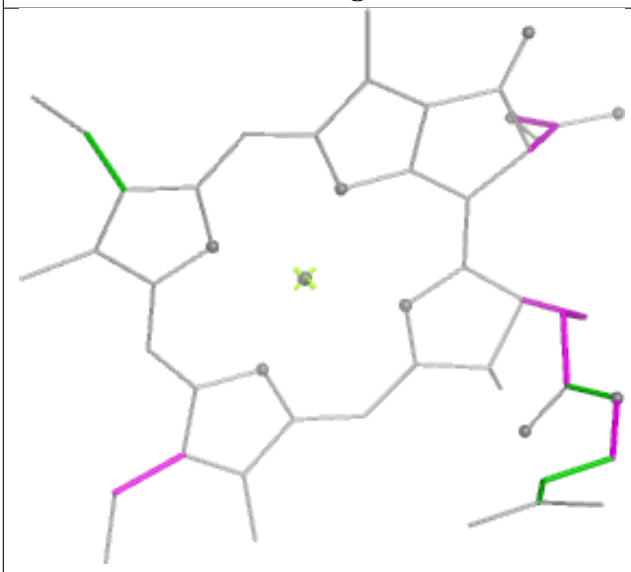
Ligand CLA 6 606



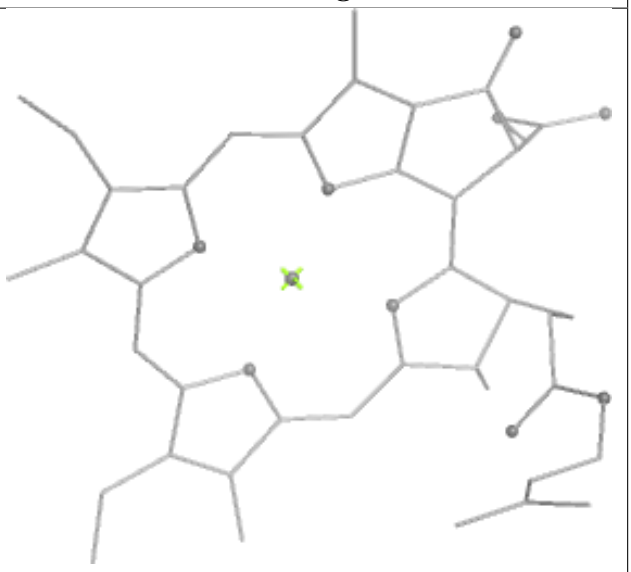
Bond lengths



Bond angles

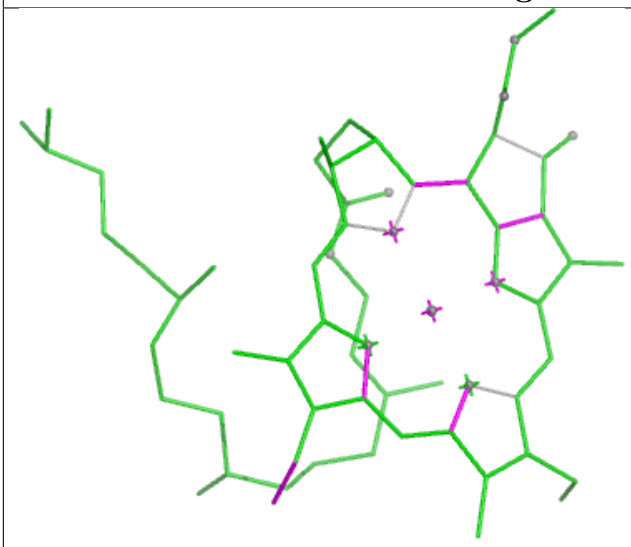


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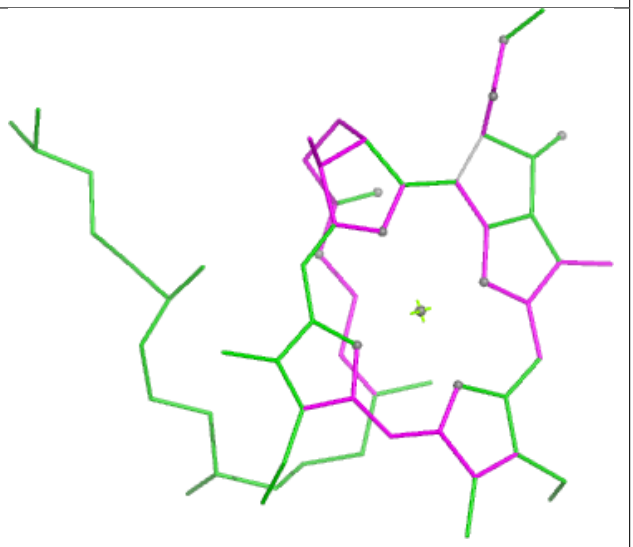


Rings

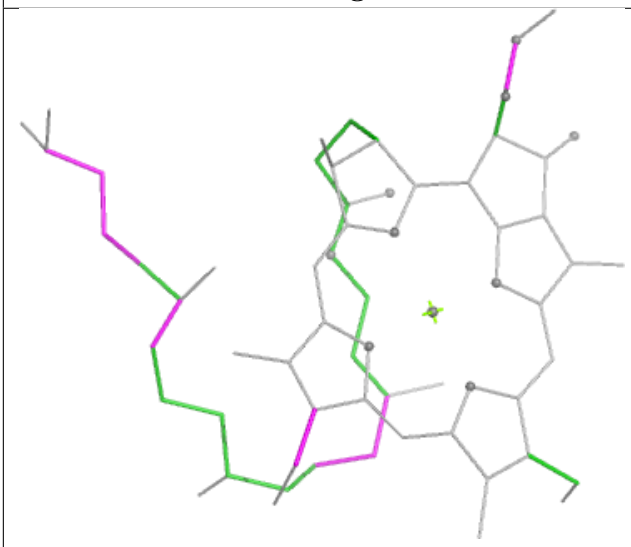
Ligand CLA B 1205



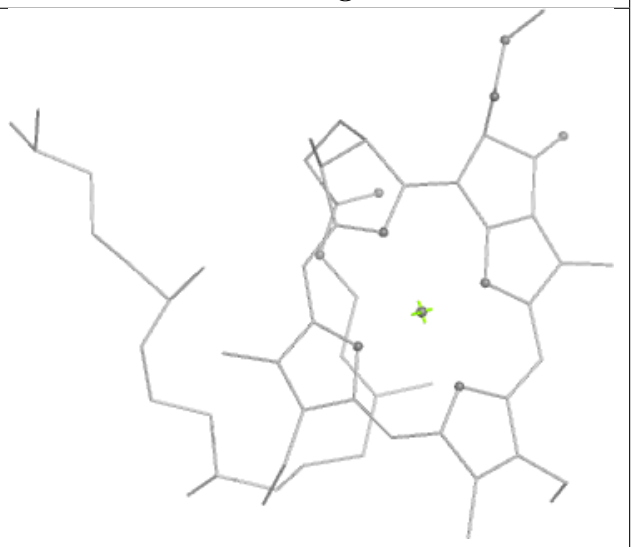
Bond lengths



Bond angles



Torsions

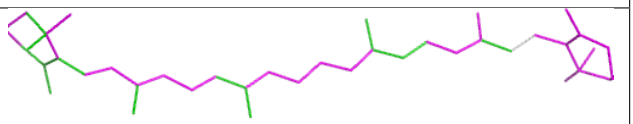


Rings

Ligand LUT 5 501



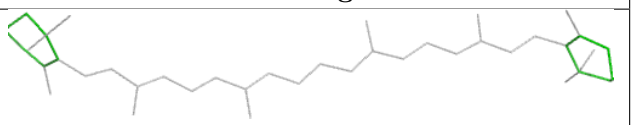
Bond lengths



Bond angles

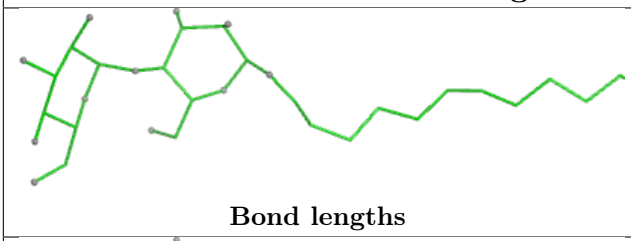


Torsions

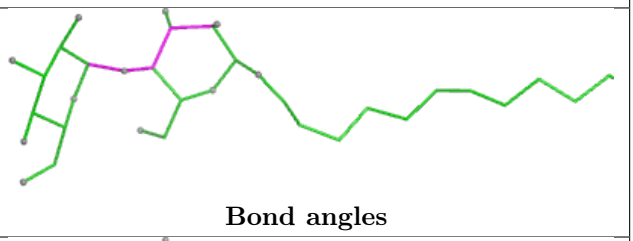


Rings

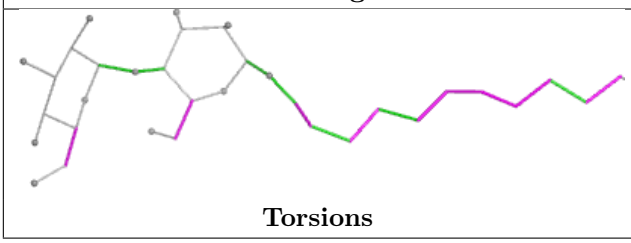
Ligand LMU A 5004



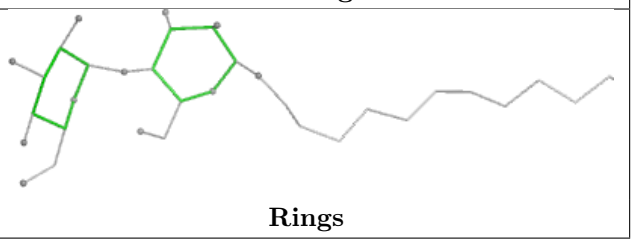
Bond lengths



Bond angles

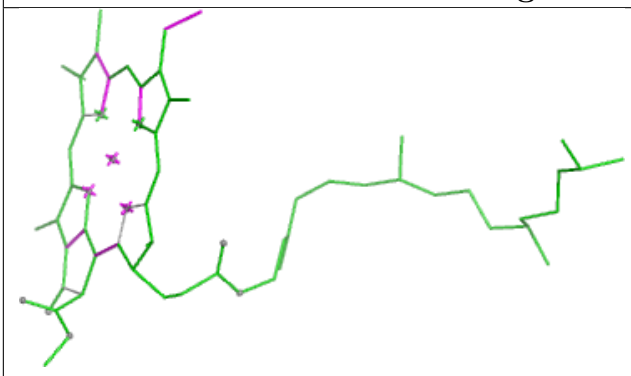


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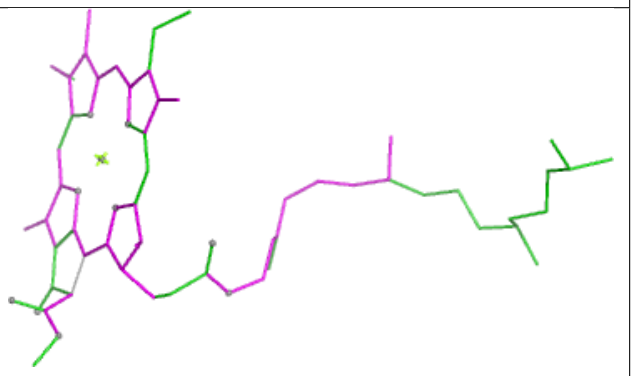


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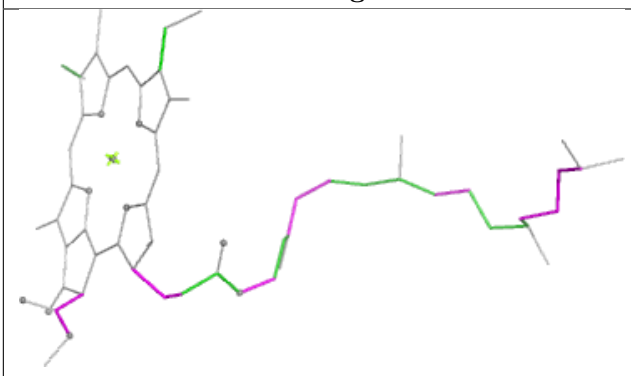
Ligand CLA L 1502



Bond lengths



Bond angles

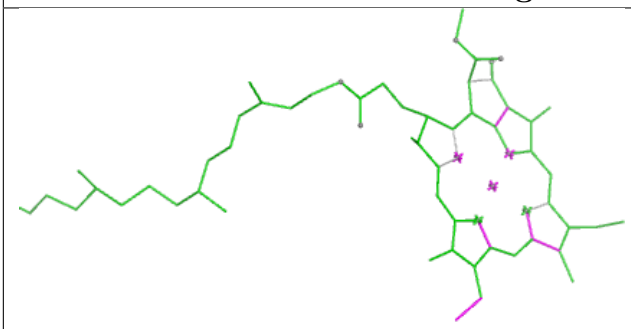


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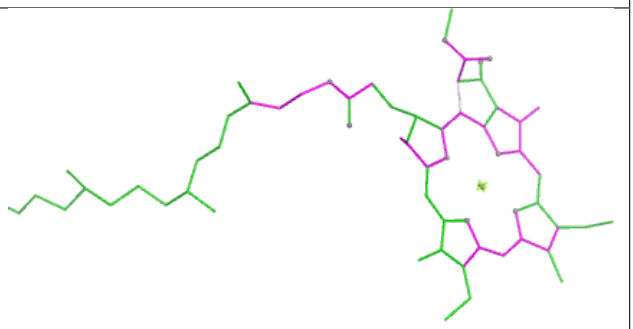


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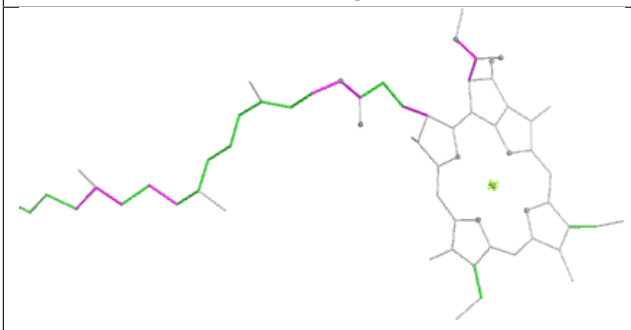
Ligand CLA B 1022



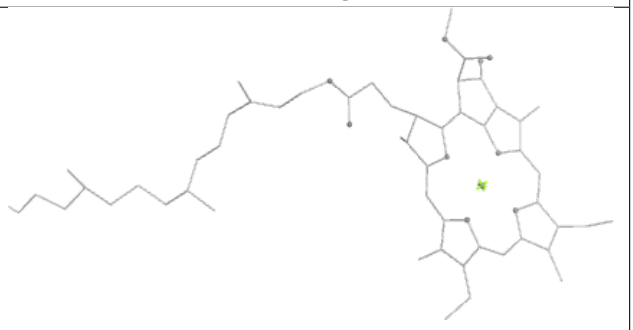
Bond lengths



Bond angles

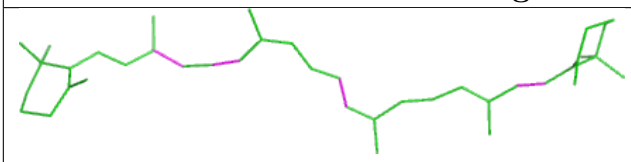


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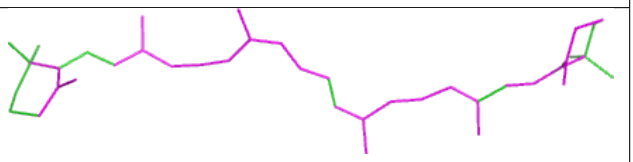


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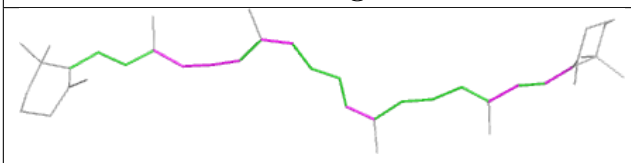
Ligand BCR G 4001



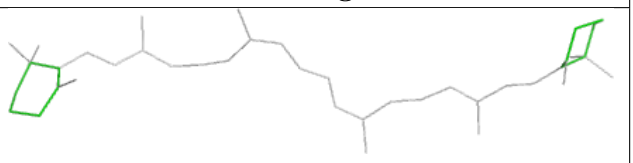
Bond lengths



Bond angles

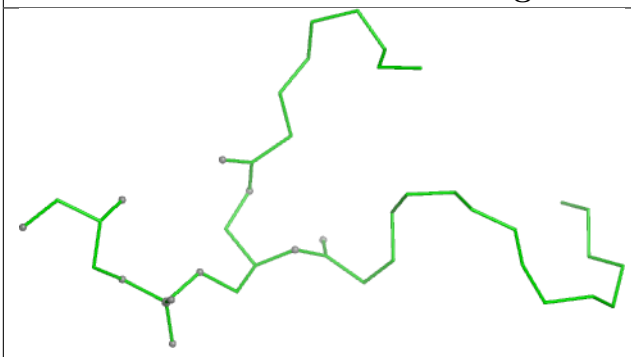


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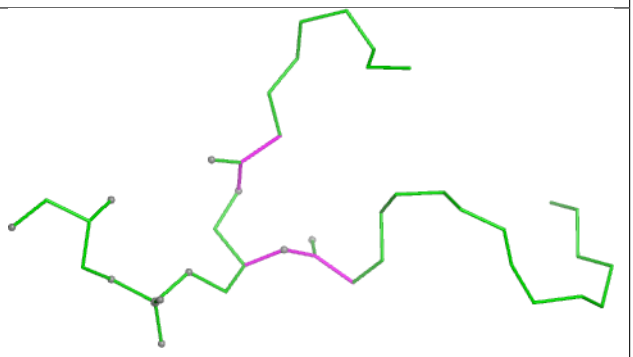


Rings

Ligand LHG B 5001



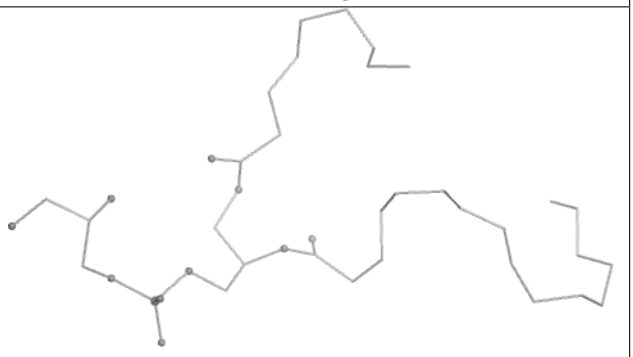
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Bond angles

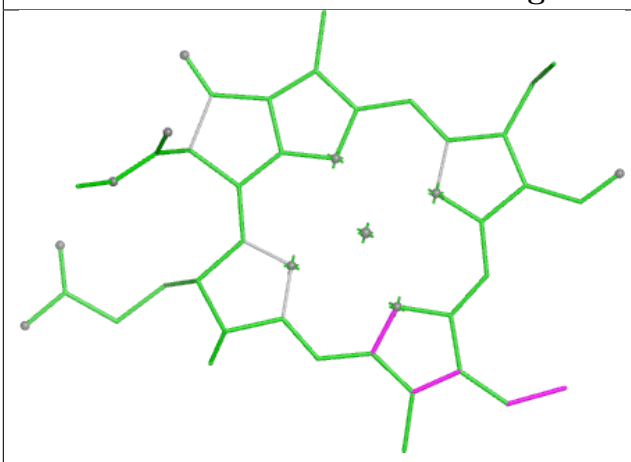


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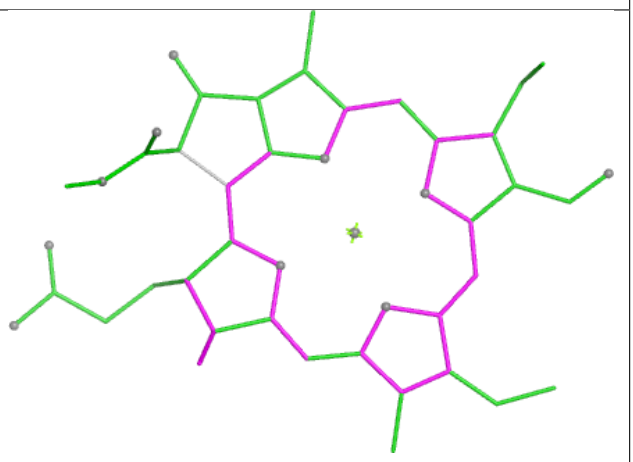


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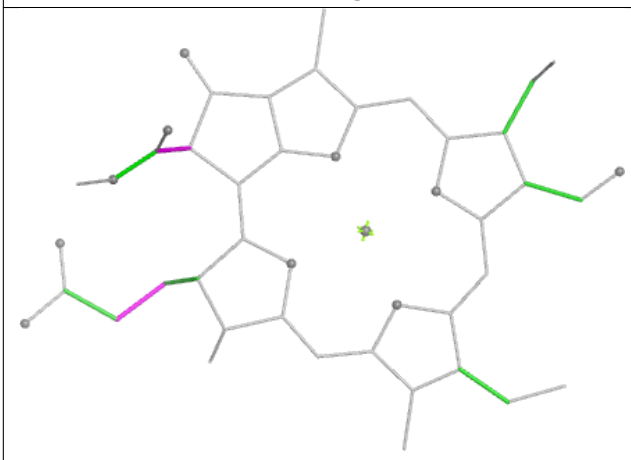
Ligand CHL 2 613



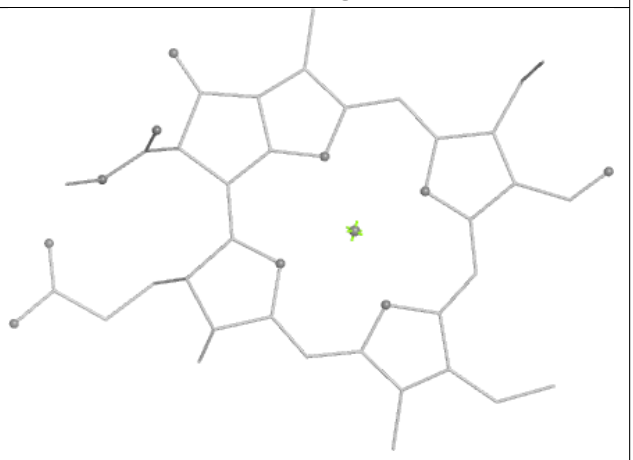
Bond lengths



Bond angles

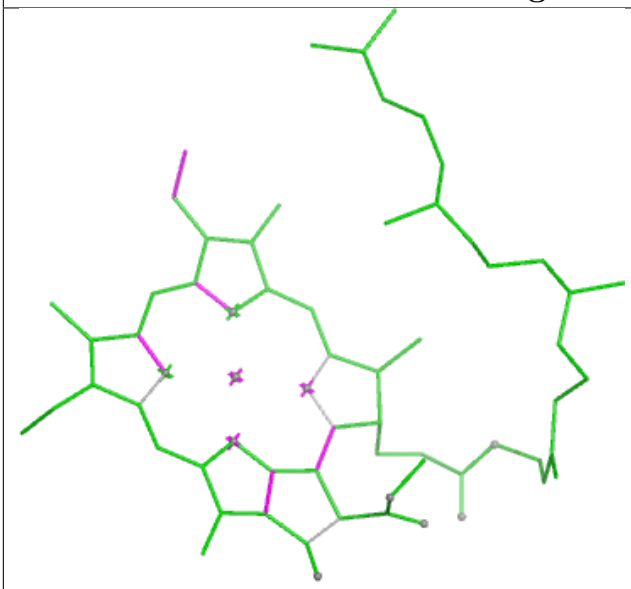


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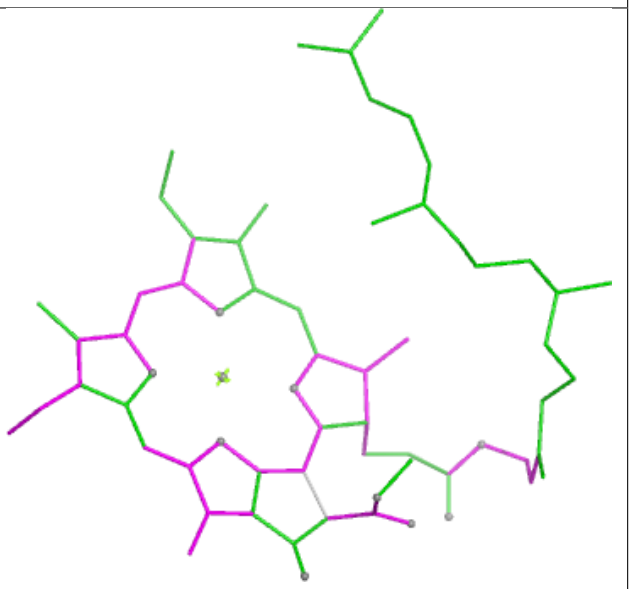


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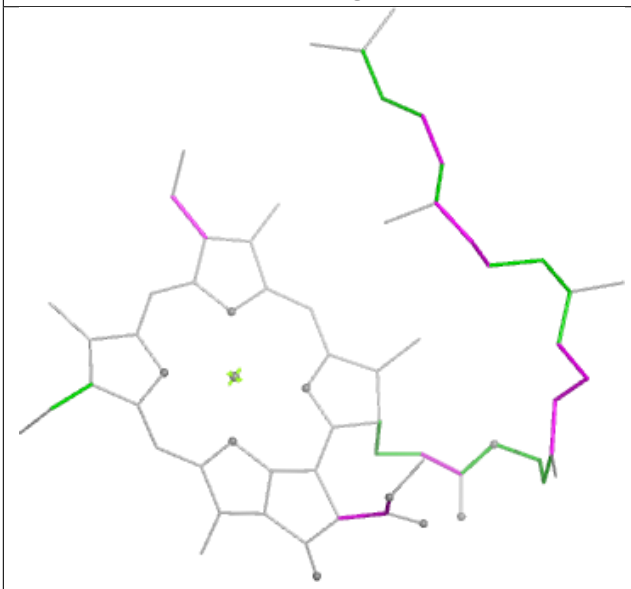
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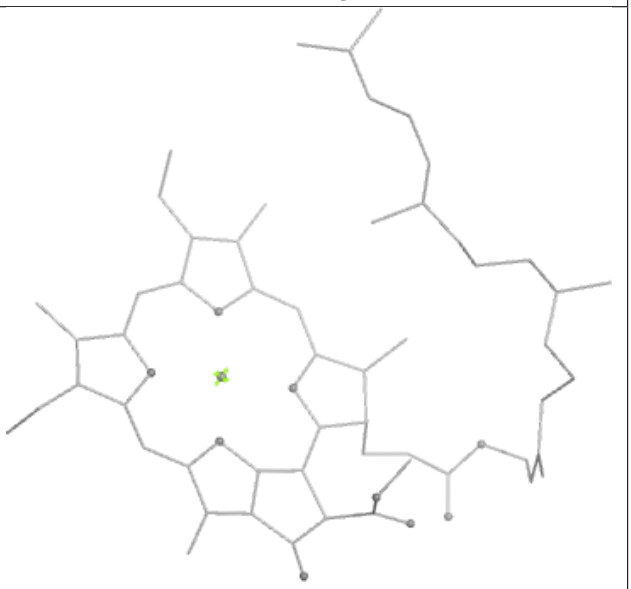
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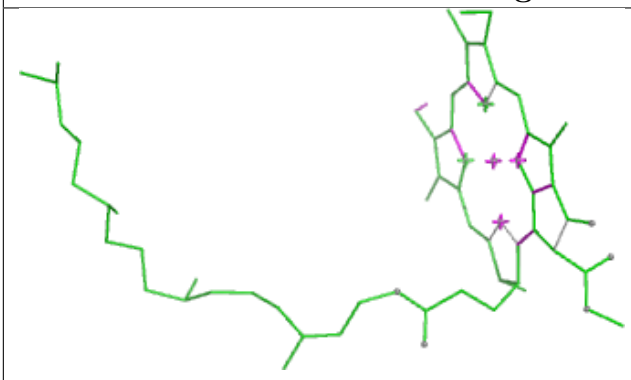


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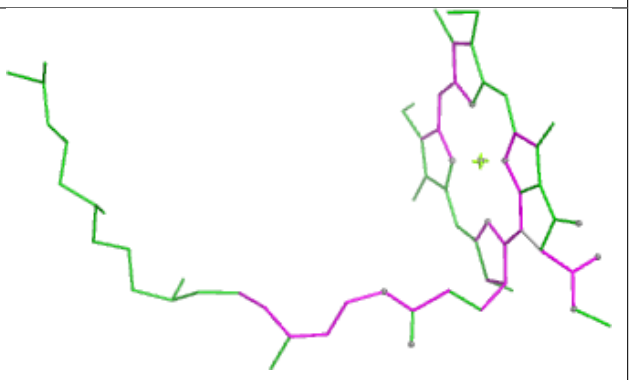


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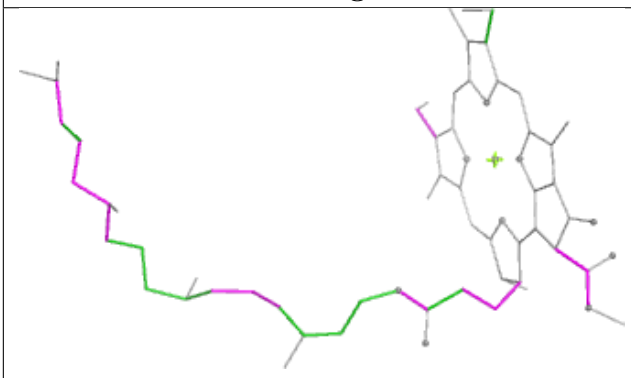
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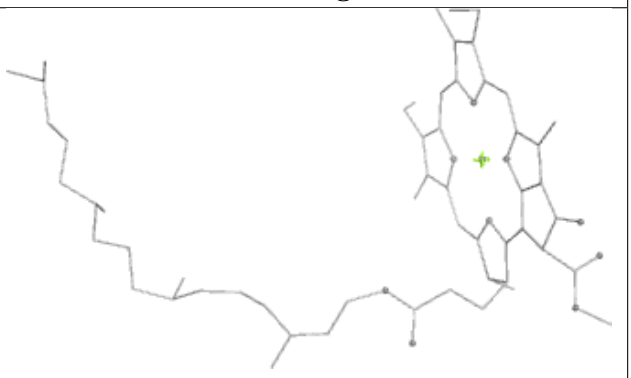
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Bond angles

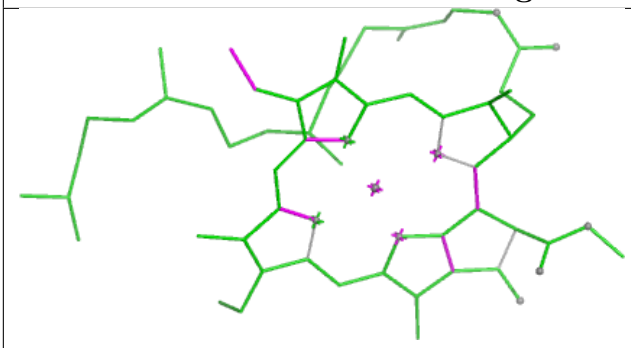


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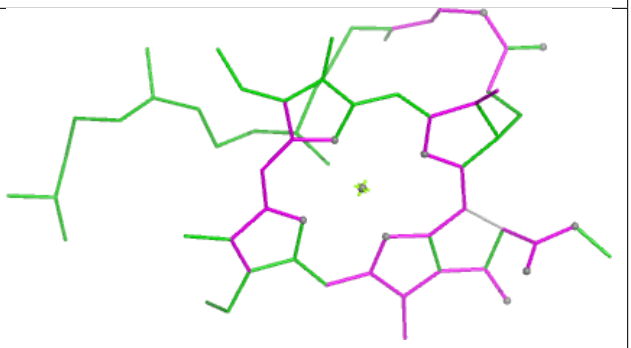


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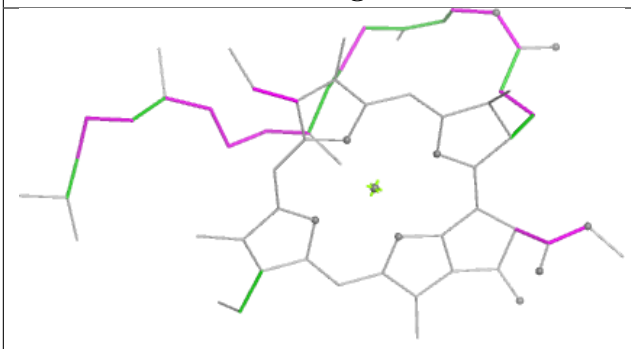
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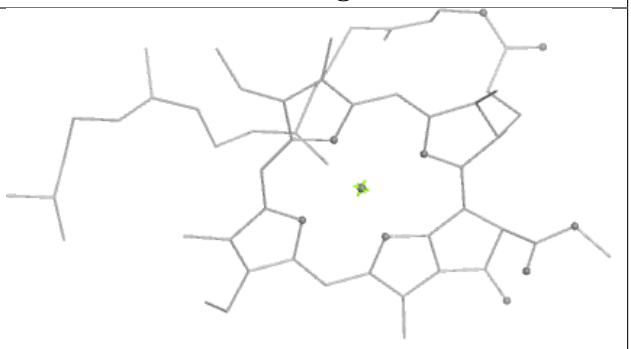
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Bond angles

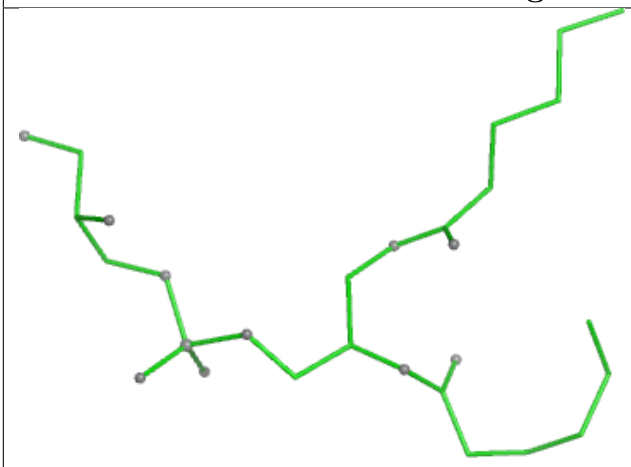


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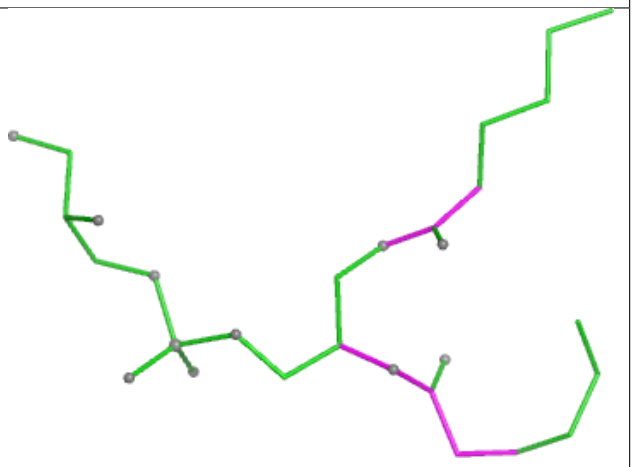


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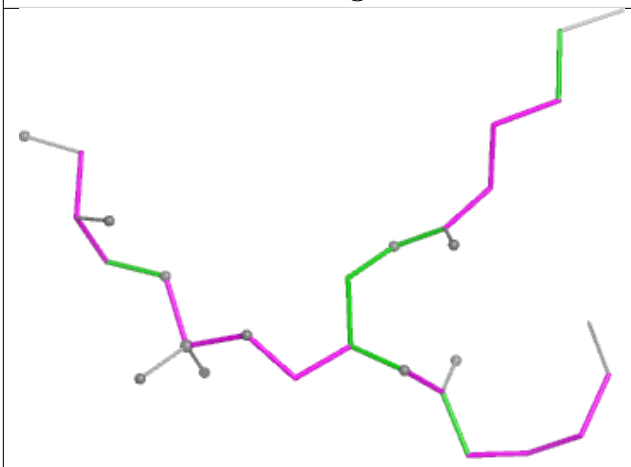
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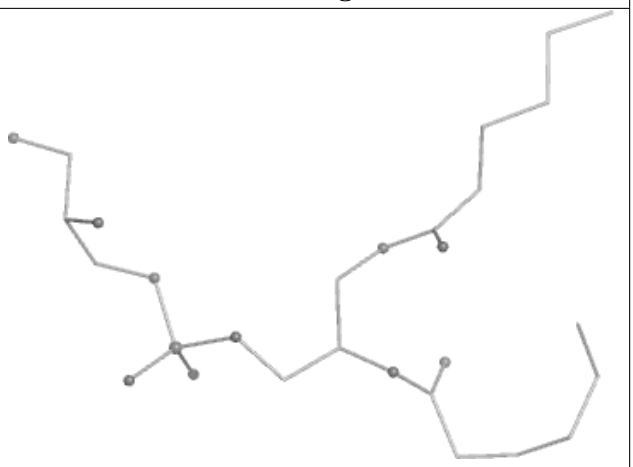
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Bond angles

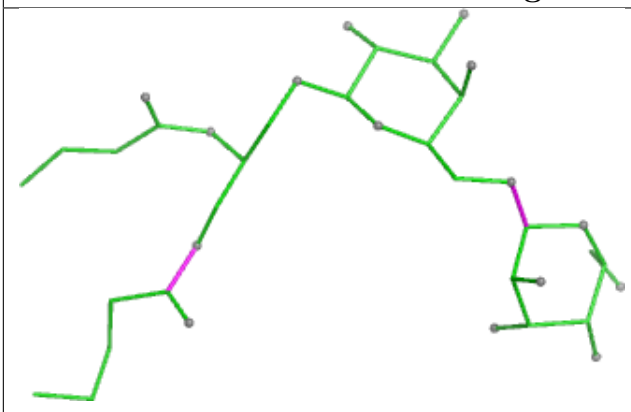


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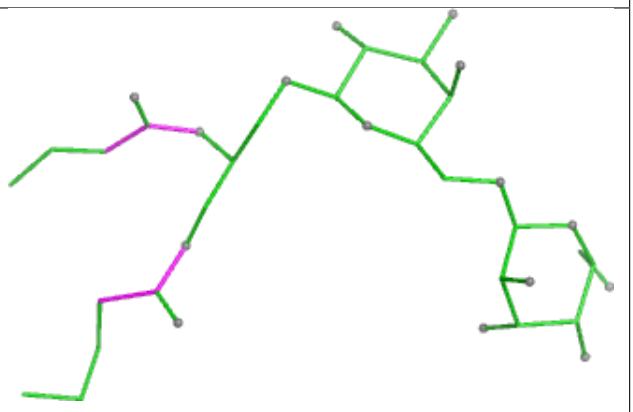


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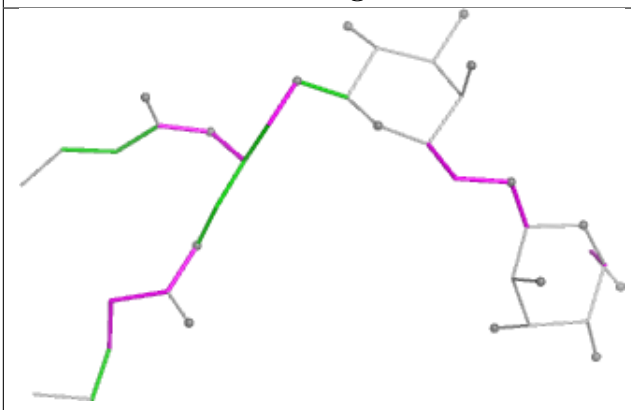
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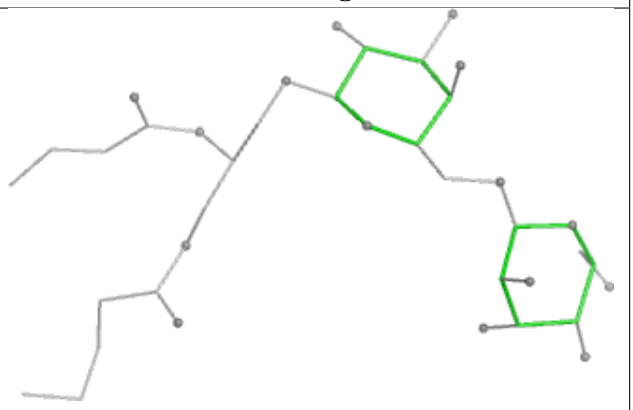
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Bond angles

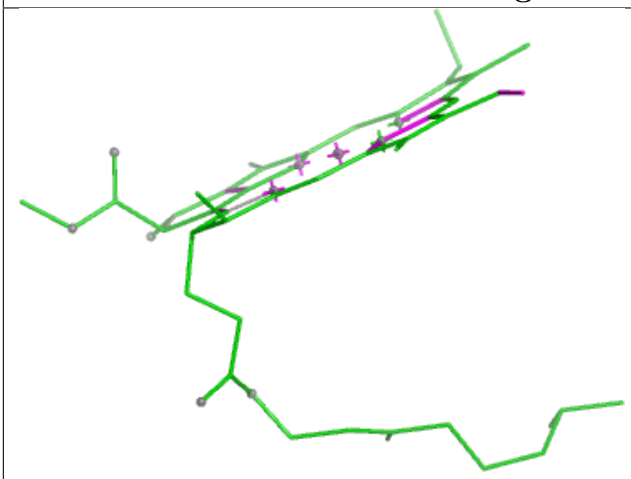


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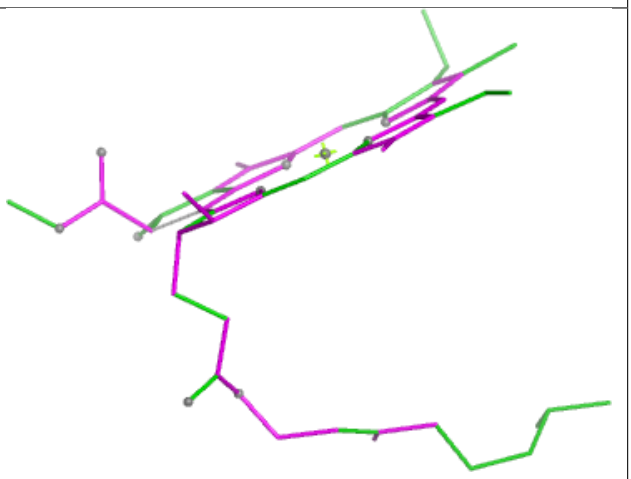


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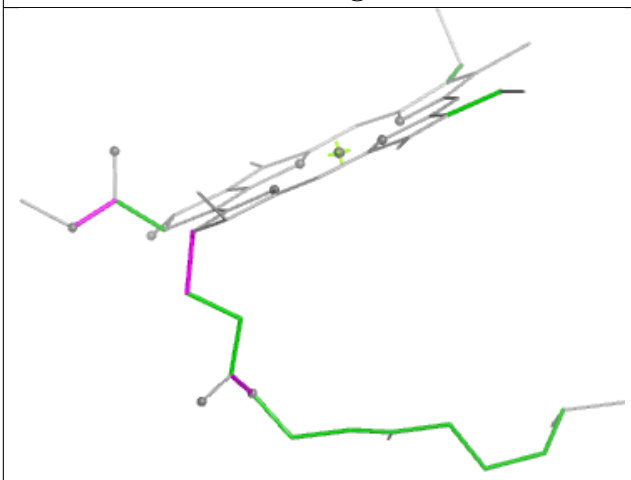
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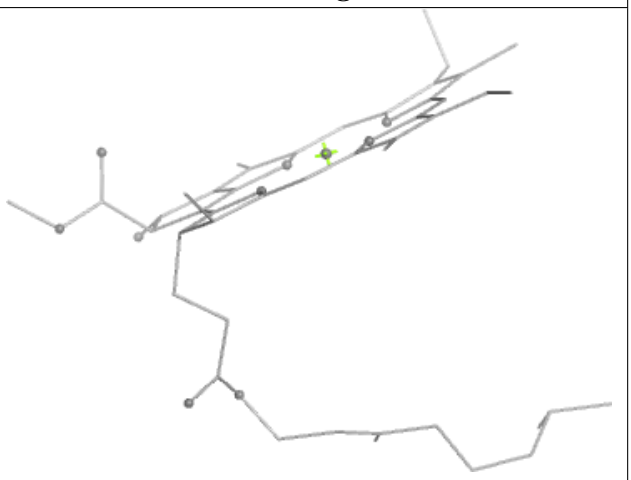
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Bond angles

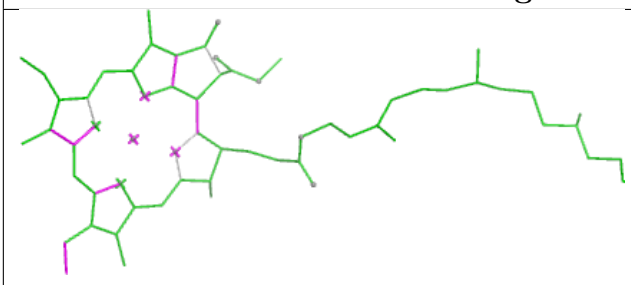


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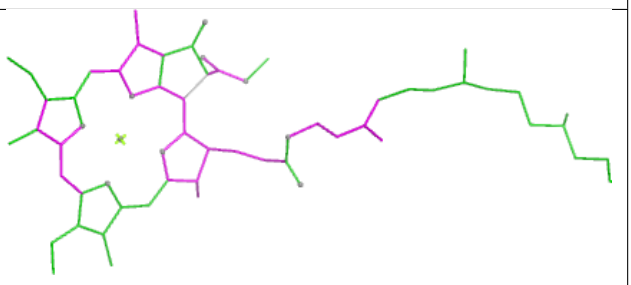


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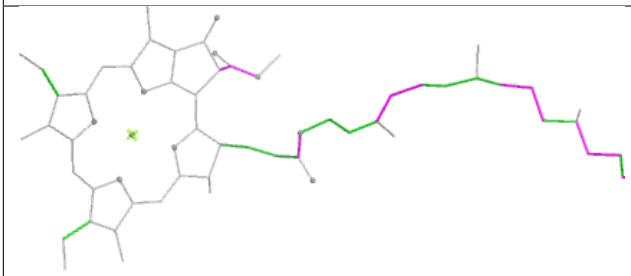
Ligand CLA A 1139



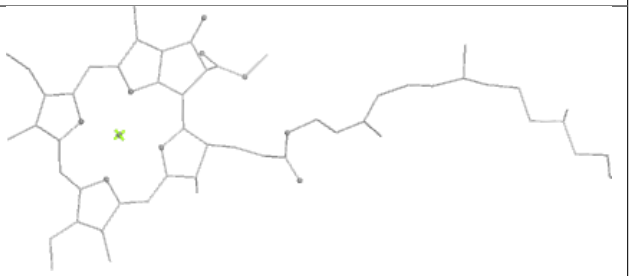
Bond lengths



Bond angles

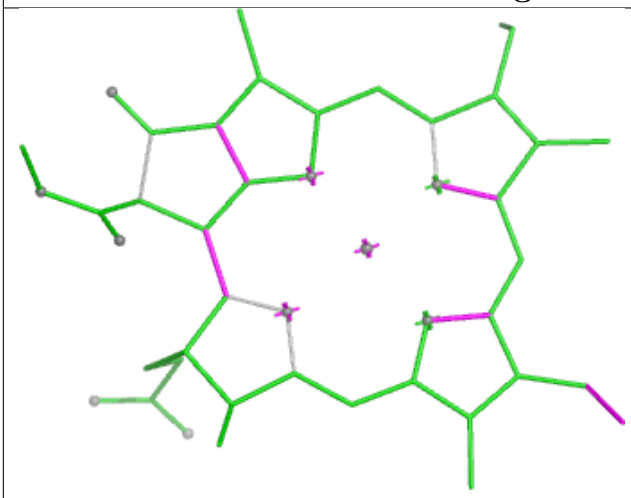


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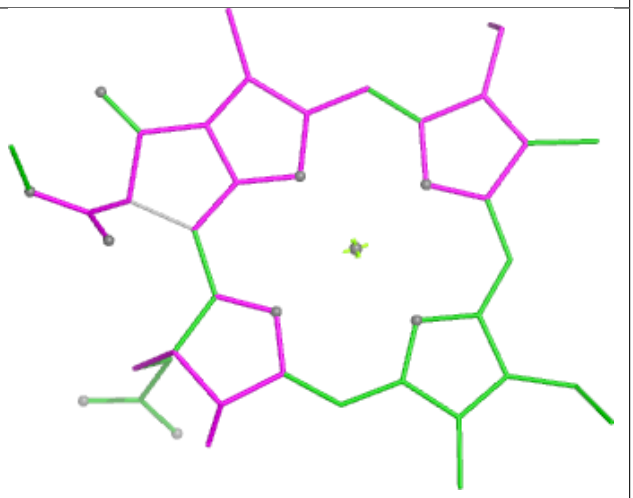


Rings

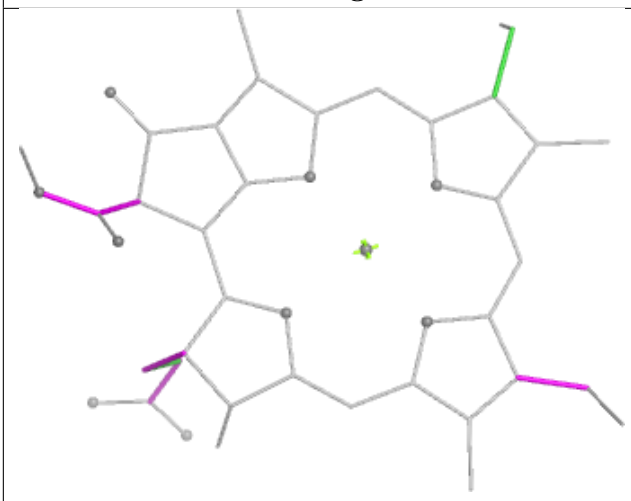
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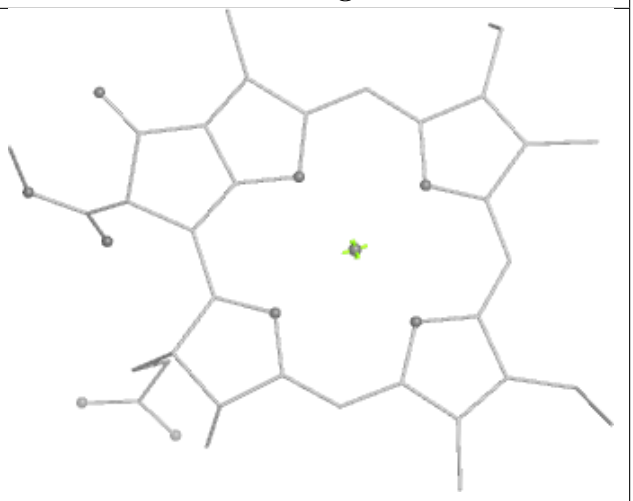
Bond lengths



Bond angles

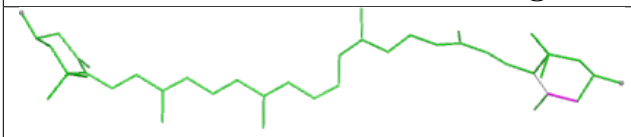


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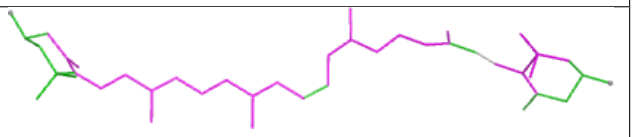


Rings

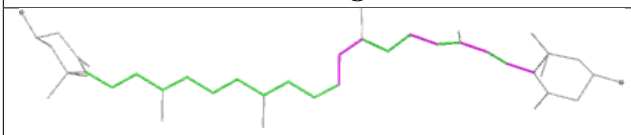
Ligand LUT 5 503



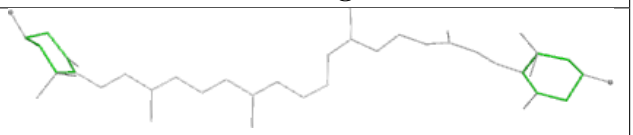
Bond lengths



Bond angles

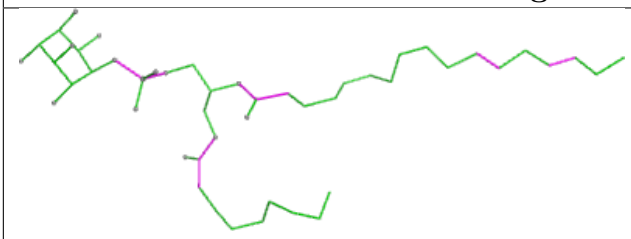


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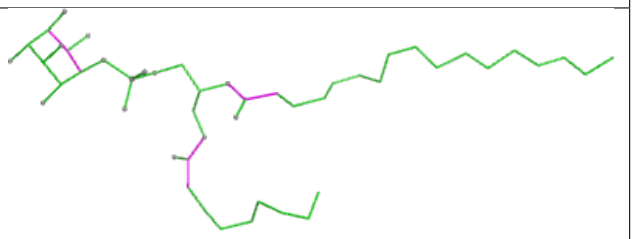


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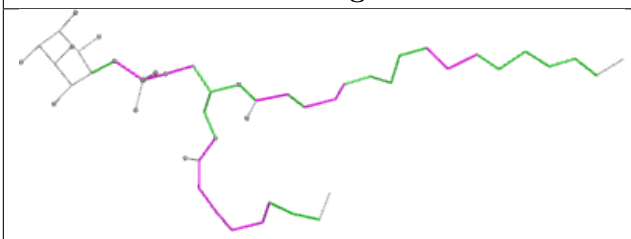
Ligand P3H 2 808



Bond lengths



Bond angles

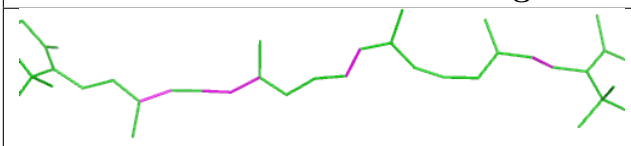


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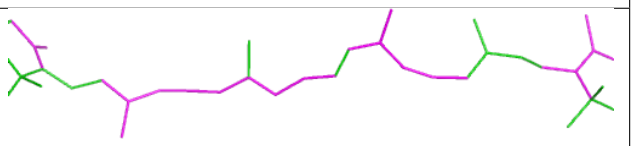


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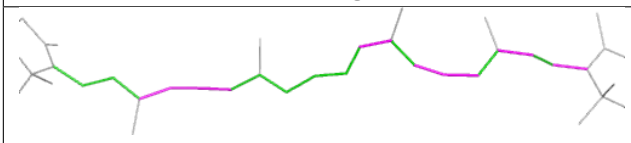
Ligand BCR A 4004



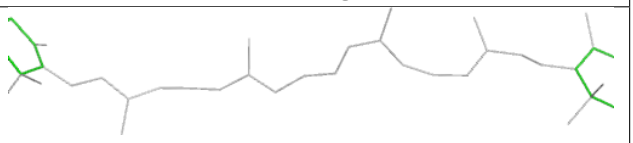
Bond lengths



Bond angles

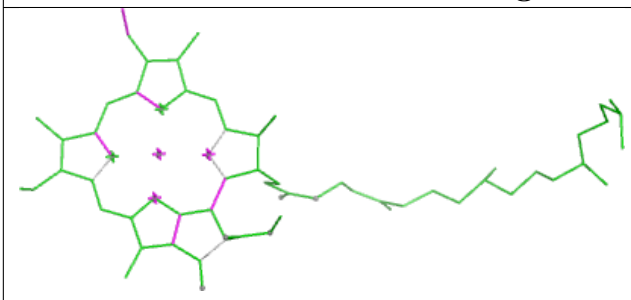


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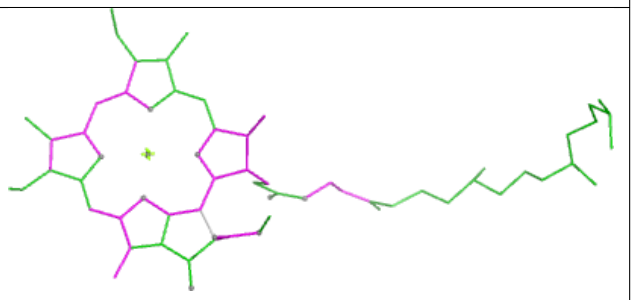


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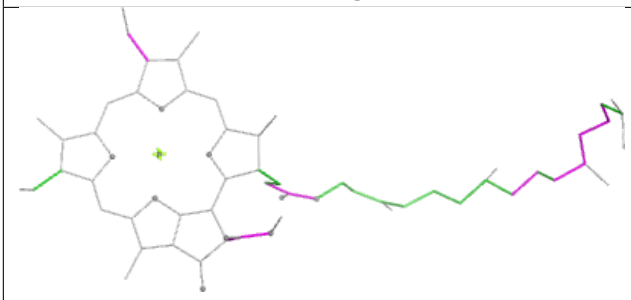
Ligand CLA B 1240



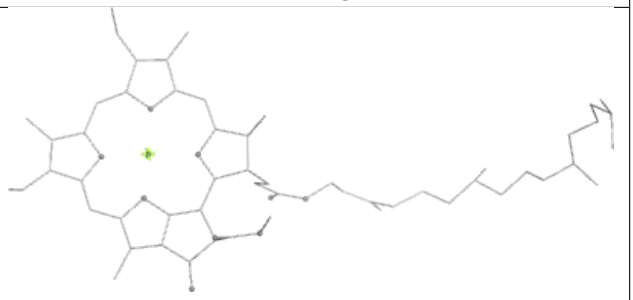
Bond lengths



Bond angles

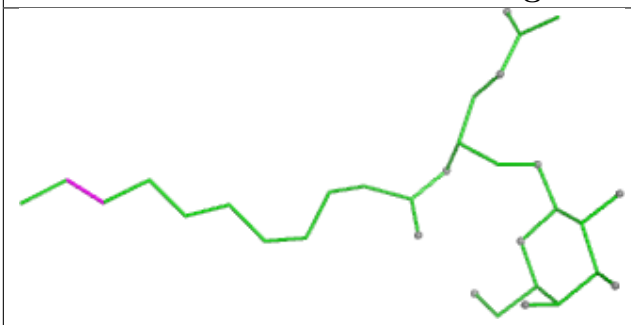


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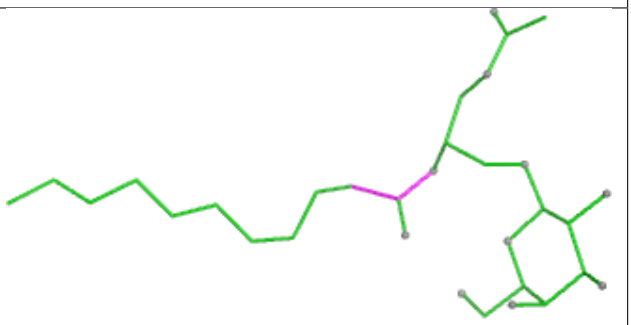


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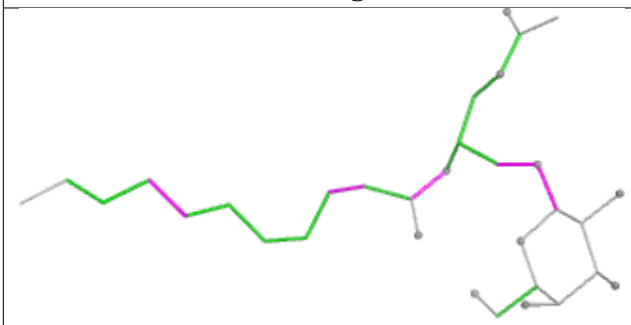
Ligand LMG 3 802



Bond lengths



Bond angles

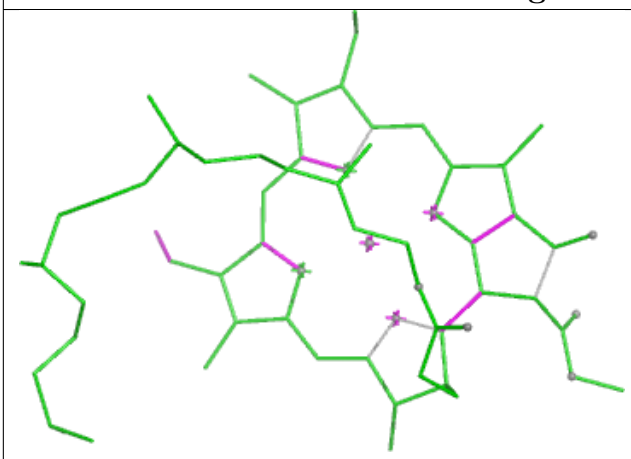


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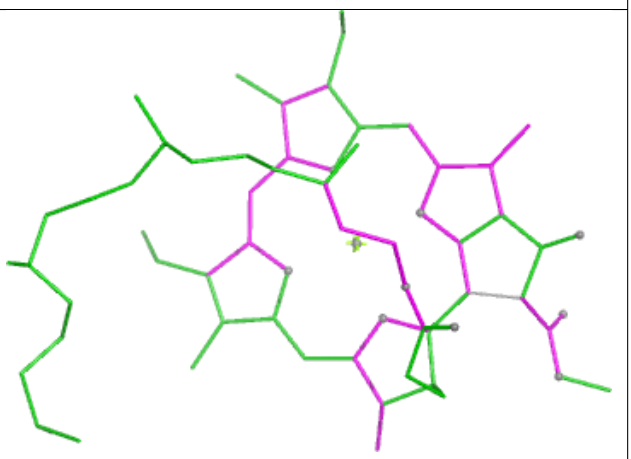


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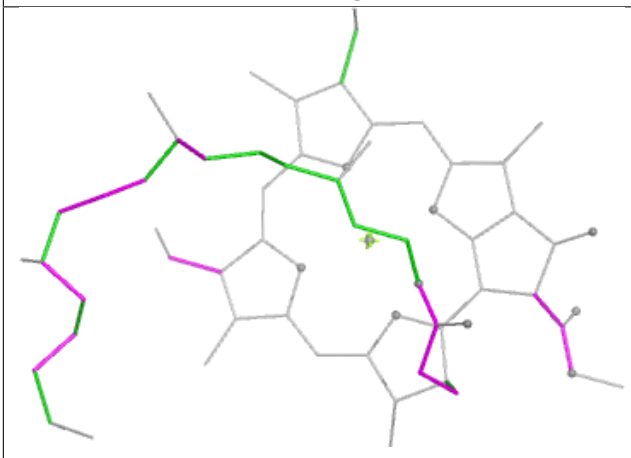
Ligand CLA 2 603



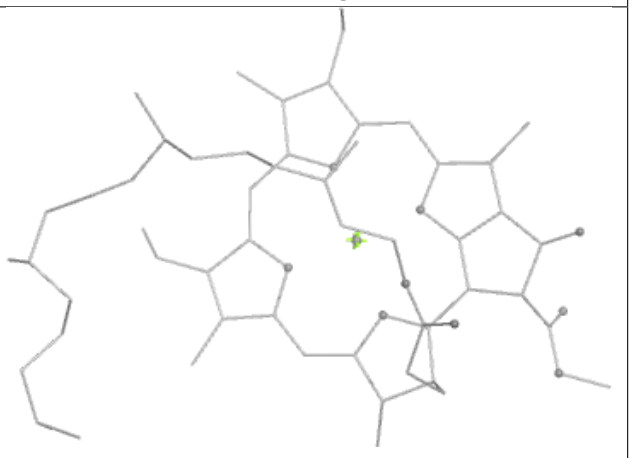
Bond lengths



Bond angles

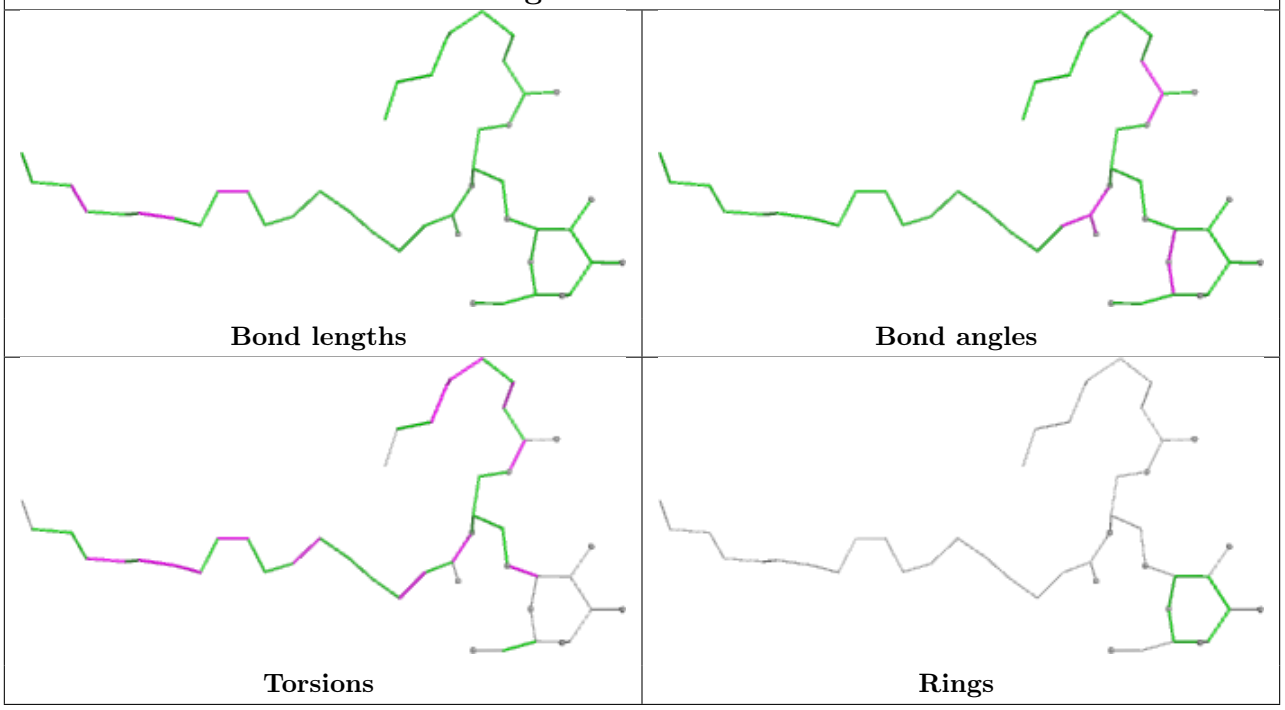


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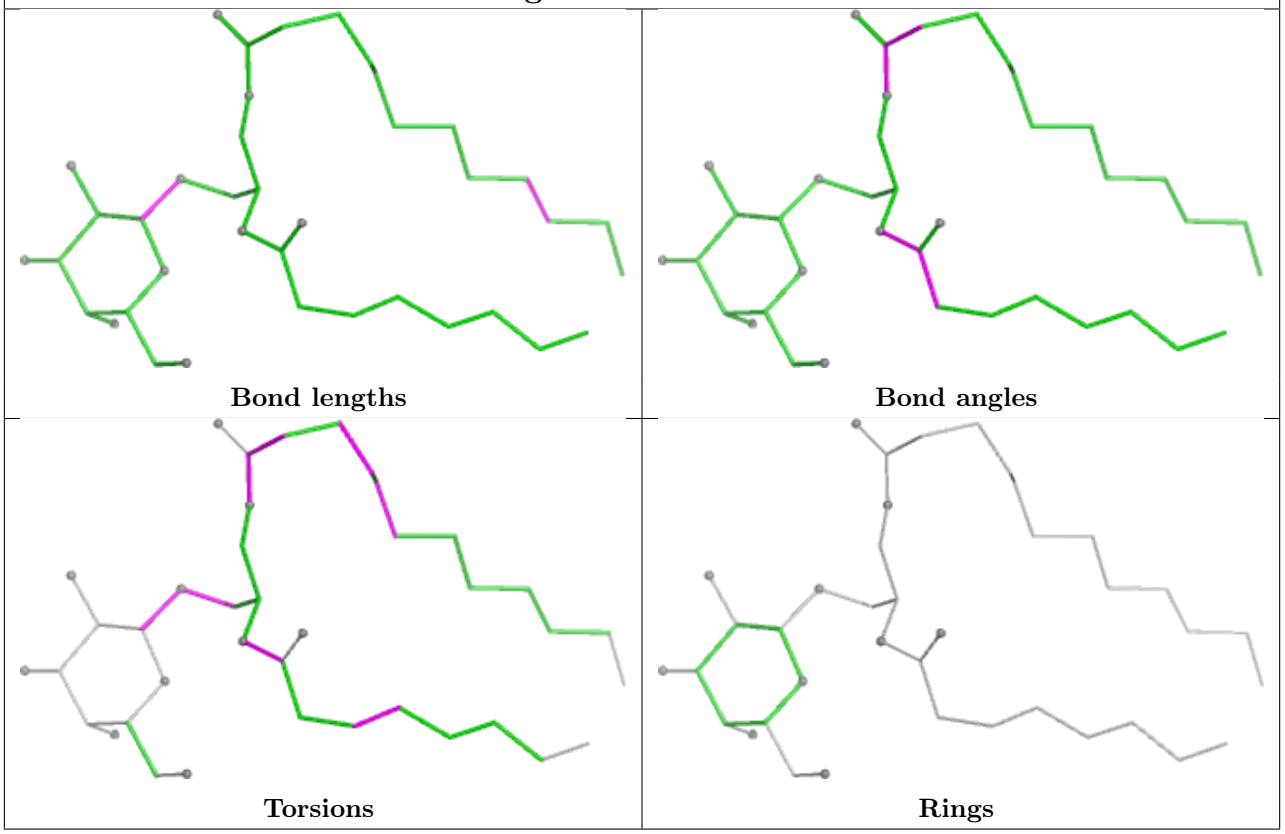


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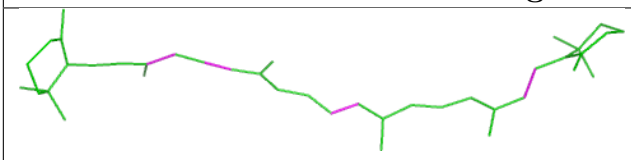
Ligand LMG 4 802



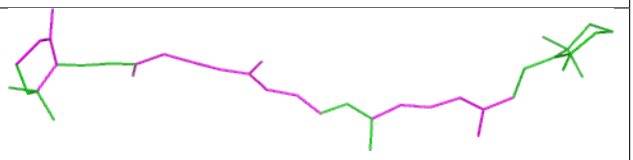
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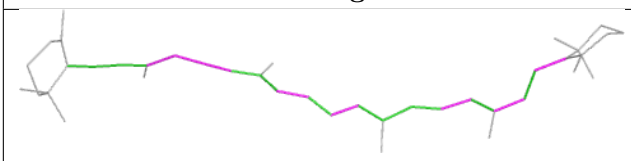
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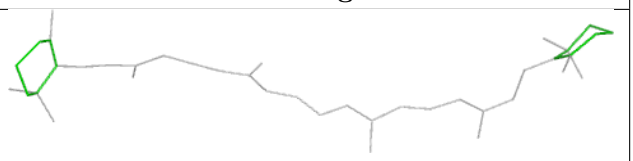
Bond lengths



Bond angles

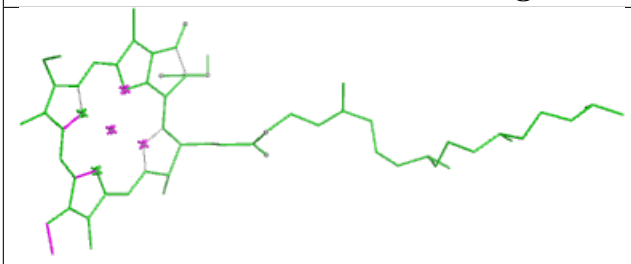


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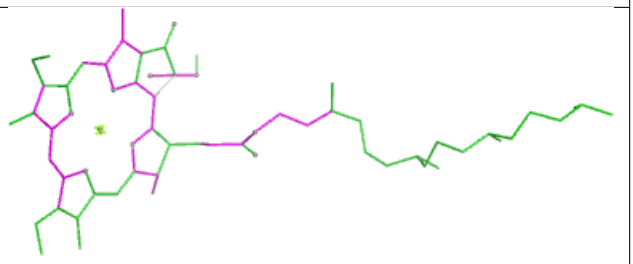


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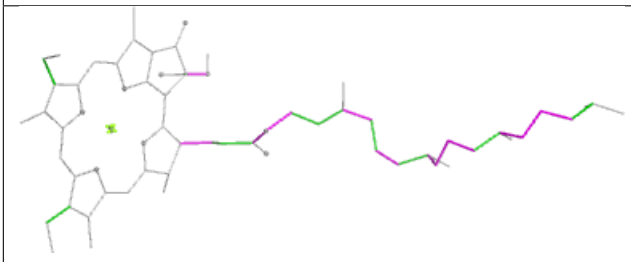
Ligand CLA A 1107



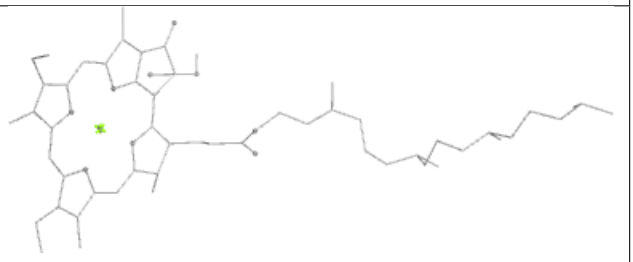
Bond lengths



Bond angles

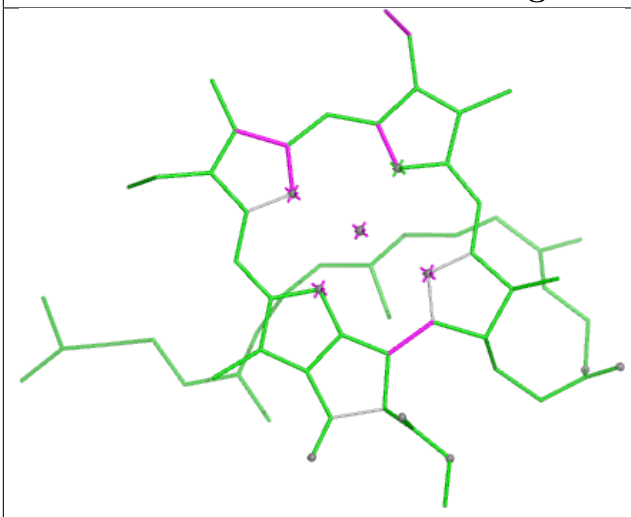


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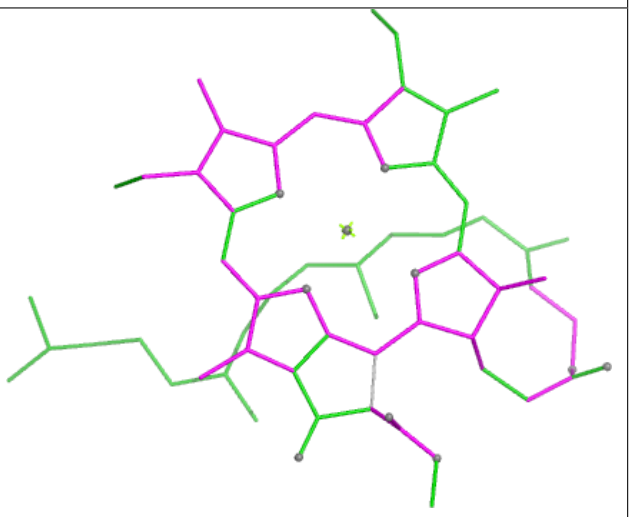


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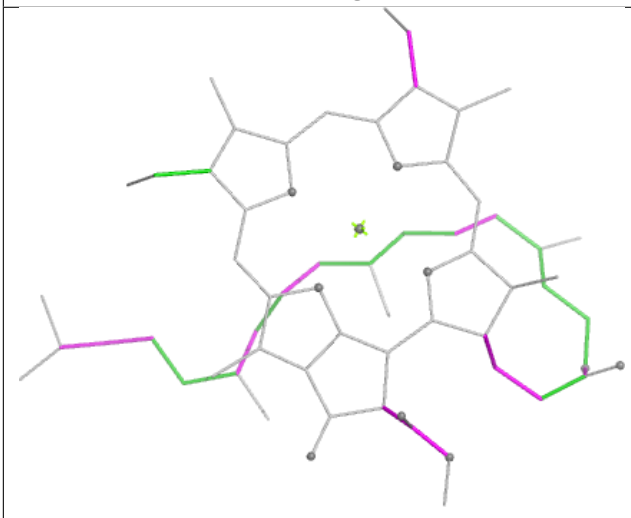
Ligand CLA 3 608



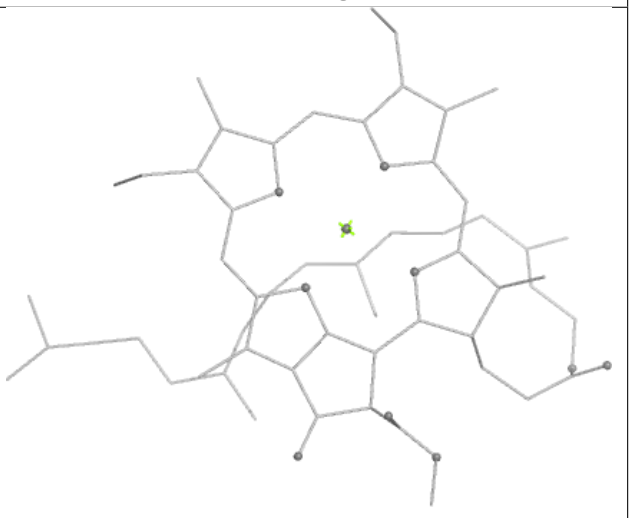
Bond lengths



Bond angles

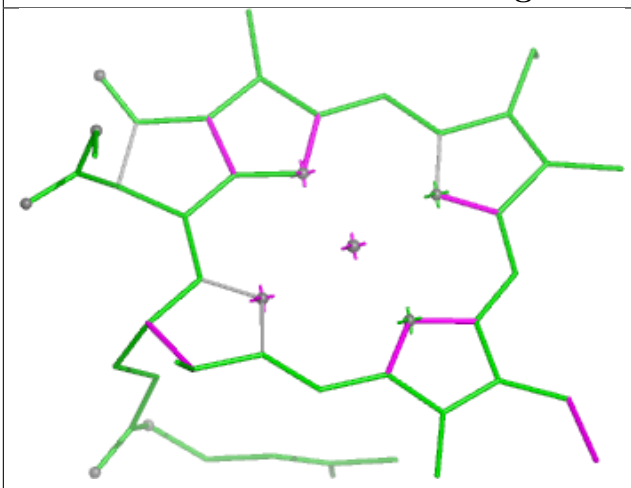


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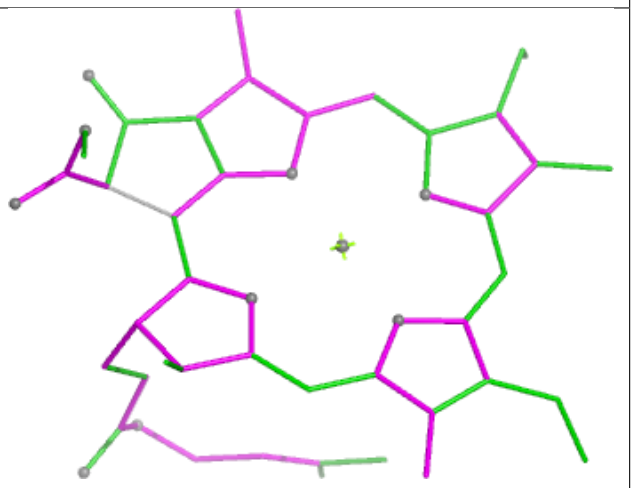


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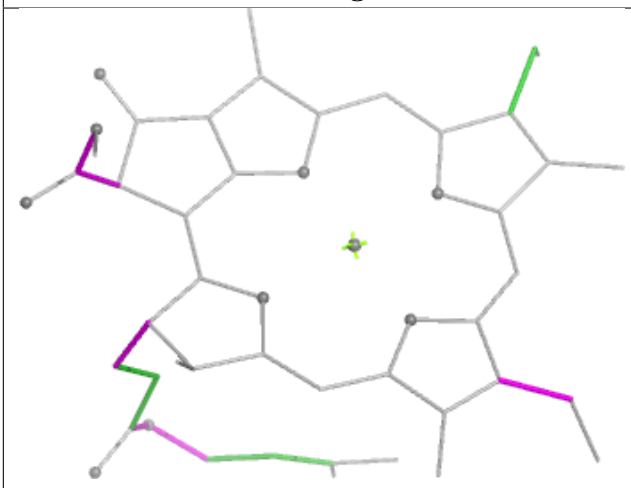
Ligand CLA A 1118



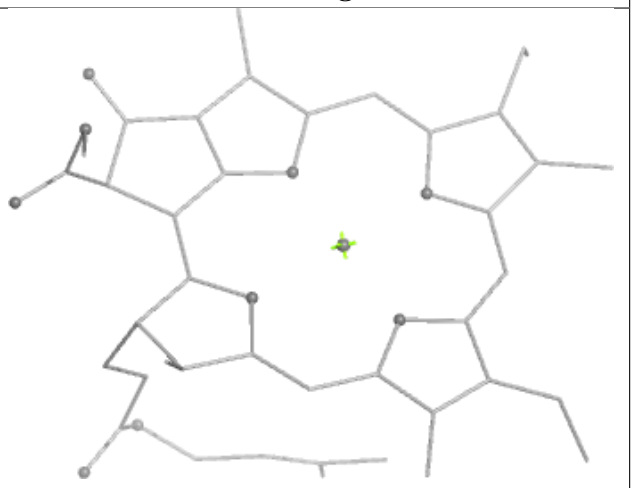
Bond lengths



Bond angles

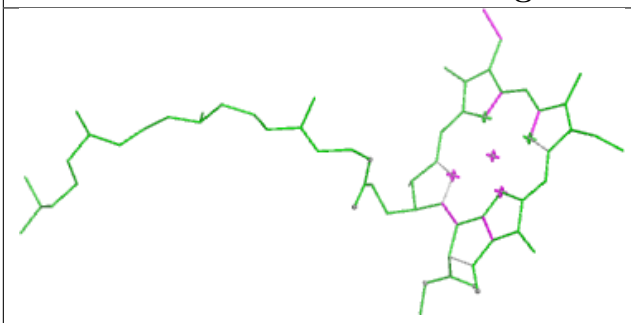


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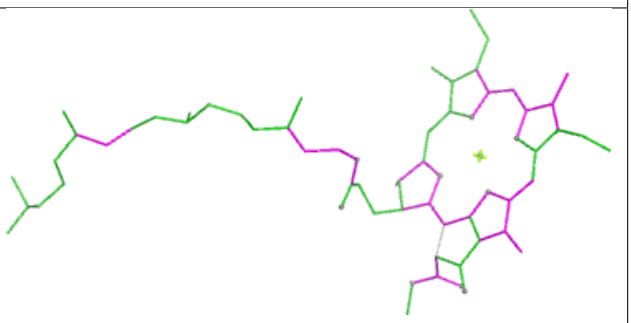


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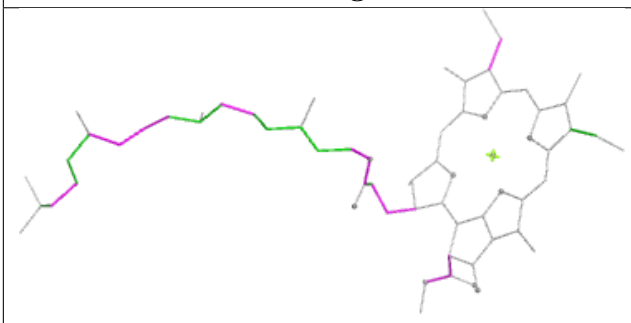
Ligand CLA A 1119



Bond lengths



Bond angles

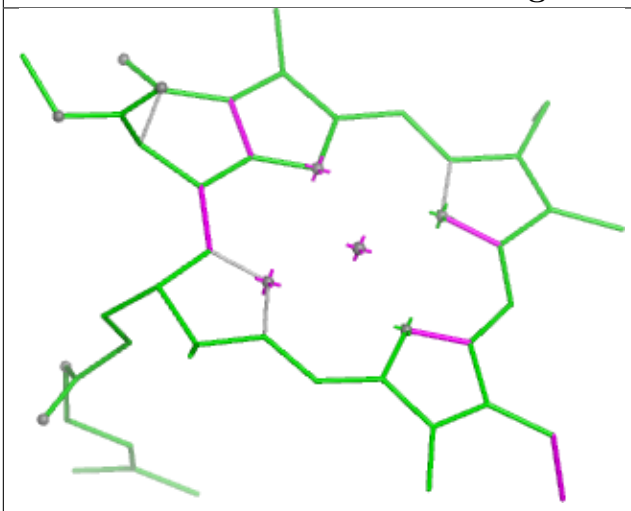


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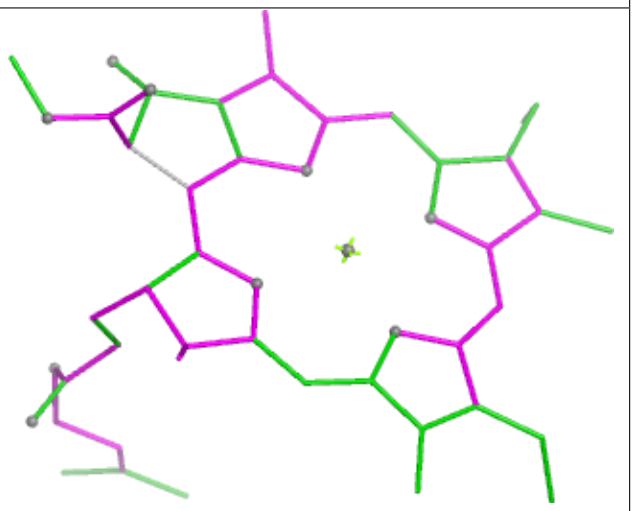


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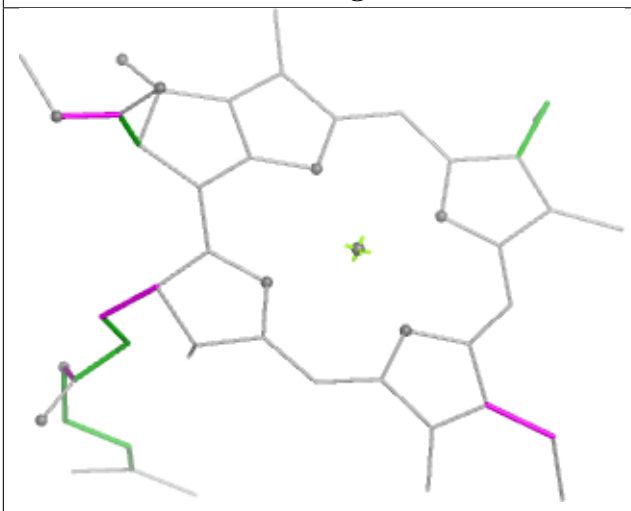
Ligand CLA 2 606



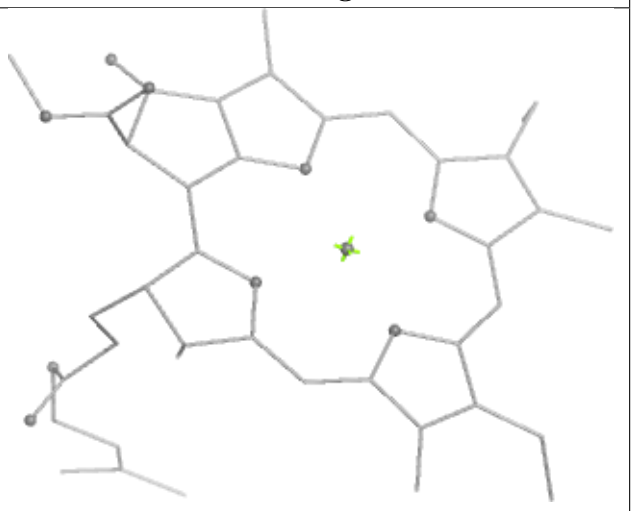
Bond lengths



Bond angles

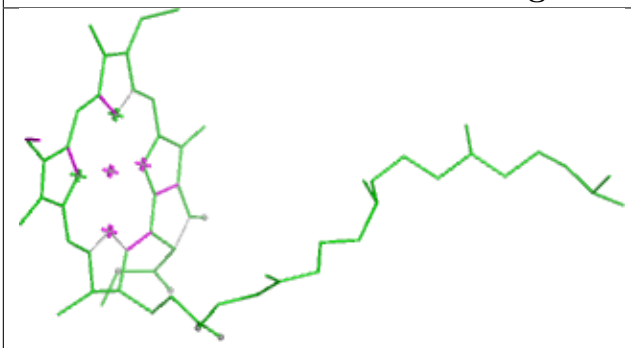


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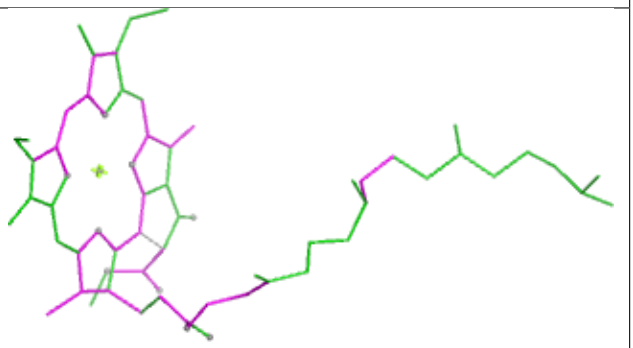


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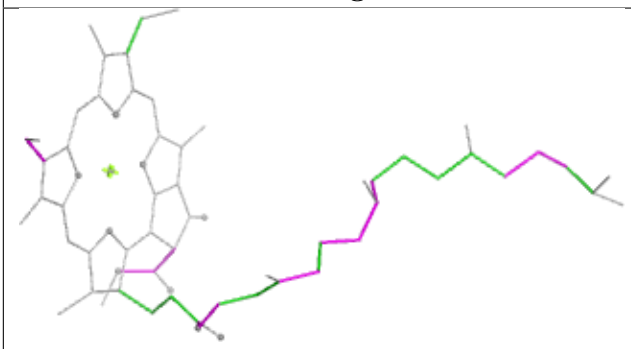
Ligand CLA 3 612



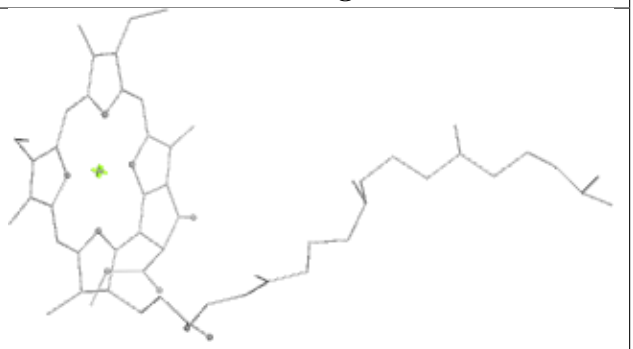
Bond lengths



Bond angles

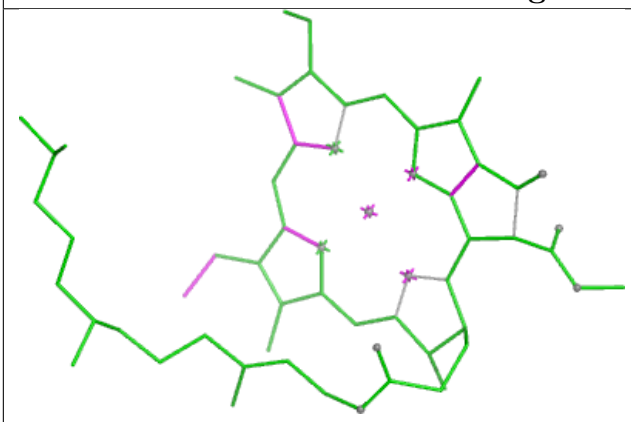


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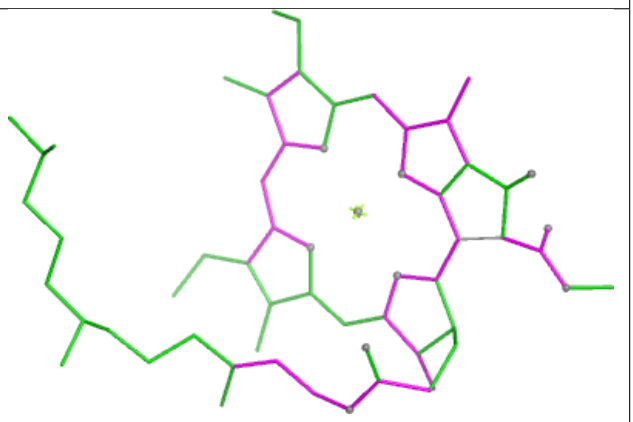


Rings

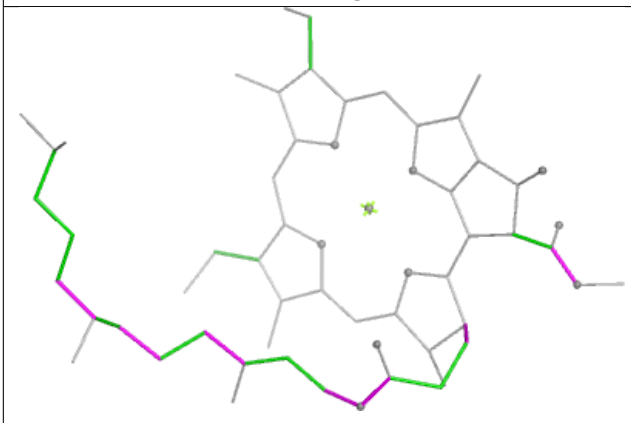
Ligand CLA 4 604



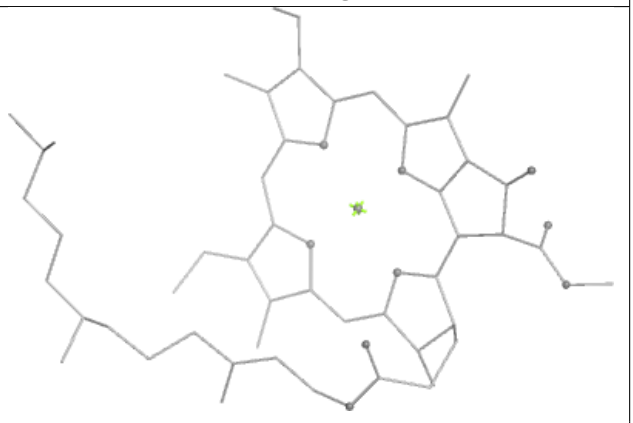
Bond lengths



Bond angles

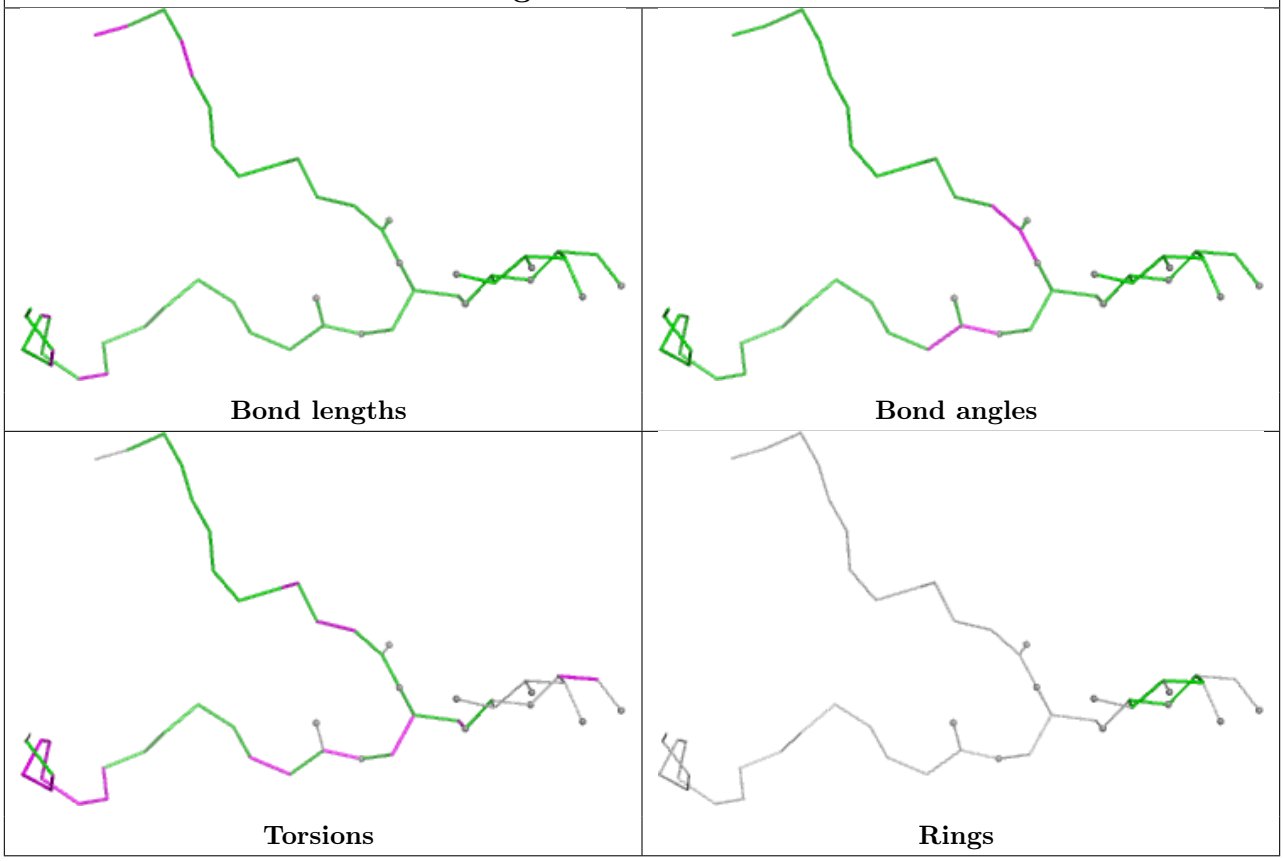


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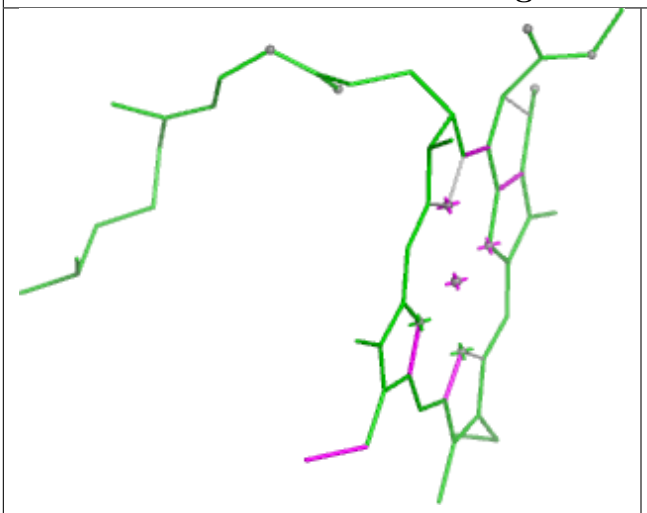


Rings

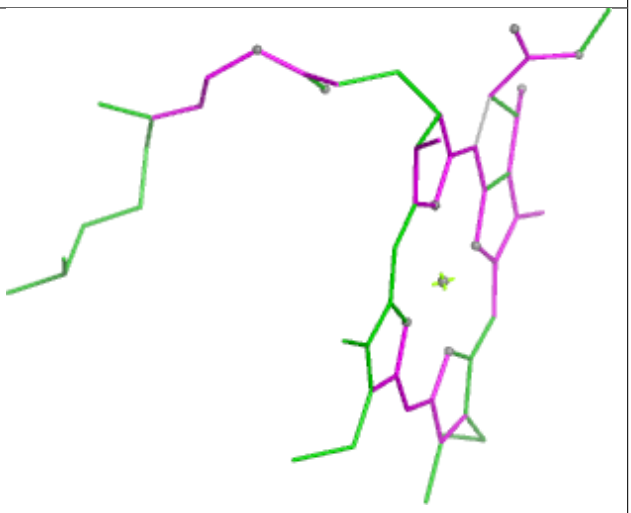
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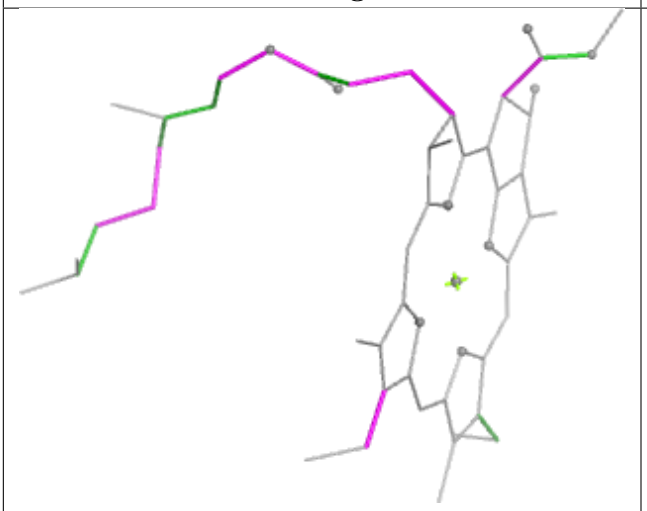
Ligand CLA B 1232



Bond lengths



Bond angles

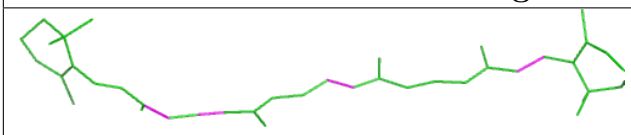


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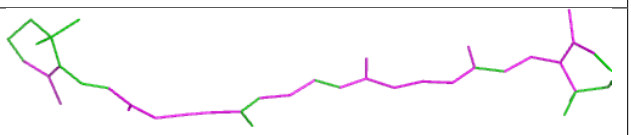


Rings

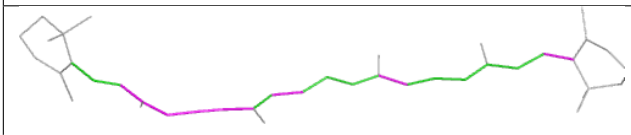
Ligand BCR K 4001



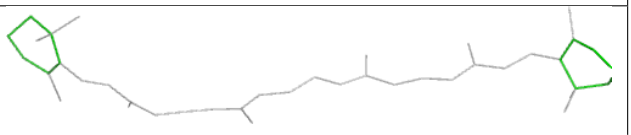
Bond lengths



Bond angles

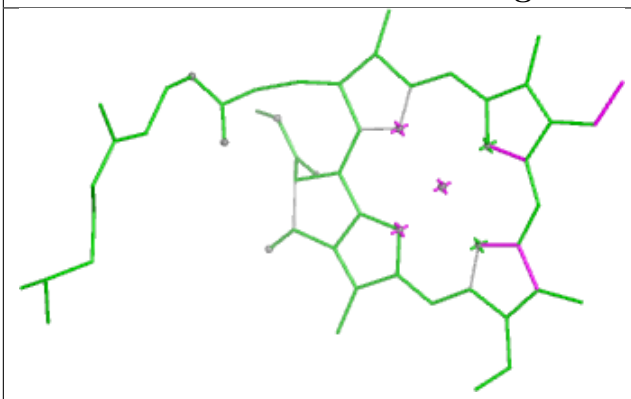


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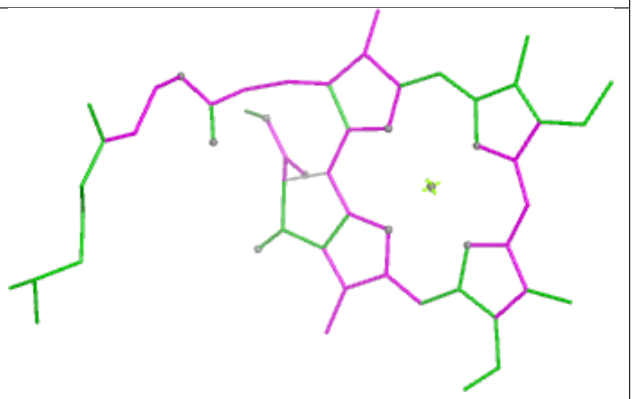


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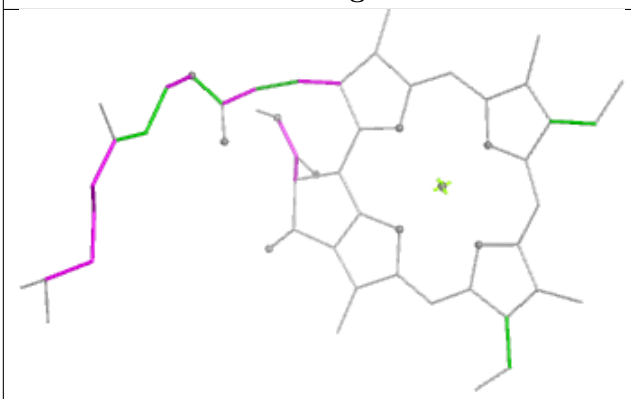
Ligand CLA K 1402



Bond lengths



Bond angles

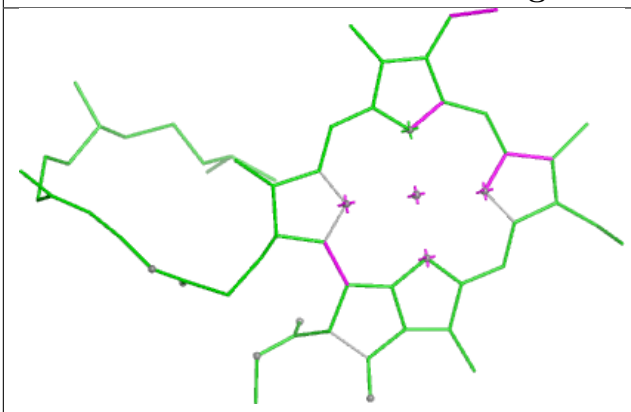


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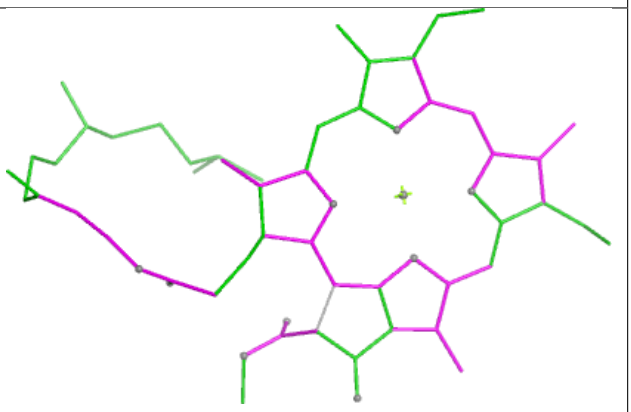


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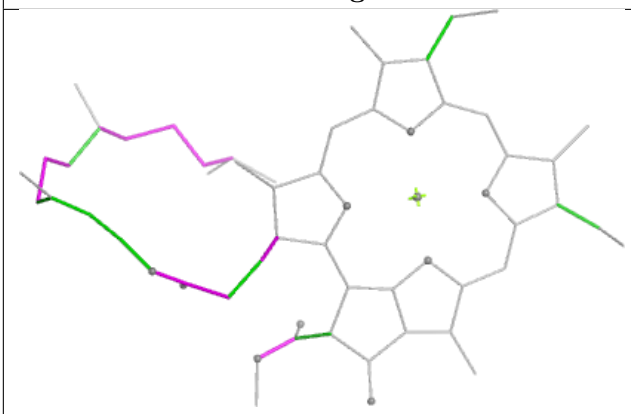
Ligand CLA 1 615



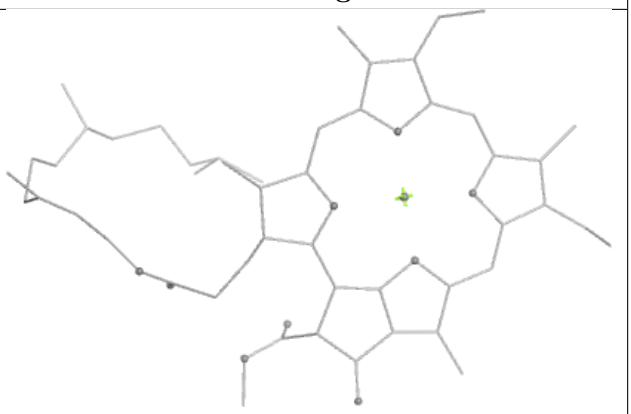
Bond lengths



Bond angles

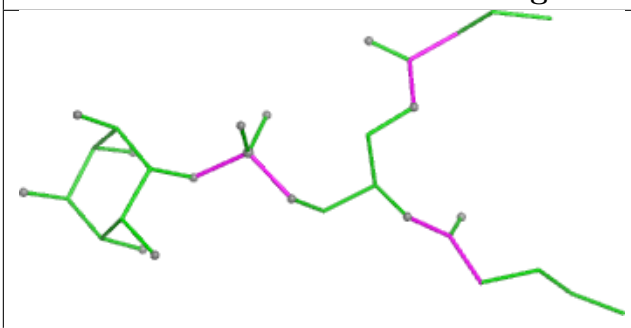


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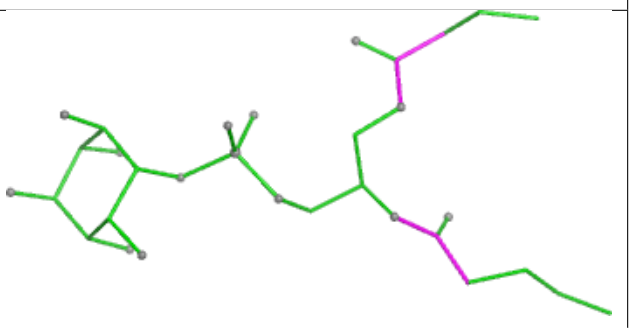


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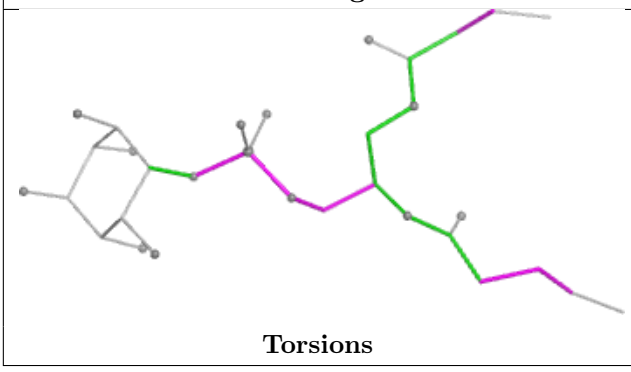
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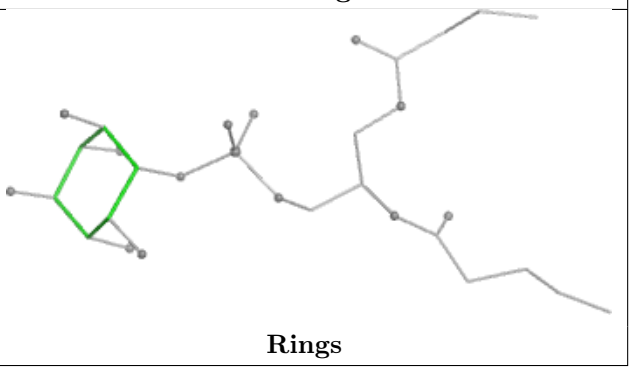
Bond lengths



Bond angles

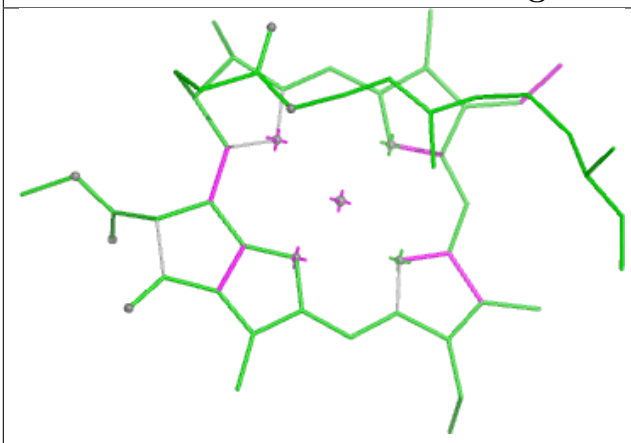


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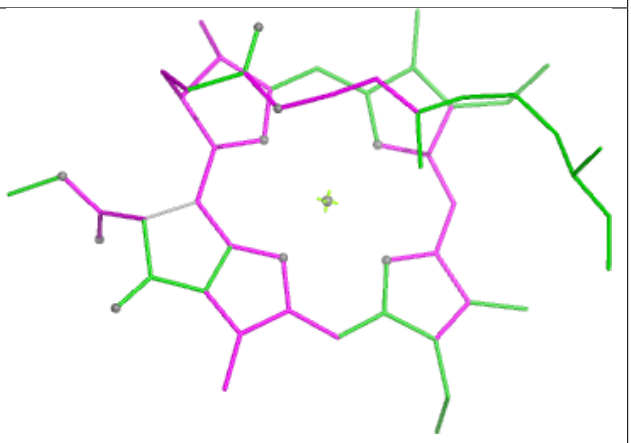


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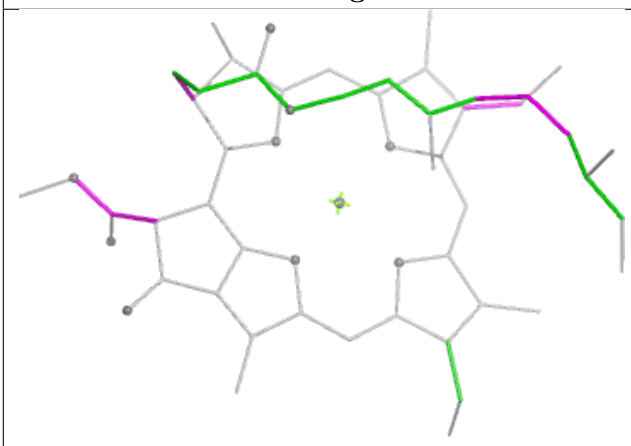
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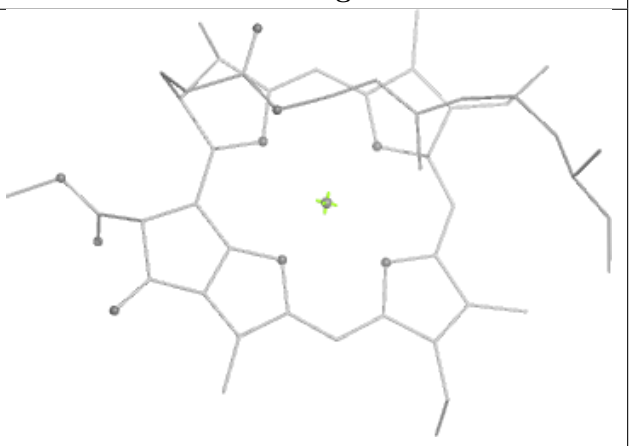
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Bond angles

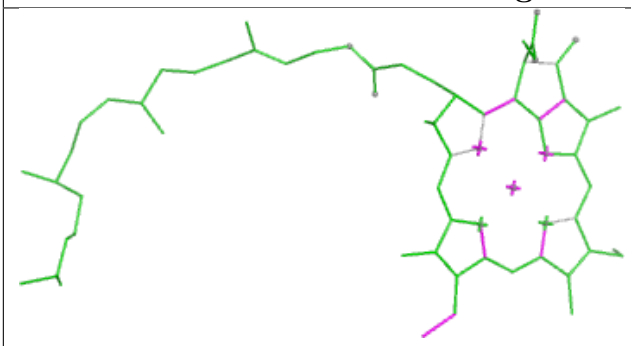


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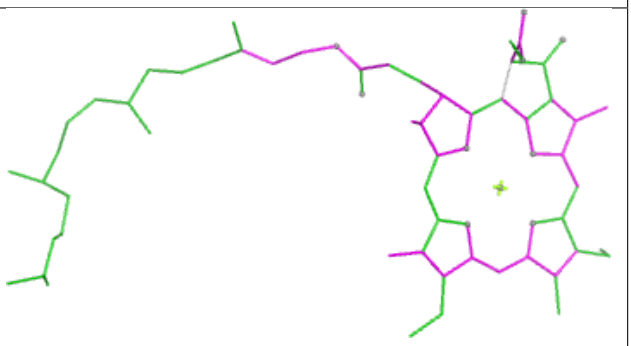


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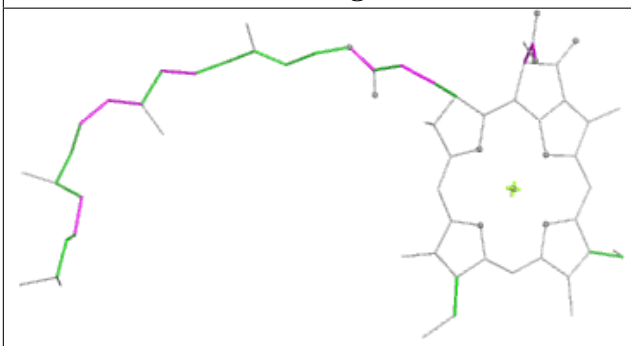
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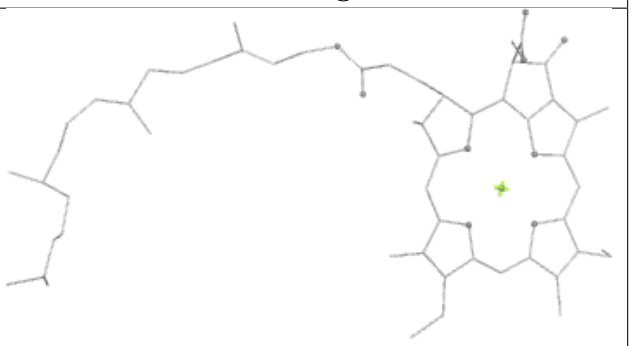
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Bond angles

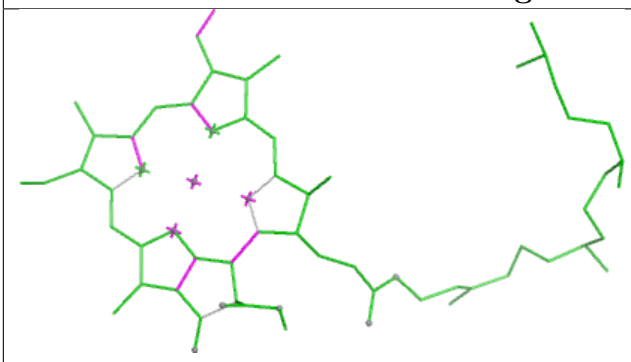


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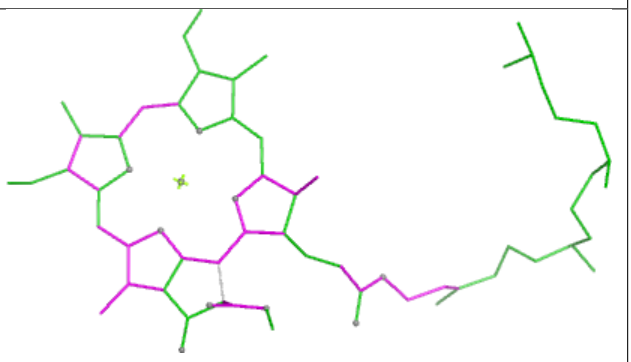


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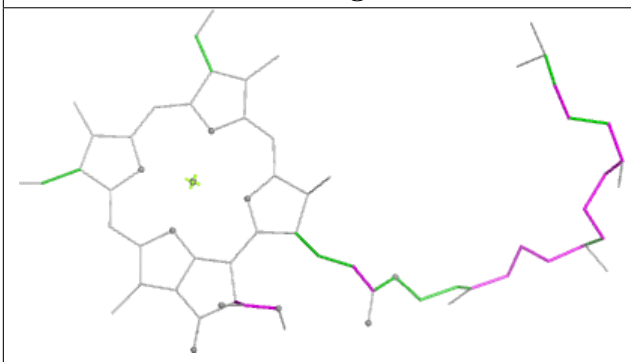
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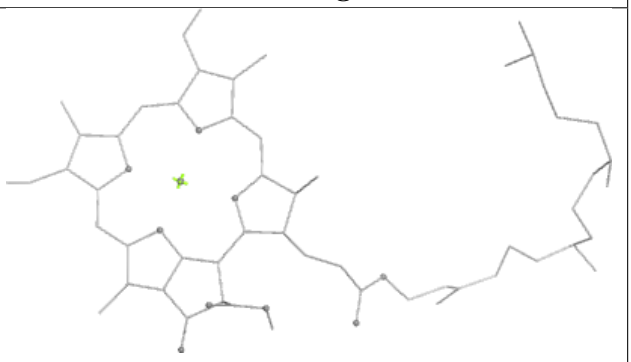
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Bond angles

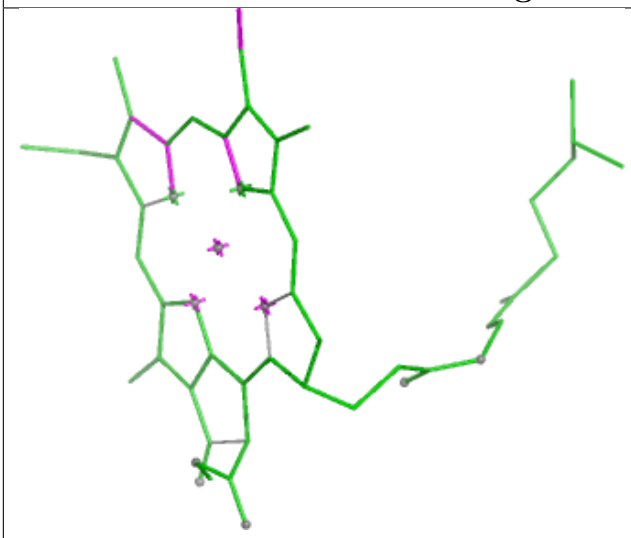


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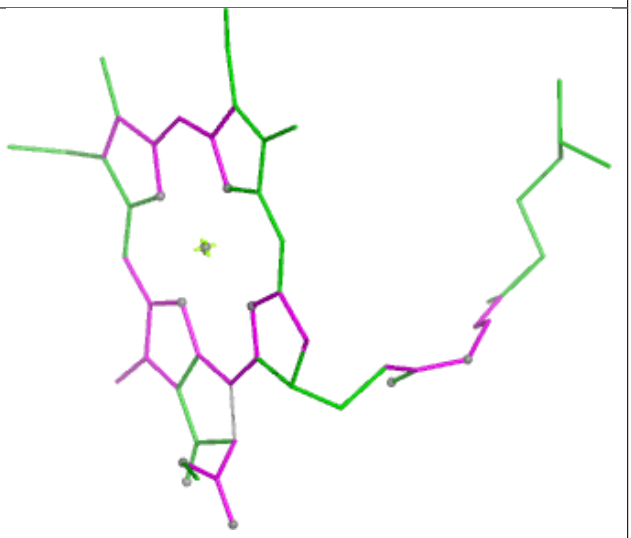


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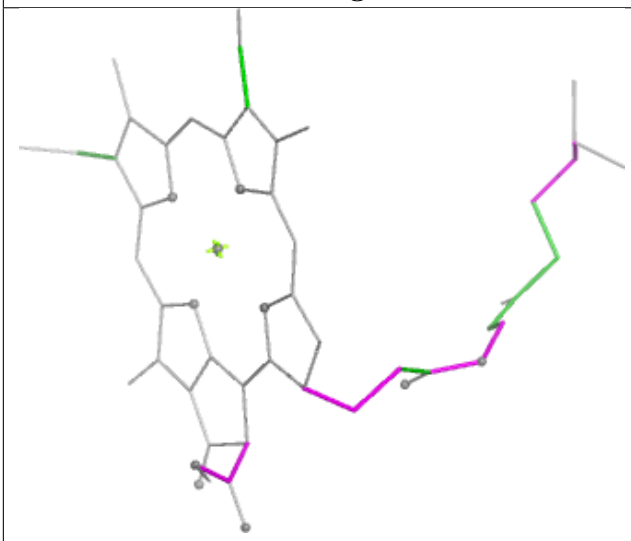
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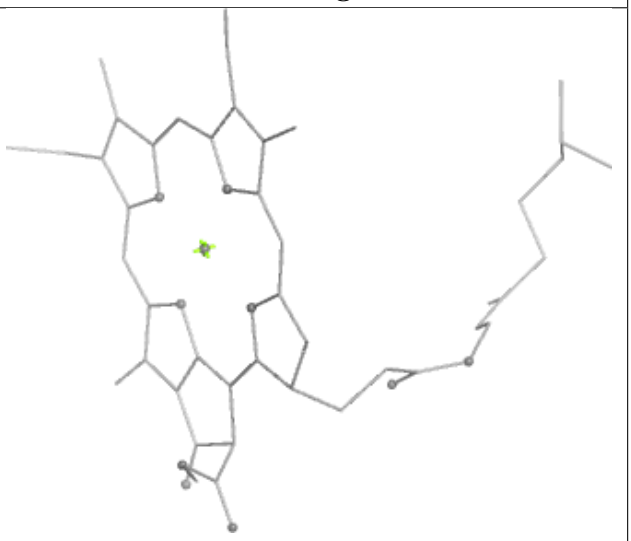
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Bond angles

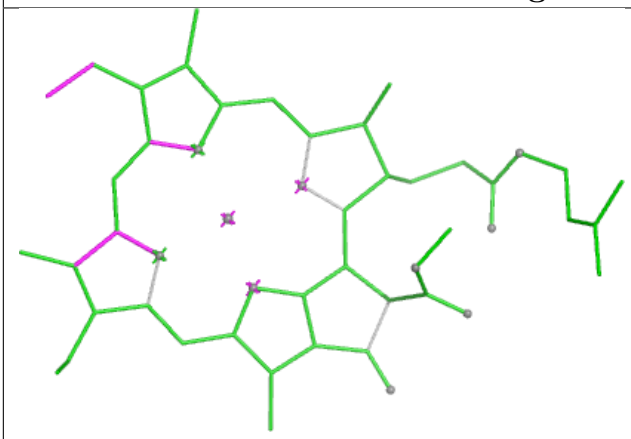


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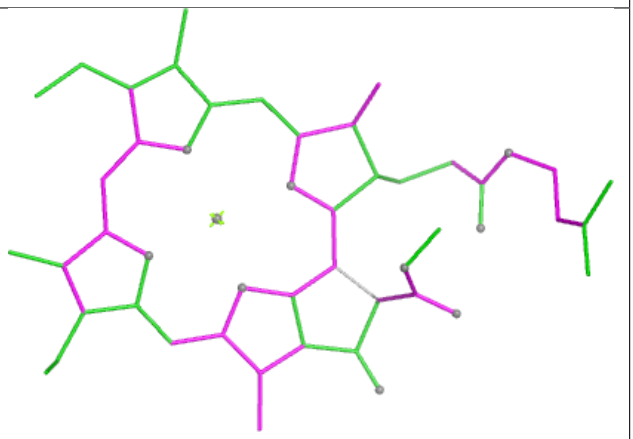


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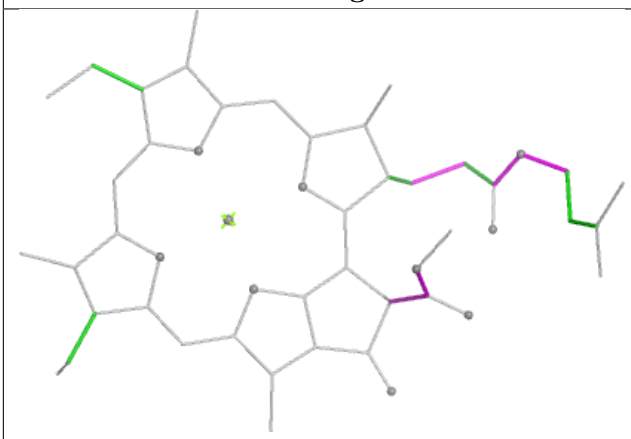
Ligand CLA 6 602



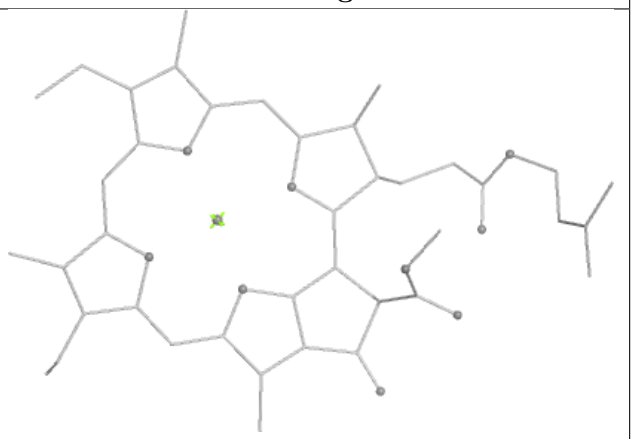
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Bond angles

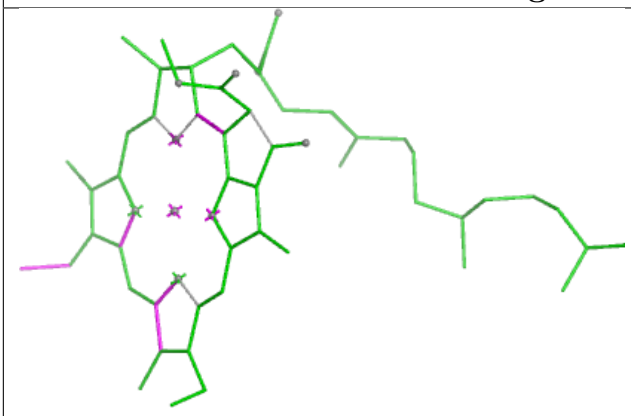


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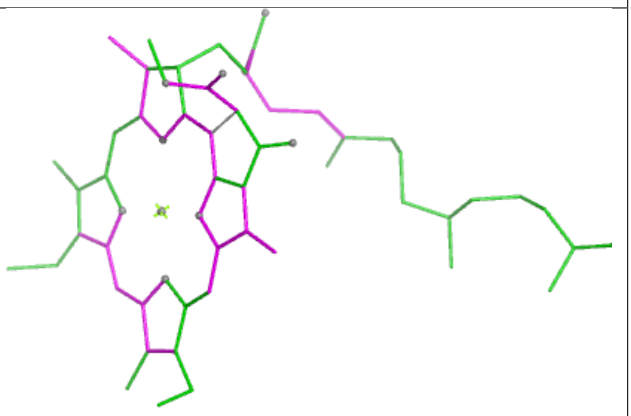


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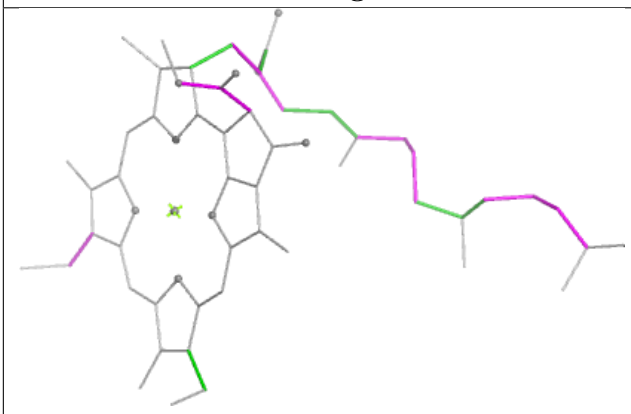
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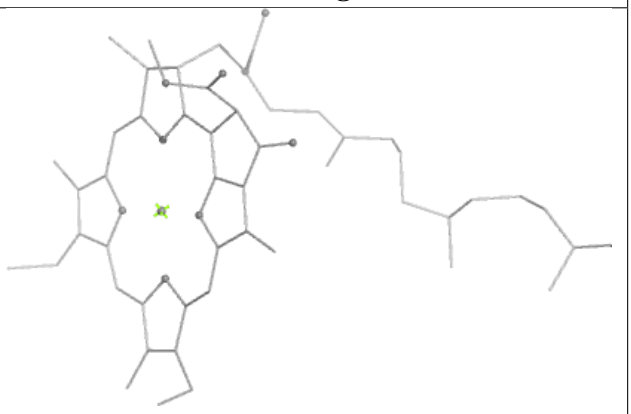
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Bond angles

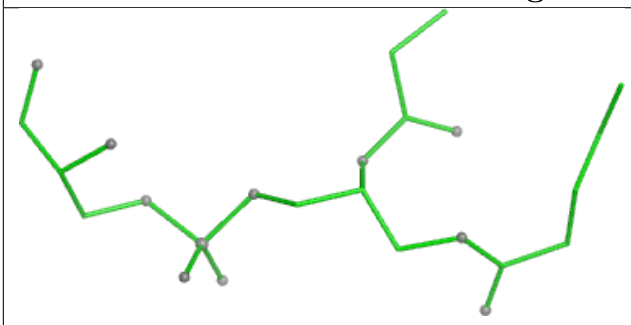


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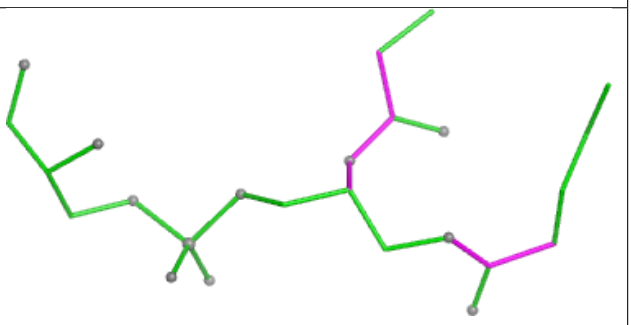


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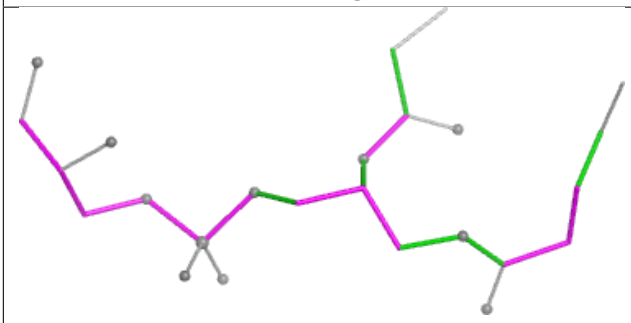
Ligand LHG 6 801



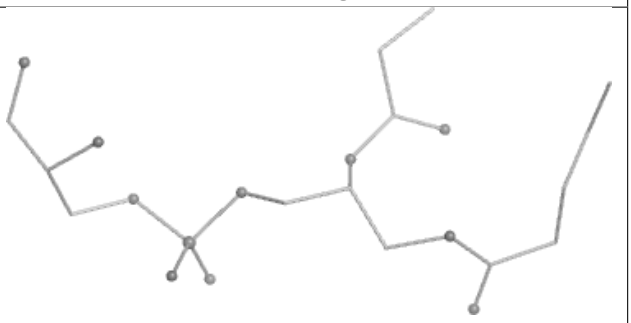
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Bond angles

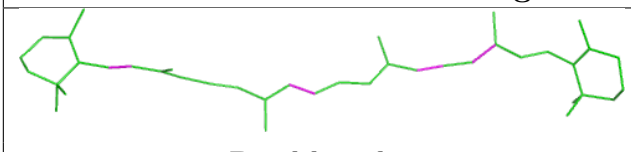


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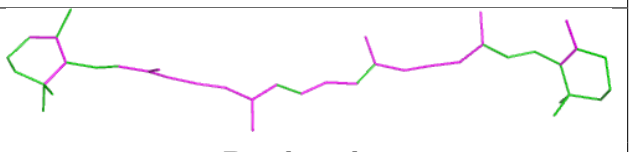


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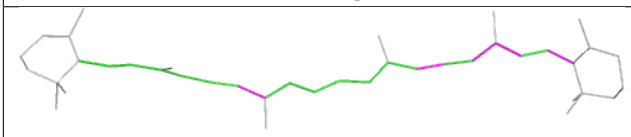
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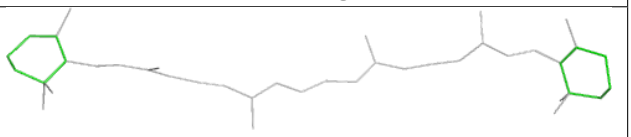
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Bond angles

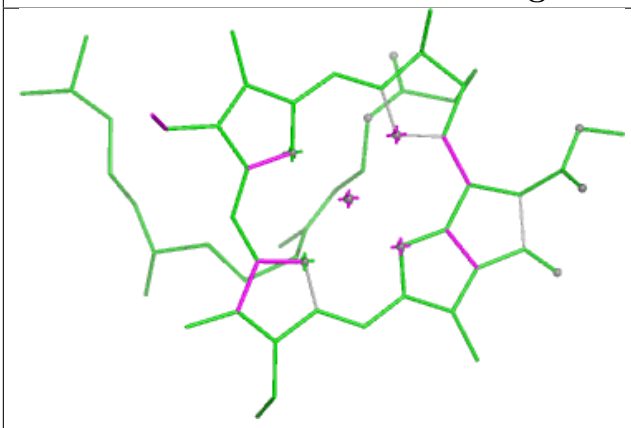


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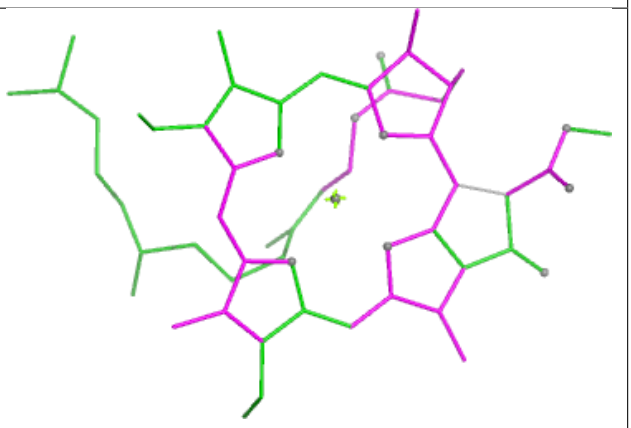


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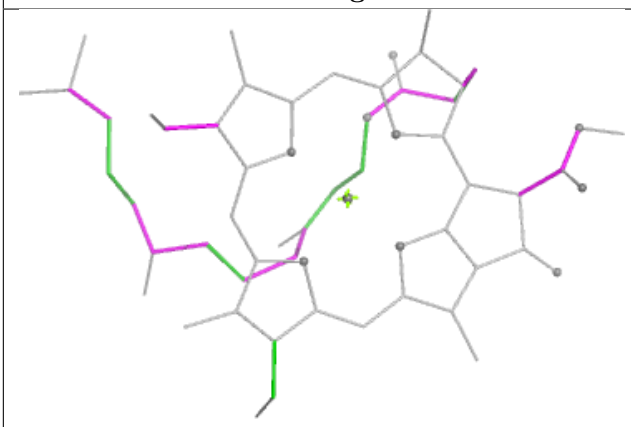
Ligand CLA 1 603



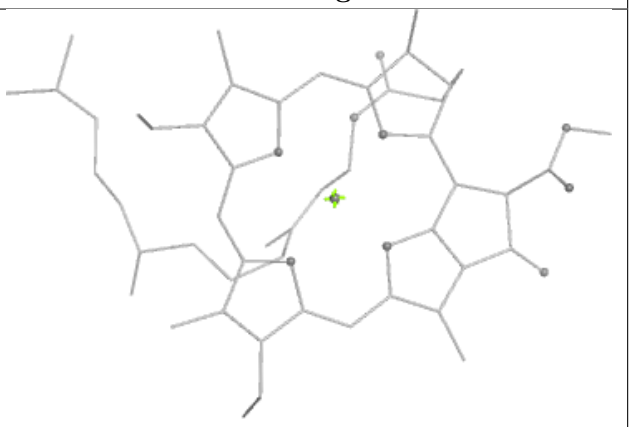
Bond lengths



Bond angles

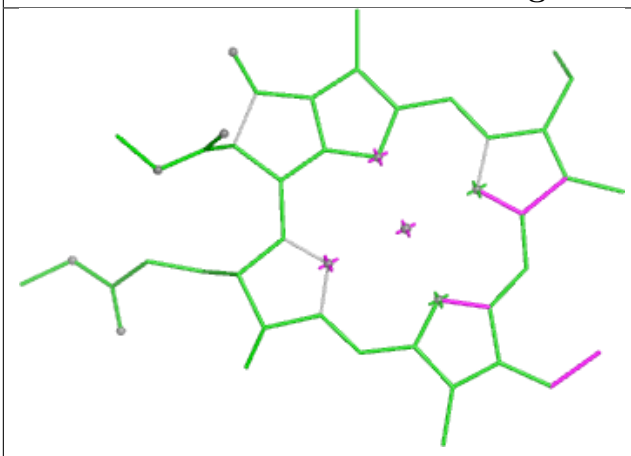


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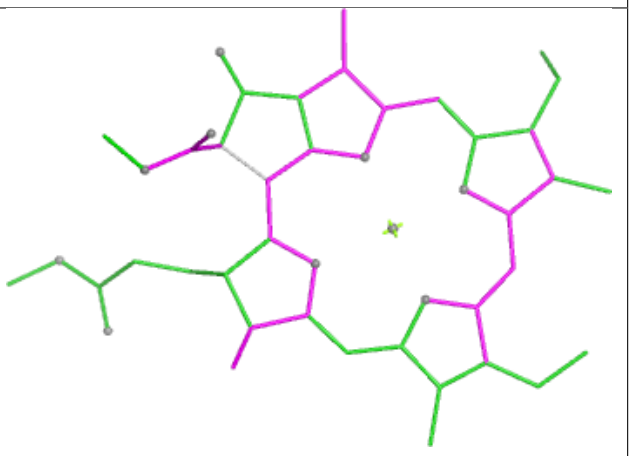


Rings

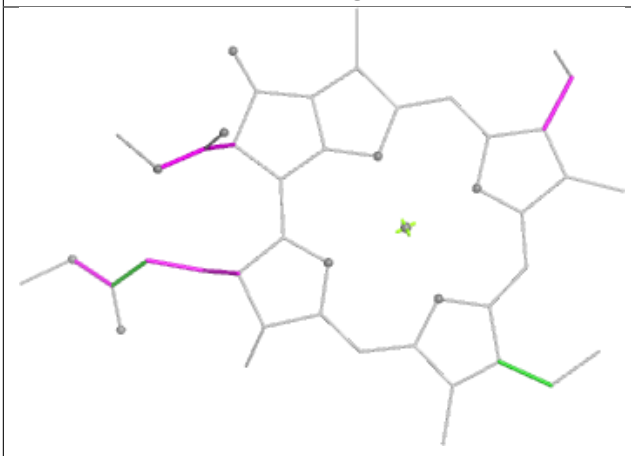
Ligand CLA 6 608



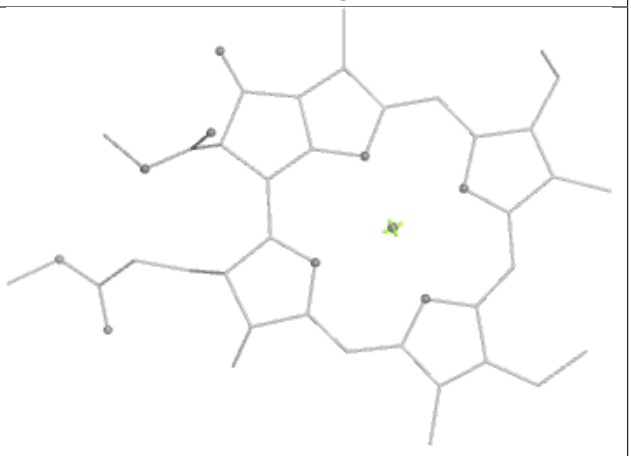
Bond lengths



Bond angles

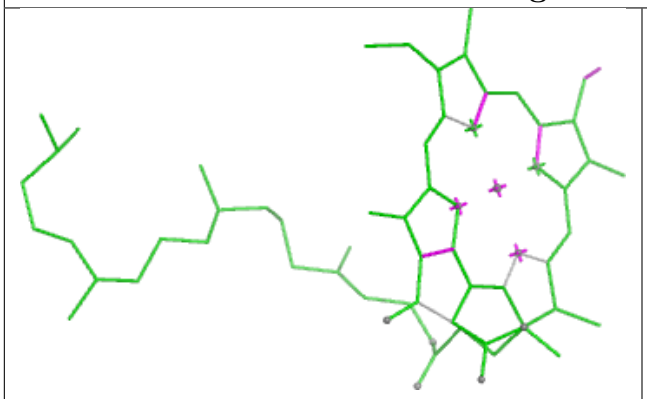


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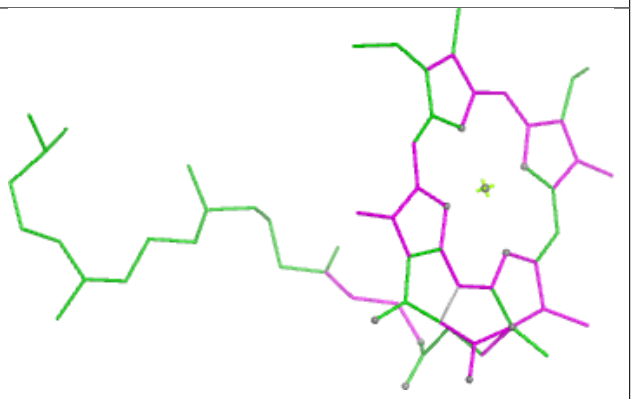


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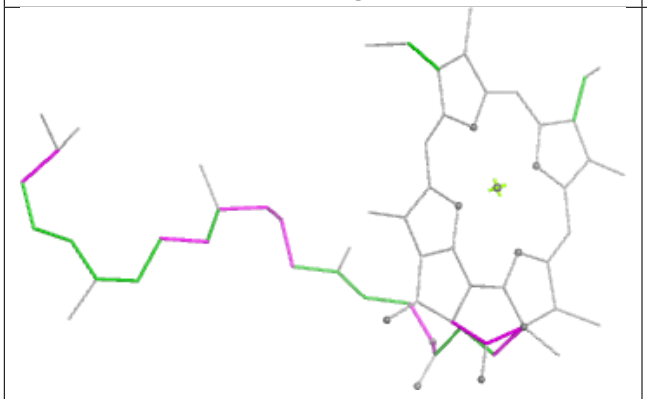
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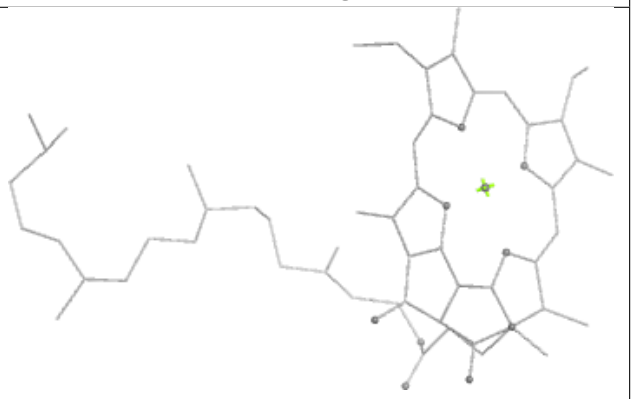
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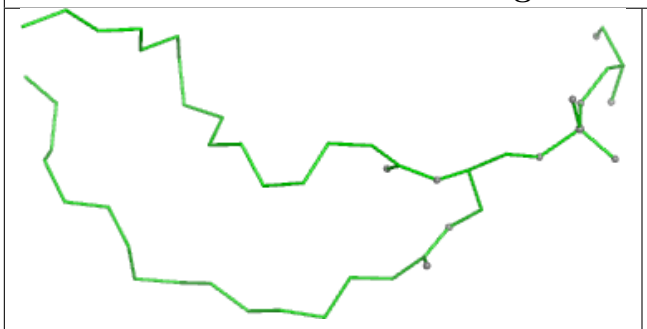


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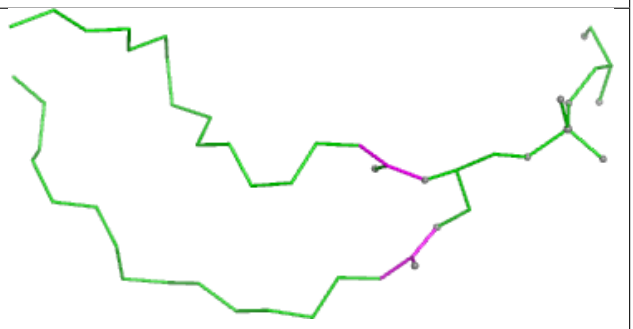


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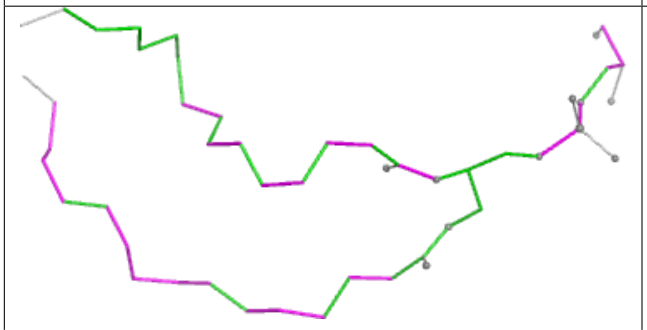
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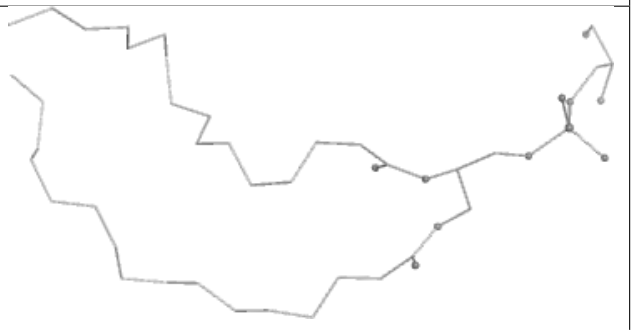
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Bond angles

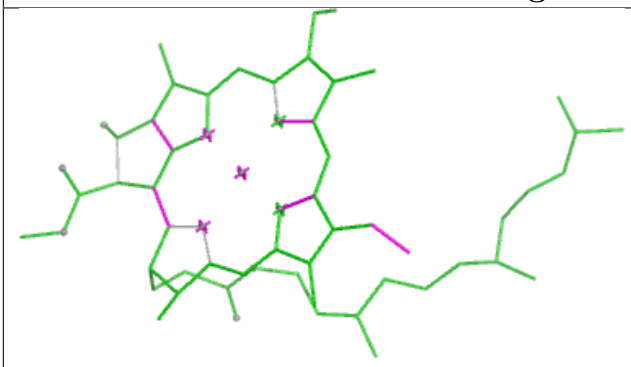


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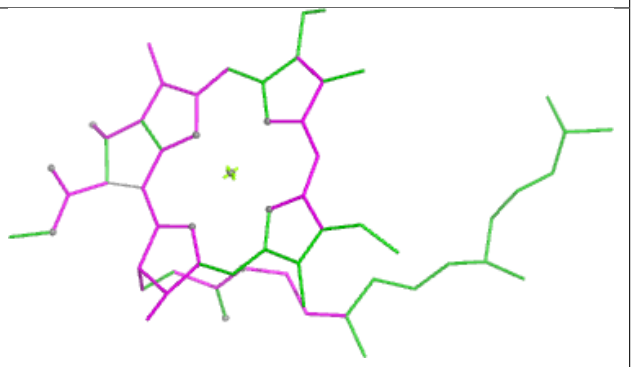


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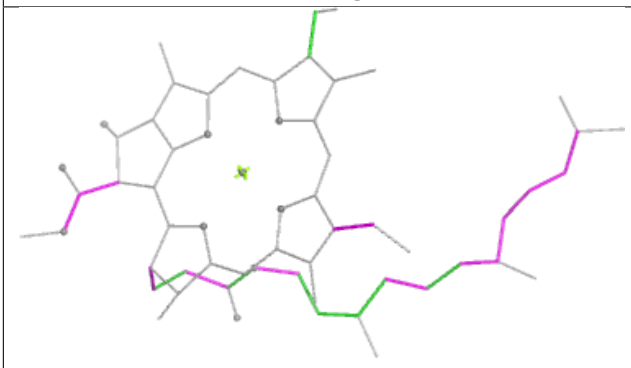
Ligand CLA 4 601



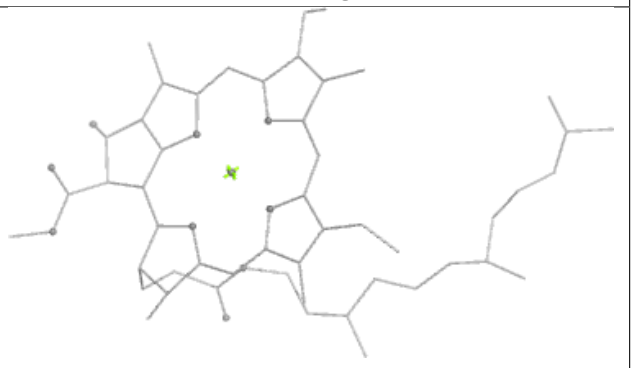
Bond lengths



Bond angles

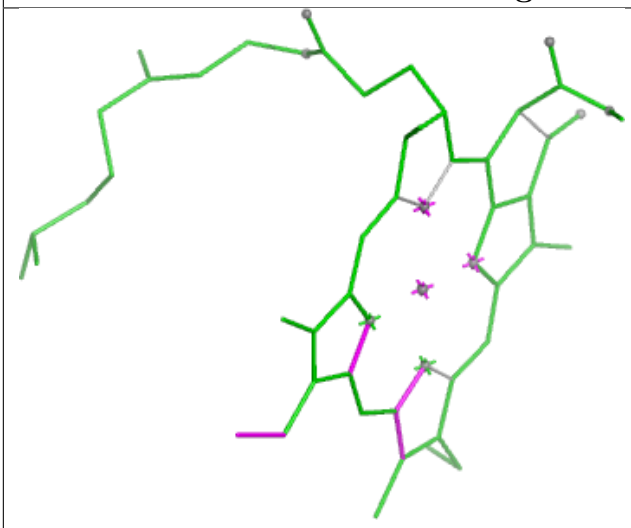


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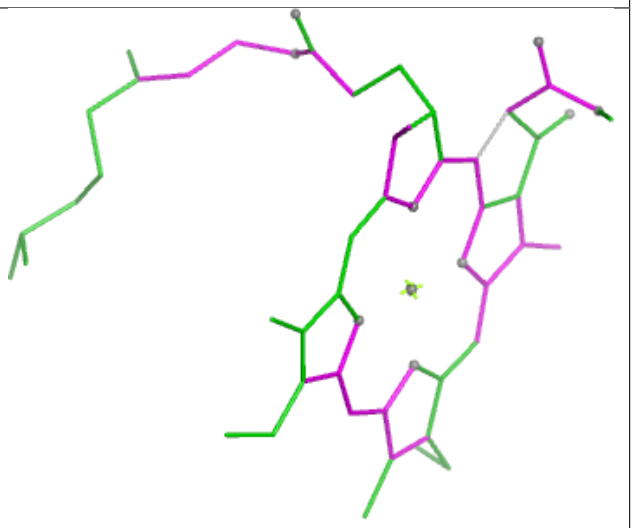


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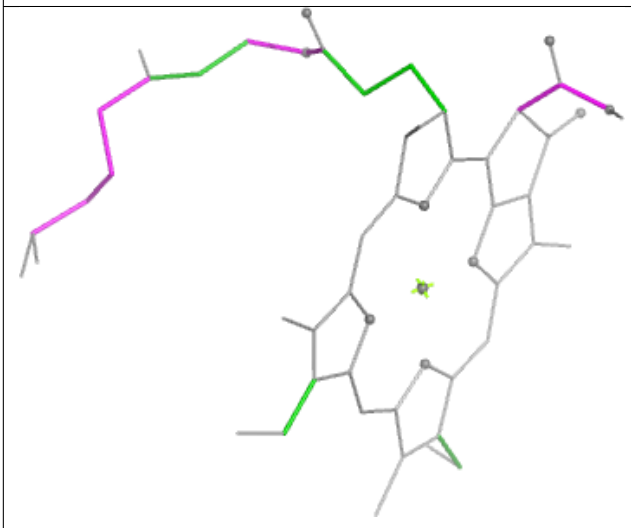
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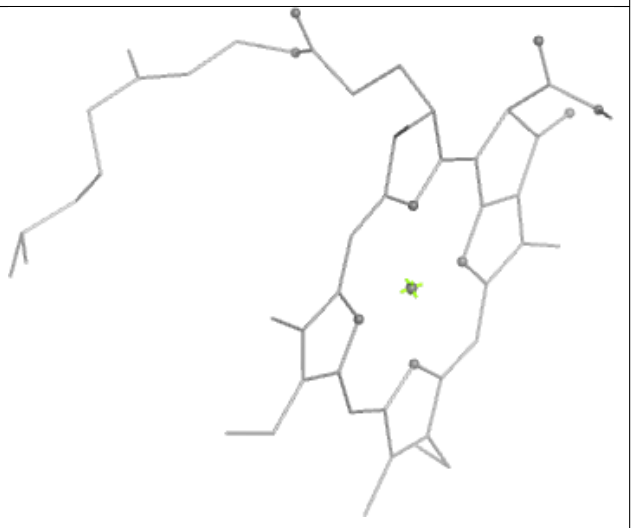
Bond lengths



Bond angles

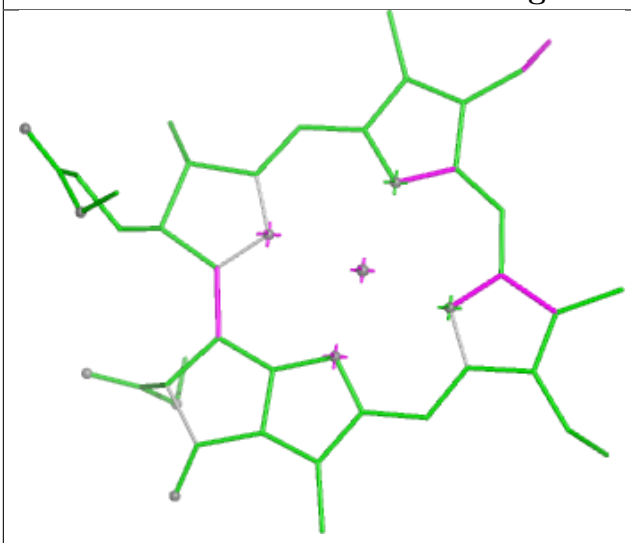


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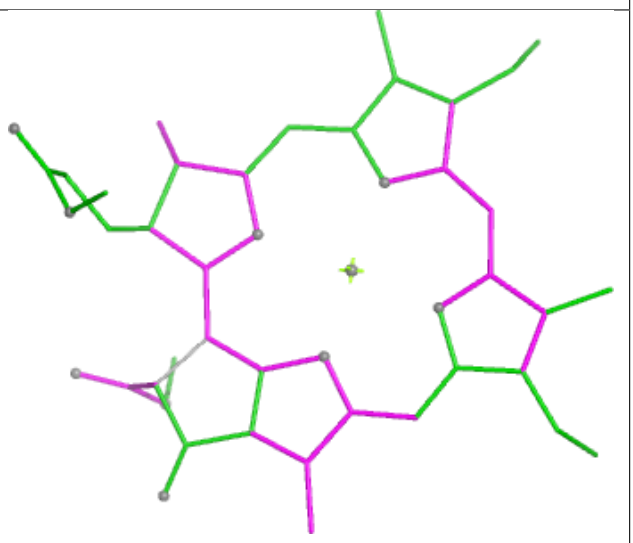


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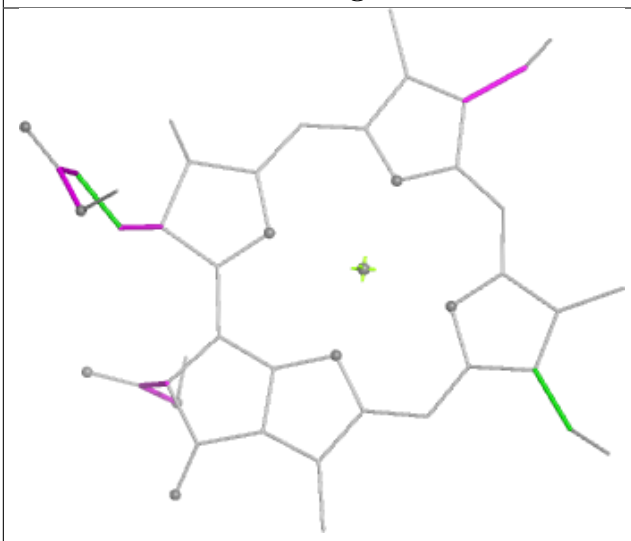
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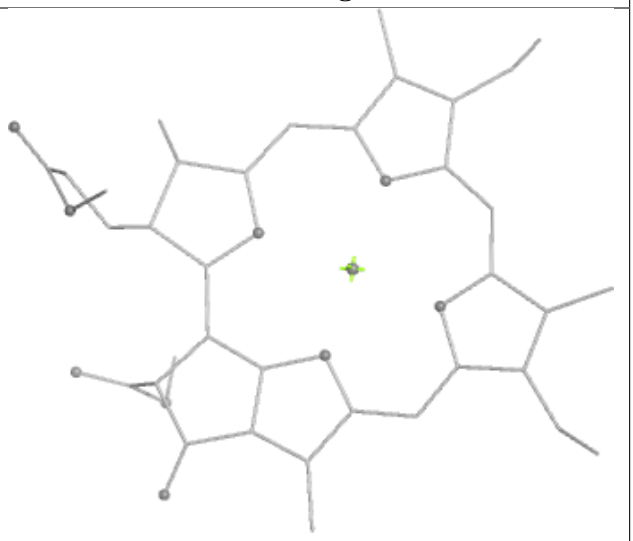
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Bond angles

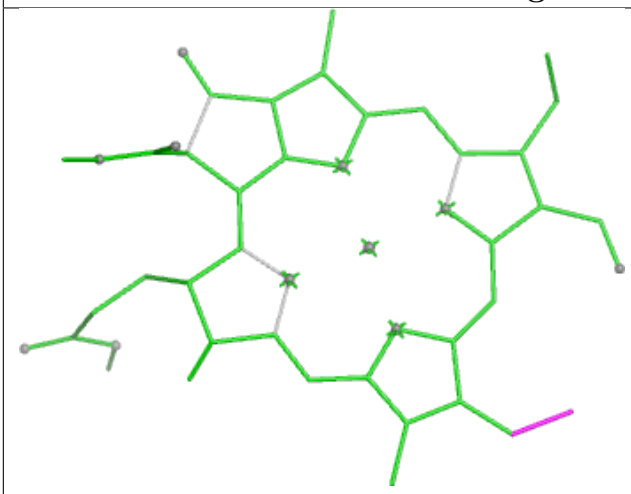


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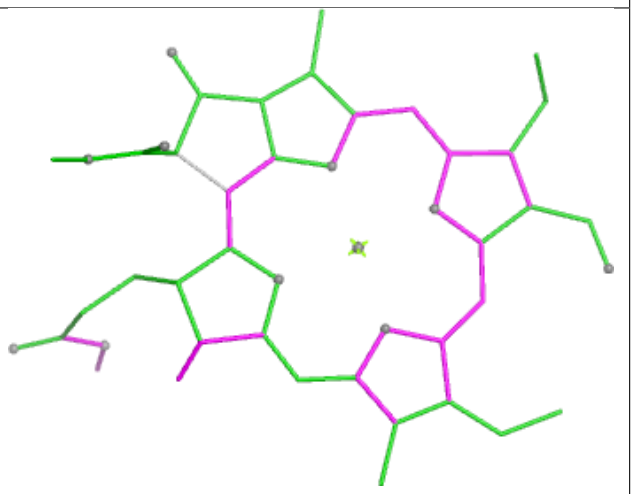


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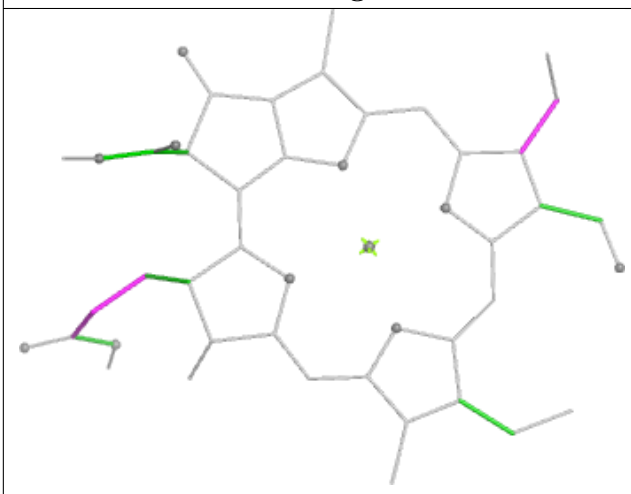
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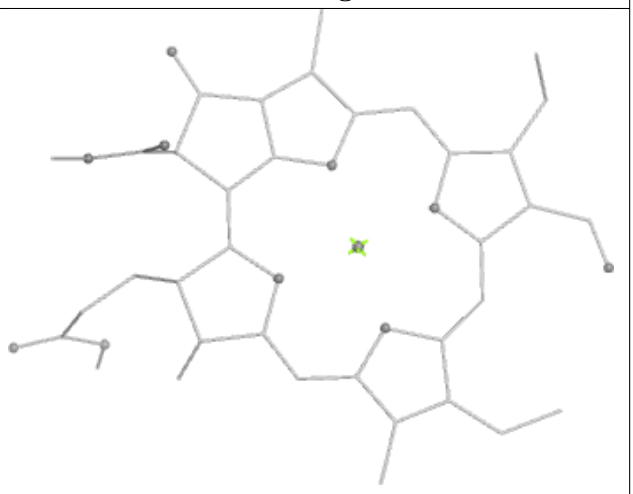
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Bond angles

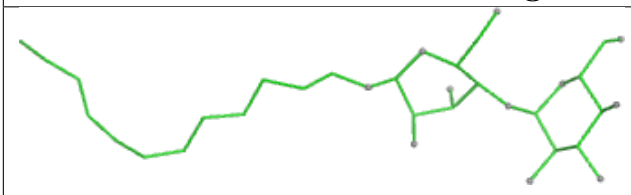


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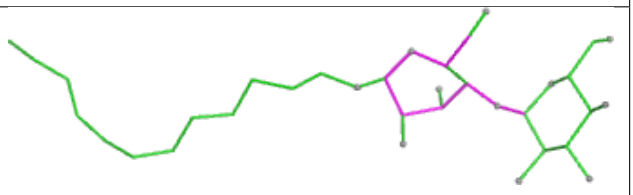


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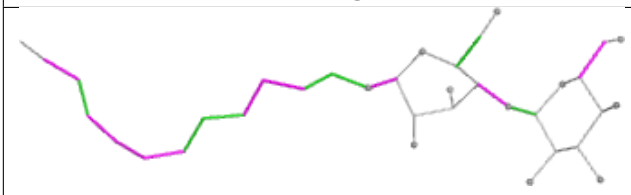
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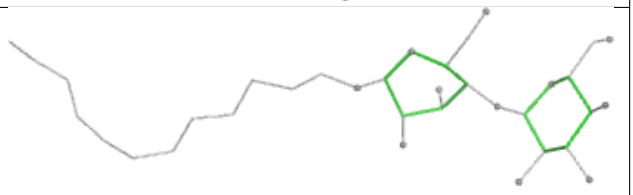
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Bond angles

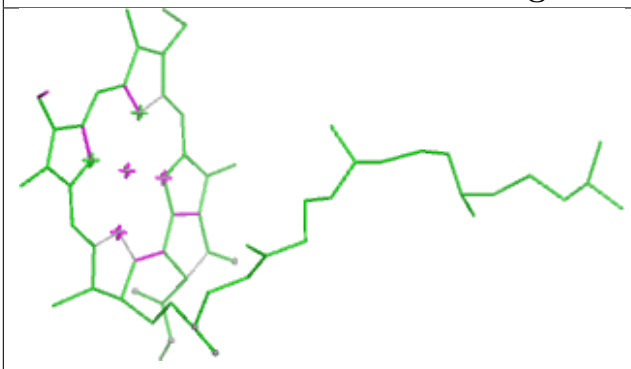


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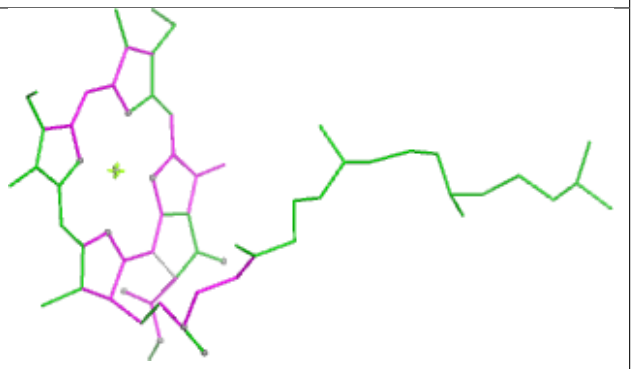


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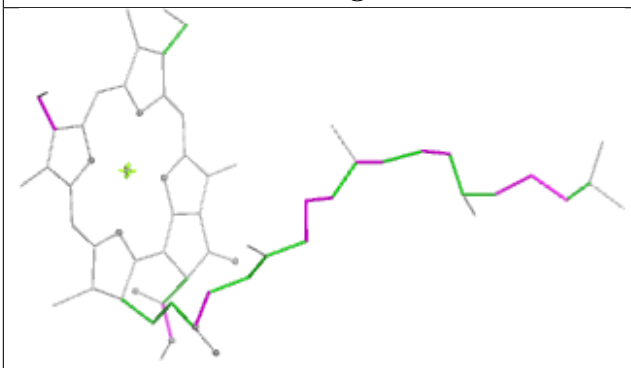
Ligand CLA 4 612



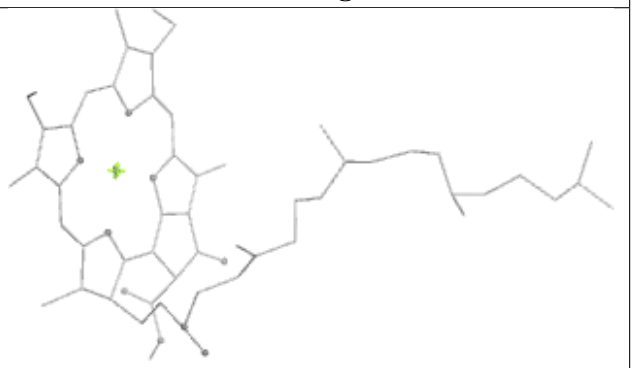
Bond lengths



Bond angles



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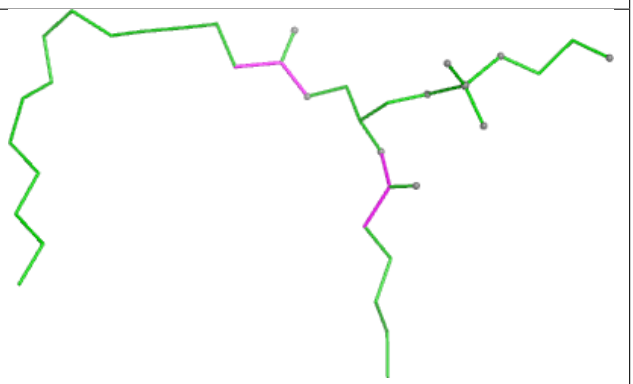


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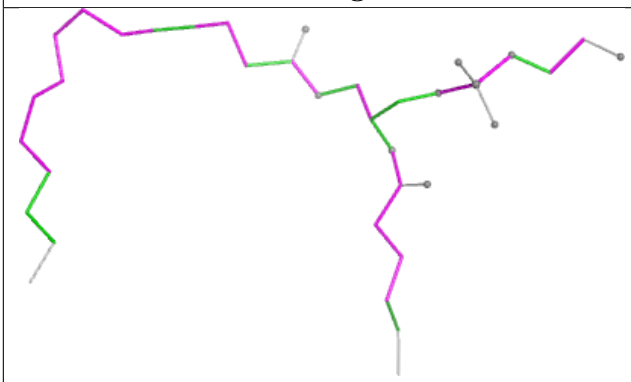
Ligand PTY 5 803



Bond lengths



Bond angles

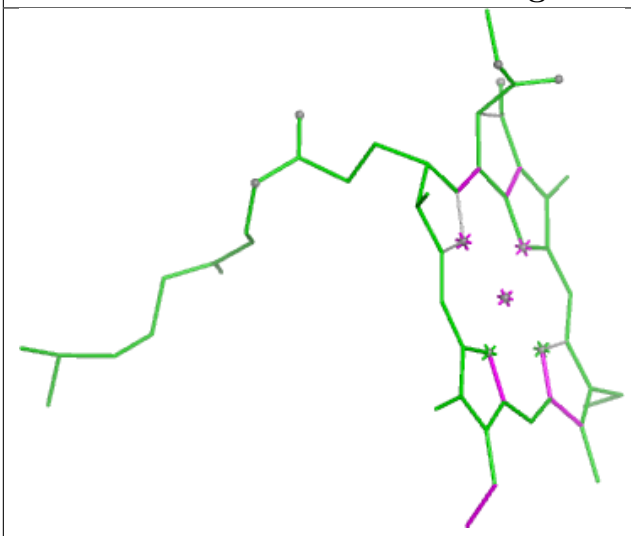


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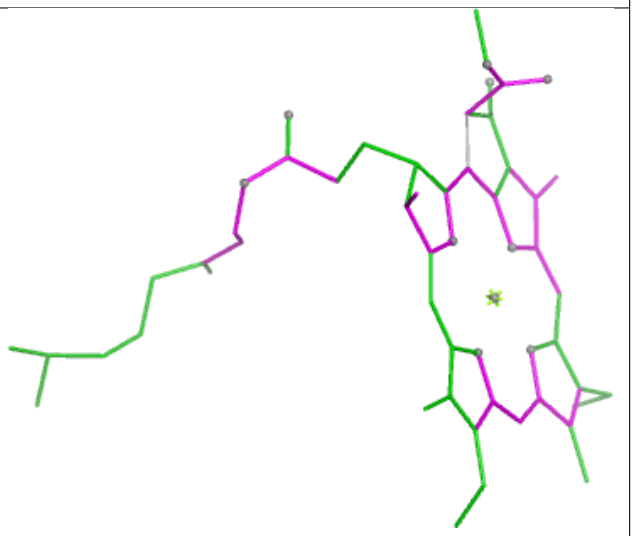


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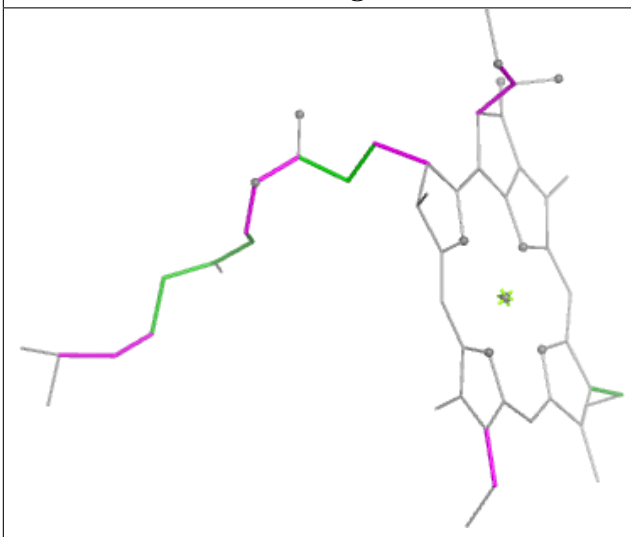
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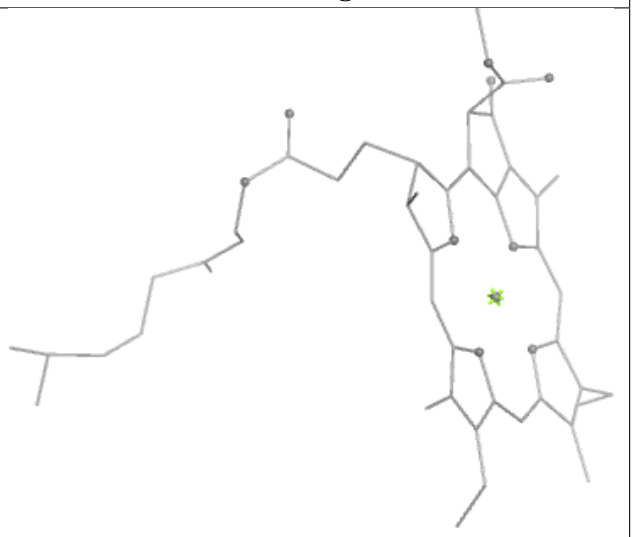
Bond lengths



Bond angles

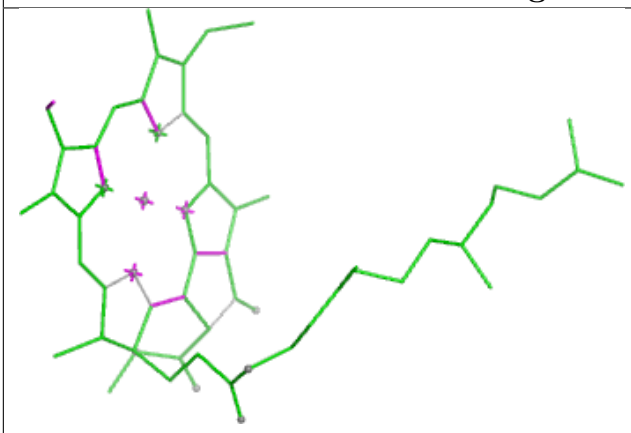


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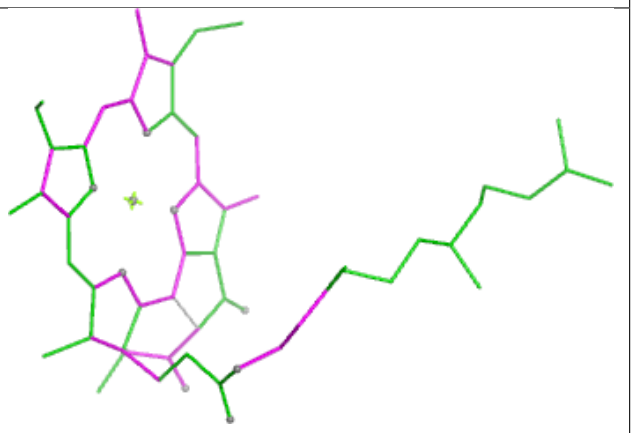


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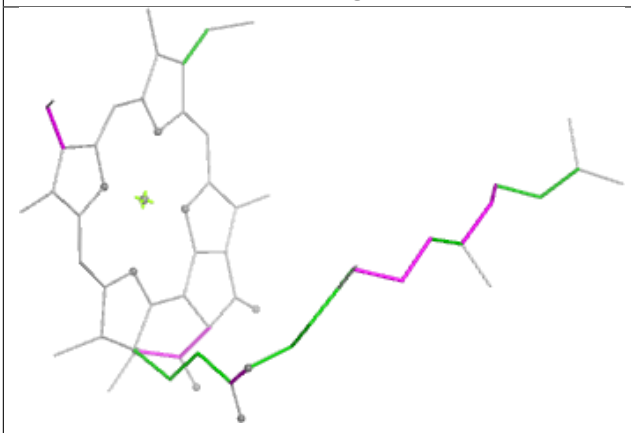
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Bond lengths



Bond angles

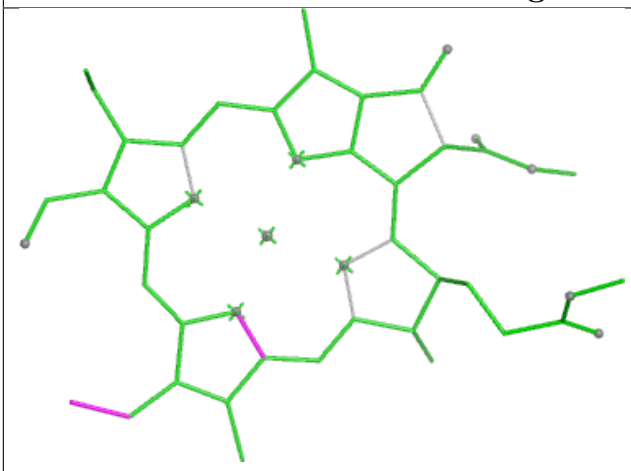


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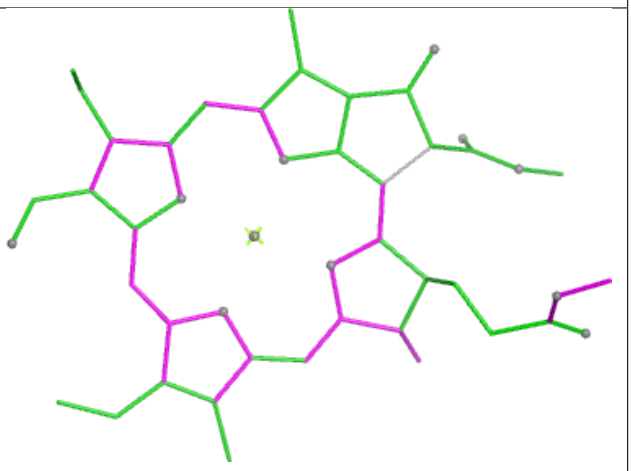


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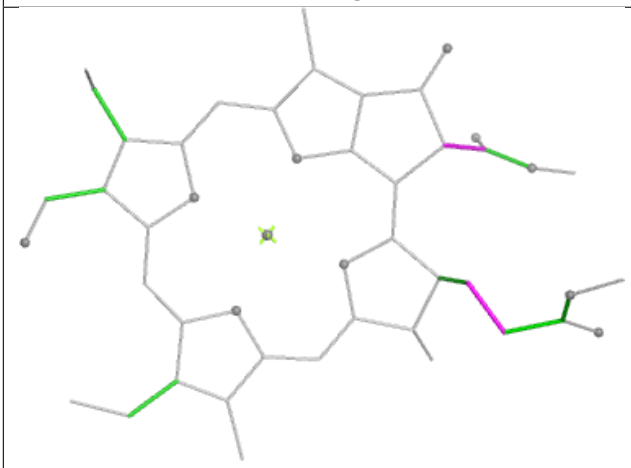
Ligand CHL 4 610



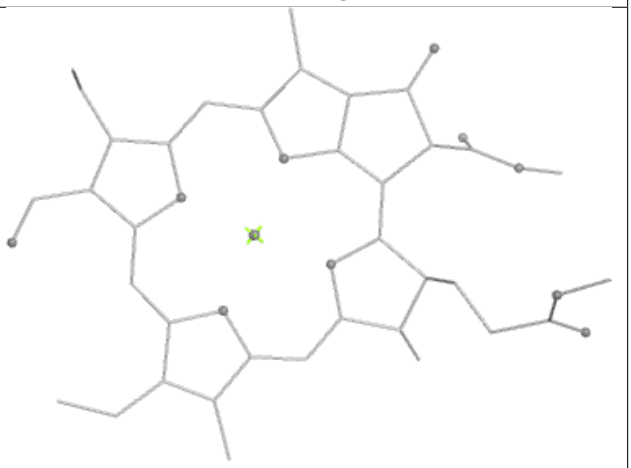
Bond lengths



Bond angles

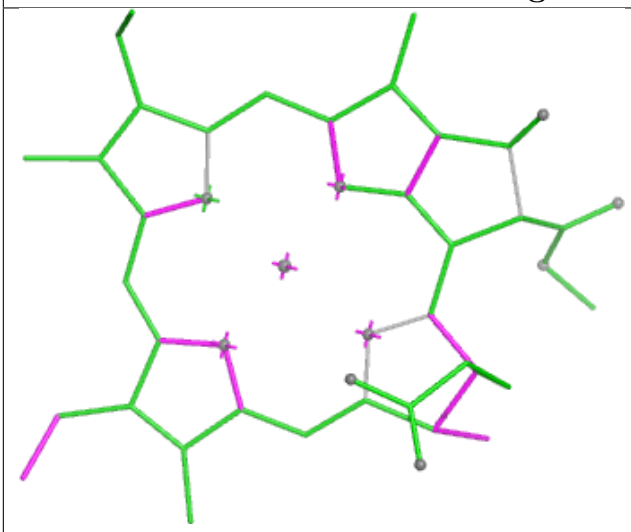


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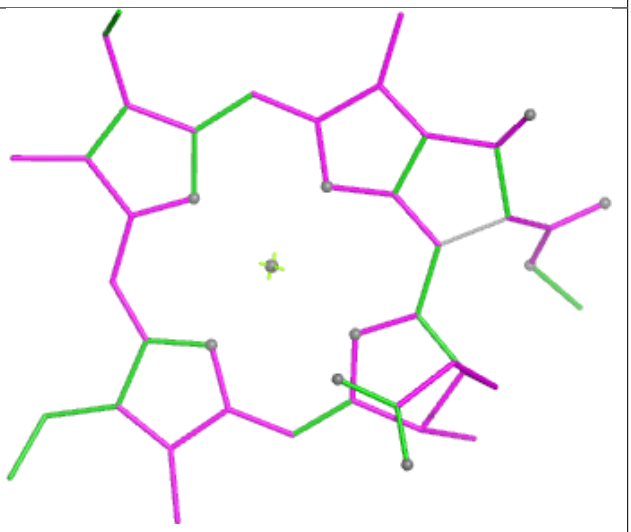


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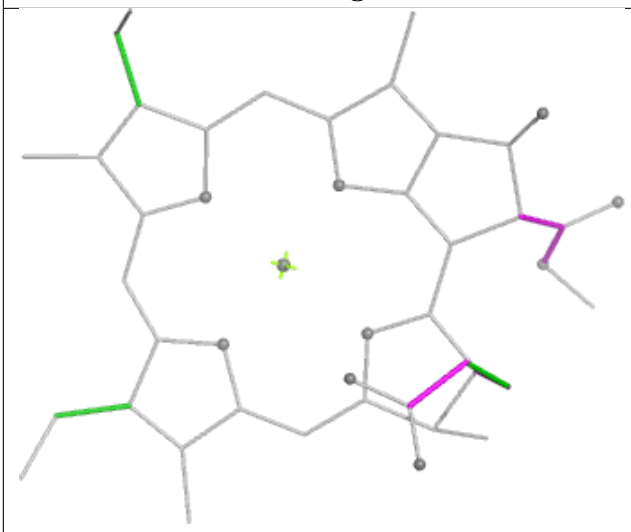
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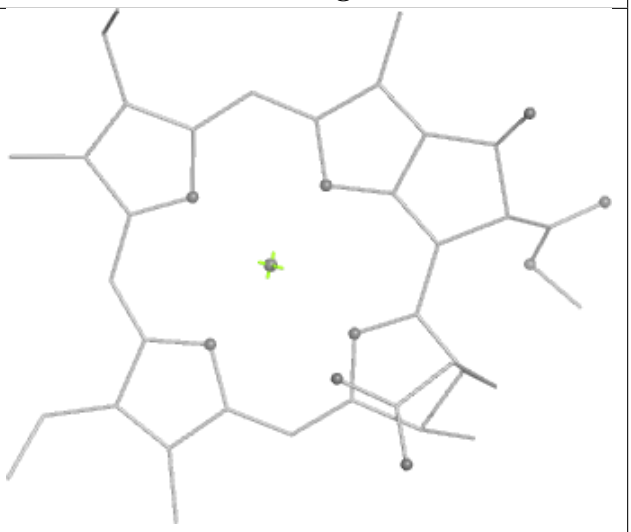
Bond lengths



Bond angles

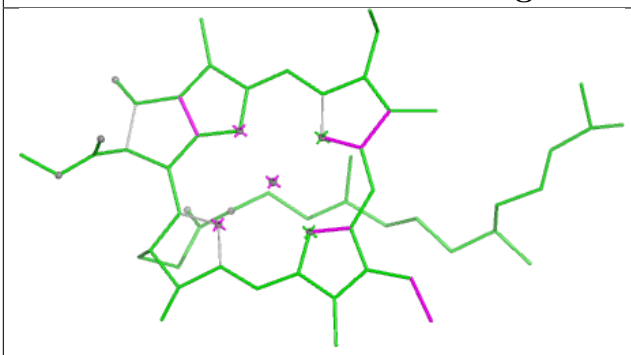


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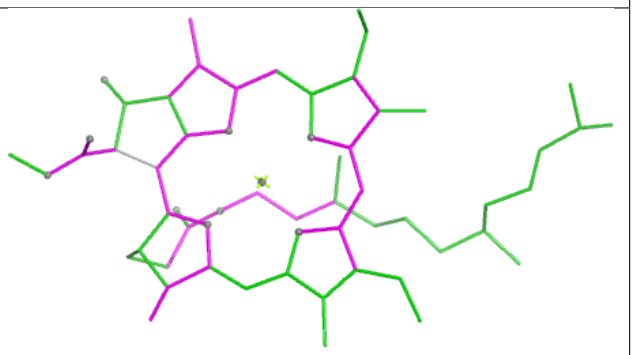


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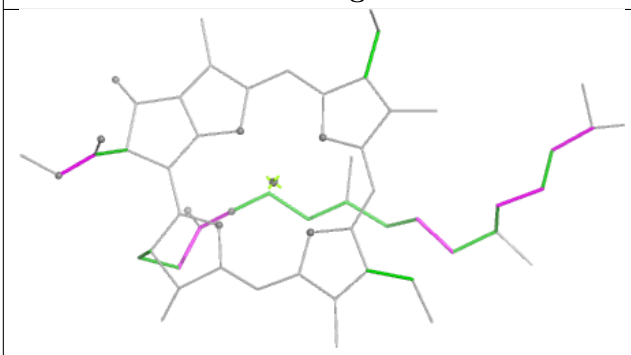
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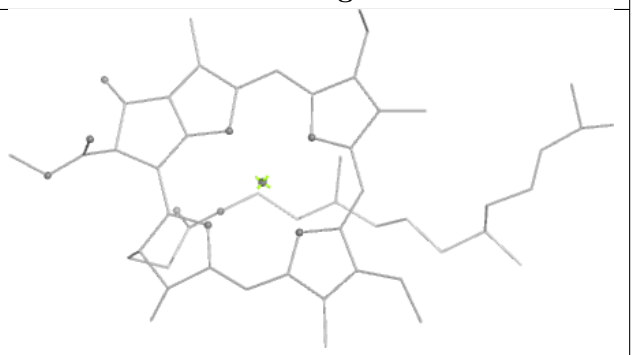
Bond lengths



Bond angles

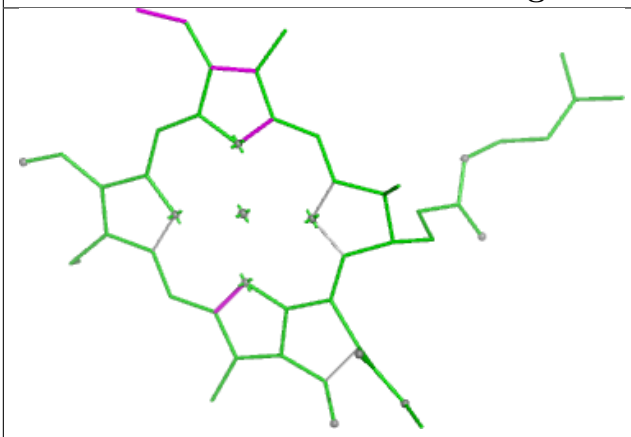


Torsions

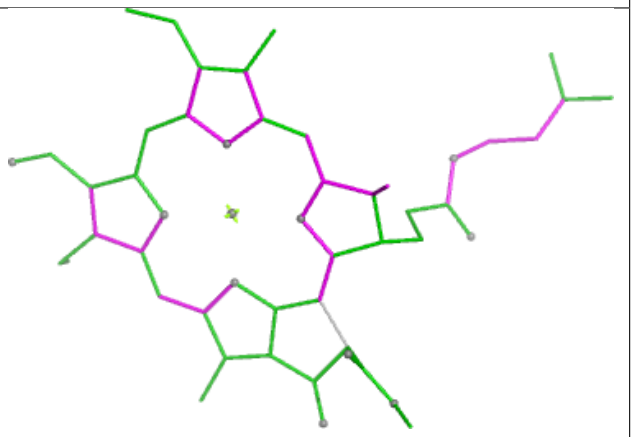


Rings

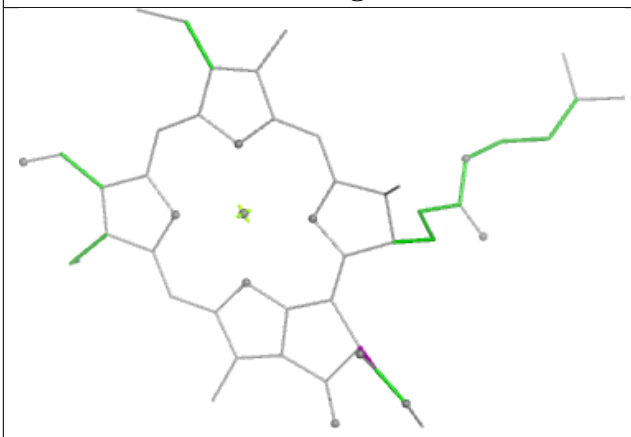
Ligand CHL 4 611



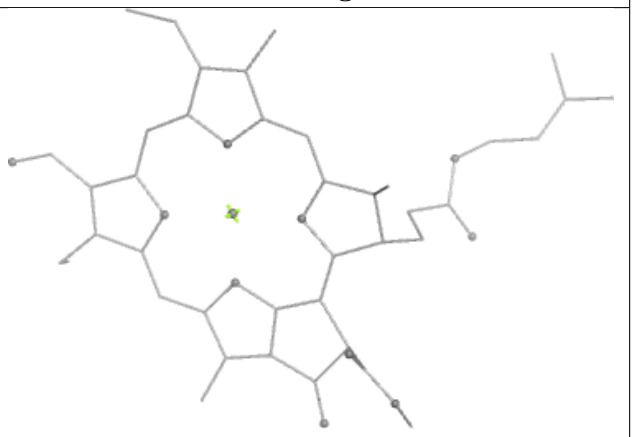
Bond lengths



Bond angles



Torsions

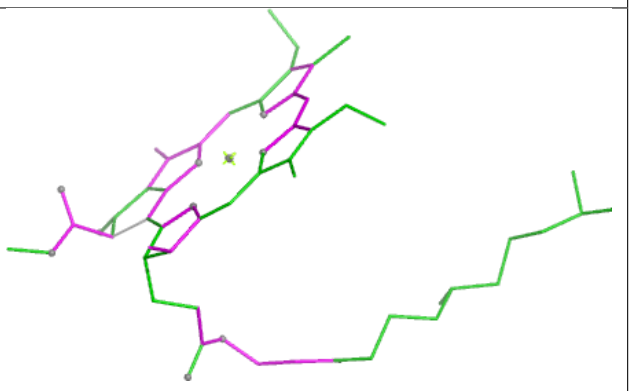


Rings

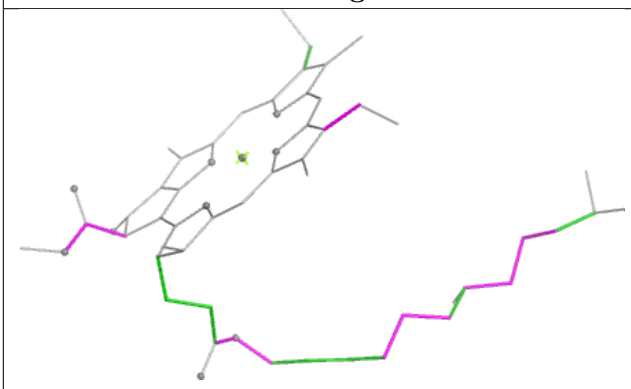
Ligand CLA B 1228



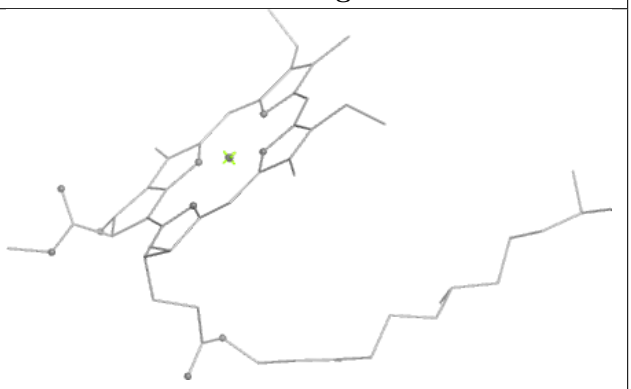
Bond lengths



Bond angles

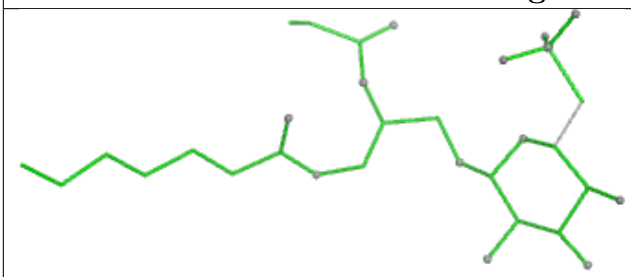


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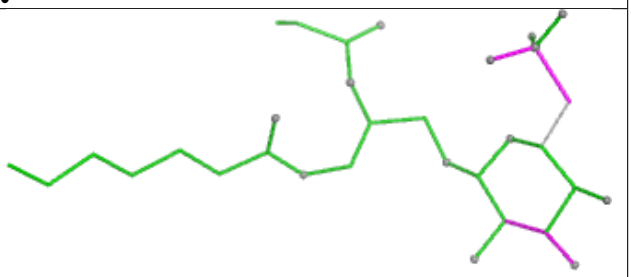


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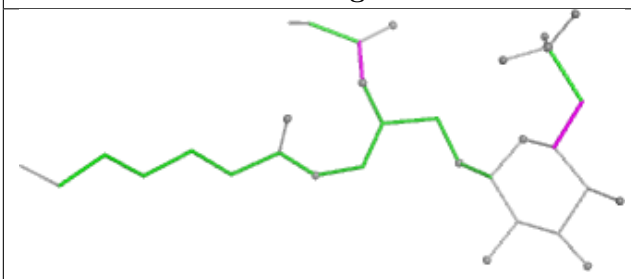
Ligand SQD 6 803



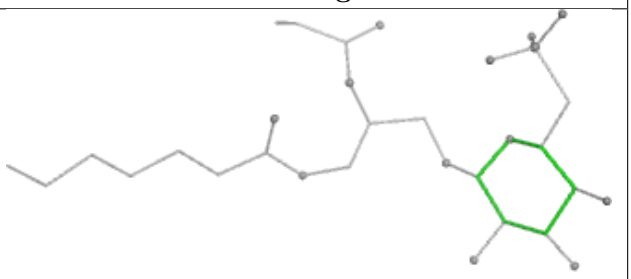
Bond lengths



Bond angles

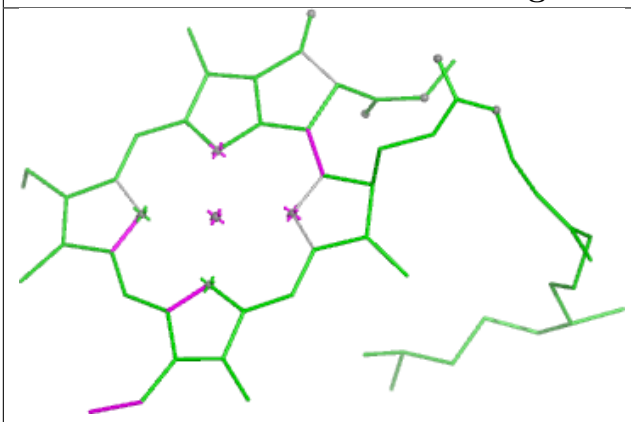


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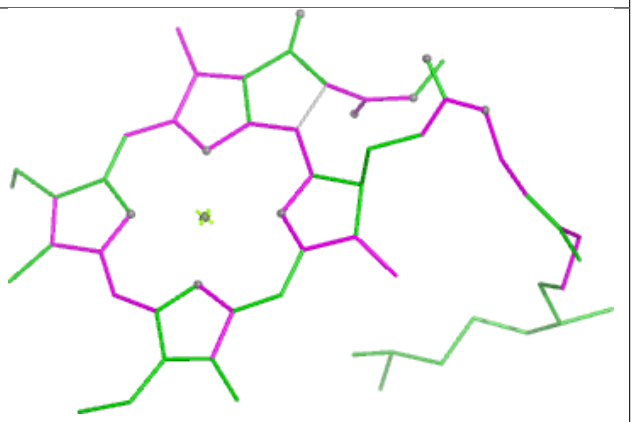


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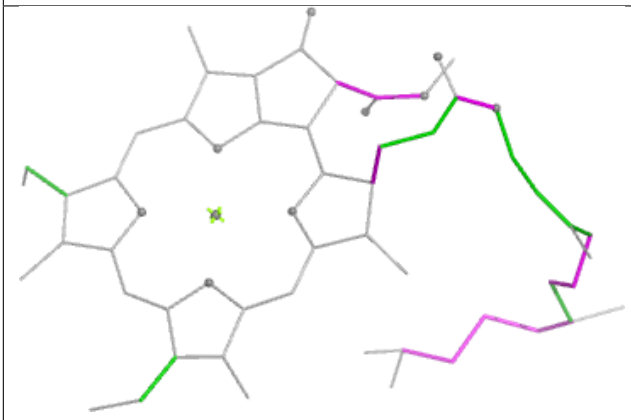
Ligand CLA 5 607



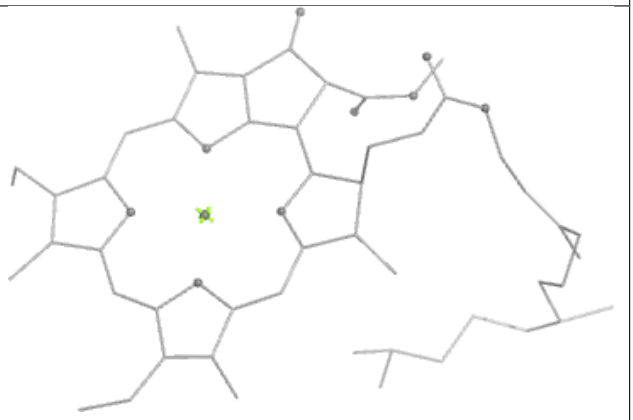
Bond lengths



Bond angles

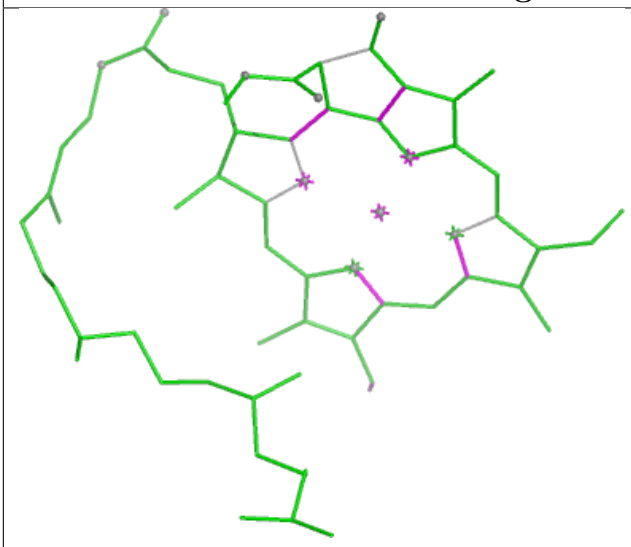


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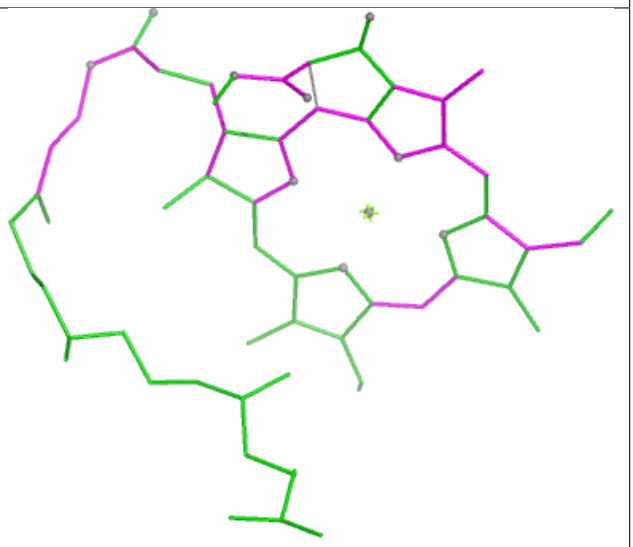


Rings

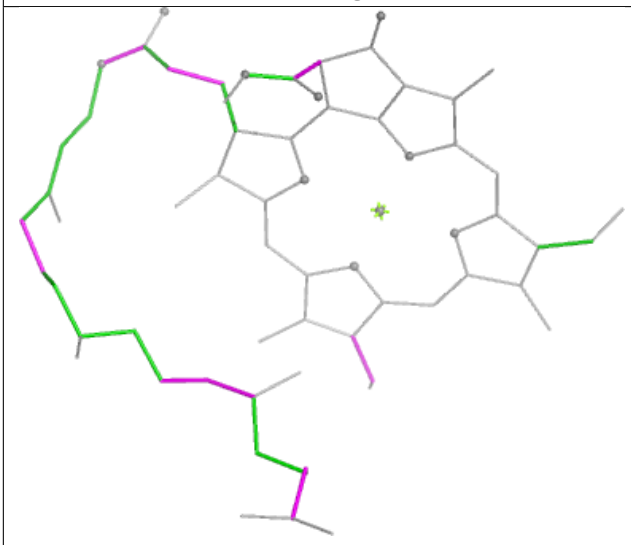
Ligand CLA A 1111



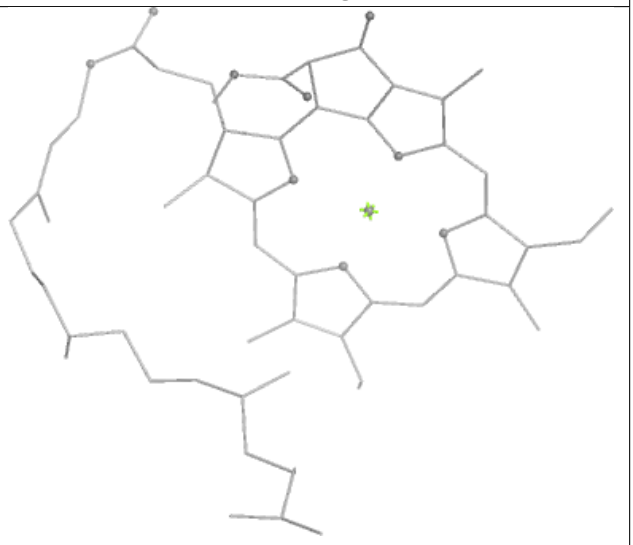
Bond lengths



Bond angles

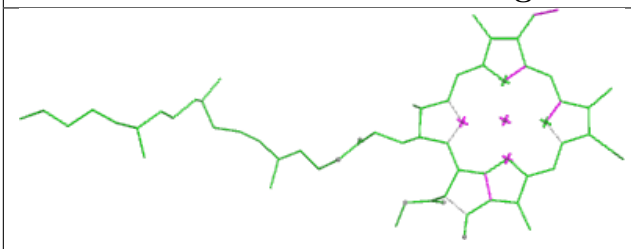


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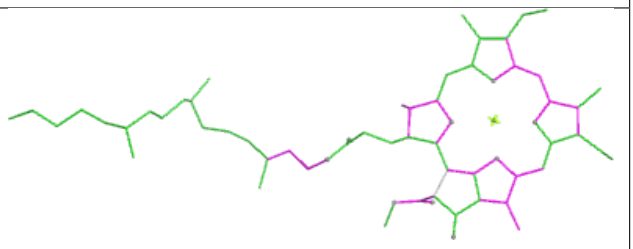


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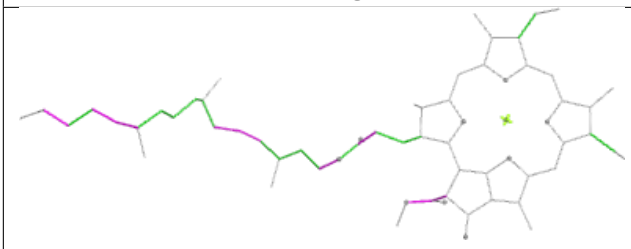
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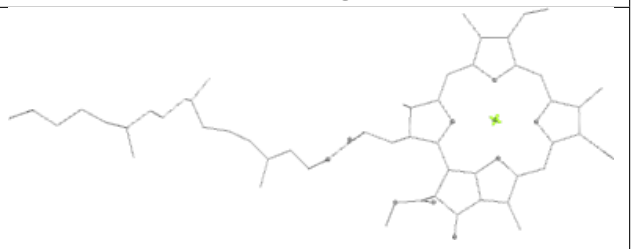
Bond lengths



Bond angles

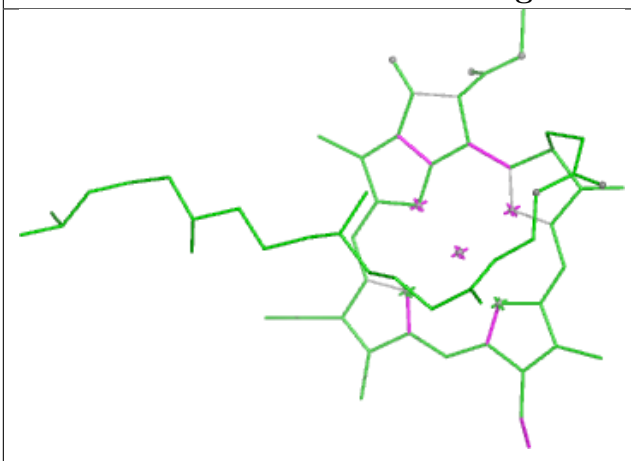


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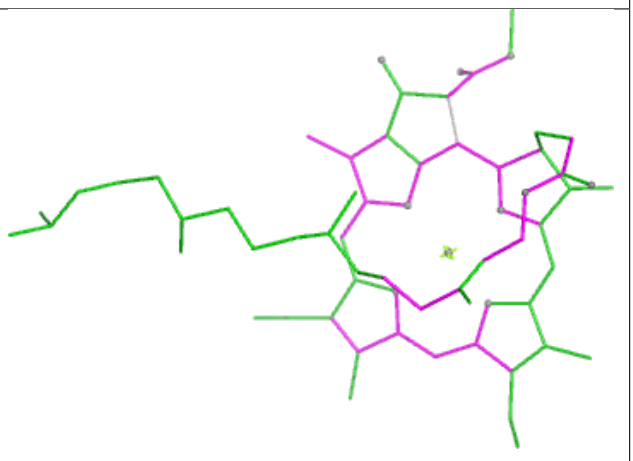


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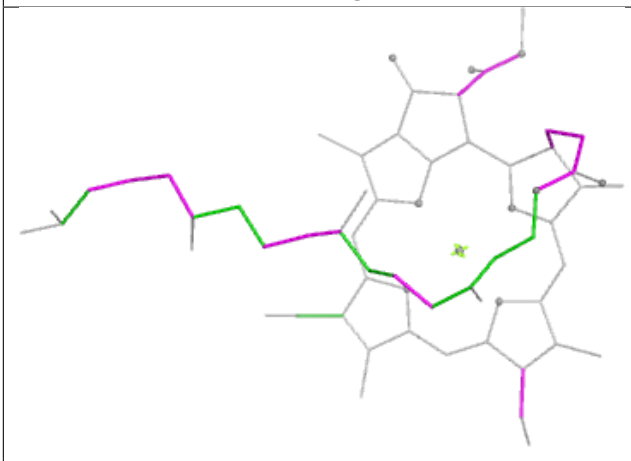
Ligand CLA B 1224



Bond lengths



Bond angles

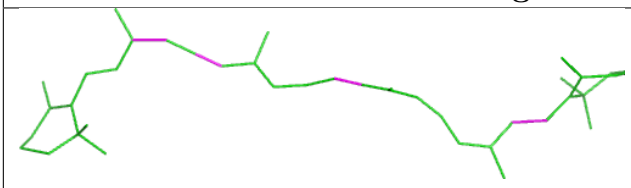


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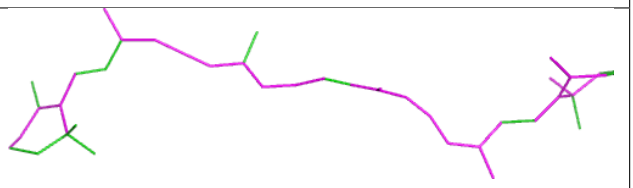


Rings

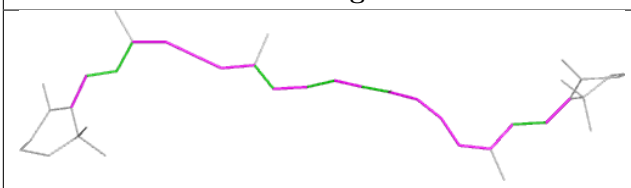
Ligand BCR H 4001



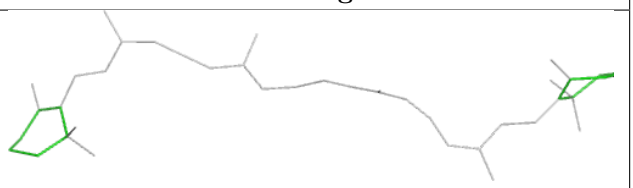
Bond lengths



Bond angles

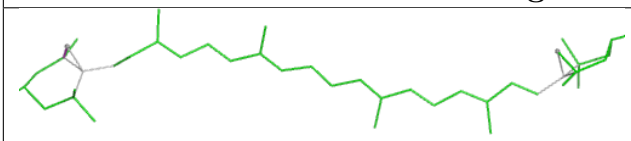


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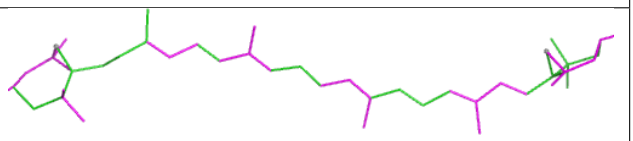


Rings

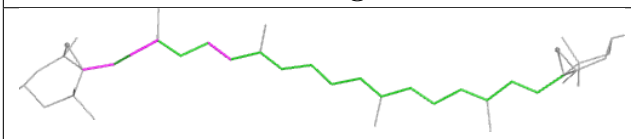
Ligand XAT 3 502



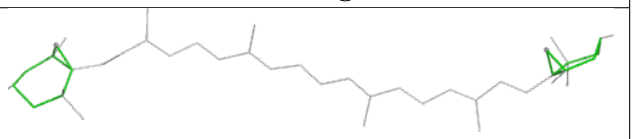
Bond lengths



Bond angles



Torsions



Rings

Ligand CLA B 1237



Bond lengths



Bond angles

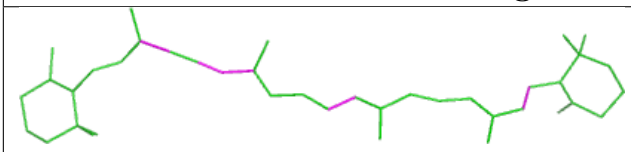


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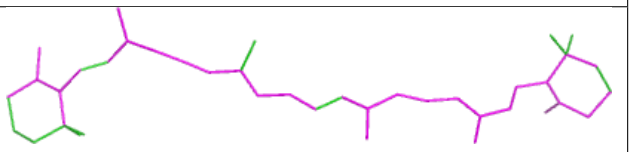


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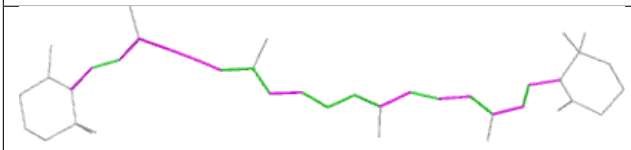
Ligand BCR B 4003



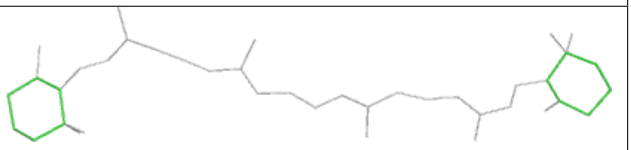
Bond lengths



Bond angles

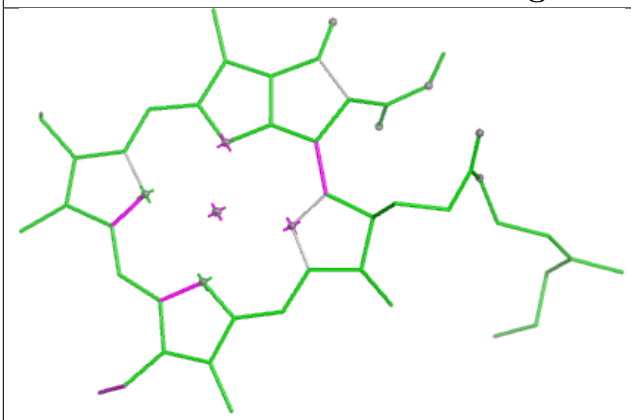


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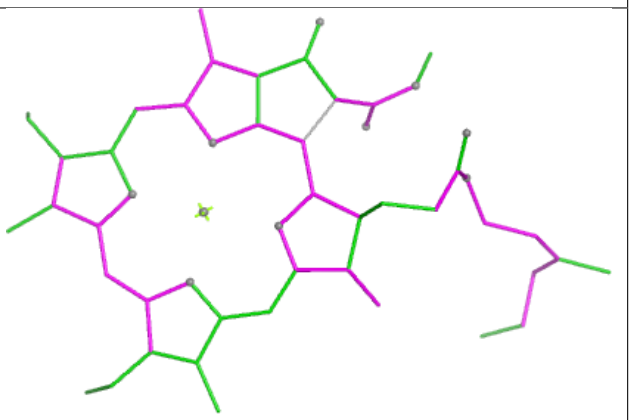


Rings

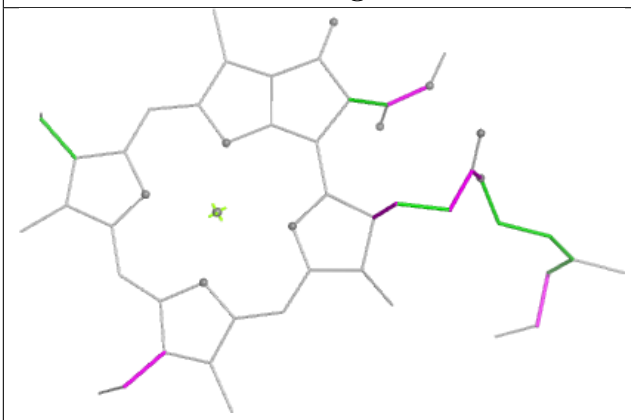
Ligand CLA 3 602



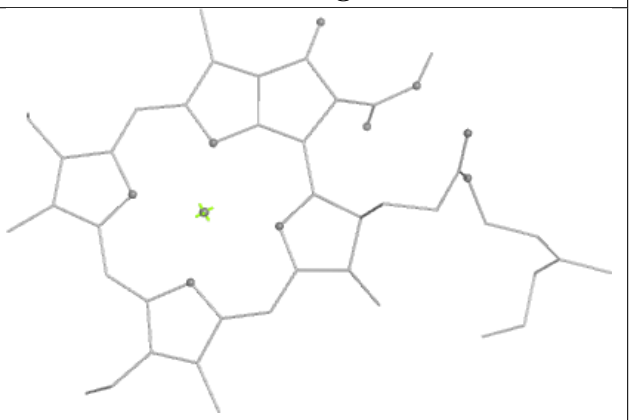
Bond lengths



Bond angles

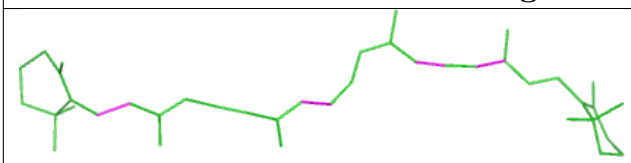


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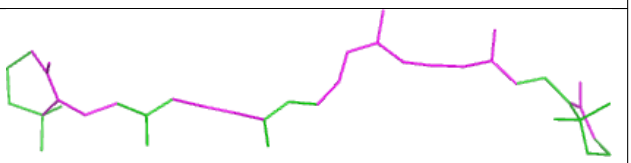


Rings

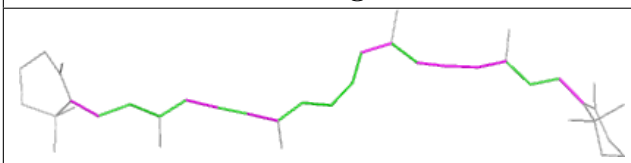
Ligand BCR I 4001



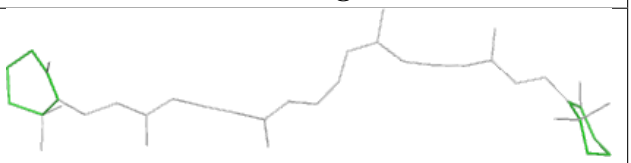
Bond lengths



Bond angles

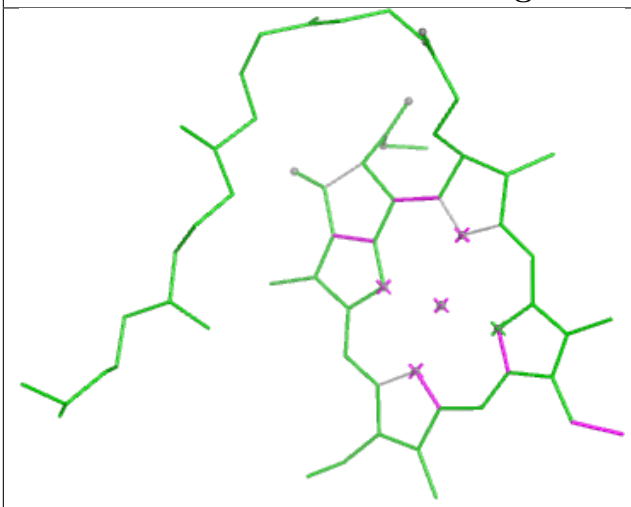


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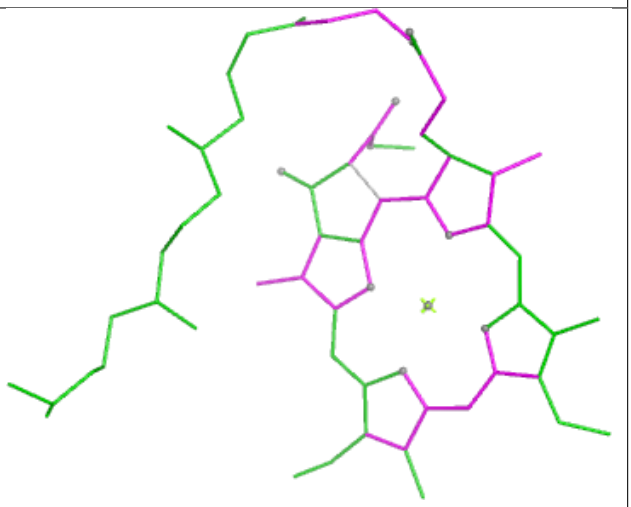


Rings

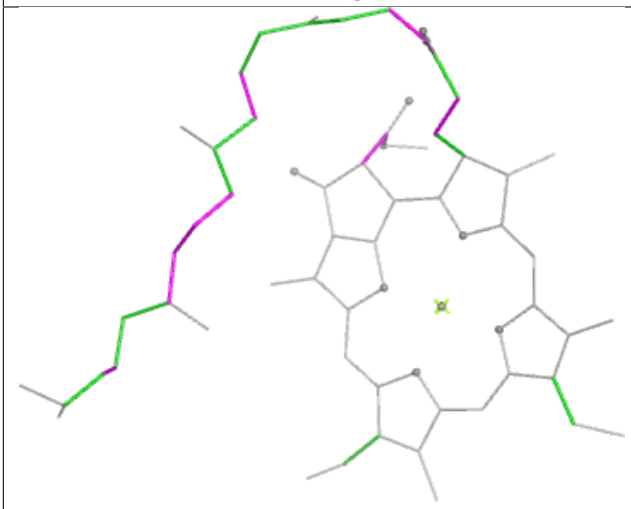
Ligand CLA A 1123



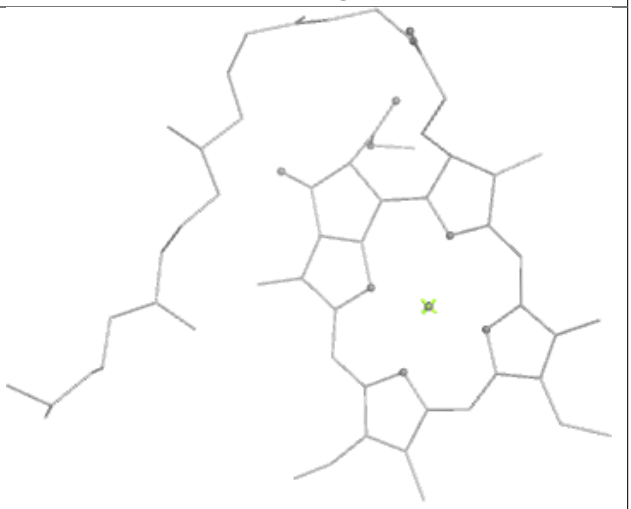
Bond lengths



Bond angles

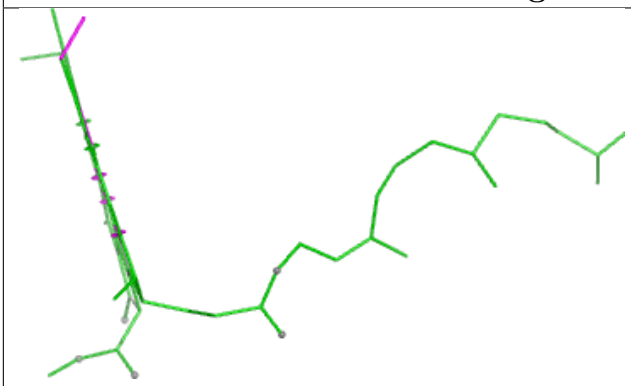


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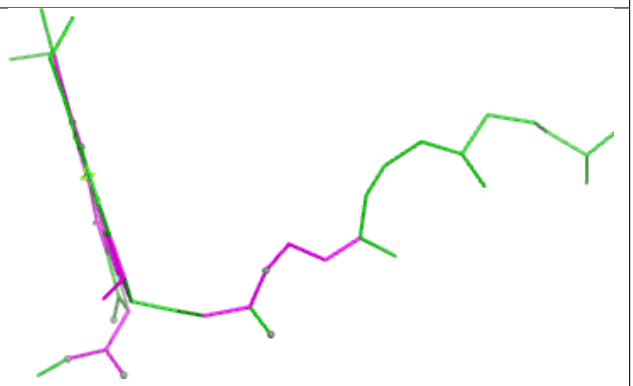


Rings

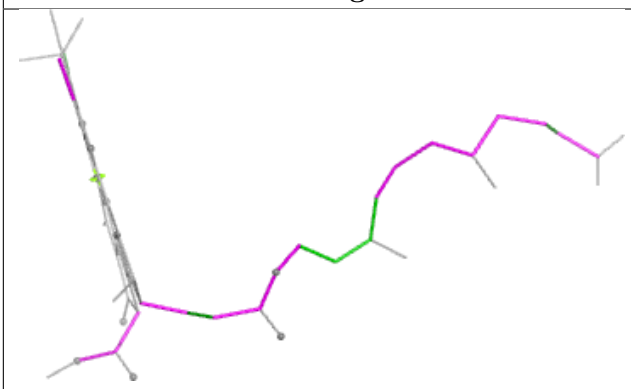
Ligand CLA 4 609



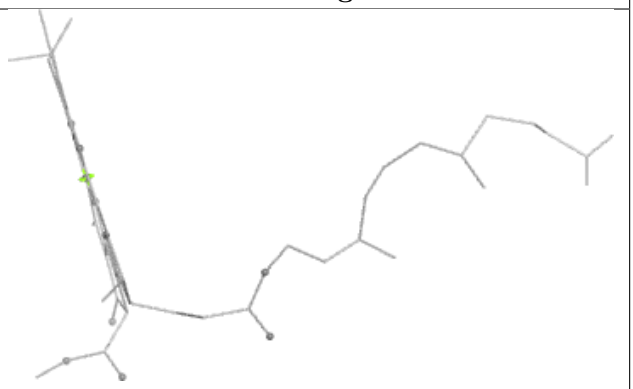
Bond lengths



Bond angles

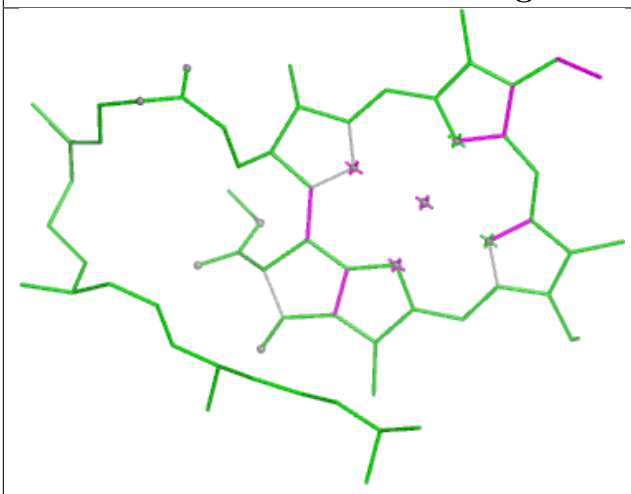


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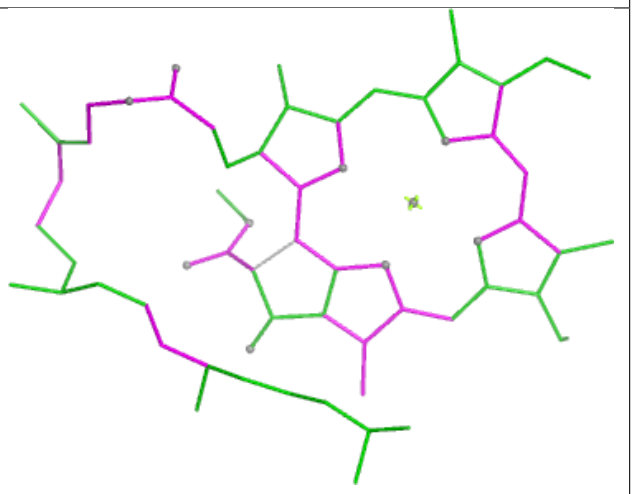


Rings

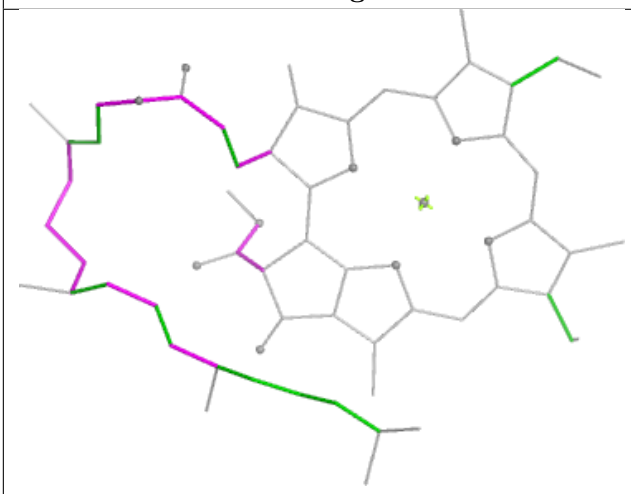
Ligand CLA B 1202



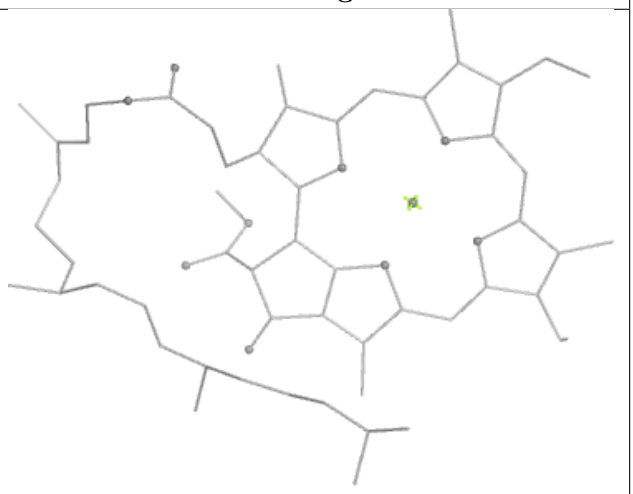
Bond lengths



Bond angles

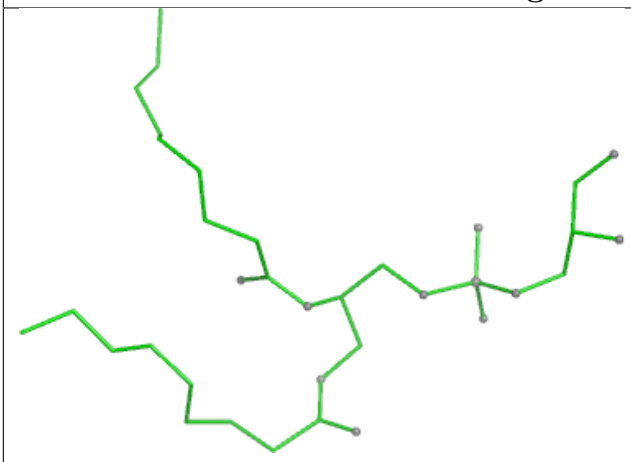


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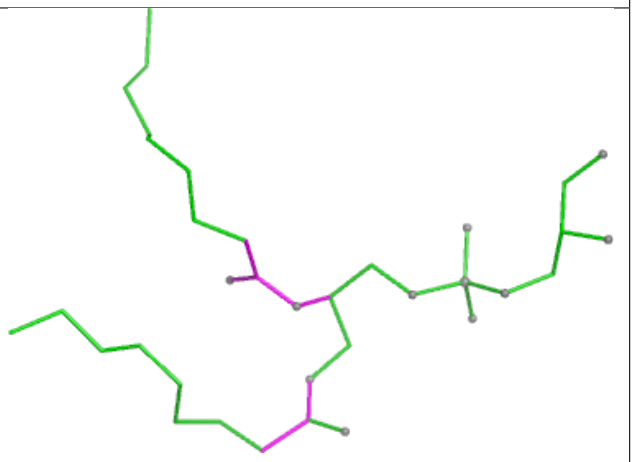


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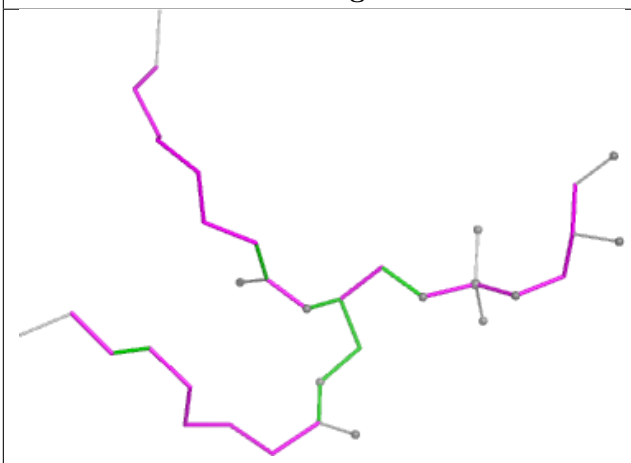
Ligand LHG 2 801



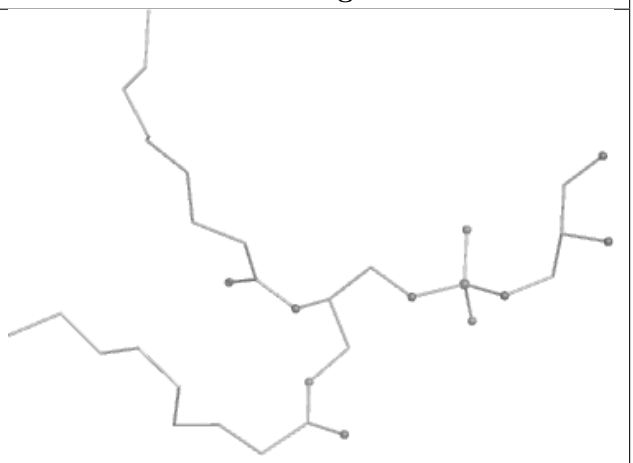
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Bond angles

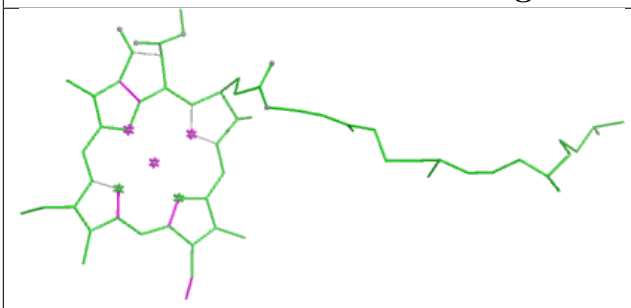


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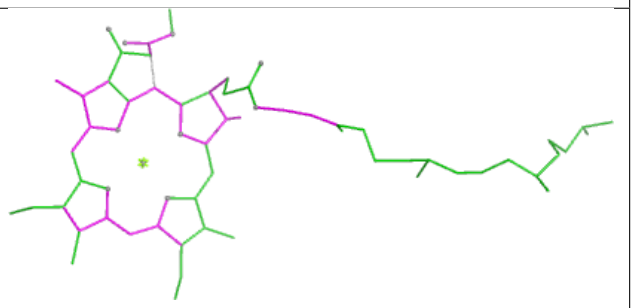


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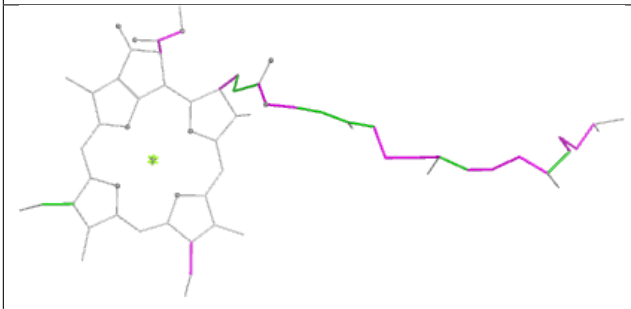
Ligand CLA A 1113



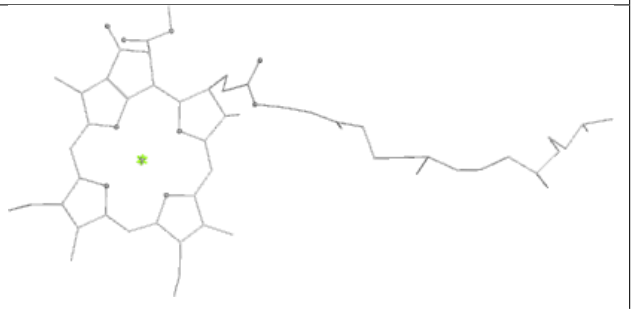
Bond lengths



Bond angles

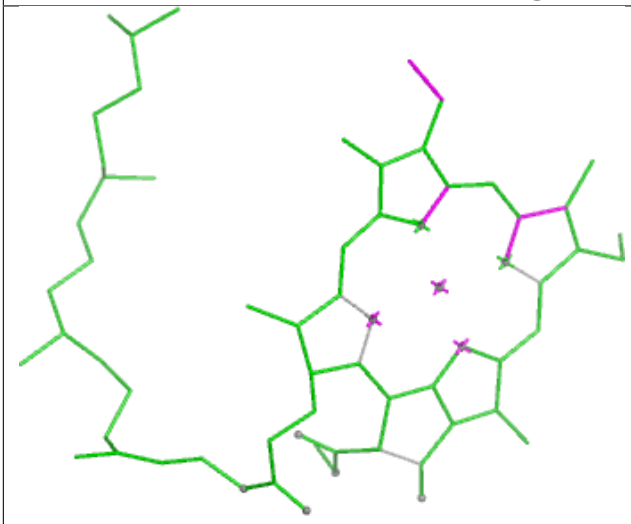


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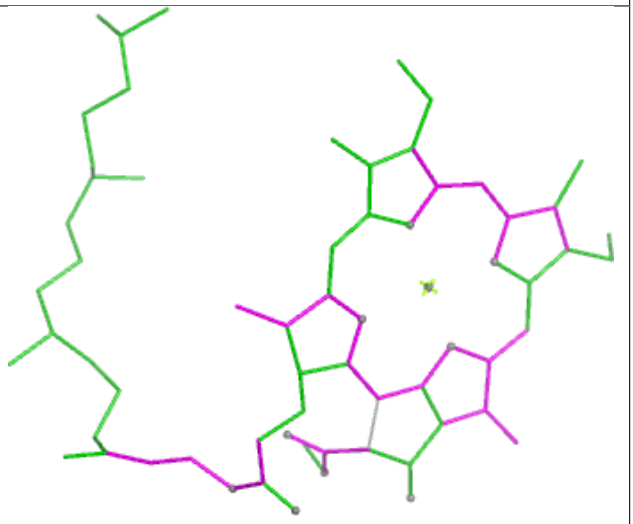


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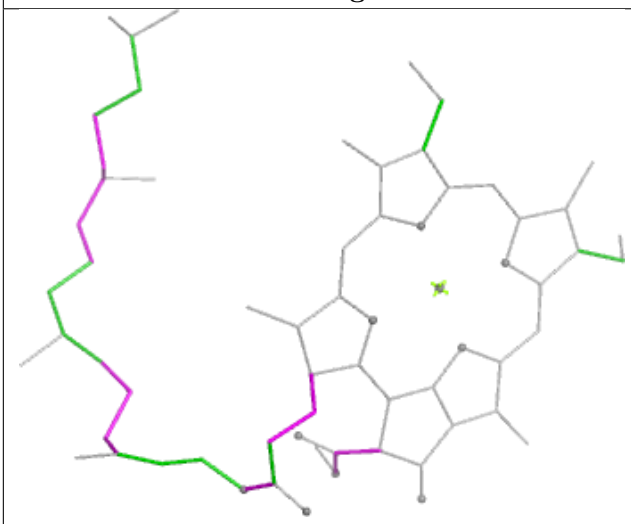
Ligand CLA 5 605



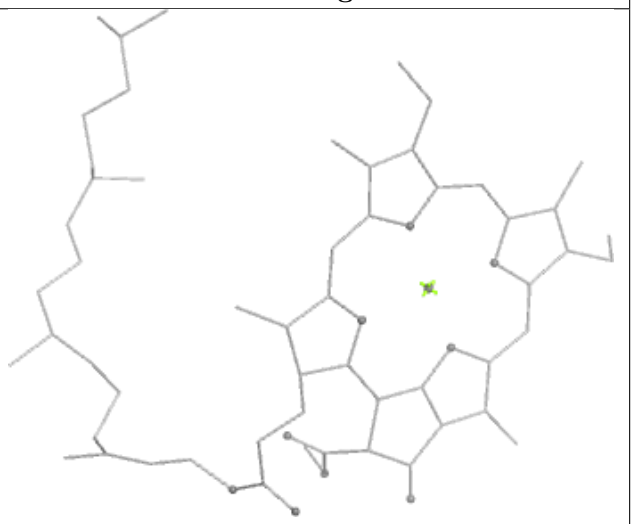
Bond lengths



Bond angles

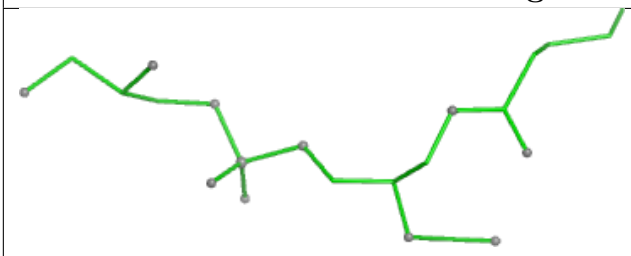


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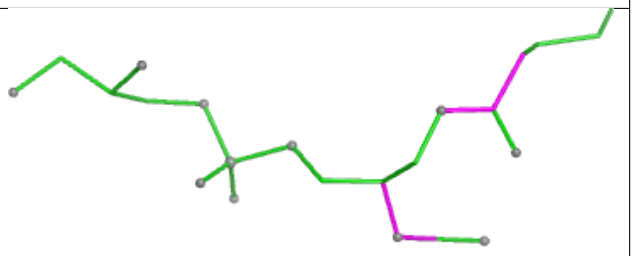


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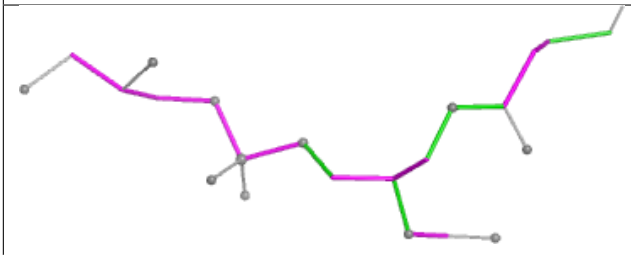
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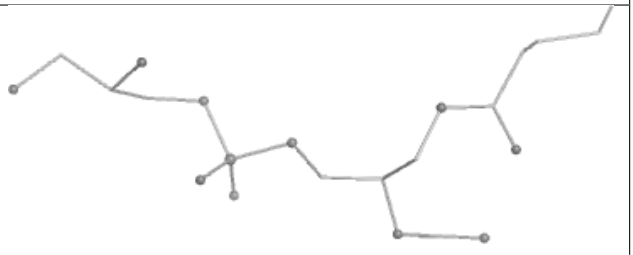
Bond lengths



Bond angles

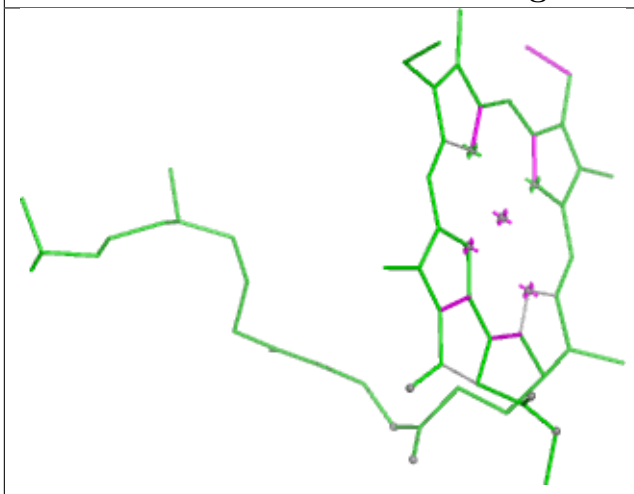


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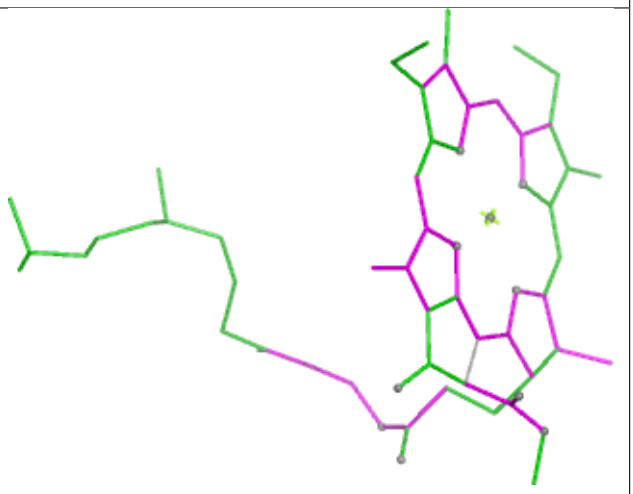


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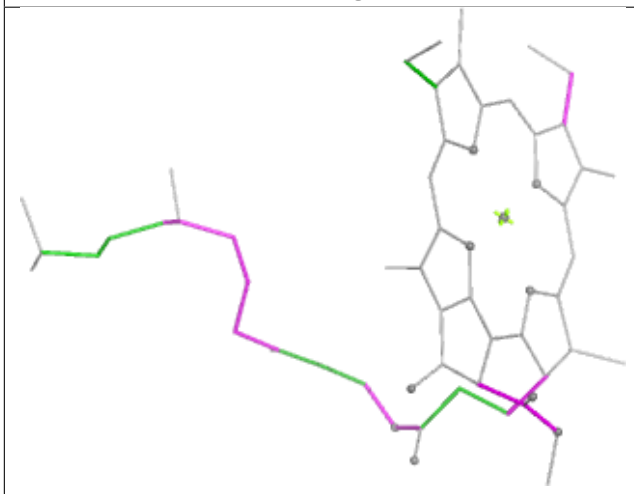
Ligand CLA 4 607



Bond lengths



Bond angles

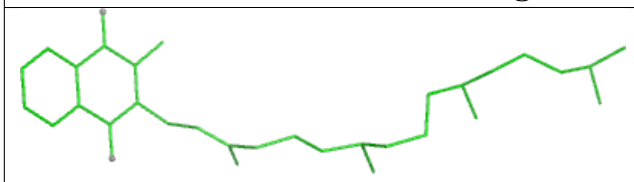


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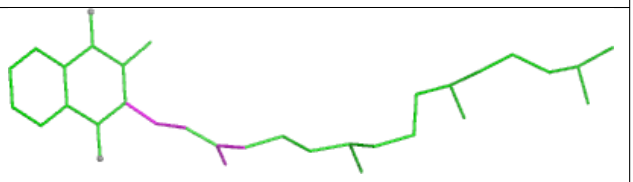


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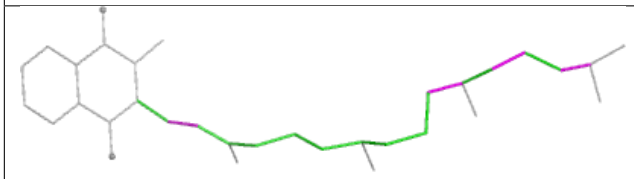
Ligand PQN A 2001



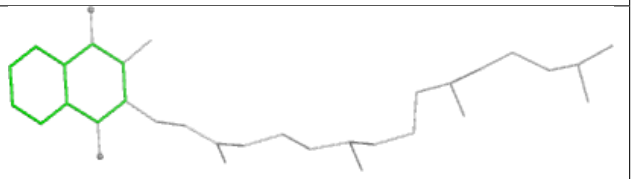
Bond lengths



Bond angles

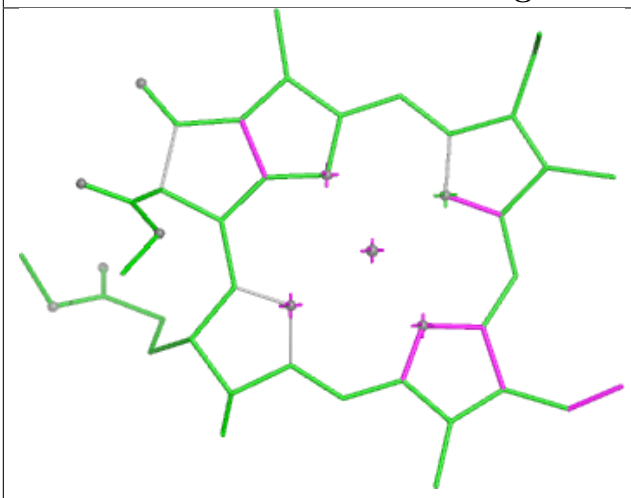


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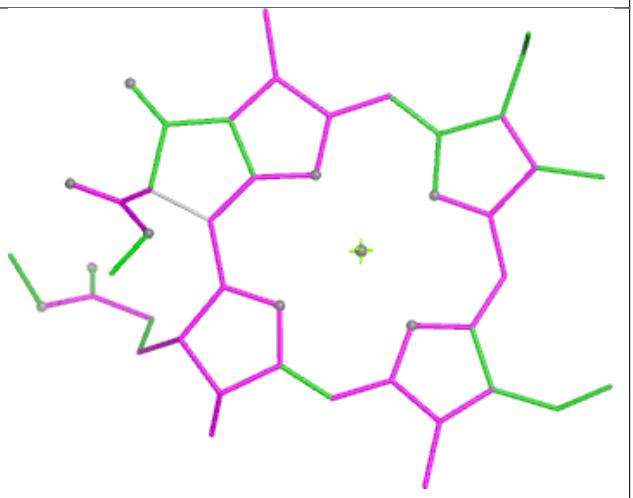


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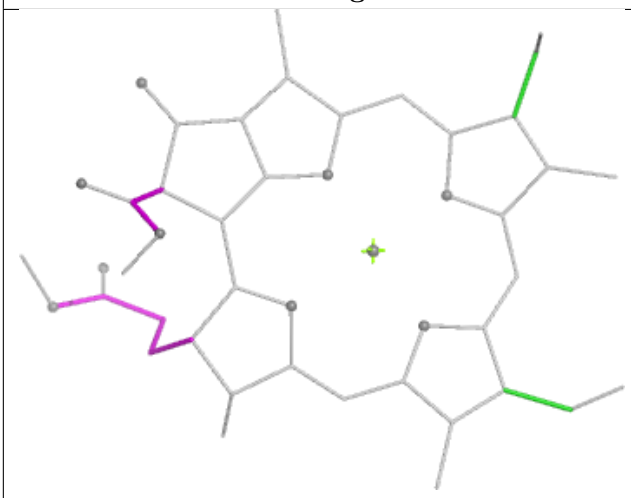
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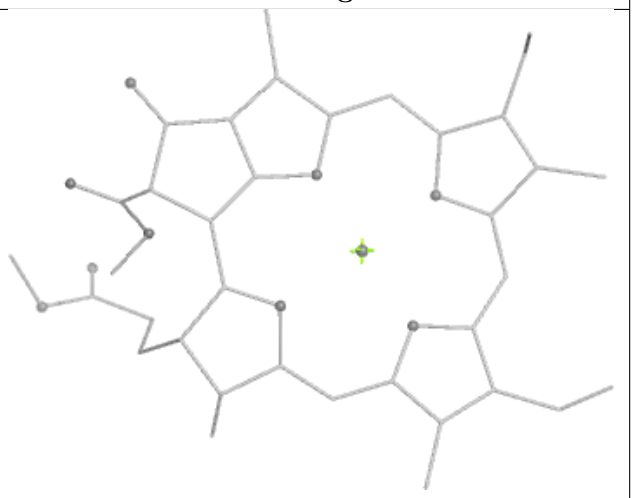
Bond lengths



Bond angles

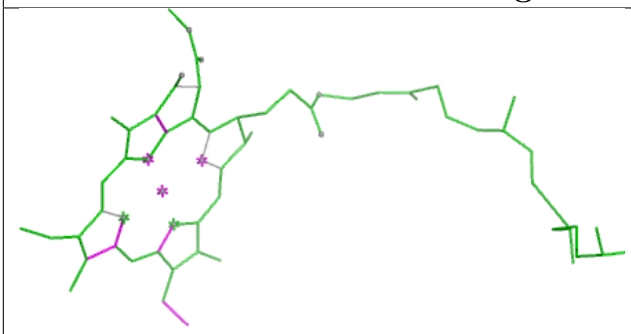


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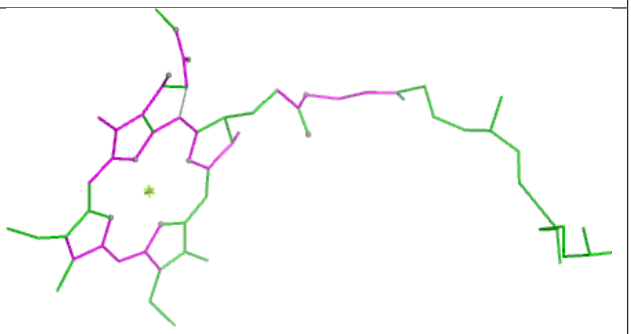


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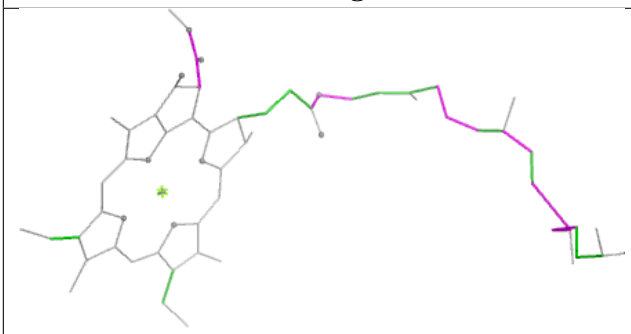
Ligand CLA A 1012



Bond lengths



Bond angles

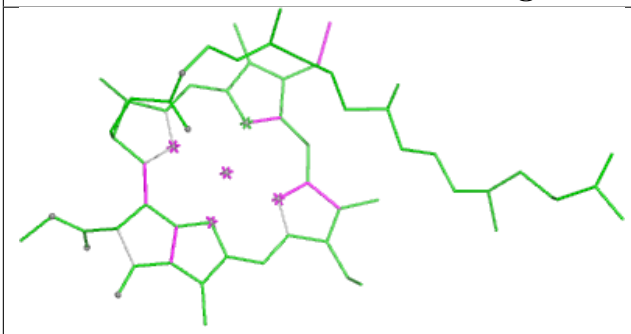


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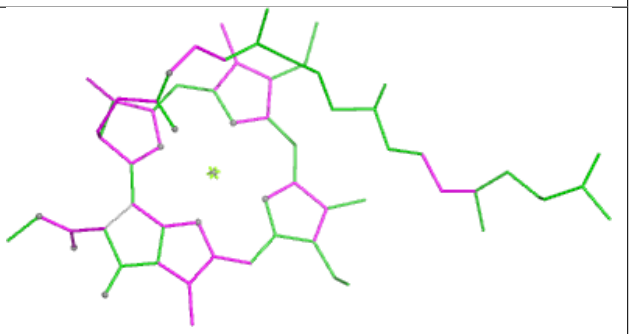


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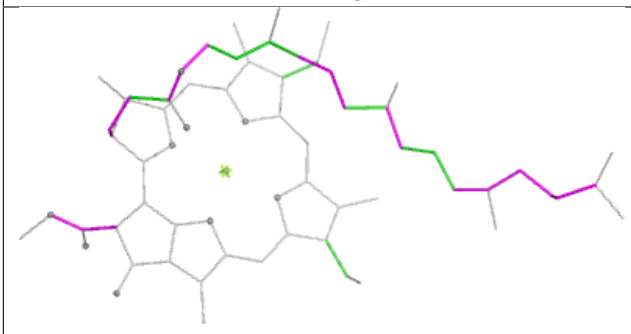
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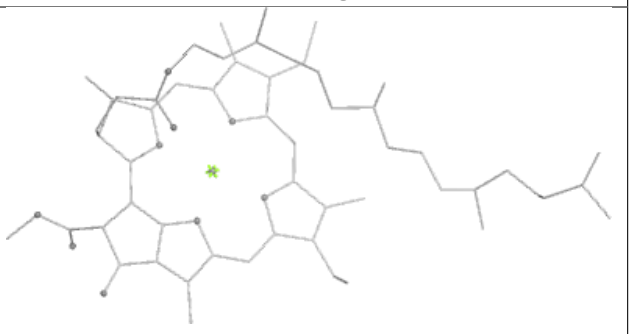
Bond lengths



Bond angles

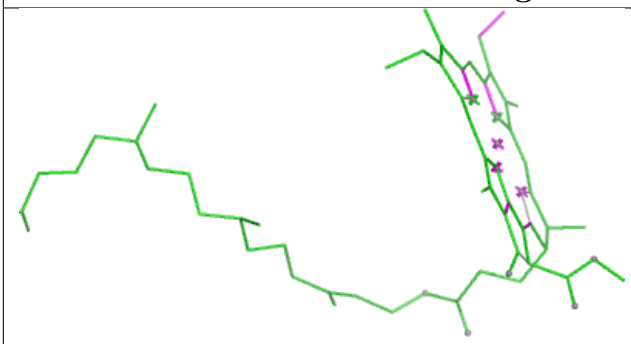


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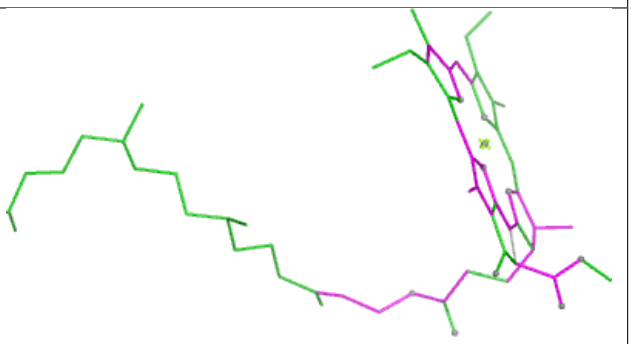


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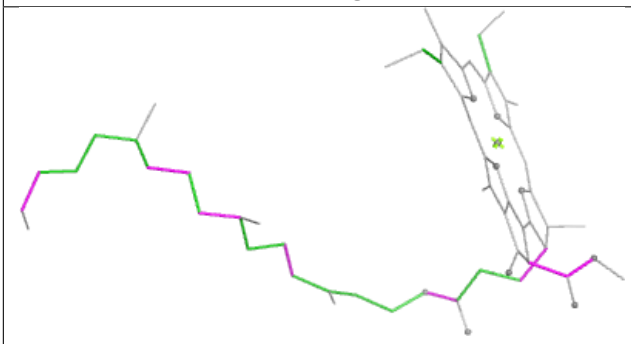
Ligand CLA A 1128



Bond lengths



Bond angles

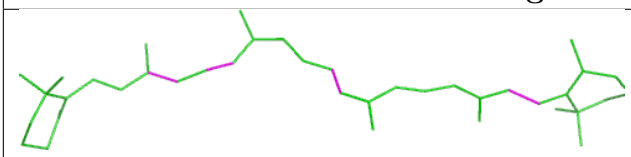


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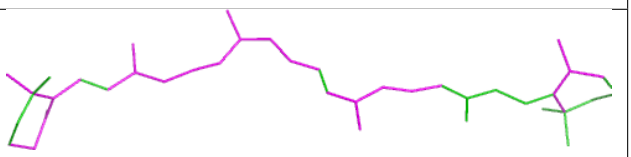


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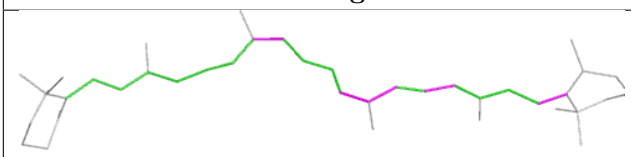
Ligand BCR 3 506



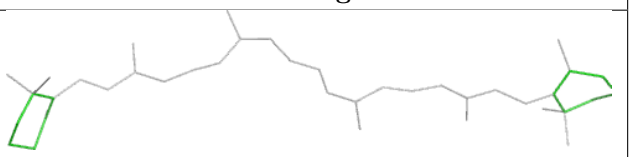
Bond lengths



Bond angles

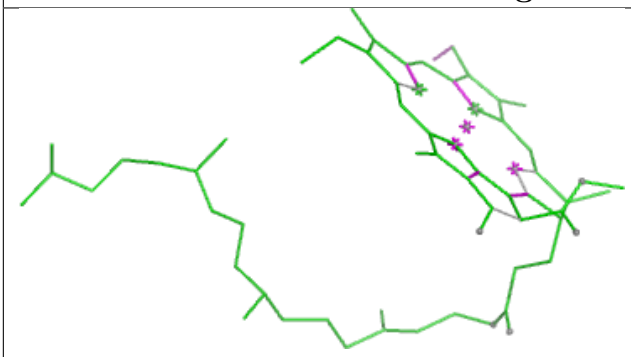


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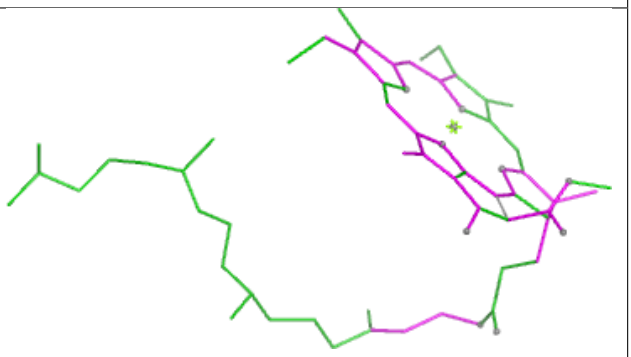


Rings

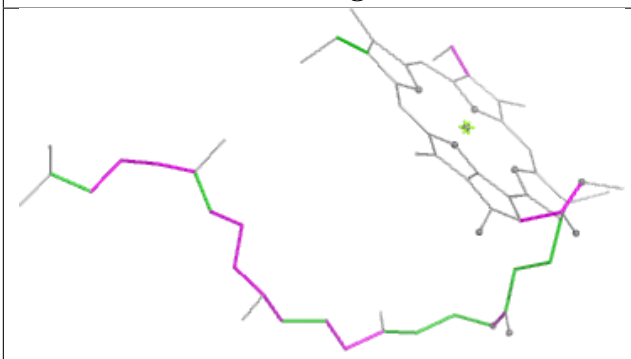
Ligand CLA B 1227



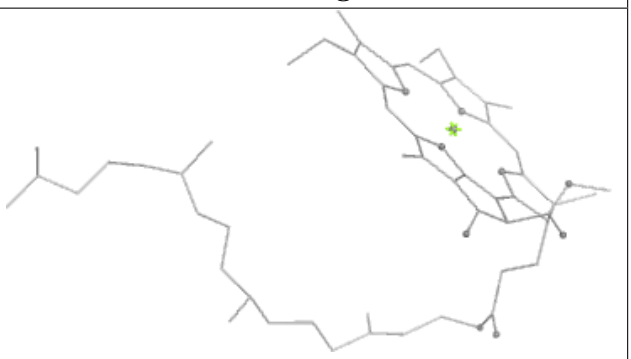
Bond lengths



Bond angles

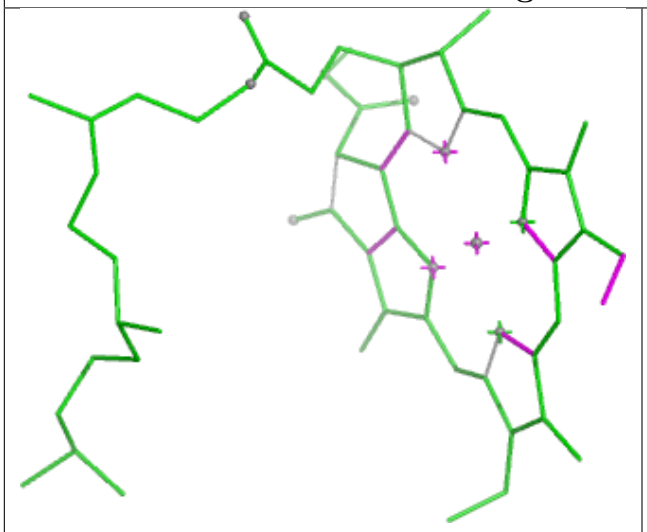


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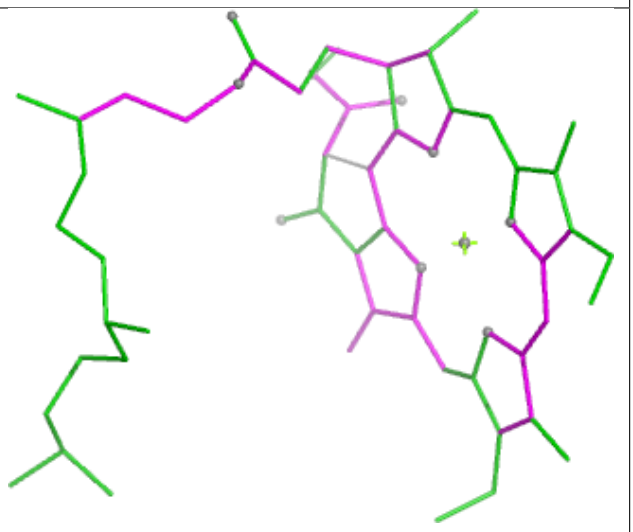


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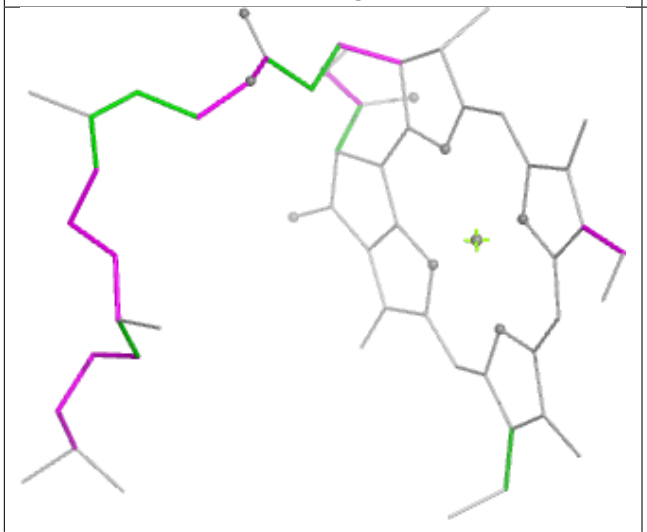
Ligand CLA B 1231



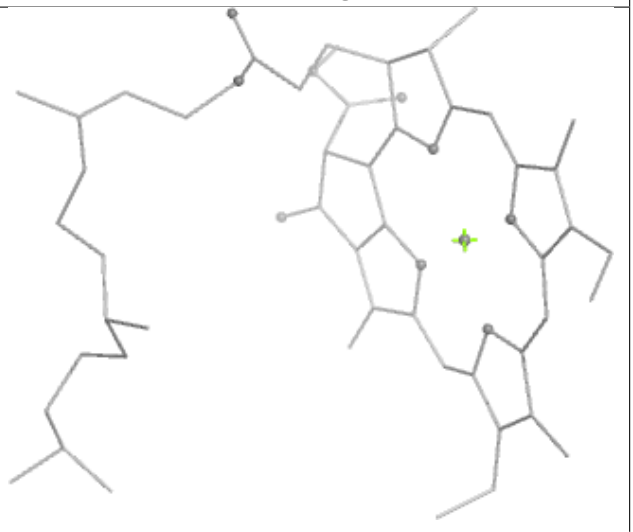
Bond lengths



Bond angles

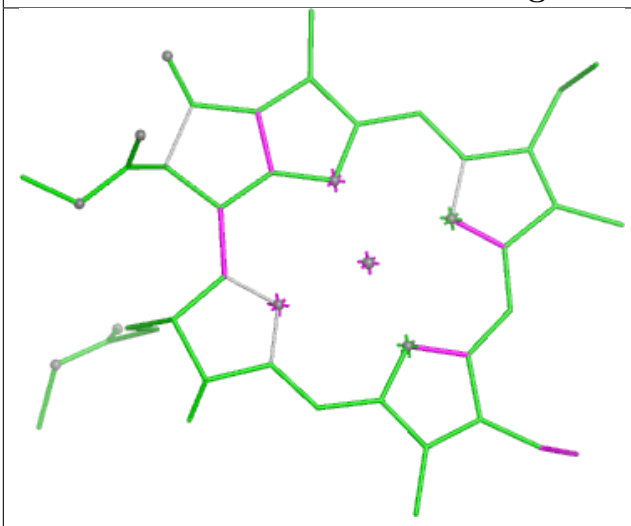


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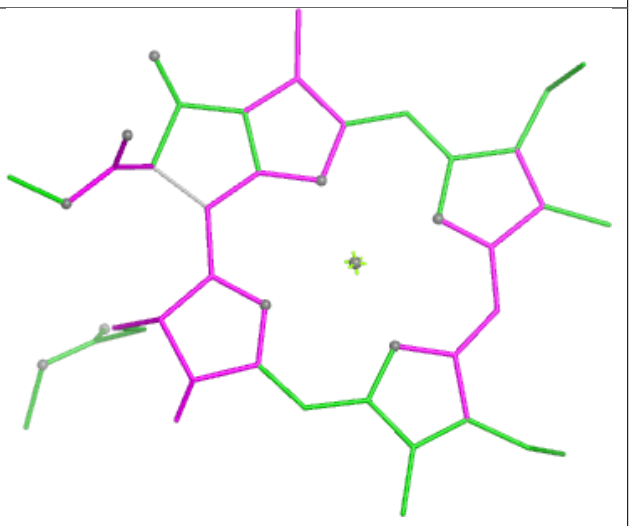


Rings

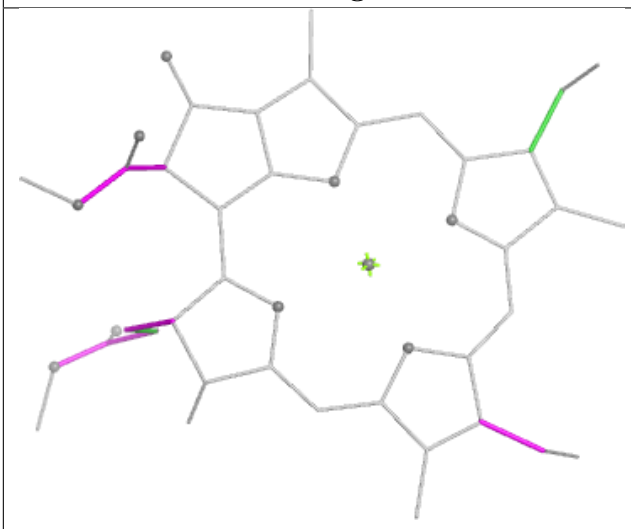
Ligand CLA 1 607



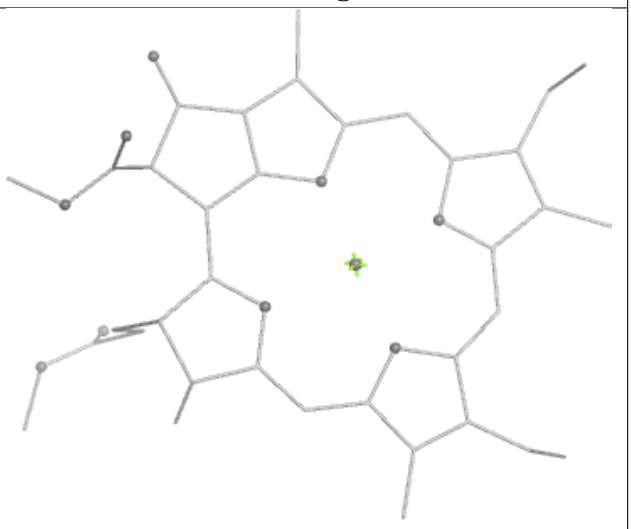
Bond lengths



Bond angles

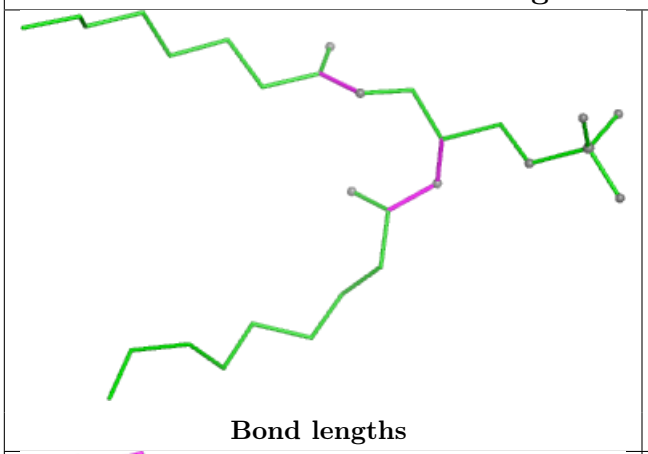


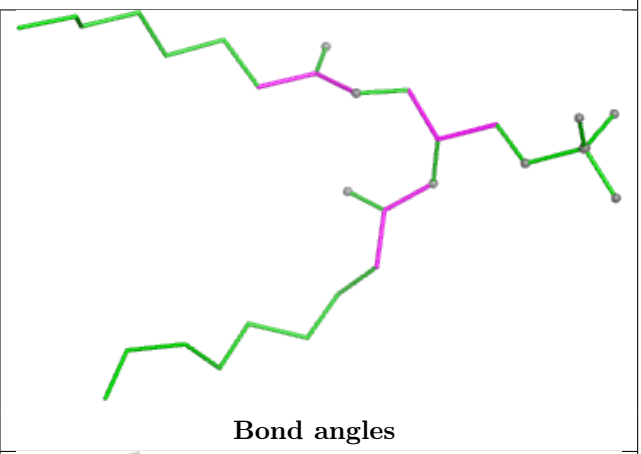
Torsions

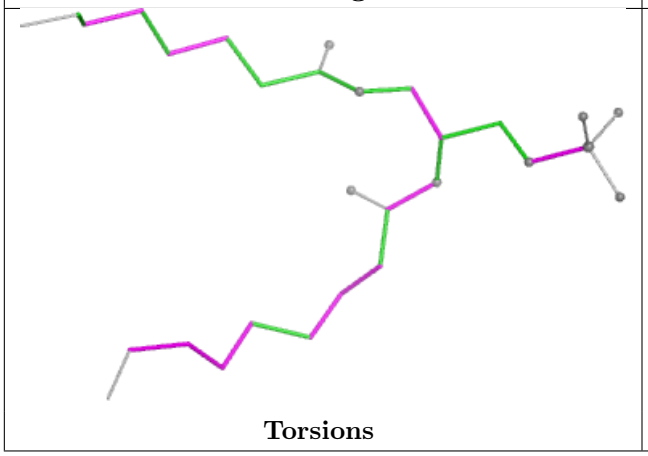


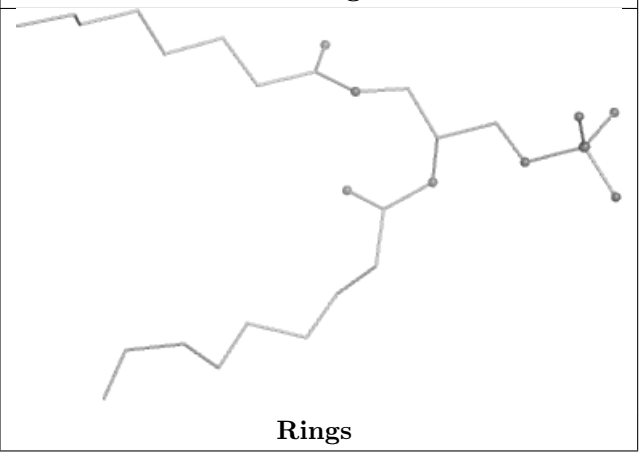
Rings

Ligand 3PH 5 807

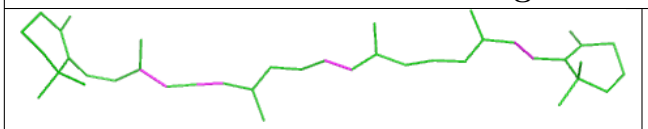

Bond lengths

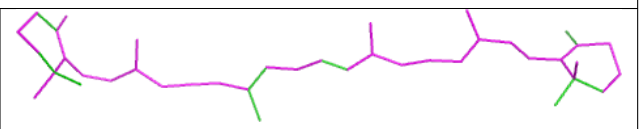

Bond angles

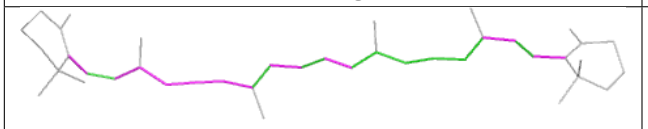

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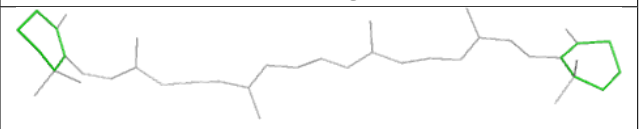

Rings

Ligand BCR A 4002

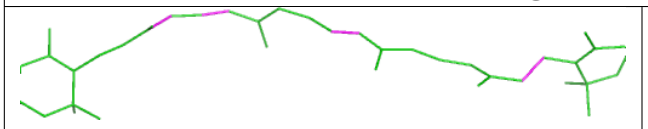

Bond lengths

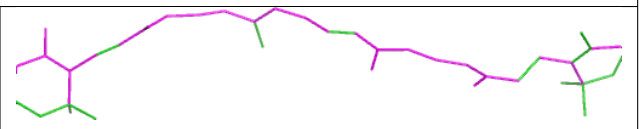

Bond angles

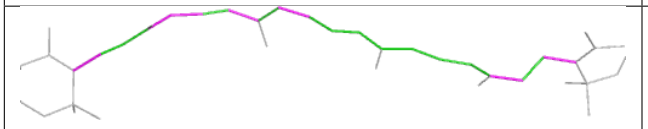

Torsions


Rings

Ligand BCR 1 504

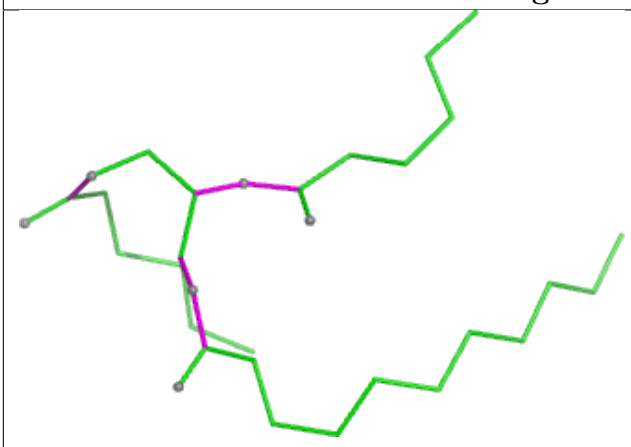

Bond lengths


Bond angles

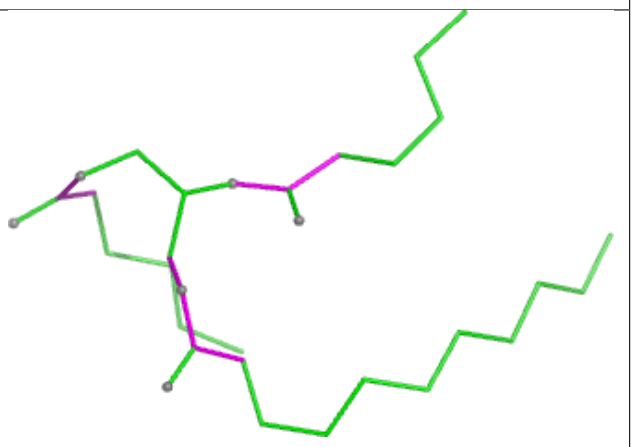

Torsions


Rings

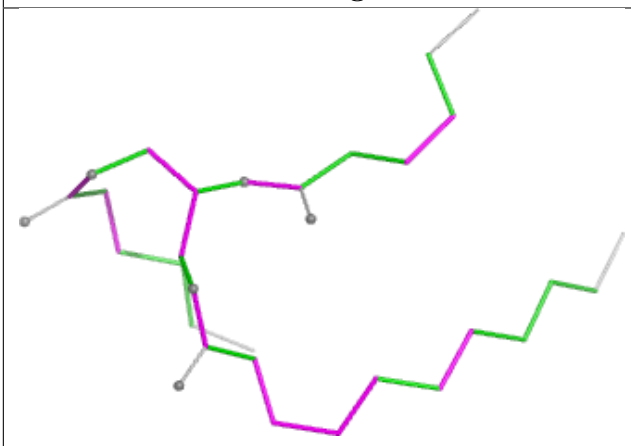
Ligand 4RF 5 805



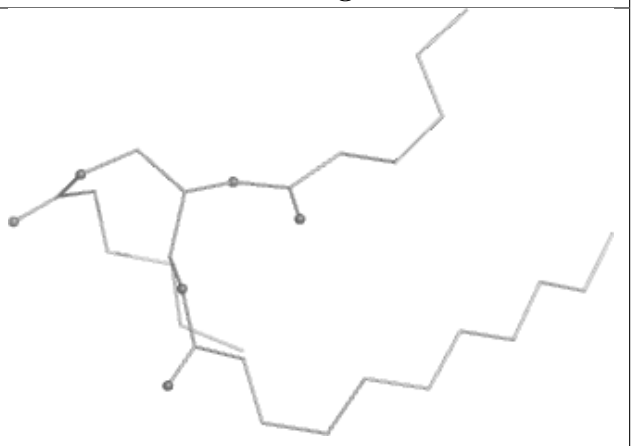
Bond lengths



Bond angles

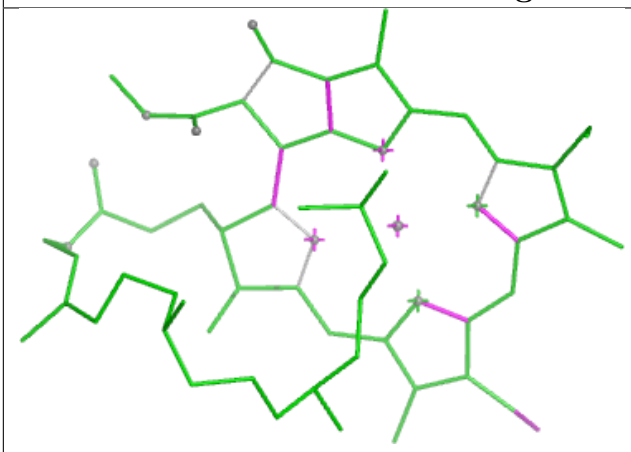


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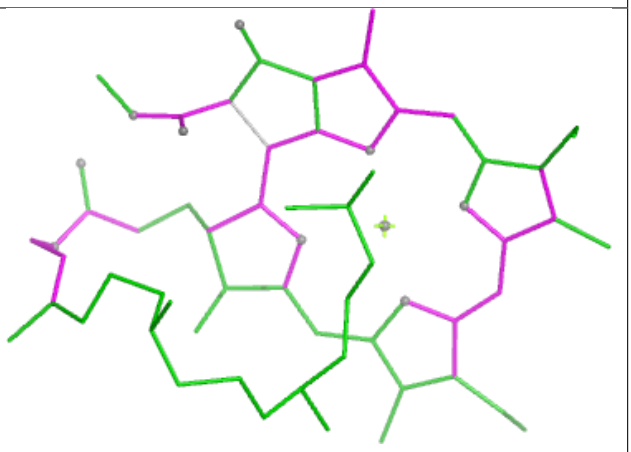


Rings

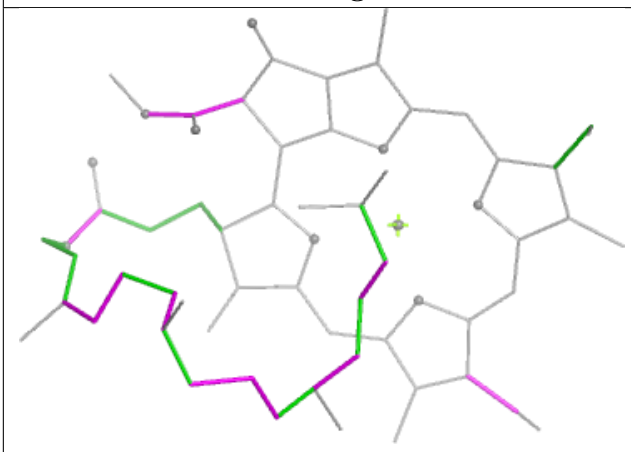
Ligand CLA B 1203



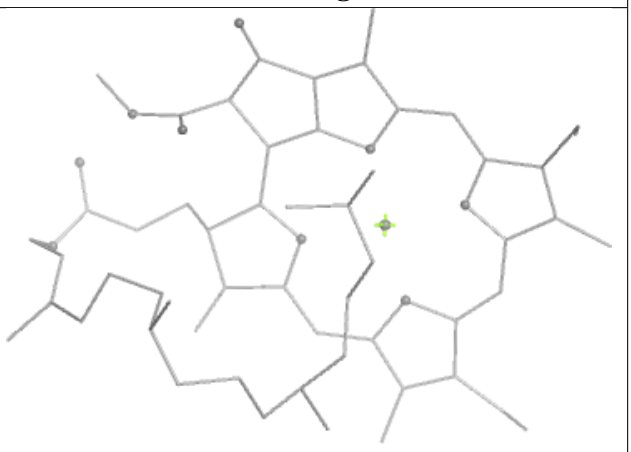
Bond lengths



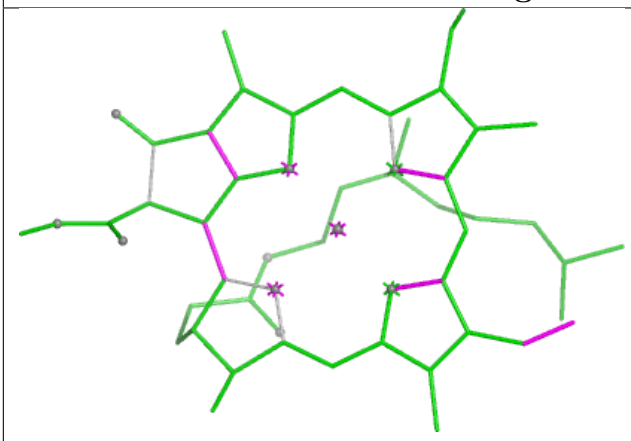
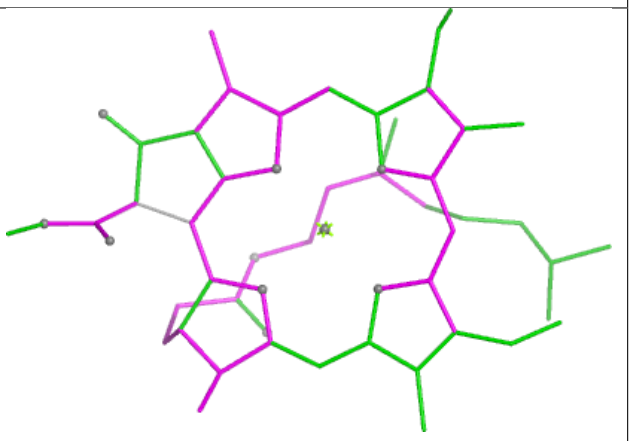
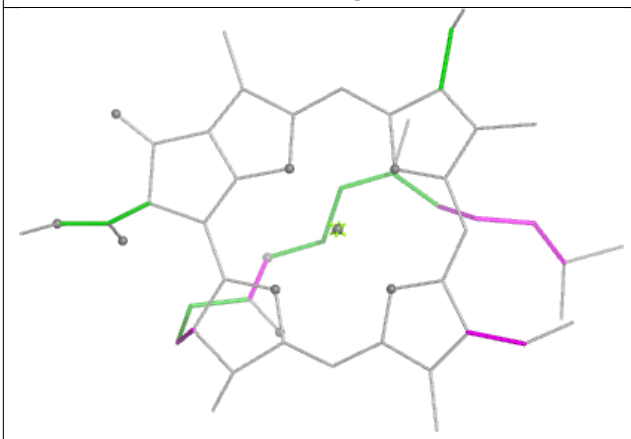
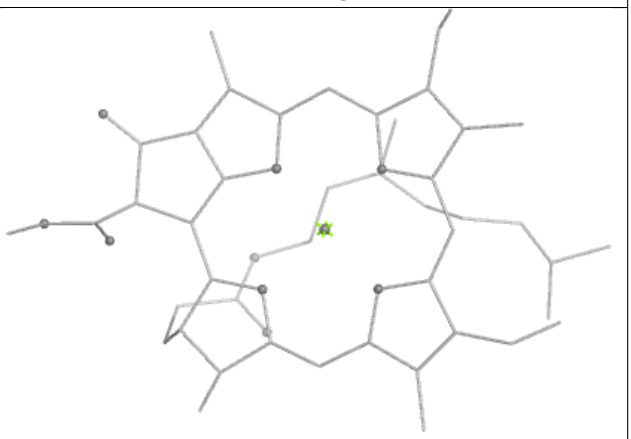
Bond angles



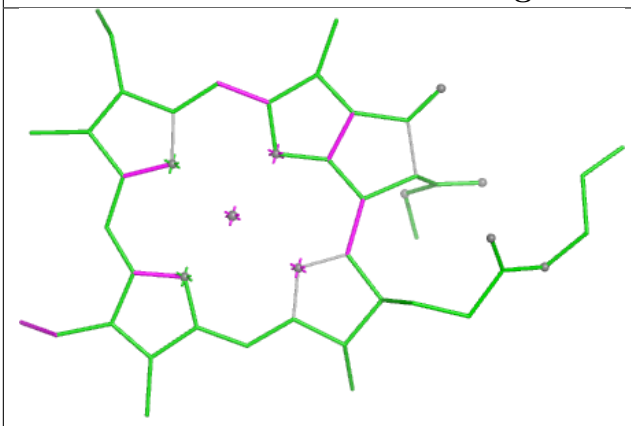
Torsions



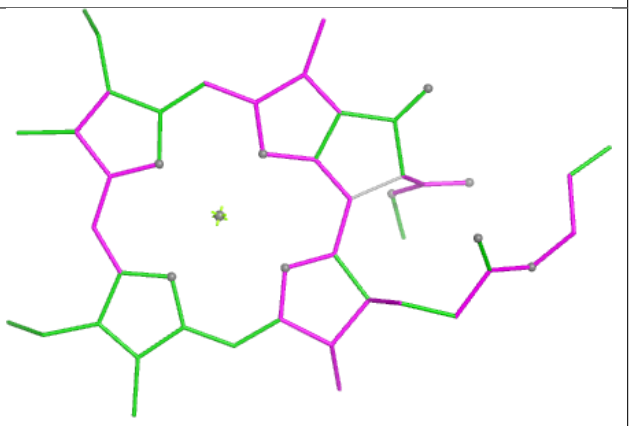
Rings

Ligand CLA A 1110	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

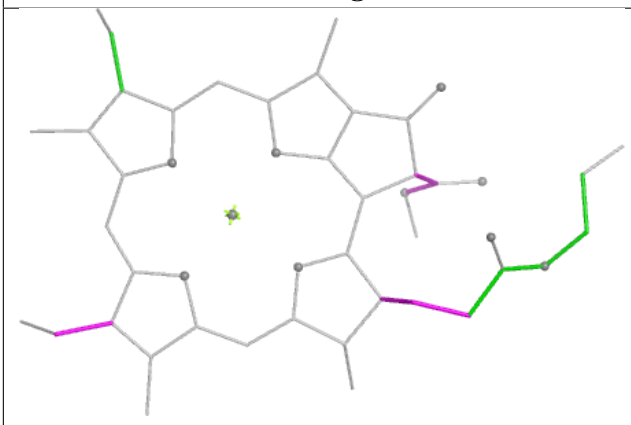
Ligand CLA K 1403



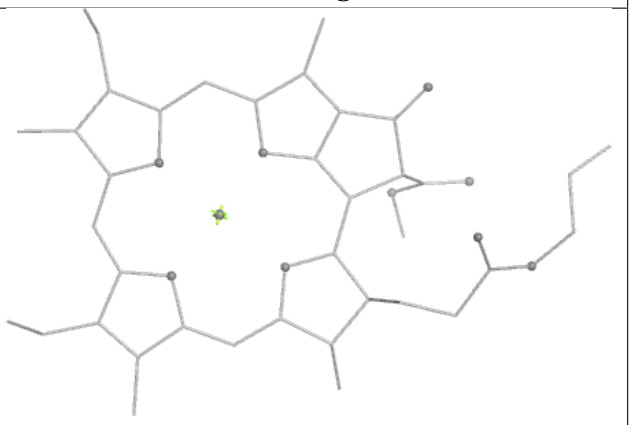
Bond lengths



Bond angles

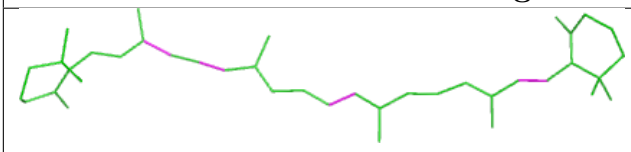


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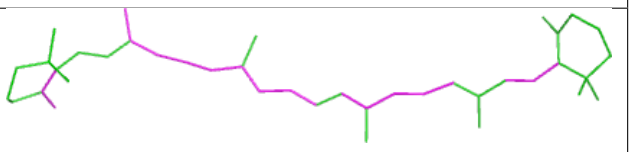


Rings

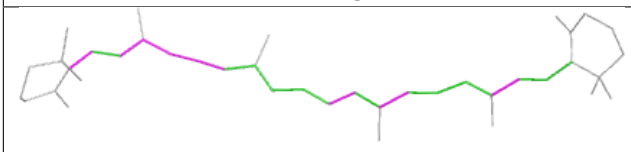
Ligand BCR B 4002



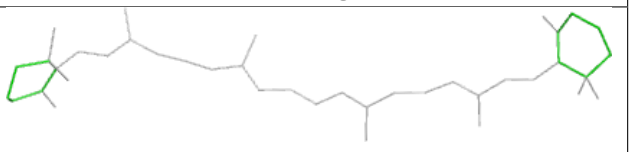
Bond lengths



Bond angles

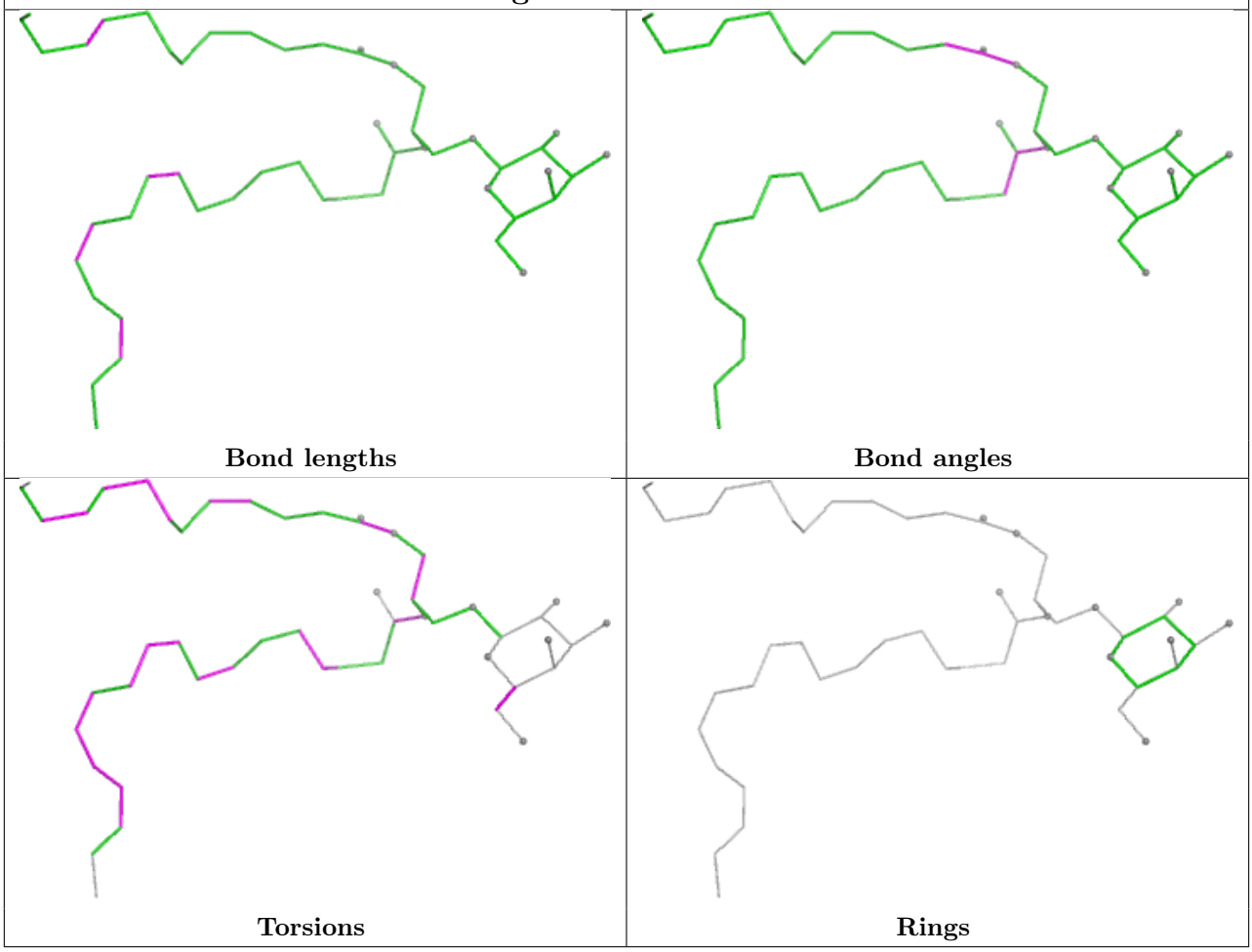


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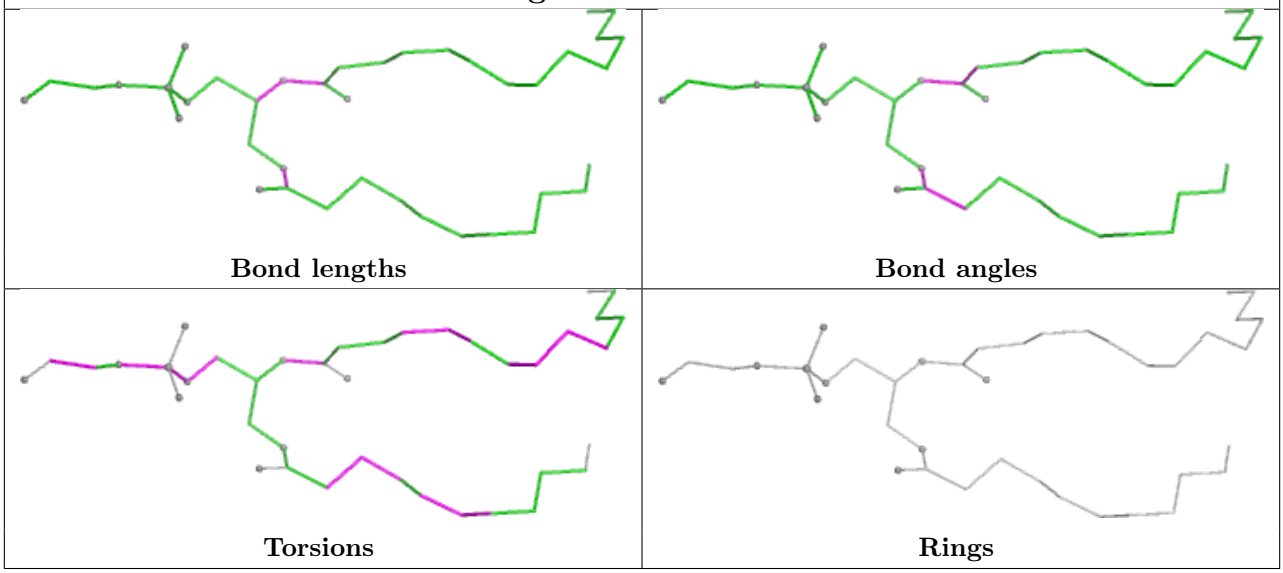


Rings

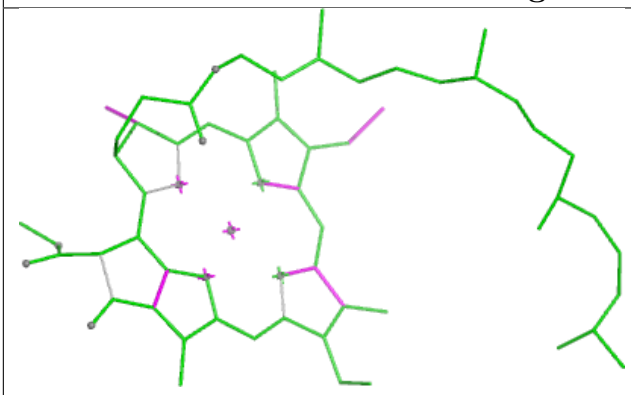
Ligand LMG 3 803



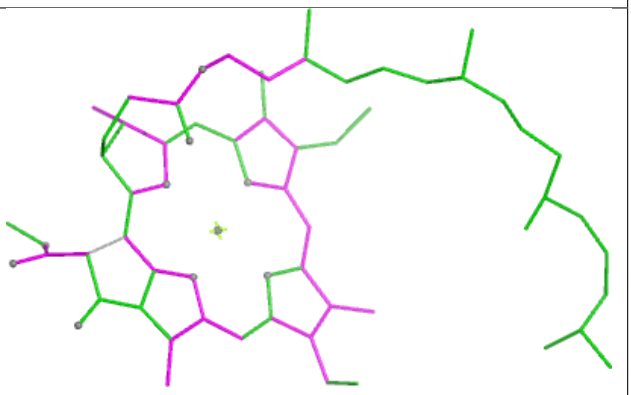
Ligand PTY 1 805



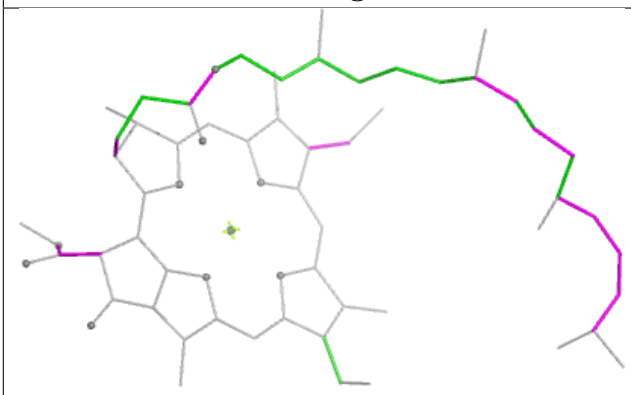
Ligand CLA 2 604



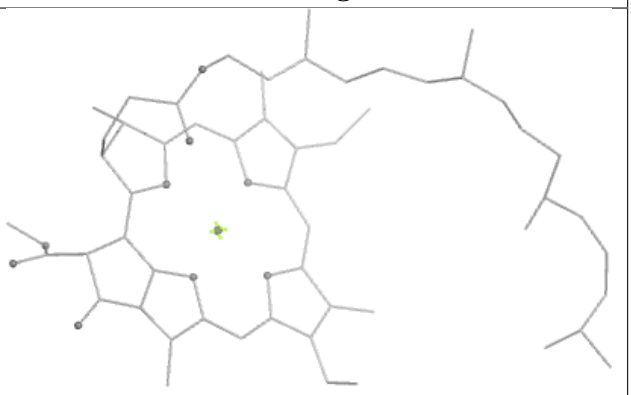
Bond lengths



Bond angles

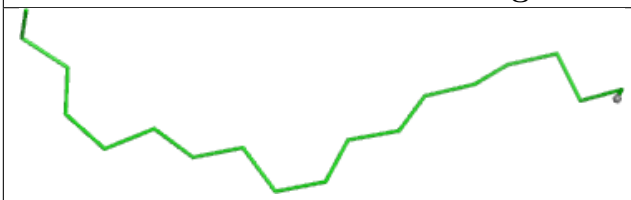


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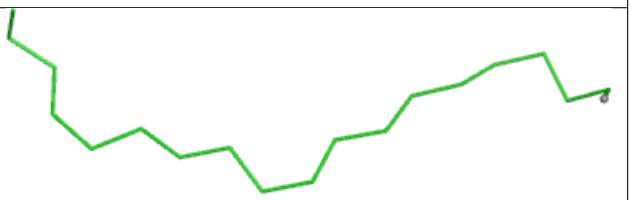


Rings

Ligand OCD A 5003



Bond lengths



Bond angles

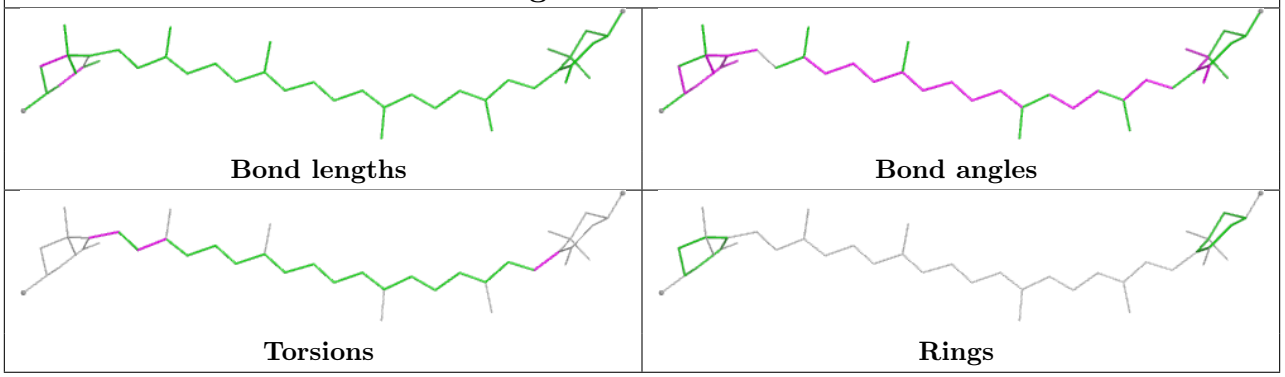


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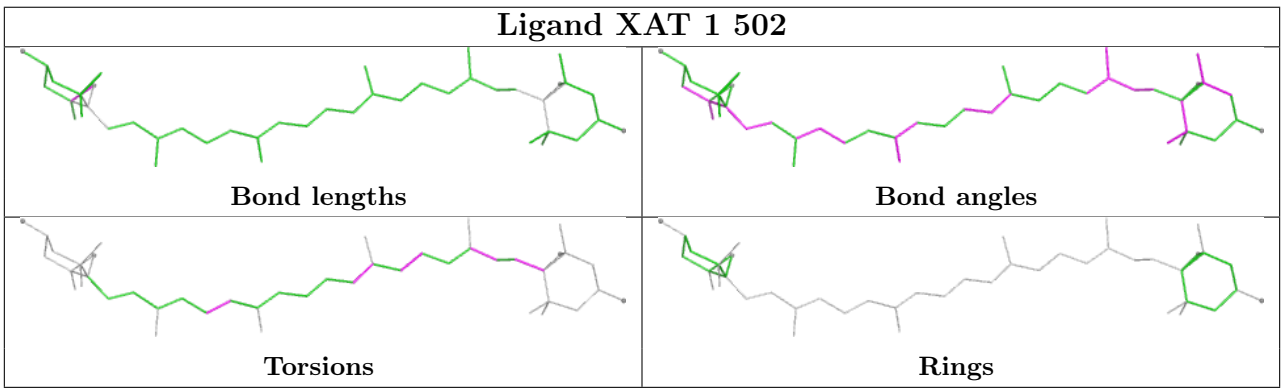


Rings

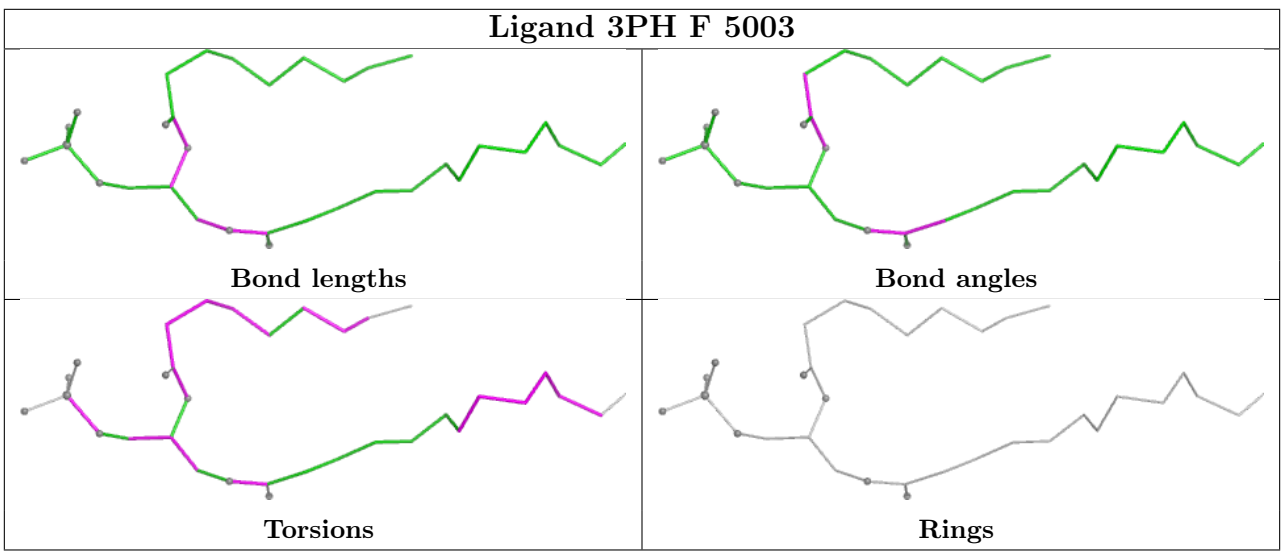
Ligand LUT 4 501



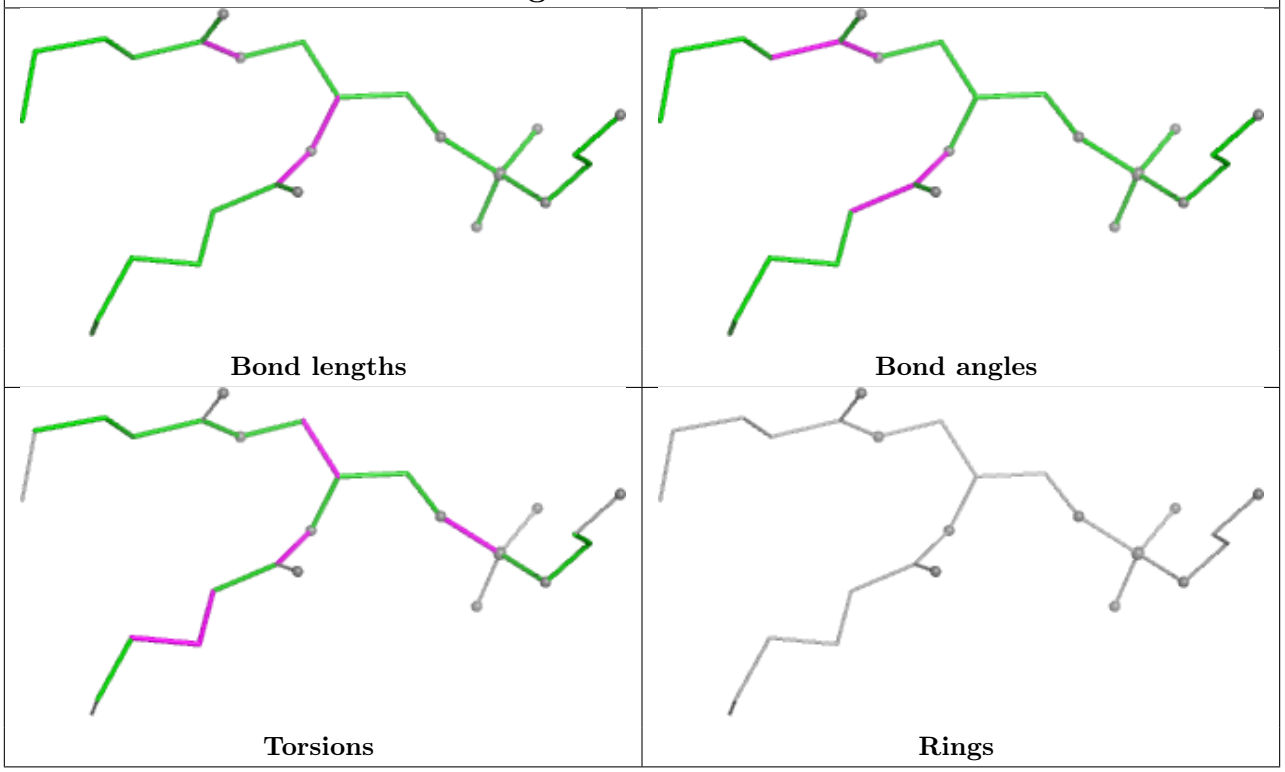
Ligand XAT 1 502



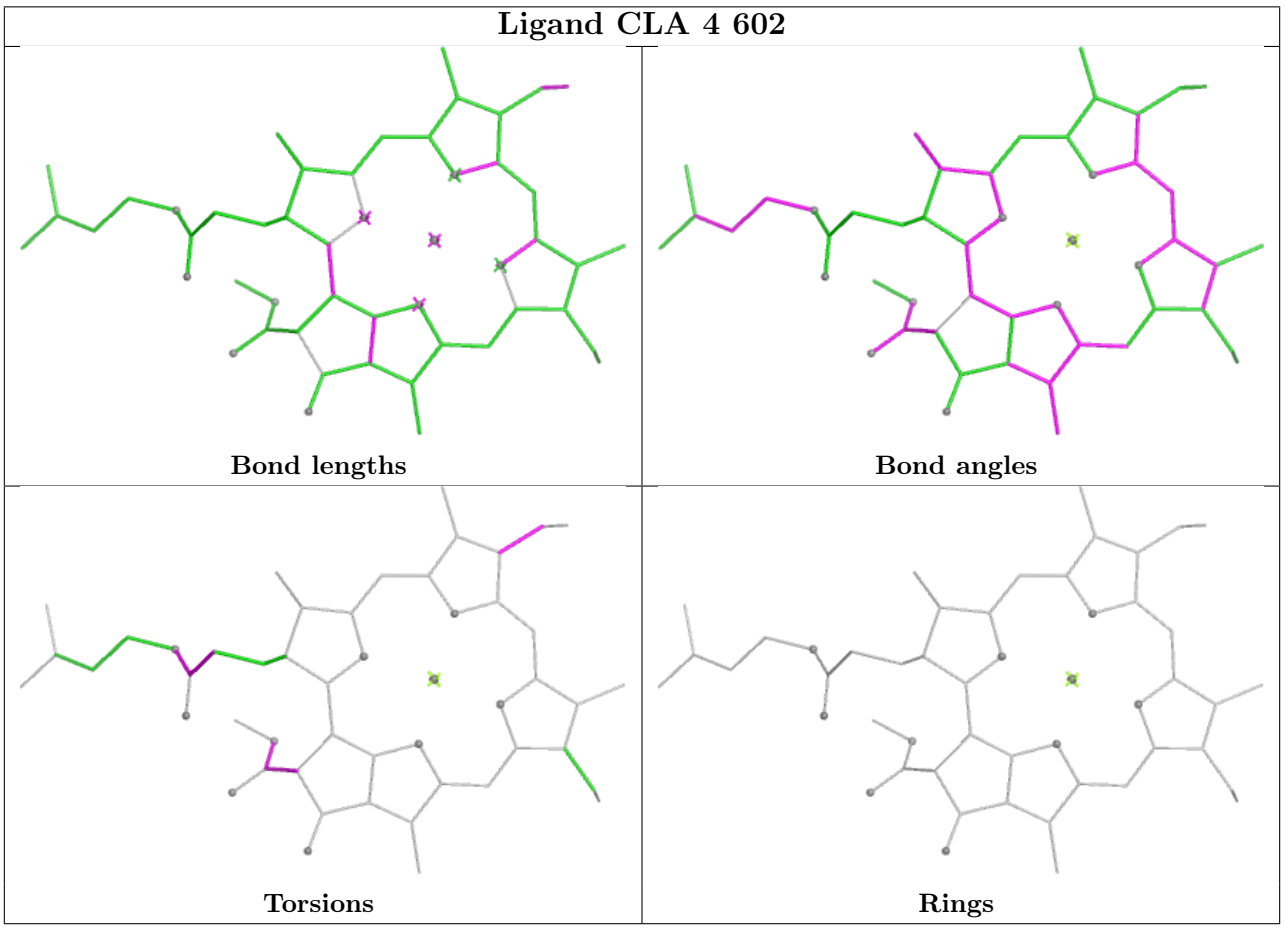
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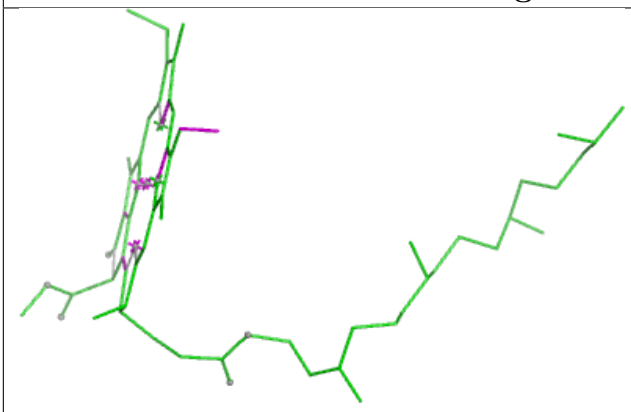
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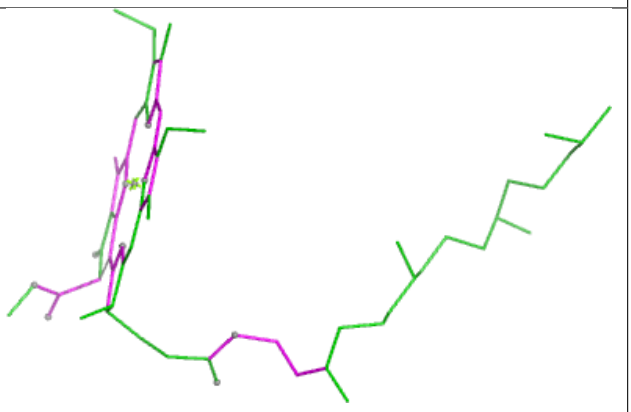
Ligand CLA 4 602



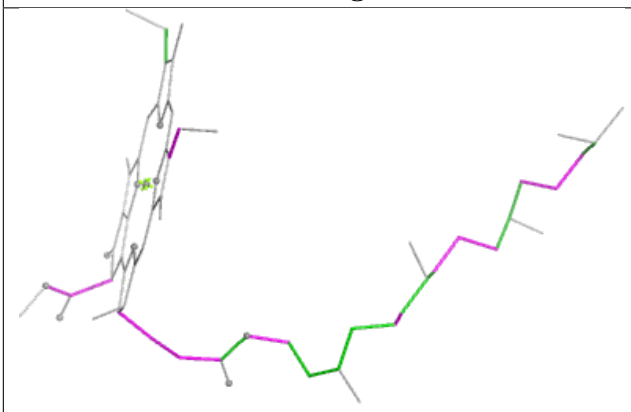
Ligand CLA A 1102



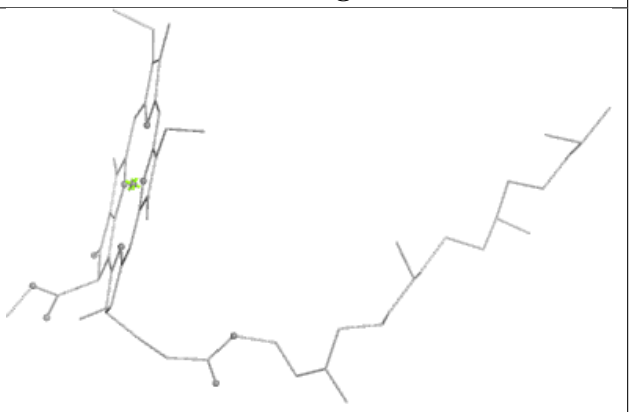
Bond lengths



Bond angles

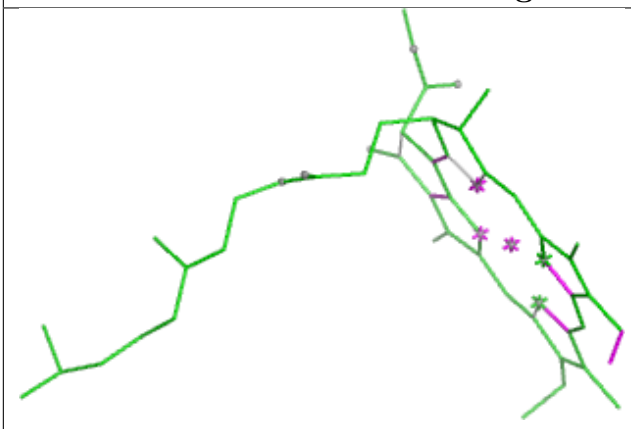


Torsions

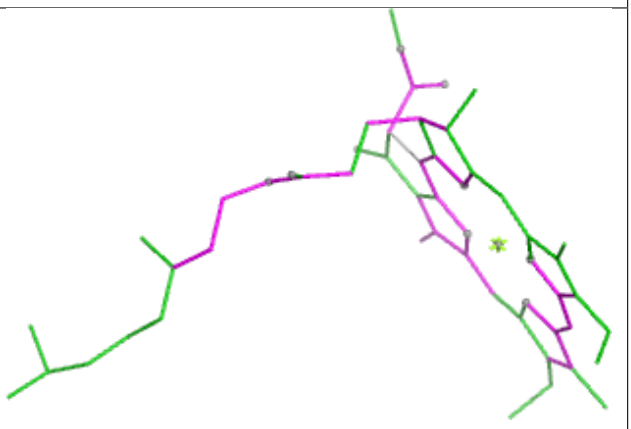


Rings

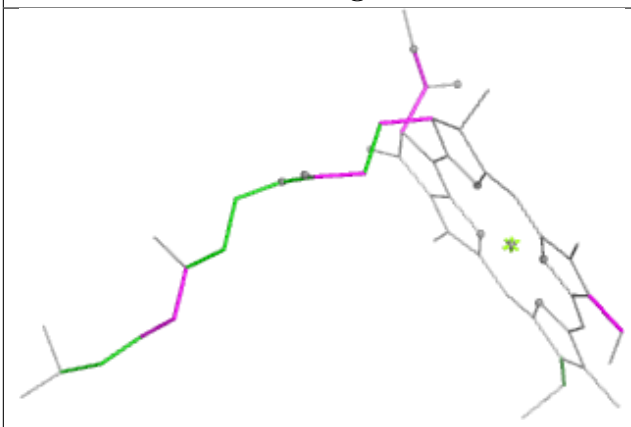
Ligand CLA B 1236



Bond lengths



Bond angles

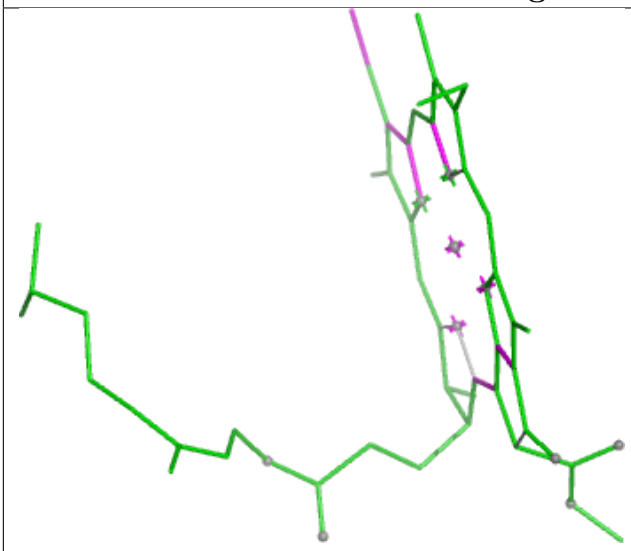


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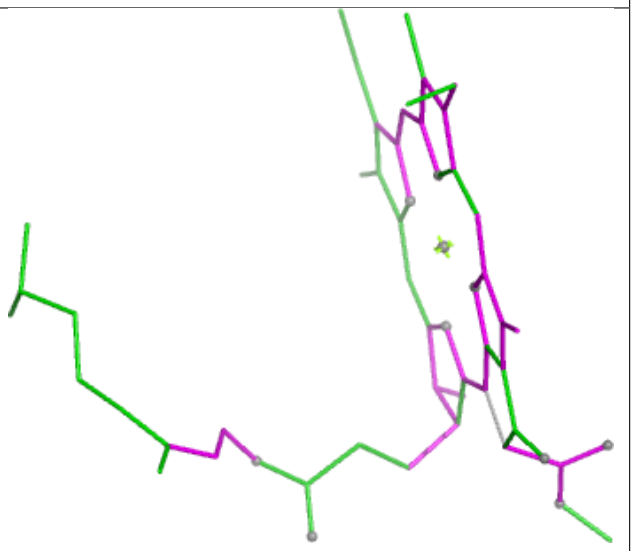


Rings

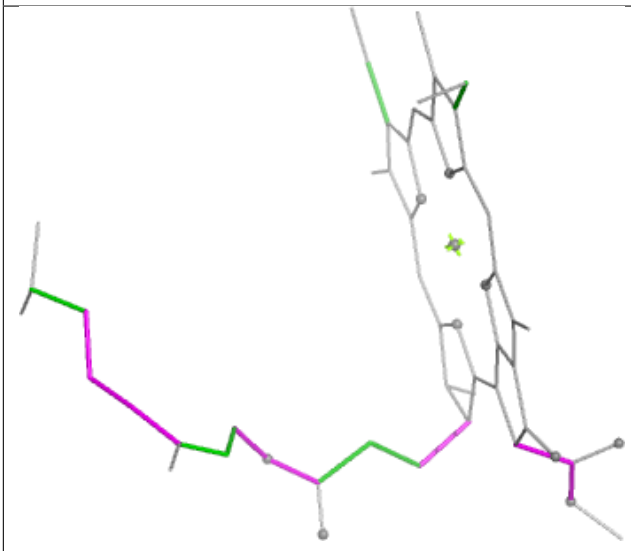
Ligand CLA 5 608



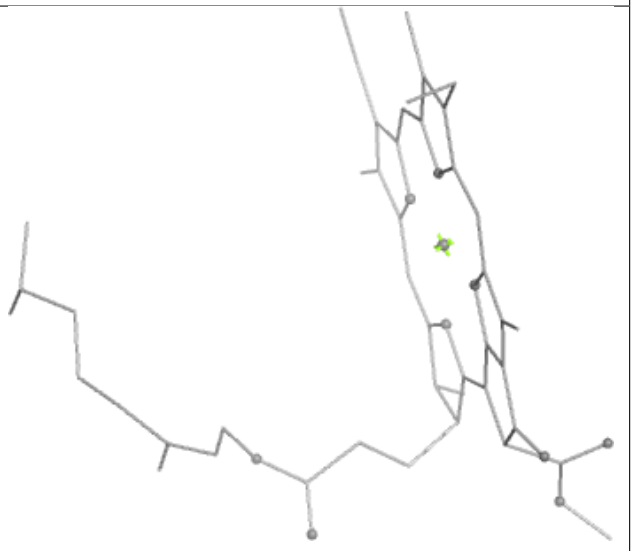
Bond lengths



Bond angles

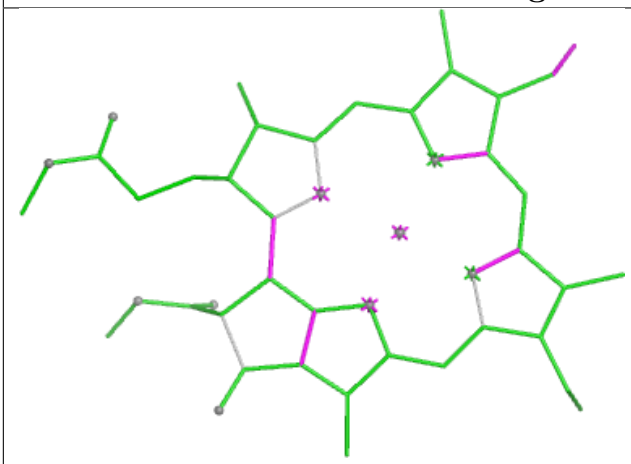


Torsions

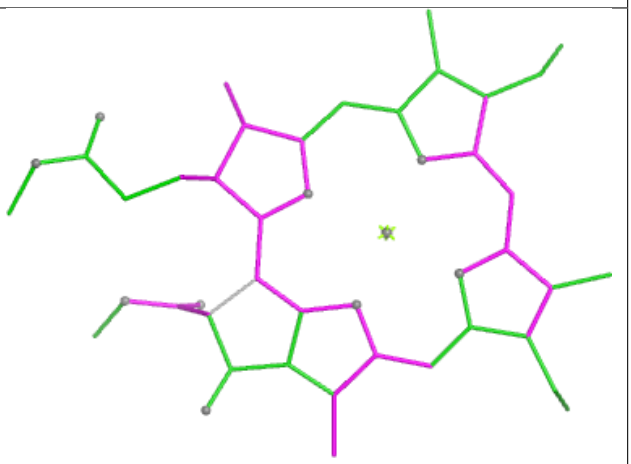


Rings

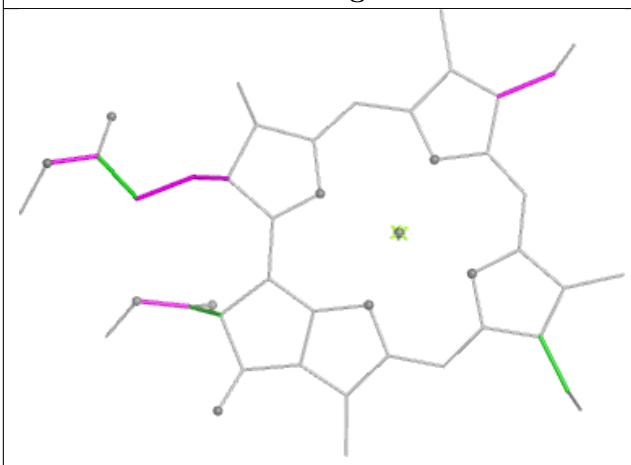
Ligand CLA 1 602



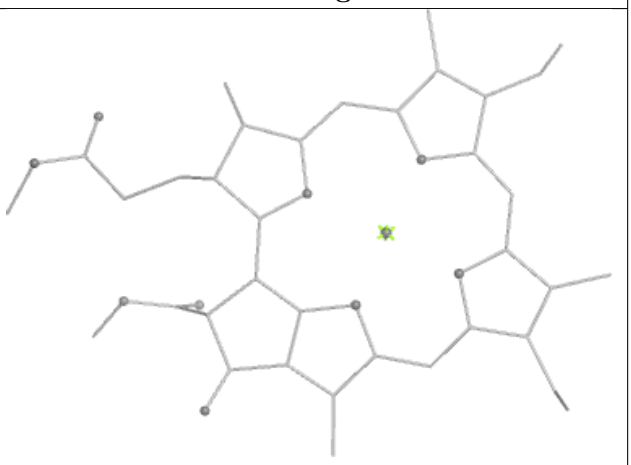
Bond lengths



Bond angles

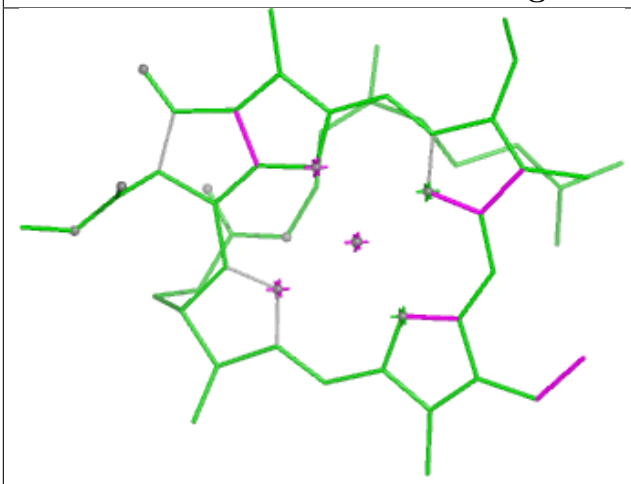


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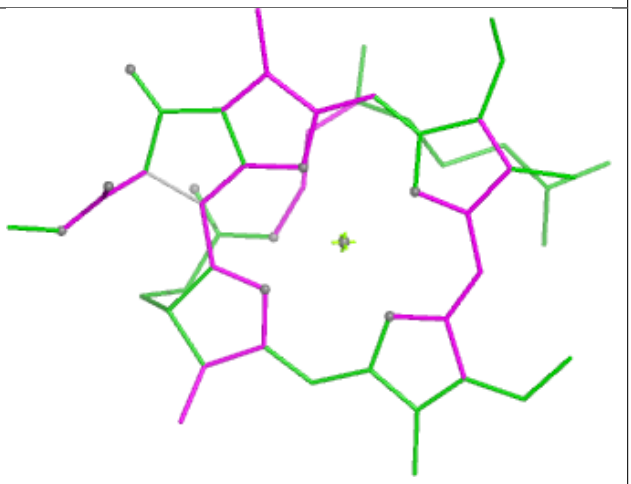


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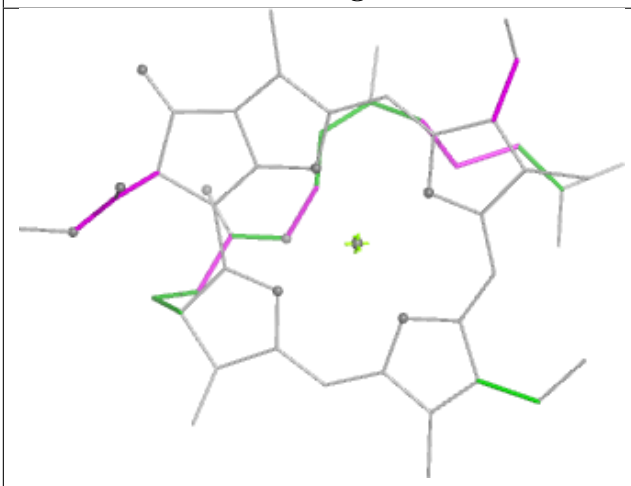
Ligand CLA 6 603



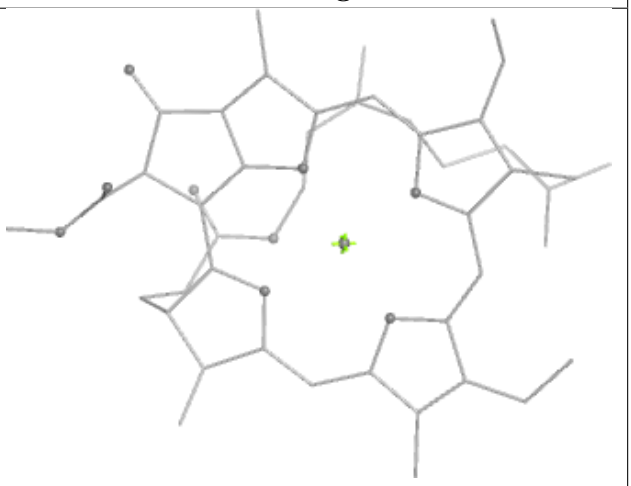
Bond lengths



Bond angles

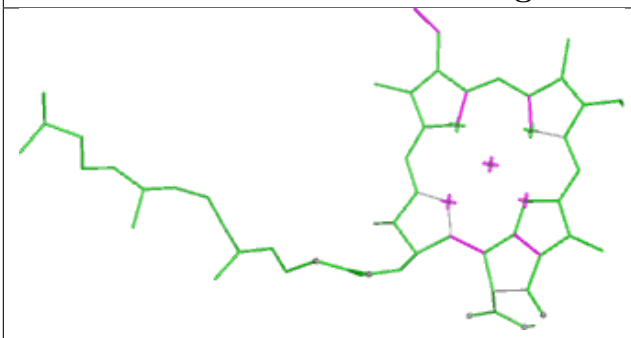


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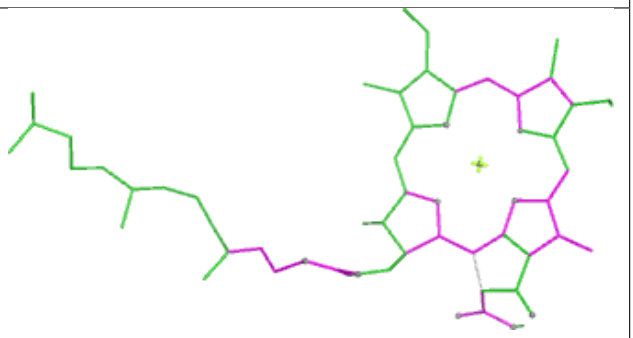


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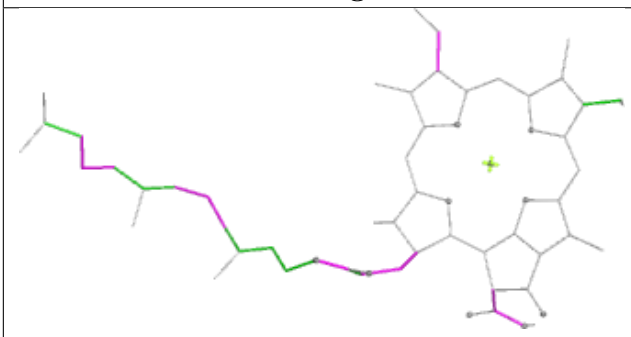
Ligand CLA A 1141



Bond lengths



Bond angles

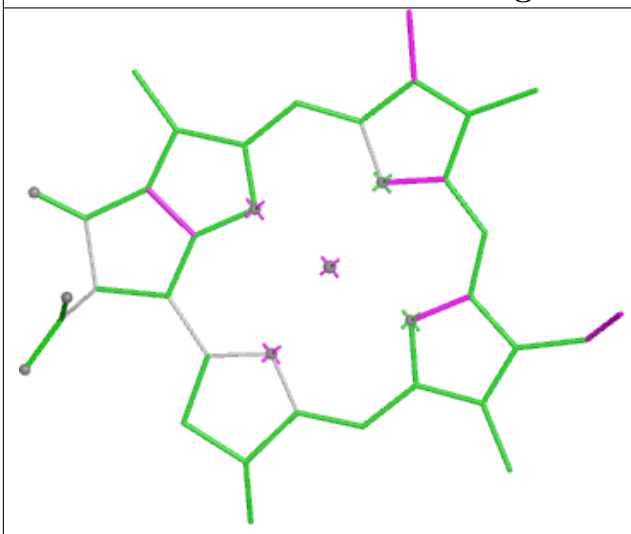


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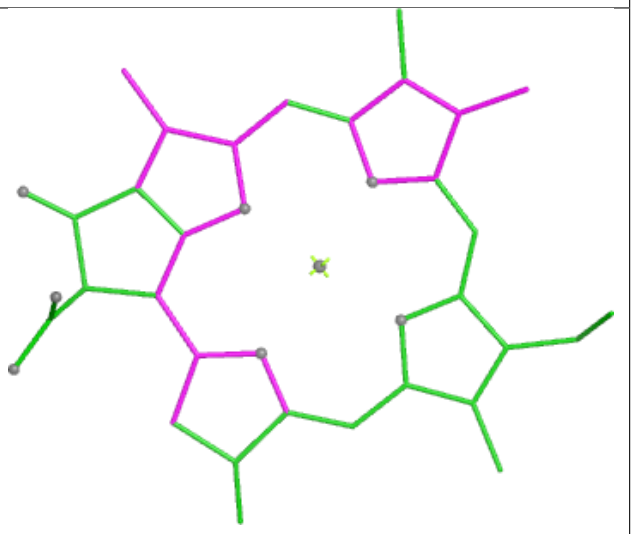


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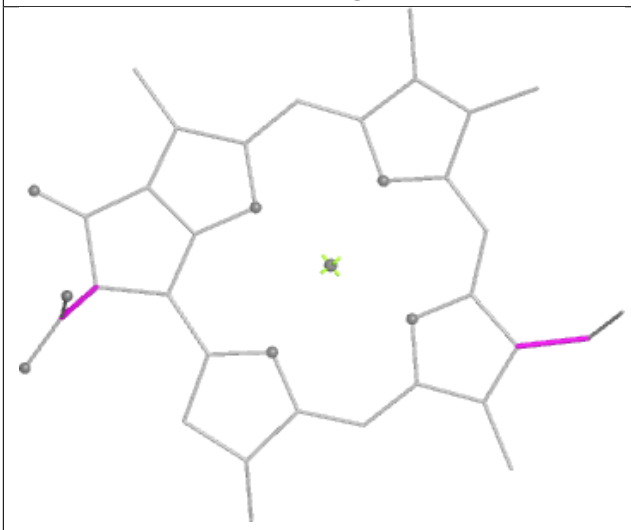
Ligand CLA O 1801



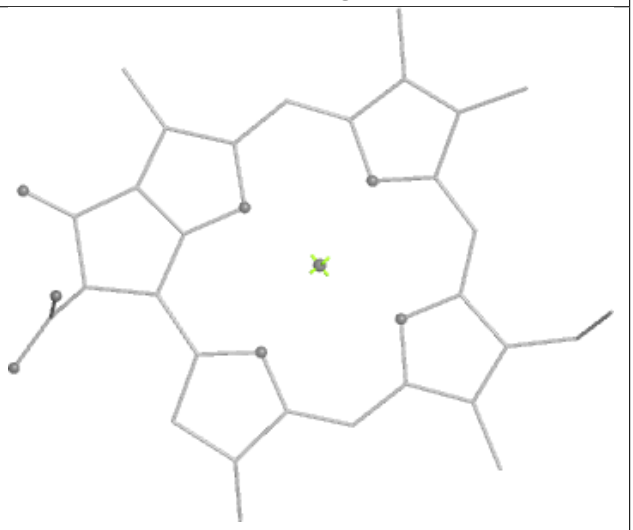
Bond lengths



Bond angles

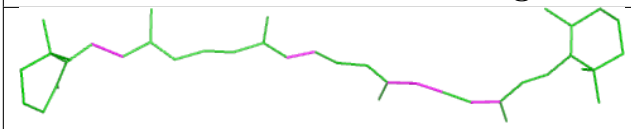


Torsions



Rings

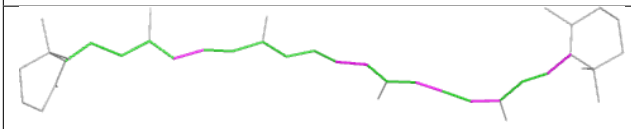
Ligand BCR A 4005



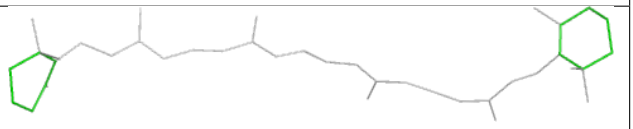
Bond lengths



Bond angles

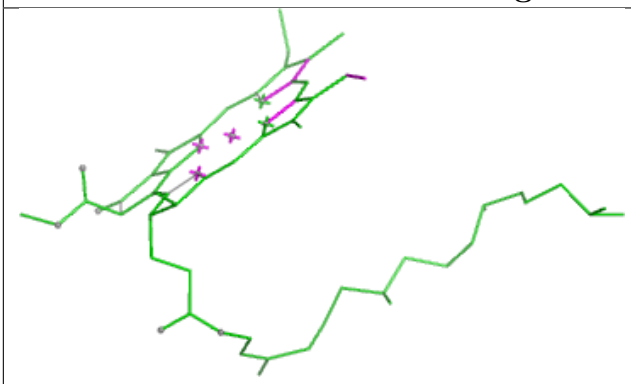


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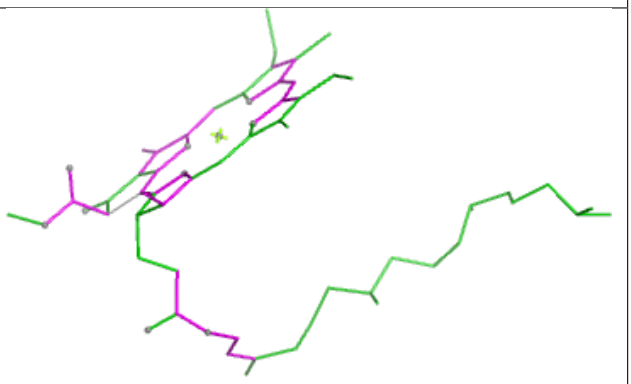


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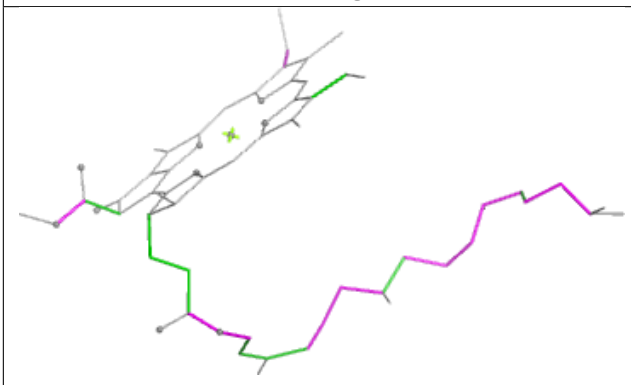
Ligand CLA A 1112



Bond lengths



Bond angles

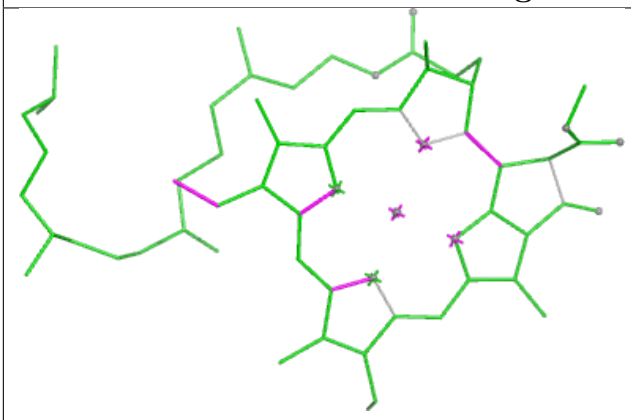


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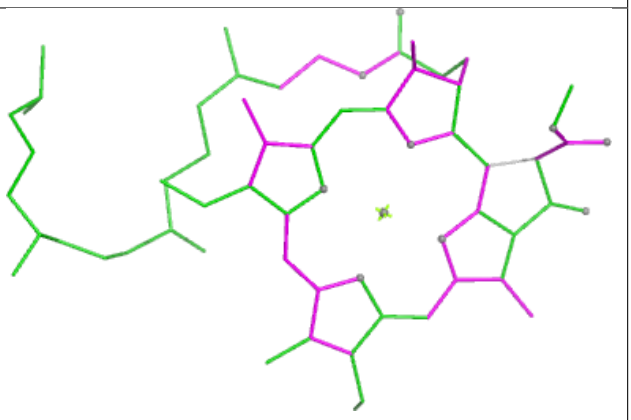


Rings

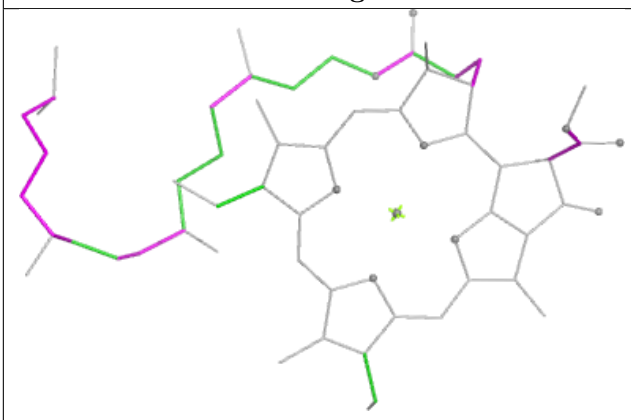
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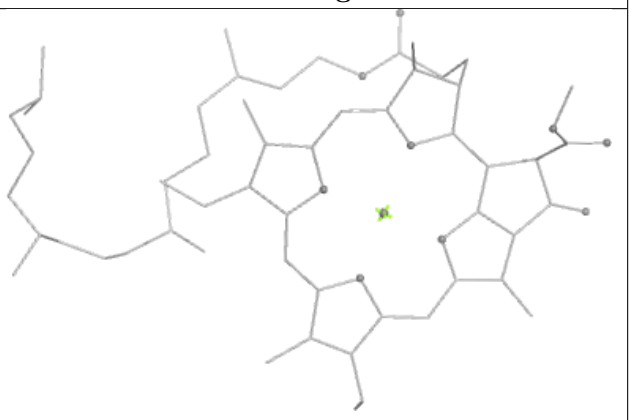
Bond lengths



Bond angles

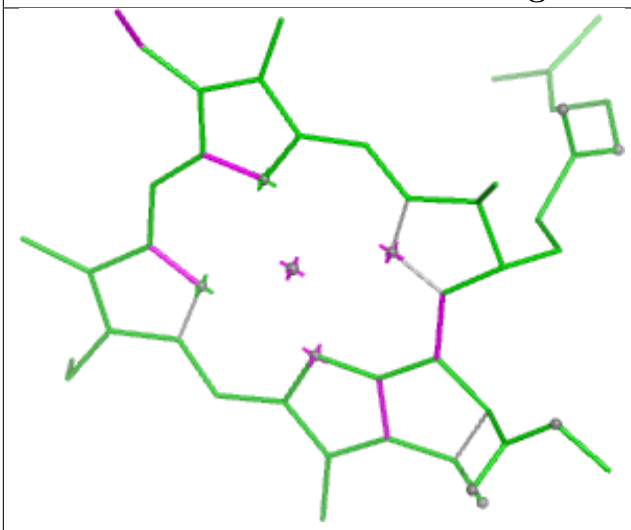


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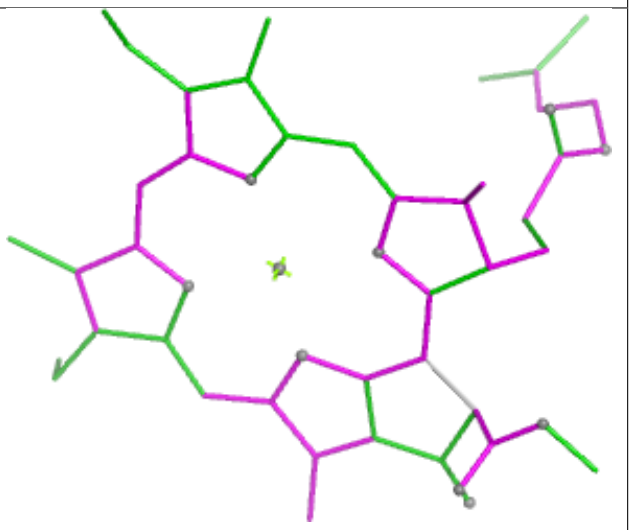


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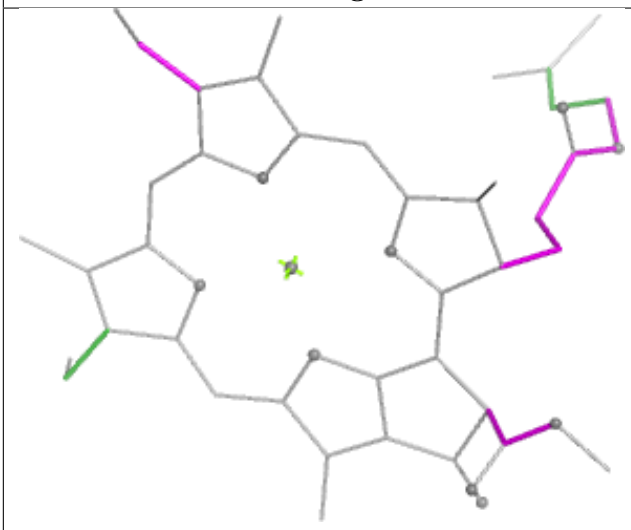
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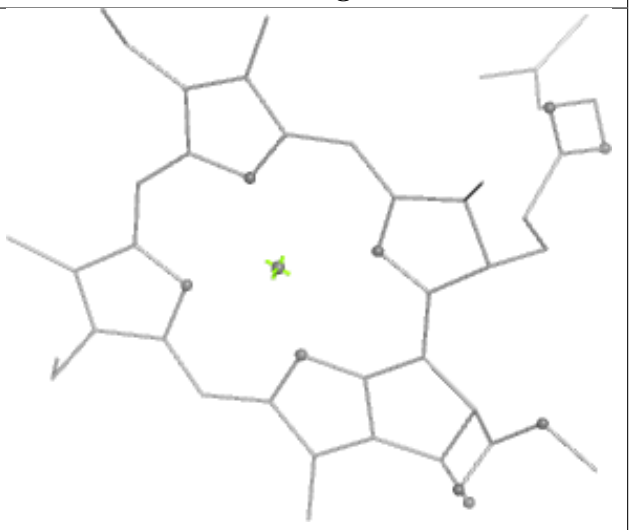
Bond lengths



Bond angles

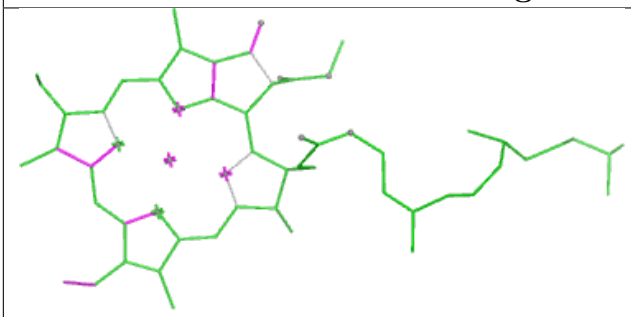


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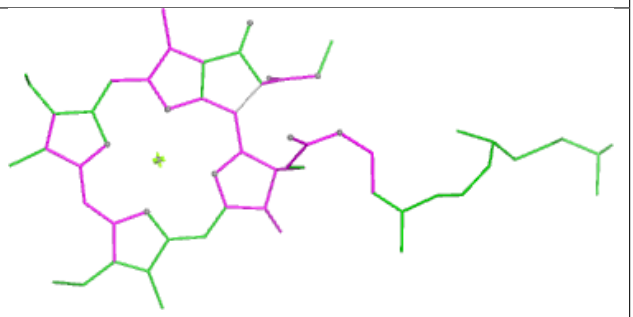


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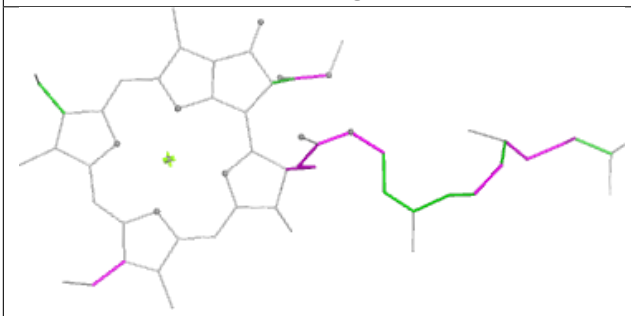
Ligand CLA O 1803



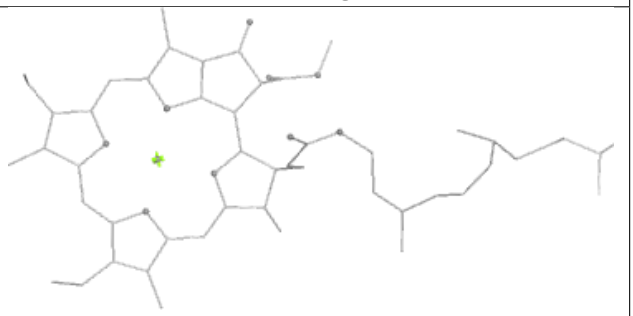
Bond lengths



Bond angles

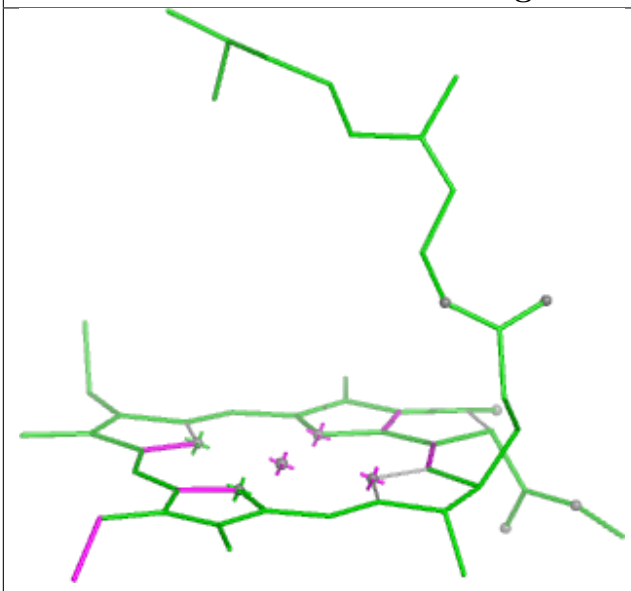


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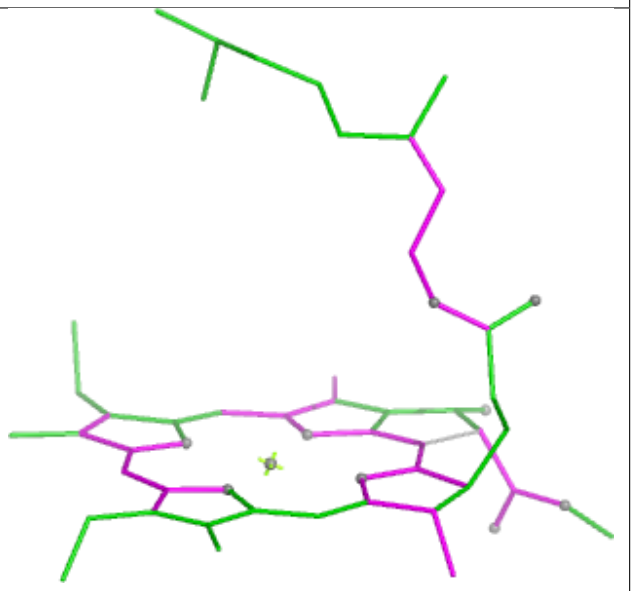


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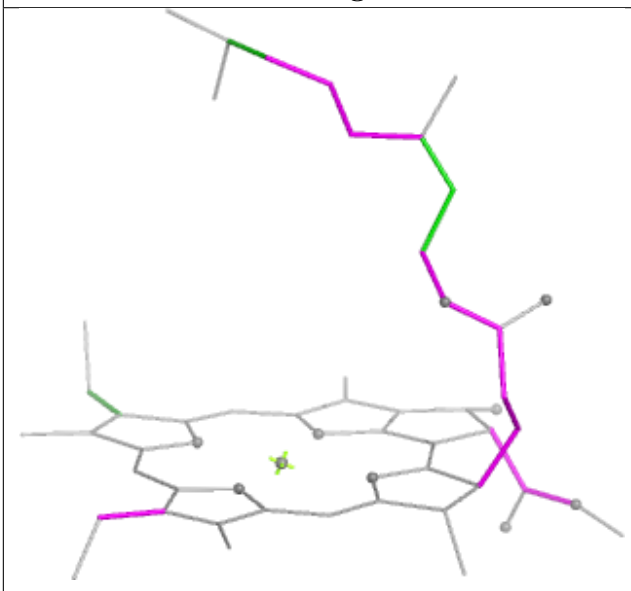
Ligand CLA A 1108



Bond lengths



Bond angles

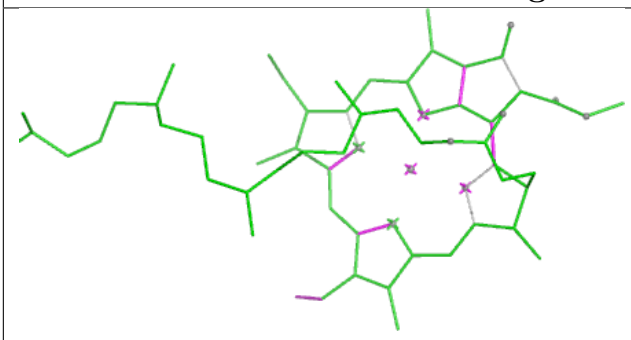


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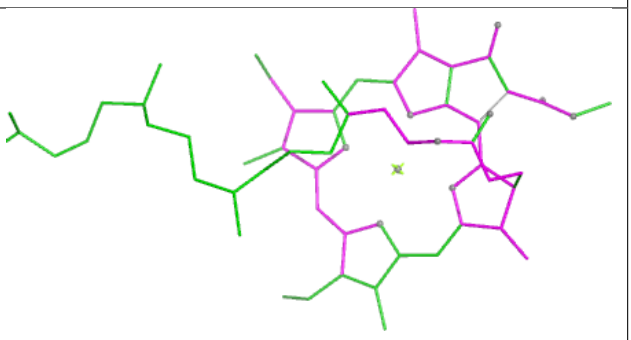


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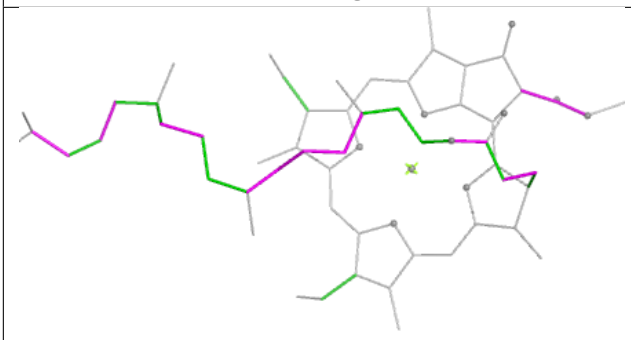
Ligand CLA 3 603



Bond lengths



Bond angles

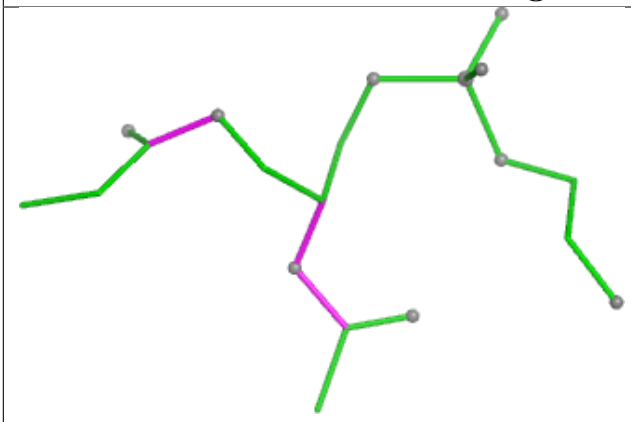


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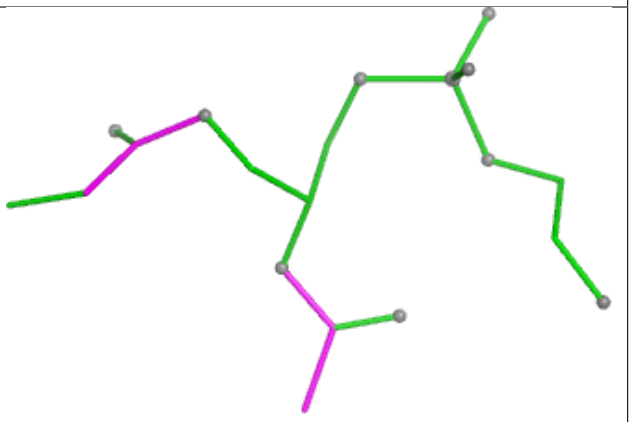


Rings

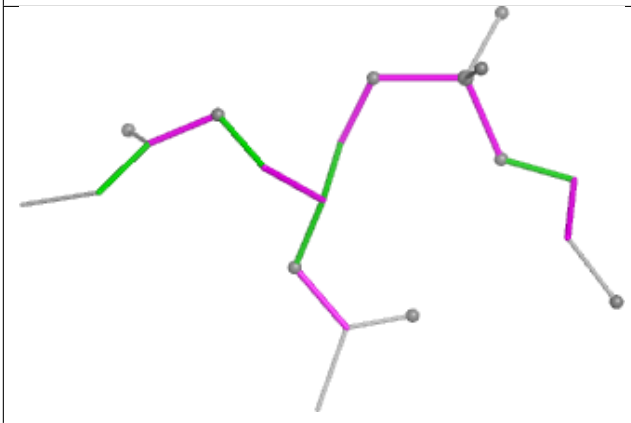
Ligand PTY 3 808



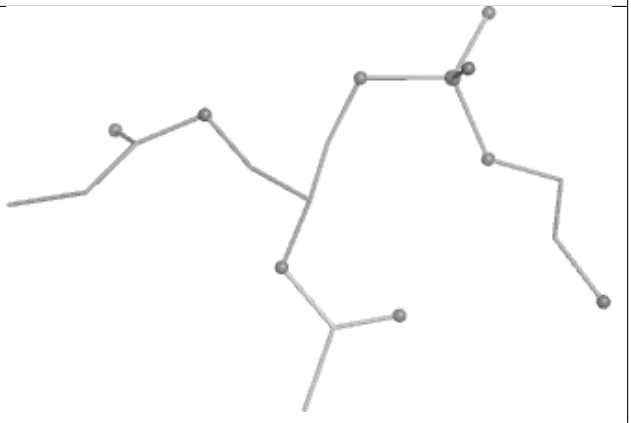
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Bond angles

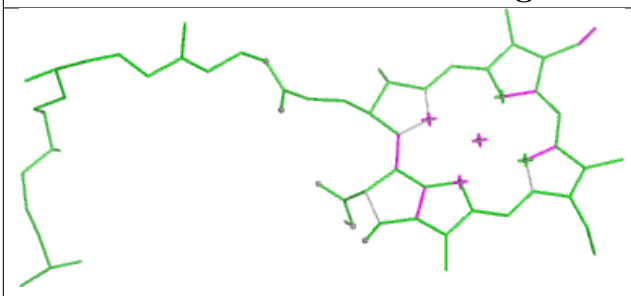


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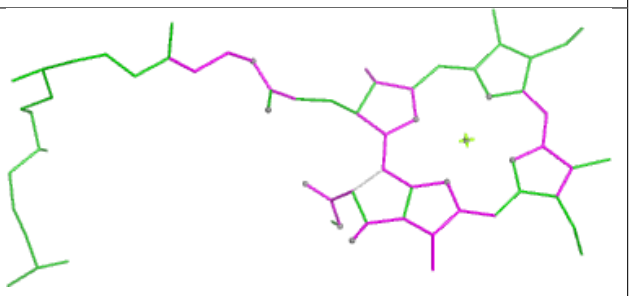


Rings

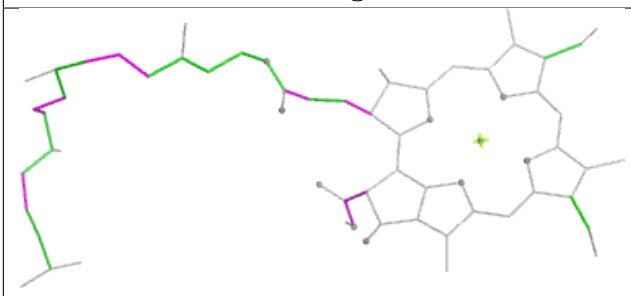
Ligand CLA B 1223



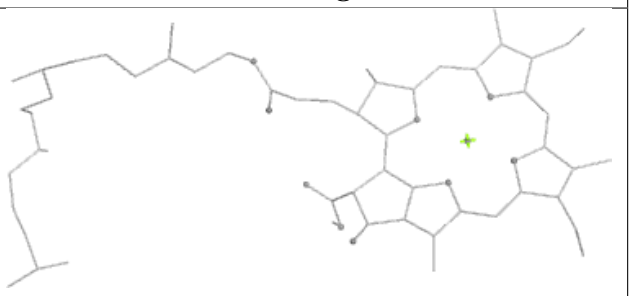
Bond lengths



Bond angles

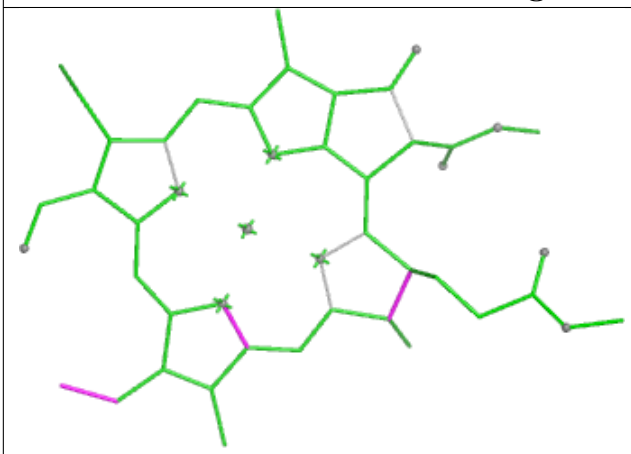


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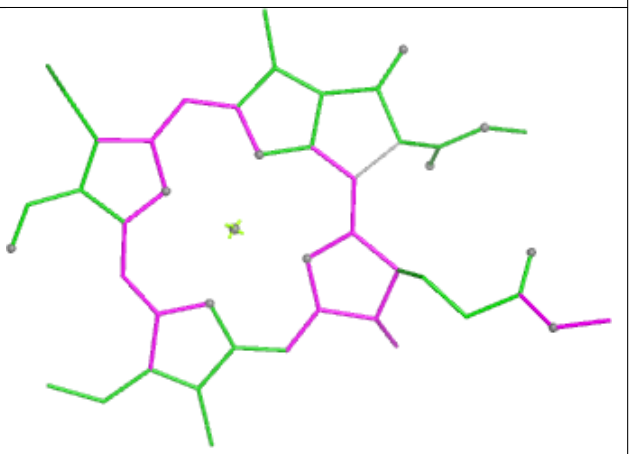


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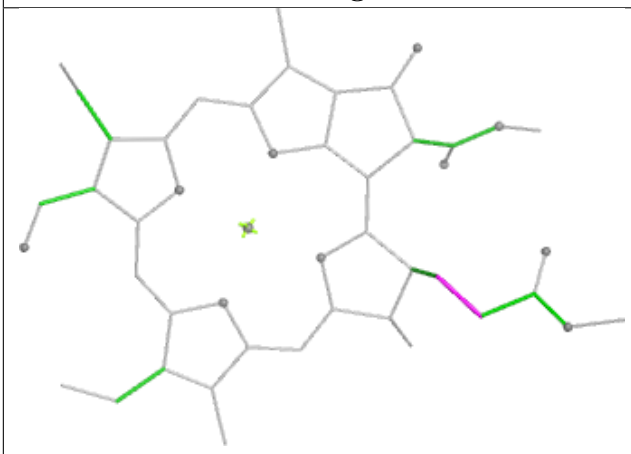
Ligand CHL 1 610



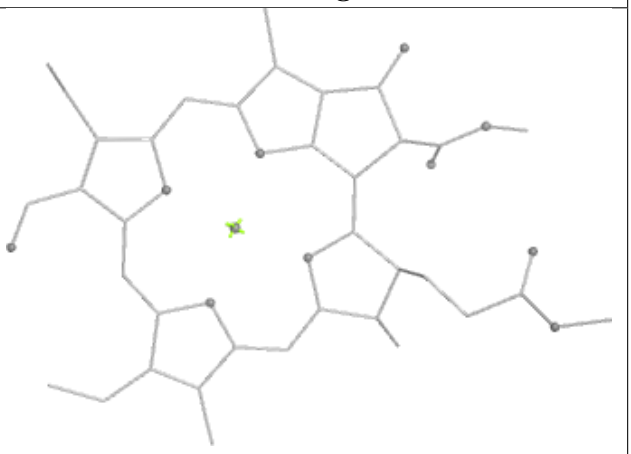
Bond lengths



Bond angles

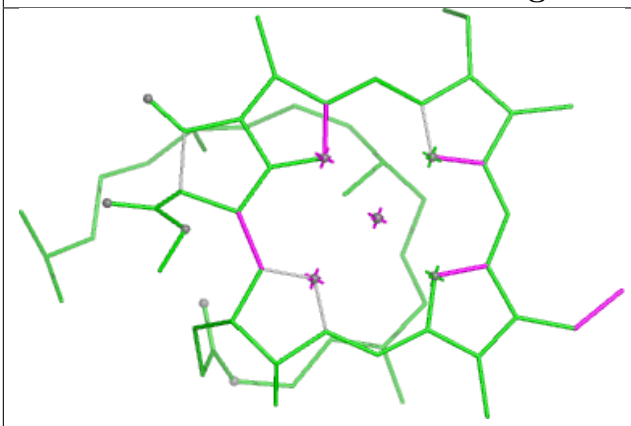


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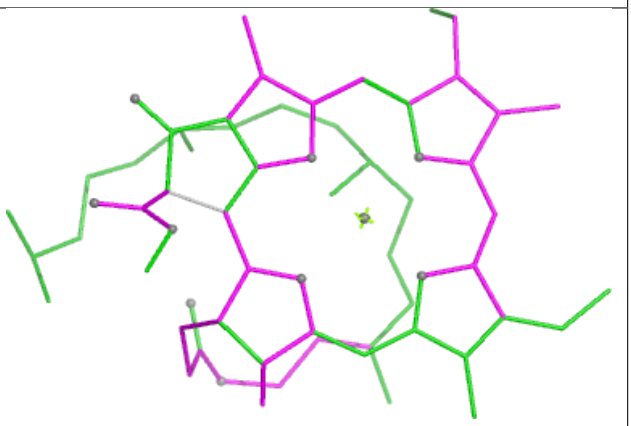


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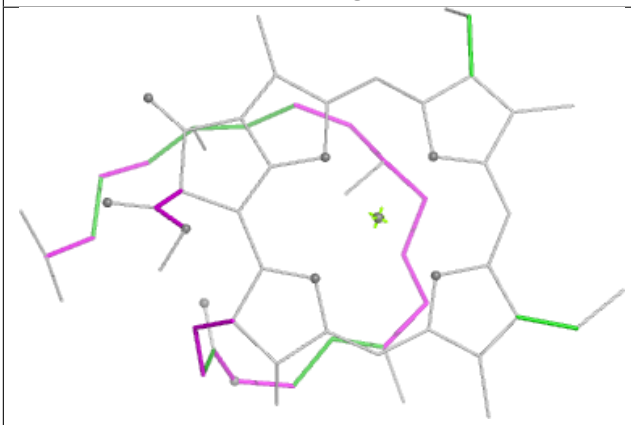
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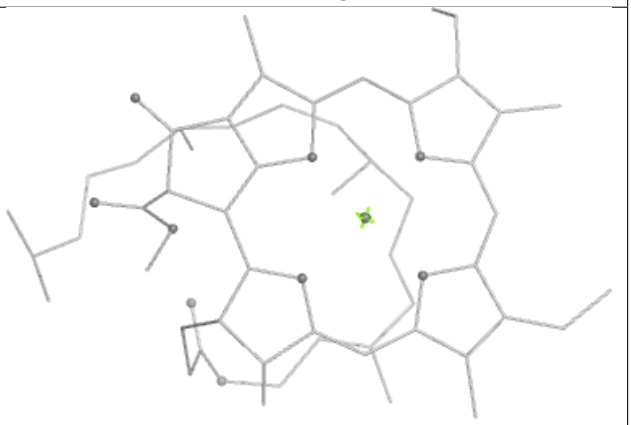
Bond lengths



Bond angles

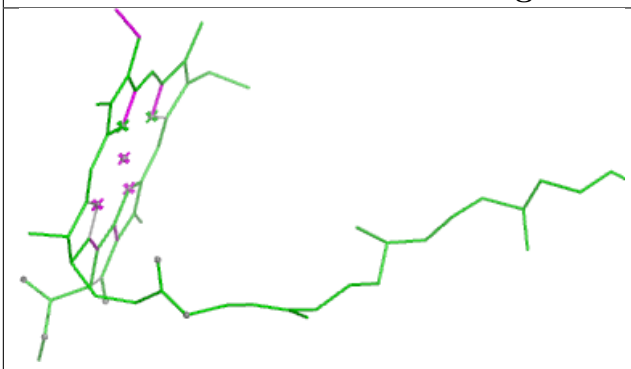


Torsions

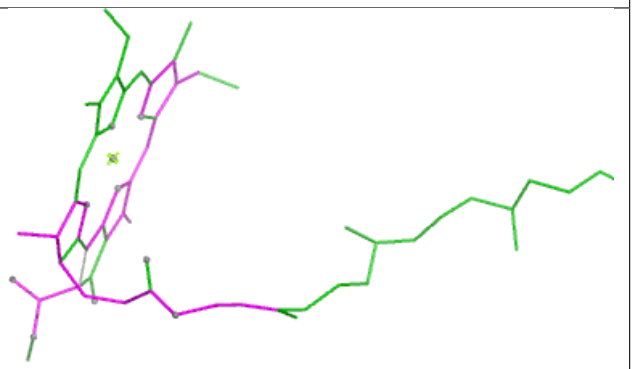


Rings

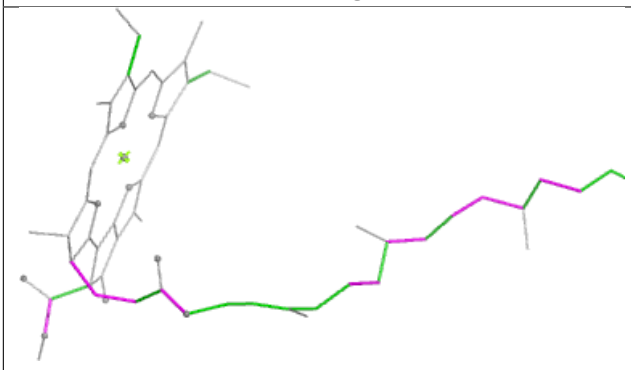
Ligand CLA B 1226



Bond lengths



Bond angles

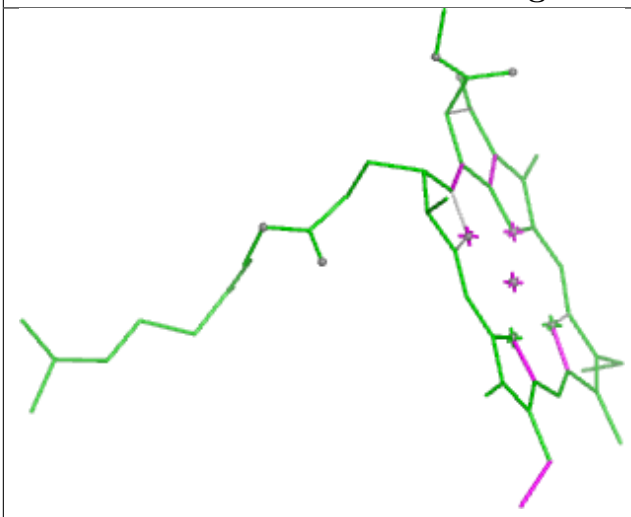


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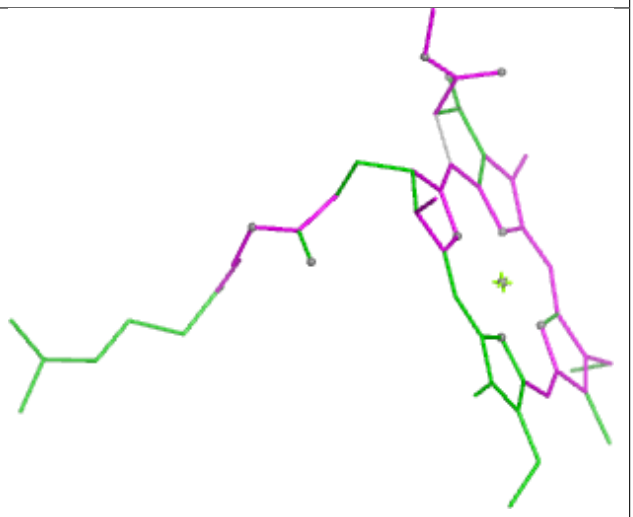


Rings

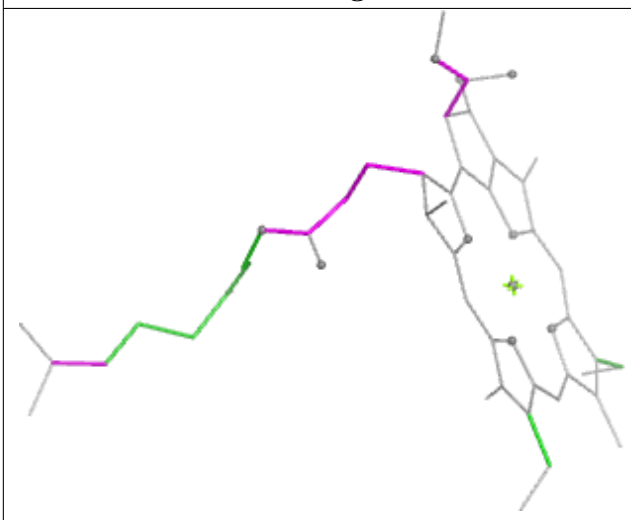
Ligand CLA 3 606



Bond lengths



Bond angles

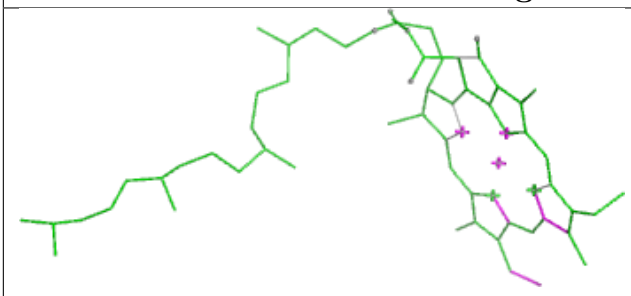


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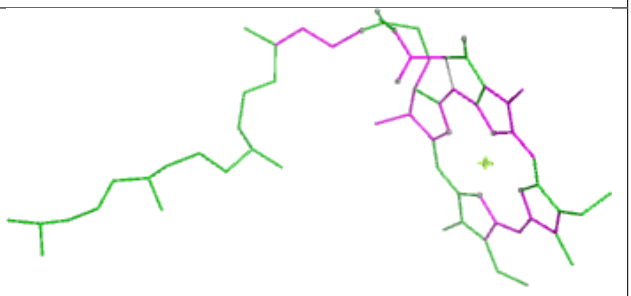


Rings

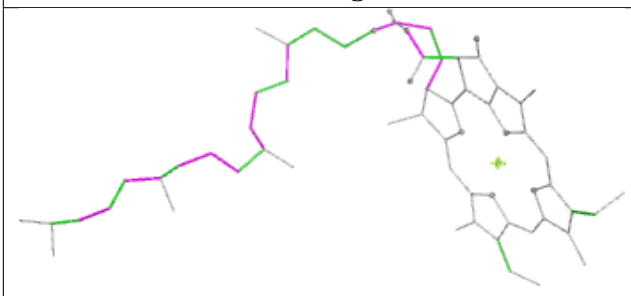
Ligand CLA B 1207



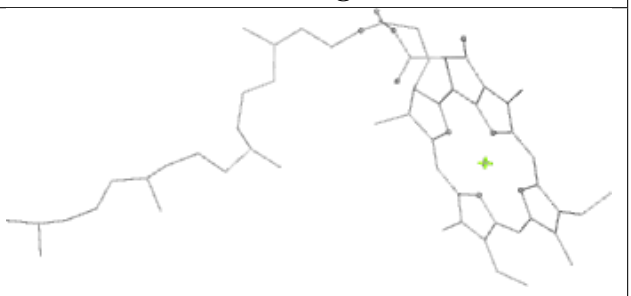
Bond lengths



Bond angles

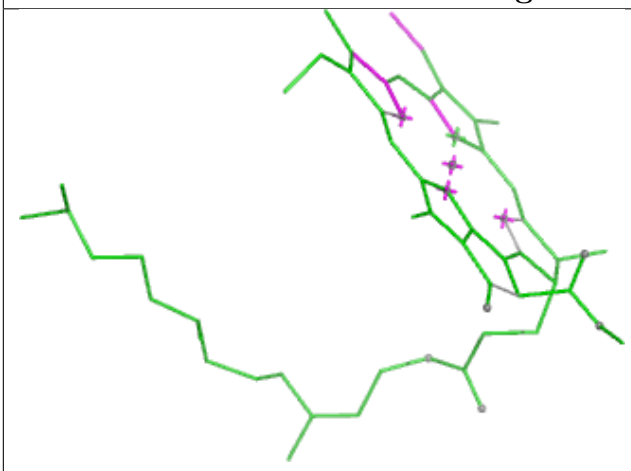


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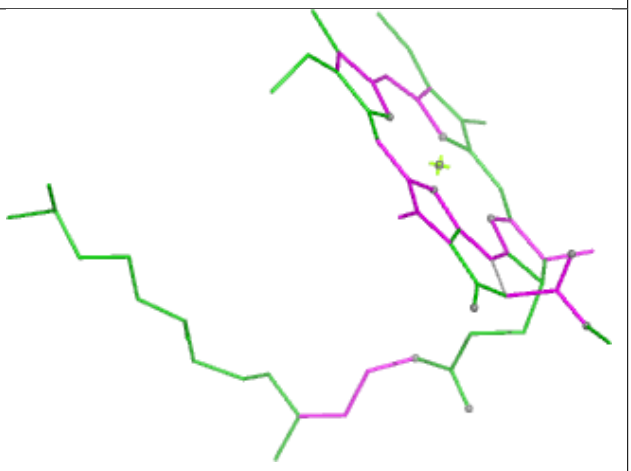


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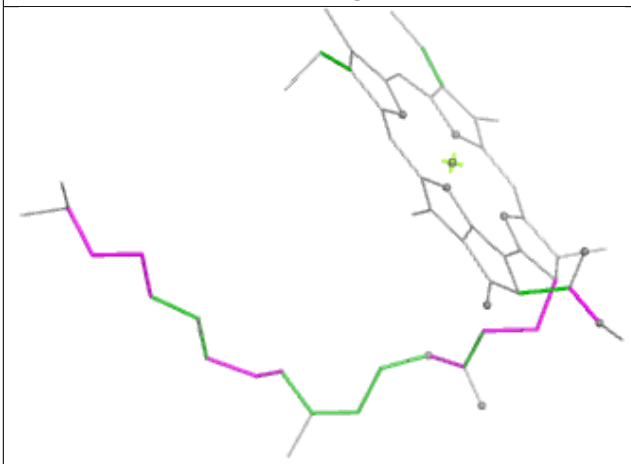
Ligand CLA B 1208



Bond lengths



Bond angles

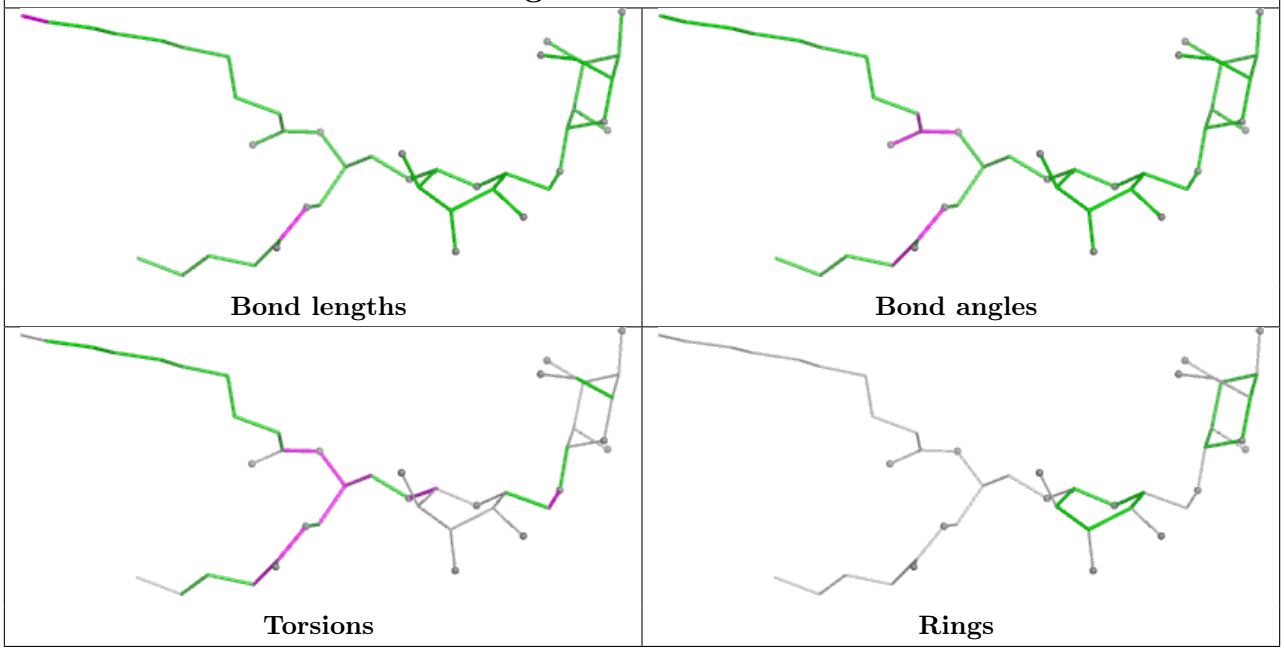


Torsions



Rings

Ligand DGD 3 805



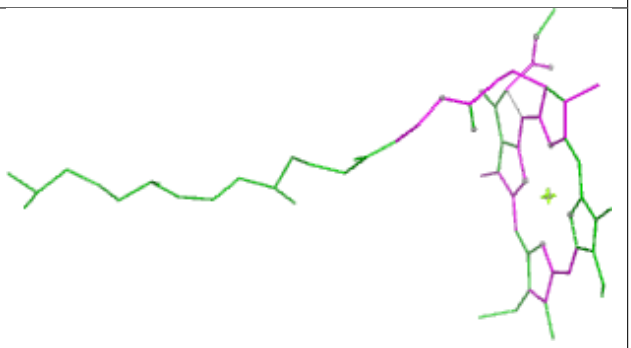
Ligand LUT 6 501



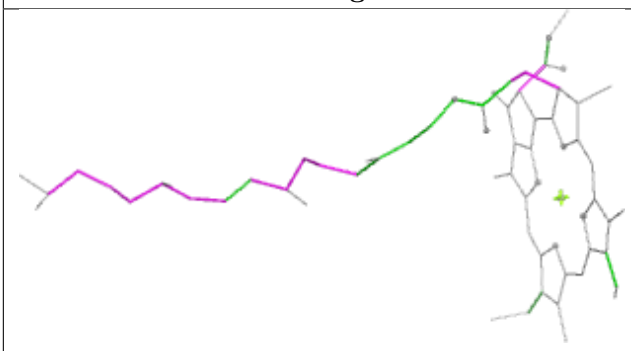
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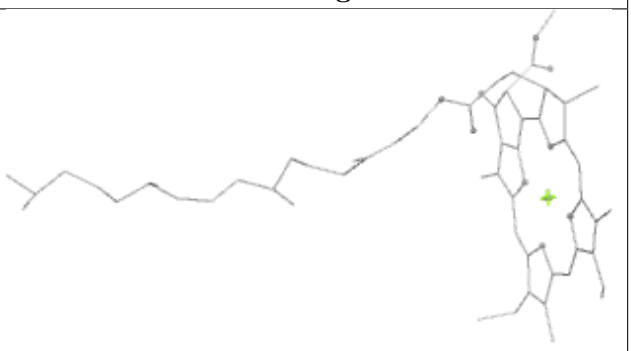
Bond lengths



Bond angles

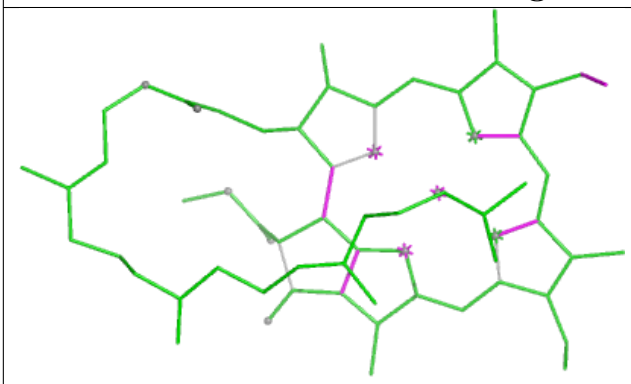


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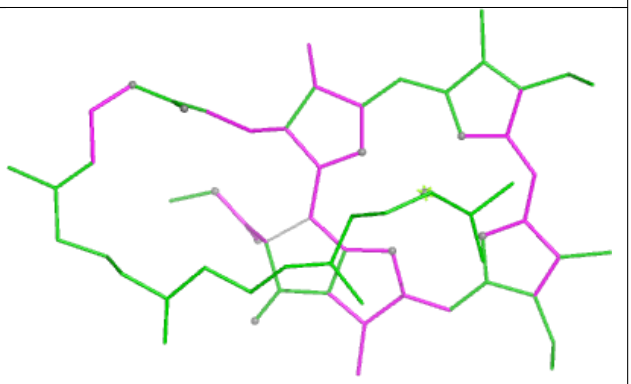


Rings

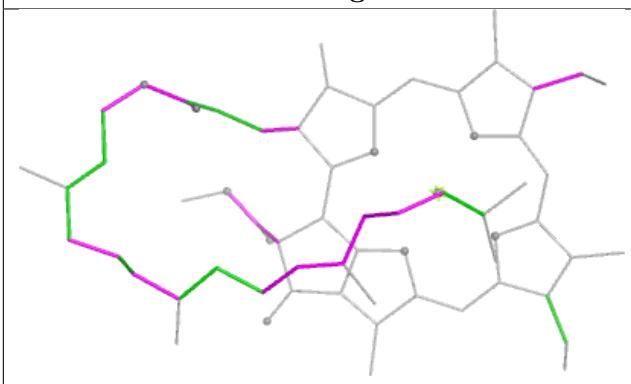
Ligand CLA 2 615



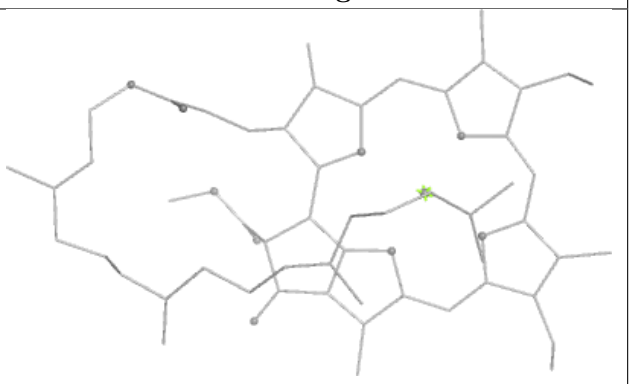
Bond lengths



Bond angles

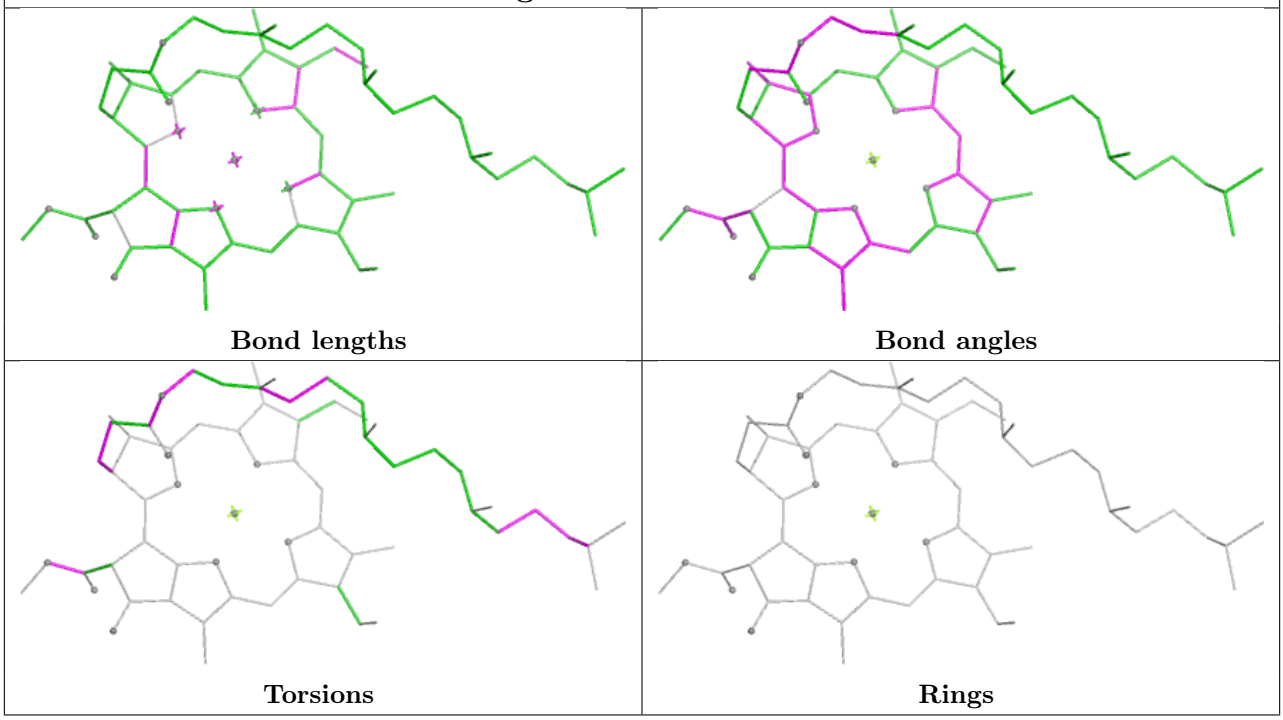


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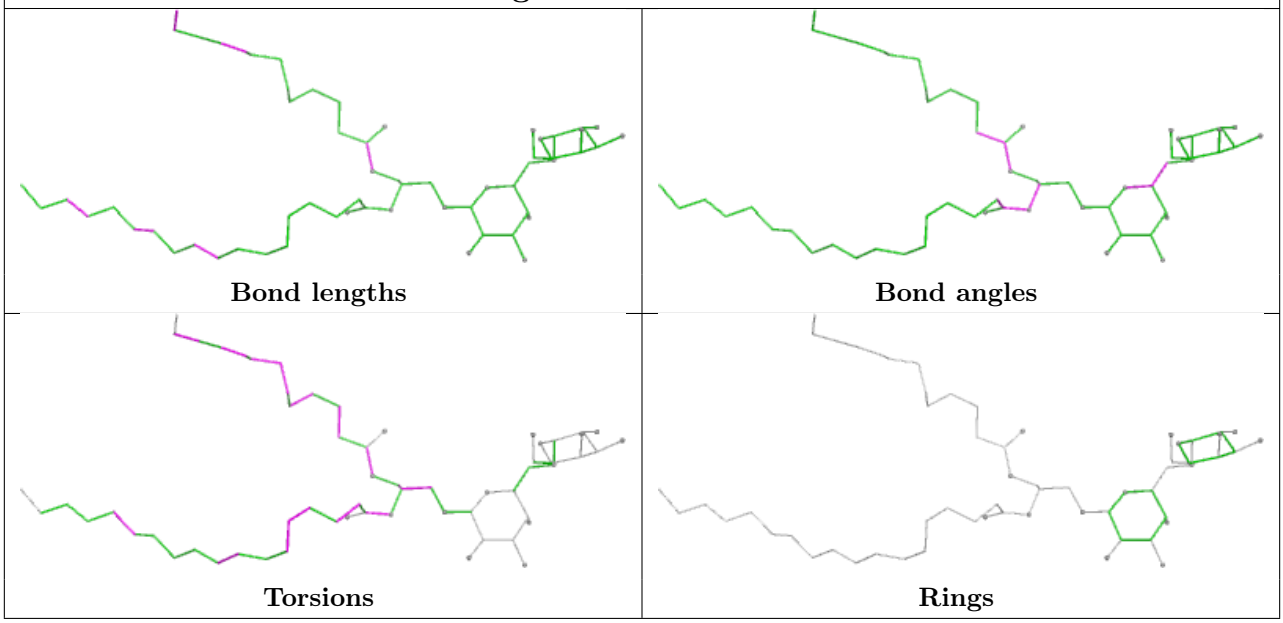


Rings

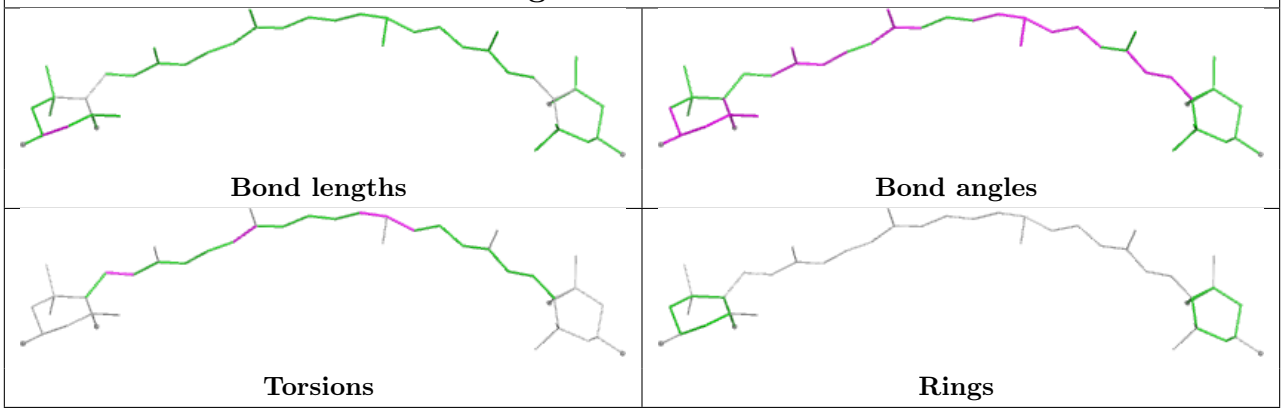
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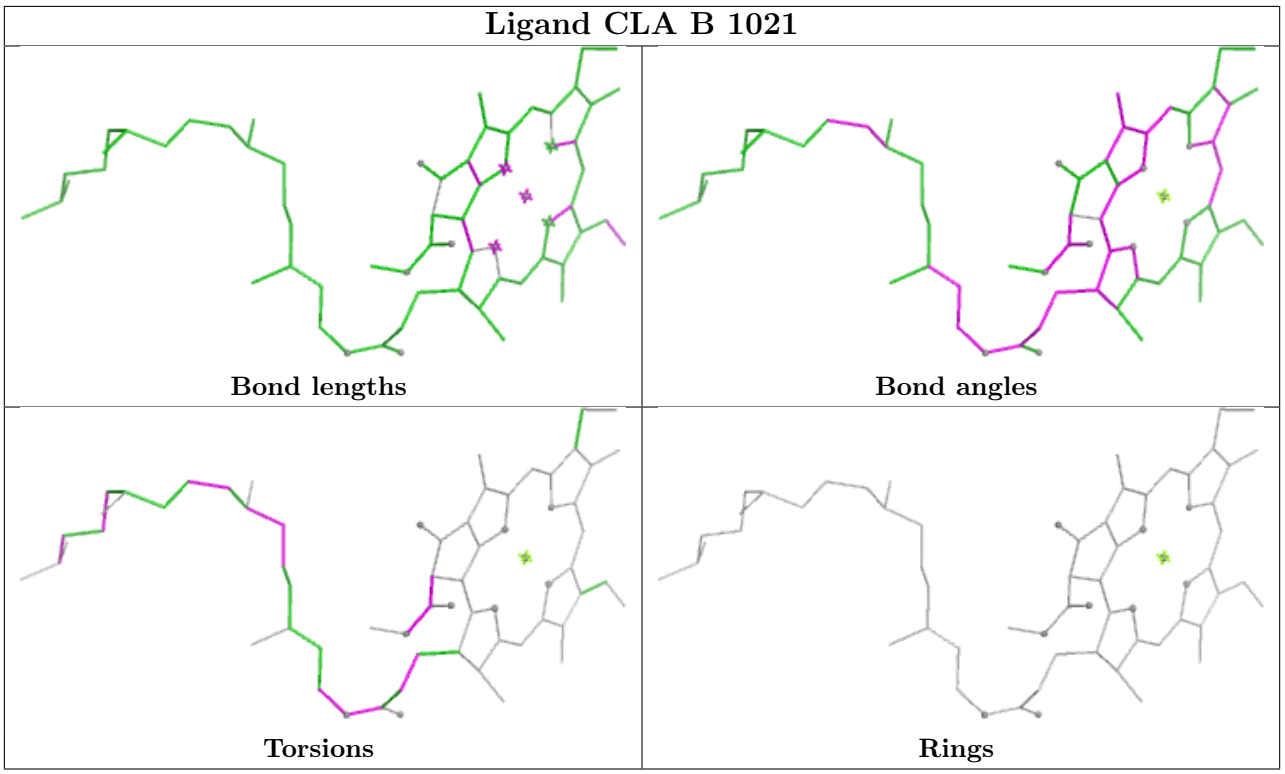
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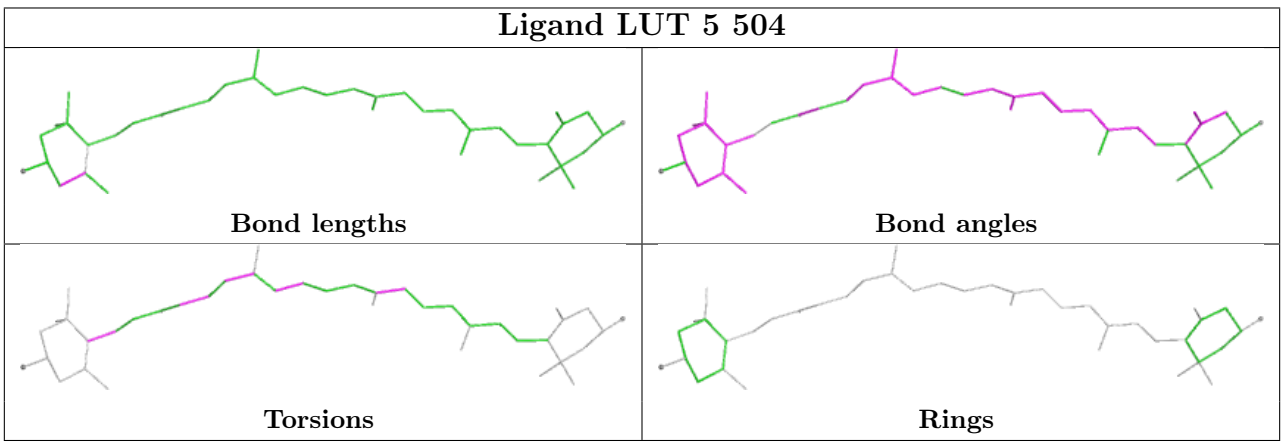
Ligand XAT 6 504



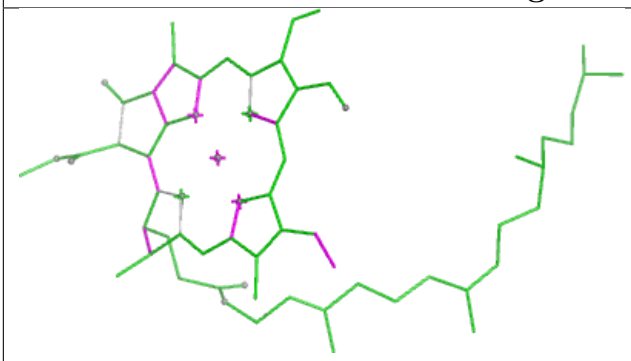
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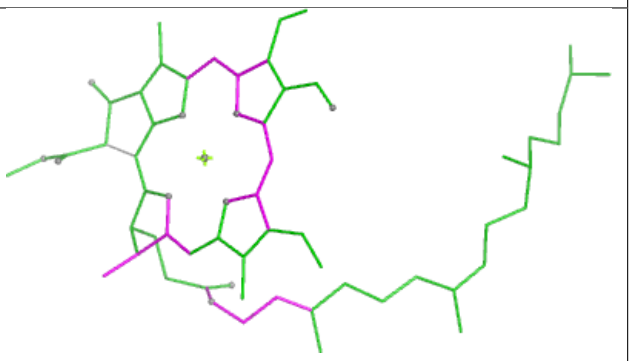
Ligand LUT 5 504



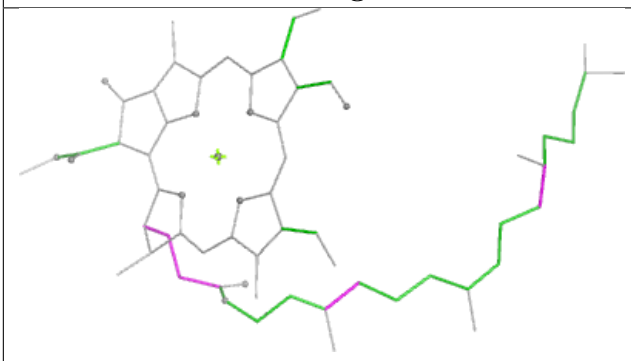
Ligand CHL 3 604



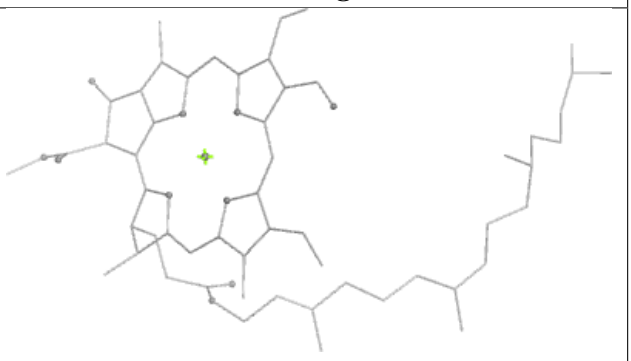
Bond lengths



Bond angles

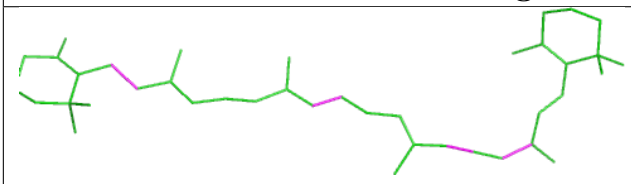


Torsions

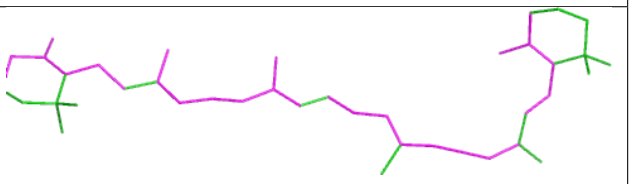


Rings

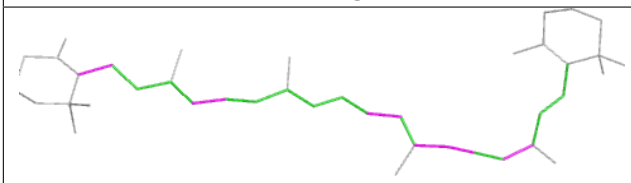
Ligand BCR F 4001



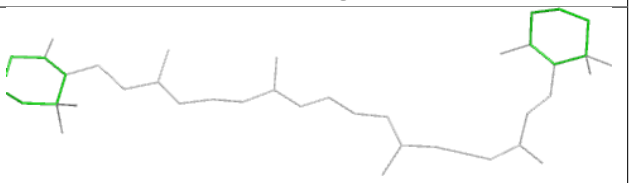
Bond lengths



Bond angles

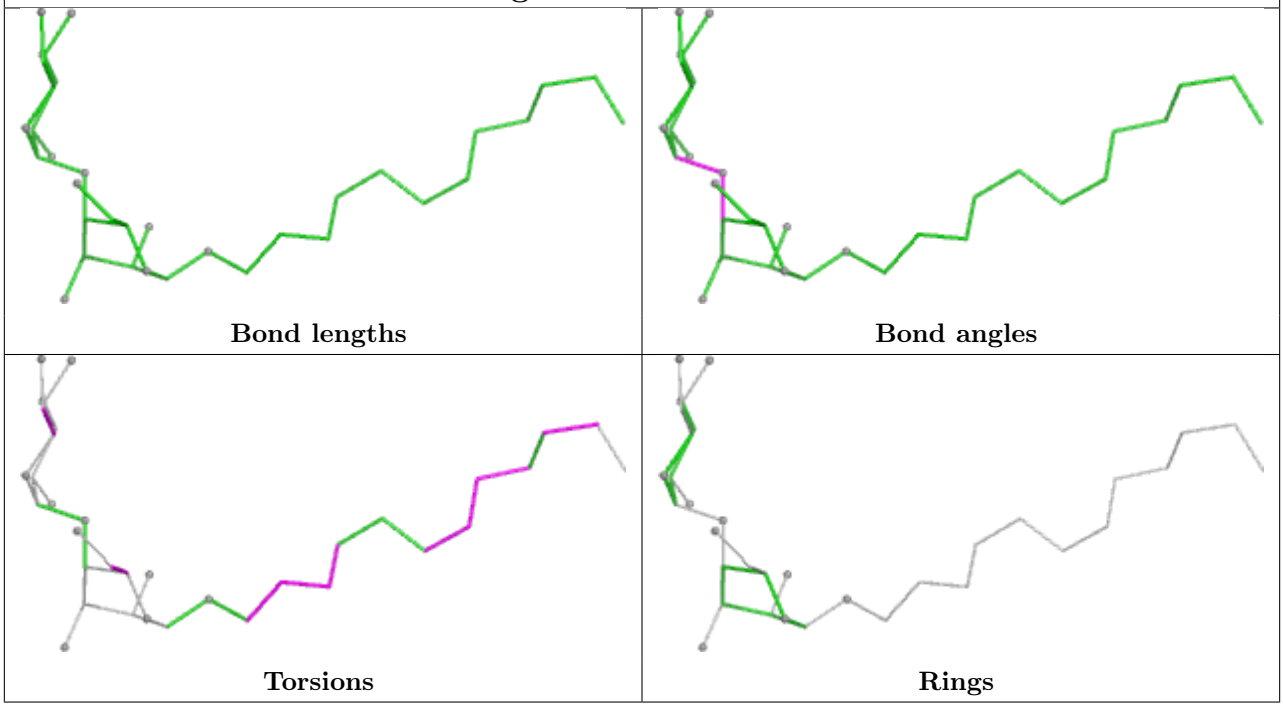


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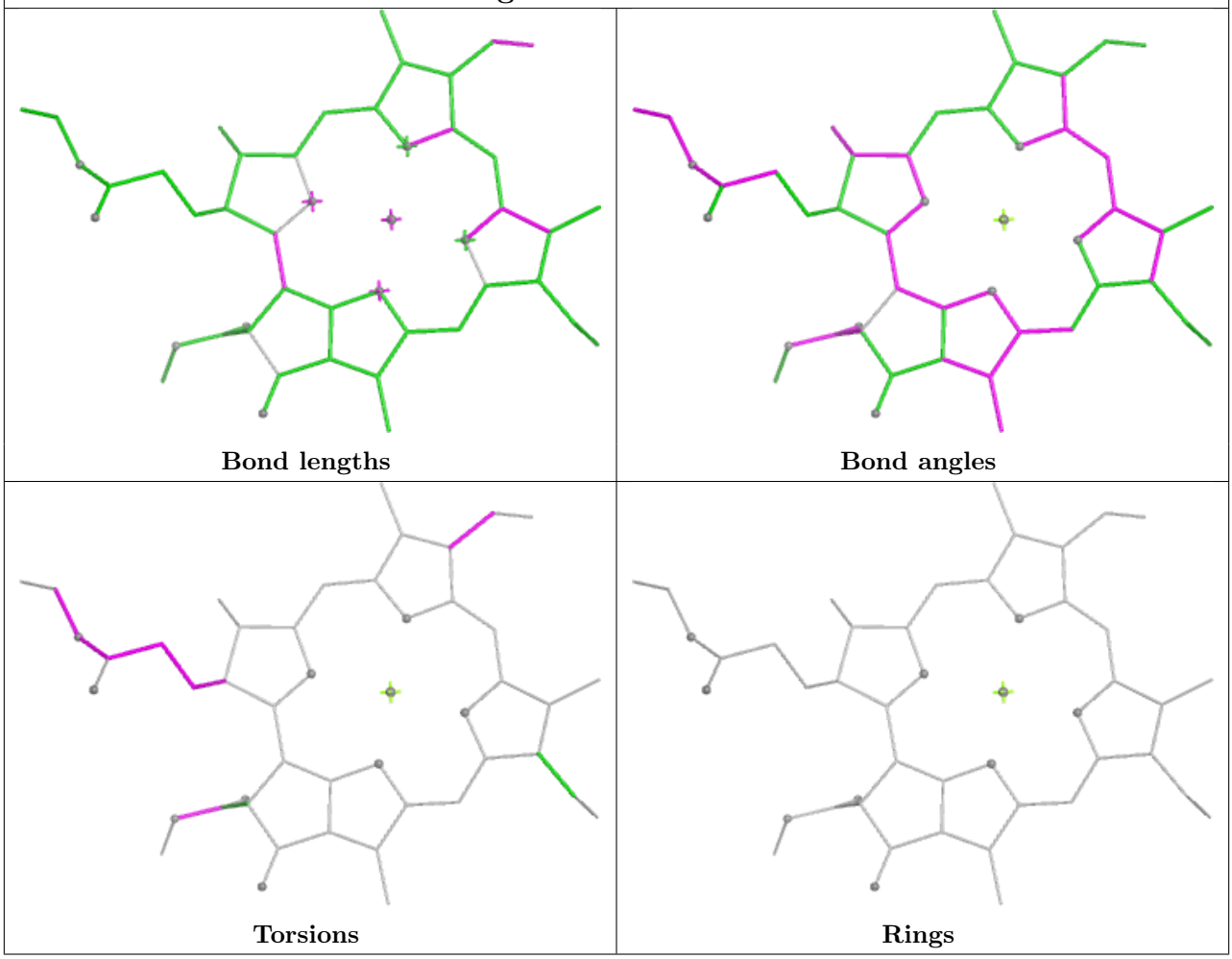


Rings

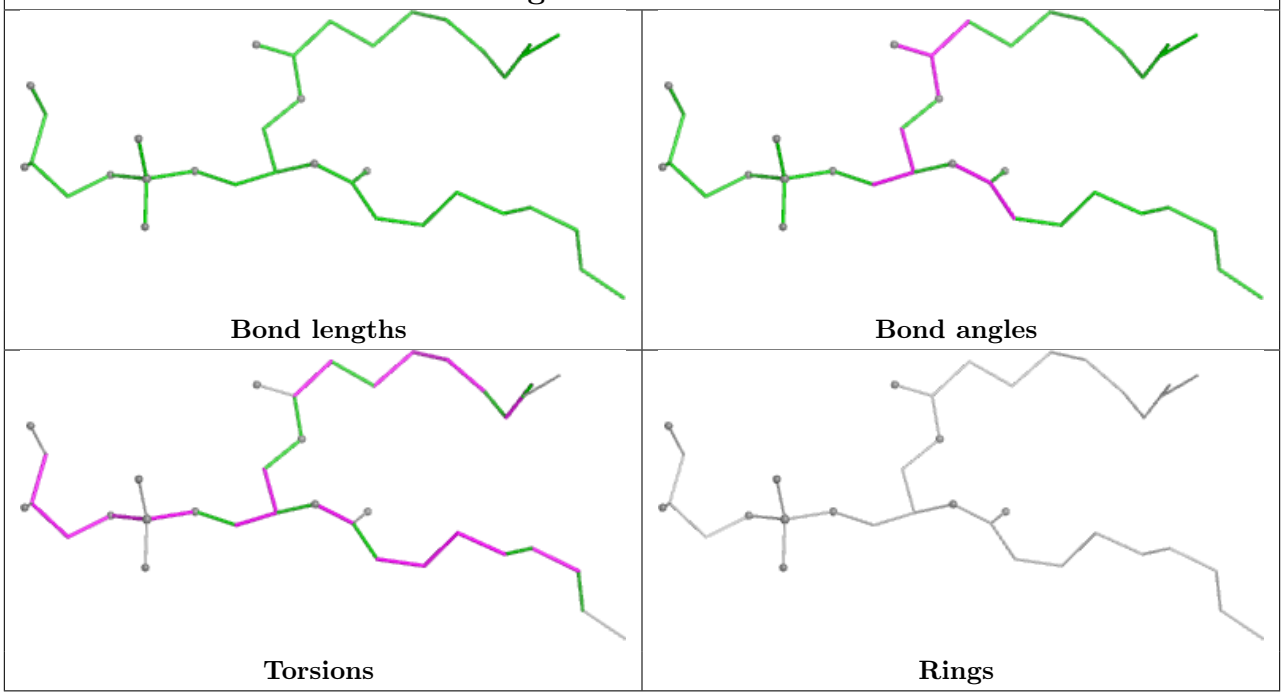
Ligand LMU A 5005



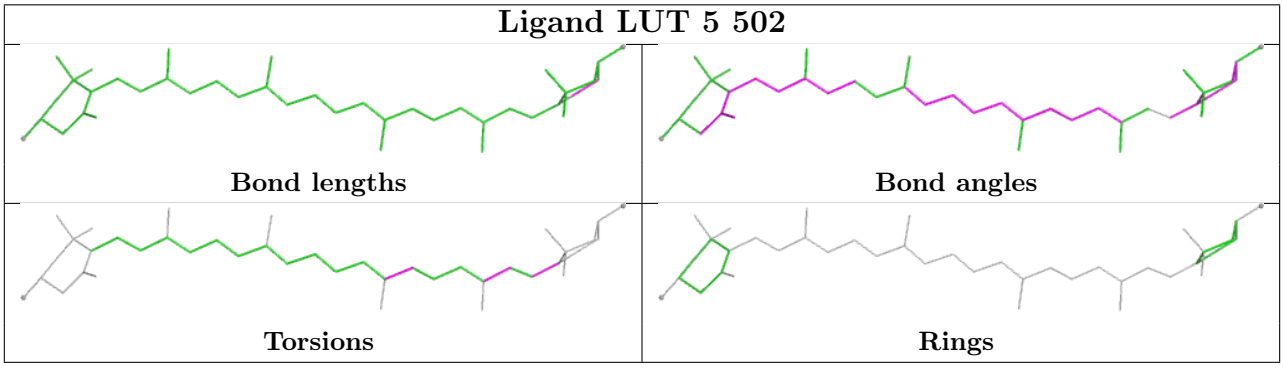
Ligand CLA F 1301



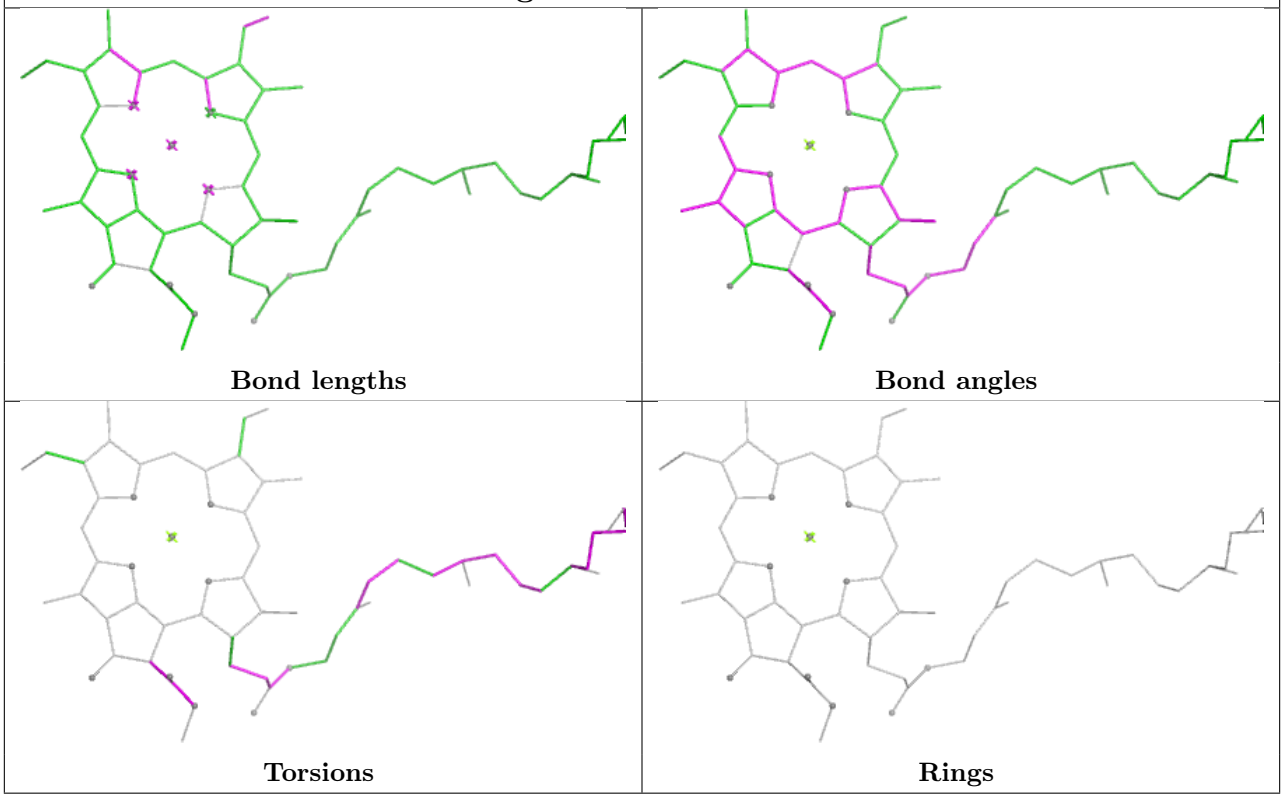
Ligand LHG 2 803



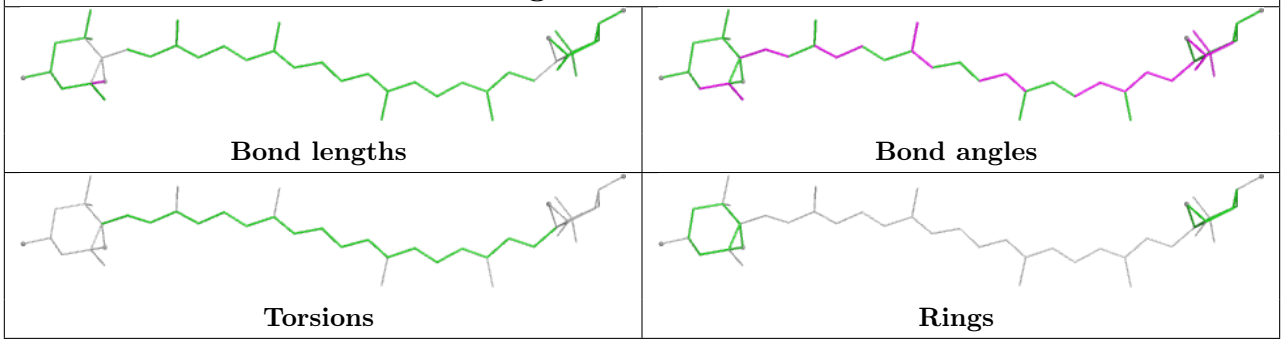
Ligand LUT 5 502



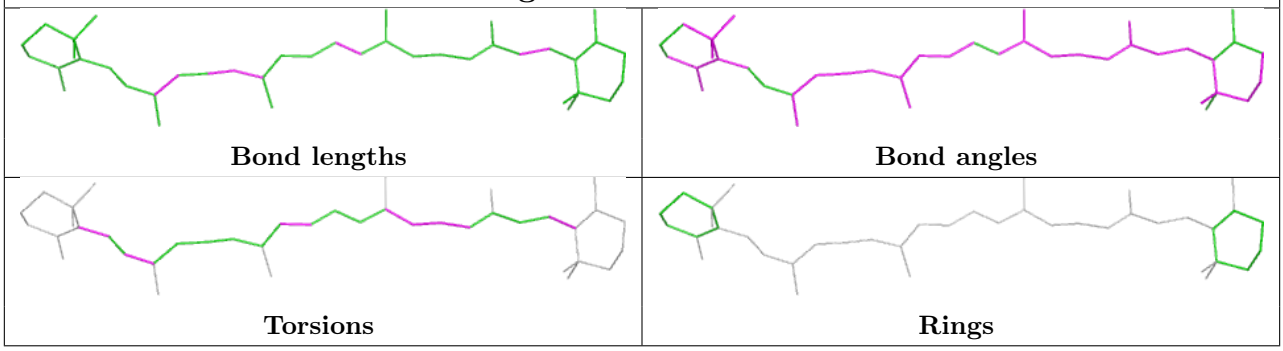
Ligand CLA B 1023



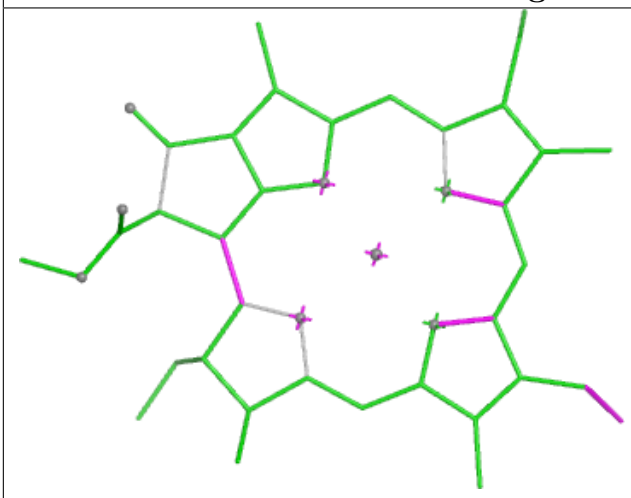
Ligand XAT 6 502



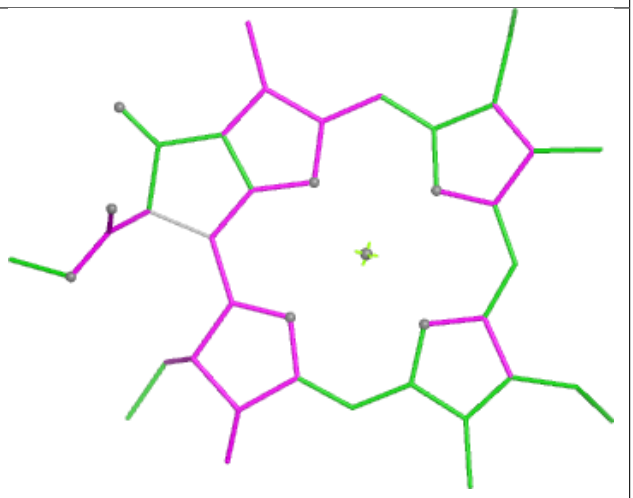
Ligand BCR J 4001



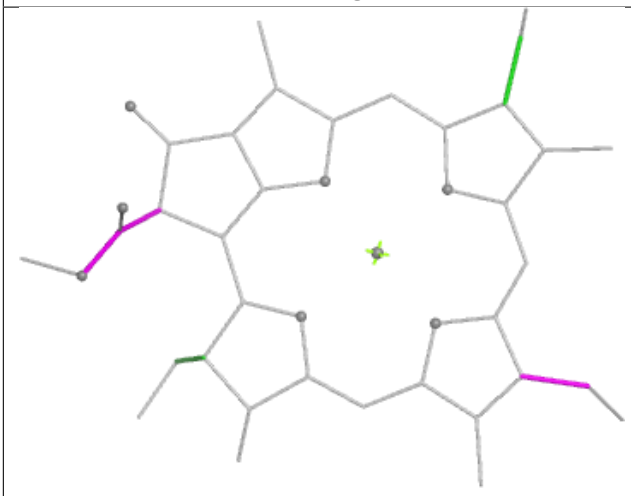
Ligand CLA 3 614



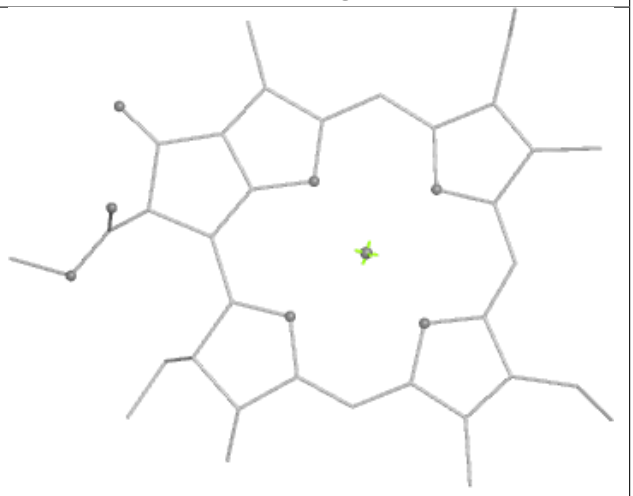
Bond lengths



Bond angles

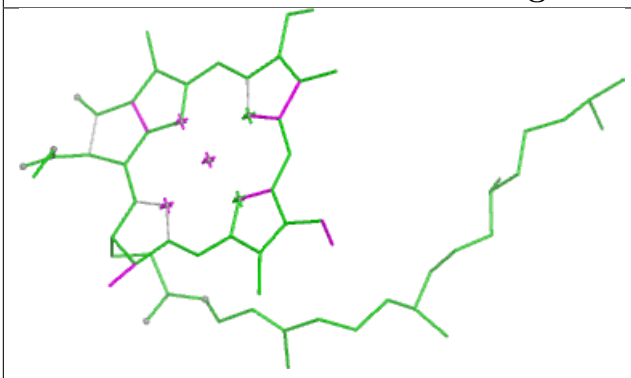


Torsions

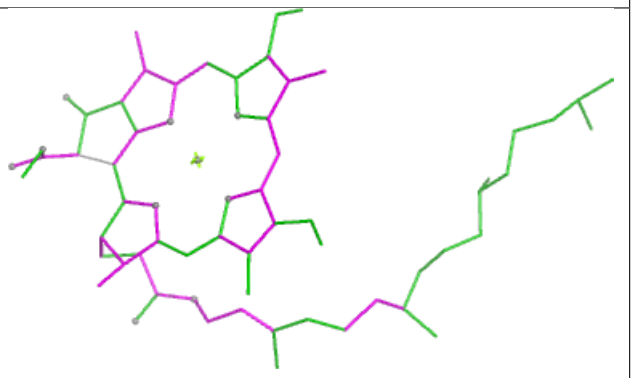


Rings

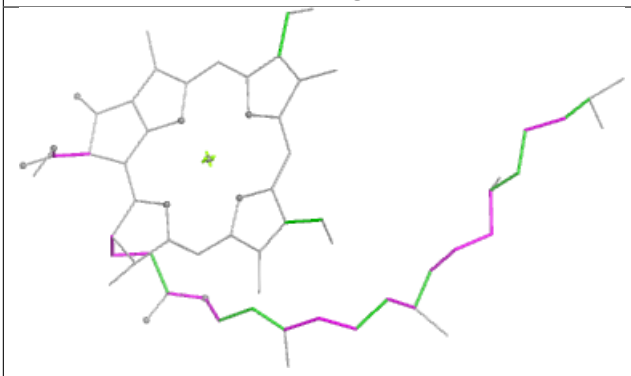
Ligand CLA 1 604



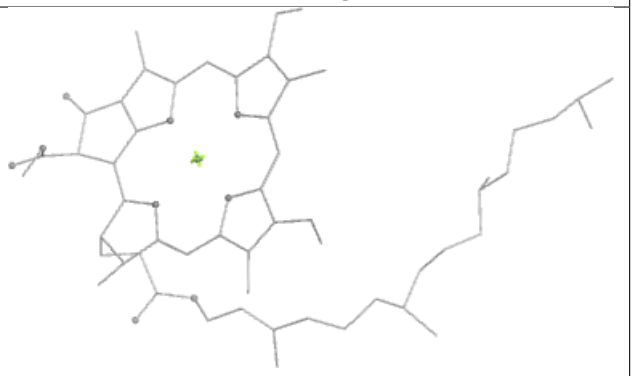
Bond lengths



Bond angles

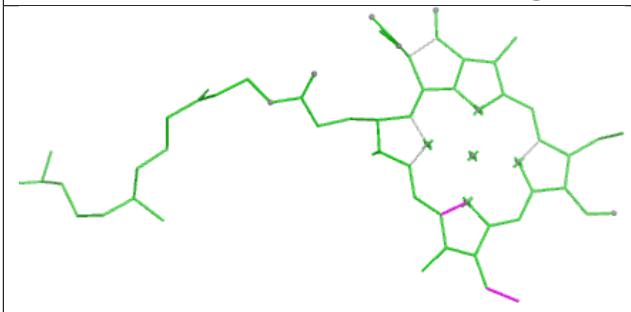


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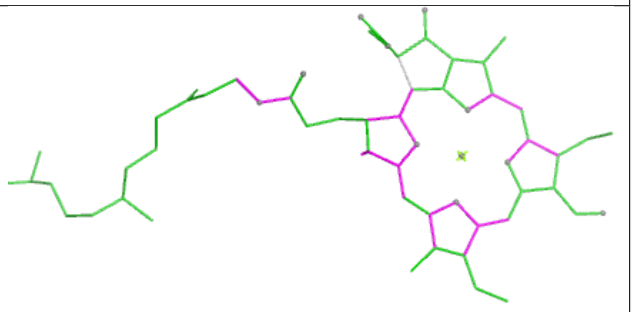


Rings

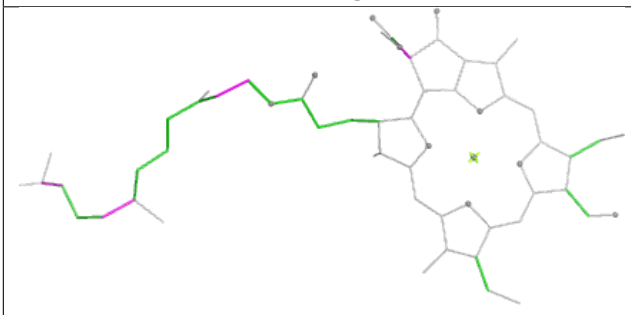
Ligand CHL 4 613



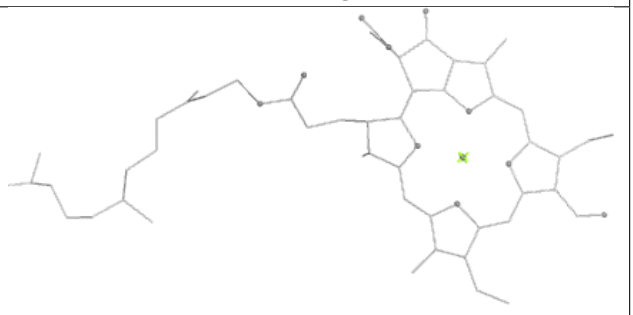
Bond lengths



Bond angles

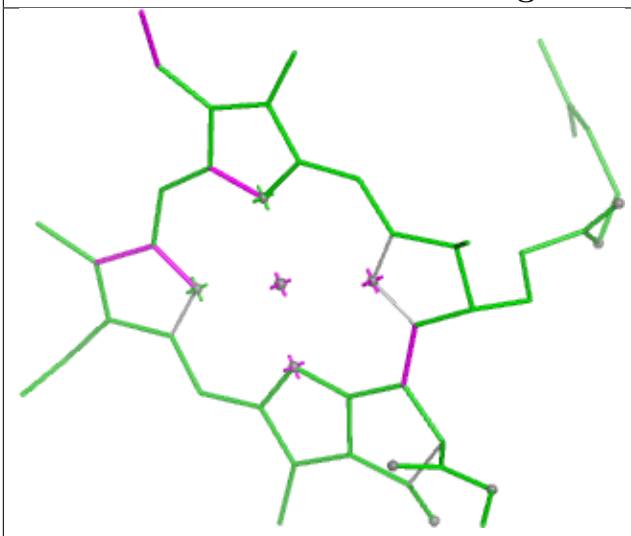


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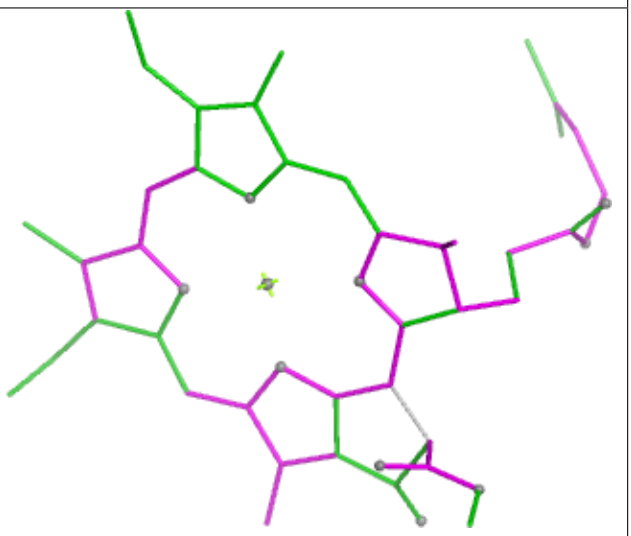


Rings

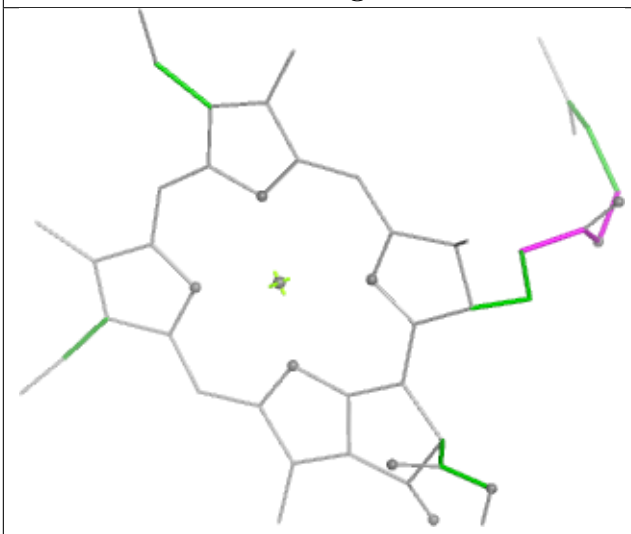
Ligand CLA L 1503



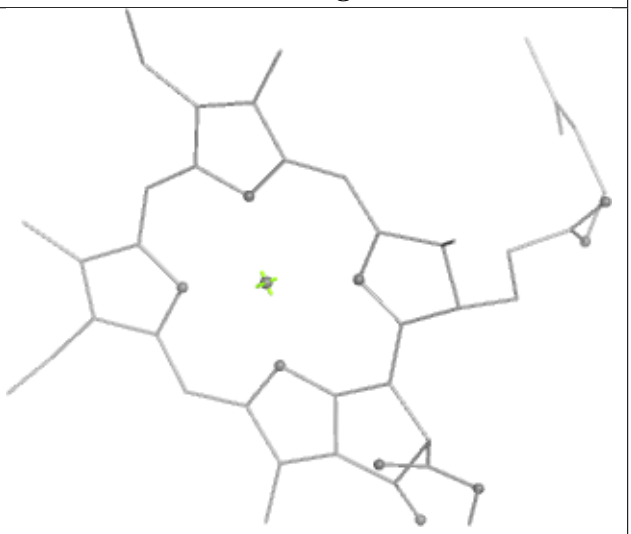
Bond lengths



Bond angles

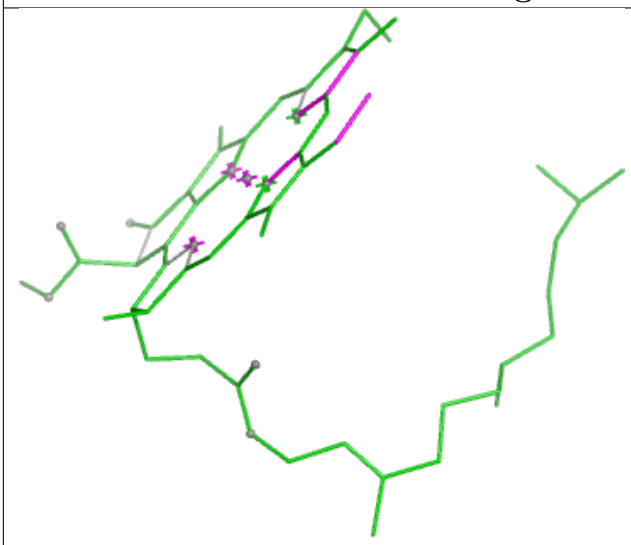


Torsions

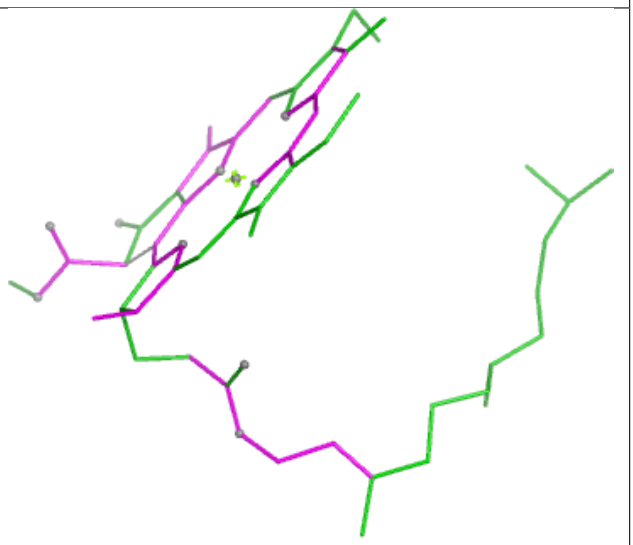


Rings

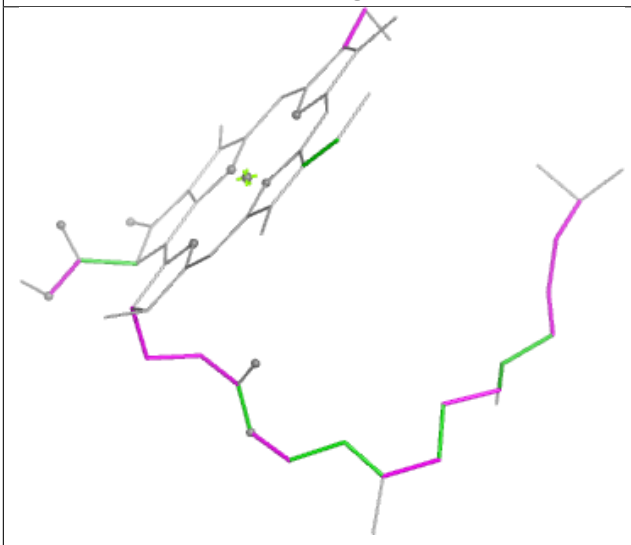
Ligand CLA A 1121



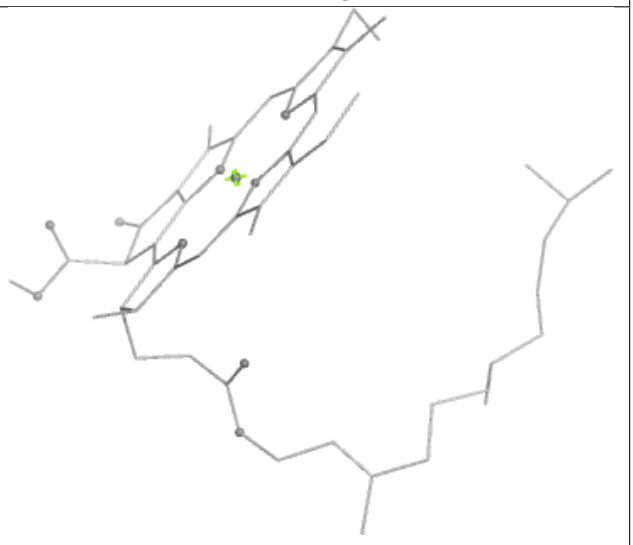
Bond lengths



Bond angles

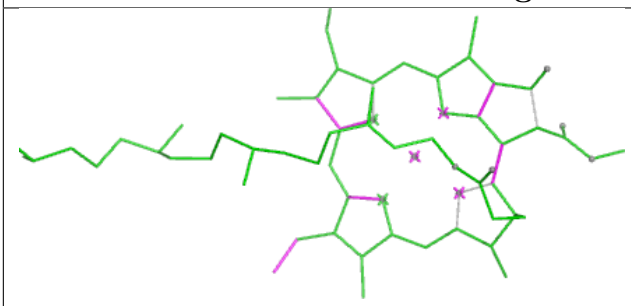


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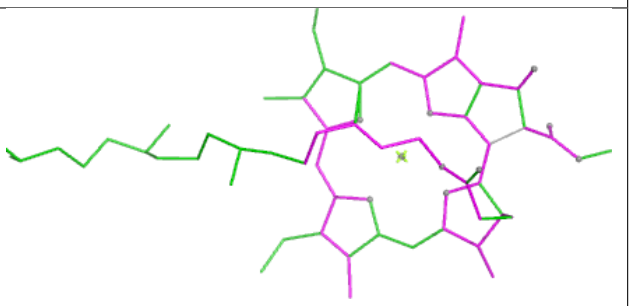


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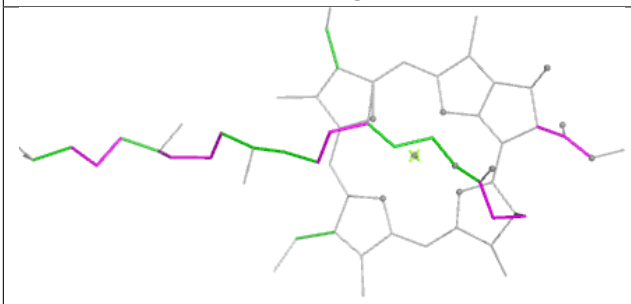
Ligand CLA A 1136



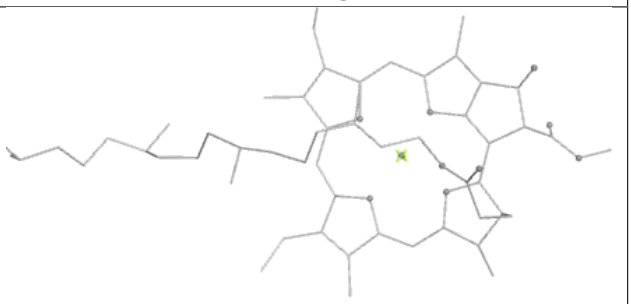
Bond lengths



Bond angles

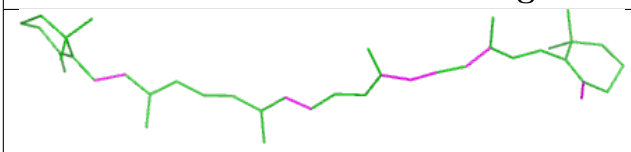


Torsions



Rings

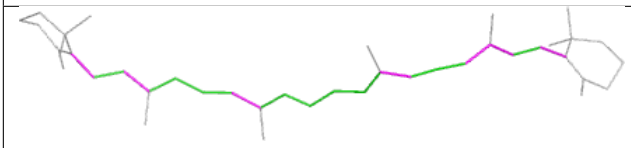
Ligand BCR J 4002



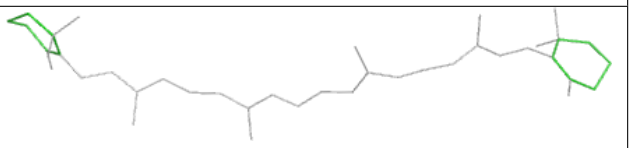
Bond lengths



Bond angles

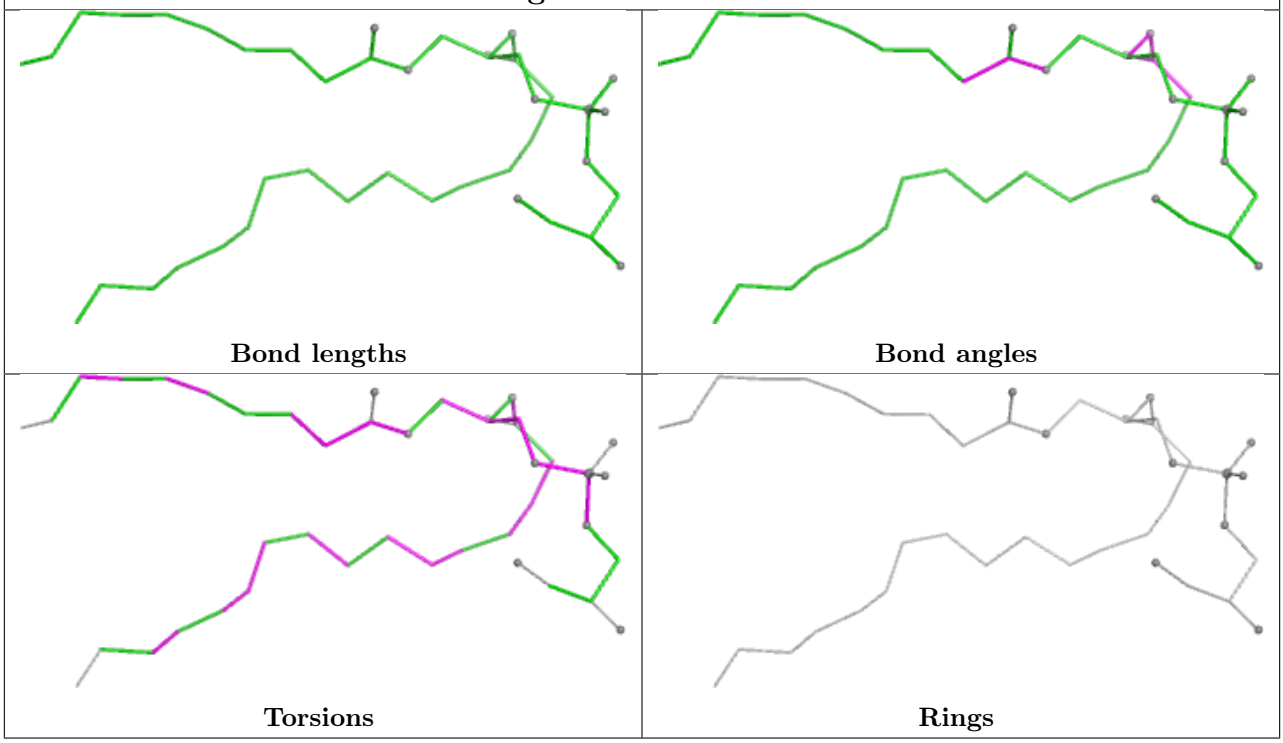


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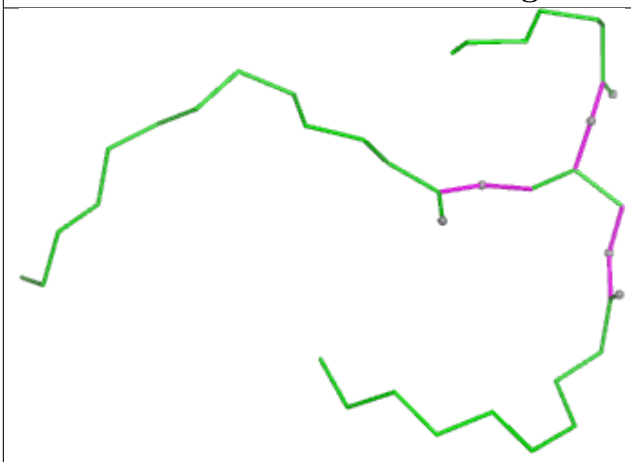


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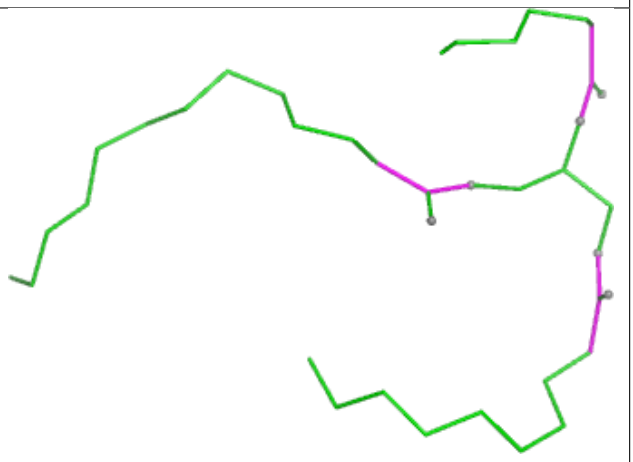
Ligand LHG 2 802



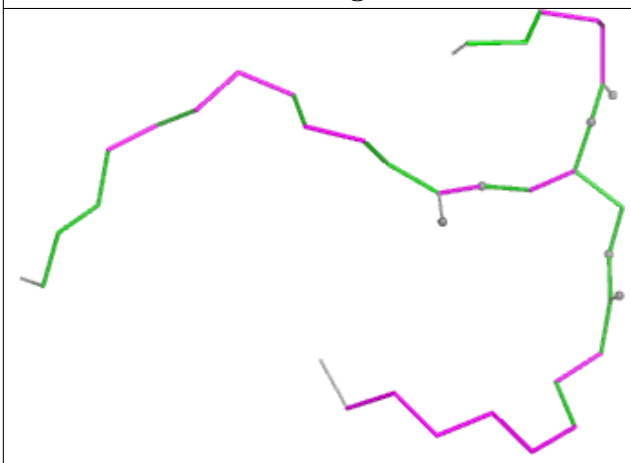
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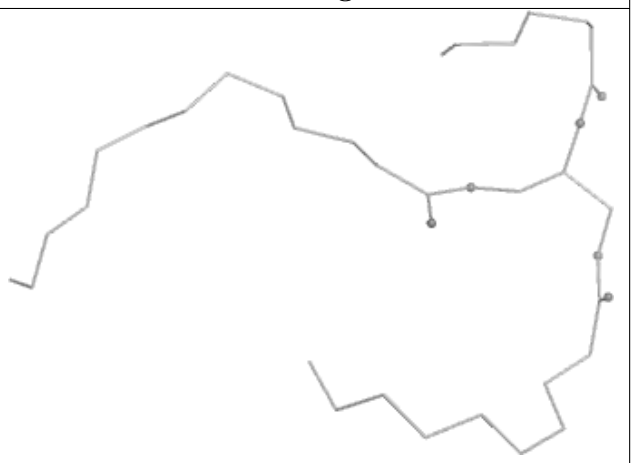
Bond lengths



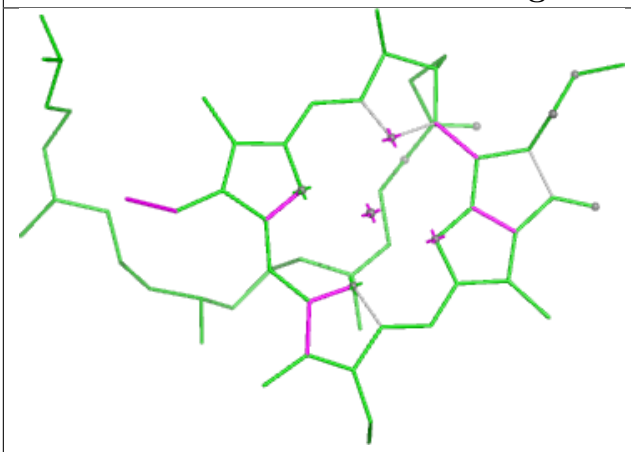
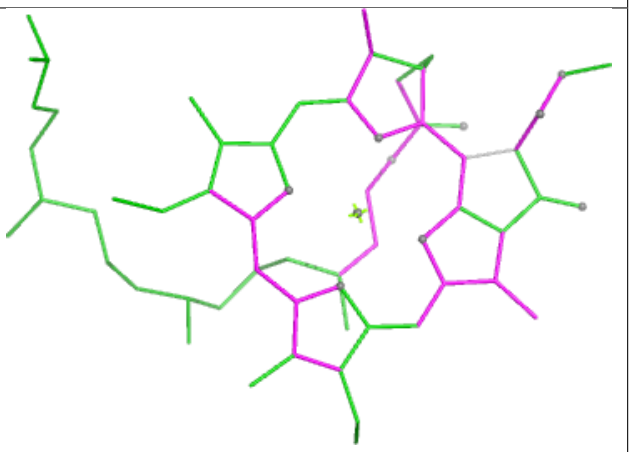
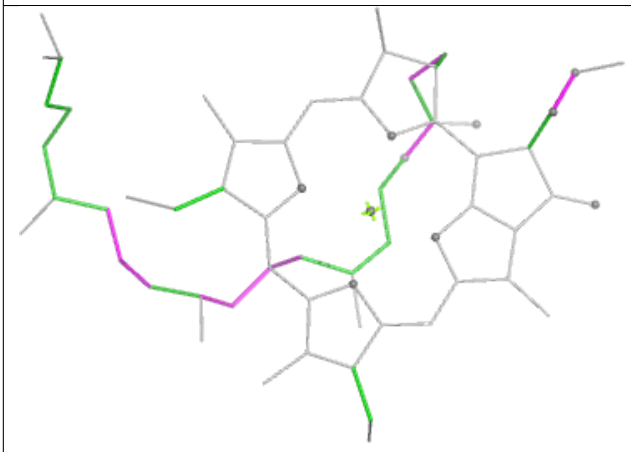
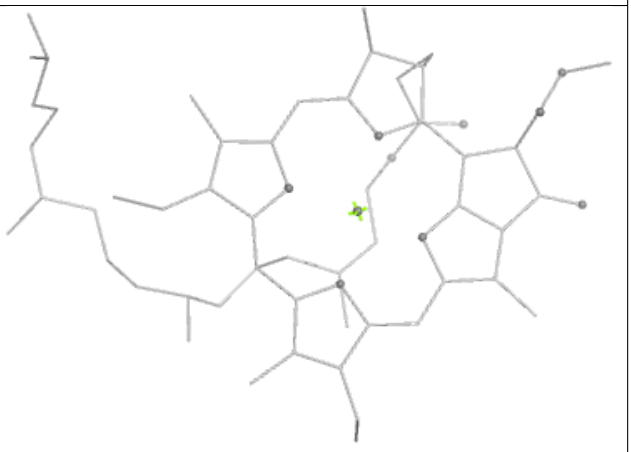
Bond angles

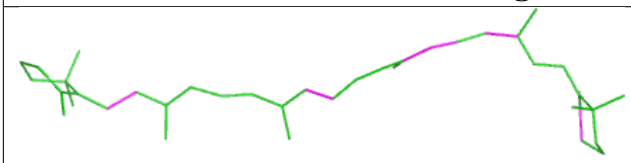
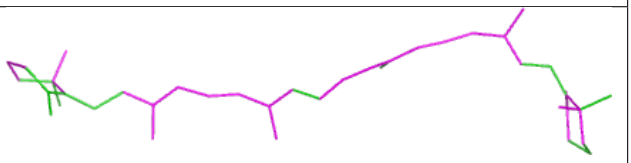
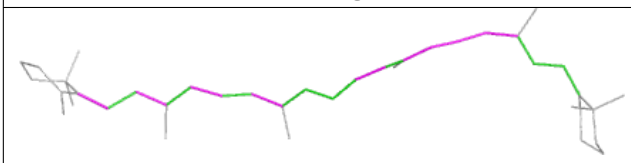
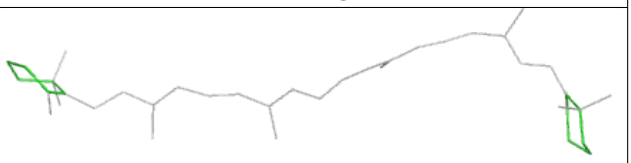


Torsions

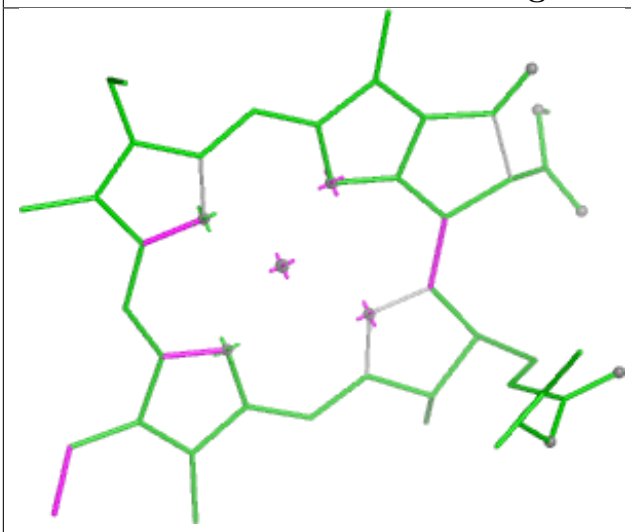


Rings

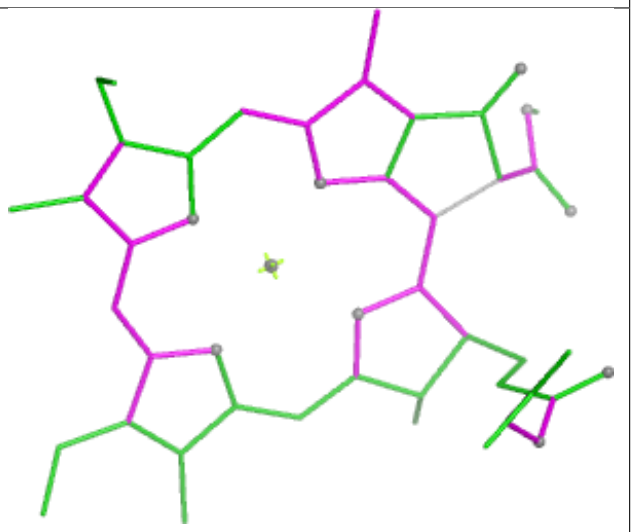
Ligand CLA 4 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR O 4001	
 Bond lengths	 Bond angles
 Torsions	 Rings

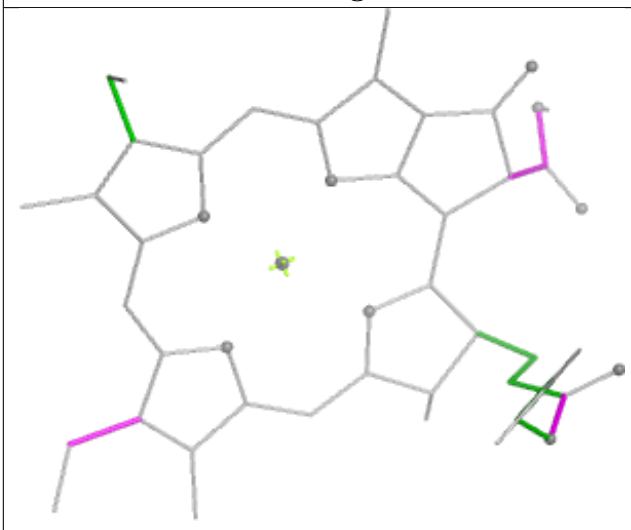
Ligand CLA 1 606



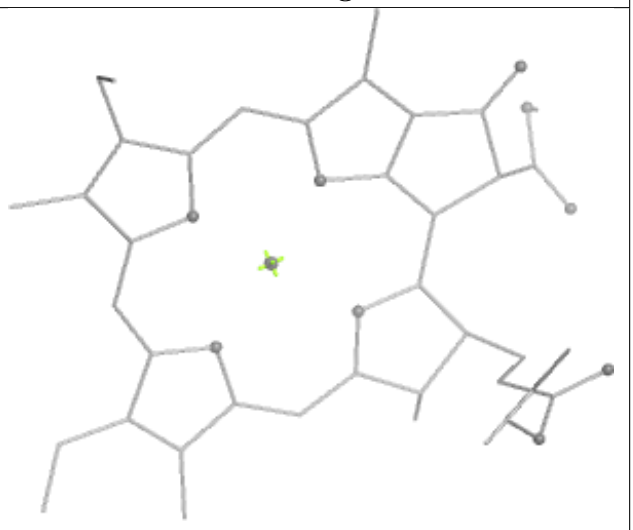
Bond lengths



Bond angles

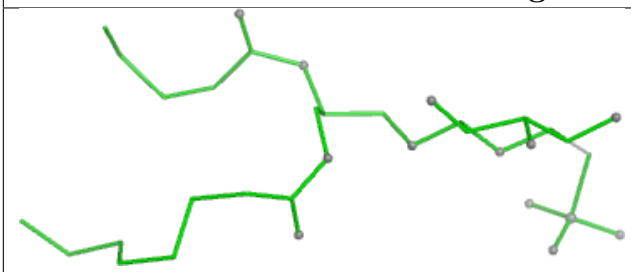


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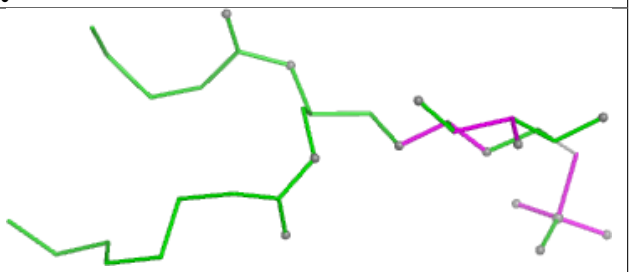


Rings

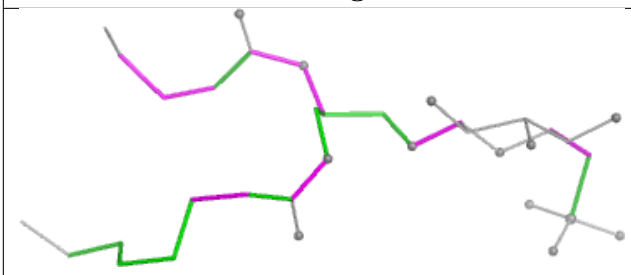
Ligand SQD 3 806



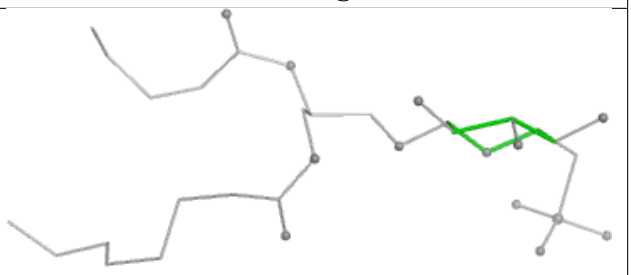
Bond lengths



Bond angles

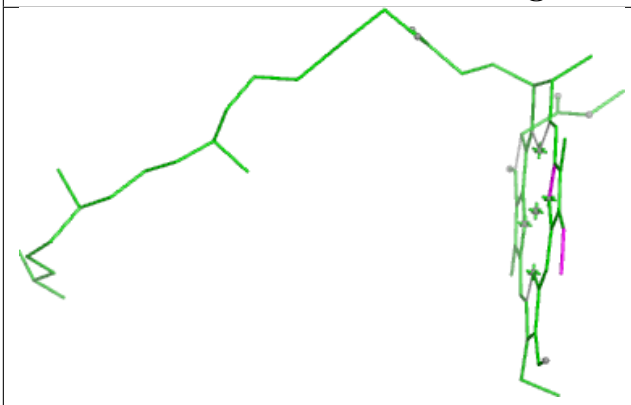


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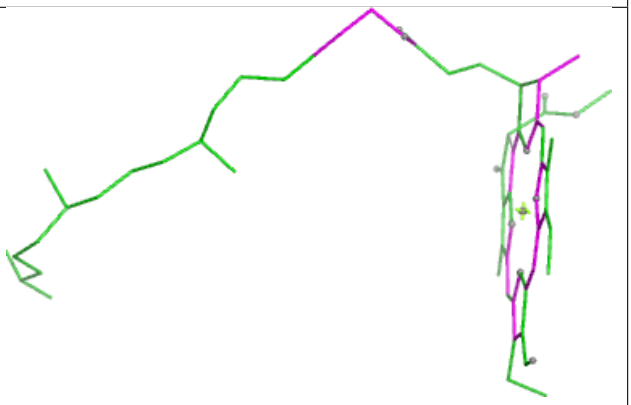


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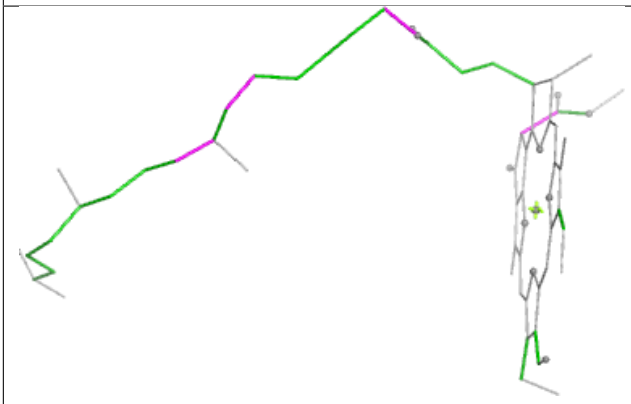
Ligand CHL 1 609



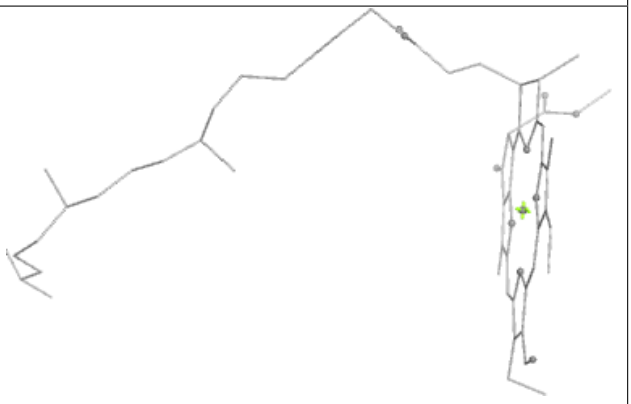
Bond lengths



Bond angles

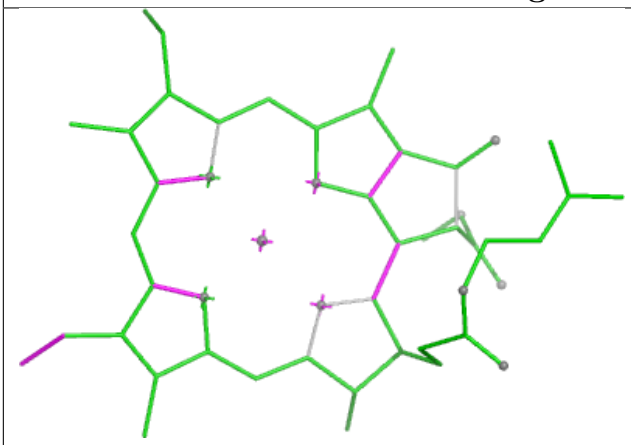


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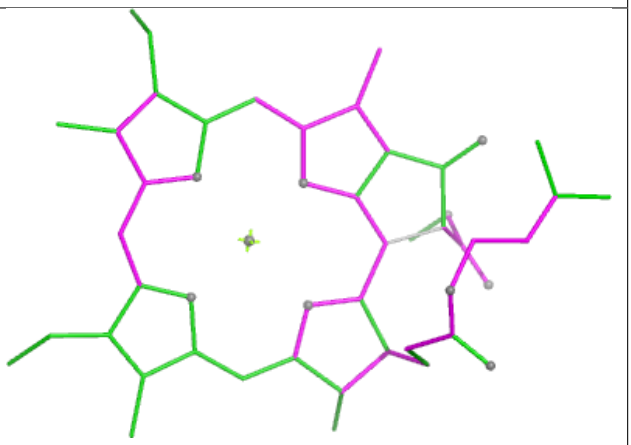


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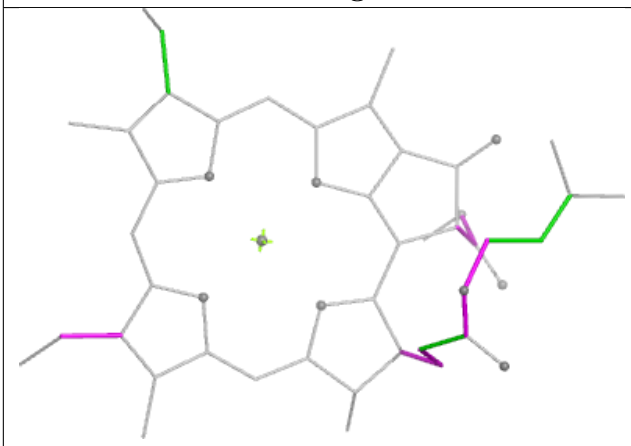
Ligand CLA 4 606



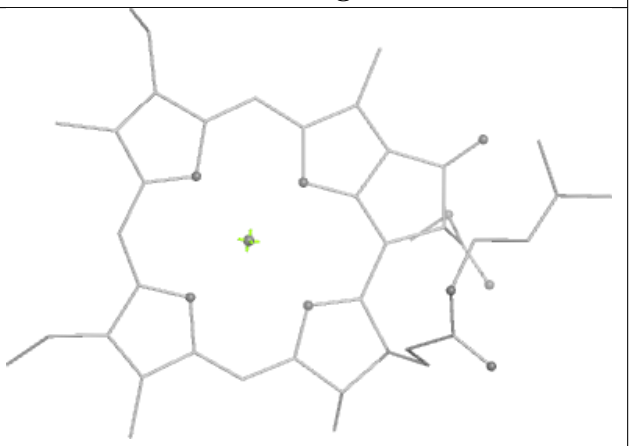
Bond lengths



Bond angles

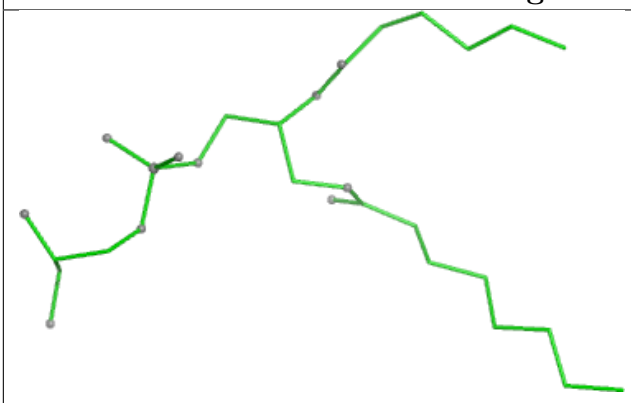


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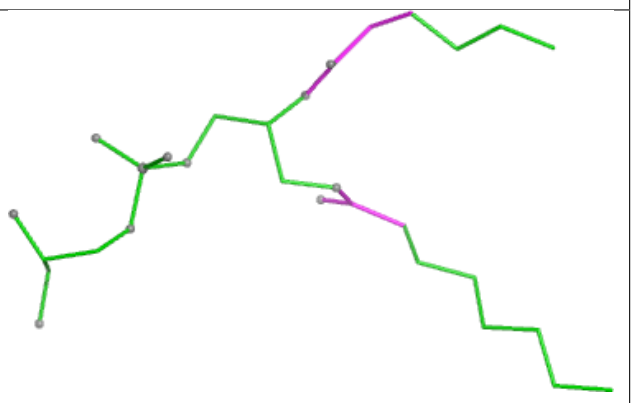


Rings

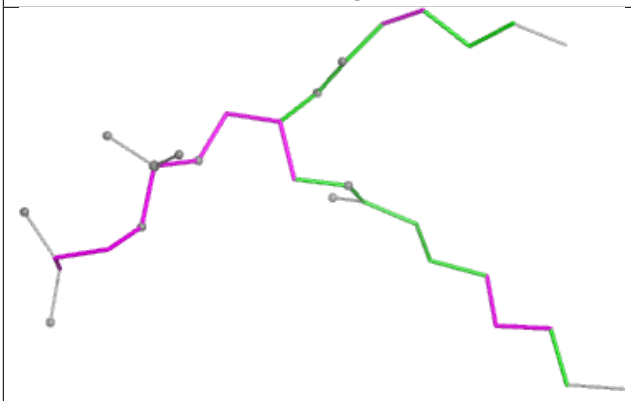
Ligand LHG 1 803



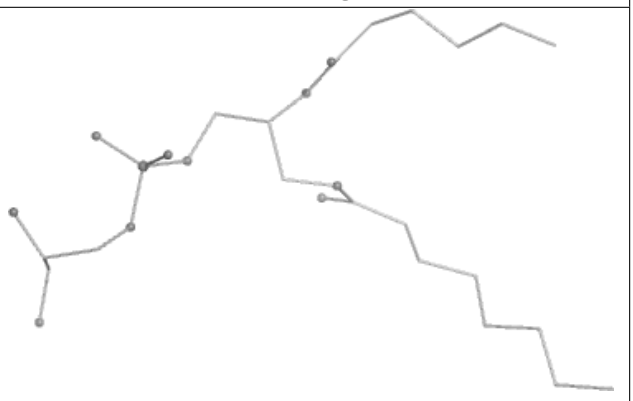
Bond lengths



Bond angles

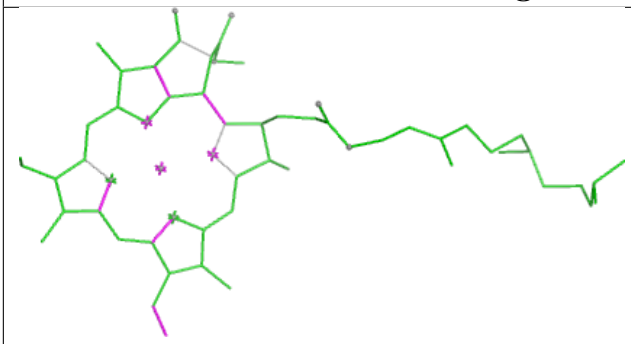


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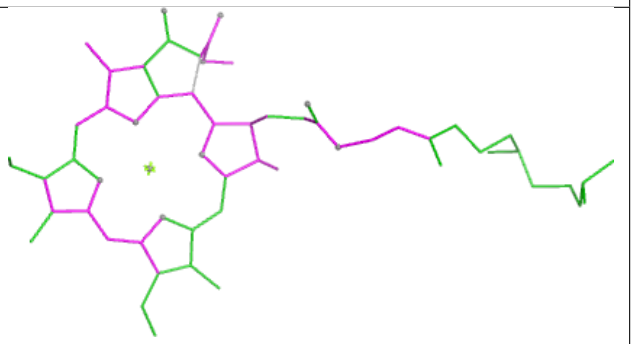


Rings

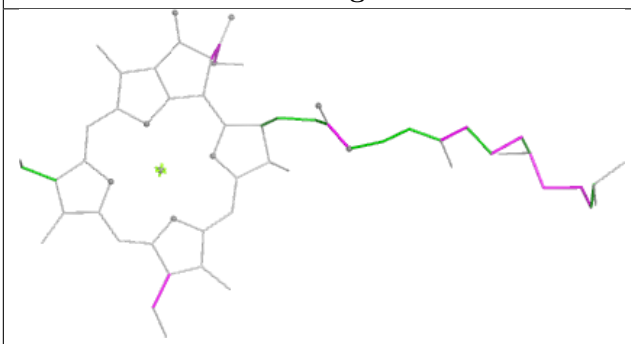
Ligand CLA A 1124



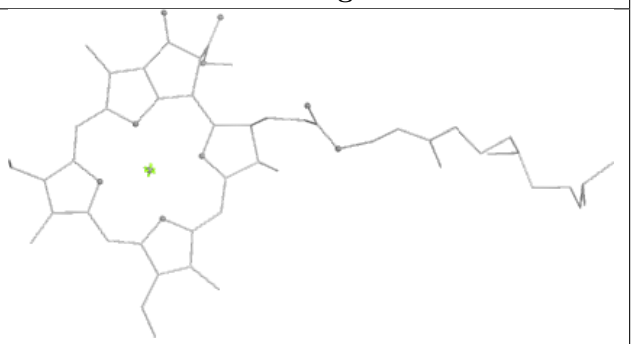
Bond lengths



Bond angles

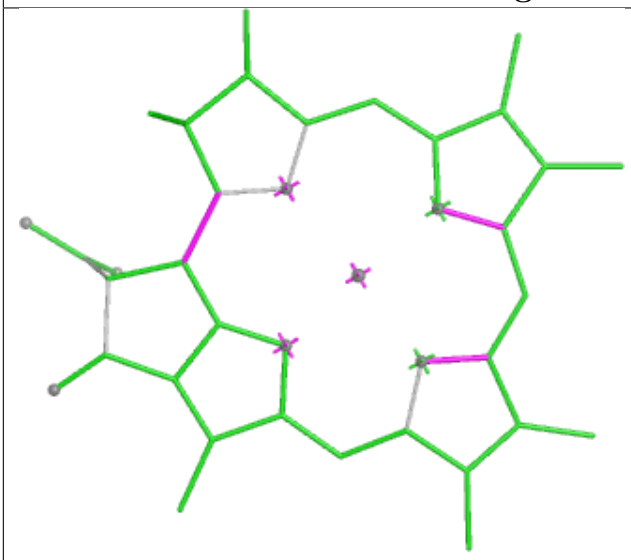


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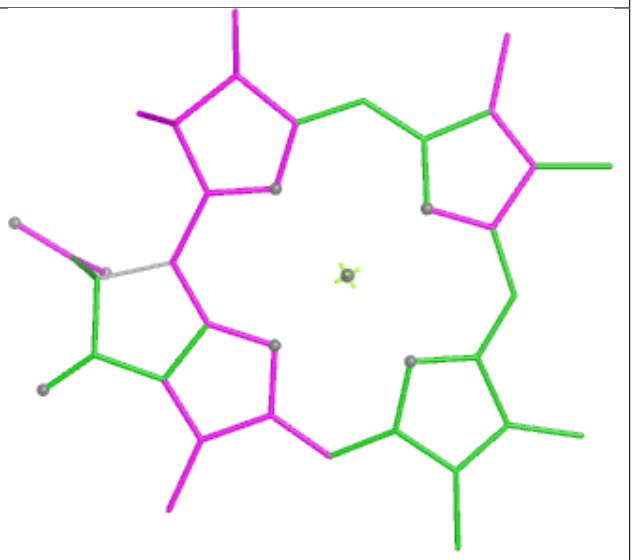


Rings

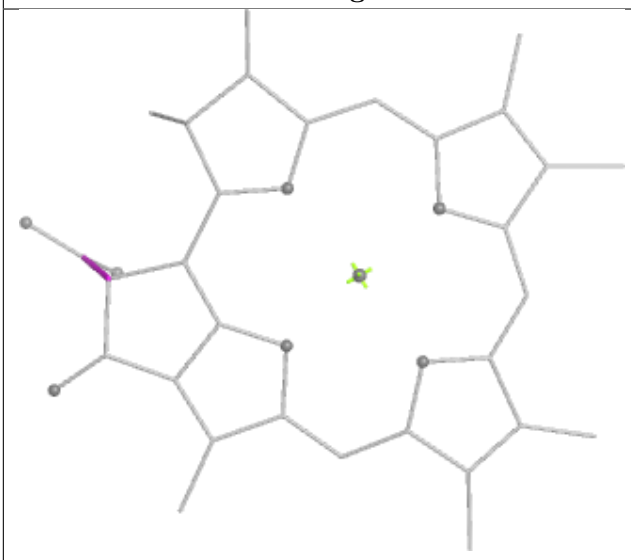
Ligand CLA O 1802



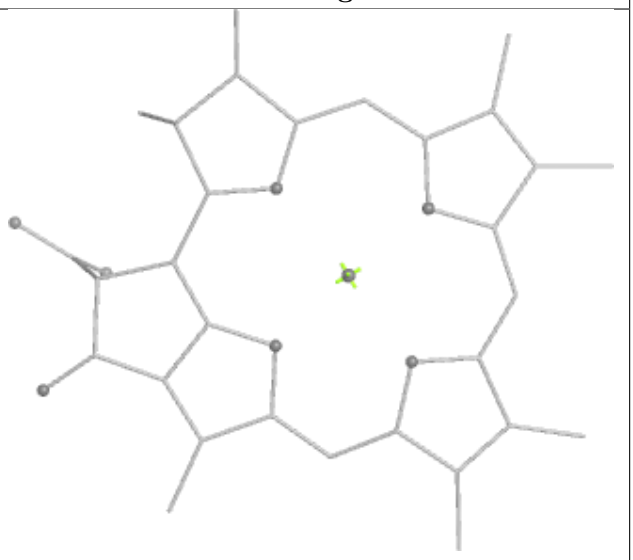
Bond lengths



Bond angles

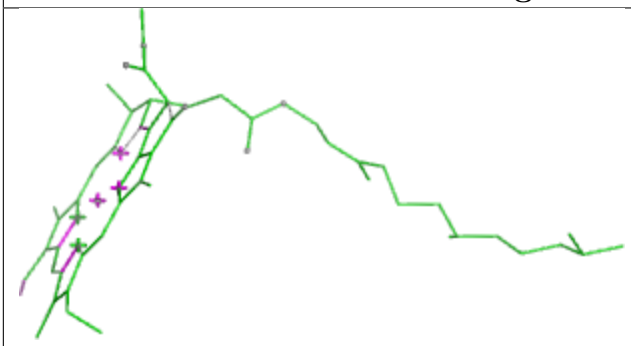


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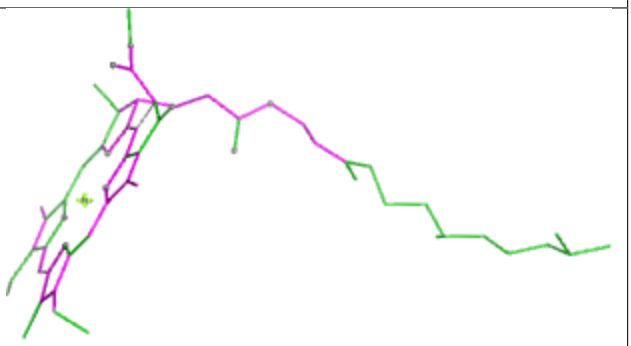


Rings

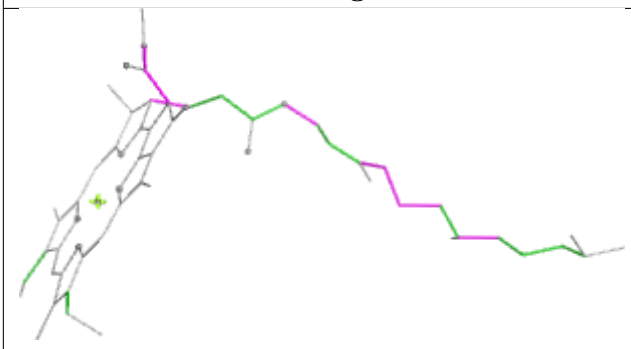
Ligand CLA A 1137



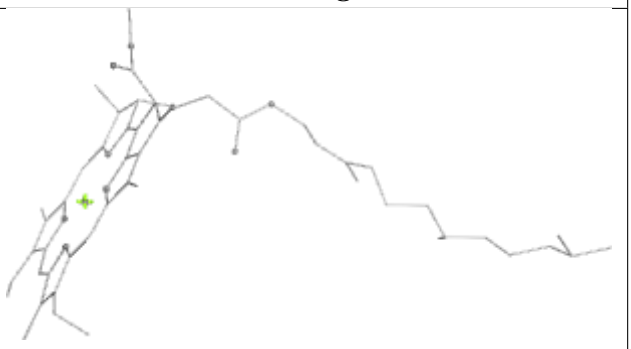
Bond lengths



Bond angles

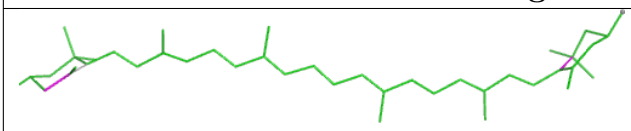


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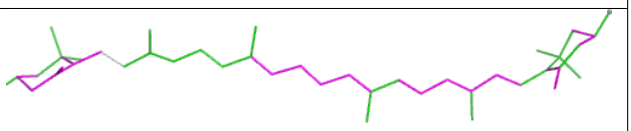


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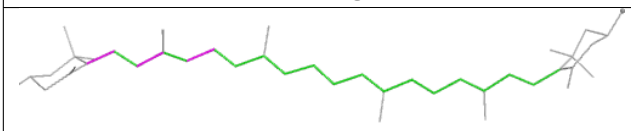
Ligand LUT 3 501



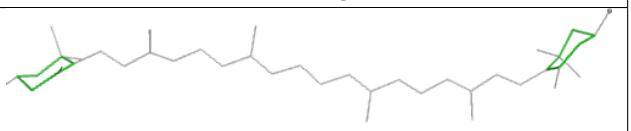
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Bond angles

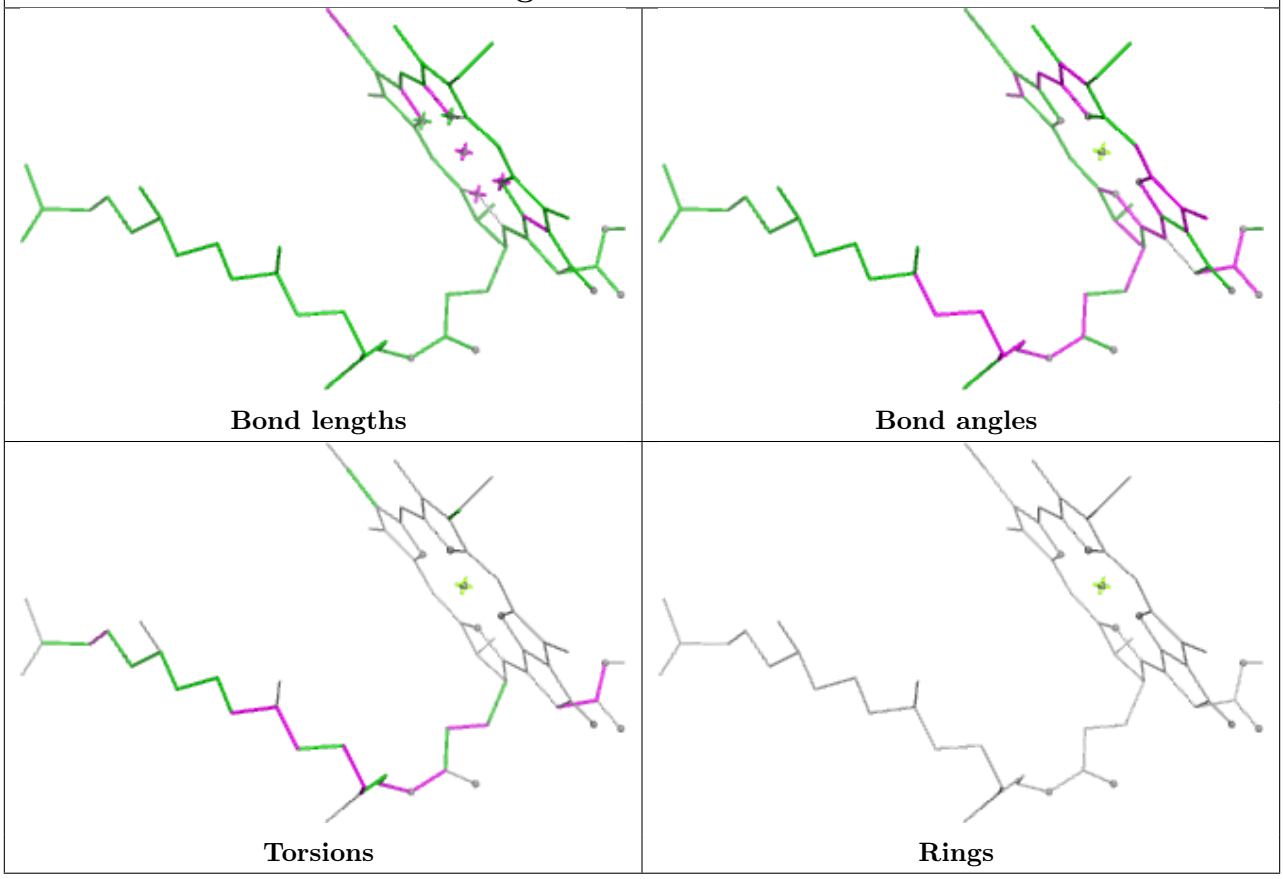


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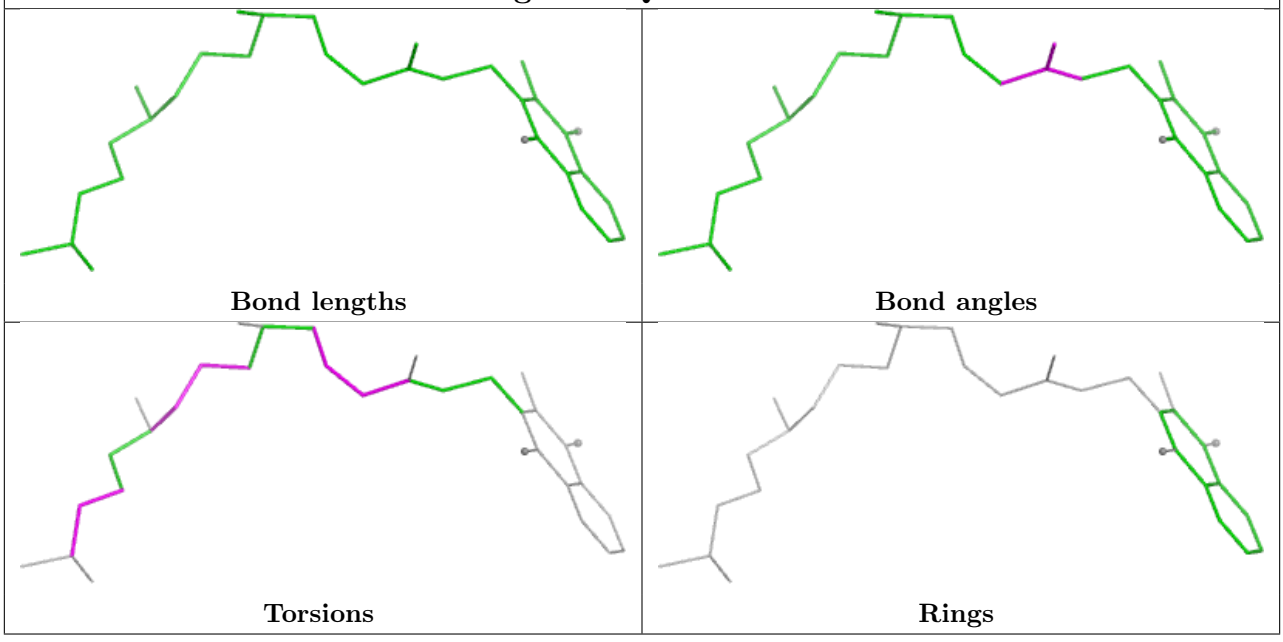


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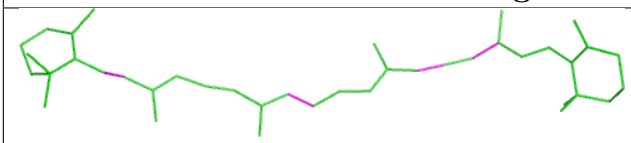
Ligand CLA B 1211



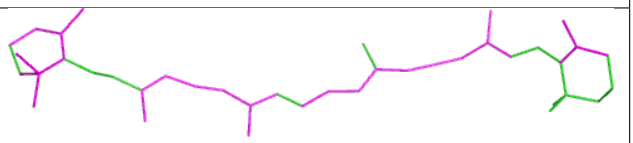
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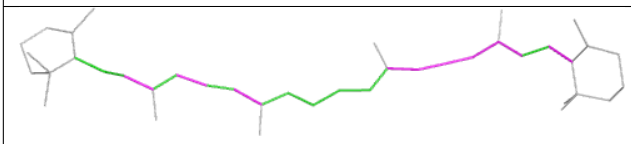
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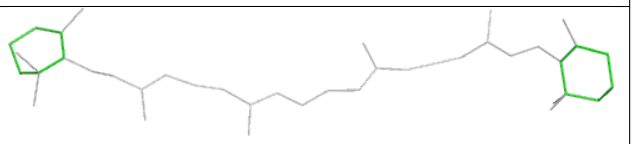
Bond lengths



Bond angles

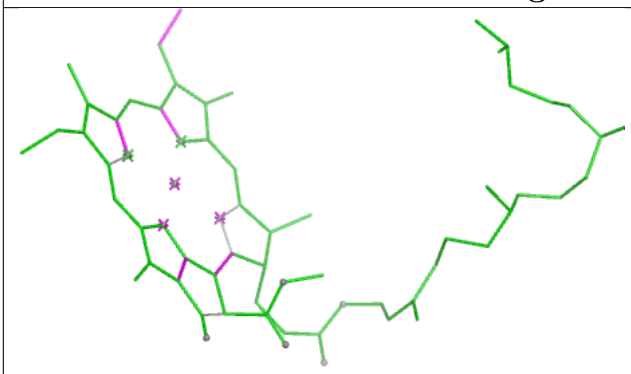


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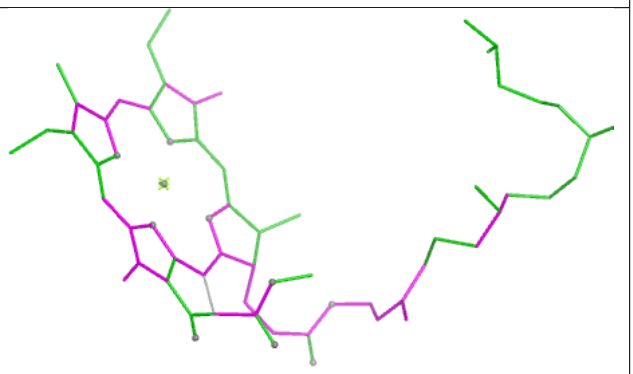


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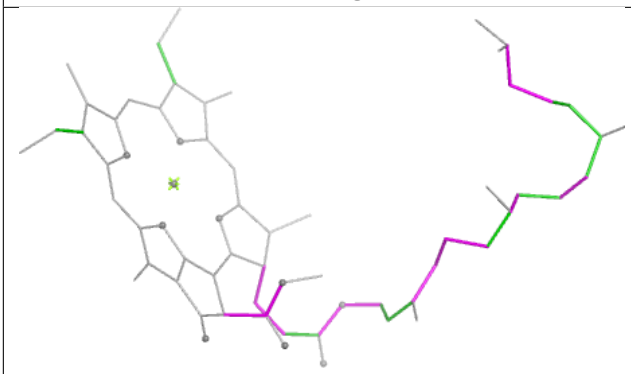
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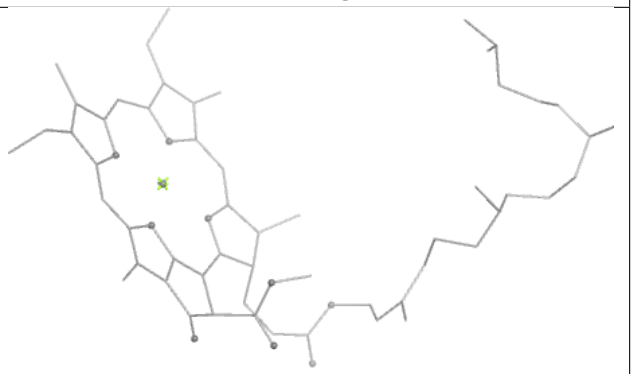
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Bond angles

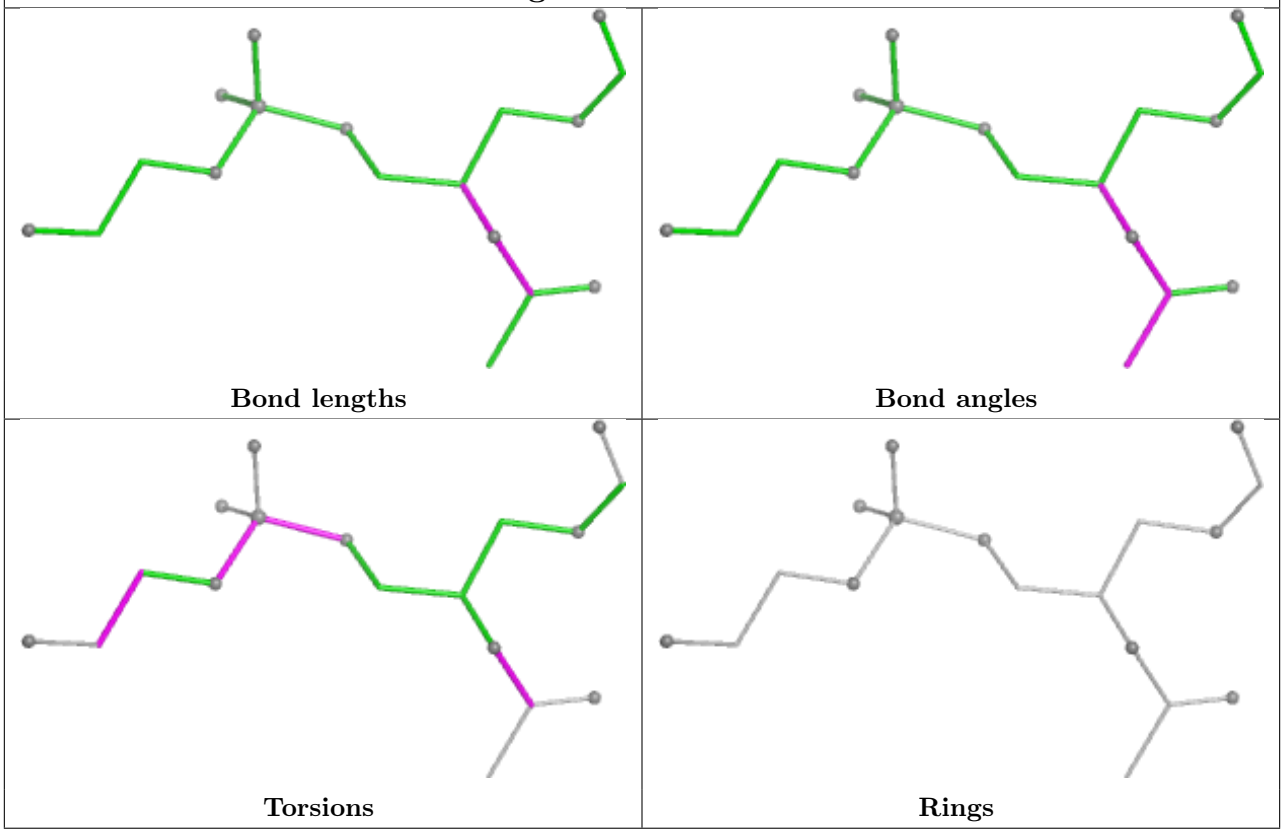


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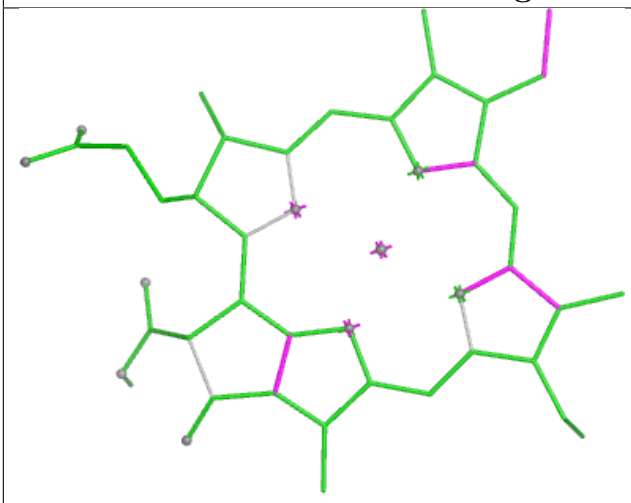


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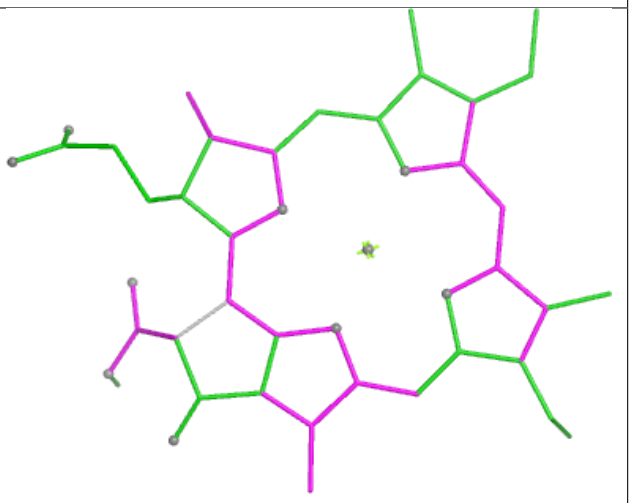
Ligand PTY 1 806



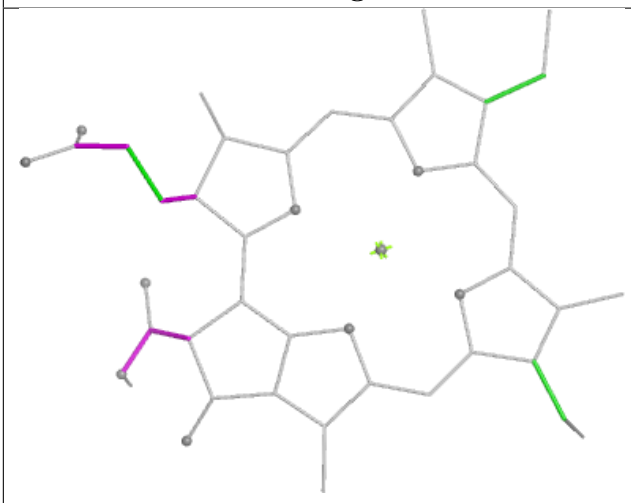
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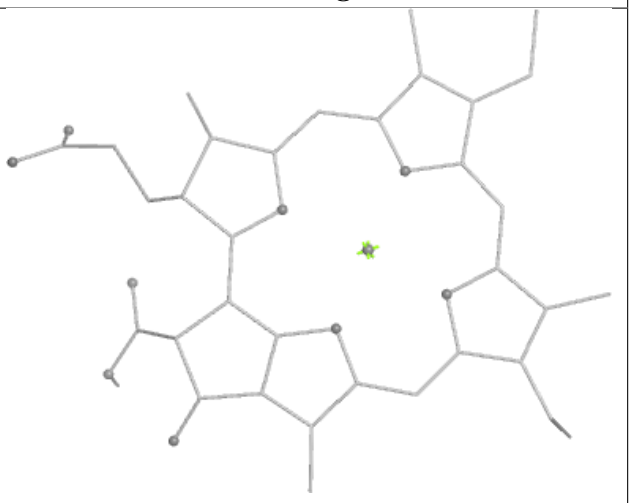
Bond lengths



Bond angles

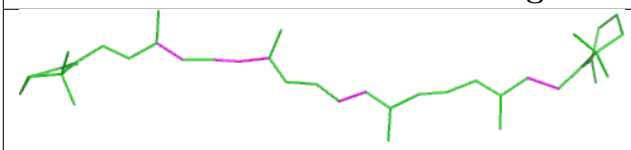


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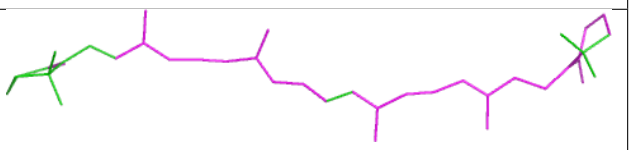


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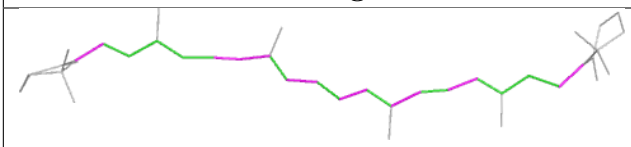
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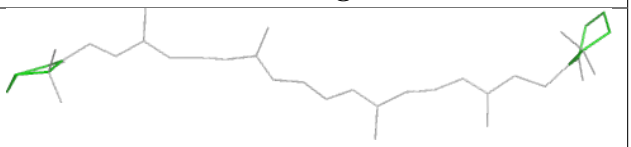
Bond lengths



Bond angles

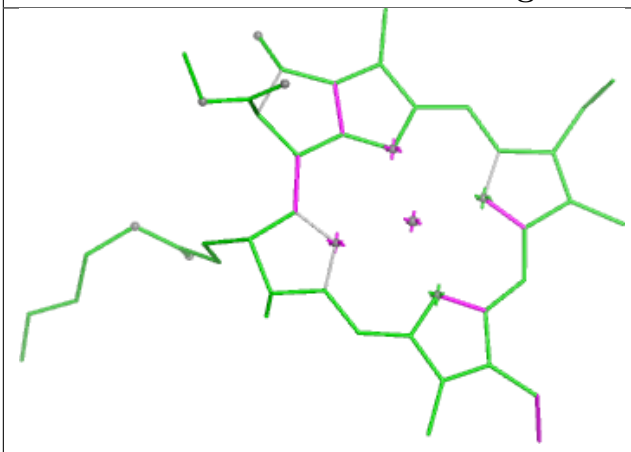


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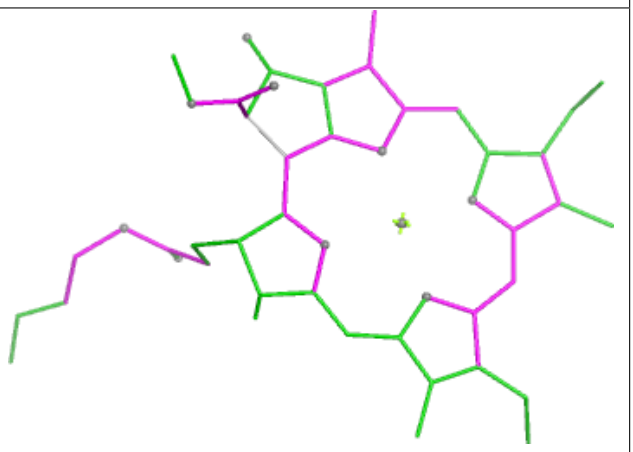


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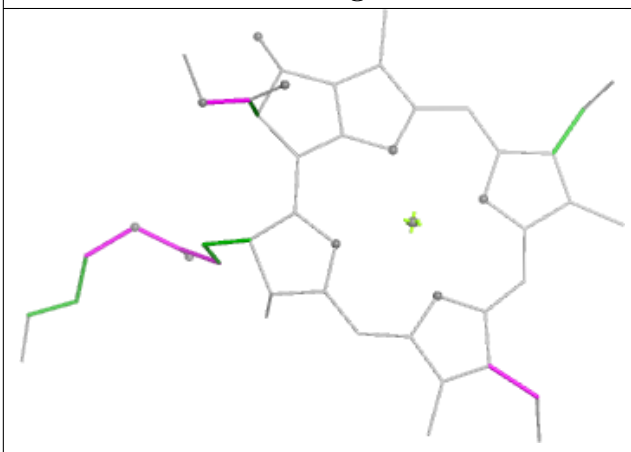
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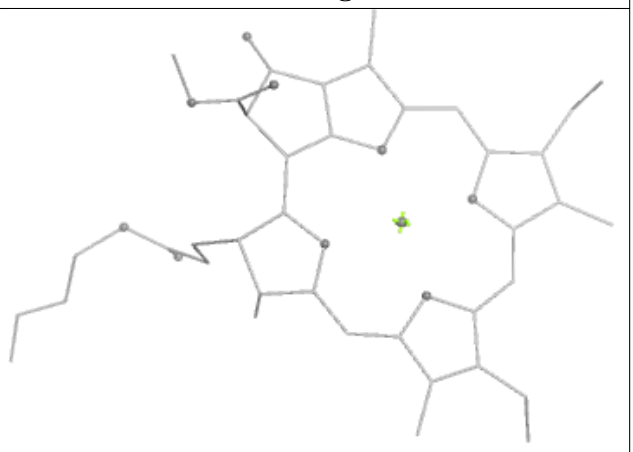
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Bond angles

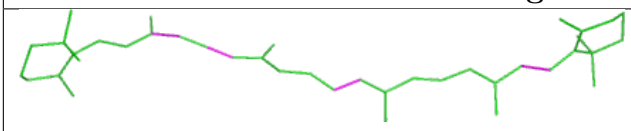


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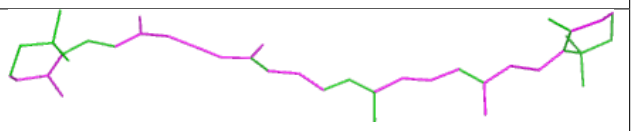


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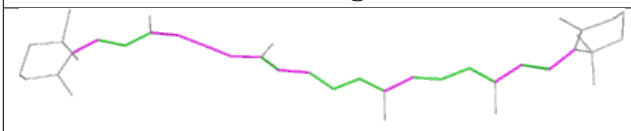
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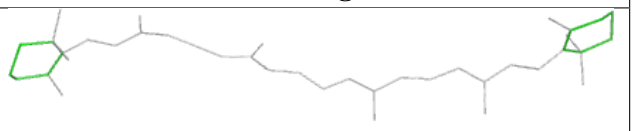
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Bond angles

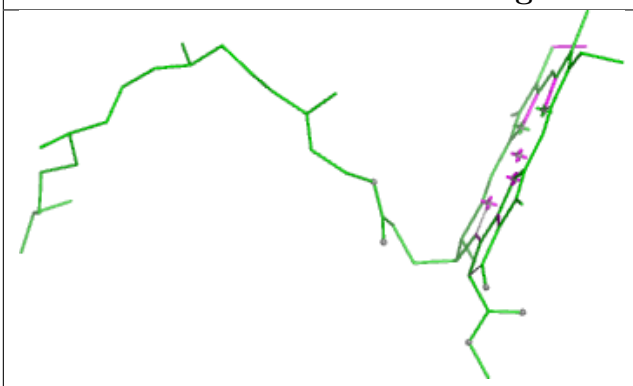


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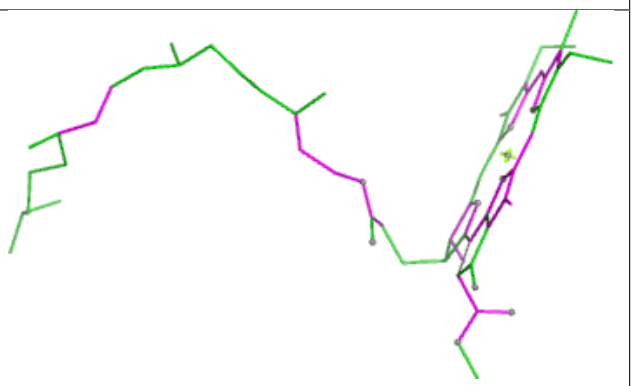


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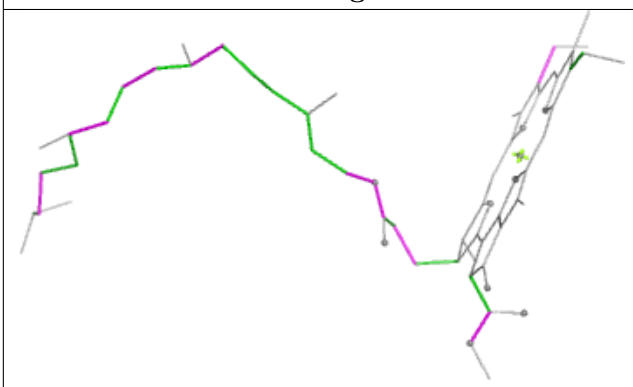
Ligand CLA B 1238



Bond lengths



Bond angles

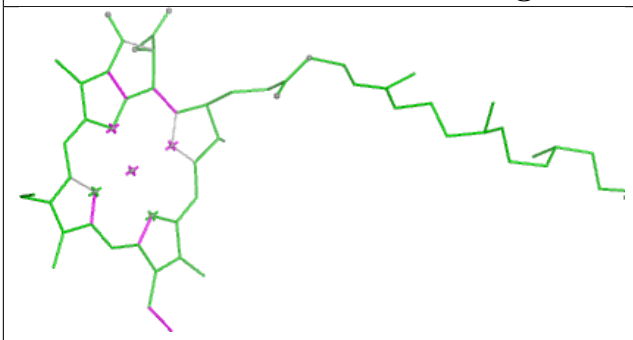


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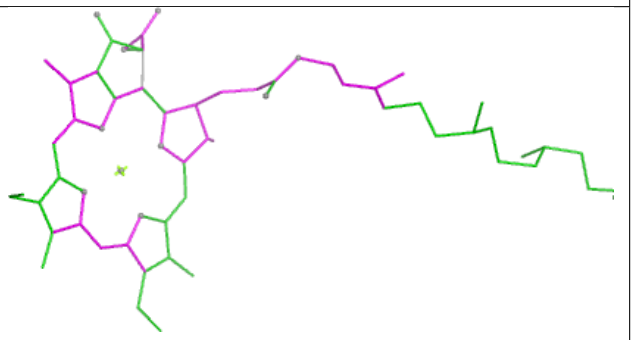


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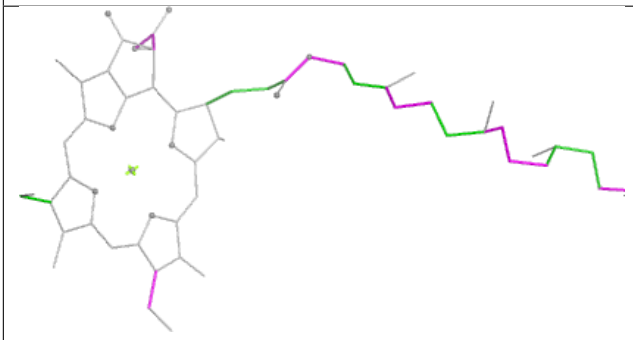
Ligand CLA B 1230



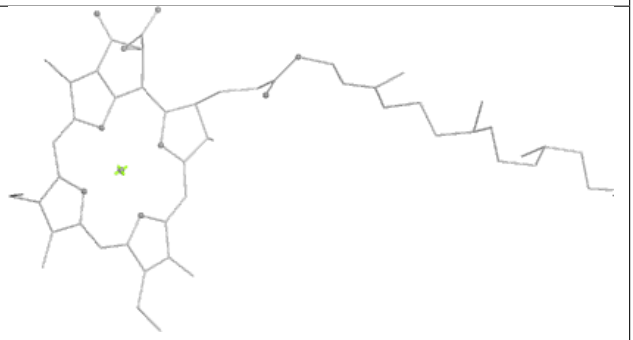
Bond lengths



Bond angles

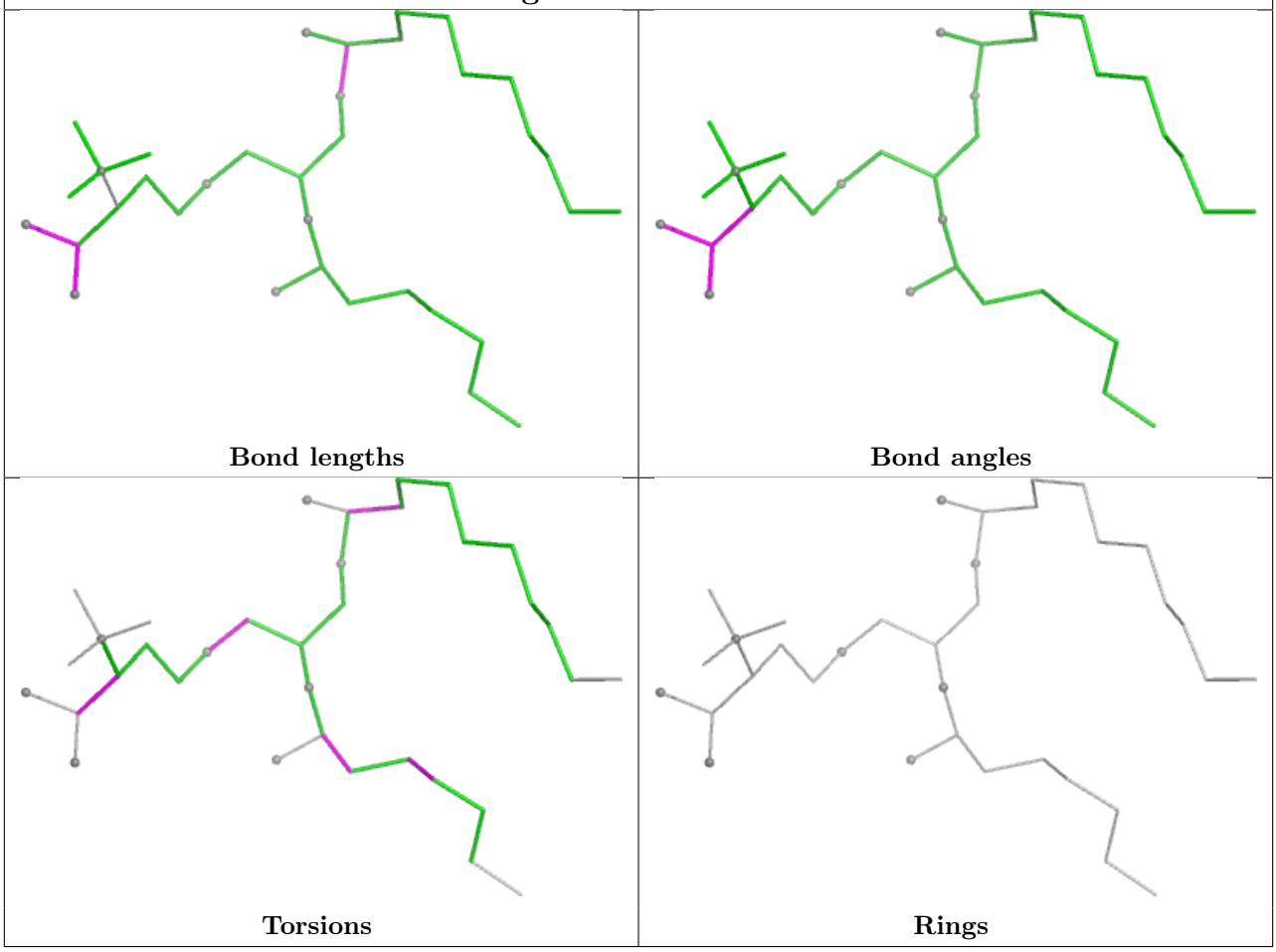


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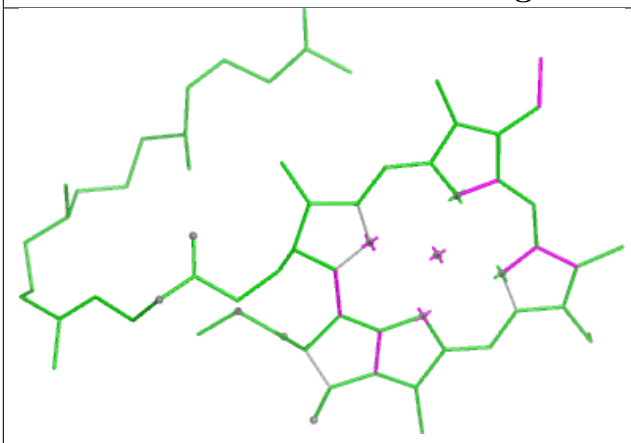


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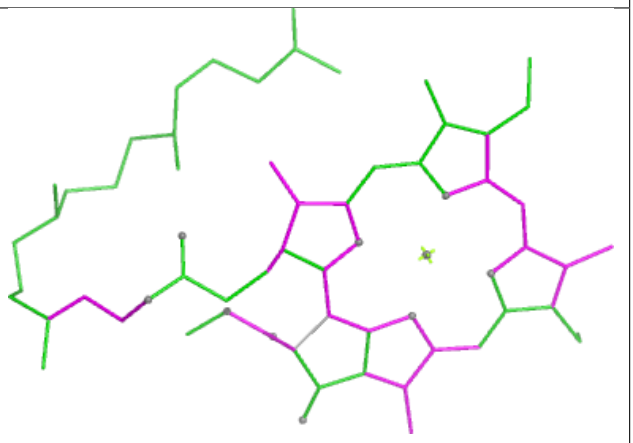
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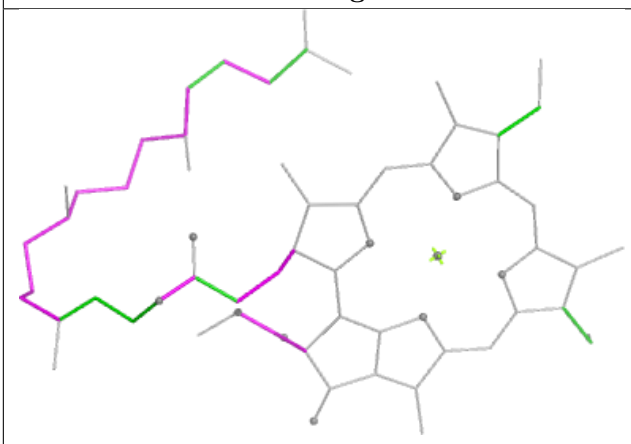
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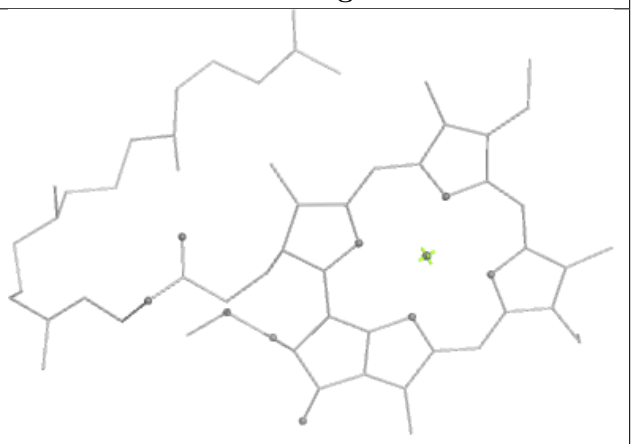
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Bond angles

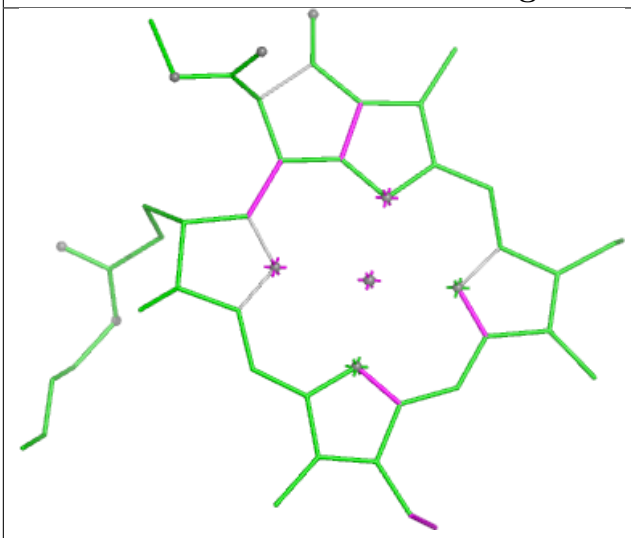


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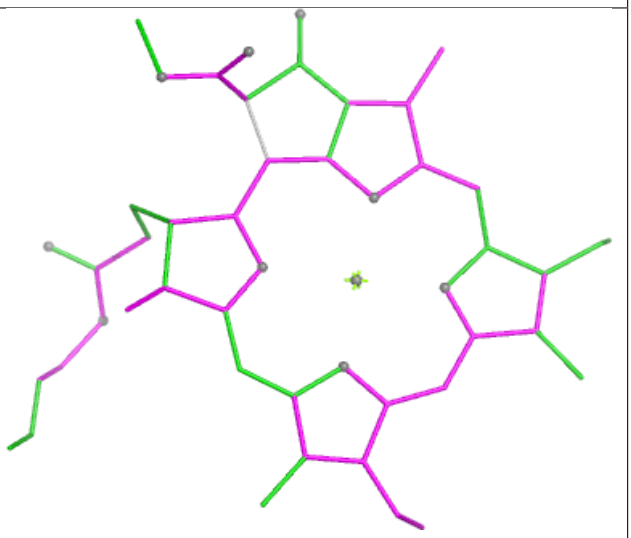


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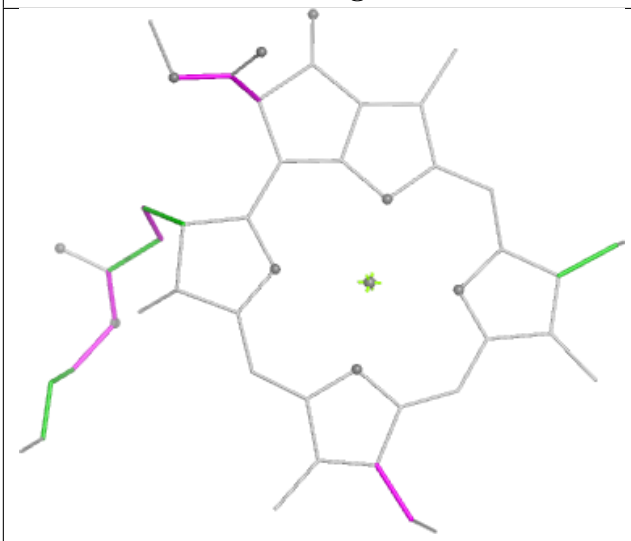
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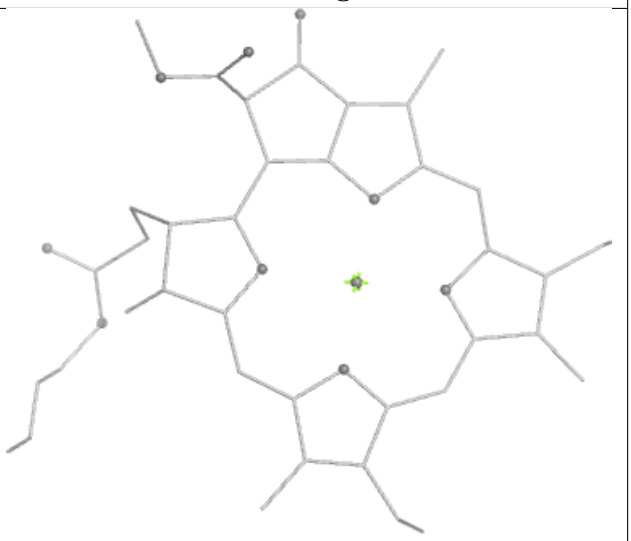
Bond lengths



Bond angles

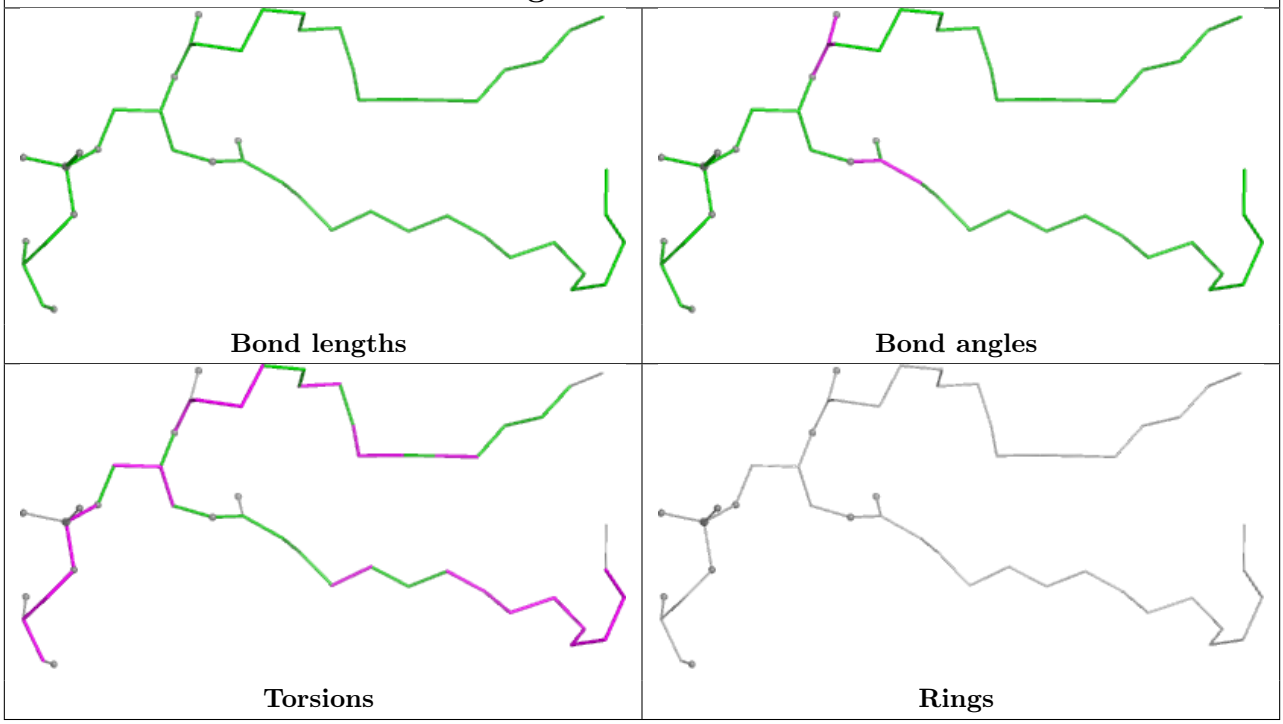


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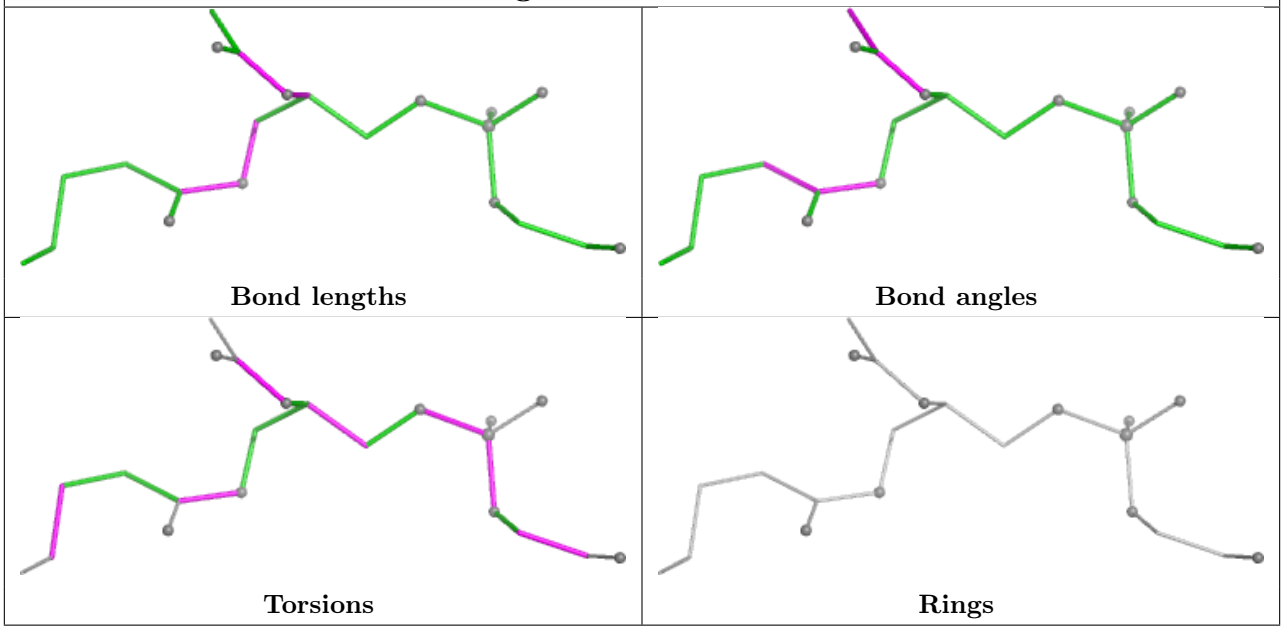


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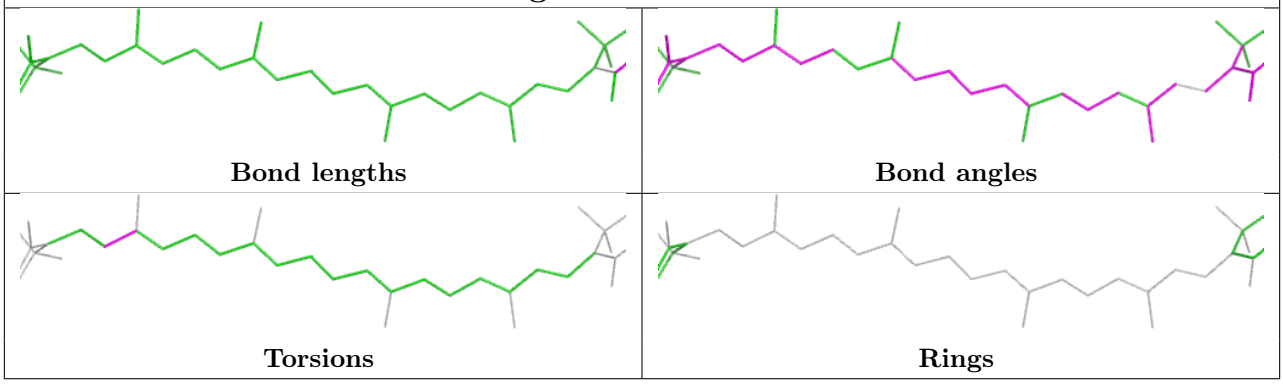
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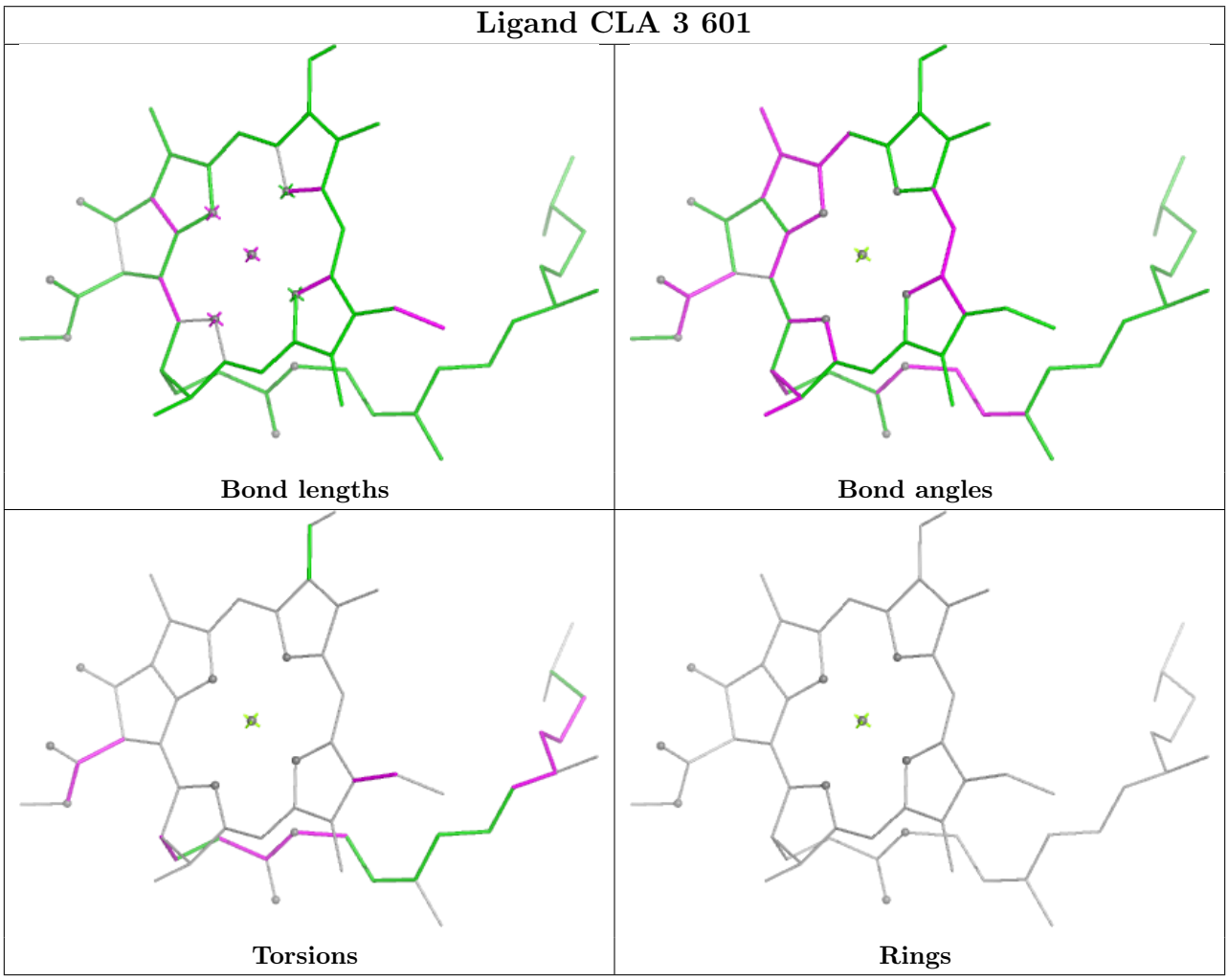
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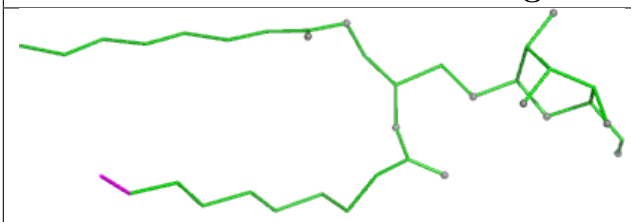
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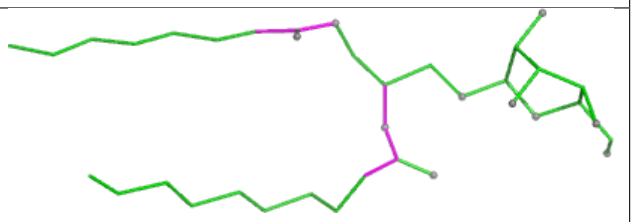
Ligand CLA 3 601



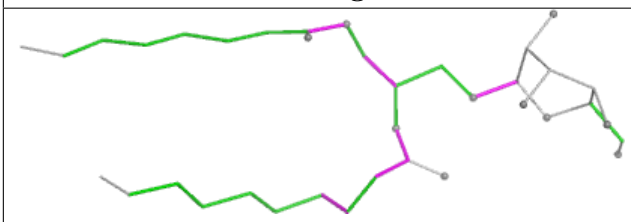
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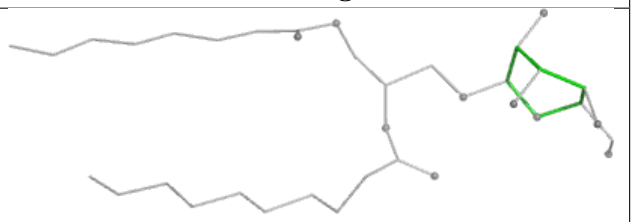
Bond lengths



Bond angles

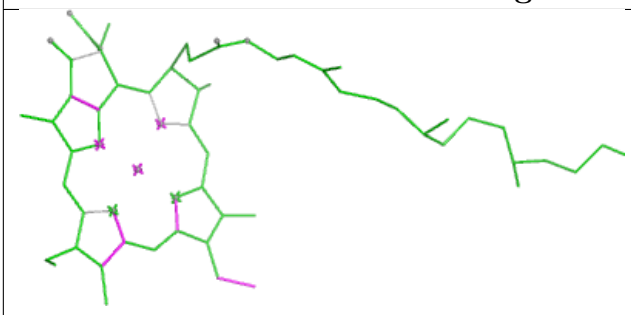


Torsions

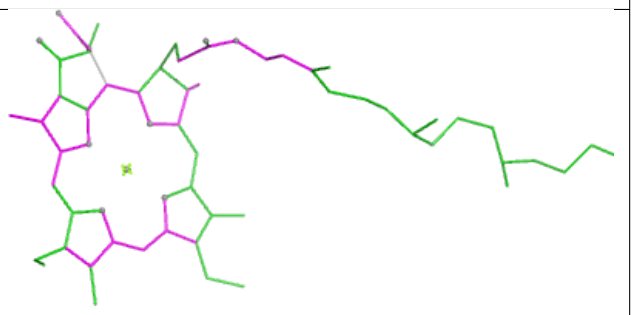


Rings

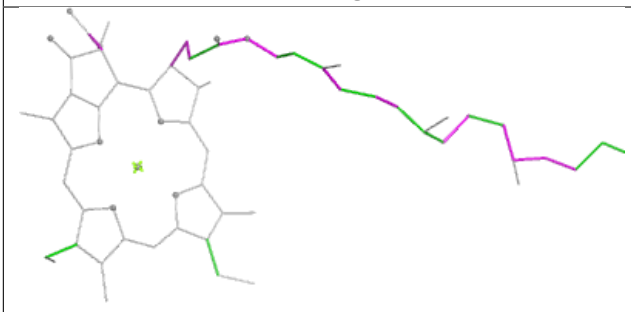
Ligand CLA A 1132



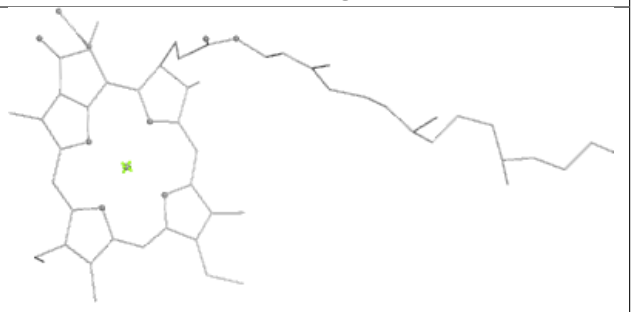
Bond lengths



Bond angles

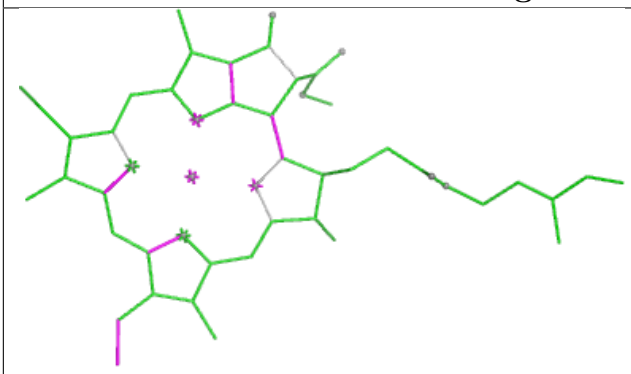


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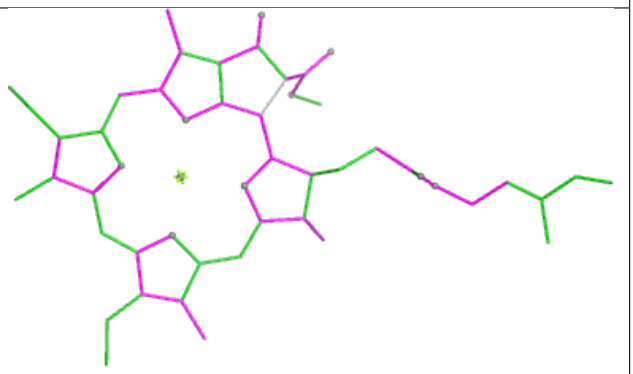


Rings

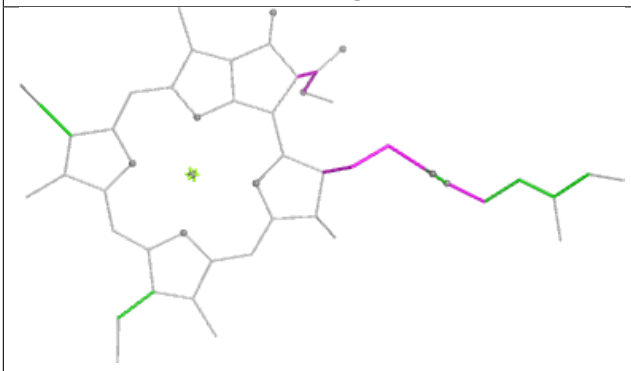
Ligand CLA A 1135



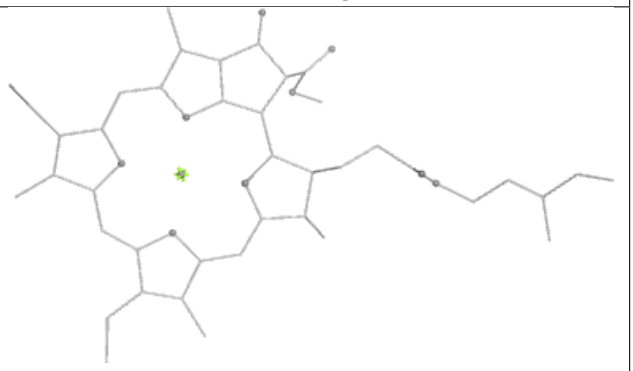
Bond lengths



Bond angles

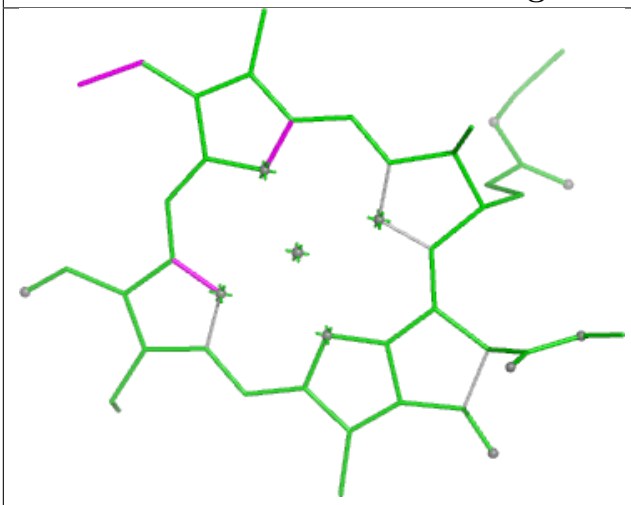


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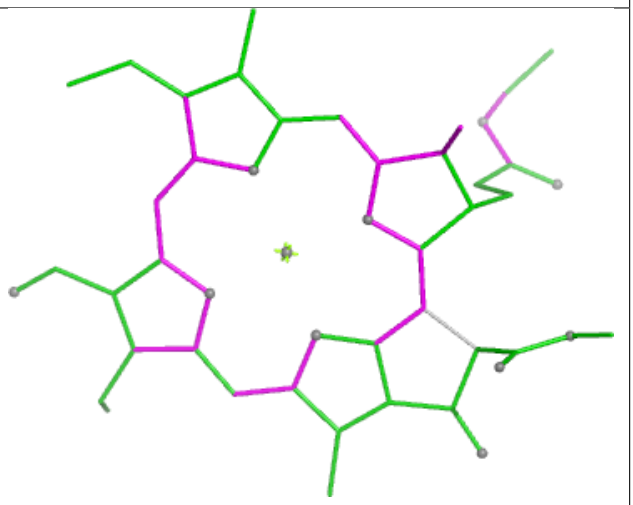


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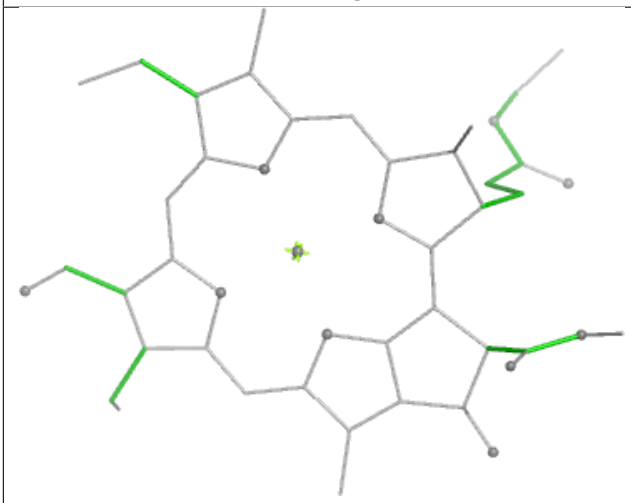
Ligand CHL 2 611



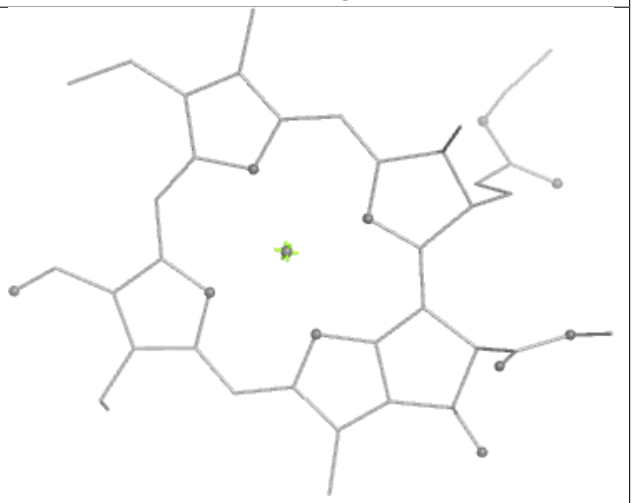
Bond lengths



Bond angles

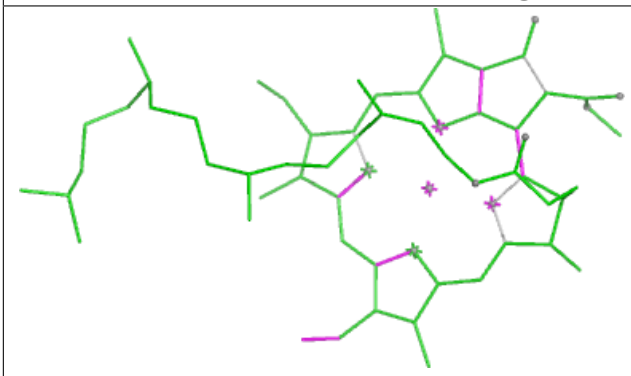


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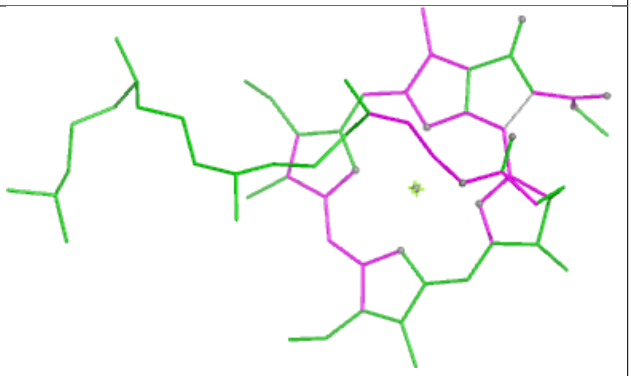


Rings

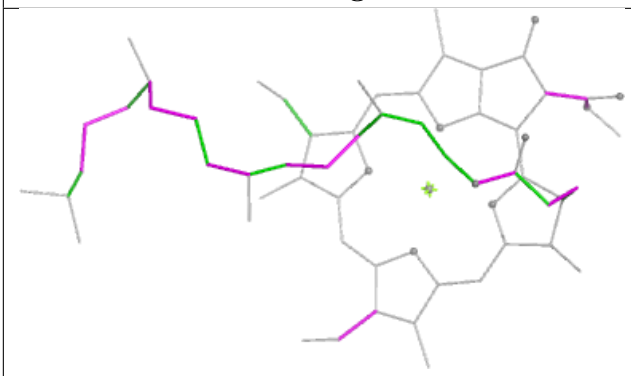
Ligand CLA B 1204



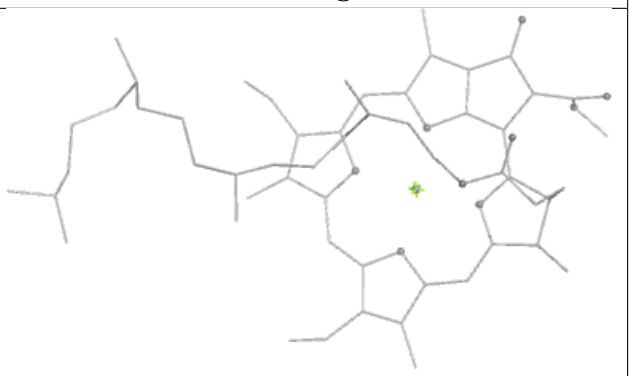
Bond lengths



Bond angles

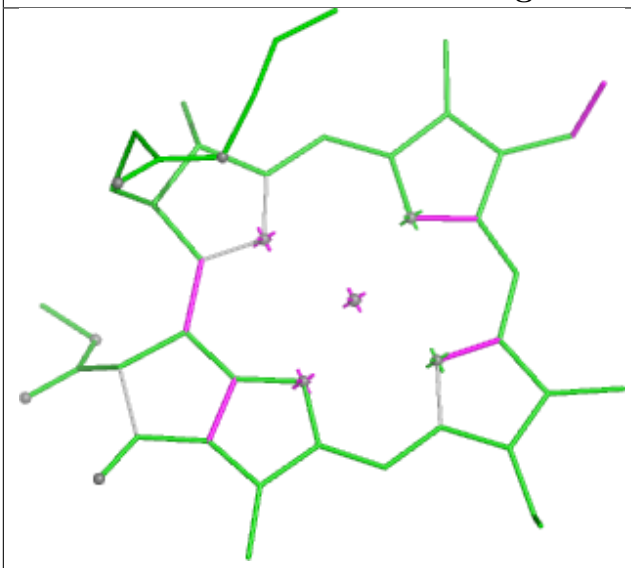


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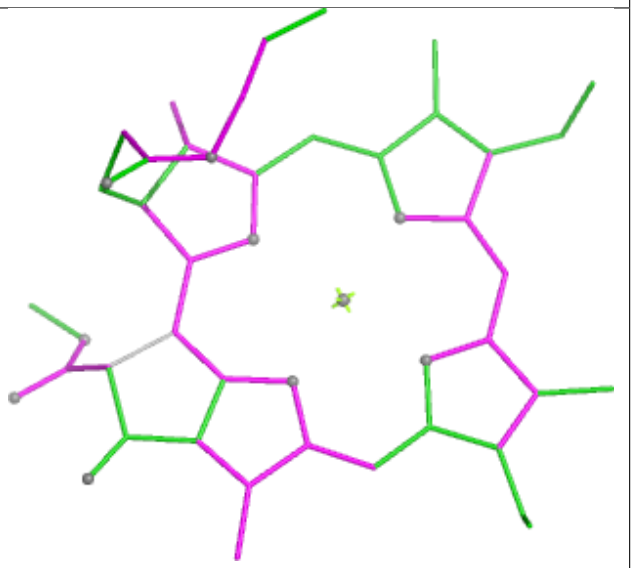


Rings

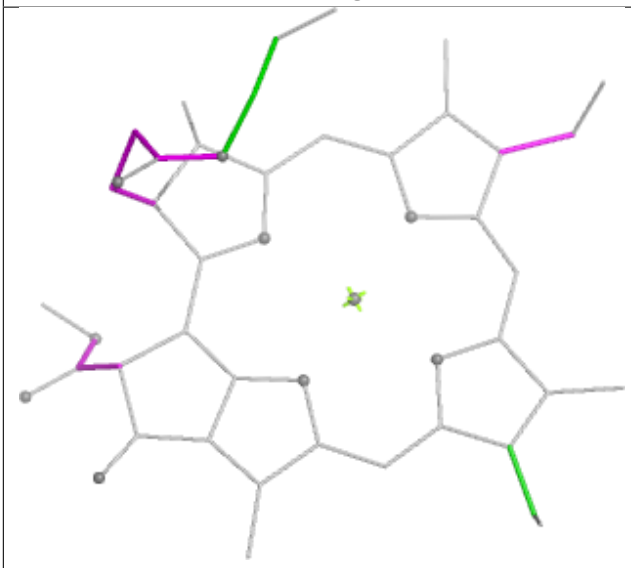
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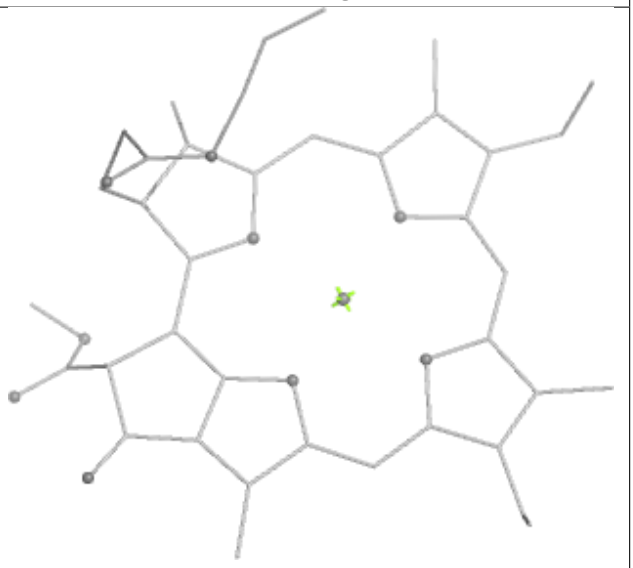
Bond lengths



Bond angles

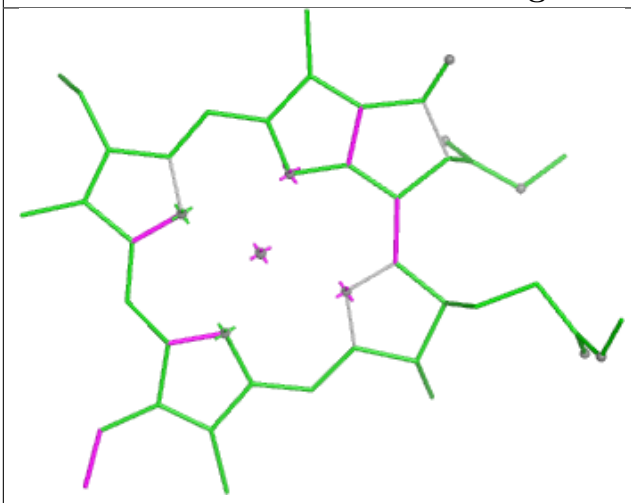


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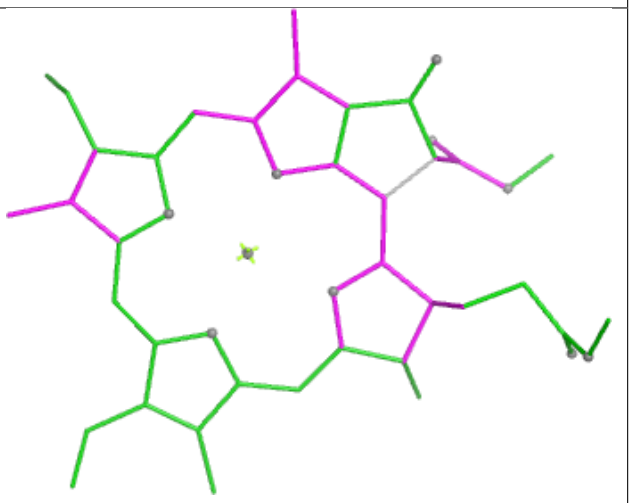


Rings

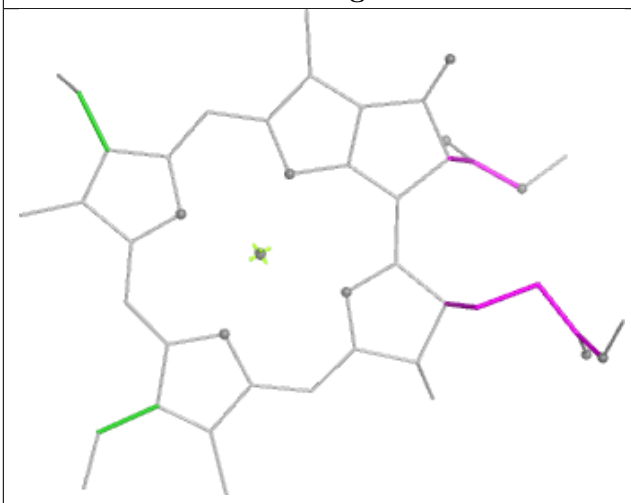
Ligand CLA 3 613



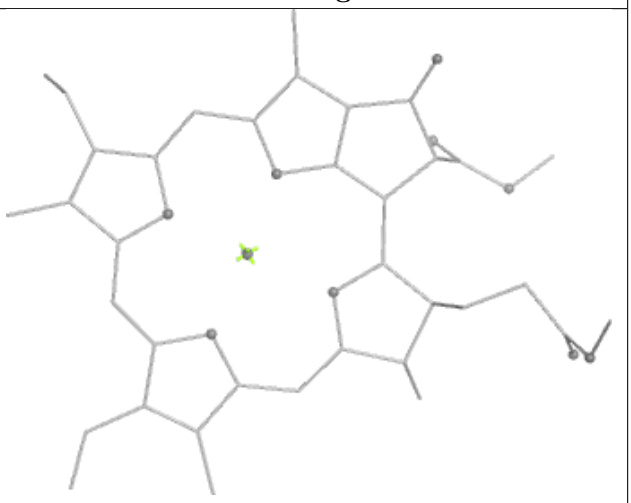
Bond lengths



Bond angles

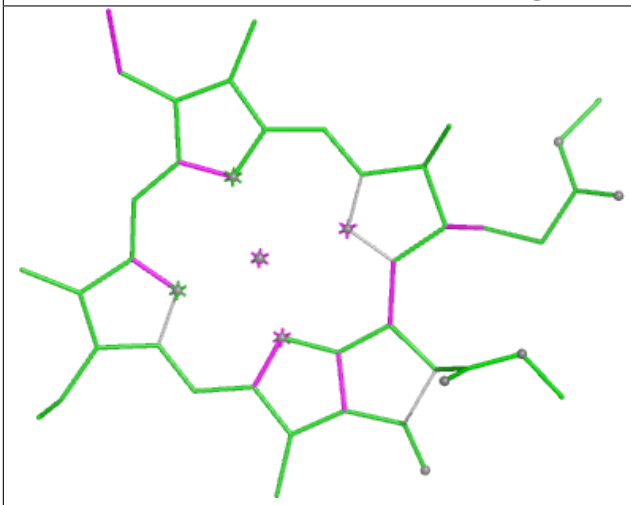


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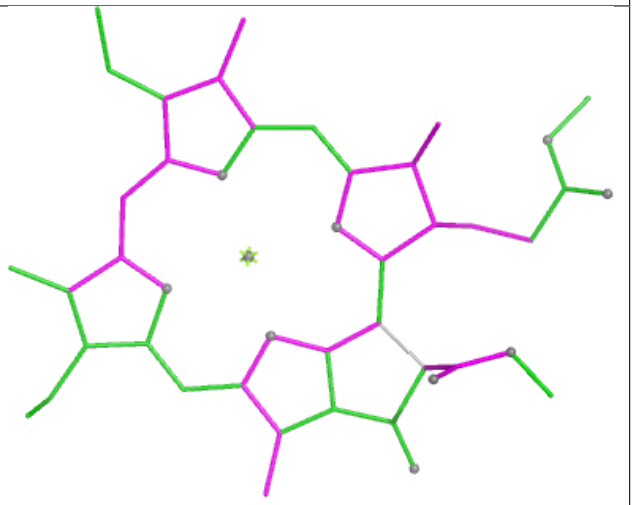


Rings

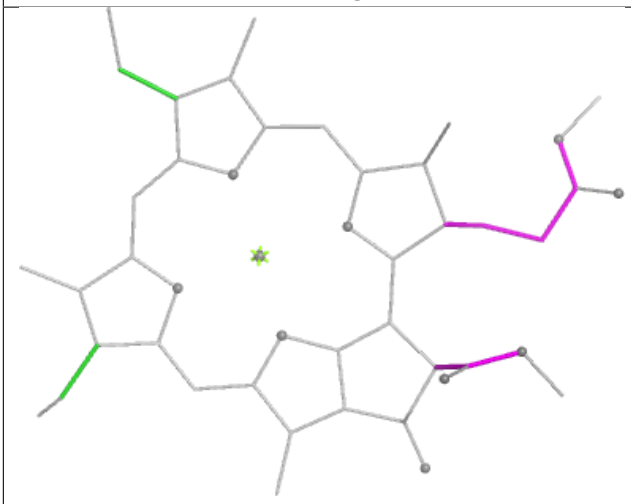
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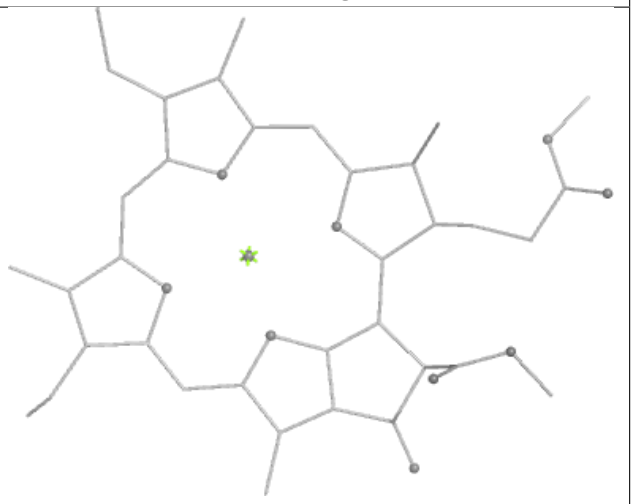
Bond lengths



Bond angles

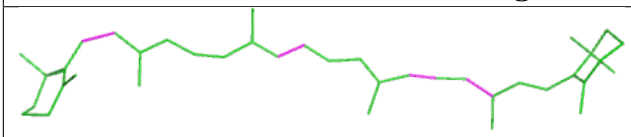


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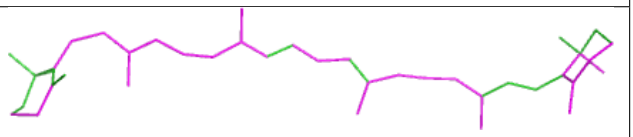


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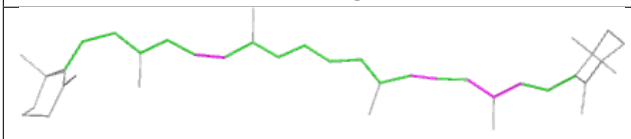
Ligand BCR A 4003



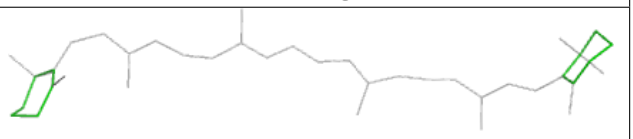
Bond lengths



Bond angles

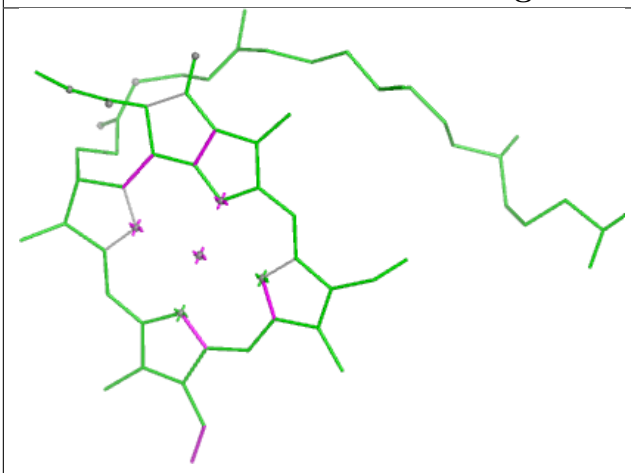


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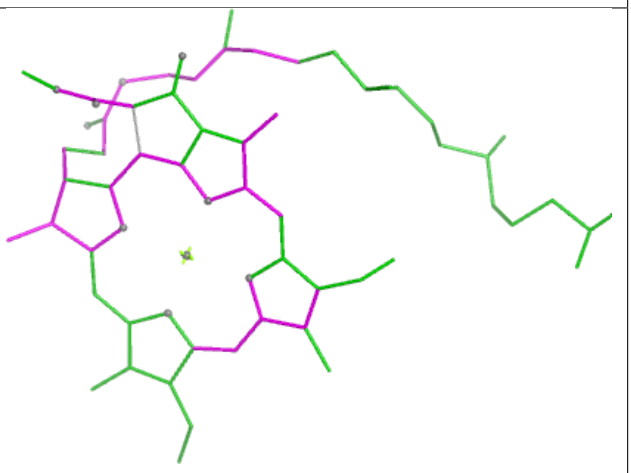


Rings

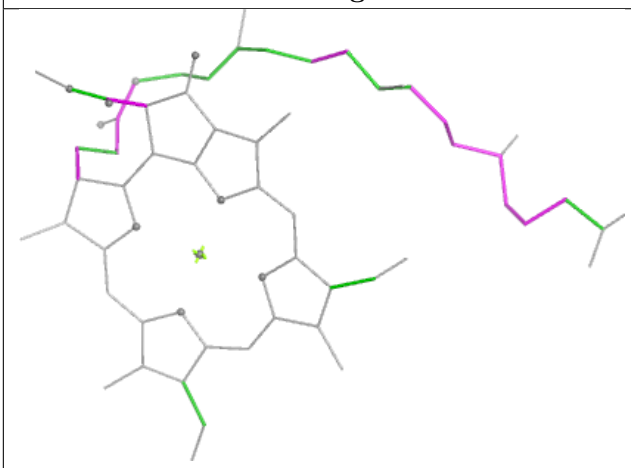
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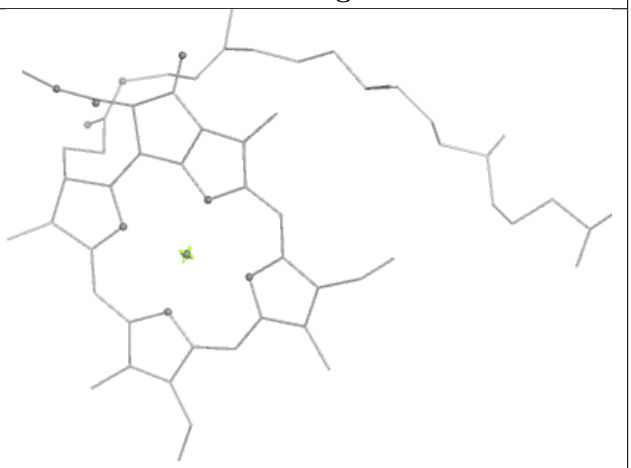
Bond lengths



Bond angles

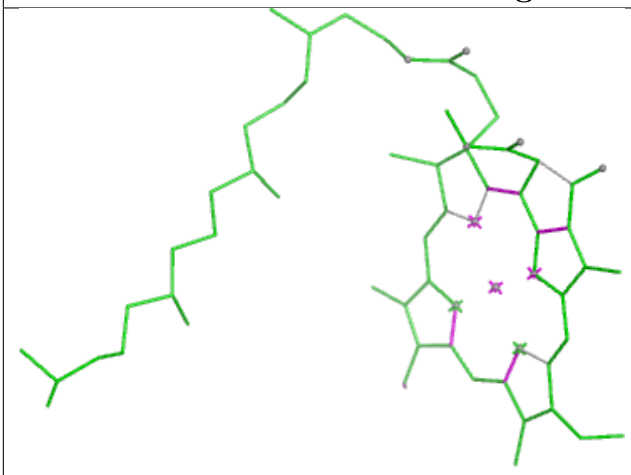


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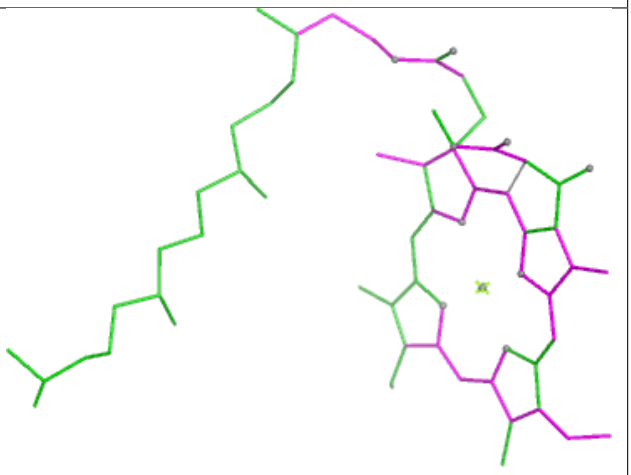


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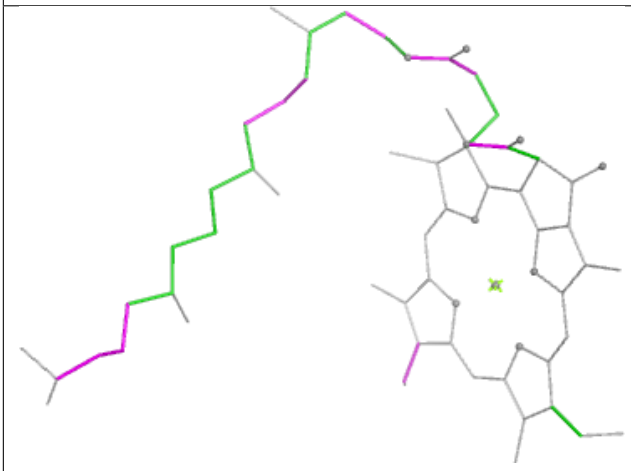
Ligand CLA B 1221



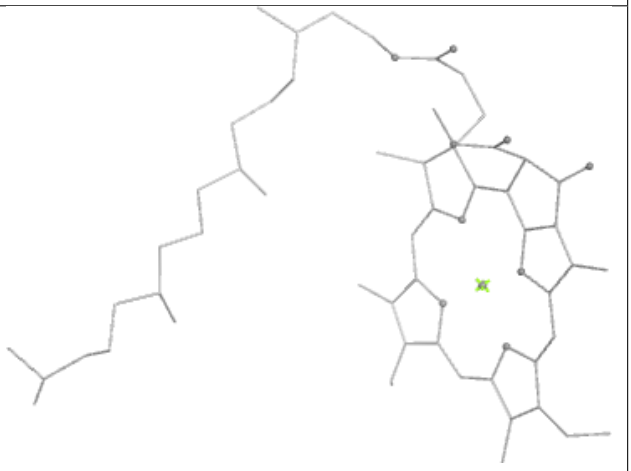
Bond lengths



Bond angles

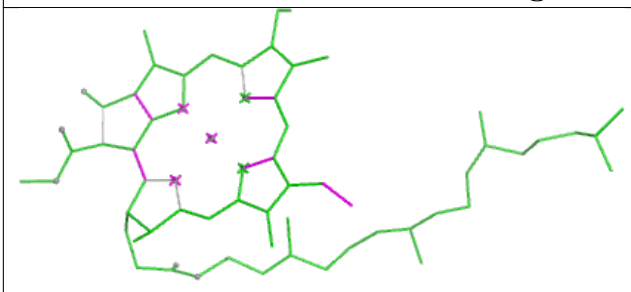


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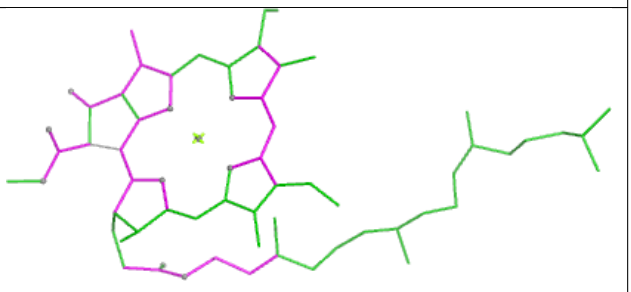


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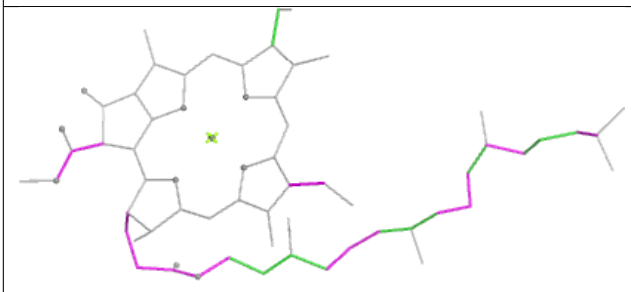
Ligand CLA 2 601



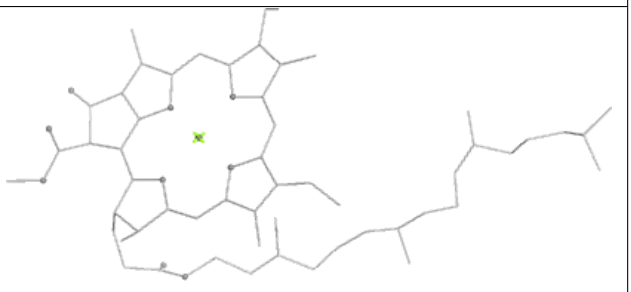
Bond lengths



Bond angles

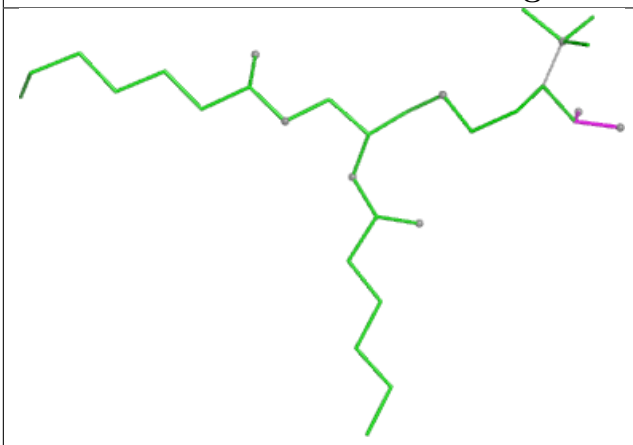


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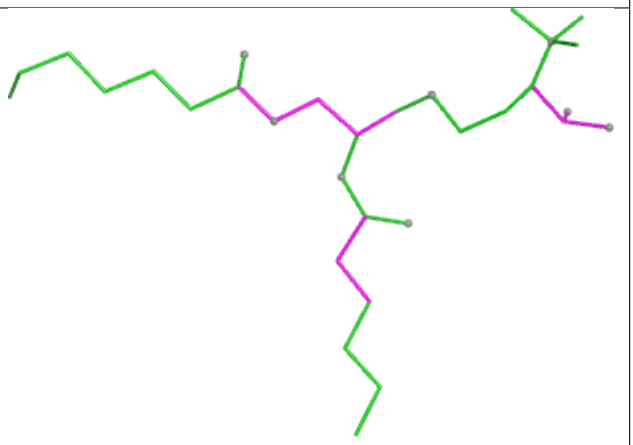


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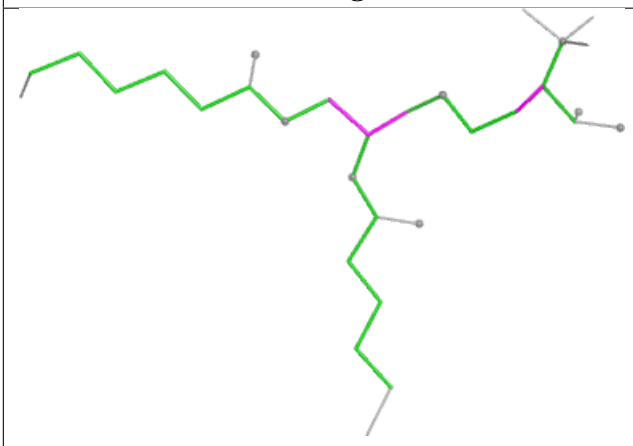
Ligand LMK 2 807



Bond lengths



Bond angles

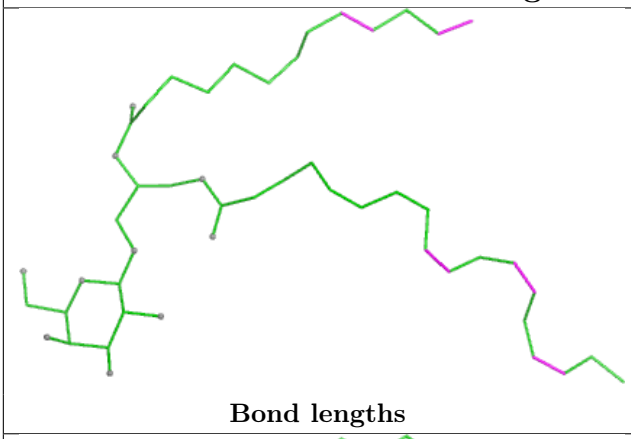


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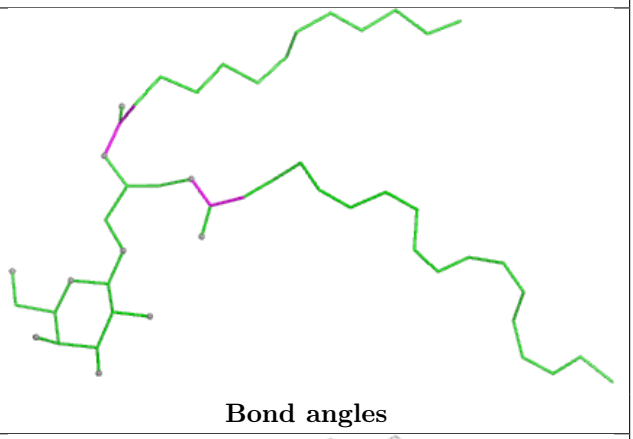


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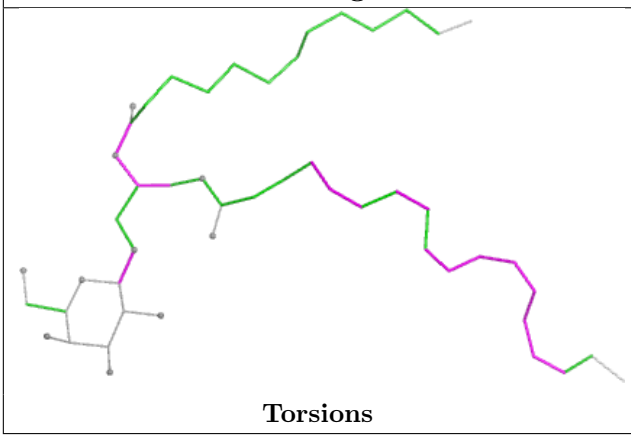
Ligand LMG 2 804



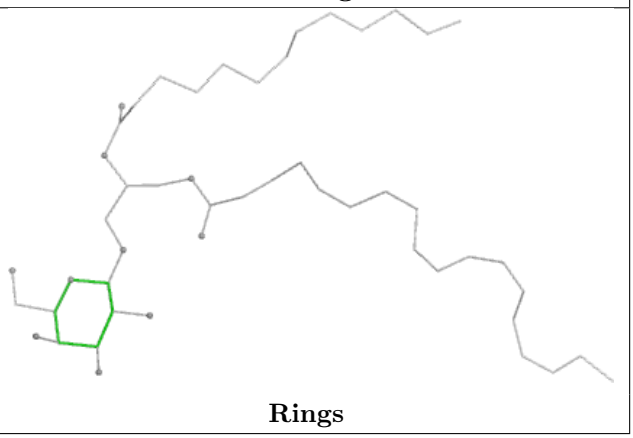
Bond lengths



Bond angles

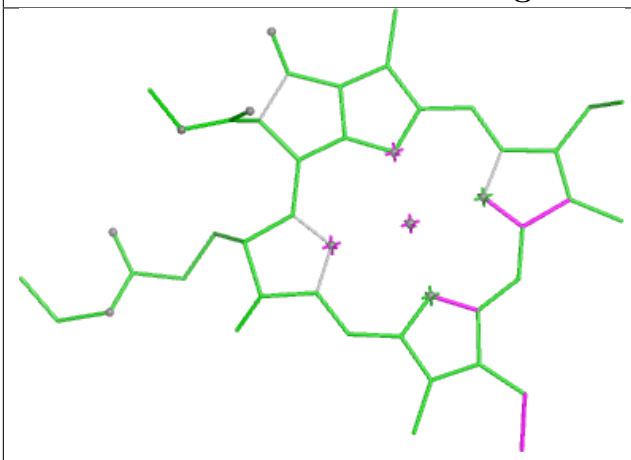


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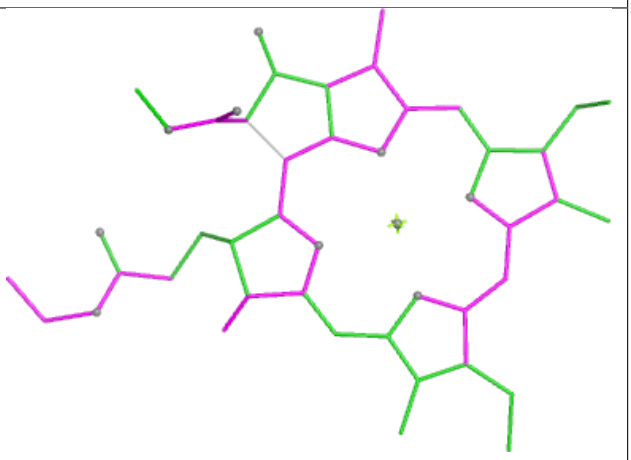


Rings

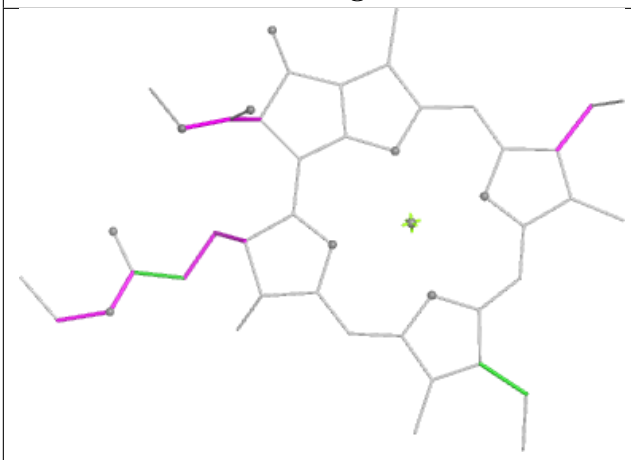
Ligand CLA G 1601



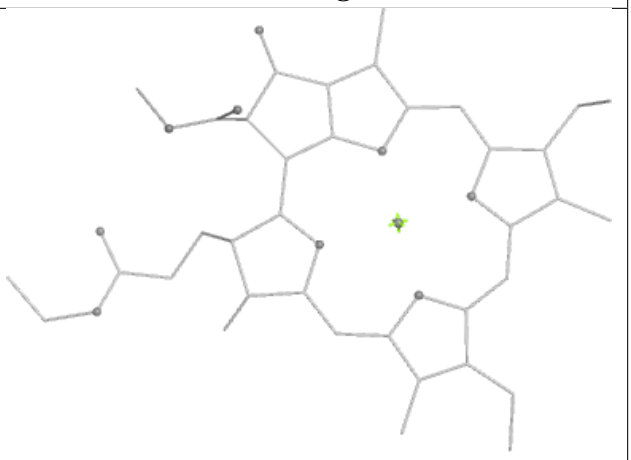
Bond lengths



Bond angles

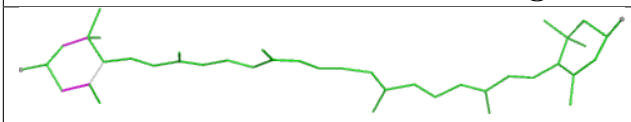


Torsions

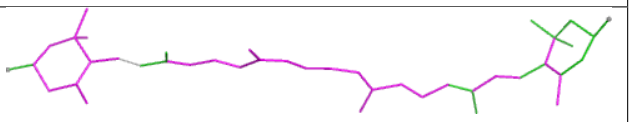


Rings

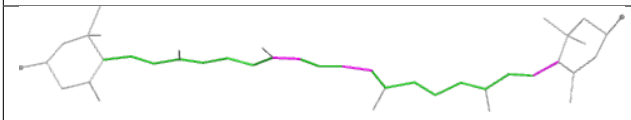
Ligand LUT 1 501



Bond lengths



Bond angles

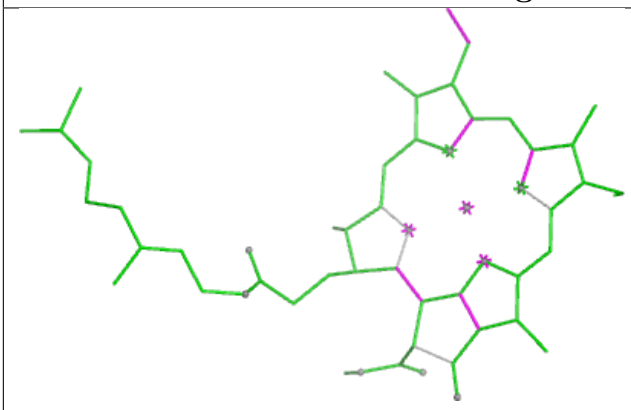


Torsions

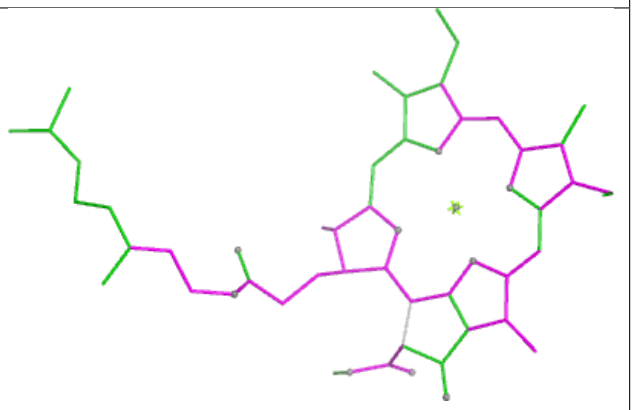


Rings

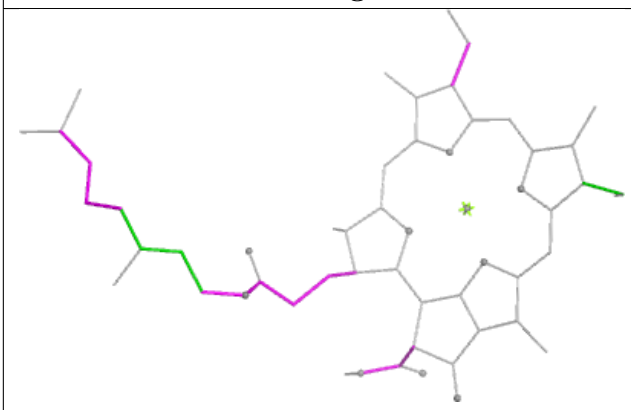
Ligand CLA B 1220



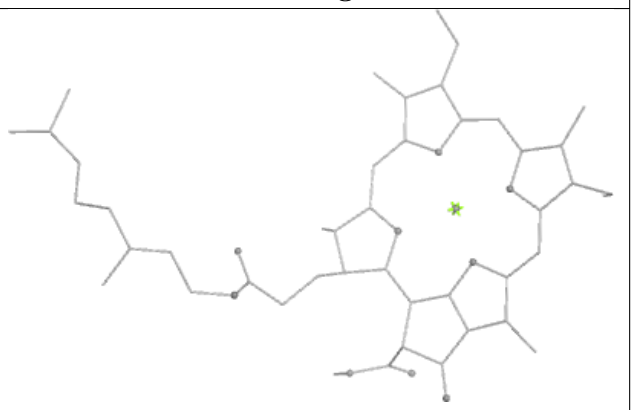
Bond lengths



Bond angles

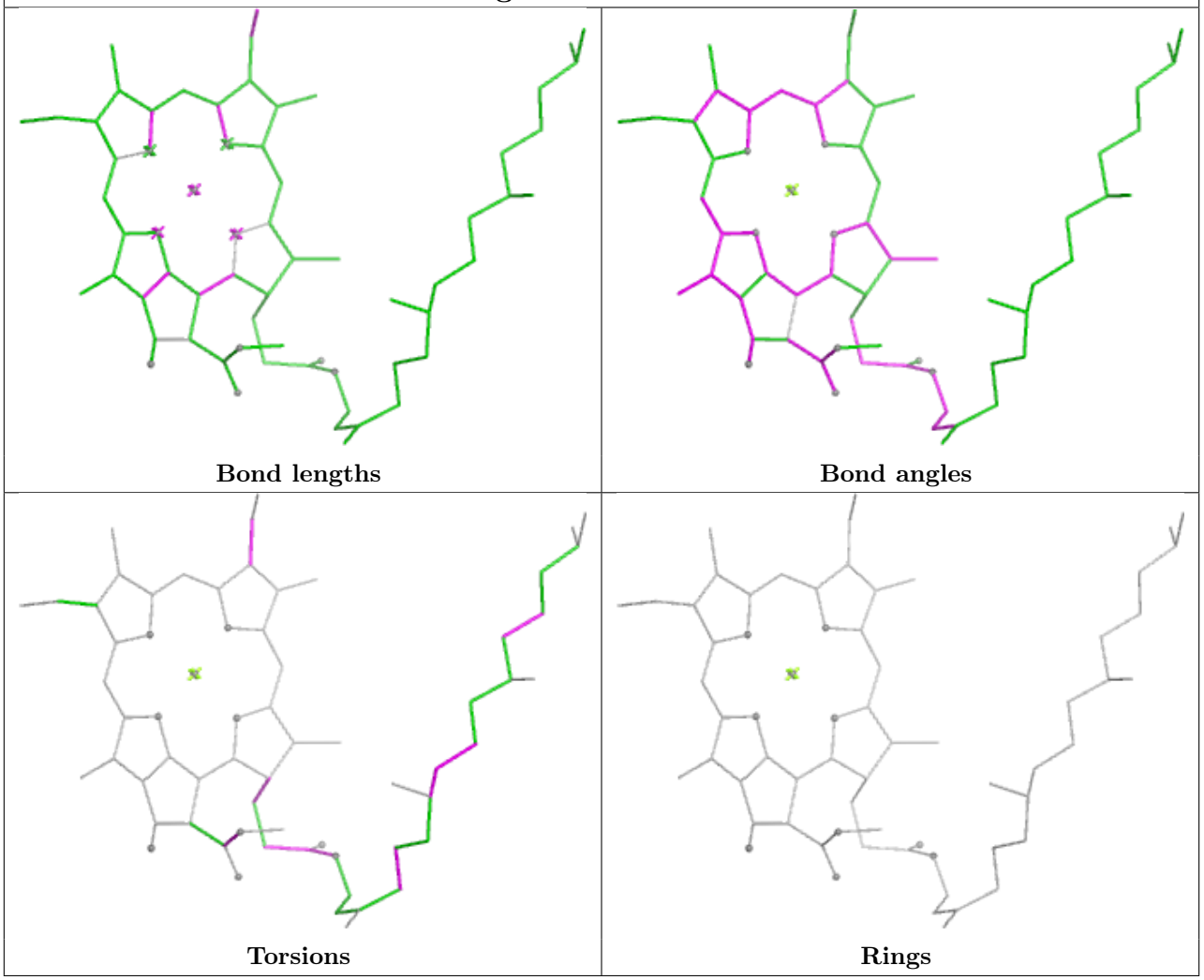


Torsions



Rings

Ligand CLA 4 605



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.

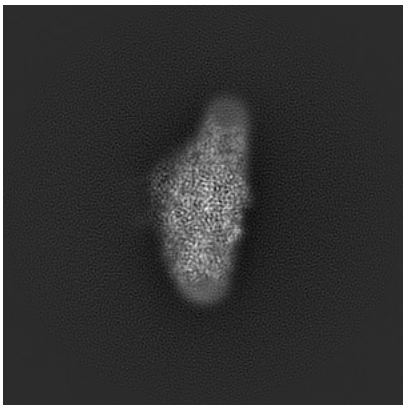
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10236. These allow visual inspection of the internal detail of the map and identification of artifacts.

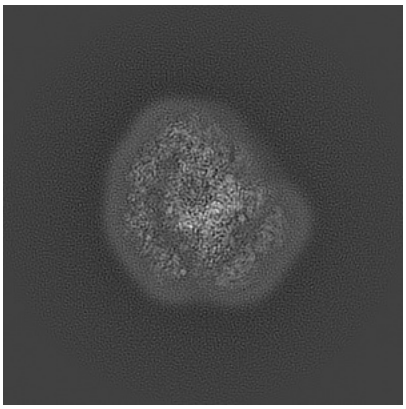
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

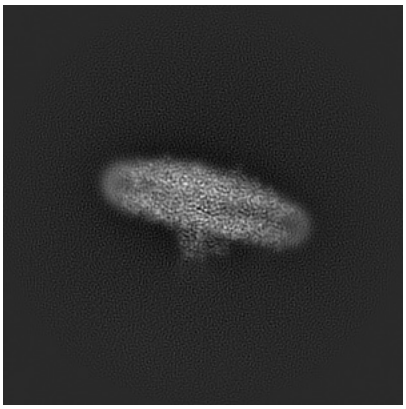
6.1.1 Primary map



X

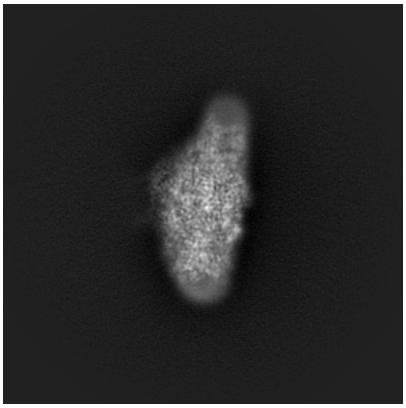


Y

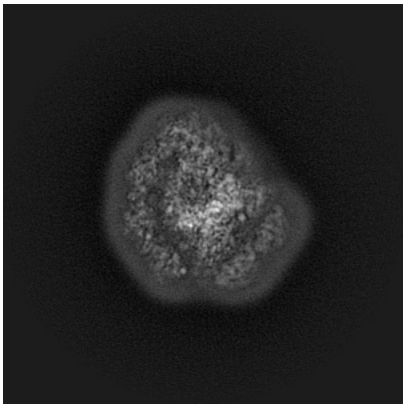


Z

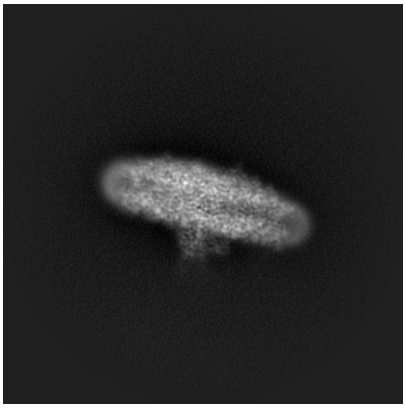
6.1.2 Raw map



X



Y

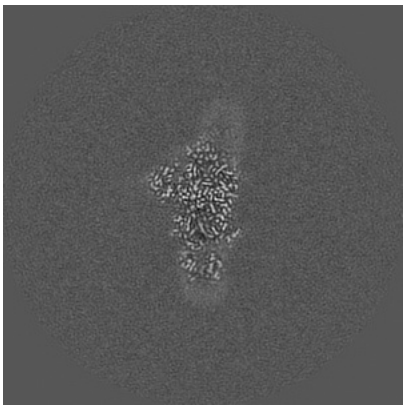


Z

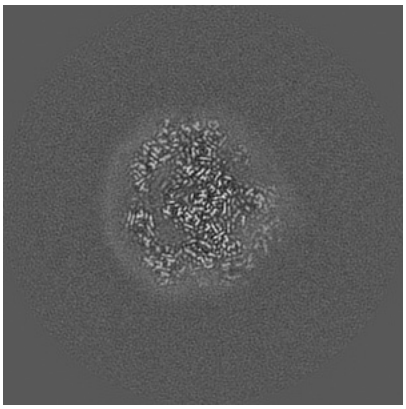
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

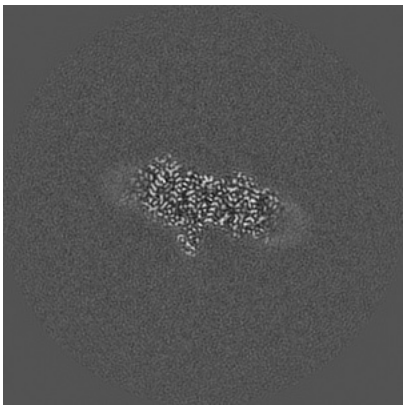
6.2.1 Primary map



X Index: 180

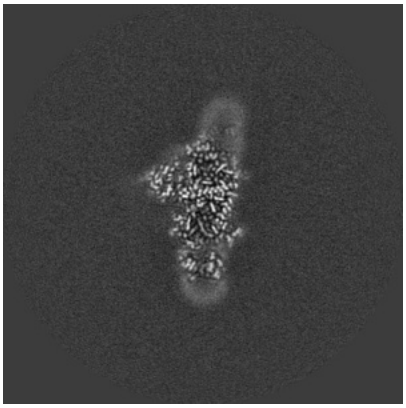


Y Index: 180

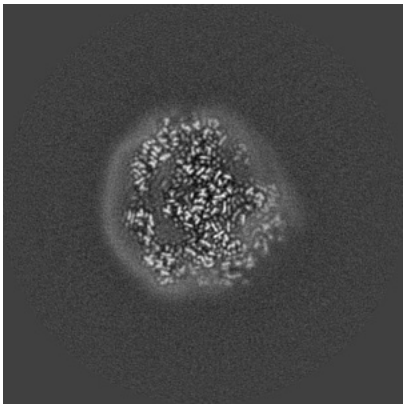


Z Index: 180

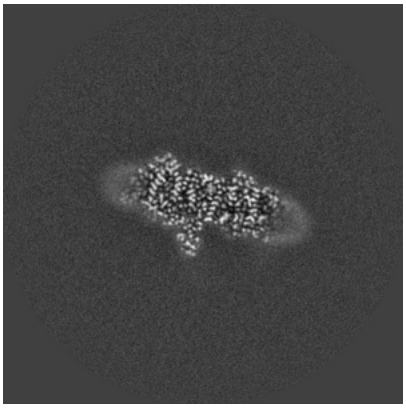
6.2.2 Raw map



X Index: 180



Y Index: 180

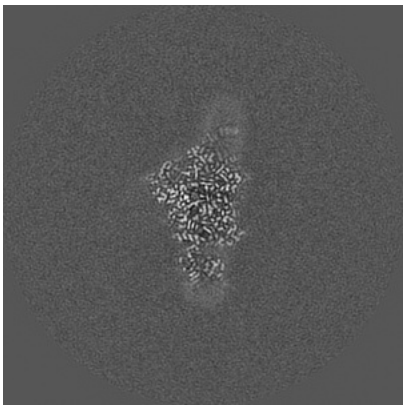


Z Index: 180

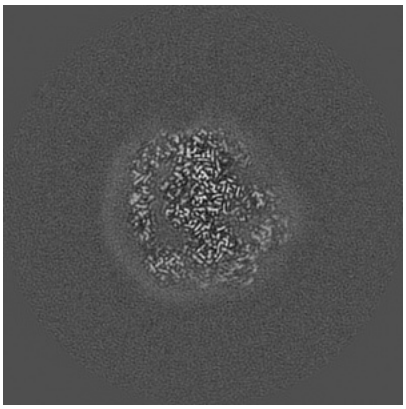
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

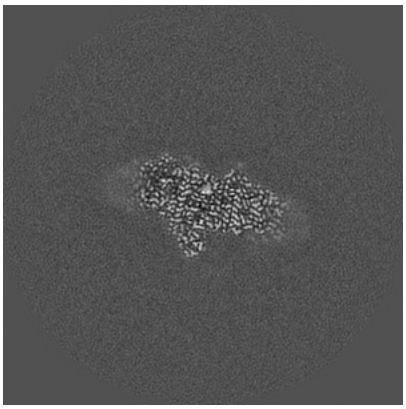
6.3.1 Primary map



X Index: 177

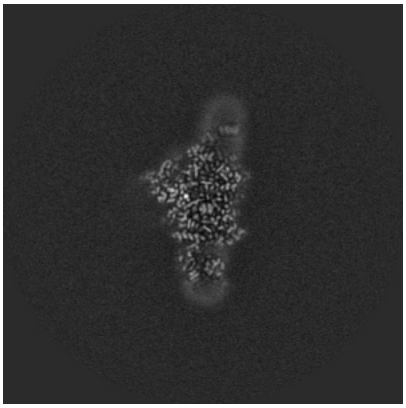


Y Index: 184

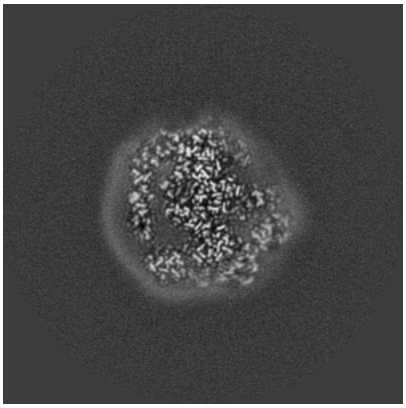


Z Index: 185

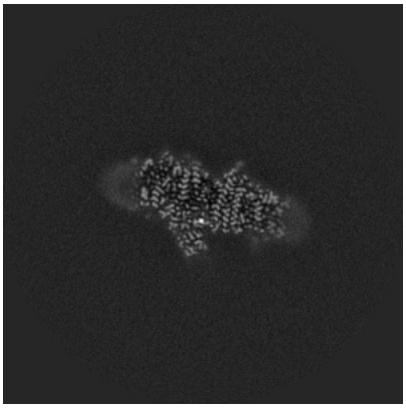
6.3.2 Raw map



X Index: 177



Y Index: 184

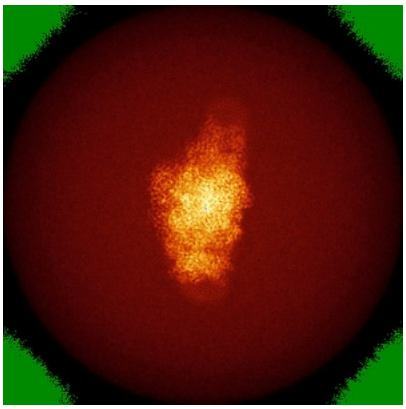


Z Index: 186

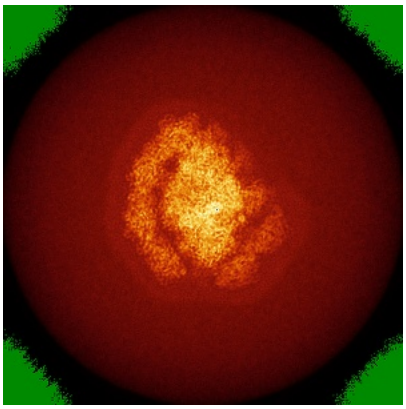
The images above show the largest variance slices of the map in three orthogonal directions.

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

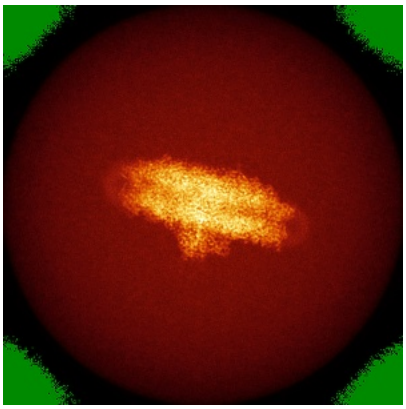
6.4.1 Primary map



X

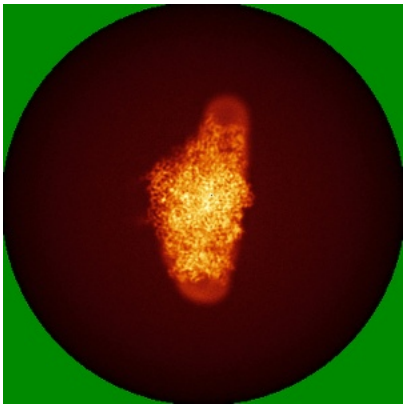


Y

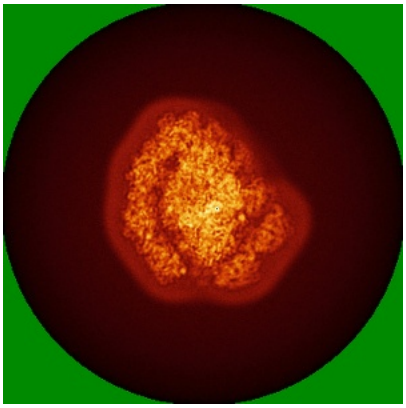


Z

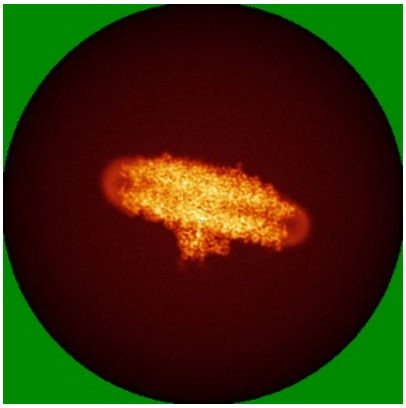
6.4.2 Raw map



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



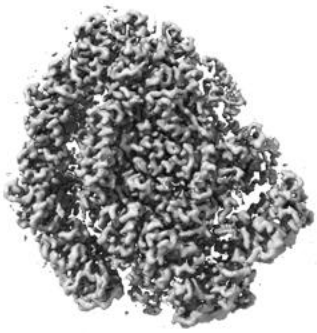
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0247. 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.

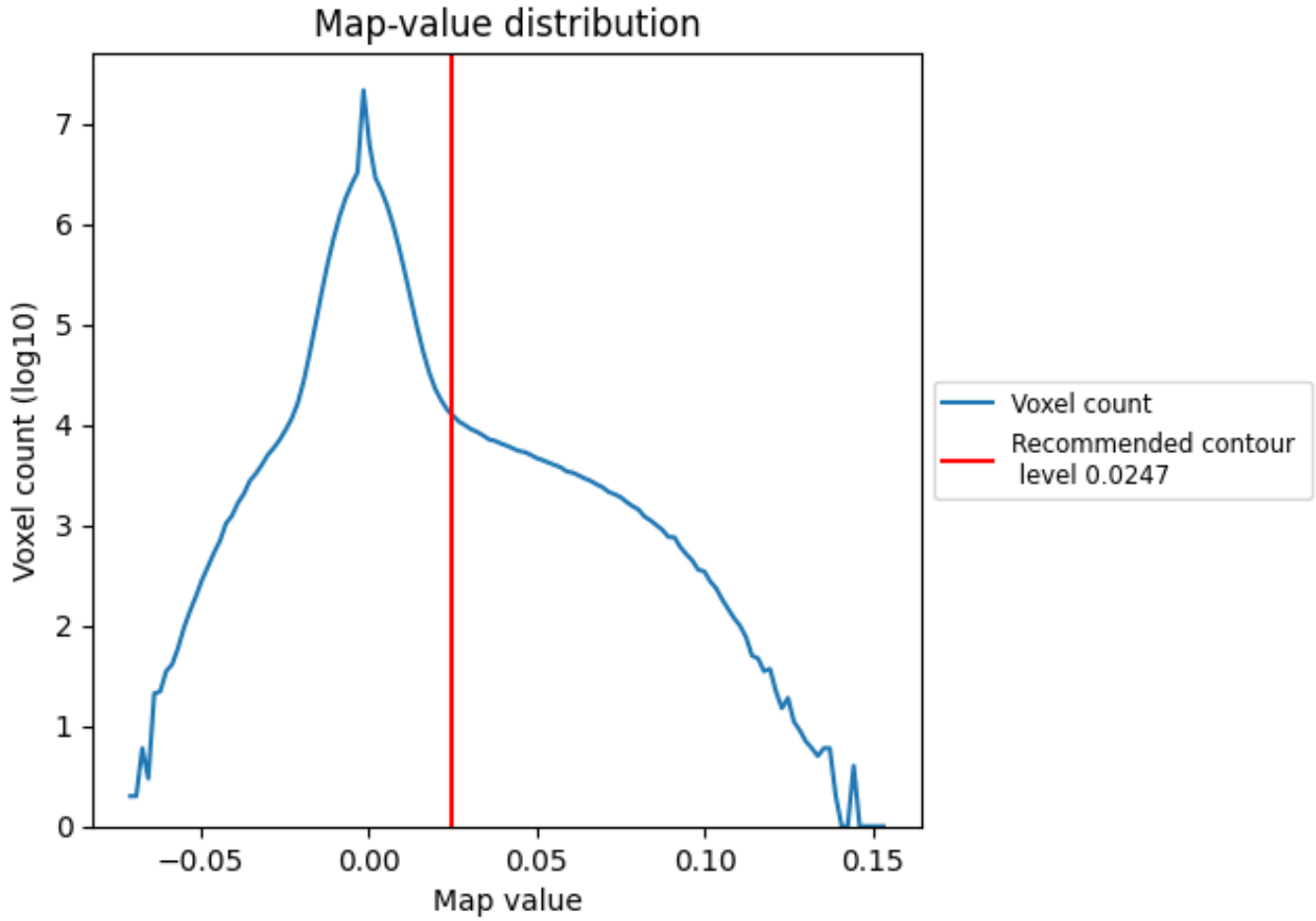
6.6 Mask visualisation (i)

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

7 Map analysis

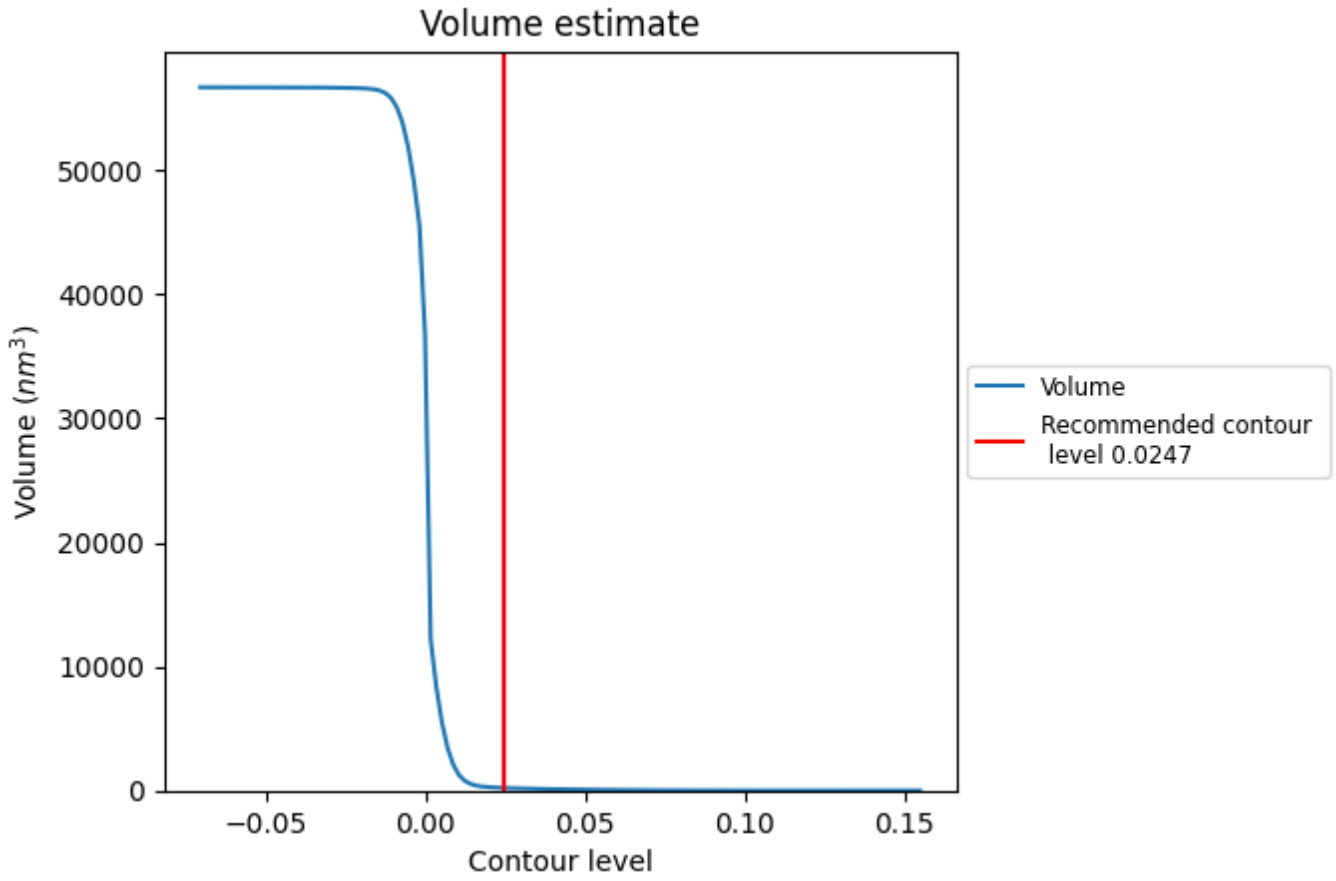
This section contains the results of statistical analysis of the map.

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.

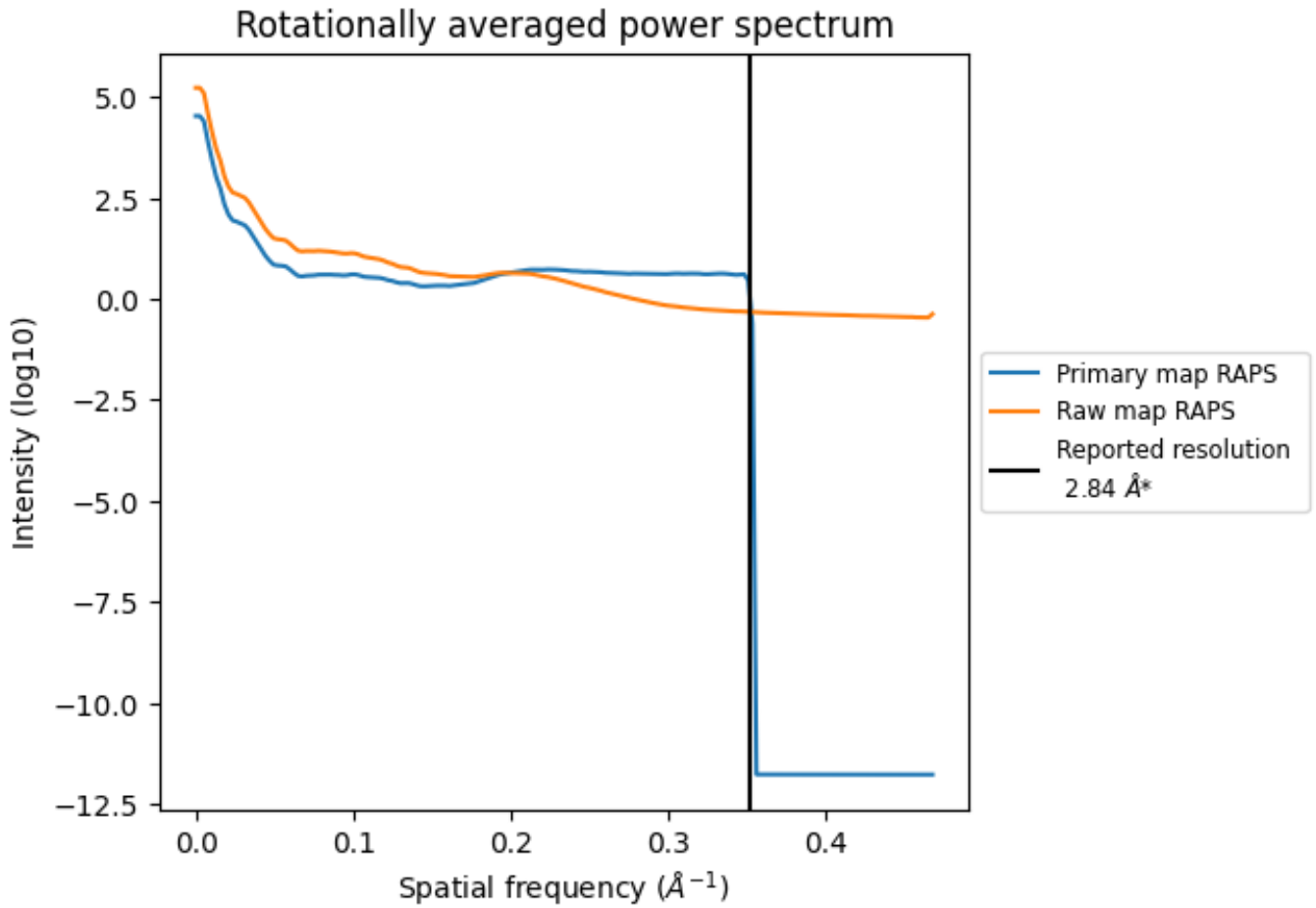
7.2 Volume estimate



The volume at the recommended contour level is 209 nm^3; this corresponds to an approximate mass of 188 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)

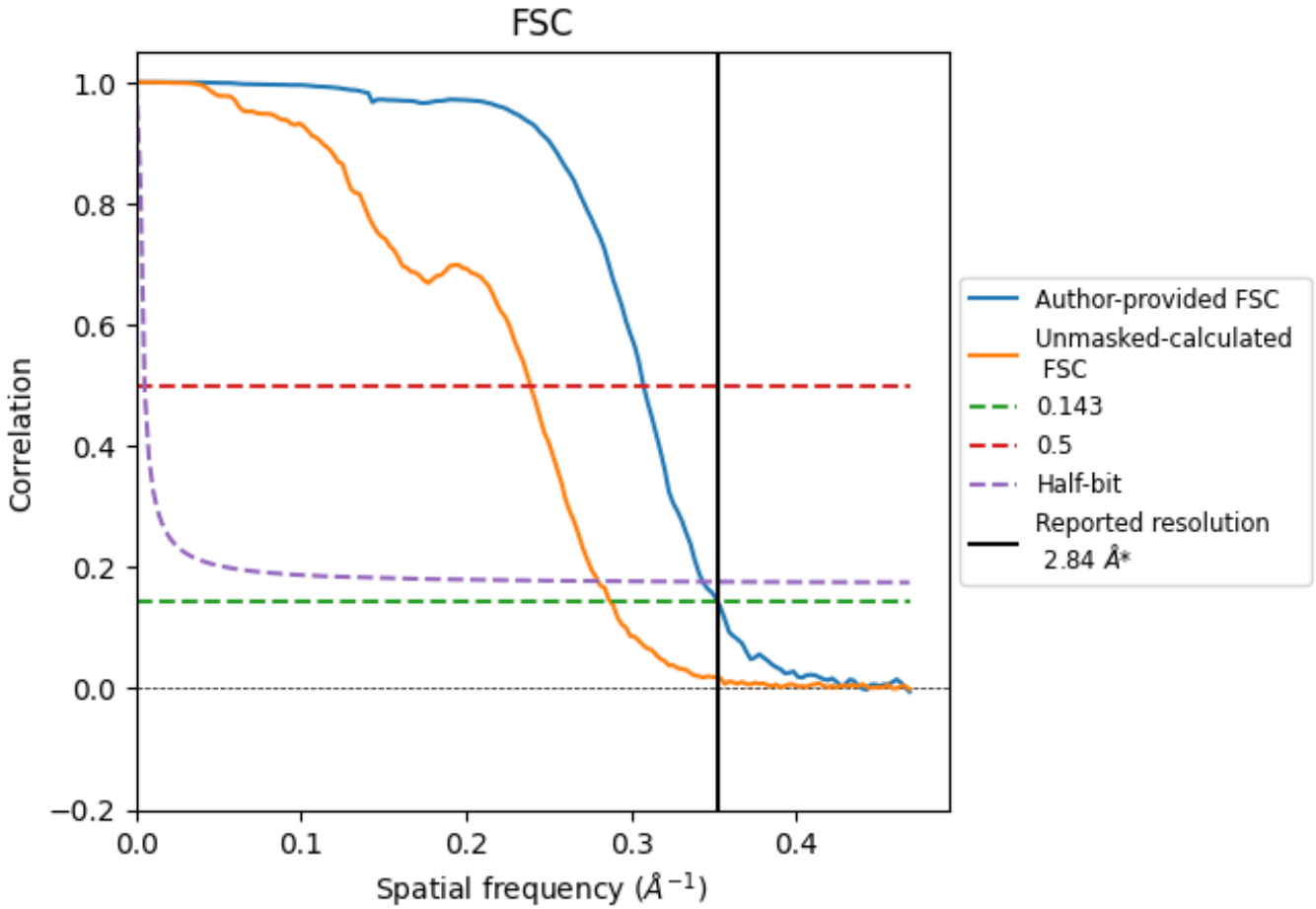


*Reported resolution corresponds to spatial frequency of 0.352 $Å^{-1}$

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 0.352 Å^{-1}

8.2 Resolution estimates (i)

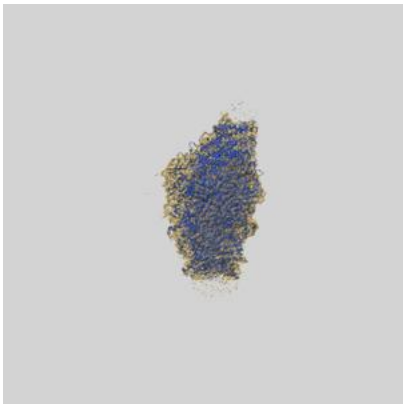
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.84	3.25	2.91
Unmasked-calculated*	3.48	4.19	3.57

*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 3.48 differs from the reported value 2.84 by more than 10 %

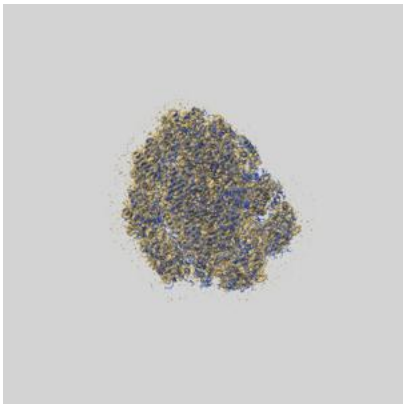
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10236 and PDB model 6SL5. Per-residue inclusion information can be found in section 3 on page 33.

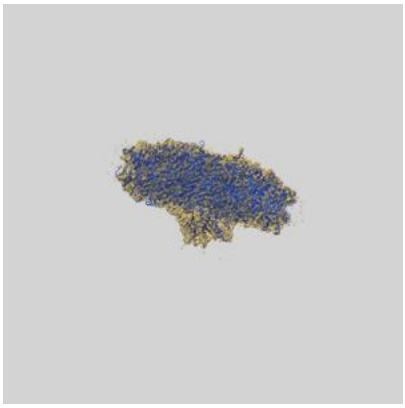
9.1 Map-model overlay



X



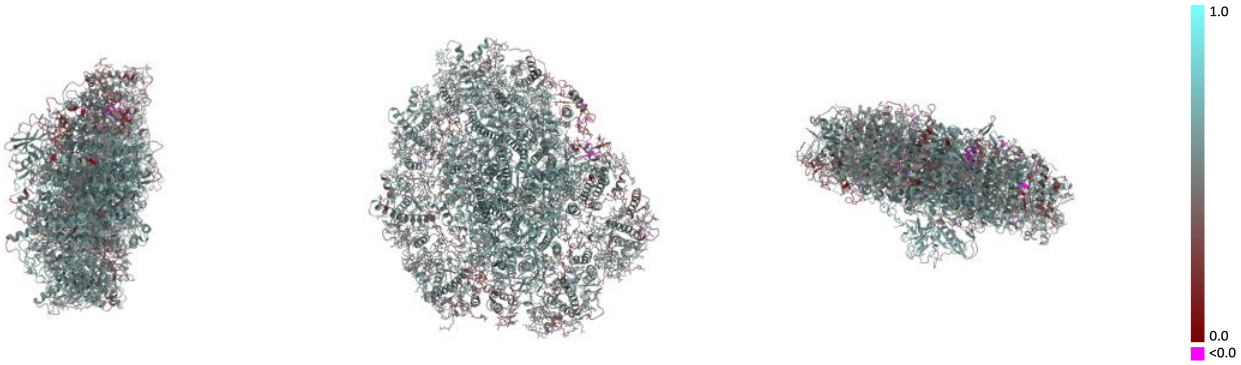
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0247 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.

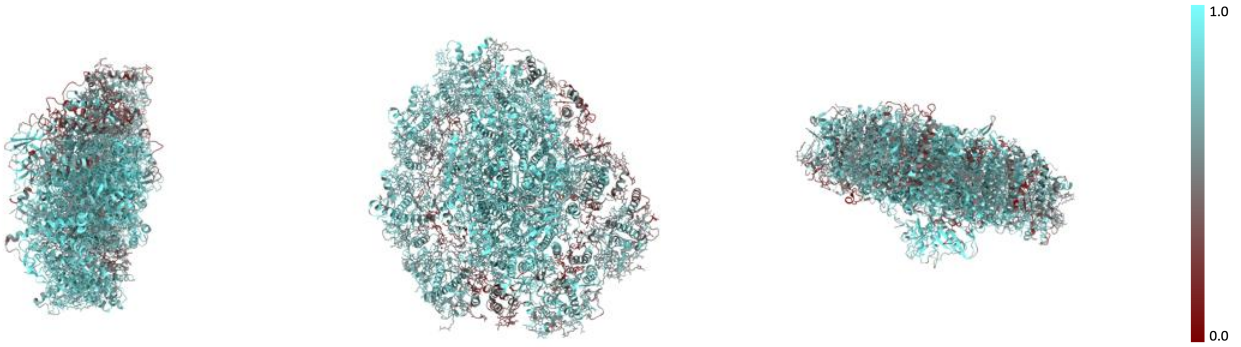
9.2 Q-score mapped to coordinate model (i)



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.

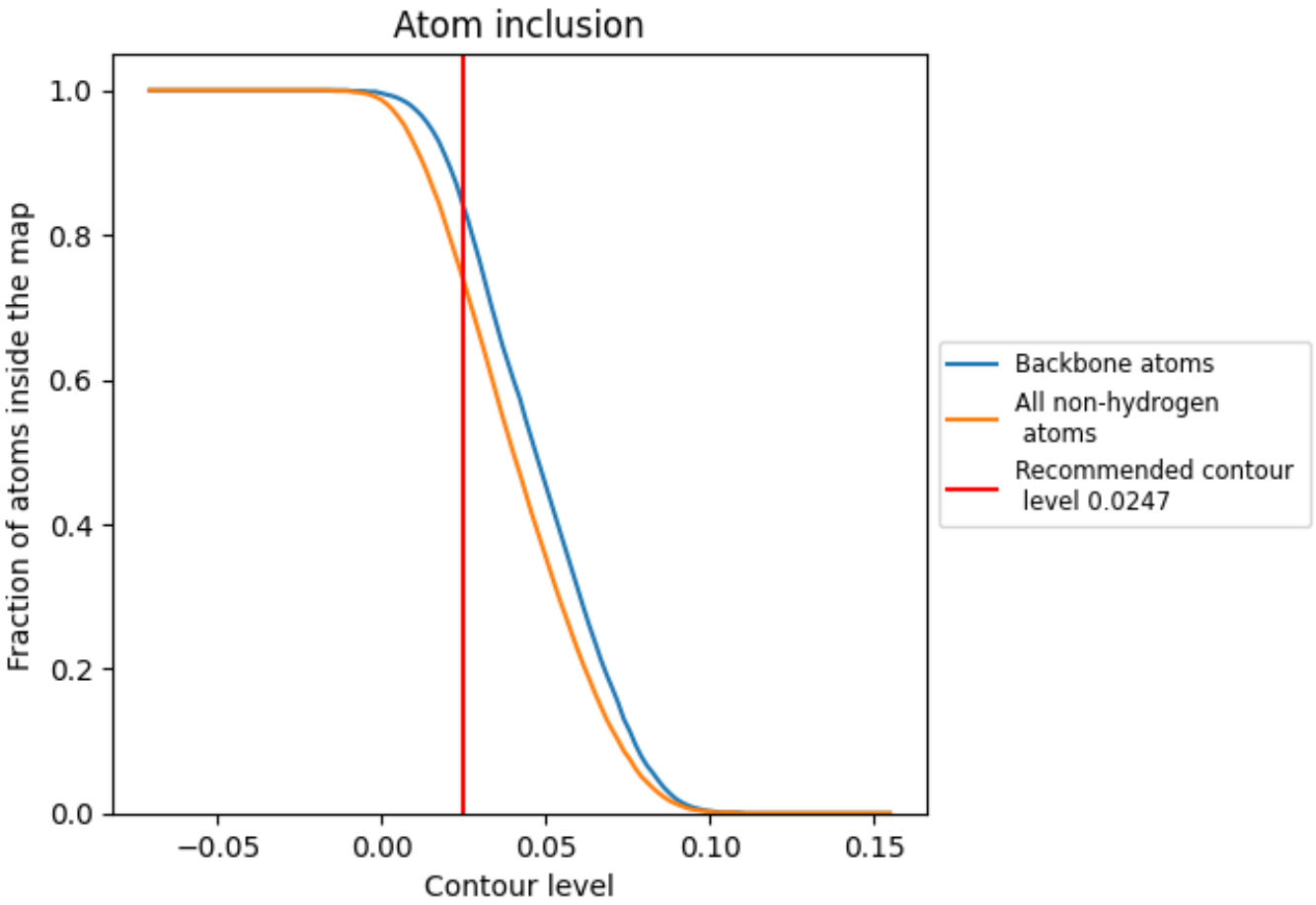
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0247).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 74% 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 (0.0247) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7400	0.5300
1	0.6550	0.4930
2	0.7430	0.5330
3	0.7530	0.5240
4	0.7140	0.4980
5	0.5470	0.4550
6	0.6290	0.4660
A	0.8750	0.5960
B	0.8640	0.5930
C	0.9150	0.6030
D	0.8050	0.5410
E	0.8020	0.5550
F	0.7420	0.5350
G	0.2700	0.3280
H	0.3330	0.3910
I	0.7370	0.5120
J	0.7720	0.5060
K	0.5120	0.4340
L	0.5980	0.4500
O	0.3310	0.3300

