Full wwPDB EM Validation Report ⓘ

Sep 9, 2026 – 01:48 pm BST

PDB ID	:	8ASP / pdb_00008asp
EMDB ID	:	EMD-15621
Title	:	RCII/PSI complex, focused refinement of PSI
Authors	:	Zhao, Z.; Vercellino, I.; Knoppova, J.; Sobotka, R.; Murray, J.W.; Nixon, P.J.; Sazanov, L.A.; Komenda, J.
Deposited on	:	2022-08-20
Resolution	:	2.90 Å(reported)
Based on initial models	:	2XBG, 6WJ6, 5OY0

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:

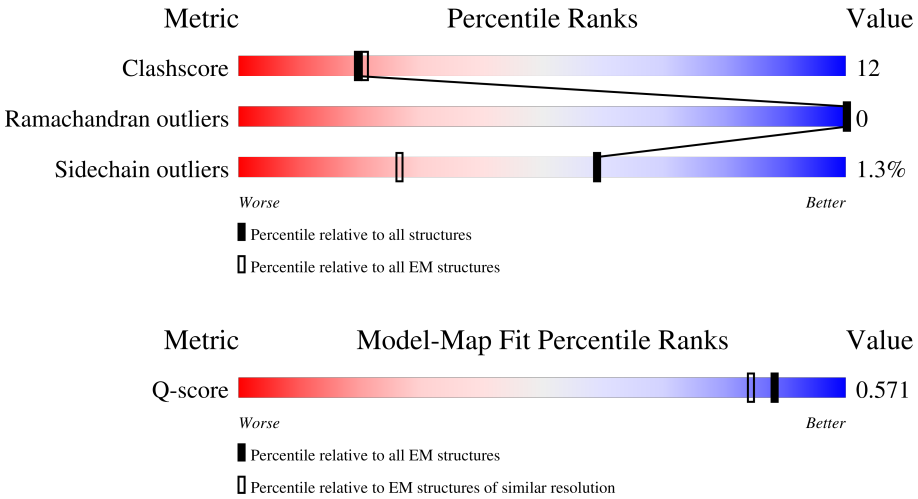
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.90 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.



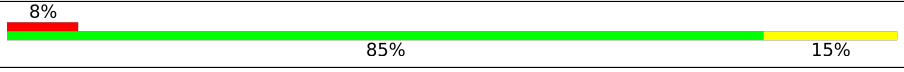
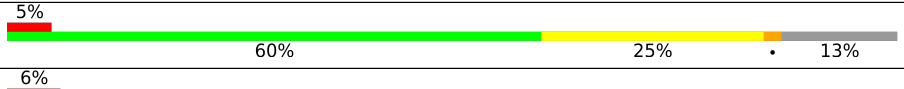
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	751	77% 21%
2	b	731	80% 20%
3	c	81	83% 16%
4	d	141	77% 21%

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Mol	Chain	Length	Quality of chain
5	e	74	
6	f	165	
7	i	40	
8	j	40	
9	k	88	
10	l	157	
11	m	31	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 24596 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	5786	3791	982	986	27	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	729	5770	3798	967	990	15	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	369	103	117	11	0	0

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	139	1087	688	188	208	3	0	0

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	e	69	538	337	95	106	0	0

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	142	1108	715	184	204	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	i	40	Total	C	N	O	S	0	0
			311	209	44	55	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	j	40	Total	C	N	O	S	0	0
			319	215	47	54	3		

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	k	77	Total	C	N	O	S	0	0
			535	350	89	92	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	87	GLY	-	expression tag	UNP P72712
k	88	VAL	-	expression tag	UNP P72712

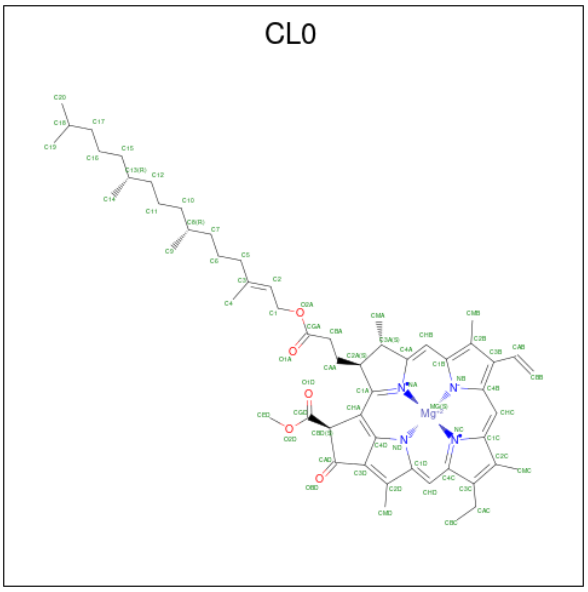
- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	143	Total	C	N	O	S	0	0
			1069	697	173	197	2		

- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

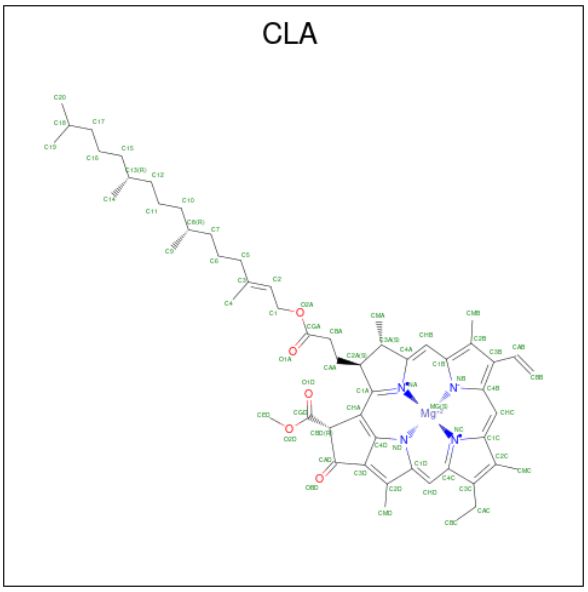
Mol	Chain	Residues	Atoms					AltConf	Trace
11	m	31	Total	C	N	O	S	0	0
			238	159	36	42	1		

- Molecule 12 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 13 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					AltConf
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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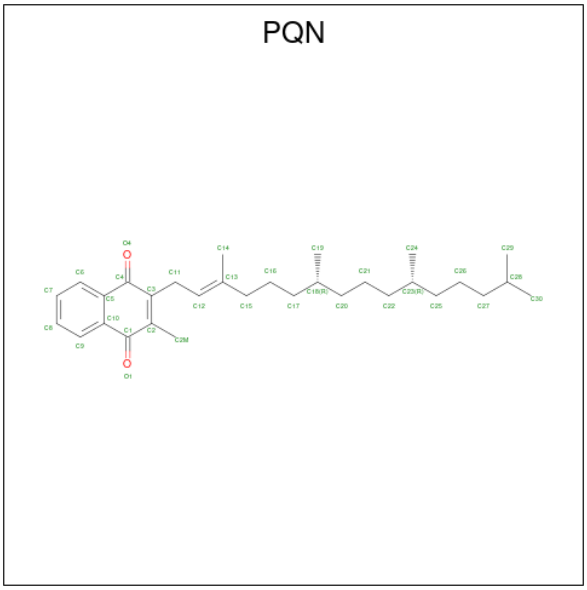
Mol	Chain	Residues	Atoms					AltConf
13	b	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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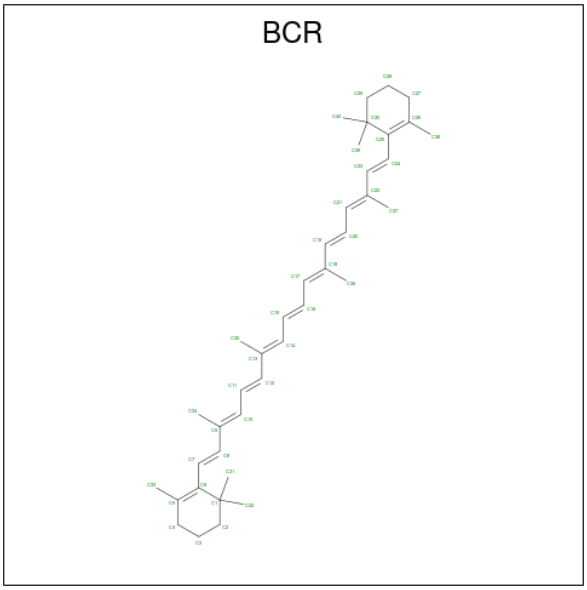
Mol	Chain	Residues	Atoms					AltConf
13	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	j	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	j	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	k	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	k	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

- Molecule 14 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
14	a	1	Total	C	O	0
			33	31	2	
14	b	1	Total	C	O	0
			33	31	2	

- Molecule 15 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



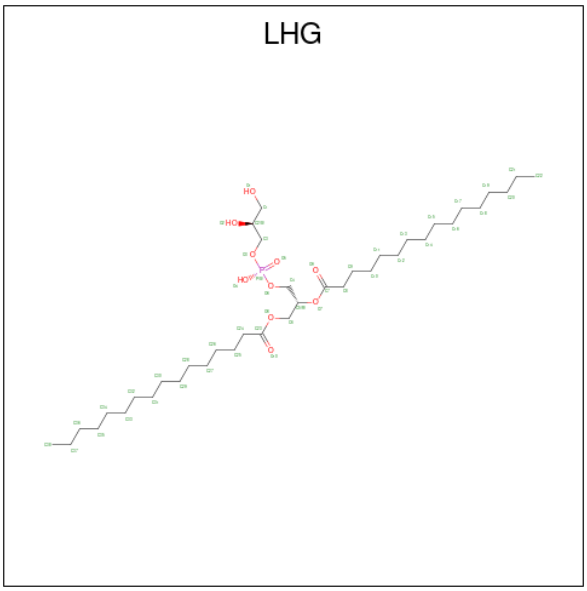
Mol	Chain	Residues	Atoms	AltConf
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 25 25	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	f	1	Total C 40 40	0
15	i	1	Total C 40 40	0
15	i	1	Total C 40 40	0

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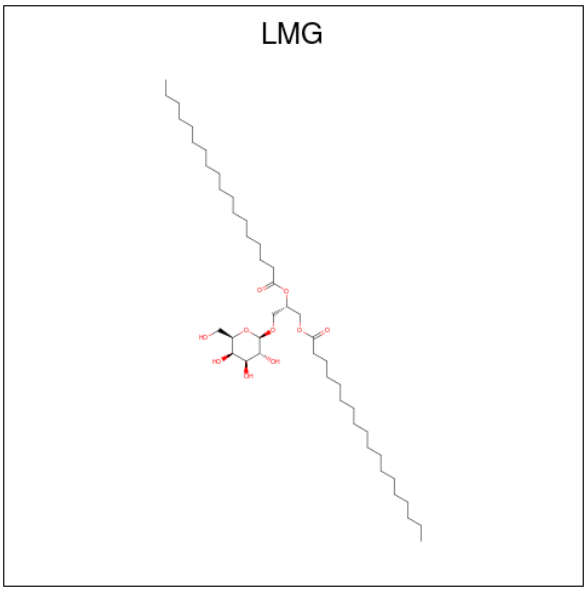
Mol	Chain	Residues	Atoms	AltConf
15	j	1	Total C 40 40	0
15	j	1	Total C 40 40	0
15	k	1	Total C 40 40	0
15	k	1	Total C 40 40	0

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



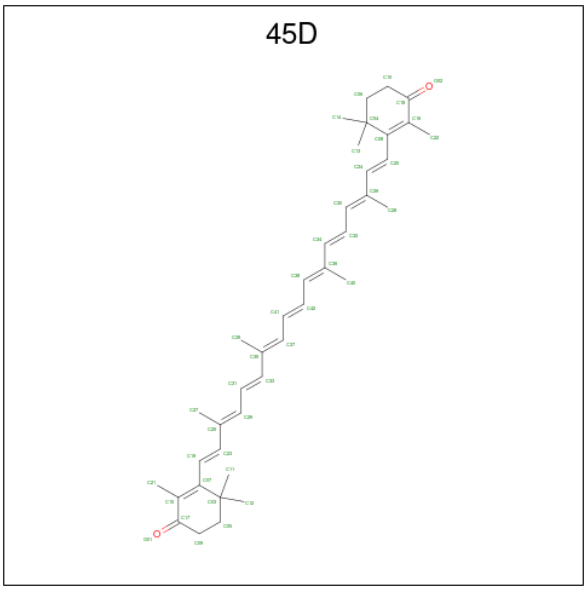
Mol	Chain	Residues	Atoms	AltConf
16	a	1	Total C O P 49 38 10 1	0
16	a	1	Total C O P 49 38 10 1	0
16	a	1	Total C O P 49 38 10 1	0
16	b	1	Total C O P 38 27 10 1	0
16	f	1	Total C O P 49 38 10 1	0

- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



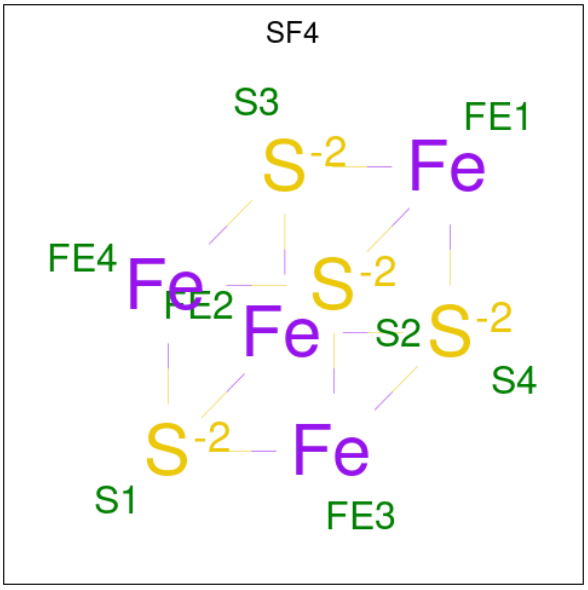
Mol	Chain	Residues	Atoms			AltConf
17	a	1	Total	C	O	0
			50	40	10	
17	a	1	Total	C	O	0
			40	30	10	
17	b	1	Total	C	O	0
			55	45	10	
17	b	1	Total	C	O	0
			55	45	10	

- Molecule 18 is beta,beta-carotene-4,4'-dione (CCD ID: 45D) (formula: $C_{40}H_{52}O_2$).



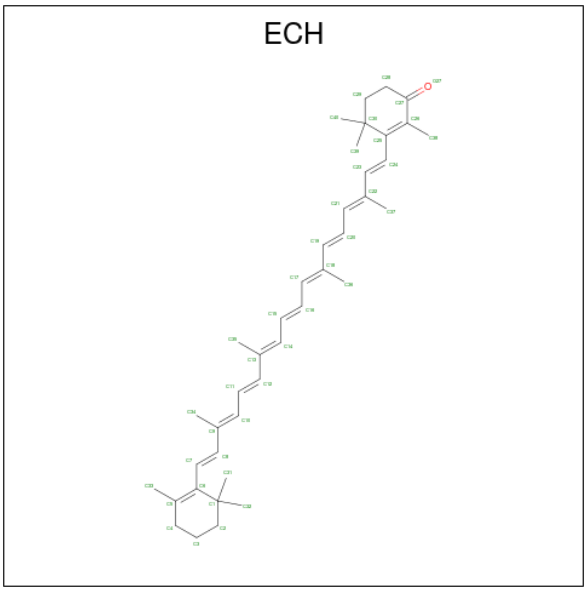
Mol	Chain	Residues	Atoms			AltConf
18	a	1	Total	C	O	0
			42	40	2	

- Molecule 19 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



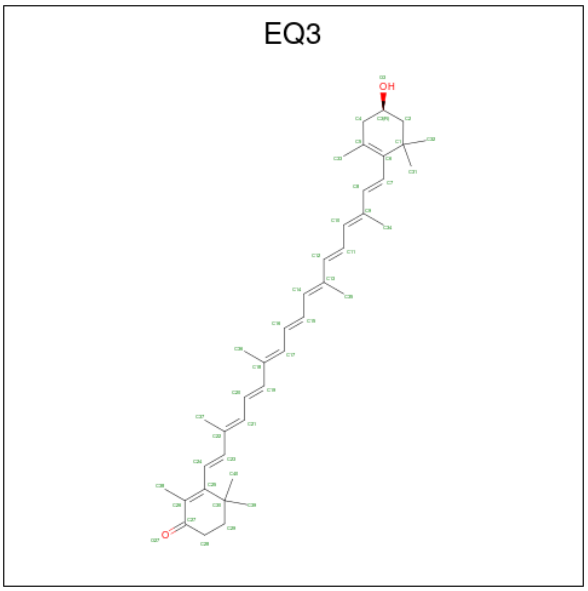
Mol	Chain	Residues	Atoms			AltConf
19	b	1	Total	Fe	S	0
			8	4	4	
19	c	1	Total	Fe	S	0
			8	4	4	
19	c	1	Total	Fe	S	0
			8	4	4	

- Molecule 20 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: $C_{40}H_{54}O$).



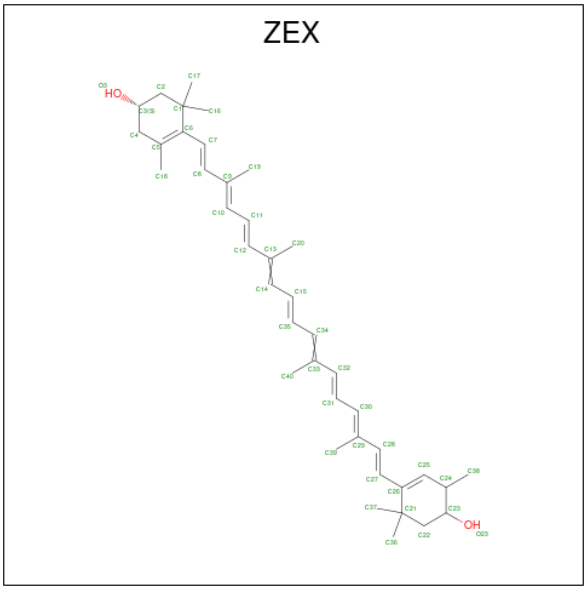
Mol	Chain	Residues	Atoms			AltConf
20	b	1	Total	C	O	0
			41	40	1	
20	m	1	Total	C	O	0
			41	40	1	

- Molecule 21 is (3'R)-3'-hydroxy-beta,beta-caroten-4-one (CCD ID: EQ3) (formula: $C_{40}H_{54}O_2$).



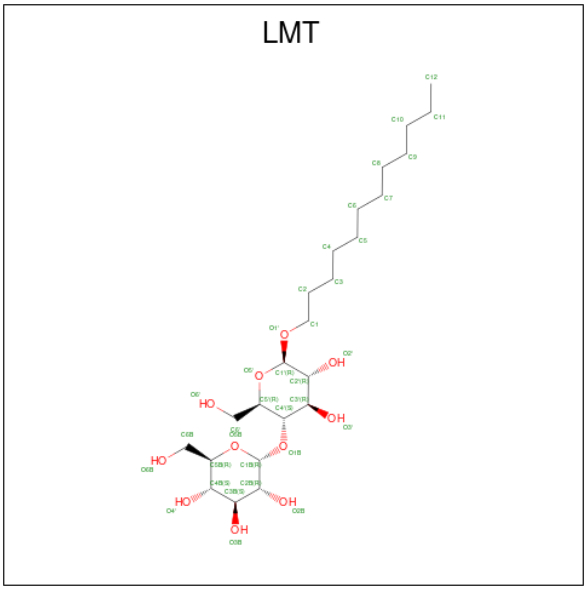
Mol	Chain	Residues	Atoms			AltConf
21	b	1	Total	C	O	0
			42	40	2	

- Molecule 22 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (CCD ID: ZEX) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
22	b	1	Total	C	O	0
			42	40	2	
22	f	1	Total	C	O	0
			42	40	2	

- Molecule 23 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
23	j	1	Total	C	O	0
			35	24	11	

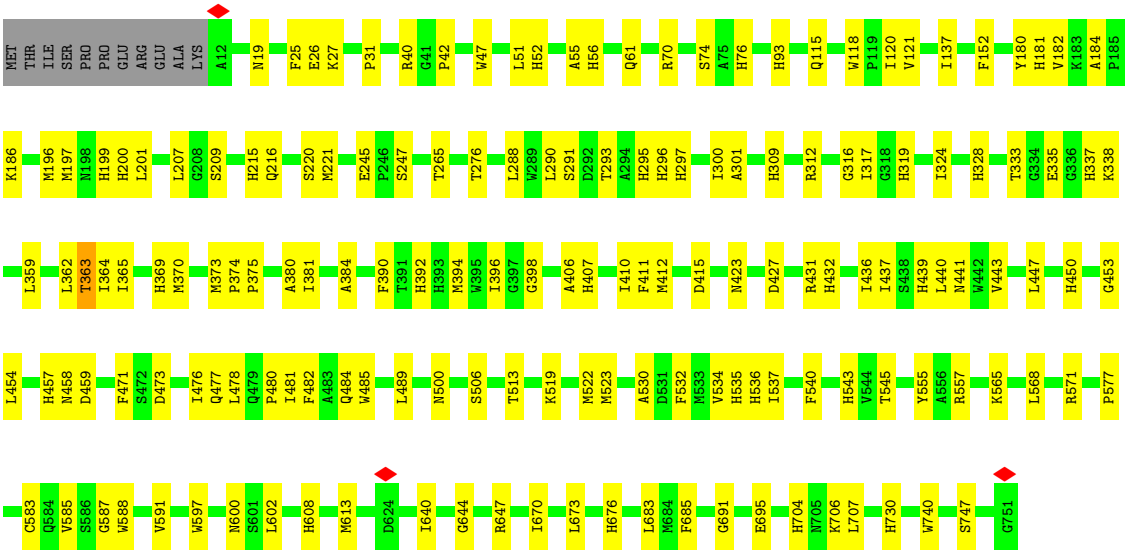
3 Residue-property plots (i)

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:

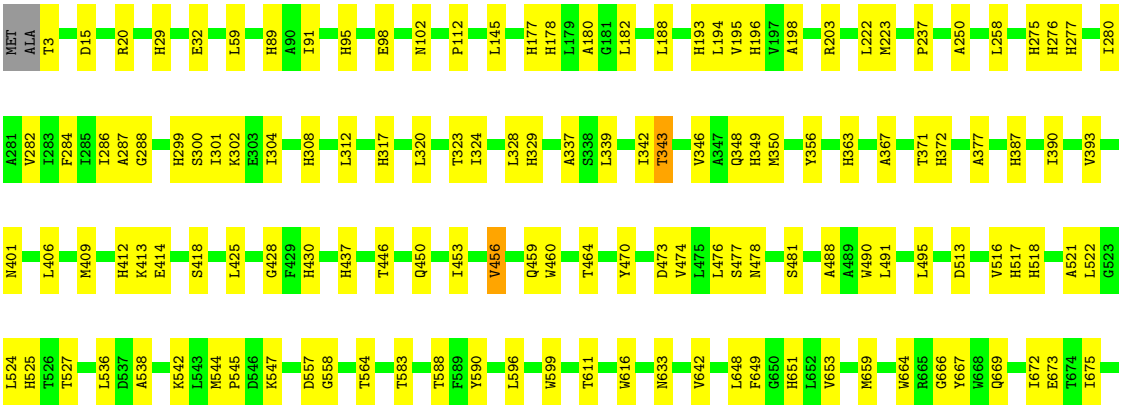




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:



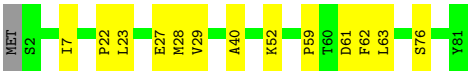




• Molecule 3: Photosystem I iron-sulfur center

Chain c:

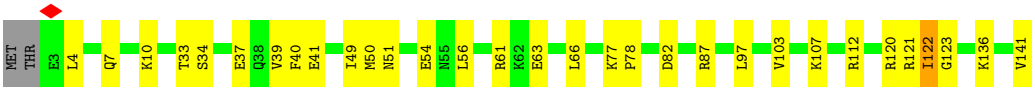




• Molecule 4: Photosystem I reaction center subunit II

Chain d:

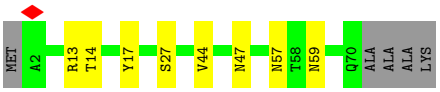




• Molecule 5: Photosystem I reaction center subunit IV

Chain e:

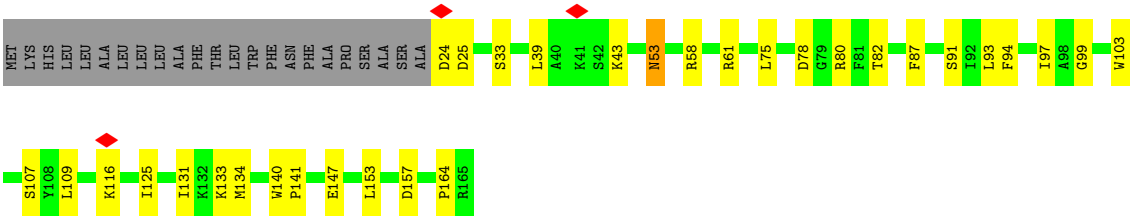




• Molecule 6: Photosystem I reaction center subunit III

Chain f:

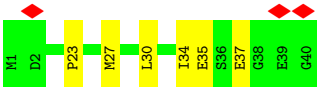




• Molecule 7: Photosystem I reaction center subunit VIII

Chain i:

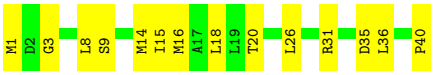




• Molecule 8: Photosystem I reaction center subunit IX

Chain j:

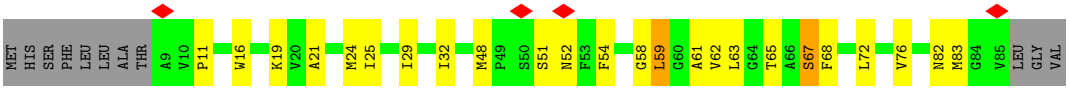




• Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain k:



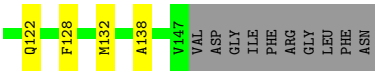


• Molecule 10: Photosystem I reaction center subunit XI

Chain l:



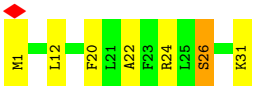




• Molecule 11: Photosystem I reaction center subunit XII

Chain m:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	178513	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	90.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.526	Depositor
Minimum map value	-0.118	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.077	Depositor
Map size (Å)	488.0, 488.0, 488.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.22, 1.22, 1.22	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, LHG, CL0, SF4, EQ3, BCR, PQN, LMG, 45D, ECH, LMT, ZEX

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	0.14	0/5984	0.29	0/8158
2	b	0.13	0/5981	0.29	0/8178
3	c	0.12	0/610	0.27	0/826
4	d	0.11	0/1111	0.30	0/1497
5	e	0.13	0/547	0.44	0/741
6	f	0.14	0/1138	0.34	0/1546
7	i	0.13	0/322	0.34	0/438
8	j	0.12	0/328	0.29	0/443
9	k	0.15	0/546	0.42	0/741
10	l	0.13	0/1097	0.33	0/1493
11	m	0.15	0/241	0.35	0/326
All	All	0.14	0/17905	0.31	0/24387

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	5786	0	5640	145	0
2	b	5770	0	5547	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	600	0	581	11	0
4	d	1087	0	1082	21	0
5	e	538	0	514	5	0
6	f	1108	0	1100	27	0
7	i	311	0	304	5	0
8	j	319	0	328	16	0
9	k	535	0	559	21	0
10	l	1069	0	1044	24	0
11	m	238	0	260	5	0
12	a	65	0	72	5	0
13	a	2637	0	2754	155	0
13	b	2475	0	2528	150	0
13	f	160	0	144	6	0
13	j	101	0	82	2	0
13	k	156	0	138	8	0
13	l	167	0	154	8	0
14	a	33	0	46	1	0
14	b	33	0	46	3	0
15	a	185	0	257	15	0
15	b	200	0	280	17	0
15	f	40	0	56	4	0
15	i	80	0	112	8	0
15	j	80	0	112	7	0
15	k	80	0	112	7	0
16	a	147	0	222	7	0
16	b	38	0	49	2	0
16	f	49	0	74	4	0
17	a	90	0	123	10	0
17	b	110	0	172	5	0
18	a	42	0	52	2	0
19	b	8	0	0	0	0
19	c	16	0	0	0	0
20	b	41	0	54	3	0
20	m	41	0	54	3	0
21	b	42	0	0	0	0
22	b	42	0	56	2	0
22	f	42	0	56	2	0
23	j	35	0	45	0	0
All	All	24596	0	24809	616	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (616) 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)
1:a:392:HIS:HE1	13:a:828:CLA:ND	1.66	0.94
1:a:407:HIS:HE1	13:a:830:CLA:NA	1.78	0.81
2:b:275:HIS:HE1	13:b:817:CLA:ND	1.78	0.80
13:b:811:CLA:HHC	13:b:811:CLA:HBB1	1.64	0.80
2:b:387:HIS:HE1	13:b:830:CLA:NA	1.80	0.79
1:a:93:HIS:HE1	13:a:807:CLA:NA	1.80	0.79
1:a:52:HIS:HE1	13:a:803:CLA:ND	1.83	0.76
13:b:818:CLA:HBA2	13:b:827:CLA:HBB2	1.69	0.74
10:l:57:HIS:HE1	13:l:1502:CLA:ND	1.84	0.74
2:b:95:HIS:HE1	13:b:811:CLA:NB	1.86	0.72
2:b:709:HIS:HE1	13:b:841:CLA:ND	1.87	0.72
4:d:37:GLU:HA	4:d:50:MET:O	1.89	0.71
10:l:118:ASP:OD1	10:l:122:GLN:NE2	2.23	0.71
13:b:807:CLA:H162	13:b:829:CLA:HBB2	1.73	0.71
3:c:61:ASP:OD1	3:c:62:PHE:N	2.24	0.70
2:b:346:VAL:O	2:b:350:MET:HB2	1.91	0.70
2:b:409:MET:HG3	15:b:849:BCR:H402	1.72	0.70
4:d:103:VAL:HG13	4:d:107:LYS:HE2	1.74	0.69
1:a:704:HIS:HE1	13:a:840:CLA:ND	1.91	0.68
13:b:830:CLA:H91	17:b:850:LMG:H262	1.75	0.68
13:a:834:CLA:H2	10:l:64:PRO:HB2	1.75	0.68
13:a:830:CLA:HBA1	13:a:830:CLA:HBD	1.77	0.67
13:a:828:CLA:H61	18:a:856:45D:H221	1.76	0.66
13:b:829:CLA:H8	15:b:845:BCR:H21C	1.78	0.66
4:d:34:SER:HB2	4:d:50:MET:HE3	1.77	0.66
4:d:61:ARG:NH2	4:d:63:GLU:OE1	2.29	0.66
9:k:51:SER:O	9:k:52:ASN:ND2	2.29	0.66
1:a:484:GLN:HB3	17:a:852:LMG:HC5	1.78	0.66
1:a:337:HIS:CD2	13:a:824:CLA:ND	2.64	0.65
2:b:32:GLU:OE2	2:b:329:HIS:NE2	2.29	0.65
9:k:32:ILE:HD11	13:k:4004:CLA:HAC2	1.79	0.65
13:a:840:CLA:H171	13:f:201:CLA:H51	1.78	0.65
10:l:57:HIS:HE1	13:l:1502:CLA:C4D	2.09	0.65
1:a:557:ARG:NH2	4:d:41:GLU:OE1	2.28	0.65
2:b:473:ASP:OD1	2:b:478:ASN:ND2	2.22	0.65
1:a:74:SER:OG	1:a:180:TYR:HB2	1.98	0.64
13:a:831:CLA:HAA2	10:l:8:VAL:HG21	1.79	0.64
8:j:16:MET:O	8:j:20:THR:HG23	1.96	0.64
1:a:480:PRO:HG3	1:a:532:PHE:HB2	1.79	0.64
1:a:673:LEU:HB3	13:b:801:CLA:H11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:684:LEU:HD12	13:l:1502:CLA:H42	1.79	0.64
1:a:647:ARG:NH1	2:b:633:ASN:OD1	2.30	0.63
13:b:830:CLA:HBA1	13:b:830:CLA:HBD	1.79	0.63
2:b:542:LYS:NZ	5:e:17:TYR:O	2.30	0.63
13:a:854:CLA:H11	2:b:648:LEU:HB3	1.80	0.63
1:a:295:HIS:HE1	13:a:817:CLA:ND	1.97	0.62
1:a:120:ILE:HG13	1:a:121:VAL:HG13	1.82	0.62
2:b:557:ASP:HB3	2:b:564:THR:HG21	1.81	0.62
13:b:818:CLA:HBC1	13:b:825:CLA:H191	1.81	0.62
13:b:808:CLA:H2	13:b:808:CLA:C4D	2.29	0.62
1:a:295:HIS:HE1	13:a:817:CLA:C4D	2.13	0.62
13:a:803:CLA:H192	13:a:841:CLA:H143	1.81	0.62
2:b:659:MET:HB2	13:b:804:CLA:C2C	2.30	0.62
13:b:804:CLA:H143	15:b:848:BCR:H362	1.82	0.62
2:b:275:HIS:HE1	13:b:817:CLA:C4D	2.12	0.61
13:a:830:CLA:O2D	13:a:830:CLA:H2A	2.00	0.61
10:l:44:LEU:HD22	10:l:48:LEU:HD23	1.81	0.61
2:b:544:MET:HE1	2:b:557:ASP:HB2	1.83	0.61
13:a:835:CLA:H43	13:k:4002:CLA:H143	1.83	0.61
2:b:195:VAL:HG11	13:b:816:CLA:HBC2	1.83	0.60
6:f:87:PHE:O	6:f:91:SER:OG	2.16	0.60
13:a:840:CLA:HED2	2:b:418:SER:HB2	1.82	0.60
1:a:473:ASP:O	1:a:477:GLN:NE2	2.33	0.60
9:k:21:ALA:O	9:k:25:ILE:HD12	2.01	0.60
13:a:823:CLA:HBD	13:a:823:CLA:HBA1	1.83	0.60
2:b:339:LEU:O	2:b:343:THR:OG1	2.19	0.60
15:b:847:BCR:H23C	15:b:849:BCR:H393	1.83	0.60
4:d:87:ARG:HB2	4:d:97:LEU:HD11	1.84	0.60
1:a:297:HIS:HE1	13:a:819:CLA:NA	2.00	0.60
1:a:181:HIS:HE1	13:a:811:CLA:NA	2.00	0.60
13:a:802:CLA:H12	2:b:425:LEU:HD23	1.84	0.59
1:a:392:HIS:HE1	13:a:828:CLA:C1D	2.14	0.59
1:a:447:LEU:HB3	1:a:540:PHE:HB2	1.85	0.59
13:a:805:CLA:H2A	13:a:805:CLA:HED3	1.85	0.59
13:a:805:CLA:H41	15:a:845:BCR:H402	1.85	0.59
13:b:831:CLA:HAC1	15:b:849:BCR:H383	1.83	0.59
6:f:97:ILE:HG23	13:f:203:CLA:HAA1	1.85	0.59
6:f:147:GLU:HB3	6:f:153:LEU:HB2	1.84	0.59
2:b:89:HIS:CD2	13:b:809:CLA:NA	2.71	0.59
2:b:371:THR:HG23	2:b:588:THR:HG21	1.85	0.59
2:b:196:HIS:HE1	13:b:816:CLA:NA	1.96	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:571:ARG:NH2	16:a:849:LHG:O2	2.36	0.58
2:b:203:ARG:HG2	2:b:250:ALA:HB1	1.86	0.58
4:d:10:LYS:HD3	4:d:49:ILE:HG13	1.83	0.58
1:a:585:VAL:HG22	2:b:666:GLY:HA3	1.85	0.58
13:a:803:CLA:HBB1	15:j:105:BCR:H292	1.85	0.58
16:a:851:LHG:H211	16:a:851:LHG:H332	1.86	0.58
6:f:107:SER:HB2	6:f:133:LYS:HE3	1.84	0.58
2:b:659:MET:HB2	13:b:804:CLA:C1C	2.33	0.58
6:f:58:ARG:NH1	8:j:35:ASP:OD2	2.37	0.57
13:b:824:CLA:H51	13:b:825:CLA:H142	1.86	0.57
10:l:41:ARG:O	10:l:49:ARG:NH2	2.37	0.57
2:b:98:GLU:OE2	2:b:102:ASN:ND2	2.37	0.57
13:a:822:CLA:HMD2	15:k:4001:BCR:H24C	1.85	0.57
1:a:27:LYS:HD2	13:a:811:CLA:HAA2	1.87	0.57
1:a:40:ARG:NH1	1:a:40:ARG:HB2	2.20	0.57
2:b:356:TYR:OH	13:b:829:CLA:OBD	2.19	0.57
13:b:810:CLA:H142	17:b:850:LMG:H242	1.85	0.57
2:b:349:HIS:CD2	13:b:827:CLA:NC	2.73	0.56
1:a:437:ILE:HG13	1:a:555:TYR:HE2	1.70	0.56
13:b:830:CLA:O2D	13:b:830:CLA:H2A	2.05	0.56
13:b:834:CLA:H62	15:f:202:BCR:HC22	1.86	0.56
1:a:25:PHE:HB2	8:j:1:MET:HG2	1.88	0.56
17:a:850:LMG:HC91	17:a:850:LMG:H352	1.86	0.56
16:a:851:LHG:H302	16:a:851:LHG:H172	1.86	0.56
13:b:804:CLA:HBC2	13:b:804:CLA:HHD	1.86	0.56
1:a:333:THR:HG21	16:a:851:LHG:HC11	1.87	0.56
1:a:427:ASP:OD2	1:a:431:ARG:NH1	2.39	0.56
13:b:818:CLA:H161	13:b:836:CLA:HBA1	1.87	0.56
3:c:63:LEU:H	3:c:63:LEU:HD22	1.71	0.56
1:a:93:HIS:HE1	13:a:807:CLA:C1A	2.17	0.56
1:a:196:MET:HB2	13:a:813:CLA:HBC2	1.87	0.56
1:a:56:HIS:HE1	13:a:804:CLA:C1C	2.19	0.56
2:b:516:VAL:HG21	2:b:590:TYR:HB2	1.87	0.56
11:m:20:PHE:CZ	11:m:24:ARG:HD2	2.41	0.56
1:a:704:HIS:HE1	13:a:840:CLA:C4D	2.18	0.56
2:b:286:ILE:HD13	15:b:844:BCR:H17C	1.87	0.56
8:j:31:ARG:HD3	15:j:105:BCR:H312	1.88	0.56
2:b:91:ILE:HB	2:b:112:PRO:HB2	1.87	0.56
1:a:362:LEU:HD11	13:a:819:CLA:H71	1.88	0.55
13:b:826:CLA:HAA2	13:b:827:CLA:OBD	2.06	0.55
5:e:13:ARG:O	5:e:14:THR:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:393:VAL:HG23	2:b:538:ALA:HB1	1.88	0.55
1:a:216:GLN:HA	1:a:220:SER:HB2	1.88	0.55
13:b:820:CLA:HBB1	13:b:825:CLA:H62	1.87	0.55
1:a:450:HIS:O	1:a:454:LEU:HG	2.07	0.55
13:b:842:CLA:HBB2	15:b:849:BCR:H14C	1.87	0.55
1:a:670:ILE:HG23	13:b:801:CLA:H62	1.89	0.55
13:b:808:CLA:HHB	13:b:809:CLA:HMB3	1.89	0.55
1:a:215:HIS:HB2	13:a:814:CLA:CHC	2.37	0.55
2:b:367:ALA:HB1	2:b:722:LEU:HD11	1.88	0.55
10:l:62:ILE:HG21	10:l:138:ALA:HB1	1.89	0.55
11:m:1:MET:HE2	11:m:1:MET:HA	1.88	0.55
1:a:691:GLY:N	2:b:564:THR:O	2.40	0.55
1:a:432:HIS:CE1	1:a:436:ILE:HD11	2.42	0.54
9:k:54:PHE:HZ	15:k:4005:BCR:H393	1.72	0.54
9:k:19:LYS:H	9:k:19:LYS:HD2	1.71	0.54
10:l:9:GLN:O	10:l:21:SER:N	2.40	0.54
1:a:398:GLY:HA3	1:a:602:LEU:HD11	1.90	0.54
13:a:808:CLA:H2	13:a:828:CLA:H43	1.88	0.54
1:a:245:GLU:OE2	1:a:247:SER:OG	2.23	0.54
15:a:844:BCR:H392	15:k:4001:BCR:HC8	1.88	0.54
1:a:583:CYS:HB2	2:b:664:TRP:HB3	1.89	0.54
2:b:276:HIS:HB2	13:b:818:CLA:C1B	2.37	0.54
2:b:684:LEU:HD11	10:l:37:LEU:HD13	1.89	0.54
1:a:373:MET:HG2	1:a:506:SER:HB2	1.90	0.54
13:b:828:CLA:HBC3	17:b:850:LMG:H442	1.88	0.54
2:b:557:ASP:OD1	3:c:52:LYS:NZ	2.37	0.54
6:f:53:ASN:OD1	6:f:53:ASN:N	2.41	0.54
1:a:485:TRP:HE1	17:a:852:LMG:H171	1.73	0.54
2:b:343:THR:HB	2:b:377:ALA:HB2	1.90	0.53
2:b:518:HIS:HE1	13:b:838:CLA:ND	2.06	0.53
13:b:805:CLA:H13	20:m:101:ECH:H17	1.90	0.53
13:a:839:CLA:HHC	13:a:839:CLA:HBB1	1.89	0.53
3:c:62:PHE:HD2	4:d:122:ILE:HG21	1.72	0.53
1:a:384:ALA:HA	1:a:747:SER:HB2	1.91	0.53
2:b:312:LEU:HD13	16:b:851:LHG:HC42	1.90	0.53
13:b:806:CLA:H8	13:b:825:CLA:HBA1	1.91	0.53
13:b:823:CLA:HHC	13:b:823:CLA:HBB1	1.90	0.53
9:k:25:ILE:HD12	9:k:25:ILE:H	1.74	0.53
1:a:216:GLN:O	1:a:221:MET:HG3	2.09	0.53
1:a:613:MET:HE3	1:a:613:MET:HA	1.90	0.53
2:b:277:HIS:HD2	2:b:280:ILE:HD11	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:718:TYR:HB2	13:b:803:CLA:HED3	1.91	0.53
6:f:93:LEU:HD13	13:j:104:CLA:HBB2	1.90	0.53
2:b:323:THR:OG1	2:b:401:ASN:OD1	2.25	0.52
13:a:807:CLA:H41	13:a:807:CLA:H92	1.91	0.52
13:b:808:CLA:HBC2	11:m:12:LEU:HD23	1.91	0.52
2:b:299:HIS:HB3	2:b:304:ILE:HD11	1.90	0.52
1:a:369:HIS:CD2	13:a:827:CLA:NC	2.77	0.52
2:b:15:ASP:HB3	2:b:20:ARG:HB2	1.92	0.52
6:f:39:LEU:O	6:f:43:LYS:NZ	2.40	0.52
13:a:841:CLA:H62	8:j:16:MET:HE1	1.92	0.52
6:f:125:ILE:O	8:j:9:SER:OG	2.27	0.52
1:a:118:TRP:HE1	15:a:848:BCR:H332	1.73	0.52
1:a:453:GLY:HA3	13:a:834:CLA:HAB	1.91	0.52
1:a:207:LEU:HD22	15:a:844:BCR:H361	1.92	0.51
2:b:413:LYS:HB2	2:b:536:LEU:HD13	1.90	0.51
1:a:31:PRO:HB2	1:a:51:LEU:HD11	1.93	0.51
1:a:199:HIS:HE1	13:a:812:CLA:NA	2.08	0.51
2:b:301:ILE:HG21	13:b:825:CLA:HAC1	1.92	0.51
13:b:818:CLA:H51	13:b:835:CLA:HAA2	1.92	0.51
13:f:201:CLA:H41	8:j:18:LEU:HD13	1.92	0.51
13:a:820:CLA:H152	13:a:820:CLA:HAB	1.93	0.51
1:a:55:ALA:O	1:a:61:GLN:NE2	2.43	0.51
1:a:597:TRP:HE1	13:b:804:CLA:C1D	2.24	0.51
2:b:95:HIS:HE1	13:b:811:CLA:C4B	2.24	0.51
2:b:308:HIS:HE1	13:b:823:CLA:C4D	2.24	0.51
2:b:412:HIS:CE1	13:b:831:CLA:ND	2.78	0.51
13:b:824:CLA:H2A	13:b:824:CLA:HED3	1.93	0.51
13:a:826:CLA:HBB1	13:a:839:CLA:HHB	1.92	0.51
13:a:832:CLA:H143	13:a:838:CLA:H202	1.93	0.51
6:f:25:ASP:OD2	6:f:80:ARG:NH2	2.44	0.51
1:a:276:THR:N	1:a:291:SER:OG	2.42	0.51
1:a:364:ILE:HG12	1:a:394:MET:HE3	1.93	0.51
3:c:23:LEU:HA	4:d:66:LEU:HD13	1.93	0.51
2:b:196:HIS:HE1	13:b:816:CLA:C1A	2.25	0.50
13:b:834:CLA:H92	13:f:203:CLA:HMB3	1.92	0.50
1:a:209:SER:HB2	1:a:301:ALA:HB2	1.92	0.50
1:a:565:LYS:NZ	1:a:585:VAL:O	2.36	0.50
1:a:500:ASN:HB2	13:a:836:CLA:HED2	1.92	0.50
13:a:802:CLA:CGA	13:a:802:CLA:H3A	2.41	0.50
13:k:4004:CLA:HBC2	13:k:4004:CLA:HHD	1.92	0.50
13:a:826:CLA:HAA2	13:a:827:CLA:OBD	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:m:31:LYS:HB2	11:m:31:LYS:NZ	2.26	0.50
13:b:841:CLA:H152	15:i:102:BCR:H15C	1.93	0.50
1:a:76:HIS:CE1	13:a:805:CLA:ND	2.80	0.50
2:b:680:GLU:O	2:b:686:ASN:ND2	2.38	0.50
13:b:840:CLA:HBB2	14:b:843:PQN:H141	1.92	0.50
2:b:317:HIS:CD2	13:b:824:CLA:ND	2.79	0.50
2:b:339:LEU:HD12	2:b:342:ILE:HD11	1.93	0.50
7:i:23:PRO:O	7:i:27:MET:HG2	2.12	0.50
2:b:659:MET:HB2	13:b:804:CLA:C3C	2.42	0.49
1:a:522:MET:HE3	1:a:523:MET:N	2.27	0.49
13:b:809:CLA:O1A	13:b:828:CLA:HBD	2.12	0.49
9:k:48:MET:SD	9:k:62:VAL:HG21	2.51	0.49
8:j:26:LEU:HD13	15:j:101:BCR:HC7	1.94	0.49
1:a:40:ARG:HB2	1:a:40:ARG:HH11	1.76	0.49
1:a:740:TRP:NE1	13:a:828:CLA:O1A	2.44	0.49
4:d:39:VAL:HG22	4:d:49:ILE:HG22	1.94	0.49
10:l:9:GLN:HG3	10:l:21:SER:HB3	1.93	0.49
13:a:813:CLA:H43	15:a:845:BCR:H19C	1.95	0.49
13:b:817:CLA:CHD	13:b:818:CLA:HBB2	2.43	0.49
2:b:490:TRP:CG	13:b:818:CLA:H42	2.48	0.49
2:b:713:GLY:O	2:b:717:THR:OG1	2.22	0.49
3:c:22:PRO:HG2	3:c:23:LEU:HD12	1.94	0.49
13:a:827:CLA:HBB1	13:a:835:CLA:HAA2	1.95	0.49
2:b:180:ALA:HB2	2:b:288:GLY:HA3	1.95	0.49
2:b:446:THR:O	2:b:446:THR:OG1	2.24	0.49
1:a:364:ILE:HG23	1:a:394:MET:HE1	1.94	0.48
1:a:600:ASN:HD21	12:a:801:CL0:H68	1.77	0.48
22:b:854:ZEX:H25	8:j:40:PRO:HD2	1.94	0.48
9:k:24:MET:HE2	9:k:24:MET:HA	1.94	0.48
9:k:63:LEU:O	9:k:67:SER:OG	2.30	0.48
13:a:808:CLA:H152	15:j:101:BCR:H402	1.94	0.48
10:l:86:LEU:HD22	10:l:132:MET:SD	2.53	0.48
1:a:683:LEU:HB2	13:a:802:CLA:HMC2	1.95	0.48
2:b:282:VAL:O	2:b:286:ILE:HG12	2.14	0.48
4:d:77:LYS:HB3	4:d:78:PRO:HD3	1.96	0.48
1:a:335:GLU:HG2	1:a:423:ASN:HB3	1.94	0.48
13:a:823:CLA:O1D	13:a:823:CLA:H2A	2.12	0.48
2:b:437:HIS:HE1	13:b:834:CLA:C1A	2.11	0.48
4:d:120:ARG:NH2	4:d:141:VAL:OXT	2.38	0.48
13:a:832:CLA:HBB1	13:a:855:CLA:HAA2	1.96	0.48
1:a:450:HIS:HE1	13:a:833:CLA:NA	2.06	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:808:CLA:HBA2	13:a:808:CLA:H3A	1.32	0.48
13:a:819:CLA:H203	13:a:827:CLA:H3A	1.95	0.48
13:a:828:CLA:H141	13:a:828:CLA:H162	1.67	0.48
18:a:856:45D:H231	18:a:856:45D:H122	1.95	0.48
1:a:706:LYS:NZ	6:f:157:ASP:OD1	2.34	0.48
17:a:852:LMG:H111	17:a:852:LMG:HC8	1.59	0.48
13:a:855:CLA:HBB2	15:i:102:BCR:H372	1.96	0.48
1:a:288:LEU:HG	1:a:375:PRO:HA	1.96	0.48
12:a:801:CL0:CGD	12:a:801:CL0:H8	2.44	0.48
13:a:818:CLA:HBA2	13:a:818:CLA:H3A	1.45	0.48
13:a:819:CLA:H3A	13:a:819:CLA:HBA2	1.51	0.48
2:b:412:HIS:CD2	13:b:831:CLA:C4A	2.95	0.48
13:b:814:CLA:H61	13:b:814:CLA:H92	1.65	0.48
1:a:432:HIS:CE1	13:a:831:CLA:ND	2.82	0.47
2:b:277:HIS:CD2	2:b:280:ILE:HD11	2.49	0.47
9:k:76:VAL:HG22	13:k:4002:CLA:HAB	1.96	0.47
13:a:821:CLA:H143	13:a:824:CLA:H112	1.95	0.47
13:a:839:CLA:H161	13:a:839:CLA:H192	1.74	0.47
13:f:201:CLA:H2	8:j:15:ILE:HD12	1.95	0.47
13:a:838:CLA:H3A	13:a:838:CLA:HBA2	1.67	0.47
2:b:177:HIS:HE1	13:b:813:CLA:NA	2.11	0.47
13:b:815:CLA:HBA1	20:b:846:ECH:H38B	1.96	0.47
13:a:805:CLA:H3A	13:a:805:CLA:HBA1	1.42	0.47
2:b:223:MET:HE2	2:b:223:MET:HB2	1.81	0.47
2:b:302:LYS:HB2	2:b:302:LYS:HE3	1.71	0.47
11:m:22:ALA:O	11:m:26:SER:OG	2.32	0.47
2:b:337:ALA:HB2	15:b:847:BCR:H372	1.95	0.47
13:b:825:CLA:H141	13:b:825:CLA:H162	1.59	0.47
1:a:70:ARG:HG2	1:a:184:ALA:HB1	1.96	0.47
1:a:215:HIS:HE1	13:a:814:CLA:C1A	2.19	0.47
1:a:482:PHE:HB3	13:a:837:CLA:H42	1.97	0.47
13:a:829:CLA:O1A	15:a:845:BCR:H393	2.14	0.47
13:b:837:CLA:H51	13:b:837:CLA:H12	1.69	0.47
3:c:7:ILE:HG12	3:c:40:ALA:HB3	1.96	0.47
6:f:58:ARG:HD3	8:j:35:ASP:OD2	2.14	0.47
1:a:152:PHE:CD1	13:a:814:CLA:HED1	2.50	0.47
1:a:450:HIS:HE1	13:a:833:CLA:C1A	2.27	0.47
1:a:485:TRP:CD2	17:a:852:LMG:H312	2.50	0.47
1:a:730:HIS:HE1	13:a:841:CLA:C4D	2.26	0.47
1:a:381:ILE:O	1:a:519:LYS:NZ	2.33	0.47
2:b:667:TYR:OH	13:b:804:CLA:OBD	2.19	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:l:26:ASP:O	10:l:31:ARG:NH1	2.48	0.47
1:a:476:ILE:H	1:a:476:ILE:HG13	1.58	0.47
1:a:476:ILE:HA	17:a:850:LMG:HC2	1.97	0.47
13:a:802:CLA:HBA2	2:b:425:LEU:HD23	1.96	0.47
13:a:840:CLA:H102	13:b:833:CLA:H43	1.97	0.47
13:b:804:CLA:CGA	13:b:804:CLA:H3A	2.45	0.47
13:b:817:CLA:HBA2	13:b:817:CLA:H3A	1.73	0.47
6:f:24:ASP:OD1	16:f:206:LHG:O2	2.27	0.47
9:k:11:PRO:HB3	9:k:82:ASN:OD1	2.15	0.47
9:k:54:PHE:HB3	13:k:4004:CLA:HBC3	1.96	0.47
10:l:36:ASN:HB3	13:l:1501:CLA:HAC1	1.96	0.47
12:a:801:CL0:NA	13:b:803:CLA:HAB	2.30	0.47
13:a:828:CLA:H3A	13:a:828:CLA:HBA2	1.70	0.47
13:a:840:CLA:CHA	13:a:840:CLA:H11	2.45	0.47
13:a:855:CLA:H3A	13:a:855:CLA:HBA2	1.60	0.47
13:b:806:CLA:H122	13:b:806:CLA:HBD	1.97	0.47
13:b:835:CLA:H3A	13:b:835:CLA:HBA2	1.34	0.47
13:b:839:CLA:CHA	13:b:839:CLA:HBA1	2.45	0.47
1:a:439:HIS:HE1	13:a:832:CLA:NA	2.12	0.46
2:b:188:LEU:HG	13:b:816:CLA:HBB2	1.97	0.46
2:b:406:LEU:HD13	13:b:824:CLA:HBC1	1.96	0.46
2:b:456:VAL:HG11	6:f:78:ASP:HB3	1.96	0.46
15:i:102:BCR:H383	10:l:96:LEU:HD21	1.97	0.46
17:a:850:LMG:H311	17:a:850:LMG:H341	1.61	0.46
1:a:297:HIS:HA	1:a:300:ILE:HG12	1.97	0.46
1:a:676:HIS:CD2	12:a:801:CL0:NB	2.82	0.46
2:b:284:PHE:HE1	13:b:820:CLA:HAB	1.79	0.46
6:f:61:ARG:NH1	8:j:35:ASP:O	2.48	0.46
1:a:197:MET:HG3	1:a:201:LEU:HD12	1.96	0.46
1:a:577:PRO:HD3	2:b:558:GLY:HA2	1.96	0.46
2:b:488:ALA:HB3	2:b:491:LEU:HG	1.97	0.46
13:a:822:CLA:H3A	13:a:822:CLA:HBA2	1.40	0.46
13:b:834:CLA:H3A	13:b:834:CLA:HBA2	1.49	0.46
13:b:830:CLA:HBB1	13:b:830:CLA:HMB1	1.97	0.46
13:b:841:CLA:H91	15:i:101:BCR:H19C	1.98	0.46
1:a:535:HIS:CD2	13:a:837:CLA:NB	2.83	0.46
2:b:287:ALA:HB2	13:b:820:CLA:HBC2	1.97	0.46
13:b:811:CLA:HBA1	13:b:811:CLA:H3A	1.67	0.46
4:d:121:ARG:HG3	4:d:123:GLY:H	1.81	0.46
1:a:309:HIS:HD2	13:a:820:CLA:C1A	2.28	0.46
13:a:820:CLA:H12	9:k:59:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:830:CLA:H102	16:a:849:LHG:H182	1.98	0.46
13:a:834:CLA:H92	13:a:834:CLA:H61	1.71	0.46
2:b:387:HIS:HA	2:b:390:ILE:HD12	1.98	0.46
2:b:348:GLN:HG3	13:b:826:CLA:HED1	1.98	0.46
2:b:430:HIS:HE1	13:b:833:CLA:C4D	2.28	0.46
2:b:459:GLN:HG2	2:b:470:TYR:CZ	2.51	0.46
4:d:7:GLN:HB2	4:d:51:ASN:HD21	1.81	0.46
1:a:42:PRO:HB3	1:a:47:TRP:CD2	2.51	0.45
1:a:457:HIS:HE1	13:a:834:CLA:C1A	2.16	0.45
1:a:489:LEU:HD21	17:a:852:LMG:H182	1.98	0.45
13:a:834:CLA:HAA1	10:l:69:GLY:HA2	1.97	0.45
13:b:807:CLA:HBA1	13:b:807:CLA:H11	1.66	0.45
13:b:815:CLA:H112	13:b:815:CLA:H72	1.51	0.45
13:a:805:CLA:HBC2	13:a:830:CLA:HMA1	1.97	0.45
13:a:820:CLA:H3A	13:a:820:CLA:HBA2	1.51	0.45
2:b:524:LEU:HD23	2:b:583:THR:HG21	1.98	0.45
13:b:801:CLA:H202	13:b:801:CLA:H162	1.79	0.45
13:b:822:CLA:H2A	13:b:822:CLA:HED3	1.97	0.45
2:b:478:ASN:HB3	2:b:481:SER:HB2	1.98	0.45
2:b:544:MET:HE3	2:b:544:MET:HB2	1.67	0.45
6:f:93:LEU:O	6:f:97:ILE:HG12	2.16	0.45
6:f:116:LYS:HE3	6:f:116:LYS:HA	1.97	0.45
10:l:48:LEU:O	10:l:52:GLU:HG2	2.16	0.45
13:l:1502:CLA:H3A	13:l:1502:CLA:HBA2	1.66	0.45
1:a:328:HIS:HE1	13:a:823:CLA:C4D	2.30	0.45
13:a:806:CLA:H151	13:a:829:CLA:HBB2	1.98	0.45
2:b:590:TYR:HA	2:b:616:TRP:HH2	1.82	0.45
8:j:35:ASP:OD1	8:j:35:ASP:N	2.50	0.45
13:l:1501:CLA:H3A	13:l:1501:CLA:HBA2	1.39	0.45
13:l:1502:CLA:H141	13:l:1502:CLA:H161	1.67	0.45
7:i:35:GLU:HA	7:i:35:GLU:OE1	2.17	0.45
1:a:730:HIS:HE1	13:a:841:CLA:ND	2.14	0.45
2:b:513:ASP:HA	2:b:516:VAL:HG12	1.97	0.45
2:b:525:HIS:CD2	13:b:839:CLA:NB	2.81	0.45
6:f:103:TRP:CH2	6:f:147:GLU:HG3	2.52	0.45
1:a:457:HIS:HE1	13:a:834:CLA:C4D	2.29	0.45
1:a:534:VAL:HG11	1:a:608:HIS:CG	2.52	0.45
13:a:855:CLA:H41	13:a:855:CLA:H62	1.45	0.45
2:b:178:HIS:CD2	13:b:814:CLA:NB	2.84	0.45
13:b:801:CLA:HMB1	13:b:801:CLA:HBB1	1.99	0.45
1:a:56:HIS:HE1	13:a:804:CLA:NC	2.06	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:806:CLA:H62	13:a:806:CLA:H41	1.56	0.45
1:a:411:PHE:CD1	1:a:415:ASP:HB2	2.51	0.45
13:a:819:CLA:HAB	13:a:819:CLA:H8	1.98	0.45
13:a:825:CLA:HBA1	13:a:829:CLA:H191	1.98	0.45
2:b:642:VAL:HG21	13:b:809:CLA:HAC1	1.99	0.45
13:b:840:CLA:H3A	13:b:840:CLA:HBA2	1.67	0.45
2:b:324:ILE:HD12	13:b:825:CLA:HMC1	1.98	0.45
13:b:839:CLA:H2	15:b:847:BCR:H352	1.99	0.45
13:a:814:CLA:H3A	13:a:814:CLA:HBA2	1.43	0.44
13:b:810:CLA:H102	13:b:810:CLA:H62	1.57	0.44
13:a:824:CLA:H141	16:a:851:LHG:H171	1.98	0.44
2:b:363:HIS:HB3	2:b:599:TRP:CZ3	2.51	0.44
2:b:525:HIS:HE1	13:b:839:CLA:C4D	2.30	0.44
1:a:359:LEU:O	1:a:363:THR:HG23	2.16	0.44
13:a:823:CLA:C4A	13:a:823:CLA:H2	2.47	0.44
13:b:836:CLA:H3A	13:b:836:CLA:HBA2	1.55	0.44
8:j:8:LEU:O	8:j:14:MET:HE3	2.18	0.44
1:a:450:HIS:HA	13:a:834:CLA:HBB2	2.00	0.44
13:a:810:CLA:CHA	13:a:810:CLA:HBA1	2.47	0.44
13:b:823:CLA:CHA	13:b:823:CLA:HBA1	2.48	0.44
5:e:44:VAL:HG12	5:e:57:ASN:HB3	1.98	0.44
1:a:370:MET:HE2	1:a:370:MET:HB3	1.88	0.44
1:a:458:ASN:OD1	1:a:471:PHE:N	2.40	0.44
13:a:817:CLA:HBD	9:k:11:PRO:HG2	1.99	0.44
13:a:835:CLA:H41	13:a:835:CLA:H62	1.69	0.44
13:b:804:CLA:H143	13:b:804:CLA:H111	1.75	0.44
1:a:406:ALA:O	1:a:410:ILE:HG13	2.18	0.44
1:a:695:GLU:OE2	2:b:547:LYS:NZ	2.41	0.44
13:a:812:CLA:H41	13:a:812:CLA:H62	1.72	0.44
13:b:833:CLA:HBB1	15:f:202:BCR:H323	1.99	0.44
13:b:817:CLA:C4D	13:b:817:CLA:H2	2.48	0.44
20:b:846:ECH:H21	20:b:846:ECH:H24	1.75	0.44
6:f:140:TRP:CD1	6:f:141:PRO:HD3	2.52	0.44
1:a:335:GLU:OE1	1:a:338:LYS:NZ	2.45	0.44
1:a:513:THR:HG23	1:a:523:MET:HB3	1.99	0.44
1:a:543:HIS:CD2	13:a:839:CLA:NB	2.84	0.44
1:a:587:GLY:O	1:a:591:VAL:HG23	2.18	0.44
1:a:392:HIS:O	1:a:396:ILE:HG12	2.17	0.44
1:a:450:HIS:HE1	13:a:833:CLA:C4D	2.31	0.44
1:a:707:LEU:HD12	13:a:840:CLA:HMA1	2.00	0.44
2:b:3:THR:N	7:i:37:GLU:OE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:b:852:LMG:H241	17:b:852:LMG:H212	1.82	0.44
13:a:830:CLA:H61	13:a:830:CLA:H41	1.74	0.43
13:a:833:CLA:H143	14:b:843:PQN:H191	2.00	0.43
13:a:841:CLA:H143	13:a:841:CLA:H111	1.72	0.43
1:a:374:PRO:HG3	1:a:380:ALA:HB2	2.00	0.43
1:a:374:PRO:HA	1:a:375:PRO:HD3	1.85	0.43
2:b:59:LEU:HD12	20:m:101:ECH:H37A	1.98	0.43
13:b:803:CLA:H61	13:b:803:CLA:H41	1.50	0.43
13:b:830:CLA:H2A	13:b:830:CLA:CED	2.48	0.43
1:a:440:LEU:O	1:a:443:VAL:HG12	2.18	0.43
2:b:194:LEU:HA	2:b:198:ALA:HB3	1.99	0.43
2:b:372:HIS:HE1	13:b:828:CLA:C1D	2.16	0.43
15:i:101:BCR:H20C	15:i:101:BCR:H361	1.85	0.43
1:a:207:LEU:HD23	1:a:207:LEU:HA	1.84	0.43
1:a:458:ASN:HD22	1:a:640:ILE:HB	1.82	0.43
13:a:828:CLA:H202	13:a:828:CLA:H161	1.73	0.43
13:b:805:CLA:HHC	13:b:807:CLA:OBD	2.19	0.43
13:a:802:CLA:O2A	2:b:428:GLY:HA3	2.18	0.43
13:a:816:CLA:HBB2	15:a:844:BCR:H352	2.00	0.43
22:f:205:ZEX:H11	22:f:205:ZEX:H191	1.86	0.43
16:f:206:LHG:H182	16:f:206:LHG:H261	1.99	0.43
13:k:4004:CLA:H3A	13:k:4004:CLA:O2A	2.19	0.43
13:l:1501:CLA:HBB1	13:l:1502:CLA:HAA2	2.00	0.43
1:a:312:ARG:HD3	1:a:316:GLY:HA2	2.01	0.43
13:a:814:CLA:O1A	15:a:844:BCR:H342	2.19	0.43
13:a:824:CLA:HED3	13:a:824:CLA:H2A	2.00	0.43
13:a:833:CLA:H62	13:a:833:CLA:H102	1.72	0.43
2:b:460:TRP:O	2:b:464:THR:HG23	2.19	0.43
4:d:33:THR:HG22	4:d:54:GLU:OE1	2.18	0.43
2:b:409:MET:HE2	13:b:824:CLA:HMC2	2.00	0.43
2:b:521:ALA:HB2	13:b:838:CLA:HMA1	2.00	0.43
2:b:669:GLN:O	2:b:673:GLU:HG2	2.18	0.43
4:d:40:PHE:CE1	4:d:50:MET:HB3	2.54	0.43
13:f:201:CLA:H41	13:f:201:CLA:H61	1.65	0.43
10:l:25:SER:OG	10:l:26:ASP:OD1	2.18	0.43
10:l:82:LEU:O	10:l:86:LEU:HG	2.18	0.43
13:a:802:CLA:H3A	13:a:802:CLA:C2	2.49	0.43
2:b:518:HIS:CD2	13:b:838:CLA:NB	2.87	0.43
2:b:545:PRO:HB3	6:f:164:PRO:HG2	2.00	0.43
2:b:672:ILE:HA	2:b:675:ILE:HD12	2.01	0.43
13:b:838:CLA:H62	13:b:838:CLA:H41	1.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:k:21:ALA:O	9:k:24:MET:N	2.52	0.43
1:a:293:THR:HG23	13:a:819:CLA:HMA3	2.00	0.43
13:b:809:CLA:H8	13:b:809:CLA:H51	1.59	0.43
13:b:823:CLA:HMC2	15:b:849:BCR:HC8	2.00	0.43
13:a:810:CLA:H2	13:a:810:CLA:H61	1.69	0.43
13:a:817:CLA:HBA2	13:a:817:CLA:H3A	1.84	0.43
13:a:832:CLA:H41	13:a:832:CLA:H61	1.78	0.43
15:b:847:BCR:H15C	15:b:847:BCR:H351	1.83	0.43
6:f:140:TRP:CG	6:f:141:PRO:HD3	2.53	0.43
1:a:297:HIS:CD2	1:a:300:ILE:HD11	2.54	0.42
15:a:846:BCR:H20C	15:a:846:BCR:H361	1.85	0.42
13:b:816:CLA:HBB1	15:b:844:BCR:H323	2.00	0.42
13:b:825:CLA:H151	13:b:825:CLA:H112	1.69	0.42
3:c:61:ASP:HB3	5:e:59:ASN:CG	2.43	0.42
10:l:112:ASP:HB3	10:l:115:GLN:HB2	2.01	0.42
1:a:296:HIS:HB2	13:a:818:CLA:C1B	2.49	0.42
2:b:188:LEU:HG	13:b:816:CLA:CBB	2.50	0.42
9:k:83:MET:HE3	13:k:4002:CLA:HMA1	2.01	0.42
13:b:839:CLA:H42	16:b:851:LHG:H381	2.01	0.42
4:d:136:LYS:HA	4:d:136:LYS:HD3	1.58	0.42
1:a:200:HIS:CD2	13:a:813:CLA:NB	2.87	0.42
1:a:319:HIS:CD2	13:a:822:CLA:ND	2.87	0.42
1:a:707:LEU:HD11	22:f:205:ZEX:H192	2.01	0.42
13:a:826:CLA:HAB	15:a:847:BCR:H311	2.01	0.42
13:a:840:CLA:H3A	13:a:840:CLA:HBA2	1.84	0.42
2:b:697:LEU:HD21	14:b:843:PQN:H151	2.01	0.42
13:b:824:CLA:C3C	15:b:849:BCR:H372	2.49	0.42
1:a:543:HIS:HE1	13:a:839:CLA:C4D	2.32	0.42
13:a:802:CLA:H8	13:a:802:CLA:H122	1.90	0.42
13:a:812:CLA:H3A	13:a:812:CLA:HBA2	1.64	0.42
2:b:237:PRO:HB2	2:b:258:LEU:HD11	2.01	0.42
13:b:821:CLA:H141	13:b:821:CLA:H161	1.79	0.42
3:c:29:VAL:HG12	4:d:112:ARG:HB3	2.00	0.42
6:f:103:TRP:HH2	6:f:147:GLU:HG3	1.85	0.42
9:k:58:GLY:O	9:k:62:VAL:HG23	2.19	0.42
15:k:4005:BCR:H15C	15:k:4005:BCR:H351	1.85	0.42
10:l:93:THR:HG21	10:l:128:PHE:HB2	2.02	0.42
12:a:801:CL0:H41	12:a:801:CL0:H49	1.78	0.42
20:b:846:ECH:H36	20:b:846:ECH:H20	1.79	0.42
4:d:4:LEU:HB3	4:d:56:LEU:HD11	2.00	0.42
1:a:265:THR:HB	9:k:16:TRP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:808:CLA:H93	13:a:830:CLA:H203	2.02	0.42
2:b:474:VAL:O	2:b:477:SER:OG	2.32	0.42
1:a:390:PHE:O	1:a:394:MET:HB2	2.19	0.42
1:a:412:MET:HE2	1:a:412:MET:HB2	1.93	0.42
1:a:478:LEU:HD21	17:a:850:LMG:H131	2.01	0.42
13:a:834:CLA:H2	10:l:64:PRO:CB	2.47	0.42
2:b:413:LYS:HG3	2:b:414:GLU:N	2.35	0.42
2:b:450:GLN:OE1	2:b:611:THR:OG1	2.33	0.42
13:b:808:CLA:H41	13:b:808:CLA:H62	1.54	0.42
13:b:812:CLA:HBD	13:b:812:CLA:HBA1	2.01	0.42
15:b:849:BCR:H361	15:b:849:BCR:H20C	1.78	0.42
22:b:854:ZEX:H11	22:b:854:ZEX:H191	1.88	0.42
6:f:94:PHE:HB2	15:f:202:BCR:H321	2.02	0.42
6:f:131:ILE:HA	6:f:134:MET:HB2	2.01	0.42
20:m:101:ECH:H20	20:m:101:ECH:H36	1.84	0.42
13:a:820:CLA:H2	13:a:820:CLA:H62	1.83	0.42
13:b:818:CLA:H101	13:b:818:CLA:H62	1.70	0.42
6:f:109:LEU:HD12	6:f:109:LEU:HA	1.90	0.42
16:f:206:LHG:H111	16:f:206:LHG:HC81	1.83	0.42
16:f:206:LHG:H122	16:f:206:LHG:HC92	1.70	0.42
13:a:817:CLA:C4D	13:a:817:CLA:H12	2.49	0.42
13:a:820:CLA:H91	13:a:820:CLA:H162	2.02	0.42
13:a:832:CLA:H3A	13:a:832:CLA:HBA2	1.55	0.42
15:a:847:BCR:H20C	15:a:847:BCR:H361	1.88	0.42
2:b:222:LEU:HD23	2:b:222:LEU:HA	1.80	0.42
13:b:801:CLA:O1D	13:b:803:CLA:H71	2.20	0.42
13:b:812:CLA:HBA1	13:b:812:CLA:CHA	2.50	0.42
4:d:33:THR:HG23	4:d:82:ASP:OD2	2.20	0.42
6:f:99:GLY:HA3	6:f:140:TRP:CE2	2.55	0.42
15:j:105:BCR:H24C	15:j:105:BCR:H371	1.81	0.42
9:k:68:PHE:CE2	9:k:72:LEU:HD11	2.55	0.42
13:k:4002:CLA:H202	13:k:4002:CLA:H161	1.78	0.42
1:a:530:ALA:O	1:a:534:VAL:HG23	2.19	0.41
13:a:804:CLA:H141	13:a:804:CLA:H162	1.86	0.41
2:b:193:HIS:HB2	13:b:815:CLA:CHC	2.49	0.41
15:i:102:BCR:H401	10:l:92:ALA:HB1	2.02	0.41
15:j:101:BCR:H15C	15:j:101:BCR:H351	1.84	0.41
1:a:115:GLN:HB3	1:a:137:ILE:HB	2.03	0.41
13:a:808:CLA:CHC	13:a:809:CLA:HMD2	2.49	0.41
13:b:808:CLA:H3A	13:b:808:CLA:HBA2	1.74	0.41
9:k:29:ILE:HD13	9:k:29:ILE:HA	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:a:849:LHG:H242	16:a:849:LHG:HC62	1.75	0.41
2:b:178:HIS:O	2:b:182:LEU:HB3	2.20	0.41
2:b:320:LEU:HD23	2:b:320:LEU:HA	1.86	0.41
13:b:822:CLA:H3A	13:b:822:CLA:HBA2	1.44	0.41
13:b:830:CLA:H91	17:b:850:LMG:H232	2.02	0.41
13:b:834:CLA:HED3	13:b:834:CLA:H2A	2.01	0.41
15:f:202:BCR:H20C	15:f:202:BCR:H361	1.89	0.41
8:j:1:MET:HG3	8:j:3:GLY:H	1.86	0.41
13:j:103:CLA:HBA2	13:j:103:CLA:H3A	1.69	0.41
10:l:88:LEU:HD12	10:l:88:LEU:HA	1.87	0.41
1:a:19:ASN:N	1:a:182:VAL:O	2.41	0.41
2:b:3:THR:HA	7:i:37:GLU:HA	2.01	0.41
2:b:491:LEU:HD23	2:b:491:LEU:HA	1.88	0.41
13:b:804:CLA:HED2	13:b:804:CLA:HBD	1.94	0.41
13:b:807:CLA:H41	13:b:807:CLA:H61	1.76	0.41
13:b:833:CLA:H62	13:b:833:CLA:H2	1.81	0.41
1:a:565:LYS:HA	1:a:568:LEU:HD12	2.03	0.41
13:a:806:CLA:H42	13:a:830:CLA:H51	2.02	0.41
2:b:651:HIS:CD2	13:b:803:CLA:NB	2.89	0.41
13:b:801:CLA:H41	13:b:801:CLA:H61	1.53	0.41
13:b:838:CLA:H141	13:b:838:CLA:H162	1.77	0.41
3:c:27:GLU:OE2	4:d:112:ARG:NE	2.53	0.41
15:i:102:BCR:H20C	15:i:102:BCR:H361	1.84	0.41
2:b:328:LEU:HD13	13:b:806:CLA:HAC1	2.03	0.41
13:b:806:CLA:H2	13:b:806:CLA:HBA2	2.02	0.41
13:b:816:CLA:H41	13:b:816:CLA:H62	1.58	0.41
13:b:833:CLA:H143	13:b:833:CLA:H112	1.85	0.41
7:i:30:LEU:O	7:i:34:ILE:HG12	2.20	0.41
15:i:101:BCR:H15C	15:i:101:BCR:H351	1.91	0.41
15:j:105:BCR:H15C	15:j:105:BCR:H351	1.87	0.41
1:a:26:GLU:H	1:a:26:GLU:HG2	1.68	0.41
1:a:536:HIS:CD2	13:a:838:CLA:NB	2.89	0.41
13:a:810:CLA:H43	13:a:812:CLA:ND	2.36	0.41
13:a:839:CLA:HHC	13:a:839:CLA:CBB	2.50	0.41
2:b:29:HIS:HE1	13:b:805:CLA:C1C	2.34	0.41
1:a:317:ILE:HD11	15:k:4001:BCR:H392	2.02	0.41
13:a:817:CLA:H142	13:a:817:CLA:H112	1.67	0.41
2:b:596:LEU:HD23	2:b:730:PHE:HE2	1.85	0.41
3:c:59:PRO:HA	5:e:47:ASN:ND2	2.36	0.41
9:k:61:ALA:O	9:k:65:THR:HG22	2.21	0.41
1:a:296:HIS:HE1	13:a:818:CLA:C1D	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:481:ILE:HB	17:a:852:LMG:O10	2.20	0.41
13:a:809:CLA:HMB3	13:a:809:CLA:HBB1	2.03	0.41
2:b:659:MET:HB2	13:b:804:CLA:C4C	2.50	0.41
13:b:803:CLA:H143	13:b:803:CLA:H111	1.79	0.41
13:b:809:CLA:CGA	13:b:809:CLA:C1A	2.99	0.41
13:b:810:CLA:H151	13:b:810:CLA:H112	1.76	0.41
13:b:819:CLA:H3A	13:b:819:CLA:HBA2	1.51	0.41
1:a:42:PRO:HB3	1:a:47:TRP:CE3	2.56	0.41
15:a:844:BCR:H361	15:a:844:BCR:H20C	1.81	0.41
13:b:814:CLA:H62	13:b:814:CLA:H2	1.62	0.41
15:b:845:BCR:H15C	15:b:845:BCR:H351	1.87	0.41
8:j:36:LEU:HD23	8:j:36:LEU:HA	1.92	0.41
1:a:290:LEU:HD23	1:a:290:LEU:HA	1.95	0.40
1:a:319:HIS:HB3	1:a:324:ILE:HD11	2.03	0.40
1:a:432:HIS:CD2	13:a:831:CLA:C4A	3.05	0.40
1:a:441:ASN:OD1	1:a:441:ASN:C	2.63	0.40
1:a:571:ARG:HG3	1:a:588:TRP:CG	2.56	0.40
1:a:644:GLY:HA2	1:a:647:ARG:HH21	1.85	0.40
1:a:685:PHE:HA	14:a:843:PQN:H9	2.03	0.40
13:a:808:CLA:H102	13:a:808:CLA:H62	1.83	0.40
13:a:808:CLA:H111	13:a:808:CLA:H91	1.87	0.40
2:b:59:LEU:HD23	2:b:59:LEU:HA	1.90	0.40
2:b:276:HIS:HE1	13:b:818:CLA:C1D	2.15	0.40
15:k:4001:BCR:H15C	15:k:4001:BCR:H351	1.86	0.40
13:a:821:CLA:H62	13:a:821:CLA:H2	1.66	0.40
13:a:837:CLA:H3A	13:a:838:CLA:HAA2	2.02	0.40
13:b:831:CLA:HBA2	13:b:831:CLA:H3A	1.41	0.40
13:a:834:CLA:CHA	13:a:834:CLA:HBA1	2.50	0.40
15:a:845:BCR:H361	15:a:845:BCR:H20C	1.84	0.40
2:b:145:LEU:HD12	2:b:145:LEU:HA	1.86	0.40
2:b:649:PHE:O	2:b:653:VAL:HG23	2.20	0.40
13:b:809:CLA:H142	13:b:809:CLA:H111	1.92	0.40
15:b:844:BCR:H11C	15:b:844:BCR:H341	1.92	0.40
13:b:828:CLA:H3A	13:b:828:CLA:HBA2	1.37	0.40
13:a:812:CLA:HBA2	13:a:812:CLA:H12	1.82	0.40
13:a:831:CLA:H52	13:a:831:CLA:H12	1.80	0.40
15:a:847:BCR:H11C	15:a:847:BCR:H341	1.98	0.40
15:a:847:BCR:H15C	15:a:847:BCR:H351	1.87	0.40
13:a:854:CLA:H193	15:b:848:BCR:H321	2.04	0.40
2:b:453:ILE:HD13	6:f:75:LEU:HB2	2.04	0.40
13:b:821:CLA:HBA2	13:b:821:CLA:H3A	1.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:b:841:CLA:H61	13:b:841:CLA:H41	1.81	0.40
15:k:4001:BCR:H20C	15:k:4001:BCR:H361	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	738/751 (98%)	717 (97%)	21 (3%)	0	100	100
2	b	727/731 (100%)	705 (97%)	22 (3%)	0	100	100
3	c	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	d	137/141 (97%)	132 (96%)	5 (4%)	0	100	100
5	e	67/74 (90%)	65 (97%)	2 (3%)	0	100	100
6	f	140/165 (85%)	139 (99%)	1 (1%)	0	100	100
7	i	38/40 (95%)	38 (100%)	0	0	100	100
8	j	38/40 (95%)	36 (95%)	2 (5%)	0	100	100
9	k	75/88 (85%)	70 (93%)	5 (7%)	0	100	100
10	l	141/157 (90%)	136 (96%)	5 (4%)	0	100	100
11	m	29/31 (94%)	29 (100%)	0	0	100	100
All	All	2208/2299 (96%)	2144 (97%)	64 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	592/603 (98%)	586 (99%)	6 (1%)	68 89
2	b	582/583 (100%)	574 (99%)	8 (1%)	59 85
3	c	68/69 (99%)	66 (97%)	2 (3%)	37 71
4	d	114/116 (98%)	113 (99%)	1 (1%)	70 90
5	e	57/60 (95%)	56 (98%)	1 (2%)	51 80
6	f	119/137 (87%)	116 (98%)	3 (2%)	42 74
7	i	32/32 (100%)	32 (100%)	0	100 100
8	j	35/35 (100%)	35 (100%)	0	100 100
9	k	54/63 (86%)	52 (96%)	2 (4%)	30 64
10	l	107/118 (91%)	107 (100%)	0	100 100
11	m	25/25 (100%)	24 (96%)	1 (4%)	28 62
All	All	1785/1841 (97%)	1761 (99%)	24 (1%)	59 86

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	186	LYS
1	a	363	THR
1	a	365	ILE
1	a	459	ASP
1	a	537	ILE
1	a	545	THR
2	b	300	SER
2	b	343	THR
2	b	456	VAL
2	b	476	LEU
2	b	495	LEU
2	b	517	HIS
2	b	522	LEU
2	b	527	THR
3	c	28	MET
3	c	76	SER
4	d	122	ILE
5	e	27	SER
6	f	33	SER
6	f	53	ASN

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Mol	Chain	Res	Type
6	f	82	THR
9	k	59	LEU
9	k	67	SER
11	m	26	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	192	ASN
1	a	216	GLN
1	a	240	HIS
1	a	282	ASN
2	b	366	GLN
2	b	582	ASN
2	b	627	GLN
2	b	669	GLN
3	c	16	GLN
3	c	38	GLN
4	d	7	GLN
4	d	95	GLN
5	e	4	ASN
6	f	121	GLN
9	k	70	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

134 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	CLA	b	840	-	69,73,73	1.25	9 (13%)	83,113,113	1.30	8 (9%)
17	LMG	b	852	-	55,55,55	0.78	1 (1%)	63,63,63	1.33	9 (14%)
13	CLA	b	822	2	64,68,73	1.31	7 (10%)	77,107,113	1.33	4 (5%)
13	CLA	b	825	-	69,73,73	1.25	8 (11%)	83,113,113	1.28	5 (6%)
13	CLA	a	819	1	69,73,73	1.25	9 (13%)	83,113,113	1.26	9 (10%)
13	CLA	a	817	1	69,73,73	1.24	7 (10%)	83,113,113	1.29	6 (7%)
13	CLA	b	841	2	69,73,73	1.26	8 (11%)	83,113,113	1.29	5 (6%)
13	CLA	a	824	1	64,68,73	1.30	8 (12%)	77,107,113	1.35	5 (6%)
13	CLA	a	820	1	69,73,73	1.26	8 (11%)	83,113,113	1.29	4 (4%)
15	BCR	i	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.23	7 (12%)
21	EQ3	b	853	-	43,43,43	1.66	9 (20%)	56,60,60	1.54	11 (19%)
13	CLA	a	809	1	55,59,73	1.40	8 (14%)	66,96,113	1.45	6 (9%)
13	CLA	b	834	2	69,73,73	1.25	8 (11%)	83,113,113	1.32	6 (7%)
16	LHG	b	851	13	37,37,48	0.69	1 (2%)	40,43,54	1.20	3 (7%)
13	CLA	b	830	2	69,73,73	1.24	9 (13%)	83,113,113	1.39	7 (8%)
13	CLA	b	826	-	59,63,73	1.35	8 (13%)	71,101,113	1.35	6 (8%)
13	CLA	a	841	1	69,73,73	1.26	9 (13%)	83,113,113	1.27	7 (8%)
13	CLA	a	828	1	69,73,73	1.24	7 (10%)	83,113,113	1.30	6 (7%)
13	CLA	b	837	2	56,60,73	1.38	8 (14%)	67,97,113	1.44	8 (11%)
13	CLA	k	4003	9	50,54,73	1.46	9 (18%)	60,90,113	1.42	6 (10%)
13	CLA	a	803	1	69,73,73	1.26	10 (14%)	83,113,113	1.29	7 (8%)
19	SF4	c	102	3	0,12,12	-	-	-		
13	CLA	b	821	2	69,73,73	1.25	8 (11%)	83,113,113	1.27	5 (6%)
13	CLA	l	1502	10	69,73,73	1.24	10 (14%)	83,113,113	1.31	5 (6%)
13	CLA	k	4004	9	49,53,73	1.48	7 (14%)	59,89,113	1.55	7 (11%)
16	LHG	a	849	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
16	LHG	a	851	13	48,48,48	0.59	1 (2%)	51,54,54	1.27	6 (11%)
13	CLA	a	826	-	69,73,73	1.24	8 (11%)	83,113,113	1.30	7 (8%)
15	BCR	b	845	-	41,41,41	1.13	2 (4%)	56,56,56	1.17	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	b	819	2	69,73,73	1.25	9 (13%)	83,113,113	1.26	6 (7%)
15	BCR	f	202	-	41,41,41	1.14	2 (4%)	56,56,56	1.19	6 (10%)
13	CLA	a	854	-	69,73,73	1.25	8 (11%)	83,113,113	1.22	5 (6%)
13	CLA	b	824	2	61,65,73	1.34	8 (13%)	73,103,113	1.35	7 (9%)
15	BCR	a	848	-	25,25,41	1.16	1 (4%)	33,33,56	1.30	5 (15%)
15	BCR	i	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.21	5 (8%)
15	BCR	b	848	-	41,41,41	1.15	2 (4%)	56,56,56	1.16	5 (8%)
13	CLA	b	815	2	69,73,73	1.25	8 (11%)	83,113,113	1.29	5 (6%)
23	LMT	j	102	-	36,36,36	1.17	5 (13%)	47,47,47	0.98	2 (4%)
13	CLA	a	815	1	50,54,73	1.44	8 (16%)	60,90,113	1.43	5 (8%)
13	CLA	a	804	1	69,73,73	1.26	7 (10%)	83,113,113	1.25	6 (7%)
13	CLA	a	831	1	60,64,73	1.34	9 (15%)	72,102,113	1.36	6 (8%)
13	CLA	b	808	2	69,73,73	1.24	8 (11%)	83,113,113	1.26	6 (7%)
19	SF4	b	802	1,2	0,12,12	-	-	-		
13	CLA	b	803	2	69,73,73	1.25	9 (13%)	83,113,113	1.21	5 (6%)
15	BCR	j	105	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	6 (10%)
13	CLA	a	816	-	50,54,73	1.46	8 (16%)	60,90,113	1.44	4 (6%)
13	CLA	b	831	2	55,59,73	1.42	6 (10%)	66,96,113	1.37	7 (10%)
13	CLA	a	811	1	69,73,73	1.24	8 (11%)	83,113,113	1.27	5 (6%)
13	CLA	j	103	8	59,63,73	1.36	7 (11%)	71,101,113	1.29	5 (7%)
13	CLA	a	840	1	69,73,73	1.24	7 (10%)	83,113,113	1.32	6 (7%)
13	CLA	f	201	-	69,73,73	1.26	9 (13%)	83,113,113	1.29	5 (6%)
13	CLA	a	822	1	69,73,73	1.24	7 (10%)	83,113,113	1.29	8 (9%)
13	CLA	f	203	-	54,58,73	1.42	7 (12%)	65,95,113	1.38	7 (10%)
13	CLA	j	104	8	50,54,73	1.46	8 (16%)	60,90,113	1.36	4 (6%)
20	ECH	b	846	-	42,42,42	1.74	8 (19%)	55,58,58	2.33	14 (25%)
13	CLA	b	838	2	69,73,73	1.24	8 (11%)	83,113,113	1.30	6 (7%)
15	BCR	a	847	-	41,41,41	1.16	2 (4%)	56,56,56	1.25	6 (10%)
13	CLA	a	808	1	69,73,73	1.25	8 (11%)	83,113,113	1.30	7 (8%)
14	PQN	b	843	-	34,34,34	0.39	0	42,45,45	0.38	0
13	CLA	b	811	2	60,64,73	1.36	7 (11%)	72,102,113	1.31	6 (8%)
15	BCR	b	849	-	41,41,41	1.11	2 (4%)	56,56,56	1.17	5 (8%)
13	CLA	a	834	1	69,73,73	1.24	9 (13%)	83,113,113	1.33	5 (6%)
13	CLA	a	830	1	69,73,73	1.24	9 (13%)	83,113,113	1.39	8 (9%)
16	LHG	f	206	-	48,48,48	0.61	1 (2%)	51,54,54	1.24	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	b	812	2	60,64,73	1.34	8 (13%)	72,102,113	1.37	4 (5%)
15	BCR	b	844	-	41,41,41	1.18	2 (4%)	56,56,56	1.25	7 (12%)
13	CLA	a	838	1	69,73,73	1.26	8 (11%)	83,113,113	1.26	7 (8%)
13	CLA	b	833	2	69,73,73	1.26	8 (11%)	83,113,113	1.26	6 (7%)
13	CLA	a	805	1	69,73,73	1.24	8 (11%)	83,113,113	1.34	7 (8%)
13	CLA	a	839	1	69,73,73	1.26	8 (11%)	83,113,113	1.27	4 (4%)
13	CLA	a	832	1	64,68,73	1.29	8 (12%)	77,107,113	1.34	8 (10%)
13	CLA	b	801	-	69,73,73	1.25	7 (10%)	83,113,113	1.24	6 (7%)
13	CLA	a	802	-	69,73,73	1.24	9 (13%)	83,113,113	1.28	5 (6%)
13	CLA	a	821	-	69,73,73	1.25	9 (13%)	83,113,113	1.29	8 (9%)
13	CLA	a	823	1	69,73,73	1.24	9 (13%)	83,113,113	1.35	7 (8%)
13	CLA	b	816	2	59,63,73	1.35	9 (15%)	71,101,113	1.33	7 (9%)
13	CLA	b	827	2	69,73,73	1.25	9 (13%)	83,113,113	1.25	5 (6%)
15	BCR	b	847	-	41,41,41	1.12	2 (4%)	56,56,56	1.24	6 (10%)
12	CL0	a	801	1	69,73,73	1.25	9 (13%)	83,113,113	1.26	6 (7%)
14	PQN	a	843	-	34,34,34	0.38	0	42,45,45	0.40	0
15	BCR	k	4005	-	41,41,41	1.11	2 (4%)	56,56,56	1.19	6 (10%)
19	SF4	c	101	3	0,12,12	-	-	-		
22	ZEX	b	854	-	42,43,43	1.67	8 (19%)	55,60,60	1.61	12 (21%)
13	CLA	b	828	2	69,73,73	1.24	7 (10%)	83,113,113	1.29	6 (7%)
15	BCR	a	844	-	41,41,41	1.16	2 (4%)	56,56,56	1.20	5 (8%)
13	CLA	a	833	1	69,73,73	1.26	9 (13%)	83,113,113	1.24	7 (8%)
13	CLA	b	817	2	60,64,73	1.31	8 (13%)	72,102,113	1.36	7 (9%)
13	CLA	b	805	2	69,73,73	1.26	7 (10%)	83,113,113	1.30	8 (9%)
13	CLA	a	818	1	69,73,73	1.25	10 (14%)	83,113,113	1.29	5 (6%)
13	CLA	b	810	2	69,73,73	1.25	9 (13%)	83,113,113	1.29	6 (7%)
13	CLA	b	823	2	50,54,73	1.47	7 (14%)	60,90,113	1.42	4 (6%)
13	CLA	a	827	1	69,73,73	1.25	9 (13%)	83,113,113	1.30	6 (7%)
13	CLA	a	842	16	49,53,73	1.47	7 (14%)	59,89,113	1.45	5 (8%)
22	ZEX	f	205	-	42,43,43	1.67	8 (19%)	55,60,60	1.59	11 (20%)
13	CLA	b	829	2	69,73,73	1.24	8 (11%)	83,113,113	1.25	6 (7%)
13	CLA	a	814	1	51,55,73	1.45	7 (13%)	61,91,113	1.46	7 (11%)
13	CLA	b	839	2	54,58,73	1.42	8 (14%)	65,95,113	1.39	5 (7%)
13	CLA	a	837	1	55,59,73	1.38	7 (12%)	66,96,113	1.42	6 (9%)
13	CLA	a	807	1	69,73,73	1.25	8 (11%)	83,113,113	1.33	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	b	809	2	69,73,73	1.24	10 (14%)	83,113,113	1.29	6 (7%)
17	LMG	a	852	-	40,40,55	0.83	0	48,48,63	1.24	4 (8%)
13	CLA	k	4002	-	69,73,73	1.26	8 (11%)	83,113,113	1.29	5 (6%)
15	BCR	a	845	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
15	BCR	k	4001	-	41,41,41	1.16	2 (4%)	56,56,56	1.25	6 (10%)
13	CLA	f	204	6	49,53,73	1.49	7 (14%)	59,89,113	1.46	5 (8%)
13	CLA	a	825	-	69,73,73	1.24	8 (11%)	83,113,113	1.33	6 (7%)
13	CLA	b	806	2	69,73,73	1.24	8 (11%)	83,113,113	1.35	6 (7%)
13	CLA	a	810	1	57,61,73	1.36	8 (14%)	68,98,113	1.36	6 (8%)
13	CLA	a	855	-	69,73,73	1.25	8 (11%)	83,113,113	1.28	5 (6%)
13	CLA	b	835	-	69,73,73	1.25	8 (11%)	83,113,113	1.29	5 (6%)
13	CLA	b	836	-	54,58,73	1.41	8 (14%)	65,95,113	1.41	6 (9%)
15	BCR	a	846	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	8 (14%)
13	CLA	a	829	1	69,73,73	1.25	8 (11%)	83,113,113	1.24	5 (6%)
18	45D	a	856	-	43,43,43	1.73	10 (23%)	54,60,60	1.61	10 (18%)
17	LMG	b	850	-	55,55,55	0.70	0	63,63,63	1.38	8 (12%)
13	CLA	a	812	1	56,60,73	1.40	9 (16%)	67,97,113	1.39	8 (11%)
13	CLA	a	835	1	69,73,73	1.24	8 (11%)	83,113,113	1.30	7 (8%)
13	CLA	b	818	2	69,73,73	1.26	8 (11%)	83,113,113	1.31	6 (7%)
13	CLA	b	813	2	54,58,73	1.41	9 (16%)	65,95,113	1.41	7 (10%)
13	CLA	l	1503	-	56,60,73	1.39	8 (14%)	67,97,113	1.40	6 (8%)
13	CLA	b	814	2	69,73,73	1.26	8 (11%)	83,113,113	1.31	5 (6%)
13	CLA	b	804	-	69,73,73	1.24	7 (10%)	83,113,113	1.27	8 (9%)
13	CLA	a	806	1	69,73,73	1.25	7 (10%)	83,113,113	1.31	5 (6%)
13	CLA	a	813	1	69,73,73	1.24	9 (13%)	83,113,113	1.33	7 (8%)
13	CLA	b	807	2	69,73,73	1.26	7 (10%)	83,113,113	1.28	6 (7%)
16	LHG	a	853	-	48,48,48	0.60	0	51,54,54	1.26	6 (11%)
13	CLA	a	836	1	59,63,73	1.36	8 (13%)	71,101,113	1.34	6 (8%)
13	CLA	l	1501	-	54,58,73	1.41	7 (12%)	65,95,113	1.41	6 (9%)
15	BCR	j	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	b	832	2	54,58,73	1.41	8 (14%)	65,95,113	1.40	9 (13%)
13	CLA	b	842	16	50,54,73	1.45	7 (14%)	60,90,113	1.44	4 (6%)
17	LMG	a	850	-	50,50,55	0.78	0	58,58,63	1.31	7 (12%)
20	ECH	m	101	-	42,42,42	1.79	9 (21%)	55,58,58	1.86	13 (23%)
13	CLA	b	820	-	64,68,73	1.30	9 (14%)	77,107,113	1.29	6 (7%)

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
13	CLA	b	840	-	-	18/39/115/115	-
17	LMG	b	852	-	-	22/50/70/70	0/1/1/1
13	CLA	b	822	2	-	16/33/109/115	-
13	CLA	b	825	-	-	14/39/115/115	-
13	CLA	a	819	1	-	15/39/115/115	-
13	CLA	a	817	1	-	14/39/115/115	-
13	CLA	b	841	2	-	18/39/115/115	-
13	CLA	a	824	1	-	11/33/109/115	-
13	CLA	a	820	1	-	26/39/115/115	-
15	BCR	i	102	-	-	11/29/63/63	0/2/2/2
21	EQ3	b	853	-	-	2/29/68/68	0/2/2/2
13	CLA	a	809	1	-	4/23/99/115	-
13	CLA	b	834	2	-	14/39/115/115	-
16	LHG	b	851	13	-	25/42/42/53	-
13	CLA	b	830	2	-	16/39/115/115	-
13	CLA	b	826	-	-	6/27/103/115	-
13	CLA	a	841	1	-	15/39/115/115	-
13	CLA	a	828	1	-	12/39/115/115	-
13	CLA	b	837	2	-	6/24/100/115	-
13	CLA	k	4003	9	-	11/17/93/115	-
13	CLA	a	803	1	-	6/39/115/115	-
19	SF4	c	102	3	-	-	0/6/5/5
13	CLA	b	821	2	-	13/39/115/115	-
13	CLA	l	1502	10	-	15/39/115/115	-
13	CLA	k	4004	9	-	7/15/91/115	-
16	LHG	a	849	-	-	31/53/53/53	-
16	LHG	a	851	13	-	19/53/53/53	-
13	CLA	a	826	-	-	11/39/115/115	-
15	BCR	b	845	-	-	5/29/63/63	0/2/2/2
13	CLA	b	819	2	-	15/39/115/115	-
15	BCR	f	202	-	-	8/29/63/63	0/2/2/2
13	CLA	a	854	-	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	b	824	2	-	12/30/106/115	-
15	BCR	a	848	-	-	8/18/35/63	0/1/1/2
15	BCR	i	101	-	-	7/29/63/63	0/2/2/2
15	BCR	b	848	-	-	8/29/63/63	0/2/2/2
13	CLA	b	815	2	-	10/39/115/115	-
23	LMT	j	102	-	-	15/21/61/61	0/2/2/2
13	CLA	a	815	1	-	5/17/93/115	-
13	CLA	a	804	1	-	12/39/115/115	-
13	CLA	a	831	1	-	11/29/105/115	-
13	CLA	b	808	2	-	17/39/115/115	-
19	SF4	b	802	1,2	-	-	0/6/5/5
13	CLA	b	803	2	-	20/39/115/115	-
15	BCR	j	105	-	-	5/29/63/63	0/2/2/2
13	CLA	a	816	-	-	7/17/93/115	-
13	CLA	b	831	2	-	10/23/99/115	-
13	CLA	a	811	1	-	15/39/115/115	-
13	CLA	j	103	8	-	11/27/103/115	-
13	CLA	a	840	1	-	20/39/115/115	-
13	CLA	f	201	-	-	20/39/115/115	-
13	CLA	a	822	1	-	13/39/115/115	-
13	CLA	f	203	-	-	4/21/97/115	-
13	CLA	j	104	8	-	8/17/93/115	-
20	ECH	b	846	-	-	10/29/66/66	0/2/2/2
13	CLA	b	838	2	-	15/39/115/115	-
15	BCR	a	847	-	-	10/29/63/63	0/2/2/2
13	CLA	a	808	1	-	13/39/115/115	-
14	PQN	b	843	-	-	1/23/43/43	0/2/2/2
13	CLA	b	811	2	-	9/29/105/115	-
15	BCR	b	849	-	-	14/29/63/63	0/2/2/2
13	CLA	a	834	1	-	16/39/115/115	-
13	CLA	a	830	1	-	12/39/115/115	-
16	LHG	f	206	-	-	20/53/53/53	-
13	CLA	b	812	2	-	7/29/105/115	-
15	BCR	b	844	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	a	838	1	-	17/39/115/115	-
13	CLA	b	833	2	-	15/39/115/115	-
13	CLA	a	805	1	-	11/39/115/115	-
13	CLA	a	839	1	-	19/39/115/115	-
13	CLA	a	832	1	-	14/33/109/115	-
13	CLA	b	801	-	-	14/39/115/115	-
13	CLA	a	802	-	-	10/39/115/115	-
13	CLA	a	821	-	-	13/39/115/115	-
13	CLA	a	823	1	-	20/39/115/115	-
13	CLA	b	816	2	-	12/27/103/115	-
13	CLA	b	827	2	-	7/39/115/115	-
15	BCR	b	847	-	-	6/29/63/63	0/2/2/2
12	CL0	a	801	1	-	10/39/115/115	-
14	PQN	a	843	-	-	1/23/43/43	0/2/2/2
15	BCR	k	4005	-	-	4/29/63/63	0/2/2/2
19	SF4	c	101	3	-	-	0/6/5/5
22	ZEX	b	854	-	-	3/29/67/67	0/2/2/2
13	CLA	b	828	2	-	15/39/115/115	-
15	BCR	a	844	-	-	6/29/63/63	0/2/2/2
13	CLA	a	833	1	-	18/39/115/115	-
13	CLA	b	817	2	-	9/29/105/115	-
13	CLA	b	805	2	-	12/39/115/115	-
13	CLA	a	818	1	-	25/39/115/115	-
13	CLA	b	810	2	-	13/39/115/115	-
13	CLA	b	823	2	-	4/17/93/115	-
13	CLA	a	827	1	-	18/39/115/115	-
13	CLA	a	842	16	-	6/15/91/115	-
22	ZEX	f	205	-	-	6/29/67/67	0/2/2/2
13	CLA	b	829	2	-	10/39/115/115	-
13	CLA	a	814	1	-	11/18/94/115	-
13	CLA	b	839	2	-	7/21/97/115	-
13	CLA	a	837	1	-	5/23/99/115	-
13	CLA	a	807	1	-	16/39/115/115	-
13	CLA	b	809	2	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	LMG	a	852	-	-	19/35/55/70	0/1/1/1
13	CLA	k	4002	-	-	12/39/115/115	-
15	BCR	a	845	-	-	6/29/63/63	0/2/2/2
15	BCR	k	4001	-	-	8/29/63/63	0/2/2/2
13	CLA	f	204	6	-	7/15/91/115	-
13	CLA	a	825	-	-	13/39/115/115	-
13	CLA	b	806	2	-	12/39/115/115	-
13	CLA	a	810	1	-	10/25/101/115	-
13	CLA	a	855	-	-	17/39/115/115	-
13	CLA	b	835	-	-	19/39/115/115	-
13	CLA	b	836	-	-	9/21/97/115	-
15	BCR	a	846	-	-	6/29/63/63	0/2/2/2
13	CLA	a	829	1	-	15/39/115/115	-
18	45D	a	856	-	-	4/29/69/69	0/2/2/2
17	LMG	b	850	-	-	24/50/70/70	0/1/1/1
13	CLA	a	812	1	-	9/24/100/115	-
13	CLA	a	835	1	-	15/39/115/115	-
13	CLA	b	818	2	-	9/39/115/115	-
13	CLA	b	813	2	-	7/21/97/115	-
13	CLA	l	1503	-	-	6/24/100/115	-
13	CLA	b	814	2	-	16/39/115/115	-
13	CLA	b	804	-	-	18/39/115/115	-
13	CLA	a	806	1	-	12/39/115/115	-
13	CLA	a	813	1	-	13/39/115/115	-
13	CLA	b	807	2	-	14/39/115/115	-
16	LHG	a	853	-	-	30/53/53/53	-
13	CLA	a	836	1	-	8/27/103/115	-
13	CLA	l	1501	-	-	10/21/97/115	-
15	BCR	j	101	-	-	6/29/63/63	0/2/2/2
13	CLA	b	832	2	-	5/21/97/115	-
13	CLA	b	842	16	-	9/17/93/115	-
17	LMG	a	850	-	-	27/45/65/70	0/1/1/1
20	ECH	m	101	-	-	6/29/66/66	0/2/2/2
13	CLA	b	820	-	-	7/33/109/115	-

All (870) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	m	101	ECH	C14-C13	4.10	1.41	1.35
20	m	101	ECH	C17-C18	4.10	1.41	1.35
20	m	101	ECH	C21-C22	4.10	1.41	1.35
13	b	818	CLA	C1D-ND	4.07	1.42	1.37
20	m	101	ECH	C10-C9	4.04	1.41	1.35
20	b	846	ECH	C21-C22	4.02	1.41	1.35
13	a	828	CLA	C1D-ND	4.02	1.42	1.37
22	f	205	ZEX	C34-C33	4.00	1.41	1.35
22	f	205	ZEX	C30-C29	3.98	1.41	1.35
20	b	846	ECH	C17-C18	3.97	1.41	1.35
13	b	814	CLA	C1D-ND	3.94	1.42	1.37
20	b	846	ECH	C10-C9	3.93	1.41	1.35
13	b	828	CLA	C1D-ND	3.92	1.42	1.37
22	b	854	ZEX	C30-C29	3.92	1.41	1.35
13	b	835	CLA	C1D-ND	3.91	1.42	1.37
18	a	856	45D	C37-C35	3.91	1.41	1.35
13	a	836	CLA	C1D-ND	3.91	1.42	1.37
13	a	816	CLA	C1D-ND	3.91	1.42	1.37
22	f	205	ZEX	C14-C13	3.90	1.41	1.35
13	l	1501	CLA	C1D-ND	3.90	1.42	1.37
18	a	856	45D	C38-C36	3.89	1.40	1.35
13	a	824	CLA	C1D-ND	3.89	1.42	1.37
13	b	831	CLA	C1D-ND	3.89	1.42	1.37
13	a	834	CLA	C1D-ND	3.88	1.42	1.37
22	b	854	ZEX	C14-C13	3.88	1.40	1.35
20	b	846	ECH	C14-C13	3.88	1.40	1.35
13	a	839	CLA	C1D-ND	3.88	1.42	1.37
13	a	818	CLA	C1D-ND	3.87	1.42	1.37
13	f	203	CLA	C1D-ND	3.87	1.42	1.37
13	a	802	CLA	C1D-ND	3.86	1.42	1.37
22	b	854	ZEX	C34-C33	3.86	1.40	1.35
13	k	4003	CLA	C1D-ND	3.86	1.42	1.37
13	j	103	CLA	C1D-ND	3.85	1.42	1.37
13	a	813	CLA	C1D-ND	3.85	1.42	1.37
13	b	822	CLA	C1D-ND	3.84	1.42	1.37
13	b	821	CLA	C1D-ND	3.84	1.42	1.37
13	b	827	CLA	C1D-ND	3.84	1.42	1.37
22	f	205	ZEX	C10-C9	3.84	1.40	1.35
13	b	803	CLA	C1D-ND	3.83	1.42	1.37
13	j	104	CLA	C1D-ND	3.83	1.42	1.37
13	b	819	CLA	C1D-ND	3.82	1.42	1.37
13	b	837	CLA	C1D-ND	3.82	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	825	CLA	C1D-ND	3.82	1.42	1.37
13	b	811	CLA	C1D-ND	3.81	1.42	1.37
13	f	204	CLA	C1D-ND	3.81	1.42	1.37
13	k	4002	CLA	C1D-ND	3.81	1.42	1.37
18	a	856	45D	C30-C26	3.81	1.40	1.35
13	a	837	CLA	C1D-ND	3.81	1.42	1.37
13	a	833	CLA	C1D-ND	3.81	1.42	1.37
13	a	820	CLA	C1D-ND	3.81	1.42	1.37
18	a	856	45D	C29-C25	3.80	1.40	1.35
12	a	801	CL0	C1D-ND	3.80	1.42	1.37
13	a	838	CLA	C1D-ND	3.80	1.42	1.37
13	b	801	CLA	C1D-ND	3.80	1.42	1.37
13	b	808	CLA	C1D-ND	3.80	1.42	1.37
13	a	821	CLA	C1D-ND	3.80	1.42	1.37
13	a	827	CLA	C1D-ND	3.80	1.42	1.37
13	a	841	CLA	C1D-ND	3.80	1.42	1.37
13	a	840	CLA	C1D-ND	3.79	1.42	1.37
13	b	842	CLA	C1D-ND	3.79	1.42	1.37
13	a	812	CLA	C1D-ND	3.79	1.42	1.37
13	a	855	CLA	C1D-ND	3.79	1.42	1.37
13	b	807	CLA	C1D-ND	3.79	1.42	1.37
13	b	834	CLA	C1D-ND	3.79	1.42	1.37
13	a	823	CLA	C1D-ND	3.79	1.42	1.37
13	b	824	CLA	C1D-ND	3.79	1.42	1.37
13	f	201	CLA	C1D-ND	3.79	1.42	1.37
13	b	815	CLA	C1D-ND	3.79	1.42	1.37
13	b	817	CLA	C1D-ND	3.79	1.42	1.37
13	b	836	CLA	C1D-ND	3.78	1.42	1.37
13	a	835	CLA	C1D-ND	3.78	1.42	1.37
13	b	839	CLA	C1D-ND	3.78	1.42	1.37
13	a	817	CLA	C1D-ND	3.78	1.42	1.37
13	a	805	CLA	C1D-ND	3.78	1.42	1.37
13	b	838	CLA	C1D-ND	3.78	1.42	1.37
13	b	806	CLA	C1D-ND	3.77	1.42	1.37
13	a	822	CLA	C1D-ND	3.77	1.42	1.37
13	b	810	CLA	C1D-ND	3.77	1.42	1.37
13	b	820	CLA	C1D-ND	3.77	1.42	1.37
13	l	1503	CLA	C1D-ND	3.76	1.42	1.37
13	a	814	CLA	C1D-ND	3.76	1.42	1.37
13	a	809	CLA	C1D-ND	3.76	1.42	1.37
13	a	810	CLA	C1D-ND	3.76	1.42	1.37
13	a	811	CLA	C1D-ND	3.76	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	825	CLA	C1D-ND	3.75	1.42	1.37
13	a	815	CLA	C1D-ND	3.75	1.42	1.37
13	a	804	CLA	C1D-ND	3.75	1.42	1.37
13	b	826	CLA	C1D-ND	3.75	1.42	1.37
13	a	842	CLA	C1D-ND	3.74	1.42	1.37
13	b	833	CLA	C1D-ND	3.74	1.42	1.37
13	a	803	CLA	C1D-ND	3.73	1.42	1.37
13	a	806	CLA	C1D-ND	3.73	1.42	1.37
13	a	830	CLA	C1D-ND	3.73	1.42	1.37
13	a	832	CLA	C1D-ND	3.73	1.42	1.37
13	b	832	CLA	C1D-ND	3.73	1.42	1.37
13	b	823	CLA	C1D-ND	3.73	1.42	1.37
13	a	807	CLA	C1D-ND	3.72	1.42	1.37
21	b	853	EQ3	C21-C22	3.71	1.40	1.35
13	b	805	CLA	C1D-ND	3.71	1.42	1.37
21	b	853	EQ3	C17-C18	3.71	1.40	1.35
15	b	844	BCR	C1-C6	-3.70	1.48	1.53
13	b	830	CLA	C1D-ND	3.70	1.42	1.37
13	b	840	CLA	C1D-ND	3.70	1.42	1.37
22	b	854	ZEX	C10-C9	3.70	1.40	1.35
13	b	841	CLA	C1D-ND	3.70	1.42	1.37
13	a	808	CLA	C1D-ND	3.70	1.42	1.37
13	a	829	CLA	C1D-ND	3.70	1.42	1.37
13	b	812	CLA	C1D-ND	3.69	1.42	1.37
13	a	819	CLA	C1D-ND	3.69	1.42	1.37
13	a	854	CLA	C1D-ND	3.69	1.42	1.37
13	b	816	CLA	C1D-ND	3.67	1.42	1.37
15	j	105	BCR	C1-C6	-3.67	1.48	1.53
13	k	4004	CLA	C1D-ND	3.67	1.42	1.37
13	b	813	CLA	C1D-ND	3.67	1.42	1.37
13	b	804	CLA	C1D-ND	3.66	1.42	1.37
13	b	811	CLA	C4B-NB	3.66	1.42	1.37
13	b	829	CLA	C1D-ND	3.66	1.42	1.37
15	k	4001	BCR	C1-C6	-3.66	1.48	1.53
15	a	847	BCR	C1-C6	-3.65	1.48	1.53
13	a	831	CLA	C1D-ND	3.65	1.42	1.37
21	b	853	EQ3	C14-C13	3.64	1.40	1.35
13	b	809	CLA	C1D-ND	3.62	1.42	1.37
13	b	823	CLA	C4B-NB	3.62	1.42	1.37
13	a	826	CLA	C1D-ND	3.56	1.42	1.37
21	b	853	EQ3	C10-C9	3.54	1.40	1.35
15	j	101	BCR	C1-C6	-3.54	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	l	1502	CLA	C1D-ND	3.53	1.42	1.37
15	a	846	BCR	C1-C6	-3.53	1.48	1.53
13	a	804	CLA	C4B-NB	3.51	1.42	1.37
13	b	839	CLA	C4B-NB	3.51	1.42	1.37
20	m	101	ECH	C25-C26	3.49	1.40	1.35
15	a	844	BCR	C1-C6	-3.48	1.49	1.53
13	b	805	CLA	C4B-NB	3.47	1.42	1.37
13	a	839	CLA	C4B-NB	3.47	1.42	1.37
15	a	848	BCR	C1-C6	-3.46	1.49	1.53
15	a	845	BCR	C1-C6	-3.46	1.49	1.53
13	b	841	CLA	C4B-NB	3.46	1.42	1.37
13	b	833	CLA	C4B-NB	3.45	1.42	1.37
13	a	833	CLA	C4B-NB	3.41	1.42	1.37
15	f	202	BCR	C1-C6	-3.41	1.49	1.53
13	b	803	CLA	C4B-NB	3.39	1.41	1.37
13	l	1501	CLA	C4B-NB	3.39	1.41	1.37
13	f	204	CLA	C4B-NB	3.38	1.41	1.37
15	b	848	BCR	C30-C25	-3.37	1.49	1.53
15	b	845	BCR	C1-C6	-3.36	1.49	1.53
13	a	820	CLA	C4B-NB	3.35	1.41	1.37
13	a	841	CLA	C4B-NB	3.35	1.41	1.37
13	b	801	CLA	C4B-NB	3.34	1.41	1.37
13	b	831	CLA	C4B-NB	3.34	1.41	1.37
13	b	816	CLA	C4B-NB	3.34	1.41	1.37
13	a	814	CLA	C4B-NB	3.33	1.41	1.37
15	b	849	BCR	C1-C6	-3.32	1.49	1.53
13	b	824	CLA	C4B-NB	3.32	1.41	1.37
13	a	812	CLA	C4B-NB	3.32	1.41	1.37
13	j	104	CLA	C4B-NB	3.32	1.41	1.37
13	b	836	CLA	C4B-NB	3.32	1.41	1.37
13	a	823	CLA	C4B-NB	3.32	1.41	1.37
13	f	203	CLA	C4B-NB	3.31	1.41	1.37
13	j	103	CLA	C4B-NB	3.30	1.41	1.37
13	b	813	CLA	C4B-NB	3.29	1.41	1.37
13	a	803	CLA	C4B-NB	3.29	1.41	1.37
13	a	854	CLA	C4B-NB	3.29	1.41	1.37
15	a	844	BCR	C30-C25	-3.29	1.49	1.53
13	a	838	CLA	C4B-NB	3.28	1.41	1.37
13	a	818	CLA	C4B-NB	3.28	1.41	1.37
13	b	822	CLA	C4B-NB	3.27	1.41	1.37
13	l	1502	CLA	C4B-NB	3.27	1.41	1.37
15	b	844	BCR	C30-C25	-3.27	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	k	4003	CLA	C4B-NB	3.27	1.41	1.37
13	a	840	CLA	C4B-NB	3.27	1.41	1.37
13	b	823	CLA	C3B-C4B	3.26	1.50	1.42
13	b	821	CLA	C4B-NB	3.25	1.41	1.37
13	a	836	CLA	C4B-NB	3.25	1.41	1.37
13	b	827	CLA	C4B-NB	3.25	1.41	1.37
13	b	840	CLA	C4B-NB	3.25	1.41	1.37
13	b	828	CLA	C4B-NB	3.24	1.41	1.37
15	j	105	BCR	C30-C25	-3.24	1.49	1.53
13	f	201	CLA	C4B-NB	3.24	1.41	1.37
13	b	810	CLA	C4B-NB	3.23	1.41	1.37
13	a	816	CLA	C4B-NB	3.23	1.41	1.37
15	i	101	BCR	C30-C25	-3.22	1.49	1.53
13	a	806	CLA	C4B-NB	3.22	1.41	1.37
13	a	831	CLA	C4B-NB	3.22	1.41	1.37
13	b	811	CLA	C3B-C4B	3.21	1.50	1.42
13	a	819	CLA	C4B-NB	3.21	1.41	1.37
13	a	807	CLA	C4B-NB	3.20	1.41	1.37
13	b	834	CLA	C4B-NB	3.20	1.41	1.37
13	a	829	CLA	C4B-NB	3.20	1.41	1.37
13	b	807	CLA	C4B-NB	3.20	1.41	1.37
13	b	842	CLA	C4B-NB	3.20	1.41	1.37
13	k	4004	CLA	C4B-NB	3.20	1.41	1.37
13	k	4002	CLA	C4B-NB	3.20	1.41	1.37
13	b	814	CLA	C4B-NB	3.19	1.41	1.37
13	b	838	CLA	C4B-NB	3.19	1.41	1.37
13	l	1503	CLA	C4B-NB	3.19	1.41	1.37
15	i	102	BCR	C1-C6	-3.19	1.49	1.53
13	a	835	CLA	C4B-NB	3.18	1.41	1.37
13	a	828	CLA	C4B-NB	3.18	1.41	1.37
15	b	847	BCR	C1-C6	-3.18	1.49	1.53
12	a	801	CL0	C4B-NB	3.18	1.41	1.37
13	b	819	CLA	C4B-NB	3.18	1.41	1.37
13	b	809	CLA	C4B-NB	3.17	1.41	1.37
15	i	101	BCR	C1-C6	-3.17	1.49	1.53
13	a	809	CLA	C4B-NB	3.17	1.41	1.37
13	b	809	CLA	C4D-ND	-3.17	1.33	1.37
13	b	812	CLA	C4B-NB	3.17	1.41	1.37
13	a	855	CLA	C4B-NB	3.16	1.41	1.37
13	a	830	CLA	C4B-NB	3.16	1.41	1.37
15	k	4005	BCR	C1-C6	-3.16	1.49	1.53
13	a	817	CLA	C4B-NB	3.16	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	810	CLA	C4B-NB	3.15	1.41	1.37
13	a	808	CLA	C4B-NB	3.15	1.41	1.37
13	a	822	CLA	C4B-NB	3.15	1.41	1.37
13	a	834	CLA	C4B-NB	3.14	1.41	1.37
13	a	805	CLA	C4B-NB	3.14	1.41	1.37
13	a	811	CLA	C4B-NB	3.14	1.41	1.37
13	a	842	CLA	C4B-NB	3.14	1.41	1.37
13	b	808	CLA	C4B-NB	3.14	1.41	1.37
13	a	825	CLA	C4B-NB	3.13	1.41	1.37
13	b	830	CLA	C4B-NB	3.13	1.41	1.37
15	k	4001	BCR	C30-C25	-3.13	1.49	1.53
15	b	848	BCR	C1-C6	-3.13	1.49	1.53
15	b	849	BCR	C30-C25	-3.13	1.49	1.53
13	b	815	CLA	C4B-NB	3.12	1.41	1.37
13	a	854	CLA	C4D-ND	-3.12	1.33	1.37
13	a	832	CLA	C4B-NB	3.12	1.41	1.37
13	b	807	CLA	C4D-ND	-3.12	1.33	1.37
13	b	817	CLA	C4B-NB	3.12	1.41	1.37
13	b	832	CLA	C4B-NB	3.12	1.41	1.37
15	f	202	BCR	C30-C25	-3.12	1.49	1.53
13	b	833	CLA	C3B-C4B	3.12	1.50	1.42
13	a	802	CLA	C4B-NB	3.12	1.41	1.37
15	j	101	BCR	C30-C25	-3.11	1.49	1.53
13	a	826	CLA	C4B-NB	3.11	1.41	1.37
13	b	806	CLA	C4D-ND	-3.11	1.33	1.37
13	b	812	CLA	C4D-ND	-3.11	1.33	1.37
13	b	816	CLA	C3B-C4B	3.10	1.50	1.42
13	b	825	CLA	C4B-NB	3.10	1.41	1.37
13	b	839	CLA	C4D-ND	-3.10	1.33	1.37
15	b	845	BCR	C30-C25	-3.09	1.49	1.53
13	a	839	CLA	C3B-C4B	3.09	1.50	1.42
20	b	846	ECH	C23-C22	-3.09	1.39	1.45
13	a	813	CLA	C4B-NB	3.09	1.41	1.37
13	b	829	CLA	C4B-NB	3.09	1.41	1.37
13	a	815	CLA	C4B-NB	3.09	1.41	1.37
13	a	806	CLA	C4D-ND	-3.09	1.33	1.37
13	a	838	CLA	C4D-ND	-3.08	1.33	1.37
13	b	831	CLA	C4D-ND	-3.08	1.33	1.37
13	b	818	CLA	C4B-NB	3.08	1.41	1.37
13	b	837	CLA	C4B-NB	3.08	1.41	1.37
15	a	846	BCR	C30-C25	-3.07	1.49	1.53
15	k	4005	BCR	C30-C25	-3.07	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	203	CLA	C4D-ND	-3.07	1.33	1.37
13	a	821	CLA	C4B-NB	3.07	1.41	1.37
13	b	806	CLA	C4B-NB	3.07	1.41	1.37
13	b	824	CLA	C4D-ND	-3.07	1.33	1.37
13	a	827	CLA	C4D-ND	-3.07	1.33	1.37
13	b	804	CLA	C4B-NB	3.07	1.41	1.37
13	b	835	CLA	C4B-NB	3.07	1.41	1.37
13	a	808	CLA	C4D-ND	-3.07	1.33	1.37
13	a	803	CLA	C4D-ND	-3.06	1.33	1.37
13	b	820	CLA	C4B-NB	3.06	1.41	1.37
13	b	820	CLA	C4D-ND	-3.06	1.33	1.37
13	b	826	CLA	C4B-NB	3.06	1.41	1.37
13	b	840	CLA	C4D-ND	-3.06	1.33	1.37
13	a	837	CLA	C4D-ND	-3.06	1.33	1.37
13	a	827	CLA	C4B-NB	3.05	1.41	1.37
13	a	824	CLA	C4B-NB	3.05	1.41	1.37
13	b	838	CLA	C4D-ND	-3.05	1.33	1.37
13	a	819	CLA	C4D-ND	-3.05	1.33	1.37
13	b	829	CLA	C4D-ND	-3.05	1.33	1.37
13	a	831	CLA	C4D-ND	-3.04	1.33	1.37
13	b	811	CLA	C4D-ND	-3.03	1.33	1.37
13	b	826	CLA	C4D-ND	-3.03	1.33	1.37
13	b	827	CLA	C4D-ND	-3.02	1.33	1.37
13	b	835	CLA	C4D-ND	-3.02	1.33	1.37
13	b	842	CLA	C4D-ND	-3.01	1.33	1.37
13	a	803	CLA	C3B-C4B	3.01	1.49	1.42
13	a	809	CLA	C4D-ND	-3.01	1.33	1.37
13	a	807	CLA	C4D-ND	-3.01	1.33	1.37
13	j	103	CLA	C3B-C4B	3.01	1.49	1.42
13	b	808	CLA	C4D-ND	-3.00	1.33	1.37
13	l	1503	CLA	C4D-ND	-3.00	1.33	1.37
13	a	804	CLA	C4D-ND	-3.00	1.33	1.37
13	a	821	CLA	C4D-ND	-3.00	1.33	1.37
13	a	826	CLA	C4D-ND	-3.00	1.33	1.37
15	b	847	BCR	C30-C25	-2.99	1.49	1.53
13	b	813	CLA	C4D-ND	-2.99	1.33	1.37
13	b	825	CLA	C4D-ND	-2.98	1.33	1.37
13	b	801	CLA	C4D-ND	-2.98	1.33	1.37
18	a	856	45D	C24-C26	-2.98	1.39	1.45
13	a	805	CLA	C4D-ND	-2.98	1.33	1.37
13	a	855	CLA	C4D-ND	-2.98	1.33	1.37
13	b	833	CLA	C4D-ND	-2.98	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	841	CLA	C4D-ND	-2.98	1.33	1.37
13	a	822	CLA	C4D-ND	-2.98	1.33	1.37
13	a	812	CLA	C3B-C4B	2.98	1.49	1.42
13	b	821	CLA	C4D-ND	-2.98	1.33	1.37
13	a	836	CLA	C4D-ND	-2.97	1.33	1.37
13	b	805	CLA	C4D-ND	-2.97	1.33	1.37
13	a	837	CLA	C4B-NB	2.97	1.41	1.37
13	a	829	CLA	C4D-ND	-2.97	1.33	1.37
13	b	834	CLA	C4D-ND	-2.97	1.33	1.37
13	b	832	CLA	C4D-ND	-2.97	1.33	1.37
13	f	204	CLA	C3B-C4B	2.96	1.49	1.42
13	a	808	CLA	C3B-C4B	2.96	1.49	1.42
21	b	853	EQ3	C23-C22	-2.96	1.39	1.45
13	b	818	CLA	C4D-ND	-2.96	1.33	1.37
13	a	841	CLA	C4D-ND	-2.96	1.33	1.37
13	b	810	CLA	C4D-ND	-2.96	1.33	1.37
13	a	835	CLA	C4D-ND	-2.96	1.33	1.37
13	a	842	CLA	C4D-ND	-2.96	1.33	1.37
13	b	816	CLA	C4D-ND	-2.96	1.33	1.37
13	b	813	CLA	C3B-C4B	2.96	1.49	1.42
13	a	811	CLA	C4D-ND	-2.95	1.33	1.37
13	a	816	CLA	C4D-ND	-2.95	1.33	1.37
13	k	4003	CLA	C4D-ND	-2.95	1.33	1.37
13	a	814	CLA	C4D-ND	-2.94	1.33	1.37
13	a	812	CLA	C4D-ND	-2.94	1.33	1.37
12	a	801	CL0	C4D-ND	-2.94	1.33	1.37
13	b	840	CLA	C3B-C4B	2.94	1.49	1.42
13	a	815	CLA	C4D-ND	-2.94	1.33	1.37
13	a	839	CLA	C4D-ND	-2.94	1.33	1.37
13	b	836	CLA	C4D-ND	-2.94	1.33	1.37
15	a	845	BCR	C30-C25	-2.93	1.49	1.53
13	b	819	CLA	C4D-ND	-2.93	1.33	1.37
21	b	853	EQ3	C8-C9	-2.93	1.39	1.45
13	b	837	CLA	C4D-ND	-2.92	1.33	1.37
13	a	832	CLA	C4D-ND	-2.92	1.33	1.37
13	b	805	CLA	C3B-C4B	2.92	1.49	1.42
13	a	813	CLA	C4D-ND	-2.92	1.33	1.37
13	b	822	CLA	C4D-ND	-2.92	1.33	1.37
13	b	839	CLA	C3B-C4B	2.92	1.49	1.42
13	l	1501	CLA	C3B-C4B	2.92	1.49	1.42
13	b	814	CLA	C4D-ND	-2.92	1.33	1.37
13	k	4003	CLA	C3B-C4B	2.92	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	823	CLA	C4D-ND	-2.92	1.33	1.37
22	b	854	ZEX	C8-C9	-2.92	1.39	1.45
13	j	104	CLA	C3B-C4B	2.91	1.49	1.42
13	k	4002	CLA	C4D-ND	-2.91	1.33	1.37
13	b	809	CLA	C3B-C4B	2.91	1.49	1.42
13	a	833	CLA	C4D-ND	-2.91	1.33	1.37
18	a	856	45D	C23-C25	-2.91	1.39	1.45
13	b	803	CLA	C4D-ND	-2.91	1.33	1.37
13	l	1502	CLA	C4D-ND	-2.91	1.33	1.37
13	a	841	CLA	C3B-C4B	2.91	1.49	1.42
13	a	802	CLA	C3B-C4B	2.90	1.49	1.42
13	b	804	CLA	C3B-C4B	2.90	1.49	1.42
13	f	201	CLA	C4D-ND	-2.90	1.33	1.37
13	a	804	CLA	C3B-C4B	2.90	1.49	1.42
13	a	817	CLA	C4D-ND	-2.89	1.33	1.37
13	a	810	CLA	C4D-ND	-2.89	1.33	1.37
13	b	804	CLA	C4D-ND	-2.89	1.33	1.37
13	b	828	CLA	C4D-ND	-2.89	1.33	1.37
13	b	825	CLA	C3B-C4B	2.89	1.49	1.42
13	a	821	CLA	C3B-C4B	2.89	1.49	1.42
13	a	825	CLA	C4D-ND	-2.88	1.33	1.37
13	a	824	CLA	C4D-ND	-2.88	1.33	1.37
13	f	201	CLA	C3B-C4B	2.88	1.49	1.42
13	a	818	CLA	C4D-ND	-2.88	1.33	1.37
13	b	815	CLA	C4D-ND	-2.88	1.33	1.37
13	f	204	CLA	C4D-ND	-2.88	1.33	1.37
13	b	832	CLA	C3B-C4B	2.88	1.49	1.42
13	a	823	CLA	C3B-C4B	2.87	1.49	1.42
13	b	830	CLA	C4D-ND	-2.87	1.33	1.37
13	a	830	CLA	C4D-ND	-2.87	1.33	1.37
13	j	103	CLA	C4D-ND	-2.87	1.33	1.37
13	a	840	CLA	C4D-ND	-2.87	1.33	1.37
13	b	814	CLA	C3B-C4B	2.87	1.49	1.42
13	b	818	CLA	C3B-C4B	2.87	1.49	1.42
13	a	820	CLA	C4D-ND	-2.87	1.33	1.37
13	a	842	CLA	C3B-C4B	2.86	1.49	1.42
13	a	838	CLA	C3B-C4B	2.86	1.49	1.42
13	a	807	CLA	C3B-C4B	2.86	1.49	1.42
13	a	813	CLA	C3B-C4B	2.86	1.49	1.42
13	a	809	CLA	C3B-C4B	2.86	1.49	1.42
13	b	824	CLA	C3B-C4B	2.85	1.49	1.42
13	a	814	CLA	C3B-C4B	2.85	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	806	CLA	C3B-C4B	2.85	1.49	1.42
13	k	4004	CLA	C4D-ND	-2.85	1.33	1.37
13	a	819	CLA	C3B-C4B	2.85	1.49	1.42
13	a	811	CLA	C3B-C4B	2.85	1.49	1.42
13	b	830	CLA	C3B-C4B	2.85	1.49	1.42
13	b	837	CLA	C3B-C4B	2.85	1.49	1.42
13	b	834	CLA	C3B-C4B	2.85	1.49	1.42
13	b	817	CLA	C4D-ND	-2.85	1.33	1.37
13	b	807	CLA	C3B-C4B	2.85	1.49	1.42
13	b	820	CLA	C3B-C4B	2.84	1.49	1.42
13	b	841	CLA	C3B-C4B	2.84	1.49	1.42
13	b	828	CLA	C3B-C4B	2.84	1.49	1.42
13	a	835	CLA	C3B-C4B	2.84	1.49	1.42
13	k	4002	CLA	C3B-C4B	2.84	1.49	1.42
15	a	847	BCR	C30-C25	-2.84	1.49	1.53
13	b	826	CLA	C3B-C4B	2.84	1.49	1.42
13	b	821	CLA	C3B-C4B	2.83	1.49	1.42
13	b	806	CLA	C3B-C4B	2.83	1.49	1.42
13	b	815	CLA	C3B-C4B	2.83	1.49	1.42
13	b	803	CLA	C3B-C4B	2.83	1.49	1.42
13	a	826	CLA	C3B-C4B	2.83	1.49	1.42
13	a	815	CLA	C3B-C4B	2.83	1.49	1.42
13	b	829	CLA	C3B-C4B	2.83	1.49	1.42
13	b	836	CLA	C3B-C4B	2.83	1.49	1.42
13	k	4004	CLA	C3B-C4B	2.83	1.49	1.42
13	b	835	CLA	C3B-C4B	2.82	1.49	1.42
13	l	1503	CLA	C3B-C4B	2.82	1.49	1.42
13	a	822	CLA	C3B-C4B	2.82	1.49	1.42
13	b	819	CLA	C3B-C4B	2.82	1.49	1.42
20	m	101	ECH	C23-C22	-2.81	1.39	1.45
13	b	822	CLA	C3B-C4B	2.81	1.49	1.42
13	a	823	CLA	C4D-ND	-2.81	1.33	1.37
13	b	842	CLA	C3B-C4B	2.81	1.49	1.42
13	b	801	CLA	C3B-C4B	2.81	1.49	1.42
13	b	817	CLA	C3B-C4B	2.81	1.49	1.42
13	a	828	CLA	C3B-C4B	2.80	1.49	1.42
13	a	833	CLA	C3B-C4B	2.80	1.49	1.42
13	b	827	CLA	C3B-C4B	2.80	1.49	1.42
13	a	820	CLA	C3B-C4B	2.80	1.49	1.42
13	a	810	CLA	C3B-C4B	2.80	1.49	1.42
13	j	104	CLA	C4D-ND	-2.80	1.33	1.37
13	a	832	CLA	C3B-C4B	2.80	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	834	CLA	C3B-C4B	2.80	1.49	1.42
22	f	205	ZEX	C8-C9	-2.80	1.39	1.45
13	a	836	CLA	C3B-C4B	2.79	1.49	1.42
13	a	834	CLA	C4D-ND	-2.79	1.33	1.37
13	a	840	CLA	C3B-C4B	2.79	1.49	1.42
13	a	829	CLA	C3B-C4B	2.79	1.49	1.42
13	b	831	CLA	C3B-C4B	2.79	1.49	1.42
13	a	830	CLA	C3B-C4B	2.79	1.49	1.42
13	a	805	CLA	C3B-C4B	2.78	1.49	1.42
13	a	855	CLA	C3B-C4B	2.78	1.49	1.42
13	a	816	CLA	C3B-C4B	2.77	1.49	1.42
13	a	854	CLA	C3B-C4B	2.77	1.49	1.42
13	a	824	CLA	C3B-C4B	2.77	1.49	1.42
13	a	827	CLA	C3B-C4B	2.77	1.49	1.42
13	a	817	CLA	C3B-C4B	2.76	1.49	1.42
22	b	854	ZEX	C28-C29	-2.76	1.40	1.45
13	a	818	CLA	C3B-C4B	2.76	1.49	1.42
13	b	812	CLA	C3B-C4B	2.76	1.49	1.42
13	a	802	CLA	C4D-ND	-2.76	1.33	1.37
13	b	838	CLA	C3B-C4B	2.75	1.49	1.42
13	a	828	CLA	C4D-ND	-2.75	1.33	1.37
13	b	810	CLA	C3B-C4B	2.75	1.49	1.42
13	a	825	CLA	C3B-C4B	2.75	1.49	1.42
13	b	808	CLA	C3B-C4B	2.75	1.49	1.42
13	l	1502	CLA	C3B-C4B	2.75	1.49	1.42
20	b	846	ECH	C8-C9	-2.74	1.40	1.45
13	a	831	CLA	C3B-C4B	2.73	1.49	1.42
13	j	104	CLA	C1B-C2B	2.73	1.49	1.43
13	b	831	CLA	C1B-C2B	2.72	1.49	1.43
22	f	205	ZEX	C28-C29	-2.72	1.40	1.45
13	a	816	CLA	C1B-C2B	2.72	1.49	1.43
20	m	101	ECH	C8-C9	-2.72	1.40	1.45
13	f	203	CLA	C3B-C4B	2.71	1.49	1.42
13	l	1501	CLA	C1B-C2B	2.71	1.49	1.43
13	l	1502	CLA	C1B-C2B	2.71	1.49	1.43
13	a	820	CLA	C1B-C2B	2.71	1.49	1.43
12	a	801	CL0	C1B-C2B	2.71	1.49	1.43
13	b	838	CLA	C1B-C2B	2.71	1.49	1.43
13	a	837	CLA	C1B-C2B	2.71	1.49	1.43
13	k	4004	CLA	C1B-C2B	2.71	1.49	1.43
13	a	836	CLA	C1B-C2B	2.71	1.49	1.43
13	k	4002	CLA	C1B-C2B	2.71	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	801	CL0	C3B-C4B	2.70	1.49	1.42
13	a	817	CLA	C1B-C2B	2.70	1.49	1.43
13	a	814	CLA	C1B-C2B	2.70	1.49	1.43
13	f	203	CLA	C1B-C2B	2.70	1.49	1.43
13	b	807	CLA	C1B-C2B	2.70	1.49	1.43
13	l	1501	CLA	C4D-ND	-2.70	1.34	1.37
13	b	834	CLA	C1B-C2B	2.69	1.49	1.43
13	a	815	CLA	C1B-C2B	2.69	1.49	1.43
13	l	1503	CLA	C1B-C2B	2.69	1.49	1.43
13	a	829	CLA	C1B-C2B	2.69	1.49	1.43
13	b	808	CLA	C1B-C2B	2.69	1.49	1.43
13	b	822	CLA	C1B-C2B	2.68	1.49	1.43
18	a	856	45D	C08-C16	2.68	1.39	1.35
13	f	201	CLA	C1B-C2B	2.68	1.49	1.43
13	b	826	CLA	C1B-C2B	2.68	1.49	1.43
13	a	827	CLA	C1B-C2B	2.68	1.49	1.43
13	b	828	CLA	C1B-C2B	2.67	1.49	1.43
13	a	823	CLA	C1B-C2B	2.66	1.49	1.43
13	a	824	CLA	C1B-C2B	2.66	1.49	1.43
13	a	840	CLA	C1B-C2B	2.66	1.49	1.43
13	a	825	CLA	C1B-C2B	2.66	1.49	1.43
13	b	812	CLA	C1B-C2B	2.66	1.49	1.43
13	b	842	CLA	C1B-C2B	2.65	1.49	1.43
13	a	805	CLA	C1B-C2B	2.65	1.49	1.43
13	b	815	CLA	C1B-C2B	2.64	1.49	1.43
13	a	831	CLA	C1B-C2B	2.64	1.49	1.43
13	a	802	CLA	C1B-C2B	2.64	1.49	1.43
13	a	842	CLA	C1B-C2B	2.64	1.49	1.43
13	a	828	CLA	C1B-C2B	2.64	1.49	1.43
13	b	832	CLA	C1B-C2B	2.63	1.49	1.43
13	b	806	CLA	C1B-C2B	2.63	1.49	1.43
13	b	819	CLA	C1B-C2B	2.63	1.49	1.43
13	a	822	CLA	C1B-C2B	2.63	1.49	1.43
23	j	102	LMT	O3'-C3'	-2.63	1.36	1.43
13	b	824	CLA	C1B-C2B	2.63	1.49	1.43
13	a	855	CLA	C1B-C2B	2.63	1.49	1.43
13	k	4003	CLA	C1B-C2B	2.62	1.49	1.43
13	a	841	CLA	C1B-C2B	2.62	1.49	1.43
13	a	804	CLA	C1B-C2B	2.62	1.49	1.43
13	b	814	CLA	C1B-C2B	2.62	1.49	1.43
13	a	806	CLA	C1B-C2B	2.62	1.49	1.43
13	b	817	CLA	C1B-C2B	2.62	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	834	CLA	C1B-C2B	2.62	1.49	1.43
13	b	825	CLA	C1B-C2B	2.62	1.49	1.43
13	b	810	CLA	C1B-C2B	2.61	1.49	1.43
13	b	820	CLA	C1B-C2B	2.61	1.49	1.43
13	a	818	CLA	C1B-C2B	2.61	1.49	1.43
13	a	809	CLA	C1B-C2B	2.61	1.49	1.43
13	b	835	CLA	C1B-C2B	2.61	1.49	1.43
13	b	804	CLA	C1B-C2B	2.61	1.49	1.43
13	f	204	CLA	C1B-C2B	2.60	1.49	1.43
15	i	102	BCR	C30-C25	-2.60	1.50	1.53
13	a	833	CLA	C1B-C2B	2.59	1.49	1.43
13	b	821	CLA	C1B-C2B	2.59	1.49	1.43
13	a	810	CLA	C1B-C2B	2.59	1.49	1.43
13	a	813	CLA	C1B-C2B	2.59	1.49	1.43
13	b	836	CLA	C1B-C2B	2.59	1.49	1.43
13	j	103	CLA	C1B-C2B	2.59	1.49	1.43
13	a	835	CLA	C1B-C2B	2.59	1.49	1.43
13	a	807	CLA	C1B-C2B	2.58	1.49	1.43
13	b	813	CLA	C1B-C2B	2.58	1.49	1.43
13	b	818	CLA	C1B-C2B	2.58	1.49	1.43
13	a	811	CLA	C1B-C2B	2.58	1.49	1.43
13	b	830	CLA	C1B-C2B	2.58	1.49	1.43
13	b	811	CLA	C1B-C2B	2.58	1.49	1.43
13	b	827	CLA	C1B-C2B	2.57	1.49	1.43
13	a	837	CLA	C3B-C4B	2.57	1.48	1.42
13	a	803	CLA	C1B-C2B	2.57	1.49	1.43
13	b	829	CLA	C1B-C2B	2.56	1.49	1.43
13	a	808	CLA	C1B-C2B	2.56	1.49	1.43
13	b	805	CLA	C1B-C2B	2.56	1.49	1.43
13	b	841	CLA	C1B-C2B	2.56	1.49	1.43
13	a	838	CLA	C1B-C2B	2.55	1.49	1.43
13	b	840	CLA	C1B-C2B	2.55	1.49	1.43
13	b	823	CLA	C1B-C2B	2.55	1.49	1.43
13	b	809	CLA	C1B-C2B	2.54	1.49	1.43
13	b	839	CLA	C1B-C2B	2.54	1.49	1.43
13	b	837	CLA	C1B-C2B	2.54	1.49	1.43
13	b	801	CLA	C1B-C2B	2.54	1.49	1.43
13	a	826	CLA	C1B-C2B	2.54	1.49	1.43
13	a	821	CLA	C1B-C2B	2.54	1.49	1.43
13	b	803	CLA	C1B-C2B	2.53	1.49	1.43
13	a	832	CLA	C1B-C2B	2.53	1.49	1.43
13	b	816	CLA	C1B-C2B	2.52	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	839	CLA	C1B-C2B	2.51	1.49	1.43
13	a	854	CLA	C1B-C2B	2.48	1.49	1.43
13	a	812	CLA	C1B-C2B	2.48	1.49	1.43
21	b	853	EQ3	C25-C26	2.47	1.39	1.35
13	a	830	CLA	C1B-C2B	2.47	1.49	1.43
13	b	833	CLA	C1B-C2B	2.46	1.49	1.43
13	a	819	CLA	C1B-C2B	2.46	1.49	1.43
21	b	853	EQ3	C19-C18	-2.45	1.40	1.45
20	b	846	ECH	C19-C18	-2.44	1.40	1.45
20	b	846	ECH	C12-C13	-2.43	1.40	1.45
21	b	853	EQ3	C12-C13	-2.41	1.40	1.45
22	b	854	ZEX	C32-C33	-2.41	1.40	1.45
13	b	805	CLA	CHC-C1C	2.40	1.43	1.38
22	b	854	ZEX	C12-C13	-2.40	1.40	1.45
18	a	856	45D	C33-C35	-2.40	1.40	1.45
13	a	804	CLA	CHC-C1C	2.39	1.43	1.38
23	j	102	LMT	O2B-C2B	-2.39	1.37	1.43
16	a	849	LHG	O7-C5	-2.36	1.40	1.46
22	f	205	ZEX	C12-C13	-2.33	1.40	1.45
18	a	856	45D	C34-C36	-2.31	1.41	1.45
23	j	102	LMT	O3B-C3B	-2.29	1.37	1.43
13	b	841	CLA	CMB-C2B	-2.27	1.46	1.50
23	j	102	LMT	O2'-C2'	-2.26	1.37	1.43
13	a	808	CLA	CHC-C1C	2.26	1.43	1.38
13	b	830	CLA	CMD-C2D	-2.26	1.46	1.50
13	b	824	CLA	CHC-C1C	2.25	1.43	1.38
13	b	826	CLA	CHC-C1C	2.25	1.43	1.38
13	b	814	CLA	CHC-C1C	2.24	1.43	1.38
20	m	101	ECH	C12-C13	-2.24	1.41	1.45
13	j	104	CLA	CHC-C1C	2.24	1.43	1.38
13	b	804	CLA	CMC-C2C	-2.23	1.46	1.50
13	a	802	CLA	CHC-C1C	2.23	1.43	1.38
13	a	806	CLA	CHC-C1C	2.23	1.43	1.38
13	b	821	CLA	CHC-C1C	2.23	1.43	1.38
13	b	840	CLA	CHC-C1C	2.22	1.43	1.38
13	a	832	CLA	CHC-C1C	2.22	1.43	1.38
13	b	832	CLA	CHC-C1C	2.22	1.43	1.38
22	f	205	ZEX	C32-C33	-2.21	1.41	1.45
13	b	833	CLA	CHC-C1C	2.21	1.43	1.38
13	a	809	CLA	CMD-C2D	-2.21	1.46	1.50
13	a	810	CLA	CHC-C1C	2.21	1.43	1.38
13	a	814	CLA	CHC-C1C	2.21	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	806	CLA	CHC-C1C	2.21	1.43	1.38
13	a	826	CLA	CHC-C1C	2.20	1.43	1.38
16	b	851	LHG	O7-C5	-2.20	1.41	1.46
13	a	826	CLA	MG-NB	-2.20	2.01	2.05
13	b	825	CLA	CHC-C1C	2.20	1.43	1.38
13	a	828	CLA	CHC-C1C	2.20	1.43	1.38
13	f	204	CLA	CHC-C1C	2.19	1.43	1.38
13	b	823	CLA	CHC-C1C	2.19	1.43	1.38
13	b	807	CLA	CHC-C1C	2.19	1.43	1.38
13	b	820	CLA	CHC-C1C	2.19	1.43	1.38
13	a	819	CLA	MG-NB	-2.19	2.01	2.05
13	j	103	CLA	CHC-C1C	2.18	1.43	1.38
13	a	838	CLA	CHC-C1C	2.18	1.43	1.38
13	f	201	CLA	CHC-C1C	2.18	1.43	1.38
13	b	835	CLA	CHC-C1C	2.18	1.42	1.38
13	b	801	CLA	CHC-C1C	2.18	1.42	1.38
13	l	1501	CLA	CHC-C1C	2.18	1.42	1.38
13	a	835	CLA	CHC-C1C	2.17	1.42	1.38
13	a	807	CLA	CHC-C1C	2.17	1.42	1.38
13	b	815	CLA	CHC-C1C	2.17	1.42	1.38
13	a	837	CLA	MG-NB	-2.17	2.01	2.05
13	a	827	CLA	CMC-C2C	-2.17	1.46	1.50
13	a	818	CLA	CHC-C1C	2.17	1.42	1.38
13	k	4002	CLA	CHC-C1C	2.17	1.42	1.38
13	a	822	CLA	CHC-C1C	2.17	1.42	1.38
13	a	813	CLA	CHC-C1C	2.17	1.42	1.38
13	a	841	CLA	CHC-C1C	2.17	1.42	1.38
13	a	842	CLA	CHC-C1C	2.17	1.42	1.38
13	a	809	CLA	CHC-C1C	2.17	1.42	1.38
13	b	842	CLA	CHC-C1C	2.17	1.42	1.38
13	a	827	CLA	CHC-C1C	2.17	1.42	1.38
13	a	832	CLA	MG-NB	-2.17	2.01	2.05
13	b	819	CLA	MG-NB	-2.16	2.01	2.05
13	b	837	CLA	CHC-C1C	2.16	1.42	1.38
13	b	803	CLA	CHC-C1C	2.16	1.42	1.38
13	a	821	CLA	CHC-C1C	2.16	1.42	1.38
13	b	827	CLA	CHC-C1C	2.16	1.42	1.38
13	b	821	CLA	MG-NB	-2.16	2.01	2.05
13	b	822	CLA	CHC-C1C	2.16	1.42	1.38
13	a	811	CLA	CHC-C1C	2.16	1.42	1.38
13	a	812	CLA	CHC-C1C	2.16	1.42	1.38
23	j	102	LMT	O4'-C4B	-2.16	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	817	CLA	CHC-C1C	2.15	1.42	1.38
13	b	817	CLA	CHC-C1C	2.15	1.42	1.38
13	b	839	CLA	CHC-C1C	2.15	1.42	1.38
13	b	830	CLA	CHC-C1C	2.15	1.42	1.38
13	b	834	CLA	CHC-C1C	2.15	1.42	1.38
13	a	830	CLA	CMB-C2B	-2.15	1.46	1.50
13	a	829	CLA	CHC-C1C	2.15	1.42	1.38
13	a	833	CLA	CHC-C1C	2.15	1.42	1.38
13	b	836	CLA	CHC-C1C	2.15	1.42	1.38
13	b	829	CLA	CMD-C2D	-2.14	1.46	1.50
13	b	804	CLA	CHC-C1C	2.14	1.42	1.38
13	a	855	CLA	CHC-C1C	2.14	1.42	1.38
13	a	827	CLA	MG-NB	-2.14	2.01	2.05
13	b	825	CLA	MG-NB	-2.14	2.01	2.05
16	f	206	LHG	O7-C5	-2.14	1.41	1.46
13	l	1503	CLA	CHC-C1C	2.14	1.42	1.38
13	a	803	CLA	CHC-C1C	2.14	1.42	1.38
13	b	828	CLA	CHC-C1C	2.14	1.42	1.38
13	b	837	CLA	MG-NB	-2.14	2.01	2.05
13	b	824	CLA	CMD-C2D	-2.14	1.46	1.50
13	b	816	CLA	CHC-C1C	2.14	1.42	1.38
13	b	816	CLA	CMB-C2B	-2.13	1.46	1.50
13	b	829	CLA	MG-NB	-2.13	2.01	2.05
13	a	830	CLA	MG-NB	-2.13	2.01	2.05
13	a	805	CLA	CHC-C1C	2.13	1.42	1.38
13	b	827	CLA	MG-NB	-2.13	2.01	2.05
13	a	820	CLA	CHC-C1C	2.13	1.42	1.38
13	k	4003	CLA	CHC-C1C	2.13	1.42	1.38
13	b	812	CLA	CHC-C1C	2.13	1.42	1.38
13	a	819	CLA	CHC-C1C	2.13	1.42	1.38
13	a	831	CLA	CMD-C2D	-2.13	1.46	1.50
13	a	834	CLA	CHC-C1C	2.13	1.42	1.38
13	b	811	CLA	CHC-C1C	2.13	1.42	1.38
13	b	829	CLA	CHC-C1C	2.13	1.42	1.38
13	b	827	CLA	CMC-C2C	-2.13	1.46	1.50
13	a	824	CLA	CHC-C1C	2.12	1.42	1.38
13	b	831	CLA	CHC-C1C	2.12	1.42	1.38
20	m	101	ECH	C19-C18	-2.12	1.41	1.45
13	a	838	CLA	MG-NB	-2.12	2.01	2.05
13	b	841	CLA	MG-NB	-2.12	2.01	2.05
13	a	841	CLA	MG-NB	-2.12	2.01	2.05
13	b	809	CLA	MG-NB	-2.12	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	856	45D	C07-C15	2.12	1.38	1.35
13	b	830	CLA	CMB-C2B	-2.12	1.46	1.50
13	a	802	CLA	CMC-C2C	-2.12	1.46	1.50
13	f	203	CLA	CHC-C1C	2.12	1.42	1.38
13	b	809	CLA	CMD-C2D	-2.11	1.46	1.50
13	a	815	CLA	CHC-C1C	2.11	1.42	1.38
13	a	812	CLA	CMB-C2B	-2.11	1.46	1.50
13	a	805	CLA	CMD-C2D	-2.11	1.46	1.50
13	a	816	CLA	CHC-C1C	2.10	1.42	1.38
13	a	813	CLA	MG-NB	-2.10	2.01	2.05
13	b	838	CLA	CHC-C1C	2.10	1.42	1.38
13	a	821	CLA	MG-NB	-2.10	2.01	2.05
13	b	832	CLA	MG-NB	-2.10	2.01	2.05
13	a	807	CLA	MG-NB	-2.10	2.01	2.05
13	l	1503	CLA	MG-NB	-2.10	2.01	2.05
13	a	833	CLA	MG-NB	-2.10	2.01	2.05
13	b	838	CLA	MG-NB	-2.10	2.01	2.05
13	a	840	CLA	CHC-C1C	2.10	1.42	1.38
13	b	819	CLA	CHC-C1C	2.10	1.42	1.38
13	a	834	CLA	MG-NB	-2.10	2.01	2.05
13	a	814	CLA	MG-NB	-2.10	2.01	2.05
13	b	815	CLA	CMD-C2D	-2.10	1.46	1.50
12	a	801	CL0	CHC-C1C	2.09	1.42	1.38
13	b	813	CLA	CMB-C2B	-2.09	1.46	1.50
13	b	809	CLA	CMC-C2C	-2.09	1.46	1.50
13	a	809	CLA	MG-NB	-2.09	2.01	2.05
13	a	820	CLA	MG-NB	-2.09	2.01	2.05
13	b	810	CLA	MG-NB	-2.09	2.01	2.05
13	a	812	CLA	MG-NB	-2.09	2.01	2.05
13	a	826	CLA	CMD-C2D	-2.09	1.46	1.50
13	b	810	CLA	CMD-C2D	-2.08	1.46	1.50
13	b	810	CLA	CHC-C1C	2.08	1.42	1.38
13	a	830	CLA	CHC-C1C	2.08	1.42	1.38
13	b	817	CLA	MG-NB	-2.08	2.01	2.05
13	b	813	CLA	CHC-C1C	2.08	1.42	1.38
13	b	836	CLA	MG-NB	-2.08	2.01	2.05
13	b	824	CLA	MG-NB	-2.08	2.01	2.05
13	a	831	CLA	CHC-C1C	2.08	1.42	1.38
13	b	820	CLA	MG-NB	-2.08	2.01	2.05
13	a	817	CLA	MG-NB	-2.08	2.01	2.05
13	b	839	CLA	MG-NB	-2.08	2.01	2.05
13	k	4004	CLA	CHC-C1C	2.08	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	a	851	LHG	O7-C5	-2.08	1.41	1.46
17	b	852	LMG	O7-C8	-2.08	1.41	1.46
13	a	836	CLA	CHC-C1C	2.08	1.42	1.38
13	b	809	CLA	CHC-C1C	2.08	1.42	1.38
13	b	830	CLA	MG-NB	-2.08	2.01	2.05
13	b	836	CLA	CMB-C2B	-2.07	1.46	1.50
13	b	803	CLA	CMD-C2D	-2.07	1.46	1.50
13	a	824	CLA	MG-NB	-2.07	2.01	2.05
13	a	833	CLA	CMB-C2B	-2.07	1.46	1.50
13	b	822	CLA	MG-NB	-2.07	2.01	2.05
13	a	819	CLA	CMB-C2B	-2.07	1.46	1.50
13	b	842	CLA	MG-NB	-2.07	2.01	2.05
13	f	201	CLA	MG-NB	-2.07	2.01	2.05
13	b	815	CLA	MG-NB	-2.07	2.01	2.05
13	a	803	CLA	MG-NB	-2.07	2.01	2.05
13	l	1502	CLA	MG-NB	-2.07	2.01	2.05
13	a	830	CLA	CMD-C2D	-2.07	1.46	1.50
13	b	813	CLA	MG-NB	-2.07	2.01	2.05
13	a	823	CLA	CHC-C1C	2.07	1.42	1.38
13	l	1502	CLA	CHC-C1C	2.07	1.42	1.38
13	b	806	CLA	MG-NB	-2.07	2.01	2.05
13	a	821	CLA	CMB-C2B	-2.07	1.46	1.50
13	a	840	CLA	MG-NB	-2.07	2.01	2.05
13	b	818	CLA	MG-NB	-2.07	2.01	2.05
13	a	837	CLA	CMD-C2D	-2.07	1.46	1.50
13	f	201	CLA	CMD-C2D	-2.07	1.46	1.50
13	a	818	CLA	MG-NB	-2.06	2.01	2.05
13	a	804	CLA	MG-NB	-2.06	2.01	2.05
13	f	203	CLA	MG-NB	-2.06	2.01	2.05
13	a	835	CLA	CMB-C2B	-2.06	1.46	1.50
13	b	818	CLA	CMB-C2B	-2.06	1.46	1.50
13	a	829	CLA	CMD-C2D	-2.06	1.46	1.50
13	b	814	CLA	MG-NB	-2.06	2.01	2.05
13	b	834	CLA	MG-NB	-2.06	2.01	2.05
13	a	813	CLA	CMC-C2C	-2.06	1.46	1.50
13	b	808	CLA	MG-NB	-2.06	2.01	2.05
13	a	825	CLA	MG-NB	-2.06	2.01	2.05
13	b	841	CLA	CMD-C2D	-2.06	1.46	1.50
13	b	816	CLA	CMD-C2D	-2.06	1.46	1.50
13	a	854	CLA	CHC-C1C	2.06	1.42	1.38
13	a	841	CLA	CMB-C2B	-2.05	1.46	1.50
13	a	836	CLA	MG-NB	-2.05	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	806	CLA	CMD-C2D	-2.05	1.46	1.50
13	k	4003	CLA	MG-NB	-2.05	2.01	2.05
13	b	814	CLA	CMD-C2D	-2.05	1.46	1.50
13	b	810	CLA	CMB-C2B	-2.05	1.46	1.50
13	a	839	CLA	CMD-C2D	-2.05	1.46	1.50
13	a	855	CLA	CMB-C2B	-2.05	1.46	1.50
13	a	829	CLA	MG-NB	-2.05	2.01	2.05
13	a	825	CLA	CHC-C1C	2.05	1.42	1.38
13	a	822	CLA	MG-NB	-2.05	2.01	2.05
13	b	835	CLA	MG-NB	-2.05	2.01	2.05
13	a	823	CLA	CMD-C2D	-2.04	1.46	1.50
13	b	809	CLA	CMB-C2B	-2.04	1.46	1.50
13	b	838	CLA	CMD-C2D	-2.04	1.46	1.50
13	a	807	CLA	CMD-C2D	-2.04	1.46	1.50
13	a	824	CLA	CMD-C2D	-2.04	1.46	1.50
12	a	801	CL0	CMD-C2D	-2.04	1.46	1.50
13	a	833	CLA	CMD-C2D	-2.04	1.46	1.50
13	b	803	CLA	MG-NB	-2.04	2.01	2.05
13	b	813	CLA	CMD-C2D	-2.04	1.46	1.50
13	a	821	CLA	CMD-C2D	-2.04	1.46	1.50
13	a	841	CLA	CMD-C2D	-2.04	1.46	1.50
13	b	816	CLA	MG-NB	-2.04	2.01	2.05
13	a	811	CLA	CMD-C2D	-2.04	1.46	1.50
13	k	4003	CLA	CMD-C2D	-2.04	1.46	1.50
13	b	826	CLA	MG-NB	-2.04	2.01	2.05
13	a	831	CLA	MG-NB	-2.03	2.01	2.05
13	a	831	CLA	CMB-C2B	-2.03	1.46	1.50
13	b	808	CLA	CHC-C1C	2.03	1.42	1.38
13	b	812	CLA	CMD-C2D	-2.03	1.46	1.50
13	b	832	CLA	CMD-C2D	-2.03	1.46	1.50
13	a	818	CLA	CMD-C2D	-2.03	1.46	1.50
13	b	820	CLA	CMB-C2B	-2.03	1.46	1.50
13	a	818	CLA	CMB-C2B	-2.03	1.46	1.50
13	a	839	CLA	MG-NB	-2.03	2.01	2.05
13	b	805	CLA	MG-NB	-2.03	2.01	2.05
12	a	801	CL0	CMB-C2B	-2.03	1.46	1.50
13	a	825	CLA	CMD-C2D	-2.03	1.46	1.50
13	l	1502	CLA	CMB-C2B	-2.03	1.46	1.50
13	a	832	CLA	CMD-C2D	-2.03	1.46	1.50
13	b	840	CLA	MG-NB	-2.03	2.01	2.05
13	b	808	CLA	CMD-C2D	-2.03	1.46	1.50
13	a	836	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	820	CLA	CMD-C2D	-2.03	1.46	1.50
13	b	839	CLA	CMB-C2B	-2.03	1.46	1.50
13	a	854	CLA	MG-NB	-2.03	2.01	2.05
13	a	855	CLA	MG-NB	-2.03	2.01	2.05
13	b	803	CLA	CMB-C2B	-2.03	1.46	1.50
13	l	1502	CLA	CMD-C2D	-2.03	1.46	1.50
13	a	839	CLA	CHC-C1C	2.03	1.42	1.38
13	a	816	CLA	MG-NB	-2.03	2.01	2.05
13	a	802	CLA	CMD-C2D	-2.03	1.46	1.50
13	a	808	CLA	MG-NB	-2.03	2.01	2.05
13	a	803	CLA	CMB-C2B	-2.03	1.46	1.50
13	a	808	CLA	CMD-C2D	-2.03	1.46	1.50
13	b	826	CLA	CMD-C2D	-2.03	1.46	1.50
13	f	201	CLA	CMB-C2B	-2.03	1.46	1.50
13	a	820	CLA	CMD-C2D	-2.02	1.46	1.50
13	b	817	CLA	CMD-C2D	-2.02	1.46	1.50
13	b	840	CLA	CMD-C2D	-2.02	1.46	1.50
13	k	4002	CLA	CMD-C2D	-2.02	1.46	1.50
13	a	815	CLA	MG-NB	-2.02	2.01	2.05
13	j	103	CLA	MG-NB	-2.02	2.01	2.05
13	a	838	CLA	CMD-C2D	-2.02	1.46	1.50
13	b	835	CLA	CMD-C2D	-2.02	1.46	1.50
13	a	803	CLA	CMD-C2D	-2.02	1.46	1.50
13	b	833	CLA	CMD-C2D	-2.02	1.46	1.50
12	a	801	CL0	MG-NB	-2.02	2.01	2.05
13	b	821	CLA	CMB-C2B	-2.02	1.46	1.50
13	b	819	CLA	CMB-C2B	-2.02	1.46	1.50
13	a	835	CLA	CMD-C2D	-2.02	1.46	1.50
13	b	811	CLA	CMD-C2D	-2.02	1.46	1.50
13	a	812	CLA	CMD-C2D	-2.02	1.46	1.50
13	b	818	CLA	CMD-C2D	-2.02	1.46	1.50
13	b	823	CLA	CMD-C2D	-2.02	1.46	1.50
13	a	811	CLA	MG-NB	-2.02	2.01	2.05
13	f	204	CLA	MG-NB	-2.02	2.01	2.05
13	a	819	CLA	CMD-C2D	-2.02	1.46	1.50
13	b	825	CLA	CMD-C2D	-2.02	1.46	1.50
13	a	813	CLA	CMD-C2D	-2.02	1.46	1.50
13	b	801	CLA	MG-NB	-2.02	2.01	2.05
13	a	828	CLA	CMD-C2D	-2.02	1.46	1.50
13	a	834	CLA	CMB-C2B	-2.02	1.46	1.50
13	a	834	CLA	CMD-C2D	-2.02	1.46	1.50
13	b	812	CLA	MG-NB	-2.02	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	k	4003	CLA	CMB-C2B	-2.02	1.46	1.50
13	a	842	CLA	MG-NB	-2.02	2.01	2.05
13	k	4004	CLA	MG-NB	-2.02	2.01	2.05
13	a	823	CLA	CMB-C2B	-2.02	1.46	1.50
13	l	1501	CLA	MG-NB	-2.02	2.01	2.05
13	a	810	CLA	CMD-C2D	-2.01	1.46	1.50
13	b	807	CLA	MG-NB	-2.01	2.01	2.05
13	a	805	CLA	CMC-C2C	-2.01	1.46	1.50
13	l	1503	CLA	CMD-C2D	-2.01	1.46	1.50
13	a	816	CLA	CMB-C2B	-2.01	1.46	1.50
13	b	840	CLA	CMB-C2B	-2.01	1.46	1.50
13	b	833	CLA	MG-NB	-2.01	2.01	2.05
13	b	837	CLA	CMD-C2D	-2.01	1.46	1.50
13	a	802	CLA	CMB-C2B	-2.01	1.46	1.50
13	a	854	CLA	CMD-C2D	-2.01	1.46	1.50
13	a	806	CLA	MG-NB	-2.01	2.01	2.05
13	a	823	CLA	MG-NB	-2.01	2.01	2.05
13	j	104	CLA	CMD-C2D	-2.01	1.46	1.50
13	k	4002	CLA	MG-NB	-2.01	2.01	2.05
13	a	815	CLA	CMD-C2D	-2.01	1.46	1.50
13	b	827	CLA	CMD-C2D	-2.01	1.46	1.50
13	j	104	CLA	MG-NB	-2.00	2.01	2.05
13	a	827	CLA	CMD-C2D	-2.00	1.46	1.50
13	b	828	CLA	CMC-C2C	-2.00	1.46	1.50
13	a	818	CLA	CMC-C2C	-2.00	1.46	1.50
13	b	819	CLA	CMD-C2D	-2.00	1.46	1.50
13	a	803	CLA	CMC-C2C	-2.00	1.46	1.50
13	a	810	CLA	CMC-C2C	-2.00	1.46	1.50
13	l	1502	CLA	CMC-C2C	-2.00	1.46	1.50
13	b	834	CLA	CMB-C2B	-2.00	1.46	1.50

All (806) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	b	846	ECH	C15-C16-C17	8.45	140.79	123.47
13	a	840	CLA	C4A-NA-C1A	7.33	110.00	106.71
13	a	805	CLA	C4A-NA-C1A	7.31	109.99	106.71
13	l	1502	CLA	C4A-NA-C1A	7.28	109.98	106.71
13	b	806	CLA	C4A-NA-C1A	7.06	109.88	106.71
13	b	838	CLA	C4A-NA-C1A	7.03	109.87	106.71
13	a	823	CLA	C4A-NA-C1A	6.99	109.85	106.71
13	b	830	CLA	C4A-NA-C1A	6.99	109.85	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	839	CLA	C4A-NA-C1A	6.99	109.85	106.71
13	a	809	CLA	C4A-NA-C1A	6.98	109.85	106.71
13	a	825	CLA	C4A-NA-C1A	6.98	109.84	106.71
13	a	837	CLA	C4A-NA-C1A	6.96	109.84	106.71
13	a	817	CLA	C4A-NA-C1A	6.94	109.83	106.71
13	b	822	CLA	C4A-NA-C1A	6.91	109.81	106.71
13	a	807	CLA	C4A-NA-C1A	6.88	109.80	106.71
13	k	4004	CLA	C4A-NA-C1A	6.88	109.80	106.71
13	b	841	CLA	C4A-NA-C1A	6.87	109.80	106.71
13	a	816	CLA	C4A-NA-C1A	6.87	109.80	106.71
13	b	840	CLA	C4A-NA-C1A	6.87	109.80	106.71
13	b	828	CLA	C4A-NA-C1A	6.86	109.79	106.71
13	a	818	CLA	C4A-NA-C1A	6.84	109.78	106.71
13	a	855	CLA	C4A-NA-C1A	6.84	109.78	106.71
13	a	815	CLA	C4A-NA-C1A	6.83	109.78	106.71
13	b	808	CLA	C4A-NA-C1A	6.82	109.77	106.71
13	b	823	CLA	C4A-NA-C1A	6.82	109.77	106.71
13	l	1503	CLA	C4A-NA-C1A	6.82	109.77	106.71
13	b	842	CLA	C4A-NA-C1A	6.80	109.76	106.71
13	f	201	CLA	C4A-NA-C1A	6.78	109.76	106.71
13	b	817	CLA	C4A-NA-C1A	6.78	109.75	106.71
13	a	834	CLA	C4A-NA-C1A	6.78	109.75	106.71
13	a	841	CLA	C4A-NA-C1A	6.78	109.75	106.71
13	b	812	CLA	C4A-NA-C1A	6.78	109.75	106.71
13	a	820	CLA	C4A-NA-C1A	6.76	109.75	106.71
13	a	835	CLA	C4A-NA-C1A	6.74	109.73	106.71
13	a	806	CLA	C4A-NA-C1A	6.70	109.72	106.71
13	a	824	CLA	C4A-NA-C1A	6.70	109.72	106.71
13	b	835	CLA	C4A-NA-C1A	6.70	109.72	106.71
13	a	828	CLA	C4A-NA-C1A	6.69	109.71	106.71
13	a	822	CLA	C4A-NA-C1A	6.68	109.71	106.71
13	a	813	CLA	C4A-NA-C1A	6.67	109.70	106.71
13	b	809	CLA	C4A-NA-C1A	6.67	109.70	106.71
13	l	1501	CLA	C4A-NA-C1A	6.67	109.70	106.71
13	a	827	CLA	C4A-NA-C1A	6.67	109.70	106.71
13	a	838	CLA	C4A-NA-C1A	6.66	109.70	106.71
13	b	839	CLA	C4A-NA-C1A	6.65	109.70	106.71
13	b	810	CLA	C4A-NA-C1A	6.64	109.69	106.71
13	b	813	CLA	C4A-NA-C1A	6.63	109.69	106.71
13	b	834	CLA	C4A-NA-C1A	6.62	109.68	106.71
13	f	204	CLA	C4A-NA-C1A	6.62	109.68	106.71
13	a	814	CLA	C4A-NA-C1A	6.62	109.68	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	b	805	CLA	C4A-NA-C1A	6.60	109.67	106.71
13	a	836	CLA	C4A-NA-C1A	6.59	109.67	106.71
13	a	832	CLA	C4A-NA-C1A	6.58	109.67	106.71
13	b	825	CLA	C4A-NA-C1A	6.58	109.66	106.71
13	a	831	CLA	C4A-NA-C1A	6.56	109.65	106.71
13	k	4002	CLA	C4A-NA-C1A	6.54	109.65	106.71
13	b	836	CLA	C4A-NA-C1A	6.54	109.65	106.71
13	b	814	CLA	C4A-NA-C1A	6.53	109.64	106.71
13	a	808	CLA	C4A-NA-C1A	6.51	109.63	106.71
13	a	803	CLA	C4A-NA-C1A	6.51	109.63	106.71
12	a	801	CL0	C4A-NA-C1A	6.51	109.63	106.71
13	b	811	CLA	C4A-NA-C1A	6.50	109.63	106.71
13	b	824	CLA	C4A-NA-C1A	6.48	109.62	106.71
13	b	807	CLA	C4A-NA-C1A	6.48	109.62	106.71
13	j	103	CLA	C4A-NA-C1A	6.47	109.61	106.71
13	a	811	CLA	C4A-NA-C1A	6.45	109.60	106.71
13	k	4003	CLA	C4A-NA-C1A	6.45	109.60	106.71
13	b	815	CLA	C4A-NA-C1A	6.44	109.60	106.71
13	b	820	CLA	C4A-NA-C1A	6.44	109.60	106.71
13	a	829	CLA	C4A-NA-C1A	6.43	109.60	106.71
13	a	842	CLA	C4A-NA-C1A	6.42	109.59	106.71
13	b	833	CLA	C4A-NA-C1A	6.42	109.59	106.71
13	a	826	CLA	C4A-NA-C1A	6.41	109.59	106.71
13	b	826	CLA	C4A-NA-C1A	6.41	109.59	106.71
13	b	837	CLA	C4A-NA-C1A	6.39	109.58	106.71
13	a	802	CLA	C4A-NA-C1A	6.39	109.58	106.71
13	a	812	CLA	C4A-NA-C1A	6.39	109.58	106.71
13	b	818	CLA	C4A-NA-C1A	6.39	109.58	106.71
13	a	830	CLA	C4A-NA-C1A	6.38	109.57	106.71
13	a	821	CLA	C4A-NA-C1A	6.35	109.56	106.71
13	b	821	CLA	C4A-NA-C1A	6.35	109.56	106.71
13	b	827	CLA	C4A-NA-C1A	6.34	109.56	106.71
13	b	831	CLA	C4A-NA-C1A	6.33	109.55	106.71
13	b	819	CLA	C4A-NA-C1A	6.32	109.55	106.71
13	a	804	CLA	C4A-NA-C1A	6.32	109.55	106.71
13	b	816	CLA	C4A-NA-C1A	6.31	109.54	106.71
13	b	832	CLA	C4A-NA-C1A	6.21	109.50	106.71
13	f	203	CLA	C4A-NA-C1A	6.21	109.50	106.71
13	b	801	CLA	C4A-NA-C1A	6.17	109.48	106.71
13	a	833	CLA	C4A-NA-C1A	6.16	109.47	106.71
13	j	104	CLA	C4A-NA-C1A	6.10	109.45	106.71
13	b	829	CLA	C4A-NA-C1A	6.05	109.42	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	810	CLA	C4A-NA-C1A	5.99	109.40	106.71
13	a	854	CLA	C4A-NA-C1A	5.84	109.33	106.71
13	a	819	CLA	C4A-NA-C1A	5.76	109.30	106.71
13	b	803	CLA	C4A-NA-C1A	5.49	109.17	106.71
13	b	804	CLA	C4A-NA-C1A	5.43	109.15	106.71
18	a	856	45D	C42-C41-C37	5.15	134.03	123.47
20	b	846	ECH	C12-C13-C14	5.02	126.65	118.94
20	m	101	ECH	C15-C16-C17	4.79	133.30	123.47
20	b	846	ECH	C19-C18-C17	4.71	126.17	118.94
22	f	205	ZEX	C35-C15-C14	4.48	132.64	123.47
20	b	846	ECH	C35-C13-C14	-4.44	116.70	122.92
20	b	846	ECH	C36-C18-C17	-4.28	116.93	122.92
20	m	101	ECH	C37-C22-C21	-4.26	116.96	122.92
16	a	851	LHG	O4-P-O5	4.23	133.17	112.24
16	a	849	LHG	O4-P-O5	4.23	133.14	112.24
16	f	206	LHG	O4-P-O5	4.21	133.04	112.24
16	b	851	LHG	O4-P-O5	4.20	133.01	112.24
16	a	853	LHG	O4-P-O5	4.20	132.98	112.24
22	f	205	ZEX	C19-C9-C10	-4.19	117.05	122.92
22	f	205	ZEX	C39-C29-C30	-4.13	117.13	122.92
20	b	846	ECH	C24-C23-C22	-4.12	120.01	126.23
20	b	846	ECH	C1-C6-C5	-4.12	116.82	122.61
18	a	856	45D	C28-C26-C30	-4.10	117.18	122.92
22	b	854	ZEX	C19-C9-C10	-4.07	117.22	122.92
22	b	854	ZEX	C39-C29-C30	-4.07	117.23	122.92
20	m	101	ECH	C34-C9-C10	-4.06	117.23	122.92
18	a	856	45D	C27-C25-C29	-4.02	117.29	122.92
21	b	853	EQ3	C34-C9-C10	-3.86	117.52	122.92
21	b	853	EQ3	C37-C22-C21	-3.83	117.56	122.92
20	m	101	ECH	C23-C22-C21	3.82	124.80	118.94
20	m	101	ECH	C36-C18-C17	-3.79	117.61	122.92
20	b	846	ECH	C34-C9-C10	-3.75	117.67	122.92
20	m	101	ECH	C19-C18-C17	3.73	124.66	118.94
20	m	101	ECH	C1-C6-C5	-3.68	117.42	122.61
20	b	846	ECH	C10-C11-C12	3.67	134.68	123.22
20	b	846	ECH	C37-C22-C21	-3.63	117.84	122.92
22	b	854	ZEX	C35-C15-C14	3.60	130.84	123.47
13	a	830	CLA	O2D-CGD-O1D	-3.56	116.89	123.84
20	b	846	ECH	C15-C14-C13	3.48	132.28	127.31
13	b	814	CLA	O2D-CGD-O1D	-3.45	117.10	123.84
13	a	830	CLA	CAA-C2A-C3A	-3.41	103.44	112.78
21	b	853	EQ3	C15-C16-C17	3.41	130.46	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	813	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
22	f	205	ZEX	C40-C33-C34	-3.32	118.28	122.92
13	b	830	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
21	b	853	EQ3	C35-C13-C14	-3.30	118.30	122.92
13	k	4004	CLA	CAC-C3C-C4C	3.29	129.07	124.81
15	b	847	BCR	C15-C16-C17	-3.28	116.75	123.47
20	m	101	ECH	C35-C13-C14	-3.28	118.33	122.92
13	a	814	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
22	b	854	ZEX	C20-C13-C14	-3.22	118.42	122.92
22	b	854	ZEX	C27-C26-C25	-3.21	117.65	122.84
13	b	837	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
13	a	831	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
21	b	853	EQ3	C16-C15-C14	3.19	130.01	123.47
13	a	834	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
13	a	823	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
13	a	825	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
21	b	853	EQ3	C36-C18-C17	-3.17	118.48	122.92
22	b	854	ZEX	C15-C35-C34	3.17	129.97	123.47
22	b	854	ZEX	C40-C33-C34	-3.16	118.49	122.92
22	f	205	ZEX	C20-C13-C14	-3.11	118.57	122.92
13	b	834	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
13	k	4002	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
13	a	818	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
20	b	846	ECH	C30-C25-C24	3.06	124.43	115.78
13	a	807	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
13	a	804	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
13	a	837	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
13	b	805	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
13	a	802	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
13	b	804	CLA	CAC-C3C-C4C	3.00	128.71	124.81
22	f	205	ZEX	C15-C35-C34	3.00	129.62	123.47
13	a	808	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
13	b	808	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
18	a	856	45D	C40-C36-C38	-2.99	118.73	122.92
12	a	801	CL0	O2D-CGD-O1D	-2.99	117.99	123.84
13	b	803	CLA	CAA-CBA-CGA	-2.99	104.52	113.25
13	b	825	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
13	b	817	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
13	b	811	CLA	C3B-C4B-NB	-2.98	107.75	110.52
13	a	803	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
13	b	830	CLA	CHB-C4A-NA	2.98	128.63	124.51
13	a	838	CLA	C3B-C4B-NB	-2.96	107.77	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a	846	BCR	C15-C16-C17	-2.95	117.43	123.47
20	m	101	ECH	C16-C15-C14	2.94	129.50	123.47
13	b	818	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
13	b	840	CLA	C3B-C4B-NB	-2.94	107.79	110.52
13	b	838	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
22	f	205	ZEX	C32-C33-C34	2.93	123.44	118.94
13	a	838	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
13	b	833	CLA	C3B-C4B-NB	-2.93	107.80	110.52
18	a	856	45D	C39-C35-C37	-2.92	118.83	122.92
13	b	809	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
13	a	823	CLA	CHB-C4A-NA	2.92	128.54	124.51
13	a	839	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
20	m	101	ECH	C12-C13-C14	2.91	123.41	118.94
13	f	204	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
13	k	4004	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
13	a	832	CLA	C3B-C4B-NB	-2.91	107.82	110.52
13	a	819	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
13	b	804	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
15	j	101	BCR	C15-C16-C17	-2.90	117.53	123.47
13	b	813	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
13	a	824	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
13	a	812	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
13	b	815	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
13	b	822	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
13	a	833	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
13	b	816	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
13	b	805	CLA	C3B-C4B-NB	-2.89	107.83	110.52
13	a	828	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
13	a	805	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
13	a	836	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
13	a	817	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
13	b	816	CLA	C3B-C4B-NB	-2.88	107.84	110.52
13	a	827	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
13	a	820	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
13	a	803	CLA	C3B-C4B-NB	-2.87	107.85	110.52
15	b	844	BCR	C33-C5-C6	-2.87	121.31	124.53
13	b	841	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
13	b	823	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
13	f	203	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
13	a	830	CLA	CHB-C4A-NA	2.86	128.47	124.51
15	a	847	BCR	C33-C5-C6	-2.86	121.32	124.53
13	b	821	CLA	O2D-CGD-O1D	-2.86	118.25	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	826	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
13	b	821	CLA	C3B-C4B-NB	-2.86	107.87	110.52
13	a	842	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
21	b	853	EQ3	C12-C13-C14	2.85	123.32	118.94
13	b	839	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
13	b	829	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
13	l	1501	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
15	a	846	BCR	C15-C14-C13	-2.85	123.24	127.31
13	l	1502	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
13	b	811	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
13	b	819	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
13	b	806	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
13	b	809	CLA	C3B-C4B-NB	-2.83	107.89	110.52
13	a	840	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
13	k	4003	CLA	C3B-C4B-NB	-2.83	107.89	110.52
13	b	801	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
13	b	840	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
13	b	828	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
13	b	824	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
13	b	826	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
13	a	854	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
13	a	804	CLA	C3B-C4B-NB	-2.81	107.90	110.52
13	a	835	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
13	b	842	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
13	a	827	CLA	C3B-C4B-NB	-2.81	107.91	110.52
13	a	830	CLA	O2D-CGD-CBD	2.81	116.27	111.27
13	l	1503	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
13	a	832	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
13	b	813	CLA	C3B-C4B-NB	-2.81	107.91	110.52
13	f	201	CLA	C3B-C4B-NB	-2.81	107.91	110.52
13	k	4003	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
13	b	814	CLA	O2D-CGD-CBD	2.81	116.26	111.27
23	j	102	LMT	C1'-O5'-C5'	-2.81	108.18	113.69
13	a	811	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
13	b	827	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
15	b	844	BCR	C15-C16-C17	-2.80	117.73	123.47
13	a	810	CLA	CAA-C2A-C3A	-2.80	105.11	112.78
13	b	804	CLA	C3B-C4B-NB	-2.80	107.92	110.52
13	f	204	CLA	C3B-C4B-NB	-2.80	107.92	110.52
15	b	847	BCR	C15-C14-C13	-2.80	123.32	127.31
13	b	818	CLA	C3B-C4B-NB	-2.80	107.92	110.52
13	b	833	CLA	O2D-CGD-O1D	-2.80	118.37	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	816	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
13	a	841	CLA	C3B-C4B-NB	-2.79	107.93	110.52
13	b	812	CLA	CHB-C4A-NA	2.78	128.36	124.51
13	a	809	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
13	b	831	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
13	b	836	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
13	b	820	CLA	C3B-C4B-NB	-2.77	107.94	110.52
13	f	201	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
22	b	854	ZEX	C12-C13-C14	2.77	123.19	118.94
13	a	841	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
13	a	815	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
13	j	104	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
13	b	812	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
17	b	850	LMG	O6-C1-O1	-2.76	103.43	109.97
20	b	846	ECH	C37-C22-C23	2.75	122.42	118.08
13	a	835	CLA	C3B-C4B-NB	-2.75	107.96	110.52
13	a	810	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
13	a	855	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
13	a	834	CLA	CHB-C4A-NA	2.75	128.31	124.51
13	a	826	CLA	C3B-C4B-NB	-2.75	107.97	110.52
13	b	824	CLA	C3B-C4B-NB	-2.74	107.97	110.52
13	a	822	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
13	b	818	CLA	CHB-C4A-NA	2.73	128.29	124.51
13	b	810	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
22	f	205	ZEX	C27-C26-C25	-2.73	118.44	122.84
13	a	835	CLA	CHB-C4A-NA	2.72	128.28	124.51
13	b	814	CLA	C3B-C4B-NB	-2.72	107.99	110.52
13	a	806	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
13	b	803	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
13	b	832	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
13	b	835	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
15	k	4001	BCR	C15-C14-C13	-2.71	123.44	127.31
13	a	805	CLA	CHB-C4A-NA	2.70	128.25	124.51
13	a	806	CLA	C3B-C4B-NB	-2.70	108.01	110.52
16	a	851	LHG	O8-C23-C24	2.70	120.38	111.91
13	j	103	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
13	a	810	CLA	CHB-C4A-NA	2.69	128.23	124.51
13	b	830	CLA	CAA-C2A-C3A	-2.69	105.41	112.78
13	b	806	CLA	CHB-C4A-NA	2.69	128.23	124.51
15	j	105	BCR	C33-C5-C6	-2.69	121.51	124.53
15	b	844	BCR	C24-C23-C22	-2.68	122.19	126.23
18	a	856	45D	C03-C07-C19	2.68	123.35	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	801	CL0	C3B-C4B-NB	-2.67	108.03	110.52
13	b	823	CLA	C3B-C4B-NB	-2.67	108.04	110.52
13	b	820	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
13	a	813	CLA	CHB-C4A-NA	2.67	128.20	124.51
15	k	4005	BCR	C15-C16-C17	-2.66	118.02	123.47
13	a	809	CLA	CHB-C4A-NA	2.66	128.19	124.51
15	b	845	BCR	C33-C5-C6	-2.65	121.55	124.53
13	a	829	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
13	a	825	CLA	CHB-C4A-NA	2.65	128.18	124.51
13	a	802	CLA	C3B-C4B-NB	-2.65	108.05	110.52
22	f	205	ZEX	C28-C29-C30	2.65	123.00	118.94
13	a	812	CLA	C3B-C4B-NB	-2.65	108.06	110.52
13	j	104	CLA	C3B-C4B-NB	-2.65	108.06	110.52
15	j	101	BCR	C15-C14-C13	-2.64	123.54	127.31
15	j	105	BCR	C15-C16-C17	-2.64	118.06	123.47
13	a	820	CLA	CHB-C4A-NA	2.64	128.16	124.51
17	a	850	LMG	O6-C1-O1	-2.64	103.72	109.97
13	l	1501	CLA	C1-C2-C3	-2.64	122.49	126.75
13	b	825	CLA	CHB-C4A-NA	2.63	128.16	124.51
13	b	803	CLA	C3B-C4B-NB	-2.63	108.07	110.52
22	f	205	ZEX	C12-C13-C14	2.63	122.98	118.94
13	b	842	CLA	C3B-C4B-NB	-2.63	108.07	110.52
13	b	825	CLA	C3B-C4B-NB	-2.63	108.08	110.52
13	a	818	CLA	C3B-C4B-NB	-2.63	108.08	110.52
13	b	833	CLA	CHB-C4A-NA	2.62	128.14	124.51
13	a	837	CLA	CHB-C4A-NA	2.62	128.14	124.51
15	a	848	BCR	C15-C16-C17	-2.62	118.11	123.47
16	a	853	LHG	O8-C23-C24	2.62	120.12	111.91
22	b	854	ZEX	C32-C33-C34	2.62	122.96	118.94
13	b	816	CLA	CHB-C4A-NA	2.61	128.12	124.51
13	a	821	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
13	j	103	CLA	C3B-C4B-NB	-2.61	108.09	110.52
13	l	1502	CLA	CHB-C4A-NA	2.60	128.11	124.51
13	b	837	CLA	C3B-C4B-NB	-2.60	108.10	110.52
13	a	824	CLA	CHB-C4A-NA	2.60	128.11	124.51
13	l	1503	CLA	CHB-C4A-NA	2.60	128.11	124.51
16	f	206	LHG	O8-C23-C24	2.60	120.07	111.91
13	b	822	CLA	C3B-C4B-NB	-2.60	108.10	110.52
13	a	818	CLA	CHB-C4A-NA	2.60	128.10	124.51
13	a	830	CLA	C3B-C4B-NB	-2.60	108.11	110.52
13	b	837	CLA	CHB-C4A-NA	2.60	128.10	124.51
13	b	834	CLA	C3B-C4B-NB	-2.59	108.11	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	840	CLA	CHB-C4A-NA	2.59	128.10	124.51
13	b	807	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
13	a	839	CLA	CHB-C4A-NA	2.59	128.10	124.51
21	b	853	EQ3	C37-C22-C23	2.59	122.16	118.08
13	f	204	CLA	CHB-C4A-NA	2.59	128.10	124.51
13	k	4003	CLA	CHB-C4A-NA	2.59	128.10	124.51
13	b	835	CLA	C3B-C4B-NB	-2.59	108.11	110.52
13	b	836	CLA	C1-C2-C3	-2.58	122.57	126.75
15	k	4001	BCR	C27-C26-C25	2.58	126.48	122.73
13	b	821	CLA	CHB-C4A-NA	2.58	128.08	124.51
13	b	842	CLA	CHB-C4A-NA	2.58	128.08	124.51
13	a	816	CLA	CHB-C4A-NA	2.58	128.07	124.51
13	b	823	CLA	CHB-C4A-NA	2.58	128.07	124.51
13	b	807	CLA	C3B-C4B-NB	-2.57	108.13	110.52
13	a	820	CLA	C3B-C4B-NB	-2.57	108.13	110.52
13	a	808	CLA	C3B-C4B-NB	-2.57	108.13	110.52
13	k	4004	CLA	CHB-C4A-NA	2.57	128.06	124.51
13	a	821	CLA	C3B-C4B-NB	-2.57	108.14	110.52
13	b	807	CLA	CHB-C4A-NA	2.56	128.06	124.51
13	k	4002	CLA	CHB-C4A-NA	2.56	128.06	124.51
13	a	811	CLA	C3B-C4B-NB	-2.56	108.14	110.52
13	a	817	CLA	C3B-C4B-NB	-2.56	108.14	110.52
13	a	832	CLA	CHB-C4A-NA	2.56	128.05	124.51
13	a	842	CLA	CHB-C4A-NA	2.56	128.05	124.51
21	b	853	EQ3	C19-C18-C17	2.56	122.87	118.94
13	a	817	CLA	CHB-C4A-NA	2.56	128.05	124.51
13	b	814	CLA	CHB-C4A-NA	2.56	128.05	124.51
21	b	853	EQ3	C24-C23-C22	2.56	130.10	126.23
20	m	101	ECH	C21-C20-C19	2.56	131.19	123.22
15	k	4001	BCR	C11-C10-C9	-2.56	123.66	127.31
13	b	806	CLA	C3B-C4B-NB	-2.56	108.14	110.52
13	a	806	CLA	CHB-C4A-NA	2.55	128.04	124.51
16	a	849	LHG	O8-C23-C24	2.55	119.91	111.91
15	b	847	BCR	C2-C1-C6	2.55	114.41	110.48
16	b	851	LHG	O8-C23-C24	2.55	119.91	111.91
15	b	844	BCR	C27-C26-C25	2.55	126.43	122.73
13	a	807	CLA	C3B-C4B-NB	-2.54	108.15	110.52
13	b	835	CLA	CHB-C4A-NA	2.54	128.03	124.51
13	a	807	CLA	CHB-C4A-NA	2.54	128.03	124.51
13	k	4002	CLA	C3B-C4B-NB	-2.54	108.16	110.52
13	a	821	CLA	CHB-C4A-NA	2.54	128.03	124.51
13	b	840	CLA	CHB-C4A-NA	2.54	128.03	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	b	815	CLA	C3B-C4B-NB	-2.54	108.16	110.52
13	b	801	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
13	b	817	CLA	C3B-C4B-NB	-2.54	108.16	110.52
13	b	836	CLA	C3B-C4B-NB	-2.54	108.16	110.52
13	f	201	CLA	CHB-C4A-NA	2.53	128.02	124.51
13	b	810	CLA	C3B-C4B-NB	-2.53	108.16	110.52
13	a	842	CLA	C3B-C4B-NB	-2.53	108.17	110.52
15	b	845	BCR	C15-C16-C17	-2.53	118.29	123.47
13	a	814	CLA	C3B-C4B-NB	-2.52	108.17	110.52
17	a	852	LMG	O6-C1-O1	-2.52	104.00	109.97
13	a	808	CLA	CHB-C4A-NA	2.52	128.00	124.51
13	l	1501	CLA	CHB-C4A-NA	2.52	128.00	124.51
13	a	841	CLA	CHB-C4A-NA	2.52	128.00	124.51
13	b	820	CLA	CHB-C4A-NA	2.52	127.99	124.51
13	a	813	CLA	C3B-C4B-NB	-2.51	108.18	110.52
17	b	850	LMG	O1-C7-C8	-2.51	104.84	110.90
13	b	832	CLA	C3B-C4B-NB	-2.51	108.18	110.52
13	a	815	CLA	CHB-C4A-NA	2.51	127.98	124.51
13	a	827	CLA	CHB-C4A-NA	2.51	127.98	124.51
15	k	4001	BCR	C33-C5-C6	-2.50	121.72	124.53
13	a	840	CLA	C3B-C4B-NB	-2.50	108.19	110.52
22	b	854	ZEX	C39-C29-C28	2.50	122.02	118.08
13	b	815	CLA	CHB-C4A-NA	2.50	127.97	124.51
13	b	831	CLA	C3B-C4B-NB	-2.50	108.20	110.52
15	i	102	BCR	C2-C1-C6	2.50	114.32	110.48
13	a	811	CLA	CHB-C4A-NA	2.49	127.96	124.51
13	a	855	CLA	CHB-C4A-NA	2.49	127.95	124.51
13	a	817	CLA	O2A-CGA-O1A	-2.49	117.32	123.59
15	i	101	BCR	C15-C16-C17	-2.48	118.39	123.47
13	a	822	CLA	CHB-C4A-NA	2.48	127.94	124.51
13	a	855	CLA	C3B-C4B-NB	-2.48	108.22	110.52
15	a	848	BCR	C33-C5-C6	-2.48	121.75	124.53
13	b	805	CLA	CHB-C4A-NA	2.48	127.94	124.51
13	a	831	CLA	O2D-CGD-CBD	2.48	115.67	111.27
13	f	203	CLA	C1-C2-C3	-2.48	122.75	126.75
13	l	1502	CLA	C3B-C4B-NB	-2.48	108.22	110.52
15	j	101	BCR	C33-C5-C6	-2.48	121.75	124.53
13	b	838	CLA	O2A-CGA-O1A	-2.47	117.35	123.59
13	b	840	CLA	C1-C2-C3	-2.47	121.76	126.04
13	a	838	CLA	CHB-C4A-NA	2.47	127.93	124.51
15	j	105	BCR	C27-C26-C25	2.47	126.31	122.73
15	b	844	BCR	C15-C14-C13	-2.46	123.79	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	b	813	CLA	CHB-C4A-NA	2.46	127.92	124.51
15	a	844	BCR	C33-C5-C6	-2.46	121.77	124.53
13	b	828	CLA	CHB-C4A-NA	2.46	127.91	124.51
15	a	848	BCR	C15-C14-C13	-2.46	123.80	127.31
15	k	4005	BCR	C2-C1-C6	2.46	114.26	110.48
13	a	816	CLA	C3B-C4B-NB	-2.46	108.24	110.52
13	b	832	CLA	CHB-C4A-NA	2.46	127.91	124.51
15	a	845	BCR	C33-C5-C6	-2.46	121.77	124.53
13	b	822	CLA	CHB-C4A-NA	2.46	127.91	124.51
15	b	848	BCR	C27-C26-C25	2.45	126.29	122.73
16	a	849	LHG	C11-C10-C9	-2.45	101.99	114.42
16	a	851	LHG	C20-C19-C18	-2.45	102.00	114.42
13	b	813	CLA	C1-C2-C3	-2.45	122.80	126.75
15	a	846	BCR	C33-C5-C6	-2.44	121.78	124.53
13	b	819	CLA	C3B-C4B-NB	-2.44	108.25	110.52
13	b	829	CLA	C3B-C4B-NB	-2.44	108.25	110.52
17	b	852	LMG	C1-O6-C5	-2.44	108.89	113.69
12	a	801	CL0	CAA-CBA-CGA	-2.44	106.12	113.25
15	k	4005	BCR	C15-C14-C13	-2.44	123.83	127.31
15	b	847	BCR	C27-C26-C25	2.44	126.27	122.73
13	b	838	CLA	C3B-C4B-NB	-2.44	108.25	110.52
13	b	810	CLA	CHB-C4A-NA	2.44	127.88	124.51
15	k	4005	BCR	C27-C26-C25	2.44	126.27	122.73
15	j	101	BCR	C27-C26-C25	2.43	126.26	122.73
16	a	851	LHG	C11-C10-C9	-2.43	102.08	114.42
13	b	826	CLA	CHB-C4A-NA	2.43	127.87	124.51
13	l	1503	CLA	C3B-C4B-NB	-2.43	108.26	110.52
17	b	850	LMG	O1-C1-C2	-2.43	104.51	108.30
16	a	853	LHG	C11-C10-C9	-2.43	102.11	114.42
13	a	829	CLA	CHB-C4A-NA	2.42	127.86	124.51
13	b	841	CLA	CHB-C4A-NA	2.42	127.86	124.51
15	a	847	BCR	C15-C16-C17	-2.42	118.51	123.47
13	a	828	CLA	CHD-C1D-ND	-2.42	122.23	124.45
15	a	845	BCR	C15-C16-C17	-2.42	118.51	123.47
13	a	813	CLA	O2D-CGD-CBD	2.42	115.57	111.27
15	a	845	BCR	C28-C27-C26	-2.42	109.76	114.08
17	a	850	LMG	C40-C39-C38	-2.42	102.16	114.42
13	a	828	CLA	CHB-C4A-NA	2.42	127.85	124.51
13	b	817	CLA	CHB-C4A-NA	2.42	127.85	124.51
13	b	812	CLA	C3B-C4B-NB	-2.41	108.28	110.52
13	b	839	CLA	CHB-C4A-NA	2.41	127.85	124.51
21	b	853	EQ3	C34-C9-C8	2.41	121.88	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	834	CLA	O2D-CGD-CBD	2.41	115.55	111.27
13	a	839	CLA	C3B-C4B-NB	-2.41	108.28	110.52
13	a	803	CLA	CHB-C4A-NA	2.41	127.84	124.51
13	a	826	CLA	CHB-C4A-NA	2.40	127.84	124.51
13	b	811	CLA	CHB-C4A-NA	2.40	127.84	124.51
13	b	829	CLA	CHB-C4A-NA	2.40	127.84	124.51
15	a	844	BCR	C27-C26-C25	2.40	126.22	122.73
13	a	802	CLA	CHB-C4A-NA	2.40	127.83	124.51
13	b	838	CLA	CHB-C4A-NA	2.40	127.83	124.51
13	a	814	CLA	CHB-C4A-NA	2.40	127.83	124.51
16	f	206	LHG	C20-C19-C18	-2.40	102.25	114.42
15	b	849	BCR	C27-C26-C25	2.40	126.21	122.73
13	a	812	CLA	CHB-C4A-NA	2.40	127.83	124.51
13	a	837	CLA	C3B-C4B-NB	-2.40	108.29	110.52
16	a	849	LHG	C20-C19-C18	-2.40	102.26	114.42
13	b	809	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
22	b	854	ZEX	C27-C28-C29	2.39	129.85	126.23
13	a	831	CLA	C3B-C4B-NB	-2.39	108.29	110.52
13	b	824	CLA	CHB-C4A-NA	2.39	127.82	124.51
13	b	804	CLA	CHD-C1D-ND	-2.39	122.26	124.45
13	b	809	CLA	CHB-C4A-NA	2.39	127.81	124.51
15	f	202	BCR	C27-C26-C25	2.38	126.19	122.73
13	a	833	CLA	C3B-C4B-NB	-2.38	108.30	110.52
13	k	4004	CLA	C3B-C4B-NB	-2.38	108.30	110.52
13	b	808	CLA	CHB-C4A-NA	2.38	127.81	124.51
13	a	827	CLA	C1-C2-C3	-2.38	121.92	126.04
13	a	824	CLA	C3B-C4B-NB	-2.38	108.31	110.52
13	b	834	CLA	CHB-C4A-NA	2.38	127.80	124.51
13	a	823	CLA	C3B-C4B-NB	-2.37	108.31	110.52
13	b	836	CLA	CHB-C4A-NA	2.37	127.79	124.51
17	b	852	LMG	C40-C39-C38	-2.37	102.39	114.42
13	b	837	CLA	C1-C2-C3	-2.37	121.94	126.04
18	a	856	45D	C33-C35-C37	2.37	122.58	118.94
13	a	819	CLA	C3B-C4B-NB	-2.37	108.32	110.52
13	b	826	CLA	C3B-C4B-NB	-2.37	108.32	110.52
13	a	805	CLA	C3B-C4B-NB	-2.37	108.32	110.52
13	a	834	CLA	C3B-C4B-NB	-2.37	108.32	110.52
13	a	836	CLA	CHB-C4A-NA	2.37	127.78	124.51
16	a	853	LHG	C20-C19-C18	-2.37	102.42	114.42
13	b	827	CLA	CHB-C4A-NA	2.37	127.78	124.51
16	f	206	LHG	C11-C10-C9	-2.36	102.42	114.42
13	b	830	CLA	CMB-C2B-C1B	-2.36	121.77	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	b	808	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
13	b	821	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
15	k	4001	BCR	C24-C23-C22	-2.36	122.67	126.23
13	b	824	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
13	j	103	CLA	CHB-C4A-NA	2.35	127.76	124.51
13	b	830	CLA	C3B-C4B-NB	-2.35	108.34	110.52
13	b	803	CLA	C1-C2-C3	-2.35	121.98	126.04
13	b	819	CLA	CHB-C4A-NA	2.34	127.75	124.51
15	j	105	BCR	C24-C23-C22	-2.34	122.70	126.23
17	b	850	LMG	C40-C39-C38	-2.34	102.54	114.42
13	a	825	CLA	O2D-CGD-CBD	2.34	115.43	111.27
13	a	804	CLA	CHB-C4A-NA	2.34	127.75	124.51
13	l	1501	CLA	C3B-C4B-NB	-2.34	108.34	110.52
15	b	848	BCR	C2-C1-C6	2.34	114.08	110.48
13	a	802	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
15	i	101	BCR	C27-C26-C25	2.33	126.12	122.73
13	a	832	CLA	C1-C2-C3	-2.33	122.01	126.04
13	a	810	CLA	C3B-C4B-NB	-2.33	108.35	110.52
18	a	856	45D	C34-C36-C38	2.33	122.51	118.94
13	b	837	CLA	O2D-CGD-CBD	2.33	115.40	111.27
13	a	831	CLA	CHB-C4A-NA	2.33	127.73	124.51
15	i	102	BCR	C33-C5-C6	-2.33	121.92	124.53
13	a	819	CLA	CHB-C4A-NA	2.32	127.73	124.51
13	a	854	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
15	a	846	BCR	C27-C26-C25	2.32	126.10	122.73
13	b	834	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
22	f	205	ZEX	C8-C9-C10	2.32	122.50	118.94
17	b	850	LMG	C38-C37-C36	-2.31	102.67	114.42
15	j	105	BCR	C15-C14-C13	-2.31	124.01	127.31
15	a	844	BCR	C24-C23-C22	-2.31	122.74	126.23
13	b	817	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
17	b	852	LMG	C38-C37-C36	-2.31	102.70	114.42
13	j	104	CLA	CHB-C4A-NA	2.31	127.70	124.51
15	b	849	BCR	C33-C5-C6	-2.30	121.94	124.53
18	a	856	45D	C24-C26-C30	2.30	122.47	118.94
13	b	841	CLA	C3B-C4B-NB	-2.30	108.38	110.52
20	m	101	ECH	C24-C23-C22	2.30	129.71	126.23
13	b	804	CLA	CHB-C4A-NA	2.29	127.68	124.51
13	a	833	CLA	CHB-C4A-NA	2.29	127.68	124.51
20	m	101	ECH	C8-C9-C10	2.29	122.45	118.94
13	a	812	CLA	C1-C2-C3	-2.29	122.08	126.04
13	b	807	CLA	C1-C2-C3	-2.29	122.09	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	b	827	CLA	C3B-C4B-NB	-2.28	108.40	110.52
12	a	801	CL0	CHB-C4A-NA	2.28	127.67	124.51
17	b	850	LMG	O3-C3-C2	-2.28	105.08	110.35
13	a	822	CLA	C3B-C4B-NB	-2.28	108.40	110.52
13	a	825	CLA	C3B-C4B-NB	-2.28	108.40	110.52
15	k	4001	BCR	C15-C16-C17	-2.28	118.80	123.47
13	b	824	CLA	C1-C2-C3	-2.28	122.10	126.04
13	b	815	CLA	C1-C2-C3	-2.28	122.11	126.04
13	b	835	CLA	CHD-C1D-ND	-2.27	122.36	124.45
13	a	815	CLA	C3B-C4B-NB	-2.27	108.41	110.52
17	b	852	LMG	O6-C1-O1	-2.27	104.61	109.97
15	i	102	BCR	C15-C14-C13	-2.26	124.08	127.31
13	a	804	CLA	CHD-C1D-ND	-2.26	122.38	124.45
13	b	837	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
13	a	835	CLA	CHD-C1D-ND	-2.26	122.38	124.45
13	b	828	CLA	CHD-C1D-ND	-2.26	122.38	124.45
15	f	202	BCR	C24-C23-C22	-2.26	122.82	126.23
13	a	809	CLA	C3B-C4B-NB	-2.26	108.42	110.52
13	a	819	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
15	a	847	BCR	C15-C14-C13	-2.25	124.09	127.31
13	b	818	CLA	CHD-C1D-ND	-2.25	122.39	124.45
15	a	846	BCR	C11-C10-C9	-2.25	124.10	127.31
13	a	822	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
17	b	852	LMG	C42-C41-C40	-2.25	103.01	114.42
16	a	853	LHG	C27-C26-C25	-2.25	103.02	114.42
15	i	102	BCR	C15-C16-C17	-2.25	118.88	123.47
13	b	829	CLA	CMB-C2B-C1B	-2.24	121.95	125.37
13	a	806	CLA	CHD-C1D-ND	-2.24	122.39	124.45
15	a	844	BCR	C15-C16-C17	-2.24	118.88	123.47
15	b	849	BCR	C15-C14-C13	-2.24	124.12	127.31
17	b	850	LMG	C42-C41-C40	-2.24	103.07	114.42
13	a	813	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
13	a	809	CLA	CMB-C2B-C1B	-2.23	121.97	125.37
16	a	851	LHG	C18-C17-C16	-2.23	103.09	114.42
13	a	803	CLA	CHD-C1D-ND	-2.23	122.40	124.45
13	b	831	CLA	CHB-C4A-NA	2.23	127.60	124.51
13	b	840	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
13	a	807	CLA	CMB-C2B-C1B	-2.23	121.98	125.37
15	b	845	BCR	C15-C14-C13	-2.23	124.13	127.31
15	b	848	BCR	C15-C16-C17	-2.22	118.92	123.47
16	a	851	LHG	C27-C26-C25	-2.22	103.16	114.42
13	a	808	CLA	CHD-C1D-ND	-2.22	122.42	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	b	832	CLA	CMB-C2B-C1B	-2.22	121.99	125.37
13	b	839	CLA	C1-C2-C3	-2.21	123.17	126.75
13	b	805	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
13	a	826	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
13	a	809	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
17	b	850	LMG	O2-C2-C1	-2.21	104.68	110.05
13	b	805	CLA	CHD-C1D-ND	-2.21	122.43	124.45
13	a	812	CLA	CHB-C1B-NB	2.21	126.59	124.26
17	a	850	LMG	C38-C37-C36	-2.21	103.23	114.42
16	a	849	LHG	C18-C17-C16	-2.20	103.23	114.42
13	f	203	CLA	CHB-C4A-NA	2.20	127.56	124.51
13	b	832	CLA	C1-C2-C3	-2.20	123.19	126.75
13	a	840	CLA	CHD-C1D-ND	-2.20	122.43	124.45
17	a	852	LMG	O3-C3-C2	-2.20	105.25	110.35
13	a	840	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
15	b	845	BCR	C27-C26-C25	2.20	125.93	122.73
17	a	850	LMG	C42-C41-C40	-2.20	103.26	114.42
13	b	817	CLA	CHD-C1D-ND	-2.20	122.43	124.45
13	a	828	CLA	C1-C2-C3	-2.19	122.25	126.04
15	i	101	BCR	C33-C5-C6	-2.19	122.06	124.53
13	b	831	CLA	C1-C2-C3	-2.19	122.25	126.04
15	b	849	BCR	C15-C16-C17	-2.19	118.99	123.47
13	b	805	CLA	CHB-C1B-NB	2.19	126.57	124.26
13	b	833	CLA	CHB-C1B-NB	2.19	126.57	124.26
22	b	854	ZEX	C8-C9-C10	2.19	122.30	118.94
13	b	830	CLA	O2D-CGD-CBD	2.19	115.15	111.27
13	b	833	CLA	CHD-C1D-ND	-2.18	122.45	124.45
13	b	837	CLA	CMB-C2B-C1B	-2.18	122.05	125.37
13	b	827	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
13	a	837	CLA	CHC-C4B-NB	2.18	126.56	124.26
15	f	202	BCR	C33-C5-C6	-2.18	122.08	124.53
13	a	826	CLA	C1-C2-C3	-2.18	122.28	126.04
17	a	850	LMG	O3-C3-C2	-2.18	105.32	110.35
16	b	851	LHG	C27-C26-C25	-2.17	103.40	114.42
15	i	102	BCR	C28-C27-C26	-2.17	110.20	114.08
13	a	803	CLA	C1-C2-C3	-2.17	122.29	126.04
16	a	849	LHG	C27-C26-C25	-2.17	103.40	114.42
16	a	853	LHG	C18-C17-C16	-2.17	103.41	114.42
13	b	839	CLA	C3B-C4B-NB	-2.17	108.51	110.52
13	a	842	CLA	CHD-C1D-ND	-2.17	122.46	124.45
13	b	826	CLA	CHD-C1D-ND	-2.17	122.46	124.45
15	a	847	BCR	C27-C26-C25	2.16	125.87	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	822	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
13	a	823	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
17	b	852	LMG	O2-C2-C1	-2.16	104.80	110.05
13	b	838	CLA	CHD-C1D-ND	-2.16	122.47	124.45
13	a	814	CLA	CHD-C1D-ND	-2.16	122.47	124.45
15	b	844	BCR	C11-C10-C9	-2.16	124.23	127.31
13	b	801	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
13	b	813	CLA	CHB-C1B-NB	2.15	126.54	124.26
15	a	848	BCR	C7-C8-C9	-2.15	122.98	126.23
13	b	801	CLA	CHB-C4A-NA	2.15	127.49	124.51
16	f	206	LHG	C18-C17-C16	-2.15	103.50	114.42
13	b	806	CLA	CMB-C2B-C1B	-2.15	122.09	125.37
13	a	821	CLA	CHD-C1D-ND	-2.15	122.48	124.45
13	f	203	CLA	CHD-C1D-ND	-2.15	122.48	124.45
13	a	812	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
13	a	803	CLA	CHB-C1B-NB	2.15	126.53	124.26
13	b	816	CLA	CHB-C1B-NB	2.15	126.53	124.26
13	a	825	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
13	a	805	CLA	C1-C2-C3	-2.14	122.34	126.04
15	b	848	BCR	C33-C5-C6	-2.14	122.12	124.53
15	j	101	BCR	C11-C10-C9	-2.14	124.26	127.31
13	a	813	CLA	CMB-C2B-C1B	-2.14	122.12	125.37
13	a	819	CLA	CHB-C1B-NB	2.14	126.52	124.26
13	b	808	CLA	C3B-C4B-NB	-2.14	108.53	110.52
15	b	849	BCR	C24-C23-C22	-2.13	123.01	126.23
13	b	807	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
15	a	846	BCR	C24-C23-C22	-2.13	123.02	126.23
16	f	206	LHG	C27-C26-C25	-2.13	103.63	114.42
15	a	845	BCR	C8-C7-C6	-2.13	121.23	127.20
13	b	826	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
13	a	833	CLA	C1-C2-C3	-2.12	122.37	126.04
17	b	852	LMG	O1-C7-C8	-2.12	105.77	110.90
13	a	814	CLA	O2D-CGD-CBD	2.12	115.04	111.27
13	a	823	CLA	CBA-CAA-C2A	2.12	120.11	113.86
17	a	850	LMG	O1-C7-C8	-2.12	105.79	110.90
13	a	821	CLA	CHB-C1B-NB	2.11	126.50	124.26
13	a	805	CLA	CMB-C2B-C1B	-2.11	122.15	125.37
13	a	854	CLA	CMB-C2B-C1B	-2.11	122.15	125.37
20	b	846	ECH	C34-C9-C8	2.11	121.41	118.08
13	b	817	CLA	CMB-C2B-C1B	-2.11	122.15	125.37
13	b	810	CLA	C1-C2-C3	-2.11	122.39	126.04
13	a	819	CLA	C1-C2-C3	-2.11	122.40	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	i	101	BCR	C15-C14-C13	-2.11	124.30	127.31
15	i	101	BCR	C8-C7-C6	-2.11	121.28	127.20
15	f	202	BCR	C8-C7-C6	-2.11	121.29	127.20
13	a	854	CLA	CHD-C1D-ND	-2.10	122.52	124.45
15	a	848	BCR	C11-C10-C9	-2.10	124.31	127.31
18	a	856	45D	C41-C42-C38	2.10	127.77	123.47
13	a	829	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
13	a	823	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
13	b	818	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
13	a	841	CLA	C1-C2-C3	-2.10	122.42	126.04
17	a	850	LMG	O2-C2-C1	-2.09	104.96	110.05
15	k	4005	BCR	C33-C5-C6	-2.09	122.18	124.53
13	a	838	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
13	a	819	CLA	CHD-C1D-ND	-2.09	122.53	124.45
13	a	829	CLA	C3B-C4B-NB	-2.09	108.57	110.52
13	b	820	CLA	CHD-C1D-ND	-2.09	122.53	124.45
15	a	847	BCR	C24-C23-C22	-2.09	123.08	126.23
13	a	835	CLA	C1-C2-C3	-2.09	122.43	126.04
13	a	836	CLA	C1-C2-C3	-2.09	122.43	126.04
13	a	838	CLA	CHB-C1B-NB	2.08	126.46	124.26
13	a	835	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
13	b	816	CLA	CHD-C1D-ND	-2.08	122.54	124.45
13	l	1503	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
13	a	815	CLA	CMB-C2B-C1B	-2.08	122.20	125.37
13	a	821	CLA	CMB-C2B-C1B	-2.08	122.20	125.37
15	b	847	BCR	C33-C5-C6	-2.08	122.19	124.53
15	k	4005	BCR	C24-C23-C22	-2.08	123.10	126.23
13	b	832	CLA	CHD-C1D-ND	-2.08	122.55	124.45
13	f	203	CLA	C3B-C4B-NB	-2.08	108.59	110.52
13	a	836	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
13	b	831	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
13	k	4004	CLA	CAC-C3C-C2C	-2.08	123.98	127.53
15	j	101	BCR	C24-C23-C22	-2.08	123.10	126.23
13	a	812	CLA	CHD-C1D-ND	-2.07	122.55	124.45
13	a	830	CLA	CMB-C2B-C1B	-2.07	122.21	125.37
13	a	804	CLA	CHB-C1B-NB	2.07	126.45	124.26
13	k	4003	CLA	CHB-C1B-NB	2.07	126.45	124.26
17	a	852	LMG	O2-C2-C1	-2.07	105.01	110.05
15	i	102	BCR	C11-C10-C9	-2.07	124.36	127.31
13	b	806	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
15	a	846	BCR	C7-C8-C9	-2.07	123.11	126.23
13	a	819	CLA	CMB-C2B-C1B	-2.07	122.22	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	817	CLA	CHD-C1D-ND	-2.07	122.56	124.45
13	b	831	CLA	CHB-C1B-NB	2.07	126.44	124.26
13	a	828	CLA	CMB-C2B-C1B	-2.06	122.22	125.37
12	a	801	CL0	CHC-C4B-NB	2.06	126.44	124.26
13	b	809	CLA	CHB-C1B-NB	2.06	126.44	124.26
13	b	811	CLA	CHB-C1B-NB	2.06	126.44	124.26
13	k	4002	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
15	f	202	BCR	C16-C15-C14	-2.06	119.25	123.47
13	b	841	CLA	CHD-C1D-ND	-2.06	122.56	124.45
15	b	844	BCR	C38-C26-C25	-2.06	122.21	124.53
13	a	830	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
13	a	832	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
13	f	203	CLA	CHC-C4B-NB	2.06	126.44	124.26
13	a	836	CLA	C3B-C4B-NB	-2.06	108.60	110.52
13	a	838	CLA	CHD-C1D-ND	-2.06	122.56	124.45
13	b	819	CLA	CHD-C1D-ND	-2.06	122.56	124.45
13	a	841	CLA	CHD-C1D-ND	-2.06	122.56	124.45
13	l	1502	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
15	a	845	BCR	C24-C23-C22	-2.06	123.13	126.23
15	a	847	BCR	C8-C7-C6	-2.05	121.43	127.20
13	b	832	CLA	CHB-C1B-NB	2.05	126.43	124.26
13	a	814	CLA	CMB-C2B-C1B	-2.05	122.24	125.37
13	a	807	CLA	CHD-C1D-ND	-2.05	122.57	124.45
15	b	848	BCR	C15-C14-C13	-2.05	124.39	127.31
13	b	829	CLA	CMB-C2B-C3B	2.05	131.55	126.59
13	a	833	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
13	k	4004	CLA	CHD-C1D-ND	-2.05	122.57	124.45
13	b	805	CLA	C1-C2-C3	-2.05	122.51	126.04
13	a	827	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
13	a	831	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
13	b	832	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
13	a	811	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
13	b	828	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
15	a	844	BCR	C15-C14-C13	-2.04	124.39	127.31
17	b	852	LMG	O3-C3-C2	-2.04	105.63	110.35
13	b	840	CLA	CHB-C1B-NB	2.04	126.42	124.26
13	l	1503	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
13	a	808	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
13	b	828	CLA	C3B-C4B-NB	-2.04	108.62	110.52
23	j	102	LMT	O5B-C5B-C4B	2.04	113.39	109.69
13	b	811	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
13	a	832	CLA	CHD-C1D-ND	-2.03	122.58	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	b	804	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
13	a	821	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
15	a	846	BCR	C35-C13-C14	-2.03	120.08	122.92
13	a	808	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
13	a	810	CLA	C2A-C1A-CHA	2.03	127.41	123.86
17	a	852	LMG	O1-C7-C8	-2.03	106.00	110.90
13	b	801	CLA	CMB-C2B-C3B	2.03	131.50	126.59
13	l	1501	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
15	j	105	BCR	C8-C7-C6	-2.03	121.51	127.20
15	i	102	BCR	C27-C26-C25	2.02	125.67	122.73
13	b	836	CLA	CHB-C1B-NB	2.02	126.40	124.26
13	b	819	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
13	b	825	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
13	a	855	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
13	f	201	CLA	CAA-CBA-CGA	-2.02	107.35	113.25
13	j	103	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
13	a	837	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
13	b	816	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
13	b	813	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
13	a	833	CLA	CHD-C1D-ND	-2.01	122.60	124.45
13	k	4003	CLA	CHD-C1D-ND	-2.01	122.60	124.45
13	a	807	CLA	CHB-C1B-NB	2.01	126.39	124.26
13	a	826	CLA	CHB-C1B-NB	2.01	126.39	124.26
13	a	824	CLA	CHD-C1D-ND	-2.01	122.60	124.45
17	b	852	LMG	O7-C10-O9	-2.01	118.84	123.70
13	a	822	CLA	CHB-C1B-NB	2.01	126.39	124.26
13	b	824	CLA	CHB-C1B-NB	2.01	126.39	124.26
15	b	847	BCR	C11-C10-C9	-2.01	124.44	127.31
15	f	202	BCR	C15-C16-C17	-2.01	119.36	123.47
13	b	840	CLA	CHD-C1D-ND	-2.01	122.61	124.45
13	f	204	CLA	CHB-C1B-NB	2.01	126.38	124.26
15	a	845	BCR	C15-C14-C13	-2.01	124.44	127.31
13	b	820	CLA	CHB-C1B-NB	2.01	126.38	124.26
13	a	841	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
13	b	804	CLA	CHB-C1B-NB	2.00	126.38	124.26
13	a	832	CLA	CHB-C1B-NB	2.00	126.38	124.26
13	a	822	CLA	CMB-C2B-C3B	2.00	131.44	126.59
13	b	808	CLA	CHD-C1D-ND	-2.00	122.61	124.45
13	a	818	CLA	CAA-CBA-CGA	-2.00	107.41	113.25
13	b	810	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
13	a	805	CLA	CHD-C1D-ND	-2.00	122.62	124.45
13	b	834	CLA	CHD-C1D-ND	-2.00	122.62	124.45

There are no chirality outliers.

All (1560) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	a	802	CLA	CBA-CGA-O2A-C1
13	a	802	CLA	O1A-CGA-O2A-C1
13	a	804	CLA	CHA-CBD-CGD-O1D
13	a	805	CLA	C3A-C2A-CAA-CBA
13	a	806	CLA	C2-C3-C5-C6
13	a	806	CLA	C4-C3-C5-C6
13	a	808	CLA	C1A-C2A-CAA-CBA
13	a	808	CLA	C3A-C2A-CAA-CBA
13	a	810	CLA	C2A-CAA-CBA-CGA
13	a	810	CLA	CHA-CBD-CGD-O1D
13	a	810	CLA	CHA-CBD-CGD-O2D
13	a	812	CLA	C1A-C2A-CAA-CBA
13	a	814	CLA	C3A-C2A-CAA-CBA
13	a	814	CLA	CHA-CBD-CGD-O1D
13	a	814	CLA	CHA-CBD-CGD-O2D
13	a	815	CLA	CBD-CGD-O2D-CED
13	a	816	CLA	C1A-C2A-CAA-CBA
13	a	816	CLA	C3A-C2A-CAA-CBA
13	a	816	CLA	CBA-CGA-O2A-C1
13	a	817	CLA	C1A-C2A-CAA-CBA
13	a	818	CLA	C1A-C2A-CAA-CBA
13	a	818	CLA	C3A-C2A-CAA-CBA
13	a	818	CLA	CBD-CGD-O2D-CED
13	a	819	CLA	C1A-C2A-CAA-CBA
13	a	819	CLA	C3A-C2A-CAA-CBA
13	a	819	CLA	CHA-CBD-CGD-O1D
13	a	819	CLA	CHA-CBD-CGD-O2D
13	a	820	CLA	C1A-C2A-CAA-CBA
13	a	820	CLA	C3A-C2A-CAA-CBA
13	a	820	CLA	C2-C1-O2A-CGA
13	a	822	CLA	C1A-C2A-CAA-CBA
13	a	822	CLA	C3A-C2A-CAA-CBA
13	a	823	CLA	C1A-C2A-CAA-CBA
13	a	824	CLA	CHA-CBD-CGD-O1D
13	a	824	CLA	CHA-CBD-CGD-O2D
13	a	826	CLA	C3A-C2A-CAA-CBA
13	a	828	CLA	C1A-C2A-CAA-CBA
13	a	831	CLA	C3A-C2A-CAA-CBA
13	a	832	CLA	C1A-C2A-CAA-CBA
13	a	832	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	a	833	CLA	C4B-C3B-CAB-CBB
13	a	834	CLA	C1A-C2A-CAA-CBA
13	a	835	CLA	C2-C3-C5-C6
13	a	835	CLA	C4-C3-C5-C6
13	a	835	CLA	C6-C7-C8-C9
13	a	836	CLA	CHA-CBD-CGD-O1D
13	a	836	CLA	CHA-CBD-CGD-O2D
13	a	838	CLA	C1A-C2A-CAA-CBA
13	a	838	CLA	C3A-C2A-CAA-CBA
13	a	838	CLA	CHA-CBD-CGD-O1D
13	a	838	CLA	CHA-CBD-CGD-O2D
13	a	840	CLA	C1A-C2A-CAA-CBA
13	a	840	CLA	C3A-C2A-CAA-CBA
13	a	842	CLA	CHA-CBD-CGD-O1D
13	a	855	CLA	C1A-C2A-CAA-CBA
13	a	855	CLA	C3A-C2A-CAA-CBA
13	a	855	CLA	C4-C3-C5-C6
13	b	801	CLA	CBD-CGD-O2D-CED
13	b	801	CLA	C2-C3-C5-C6
13	b	801	CLA	C4-C3-C5-C6
13	b	803	CLA	C1A-C2A-CAA-CBA
13	b	803	CLA	C3A-C2A-CAA-CBA
13	b	803	CLA	CHA-CBD-CGD-O1D
13	b	803	CLA	CHA-CBD-CGD-O2D
13	b	803	CLA	C2-C3-C5-C6
13	b	803	CLA	C4-C3-C5-C6
13	b	804	CLA	CHA-CBD-CGD-O1D
13	b	804	CLA	CHA-CBD-CGD-O2D
13	b	804	CLA	CBD-CGD-O2D-CED
13	b	804	CLA	O1D-CGD-O2D-CED
13	b	805	CLA	C2A-CAA-CBA-CGA
13	b	807	CLA	C14-C13-C15-C16
13	b	808	CLA	C1A-C2A-CAA-CBA
13	b	808	CLA	C3A-C2A-CAA-CBA
13	b	808	CLA	C2-C3-C5-C6
13	b	808	CLA	C4-C3-C5-C6
13	b	808	CLA	C6-C7-C8-C9
13	b	810	CLA	C2A-CAA-CBA-CGA
13	b	810	CLA	CBD-CGD-O2D-CED
13	b	812	CLA	C1A-C2A-CAA-CBA
13	b	813	CLA	C1A-C2A-CAA-CBA
13	b	816	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	b	816	CLA	CBD-CGD-O2D-CED
13	b	816	CLA	C2-C3-C5-C6
13	b	816	CLA	C4-C3-C5-C6
13	b	817	CLA	C1A-C2A-CAA-CBA
13	b	818	CLA	C11-C10-C8-C9
13	b	819	CLA	C1A-C2A-CAA-CBA
13	b	819	CLA	C3A-C2A-CAA-CBA
13	b	821	CLA	C1A-C2A-CAA-CBA
13	b	821	CLA	C3A-C2A-CAA-CBA
13	b	821	CLA	C2B-C3B-CAB-CBB
13	b	821	CLA	C4B-C3B-CAB-CBB
13	b	822	CLA	C1A-C2A-CAA-CBA
13	b	822	CLA	C3A-C2A-CAA-CBA
13	b	823	CLA	C1A-C2A-CAA-CBA
13	b	823	CLA	C3A-C2A-CAA-CBA
13	b	823	CLA	CBA-CGA-O2A-C1
13	b	823	CLA	O1A-CGA-O2A-C1
13	b	824	CLA	C1A-C2A-CAA-CBA
13	b	824	CLA	C3A-C2A-CAA-CBA
13	b	825	CLA	C1A-C2A-CAA-CBA
13	b	826	CLA	C3A-C2A-CAA-CBA
13	b	828	CLA	C1A-C2A-CAA-CBA
13	b	828	CLA	C3A-C2A-CAA-CBA
13	b	830	CLA	C1A-C2A-CAA-CBA
13	b	830	CLA	C3A-C2A-CAA-CBA
13	b	831	CLA	C1A-C2A-CAA-CBA
13	b	831	CLA	C3A-C2A-CAA-CBA
13	b	831	CLA	CBD-CGD-O2D-CED
13	b	831	CLA	O1D-CGD-O2D-CED
13	b	834	CLA	C1A-C2A-CAA-CBA
13	b	834	CLA	C3A-C2A-CAA-CBA
13	b	834	CLA	CBA-CGA-O2A-C1
13	b	834	CLA	O1A-CGA-O2A-C1
13	b	834	CLA	CHA-CBD-CGD-O1D
13	b	834	CLA	CHA-CBD-CGD-O2D
13	b	835	CLA	C1A-C2A-CAA-CBA
13	b	835	CLA	C3A-C2A-CAA-CBA
13	b	836	CLA	C1A-C2A-CAA-CBA
13	b	836	CLA	C3A-C2A-CAA-CBA
13	b	838	CLA	C1A-C2A-CAA-CBA
13	b	838	CLA	C3A-C2A-CAA-CBA
13	b	839	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	b	839	CLA	C3A-C2A-CAA-CBA
13	b	840	CLA	C1A-C2A-CAA-CBA
13	b	841	CLA	CHA-CBD-CGD-O1D
13	b	841	CLA	CHA-CBD-CGD-O2D
13	b	842	CLA	C1A-C2A-CAA-CBA
13	b	842	CLA	C3A-C2A-CAA-CBA
13	b	842	CLA	CAD-CBD-CGD-O1D
13	b	842	CLA	CAD-CBD-CGD-O2D
13	f	201	CLA	C2B-C3B-CAB-CBB
13	f	201	CLA	C4B-C3B-CAB-CBB
13	f	201	CLA	CHA-CBD-CGD-O1D
13	f	201	CLA	CHA-CBD-CGD-O2D
13	j	103	CLA	C1A-C2A-CAA-CBA
13	j	104	CLA	CBA-CGA-O2A-C1
13	j	104	CLA	CHA-CBD-CGD-O1D
13	j	104	CLA	CHA-CBD-CGD-O2D
13	k	4003	CLA	C3A-C2A-CAA-CBA
13	k	4003	CLA	CBA-CGA-O2A-C1
13	k	4003	CLA	O1A-CGA-O2A-C1
13	k	4003	CLA	CHA-CBD-CGD-O1D
13	k	4003	CLA	CHA-CBD-CGD-O2D
13	l	1501	CLA	C1A-C2A-CAA-CBA
13	l	1501	CLA	C3A-C2A-CAA-CBA
13	l	1502	CLA	C1A-C2A-CAA-CBA
13	l	1502	CLA	CHA-CBD-CGD-O1D
13	l	1502	CLA	CHA-CBD-CGD-O2D
15	a	844	BCR	C1-C6-C7-C8
15	a	844	BCR	C7-C8-C9-C34
15	a	845	BCR	C1-C6-C7-C8
15	a	847	BCR	C1-C6-C7-C8
15	a	847	BCR	C7-C8-C9-C34
15	a	847	BCR	C20-C21-C22-C37
15	a	847	BCR	C21-C22-C23-C24
15	a	847	BCR	C37-C22-C23-C24
15	a	847	BCR	C23-C24-C25-C30
15	a	848	BCR	C9-C10-C11-C12
15	a	848	BCR	C11-C12-C13-C35
15	b	844	BCR	C7-C8-C9-C10
15	b	844	BCR	C7-C8-C9-C34
15	b	844	BCR	C21-C22-C23-C24
15	b	844	BCR	C37-C22-C23-C24
15	b	844	BCR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
15	b	845	BCR	C1-C6-C7-C8
15	b	847	BCR	C21-C22-C23-C24
15	b	847	BCR	C22-C23-C24-C25
15	b	848	BCR	C10-C11-C12-C13
15	b	848	BCR	C11-C12-C13-C35
15	b	848	BCR	C20-C21-C22-C37
15	b	849	BCR	C6-C7-C8-C9
15	b	849	BCR	C11-C10-C9-C8
15	b	849	BCR	C11-C12-C13-C35
15	b	849	BCR	C16-C17-C18-C36
15	b	849	BCR	C21-C22-C23-C24
15	b	849	BCR	C37-C22-C23-C24
15	f	202	BCR	C7-C8-C9-C10
15	f	202	BCR	C37-C22-C23-C24
15	i	101	BCR	C21-C22-C23-C24
15	i	102	BCR	C7-C8-C9-C10
15	i	102	BCR	C7-C8-C9-C34
15	i	102	BCR	C37-C22-C23-C24
15	j	101	BCR	C1-C6-C7-C8
15	j	105	BCR	C23-C24-C25-C30
15	k	4001	BCR	C7-C8-C9-C34
16	a	849	LHG	O2-C2-C3-O3
16	a	849	LHG	C3-O3-P-O5
16	a	849	LHG	O10-C23-O8-C6
16	a	849	LHG	C24-C23-O8-C6
16	a	853	LHG	O9-C7-O7-C5
16	a	853	LHG	C8-C7-O7-C5
16	b	851	LHG	O1-C1-C2-C3
16	b	851	LHG	C3-O3-P-O4
16	b	851	LHG	C3-O3-P-O6
16	f	206	LHG	O9-C7-O7-C5
16	f	206	LHG	O10-C23-O8-C6
17	a	850	LMG	O6-C1-O1-C7
17	a	850	LMG	O9-C10-O7-C8
17	a	850	LMG	C11-C10-O7-C8
17	a	852	LMG	C2-C1-O1-C7
17	a	852	LMG	O6-C1-O1-C7
17	a	852	LMG	O9-C10-O7-C8
17	a	852	LMG	C11-C10-O7-C8
20	b	846	ECH	C21-C22-C23-C24
20	b	846	ECH	C37-C22-C23-C24
20	m	101	ECH	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
20	m	101	ECH	C37-C22-C23-C24
23	j	102	LMT	C2'-C1'-O1'-C1
23	j	102	LMT	O5'-C1'-O1'-C1
13	b	803	CLA	O1D-CGD-O2D-CED
13	b	816	CLA	O1D-CGD-O2D-CED
13	a	805	CLA	CBD-CGD-O2D-CED
13	a	810	CLA	CBD-CGD-O2D-CED
13	a	813	CLA	CBD-CGD-O2D-CED
13	a	820	CLA	CBD-CGD-O2D-CED
13	b	803	CLA	CBD-CGD-O2D-CED
13	b	821	CLA	CBD-CGD-O2D-CED
13	b	822	CLA	CBD-CGD-O2D-CED
13	b	824	CLA	CBD-CGD-O2D-CED
13	b	835	CLA	CBD-CGD-O2D-CED
13	b	837	CLA	CBD-CGD-O2D-CED
13	f	201	CLA	CBD-CGD-O2D-CED
13	j	103	CLA	CBD-CGD-O2D-CED
13	k	4004	CLA	CBD-CGD-O2D-CED
13	l	1501	CLA	CBD-CGD-O2D-CED
13	a	812	CLA	O1A-CGA-O2A-C1
13	a	819	CLA	O1A-CGA-O2A-C1
13	b	806	CLA	O1A-CGA-O2A-C1
13	b	807	CLA	O1A-CGA-O2A-C1
13	b	839	CLA	O1A-CGA-O2A-C1
13	b	840	CLA	O1A-CGA-O2A-C1
13	l	1501	CLA	O1A-CGA-O2A-C1
17	a	850	LMG	O10-C28-O8-C9
13	j	104	CLA	O1A-CGA-O2A-C1
13	a	810	CLA	O1D-CGD-O2D-CED
13	a	815	CLA	O1D-CGD-O2D-CED
13	b	801	CLA	O1D-CGD-O2D-CED
13	k	4004	CLA	O1D-CGD-O2D-CED
13	a	815	CLA	CBA-CGA-O2A-C1
13	a	818	CLA	O1D-CGD-O2D-CED
13	a	820	CLA	O1D-CGD-O2D-CED
13	f	201	CLA	O1D-CGD-O2D-CED
13	a	812	CLA	CBA-CGA-O2A-C1
13	a	819	CLA	CBA-CGA-O2A-C1
13	b	807	CLA	CBA-CGA-O2A-C1
13	b	839	CLA	CBA-CGA-O2A-C1
17	a	850	LMG	C29-C28-O8-C9
13	a	809	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	a	822	CLA	CBD-CGD-O2D-CED
13	a	827	CLA	CBD-CGD-O2D-CED
13	b	830	CLA	CBD-CGD-O2D-CED
13	b	834	CLA	CBD-CGD-O2D-CED
13	b	836	CLA	CBD-CGD-O2D-CED
13	b	841	CLA	CBD-CGD-O2D-CED
13	a	820	CLA	O1A-CGA-O2A-C1
13	a	824	CLA	O1A-CGA-O2A-C1
13	a	831	CLA	O1A-CGA-O2A-C1
13	a	834	CLA	O1A-CGA-O2A-C1
13	a	854	CLA	O1A-CGA-O2A-C1
13	b	801	CLA	O1A-CGA-O2A-C1
13	b	804	CLA	O1A-CGA-O2A-C1
13	b	813	CLA	O1A-CGA-O2A-C1
13	b	818	CLA	O1A-CGA-O2A-C1
13	b	822	CLA	O1A-CGA-O2A-C1
13	b	825	CLA	O1A-CGA-O2A-C1
13	b	828	CLA	O1A-CGA-O2A-C1
13	b	836	CLA	O1A-CGA-O2A-C1
13	b	837	CLA	O1A-CGA-O2A-C1
13	f	203	CLA	O1A-CGA-O2A-C1
13	l	1502	CLA	O1A-CGA-O2A-C1
16	a	853	LHG	O10-C23-O8-C6
13	a	816	CLA	O1A-CGA-O2A-C1
13	b	810	CLA	O1D-CGD-O2D-CED
13	l	1501	CLA	O1D-CGD-O2D-CED
13	a	802	CLA	C3-C5-C6-C7
13	a	817	CLA	C3-C5-C6-C7
13	a	825	CLA	C3-C5-C6-C7
13	a	835	CLA	C3-C5-C6-C7
13	a	855	CLA	C3-C5-C6-C7
13	b	805	CLA	C3-C5-C6-C7
13	b	838	CLA	C3-C5-C6-C7
13	a	829	CLA	CBA-CGA-O2A-C1
13	a	834	CLA	CBA-CGA-O2A-C1
13	b	801	CLA	CBA-CGA-O2A-C1
13	b	803	CLA	CBA-CGA-O2A-C1
13	b	806	CLA	CBA-CGA-O2A-C1
13	b	808	CLA	CBA-CGA-O2A-C1
13	b	813	CLA	CBA-CGA-O2A-C1
13	b	822	CLA	CBA-CGA-O2A-C1
13	b	833	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	b	838	CLA	CBA-CGA-O2A-C1
13	b	840	CLA	CBA-CGA-O2A-C1
13	j	103	CLA	CBA-CGA-O2A-C1
13	l	1501	CLA	CBA-CGA-O2A-C1
16	f	206	LHG	C8-C7-O7-C5
13	a	824	CLA	CBD-CGD-O2D-CED
13	b	804	CLA	C2C-C3C-CAC-CBC
13	a	830	CLA	C4-C3-C5-C6
13	b	810	CLA	C4-C3-C5-C6
13	f	201	CLA	C4-C3-C5-C6
13	a	855	CLA	C2-C3-C5-C6
13	a	808	CLA	C2A-CAA-CBA-CGA
13	a	814	CLA	C2A-CAA-CBA-CGA
13	a	815	CLA	C2A-CAA-CBA-CGA
13	a	836	CLA	C2A-CAA-CBA-CGA
13	b	818	CLA	C2A-CAA-CBA-CGA
13	b	829	CLA	C2A-CAA-CBA-CGA
13	b	832	CLA	C2A-CAA-CBA-CGA
13	b	833	CLA	C2A-CAA-CBA-CGA
13	b	842	CLA	C2A-CAA-CBA-CGA
13	k	4003	CLA	C2A-CAA-CBA-CGA
13	a	811	CLA	O1A-CGA-O2A-C1
13	a	815	CLA	O1A-CGA-O2A-C1
13	a	830	CLA	C3-C5-C6-C7
13	a	839	CLA	C3-C5-C6-C7
13	a	840	CLA	C3-C5-C6-C7
13	b	801	CLA	C3-C5-C6-C7
13	a	811	CLA	CBA-CGA-O2A-C1
13	a	818	CLA	CBA-CGA-O2A-C1
13	a	820	CLA	CBA-CGA-O2A-C1
13	a	824	CLA	CBA-CGA-O2A-C1
13	a	827	CLA	CBA-CGA-O2A-C1
13	a	831	CLA	CBA-CGA-O2A-C1
13	a	838	CLA	CBA-CGA-O2A-C1
13	a	841	CLA	CBA-CGA-O2A-C1
13	a	854	CLA	CBA-CGA-O2A-C1
13	a	855	CLA	CBA-CGA-O2A-C1
13	b	804	CLA	CBA-CGA-O2A-C1
13	b	814	CLA	CBA-CGA-O2A-C1
13	b	817	CLA	CBA-CGA-O2A-C1
13	b	818	CLA	CBA-CGA-O2A-C1
13	b	825	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	b	828	CLA	CBA-CGA-O2A-C1
13	b	831	CLA	CBA-CGA-O2A-C1
13	b	835	CLA	CBA-CGA-O2A-C1
13	b	836	CLA	CBA-CGA-O2A-C1
13	b	837	CLA	CBA-CGA-O2A-C1
13	f	201	CLA	CBA-CGA-O2A-C1
13	f	203	CLA	CBA-CGA-O2A-C1
13	k	4002	CLA	CBA-CGA-O2A-C1
13	l	1502	CLA	CBA-CGA-O2A-C1
16	a	853	LHG	C24-C23-O8-C6
16	f	206	LHG	C24-C23-O8-C6
23	j	102	LMT	C4'-C5'-C6'-O6'
13	b	821	CLA	O1D-CGD-O2D-CED
13	b	837	CLA	O1D-CGD-O2D-CED
13	a	805	CLA	O1D-CGD-O2D-CED
13	j	103	CLA	O1D-CGD-O2D-CED
13	a	818	CLA	O1A-CGA-O2A-C1
13	a	822	CLA	O1A-CGA-O2A-C1
13	a	827	CLA	O1A-CGA-O2A-C1
13	a	829	CLA	O1A-CGA-O2A-C1
13	a	841	CLA	O1A-CGA-O2A-C1
13	b	803	CLA	O1A-CGA-O2A-C1
13	b	808	CLA	O1A-CGA-O2A-C1
13	b	830	CLA	O1A-CGA-O2A-C1
13	b	832	CLA	O1A-CGA-O2A-C1
13	b	833	CLA	O1A-CGA-O2A-C1
13	b	835	CLA	O1A-CGA-O2A-C1
13	b	838	CLA	O1A-CGA-O2A-C1
13	j	103	CLA	O1A-CGA-O2A-C1
13	k	4002	CLA	O1A-CGA-O2A-C1
13	a	806	CLA	CBD-CGD-O2D-CED
13	a	833	CLA	CBD-CGD-O2D-CED
13	b	814	CLA	CBD-CGD-O2D-CED
13	b	828	CLA	CBD-CGD-O2D-CED
13	b	840	CLA	CBD-CGD-O2D-CED
13	b	822	CLA	O1D-CGD-O2D-CED
16	b	851	LHG	O2-C2-C3-O3
13	k	4002	CLA	C3-C5-C6-C7
13	a	803	CLA	CBA-CGA-O2A-C1
13	a	821	CLA	CBA-CGA-O2A-C1
13	a	822	CLA	CBA-CGA-O2A-C1
13	a	823	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	a	832	CLA	CBA-CGA-O2A-C1
13	b	812	CLA	CBA-CGA-O2A-C1
13	b	816	CLA	CBA-CGA-O2A-C1
13	b	829	CLA	CBA-CGA-O2A-C1
13	b	830	CLA	CBA-CGA-O2A-C1
13	b	832	CLA	CBA-CGA-O2A-C1
17	b	852	LMG	C29-C28-O8-C9
12	a	801	CL0	O1A-CGA-O2A-C1
13	a	823	CLA	O1A-CGA-O2A-C1
13	a	838	CLA	O1A-CGA-O2A-C1
13	a	855	CLA	O1A-CGA-O2A-C1
13	b	812	CLA	O1A-CGA-O2A-C1
13	b	824	CLA	O1D-CGD-O2D-CED
13	b	835	CLA	O1D-CGD-O2D-CED
13	a	814	CLA	CBD-CGD-O2D-CED
13	f	203	CLA	CBD-CGD-O2D-CED
16	a	851	LHG	C29-C30-C31-C32
13	b	816	CLA	O1A-CGA-O2A-C1
13	f	201	CLA	O1A-CGA-O2A-C1
13	a	813	CLA	O1D-CGD-O2D-CED
13	a	834	CLA	CBD-CGD-O2D-CED
13	j	104	CLA	CBD-CGD-O2D-CED
13	a	823	CLA	C3-C5-C6-C7
13	b	814	CLA	C3-C5-C6-C7
12	a	801	CL0	CBA-CGA-O2A-C1
17	b	850	LMG	C4-C5-C6-O5
17	b	852	LMG	C4-C5-C6-O5
13	a	832	CLA	O1A-CGA-O2A-C1
13	b	817	CLA	O1A-CGA-O2A-C1
13	b	831	CLA	O1A-CGA-O2A-C1
16	b	851	LHG	C32-C33-C34-C35
17	b	850	LMG	O6-C5-C6-O5
13	b	830	CLA	C4-C3-C5-C6
13	b	838	CLA	C4-C3-C5-C6
13	a	830	CLA	C2-C3-C5-C6
13	b	830	CLA	C2-C3-C5-C6
13	b	838	CLA	C2-C3-C5-C6
13	a	820	CLA	C2A-CAA-CBA-CGA
13	a	827	CLA	C2A-CAA-CBA-CGA
23	j	102	LMT	O5'-C5'-C6'-O6'
13	a	803	CLA	O1A-CGA-O2A-C1
13	a	821	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	b	814	CLA	O1A-CGA-O2A-C1
13	b	829	CLA	O1A-CGA-O2A-C1
17	b	852	LMG	O10-C28-O8-C9
13	a	804	CLA	CBA-CGA-O2A-C1
13	a	825	CLA	CBA-CGA-O2A-C1
13	a	830	CLA	CBA-CGA-O2A-C1
13	b	842	CLA	CBA-CGA-O2A-C1
13	a	822	CLA	O1D-CGD-O2D-CED
13	a	816	CLA	CBD-CGD-O2D-CED
13	k	4004	CLA	C2C-C3C-CAC-CBC
16	a	849	LHG	C1-C2-C3-O3
17	b	852	LMG	O6-C5-C6-O5
13	a	804	CLA	O1A-CGA-O2A-C1
13	a	830	CLA	O1A-CGA-O2A-C1
13	b	810	CLA	O1A-CGA-O2A-C1
13	a	807	CLA	CBA-CGA-O2A-C1
13	a	808	CLA	CBA-CGA-O2A-C1
13	a	835	CLA	CBA-CGA-O2A-C1
13	a	836	CLA	CBA-CGA-O2A-C1
13	a	840	CLA	CBA-CGA-O2A-C1
13	b	810	CLA	CBA-CGA-O2A-C1
23	j	102	LMT	C4B-C5B-C6B-O6B
13	a	813	CLA	C13-C15-C16-C17
13	a	828	CLA	C10-C11-C12-C13
13	b	834	CLA	C15-C16-C17-C18
13	k	4002	CLA	C5-C6-C7-C8
17	a	850	LMG	C2-C1-O1-C7
17	b	850	LMG	O7-C8-C9-O8
13	a	836	CLA	O1A-CGA-O2A-C1
13	a	840	CLA	O1A-CGA-O2A-C1
13	b	810	CLA	C2-C3-C5-C6
13	f	201	CLA	C2-C3-C5-C6
13	a	807	CLA	C11-C10-C8-C9
13	a	808	CLA	C11-C12-C13-C14
13	a	817	CLA	C11-C10-C8-C9
13	a	818	CLA	C6-C7-C8-C9
13	a	818	CLA	C11-C10-C8-C9
13	a	820	CLA	C11-C10-C8-C9
13	a	825	CLA	C14-C13-C15-C16
13	a	834	CLA	C6-C7-C8-C9
13	a	838	CLA	C11-C10-C8-C9
13	a	841	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
13	b	801	CLA	C11-C10-C8-C9
13	b	805	CLA	C14-C13-C15-C16
13	b	820	CLA	C11-C10-C8-C9
13	b	830	CLA	C11-C12-C13-C14
13	a	827	CLA	O1D-CGD-O2D-CED
13	b	830	CLA	O1D-CGD-O2D-CED
13	a	807	CLA	C2A-CAA-CBA-CGA
13	l	1503	CLA	C2A-CAA-CBA-CGA
15	a	845	BCR	C37-C22-C23-C24
15	b	845	BCR	C37-C22-C23-C24
15	f	202	BCR	C7-C8-C9-C34
15	k	4001	BCR	C37-C22-C23-C24
15	i	102	BCR	C21-C22-C23-C24
17	b	852	LMG	C28-C29-C30-C31
13	a	835	CLA	O1A-CGA-O2A-C1
13	a	818	CLA	C8-C10-C11-C12
13	a	827	CLA	C8-C10-C11-C12
13	l	1503	CLA	CBA-CGA-O2A-C1
17	b	850	LMG	C29-C28-O8-C9
13	a	811	CLA	C13-C15-C16-C17
13	a	813	CLA	C15-C16-C17-C18
13	a	841	CLA	C10-C11-C12-C13
13	b	827	CLA	C8-C10-C11-C12
13	b	833	CLA	C10-C11-C12-C13
13	b	834	CLA	C5-C6-C7-C8
13	b	840	CLA	C10-C11-C12-C13
14	a	843	PQN	C18-C20-C21-C22
13	a	809	CLA	O1D-CGD-O2D-CED
17	a	852	LMG	O6-C5-C6-O5
13	a	807	CLA	C13-C15-C16-C17
13	a	832	CLA	C10-C11-C12-C13
13	a	839	CLA	C15-C16-C17-C18
13	b	804	CLA	C10-C11-C12-C13
13	b	805	CLA	C10-C11-C12-C13
13	b	806	CLA	C13-C15-C16-C17
13	b	807	CLA	C5-C6-C7-C8
13	b	808	CLA	C5-C6-C7-C8
13	b	811	CLA	C5-C6-C7-C8
13	b	841	CLA	C15-C16-C17-C18
16	a	849	LHG	O1-C1-C2-O2
16	a	853	LHG	C23-C24-C25-C26
16	b	851	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
17	a	852	LMG	C28-C29-C30-C31
13	b	804	CLA	C4C-C3C-CAC-CBC
16	a	853	LHG	C28-C29-C30-C31
13	b	841	CLA	O1D-CGD-O2D-CED
13	a	822	CLA	C13-C15-C16-C17
13	b	828	CLA	C8-C10-C11-C12
13	b	834	CLA	O1D-CGD-O2D-CED
13	b	836	CLA	O1D-CGD-O2D-CED
13	a	854	CLA	C2-C1-O2A-CGA
13	b	822	CLA	C2-C1-O2A-CGA
13	a	818	CLA	C13-C15-C16-C17
13	a	819	CLA	C15-C16-C17-C18
13	b	827	CLA	C5-C6-C7-C8
13	a	808	CLA	O1A-CGA-O2A-C1
16	a	851	LHG	C7-C8-C9-C10
16	f	206	LHG	C23-C24-C25-C26
17	a	850	LMG	C10-C11-C12-C13
13	a	811	CLA	C5-C6-C7-C8
13	a	820	CLA	C5-C6-C7-C8
13	a	808	CLA	C6-C7-C8-C10
13	a	808	CLA	C11-C12-C13-C15
13	a	833	CLA	C11-C12-C13-C15
13	a	838	CLA	C11-C10-C8-C7
13	b	807	CLA	C11-C10-C8-C7
13	b	807	CLA	C12-C13-C15-C16
13	b	825	CLA	C11-C10-C8-C7
13	b	825	CLA	C11-C12-C13-C15
13	b	833	CLA	C6-C7-C8-C10
13	b	819	CLA	C3-C5-C6-C7
13	a	807	CLA	O1A-CGA-O2A-C1
13	a	827	CLA	C10-C11-C12-C13
13	a	829	CLA	C5-C6-C7-C8
23	j	102	LMT	O5B-C5B-C6B-O6B
15	b	844	BCR	C18-C19-C20-C21
15	b	849	BCR	C10-C11-C12-C13
16	a	851	LHG	O2-C2-C3-O3
16	f	206	LHG	O2-C2-C3-O3
13	a	804	CLA	C13-C15-C16-C17
13	b	835	CLA	C13-C15-C16-C17
13	a	825	CLA	O1A-CGA-O2A-C1
13	a	818	CLA	C5-C6-C7-C8
13	b	803	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
13	b	814	CLA	C5-C6-C7-C8
13	b	830	CLA	C5-C6-C7-C8
13	k	4002	CLA	C13-C15-C16-C17
13	l	1503	CLA	O1A-CGA-O2A-C1
13	k	4004	CLA	C4C-C3C-CAC-CBC
13	a	821	CLA	C8-C10-C11-C12
13	a	823	CLA	C5-C6-C7-C8
13	a	855	CLA	C13-C15-C16-C17
13	b	807	CLA	C13-C15-C16-C17
13	b	814	CLA	C13-C15-C16-C17
16	a	851	LHG	C4-O6-P-O3
13	a	824	CLA	O1D-CGD-O2D-CED
22	b	854	ZEX	C25-C26-C27-C28
16	a	851	LHG	C23-C24-C25-C26
16	a	851	LHG	C1-C2-C3-O3
16	b	851	LHG	C1-C2-C3-O3
16	f	206	LHG	C1-C2-C3-O3
13	a	821	CLA	C10-C11-C12-C13
13	b	801	CLA	C2A-CAA-CBA-CGA
13	a	836	CLA	C6-C7-C8-C9
17	b	850	LMG	C28-C29-C30-C31
13	b	842	CLA	O1A-CGA-O2A-C1
16	f	206	LHG	C11-C12-C13-C14
23	j	102	LMT	O5B-C1B-O1B-C4'
17	a	852	LMG	C30-C31-C32-C33
15	b	847	BCR	C20-C21-C22-C37
15	b	849	BCR	C20-C21-C22-C37
15	i	101	BCR	C16-C17-C18-C36
15	i	101	BCR	C20-C21-C22-C37
15	k	4005	BCR	C16-C17-C18-C36
16	a	853	LHG	C12-C13-C14-C15
13	a	824	CLA	C11-C12-C13-C15
13	a	829	CLA	C16-C17-C18-C19
13	b	841	CLA	C16-C17-C18-C20
17	b	852	LMG	C17-C18-C19-C20
17	b	850	LMG	C32-C33-C34-C35
17	b	852	LMG	C14-C15-C16-C17
17	b	852	LMG	C18-C19-C20-C21
16	a	849	LHG	C24-C25-C26-C27
16	a	851	LHG	C28-C29-C30-C31
17	b	852	LMG	C34-C35-C36-C37
13	b	809	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
15	a	847	BCR	C20-C21-C22-C23
15	b	849	BCR	C16-C17-C18-C19
17	b	850	LMG	C30-C31-C32-C33
17	b	850	LMG	C33-C34-C35-C36
13	a	833	CLA	O1D-CGD-O2D-CED
13	b	814	CLA	C4-C3-C5-C6
16	a	851	LHG	C27-C28-C29-C30
16	a	851	LHG	C32-C33-C34-C35
13	a	805	CLA	C11-C12-C13-C14
13	a	826	CLA	C11-C10-C8-C9
13	a	829	CLA	C11-C12-C13-C14
13	f	201	CLA	C11-C12-C13-C14
16	f	206	LHG	C7-C8-C9-C10
17	a	850	LMG	C38-C39-C40-C41
17	a	852	LMG	C32-C33-C34-C35
17	b	850	LMG	C34-C35-C36-C37
13	a	834	CLA	C5-C6-C7-C8
13	a	839	CLA	C10-C11-C12-C13
13	b	810	CLA	C8-C10-C11-C12
13	b	821	CLA	C5-C6-C7-C8
13	a	804	CLA	C2A-CAA-CBA-CGA
13	j	104	CLA	C2A-CAA-CBA-CGA
15	b	845	BCR	C36-C18-C19-C20
16	a	853	LHG	C16-C17-C18-C19
17	b	850	LMG	C39-C40-C41-C42
16	a	849	LHG	O1-C1-C2-C3
13	b	829	CLA	C8-C10-C11-C12
16	a	849	LHG	C23-C24-C25-C26
23	j	102	LMT	C11-C10-C9-C8
12	a	801	CL0	C4B-C3B-CAB-CBB
13	a	818	CLA	C4B-C3B-CAB-CBB
13	a	835	CLA	C4B-C3B-CAB-CBB
13	a	824	CLA	C11-C12-C13-C14
13	a	829	CLA	C16-C17-C18-C20
13	a	833	CLA	C16-C17-C18-C20
13	b	825	CLA	C13-C15-C16-C17
16	a	849	LHG	C29-C30-C31-C32
16	a	849	LHG	C34-C35-C36-C37
17	b	850	LMG	C16-C17-C18-C19
17	b	852	LMG	C30-C31-C32-C33
16	f	206	LHG	C28-C29-C30-C31
17	a	850	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
17	a	852	LMG	C33-C34-C35-C36
17	b	850	LMG	C37-C38-C39-C40
16	a	851	LHG	C24-C25-C26-C27
16	b	851	LHG	C24-C25-C26-C27
13	b	828	CLA	O1D-CGD-O2D-CED
13	b	840	CLA	O1D-CGD-O2D-CED
13	a	823	CLA	C3A-C2A-CAA-CBA
13	a	827	CLA	C3A-C2A-CAA-CBA
13	a	837	CLA	C3A-C2A-CAA-CBA
13	a	842	CLA	C3A-C2A-CAA-CBA
13	b	806	CLA	C3A-C2A-CAA-CBA
13	b	812	CLA	C3A-C2A-CAA-CBA
13	b	817	CLA	C3A-C2A-CAA-CBA
13	b	825	CLA	C3A-C2A-CAA-CBA
13	j	103	CLA	C3A-C2A-CAA-CBA
13	b	812	CLA	C5-C6-C7-C8
16	a	853	LHG	C29-C30-C31-C32
16	a	853	LHG	C32-C33-C34-C35
16	b	851	LHG	C28-C29-C30-C31
17	a	850	LMG	C36-C37-C38-C39
13	a	806	CLA	O1D-CGD-O2D-CED
13	b	807	CLA	C16-C17-C18-C20
16	a	853	LHG	C30-C31-C32-C33
17	b	852	LMG	C32-C33-C34-C35
17	b	852	LMG	C16-C17-C18-C19
13	a	855	CLA	O2A-C1-C2-C3
15	f	202	BCR	C14-C15-C16-C17
13	a	807	CLA	C8-C10-C11-C12
13	b	806	CLA	C4-C3-C5-C6
13	b	833	CLA	C4-C3-C5-C6
13	a	839	CLA	CBA-CGA-O2A-C1
13	a	819	CLA	C2-C3-C5-C6
13	b	806	CLA	C2-C3-C5-C6
17	a	852	LMG	C31-C32-C33-C34
13	b	814	CLA	C2A-CAA-CBA-CGA
16	b	851	LHG	O1-C1-C2-O2
13	a	820	CLA	C13-C15-C16-C17
13	b	841	CLA	C16-C17-C18-C19
17	a	850	LMG	C17-C18-C19-C20
12	a	801	CL0	C2B-C3B-CAB-CBB
13	a	818	CLA	C2B-C3B-CAB-CBB
13	a	833	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	a	835	CLA	C2B-C3B-CAB-CBB
13	a	813	CLA	CBA-CGA-O2A-C1
17	a	852	LMG	C13-C14-C15-C16
12	a	801	CL0	C2-C1-O2A-CGA
13	a	818	CLA	C2-C1-O2A-CGA
13	a	823	CLA	C2-C1-O2A-CGA
13	a	829	CLA	C2-C1-O2A-CGA
13	a	838	CLA	C2-C1-O2A-CGA
13	b	804	CLA	C2-C1-O2A-CGA
13	l	1502	CLA	C2-C1-O2A-CGA
13	a	823	CLA	C8-C10-C11-C12
13	b	807	CLA	C15-C16-C17-C18
13	b	840	CLA	C8-C10-C11-C12
16	a	851	LHG	C11-C12-C13-C14
16	a	853	LHG	C7-C8-C9-C10
13	a	818	CLA	C3-C5-C6-C7
13	b	834	CLA	C3-C5-C6-C7
15	a	844	BCR	C5-C6-C7-C8
15	a	845	BCR	C5-C6-C7-C8
15	a	847	BCR	C5-C6-C7-C8
15	a	847	BCR	C23-C24-C25-C26
15	b	844	BCR	C1-C6-C7-C8
15	b	844	BCR	C5-C6-C7-C8
15	b	844	BCR	C23-C24-C25-C26
15	b	844	BCR	C23-C24-C25-C30
15	b	845	BCR	C5-C6-C7-C8
15	i	102	BCR	C23-C24-C25-C26
15	i	102	BCR	C23-C24-C25-C30
15	j	101	BCR	C5-C6-C7-C8
15	j	105	BCR	C1-C6-C7-C8
15	j	105	BCR	C5-C6-C7-C8
15	k	4005	BCR	C23-C24-C25-C30
20	b	846	ECH	C1-C6-C7-C8
20	b	846	ECH	C5-C6-C7-C8
20	m	101	ECH	C5-C6-C7-C8
13	b	814	CLA	O1D-CGD-O2D-CED
13	b	826	CLA	CBA-CGA-O2A-C1
13	a	817	CLA	C10-C11-C12-C13
13	b	805	CLA	C15-C16-C17-C18
16	a	853	LHG	C11-C10-C9-C8
23	j	102	LMT	C7-C8-C9-C10
13	a	836	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
13	a	839	CLA	C8-C10-C11-C12
16	b	851	LHG	C26-C27-C28-C29
13	a	819	CLA	C4-C3-C5-C6
13	a	805	CLA	C11-C12-C13-C15
13	a	813	CLA	C6-C7-C8-C10
13	a	817	CLA	C11-C10-C8-C7
13	a	820	CLA	C2-C3-C5-C6
13	a	826	CLA	C11-C10-C8-C7
13	a	827	CLA	C2-C3-C5-C6
13	a	829	CLA	C11-C12-C13-C15
13	a	835	CLA	C11-C12-C13-C15
13	b	814	CLA	C2-C3-C5-C6
13	b	833	CLA	C2-C3-C5-C6
13	b	841	CLA	C11-C12-C13-C15
13	f	201	CLA	C11-C12-C13-C15
13	a	807	CLA	C3-C5-C6-C7
13	a	813	CLA	O1A-CGA-O2A-C1
13	a	839	CLA	O1A-CGA-O2A-C1
13	a	828	CLA	C15-C16-C17-C18
13	a	840	CLA	C15-C16-C17-C18
13	a	832	CLA	CBD-CGD-O2D-CED
13	a	839	CLA	CBD-CGD-O2D-CED
13	a	814	CLA	CBA-CGA-O2A-C1
13	a	833	CLA	CBA-CGA-O2A-C1
13	b	828	CLA	C2A-CAA-CBA-CGA
13	l	1501	CLA	C2A-CAA-CBA-CGA
13	a	803	CLA	C15-C16-C17-C18
13	a	834	CLA	O1D-CGD-O2D-CED
16	a	849	LHG	C11-C12-C13-C14
16	a	849	LHG	C32-C33-C34-C35
13	a	821	CLA	C16-C17-C18-C20
13	k	4002	CLA	C16-C17-C18-C19
13	b	815	CLA	C15-C16-C17-C18
13	a	814	CLA	O1D-CGD-O2D-CED
13	f	203	CLA	O1D-CGD-O2D-CED
16	a	849	LHG	C15-C16-C17-C18
16	a	849	LHG	C26-C27-C28-C29
16	a	849	LHG	C8-C7-O7-C5
17	b	852	LMG	C11-C10-O7-C8
15	i	102	BCR	C18-C19-C20-C21
16	f	206	LHG	C24-C25-C26-C27
13	b	805	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
13	b	833	CLA	CBD-CGD-O2D-CED
16	f	206	LHG	C32-C33-C34-C35
13	b	820	CLA	C3-C5-C6-C7
17	a	850	LMG	O7-C8-C9-O8
13	a	836	CLA	C6-C7-C8-C10
13	j	104	CLA	O1D-CGD-O2D-CED
13	a	820	CLA	C4-C3-C5-C6
13	a	827	CLA	C4-C3-C5-C6
13	a	811	CLA	C14-C13-C15-C16
13	a	823	CLA	C14-C13-C15-C16
13	a	829	CLA	C14-C13-C15-C16
13	a	835	CLA	C11-C12-C13-C14
13	a	840	CLA	C11-C12-C13-C14
13	b	819	CLA	C11-C10-C8-C9
13	b	819	CLA	C14-C13-C15-C16
13	b	824	CLA	C11-C10-C8-C9
13	b	833	CLA	C6-C7-C8-C9
13	b	841	CLA	C11-C12-C13-C14
13	b	808	CLA	C3-C5-C6-C7
13	a	830	CLA	C2A-CAA-CBA-CGA
13	b	835	CLA	C2A-CAA-CBA-CGA
13	b	826	CLA	O1A-CGA-O2A-C1
13	a	804	CLA	C1A-C2A-CAA-CBA
13	a	805	CLA	C1A-C2A-CAA-CBA
13	a	807	CLA	C1A-C2A-CAA-CBA
13	a	809	CLA	C1A-C2A-CAA-CBA
13	a	810	CLA	C1A-C2A-CAA-CBA
13	a	814	CLA	C1A-C2A-CAA-CBA
13	a	826	CLA	C1A-C2A-CAA-CBA
13	a	827	CLA	C1A-C2A-CAA-CBA
13	a	831	CLA	C1A-C2A-CAA-CBA
13	a	837	CLA	C1A-C2A-CAA-CBA
13	a	841	CLA	C1A-C2A-CAA-CBA
13	a	842	CLA	C1A-C2A-CAA-CBA
13	b	826	CLA	C1A-C2A-CAA-CBA
13	k	4003	CLA	C1A-C2A-CAA-CBA
13	k	4004	CLA	C1A-C2A-CAA-CBA
13	a	821	CLA	C16-C17-C18-C19
13	b	807	CLA	C16-C17-C18-C19
13	b	825	CLA	C5-C6-C7-C8
12	a	801	CL0	C3-C5-C6-C7
13	a	841	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
13	b	811	CLA	C3-C5-C6-C7
13	a	803	CLA	C5-C6-C7-C8
13	a	825	CLA	C13-C15-C16-C17
13	a	816	CLA	O1D-CGD-O2D-CED
16	b	851	LHG	C33-C34-C35-C36
13	a	818	CLA	C16-C17-C18-C20
22	f	205	ZEX	C25-C26-C27-C28
17	a	850	LMG	C32-C33-C34-C35
16	a	849	LHG	C28-C29-C30-C31
16	a	853	LHG	C34-C35-C36-C37
13	b	804	CLA	C2A-CAA-CBA-CGA
13	a	833	CLA	C16-C17-C18-C19
16	b	851	LHG	C30-C31-C32-C33
13	b	826	CLA	C6-C7-C8-C10
13	a	814	CLA	O1A-CGA-O2A-C1
15	b	849	BCR	C11-C10-C9-C34
15	f	202	BCR	C35-C13-C14-C15
15	i	102	BCR	C20-C21-C22-C37
13	a	833	CLA	C4-C3-C5-C6
13	b	815	CLA	C4-C3-C5-C6
13	b	815	CLA	C2-C3-C5-C6
13	a	837	CLA	CBA-CGA-O2A-C1
13	b	811	CLA	CBA-CGA-O2A-C1
13	k	4003	CLA	CBD-CGD-O2D-CED
13	a	841	CLA	C5-C6-C7-C8
13	l	1502	CLA	C13-C15-C16-C17
16	a	849	LHG	C30-C31-C32-C33
13	a	802	CLA	C2A-CAA-CBA-CGA
13	b	824	CLA	C2A-CAA-CBA-CGA
13	a	805	CLA	C5-C6-C7-C8
13	a	855	CLA	C5-C6-C7-C8
13	b	801	CLA	C5-C6-C7-C8
13	a	822	CLA	C2-C1-O2A-CGA
13	a	824	CLA	C2-C1-O2A-CGA
13	a	825	CLA	C2-C1-O2A-CGA
13	a	855	CLA	C2-C1-O2A-CGA
13	b	803	CLA	C2-C1-O2A-CGA
13	b	808	CLA	C2-C1-O2A-CGA
13	b	825	CLA	C2-C1-O2A-CGA
13	b	838	CLA	C2-C1-O2A-CGA
16	a	849	LHG	C18-C19-C20-C21
17	a	850	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
17	b	852	LMG	C13-C14-C15-C16
13	a	829	CLA	C15-C16-C17-C18
13	a	833	CLA	O1A-CGA-O2A-C1
16	b	851	LHG	O6-C4-C5-O7
13	a	818	CLA	C16-C17-C18-C19
12	a	801	CL0	C5-C6-C7-C8
13	b	809	CLA	C5-C6-C7-C8
17	b	852	LMG	C2-C1-O1-C7
13	k	4002	CLA	C15-C16-C17-C18
13	a	806	CLA	C12-C13-C15-C16
13	a	807	CLA	C11-C12-C13-C15
13	a	811	CLA	C12-C13-C15-C16
13	a	820	CLA	C6-C7-C8-C10
13	a	820	CLA	C11-C12-C13-C15
13	a	821	CLA	C11-C12-C13-C15
13	a	823	CLA	C11-C12-C13-C15
13	a	823	CLA	C12-C13-C15-C16
13	a	829	CLA	C12-C13-C15-C16
13	a	833	CLA	C2-C3-C5-C6
13	a	833	CLA	C11-C10-C8-C7
13	a	834	CLA	C6-C7-C8-C10
13	a	839	CLA	C12-C13-C15-C16
13	a	841	CLA	C11-C12-C13-C15
13	b	801	CLA	C6-C7-C8-C10
13	b	803	CLA	C11-C10-C8-C7
13	b	804	CLA	C11-C10-C8-C7
13	b	805	CLA	C12-C13-C15-C16
13	b	814	CLA	C11-C12-C13-C15
13	b	815	CLA	C11-C10-C8-C7
13	b	815	CLA	C12-C13-C15-C16
13	b	819	CLA	C11-C10-C8-C7
13	b	819	CLA	C12-C13-C15-C16
13	b	824	CLA	C11-C10-C8-C7
13	b	828	CLA	C11-C12-C13-C15
13	b	835	CLA	C11-C10-C8-C7
13	b	835	CLA	C11-C12-C13-C15
13	b	838	CLA	C6-C7-C8-C10
13	b	840	CLA	C6-C7-C8-C10
13	f	201	CLA	C6-C7-C8-C10
13	k	4002	CLA	C12-C13-C15-C16
13	l	1502	CLA	C11-C12-C13-C15
16	f	206	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
13	a	806	CLA	C6-C7-C8-C9
13	a	806	CLA	C11-C12-C13-C14
13	a	806	CLA	C14-C13-C15-C16
13	a	807	CLA	C11-C12-C13-C14
13	a	808	CLA	C6-C7-C8-C9
13	a	811	CLA	C11-C12-C13-C14
13	a	813	CLA	C11-C12-C13-C14
13	a	817	CLA	C11-C12-C13-C14
13	a	819	CLA	C14-C13-C15-C16
13	a	820	CLA	C11-C12-C13-C14
13	a	822	CLA	C11-C10-C8-C9
13	a	830	CLA	C6-C7-C8-C9
13	a	833	CLA	C11-C10-C8-C9
13	a	839	CLA	C14-C13-C15-C16
13	a	841	CLA	C6-C7-C8-C9
13	b	801	CLA	C6-C7-C8-C9
13	b	803	CLA	C11-C10-C8-C9
13	b	803	CLA	C11-C12-C13-C14
13	b	804	CLA	C11-C10-C8-C9
13	b	815	CLA	C14-C13-C15-C16
13	b	825	CLA	C6-C7-C8-C9
13	b	825	CLA	C11-C10-C8-C9
13	b	828	CLA	C11-C12-C13-C14
13	b	833	CLA	C11-C10-C8-C9
13	b	834	CLA	C11-C10-C8-C9
13	b	835	CLA	C11-C10-C8-C9
13	b	835	CLA	C11-C12-C13-C14
13	b	838	CLA	C6-C7-C8-C9
13	f	201	CLA	C6-C7-C8-C9
13	k	4002	CLA	C6-C7-C8-C9
13	k	4002	CLA	C14-C13-C15-C16
13	l	1502	CLA	C11-C12-C13-C14
13	a	839	CLA	C5-C6-C7-C8
13	a	819	CLA	C16-C17-C18-C20
13	a	820	CLA	C16-C17-C18-C20
13	b	826	CLA	C6-C7-C8-C9
15	b	845	BCR	C21-C22-C23-C24
15	b	849	BCR	C11-C12-C13-C14
13	b	816	CLA	C3-C5-C6-C7
13	a	841	CLA	C8-C10-C11-C12
13	b	819	CLA	C13-C15-C16-C17
17	a	850	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
17	b	852	LMG	C33-C34-C35-C36
13	a	826	CLA	C4B-C3B-CAB-CBB
13	b	840	CLA	C4B-C3B-CAB-CBB
16	a	853	LHG	O6-C4-C5-C6
16	b	851	LHG	O6-C4-C5-C6
13	a	812	CLA	C4-C3-C5-C6
13	a	807	CLA	C16-C17-C18-C20
13	a	855	CLA	C16-C17-C18-C20
13	a	804	CLA	C3A-C2A-CAA-CBA
13	a	807	CLA	C3A-C2A-CAA-CBA
13	a	810	CLA	C3A-C2A-CAA-CBA
13	a	811	CLA	C3A-C2A-CAA-CBA
13	a	812	CLA	C3A-C2A-CAA-CBA
13	a	817	CLA	C3A-C2A-CAA-CBA
13	a	828	CLA	C3A-C2A-CAA-CBA
13	b	813	CLA	C3A-C2A-CAA-CBA
13	b	840	CLA	C3A-C2A-CAA-CBA
13	l	1502	CLA	C3A-C2A-CAA-CBA
17	a	850	LMG	C12-C13-C14-C15
13	a	810	CLA	CBA-CGA-O2A-C1
17	b	850	LMG	C7-C8-C9-O8
13	b	811	CLA	O1A-CGA-O2A-C1
13	b	804	CLA	O2A-C1-C2-C3
13	b	841	CLA	C10-C11-C12-C13
17	b	852	LMG	C41-C42-C43-C44
13	b	829	CLA	CBD-CGD-O2D-CED
13	f	201	CLA	C15-C16-C17-C18
13	a	837	CLA	O1A-CGA-O2A-C1
13	a	821	CLA	C2A-CAA-CBA-CGA
13	a	805	CLA	C10-C11-C12-C13
13	a	820	CLA	C16-C17-C18-C19
13	b	803	CLA	C2B-C3B-CAB-CBB
13	b	840	CLA	C2B-C3B-CAB-CBB
17	a	850	LMG	C11-C12-C13-C14
16	a	849	LHG	O7-C5-C6-O8
13	b	821	CLA	C15-C16-C17-C18
16	f	206	LHG	C30-C31-C32-C33
13	a	817	CLA	C2-C1-O2A-CGA
13	a	825	CLA	C11-C12-C13-C14
13	a	827	CLA	C14-C13-C15-C16
13	a	833	CLA	C11-C12-C13-C14
13	a	835	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
13	b	805	CLA	C6-C7-C8-C9
13	b	807	CLA	C11-C10-C8-C9
13	b	815	CLA	C6-C7-C8-C9
13	b	825	CLA	C11-C12-C13-C14
13	b	835	CLA	C14-C13-C15-C16
13	a	820	CLA	C8-C10-C11-C12
22	b	854	ZEX	C21-C26-C27-C28
22	f	205	ZEX	C21-C26-C27-C28
13	a	803	CLA	C2A-CAA-CBA-CGA
13	b	831	CLA	C2A-CAA-CBA-CGA
13	a	819	CLA	C16-C17-C18-C19
13	a	831	CLA	C3-C5-C6-C7
15	a	845	BCR	C23-C24-C25-C26
15	a	845	BCR	C23-C24-C25-C30
15	a	846	BCR	C1-C6-C7-C8
15	a	846	BCR	C5-C6-C7-C8
15	a	848	BCR	C1-C6-C7-C8
15	a	848	BCR	C5-C6-C7-C8
15	b	847	BCR	C23-C24-C25-C26
15	b	847	BCR	C23-C24-C25-C30
15	i	102	BCR	C1-C6-C7-C8
15	i	102	BCR	C5-C6-C7-C8
15	j	105	BCR	C23-C24-C25-C26
15	k	4001	BCR	C1-C6-C7-C8
15	k	4001	BCR	C5-C6-C7-C8
13	b	807	CLA	C10-C11-C12-C13
17	a	850	LMG	C19-C20-C21-C22
17	b	850	LMG	C15-C16-C17-C18
16	a	853	LHG	C33-C34-C35-C36
13	a	839	CLA	O1D-CGD-O2D-CED
15	a	848	BCR	C11-C12-C13-C14
15	a	848	BCR	C16-C17-C18-C36
15	b	848	BCR	C21-C22-C23-C24
13	a	808	CLA	C10-C11-C12-C13
13	b	822	CLA	C11-C12-C13-C15
13	k	4002	CLA	C16-C17-C18-C20
14	b	843	PQN	C13-C15-C16-C17
13	a	832	CLA	O1D-CGD-O2D-CED
17	b	850	LMG	O10-C28-O8-C9
17	b	850	LMG	C38-C39-C40-C41
17	b	852	LMG	C37-C38-C39-C40
13	a	806	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
13	a	818	CLA	C11-C10-C8-C7
13	a	819	CLA	C12-C13-C15-C16
13	a	822	CLA	C11-C10-C8-C7
13	a	825	CLA	C11-C12-C13-C15
13	a	826	CLA	C12-C13-C15-C16
13	a	827	CLA	C11-C10-C8-C7
13	a	827	CLA	C12-C13-C15-C16
13	a	830	CLA	C6-C7-C8-C10
13	a	835	CLA	C6-C7-C8-C10
13	a	841	CLA	C6-C7-C8-C10
13	b	801	CLA	C11-C10-C8-C7
13	b	806	CLA	C12-C13-C15-C16
13	b	808	CLA	C6-C7-C8-C10
13	b	815	CLA	C6-C7-C8-C10
13	b	818	CLA	C11-C10-C8-C7
13	b	825	CLA	C6-C7-C8-C10
13	b	833	CLA	C11-C10-C8-C7
13	b	835	CLA	C12-C13-C15-C16
13	k	4002	CLA	C6-C7-C8-C10
13	a	855	CLA	C16-C17-C18-C19
17	b	850	LMG	C41-C42-C43-C44
13	b	838	CLA	C5-C6-C7-C8
13	a	823	CLA	C13-C15-C16-C17
15	a	845	BCR	C20-C21-C22-C37
15	a	846	BCR	C16-C17-C18-C36
13	b	803	CLA	C3-C5-C6-C7
13	b	807	CLA	C3-C5-C6-C7
13	a	804	CLA	C16-C17-C18-C20
13	a	807	CLA	C16-C17-C18-C19
13	f	201	CLA	C16-C17-C18-C20
13	b	805	CLA	CBA-CGA-O2A-C1
17	b	850	LMG	C31-C32-C33-C34
13	a	808	CLA	C15-C16-C17-C18
13	b	819	CLA	C10-C11-C12-C13
13	a	810	CLA	O1A-CGA-O2A-C1
13	a	808	CLA	CAD-CBD-CGD-O2D
13	a	825	CLA	CAD-CBD-CGD-O2D
13	b	813	CLA	CAD-CBD-CGD-O2D
13	b	817	CLA	CAD-CBD-CGD-O2D
13	b	819	CLA	CAD-CBD-CGD-O2D
13	b	830	CLA	CAD-CBD-CGD-O2D
13	b	833	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
13	b	839	CLA	CAD-CBD-CGD-O2D
16	a	853	LHG	C6-C5-O7-C7
15	a	846	BCR	C22-C23-C24-C25
15	b	844	BCR	C6-C7-C8-C9
15	i	102	BCR	C22-C23-C24-C25
15	j	105	BCR	C6-C7-C8-C9
13	b	824	CLA	CBA-CGA-O2A-C1
17	b	852	LMG	O1-C7-C8-C9
16	a	853	LHG	O6-C4-C5-O7
13	a	802	CLA	C10-C11-C12-C13
13	a	838	CLA	C8-C10-C11-C12
13	a	838	CLA	C10-C11-C12-C13
16	a	851	LHG	C10-C11-C12-C13
13	f	204	CLA	C2A-CAA-CBA-CGA
13	f	201	CLA	C8-C10-C11-C12
23	j	102	LMT	C3-C4-C5-C6
13	b	833	CLA	O1D-CGD-O2D-CED
13	a	804	CLA	CHA-CBD-CGD-O2D
13	a	822	CLA	CHA-CBD-CGD-O1D
13	a	834	CLA	CHA-CBD-CGD-O1D
13	a	834	CLA	CHA-CBD-CGD-O2D
13	a	839	CLA	CHA-CBD-CGD-O1D
13	a	839	CLA	CHA-CBD-CGD-O2D
13	b	806	CLA	CHA-CBD-CGD-O1D
13	b	806	CLA	CHA-CBD-CGD-O2D
13	b	822	CLA	CHA-CBD-CGD-O1D
13	b	837	CLA	CHA-CBD-CGD-O1D
13	b	837	CLA	CHA-CBD-CGD-O2D
13	f	204	CLA	CHA-CBD-CGD-O1D
13	l	1501	CLA	CHA-CBD-CGD-O1D
13	l	1501	CLA	CHA-CBD-CGD-O2D
15	a	846	BCR	C12-C13-C14-C15
16	a	853	LHG	C24-C25-C26-C27
13	b	828	CLA	C4-C3-C5-C6
13	a	827	CLA	C11-C10-C8-C9
13	a	833	CLA	C14-C13-C15-C16
13	f	201	CLA	C3-C5-C6-C7
13	a	816	CLA	C2A-CAA-CBA-CGA
13	k	4004	CLA	C2A-CAA-CBA-CGA
13	b	809	CLA	C10-C11-C12-C13
13	k	4003	CLA	O1D-CGD-O2D-CED
15	j	101	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
13	a	806	CLA	C3-C5-C6-C7
16	a	853	LHG	C13-C14-C15-C16
13	a	811	CLA	C1A-C2A-CAA-CBA
13	b	806	CLA	C1A-C2A-CAA-CBA
13	b	841	CLA	C1A-C2A-CAA-CBA
13	j	104	CLA	C1A-C2A-CAA-CBA
13	a	840	CLA	C2-C1-O2A-CGA
13	b	828	CLA	C2-C1-O2A-CGA
13	a	839	CLA	C4-C3-C5-C6
23	j	102	LMT	O1'-C1-C2-C3
13	b	805	CLA	O1A-CGA-O2A-C1
13	a	823	CLA	C4B-C3B-CAB-CBB
13	a	838	CLA	C4B-C3B-CAB-CBB
13	a	841	CLA	C4B-C3B-CAB-CBB
13	b	803	CLA	C4B-C3B-CAB-CBB
13	b	809	CLA	C4B-C3B-CAB-CBB
13	b	818	CLA	C4B-C3B-CAB-CBB
13	b	839	CLA	C4B-C3B-CAB-CBB
13	b	841	CLA	C4B-C3B-CAB-CBB
13	f	204	CLA	C4B-C3B-CAB-CBB
13	j	103	CLA	C4B-C3B-CAB-CBB
13	k	4003	CLA	C4B-C3B-CAB-CBB
16	a	851	LHG	C4-O6-P-O5
16	b	851	LHG	C3-O3-P-O5
16	f	206	LHG	C3-O3-P-O4
13	a	840	CLA	C16-C17-C18-C19
13	b	821	CLA	C16-C17-C18-C20
13	b	822	CLA	C11-C12-C13-C14
13	a	825	CLA	C5-C6-C7-C8
12	a	801	CL0	CBD-CGD-O2D-CED
17	a	850	LMG	C18-C19-C20-C21
13	a	832	CLA	C3-C5-C6-C7
13	b	810	CLA	C3-C5-C6-C7
17	b	852	LMG	C42-C43-C44-C45
13	a	818	CLA	CAD-CBD-CGD-O1D
13	a	822	CLA	CAD-CBD-CGD-O1D
13	a	823	CLA	CAD-CBD-CGD-O1D
13	b	831	CLA	C2-C3-C5-C6
13	b	828	CLA	C10-C11-C12-C13
17	a	850	LMG	C37-C38-C39-C40
13	a	807	CLA	C11-C10-C8-C7
13	a	824	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
13	a	825	CLA	C12-C13-C15-C16
13	a	828	CLA	C11-C12-C13-C15
13	a	832	CLA	C11-C10-C8-C7
13	a	833	CLA	C12-C13-C15-C16
13	a	838	CLA	C11-C12-C13-C15
13	a	840	CLA	C6-C7-C8-C10
13	a	855	CLA	C11-C12-C13-C15
13	b	810	CLA	C11-C10-C8-C7
13	b	814	CLA	C12-C13-C15-C16
13	b	820	CLA	C11-C10-C8-C7
13	b	829	CLA	C11-C12-C13-C15
13	b	832	CLA	C3A-C2A-CAA-CBA
13	b	833	CLA	C12-C13-C15-C16
13	b	841	CLA	C12-C13-C15-C16
17	b	850	LMG	C42-C43-C44-C45
13	a	854	CLA	C5-C6-C7-C8
16	b	851	LHG	C8-C7-O7-C5
13	b	824	CLA	O1A-CGA-O2A-C1
16	a	853	LHG	C27-C28-C29-C30
13	a	841	CLA	C2A-CAA-CBA-CGA
13	b	829	CLA	O1D-CGD-O2D-CED
17	a	850	LMG	C42-C43-C44-C45
23	j	102	LMT	C6-C7-C8-C9
17	a	852	LMG	C4-C5-C6-O5
17	a	850	LMG	C7-C8-C9-O8
17	b	852	LMG	O1-C7-C8-O7
17	a	850	LMG	C41-C42-C43-C44
13	b	811	CLA	CAA-CBA-CGA-O2A
17	a	850	LMG	C34-C35-C36-C37
13	a	817	CLA	C14-C13-C15-C16
13	a	823	CLA	C11-C10-C8-C9
13	a	826	CLA	C14-C13-C15-C16
13	a	840	CLA	C6-C7-C8-C9
13	b	806	CLA	C14-C13-C15-C16
20	b	846	ECH	C22-C23-C24-C25
16	a	851	LHG	C15-C16-C17-C18
13	a	804	CLA	C16-C17-C18-C19
13	f	201	CLA	C16-C17-C18-C19
13	a	817	CLA	C2B-C3B-CAB-CBB
13	a	826	CLA	C2B-C3B-CAB-CBB
13	f	204	CLA	C2B-C3B-CAB-CBB
13	l	1502	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	b	828	CLA	C2-C3-C5-C6
13	b	819	CLA	C8-C10-C11-C12
13	a	832	CLA	C2A-CAA-CBA-CGA
13	b	811	CLA	C2A-CAA-CBA-CGA
13	b	816	CLA	C2A-CAA-CBA-CGA
13	a	834	CLA	C2-C1-O2A-CGA
13	b	811	CLA	C2-C1-O2A-CGA
13	b	817	CLA	C2-C1-O2A-CGA
13	l	1501	CLA	C2-C1-O2A-CGA
16	a	853	LHG	C10-C11-C12-C13
15	b	849	BCR	C15-C16-C17-C18
15	a	844	BCR	C23-C24-C25-C30
15	f	202	BCR	C1-C6-C7-C8
15	f	202	BCR	C5-C6-C7-C8
15	i	101	BCR	C1-C6-C7-C8
15	j	101	BCR	C23-C24-C25-C26
15	j	101	BCR	C23-C24-C25-C30
15	k	4005	BCR	C23-C24-C25-C26
20	m	101	ECH	C1-C6-C7-C8
20	m	101	ECH	C23-C24-C25-C26
13	b	815	CLA	C8-C10-C11-C12
17	b	850	LMG	C17-C18-C19-C20
13	a	813	CLA	C2A-CAA-CBA-CGA
16	a	849	LHG	C3-O3-P-O6
16	a	851	LHG	C3-O3-P-O6
16	a	853	LHG	C3-O3-P-O6
16	b	851	LHG	C4-O6-P-O3
16	f	206	LHG	C3-O3-P-O6
16	a	851	LHG	C31-C32-C33-C34
13	b	835	CLA	C4-C3-C5-C6
13	a	811	CLA	C11-C12-C13-C15
13	a	813	CLA	C11-C12-C13-C15
13	b	803	CLA	C11-C12-C13-C15
13	b	805	CLA	C6-C7-C8-C10
13	a	821	CLA	C11-C12-C13-C14
13	a	832	CLA	C11-C10-C8-C9
13	a	838	CLA	C11-C12-C13-C14
13	b	814	CLA	C6-C7-C8-C9
13	b	814	CLA	C14-C13-C15-C16
15	b	849	BCR	C13-C14-C15-C16
13	a	840	CLA	C16-C17-C18-C20
12	a	801	CL0	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	a	837	CLA	C2A-CAA-CBA-CGA
13	b	810	CLA	C5-C6-C7-C8
17	a	852	LMG	C34-C35-C36-C37
13	b	821	CLA	C16-C17-C18-C19
13	b	827	CLA	CBA-CGA-O2A-C1
16	a	853	LHG	C14-C15-C16-C17
15	k	4001	BCR	C7-C8-C9-C10
13	a	812	CLA	C2-C3-C5-C6
23	j	102	LMT	C5'-C4'-O1B-C1B
16	a	853	LHG	C25-C26-C27-C28
13	b	827	CLA	O1A-CGA-O2A-C1
13	a	817	CLA	C4B-C3B-CAB-CBB
13	a	831	CLA	C4B-C3B-CAB-CBB
13	b	808	CLA	C4B-C3B-CAB-CBB
13	b	831	CLA	C4B-C3B-CAB-CBB
13	l	1502	CLA	C4B-C3B-CAB-CBB
13	b	813	CLA	C2A-CAA-CBA-CGA
15	b	848	BCR	C9-C10-C11-C12
13	a	828	CLA	CBD-CGD-O2D-CED
16	f	206	LHG	C26-C27-C28-C29
13	a	840	CLA	CBD-CGD-O2D-CED
16	b	851	LHG	C7-C8-C9-C10
13	b	829	CLA	C16-C17-C18-C19
13	a	818	CLA	C4-C3-C5-C6
13	a	828	CLA	C4-C3-C5-C6
16	a	849	LHG	C12-C13-C14-C15
16	b	851	LHG	C27-C28-C29-C30
16	a	849	LHG	C35-C36-C37-C38
17	b	850	LMG	C35-C36-C37-C38
12	a	801	CL0	O1D-CGD-O2D-CED
13	a	811	CLA	C2A-CAA-CBA-CGA
13	a	812	CLA	C2A-CAA-CBA-CGA
13	a	831	CLA	C2A-CAA-CBA-CGA
13	a	854	CLA	C2A-CAA-CBA-CGA
13	a	830	CLA	C3A-C2A-CAA-CBA
13	a	834	CLA	C3A-C2A-CAA-CBA
13	b	820	CLA	C3A-C2A-CAA-CBA
13	a	823	CLA	C16-C17-C18-C20
13	b	841	CLA	C2C-C3C-CAC-CBC
16	a	849	LHG	C33-C34-C35-C36
13	a	804	CLA	C11-C10-C8-C9
13	a	813	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
13	a	819	CLA	C11-C12-C13-C14
13	a	854	CLA	C14-C13-C15-C16
13	a	855	CLA	C11-C12-C13-C14
13	b	804	CLA	C6-C7-C8-C9
13	b	804	CLA	C11-C12-C13-C14
13	b	819	CLA	C6-C7-C8-C9
13	b	825	CLA	C14-C13-C15-C16
13	b	838	CLA	C14-C13-C15-C16
13	b	840	CLA	C14-C13-C15-C16
13	a	834	CLA	C16-C17-C18-C19
17	a	850	LMG	C30-C31-C32-C33
18	a	856	45D	C28-C26-C30-C32
18	a	856	45D	C39-C35-C37-C41
20	b	846	ECH	C11-C10-C9-C34
20	b	846	ECH	C35-C13-C14-C15
21	b	853	EQ3	C11-C10-C9-C34
22	f	205	ZEX	C20-C13-C14-C15
23	j	102	LMT	C1-C2-C3-C4
16	f	206	LHG	C14-C15-C16-C17
13	b	835	CLA	C5-C6-C7-C8
13	b	820	CLA	CBD-CGD-O2D-CED
13	b	832	CLA	C1A-C2A-CAA-CBA
13	a	813	CLA	C11-C10-C8-C7
13	a	818	CLA	C11-C12-C13-C15
13	a	855	CLA	C6-C7-C8-C10
13	b	818	CLA	C11-C12-C13-C15
13	b	821	CLA	C6-C7-C8-C10
13	b	827	CLA	C11-C12-C13-C15
13	a	838	CLA	C13-C15-C16-C17
13	b	809	CLA	CBA-CGA-O2A-C1
17	a	852	LMG	C14-C15-C16-C17
13	b	836	CLA	C2A-CAA-CBA-CGA
13	a	804	CLA	C5-C6-C7-C8
16	a	849	LHG	O9-C7-O7-C5
13	a	833	CLA	C13-C15-C16-C17
13	a	817	CLA	CBA-CGA-O2A-C1
16	b	851	LHG	C29-C30-C31-C32
13	b	835	CLA	C2-C3-C5-C6
13	a	820	CLA	C2B-C3B-CAB-CBB
13	a	823	CLA	C2B-C3B-CAB-CBB
13	a	827	CLA	C2B-C3B-CAB-CBB
13	a	838	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	a	840	CLA	C2B-C3B-CAB-CBB
13	a	841	CLA	C2B-C3B-CAB-CBB
13	b	808	CLA	C2B-C3B-CAB-CBB
13	b	809	CLA	C2B-C3B-CAB-CBB
13	b	818	CLA	C2B-C3B-CAB-CBB
13	b	839	CLA	C2B-C3B-CAB-CBB
13	b	841	CLA	C2B-C3B-CAB-CBB
13	j	103	CLA	C2B-C3B-CAB-CBB
13	k	4003	CLA	C2B-C3B-CAB-CBB
13	b	822	CLA	C10-C11-C12-C13
15	i	101	BCR	C16-C17-C18-C19
18	a	856	45D	C24-C26-C30-C32
18	a	856	45D	C33-C35-C37-C41
20	b	846	ECH	C11-C10-C9-C8
20	b	846	ECH	C12-C13-C14-C15
21	b	853	EQ3	C11-C10-C9-C8
22	f	205	ZEX	C12-C13-C14-C15
16	b	851	LHG	C24-C23-O8-C6
17	a	852	LMG	C29-C28-O8-C9
15	a	848	BCR	C13-C14-C15-C16
15	j	101	BCR	C6-C7-C8-C9
13	b	840	CLA	C5-C6-C7-C8
13	b	841	CLA	C4-C3-C5-C6
13	a	828	CLA	O1D-CGD-O2D-CED
13	a	817	CLA	O1A-CGA-O2A-C1
13	b	820	CLA	O1D-CGD-O2D-CED
13	b	840	CLA	C11-C12-C13-C14
13	b	803	CLA	C8-C10-C11-C12
13	b	818	CLA	C15-C16-C17-C18
13	a	828	CLA	C2A-CAA-CBA-CGA
13	a	839	CLA	C2A-CAA-CBA-CGA
13	b	830	CLA	C2A-CAA-CBA-CGA
15	a	846	BCR	C23-C24-C25-C30
15	b	847	BCR	C1-C6-C7-C8
15	b	848	BCR	C1-C6-C7-C8
15	b	848	BCR	C23-C24-C25-C30
15	b	849	BCR	C23-C24-C25-C30
15	f	202	BCR	C23-C24-C25-C30
15	i	101	BCR	C5-C6-C7-C8
15	i	101	BCR	C23-C24-C25-C30
15	k	4001	BCR	C23-C24-C25-C30
15	k	4005	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	b	846	ECH	C23-C24-C25-C26
20	m	101	ECH	C23-C24-C25-C30
13	b	807	CLA	C4-C3-C5-C6
15	a	844	BCR	C21-C22-C23-C24
13	a	842	CLA	CAA-CBA-CGA-O2A
13	a	821	CLA	C3-C5-C6-C7
13	l	1502	CLA	C10-C11-C12-C13
13	a	808	CLA	C8-C10-C11-C12
13	a	805	CLA	CAA-CBA-CGA-O2A
13	l	1503	CLA	CAA-CBA-CGA-O2A
13	f	204	CLA	CAA-CBA-CGA-O2A
13	a	840	CLA	O1D-CGD-O2D-CED
13	a	820	CLA	C4B-C3B-CAB-CBB
13	a	827	CLA	C4B-C3B-CAB-CBB
13	a	834	CLA	C4B-C3B-CAB-CBB
13	a	840	CLA	C4B-C3B-CAB-CBB
13	k	4004	CLA	C4B-C3B-CAB-CBB
16	a	851	LHG	O6-C4-C5-C6
13	b	821	CLA	C4-C3-C5-C6
13	a	817	CLA	C12-C13-C15-C16
13	a	819	CLA	C11-C12-C13-C15
13	a	835	CLA	C12-C13-C15-C16
13	a	839	CLA	C16-C17-C18-C19
13	b	815	CLA	C16-C17-C18-C20
17	a	852	LMG	C15-C16-C17-C18
16	a	853	LHG	O7-C5-C6-O8
13	b	804	CLA	C8-C10-C11-C12
13	b	812	CLA	CAA-CBA-CGA-O2A
16	a	849	LHG	C27-C28-C29-C30
13	a	832	CLA	C4-C3-C5-C6
13	a	834	CLA	C4-C3-C5-C6
13	b	819	CLA	C5-C6-C7-C8
13	a	839	CLA	C2-C3-C5-C6
17	a	850	LMG	C14-C15-C16-C17
13	a	813	CLA	C11-C10-C8-C9
13	a	824	CLA	C6-C7-C8-C9
13	a	828	CLA	C11-C12-C13-C14
13	b	805	CLA	C11-C10-C8-C9
13	b	810	CLA	C11-C10-C8-C9
13	b	822	CLA	C11-C10-C8-C9
13	b	833	CLA	C14-C13-C15-C16
13	b	835	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
13	b	841	CLA	C14-C13-C15-C16
13	a	802	CLA	C3A-C2A-CAA-CBA
13	b	811	CLA	C3A-C2A-CAA-CBA
13	a	811	CLA	C8-C10-C11-C12
17	b	850	LMG	C36-C37-C38-C39
13	a	803	CLA	CAD-CBD-CGD-O2D
13	a	807	CLA	CAD-CBD-CGD-O2D
13	a	811	CLA	CAD-CBD-CGD-O2D
13	a	812	CLA	CAD-CBD-CGD-O2D
13	a	826	CLA	CAD-CBD-CGD-O2D
13	a	830	CLA	CAD-CBD-CGD-O2D
13	a	833	CLA	CAD-CBD-CGD-O2D
13	a	841	CLA	CAD-CBD-CGD-O2D
13	b	835	CLA	CAD-CBD-CGD-O2D
13	j	103	CLA	CAD-CBD-CGD-O2D
13	l	1503	CLA	CAD-CBD-CGD-O2D
13	b	819	CLA	CBA-CGA-O2A-C1
13	b	834	CLA	C2-C1-O2A-CGA
13	a	806	CLA	CAA-CBA-CGA-O2A
13	a	839	CLA	CAA-CBA-CGA-O2A
13	j	103	CLA	CAA-CBA-CGA-O2A
13	b	804	CLA	C4-C3-C5-C6
13	a	842	CLA	CAA-CBA-CGA-O1A
13	f	204	CLA	CAA-CBA-CGA-O1A
17	b	850	LMG	C18-C19-C20-C21
15	a	847	BCR	C7-C8-C9-C10
15	a	848	BCR	C7-C8-C9-C10
16	a	849	LHG	C4-C5-C6-O8
16	a	853	LHG	C4-C5-C6-O8
13	a	818	CLA	C15-C16-C17-C18
13	a	830	CLA	CAA-CBA-CGA-O2A
13	a	831	CLA	CAA-CBA-CGA-O2A
13	b	836	CLA	CAA-CBA-CGA-O2A
13	a	802	CLA	O2A-C1-C2-C3
13	a	807	CLA	O2A-C1-C2-C3
13	a	818	CLA	O2A-C1-C2-C3
13	a	820	CLA	O2A-C1-C2-C3
13	a	823	CLA	O2A-C1-C2-C3
13	b	808	CLA	O2A-C1-C2-C3
13	b	817	CLA	O2A-C1-C2-C3
13	b	828	CLA	O2A-C1-C2-C3
13	b	838	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
13	l	1503	CLA	O2A-C1-C2-C3
13	b	819	CLA	O1A-CGA-O2A-C1
13	a	825	CLA	C15-C16-C17-C18
13	a	811	CLA	CAA-CBA-CGA-O2A
13	b	809	CLA	O1A-CGA-O2A-C1
13	a	802	CLA	CHA-CBD-CGD-O1D
13	a	802	CLA	CHA-CBD-CGD-O2D
13	a	805	CLA	CHA-CBD-CGD-O1D
13	a	805	CLA	CHA-CBD-CGD-O2D
13	a	822	CLA	CHA-CBD-CGD-O2D
13	a	829	CLA	CHA-CBD-CGD-O1D
13	a	829	CLA	CHA-CBD-CGD-O2D
13	a	840	CLA	CHA-CBD-CGD-O1D
13	a	840	CLA	CHA-CBD-CGD-O2D
13	a	842	CLA	CHA-CBD-CGD-O2D
13	b	808	CLA	CHA-CBD-CGD-O1D
13	b	808	CLA	CHA-CBD-CGD-O2D
13	b	822	CLA	CHA-CBD-CGD-O2D
13	b	824	CLA	CHA-CBD-CGD-O2D
13	b	838	CLA	CHA-CBD-CGD-O1D
13	b	838	CLA	CHA-CBD-CGD-O2D
13	b	842	CLA	CHA-CBD-CGD-O1D
13	b	842	CLA	CHA-CBD-CGD-O2D
13	f	204	CLA	CHA-CBD-CGD-O2D
13	a	832	CLA	CAA-CBA-CGA-O2A
17	a	852	LMG	O7-C10-C11-C12
13	a	820	CLA	CAA-CBA-CGA-O2A
13	a	829	CLA	CAA-CBA-CGA-O2A
13	b	830	CLA	CAA-CBA-CGA-O2A
13	a	840	CLA	C5-C6-C7-C8
17	a	852	LMG	C10-C11-C12-C13
13	b	817	CLA	CAA-CBA-CGA-O2A
13	a	821	CLA	C2-C3-C5-C6
13	a	834	CLA	C2-C3-C5-C6
13	b	824	CLA	C2-C3-C5-C6
13	a	838	CLA	C16-C17-C18-C20
17	a	850	LMG	C31-C32-C33-C34
16	f	206	LHG	C25-C26-C27-C28
13	a	818	CLA	C11-C12-C13-C14
13	a	820	CLA	C6-C7-C8-C9
13	a	855	CLA	C6-C7-C8-C9
13	b	827	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
13	b	829	CLA	C11-C12-C13-C14
16	a	853	LHG	C9-C10-C11-C12
16	a	849	LHG	C11-C10-C9-C8
17	b	850	LMG	O7-C10-C11-C12
16	b	851	LHG	C25-C26-C27-C28
13	a	831	CLA	C2C-C3C-CAC-CBC
13	a	831	CLA	C4C-C3C-CAC-CBC
22	f	205	ZEX	C27-C28-C29-C39
13	b	836	CLA	CAA-CBA-CGA-O1A
13	b	829	CLA	C16-C17-C18-C20
16	a	851	LHG	O1-C1-C2-C3
13	b	812	CLA	CAA-CBA-CGA-O1A
15	b	848	BCR	C11-C12-C13-C14
22	f	205	ZEX	C27-C28-C29-C30
13	a	802	CLA	C1A-C2A-CAA-CBA
13	b	811	CLA	C1A-C2A-CAA-CBA
13	b	820	CLA	C1A-C2A-CAA-CBA
13	b	827	CLA	C1A-C2A-CAA-CBA
16	a	849	LHG	O9-C7-C8-C9
13	a	839	CLA	CAA-CBA-CGA-O1A
13	j	103	CLA	CAA-CBA-CGA-O1A
13	a	806	CLA	CAA-CBA-CGA-O1A
13	a	827	CLA	C13-C15-C16-C17
16	a	853	LHG	C11-C12-C13-C14
13	a	812	CLA	C4B-C3B-CAB-CBB
16	a	851	LHG	C3-O3-P-O5
16	a	853	LHG	C3-O3-P-O4
16	b	851	LHG	C4-O6-P-O5
13	a	811	CLA	CAA-CBA-CGA-O1A
13	a	832	CLA	CAA-CBA-CGA-O1A
16	f	206	LHG	O10-C23-C24-C25
15	a	844	BCR	C23-C24-C25-C26
15	k	4001	BCR	C23-C24-C25-C26
22	b	854	ZEX	C1-C6-C7-C8
13	a	829	CLA	CAA-CBA-CGA-O1A
13	a	826	CLA	C15-C16-C17-C18
13	f	201	CLA	C13-C15-C16-C17
13	a	809	CLA	CAA-CBA-CGA-O2A
13	b	808	CLA	CAA-CBA-CGA-O2A
13	l	1502	CLA	CAA-CBA-CGA-O2A
13	b	821	CLA	C13-C15-C16-C17
13	a	830	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
13	a	825	CLA	CAD-CBD-CGD-O1D
13	a	840	CLA	CAD-CBD-CGD-O1D
13	b	830	CLA	CAD-CBD-CGD-O1D
13	a	831	CLA	CAA-CBA-CGA-O1A
13	b	841	CLA	C4C-C3C-CAC-CBC
17	b	852	LMG	C31-C32-C33-C34
13	a	823	CLA	C11-C12-C13-C14
13	b	814	CLA	C11-C12-C13-C14
13	b	840	CLA	C6-C7-C8-C9
16	b	851	LHG	C11-C10-C9-C8
13	b	801	CLA	C15-C16-C17-C18
13	a	810	CLA	CAA-CBA-CGA-O2A
13	a	823	CLA	CAA-CBA-CGA-O2A
13	b	822	CLA	CAA-CBA-CGA-O2A
13	a	828	CLA	CAA-CBA-CGA-O2A
13	b	816	CLA	CAA-CBA-CGA-O2A
16	a	849	LHG	O7-C7-C8-C9
16	a	849	LHG	O8-C23-C24-C25
13	b	824	CLA	C4-C3-C5-C6
13	a	818	CLA	C2-C3-C5-C6
13	a	820	CLA	C11-C10-C8-C7
13	a	821	CLA	C12-C13-C15-C16
13	a	828	CLA	C2-C3-C5-C6
13	b	810	CLA	C6-C7-C8-C10
13	b	816	CLA	C3A-C2A-CAA-CBA
13	b	830	CLA	C11-C12-C13-C15
13	b	840	CLA	C11-C12-C13-C15
13	a	814	CLA	CAA-CBA-CGA-O2A
13	a	835	CLA	CAA-CBA-CGA-O2A
13	b	831	CLA	CAA-CBA-CGA-O2A
15	k	4001	BCR	C21-C22-C23-C24
13	a	814	CLA	CAA-CBA-CGA-O1A
13	a	820	CLA	CAA-CBA-CGA-O1A
13	a	835	CLA	CAA-CBA-CGA-O1A
13	b	830	CLA	CAA-CBA-CGA-O1A
23	j	102	LMT	C2-C1-O1'-C1'
13	b	813	CLA	CAA-CBA-CGA-O2A
13	b	834	CLA	CAA-CBA-CGA-O2A
13	b	840	CLA	CAA-CBA-CGA-O2A
13	b	814	CLA	C8-C10-C11-C12
13	b	822	CLA	C5-C6-C7-C8
13	a	826	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	b	817	CLA	CAA-CBA-CGA-O1A
13	b	822	CLA	CAA-CBA-CGA-O1A
13	l	1502	CLA	CAA-CBA-CGA-O1A
13	b	816	CLA	C5-C6-C7-C8
13	b	840	CLA	CAA-CBA-CGA-O1A
17	a	852	LMG	O9-C10-C11-C12
13	a	821	CLA	C4-C3-C5-C6
13	b	806	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

122 monomers are involved in 395 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	b	840	CLA	2	0
17	b	852	LMG	1	0
13	b	822	CLA	2	0
13	b	825	CLA	8	0
13	a	819	CLA	6	0
13	a	817	CLA	6	0
13	b	841	CLA	4	0
13	a	824	CLA	4	0
13	a	820	CLA	6	0
15	i	102	BCR	5	0
13	a	809	CLA	2	0
13	b	834	CLA	5	0
16	b	851	LHG	2	0
13	b	830	CLA	7	0
13	b	826	CLA	2	0
13	a	841	CLA	5	0
13	a	828	CLA	8	0
13	b	837	CLA	1	0
13	a	803	CLA	3	0
13	b	821	CLA	2	0
13	l	1502	CLA	6	0
13	k	4004	CLA	4	0
16	a	849	LHG	3	0
16	a	851	LHG	4	0
13	a	826	CLA	3	0
15	b	845	BCR	2	0
13	b	819	CLA	1	0
15	f	202	BCR	4	0
13	a	854	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	b	824	CLA	6	0
15	a	848	BCR	1	0
15	i	101	BCR	3	0
15	b	848	BCR	2	0
13	b	815	CLA	3	0
13	a	804	CLA	3	0
13	a	831	CLA	4	0
13	b	808	CLA	5	0
13	b	803	CLA	6	0
15	j	105	BCR	4	0
13	a	816	CLA	1	0
13	b	831	CLA	4	0
13	a	811	CLA	2	0
13	j	103	CLA	1	0
13	a	840	CLA	8	0
13	f	201	CLA	4	0
13	a	822	CLA	3	0
13	f	203	CLA	2	0
13	j	104	CLA	1	0
20	b	846	ECH	3	0
13	b	838	CLA	5	0
15	a	847	BCR	4	0
13	a	808	CLA	7	0
14	b	843	PQN	3	0
13	b	811	CLA	4	0
15	b	849	BCR	7	0
13	a	834	CLA	9	0
13	a	830	CLA	8	0
16	f	206	LHG	4	0
13	b	812	CLA	2	0
15	b	844	BCR	3	0
13	a	838	CLA	4	0
13	b	833	CLA	5	0
13	a	805	CLA	5	0
13	a	839	CLA	6	0
13	a	832	CLA	5	0
13	b	801	CLA	6	0
13	a	802	CLA	7	0
13	a	821	CLA	2	0
13	a	823	CLA	4	0
13	b	816	CLA	7	0
13	b	827	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	b	847	BCR	4	0
12	a	801	CL0	5	0
14	a	843	PQN	1	0
15	k	4005	BCR	2	0
22	b	854	ZEX	2	0
13	b	828	CLA	4	0
15	a	844	BCR	5	0
13	a	833	CLA	5	0
13	b	817	CLA	5	0
13	b	805	CLA	3	0
13	a	818	CLA	3	0
13	b	810	CLA	3	0
13	b	823	CLA	4	0
13	a	827	CLA	4	0
22	f	205	ZEX	2	0
13	b	829	CLA	3	0
13	a	814	CLA	5	0
13	b	839	CLA	5	0
13	a	837	CLA	3	0
13	a	807	CLA	3	0
13	b	809	CLA	7	0
17	a	852	LMG	6	0
13	k	4002	CLA	4	0
15	a	845	BCR	4	0
15	k	4001	BCR	5	0
13	a	825	CLA	1	0
13	b	806	CLA	4	0
13	a	810	CLA	3	0
13	a	855	CLA	4	0
13	b	835	CLA	2	0
13	b	836	CLA	2	0
15	a	846	BCR	1	0
13	a	829	CLA	3	0
18	a	856	45D	2	0
17	b	850	LMG	4	0
13	a	812	CLA	5	0
13	a	835	CLA	3	0
13	b	818	CLA	9	0
13	b	813	CLA	1	0
13	b	814	CLA	3	0
13	b	804	CLA	11	0
13	a	806	CLA	3	0

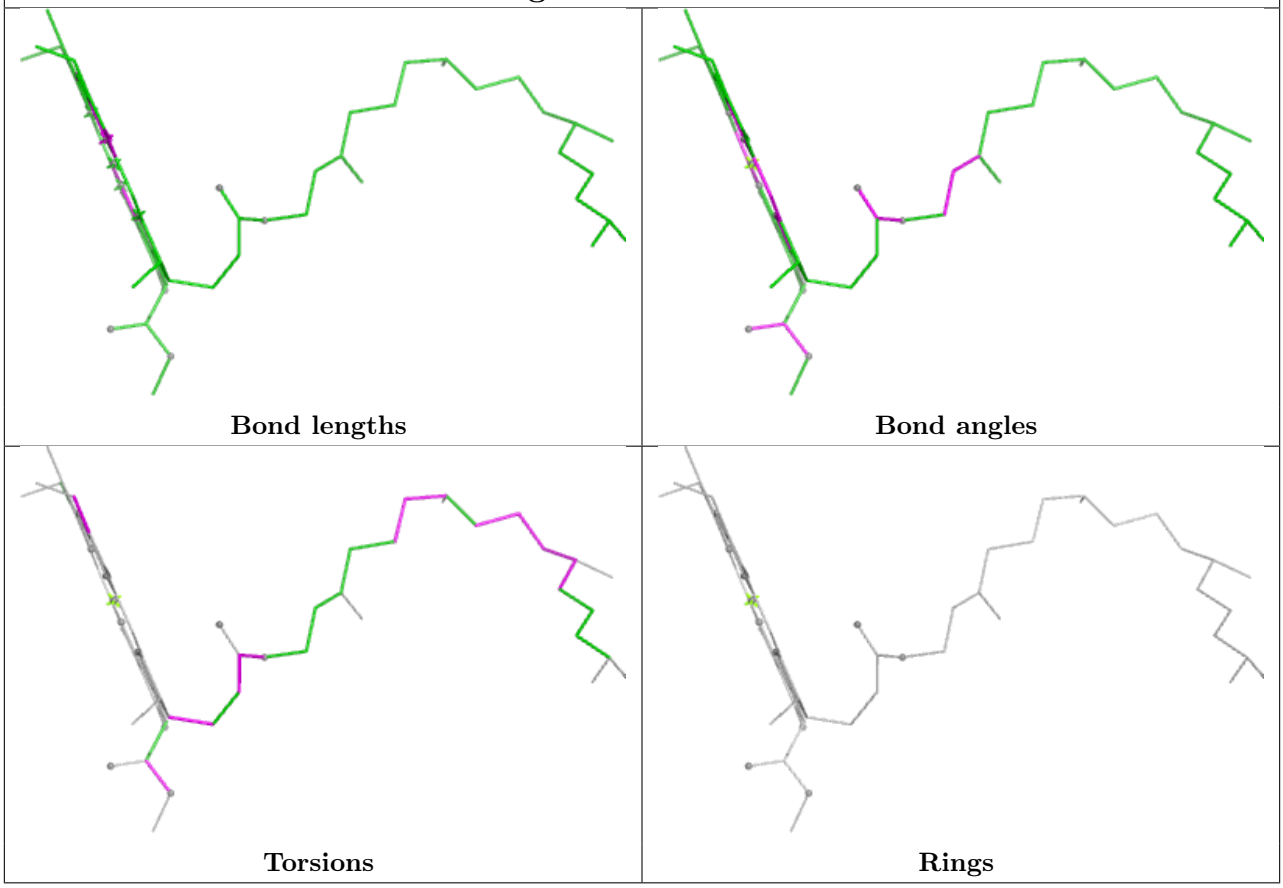
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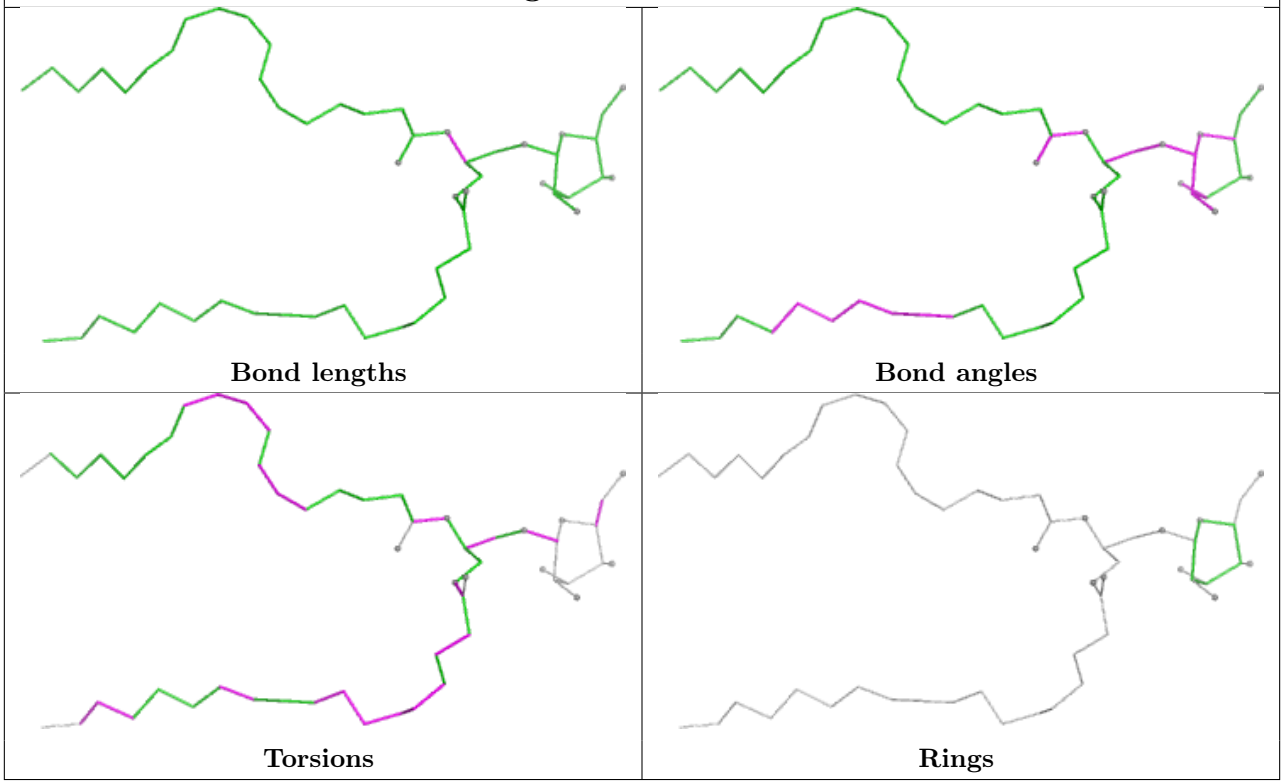
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	a	813	CLA	3	0
13	b	807	CLA	4	0
13	a	836	CLA	1	0
13	l	1501	CLA	3	0
15	j	101	BCR	3	0
13	b	842	CLA	1	0
17	a	850	LMG	4	0
20	m	101	ECH	3	0
13	b	820	CLA	3	0

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.

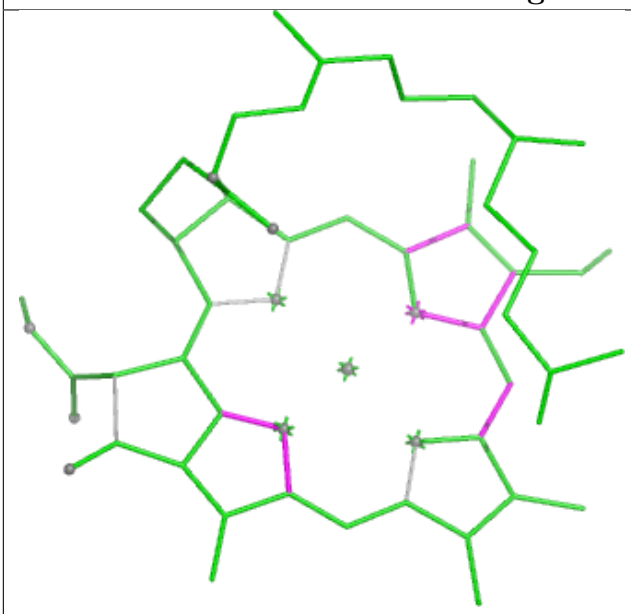
Ligand CLA b 840



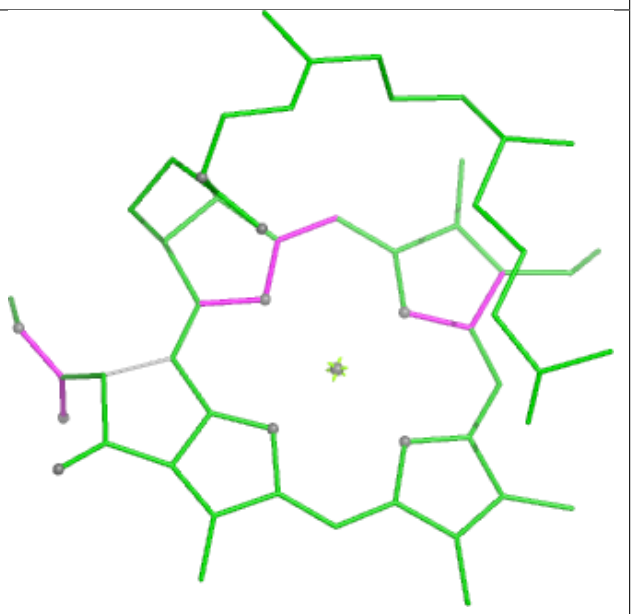
Ligand LMG b 852



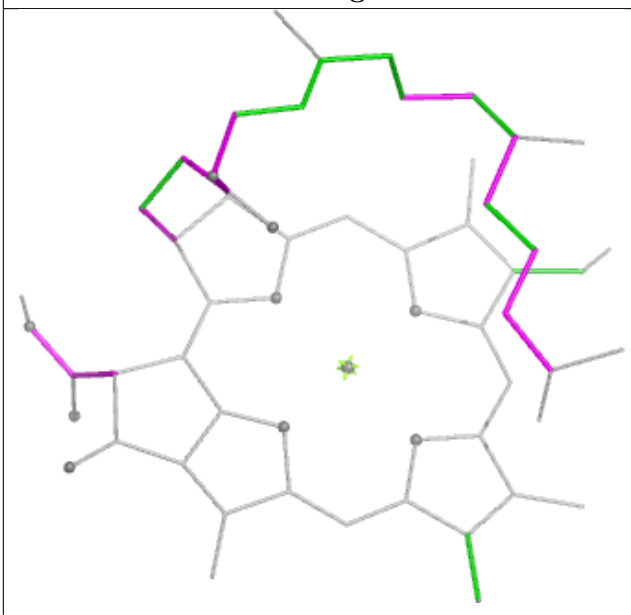
Ligand CLA b 822



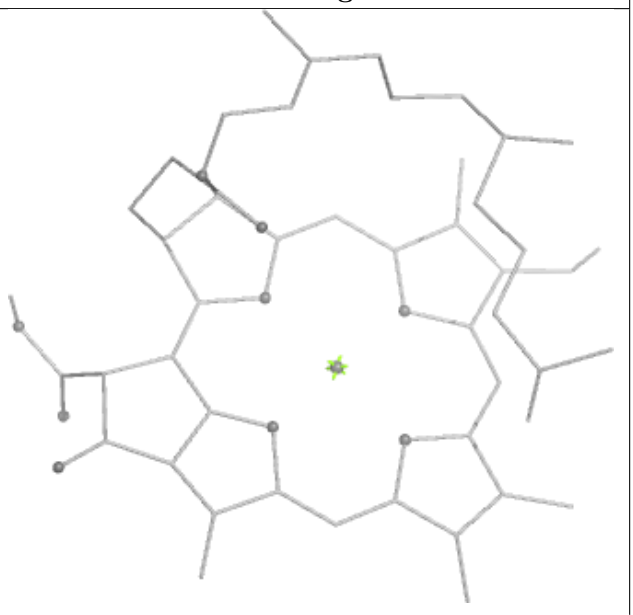
Bond lengths



Bond angles

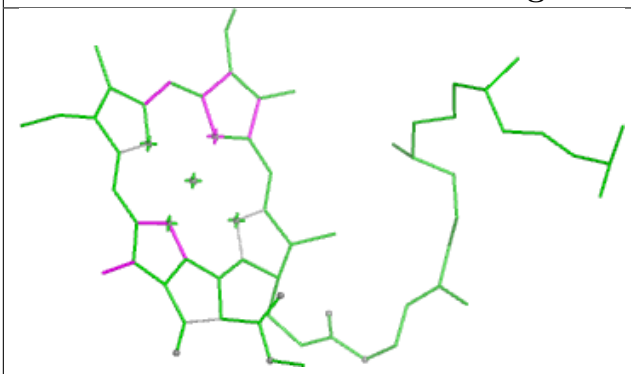


Torsions

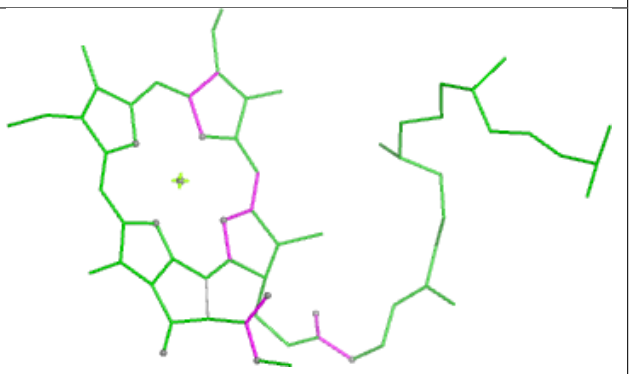


Rings

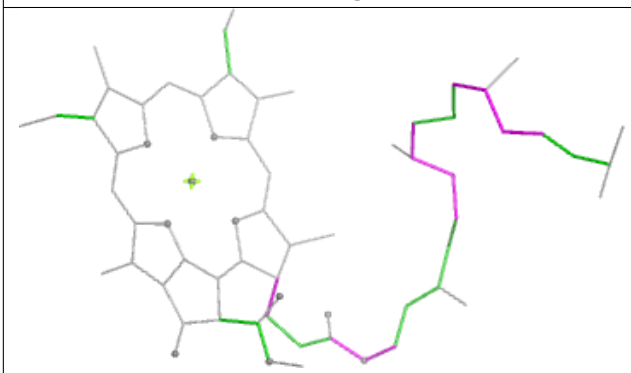
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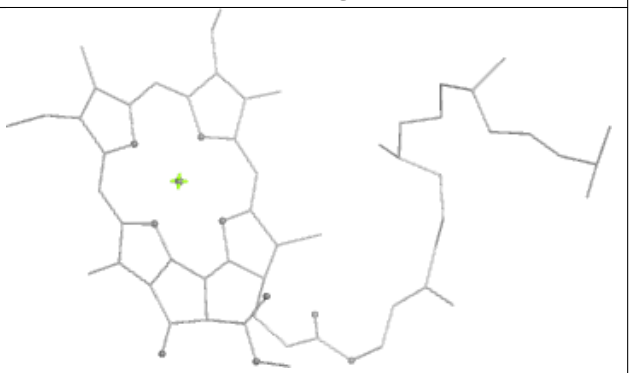
Bond lengths



Bond angles

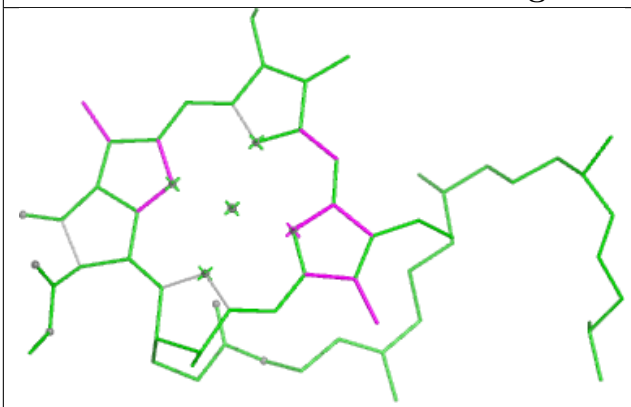


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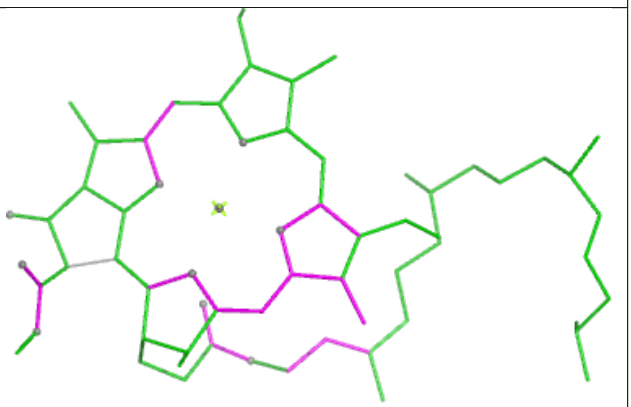


Rings

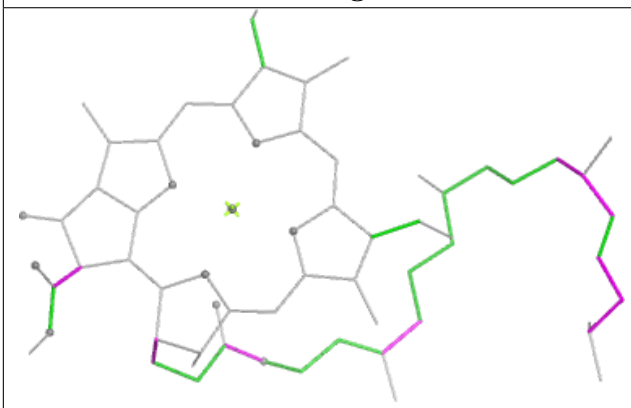
Ligand CLA a 819



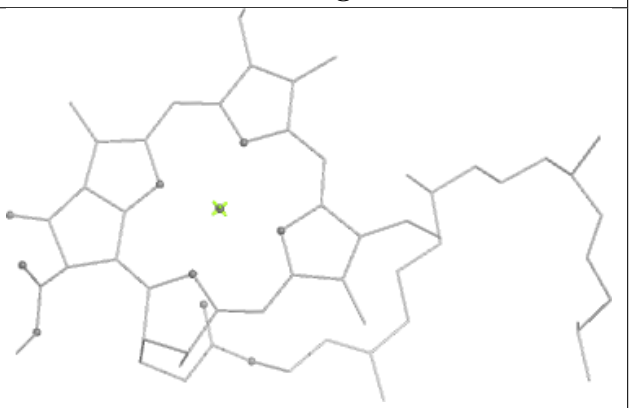
Bond lengths



Bond angles

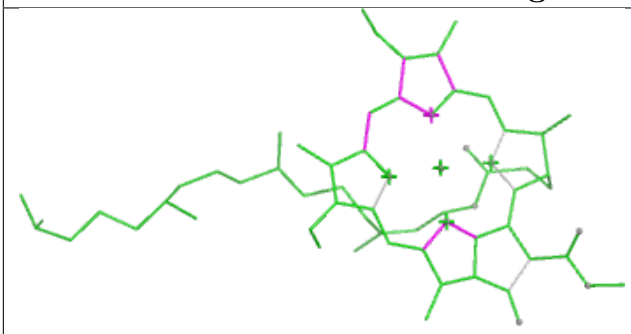


Torsions

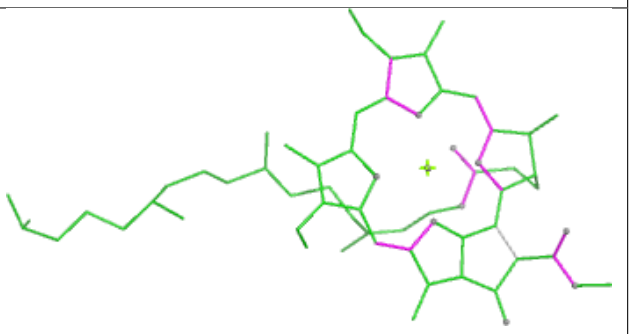


Rings

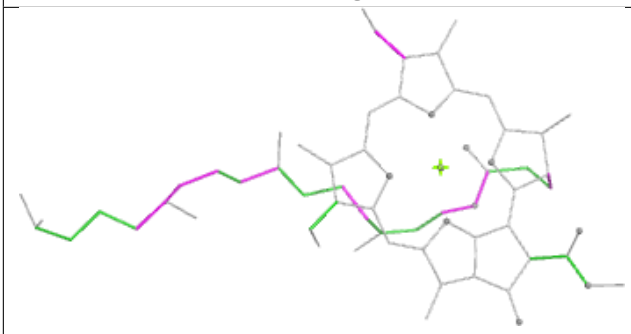
Ligand CLA a 817



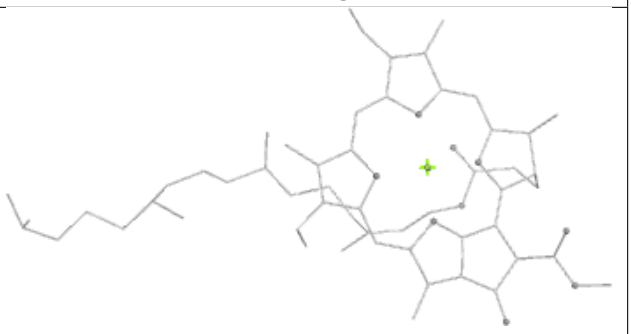
Bond lengths



Bond angles



Torsions



Rings

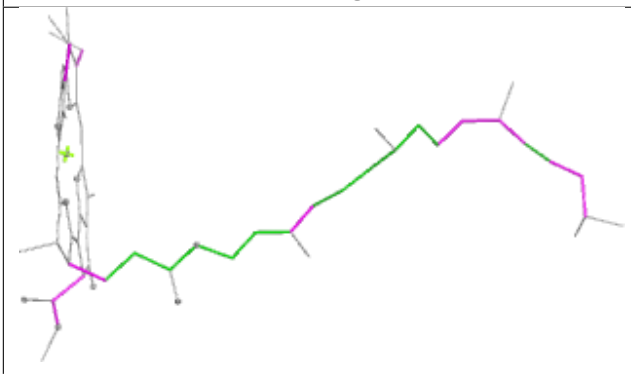
Ligand CLA b 841



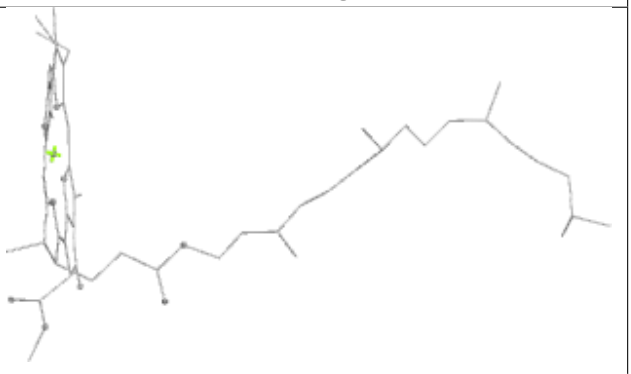
Bond lengths



Bond angles

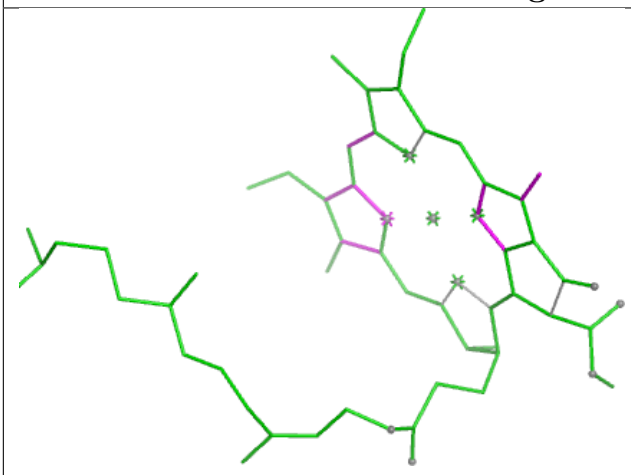


Torsions

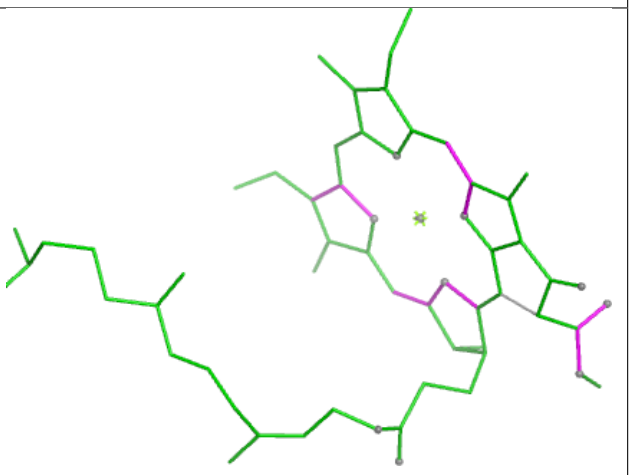


Rings

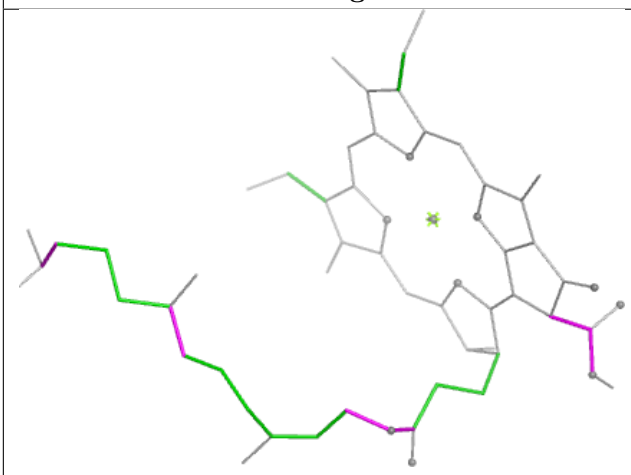
Ligand CLA a 824



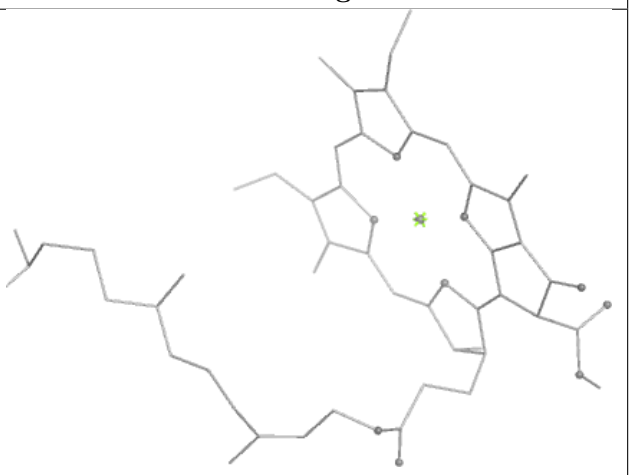
Bond lengths



Bond angles

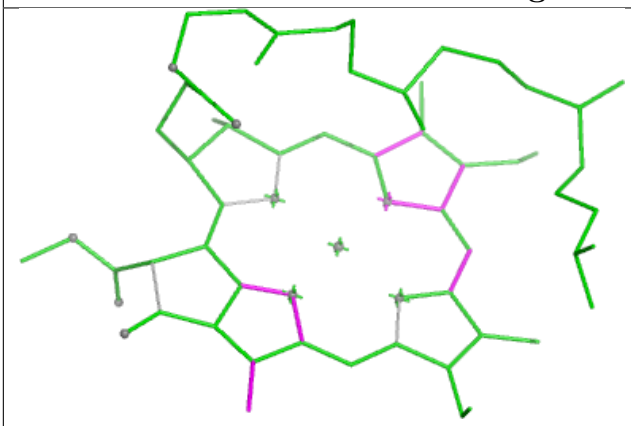


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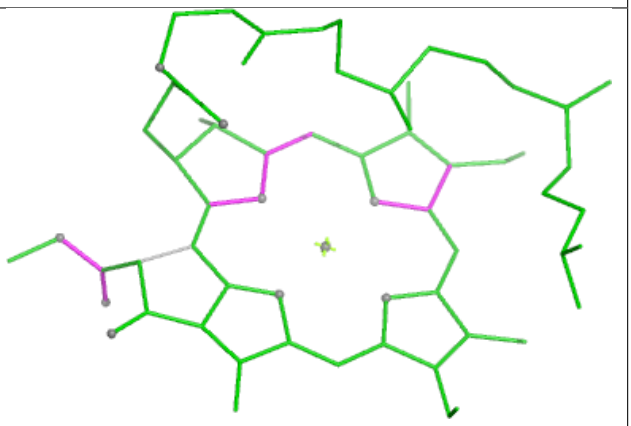


Rings

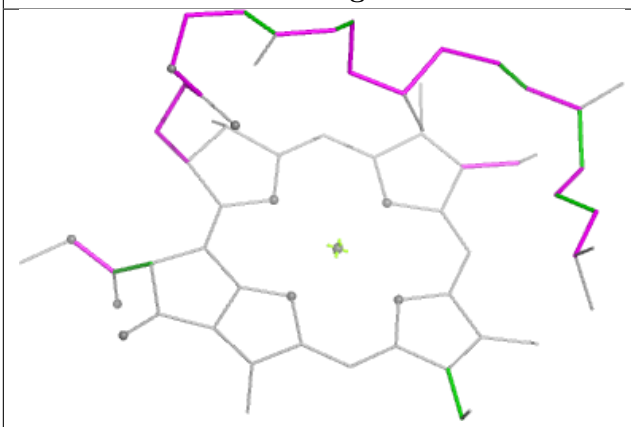
Ligand CLA a 820



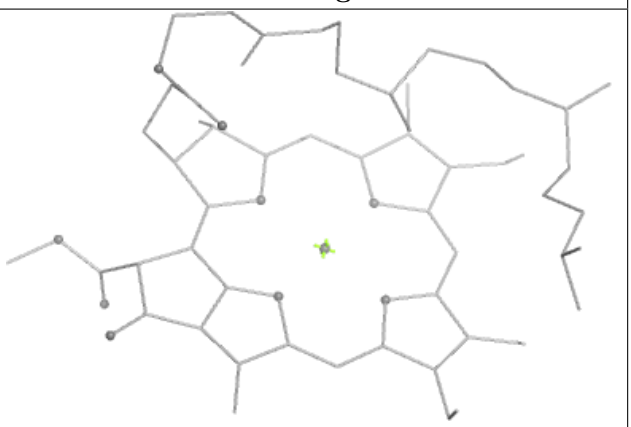
Bond lengths



Bond angles



Torsions

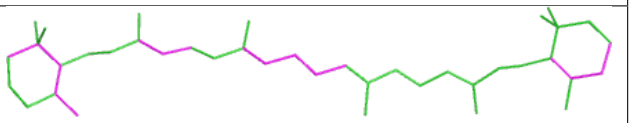


Rings

Ligand BCR i 102



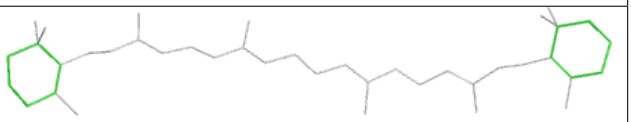
Bond lengths



Bond angles

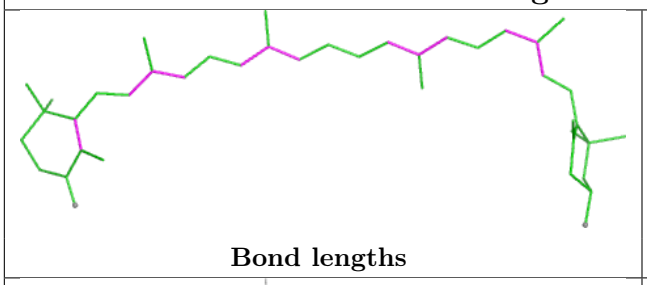


Torsions

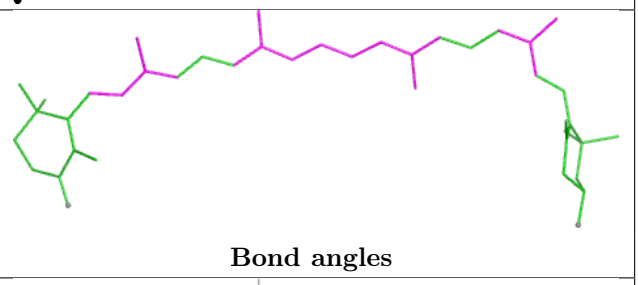


Rings

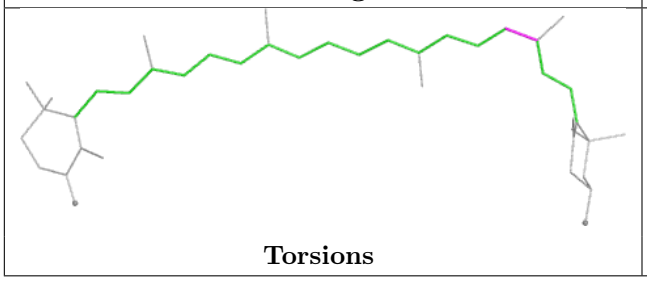
Ligand EQ3 b 853



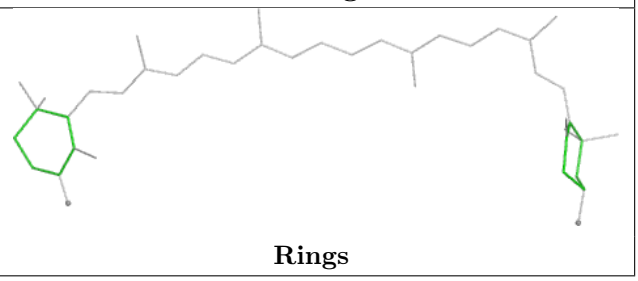
Bond lengths



Bond angles

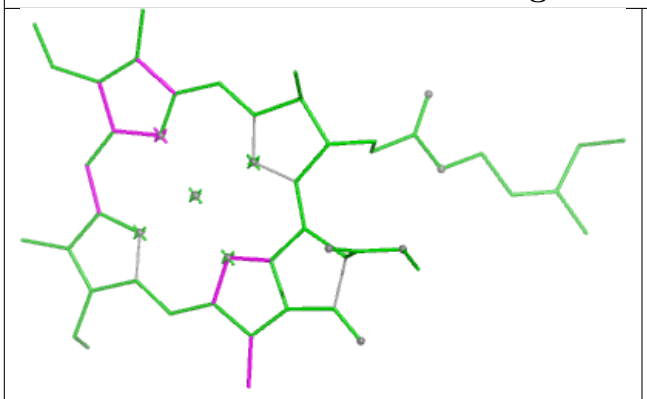


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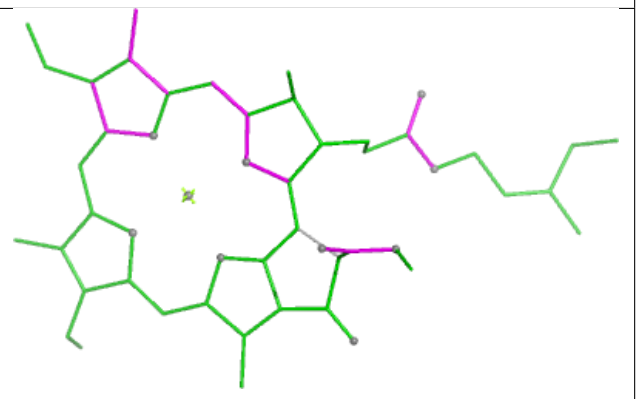


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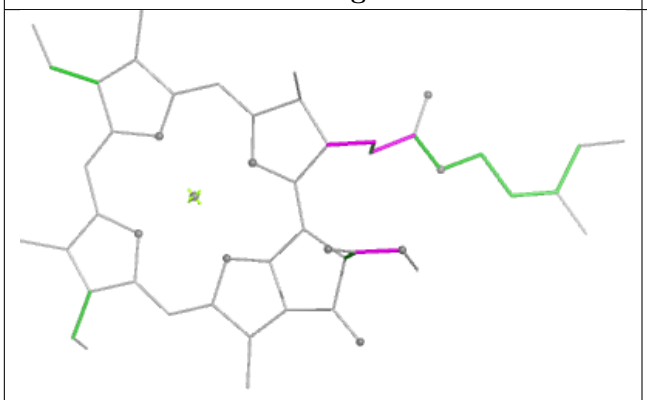
Ligand CLA a 809



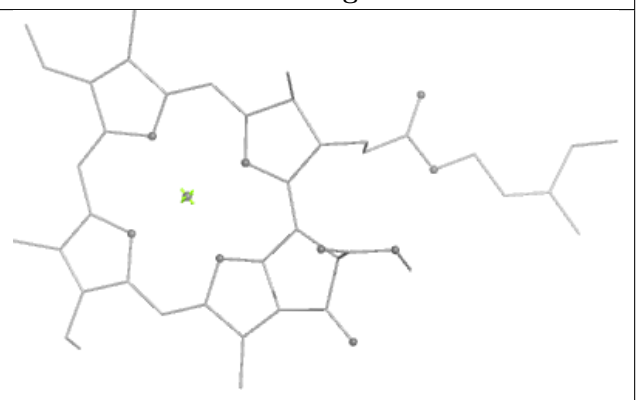
Bond lengths



Bond angles

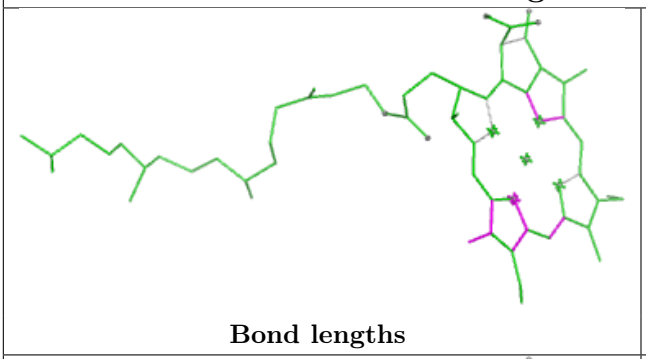


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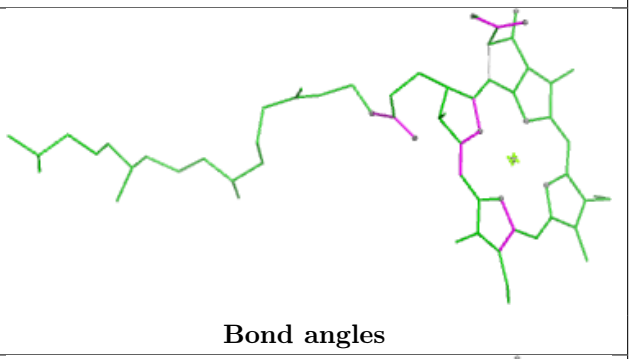


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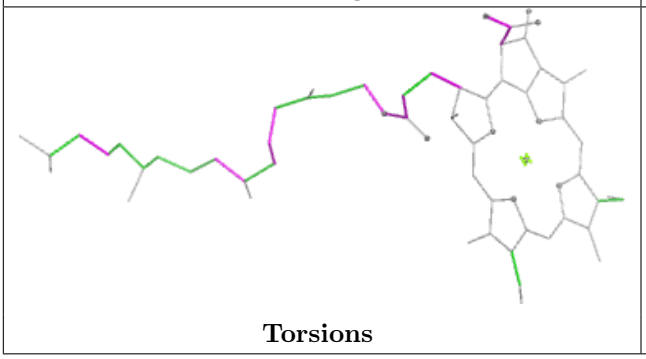
Ligand CLA b 834



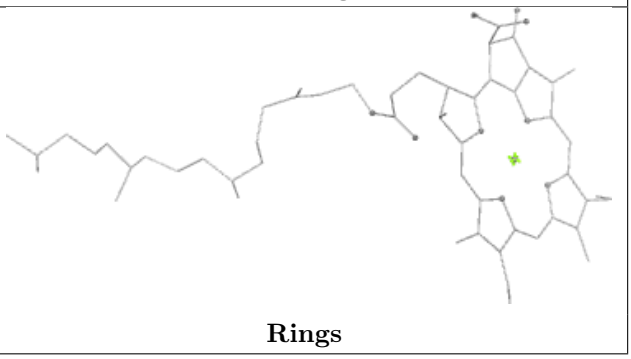
Bond lengths



Bond angles

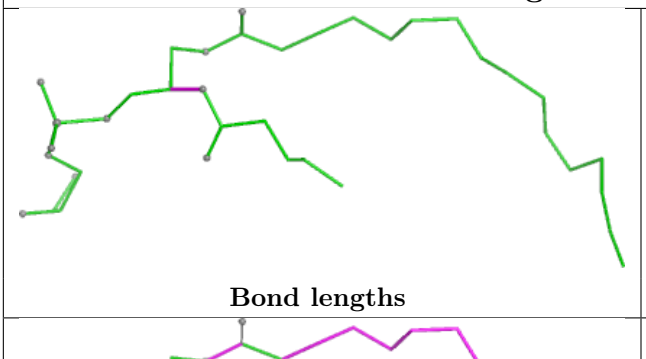


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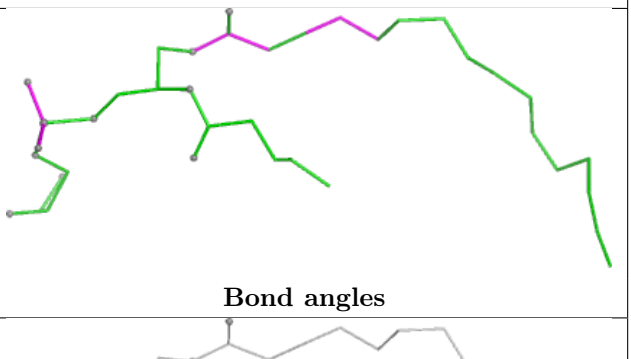


Rings

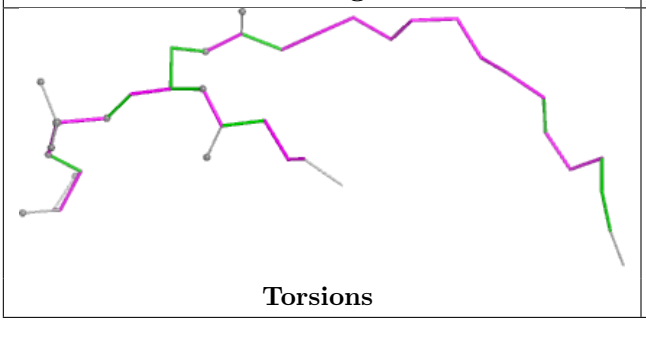
Ligand LHG b 851



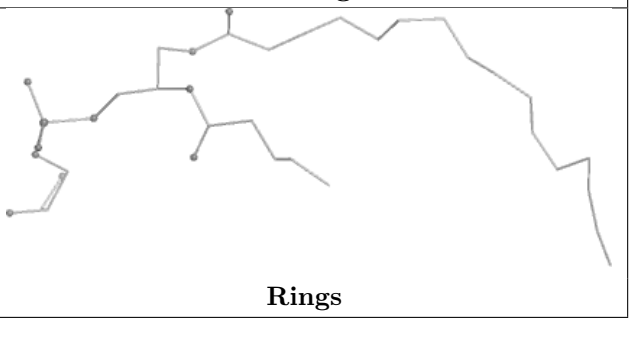
Bond lengths



Bond angles

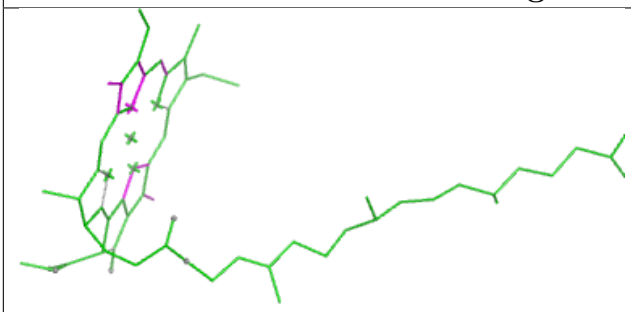


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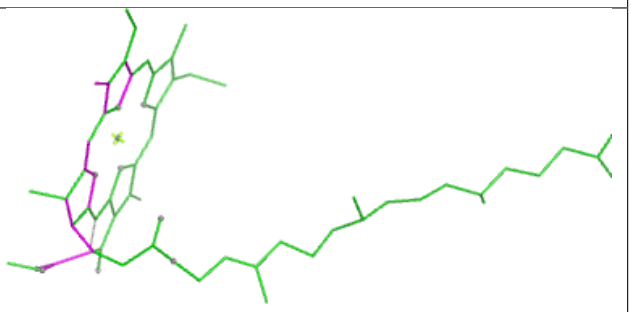


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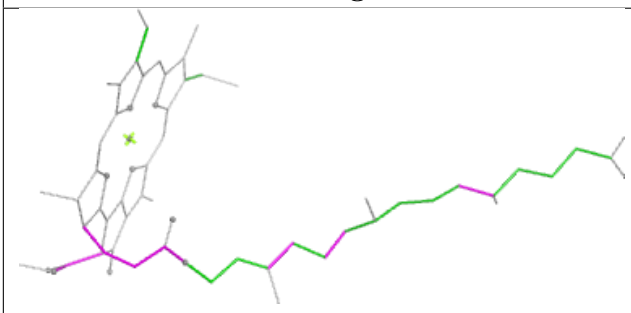
Ligand CLA b 830



Bond lengths



Bond angles

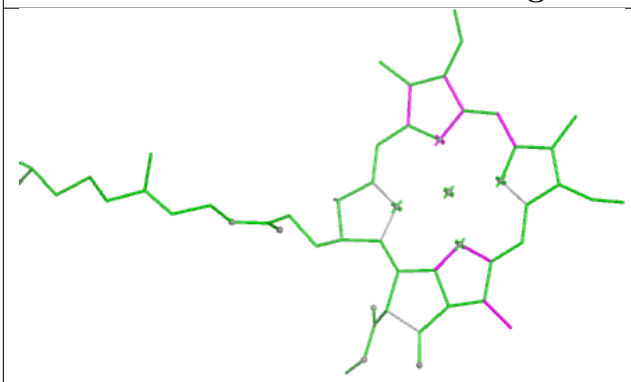


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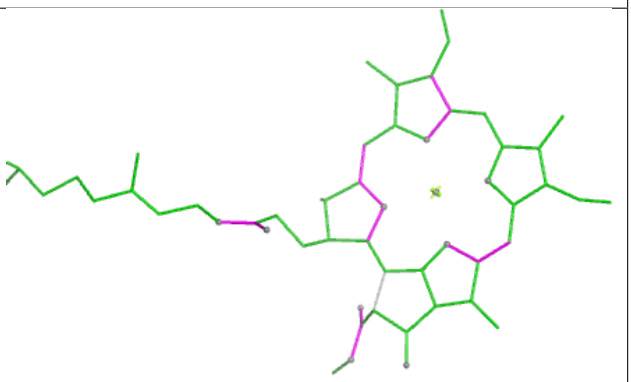


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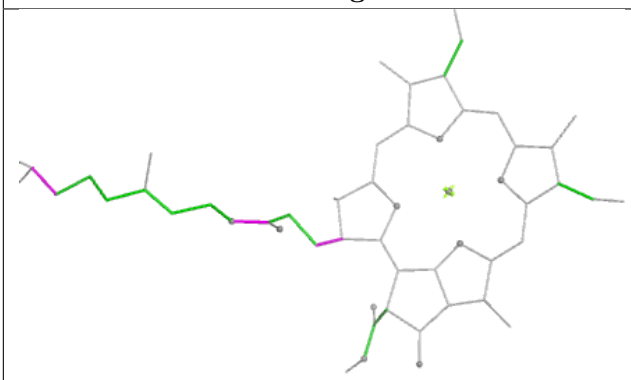
Ligand CLA b 826



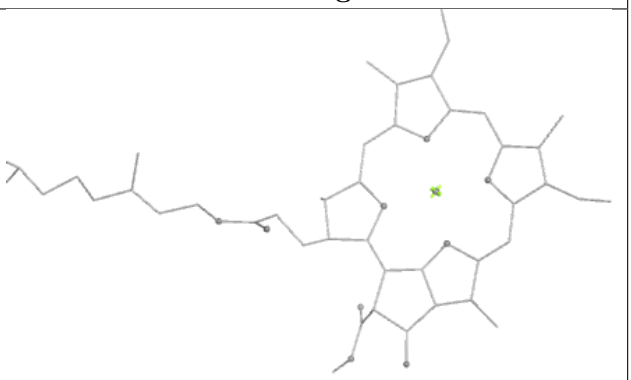
Bond lengths



Bond angles

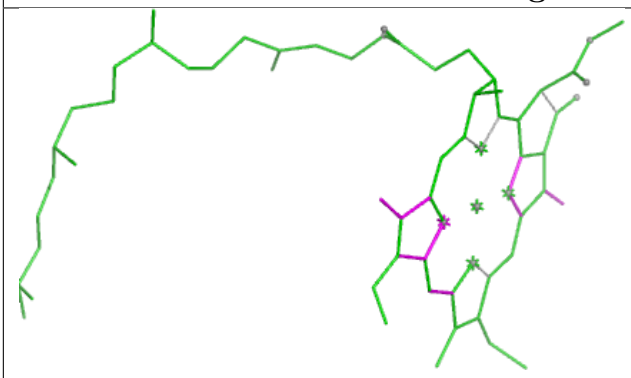


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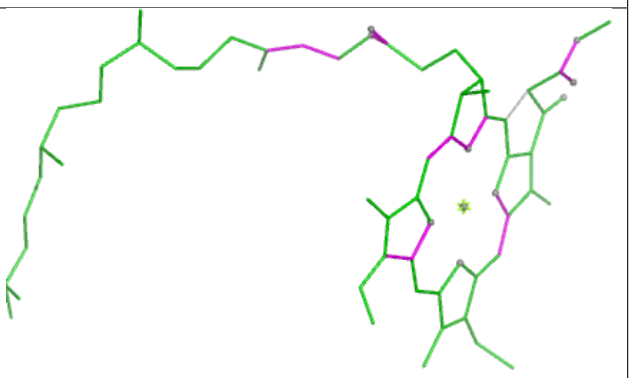


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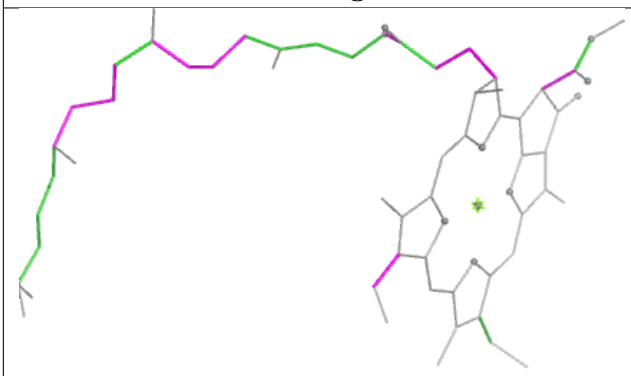
Ligand CLA a 841



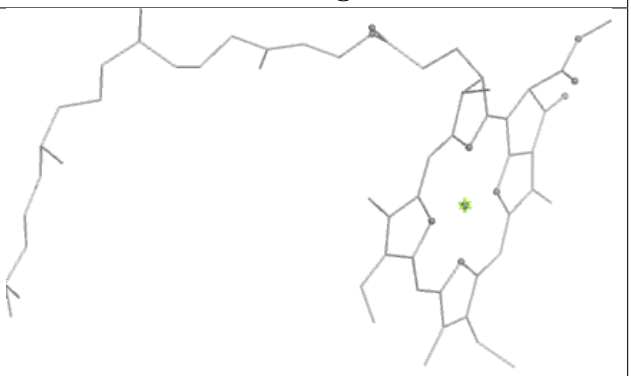
Bond lengths



Bond angles

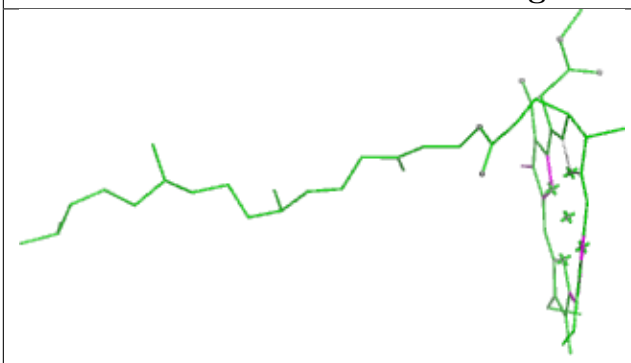


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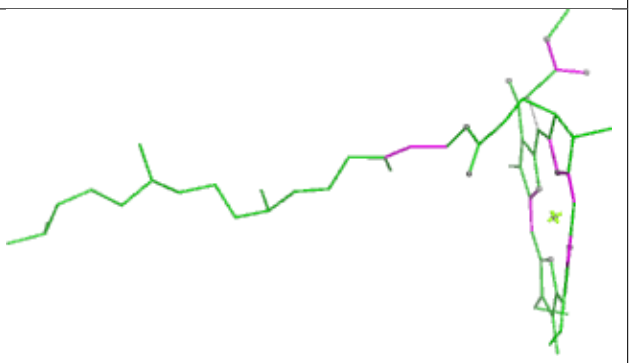


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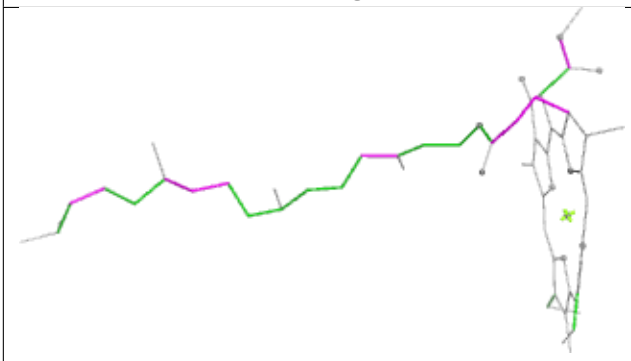
Ligand CLA a 828



Bond lengths



Bond angles

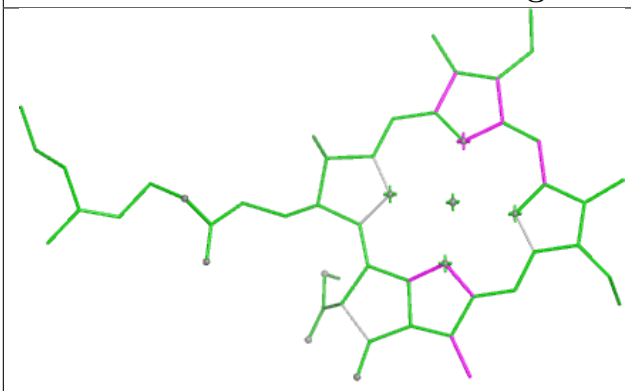


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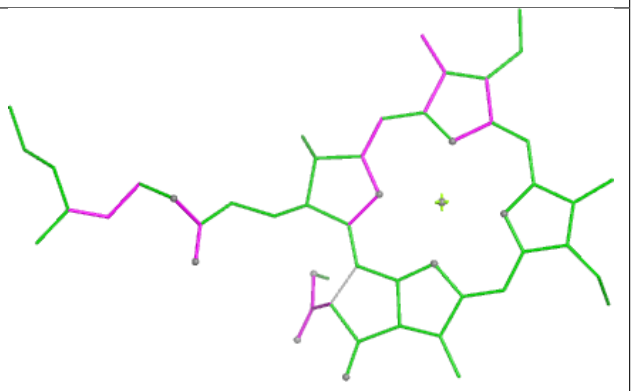


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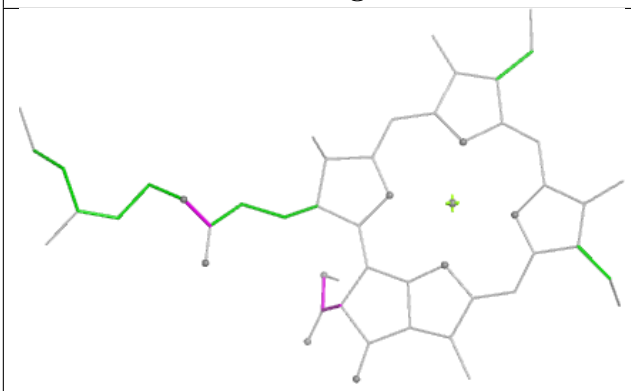
Ligand CLA b 837



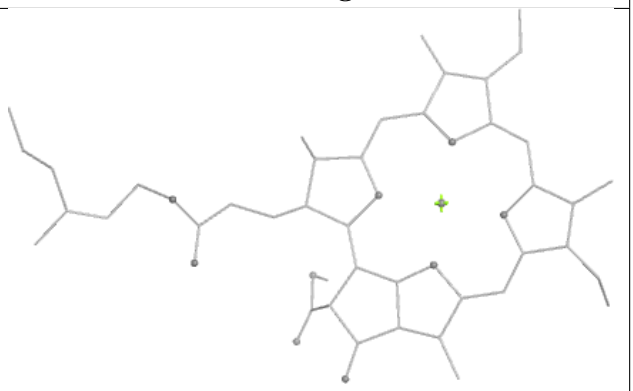
Bond lengths



Bond angles

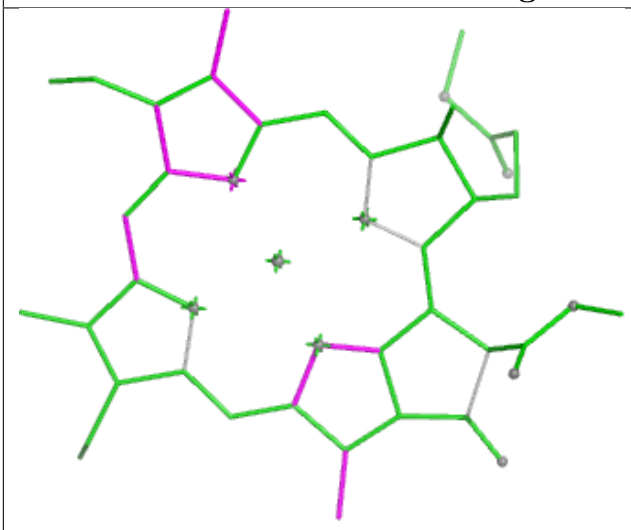


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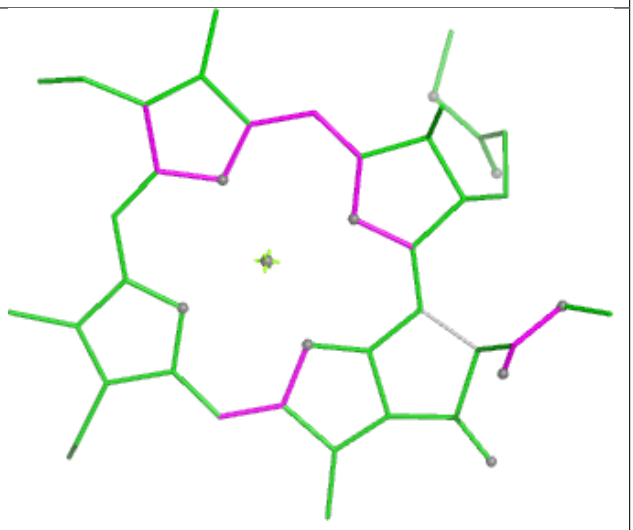


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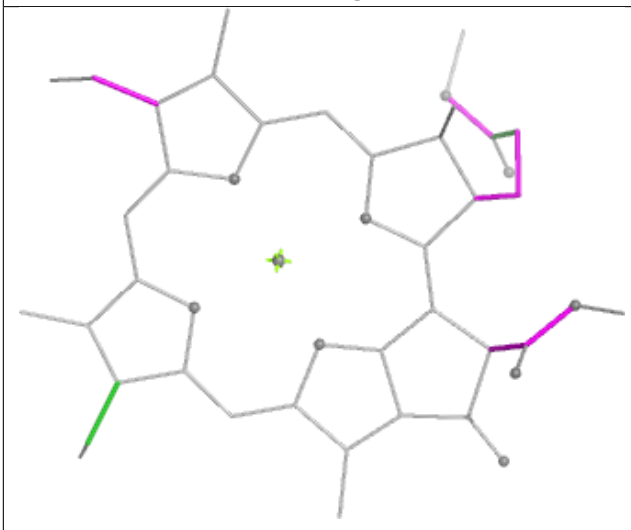
Ligand CLA k 4003



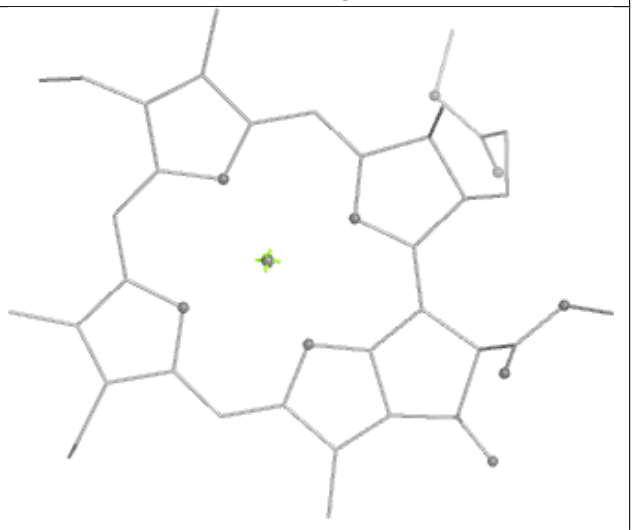
Bond lengths



Bond angles

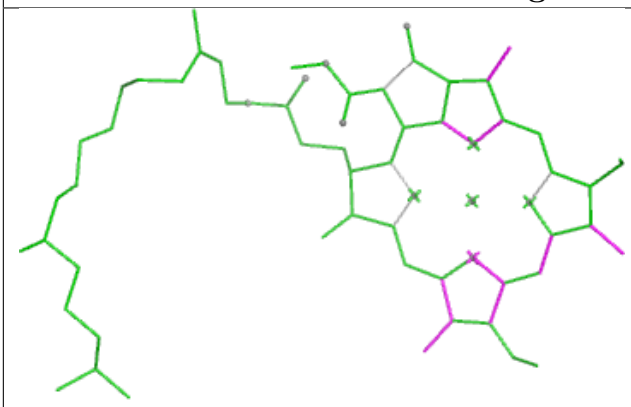


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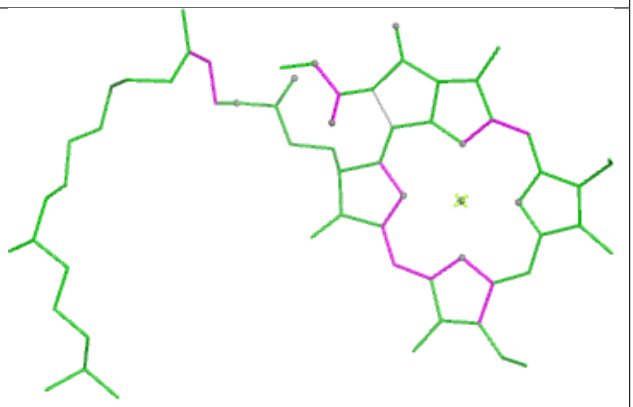


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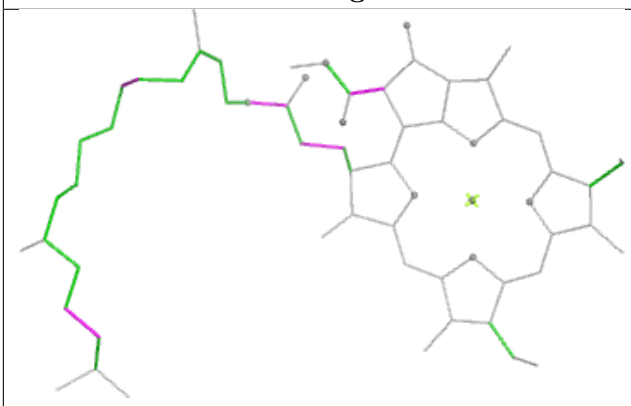
Ligand CLA a 803



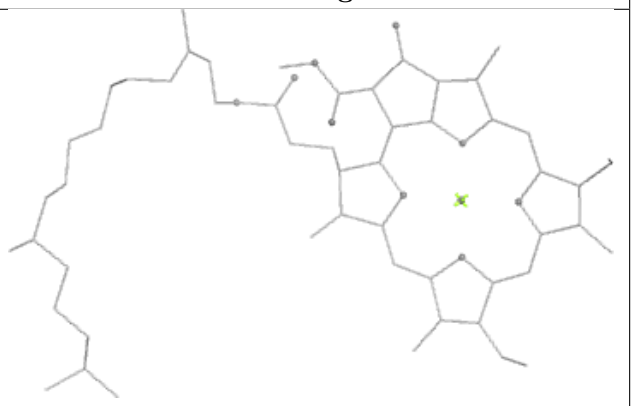
Bond lengths



Bond angles

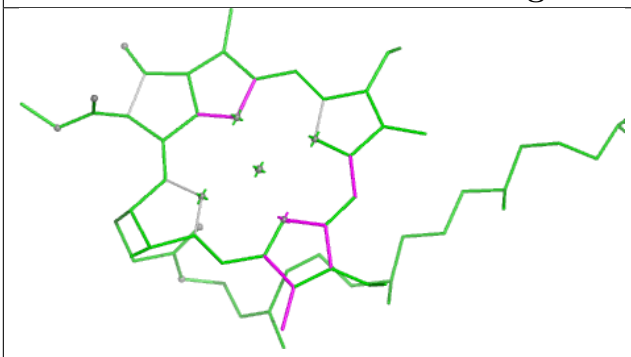


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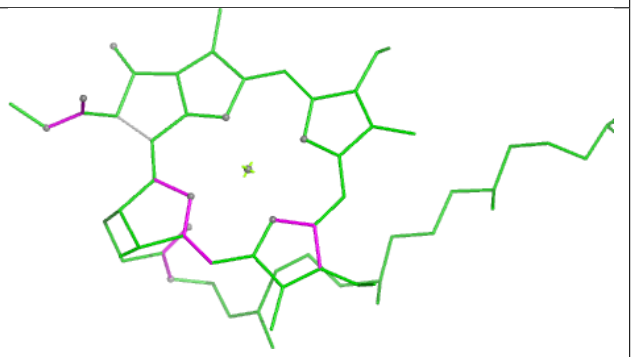


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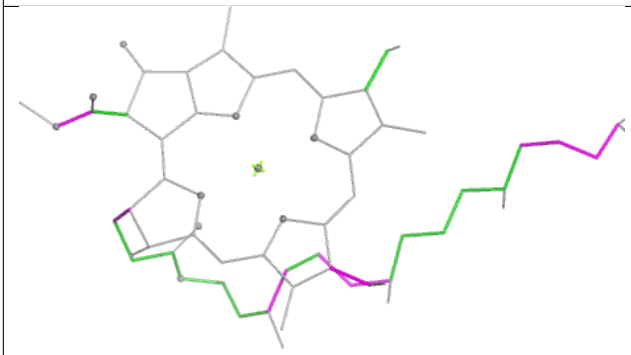
Ligand CLA b 821



Bond lengths



Bond angles

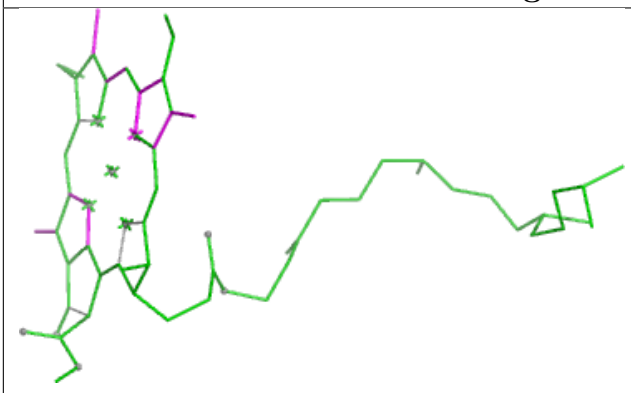


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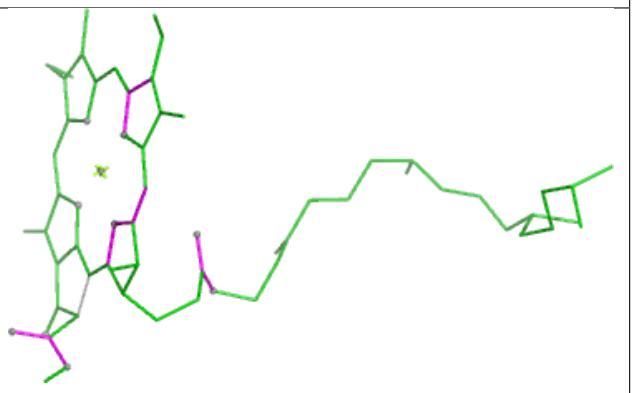


Rings

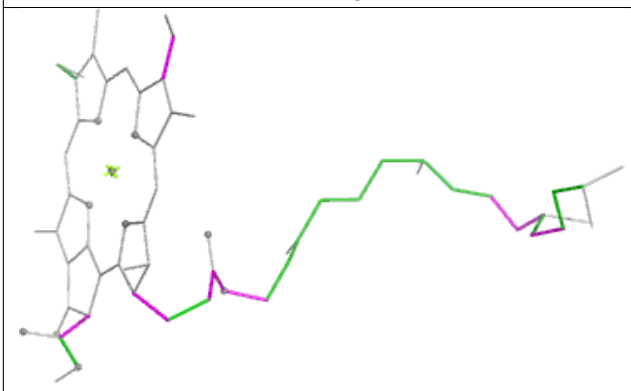
Ligand CLA l 1502



Bond lengths



Bond angles

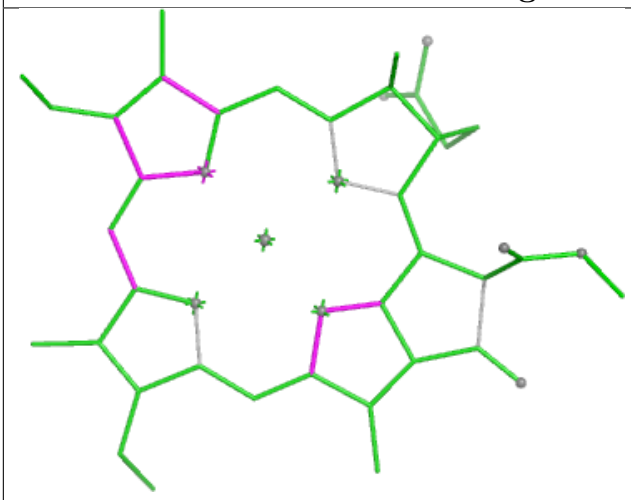


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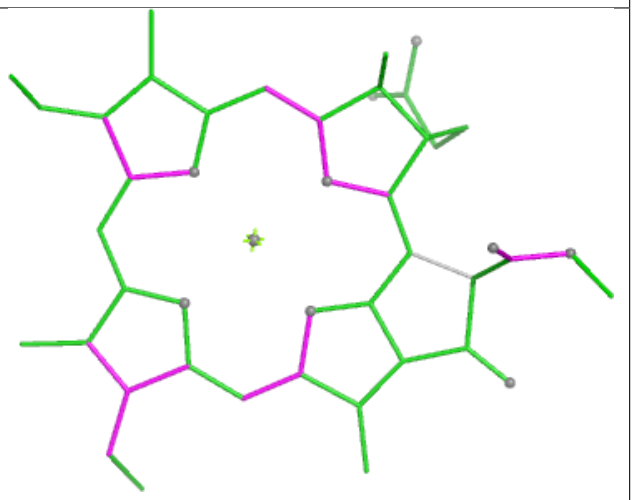


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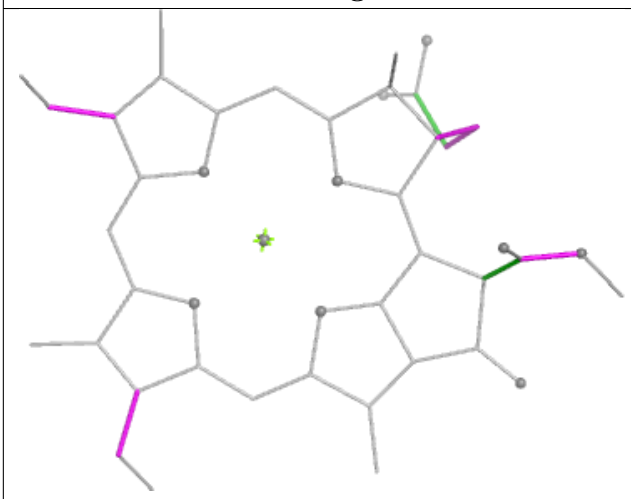
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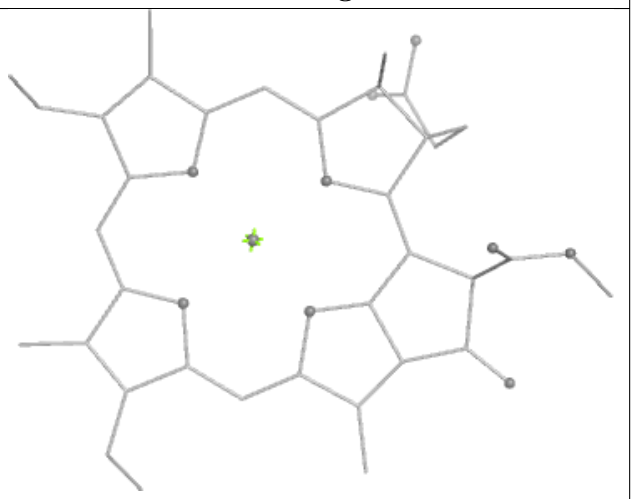
Bond lengths



Bond angles

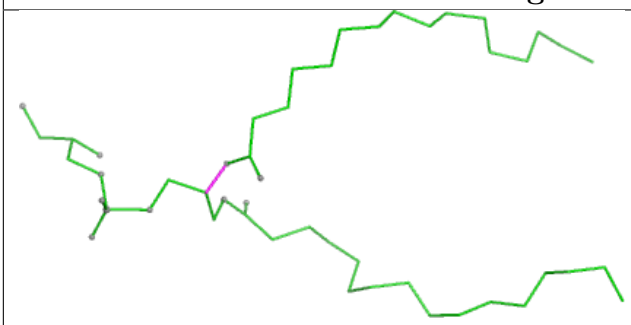


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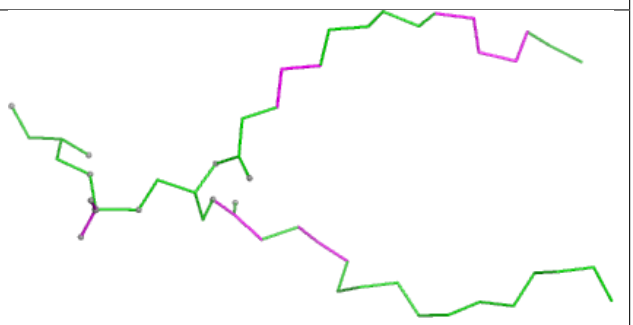


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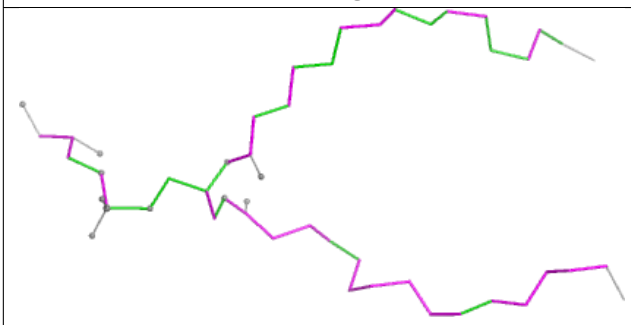
Ligand LHG a 849



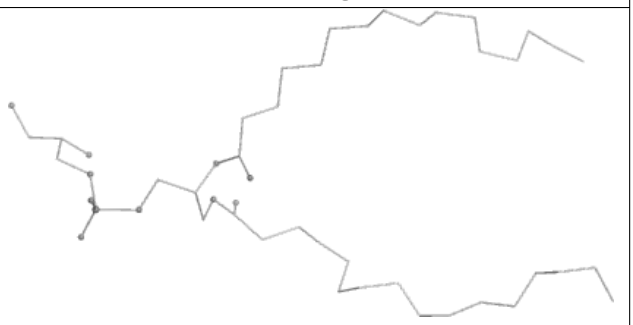
Bond lengths



Bond angles



Torsions

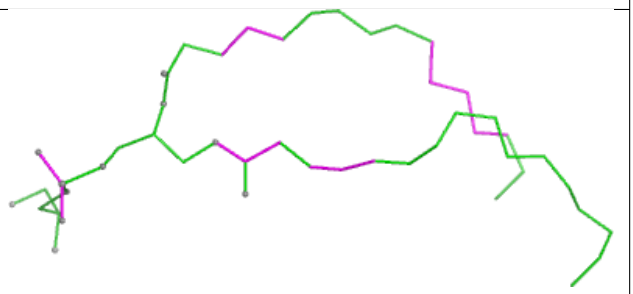


Rings

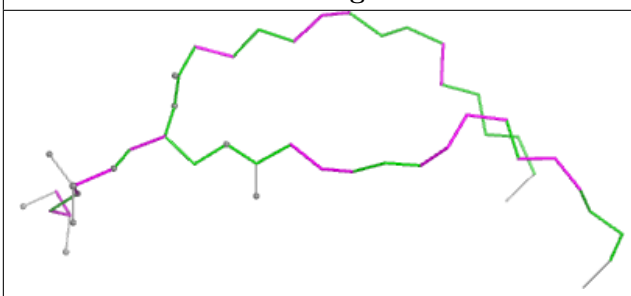
Ligand LHG a 851



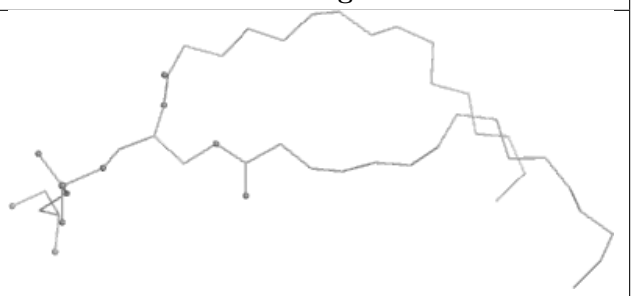
Bond lengths



Bond angles

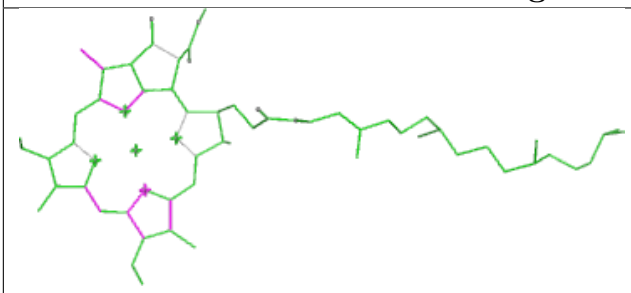


Torsions

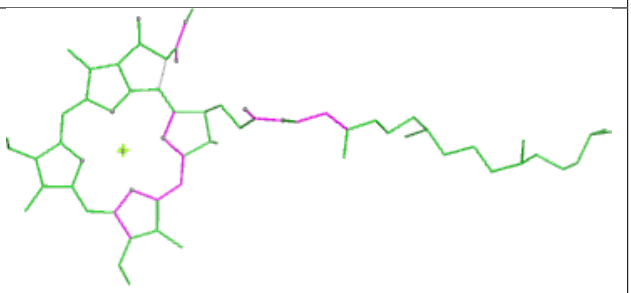


Rings

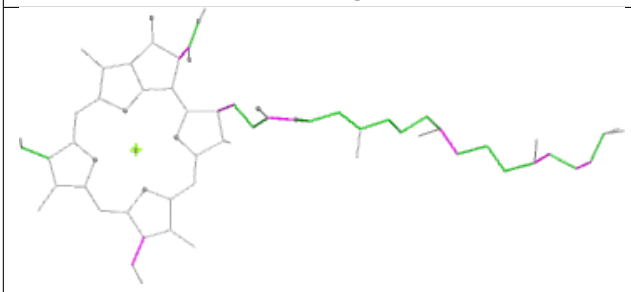
Ligand CLA a 826



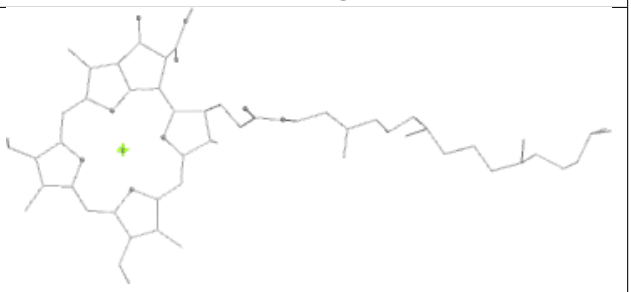
Bond lengths



Bond angles

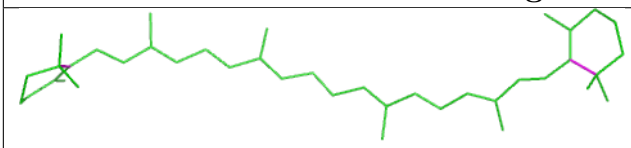


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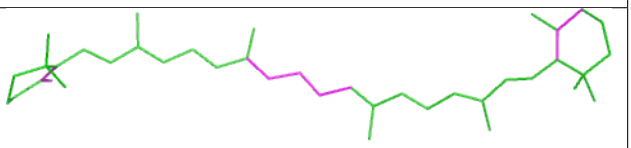


Rings

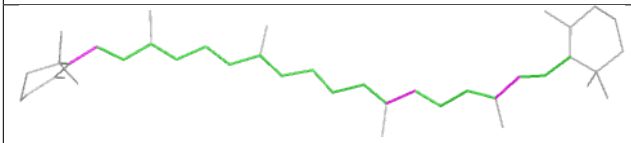
Ligand BCR b 845



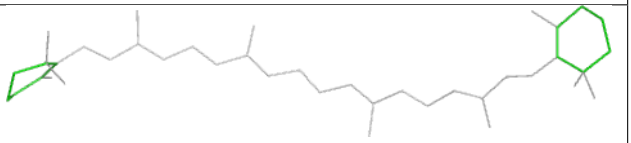
Bond lengths



Bond angles

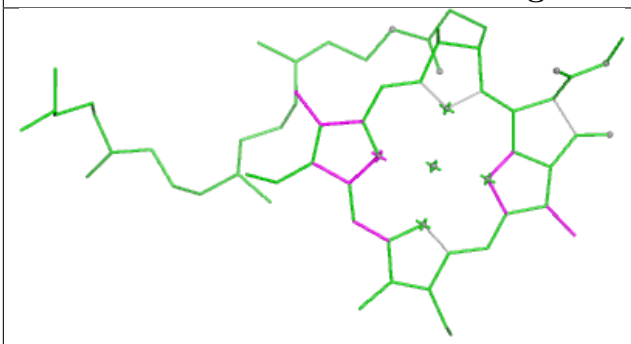


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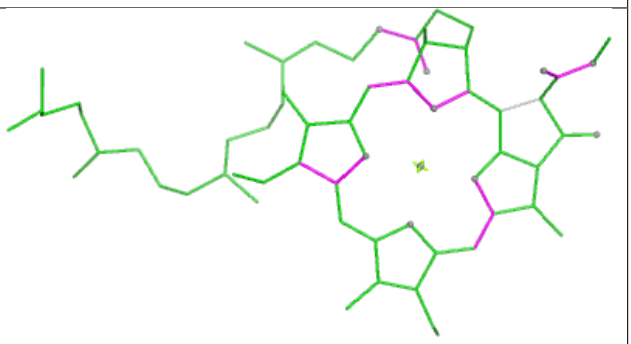


Rings

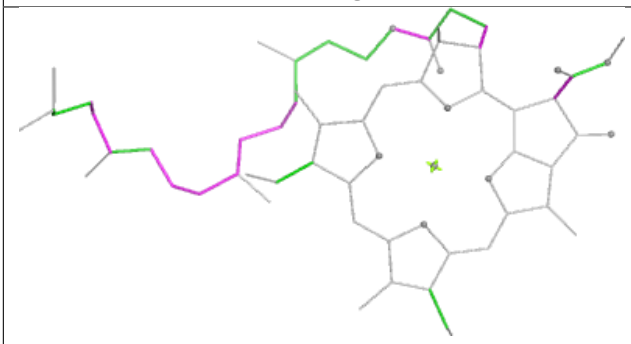
Ligand CLA b 819



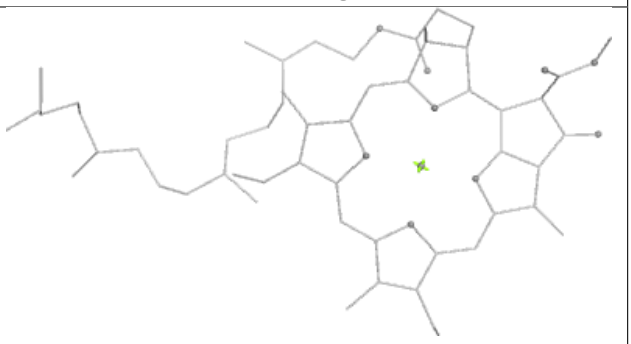
Bond lengths



Bond angles

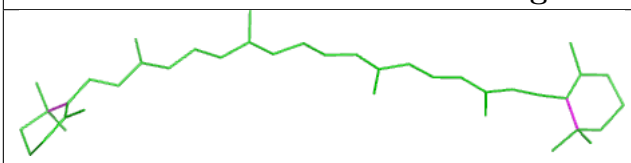


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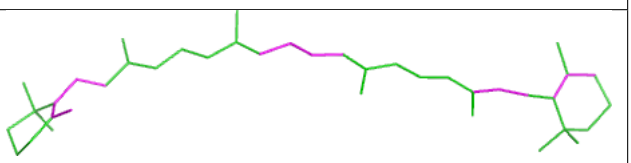


Rings

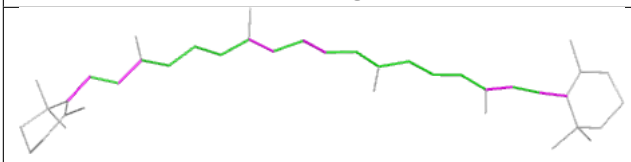
Ligand BCR f 202



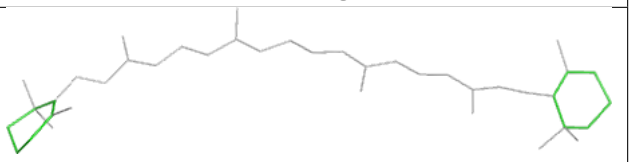
Bond lengths



Bond angles

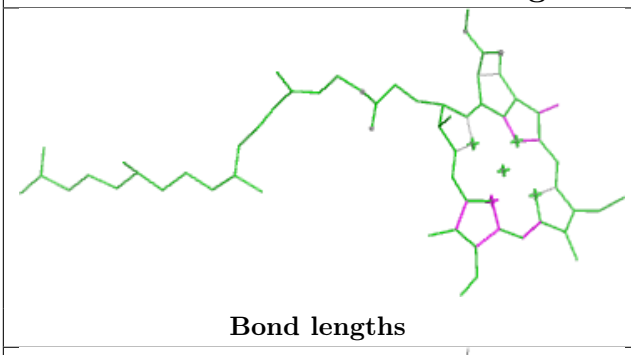


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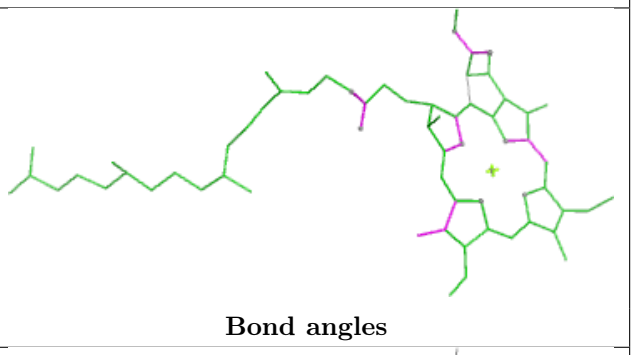


Rings

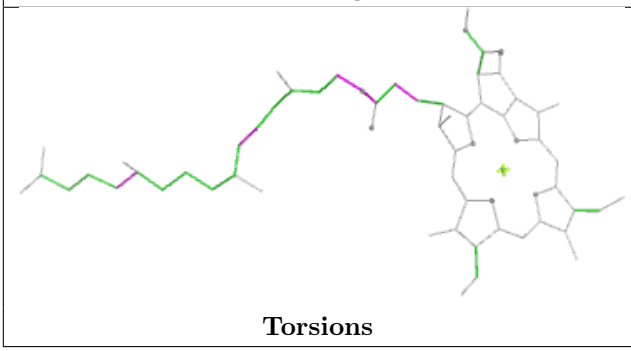
Ligand CLA a 854



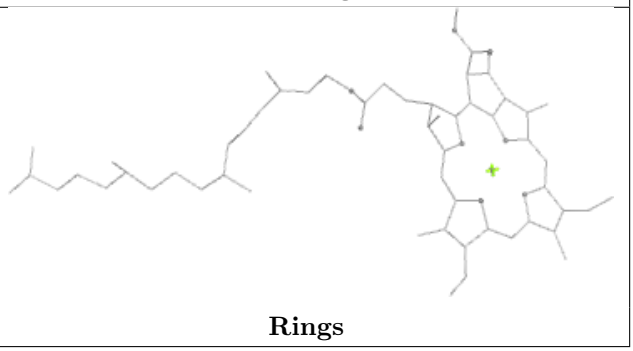
Bond lengths



Bond angles

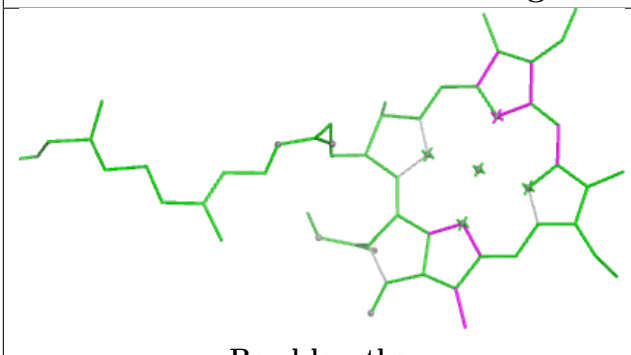


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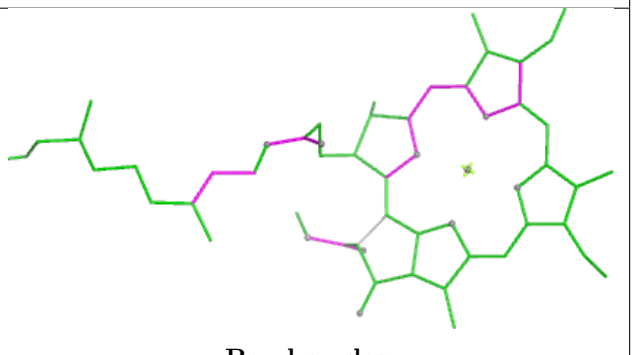


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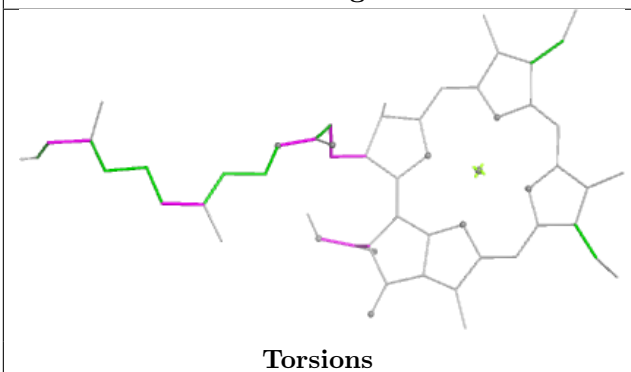
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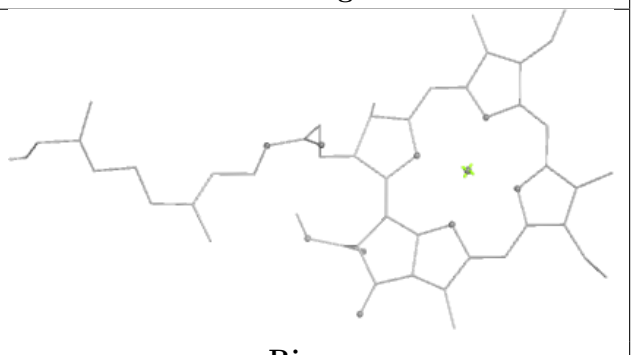
Bond lengths



Bond angles

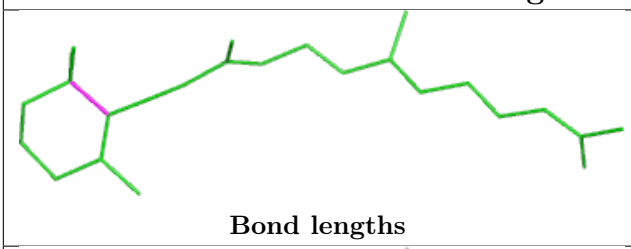


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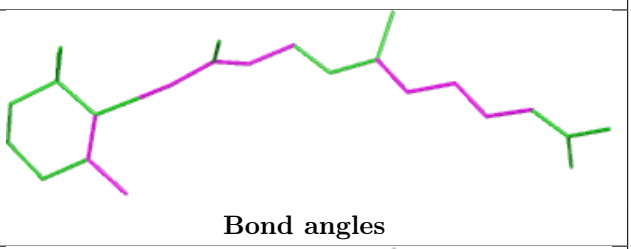


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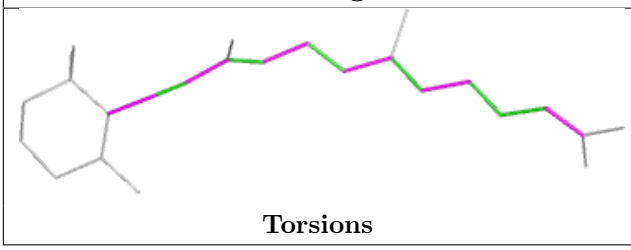
Ligand BCR a 848



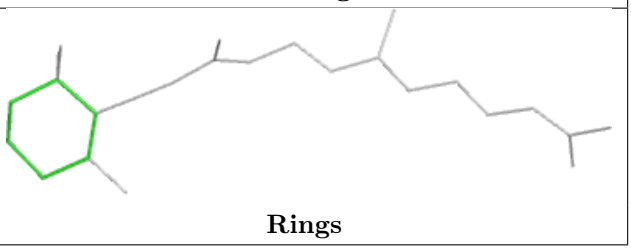
Bond lengths



Bond angles



Torsions

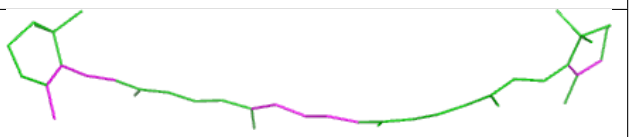


Rings

Ligand BCR i 101



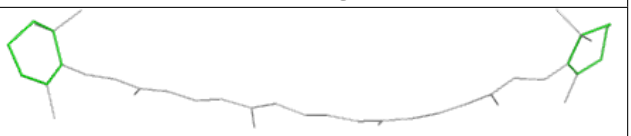
Bond lengths



Bond angles



Torsions

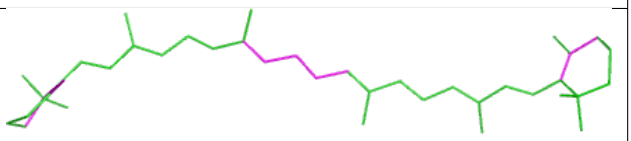


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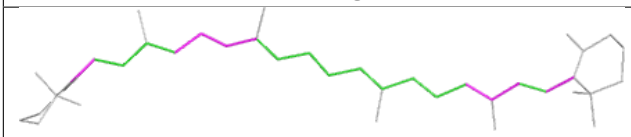
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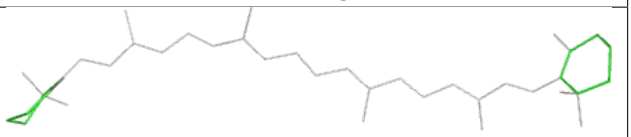
Bond lengths



Bond angles

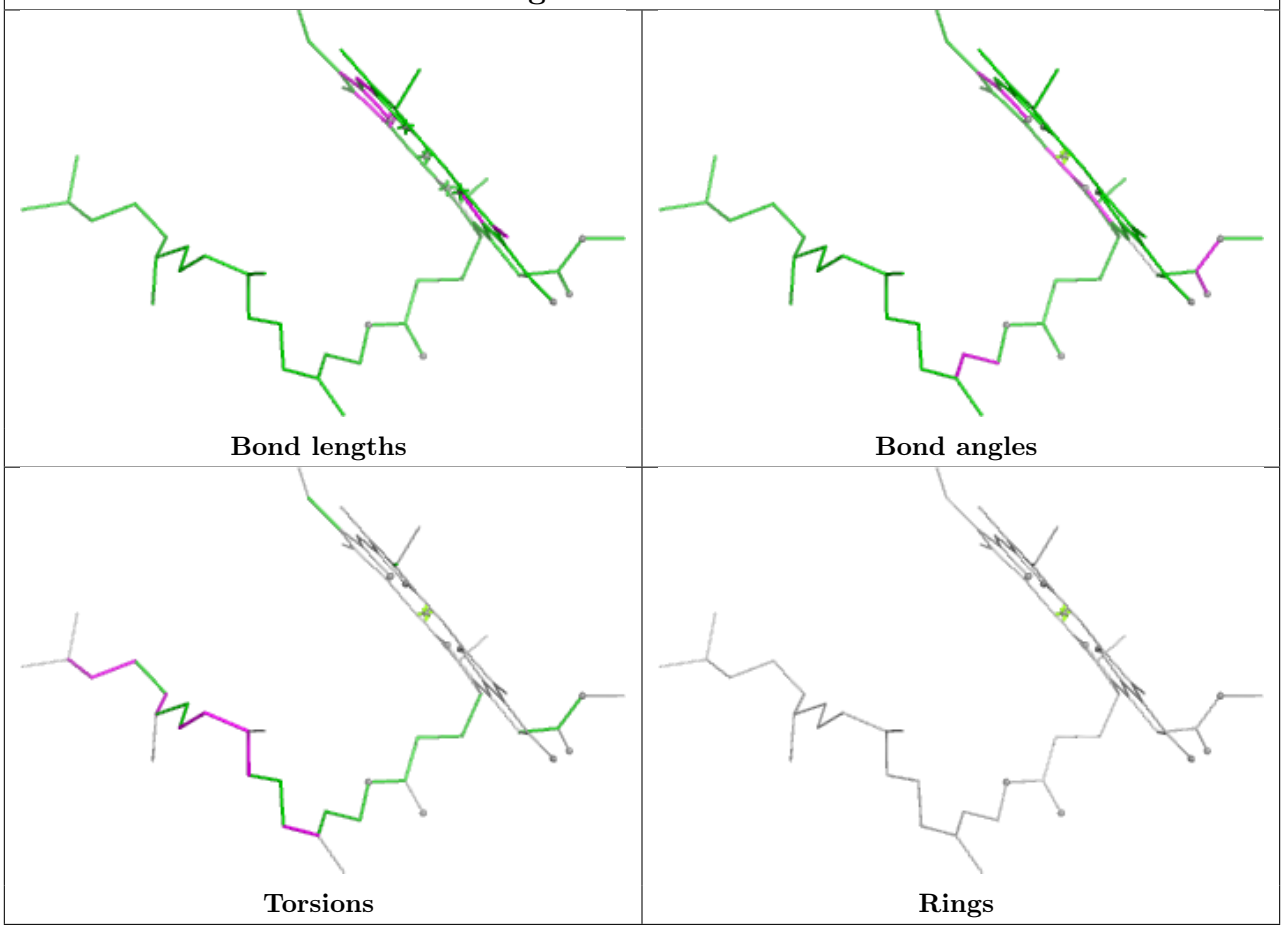


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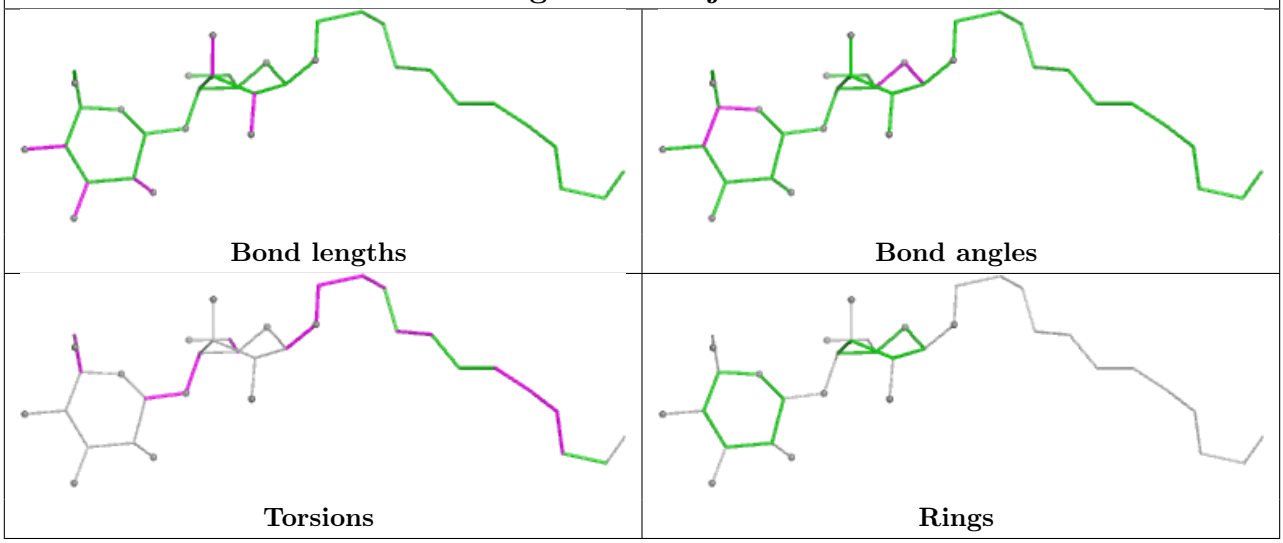


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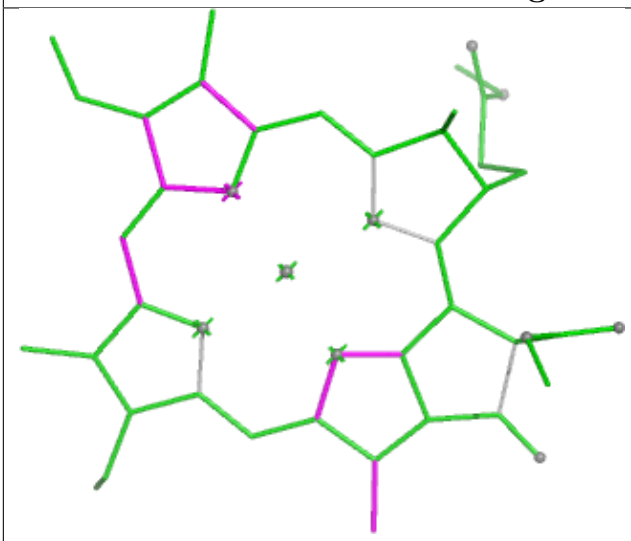
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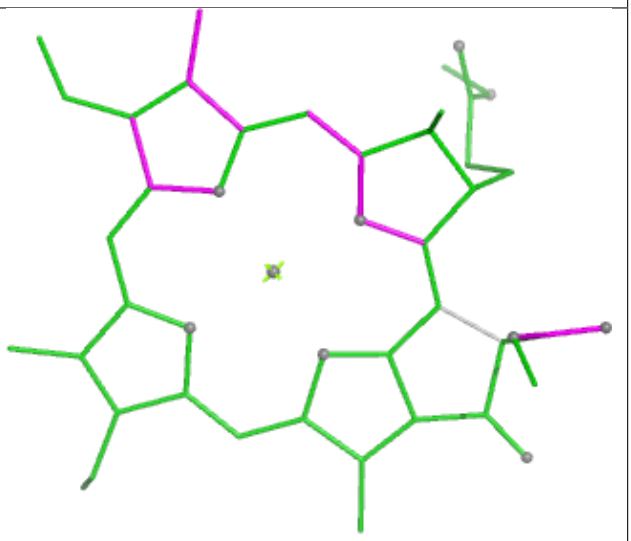
Ligand LMT j 102



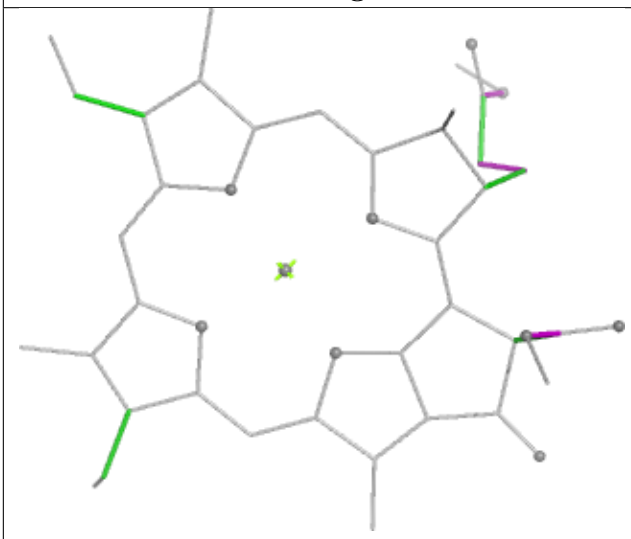
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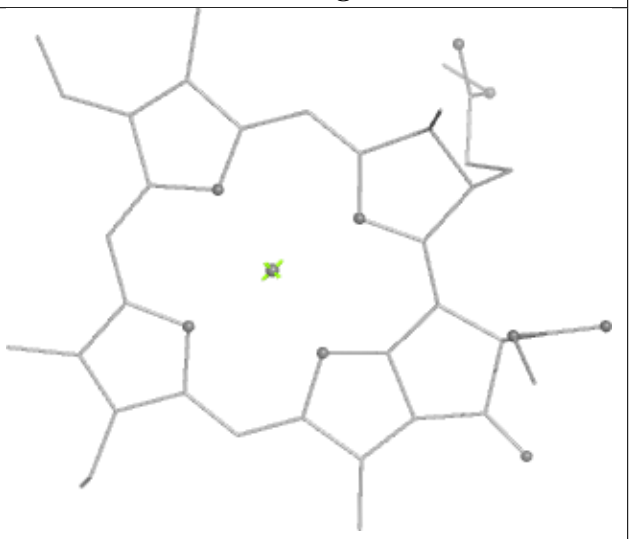
Bond lengths



Bond angles

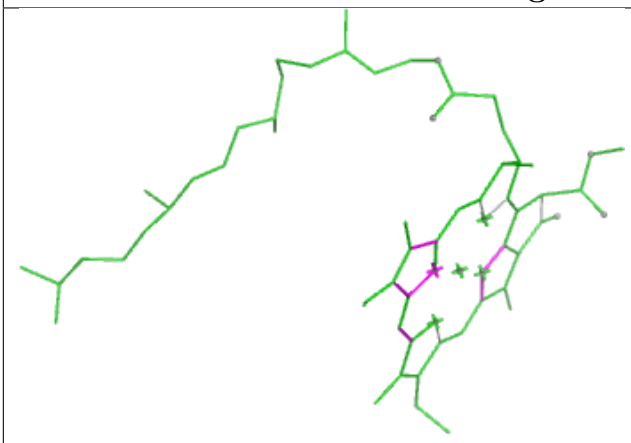


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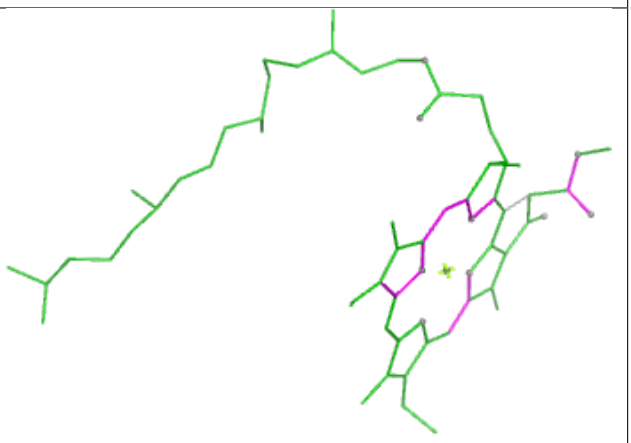


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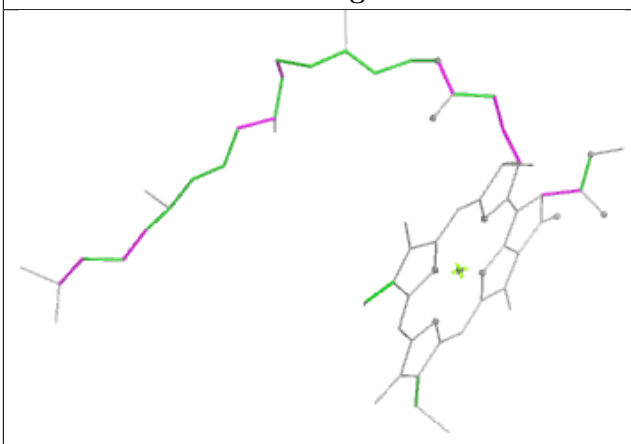
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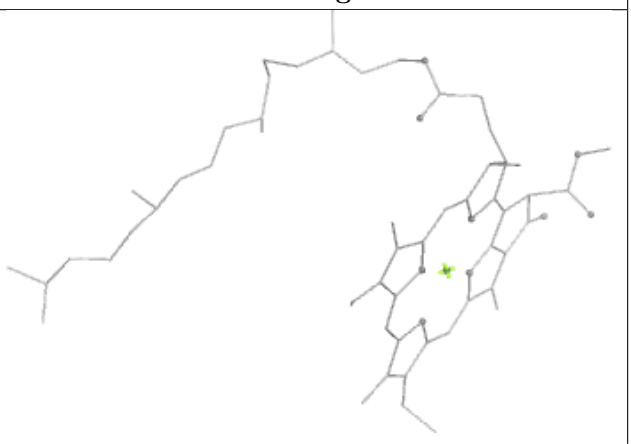
Bond lengths



Bond angles

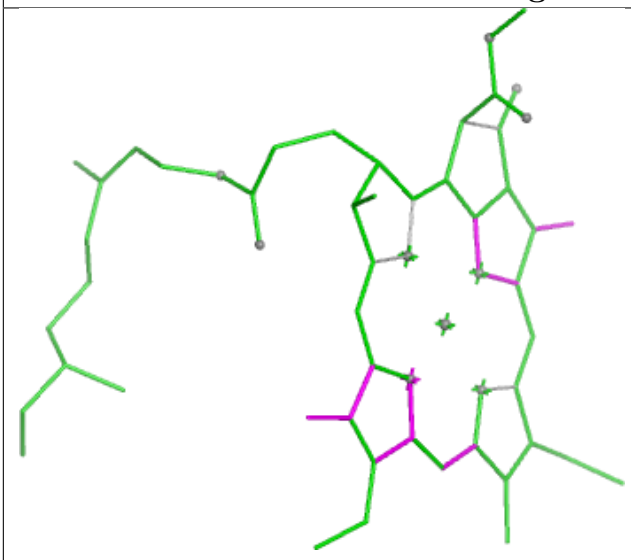


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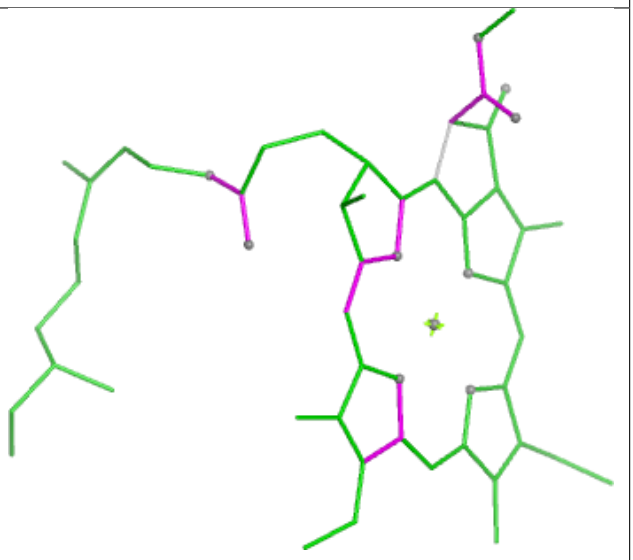


Rings

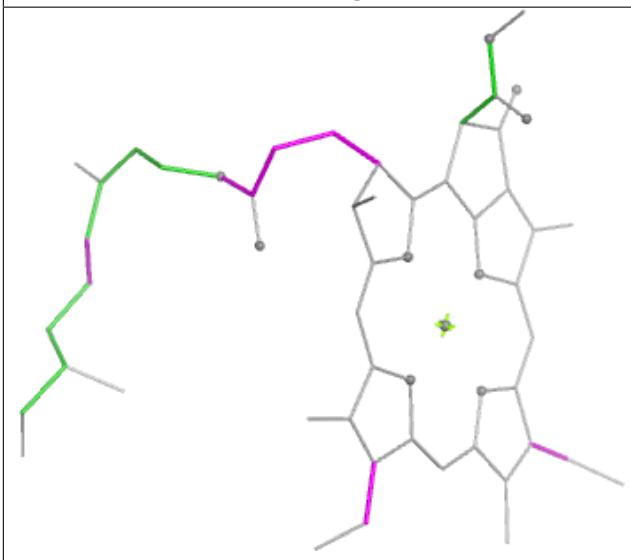
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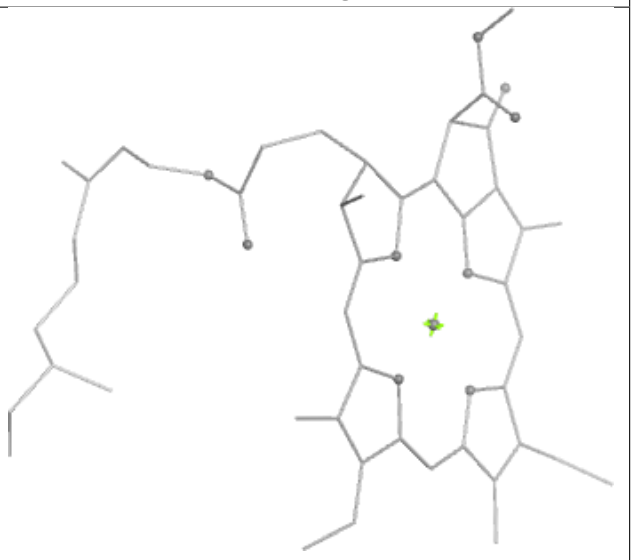
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Bond angles

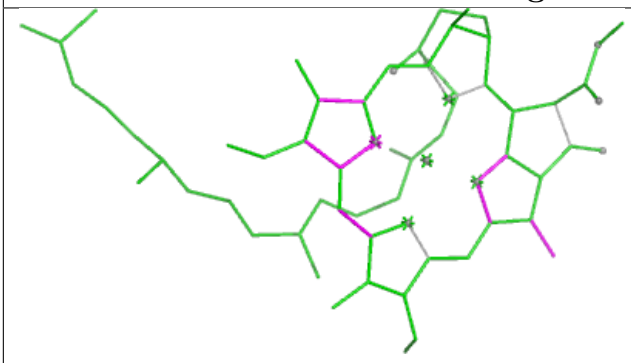


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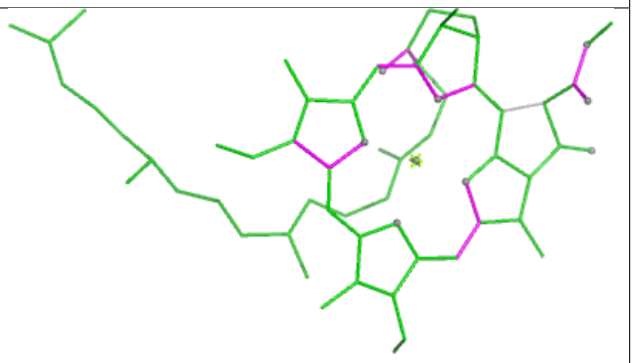


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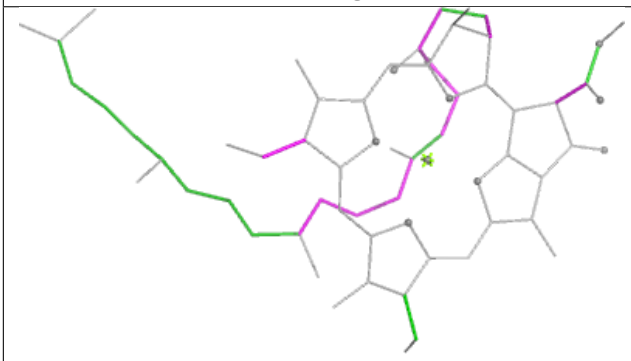
Ligand CLA b 808



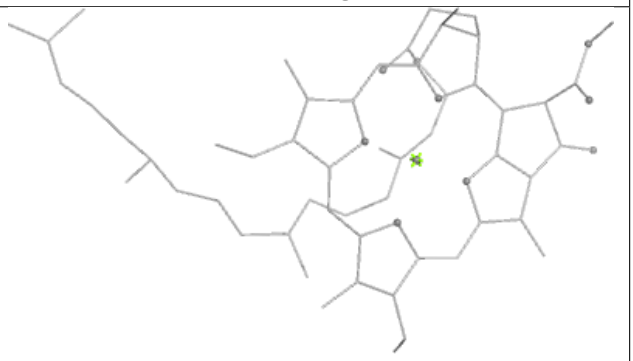
Bond lengths



Bond angles

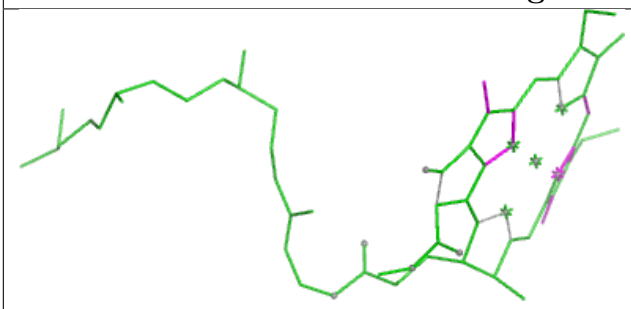


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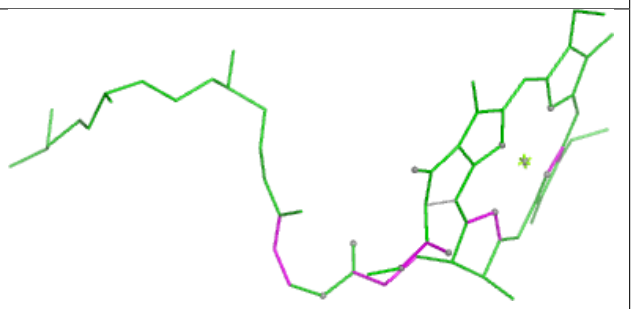


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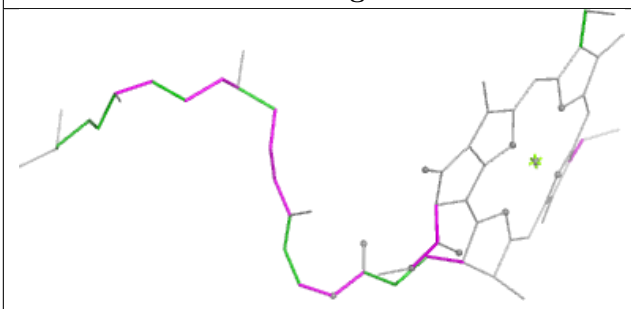
Ligand CLA b 803



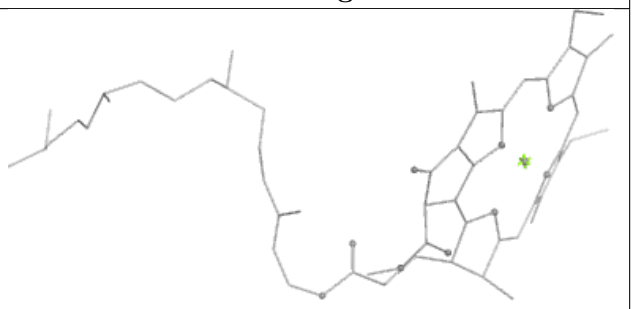
Bond lengths



Bond angles

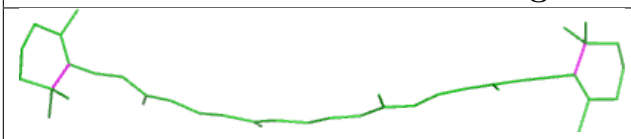


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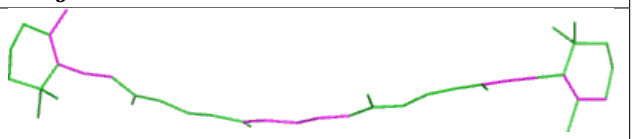


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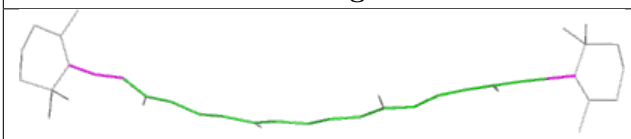
Ligand BCR j 105



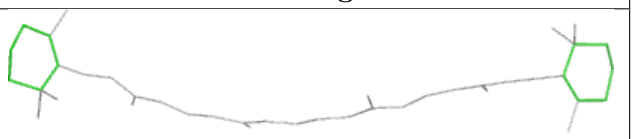
Bond lengths



Bond angles

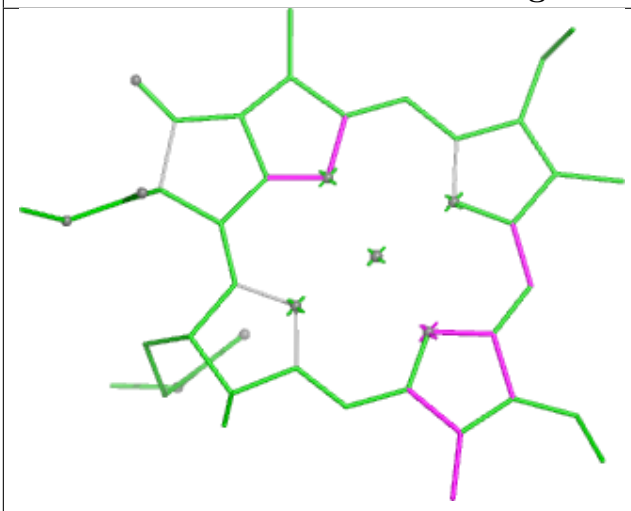


Torsions

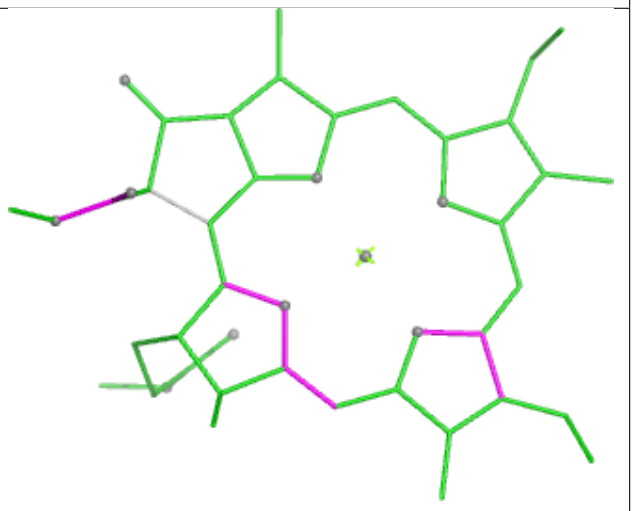


Rings

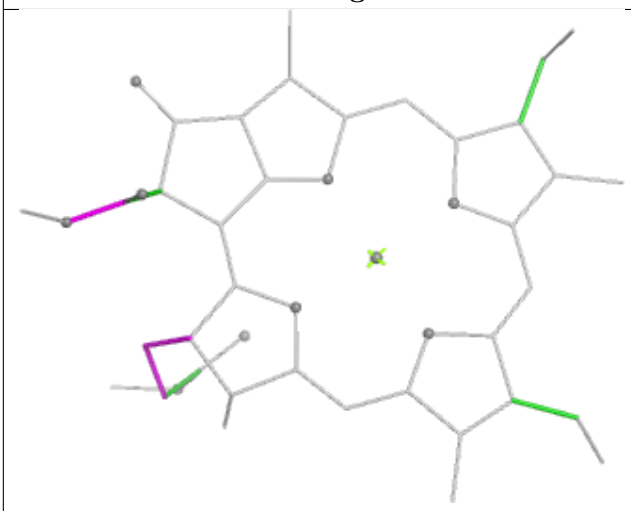
Ligand CLA a 816



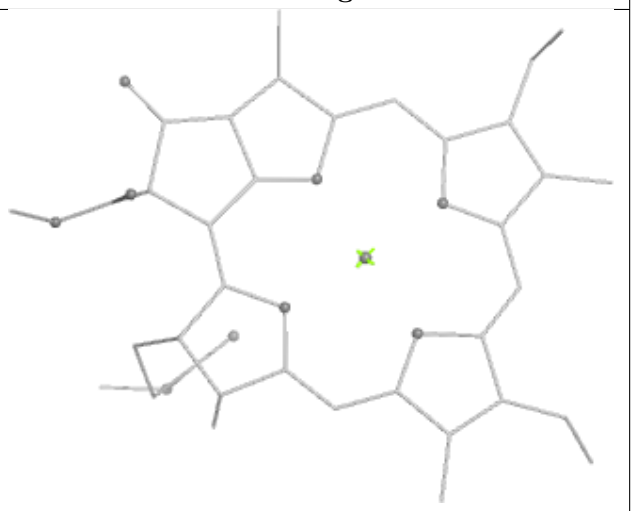
Bond lengths



Bond angles

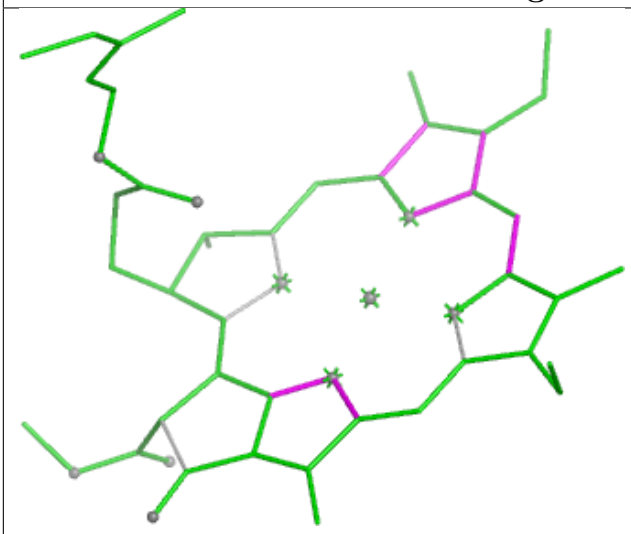


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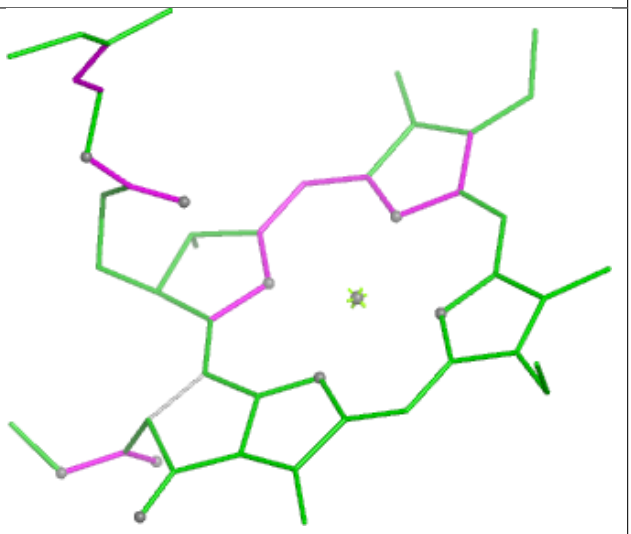


Rings

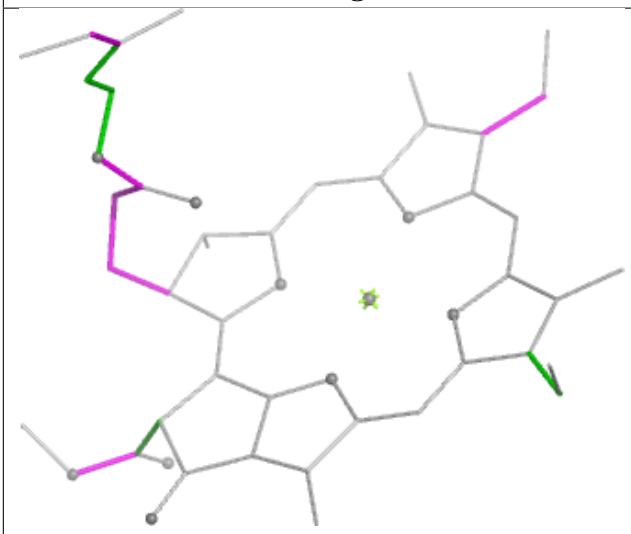
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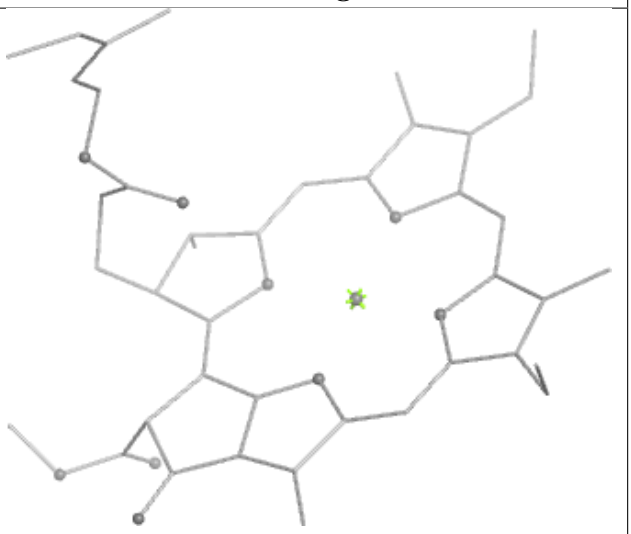
Bond lengths



Bond angles



Torsions

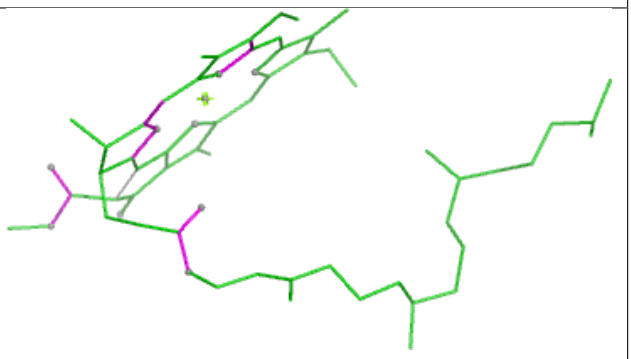


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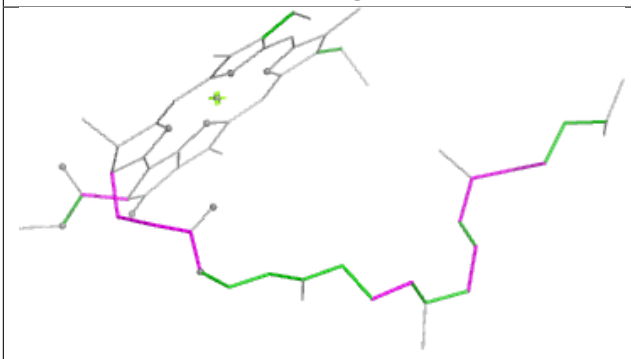
Ligand CLA a 811



Bond lengths



Bond angles

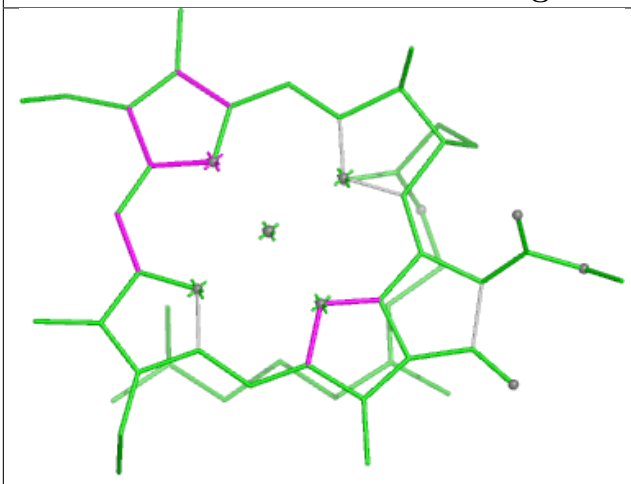


Torsions



Rings

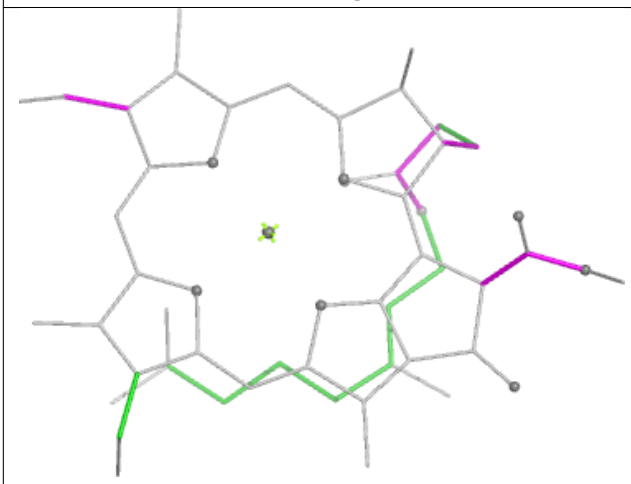
Ligand CLA j 103



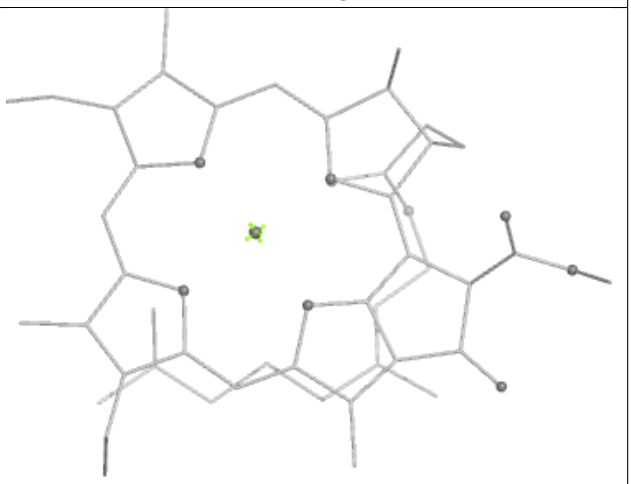
Bond lengths



Bond angles

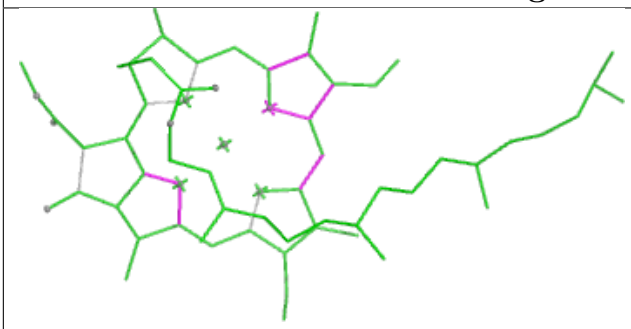


Torsions



Rings

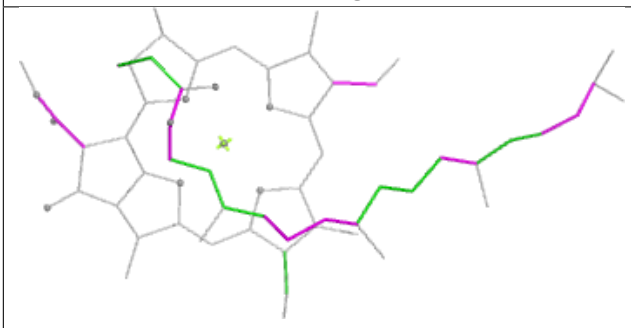
Ligand CLA a 840



Bond lengths



Bond angles

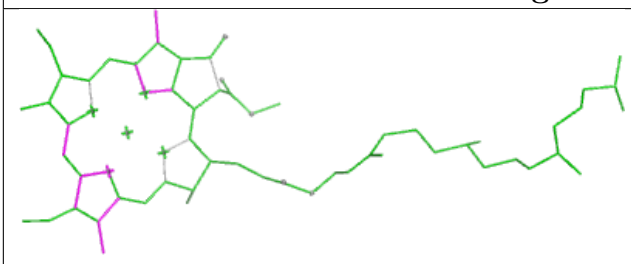


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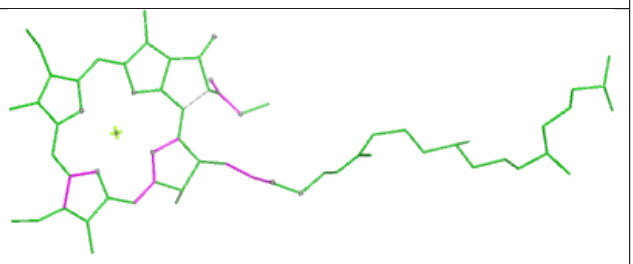


Rings

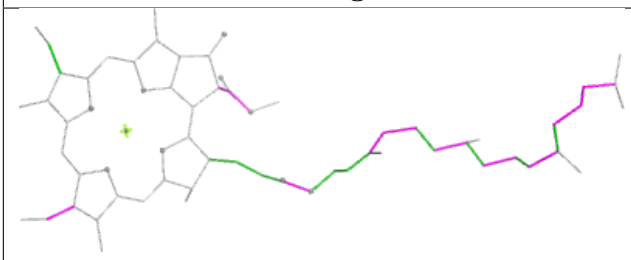
Ligand CLA f 201



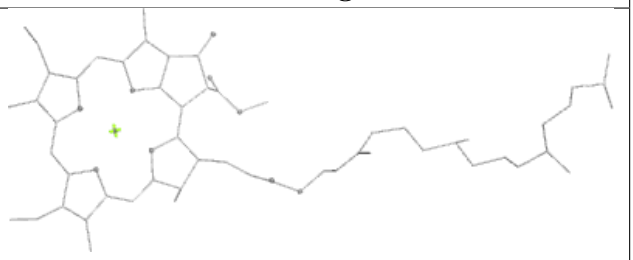
Bond lengths



Bond angles



Torsions

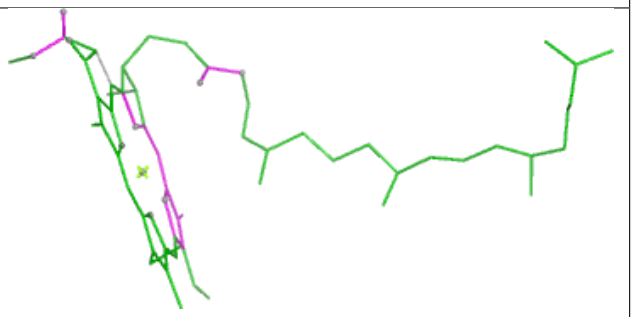


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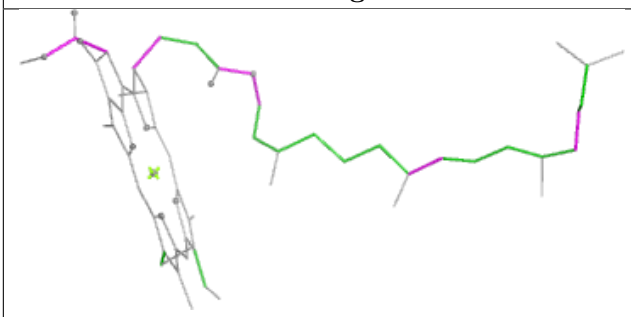
Ligand CLA a 822



Bond lengths



Bond angles

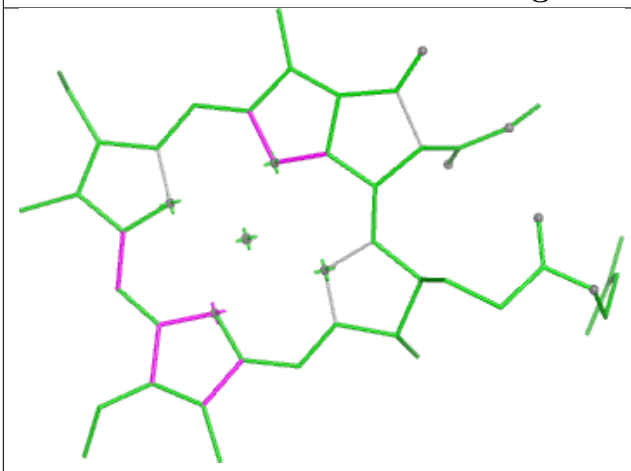


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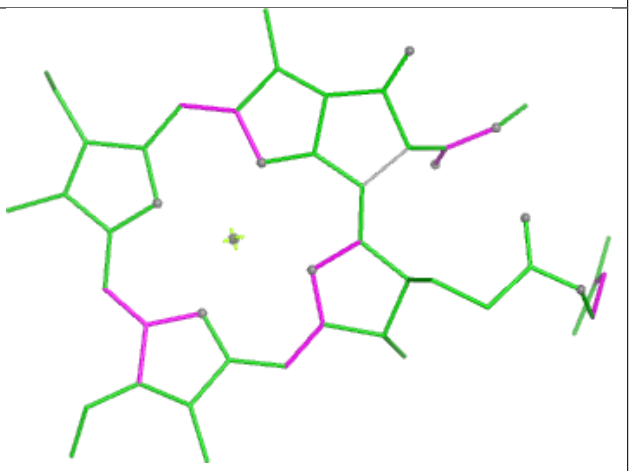


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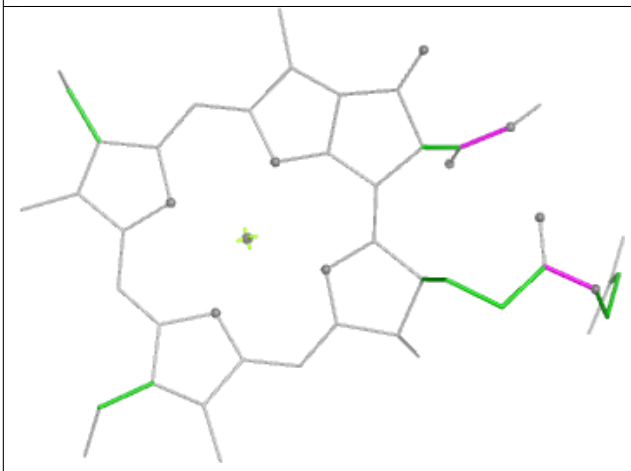
Ligand CLA f 203



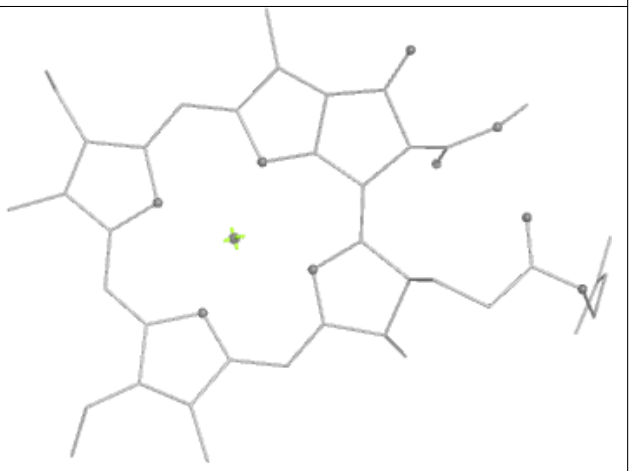
Bond lengths



Bond angles

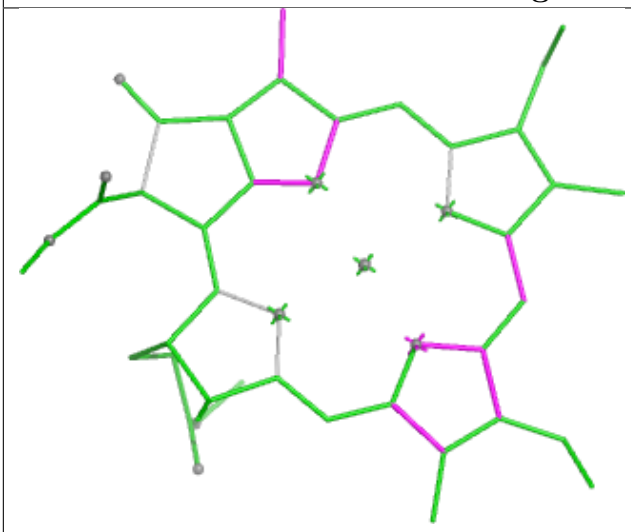


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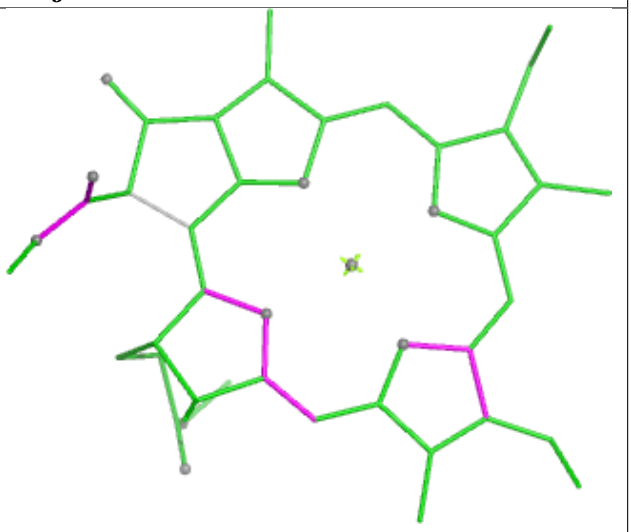


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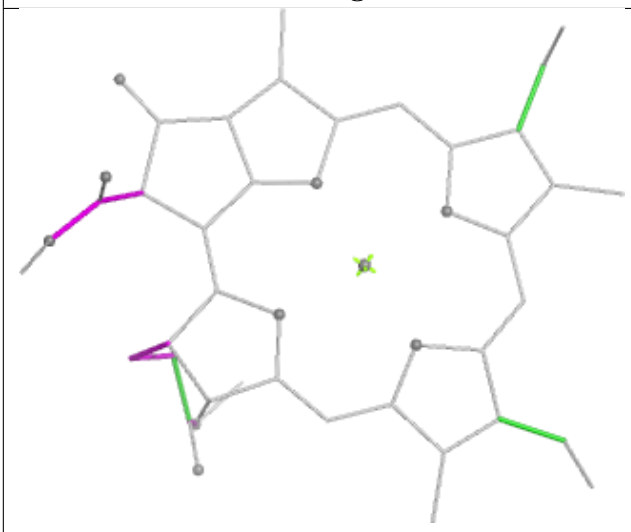
Ligand CLA j 104



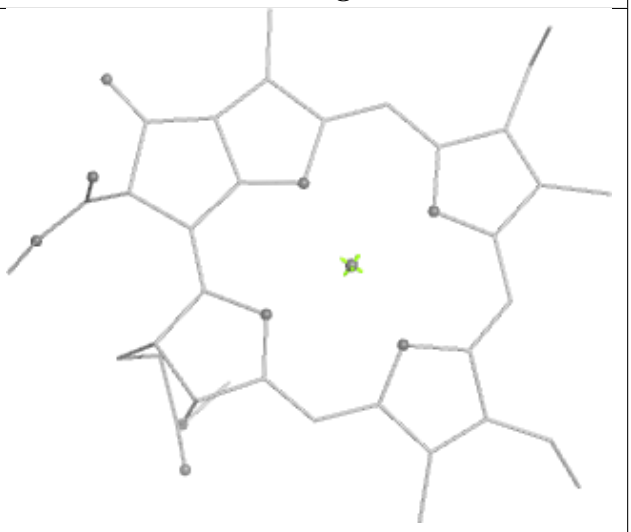
Bond lengths



Bond angles

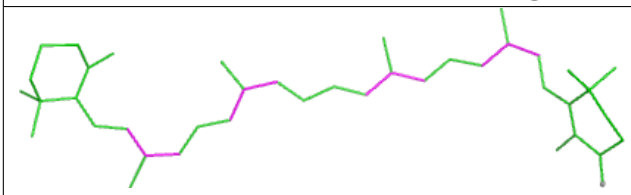


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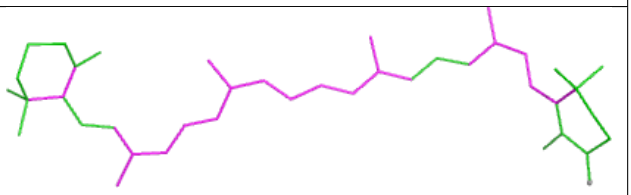


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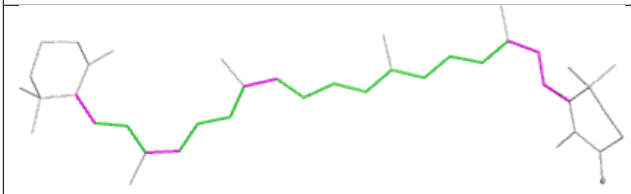
Ligand ECH b 846



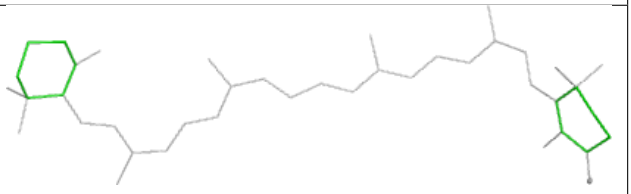
Bond lengths



Bond angles

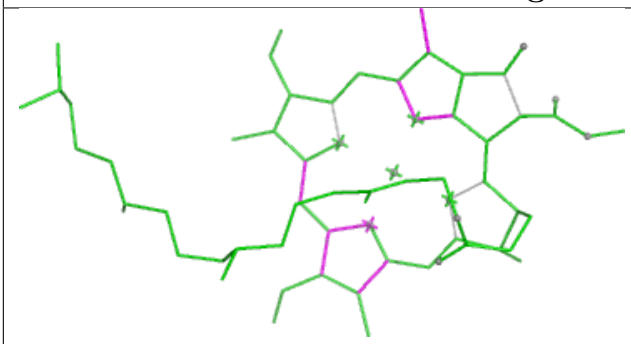


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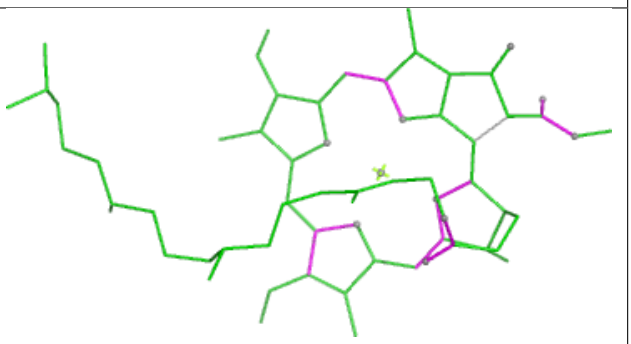


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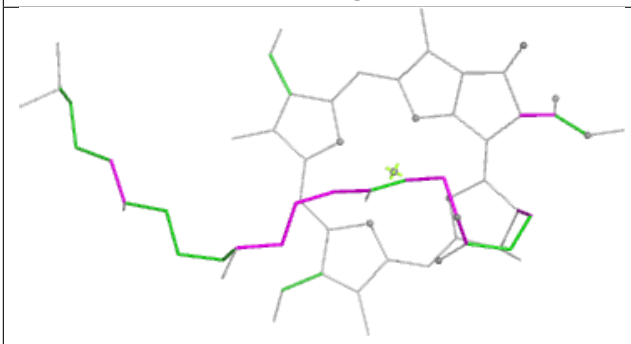
Ligand CLA b 838



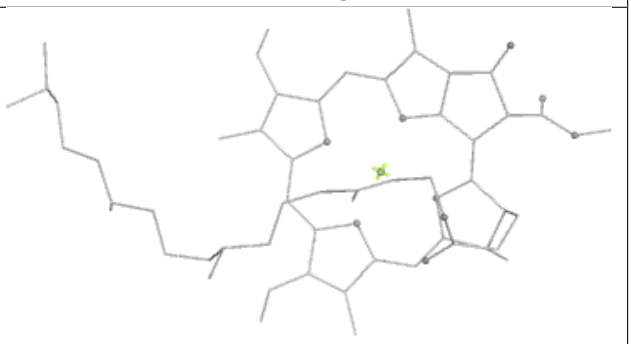
Bond lengths



Bond angles



Torsions

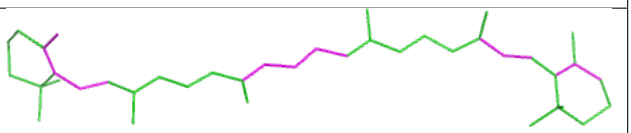


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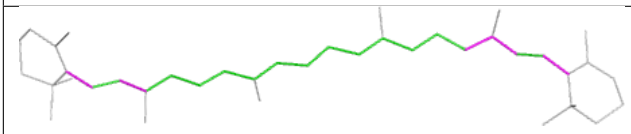
Ligand BCR a 847



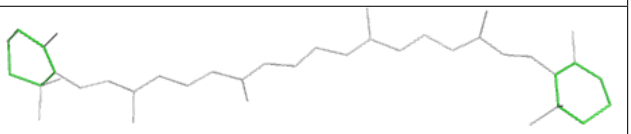
Bond lengths



Bond angles

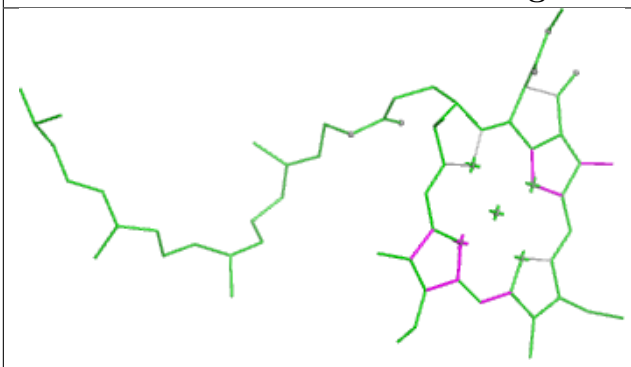


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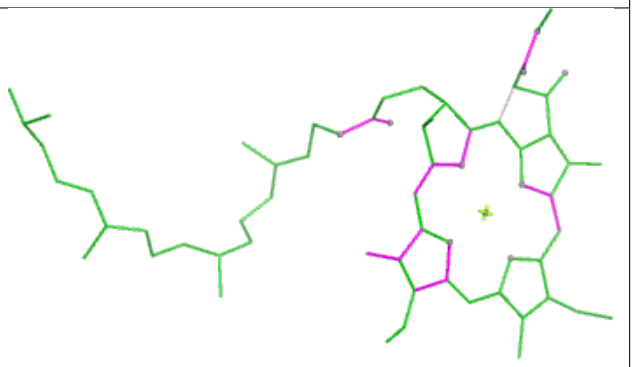


Rings

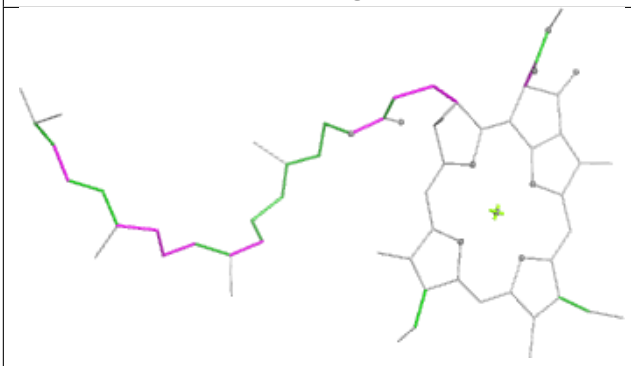
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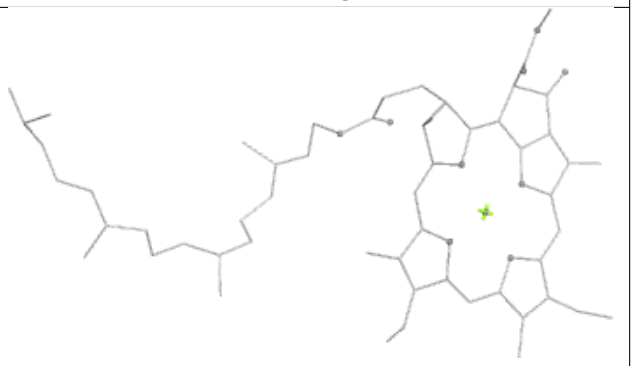
Bond lengths



Bond angles

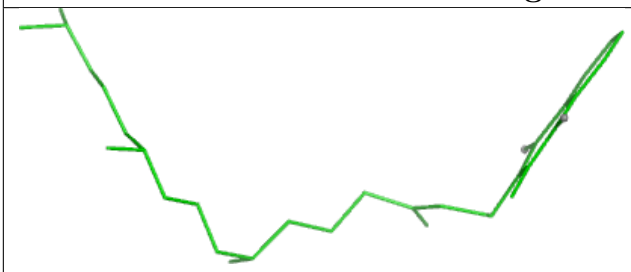


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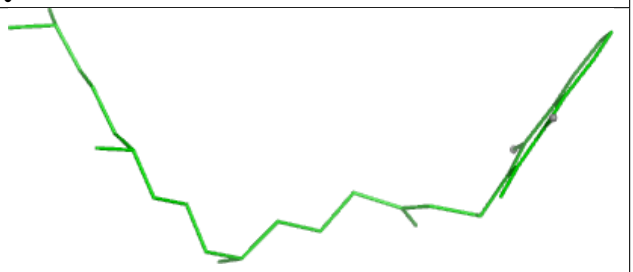


Rings

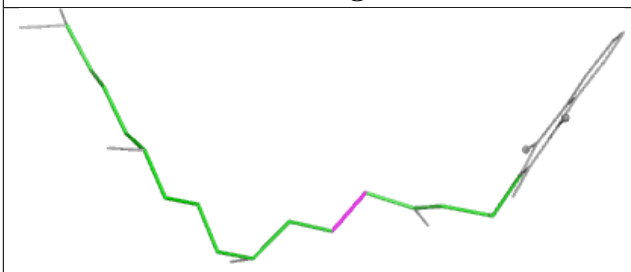
Ligand PQN b 843



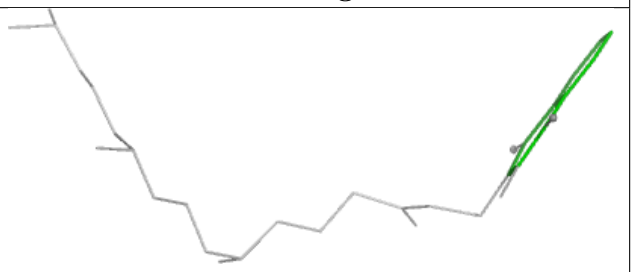
Bond lengths



Bond angles

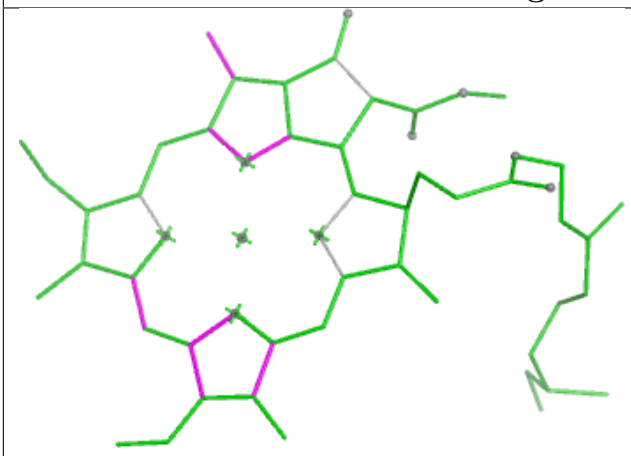


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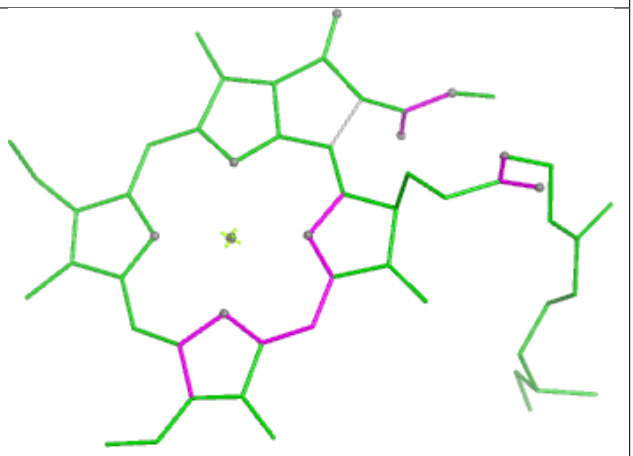


Rings

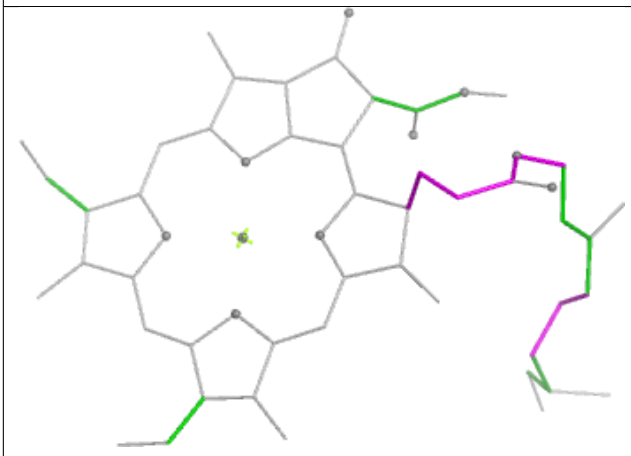
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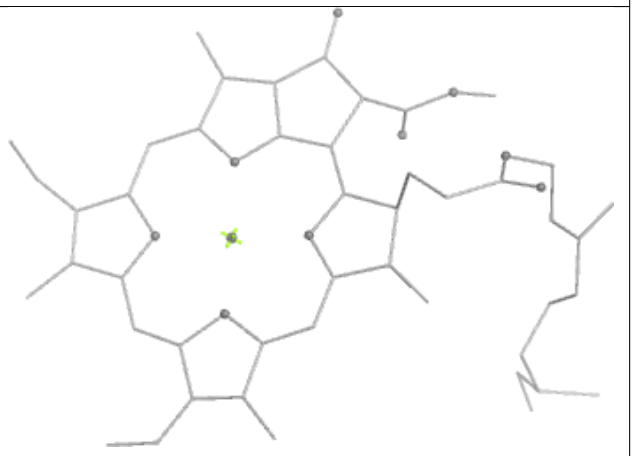
Bond lengths



Bond angles

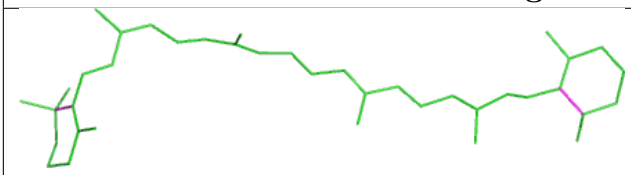


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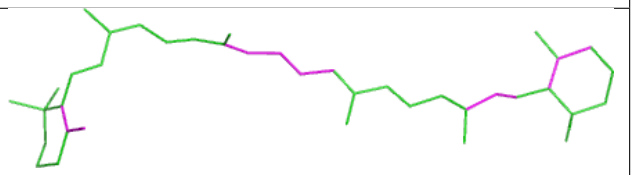


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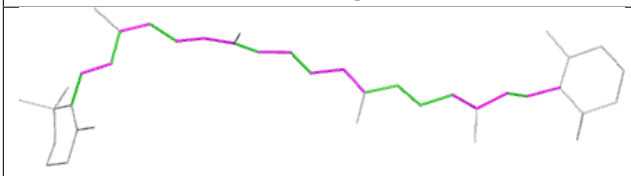
Ligand BCR b 849



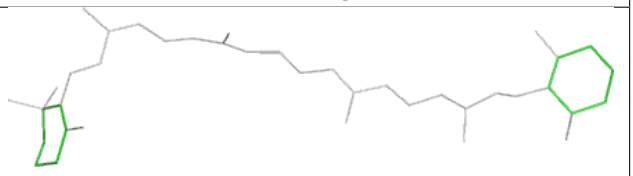
Bond lengths



Bond angles

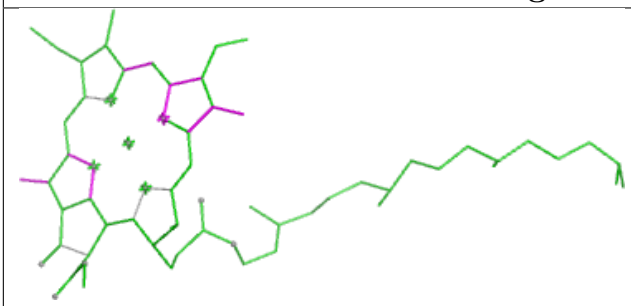


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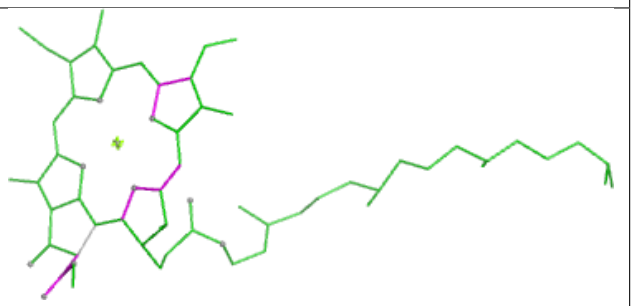


Rings

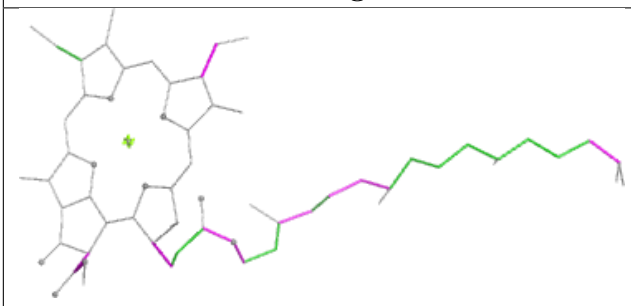
Ligand CLA a 834



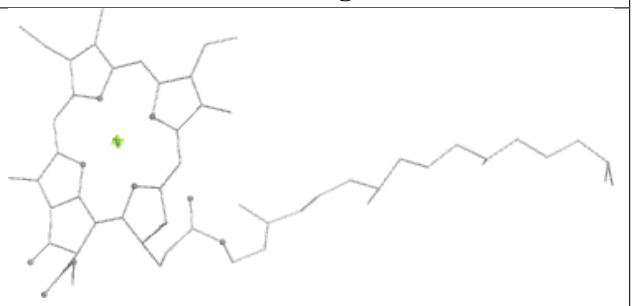
Bond lengths



Bond angles

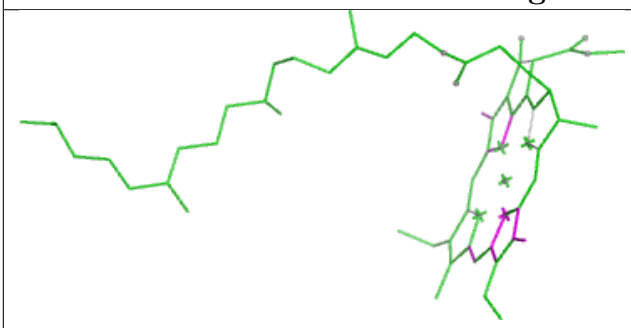


Torsions

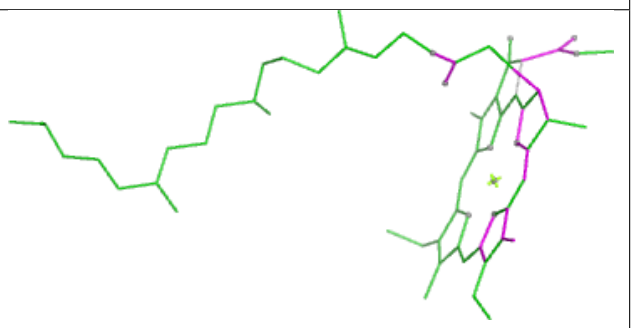


Rings

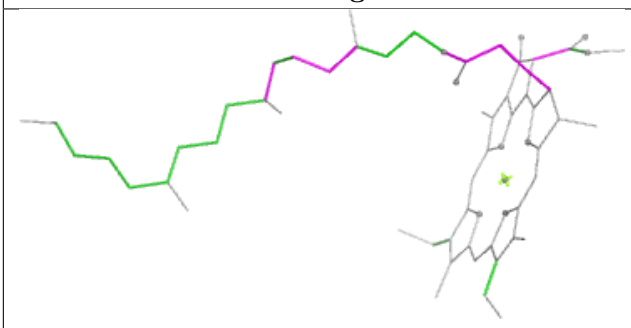
Ligand CLA a 830



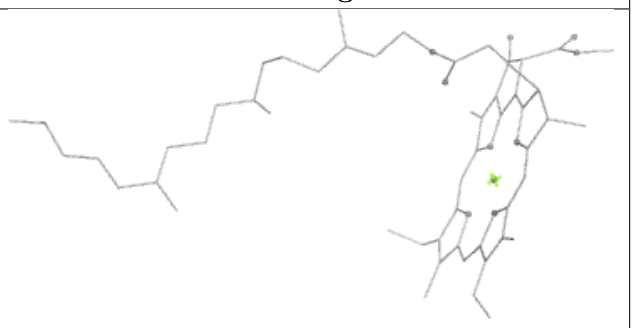
Bond lengths



Bond angles

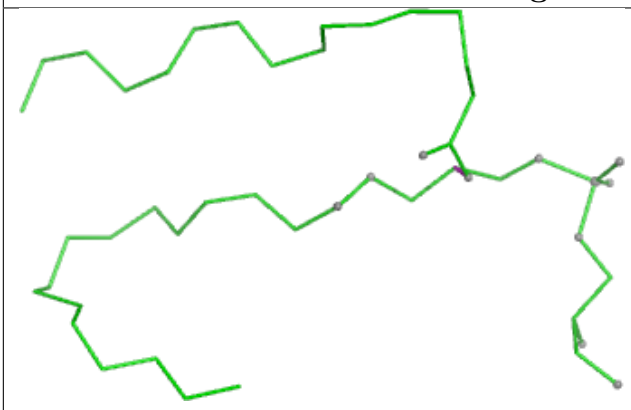


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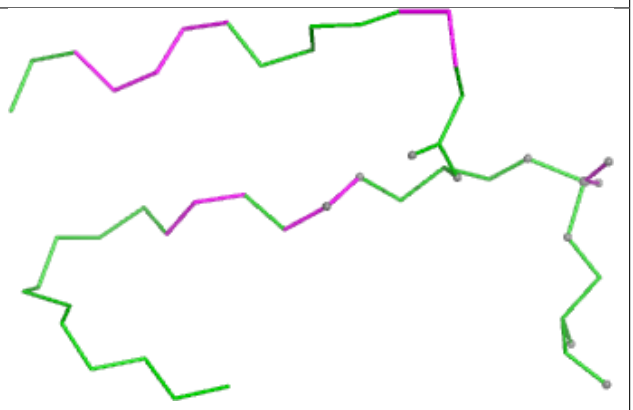


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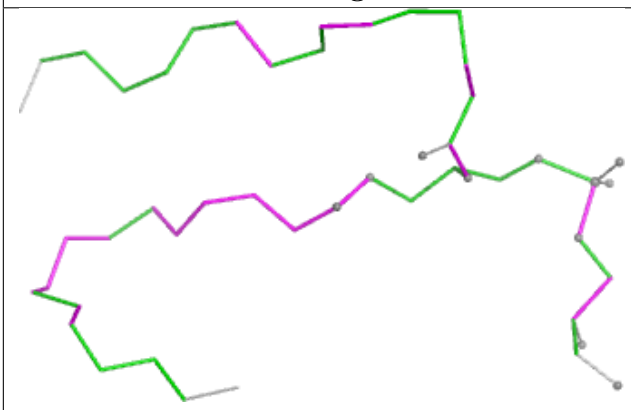
Ligand LHG f 206



Bond lengths



Bond angles

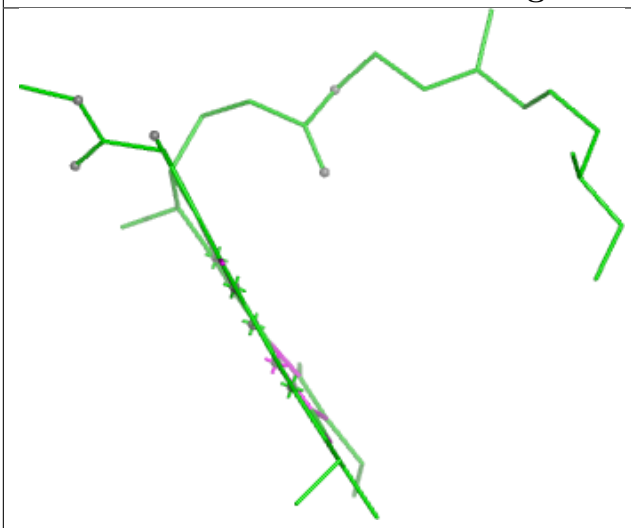


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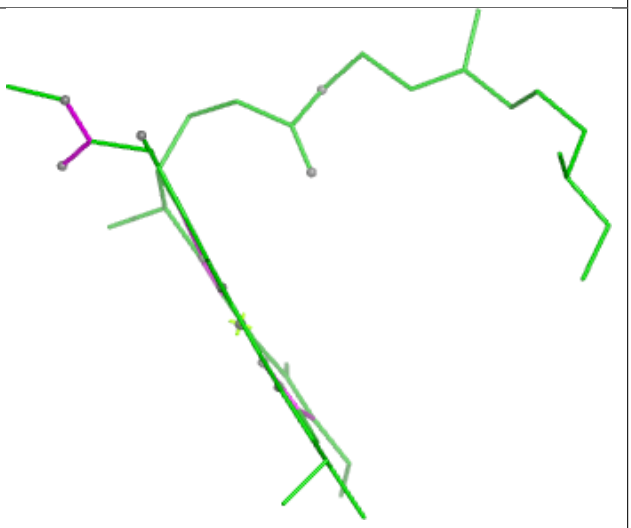


Rings

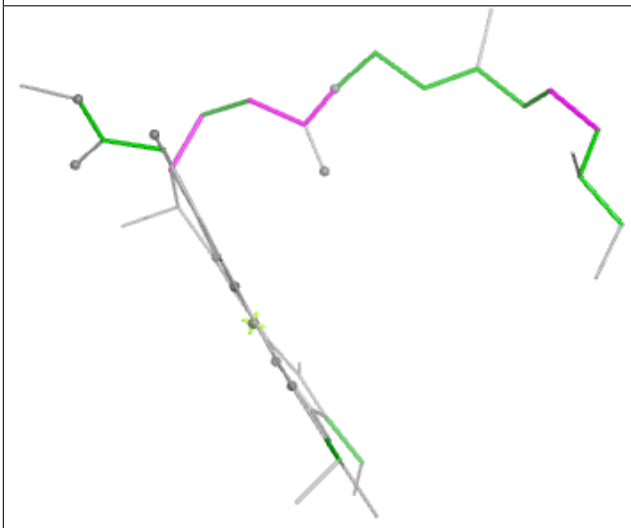
Ligand CLA b 812



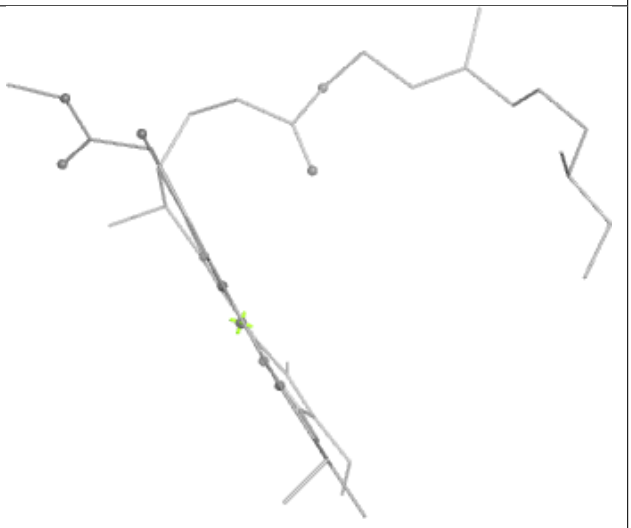
Bond lengths



Bond angles

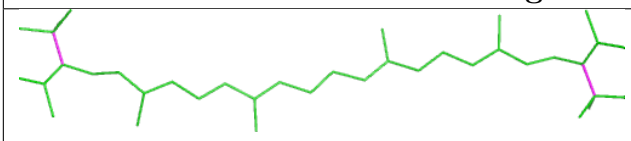


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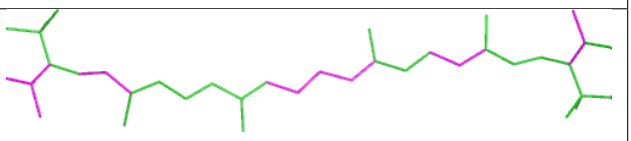


Rings

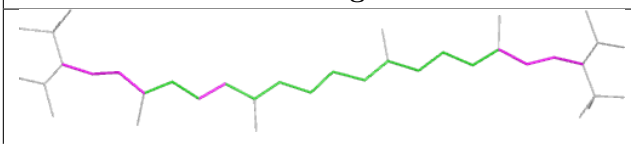
Ligand BCR b 844



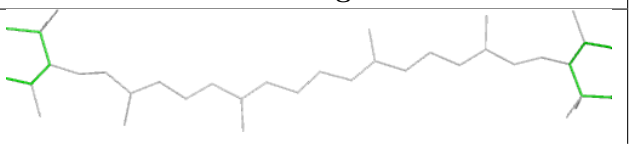
Bond lengths



Bond angles

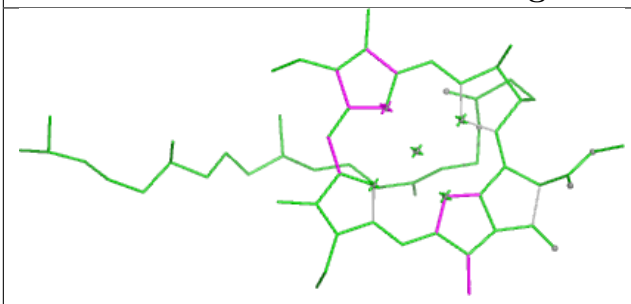


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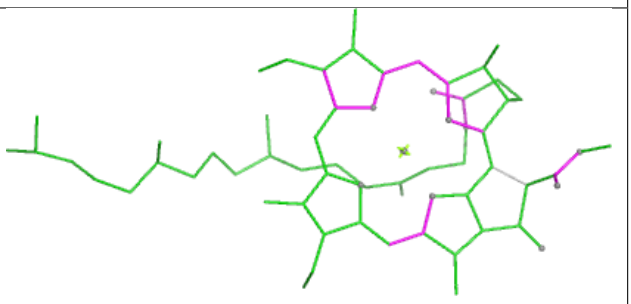


Rings

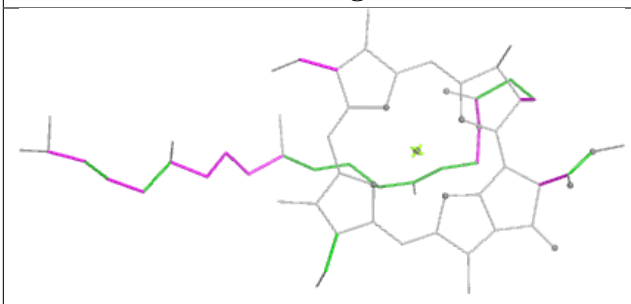
Ligand CLA a 838



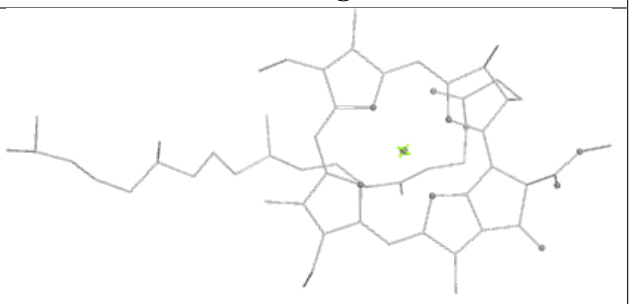
Bond lengths



Bond angles

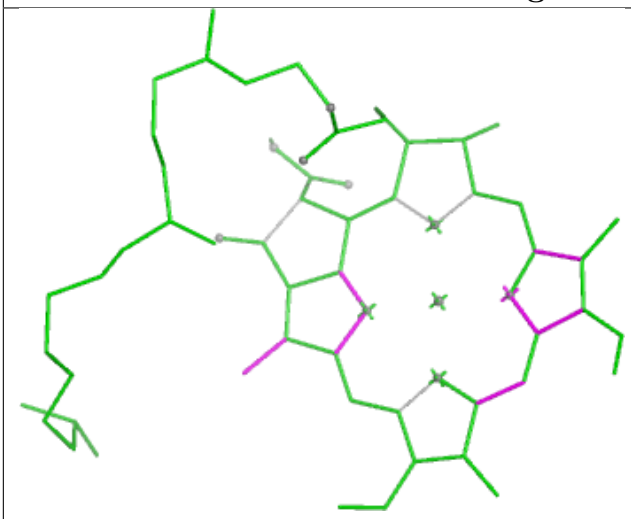


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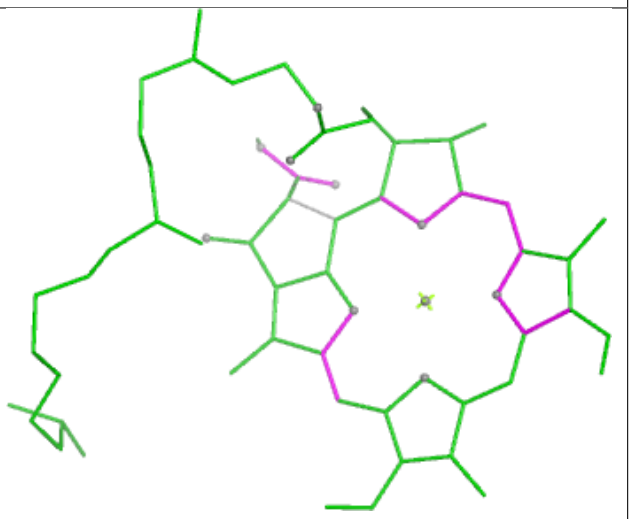


Rings

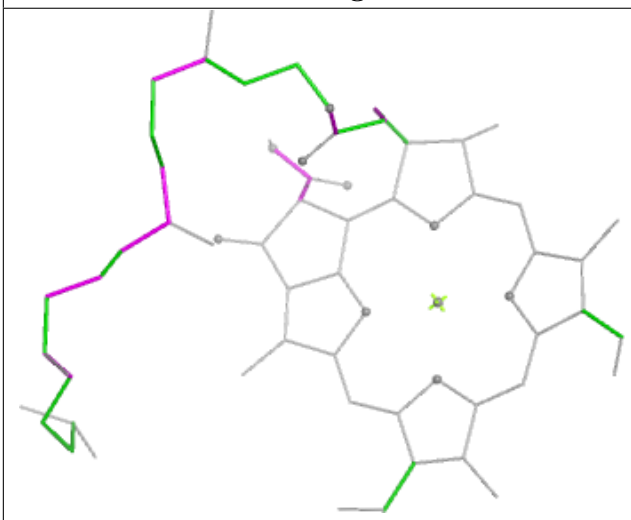
Ligand CLA b 833



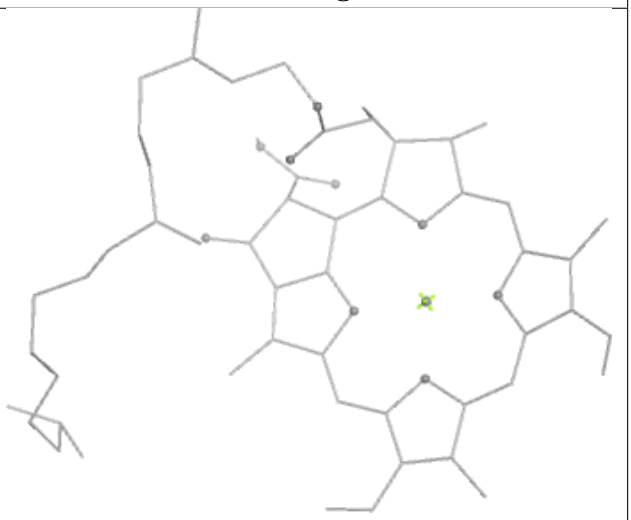
Bond lengths



Bond angles

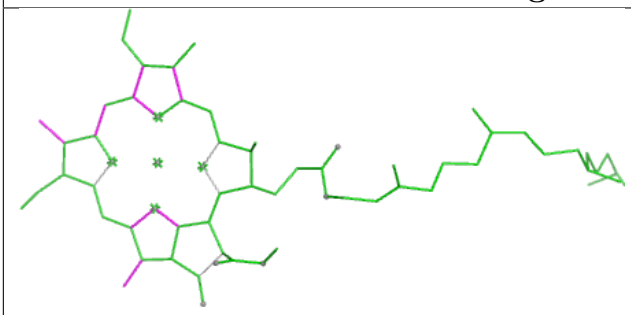


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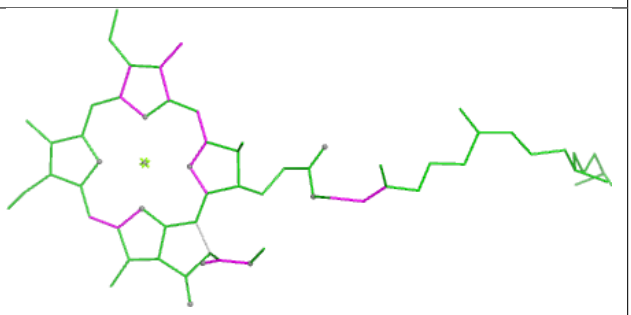


Rings

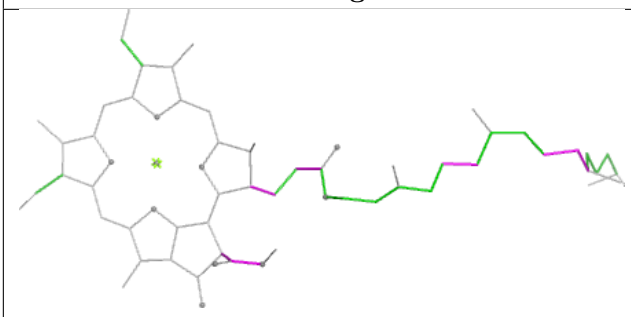
Ligand CLA a 805



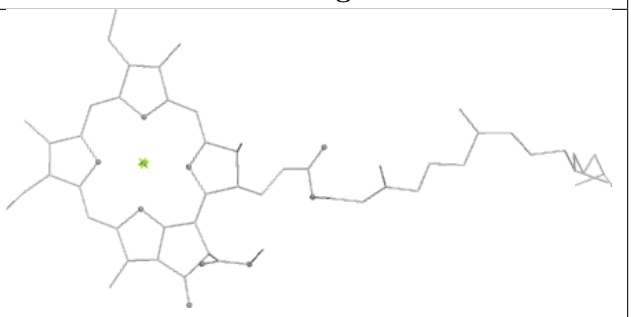
Bond lengths



Bond angles

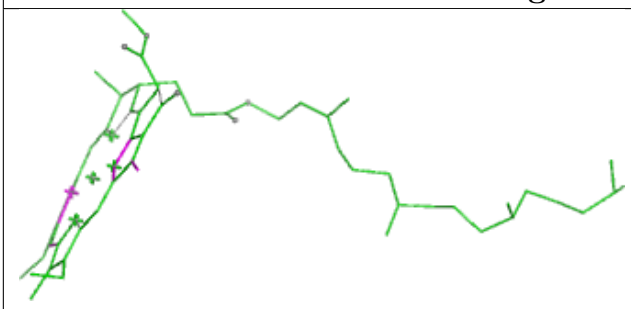


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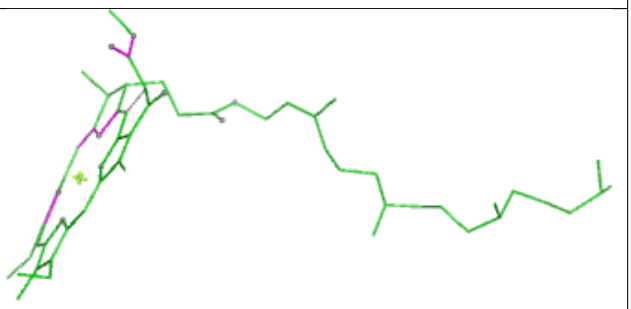


Rings

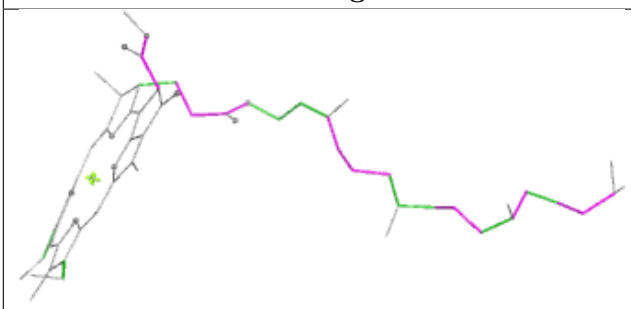
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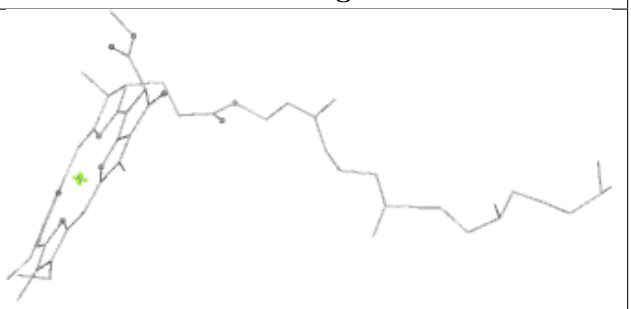
Bond lengths



Bond angles

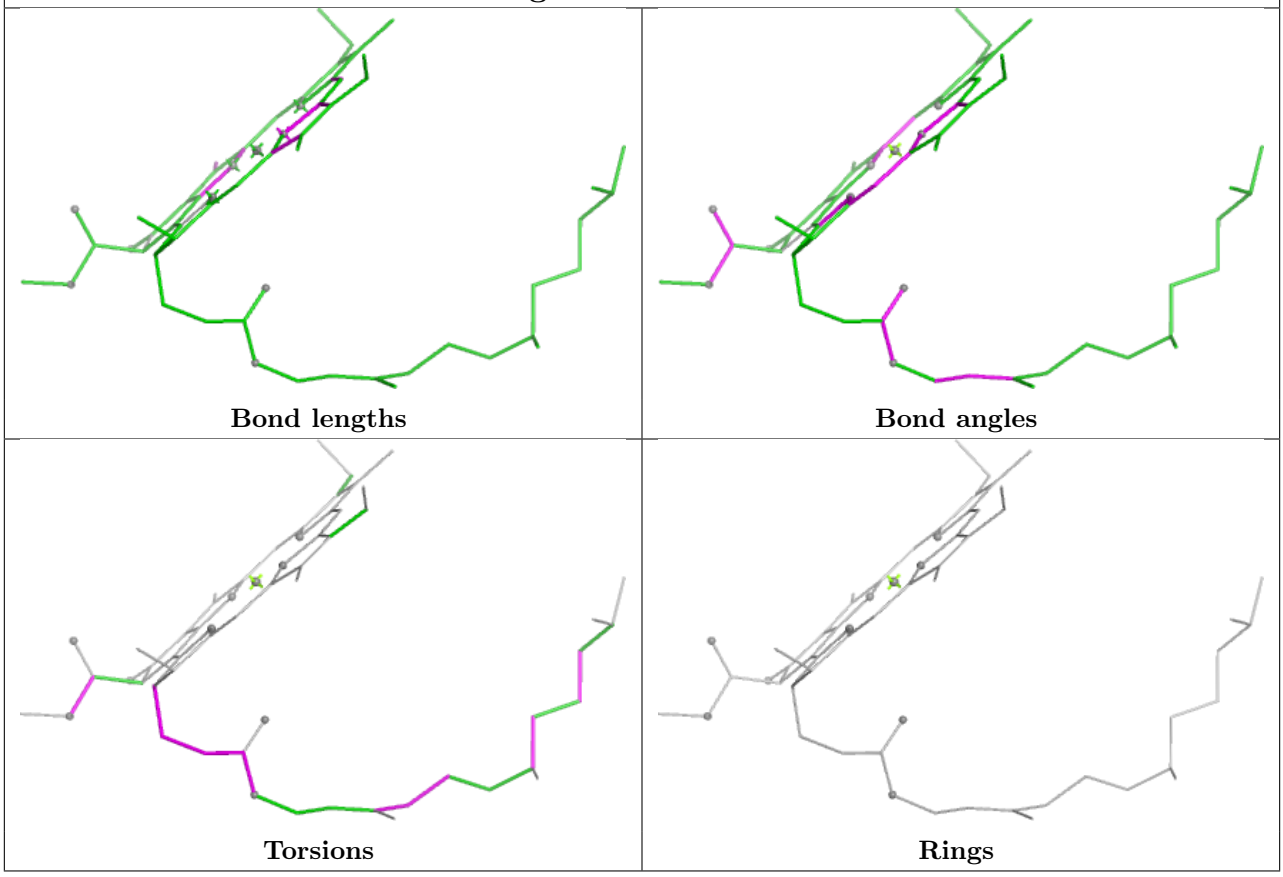


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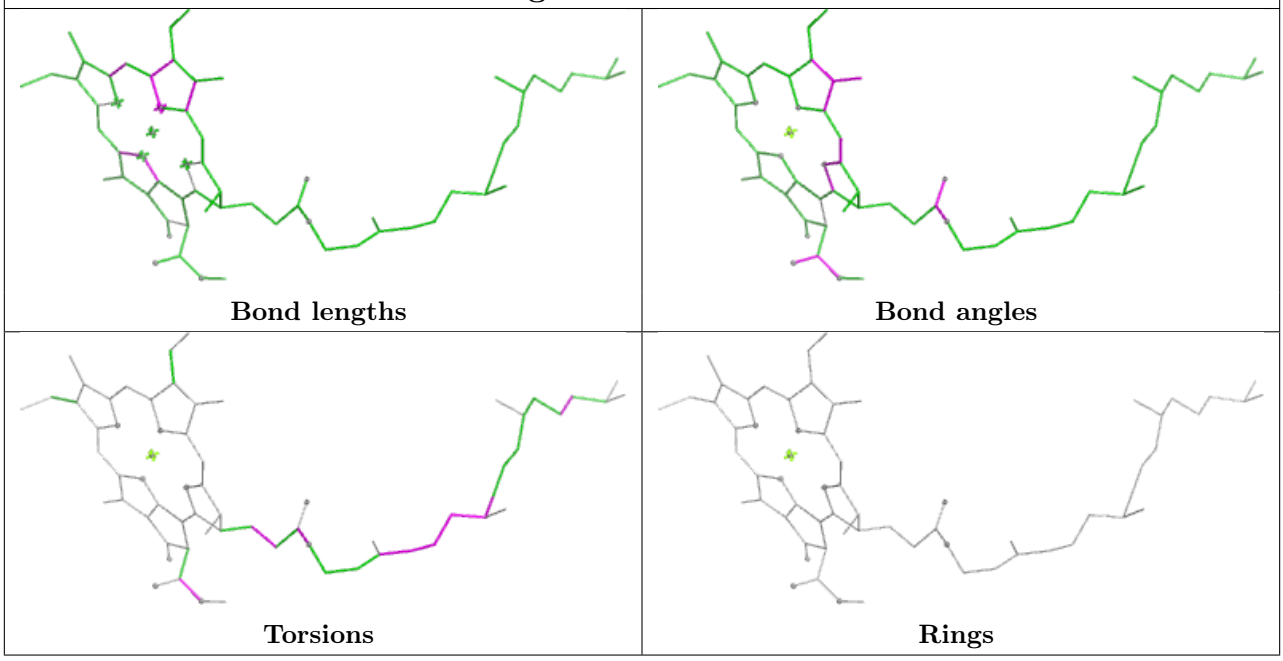


Rings

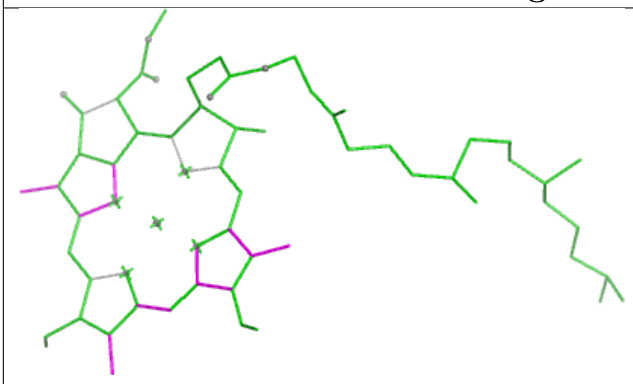
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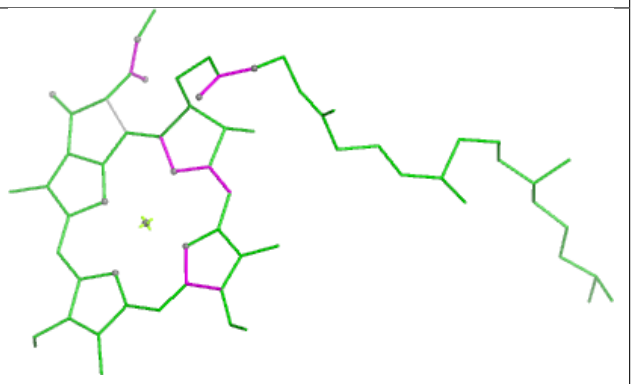
Ligand CLA b 801



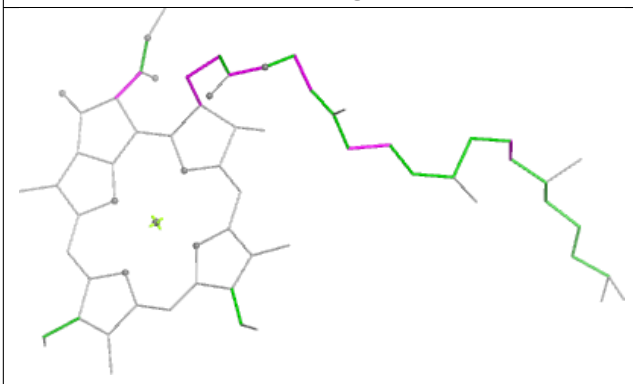
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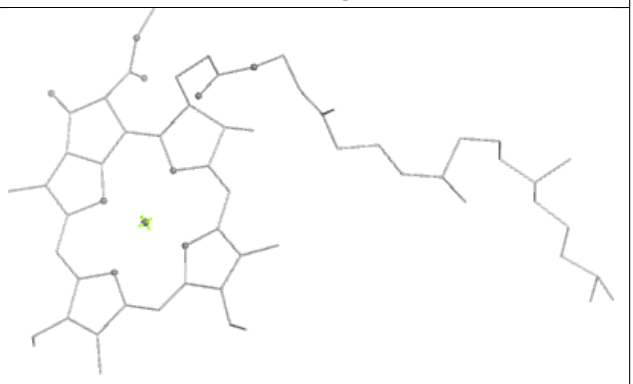
Bond lengths



Bond angles

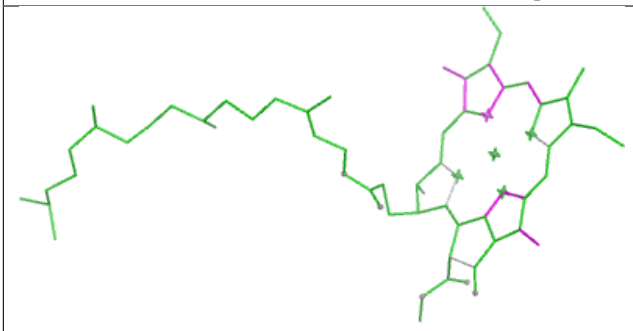


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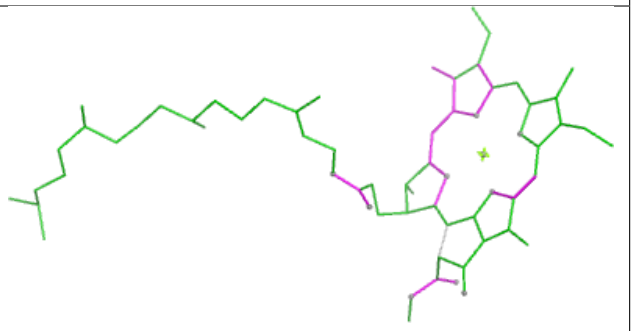


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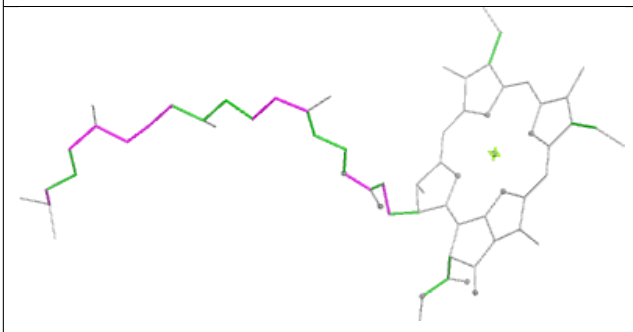
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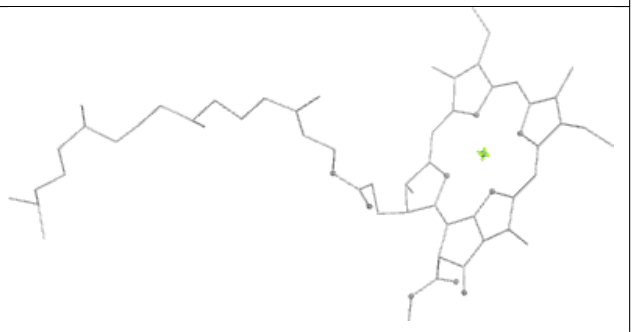
Bond lengths



Bond angles

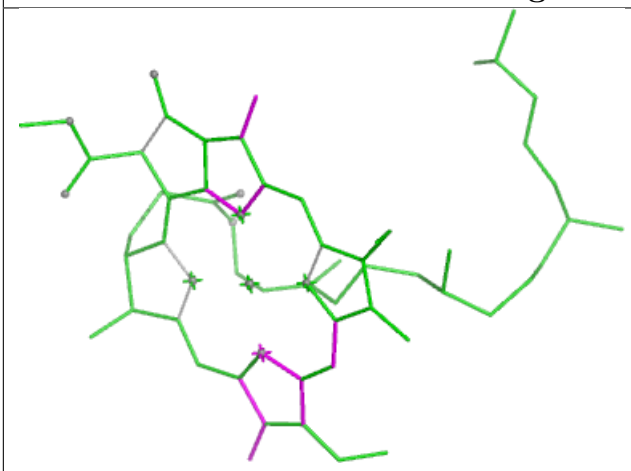


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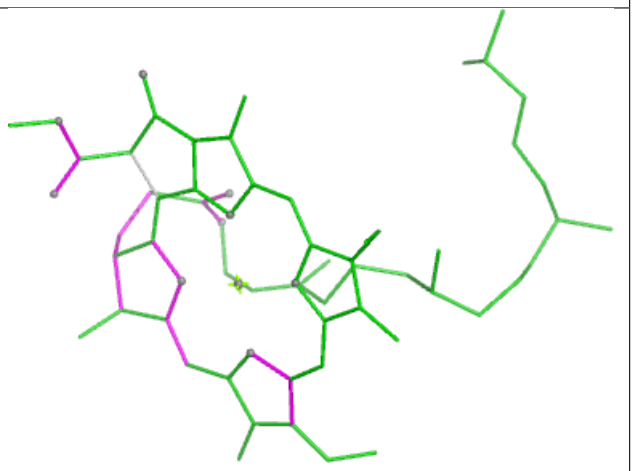


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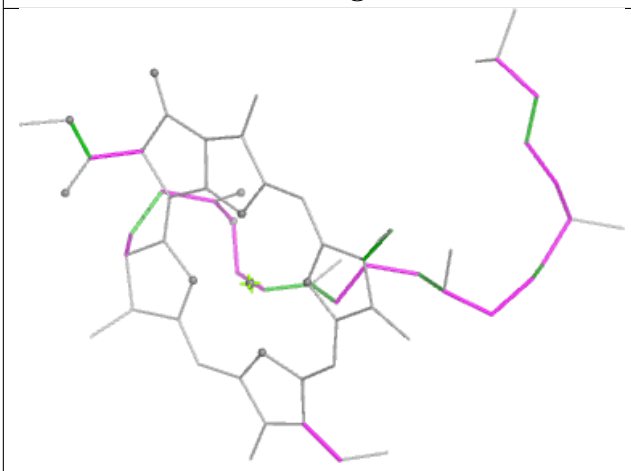
Ligand CLA a 823



Bond lengths



Bond angles

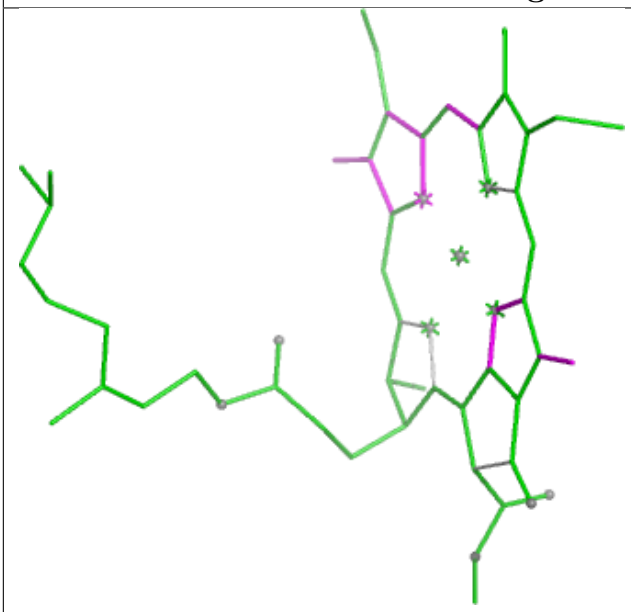


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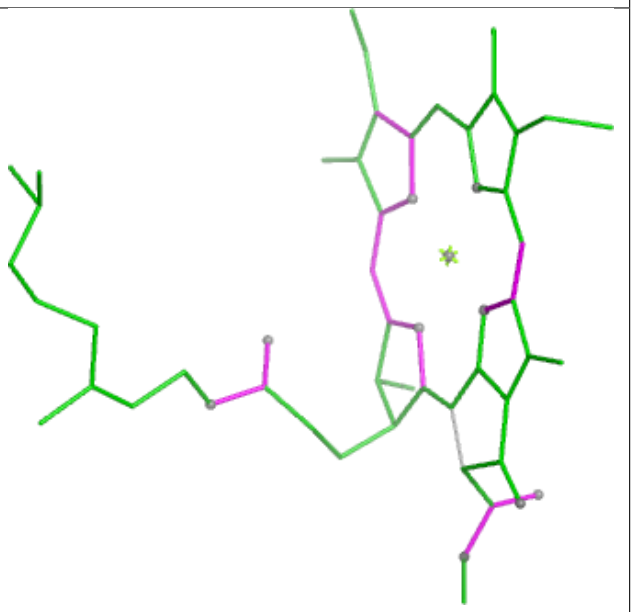


Rings

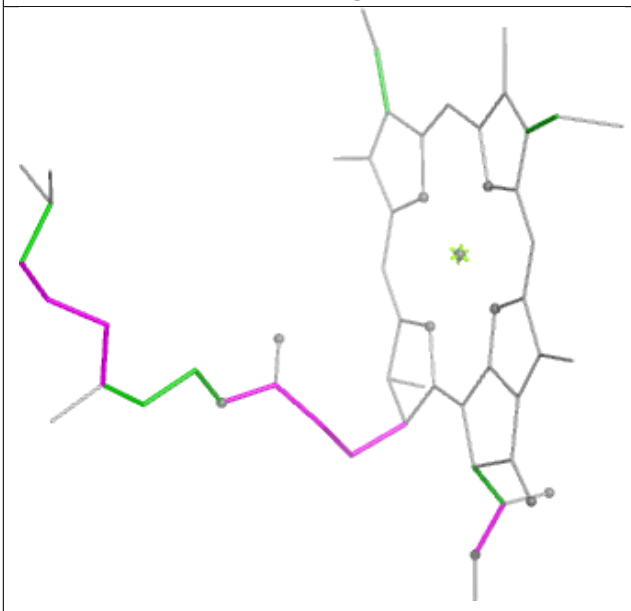
Ligand CLA b 816



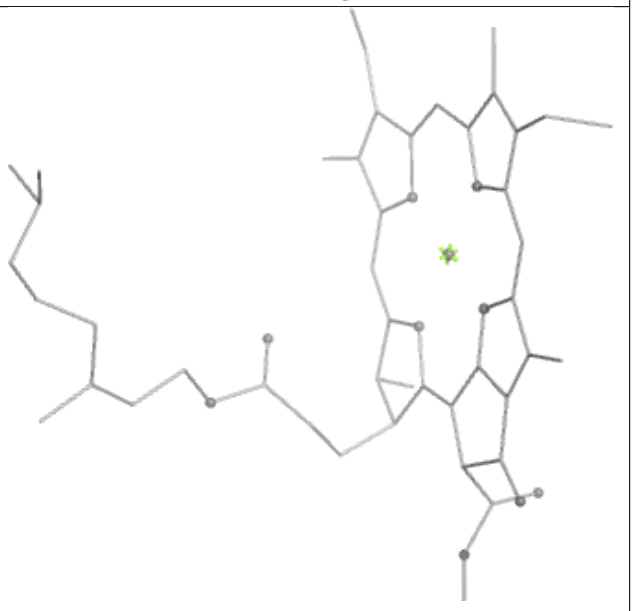
Bond lengths



Bond angles

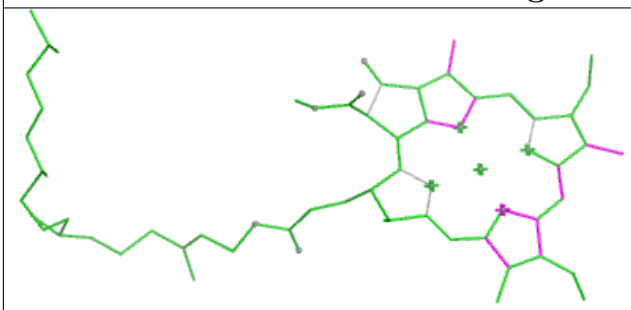


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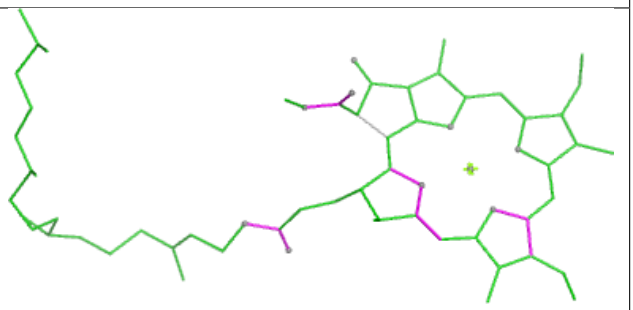


Rings

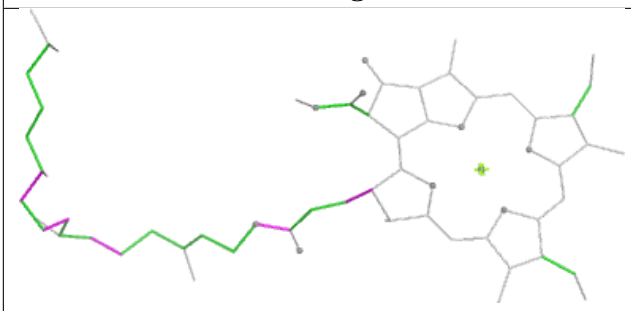
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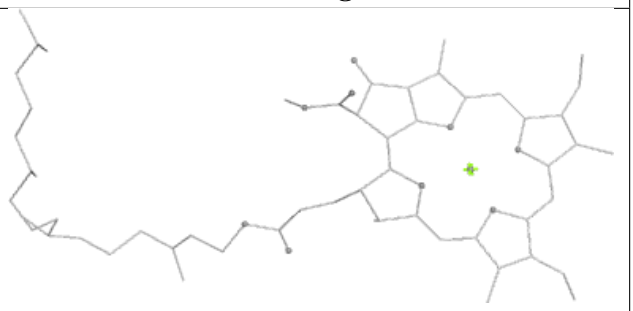
Bond lengths



Bond angles

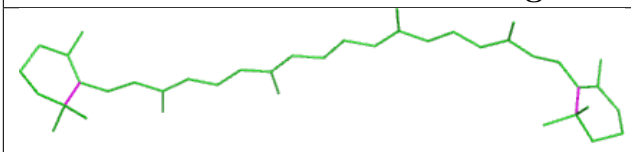


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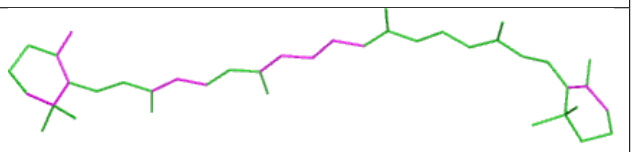


Rings

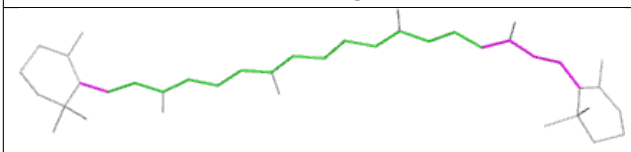
Ligand BCR b 847



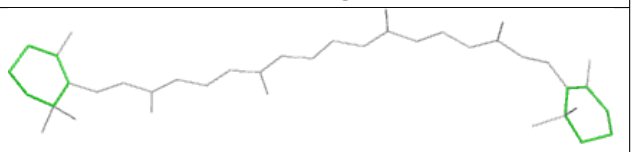
Bond lengths



Bond angles

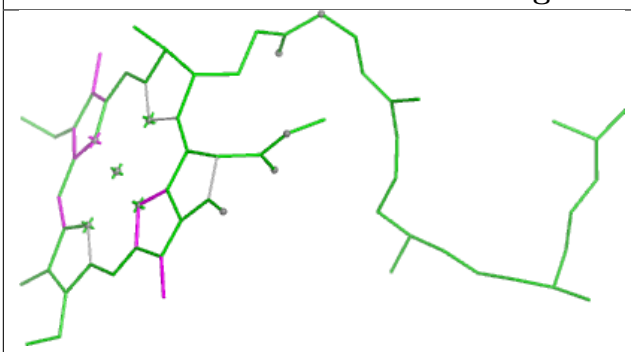


Torsions



Rings

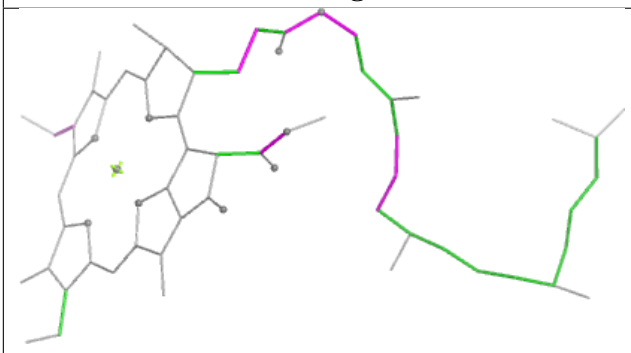
Ligand CL0 a 801



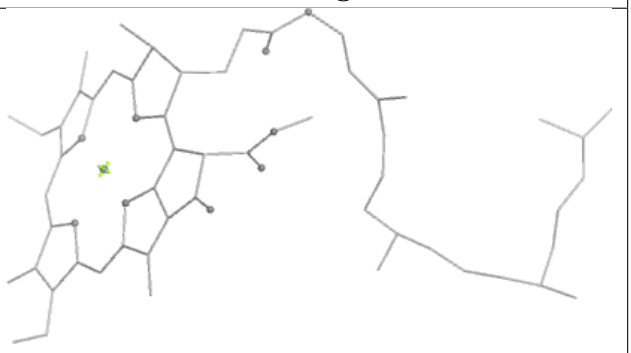
Bond lengths



Bond angles

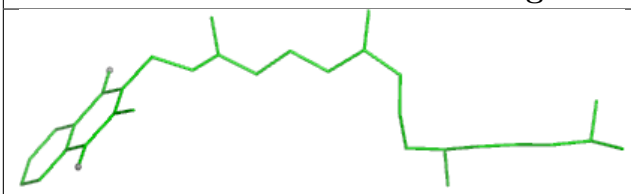


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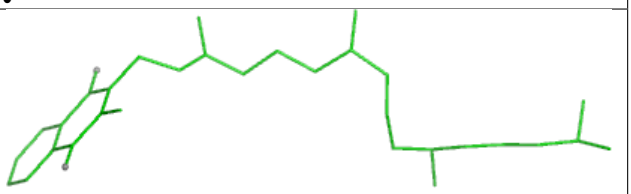


Rings

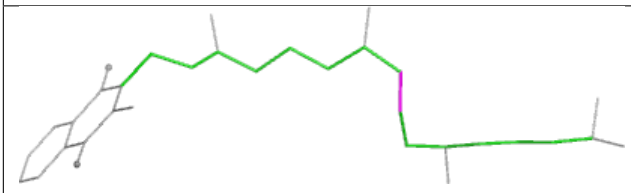
Ligand PQN a 843



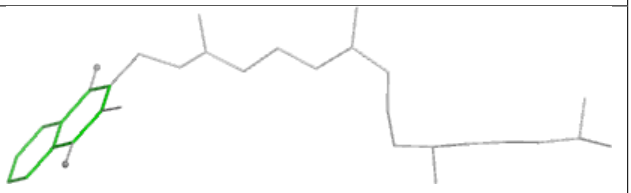
Bond lengths



Bond angles

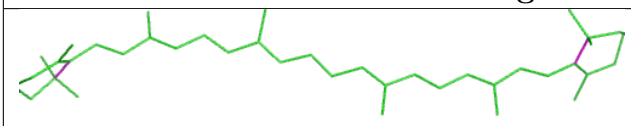


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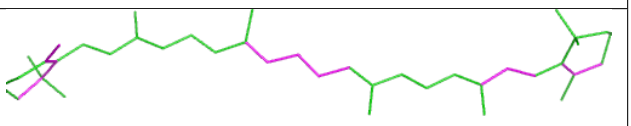


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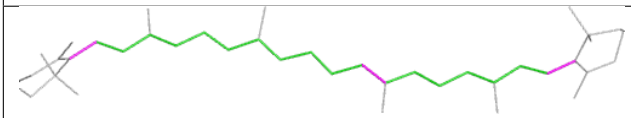
Ligand BCR k 4005



Bond lengths



Bond angles

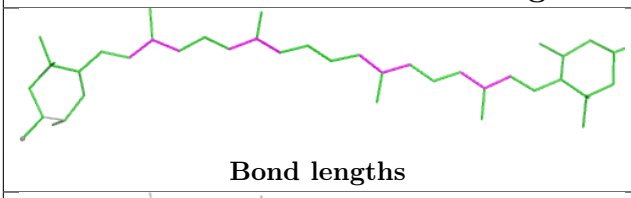


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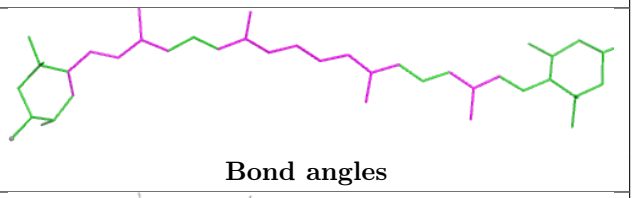


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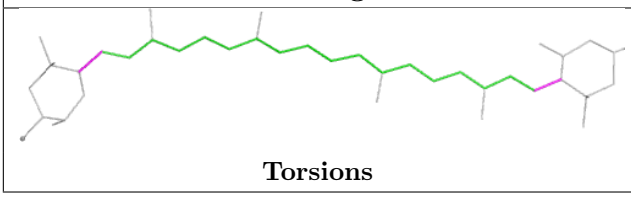
Ligand ZEX b 854



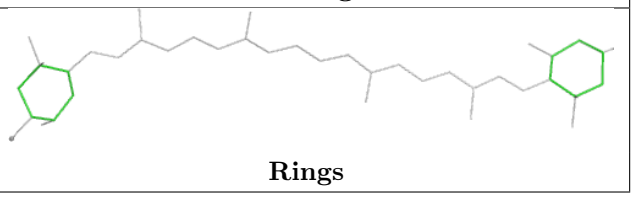
Bond lengths



Bond angles

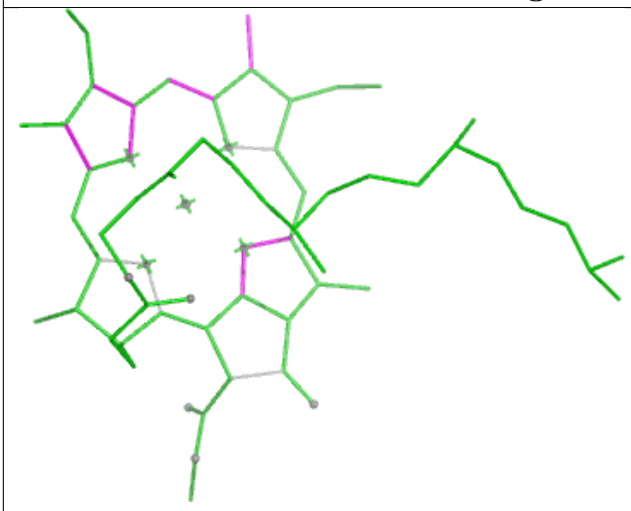


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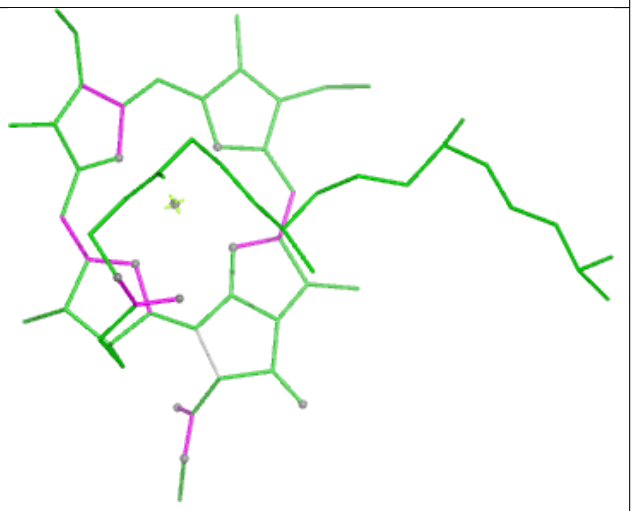


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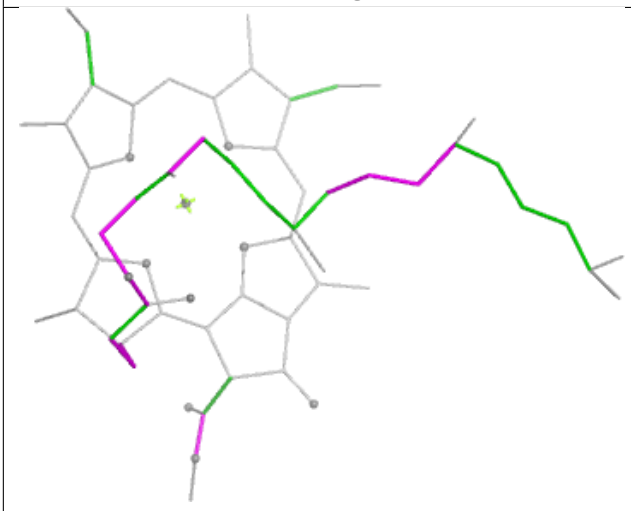
Ligand CLA b 828



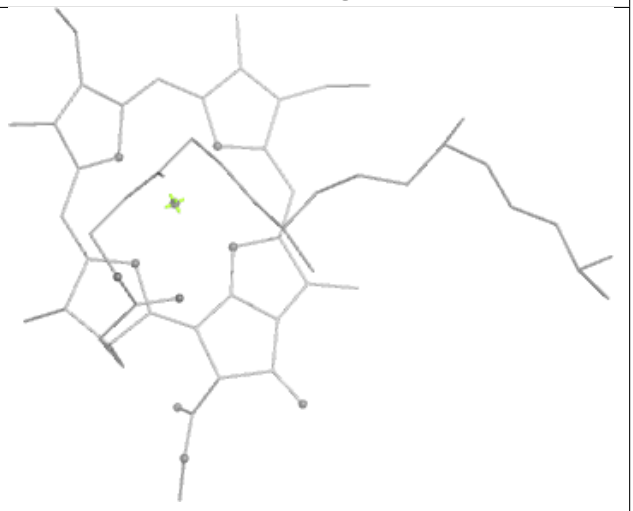
Bond lengths



Bond angles

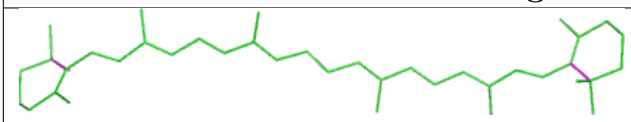


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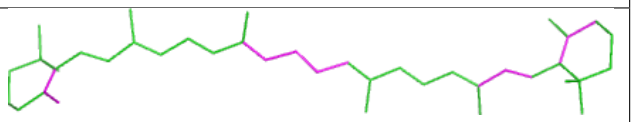


Rings

Ligand BCR a 844



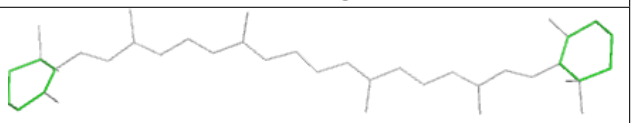
Bond lengths



Bond angles

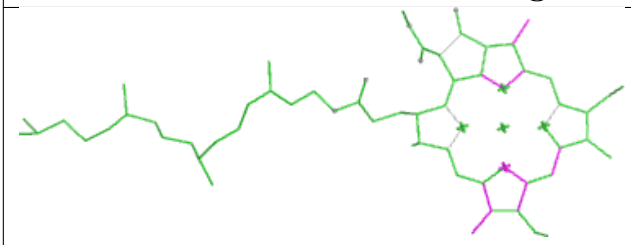


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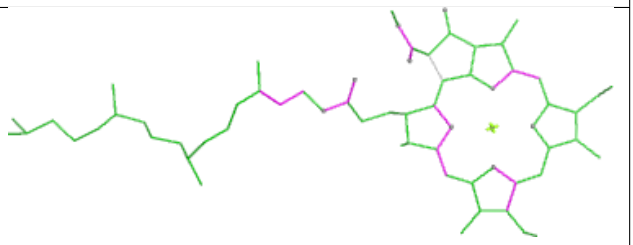


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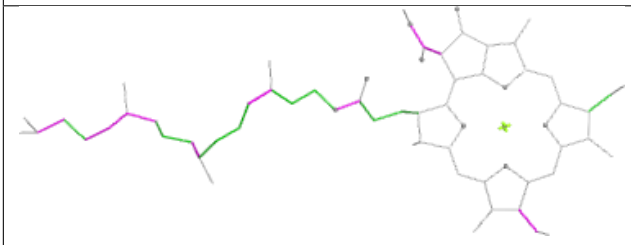
Ligand CLA a 833



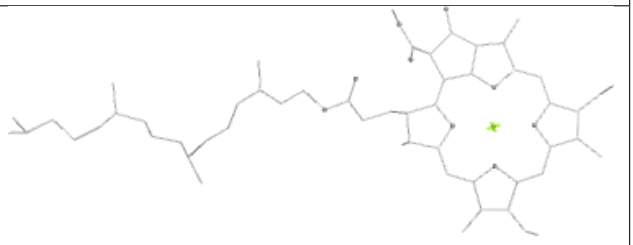
Bond lengths



Bond angles

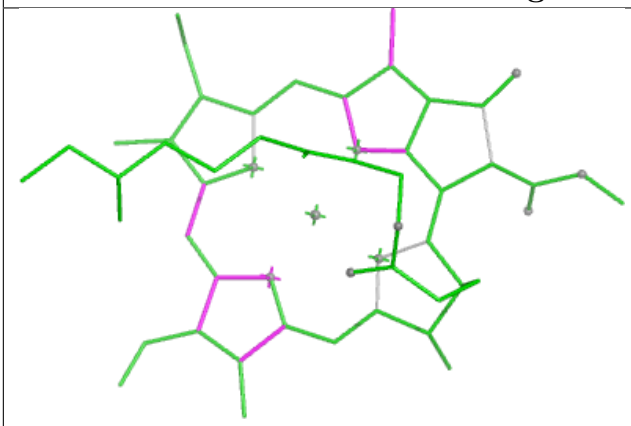


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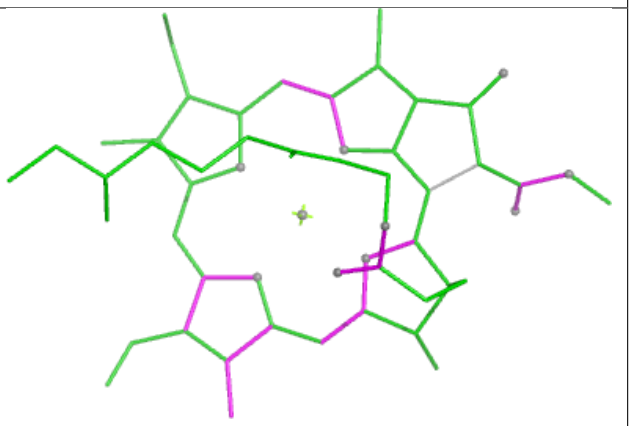


Rings

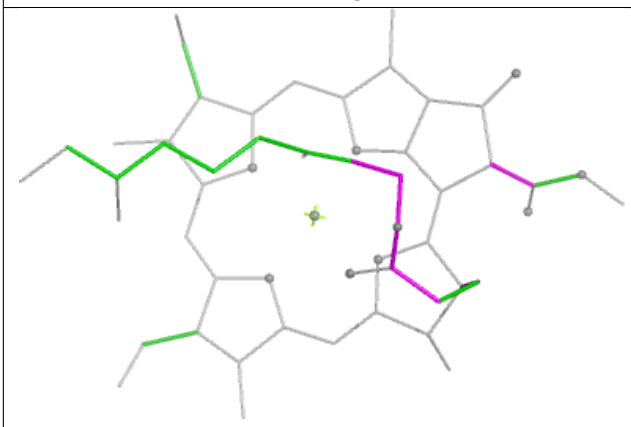
Ligand CLA b 817



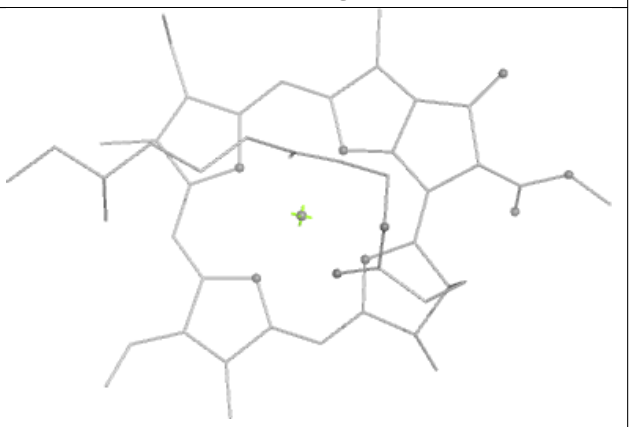
Bond lengths



Bond angles

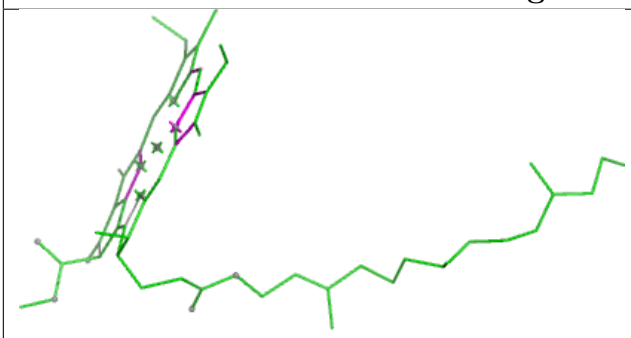


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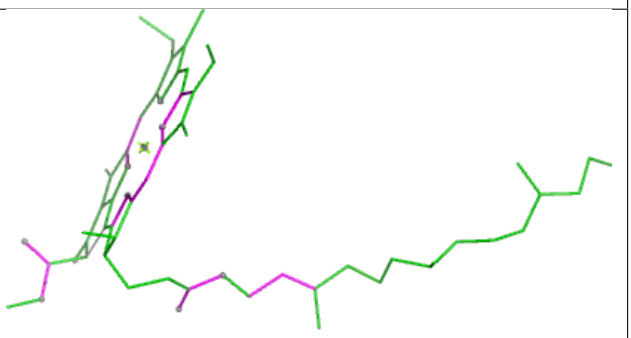


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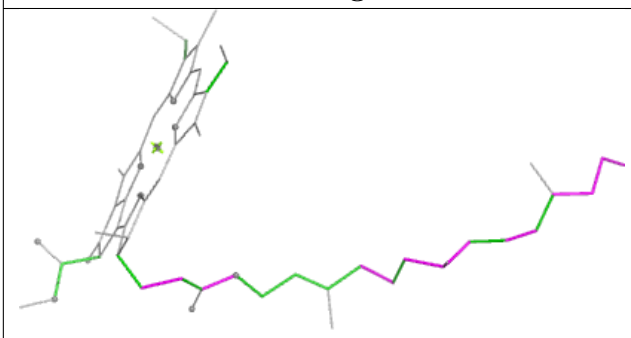
Ligand CLA b 805



Bond lengths



Bond angles

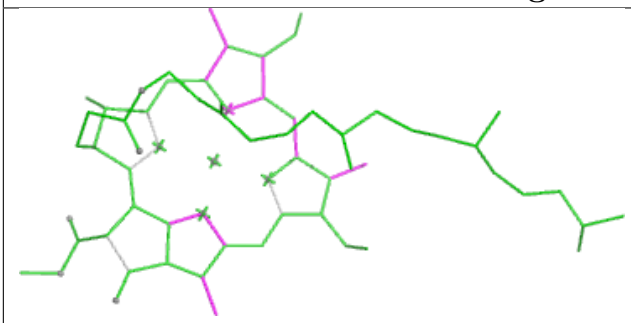


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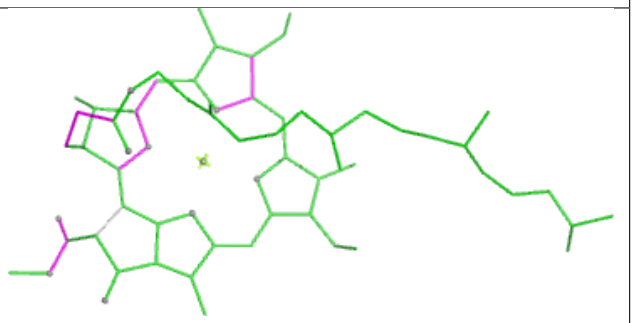


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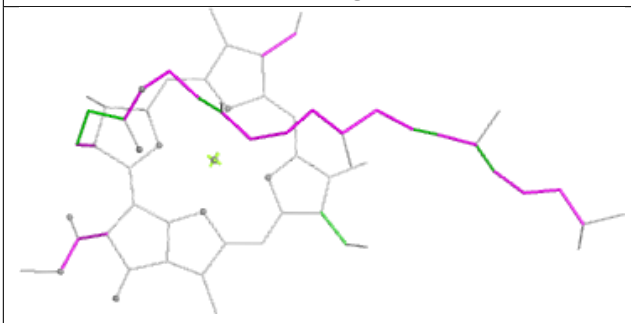
Ligand CLA a 818



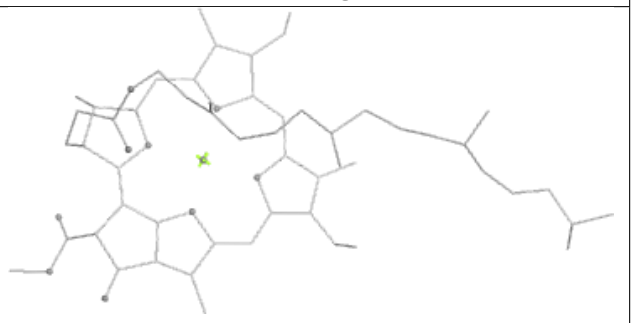
Bond lengths



Bond angles

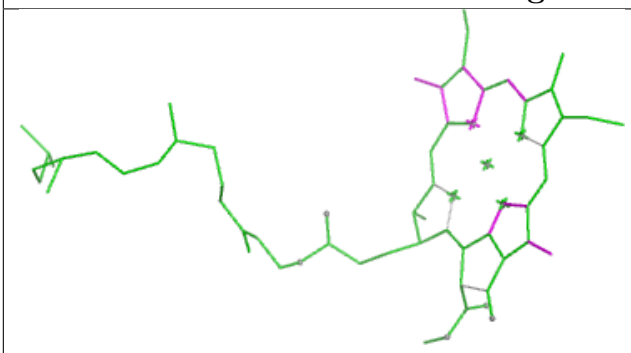


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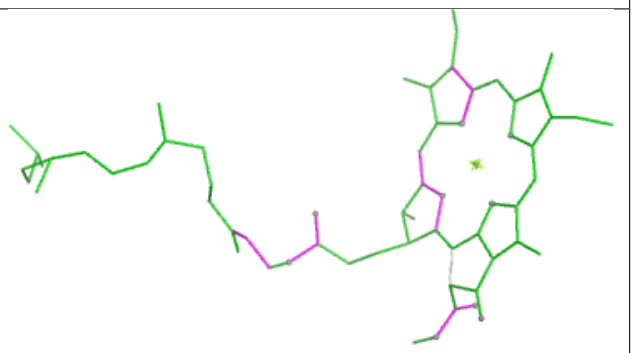


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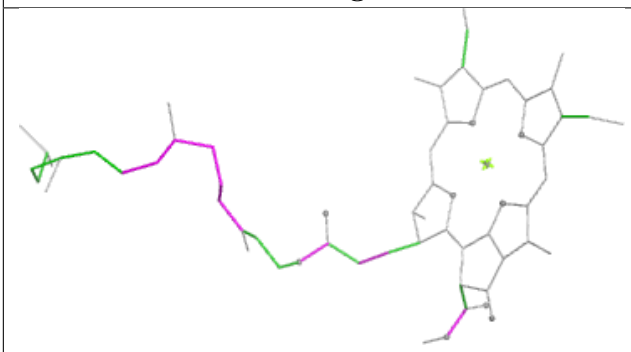
Ligand CLA b 810



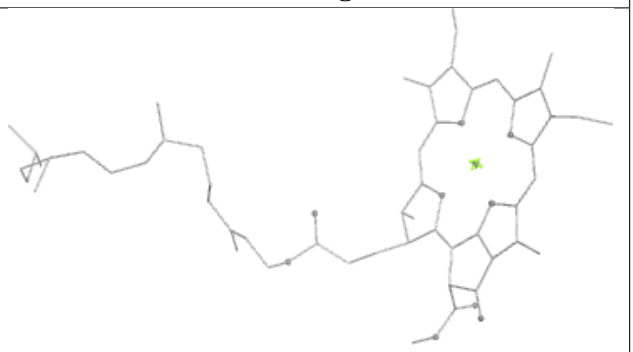
Bond lengths



Bond angles

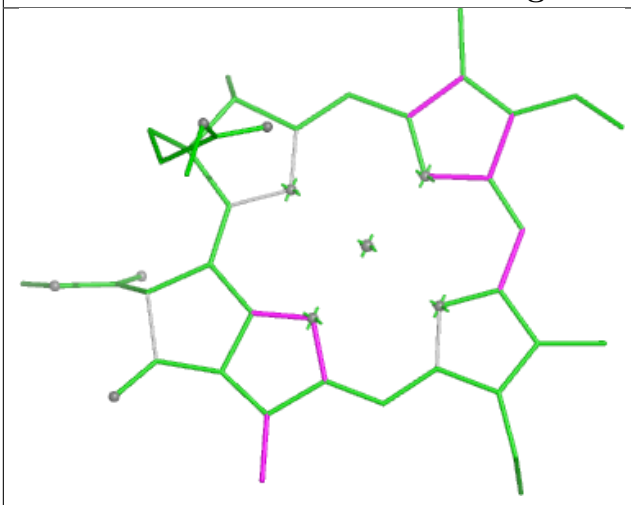


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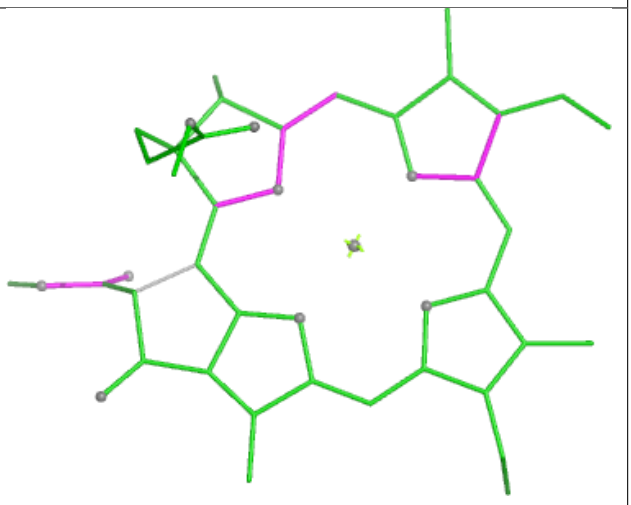


Rings

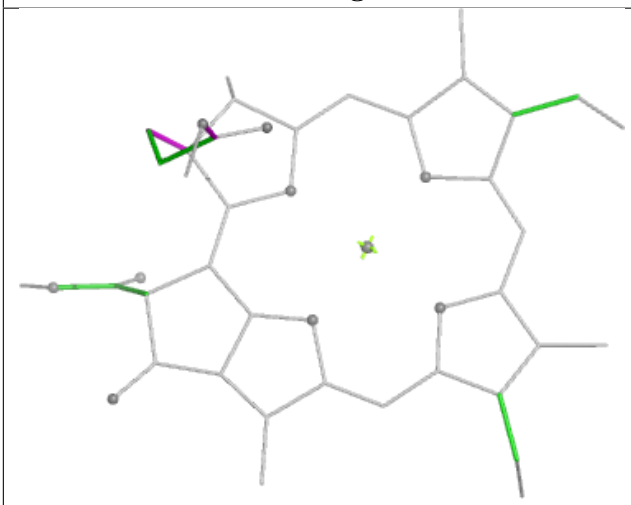
Ligand CLA b 823



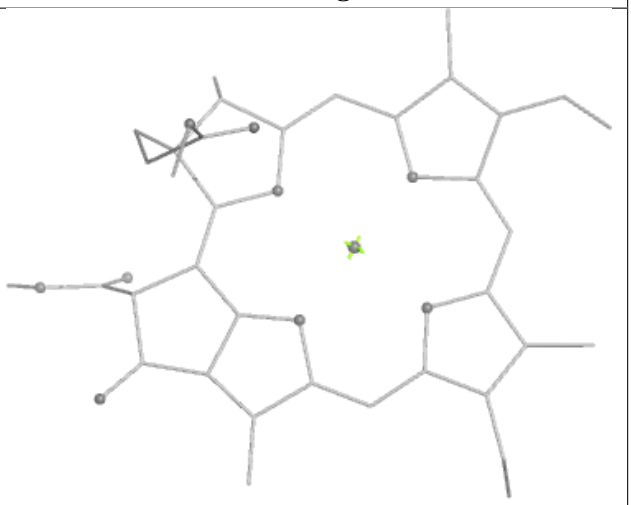
Bond lengths



Bond angles

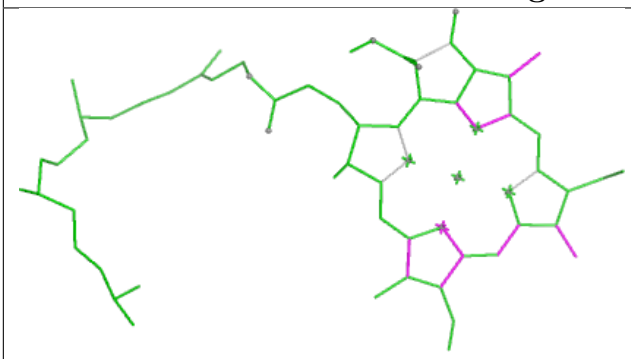


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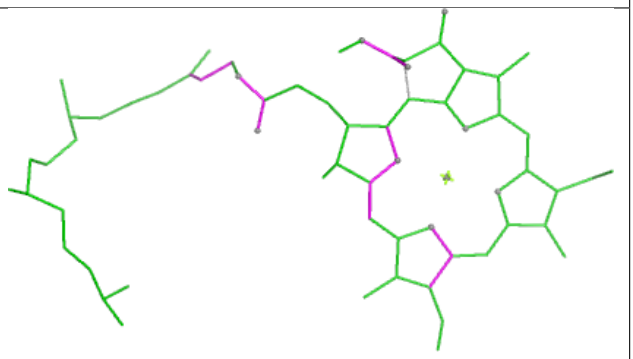


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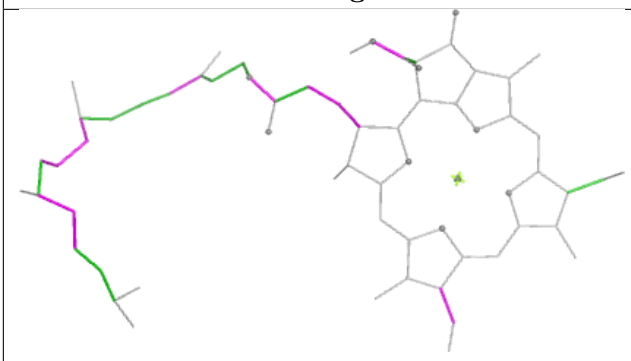
Ligand CLA a 827



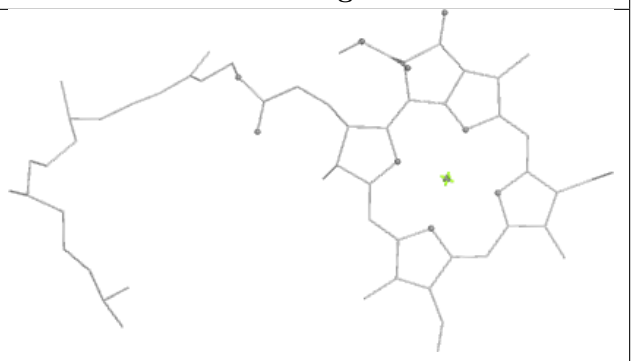
Bond lengths



Bond angles

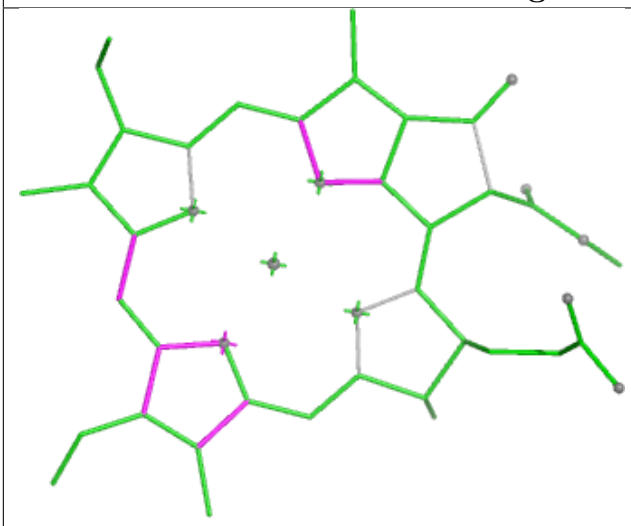


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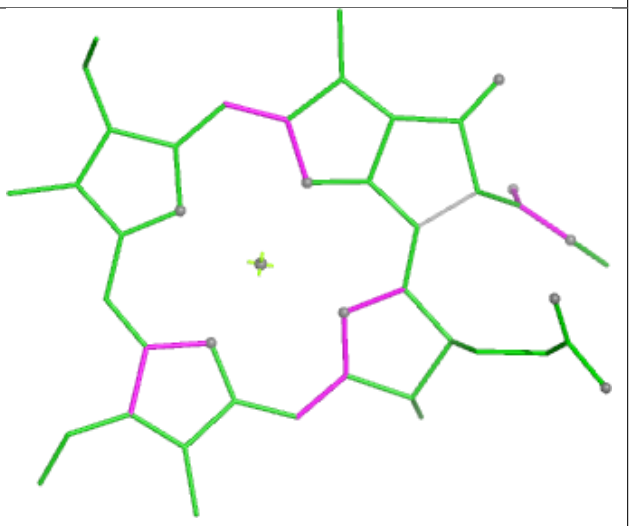


Rings

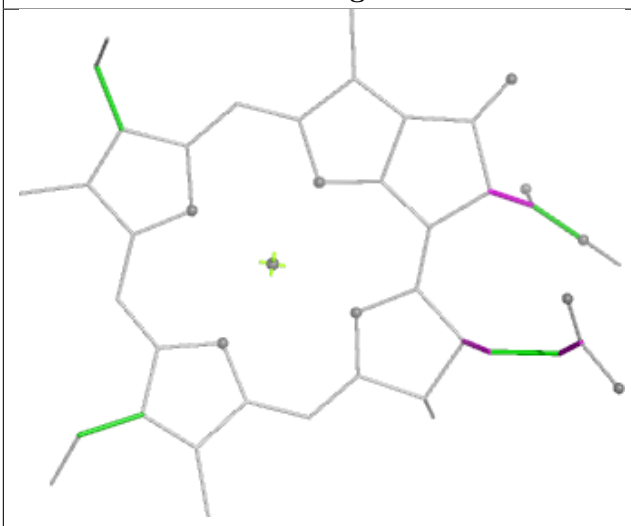
Ligand CLA a 842



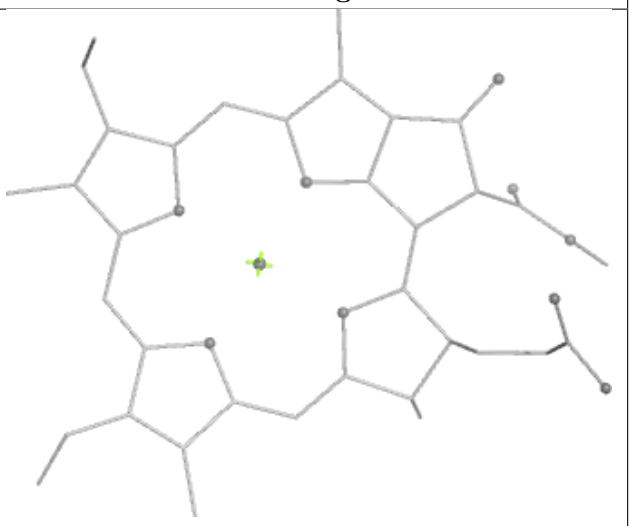
Bond lengths



Bond angles

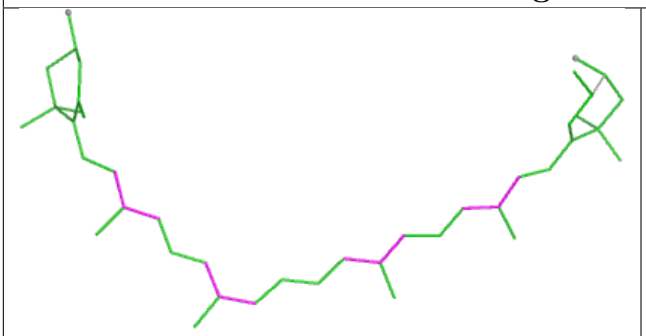


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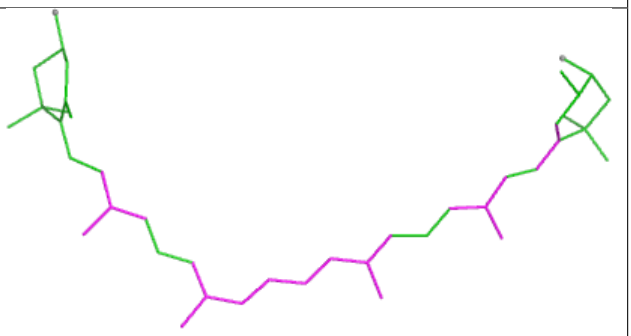


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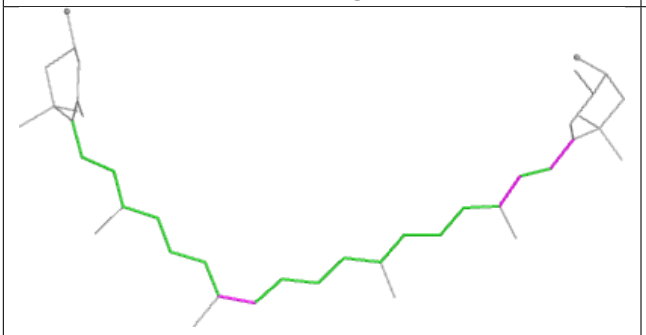
Ligand ZEX f 205



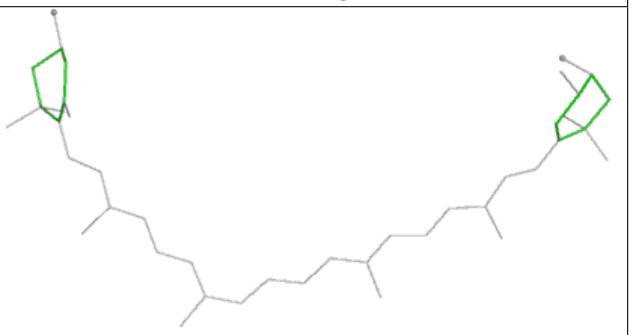
Bond lengths



Bond angles

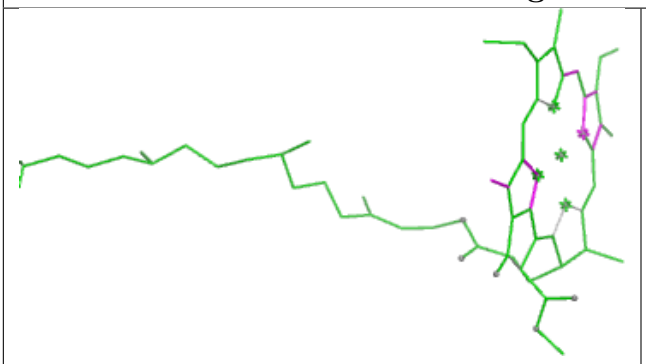


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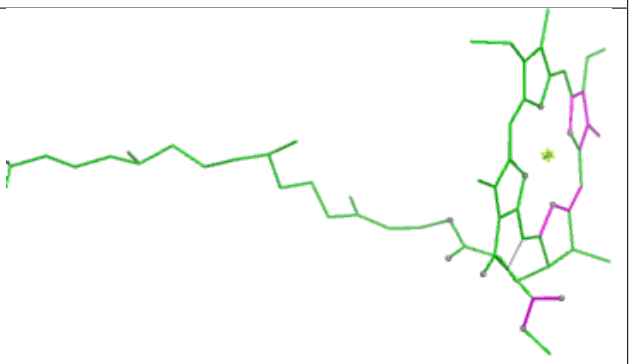


Rings

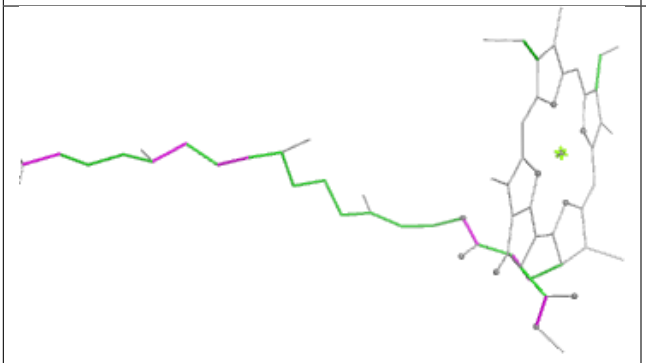
Ligand CLA b 829



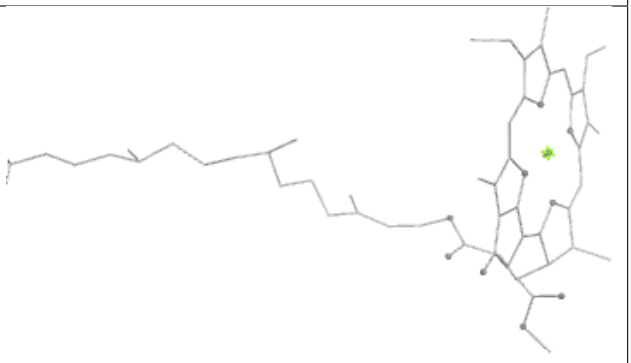
Bond lengths



Bond angles

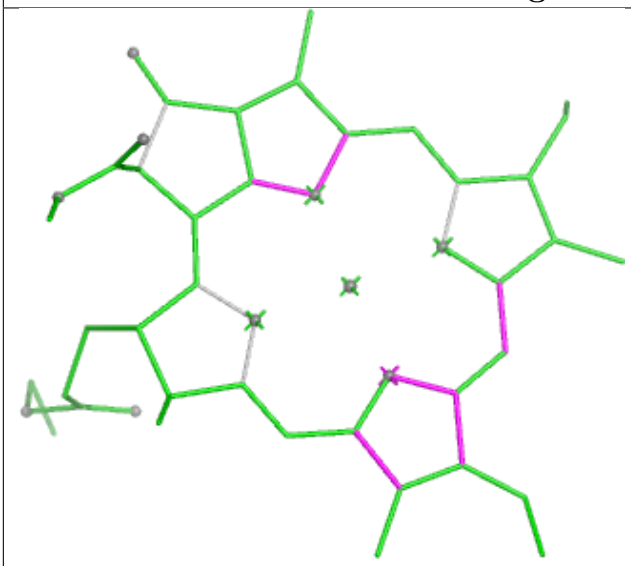


Torsions

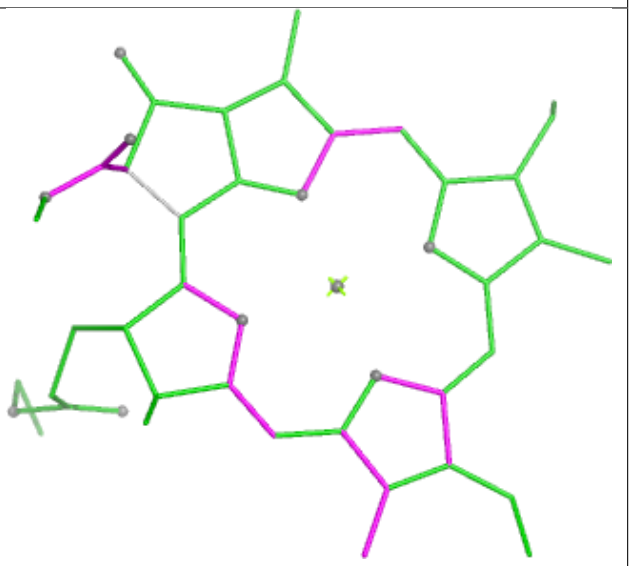


Rings

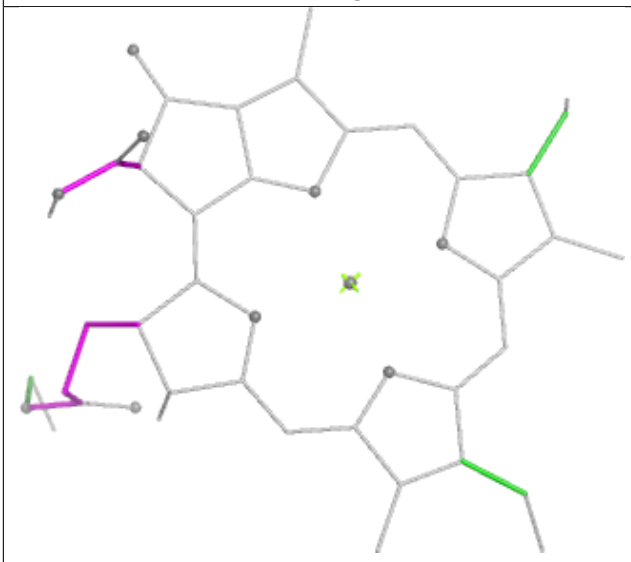
Ligand CLA a 814



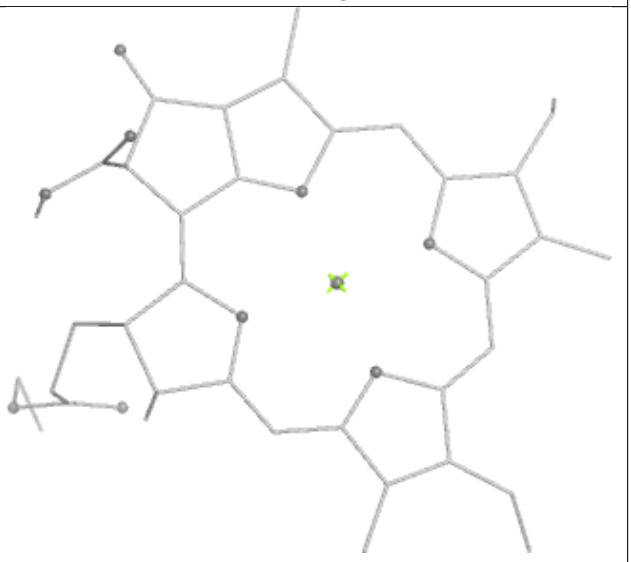
Bond lengths



Bond angles

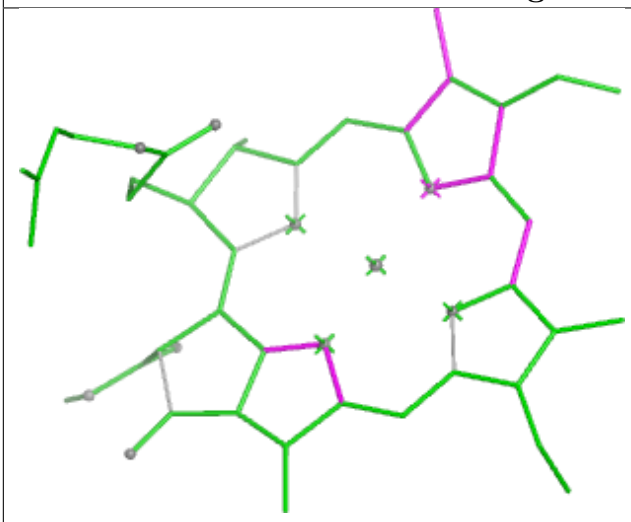


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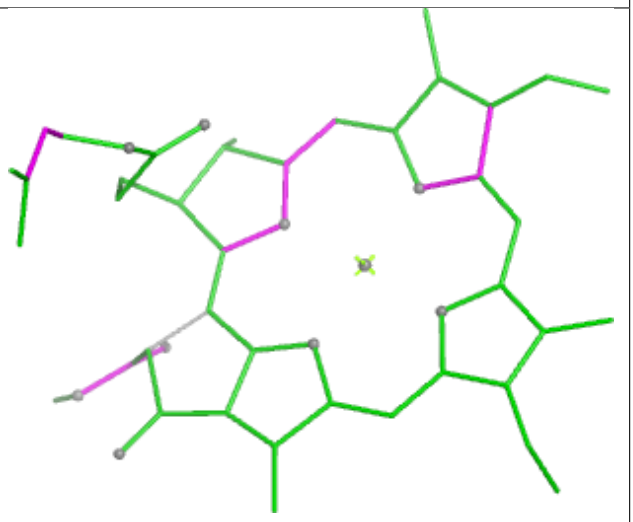


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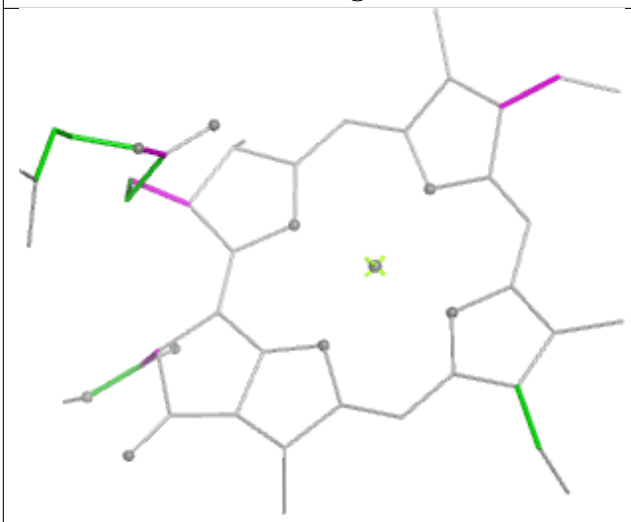
Ligand CLA b 839



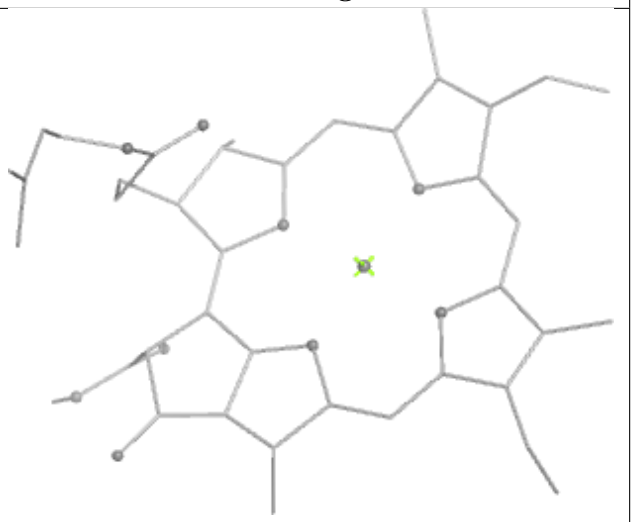
Bond lengths



Bond angles

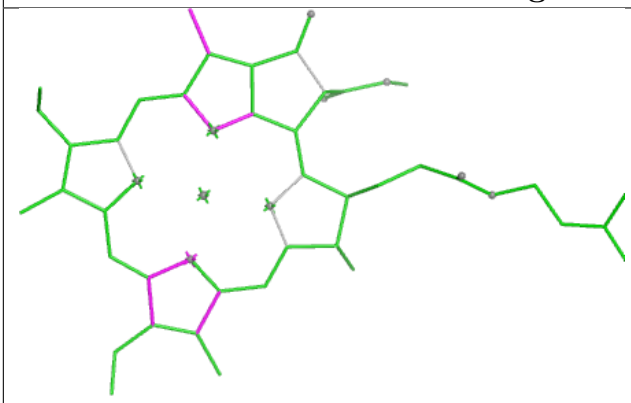


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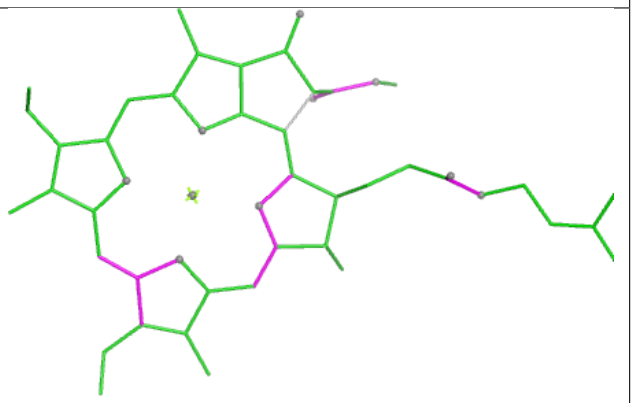


Rings

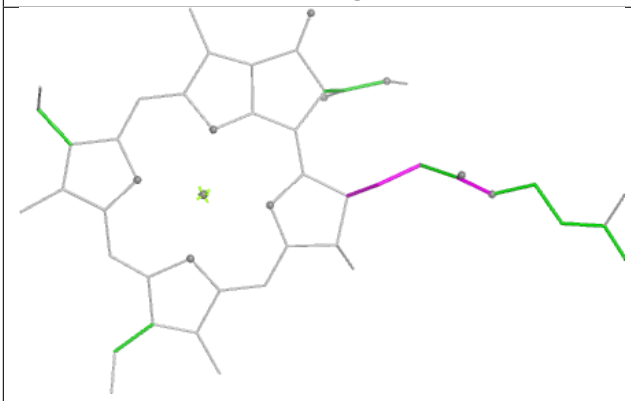
Ligand CLA a 837



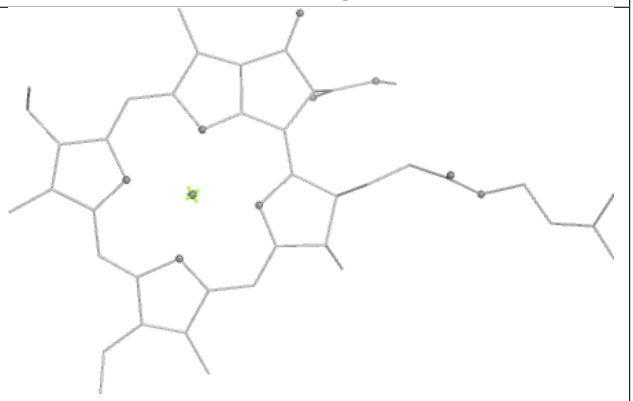
Bond lengths



Bond angles

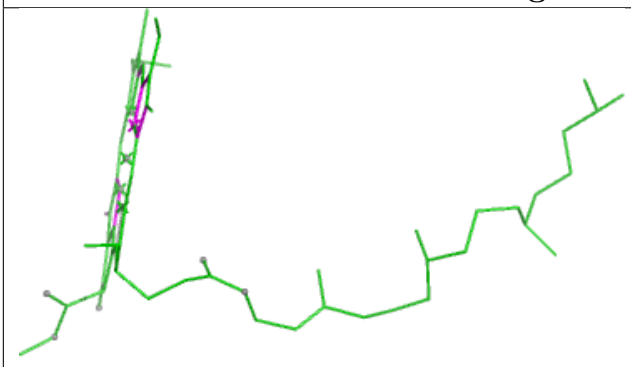


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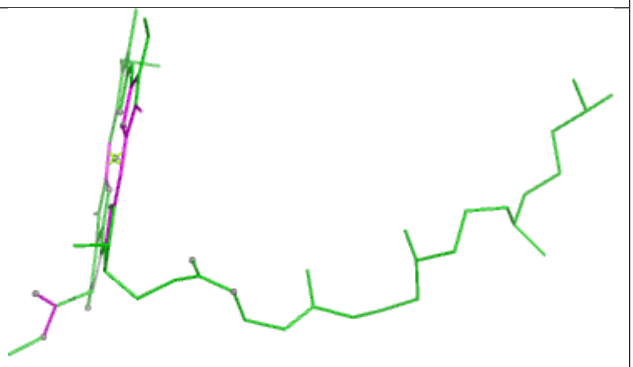


Rings

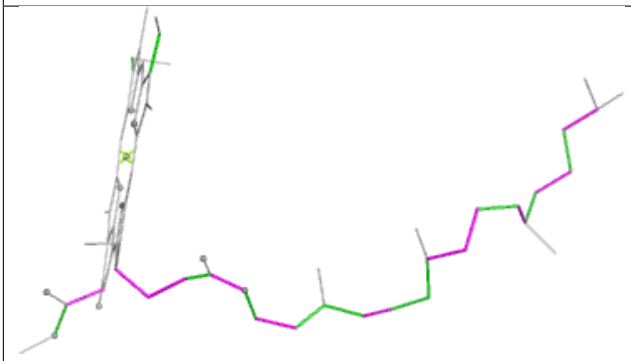
Ligand CLA a 807



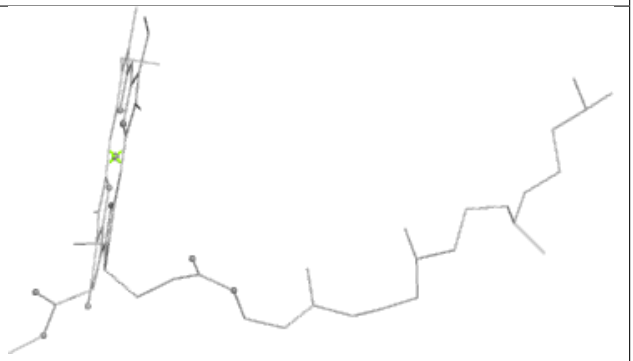
Bond lengths



Bond angles

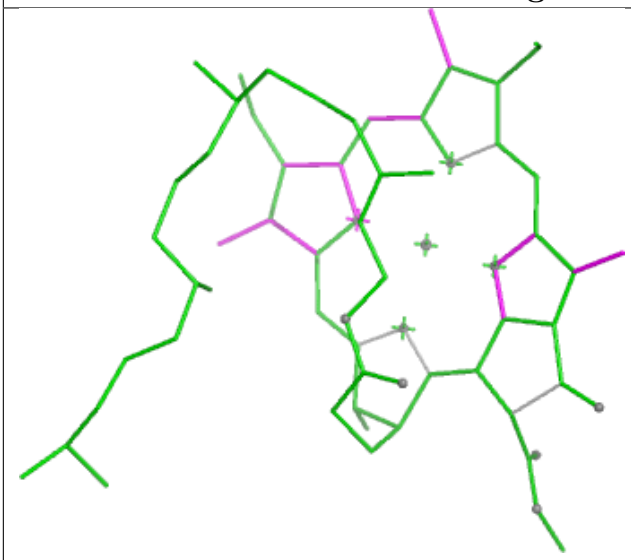


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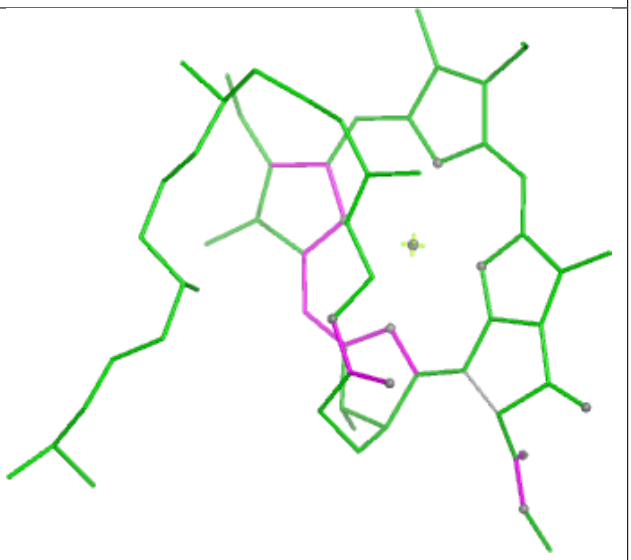


Rings

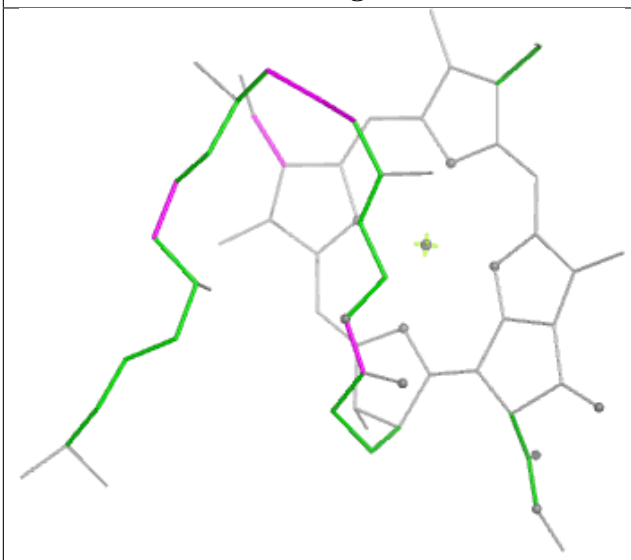
Ligand CLA b 809



Bond lengths



Bond angles

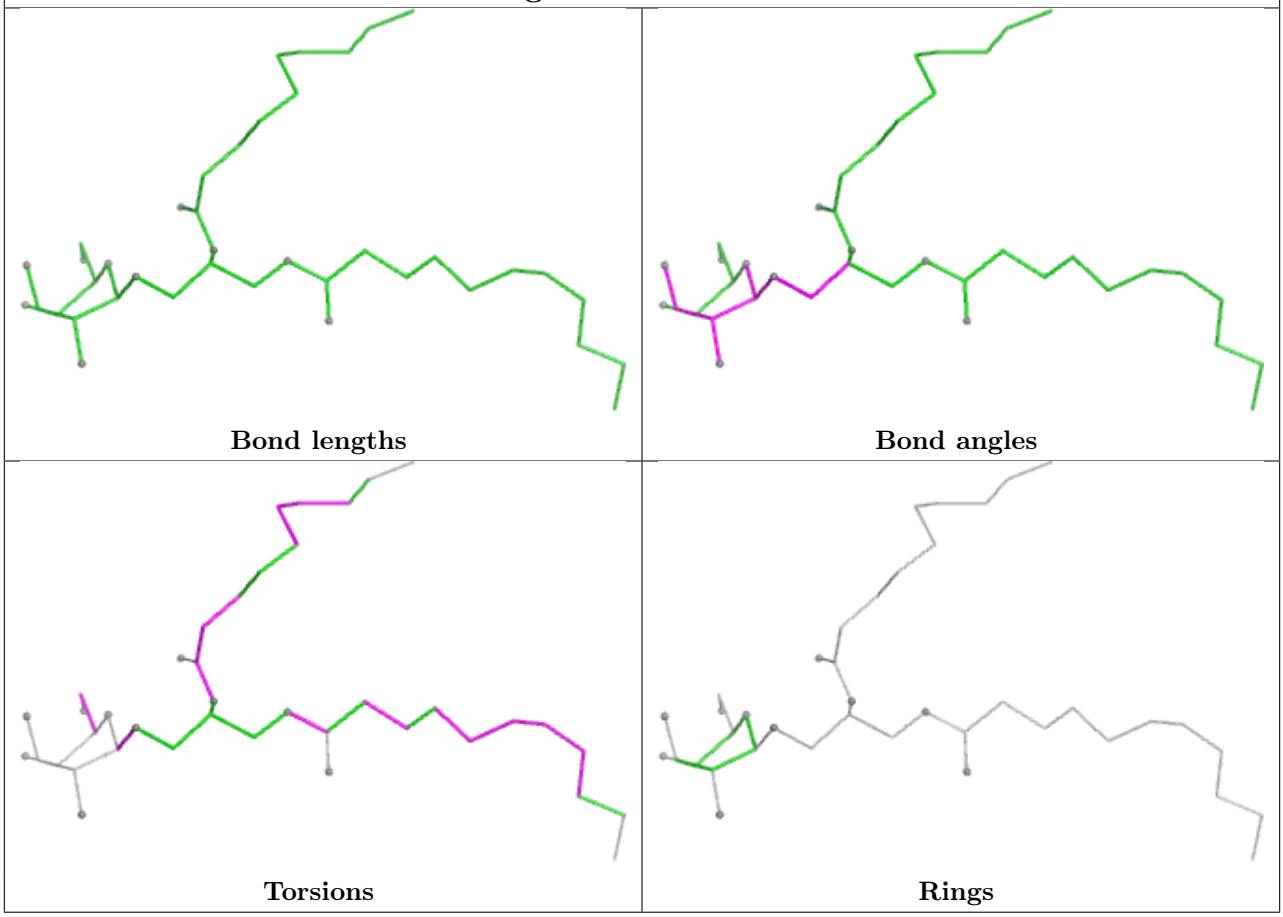


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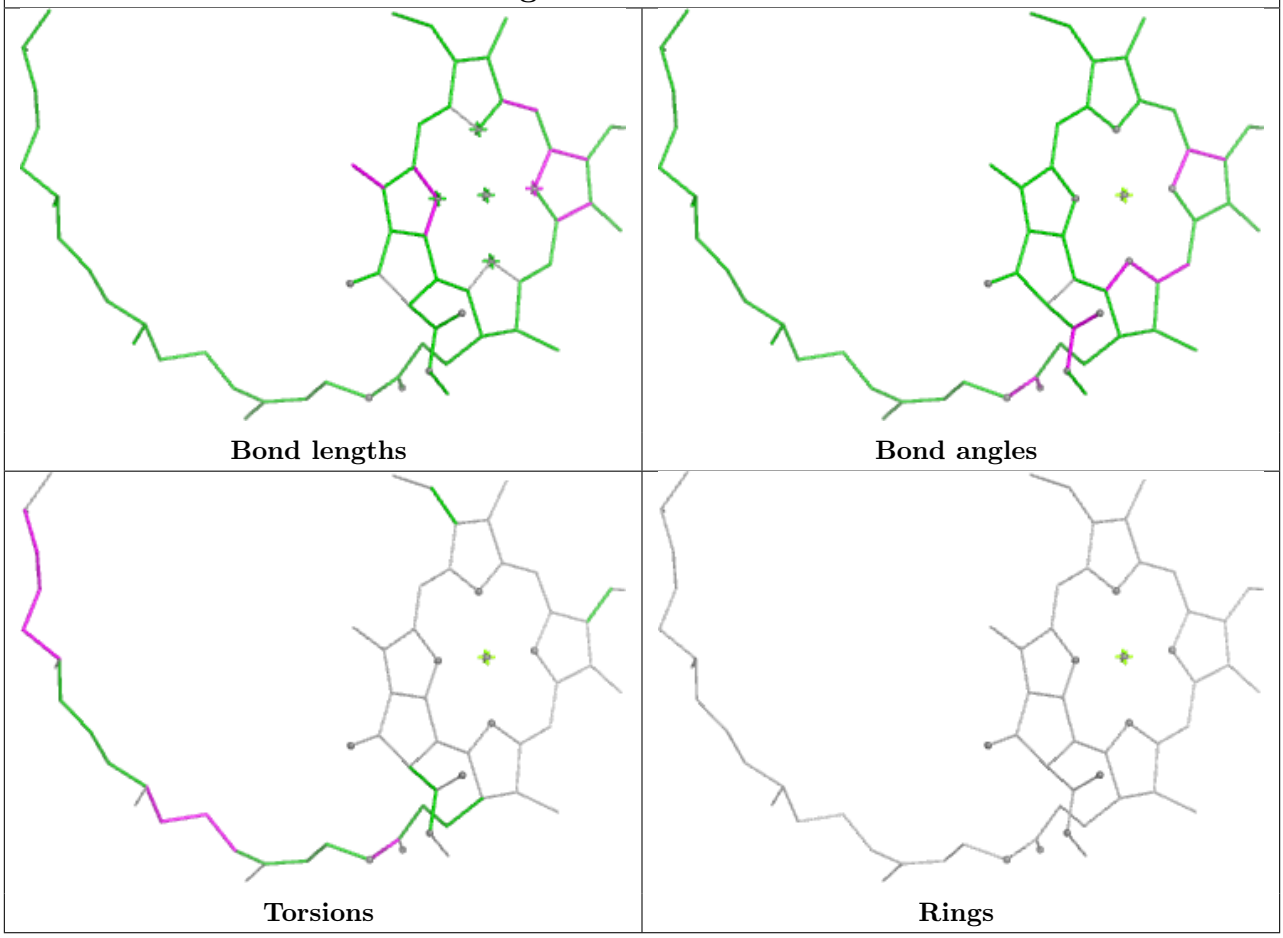


Rings

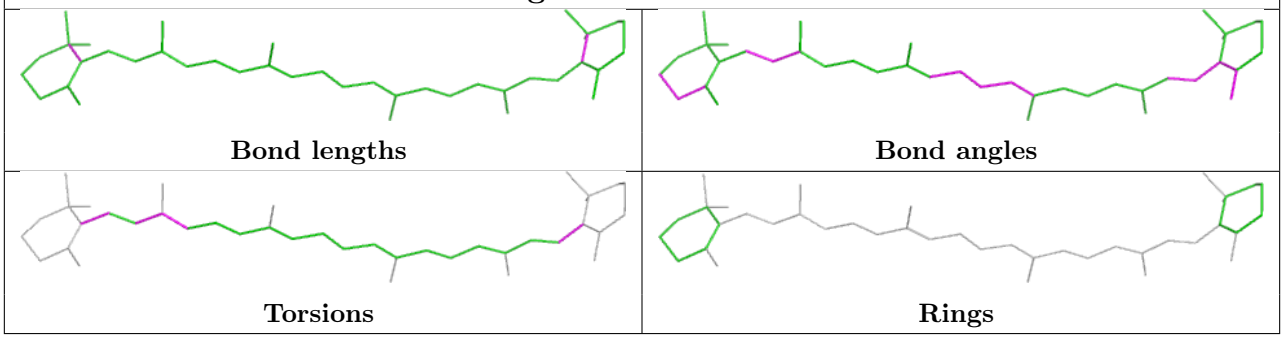
Ligand LMG a 852



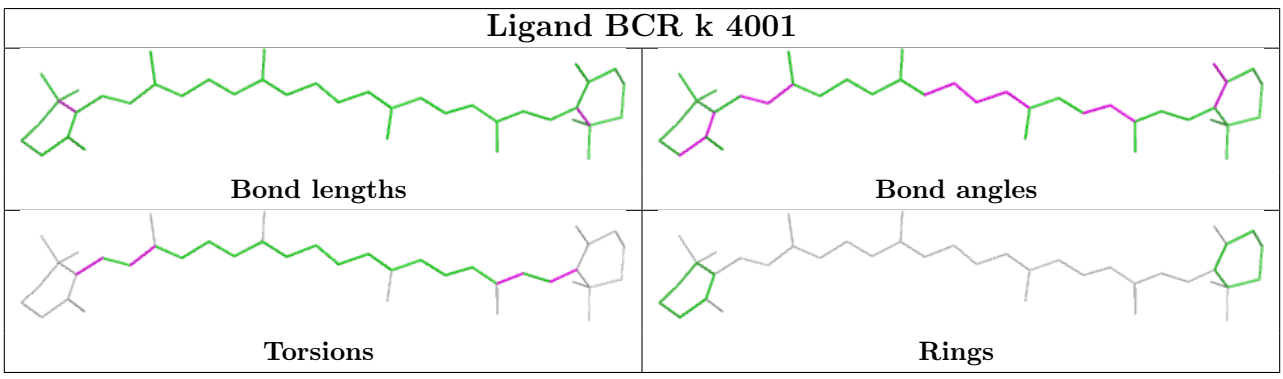
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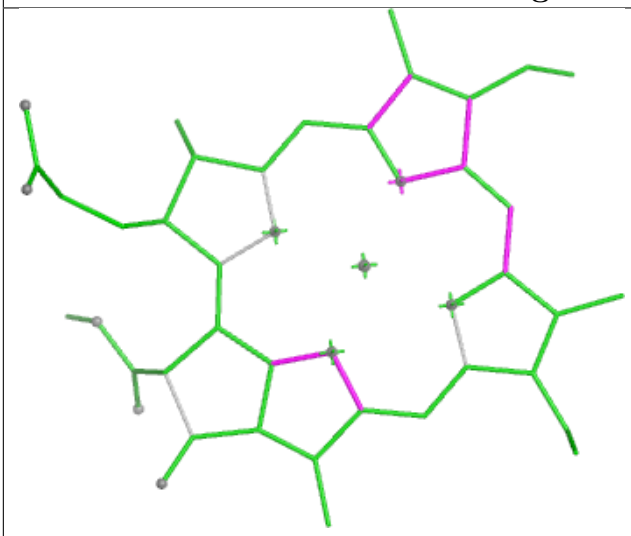
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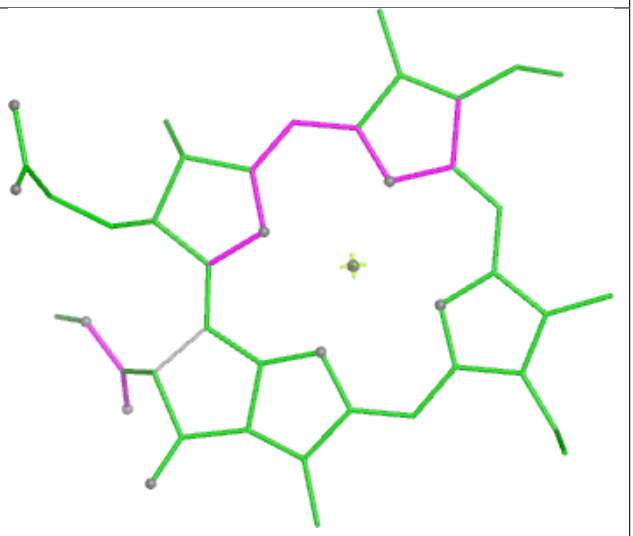
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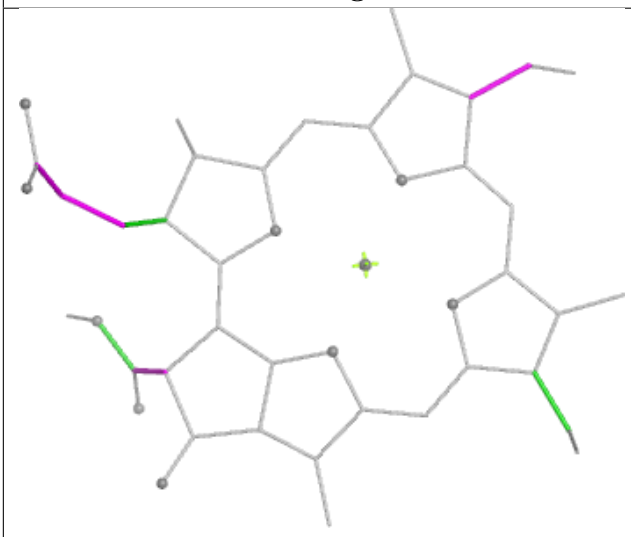
Ligand CLA f 204



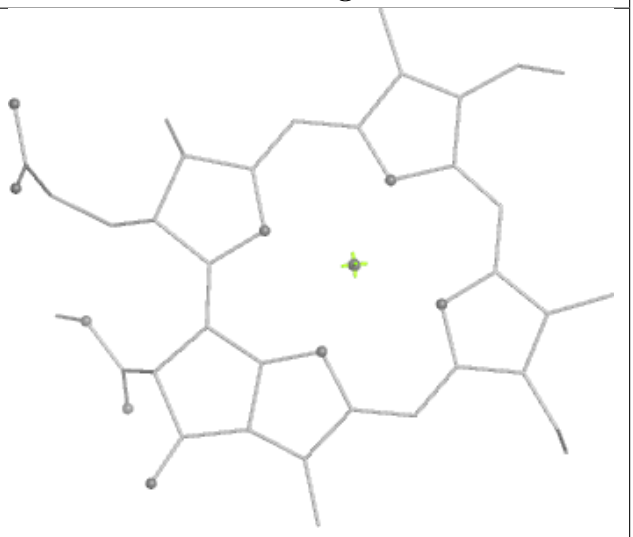
Bond lengths



Bond angles



Torsions

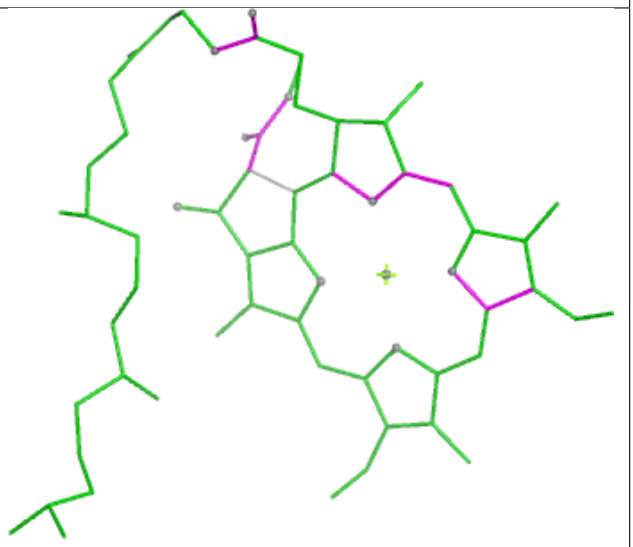


Rings

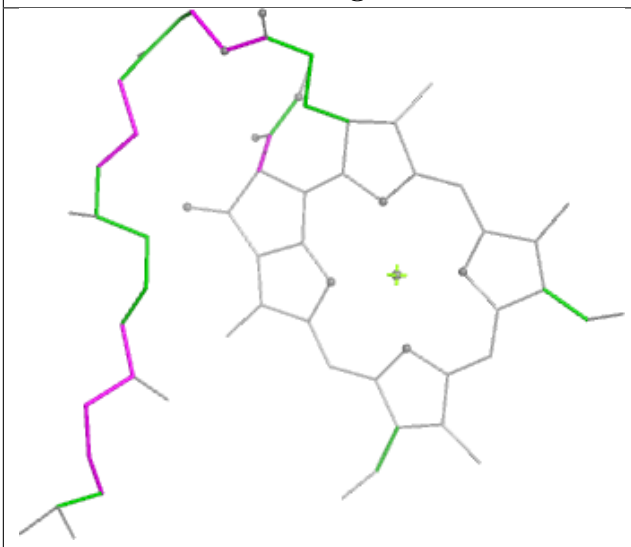
Ligand CLA a 825



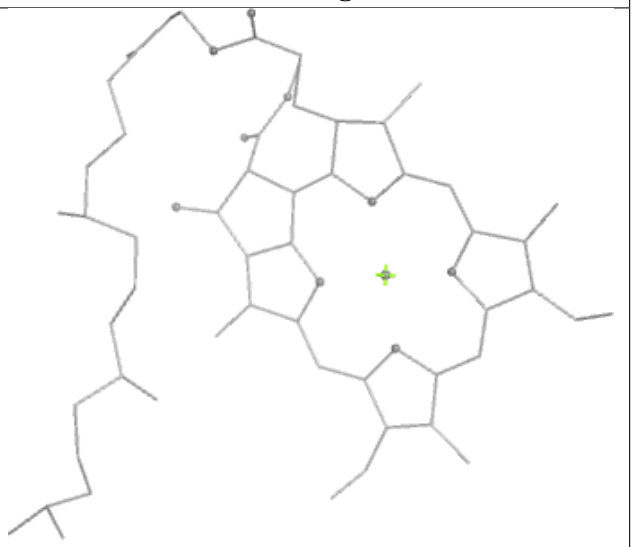
Bond lengths



Bond angles

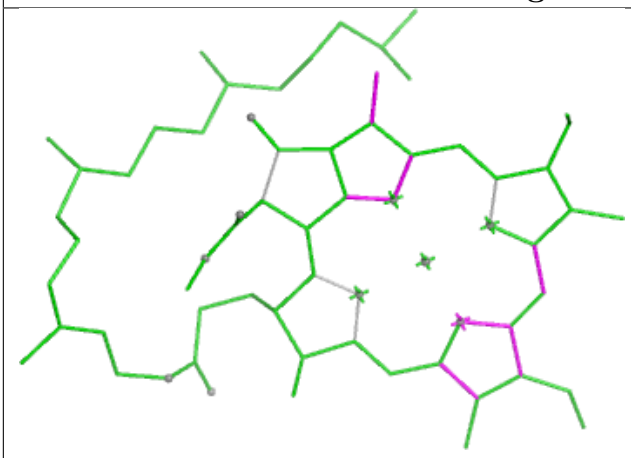


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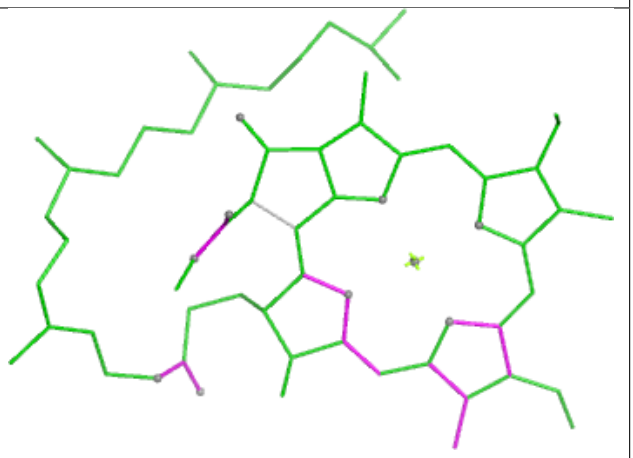


Rings

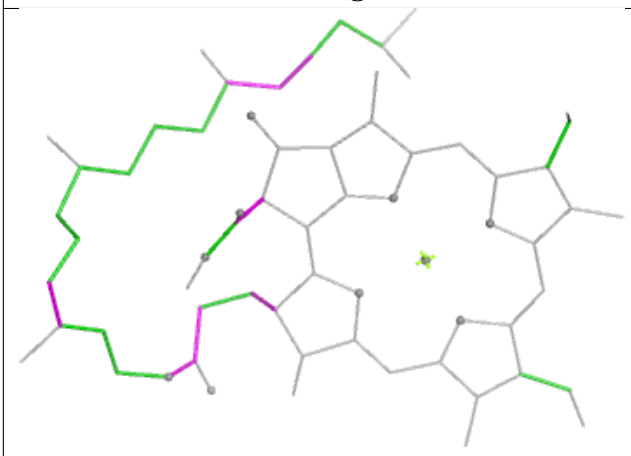
Ligand CLA b 806



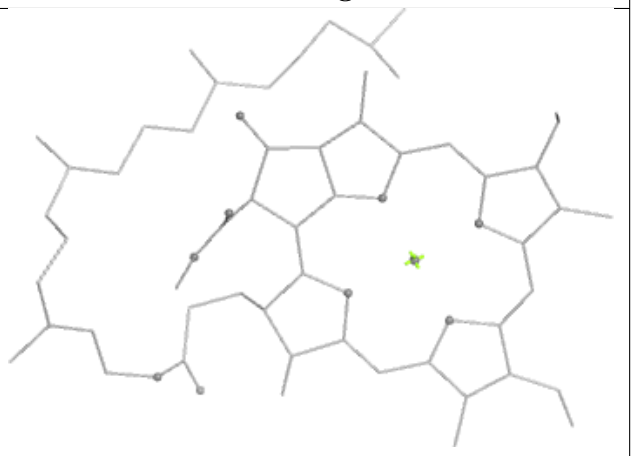
Bond lengths



Bond angles

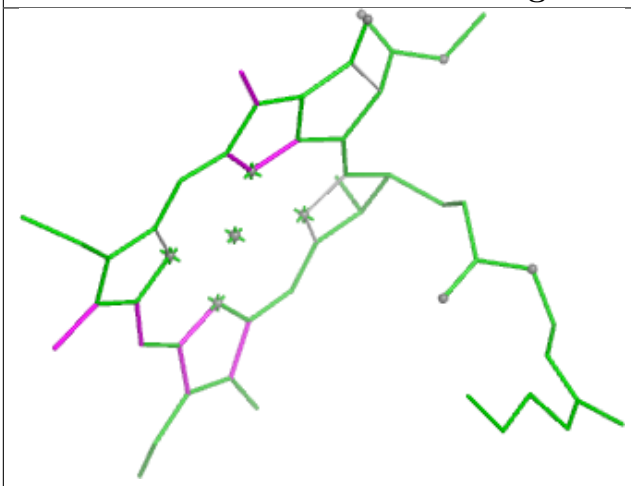


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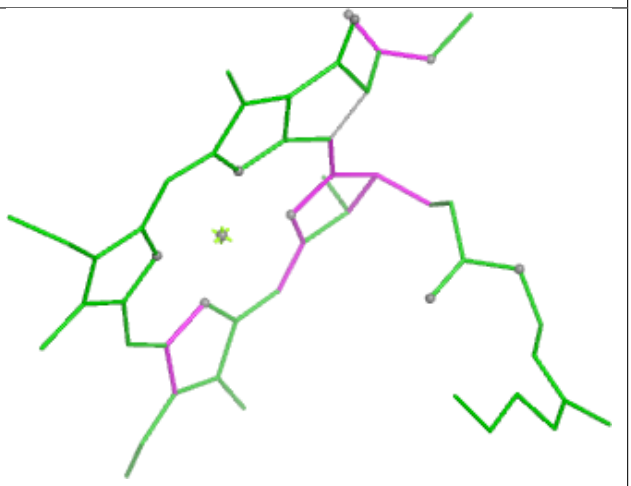


Rings

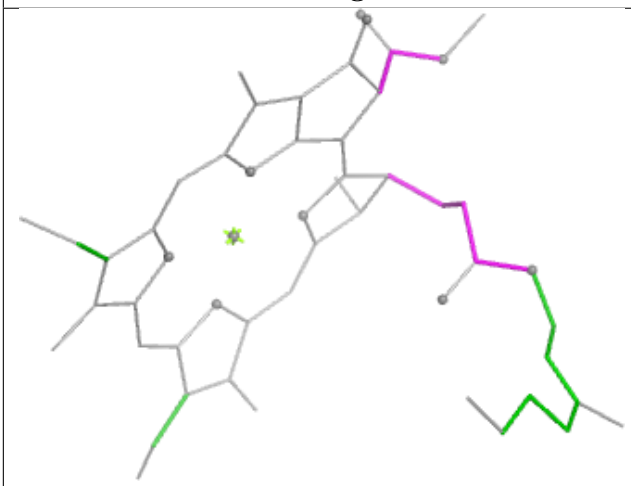
Ligand CLA a 810



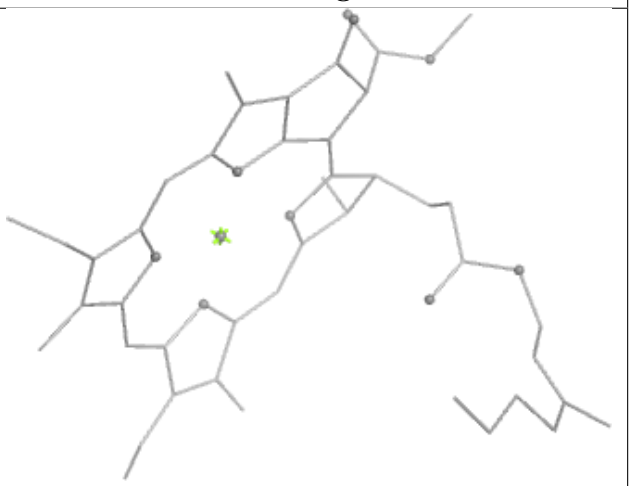
Bond lengths



Bond angles



Torsions



Rings

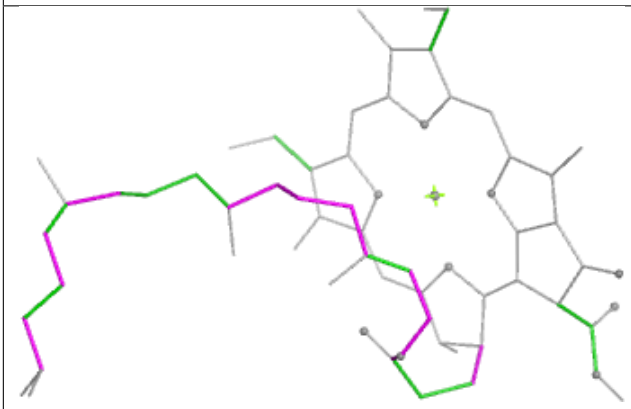
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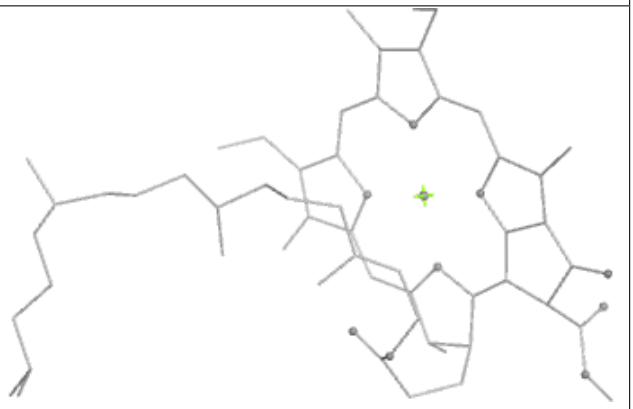
Bond lengths



Bond angles

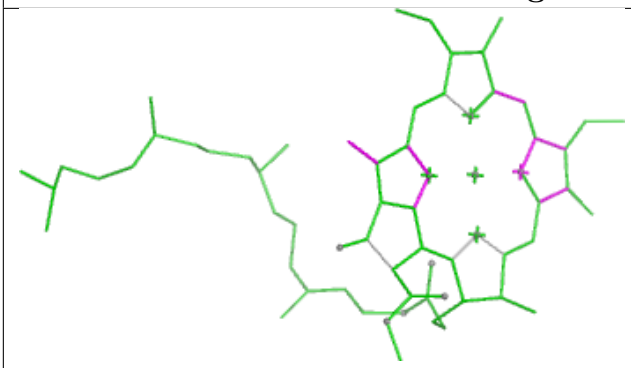


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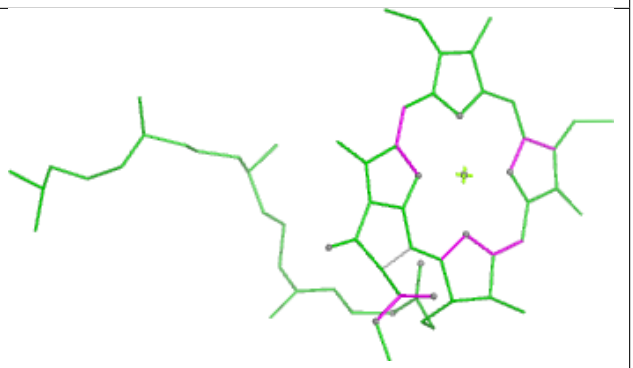


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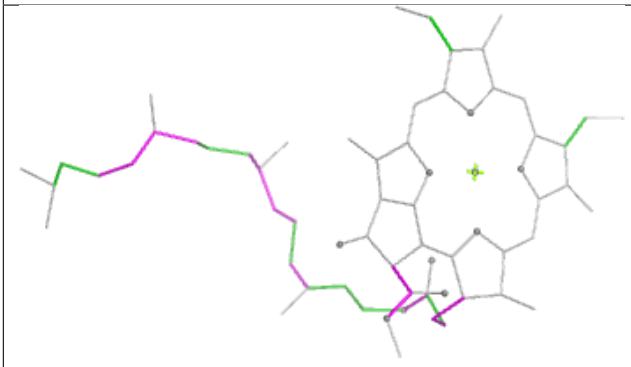
Ligand CLA b 835



Bond lengths



Bond angles

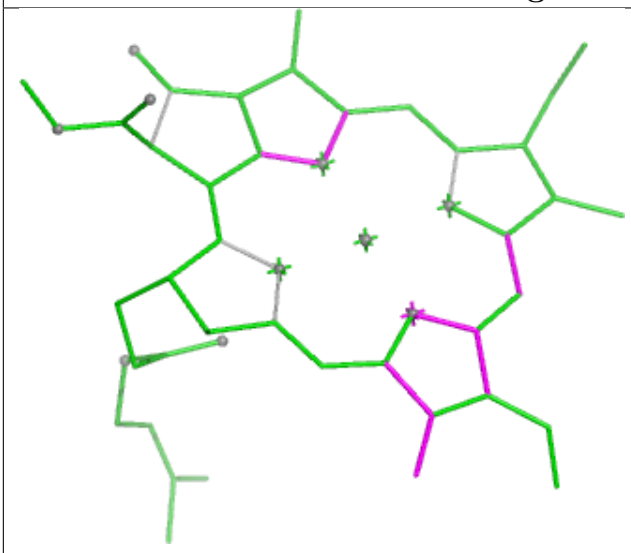


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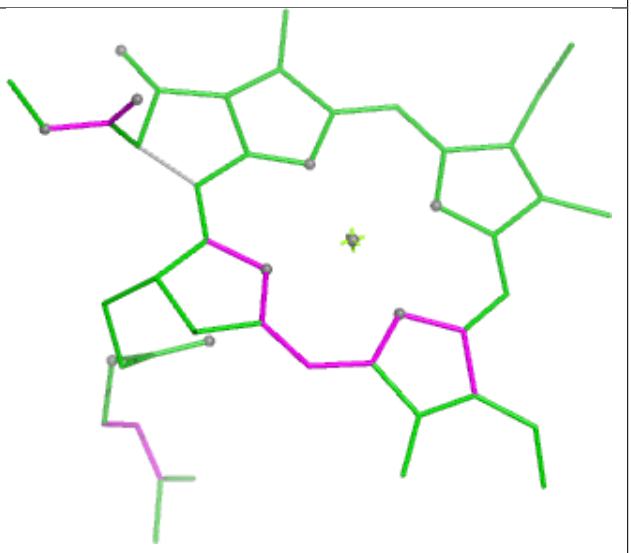


Rings

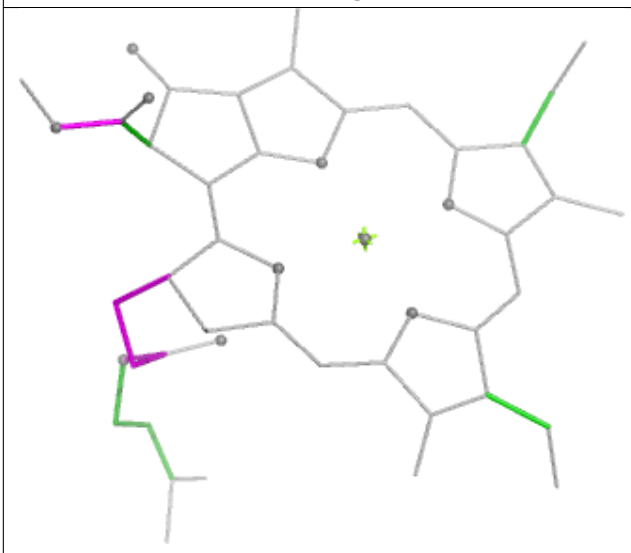
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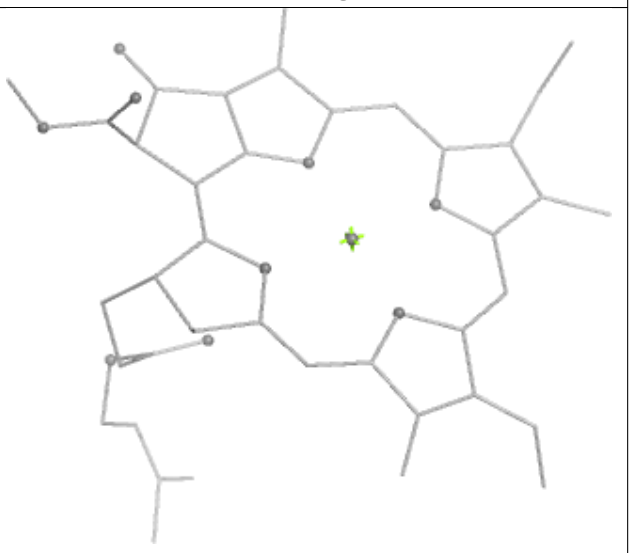
Bond lengths



Bond angles

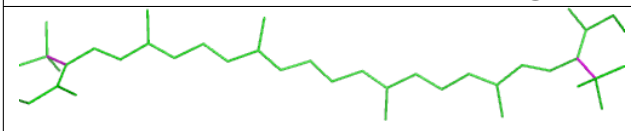


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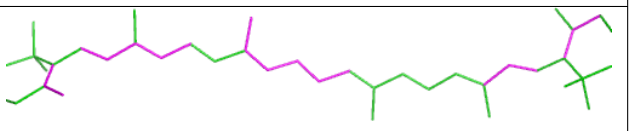


Rings

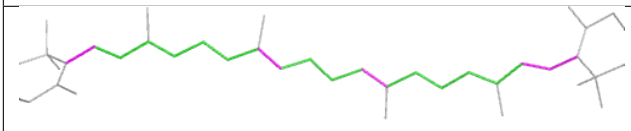
Ligand BCR a 846



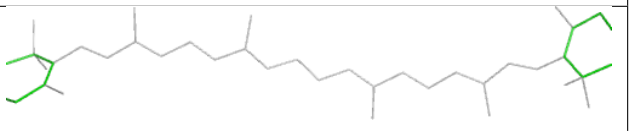
Bond lengths



Bond angles

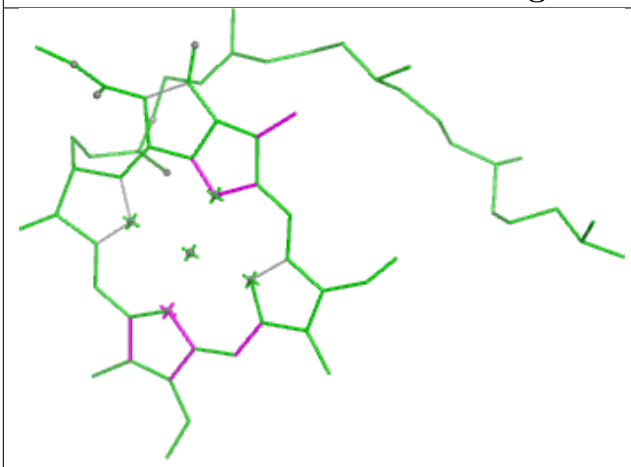


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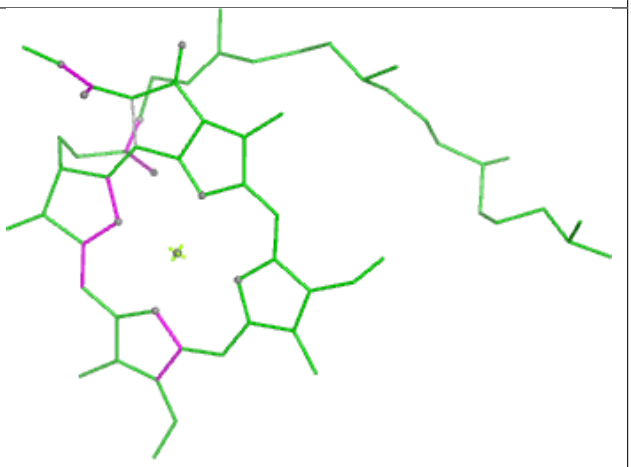


Rings

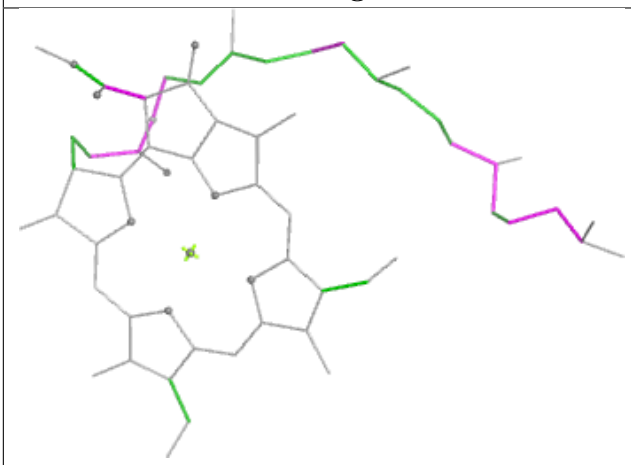
Ligand CLA a 829



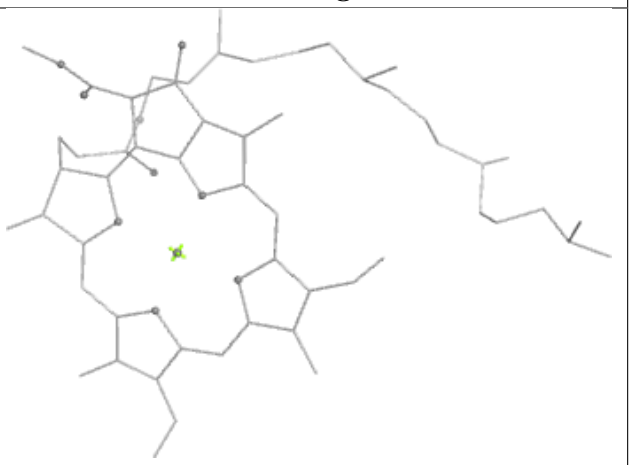
Bond lengths



Bond angles

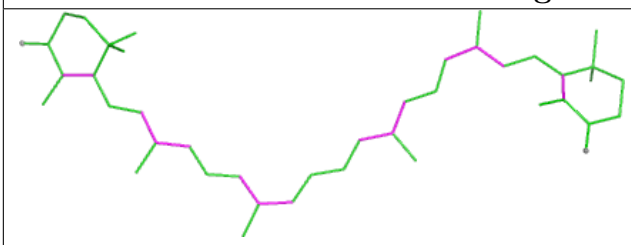


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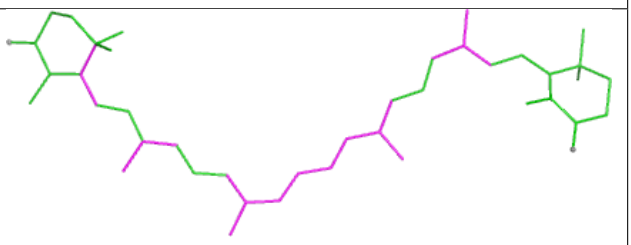


Rings

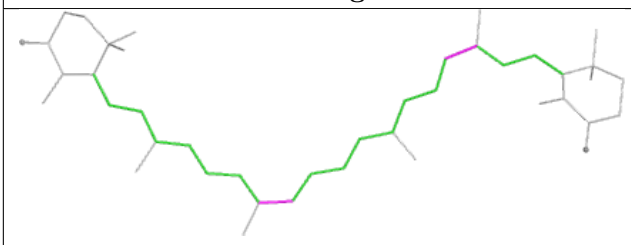
Ligand 45D a 856



Bond lengths



Bond angles

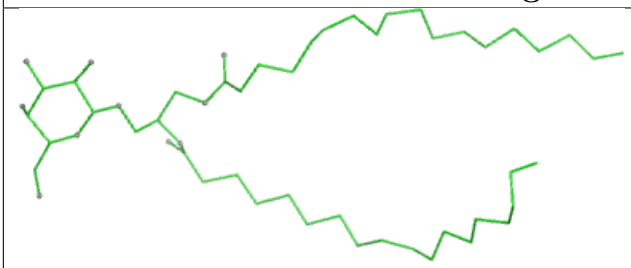


Torsions

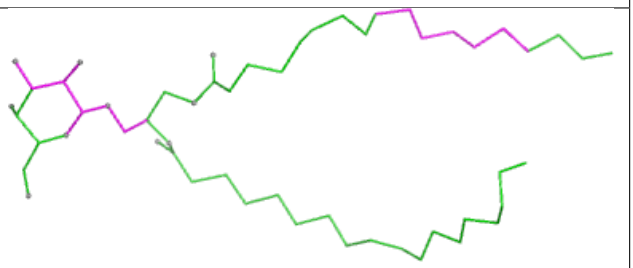


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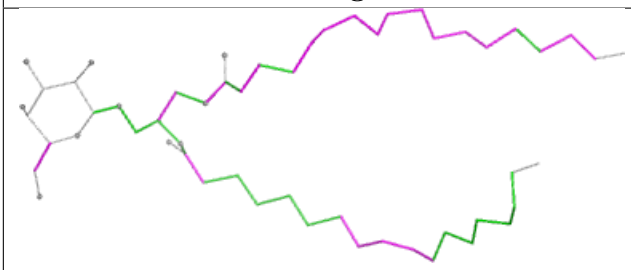
Ligand LMG b 850



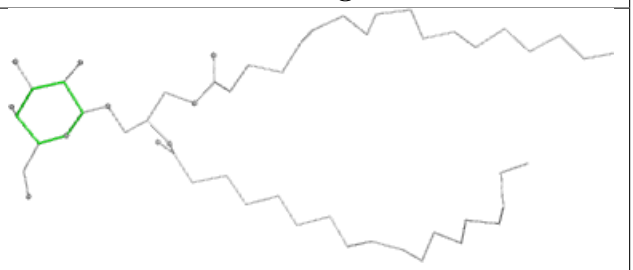
Bond lengths



Bond angles

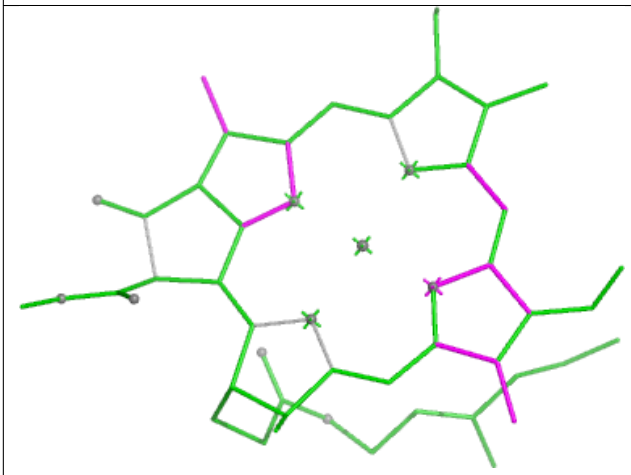


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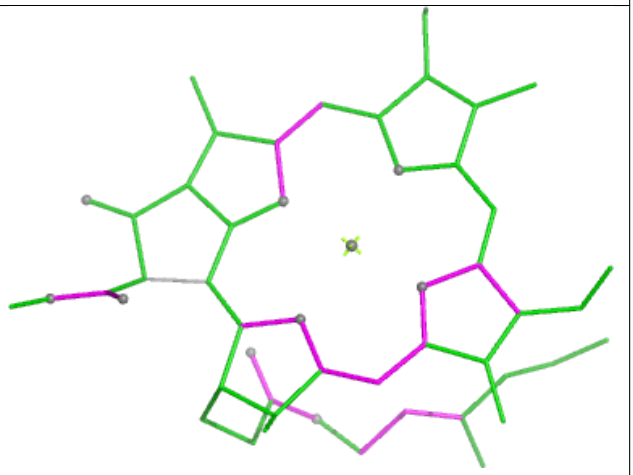


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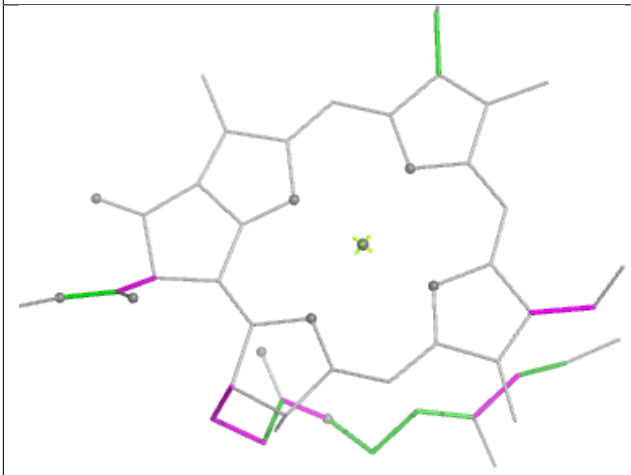
Ligand CLA a 812



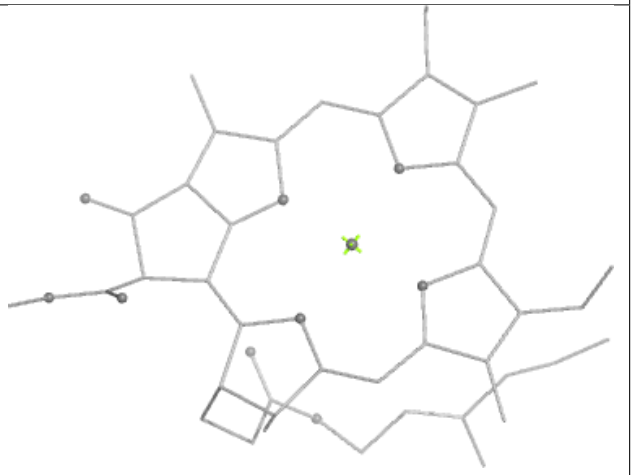
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Bond angles

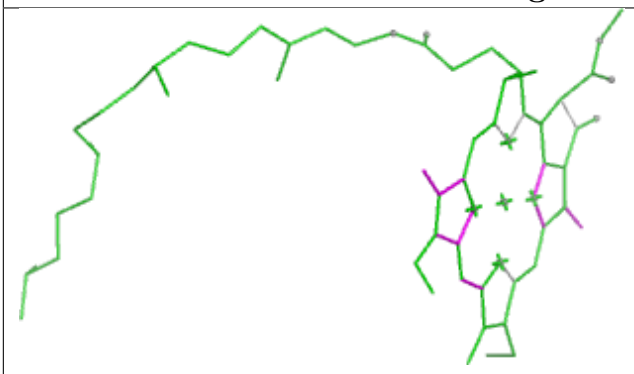


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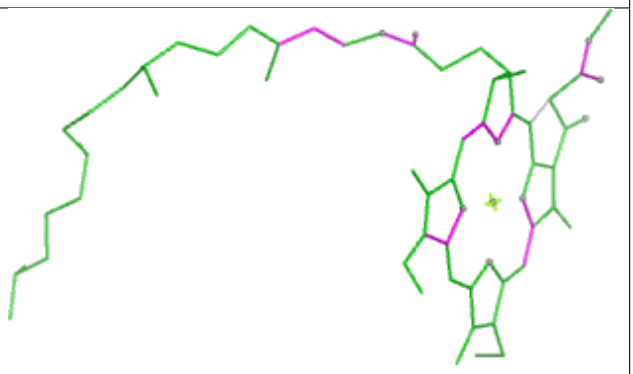


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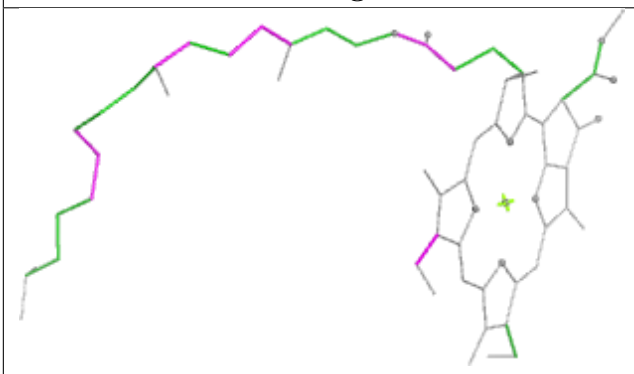
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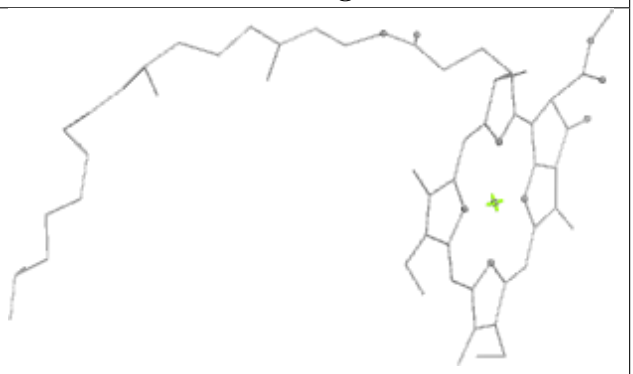
Bond lengths



Bond angles

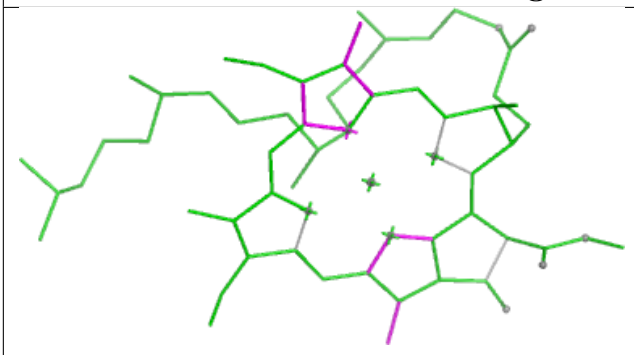


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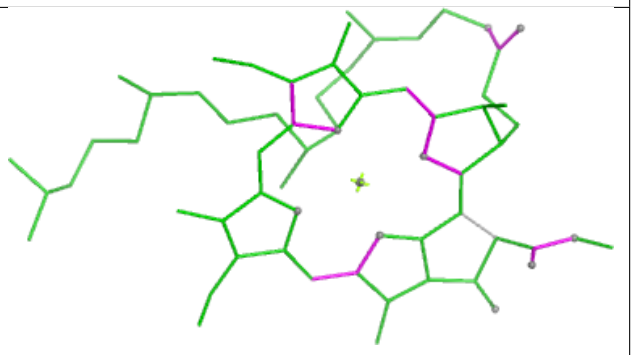


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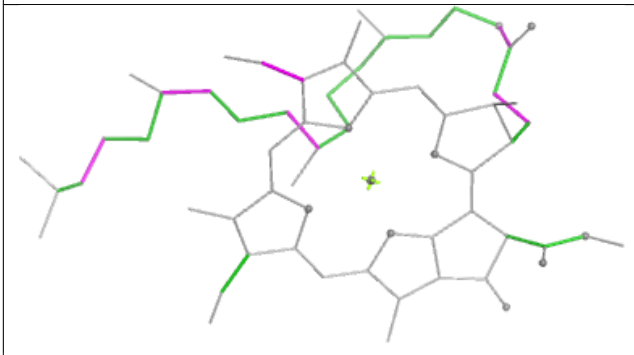
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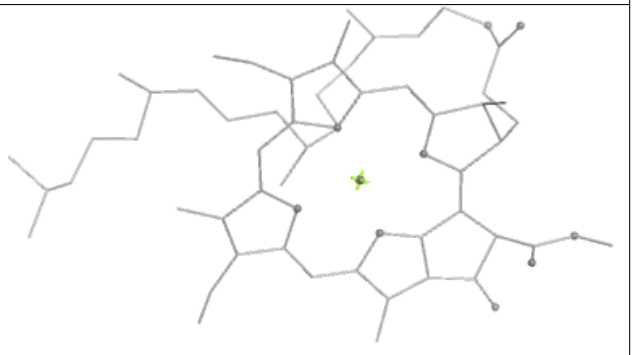
Bond lengths



Bond angles

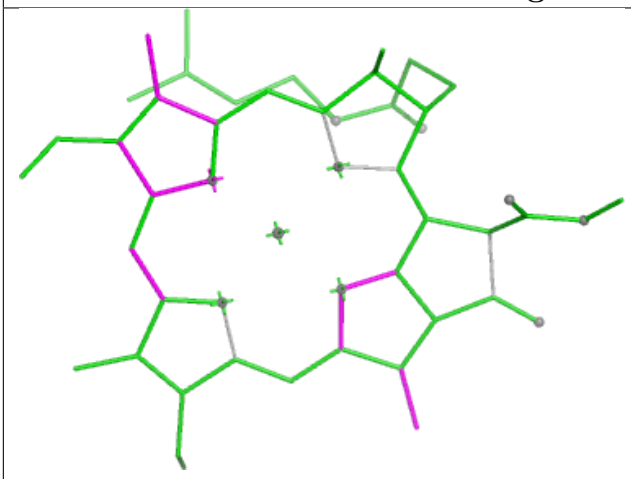


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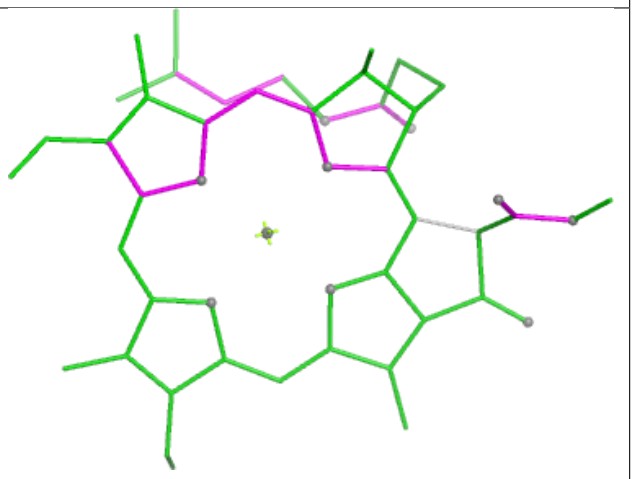


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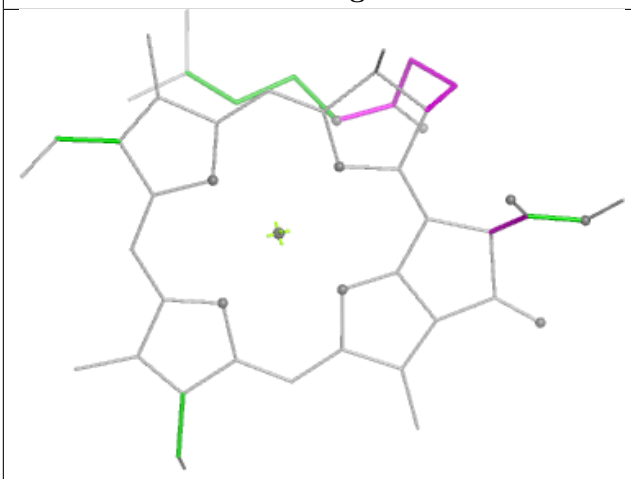
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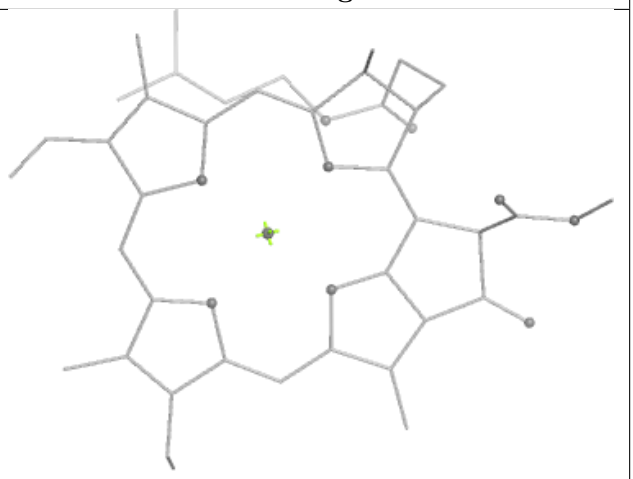
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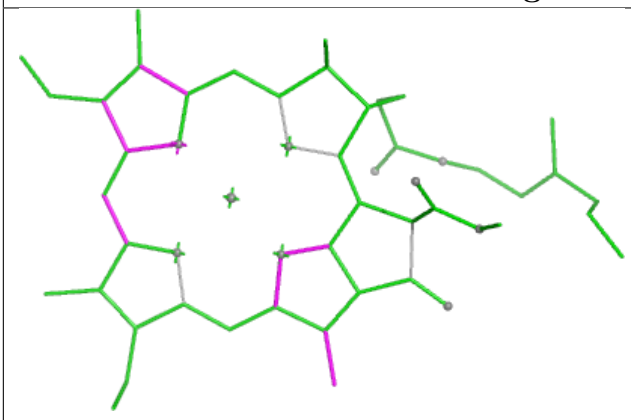


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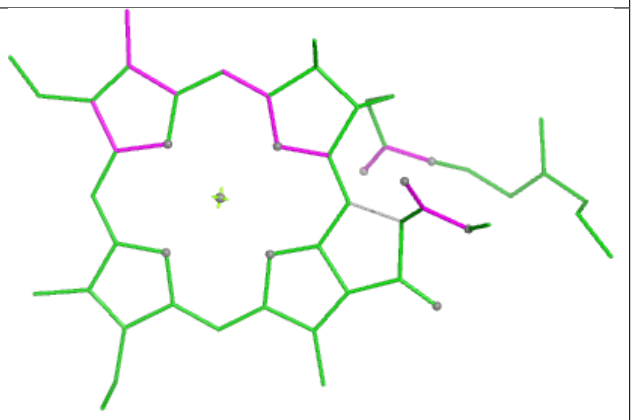


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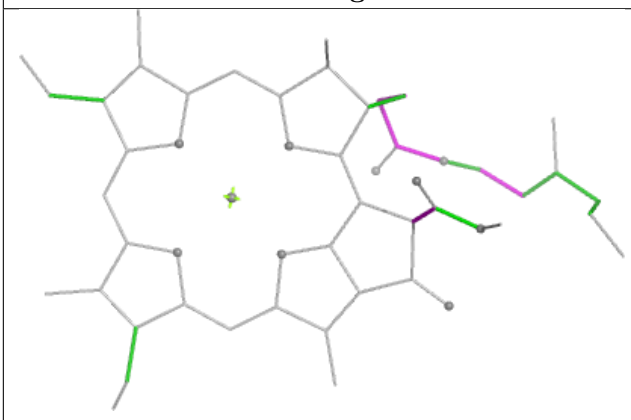
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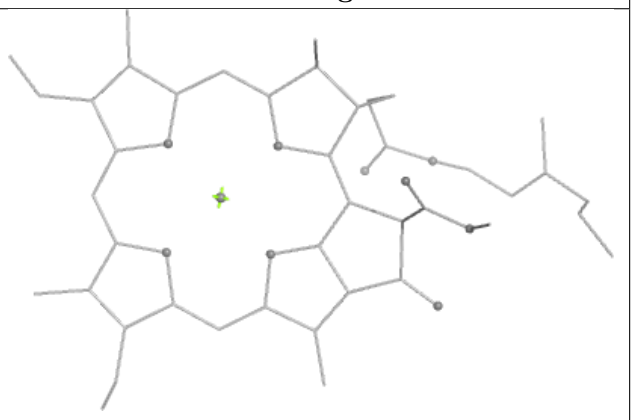
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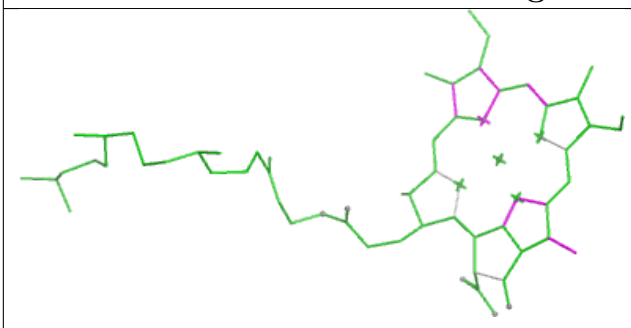


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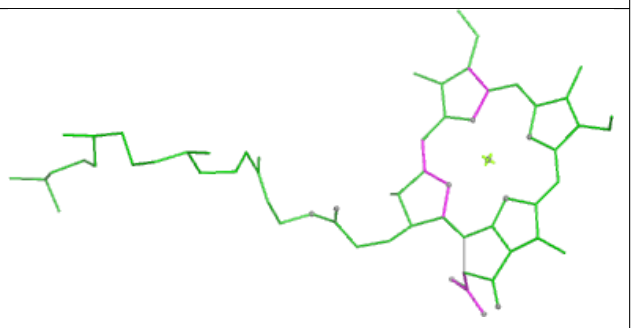


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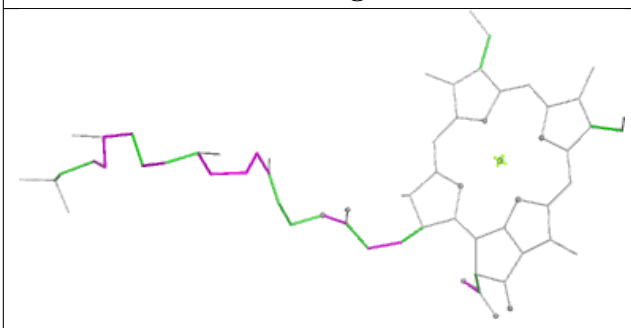
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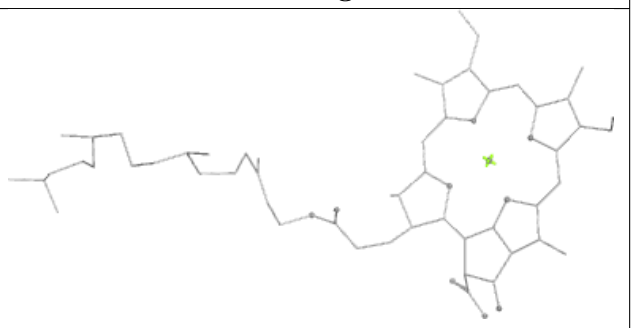
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Bond angles

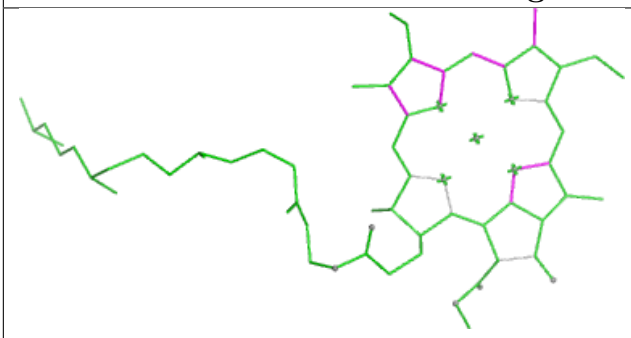


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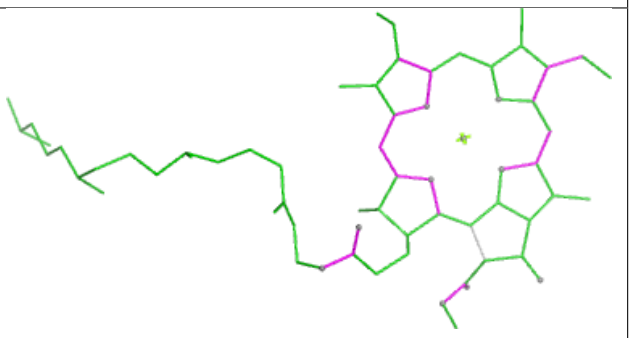


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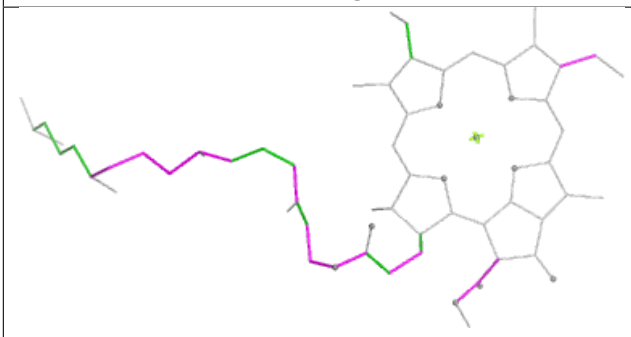
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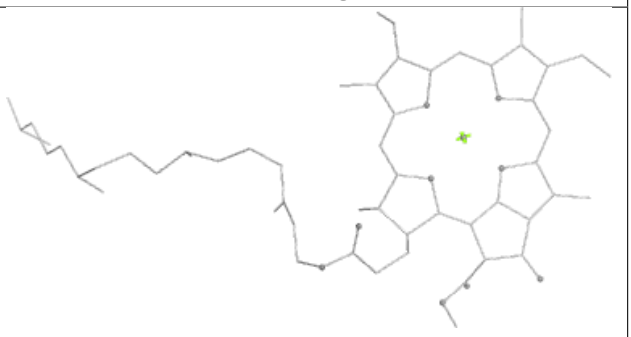
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Bond angles

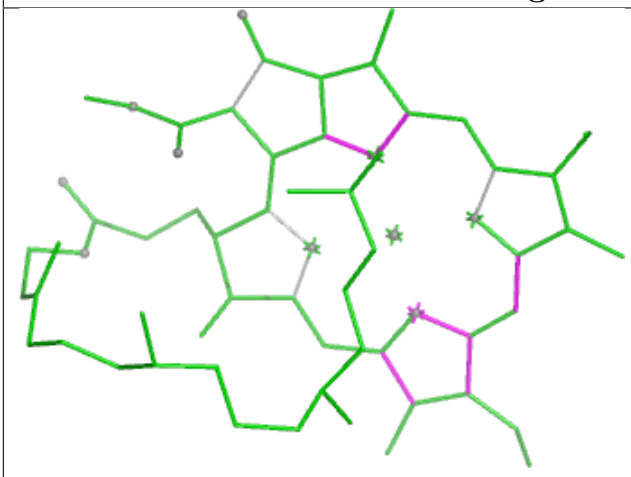


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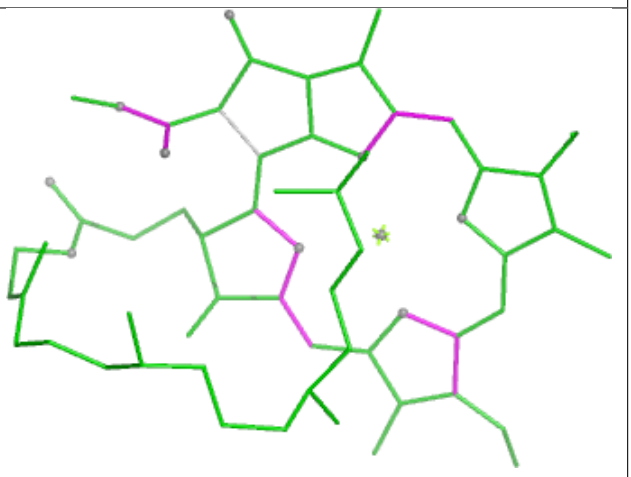


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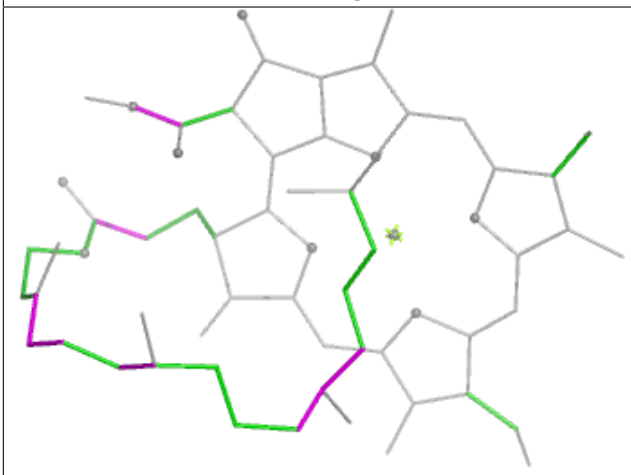
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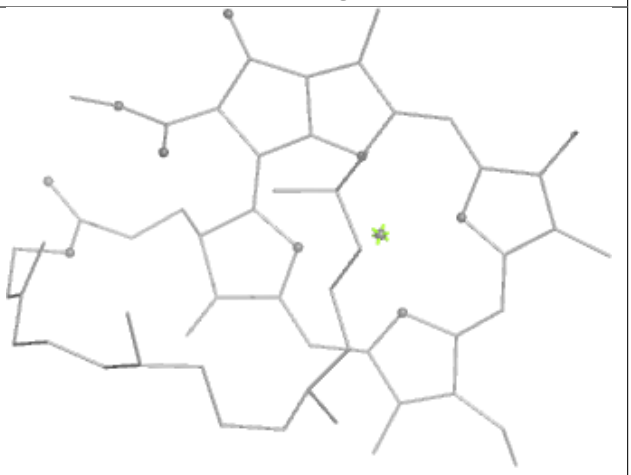
Bond lengths



Bond angles

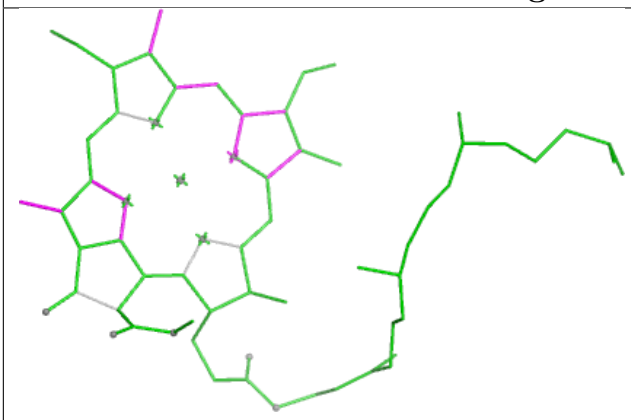


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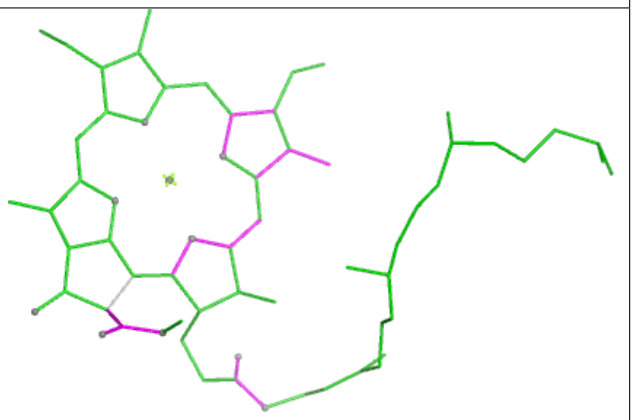


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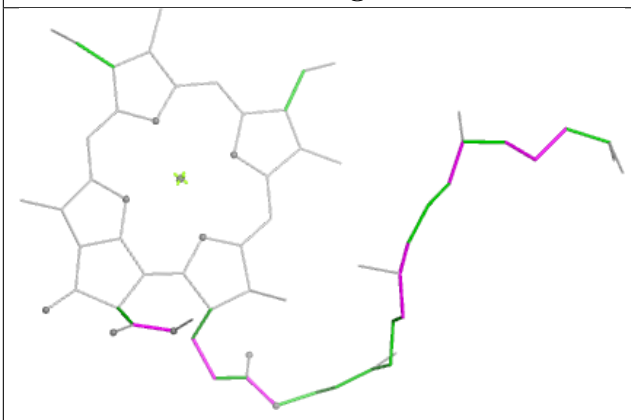
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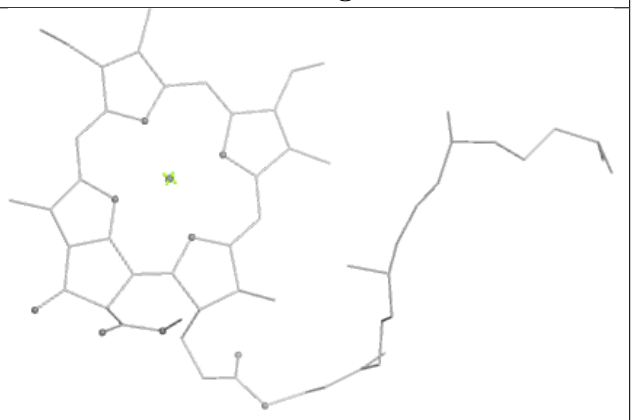
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Bond angles

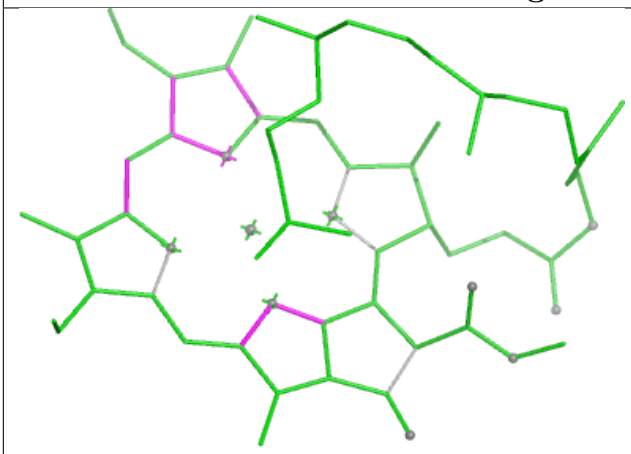


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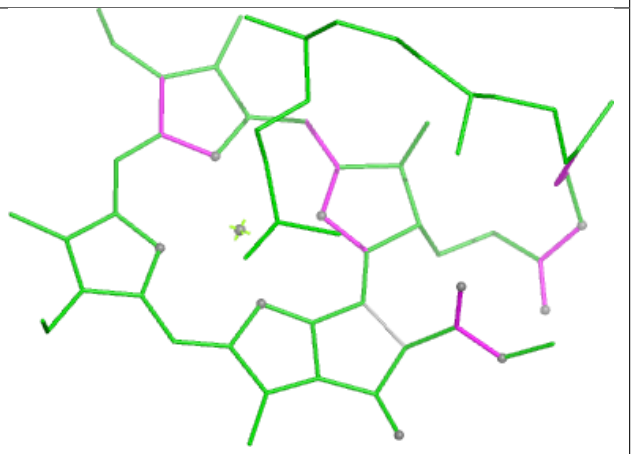


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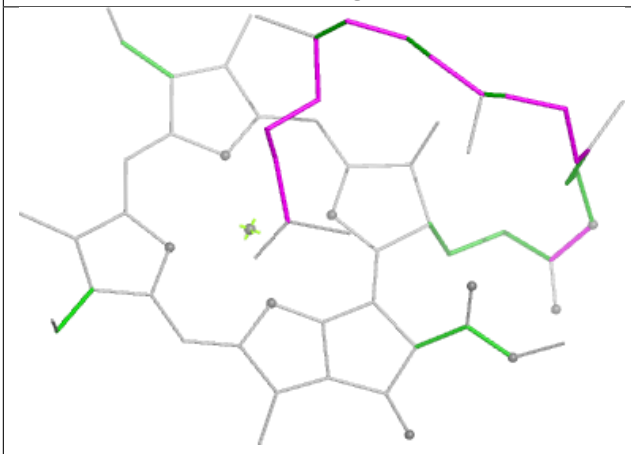
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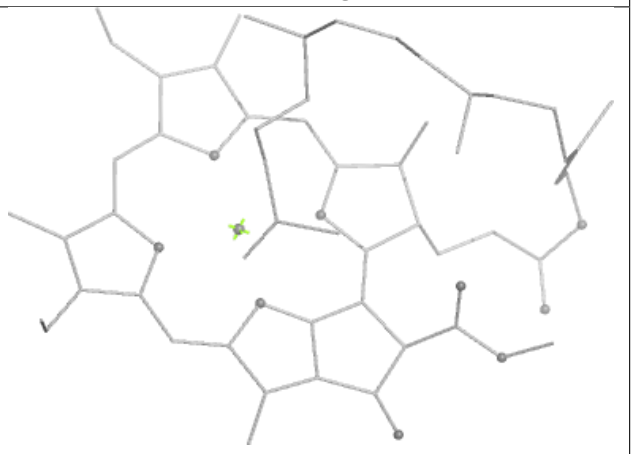
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Bond angles

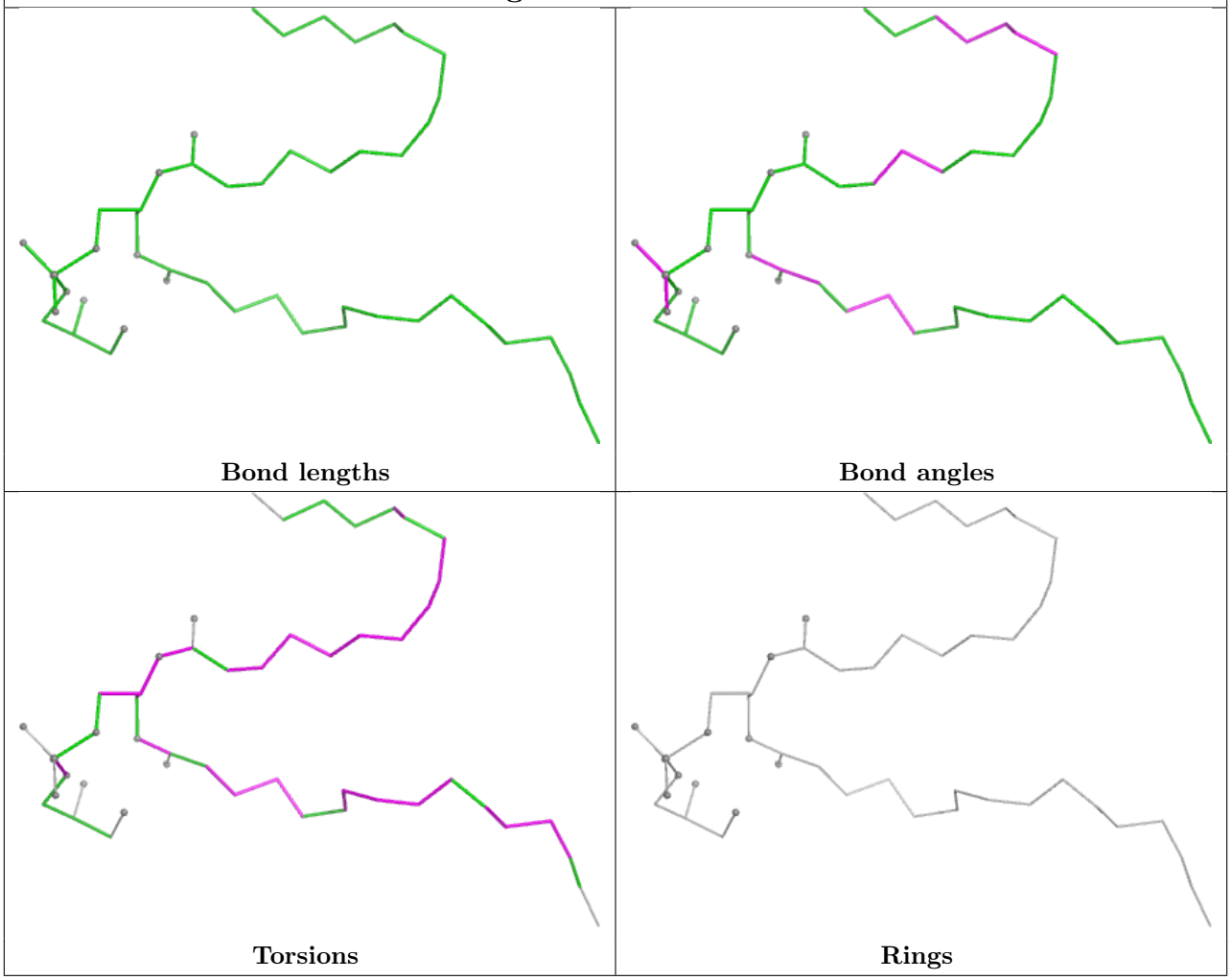


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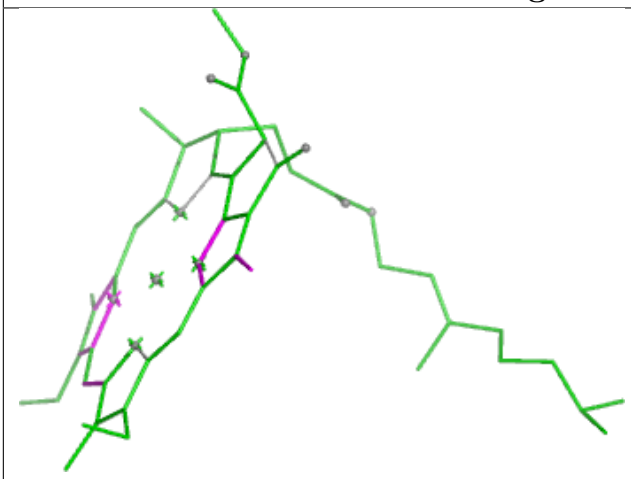


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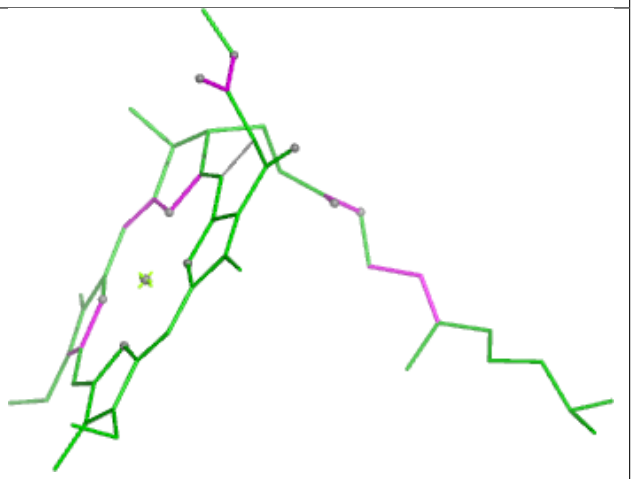
Ligand LHG a 853



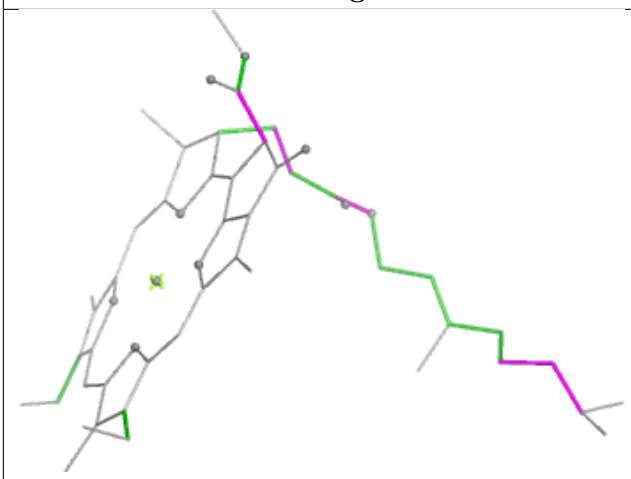
Ligand CLA a 836



Bond lengths



Bond angles

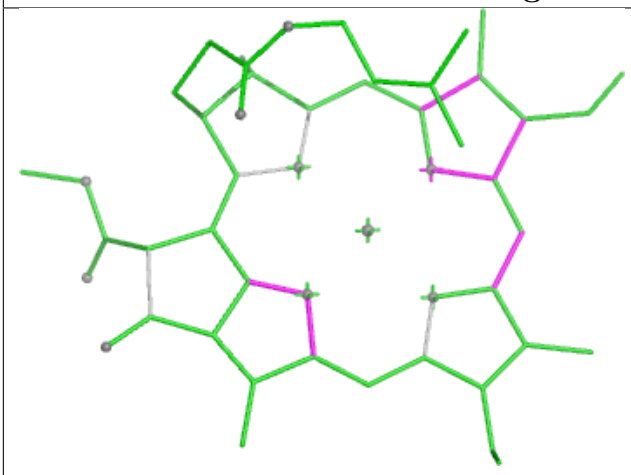


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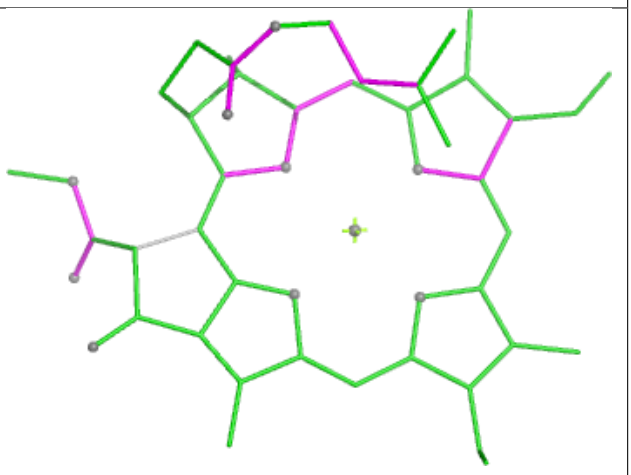


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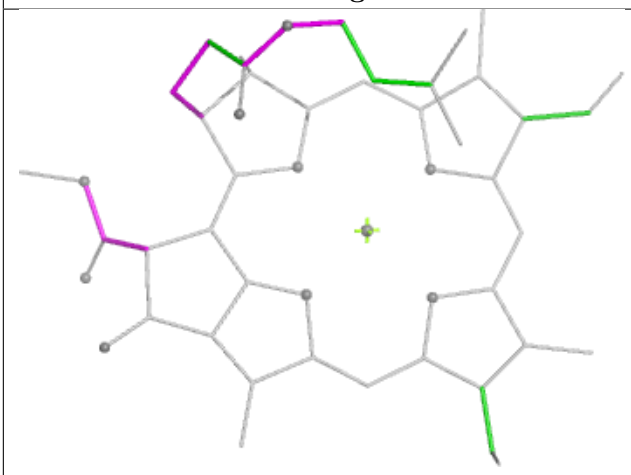
Ligand CLA l 1501



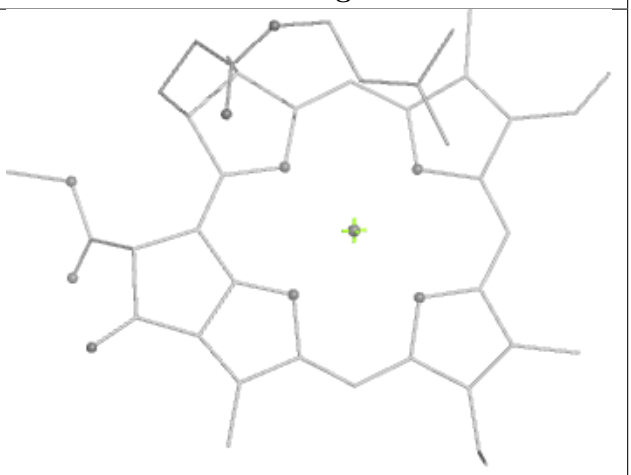
Bond lengths



Bond angles



Torsions



Rings

Ligand BCR j 101



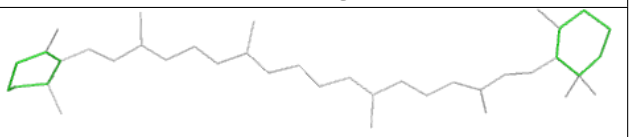
Bond lengths



Bond angles

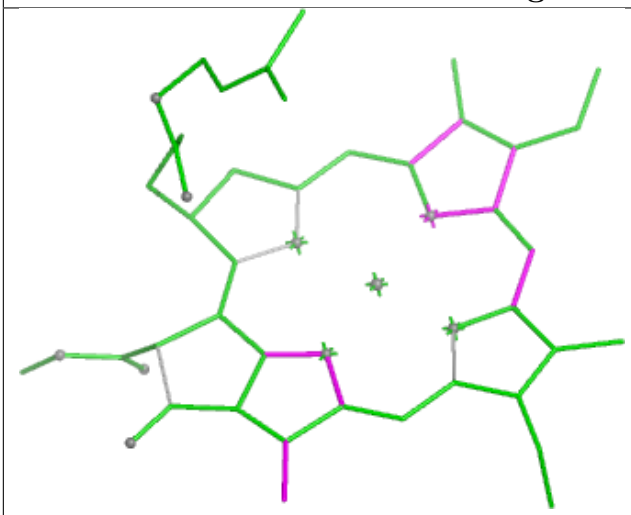


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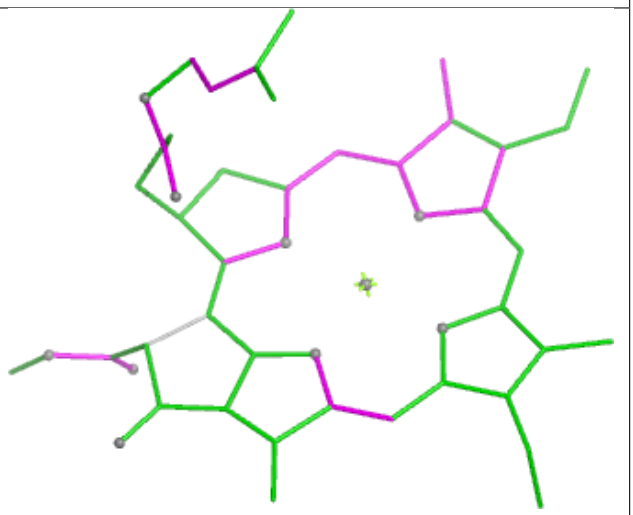


Rings

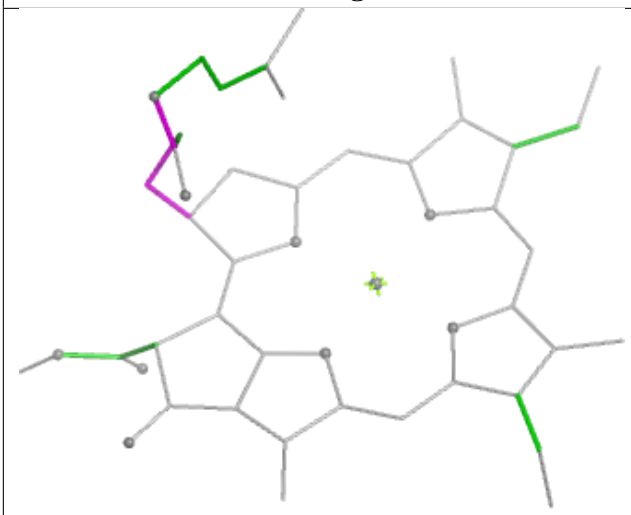
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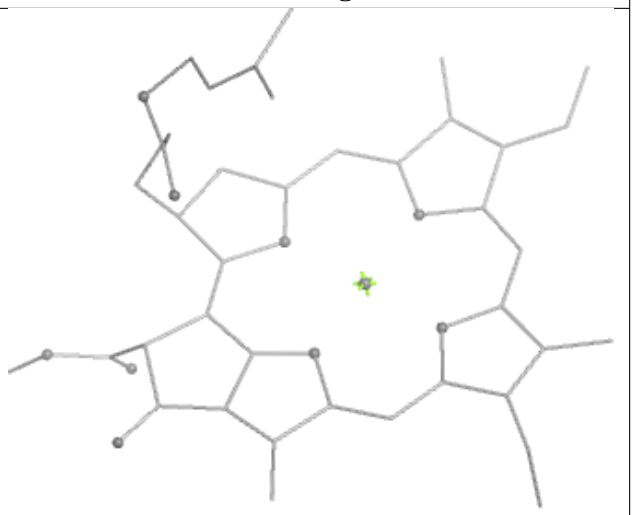
Bond lengths



Bond angles

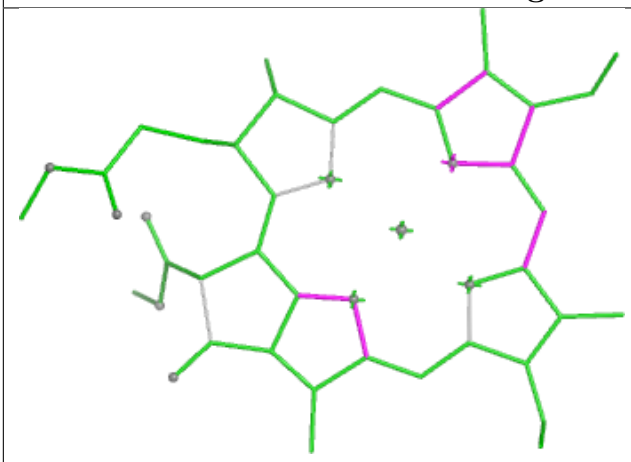


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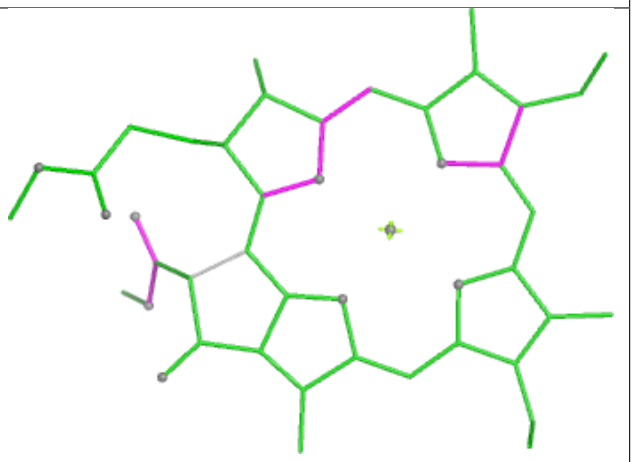


Rings

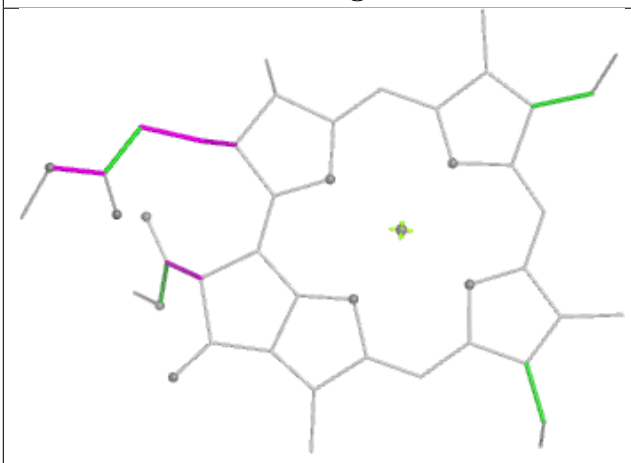
Ligand CLA b 842



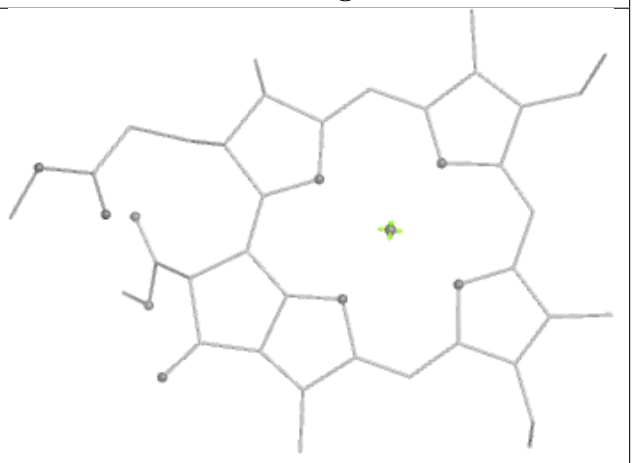
Bond lengths



Bond angles

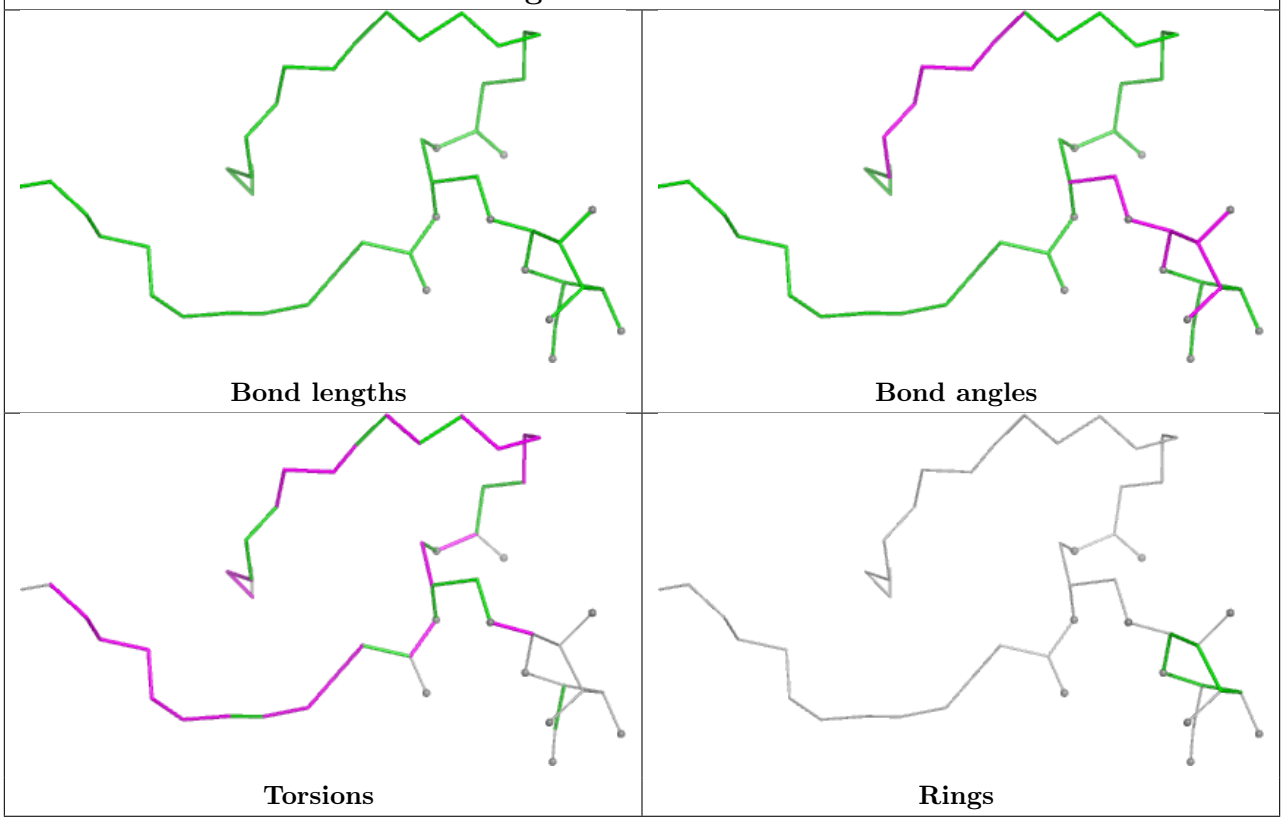


Torsions

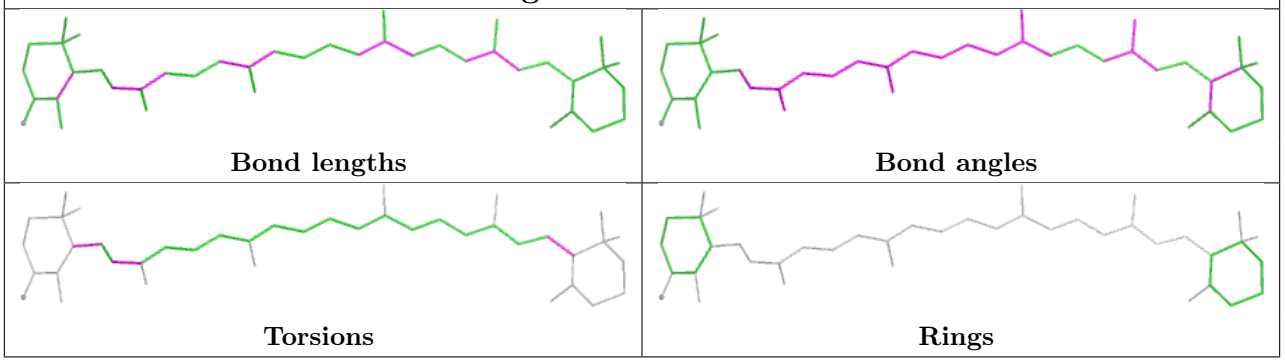


Rings

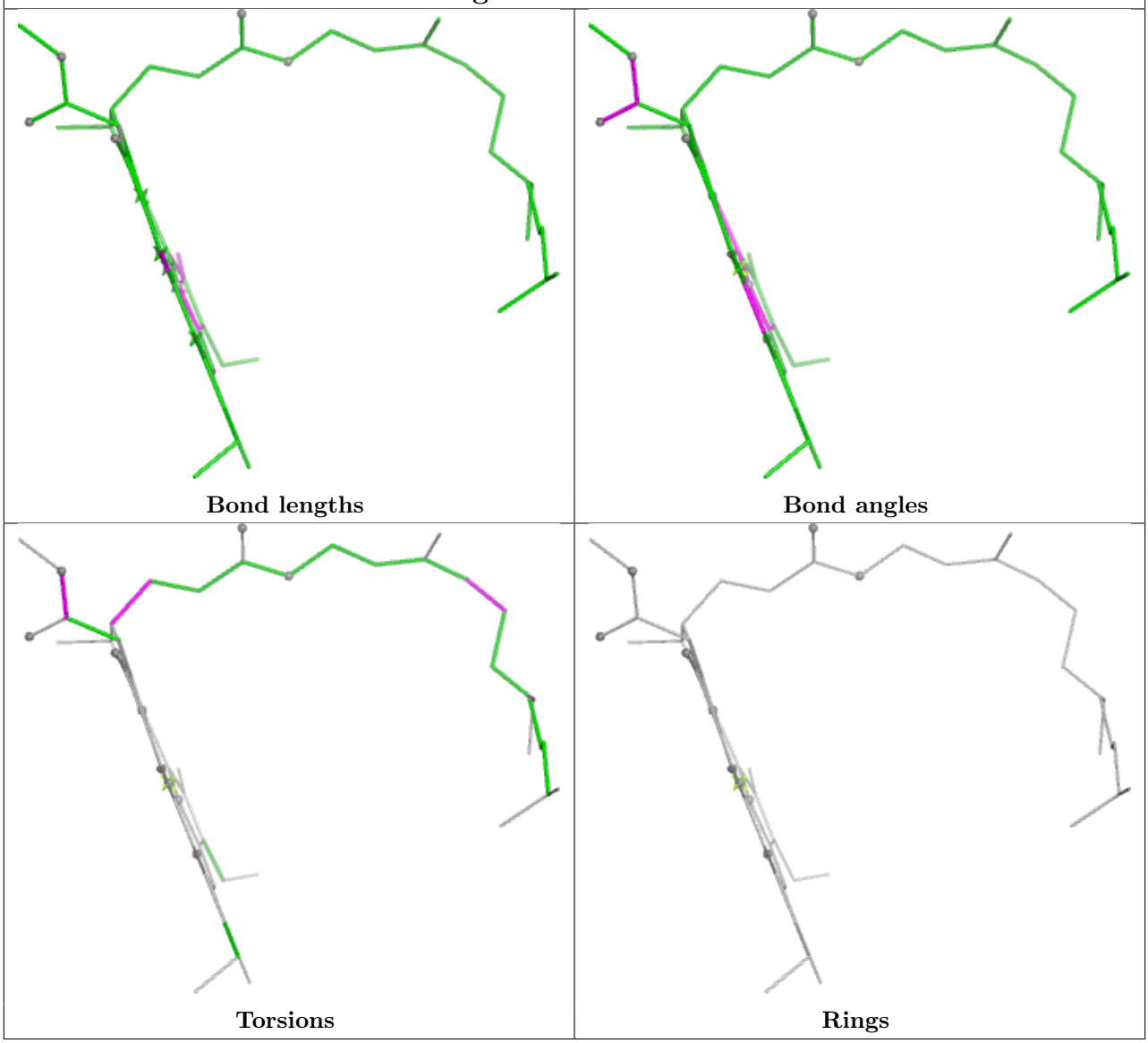
Ligand LMG a 850



Ligand ECH m 101



Ligand CLA b 820



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.

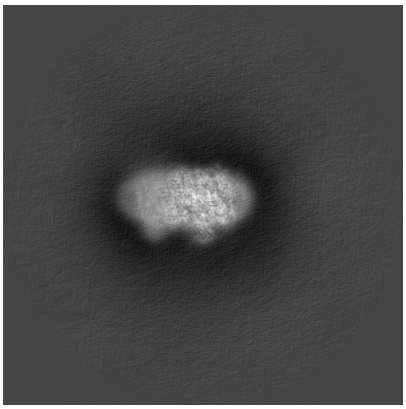
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15621. These allow visual inspection of the internal detail of the map and identification of artifacts.

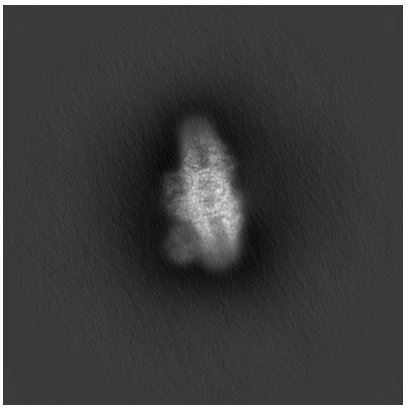
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

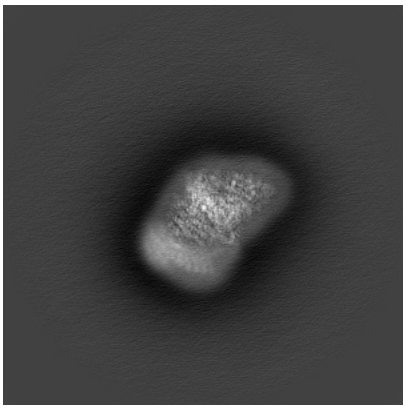
6.1.1 Primary map



X

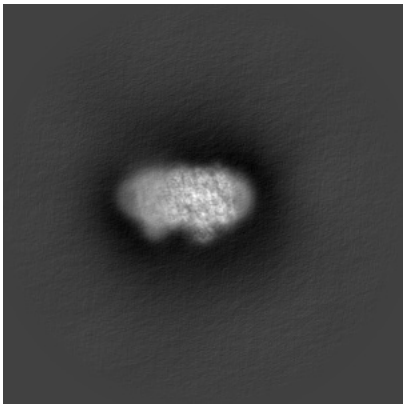


Y

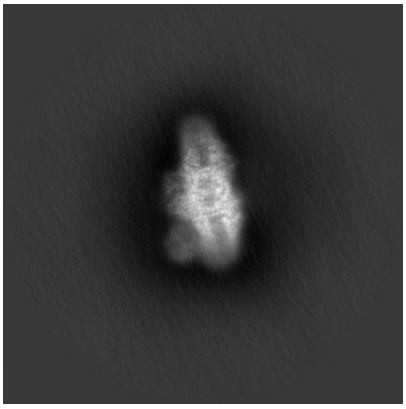


Z

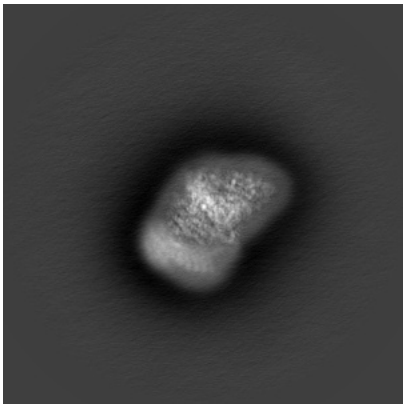
6.1.2 Raw map



X



Y

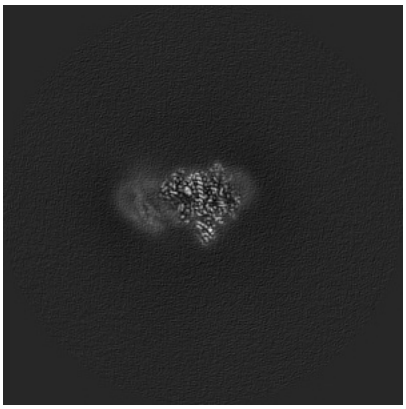


Z

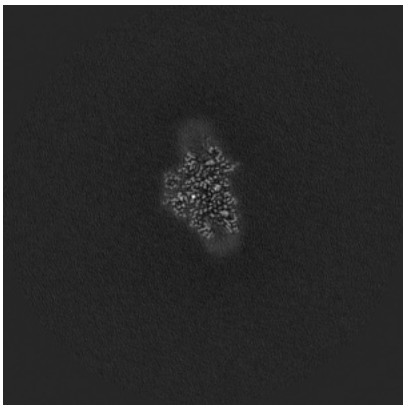
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

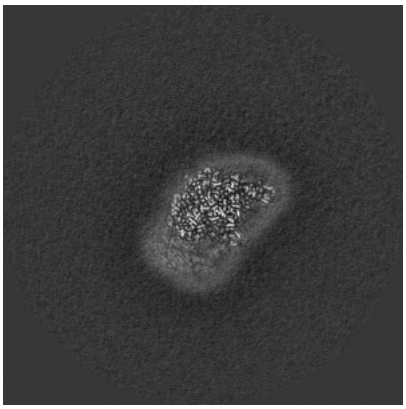
6.2.1 Primary map



X Index: 200

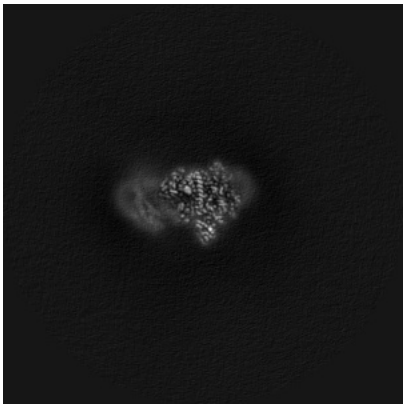


Y Index: 200

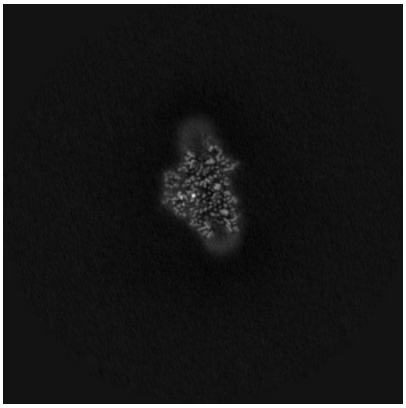


Z Index: 200

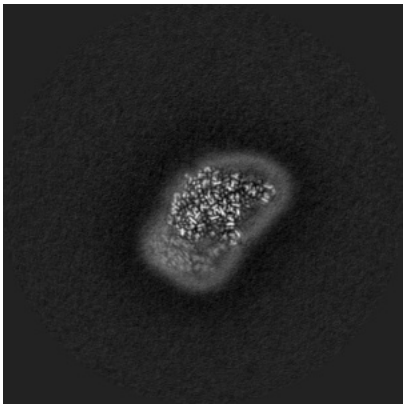
6.2.2 Raw map



X Index: 200



Y Index: 200

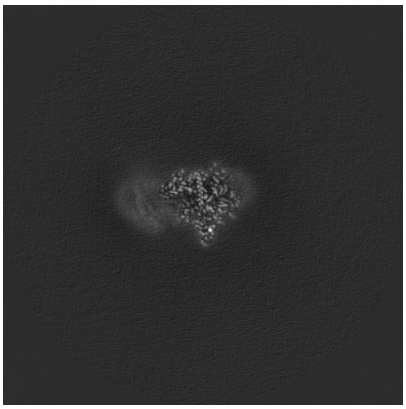


Z Index: 200

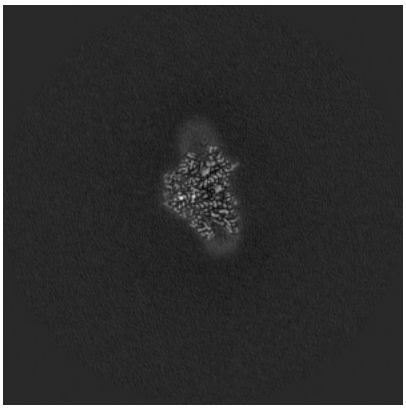
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

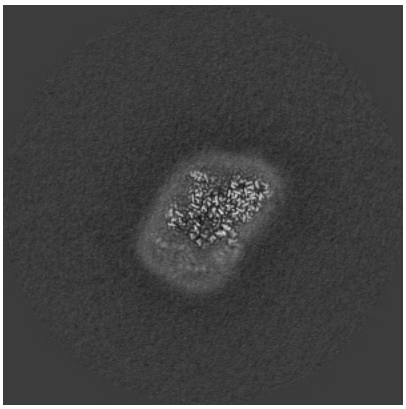
6.3.1 Primary map



X Index: 201

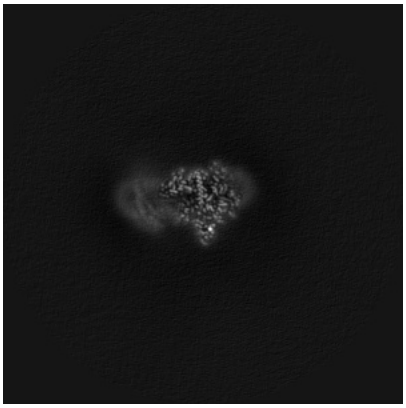


Y Index: 199

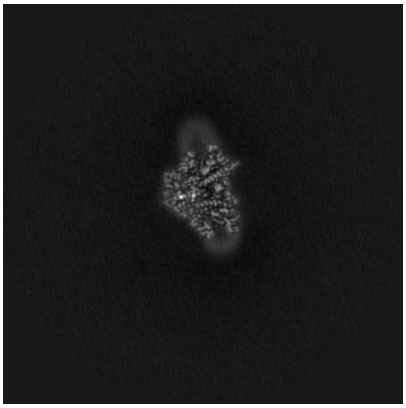


Z Index: 209

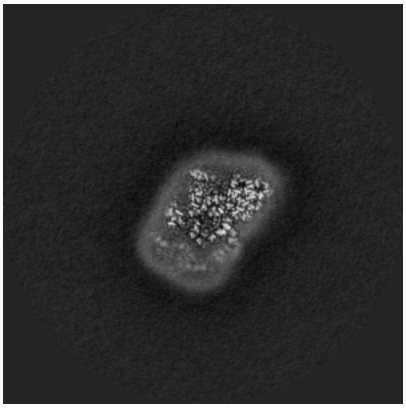
6.3.2 Raw map



X Index: 201



Y Index: 199

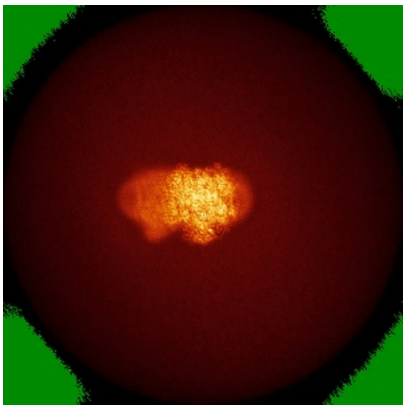


Z Index: 209

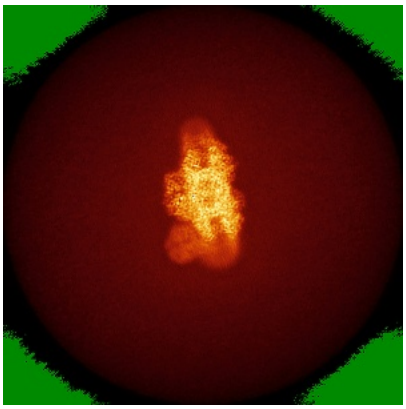
The images above show the largest variance slices of the map in three orthogonal directions.

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

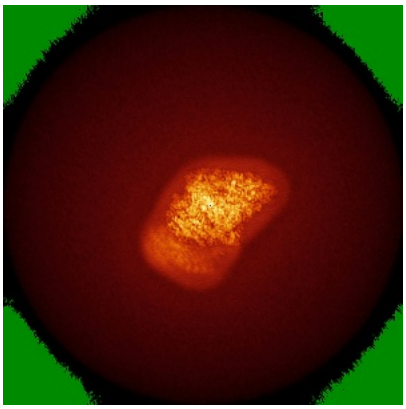
6.4.1 Primary map



X

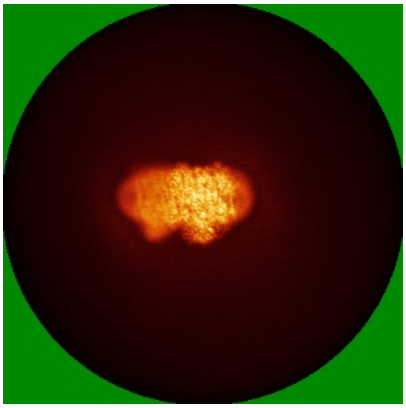


Y

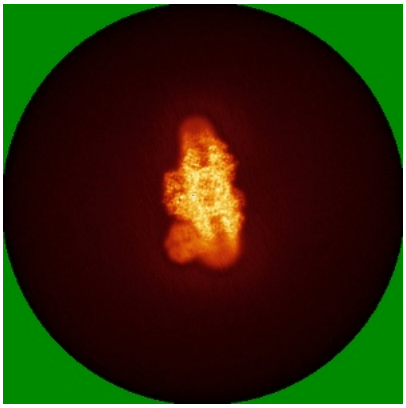


Z

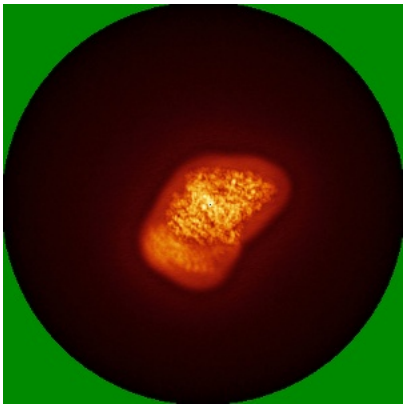
6.4.2 Raw map



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)

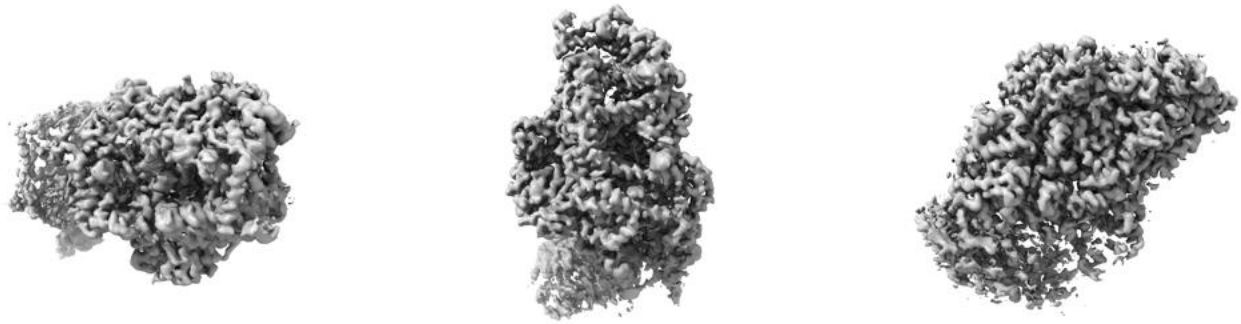
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.077. 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.

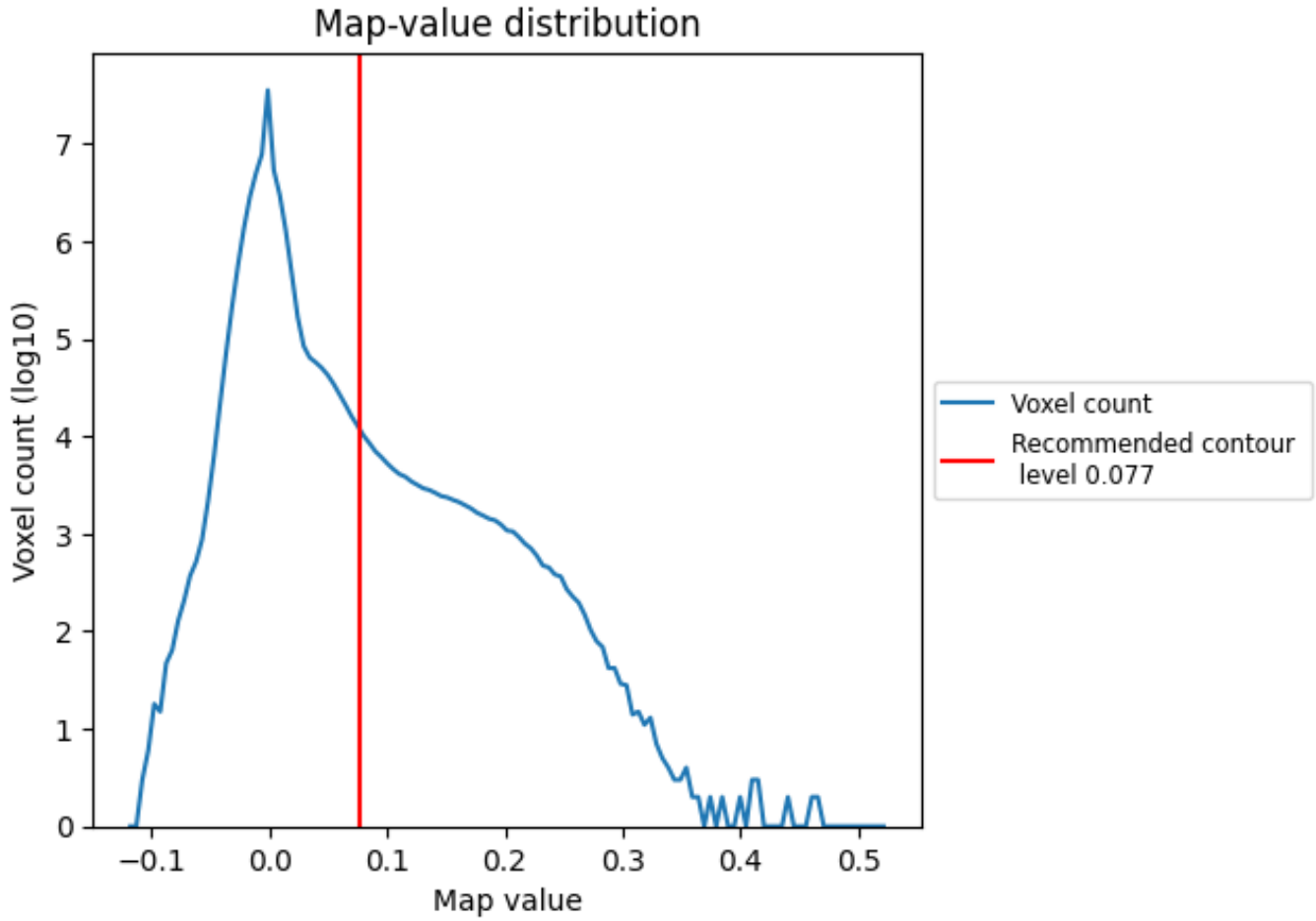
6.6 Mask visualisation (i)

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

7 Map analysis

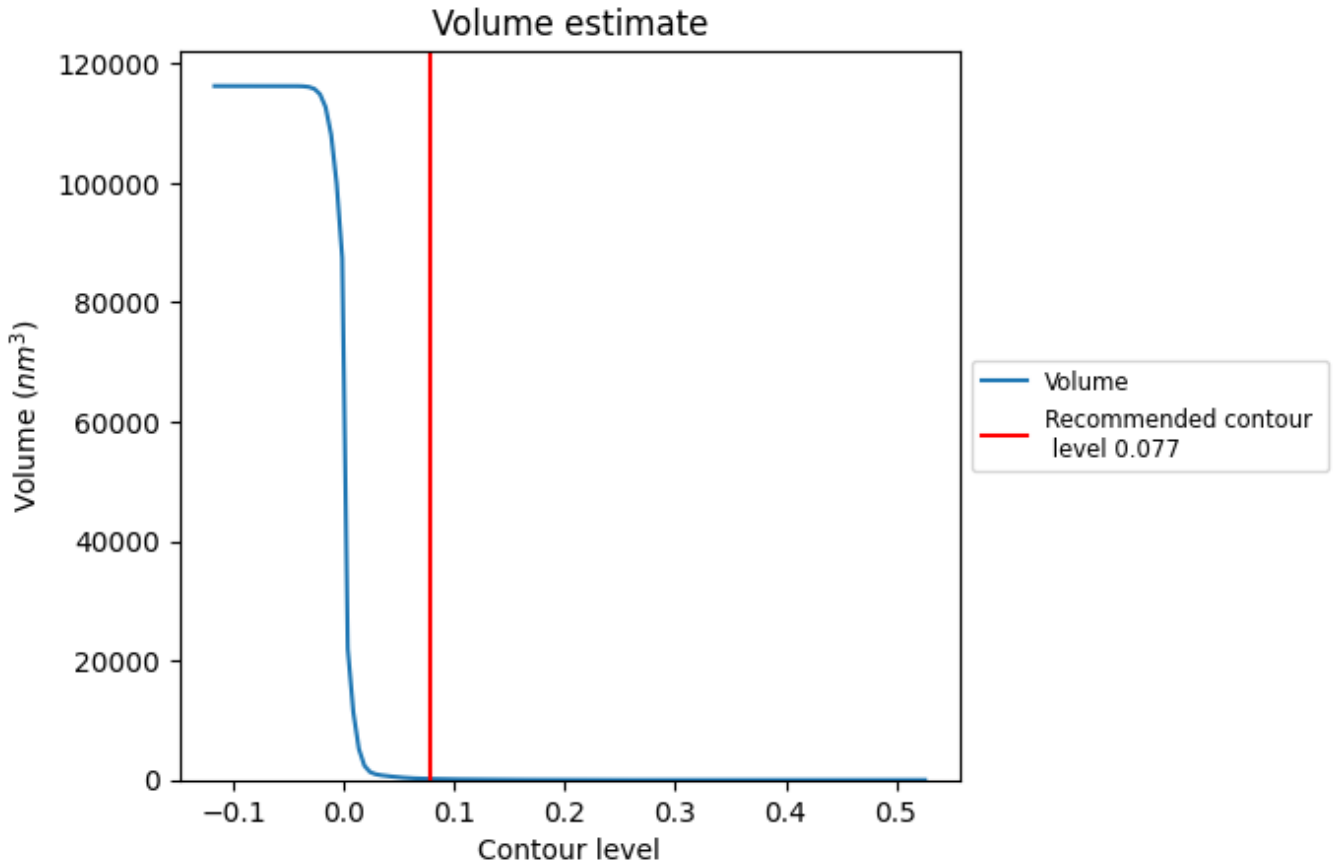
This section contains the results of statistical analysis of the map.

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.

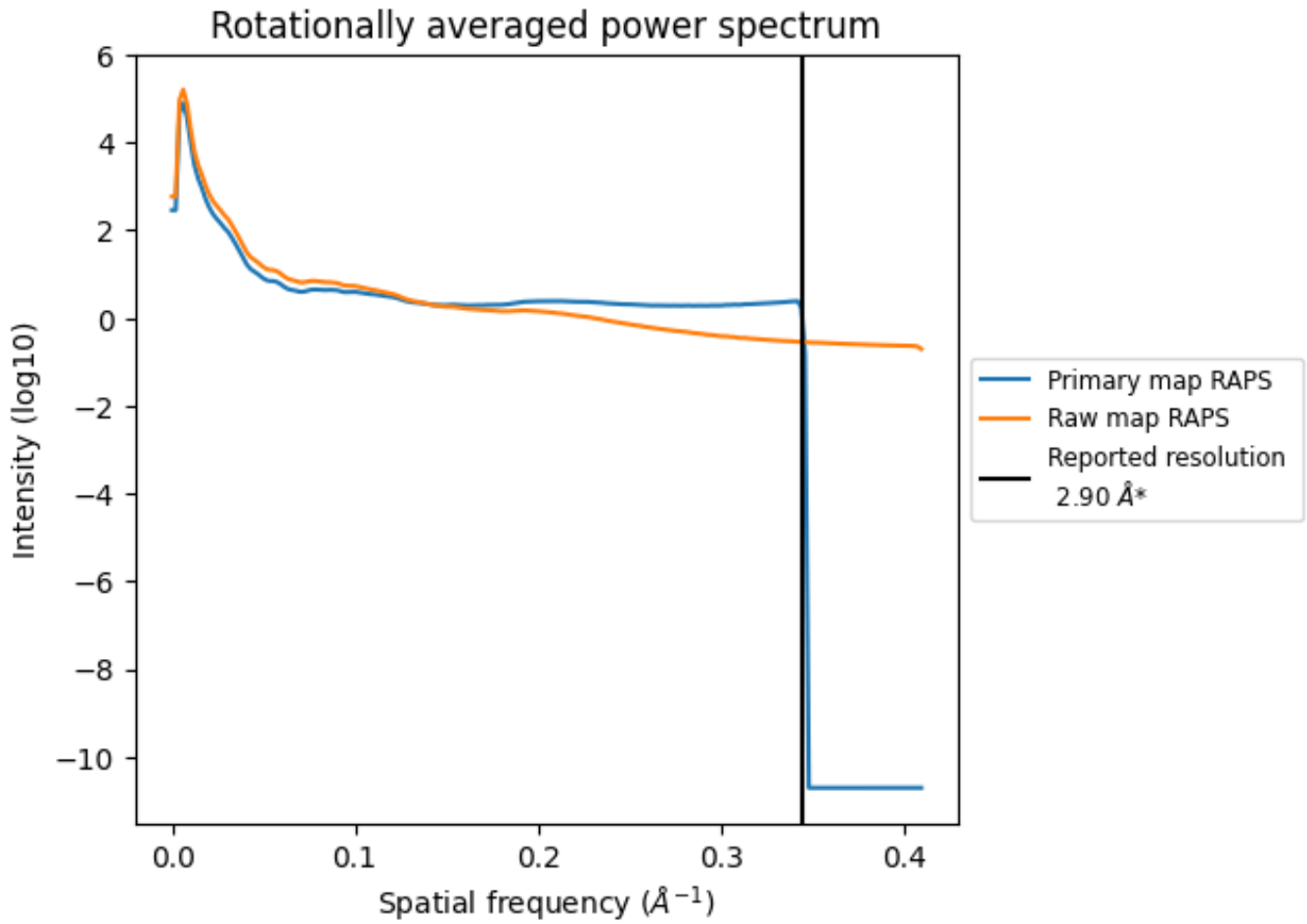
7.2 Volume estimate



The volume at the recommended contour level is 183 nm^3; this corresponds to an approximate mass of 165 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)

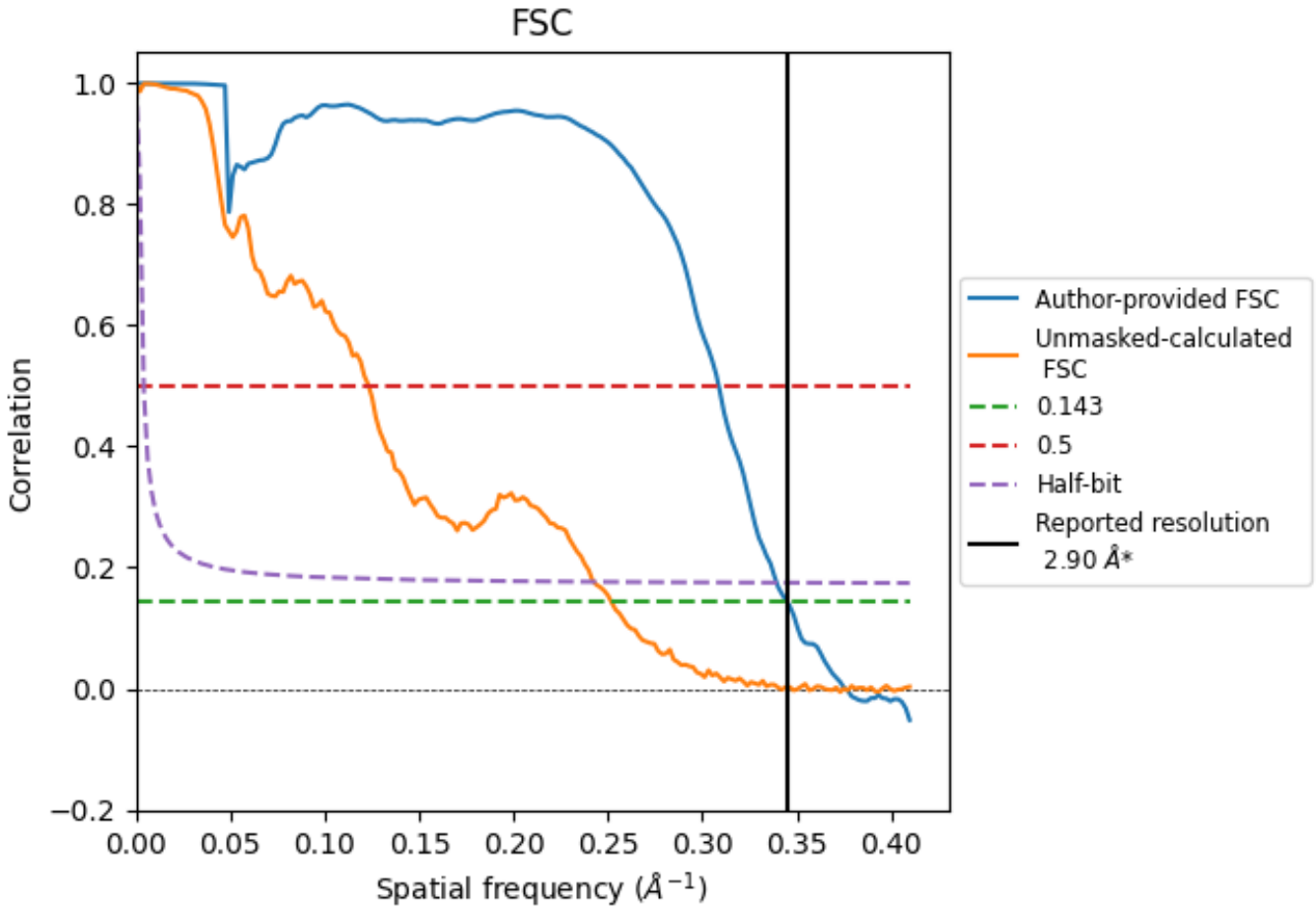


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

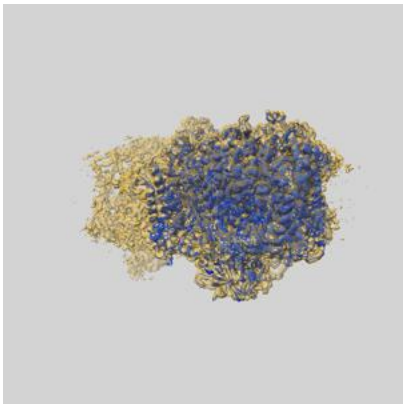
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.24	2.95
Unmasked-calculated*	3.97	8.12	4.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.97 differs from the reported value 2.9 by more than 10 %

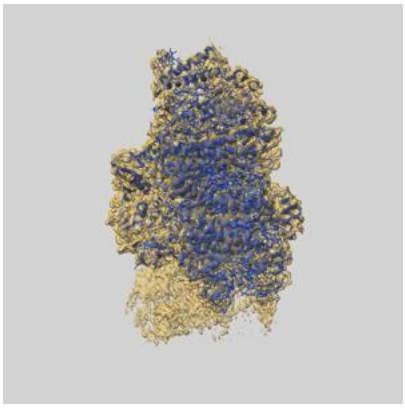
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15621 and PDB model 8ASP. Per-residue inclusion information can be found in section 3 on page 19.

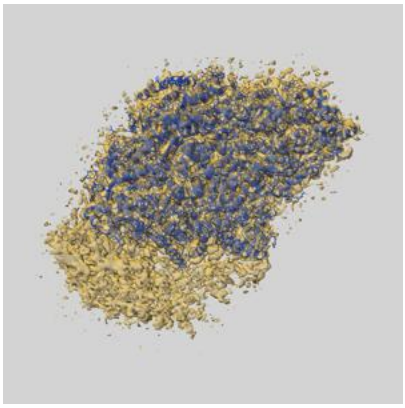
9.1 Map-model overlay



X



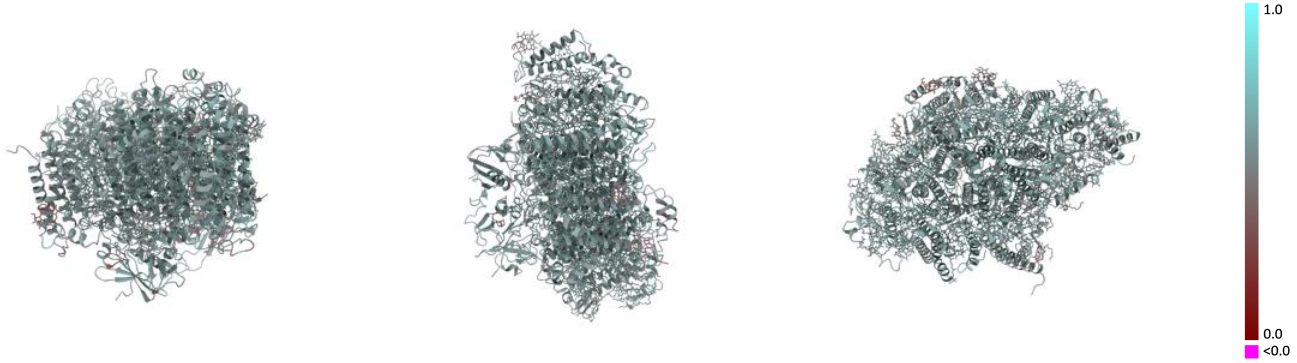
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.077 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.

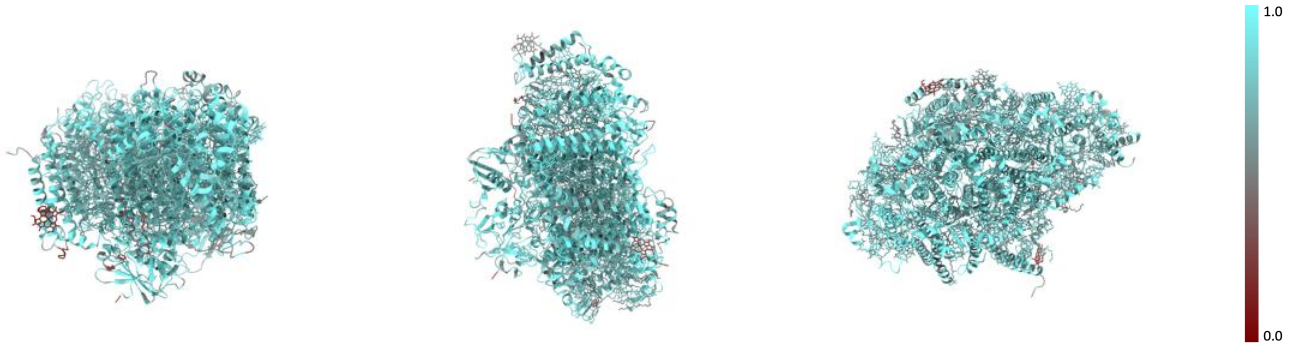
9.2 Q-score mapped to coordinate model (i)



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.

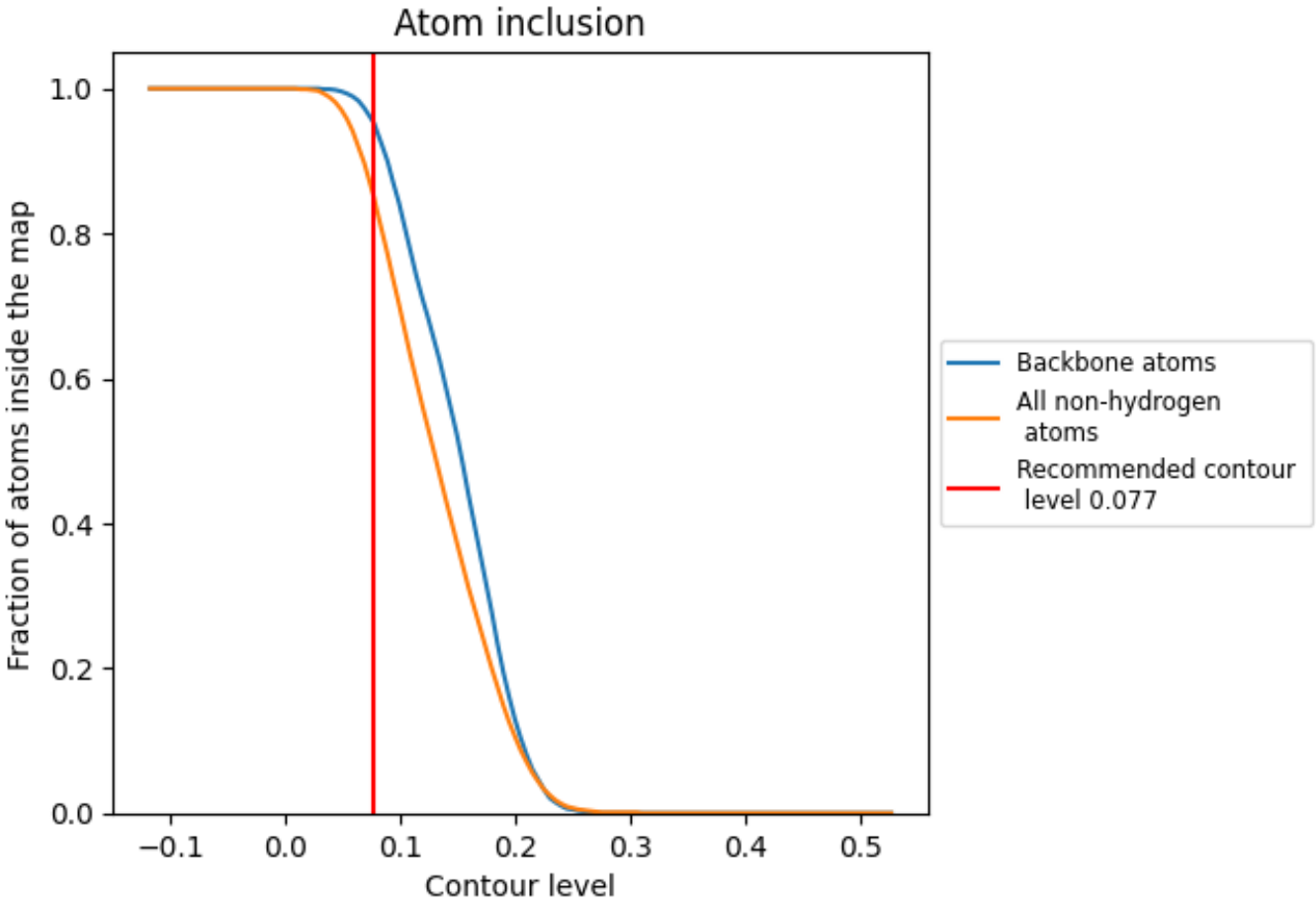
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.077).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 85% 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 (0.077) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8490	0.5710
a	0.8670	0.5810
b	0.8770	0.5800
c	0.9450	0.5740
d	0.8630	0.5670
e	0.8160	0.5560
f	0.7640	0.5490
i	0.8350	0.5750
j	0.6760	0.5200
k	0.7140	0.5370
l	0.7420	0.5220
m	0.7970	0.5590

