Full wwPDB EM Validation Report ⓘ

Sep 9, 2026 – 03:32 pm BST

PDB ID	:	6TRD / pdb_00006trd
EMDB ID	:	EMD-10559
Title	:	Cryo- EM structure of the Thermosynechococcus elongatus photosystem I in the presence of cytochrome c6
Authors	:	Koelsch, A.; Radon, C.; Baumert, A.; Buerger, J.; Mielke, T.; Lisdat, F.; Zouni, A.; Wendler, P.
Deposited on	:	2019-12-18
Resolution	:	3.16 Å(reported)
Based on initial model	:	1JB0

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:

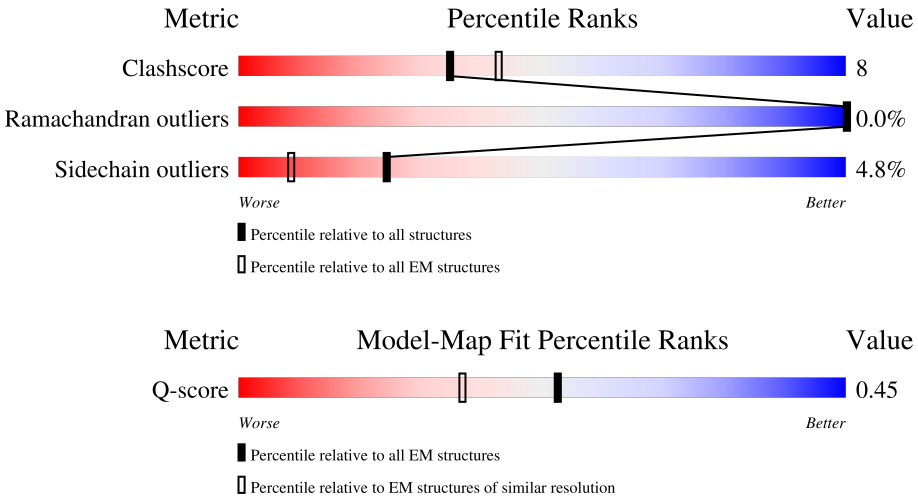
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.16 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.



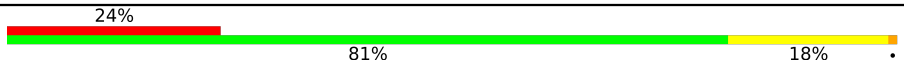
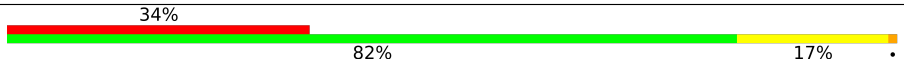
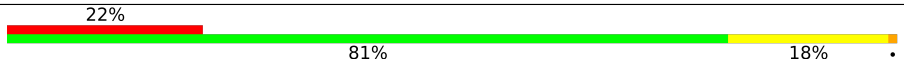
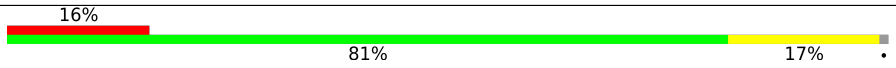
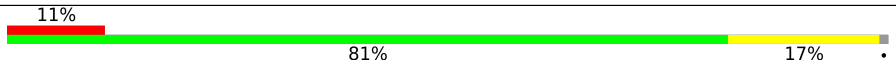
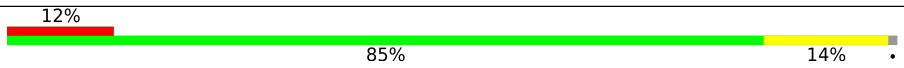
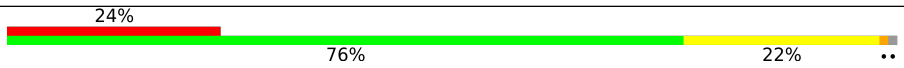
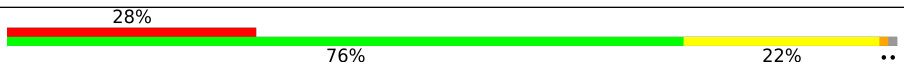
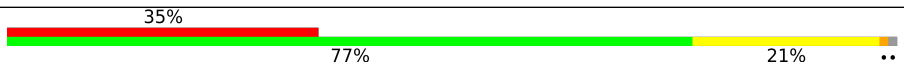
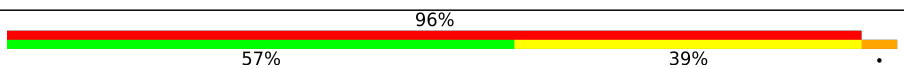
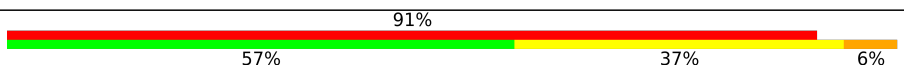
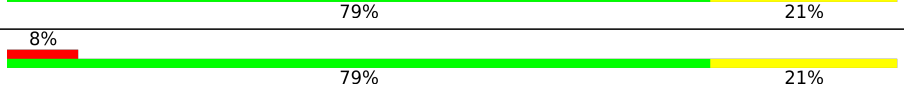
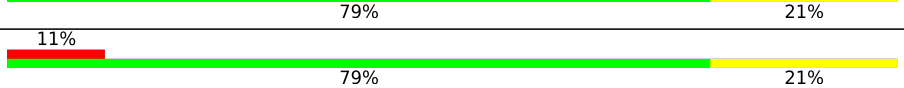
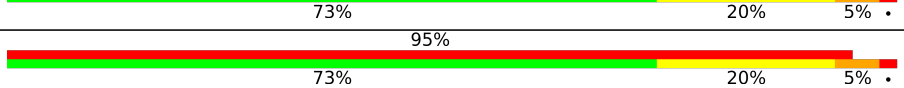
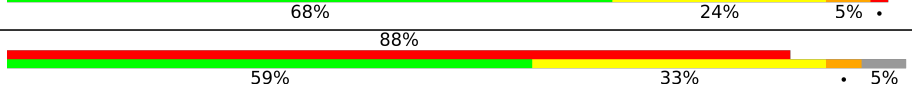
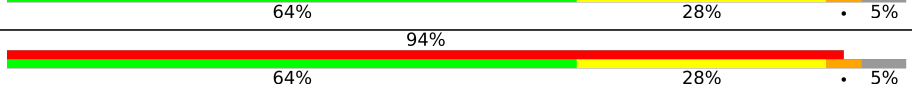
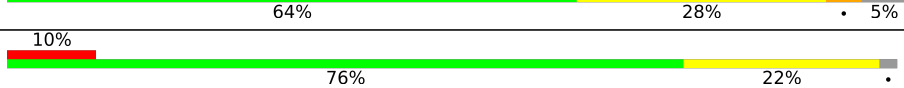
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14474 (2.66 - 3.66)

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	1	755	27% 76% 22%
1	A	755	33% 76% 21%
1	a	755	36% 76% 21%

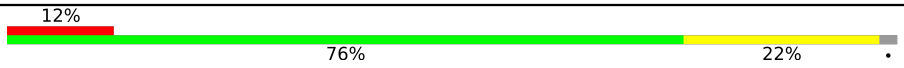
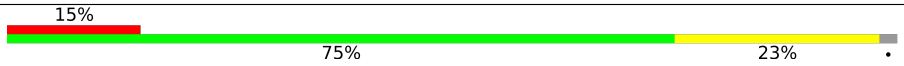
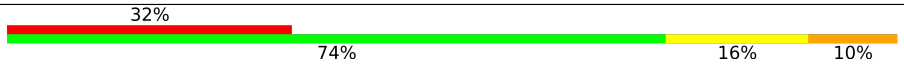
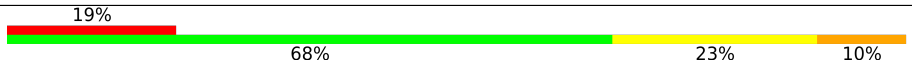
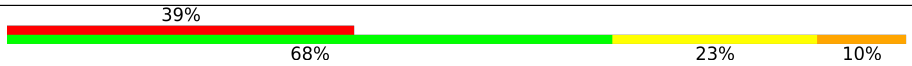
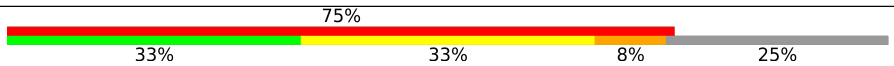
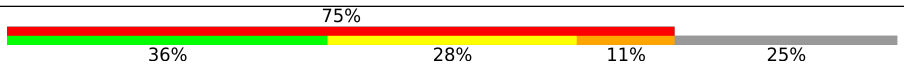
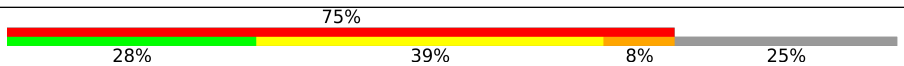
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Mol	Chain	Length	Quality of chain
2	2	741	
2	B	741	
2	b	741	
3	3	81	
3	C	81	
3	c	81	
4	4	139	
4	D	139	
4	d	139	
5	5	76	
5	E	76	
5	e	76	
6	6	141	
6	F	141	
6	f	141	
7	7	38	
7	I	38	
7	i	38	
8	8	41	
8	J	41	
8	j	41	
9	9	83	
9	K	83	
9	k	83	
10	0	155	

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Mol	Chain	Length	Quality of chain
10	L	155	
10	l	155	
11	M	31	
11	m	31	
11	y	31	
12	X	36	
12	x	36	
12	z	36	

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 74991 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
1	A	746	Total	C	N	O	S	0	0
			5826	3823	995	982	26		
1	a	746	Total	C	N	O	S	0	0
			5826	3823	995	982	26		
1	1	746	Total	C	N	O	S	0	0
			5826	3823	995	982	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	740	Total	C	N	O	S	0	0
			5894	3878	988	1007	21		
2	b	740	Total	C	N	O	S	0	0
			5894	3878	988	1007	21		
2	2	740	Total	C	N	O	S	0	0
			5894	3878	988	1007	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
3	c	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
3	3	80	Total	C	N	O	S	0	0
			598	367	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		
4	4	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	70	Total	C	N	O	0	0
			546	347	94	105		
5	e	70	Total	C	N	O	0	0
			546	347	94	105		
5	5	70	Total	C	N	O	0	0
			546	347	94	105		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		
6	f	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		
6	6	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	38	Total	C	N	O	S	0	0
			303	209	40	49	5		
7	i	38	Total	C	N	O	S	0	0
			303	209	40	49	5		
7	7	38	Total	C	N	O	S	0	0
			303	209	40	49	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	41	Total	C	N	O	S	0	0
			340	232	51	55	2		
8	j	41	Total	C	N	O	S	0	0
			340	232	51	55	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	41	Total	C	N	O	S	0	0
			340	232	51	55	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	79	Total	C	N	O	S	0	0
			571	377	92	101	1		
9	k	79	Total	C	N	O	S	0	0
			571	377	92	101	1		
9	9	79	Total	C	N	O	S	0	0
			571	377	92	101	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	152	Total	C	N	O	S	0	0
			1124	738	180	202	4		
10	l	152	Total	C	N	O	S	0	0
			1124	738	180	202	4		
10	0	152	Total	C	N	O	S	0	0
			1124	738	180	202	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	143	LEU	SER	conflict	UNP Q8DGB4
l	143	LEU	SER	conflict	UNP Q8DGB4
0	143	LEU	SER	conflict	UNP Q8DGB4

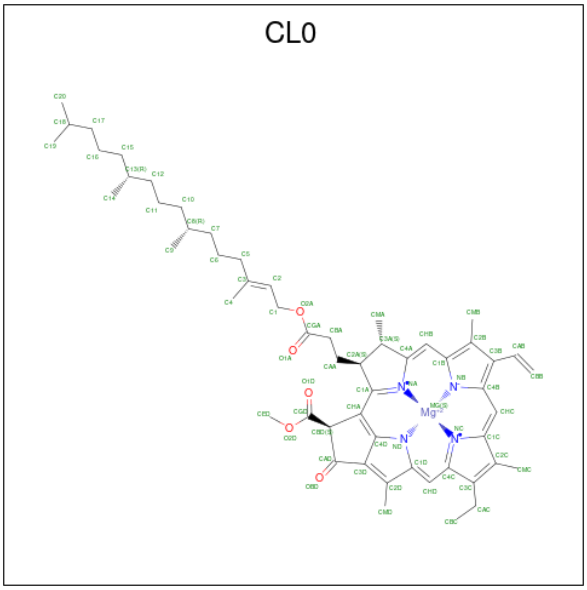
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	m	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	y	31	Total	C	N	O	S	0	0
			241	161	36	43	1		

- Molecule 12 is a protein called Photosystem I 4.8K protein.

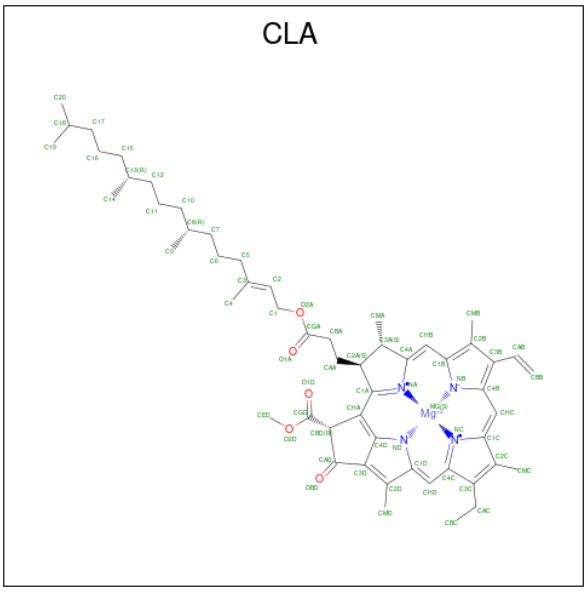
Mol	Chain	Residues	Atoms				AltConf	Trace
12	X	27	Total 228	C 163	N 33	O 32	0	0
12	x	27	Total 228	C 163	N 33	O 32	0	0
12	z	27	Total 228	C 163	N 33	O 32	0	0

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	F	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	F	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	J	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
14	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	K	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	M	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
14	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			58	48	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	f	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	j	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
14	k	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	x	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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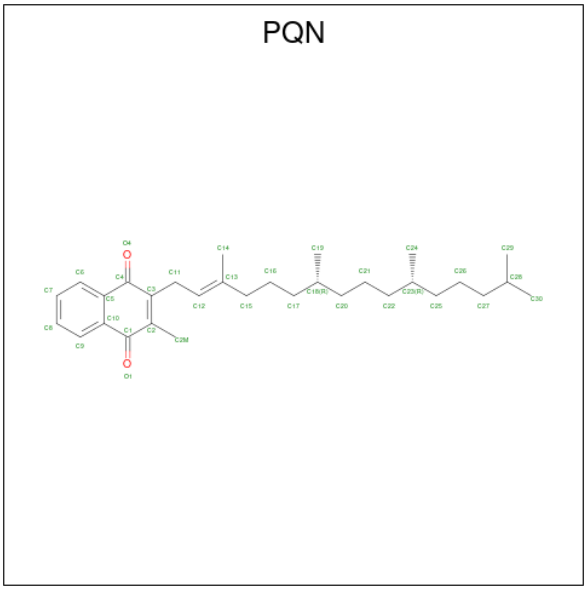
Mol	Chain	Residues	Atoms					AltConf
14	2	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	6	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	8	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
14	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	9	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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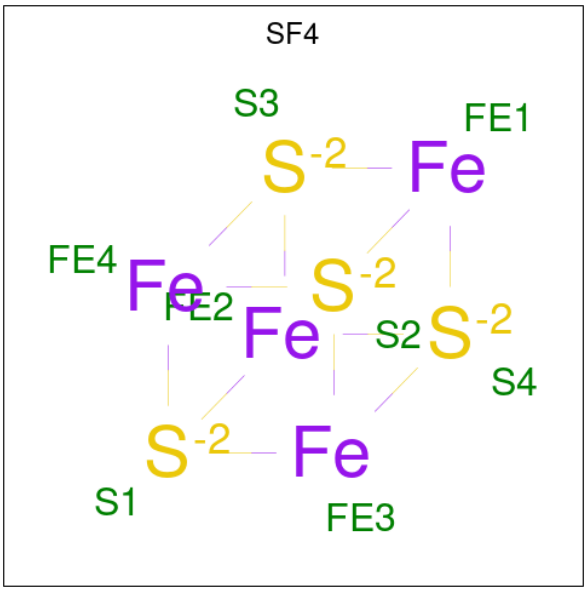
Mol	Chain	Residues	Atoms					AltConf
14	z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



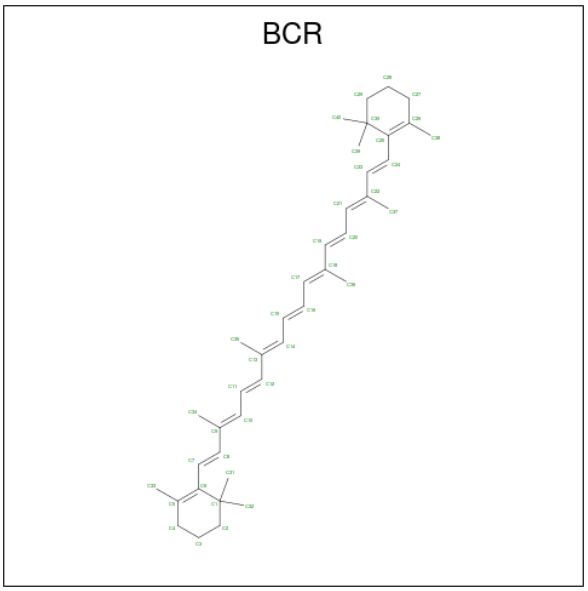
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	C	O	0
			33	31	2	
15	B	1	Total	C	O	0
			33	31	2	
15	a	1	Total	C	O	0
			33	31	2	
15	b	1	Total	C	O	0
			33	31	2	
15	1	1	Total	C	O	0
			33	31	2	
15	2	1	Total	C	O	0
			33	31	2	

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
16	A	1	Total Fe S 8 4 4	0
16	C	1	Total Fe S 8 4 4	0
16	C	1	Total Fe S 8 4 4	0
16	a	1	Total Fe S 8 4 4	0
16	c	1	Total Fe S 8 4 4	0
16	c	1	Total Fe S 8 4 4	0
16	1	1	Total Fe S 8 4 4	0
16	3	1	Total Fe S 8 4 4	0
16	3	1	Total Fe S 8 4 4	0

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 25 25	0
17	A	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	F	1	Total C 40 40	0
17	F	1	Total C 40 40	0
17	I	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	K	1	Total C 40 40	0
17	K	1	Total C 25 25	0
17	L	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	M	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 25 25	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0

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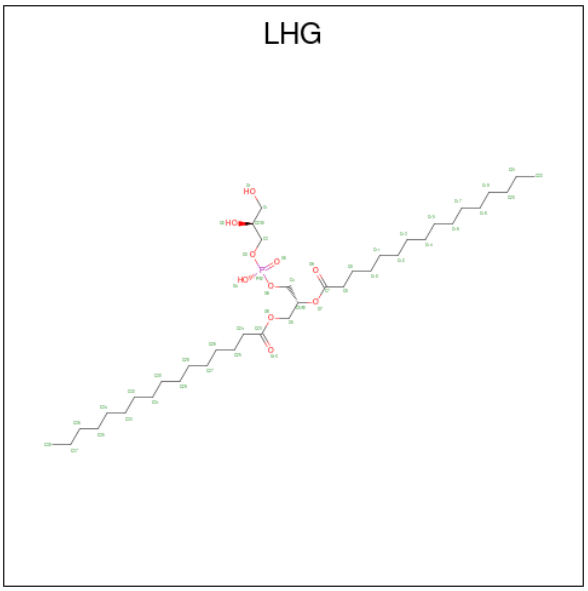
Mol	Chain	Residues	Atoms	AltConf
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	f	1	Total C 40 40	0
17	f	1	Total C 40 40	0
17	i	1	Total C 40 40	0
17	j	1	Total C 40 40	0
17	j	1	Total C 40 40	0
17	k	1	Total C 40 40	0
17	k	1	Total C 25 25	0
17	l	1	Total C 40 40	0
17	l	1	Total C 40 40	0
17	m	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 25 25	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	6	1	Total C 40 40	0
17	6	1	Total C 40 40	0
17	7	1	Total C 40 40	0
17	8	1	Total C 40 40	0
17	8	1	Total C 40 40	0
17	8	1	Total C 40 40	0
17	9	1	Total C 40 40	0
17	9	1	Total C 25 25	0
17	0	1	Total C 40 40	0
17	0	1	Total C 40 40	0
17	0	1	Total C 40 40	0
17	0	1	Total C 40 40	0
17	y	1	Total C 40 40	0

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	O	P	0
			49	38	10	1	
18	A	1	Total	C	O	P	0
			41	30	10	1	
18	B	1	Total	C	O	P	0
			49	38	10	1	
18	L	1	Total	C	O	P	0
			39	28	10	1	
18	M	1	Total	C	O	P	0
			49	38	10	1	
18	a	1	Total	C	O	P	0
			49	38	10	1	
18	a	1	Total	C	O	P	0
			41	30	10	1	
18	b	1	Total	C	O	P	0
			49	38	10	1	
18	l	1	Total	C	O	P	0
			39	28	10	1	
18	m	1	Total	C	O	P	0
			49	38	10	1	
18	1	1	Total	C	O	P	0
			49	38	10	1	
18	1	1	Total	C	O	P	0
			41	30	10	1	
18	0	1	Total	C	O	P	0
			39	28	10	1	
18	y	1	Total	C	O	P	0
			49	38	10	1	

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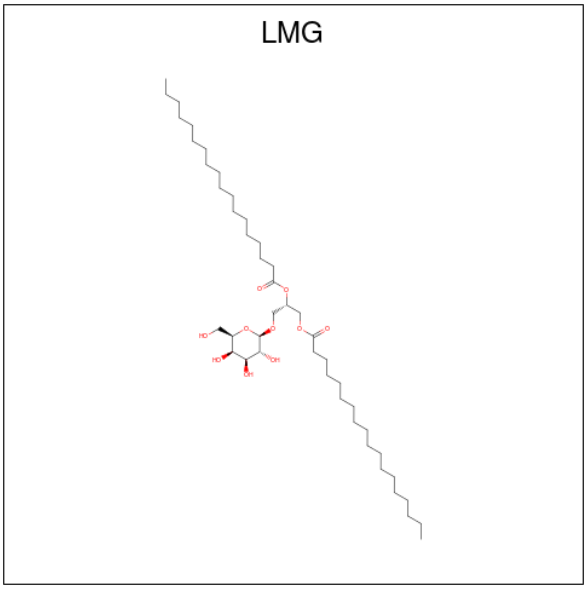
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Mol	Chain	Residues	Atoms				AltConf
18	z	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 19 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
19	B	1	Total	Ca	0
			1	1	
19	L	1	Total	Ca	0
			1	1	
19	b	1	Total	Ca	0
			1	1	
19	l	1	Total	Ca	0
			1	1	
19	2	1	Total	Ca	0
			1	1	
19	0	1	Total	Ca	0
			1	1	

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
20	B	1	Total	C	O	0
			55	45	10	
20	b	1	Total	C	O	0
			55	45	10	

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Mol	Chain	Residues	Atoms	AltConf
20	2	1	Total C O 55 45 10	0

- Molecule 21 is water.

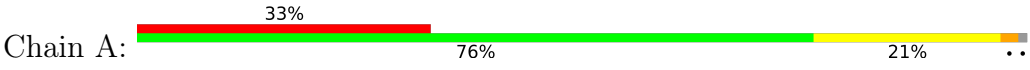
Mol	Chain	Residues	Atoms	AltConf
21	A	5	Total O 5 5	0
21	B	8	Total O 8 8	0
21	F	1	Total O 1 1	0
21	J	1	Total O 1 1	0
21	K	1	Total O 1 1	0
21	L	1	Total O 1 1	0
21	a	5	Total O 5 5	0
21	b	8	Total O 8 8	0
21	f	1	Total O 1 1	0
21	j	1	Total O 1 1	0
21	k	1	Total O 1 1	0
21	l	1	Total O 1 1	0
21	1	5	Total O 5 5	0
21	2	8	Total O 8 8	0
21	6	1	Total O 1 1	0
21	8	1	Total O 1 1	0
21	9	1	Total O 1 1	0
21	0	1	Total O 1 1	0

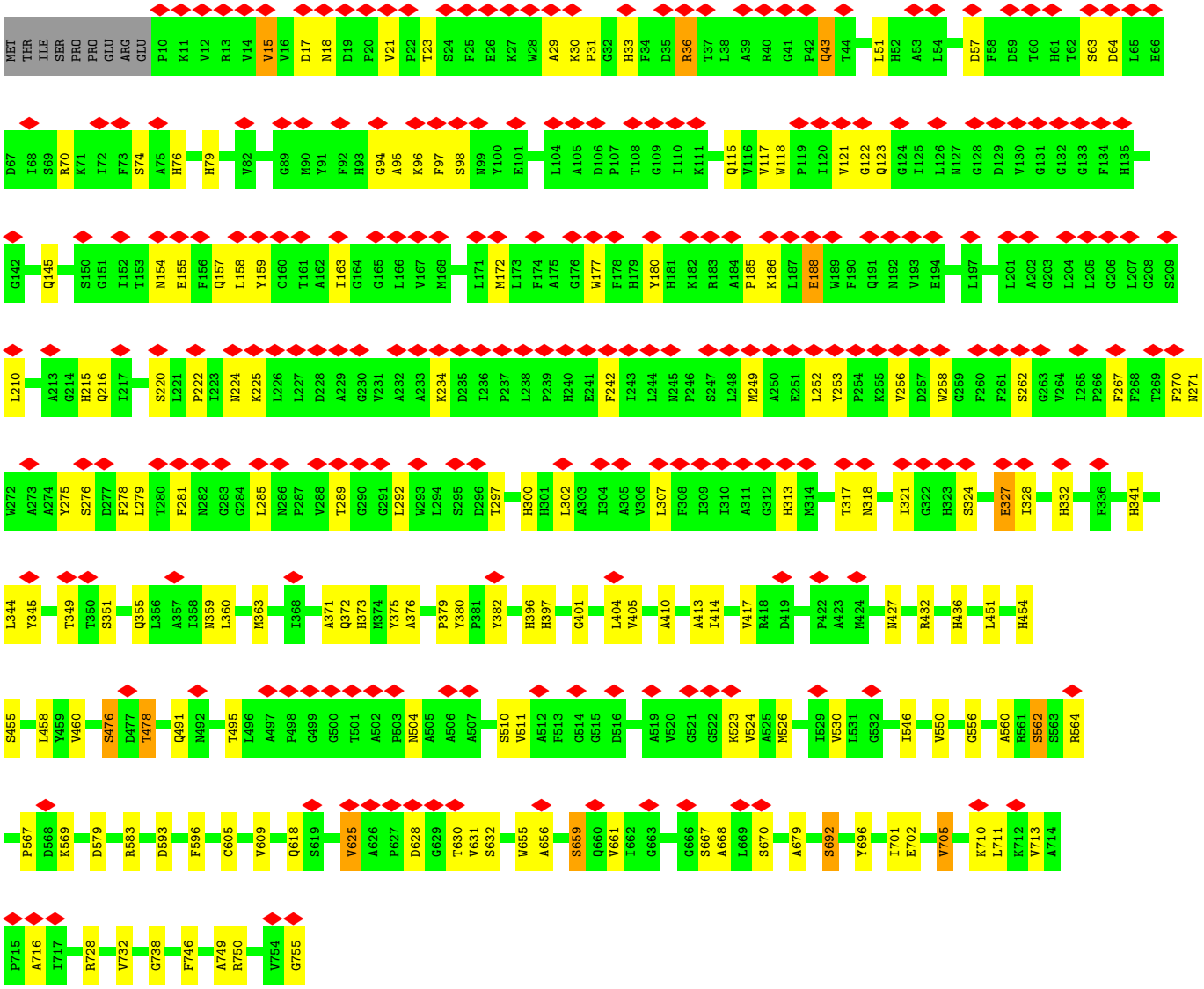
3 Residue-property plots (i)

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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

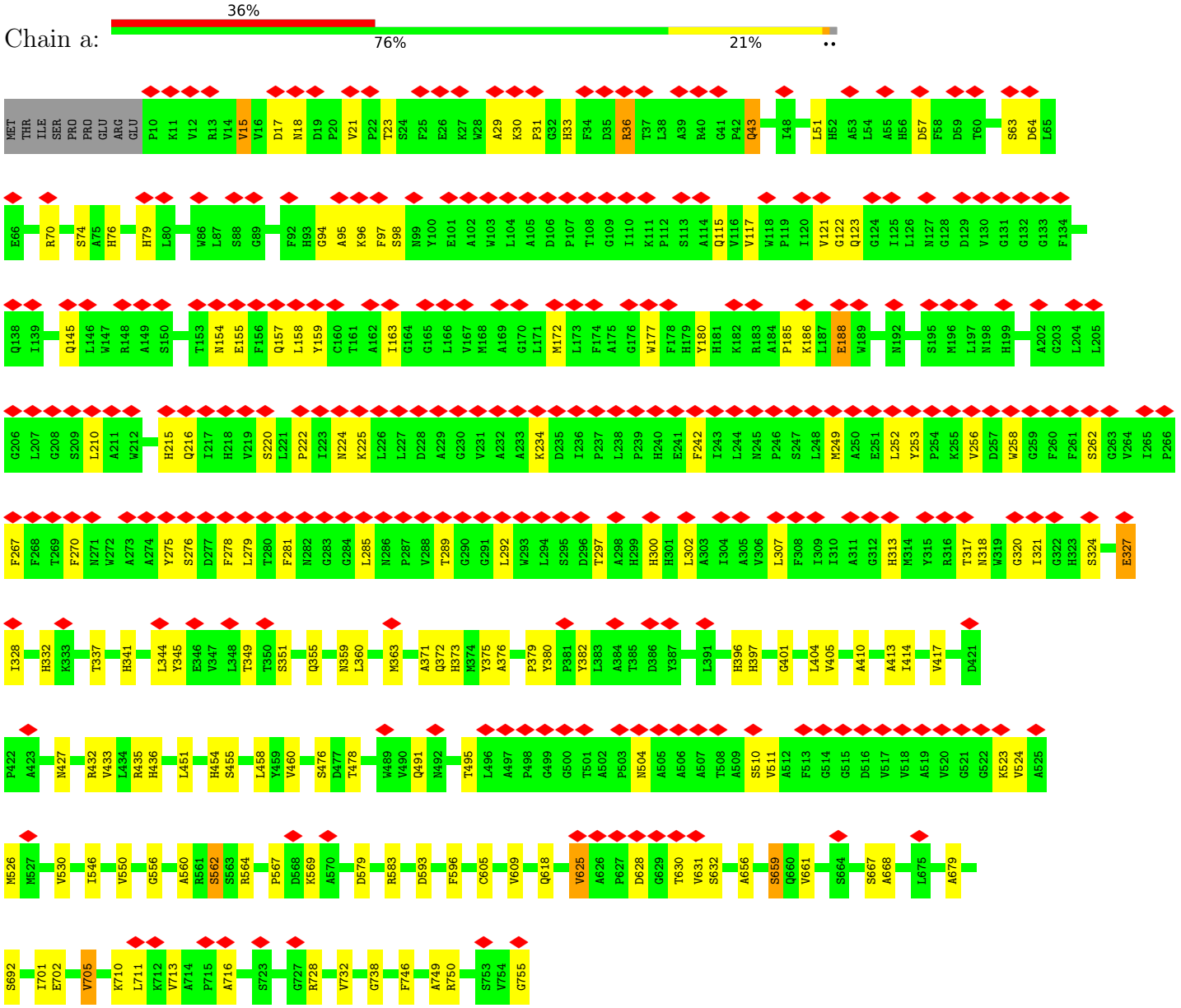
Chain A:





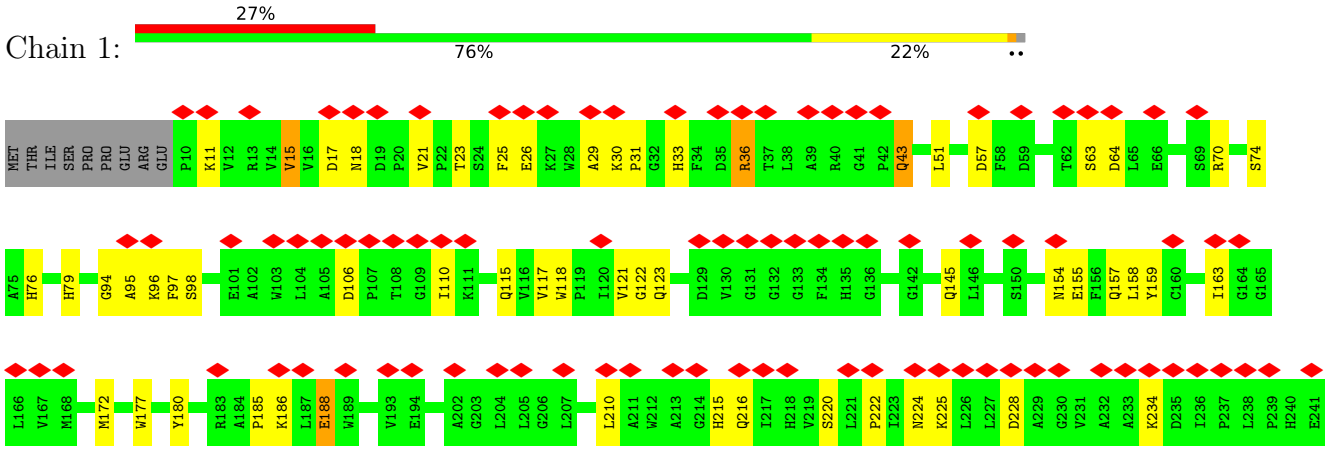
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

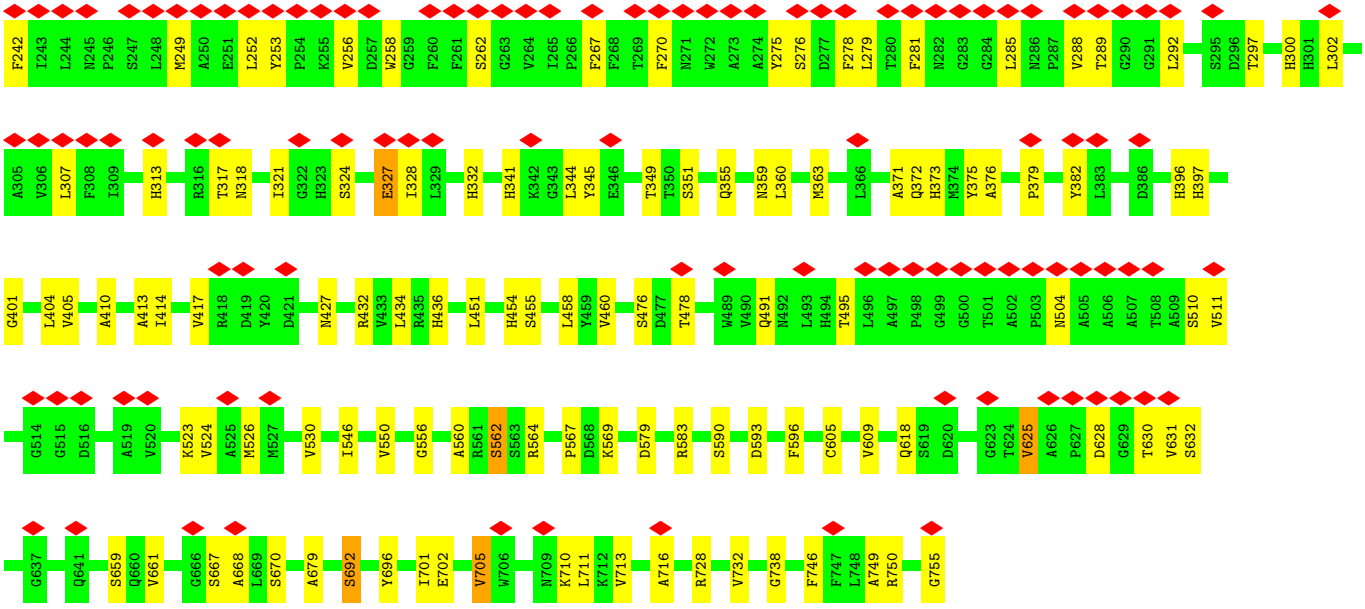
Chain a:



• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain 1:

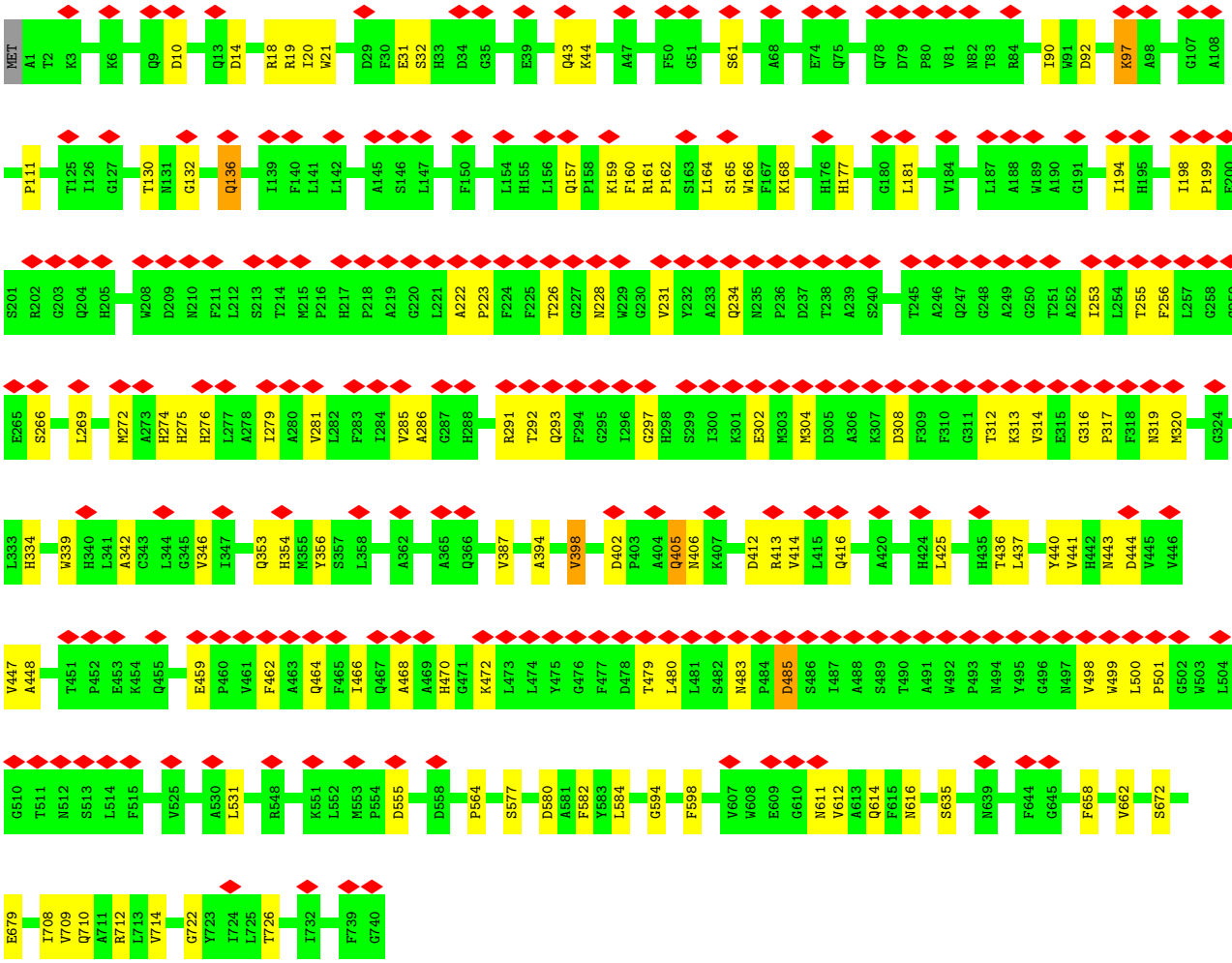




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

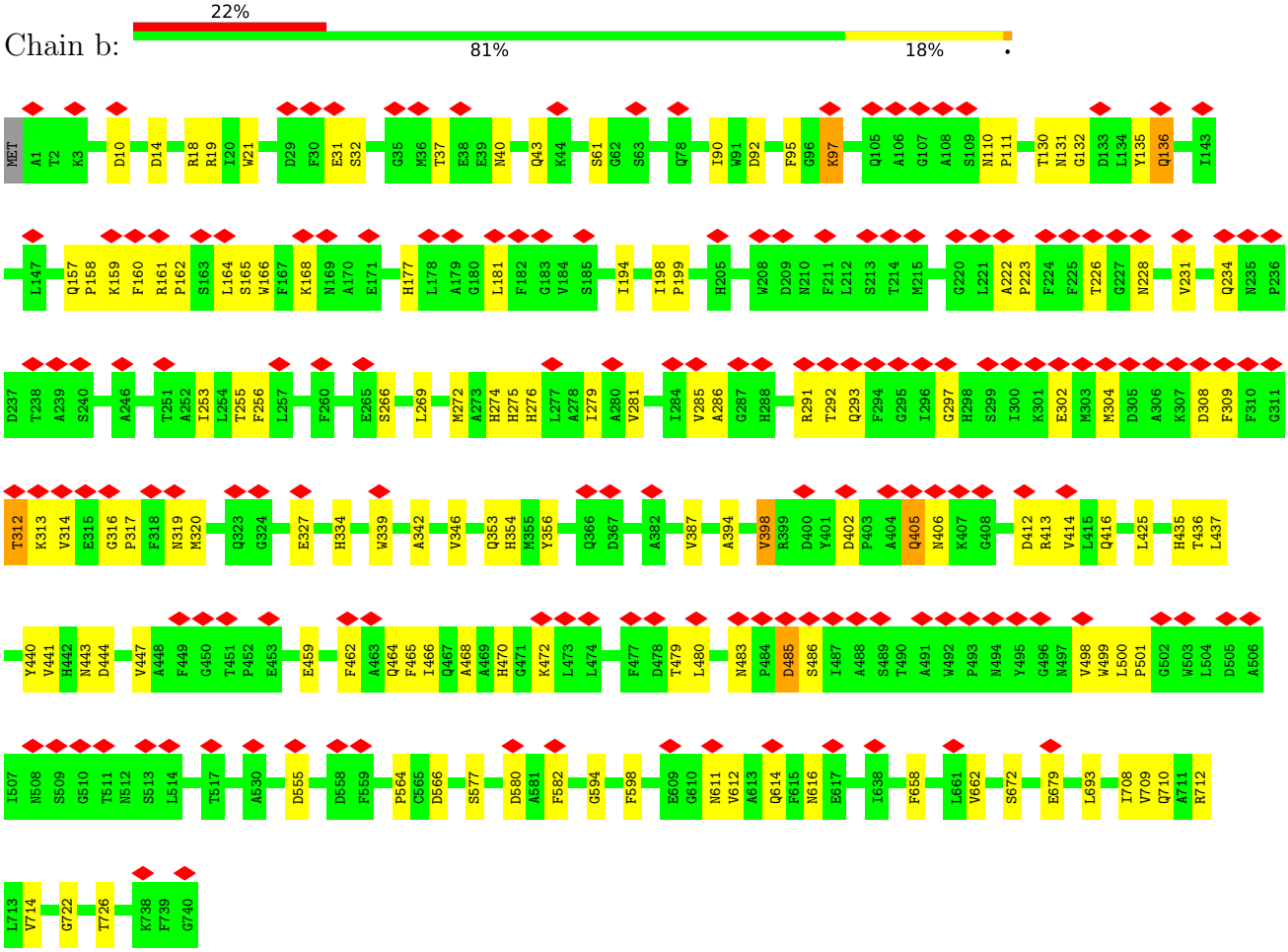
Chain B:





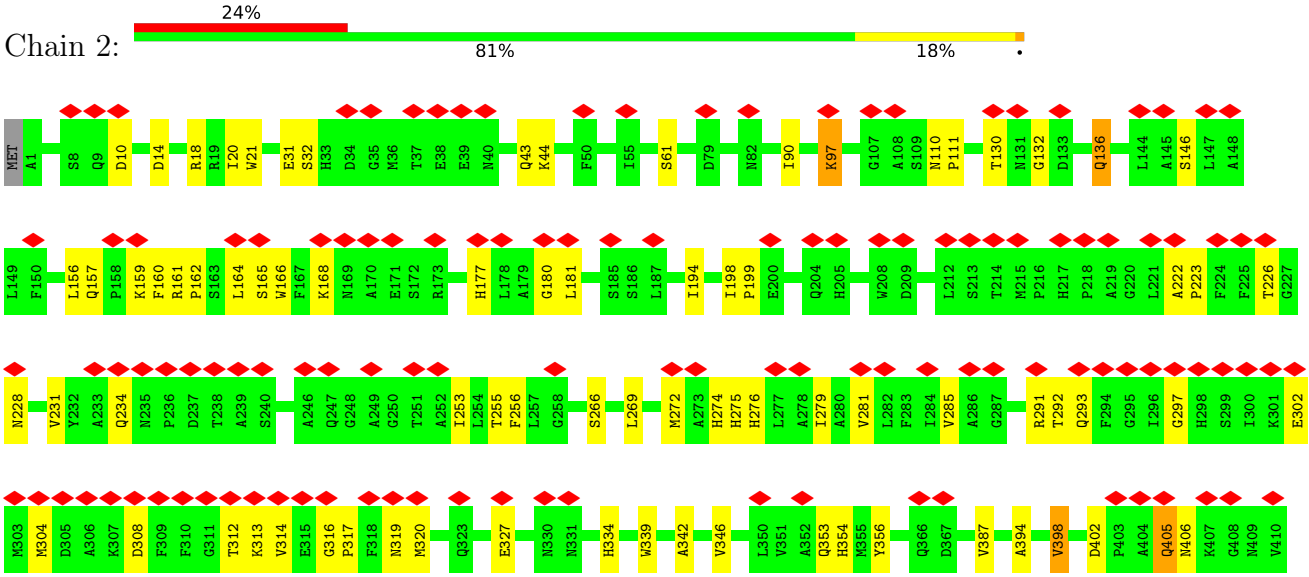
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

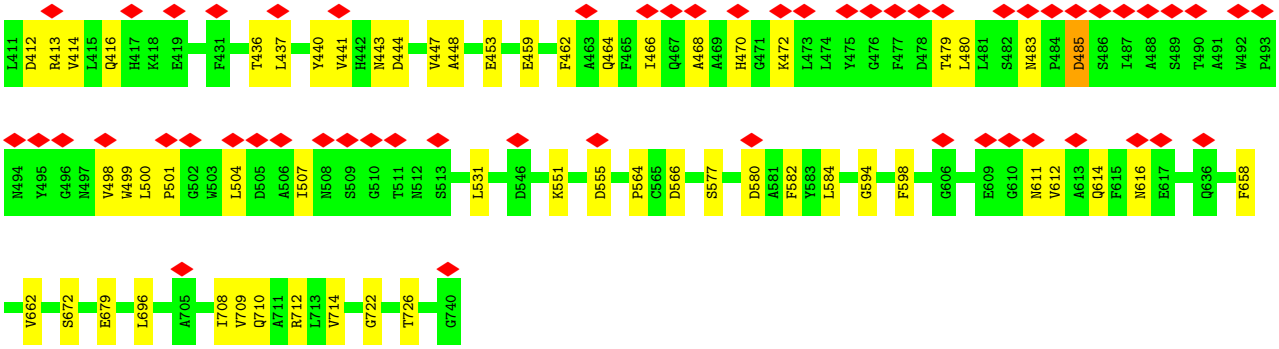
Chain b:



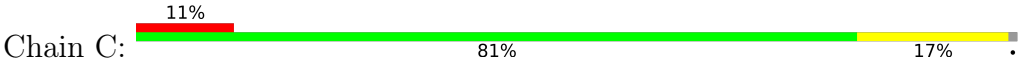
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

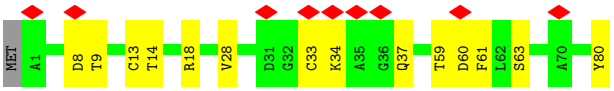
Chain 2:



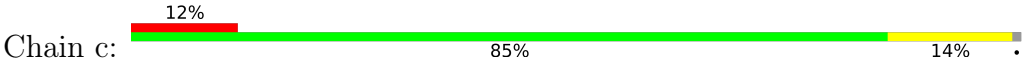


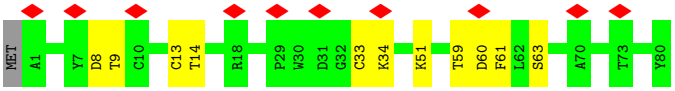
• Molecule 3: Photosystem I iron-sulfur center



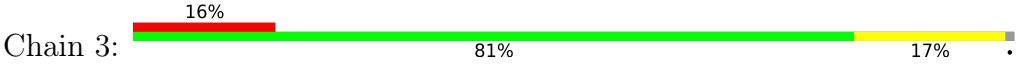


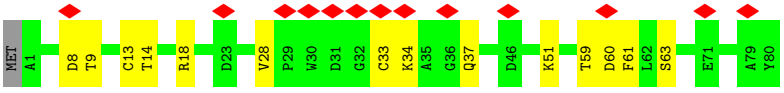
• Molecule 3: Photosystem I iron-sulfur center



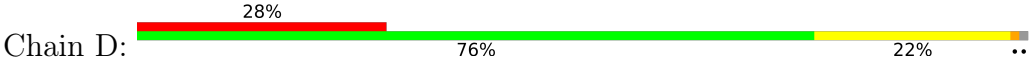


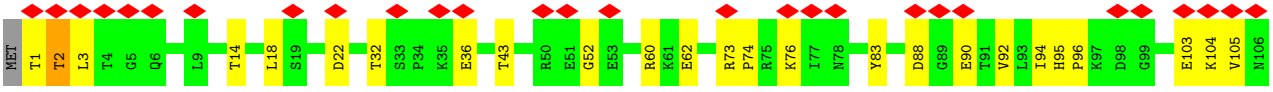
• Molecule 3: Photosystem I iron-sulfur center

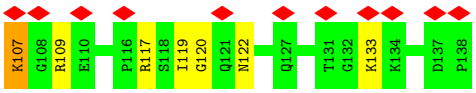




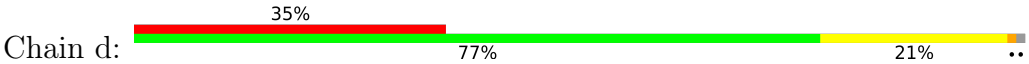
• Molecule 4: Photosystem I reaction center subunit II

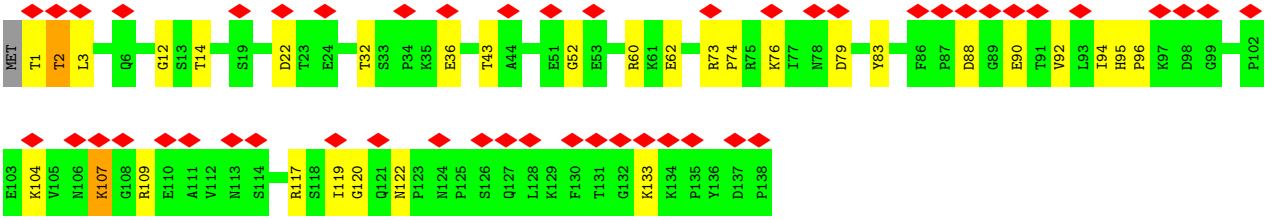






• Molecule 4: Photosystem I reaction center subunit II

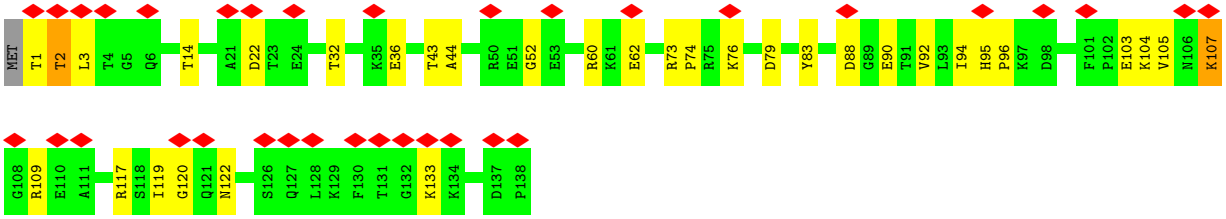




• Molecule 4: Photosystem I reaction center subunit II

Chain 4:

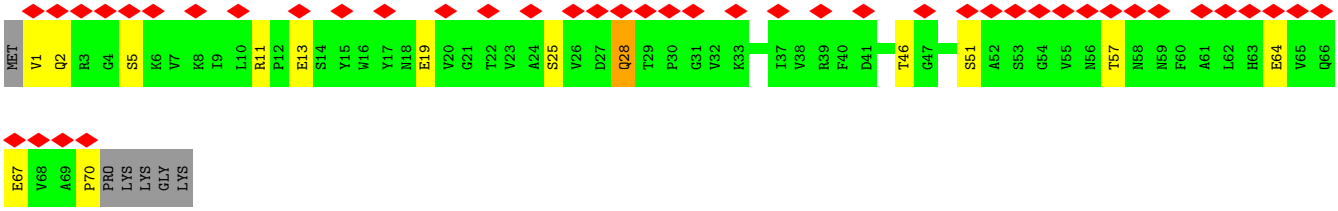




• Molecule 5: Photosystem I reaction center subunit IV

Chain E:

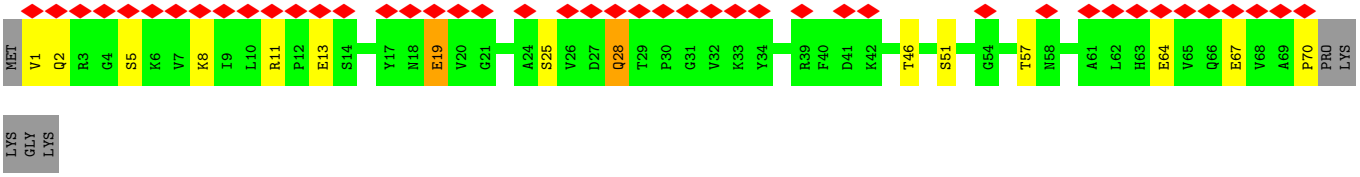




• Molecule 5: Photosystem I reaction center subunit IV

Chain e:

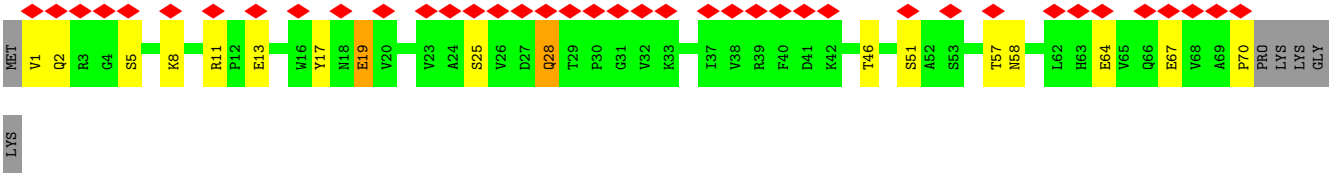




• Molecule 5: Photosystem I reaction center subunit IV

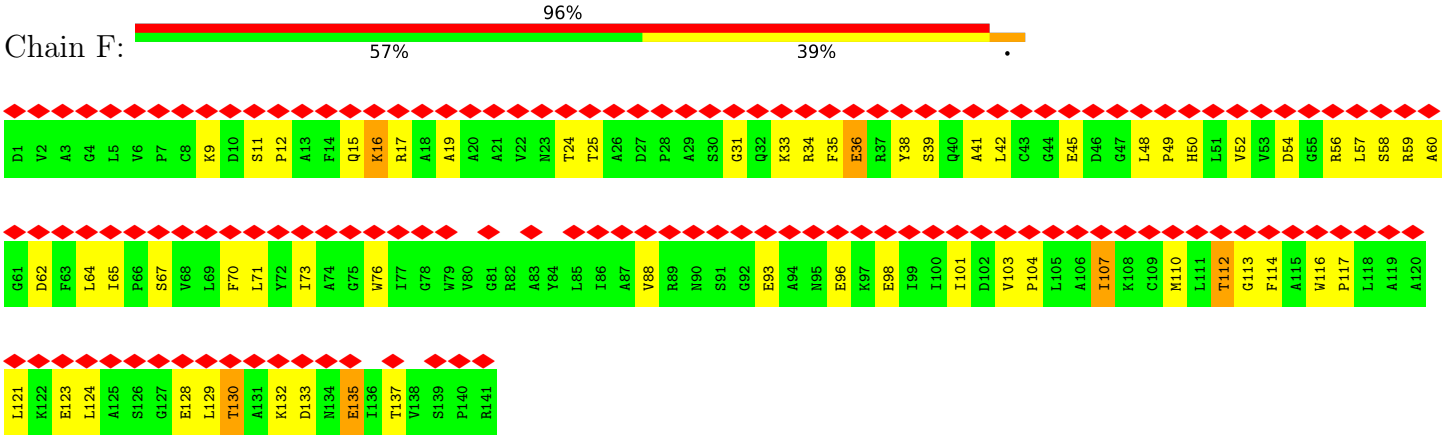
Chain 5:





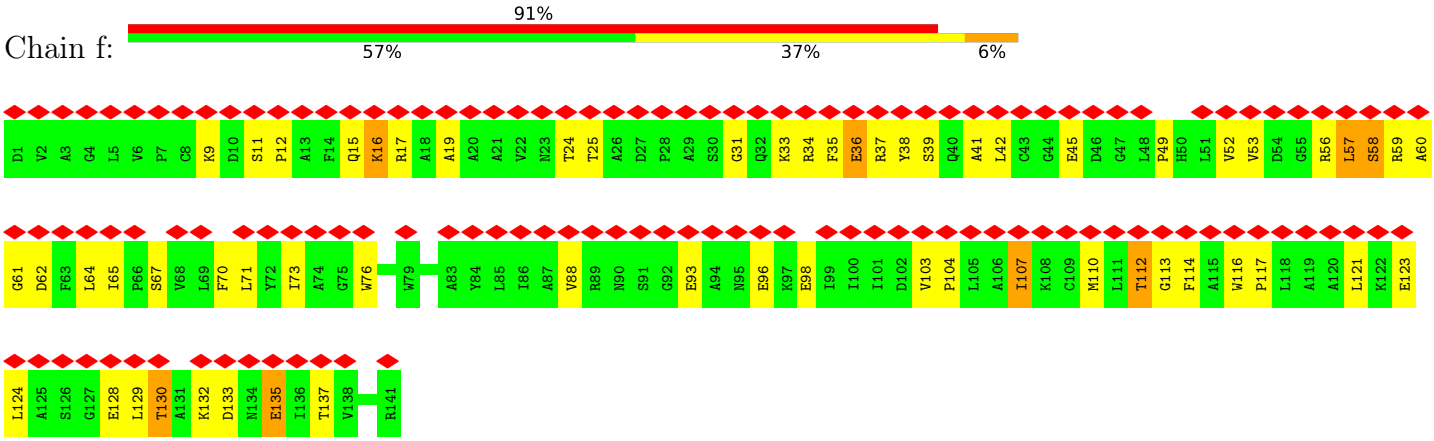
• Molecule 6: Photosystem I reaction center subunit III

Chain F:



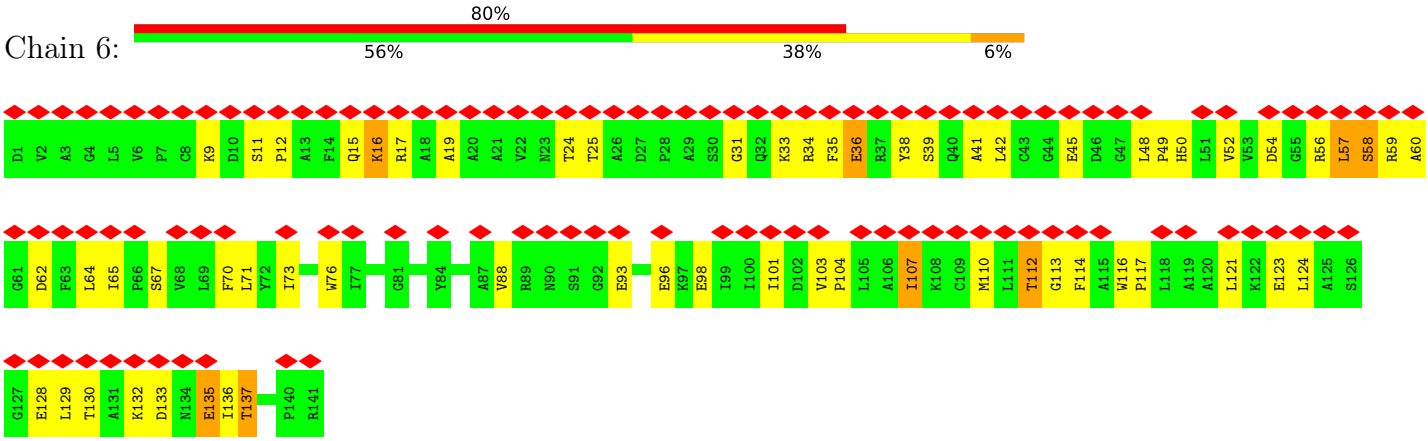
• Molecule 6: Photosystem I reaction center subunit III

Chain f:



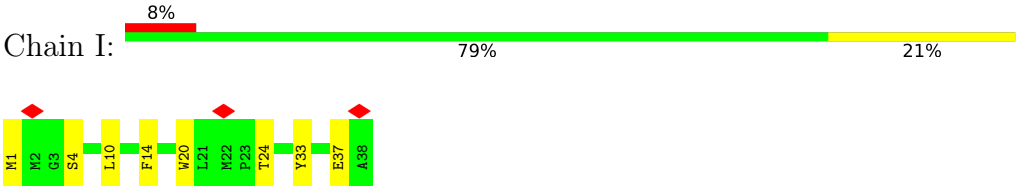
• Molecule 6: Photosystem I reaction center subunit III

Chain 6:



• Molecule 7: Photosystem I reaction center subunit VIII

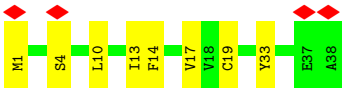
Chain I:



• Molecule 7: Photosystem I reaction center subunit VIII

Chain i:

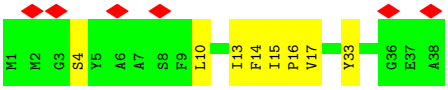




• Molecule 7: Photosystem I reaction center subunit VIII

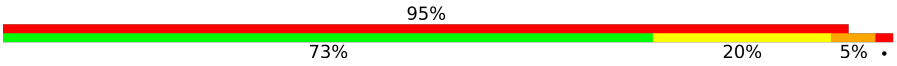
Chain 7:

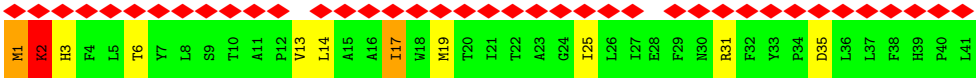




• Molecule 8: Photosystem I reaction center subunit IX

Chain J:

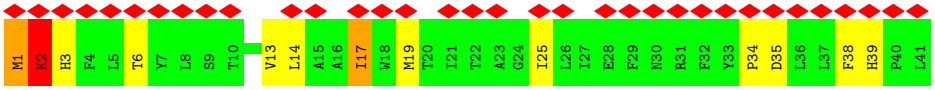




• Molecule 8: Photosystem I reaction center subunit IX

Chain j:





• Molecule 8: Photosystem I reaction center subunit IX

Chain 8:

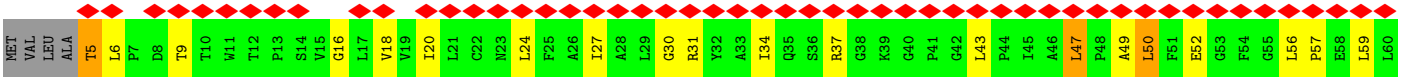


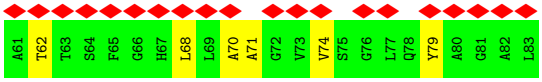


• Molecule 9: Photosystem I reaction center subunit PsaK

Chain K:

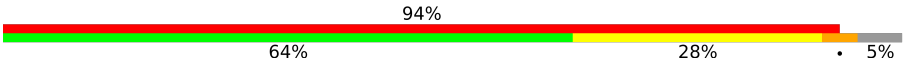


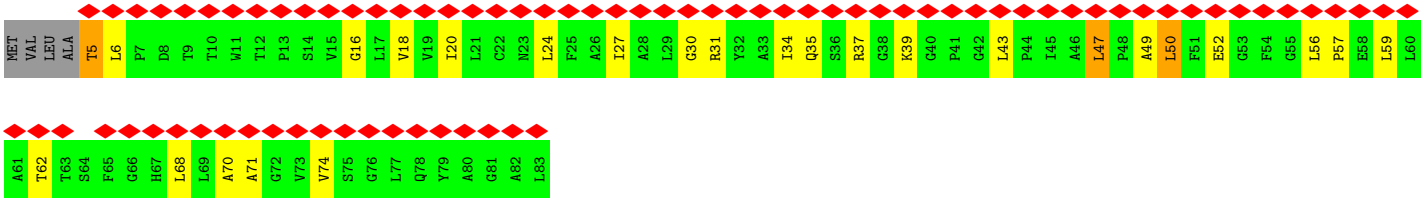




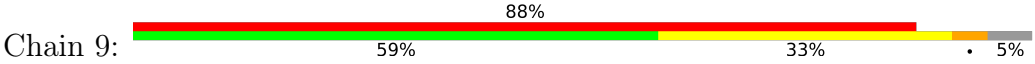
• Molecule 9: Photosystem I reaction center subunit PsaK

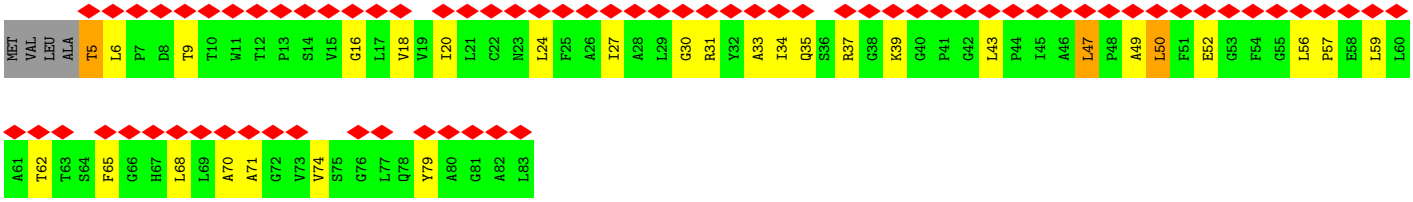
Chain k:



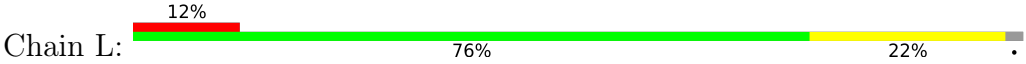


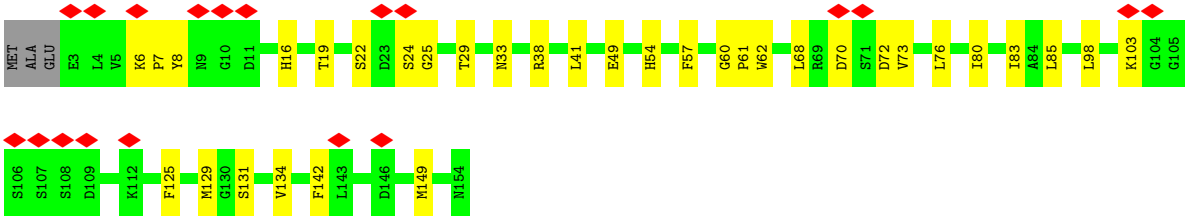
• Molecule 9: Photosystem I reaction center subunit PsaK





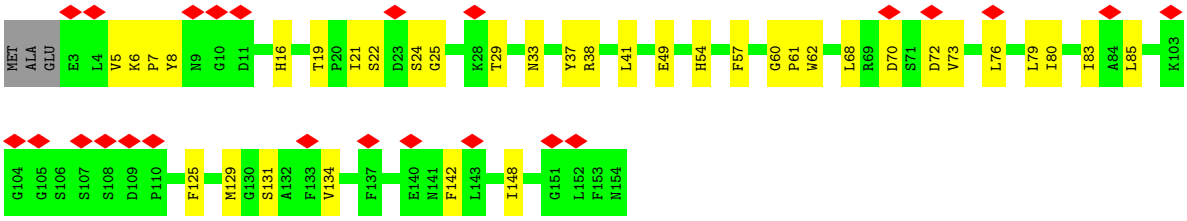
• Molecule 10: Photosystem I reaction center subunit XI



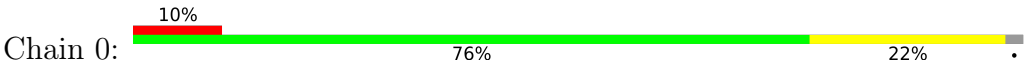


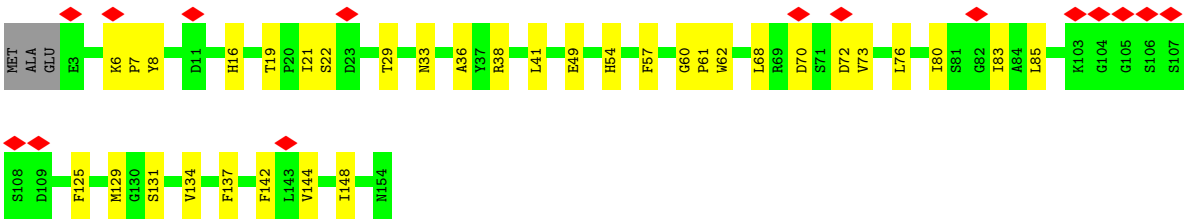
• Molecule 10: Photosystem I reaction center subunit XI





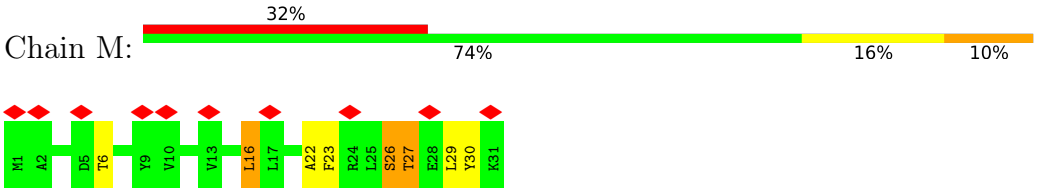
• Molecule 10: Photosystem I reaction center subunit XI





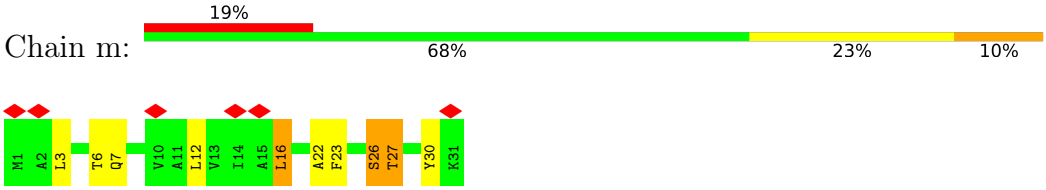
• Molecule 11: Photosystem I reaction center subunit XII

Chain M:



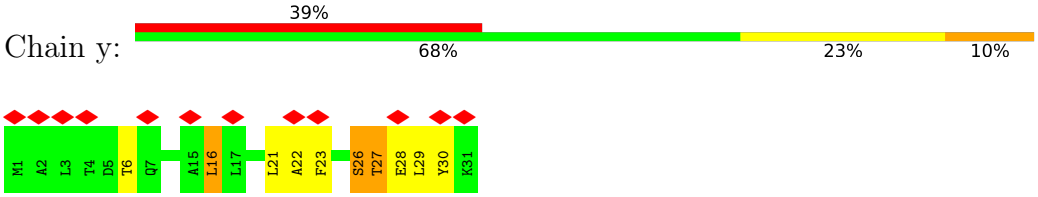
• Molecule 11: Photosystem I reaction center subunit XII

Chain m:



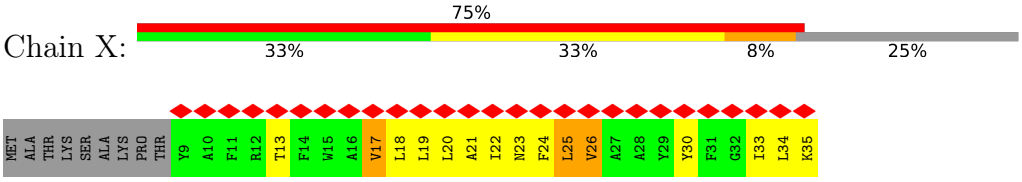
• Molecule 11: Photosystem I reaction center subunit XII

Chain y:



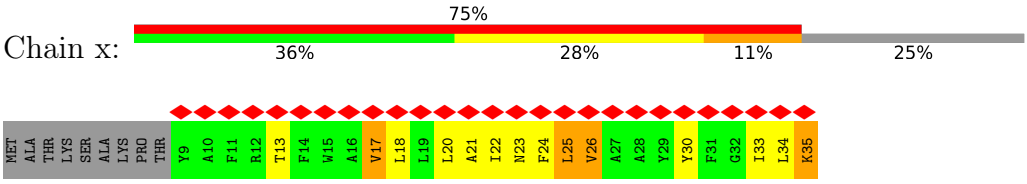
• Molecule 12: Photosystem I 4.8K protein

Chain X:



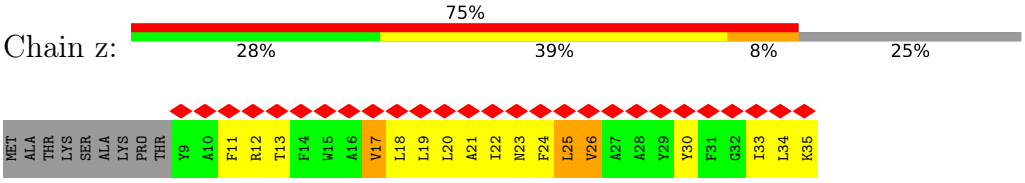
• Molecule 12: Photosystem I 4.8K protein

Chain x:



• Molecule 12: Photosystem I 4.8K protein

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	175999	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND4 was used to estimate contrast transfer function parameters. CTF correction was done in Relion 3.0.	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	32	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	351.68002, 351.68002, 351.68002	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.628, 0.628, 0.628	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL0, LHG, CA, SF4, LMG, CLA, BCR, FME, PQN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	1	0.37	0/6027	0.48	2/8220 (0.0%)
1	A	0.37	0/6027	0.48	2/8220 (0.0%)
1	a	0.37	0/6027	0.48	2/8220 (0.0%)
2	2	0.37	0/6112	0.44	1/8350 (0.0%)
2	B	0.37	0/6112	0.44	1/8350 (0.0%)
2	b	0.37	0/6112	0.44	1/8350 (0.0%)
3	3	0.36	0/608	0.41	0/824
3	C	0.36	0/608	0.41	0/824
3	c	0.36	0/608	0.41	0/824
4	4	0.36	0/1101	0.60	2/1492 (0.1%)
4	D	0.36	0/1101	0.60	2/1492 (0.1%)
4	d	0.36	0/1101	0.60	2/1492 (0.1%)
5	5	0.29	0/559	0.56	1/762 (0.1%)
5	E	0.29	0/559	0.56	1/762 (0.1%)
5	e	0.29	0/559	0.56	1/762 (0.1%)
6	6	0.37	0/1087	0.89	5/1476 (0.3%)
6	F	0.37	0/1087	0.88	5/1476 (0.3%)
6	f	0.37	0/1087	0.88	5/1476 (0.3%)
7	7	0.41	0/304	0.50	0/415
7	I	0.41	0/304	0.50	0/415
7	i	0.41	0/304	0.50	0/415
8	8	0.30	0/342	0.55	0/467
8	J	0.31	0/342	0.55	0/467
8	j	0.30	0/342	0.55	0/467
9	9	0.28	0/585	0.68	1/800 (0.1%)
9	K	0.28	0/585	0.68	1/800 (0.1%)
9	k	0.28	0/585	0.68	1/800 (0.1%)
10	0	0.43	0/1153	0.43	0/1565
10	L	0.43	0/1153	0.43	0/1565
10	l	0.43	0/1153	0.43	0/1565
11	M	0.36	0/244	0.41	0/332
11	m	0.36	0/244	0.41	0/332

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
11	y	0.36	0/244	0.41	0/332
12	X	0.39	0/236	1.29	6/321 (1.9%)
12	x	0.38	0/236	1.29	6/321 (1.9%)
12	z	0.38	0/236	1.29	6/321 (1.9%)
All	All	0.37	0/55074	0.53	54/75072 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	9	0	1
9	K	0	1
9	k	0	1
All	All	0	3

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	z	25	LEU	CA-CB-CG	11.29	155.81	116.30
12	X	25	LEU	CA-CB-CG	11.28	155.79	116.30
12	x	25	LEU	CA-CB-CG	11.28	155.77	116.30
6	f	121	LEU	CA-CB-CG	10.78	154.04	116.30
6	F	121	LEU	CA-CB-CG	10.78	154.03	116.30
6	6	121	LEU	CA-CB-CG	10.78	154.03	116.30
9	9	59	LEU	CA-CB-CG	8.17	144.88	116.30
12	z	35	LYS	CD-CE-NZ	8.16	138.01	111.90
12	x	35	LYS	CD-CE-NZ	8.15	138.00	111.90
9	K	59	LEU	CA-CB-CG	8.15	144.83	116.30
9	k	59	LEU	CA-CB-CG	8.15	144.82	116.30
12	X	35	LYS	CD-CE-NZ	8.14	137.95	111.90
4	D	107	LYS	CD-CE-NZ	-7.88	86.69	111.90
4	4	107	LYS	CD-CE-NZ	-7.88	86.69	111.90
4	d	107	LYS	CD-CE-NZ	-7.86	86.75	111.90
12	x	25	LEU	CB-CG-CD1	7.65	133.66	110.70
12	X	25	LEU	CB-CG-CD1	7.65	133.65	110.70
12	z	25	LEU	CB-CG-CD1	7.65	133.65	110.70
4	d	76	LYS	CD-CE-NZ	7.41	135.61	111.90
4	D	76	LYS	CD-CE-NZ	7.40	135.59	111.90
4	4	76	LYS	CD-CE-NZ	7.40	135.57	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	f	121	LEU	CB-CG-CD1	7.18	132.23	110.70
6	F	121	LEU	CB-CG-CD1	7.17	132.20	110.70
6	6	121	LEU	CB-CG-CD1	7.16	132.18	110.70
12	z	25	LEU	CB-CG-CD2	-6.77	90.38	110.70
12	X	25	LEU	CB-CG-CD2	-6.77	90.40	110.70
12	x	25	LEU	CB-CG-CD2	-6.77	90.40	110.70
1	a	30	LYS	CD-CE-NZ	6.57	132.93	111.90
1	A	30	LYS	CD-CE-NZ	6.56	132.90	111.90
1	1	30	LYS	CD-CE-NZ	6.56	132.90	111.90
12	z	35	LYS	CB-CG-CD	6.33	125.85	111.30
12	X	35	LYS	CB-CG-CD	6.33	125.85	111.30
12	x	35	LYS	CB-CG-CD	6.31	125.81	111.30
2	B	97	LYS	CB-CG-CD	6.25	125.66	111.30
2	2	97	LYS	CB-CG-CD	6.24	125.65	111.30
2	b	97	LYS	CB-CG-CD	6.22	125.61	111.30
6	6	121	LEU	CB-CG-CD2	-6.20	92.09	110.70
6	F	121	LEU	CB-CG-CD2	-6.19	92.13	110.70
6	f	121	LEU	CB-CG-CD2	-6.19	92.13	110.70
5	5	28	GLN	CB-CG-CD	6.12	123.00	112.60
5	E	28	GLN	CB-CG-CD	6.11	122.99	112.60
5	e	28	GLN	CB-CG-CD	6.10	122.96	112.60
1	1	188	GLU	CA-CB-CG	5.96	126.02	114.10
1	A	188	GLU	CA-CB-CG	5.95	126.01	114.10
1	a	188	GLU	CA-CB-CG	5.95	126.01	114.10
6	F	9	LYS	CD-CE-NZ	-5.68	93.72	111.90
6	6	9	LYS	CD-CE-NZ	-5.67	93.76	111.90
6	f	9	LYS	CD-CE-NZ	-5.67	93.77	111.90
6	f	57	LEU	CB-CG-CD2	5.44	127.03	110.70
6	F	57	LEU	CB-CG-CD2	5.44	127.01	110.70
6	6	57	LEU	CB-CG-CD2	5.43	126.99	110.70
12	X	25	LEU	CD1-CG-CD2	-5.06	99.67	110.80
12	x	25	LEU	CD1-CG-CD2	-5.04	99.70	110.80
12	z	25	LEU	CD1-CG-CD2	-5.04	99.71	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	9	47	LEU	Peptide
9	K	47	LEU	Peptide
9	k	47	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	5826	0	5692	121	0
1	A	5826	0	5692	120	0
1	a	5826	0	5692	114	0
2	2	5894	0	5653	100	0
2	B	5894	0	5653	92	0
2	b	5894	0	5653	102	0
3	3	598	0	580	15	0
3	C	598	0	580	13	0
3	c	598	0	580	8	0
4	4	1075	0	1077	27	0
4	D	1075	0	1077	24	0
4	d	1075	0	1077	21	0
5	5	546	0	535	11	0
5	E	546	0	535	6	0
5	e	546	0	535	5	0
6	6	1065	0	1077	53	0
6	F	1065	0	1077	48	0
6	f	1065	0	1077	50	0
7	7	303	0	305	7	0
7	I	303	0	305	8	0
7	i	303	0	305	10	0
8	8	340	0	346	13	0
8	J	340	0	346	10	0
8	j	340	0	346	12	0
9	9	571	0	593	17	0
9	K	571	0	593	16	0
9	k	571	0	593	13	0
10	0	1124	0	1127	25	0
10	L	1124	0	1127	24	0
10	l	1124	0	1127	30	0
11	M	241	0	264	5	0
11	m	241	0	264	10	0
11	y	241	0	264	8	0
12	X	228	0	234	12	0
12	x	228	0	234	16	0
12	z	228	0	234	28	0
13	1	65	0	72	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	A	65	0	72	0	0
13	a	65	0	72	2	0
14	0	195	0	216	4	0
14	1	2710	0	2873	50	0
14	2	2511	0	2634	29	0
14	6	108	0	94	2	0
14	8	127	0	91	2	0
14	9	104	0	88	1	0
14	A	2775	0	2945	47	0
14	B	2446	0	2562	32	0
14	F	153	0	127	4	0
14	J	82	0	58	1	0
14	K	104	0	88	1	0
14	L	195	0	216	4	0
14	M	36	0	24	1	0
14	X	45	0	33	3	0
14	a	2674	0	2849	41	0
14	b	2511	0	2634	39	0
14	f	108	0	94	3	0
14	j	127	0	91	2	0
14	k	104	0	88	0	0
14	l	195	0	216	4	0
14	x	45	0	33	4	0
14	z	45	0	33	3	0
15	1	33	0	46	1	0
15	2	33	0	46	0	0
15	A	33	0	46	1	0
15	B	33	0	46	0	0
15	a	33	0	46	1	0
15	b	33	0	46	0	0
16	1	8	0	0	0	0
16	3	16	0	0	0	0
16	A	8	0	0	0	0
16	C	16	0	0	0	0
16	a	8	0	0	0	0
16	c	16	0	0	0	0
17	0	160	0	224	4	0
17	1	225	0	313	5	0
17	2	240	0	336	1	0
17	6	80	0	112	2	0
17	7	40	0	56	0	0
17	8	120	0	168	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	9	65	0	89	1	0
17	A	265	0	369	7	0
17	B	280	0	392	1	0
17	F	80	0	112	1	0
17	I	40	0	56	3	0
17	J	40	0	56	0	0
17	K	65	0	89	0	0
17	L	120	0	168	1	0
17	M	40	0	56	4	0
17	a	225	0	313	5	0
17	b	280	0	392	2	0
17	f	80	0	112	1	0
17	i	40	0	56	0	0
17	j	80	0	112	0	0
17	k	65	0	89	0	0
17	l	80	0	112	1	0
17	m	40	0	56	2	0
17	y	40	0	56	2	0
18	0	39	0	51	1	0
18	1	90	0	129	1	0
18	A	90	0	129	1	0
18	B	49	0	74	3	0
18	L	39	0	51	1	0
18	M	49	0	74	1	0
18	a	90	0	129	1	0
18	b	49	0	74	3	0
18	l	39	0	51	1	0
18	m	49	0	74	1	0
18	y	49	0	74	2	0
18	z	49	0	74	13	0
19	0	1	0	0	0	0
19	2	1	0	0	0	0
19	B	1	0	0	0	0
19	L	1	0	0	0	0
19	b	1	0	0	0	0
19	l	1	0	0	0	0
20	2	55	0	86	0	0
20	B	55	0	86	0	0
20	b	55	0	86	0	0
21	0	1	0	0	0	0
21	1	5	0	0	1	0
21	2	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	6	1	0	0	0	0
21	8	1	0	0	0	0
21	9	1	0	0	0	0
21	A	5	0	0	1	0
21	B	8	0	0	0	0
21	F	1	0	0	0	0
21	J	1	0	0	0	0
21	K	1	0	0	0	0
21	L	1	0	0	0	0
21	a	5	0	0	1	0
21	b	8	0	0	0	0
21	f	1	0	0	0	0
21	j	1	0	0	0	0
21	k	1	0	0	0	0
21	l	1	0	0	0	0
All	All	74991	0	76164	1204	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 8.

All (1204) 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)
2:2:483:ASN:ND2	2:2:485:ASP:OD2	1.92	1.03
2:B:483:ASN:ND2	2:B:485:ASP:OD2	1.92	1.01
2:b:483:ASN:ND2	2:b:485:ASP:OD2	1.92	1.00
1:1:157:GLN:NE2	14:1:1616:CLA:O1D	2.05	0.90
1:A:157:GLN:NE2	14:A:815:CLA:O1D	2.05	0.90
6:F:59:ARG:NE	6:F:62:ASP:OD1	2.05	0.90
1:a:157:GLN:NE2	14:a:815:CLA:O1D	2.05	0.90
6:f:59:ARG:NE	6:f:62:ASP:OD1	2.05	0.89
7:i:33:TYR:HH	11:m:30:TYR:HH	1.02	0.89
6:6:59:ARG:NE	6:6:62:ASP:OD1	2.05	0.88
4:4:120:GLY:N	5:5:13:GLU:OE2	2.07	0.86
2:2:43:GLN:OE1	2:2:161:ARG:NH2	2.10	0.85
2:B:43:GLN:OE1	2:B:161:ARG:NH2	2.10	0.85
2:B:226:THR:OG1	2:B:228:ASN:OD1	1.95	0.85
2:b:43:GLN:OE1	2:b:161:ARG:NH2	2.10	0.84
1:1:94:GLY:O	1:1:98:SER:OG	1.96	0.84
1:A:94:GLY:O	1:A:98:SER:OG	1.96	0.83
2:b:226:THR:OG1	2:b:228:ASN:OD1	1.95	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:226:THR:OG1	2:2:228:ASN:OD1	1.95	0.83
2:2:577:SER:OG	2:2:580:ASP:OD1	1.96	0.82
1:a:94:GLY:O	1:a:98:SER:OG	1.96	0.82
10:0:16:HIS:HE2	10:0:22:SER:HG	1.23	0.82
2:B:577:SER:OG	2:B:580:ASP:OD1	1.97	0.81
2:b:577:SER:OG	2:b:580:ASP:OD1	1.96	0.81
2:2:479:THR:HG22	2:2:480:LEU:H	1.46	0.81
4:D:60:ARG:NH2	4:D:62:GLU:OE1	2.15	0.80
4:4:60:ARG:NH2	4:4:62:GLU:OE1	2.15	0.80
4:d:60:ARG:NH2	4:d:62:GLU:OE1	2.15	0.79
4:D:120:GLY:N	5:E:13:GLU:OE2	2.14	0.79
1:a:15:VAL:HG12	1:a:186:LYS:HB2	1.65	0.79
2:b:479:THR:HG22	2:b:480:LEU:H	1.47	0.78
1:A:15:VAL:HG12	1:A:186:LYS:HB2	1.65	0.78
2:B:479:THR:HG22	2:B:480:LEU:H	1.46	0.78
5:5:17:TYR:O	6:6:137:THR:OG1	2.02	0.77
2:B:479:THR:HG22	2:B:480:LEU:HD12	1.67	0.77
10:L:16:HIS:HE2	10:L:22:SER:HG	1.29	0.77
1:1:15:VAL:HG12	1:1:186:LYS:HB2	1.65	0.77
2:2:479:THR:HG22	2:2:480:LEU:HD12	1.67	0.76
3:3:8:ASP:OD2	4:4:117:ARG:N	2.18	0.76
1:A:504:ASN:ND2	14:A:818:CLA:OBD	2.19	0.76
6:6:110:MET:HE1	14:6:201:CLA:H8	1.68	0.76
1:1:504:ASN:ND2	14:1:1619:CLA:OBD	2.19	0.76
2:2:314:VAL:CG2	12:z:11:PHE:HE1	2.00	0.75
6:F:52:VAL:HG22	6:F:59:ARG:HD3	1.69	0.74
12:z:12:ARG:CZ	18:z:101:LHG:HC92	2.17	0.74
2:b:479:THR:HG22	2:b:480:LEU:HD12	1.67	0.74
1:a:504:ASN:ND2	14:a:818:CLA:OBD	2.19	0.74
3:C:8:ASP:OD2	4:D:117:ARG:N	2.20	0.74
2:2:319:ASN:HD22	12:z:11:PHE:HD1	1.36	0.74
6:6:52:VAL:HG22	6:6:59:ARG:HD3	1.69	0.74
10:l:16:HIS:HE2	10:l:22:SER:HG	1.32	0.73
11:y:23:PHE:O	11:y:27:THR:OG1	2.07	0.73
6:f:76:TRP:HZ3	6:f:114:PHE:HA	1.54	0.72
12:z:12:ARG:HG3	18:z:101:LHG:H101	1.70	0.72
11:M:23:PHE:O	11:M:27:THR:OG1	2.07	0.72
11:m:23:PHE:O	11:m:27:THR:OG1	2.07	0.72
12:z:12:ARG:HG2	18:z:101:LHG:HC61	1.71	0.72
2:2:314:VAL:HG23	12:z:11:PHE:HE1	1.54	0.72
6:f:52:VAL:HG22	6:f:59:ARG:HD3	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:76:TRP:HZ3	6:6:114:PHE:HA	1.54	0.71
3:c:13:CYS:O	3:c:14:THR:OG1	2.09	0.71
6:F:76:TRP:HZ3	6:F:114:PHE:HA	1.54	0.69
3:3:13:CYS:O	3:3:14:THR:OG1	2.09	0.69
1:a:523:LYS:NZ	1:a:755:GLY:O	2.26	0.69
1:A:270:PHE:O	9:K:9:THR:OG1	2.11	0.69
1:A:523:LYS:NZ	1:A:755:GLY:O	2.26	0.69
3:C:13:CYS:O	3:C:14:THR:OG1	2.09	0.68
9:9:5:THR:OG1	9:9:6:LEU:N	2.26	0.68
1:1:523:LYS:NZ	1:1:755:GLY:O	2.26	0.68
1:1:564:ARG:O	4:4:60:ARG:NH1	2.26	0.68
1:a:716:ALA:HB3	6:f:98:GLU:OE1	1.94	0.68
12:z:12:ARG:NE	18:z:101:LHG:O7	2.28	0.67
1:a:579:ASP:OD2	1:a:583:ARG:NH1	2.27	0.67
1:1:579:ASP:OD2	1:1:583:ARG:NH1	2.27	0.67
1:1:36:ARG:HH21	1:1:36:ARG:HB2	1.60	0.67
12:z:23:ASN:OD1	14:z:102:CLA:NA	2.28	0.67
9:K:5:THR:OG1	9:K:6:LEU:N	2.26	0.67
3:3:9:THR:O	3:3:63:SER:OG	2.13	0.67
17:0:208:BCR:H403	17:0:208:BCR:H23C	1.76	0.67
17:l:207:BCR:H403	17:l:207:BCR:H23C	1.76	0.66
1:a:121:VAL:O	6:f:24:THR:HB	1.95	0.66
6:f:96:GLU:N	6:f:96:GLU:OE2	2.28	0.66
14:1:1619:CLA:O1A	9:9:79:TYR:OH	2.13	0.66
3:C:60:ASP:OD2	5:E:11:ARG:NH1	2.29	0.66
3:c:9:THR:O	3:c:63:SER:OG	2.13	0.66
6:F:96:GLU:N	6:F:96:GLU:OE2	2.28	0.66
9:k:5:THR:OG1	9:k:6:LEU:N	2.26	0.66
1:A:579:ASP:OD2	1:A:583:ARG:NH1	2.27	0.66
12:x:23:ASN:OD1	14:x:1701:CLA:NA	2.28	0.66
3:C:9:THR:O	3:C:63:SER:OG	2.13	0.66
12:X:23:ASN:OD1	14:X:1701:CLA:NA	2.28	0.66
7:7:33:TYR:OH	11:y:30:TYR:OH	1.96	0.66
12:z:19:LEU:HD21	18:z:101:LHG:H211	1.78	0.66
17:L:206:BCR:H403	17:L:206:BCR:H23C	1.76	0.65
1:A:36:ARG:HH21	1:A:36:ARG:HB2	1.60	0.65
6:6:96:GLU:OE2	6:6:96:GLU:N	2.28	0.65
12:x:21:ALA:HA	12:x:24:PHE:HD2	1.62	0.65
1:1:225:LYS:HE2	1:1:252:LEU:HD22	1.78	0.65
1:1:249:MET:HA	1:1:249:MET:HE2	1.79	0.64
1:a:36:ARG:HH21	1:a:36:ARG:HB2	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:z:21:ALA:HA	12:z:24:PHE:HD2	1.62	0.64
1:a:225:LYS:HE2	1:a:252:LEU:HD22	1.78	0.64
17:A:851:BCR:H362	14:A:855:CLA:C4	2.28	0.64
3:C:28:VAL:HG12	4:D:109:ARG:HB3	1.79	0.64
12:X:21:ALA:HA	12:X:24:PHE:HD2	1.62	0.64
1:A:564:ARG:NH2	4:D:14:THR:O	2.31	0.63
1:A:583:ARG:NH2	4:D:62:GLU:OE2	2.31	0.63
1:1:76:HIS:ND1	14:1:1615:CLA:OBD	2.30	0.63
1:a:249:MET:HA	1:a:249:MET:HE2	1.79	0.63
1:A:249:MET:HE2	1:A:249:MET:HA	1.79	0.63
1:A:225:LYS:HE2	1:A:252:LEU:HD22	1.78	0.63
7:i:33:TYR:OH	11:m:30:TYR:OH	1.88	0.63
1:a:320:GLY:N	9:k:39:LYS:HD2	2.13	0.62
2:B:402:ASP:HB3	2:B:405:GLN:HB2	1.81	0.62
1:a:376:ALA:O	1:a:510:SER:OG	2.11	0.62
1:A:267:PHE:N	1:A:275:TYR:OH	2.33	0.62
1:a:267:PHE:N	1:a:275:TYR:OH	2.33	0.62
2:2:402:ASP:HB3	2:2:405:GLN:HB2	1.81	0.62
1:a:564:ARG:O	4:d:60:ARG:NH1	2.32	0.62
6:F:73:ILE:O	6:F:76:TRP:HB3	2.00	0.62
1:a:76:HIS:ND1	14:a:814:CLA:OBD	2.30	0.62
6:6:73:ILE:O	6:6:76:TRP:HB3	2.00	0.62
14:A:802:CLA:O1A	2:B:531:LEU:HD11	1.99	0.62
17:A:851:BCR:H362	14:A:855:CLA:H42	1.81	0.62
1:1:70:ARG:NE	1:1:185:PRO:O	2.32	0.62
6:6:54:ASP:CG	12:z:30:TYR:OH	2.43	0.62
10:0:38:ARG:NH2	10:0:49:GLU:OE1	2.33	0.62
1:1:267:PHE:N	1:1:275:TYR:OH	2.33	0.61
2:2:314:VAL:CG2	12:z:11:PHE:CE1	2.81	0.61
2:b:402:ASP:HB3	2:b:405:GLN:HB2	1.81	0.61
1:A:376:ALA:O	1:A:510:SER:OG	2.11	0.61
12:X:33:ILE:HG22	12:X:34:LEU:HD12	1.81	0.61
12:x:33:ILE:HG22	12:x:34:LEU:HD12	1.81	0.61
7:I:20:TRP:O	7:I:24:THR:OG1	2.14	0.61
10:L:38:ARG:NH2	10:L:49:GLU:OE1	2.33	0.61
14:2:811:CLA:H2A	14:2:811:CLA:O2A	2.00	0.61
6:f:73:ILE:O	6:f:76:TRP:HB3	2.00	0.61
12:X:20:LEU:HG	12:X:24:PHE:CE2	2.36	0.61
4:4:120:GLY:CA	5:5:13:GLU:OE2	2.49	0.60
12:z:33:ILE:HG22	12:z:34:LEU:HD12	1.81	0.60
14:B:810:CLA:H2A	14:B:810:CLA:O2A	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:70:ARG:NE	1:a:185:PRO:O	2.32	0.60
6:F:112:THR:O	6:F:112:THR:OG1	2.18	0.60
1:1:376:ALA:O	1:1:510:SER:OG	2.11	0.60
6:F:132:LYS:O	6:F:135:GLU:N	2.34	0.60
10:l:38:ARG:NH2	10:l:49:GLU:OE1	2.33	0.60
12:x:20:LEU:HG	12:x:24:PHE:CE2	2.36	0.60
1:1:29:ALA:HB2	8:8:3:HIS:HB3	1.83	0.60
12:z:20:LEU:HG	12:z:24:PHE:CE2	2.36	0.60
1:1:115:GLN:NE2	14:1:1611:CLA:OBD	2.35	0.60
1:1:43:GLN:OE1	1:1:43:GLN:HA	2.02	0.60
17:a:851:BCR:H362	14:b:802:CLA:C4	2.32	0.59
2:b:465:PHE:CE1	12:x:30:TYR:HA	2.36	0.59
4:4:95:HIS:HB3	4:4:96:PRO:HD3	1.84	0.59
1:A:115:GLN:NE2	14:A:810:CLA:OBD	2.35	0.59
6:F:67:SER:O	6:F:71:LEU:HD12	2.02	0.59
1:a:43:GLN:OE1	1:a:43:GLN:HA	2.02	0.59
4:d:95:HIS:HB3	4:d:96:PRO:HD3	1.84	0.59
1:A:76:HIS:ND1	14:A:814:CLA:OBD	2.30	0.59
4:D:95:HIS:HB3	4:D:96:PRO:HD3	1.84	0.59
6:f:67:SER:O	6:f:71:LEU:HD12	2.02	0.59
14:b:811:CLA:H2A	14:b:811:CLA:O2A	2.00	0.59
2:2:555:ASP:OD1	4:4:119:ILE:HG21	2.02	0.59
2:b:486:SER:HA	12:x:35:LYS:HD2	1.83	0.59
1:A:271:ASN:HA	9:K:9:THR:HG23	1.85	0.59
6:6:112:THR:O	6:6:112:THR:OG1	2.18	0.59
1:a:596:PHE:CE1	1:a:732:VAL:HB	2.38	0.59
12:z:12:ARG:NH2	18:z:101:LHG:HC92	2.18	0.59
4:D:1:THR:HG22	4:D:2:THR:H	1.68	0.58
4:d:1:THR:HG22	4:d:2:THR:H	1.68	0.58
6:6:132:LYS:O	6:6:135:GLU:N	2.34	0.58
1:A:43:GLN:OE1	1:A:43:GLN:HA	2.02	0.58
4:d:120:GLY:N	5:e:13:GLU:OE2	2.35	0.58
14:2:804:CLA:HBC3	14:2:804:CLA:HHD	1.85	0.58
2:b:693:LEU:HD23	10:l:37:TYR:CE2	2.38	0.58
14:B:803:CLA:HBC3	14:B:803:CLA:HHD	1.85	0.58
1:A:371:ALA:HB2	1:A:397:HIS:HB2	1.85	0.58
1:A:596:PHE:CE1	1:A:732:VAL:HB	2.38	0.58
1:1:596:PHE:CE1	1:1:732:VAL:HB	2.38	0.58
2:2:291:ARG:NE	2:2:297:GLY:O	2.35	0.58
6:6:67:SER:O	6:6:71:LEU:HD12	2.02	0.58
6:f:132:LYS:O	6:f:135:GLU:N	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ARG:NE	1:A:185:PRO:O	2.32	0.57
4:4:1:THR:HG22	4:4:2:THR:H	1.68	0.57
1:1:562:SER:HB2	1:1:567:PRO:O	2.04	0.57
6:6:54:ASP:OD1	12:z:30:TYR:OH	2.19	0.57
14:b:804:CLA:HBC3	14:b:804:CLA:HHD	1.85	0.57
14:A:825:CLA:HMB2	17:A:849:BCR:H362	1.86	0.57
1:a:371:ALA:HB2	1:a:397:HIS:HB2	1.85	0.57
1:a:115:GLN:NE2	14:a:810:CLA:OBD	2.35	0.57
14:a:825:CLA:HMB2	17:a:849:BCR:H362	1.86	0.57
1:1:371:ALA:HB2	1:1:397:HIS:HB2	1.85	0.57
1:A:562:SER:HB2	1:A:567:PRO:O	2.04	0.57
6:f:112:THR:O	6:f:112:THR:OG1	2.18	0.57
1:A:159:TYR:O	1:A:163:ILE:HG12	2.05	0.57
1:1:159:TYR:O	1:1:163:ILE:HG12	2.05	0.56
3:3:60:ASP:OD1	3:3:61:PHE:N	2.36	0.56
1:A:215:HIS:ND1	14:A:815:CLA:NB	2.53	0.56
1:a:562:SER:HB2	1:a:567:PRO:O	2.04	0.56
14:1:1626:CLA:HMB2	17:1:1650:BCR:H362	1.86	0.56
10:0:54:HIS:HA	10:0:57:PHE:CE1	2.41	0.56
10:L:54:HIS:HA	10:L:57:PHE:CE1	2.41	0.56
2:B:394:ALA:O	2:B:398:VAL:HG23	2.06	0.56
1:a:159:TYR:O	1:a:163:ILE:HG12	2.05	0.56
2:2:394:ALA:O	2:2:398:VAL:HG23	2.06	0.56
1:A:33:HIS:NE2	14:A:812:CLA:O1A	2.38	0.56
1:a:215:HIS:ND1	14:a:815:CLA:NB	2.53	0.56
12:x:22:ILE:O	12:x:26:VAL:HG13	2.06	0.56
1:1:215:HIS:ND1	14:1:1616:CLA:NB	2.53	0.56
1:1:454:HIS:O	1:1:458:LEU:HG	2.06	0.56
7:I:10:LEU:HD22	7:I:14:PHE:HE2	1.71	0.56
12:X:22:ILE:O	12:X:26:VAL:HG13	2.06	0.56
1:A:270:PHE:CD2	9:K:74:VAL:HG11	2.41	0.56
14:B:831:CLA:C2	6:F:124:LEU:HD11	2.35	0.56
3:C:59:THR:OG1	3:C:61:PHE:O	2.20	0.56
1:1:33:HIS:NE2	14:1:1613:CLA:O1A	2.38	0.56
6:F:132:LYS:HG2	6:F:133:ASP:H	1.72	0.55
10:l:54:HIS:HA	10:l:57:PHE:CE1	2.41	0.55
1:a:454:HIS:O	1:a:458:LEU:HG	2.06	0.55
1:1:31:PRO:HB2	1:1:51:LEU:HD11	1.89	0.55
3:3:28:VAL:HG12	4:4:109:ARG:HB3	1.88	0.55
1:a:33:HIS:NE2	14:a:812:CLA:O1A	2.38	0.55
2:2:156:LEU:HD13	11:y:28:GLU:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:291:ARG:NE	2:b:297:GLY:O	2.35	0.55
6:f:132:LYS:HG2	6:f:133:ASP:H	1.72	0.55
1:1:583:ARG:NH2	4:4:62:GLU:OE2	2.38	0.55
6:f:52:VAL:CG2	6:f:59:ARG:HD3	2.37	0.55
3:C:60:ASP:OD1	3:C:61:PHE:N	2.36	0.55
6:F:110:MET:HE1	14:F:201:CLA:H8	1.89	0.55
2:b:194:ILE:HD12	2:b:253:ILE:HB	1.89	0.55
10:l:68:LEU:HD11	10:0:148:ILE:HG22	1.88	0.55
12:z:22:ILE:O	12:z:26:VAL:HG13	2.06	0.55
1:a:31:PRO:HB2	1:a:51:LEU:HD11	1.89	0.55
2:b:555:ASP:OD2	2:b:555:ASP:O	2.25	0.55
7:i:10:LEU:HD22	7:i:14:PHE:HE2	1.71	0.55
6:6:52:VAL:CG2	6:6:59:ARG:HD3	2.37	0.55
2:B:194:ILE:HD12	2:B:253:ILE:HB	1.89	0.55
2:b:394:ALA:O	2:b:398:VAL:HG23	2.06	0.55
6:6:54:ASP:CG	12:z:30:TYR:HH	2.13	0.55
6:f:110:MET:HE1	14:f:201:CLA:H8	1.88	0.55
14:1:1634:CLA:OBD	10:0:19:THR:HG21	2.07	0.55
2:2:194:ILE:HD12	2:2:253:ILE:HB	1.89	0.55
6:F:52:VAL:CG2	6:F:59:ARG:HD3	2.37	0.54
1:1:96:LYS:HD2	1:1:97:PHE:CZ	2.43	0.54
2:2:555:ASP:O	2:2:555:ASP:OD2	2.25	0.54
1:A:454:HIS:O	1:A:458:LEU:HG	2.06	0.54
2:B:555:ASP:O	2:B:555:ASP:OD2	2.25	0.54
2:b:722:GLY:O	2:b:726:THR:HG22	2.07	0.54
6:6:132:LYS:HG2	6:6:133:ASP:H	1.71	0.54
1:A:96:LYS:HD2	1:A:97:PHE:CZ	2.43	0.54
2:b:693:LEU:HD23	10:l:37:TYR:HE2	1.72	0.54
1:a:79:HIS:CE1	14:a:806:CLA:HMA3	2.43	0.54
2:b:465:PHE:CG	12:x:30:TYR:HD1	2.25	0.54
7:7:10:LEU:HD22	7:7:14:PHE:HE2	1.71	0.54
15:1:1646:PQN:H241	15:1:1646:PQN:H271	1.90	0.54
2:2:722:GLY:O	2:2:726:THR:HG22	2.07	0.54
1:A:564:ARG:O	4:D:60:ARG:NH1	2.41	0.54
2:B:291:ARG:NE	2:B:297:GLY:O	2.35	0.54
9:K:31:ARG:O	9:K:37:ARG:NH2	2.41	0.54
14:b:839:CLA:HBC1	6:f:53:VAL:HG11	1.89	0.54
9:9:31:ARG:O	9:9:37:ARG:NH2	2.41	0.54
14:2:828:CLA:HHC	14:2:828:CLA:HBB1	1.90	0.54
2:B:31:GLU:OE2	2:B:334:HIS:NE2	2.40	0.53
1:a:96:LYS:HD2	1:a:97:PHE:CZ	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:PRO:HB2	1:A:51:LEU:HD11	1.89	0.53
1:A:716:ALA:HB3	6:F:98:GLU:OE1	2.08	0.53
15:A:845:PQN:H271	15:A:845:PQN:H241	1.90	0.53
14:b:828:CLA:HHC	14:b:828:CLA:HBB1	1.90	0.53
6:6:54:ASP:CB	12:z:30:TYR:OH	2.57	0.53
14:A:818:CLA:O1A	9:K:79:TYR:OH	2.23	0.53
2:B:157:GLN:O	2:B:159:LYS:N	2.42	0.53
15:a:845:PQN:H241	15:a:845:PQN:H271	1.90	0.53
9:k:31:ARG:O	9:k:37:ARG:NH2	2.41	0.53
1:1:79:HIS:CE1	14:1:1607:CLA:HMA3	2.43	0.53
2:B:722:GLY:O	2:B:726:THR:HG22	2.07	0.53
3:c:60:ASP:OD1	3:c:61:PHE:N	2.36	0.53
14:B:827:CLA:HHC	14:B:827:CLA:HBB1	1.90	0.53
4:4:120:GLY:HA3	5:5:13:GLU:OE2	2.08	0.53
1:A:79:HIS:CE1	14:A:806:CLA:HMA3	2.43	0.53
2:B:10:ASP:OD1	2:B:10:ASP:N	2.42	0.53
5:E:11:ARG:NE	5:E:64:GLU:OE1	2.39	0.53
5:5:11:ARG:NE	5:5:64:GLU:OE1	2.39	0.53
1:1:564:ARG:NH2	4:4:14:THR:O	2.42	0.53
2:2:31:GLU:OE2	2:2:334:HIS:NE2	2.40	0.53
12:z:12:ARG:NH2	18:z:101:LHG:C7	2.71	0.53
14:b:838:CLA:H41	14:x:1701:CLA:HED1	1.91	0.53
2:B:555:ASP:OD1	3:C:61:PHE:HE2	1.91	0.52
2:B:611:ASN:OD1	2:B:614:GLN:HB2	2.09	0.52
1:a:276:SER:O	1:a:276:SER:OG	2.24	0.52
2:b:157:GLN:O	2:b:159:LYS:N	2.42	0.52
17:A:851:BCR:H24C	14:B:833:CLA:HMC1	1.92	0.52
2:b:611:ASN:OD1	2:b:614:GLN:HB2	2.10	0.52
1:1:154:ASN:ND2	1:1:157:GLN:OE1	2.43	0.52
2:2:157:GLN:O	2:2:159:LYS:N	2.42	0.52
1:A:31:PRO:HB3	14:A:804:CLA:HAC1	1.91	0.52
1:A:710:LYS:O	6:F:130:THR:HA	2.10	0.52
1:a:31:PRO:HB3	14:a:804:CLA:HAC1	1.91	0.52
1:a:154:ASN:ND2	1:a:157:GLN:OE1	2.43	0.52
2:b:10:ASP:OD1	2:b:10:ASP:N	2.42	0.52
6:f:61:GLY:O	8:j:39:HIS:N	2.39	0.52
2:2:611:ASN:OD1	2:2:614:GLN:HB2	2.10	0.52
1:A:17:ASP:OD2	1:A:18:ASN:N	2.43	0.52
6:f:37:ARG:NH2	8:j:34:PRO:O	2.43	0.52
2:B:223:PRO:O	2:B:228:ASN:HB2	2.10	0.51
1:1:355:GLN:NE2	21:1:1702:HOH:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:PRO:HB3	1:A:249:MET:HE1	1.92	0.51
14:B:833:CLA:O1D	8:J:35:ASP:HA	2.10	0.51
1:a:596:PHE:CE1	1:a:728:ARG:O	2.63	0.51
6:f:76:TRP:HE1	14:j:1301:CLA:CAD	2.24	0.51
1:1:31:PRO:HB3	14:1:1605:CLA:HAC1	1.91	0.51
1:A:154:ASN:ND2	1:A:157:GLN:OE1	2.43	0.51
2:B:555:ASP:OD1	4:D:119:ILE:HG21	2.09	0.51
6:F:103:VAL:O	6:F:107:ILE:HG13	2.11	0.51
2:B:130:THR:HG22	2:B:132:GLY:H	1.76	0.51
9:k:30:GLY:O	9:k:34:ILE:HD12	2.10	0.51
6:6:76:TRP:HE1	14:8:1301:CLA:CAD	2.24	0.51
6:F:76:TRP:HE1	14:F:203:CLA:CAD	2.23	0.51
9:K:30:GLY:O	9:K:34:ILE:HD12	2.10	0.51
2:b:555:ASP:OD1	4:d:119:ILE:HG21	2.09	0.51
6:f:103:VAL:O	6:f:107:ILE:HG13	2.11	0.51
1:A:569:LYS:NZ	2:B:679:GLU:OE2	2.42	0.51
2:B:479:THR:CG2	2:B:480:LEU:HD12	2.40	0.51
10:L:125:PHE:O	10:L:129:MET:HG2	2.11	0.51
1:a:583:ARG:NH2	4:d:62:GLU:OE2	2.41	0.51
13:a:801:CL0:H13	14:b:802:CLA:OBD	2.11	0.51
1:A:64:ASP:OD1	1:A:64:ASP:O	2.29	0.51
1:1:596:PHE:CE1	1:1:728:ARG:O	2.63	0.51
2:2:708:ILE:HG22	2:2:712:ARG:NH1	2.26	0.51
2:2:130:THR:HG22	2:2:132:GLY:H	1.76	0.51
2:B:353:GLN:HA	2:B:356:TYR:HE1	1.75	0.51
4:D:3:LEU:HD21	4:D:83:TYR:CD1	2.46	0.51
1:A:596:PHE:CE1	1:A:728:ARG:O	2.63	0.51
17:A:851:BCR:H23C	17:A:851:BCR:H403	1.93	0.51
2:B:708:ILE:HG22	2:B:712:ARG:NH1	2.26	0.51
4:d:3:LEU:HD21	4:d:83:TYR:CD1	2.46	0.51
9:k:27:ILE:HA	9:k:62:THR:HG21	1.93	0.51
5:E:1:VAL:HG12	5:E:2:GLN:N	2.26	0.50
7:I:33:TYR:OH	11:M:30:TYR:OH	2.26	0.50
2:2:353:GLN:HA	2:2:356:TYR:HE1	1.75	0.50
10:0:76:LEU:O	10:0:80:ILE:HG13	2.11	0.50
14:b:833:CLA:CBC	6:f:71:LEU:HD11	2.41	0.50
2:2:479:THR:CG2	2:2:480:LEU:HD12	2.40	0.50
10:0:125:PHE:O	10:0:129:MET:HG2	2.11	0.50
17:1:1652:BCR:H403	17:1:1652:BCR:H23C	1.93	0.50
2:2:223:PRO:O	2:2:228:ASN:HB2	2.10	0.50
2:2:387:VAL:HG12	2:2:582:PHE:HE1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:103:VAL:O	6:6:107:ILE:HG13	2.11	0.50
10:L:76:LEU:O	10:L:80:ILE:HG13	2.11	0.50
1:a:64:ASP:OD1	1:a:64:ASP:O	2.29	0.50
1:a:222:PRO:HB3	1:a:249:MET:HE1	1.93	0.50
9:9:30:GLY:O	9:9:34:ILE:HD12	2.10	0.50
1:A:711:LEU:HD21	14:B:831:CLA:H3A	1.93	0.50
2:b:130:THR:HG22	2:b:132:GLY:H	1.76	0.50
2:b:223:PRO:O	2:b:228:ASN:HB2	2.10	0.50
14:b:811:CLA:H12	10:0:148:ILE:HD12	1.93	0.50
4:d:104:LYS:O	4:d:109:ARG:NH1	2.44	0.50
6:f:123:GLU:HB2	6:f:128:GLU:HB2	1.94	0.50
14:1:1603:CLA:O1A	2:2:531:LEU:HD11	2.11	0.50
6:6:110:MET:HE1	14:6:201:CLA:C8	2.40	0.50
2:B:316:GLY:O	2:B:319:ASN:N	2.45	0.50
2:b:566:ASP:OD1	3:c:51:LYS:NZ	2.43	0.50
2:2:316:GLY:O	2:2:319:ASN:N	2.45	0.50
6:F:124:LEU:HD12	6:F:129:LEU:CD2	2.42	0.50
17:a:851:BCR:H23C	17:a:851:BCR:H403	1.93	0.50
2:b:353:GLN:HA	2:b:356:TYR:HE1	1.75	0.50
2:b:465:PHE:CD1	12:x:30:TYR:HD1	2.30	0.50
8:8:1:FME:O	8:8:2:LYS:C	2.55	0.50
2:B:387:VAL:HG12	2:B:582:PHE:HE1	1.76	0.50
2:b:387:VAL:HG12	2:b:582:PHE:HE1	1.77	0.50
10:l:76:LEU:O	10:l:80:ILE:HG13	2.11	0.50
1:1:276:SER:O	1:1:276:SER:OG	2.24	0.50
9:9:27:ILE:HA	9:9:62:THR:HG21	1.93	0.50
2:b:708:ILE:HG22	2:b:712:ARG:NH1	2.26	0.50
1:1:64:ASP:O	1:1:64:ASP:OD1	2.29	0.50
4:4:3:LEU:HD21	4:4:83:TYR:CD1	2.46	0.50
6:6:124:LEU:HD12	6:6:129:LEU:CD2	2.42	0.50
9:K:27:ILE:HA	9:K:62:THR:HG21	1.93	0.49
1:a:17:ASP:OD2	1:a:18:ASN:N	2.43	0.49
14:b:808:CLA:HBC2	11:m:12:LEU:HD23	1.94	0.49
6:f:93:GLU:HB3	6:f:96:GLU:HB2	1.93	0.49
1:1:222:PRO:HB3	1:1:249:MET:HE1	1.92	0.49
1:1:270:PHE:O	9:9:9:THR:OG1	2.29	0.49
1:A:216:GLN:HA	1:A:220:SER:OG	2.12	0.49
2:B:308:ASP:HA	2:B:313:LYS:HA	1.94	0.49
6:F:123:GLU:HB2	6:F:128:GLU:HB2	1.94	0.49
1:1:427:ASN:OD1	1:1:432:ARG:NH1	2.44	0.49
1:A:692:SER:HB2	2:B:584:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:216:GLN:HA	1:a:220:SER:OG	2.12	0.49
17:a:851:BCR:H362	14:b:802:CLA:H42	1.93	0.49
1:1:216:GLN:HA	1:1:220:SER:OG	2.12	0.49
1:1:504:ASN:ND2	14:1:1619:CLA:O2D	2.45	0.49
2:2:10:ASP:OD1	2:2:10:ASP:N	2.42	0.49
14:1:1634:CLA:H42	10:0:21:ILE:HG23	1.93	0.49
6:6:124:LEU:HD12	6:6:129:LEU:HD22	1.95	0.49
14:A:824:CLA:H2A	14:A:824:CLA:O2D	2.13	0.49
2:b:131:ASN:HB3	11:m:3:LEU:HD11	1.93	0.49
2:b:308:ASP:HA	2:b:313:LYS:HA	1.94	0.49
6:f:33:LYS:O	6:f:36:GLU:HG3	2.13	0.49
10:l:125:PHE:O	10:l:129:MET:HG2	2.11	0.49
1:1:328:ILE:O	1:1:332:HIS:ND1	2.44	0.49
4:4:104:LYS:O	4:4:109:ARG:NH1	2.44	0.49
1:A:593:ASP:OD1	1:A:728:ARG:NH1	2.46	0.49
14:a:833:CLA:OBD	10:l:19:THR:HG21	2.13	0.49
2:b:435:HIS:HB2	17:b:852:BCR:HC42	1.94	0.49
6:f:124:LEU:HD12	6:f:129:LEU:CD2	2.42	0.49
6:6:33:LYS:O	6:6:36:GLU:HG3	2.13	0.49
6:6:123:GLU:HB2	6:6:128:GLU:HB2	1.94	0.49
14:A:833:CLA:OBD	10:L:19:THR:HG21	2.13	0.49
6:F:16:LYS:O	6:F:19:ALA:N	2.46	0.49
6:F:93:GLU:HB3	6:F:96:GLU:HB2	1.93	0.49
1:a:593:ASP:OD1	1:a:728:ARG:NH1	2.46	0.49
1:1:593:ASP:OD1	1:1:728:ARG:NH1	2.46	0.49
6:6:16:LYS:O	6:6:19:ALA:N	2.46	0.49
6:6:34:ARG:HG3	6:6:38:TYR:CE2	2.48	0.49
8:8:19:MET:HA	8:8:19:MET:HE2	1.95	0.49
2:b:316:GLY:O	2:b:319:ASN:N	2.45	0.49
5:5:1:VAL:HG12	5:5:2:GLN:N	2.26	0.49
6:F:33:LYS:O	6:F:36:GLU:HG3	2.13	0.49
7:I:37:GLU:CD	10:L:103:LYS:HZ1	2.21	0.49
1:a:328:ILE:O	1:a:332:HIS:ND1	2.44	0.49
6:f:16:LYS:O	6:f:19:ALA:N	2.46	0.49
6:f:34:ARG:HG3	6:f:38:TYR:CE2	2.48	0.49
4:D:104:LYS:O	4:D:109:ARG:NH1	2.44	0.49
6:F:34:ARG:HG3	6:F:38:TYR:CE2	2.48	0.49
14:a:824:CLA:O2D	14:a:824:CLA:H2A	2.13	0.49
3:c:8:ASP:OD2	4:d:117:ARG:N	2.46	0.49
11:m:22:ALA:O	11:m:26:SER:OG	2.31	0.49
2:2:308:ASP:HA	2:2:313:LYS:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:93:GLU:HB3	6:6:96:GLU:HB2	1.93	0.49
11:M:22:ALA:O	11:M:26:SER:OG	2.31	0.48
2:b:440:TYR:O	2:b:444:ASP:OD2	2.31	0.48
2:b:479:THR:CG2	2:b:480:LEU:HD12	2.40	0.48
5:e:1:VAL:HG12	5:e:2:GLN:N	2.26	0.48
1:1:17:ASP:OD2	1:1:18:ASN:N	2.43	0.48
1:1:460:VAL:HG12	14:1:1636:CLA:HBC2	1.94	0.48
17:1:1652:BCR:H362	14:2:802:CLA:C4	2.42	0.48
1:a:460:VAL:HG12	14:a:835:CLA:HBC2	1.94	0.48
5:e:11:ARG:NE	5:e:64:GLU:OE1	2.39	0.48
8:j:1:FME:O	8:j:2:LYS:C	2.55	0.48
1:1:25:PHE:O	8:8:3:HIS:HB2	2.12	0.48
2:2:696:LEU:HD11	10:0:36:ALA:HB1	1.94	0.48
1:A:696:TYR:OH	14:A:802:CLA:OBD	2.28	0.48
2:b:135:TYR:OH	11:m:7:GLN:O	2.32	0.48
2:B:274:HIS:HB3	14:B:817:CLA:HMB2	1.95	0.48
2:B:470:HIS:CD2	14:B:834:CLA:ND	2.81	0.48
6:F:124:LEU:HD12	6:F:129:LEU:HD22	1.95	0.48
17:F:202:BCR:H331	14:F:203:CLA:HMB3	1.93	0.48
1:a:29:ALA:HB2	8:j:3:HIS:HB3	1.94	0.48
1:1:222:PRO:CB	1:1:249:MET:HE1	2.44	0.48
2:2:274:HIS:HB3	14:2:818:CLA:HMB2	1.95	0.48
2:2:459:GLU:OE1	2:2:464:GLN:NE2	2.41	0.48
2:2:470:HIS:CD2	14:2:835:CLA:ND	2.81	0.48
8:J:19:MET:HE2	8:J:19:MET:HA	1.95	0.48
9:K:16:GLY:HA2	14:K:101:CLA:OBD	2.12	0.48
10:L:98:LEU:HD21	10:l:38:ARG:HD2	1.96	0.48
2:b:314:VAL:HG11	14:b:823:CLA:HMB3	1.95	0.48
1:1:710:LYS:HA	6:6:136:ILE:HD11	1.95	0.48
8:J:1:FME:O	8:J:2:LYS:C	2.55	0.48
14:a:823:CLA:O1D	9:k:35:GLN:OE1	2.32	0.48
2:b:31:GLU:OE2	2:b:334:HIS:NE2	2.40	0.48
2:2:479:THR:HG22	2:2:480:LEU:N	2.24	0.48
1:A:145:GLN:OE1	1:A:145:GLN:N	2.45	0.48
1:A:460:VAL:HG12	14:A:835:CLA:HBC2	1.94	0.48
12:X:13:THR:O	12:X:17:VAL:HG13	2.14	0.48
1:A:222:PRO:CB	1:A:249:MET:HE1	2.44	0.48
2:B:314:VAL:HG11	14:B:822:CLA:HMB3	1.95	0.48
1:a:413:ALA:O	1:a:417:VAL:HG23	2.14	0.48
1:a:661:VAL:HG22	1:a:749:ALA:HB3	1.96	0.48
2:b:470:HIS:CD2	14:b:835:CLA:ND	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:PHE:CE2	1:A:279:LEU:HD13	2.49	0.48
1:A:413:ALA:O	1:A:417:VAL:HG23	2.14	0.48
2:b:14:ASP:OD2	2:b:18:ARG:NH1	2.47	0.48
12:z:13:THR:O	12:z:17:VAL:HG13	2.14	0.48
1:a:289:THR:HG22	1:a:382:TYR:CZ	2.49	0.48
6:f:124:LEU:HD12	6:f:129:LEU:HD22	1.95	0.48
12:x:13:THR:O	12:x:17:VAL:HG13	2.14	0.48
14:B:832:CLA:CBC	6:F:71:LEU:HD11	2.43	0.47
2:b:710:GLN:O	2:b:714:VAL:HG23	2.14	0.47
6:f:62:ASP:HA	8:j:38:PHE:HB2	1.95	0.47
1:1:711:LEU:HD21	14:2:832:CLA:H3A	1.96	0.47
1:A:172:MET:HE1	14:A:814:CLA:H92	1.96	0.47
2:B:440:TYR:O	2:B:444:ASP:OD2	2.32	0.47
1:a:569:LYS:NZ	2:b:679:GLU:OE2	2.47	0.47
1:a:701:ILE:O	1:a:705:VAL:HG22	2.14	0.47
6:f:76:TRP:HZ3	6:f:114:PHE:CA	2.26	0.47
1:1:289:THR:HG22	1:1:382:TYR:CZ	2.49	0.47
14:1:1625:CLA:O2D	14:1:1625:CLA:H2A	2.13	0.47
14:1:1635:CLA:H191	2:2:20:ILE:HG21	1.96	0.47
1:A:253:TYR:O	1:A:258:TRP:NE1	2.43	0.47
14:A:841:CLA:HAA2	14:B:831:CLA:HMB1	1.96	0.47
1:1:413:ALA:O	1:1:417:VAL:HG23	2.14	0.47
2:2:14:ASP:OD2	2:2:18:ARG:NH1	2.47	0.47
2:2:440:TYR:O	2:2:444:ASP:OD2	2.31	0.47
6:6:56:ARG:O	6:6:59:ARG:HB3	2.14	0.47
11:y:22:ALA:O	11:y:26:SER:OG	2.31	0.47
1:a:222:PRO:CB	1:a:249:MET:HE1	2.44	0.47
6:f:56:ARG:O	6:f:59:ARG:HB3	2.14	0.47
8:j:13:VAL:O	8:j:17:ILE:HG13	2.15	0.47
8:j:19:MET:HE2	8:j:19:MET:HA	1.95	0.47
1:1:432:ARG:O	1:1:436:HIS:ND1	2.46	0.47
7:7:10:LEU:HD22	7:7:14:PHE:CE2	2.49	0.47
2:B:166:TRP:CZ2	14:B:811:CLA:HMA1	2.50	0.47
2:B:710:GLN:O	2:B:714:VAL:HG23	2.14	0.47
6:F:56:ARG:O	6:F:59:ARG:HB3	2.14	0.47
8:J:25:ILE:HD13	14:J:101:CLA:HMB2	1.97	0.47
1:a:300:HIS:HB2	14:a:819:CLA:C1B	2.45	0.47
2:b:166:TRP:CZ2	14:b:812:CLA:HMA1	2.49	0.47
2:b:436:THR:HG22	2:b:440:TYR:HE2	1.79	0.47
8:j:25:ILE:HD13	14:j:1302:CLA:HMB2	1.97	0.47
1:1:701:ILE:O	1:1:705:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:710:GLN:O	2:2:714:VAL:HG23	2.14	0.47
8:8:13:VAL:O	8:8:17:ILE:HG13	2.15	0.47
10:0:62:TRP:HH2	10:0:85:LEU:HD22	1.78	0.47
1:A:701:ILE:O	1:A:705:VAL:HG22	2.14	0.47
14:A:824:CLA:HHC	14:A:824:CLA:HBB1	1.96	0.47
6:F:54:ASP:OD1	12:X:30:TYR:HE2	1.97	0.47
7:I:10:LEU:HD22	7:I:14:PHE:CE2	2.49	0.47
1:1:661:VAL:HG22	1:1:749:ALA:HB3	1.96	0.47
14:1:1624:CLA:O1D	9:9:35:GLN:OE1	2.33	0.47
1:A:504:ASN:ND2	14:A:818:CLA:O2D	2.45	0.47
1:a:372:GLN:HG2	14:a:827:CLA:HED1	1.96	0.47
1:a:396:HIS:CE1	14:a:829:CLA:ND	2.83	0.47
1:a:656:ALA:O	1:a:659:SER:OG	2.31	0.47
2:b:274:HIS:HB3	14:b:818:CLA:HMB2	1.95	0.47
14:b:811:CLA:CBB	7:i:19:CYS:HB3	2.44	0.47
1:1:145:GLN:OE1	1:1:145:GLN:N	2.45	0.47
1:1:317:THR:HG23	1:1:318:ASN:N	2.30	0.47
14:1:1620:CLA:H143	14:9:103:CLA:H91	1.97	0.47
2:2:146:SER:O	11:y:21:LEU:HD13	2.13	0.47
10:L:62:TRP:HH2	10:L:85:LEU:HD22	1.79	0.47
17:1:1652:BCR:H362	14:2:802:CLA:H42	1.97	0.47
9:9:65:PHE:HB2	17:9:102:BCR:H23C	1.97	0.47
1:A:289:THR:HG22	1:A:382:TYR:CZ	2.49	0.47
1:A:300:HIS:HB2	14:A:819:CLA:C1B	2.44	0.47
1:A:317:THR:HG23	1:A:318:ASN:N	2.30	0.47
2:B:436:THR:HG22	2:B:440:TYR:HE2	1.79	0.47
6:F:76:TRP:HZ3	6:F:114:PHE:CA	2.26	0.47
2:b:320:MET:HE2	18:b:851:LHG:HC81	1.97	0.47
2:2:436:THR:HG22	2:2:440:TYR:HE2	1.79	0.47
14:A:834:CLA:H191	2:B:20:ILE:HG21	1.97	0.47
14:b:836:CLA:CBC	12:x:35:LYS:O	2.63	0.47
10:l:62:TRP:HH2	10:l:85:LEU:HD22	1.79	0.47
14:1:1625:CLA:HHC	14:1:1625:CLA:HBB1	1.97	0.47
1:A:276:SER:O	1:A:276:SER:OG	2.24	0.46
2:B:281:VAL:O	2:B:285:VAL:HG23	2.15	0.46
8:J:13:VAL:O	8:J:17:ILE:HG13	2.15	0.46
17:M:103:BCR:H382	17:M:103:BCR:H23C	1.97	0.46
1:1:278:PHE:CE2	1:1:279:LEU:HD13	2.49	0.46
14:1:1644:CLA:HHC	14:1:1644:CLA:HBB1	1.97	0.46
2:2:281:VAL:O	2:2:285:VAL:HG23	2.15	0.46
1:A:36:ARG:HH21	1:A:36:ARG:CB	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:ASP:OD2	2:B:18:ARG:NH1	2.47	0.46
2:B:459:GLU:OE1	2:B:464:GLN:NE2	2.41	0.46
1:a:172:MET:HE1	14:a:814:CLA:H92	1.97	0.46
1:a:491:GLN:O	1:a:495:THR:HG23	2.15	0.46
14:a:824:CLA:HHC	14:a:824:CLA:HBB1	1.96	0.46
8:j:3:HIS:HA	8:j:6:THR:HG22	1.97	0.46
1:1:172:MET:HE1	14:1:1615:CLA:H92	1.97	0.46
1:1:396:HIS:CE1	14:1:1630:CLA:ND	2.83	0.46
2:2:320:MET:HE2	18:z:101:LHG:HC81	1.97	0.46
1:A:372:GLN:HG2	14:A:827:CLA:HED1	1.96	0.46
1:A:661:VAL:HG22	1:A:749:ALA:HB3	1.96	0.46
10:L:6:LYS:HB2	10:L:7:PRO:HD2	1.97	0.46
1:a:23:THR:HG21	1:a:177:TRP:HE1	1.81	0.46
2:b:281:VAL:O	2:b:285:VAL:HG23	2.15	0.46
14:b:836:CLA:HBC1	12:x:35:LYS:O	2.14	0.46
10:l:6:LYS:HB2	10:l:7:PRO:HD2	1.97	0.46
14:l:204:CLA:HHC	14:l:204:CLA:HBB1	1.97	0.46
1:1:300:HIS:HB2	14:1:1620:CLA:C1B	2.45	0.46
1:1:372:GLN:HG2	14:1:1628:CLA:HED1	1.96	0.46
1:1:491:GLN:O	1:1:495:THR:HG23	2.16	0.46
2:2:166:TRP:CZ2	14:2:812:CLA:HMA1	2.49	0.46
2:2:314:VAL:HG11	14:2:823:CLA:HMB3	1.95	0.46
2:2:453:GLU:HA	6:6:48:LEU:HD22	1.98	0.46
6:6:76:TRP:HZ3	6:6:114:PHE:CA	2.26	0.46
17:m:102:BCR:H382	17:m:102:BCR:H23C	1.97	0.46
14:X:1701:CLA:O1D	14:X:1701:CLA:H2A	2.16	0.46
1:a:278:PHE:CE2	1:a:279:LEU:HD13	2.49	0.46
1:a:432:ARG:O	1:a:436:HIS:ND1	2.46	0.46
6:6:17:ARG:O	6:6:35:PHE:CZ	2.69	0.46
1:A:373:HIS:NE2	14:A:828:CLA:NC	2.64	0.46
14:A:843:CLA:HHC	14:A:843:CLA:HBB1	1.98	0.46
14:B:841:CLA:H91	17:I:101:BCR:H19C	1.98	0.46
9:K:49:ALA:O	9:K:50:LEU:HB2	2.16	0.46
7:i:10:LEU:HD22	7:i:14:PHE:CE2	2.49	0.46
12:x:22:ILE:HA	12:x:25:LEU:HD23	1.97	0.46
1:1:618:GLN:HE22	1:1:750:ARG:HE	1.63	0.46
1:A:396:HIS:CE1	14:A:829:CLA:ND	2.83	0.46
9:K:16:GLY:O	9:K:20:ILE:HG12	2.16	0.46
10:L:8:TYR:CD1	10:L:16:HIS:HD2	2.34	0.46
10:l:8:TYR:CD1	10:l:16:HIS:HD2	2.34	0.46
9:9:16:GLY:O	9:9:20:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:GLN:O	1:A:495:THR:HG23	2.15	0.46
1:a:373:HIS:NE2	14:a:828:CLA:NC	2.64	0.46
1:a:427:ASN:OD1	1:a:432:ARG:NH1	2.44	0.46
2:b:319:ASN:OD1	2:b:319:ASN:O	2.34	0.46
1:1:670:SER:HB2	2:2:448:ALA:HB1	1.97	0.46
9:9:49:ALA:O	9:9:50:LEU:HB2	2.16	0.46
1:A:618:GLN:HE22	1:A:750:ARG:HE	1.63	0.46
8:J:3:HIS:HA	8:J:6:THR:HG22	1.97	0.46
14:L:203:CLA:HHC	14:L:203:CLA:HBB1	1.98	0.46
1:a:317:THR:HG23	1:a:318:ASN:N	2.30	0.46
14:a:843:CLA:HHC	14:a:843:CLA:HBB1	1.98	0.46
1:a:36:ARG:HH21	1:a:36:ARG:CB	2.27	0.46
1:a:145:GLN:OE1	1:a:145:GLN:N	2.45	0.46
2:b:459:GLU:OE1	2:b:464:GLN:NE2	2.41	0.46
8:8:25:ILE:HD13	14:8:1302:CLA:HMB2	1.97	0.46
2:B:320:MET:HE2	18:B:850:LHG:HC81	1.97	0.45
12:X:20:LEU:O	12:X:24:PHE:CD2	2.69	0.45
1:a:667:SER:OG	1:a:668:ALA:N	2.50	0.45
9:k:49:ALA:O	9:k:50:LEU:HB2	2.16	0.45
10:l:76:LEU:HD13	10:0:144:VAL:HG21	1.98	0.45
1:1:36:ARG:HH21	1:1:36:ARG:CB	2.27	0.45
1:1:121:VAL:HG23	1:1:122:GLY:H	1.81	0.45
12:z:22:ILE:HA	12:z:25:LEU:HD23	1.97	0.45
2:B:387:VAL:HG12	2:B:582:PHE:CE1	2.51	0.45
14:B:834:CLA:H41	14:B:835:CLA:O1A	2.17	0.45
4:D:117:ARG:NH2	4:D:122:ASN:OD1	2.48	0.45
1:a:524:VAL:HG22	1:a:625:VAL:HG23	1.99	0.45
14:x:1701:CLA:O1D	14:x:1701:CLA:H2A	2.16	0.45
3:3:8:ASP:OD2	4:4:117:ARG:CA	2.64	0.45
12:z:20:LEU:O	12:z:24:PHE:CD2	2.69	0.45
1:A:432:ARG:O	1:A:436:HIS:ND1	2.46	0.45
14:A:807:CLA:H42	18:A:853:LHG:H261	1.99	0.45
12:X:22:ILE:HA	12:X:25:LEU:HD23	1.97	0.45
2:b:387:VAL:HG12	2:b:582:PHE:CE1	2.51	0.45
1:1:373:HIS:NE2	14:1:1629:CLA:NC	2.64	0.45
17:y:102:BCR:H382	17:y:102:BCR:H23C	1.97	0.45
14:z:102:CLA:O1D	14:z:102:CLA:H2A	2.16	0.45
6:F:34:ARG:NH1	8:J:35:ASP:OD2	2.46	0.45
1:a:504:ASN:ND2	14:a:818:CLA:O2D	2.45	0.45
1:a:546:ILE:O	1:a:550:VAL:HG23	2.16	0.45
2:b:406:ASN:OD1	2:b:406:ASN:O	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:k:16:GLY:O	9:k:20:ILE:HG12	2.16	0.45
1:1:546:ILE:O	1:1:550:VAL:HG23	2.16	0.45
14:2:808:CLA:HAA1	7:7:15:ILE:HD11	1.99	0.45
3:3:59:THR:OG1	3:3:61:PHE:O	2.20	0.45
10:0:131:SER:HA	10:0:134:VAL:HG12	1.99	0.45
1:A:524:VAL:HG22	1:A:625:VAL:HG23	1.98	0.45
1:A:546:ILE:O	1:A:550:VAL:HG23	2.16	0.45
2:b:131:ASN:HB3	11:m:3:LEU:CD1	2.47	0.45
14:b:835:CLA:H41	14:b:836:CLA:O1A	2.17	0.45
6:f:59:ARG:HG3	6:f:59:ARG:O	2.17	0.45
1:1:451:LEU:O	1:1:455:SER:OG	2.27	0.45
6:F:17:ARG:O	6:F:35:PHE:CZ	2.69	0.45
6:F:135:GLU:OE1	6:F:135:GLU:HA	2.17	0.45
9:K:70:ALA:O	9:K:71:ALA:C	2.60	0.45
1:a:253:TYR:O	1:a:258:TRP:NE1	2.43	0.45
1:a:713:VAL:HG12	1:a:713:VAL:O	2.17	0.45
2:b:90:ILE:HB	2:b:111:PRO:HB2	1.98	0.45
2:b:658:PHE:O	2:b:662:VAL:HG23	2.17	0.45
3:c:59:THR:OG1	3:c:61:PHE:O	2.20	0.45
6:f:17:ARG:O	6:f:35:PHE:CZ	2.69	0.45
10:l:38:ARG:HB3	10:l:41:LEU:HD13	1.99	0.45
12:x:20:LEU:O	12:x:24:PHE:CD2	2.69	0.45
2:2:387:VAL:HG12	2:2:582:PHE:CE1	2.51	0.45
14:2:805:CLA:O1A	11:y:30:TYR:HB2	2.17	0.45
14:2:835:CLA:H41	14:2:836:CLA:O1A	2.17	0.45
1:A:23:THR:HG21	1:A:177:TRP:HE1	1.81	0.45
1:A:427:ASN:OD1	1:A:432:ARG:NH1	2.44	0.45
1:A:451:LEU:O	1:A:455:SER:OG	2.27	0.45
1:A:655:TRP:CZ2	2:B:635:SER:HB2	2.51	0.45
2:B:319:ASN:OD1	2:B:319:ASN:O	2.34	0.45
2:B:406:ASN:OD1	2:B:406:ASN:O	2.34	0.45
9:K:70:ALA:O	9:K:74:VAL:HG12	2.17	0.45
2:b:309:PHE:N	2:b:312:THR:O	2.37	0.45
4:d:94:ILE:HG13	4:d:95:HIS:N	2.32	0.45
2:2:319:ASN:OD1	2:2:319:ASN:O	2.34	0.45
6:6:135:GLU:HA	6:6:135:GLU:OE1	2.17	0.45
8:8:3:HIS:HA	8:8:6:THR:HG22	1.97	0.45
10:0:8:TYR:CD1	10:0:16:HIS:HD2	2.34	0.45
6:f:98:GLU:HG2	14:f:201:CLA:O1D	2.17	0.45
2:2:316:GLY:O	2:2:317:PRO:C	2.60	0.45
2:2:658:PHE:O	2:2:662:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:809:CLA:C1A	14:2:809:CLA:CGA	2.95	0.45
5:5:5:SER:HB2	5:5:70:PRO:HA	1.99	0.45
6:6:60:ALA:HB1	6:6:64:LEU:HB3	1.99	0.45
10:0:6:LYS:HB2	10:0:7:PRO:HD2	1.97	0.45
14:0:205:CLA:HHC	14:0:205:CLA:HBB1	1.97	0.45
2:B:90:ILE:HB	2:B:111:PRO:HB2	1.98	0.45
6:F:60:ALA:HB1	6:F:64:LEU:HB3	1.99	0.45
1:a:618:GLN:HE22	1:a:750:ARG:HE	1.64	0.45
14:a:832:CLA:O1D	10:l:5:VAL:HG11	2.16	0.45
2:b:316:GLY:O	2:b:317:PRO:C	2.60	0.45
1:1:667:SER:OG	1:1:668:ALA:N	2.50	0.45
1:1:692:SER:HB2	2:2:584:LEU:HD21	1.99	0.45
14:1:1642:CLA:HAA2	14:2:832:CLA:HMB1	1.97	0.45
3:3:60:ASP:OD2	5:5:11:ARG:NH1	2.47	0.45
6:6:59:ARG:O	6:6:59:ARG:HG3	2.17	0.45
10:L:38:ARG:HB3	10:L:41:LEU:HD13	1.98	0.45
9:k:70:ALA:O	9:k:74:VAL:HG12	2.17	0.45
1:1:300:HIS:HB2	14:1:1620:CLA:CHB	2.47	0.45
1:1:410:ALA:O	1:1:414:ILE:HG13	2.17	0.45
2:2:90:ILE:HB	2:2:111:PRO:HB2	1.98	0.45
1:A:401:GLY:O	1:A:405:VAL:HG23	2.17	0.44
1:a:321:ILE:HD11	14:a:821:CLA:H2A	1.99	0.44
14:a:833:CLA:H42	10:l:21:ILE:HG23	1.99	0.44
2:b:136:GLN:OE1	2:b:136:GLN:HA	2.18	0.44
3:c:33:CYS:SG	3:c:34:LYS:N	2.91	0.44
5:e:5:SER:HB2	5:e:70:PRO:HA	1.99	0.44
2:2:136:GLN:OE1	2:2:136:GLN:HA	2.18	0.44
6:6:70:PHE:O	6:6:71:LEU:C	2.61	0.44
6:6:70:PHE:O	6:6:73:ILE:N	2.51	0.44
1:A:121:VAL:HG23	1:A:122:GLY:H	1.81	0.44
1:A:300:HIS:HB2	14:A:819:CLA:CHB	2.47	0.44
1:A:328:ILE:O	1:A:332:HIS:ND1	2.44	0.44
2:B:443:ASN:O	2:B:447:VAL:HG12	2.18	0.44
5:E:5:SER:HB2	5:E:70:PRO:HA	1.99	0.44
1:a:121:VAL:HG23	1:a:122:GLY:H	1.81	0.44
1:a:401:GLY:O	1:a:405:VAL:HG23	2.17	0.44
1:a:564:ARG:NH2	4:d:14:THR:O	2.50	0.44
1:1:23:THR:HG21	1:1:177:TRP:HE1	1.81	0.44
1:1:590:SER:OG	1:1:593:ASP:OD2	2.35	0.44
2:2:406:ASN:OD1	2:2:406:ASN:O	2.34	0.44
1:A:324:SER:OG	1:A:327:GLU:OE2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:SER:OG	1:A:668:ALA:N	2.50	0.44
2:B:658:PHE:O	2:B:662:VAL:HG23	2.17	0.44
3:C:18:ARG:HG2	4:D:103:GLU:HG2	1.99	0.44
6:F:76:TRP:CZ3	6:F:113:GLY:C	2.96	0.44
14:b:809:CLA:C1A	14:b:809:CLA:CGA	2.95	0.44
1:1:524:VAL:HG22	1:1:625:VAL:HG23	1.98	0.44
1:1:702:GLU:CD	2:2:551:LYS:HB3	2.41	0.44
4:4:1:THR:HG22	4:4:2:THR:N	2.32	0.44
11:y:16:LEU:HD12	17:y:102:BCR:H21C	1.99	0.44
6:F:59:ARG:O	6:F:59:ARG:HG3	2.17	0.44
1:a:410:ALA:O	1:a:414:ILE:HG13	2.17	0.44
14:l:205:CLA:HBC2	14:l:205:CLA:HHD	1.99	0.44
3:3:60:ASP:H	5:5:58:ASN:HD22	1.65	0.44
1:A:57:ASP:OD1	14:A:831:CLA:CAA	2.66	0.44
1:a:324:SER:OG	1:a:327:GLU:HB2	2.18	0.44
1:a:435:ARG:HD2	4:d:12:GLY:O	2.17	0.44
1:1:11:LYS:NZ	9:9:39:LYS:NZ	2.66	0.44
3:3:33:CYS:SG	3:3:34:LYS:N	2.91	0.44
9:9:70:ALA:O	9:9:71:ALA:C	2.60	0.44
6:F:70:PHE:O	6:F:71:LEU:C	2.61	0.44
11:M:16:LEU:HD12	17:M:103:BCR:H21C	1.99	0.44
17:a:851:BCR:H24C	14:b:834:CLA:HMC1	1.99	0.44
2:b:92:ASP:O	7:i:1:FME:HE2	2.18	0.44
4:d:73:ARG:N	4:d:74:PRO:HD2	2.33	0.44
9:k:70:ALA:O	9:k:71:ALA:C	2.60	0.44
9:9:70:ALA:O	9:9:74:VAL:HG12	2.17	0.44
1:A:321:ILE:HD11	14:A:821:CLA:H2A	1.98	0.44
2:B:231:VAL:O	2:B:234:GLN:HB2	2.18	0.44
6:F:24:THR:OG1	6:F:25:THR:N	2.51	0.44
1:a:360:LEU:HG	1:a:404:LEU:O	2.18	0.44
14:a:807:CLA:H42	18:a:853:LHG:H261	1.99	0.44
2:b:555:ASP:OD1	3:c:61:PHE:HE2	2.00	0.44
6:f:24:THR:OG1	6:f:25:THR:N	2.51	0.44
1:1:57:ASP:OD1	14:1:1632:CLA:CAA	2.66	0.44
1:1:324:SER:OG	1:1:327:GLU:HB2	2.18	0.44
1:1:401:GLY:O	1:1:405:VAL:HG23	2.17	0.44
4:4:94:ILE:HG13	4:4:95:HIS:N	2.32	0.44
2:B:157:GLN:O	2:B:161:ARG:HG3	2.18	0.44
2:B:479:THR:HG22	2:B:480:LEU:N	2.24	0.44
4:D:94:ILE:HG13	4:D:95:HIS:N	2.32	0.44
4:D:107:LYS:O	4:D:109:ARG:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:443:ASN:O	2:b:447:VAL:HG12	2.18	0.44
14:b:812:CLA:H172	14:b:815:CLA:H91	2.00	0.44
10:l:16:HIS:NE2	10:l:22:SER:OG	2.32	0.44
1:1:679:ALA:HB1	1:1:738:GLY:O	2.18	0.44
10:0:38:ARG:HB3	10:0:41:LEU:HD13	1.98	0.44
2:B:316:GLY:O	2:B:317:PRO:C	2.60	0.44
2:B:413:ARG:NH2	18:B:850:LHG:O1	2.51	0.44
2:B:498:VAL:O	2:B:501:PRO:HD2	2.18	0.44
14:B:808:CLA:C1A	14:B:808:CLA:CGA	2.95	0.44
10:L:131:SER:HA	10:L:134:VAL:HG12	1.99	0.44
1:a:297:THR:O	1:a:300:HIS:HB3	2.18	0.44
2:b:157:GLN:O	2:b:161:ARG:HG3	2.18	0.44
2:b:255:THR:HG22	2:b:256:PHE:H	1.83	0.44
2:b:292:THR:OG1	2:b:293:GLN:N	2.51	0.44
6:f:76:TRP:CZ3	6:f:113:GLY:C	2.96	0.44
1:1:321:ILE:HD11	14:1:1622:CLA:H2A	1.98	0.44
2:2:222:ALA:N	2:2:223:PRO:CD	2.81	0.44
4:4:73:ARG:N	4:4:74:PRO:HD2	2.33	0.44
14:0:206:CLA:HBC2	14:0:206:CLA:HHD	2.00	0.44
4:D:73:ARG:N	4:D:74:PRO:HD2	2.33	0.43
6:F:98:GLU:HG2	14:F:201:CLA:O1D	2.18	0.43
14:L:204:CLA:HHD	14:L:204:CLA:HBC2	1.99	0.43
1:a:605:CYS:O	1:a:609:VAL:HG23	2.18	0.43
4:d:107:LYS:O	4:d:109:ARG:N	2.51	0.43
6:f:60:ALA:HB1	6:f:64:LEU:HB3	1.99	0.43
11:m:16:LEU:HD12	17:m:102:BCR:H21C	1.99	0.43
1:1:313:HIS:CE1	14:1:1622:CLA:NC	2.85	0.43
1:1:569:LYS:NZ	2:2:679:GLU:OE2	2.49	0.43
1:1:696:TYR:OH	14:1:1603:CLA:OBD	2.28	0.43
14:1:1635:CLA:HAA1	17:0:203:BCR:C17	2.48	0.43
6:6:24:THR:OG1	6:6:25:THR:N	2.51	0.43
1:A:360:LEU:HG	1:A:404:LEU:O	2.18	0.43
1:A:713:VAL:HG12	1:A:713:VAL:O	2.17	0.43
14:A:839:CLA:O1D	14:A:839:CLA:H2A	2.18	0.43
2:B:292:THR:OG1	2:B:293:GLN:N	2.51	0.43
4:D:1:THR:HG22	4:D:2:THR:N	2.32	0.43
1:a:451:LEU:O	1:a:455:SER:OG	2.27	0.43
1:a:702:GLU:O	1:a:705:VAL:HG23	2.18	0.43
2:b:256:PHE:CD1	14:b:818:CLA:HMB3	2.53	0.43
2:b:412:ASP:O	2:b:416:GLN:HG2	2.18	0.43
14:b:805:CLA:O1A	11:m:30:TYR:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:70:PHE:O	6:f:73:ILE:N	2.51	0.43
6:f:135:GLU:OE1	6:f:135:GLU:HA	2.17	0.43
14:1:1640:CLA:O1D	14:1:1640:CLA:H2A	2.18	0.43
2:2:413:ARG:NH2	18:z:101:LHG:O1	2.51	0.43
2:2:498:VAL:O	2:2:501:PRO:HD2	2.18	0.43
1:A:313:HIS:CE1	14:A:821:CLA:NC	2.86	0.43
1:A:410:ALA:O	1:A:414:ILE:HG13	2.17	0.43
14:A:840:CLA:H2A	14:A:840:CLA:O2D	2.18	0.43
14:B:811:CLA:H172	14:B:814:CLA:H91	2.00	0.43
3:C:33:CYS:SG	3:C:34:LYS:N	2.91	0.43
1:a:355:GLN:NE2	21:a:902:HOH:O	2.51	0.43
14:1:1608:CLA:H42	18:1:1654:LHG:H261	1.99	0.43
2:2:255:THR:HG22	2:2:256:PHE:H	1.83	0.43
2:2:443:ASN:O	2:2:447:VAL:HG12	2.18	0.43
4:4:88:ASP:OD1	4:4:90:GLU:HB2	2.18	0.43
6:6:116:TRP:N	6:6:117:PRO:CD	2.82	0.43
1:A:679:ALA:HB1	1:A:738:GLY:O	2.18	0.43
1:A:702:GLU:O	1:A:705:VAL:HG23	2.18	0.43
2:B:92:ASP:O	7:I:1:FME:HE2	2.19	0.43
2:B:339:TRP:HE1	14:B:824:CLA:C2B	2.31	0.43
1:a:300:HIS:HB2	14:a:819:CLA:CHB	2.47	0.43
1:a:313:HIS:CE1	14:a:821:CLA:NC	2.86	0.43
1:a:661:VAL:HG21	1:a:746:PHE:HA	2.01	0.43
2:b:413:ARG:NH2	18:b:851:LHG:O1	2.51	0.43
10:l:131:SER:HA	10:l:134:VAL:HG12	1.99	0.43
1:1:297:THR:O	1:1:300:HIS:HB3	2.18	0.43
1:1:360:LEU:HG	1:1:404:LEU:O	2.18	0.43
2:2:412:ASP:O	2:2:416:GLN:HG2	2.18	0.43
1:A:341:HIS:HB3	1:A:344:LEU:HD12	2.01	0.43
6:F:42:LEU:HG	6:F:59:ARG:HH12	1.84	0.43
6:F:116:TRP:N	6:F:117:PRO:CD	2.82	0.43
1:a:710:LYS:O	6:f:130:THR:HA	2.19	0.43
4:d:1:THR:HG22	4:d:2:THR:N	2.32	0.43
6:f:116:TRP:N	6:f:117:PRO:CD	2.82	0.43
1:1:242:PHE:HD2	1:1:249:MET:HE3	1.84	0.43
1:1:713:VAL:HG12	1:1:713:VAL:O	2.17	0.43
2:2:292:THR:OG1	2:2:293:GLN:N	2.51	0.43
4:4:32:THR:HA	4:4:52:GLY:O	2.19	0.43
1:A:656:ALA:O	1:A:659:SER:OG	2.31	0.43
1:A:661:VAL:HG21	1:A:746:PHE:HA	2.01	0.43
2:B:222:ALA:N	2:B:223:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:ASP:O	2:B:416:GLN:HG2	2.18	0.43
1:a:57:ASP:OD1	14:a:831:CLA:CAA	2.66	0.43
14:a:840:CLA:H2A	14:a:840:CLA:O2D	2.18	0.43
4:d:88:ASP:OD1	4:d:90:GLU:HB2	2.19	0.43
10:l:68:LEU:HD23	10:l:73:VAL:HG23	2.01	0.43
10:l:79:LEU:HD23	10:0:137:PHE:CE2	2.54	0.43
1:1:372:GLN:O	1:1:375:TYR:CE1	2.72	0.43
3:3:18:ARG:HG2	4:4:103:GLU:HG2	2.00	0.43
1:A:118:TRP:CZ3	17:A:856:BCR:HC8	2.54	0.43
1:A:324:SER:OG	1:A:327:GLU:HB2	2.18	0.43
2:B:164:LEU:HD11	2:B:168:LYS:HE3	2.01	0.43
6:F:70:PHE:O	6:F:73:ILE:N	2.51	0.43
1:a:341:HIS:HB3	1:a:344:LEU:HD12	2.01	0.43
2:b:136:GLN:OE1	2:b:136:GLN:CA	2.67	0.43
2:b:231:VAL:O	2:b:234:GLN:HB2	2.18	0.43
2:b:594:GLY:O	2:b:598:PHE:CD1	2.71	0.43
1:1:253:TYR:O	1:1:258:TRP:NE1	2.43	0.43
1:1:716:ALA:HB3	6:6:98:GLU:OE1	2.18	0.43
17:1:1653:BCR:HC8	17:8:1305:BCR:H332	2.01	0.43
2:2:157:GLN:O	2:2:161:ARG:HG3	2.18	0.43
2:2:555:ASP:OD1	3:3:61:PHE:HE2	2.00	0.43
10:0:142:PHE:CD1	14:0:207:CLA:H43	2.54	0.43
12:z:19:LEU:HD21	18:z:101:LHG:C21	2.48	0.43
2:B:255:THR:HG22	2:B:256:PHE:H	1.83	0.43
1:a:242:PHE:HD2	1:a:249:MET:HE3	1.84	0.43
2:b:498:VAL:O	2:b:501:PRO:HD2	2.18	0.43
14:b:833:CLA:HHC	14:b:833:CLA:HBB1	2.00	0.43
2:2:136:GLN:OE1	2:2:136:GLN:CA	2.67	0.43
2:2:339:TRP:HE1	14:2:825:CLA:C2B	2.32	0.43
2:B:256:PHE:CD1	14:B:817:CLA:HMB3	2.53	0.43
18:M:101:LHG:H112	18:l:201:LHG:H261	2.01	0.43
1:a:70:ARG:NH2	1:a:185:PRO:O	2.51	0.43
2:b:342:ALA:O	2:b:346:VAL:HG23	2.19	0.43
6:f:42:LEU:HG	6:f:59:ARG:HH12	1.84	0.43
10:l:60:GLY:N	10:l:61:PRO:CD	2.82	0.43
1:1:605:CYS:O	1:1:609:VAL:HG23	2.18	0.43
2:2:110:ASN:OD1	2:2:110:ASN:N	2.52	0.43
6:6:76:TRP:CZ3	6:6:113:GLY:C	2.96	0.43
10:0:60:GLY:N	10:0:61:PRO:CD	2.82	0.43
1:a:292:LEU:HD12	1:a:379:PRO:HB3	2.01	0.43
1:a:596:PHE:HE1	1:a:728:ARG:O	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:a:841:CLA:O2D	14:a:841:CLA:H2A	2.19	0.43
2:b:339:TRP:HE1	14:b:825:CLA:C2B	2.31	0.43
1:1:341:HIS:HB3	1:1:344:LEU:HD12	2.01	0.43
2:2:231:VAL:O	2:2:234:GLN:HB2	2.18	0.43
2:2:342:ALA:O	2:2:346:VAL:HG23	2.19	0.43
1:A:511:VAL:HB	1:A:526:MET:HG3	2.02	0.42
14:B:832:CLA:HHC	14:B:832:CLA:HBB1	2.00	0.42
6:F:101:ILE:HG13	8:J:14:LEU:HD23	2.00	0.42
10:L:142:PHE:CD1	14:L:205:CLA:H43	2.54	0.42
1:a:281:PHE:CD1	14:a:819:CLA:HMB3	2.54	0.42
2:b:255:THR:HG22	2:b:256:PHE:N	2.34	0.42
2:b:479:THR:HG22	2:b:480:LEU:N	2.24	0.42
4:d:117:ARG:NH2	4:d:122:ASN:OD1	2.48	0.42
6:f:70:PHE:O	6:f:71:LEU:C	2.60	0.42
2:2:44:LYS:NZ	11:y:29:LEU:O	2.52	0.42
2:2:726:THR:HG23	14:2:803:CLA:O1D	2.19	0.42
14:2:812:CLA:H172	14:2:815:CLA:H91	2.00	0.42
4:4:107:LYS:O	4:4:109:ARG:N	2.51	0.42
6:6:42:LEU:HG	6:6:59:ARG:HH12	1.83	0.42
1:A:242:PHE:HD2	1:A:249:MET:HE3	1.84	0.42
1:A:605:CYS:O	1:A:609:VAL:HG23	2.18	0.42
2:B:414:VAL:HG11	17:B:846:BCR:H401	2.01	0.42
2:B:726:THR:HG23	14:B:802:CLA:O1D	2.19	0.42
6:F:103:VAL:HB	6:F:104:PRO:HD3	2.01	0.42
1:a:679:ALA:HB1	1:a:738:GLY:O	2.18	0.42
2:b:222:ALA:N	2:b:223:PRO:CD	2.81	0.42
1:1:95:ALA:HB2	1:1:158:LEU:HB2	2.02	0.42
1:1:596:PHE:HE1	1:1:728:ARG:O	2.02	0.42
1:1:702:GLU:O	1:1:705:VAL:HG23	2.18	0.42
2:2:256:PHE:CD1	14:2:818:CLA:HMB3	2.53	0.42
2:2:594:GLY:O	2:2:598:PHE:CD1	2.71	0.42
14:2:833:CLA:HHC	14:2:833:CLA:HBB1	2.00	0.42
14:2:839:CLA:C16	17:6:204:BCR:H23C	2.50	0.42
1:A:95:ALA:HB2	1:A:158:LEU:HB2	2.01	0.42
1:A:297:THR:O	1:A:300:HIS:HB3	2.18	0.42
1:A:372:GLN:O	1:A:375:TYR:CE1	2.72	0.42
2:B:320:MET:CE	18:B:850:LHG:HC81	2.49	0.42
2:B:594:GLY:O	2:B:598:PHE:CD1	2.71	0.42
14:B:814:CLA:H141	14:B:814:CLA:H161	1.86	0.42
1:a:270:PHE:CD2	9:k:74:VAL:HG11	2.54	0.42
1:a:372:GLN:O	1:a:375:TYR:CE1	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:a:839:CLA:H2A	14:a:839:CLA:O1D	2.18	0.42
6:f:70:PHE:HB2	17:f:202:BCR:C32	2.49	0.42
10:l:142:PHE:CD1	14:l:206:CLA:H43	2.54	0.42
1:1:511:VAL:HB	1:1:526:MET:HG3	2.01	0.42
14:1:1641:CLA:O2D	14:1:1641:CLA:H2A	2.18	0.42
2:2:276:HIS:HA	2:2:279:ILE:HG12	2.02	0.42
10:0:57:PHE:CD1	14:0:207:CLA:HBC2	2.54	0.42
1:A:281:PHE:CD1	14:A:819:CLA:HMB3	2.54	0.42
1:A:670:SER:HB2	2:B:448:ALA:HB1	2.02	0.42
14:B:816:CLA:H2A	14:B:816:CLA:O2D	2.20	0.42
3:C:13:CYS:C	3:C:14:THR:HG1	2.21	0.42
4:D:88:ASP:OD1	4:D:90:GLU:HB2	2.18	0.42
18:L:208:LHG:H261	18:y:101:LHG:H112	2.01	0.42
2:b:320:MET:CE	18:b:851:LHG:HC81	2.49	0.42
4:d:32:THR:HA	4:d:52:GLY:O	2.19	0.42
1:1:118:TRP:CZ3	17:8:1305:BCR:HC8	2.54	0.42
14:1:1642:CLA:H2A	14:1:1642:CLA:O2D	2.19	0.42
6:6:11:SER:O	6:6:12:PRO:C	2.62	0.42
6:6:103:VAL:HB	6:6:104:PRO:HD3	2.01	0.42
10:0:29:THR:O	10:0:33:ASN:ND2	2.52	0.42
2:B:255:THR:HG22	2:B:256:PHE:N	2.34	0.42
6:F:41:ALA:HB3	6:F:49:PRO:HB3	2.01	0.42
10:L:29:THR:O	10:L:33:ASN:ND2	2.52	0.42
10:L:60:GLY:N	10:L:61:PRO:CD	2.82	0.42
10:L:131:SER:O	10:L:134:VAL:HG12	2.20	0.42
1:a:380:TYR:OH	14:a:830:CLA:OBD	2.33	0.42
1:a:511:VAL:HB	1:a:526:MET:HG3	2.01	0.42
2:b:21:TRP:CG	2:b:710:GLN:HE22	2.38	0.42
10:l:83:ILE:HA	10:l:129:MET:HE1	2.02	0.42
1:1:292:LEU:HD12	1:1:379:PRO:HB3	2.01	0.42
2:2:164:LEU:HD11	2:2:168:LYS:HE3	2.01	0.42
2:2:320:MET:CE	18:z:101:LHG:HC81	2.49	0.42
10:0:68:LEU:HD23	10:0:73:VAL:HG23	2.01	0.42
1:A:380:TYR:OH	14:A:830:CLA:OBD	2.33	0.42
14:A:841:CLA:O2D	14:A:841:CLA:H2A	2.19	0.42
2:B:256:PHE:HE2	2:B:499:TRP:HB3	1.85	0.42
6:F:11:SER:O	6:F:12:PRO:C	2.62	0.42
10:L:57:PHE:CD1	14:L:205:CLA:HBC2	2.54	0.42
2:b:198:ILE:N	2:b:199:PRO:HD2	2.35	0.42
2:b:414:VAL:HG11	17:b:847:BCR:H401	2.01	0.42
1:1:285:LEU:HD23	1:1:292:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:661:VAL:HG21	1:1:746:PHE:HA	2.01	0.42
14:2:808:CLA:H201	18:y:101:LHG:H381	2.02	0.42
6:6:101:ILE:HG13	8:8:14:LEU:CD2	2.49	0.42
12:z:12:ARG:HH21	18:z:101:LHG:C7	2.32	0.42
1:A:292:LEU:HD12	1:A:379:PRO:HB3	2.01	0.42
2:B:136:GLN:OE1	2:B:136:GLN:CA	2.67	0.42
2:B:564:PRO:HA	2:B:712:ARG:HH22	1.85	0.42
3:C:37:GLN:OE1	4:D:105:VAL:HB	2.20	0.42
9:K:56:LEU:HB3	9:K:57:PRO:HD3	2.02	0.42
1:a:596:PHE:CZ	1:a:728:ARG:HB3	2.55	0.42
2:b:164:LEU:HD11	2:b:168:LYS:HE3	2.01	0.42
6:f:103:VAL:HB	6:f:104:PRO:HD3	2.01	0.42
9:k:34:ILE:HD12	9:k:34:ILE:H	1.85	0.42
10:l:57:PHE:CD1	14:l:206:CLA:HBC2	2.54	0.42
2:2:21:TRP:CG	2:2:710:GLN:HE22	2.38	0.42
6:6:41:ALA:HB3	6:6:49:PRO:HB3	2.01	0.42
6:6:42:LEU:HG	6:6:59:ARG:NH1	2.35	0.42
8:8:2:LYS:HE2	8:8:2:LYS:HB2	1.80	0.42
1:A:270:PHE:CE2	9:K:74:VAL:HG11	2.55	0.42
2:B:21:TRP:CG	2:B:710:GLN:HE22	2.38	0.42
2:B:136:GLN:OE1	2:B:136:GLN:HA	2.18	0.42
2:B:198:ILE:N	2:B:199:PRO:HD2	2.35	0.42
2:B:276:HIS:HA	2:B:279:ILE:HG12	2.02	0.42
4:D:32:THR:HA	4:D:52:GLY:O	2.19	0.42
4:D:120:GLY:CA	5:E:13:GLU:OE2	2.68	0.42
6:F:31:GLY:HA2	6:F:34:ARG:NH1	2.35	0.42
6:F:42:LEU:HG	6:F:59:ARG:NH1	2.35	0.42
13:a:801:CL0:CMB	14:b:802:CLA:OBD	2.68	0.42
14:a:829:CLA:O1D	14:a:829:CLA:H2A	2.20	0.42
7:i:10:LEU:O	7:i:14:PHE:CD2	2.73	0.42
3:3:37:GLN:OE1	4:4:105:VAL:HB	2.19	0.42
4:4:117:ARG:NH2	4:4:122:ASN:OD1	2.48	0.42
10:0:83:ILE:HA	10:0:129:MET:HE1	2.02	0.42
14:A:829:CLA:H2A	14:A:829:CLA:O1D	2.20	0.42
3:C:80:TYR:HB3	4:D:18:LEU:HD12	2.01	0.42
7:I:10:LEU:O	7:I:14:PHE:CD2	2.73	0.42
10:L:68:LEU:HD23	10:L:73:VAL:HG23	2.01	0.42
10:L:149:MET:HE2	7:7:16:PRO:HG3	2.02	0.42
14:b:817:CLA:O2D	14:b:817:CLA:H2A	2.20	0.42
1:1:70:ARG:NH2	1:1:185:PRO:O	2.51	0.42
6:6:16:LYS:O	6:6:17:ARG:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:z:12:ARG:CG	18:z:101:LHG:H101	2.44	0.42
1:A:279:LEU:HD21	1:A:302:LEU:HD22	2.02	0.42
1:A:345:TYR:O	1:A:349:THR:HG23	2.20	0.42
1:A:596:PHE:CZ	1:A:728:ARG:HB3	2.55	0.42
9:K:34:ILE:HD12	9:K:34:ILE:H	1.85	0.42
2:b:276:HIS:HA	2:b:279:ILE:HG12	2.02	0.42
2:b:486:SER:HA	12:x:35:LYS:CD	2.50	0.42
14:b:834:CLA:O1D	8:j:35:ASP:HA	2.20	0.42
6:f:11:SER:O	6:f:12:PRO:C	2.62	0.42
1:1:281:PHE:CD1	14:1:1620:CLA:HMB3	2.54	0.42
14:2:839:CLA:H162	17:6:204:BCR:H23C	2.01	0.42
2:B:44:LYS:NZ	11:M:29:LEU:O	2.52	0.41
2:B:437:LEU:O	2:B:441:VAL:HG23	2.20	0.41
6:f:31:GLY:HA2	6:f:34:ARG:NH1	2.35	0.41
1:1:345:TYR:O	1:1:349:THR:HG23	2.20	0.41
14:1:1601:CLA:HHC	14:1:1601:CLA:HBB1	2.02	0.41
2:2:256:PHE:HE2	2:2:499:TRP:HB3	1.85	0.41
7:7:10:LEU:O	7:7:14:PHE:CD2	2.73	0.41
10:0:131:SER:O	10:0:134:VAL:HG12	2.20	0.41
1:A:285:LEU:HD23	1:A:292:LEU:HD23	2.02	0.41
1:A:556:GLY:O	1:A:560:ALA:HB2	2.20	0.41
14:a:843:CLA:H41	14:a:843:CLA:H62	1.90	0.41
2:b:256:PHE:HE2	2:b:499:TRP:HB3	1.85	0.41
6:f:57:LEU:O	6:f:58:SER:OG	2.37	0.41
10:l:29:THR:O	10:l:33:ASN:ND2	2.52	0.41
2:2:255:THR:HG22	2:2:256:PHE:N	2.34	0.41
1:A:278:PHE:CD2	1:A:279:LEU:CD1	3.03	0.41
14:A:857:CLA:HHC	14:A:857:CLA:HBB1	2.02	0.41
2:B:286:ALA:HB2	14:B:819:CLA:HBC2	2.03	0.41
2:B:342:ALA:O	2:B:346:VAL:HG23	2.19	0.41
14:B:804:CLA:H171	17:M:103:BCR:H363	2.01	0.41
6:F:16:LYS:O	6:F:17:ARG:C	2.63	0.41
1:a:285:LEU:HD23	1:a:292:LEU:HD23	2.02	0.41
1:a:556:GLY:O	1:a:560:ALA:HB2	2.21	0.41
6:f:16:LYS:O	6:f:17:ARG:C	2.63	0.41
1:1:74:SER:HB2	1:1:180:TYR:HB2	2.03	0.41
2:2:314:VAL:O	2:2:319:ASN:HA	2.21	0.41
2:2:414:VAL:HG11	17:2:847:BCR:H401	2.01	0.41
2:2:612:VAL:HG12	2:2:616:ASN:ND2	2.36	0.41
1:A:372:GLN:HG2	14:A:827:CLA:CED	2.51	0.41
14:A:816:CLA:C4	14:A:816:CLA:O2A	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:48:LEU:O	6:F:50:HIS:ND1	2.53	0.41
1:a:359:ASN:O	1:a:363:MET:HG2	2.21	0.41
2:b:437:LEU:O	2:b:441:VAL:HG23	2.20	0.41
2:b:612:VAL:HG12	2:b:616:ASN:ND2	2.35	0.41
9:k:56:LEU:HB3	9:k:57:PRO:HD3	2.02	0.41
18:m:101:LHG:H112	18:0:202:LHG:H261	2.01	0.41
2:2:437:LEU:O	2:2:441:VAL:HG23	2.20	0.41
2:2:566:ASP:OD1	3:3:51:LYS:NZ	2.45	0.41
9:9:56:LEU:HB3	9:9:57:PRO:HD3	2.02	0.41
1:A:596:PHE:HE1	1:A:728:ARG:O	2.02	0.41
2:B:272:MET:O	2:B:275:HIS:HB3	2.20	0.41
2:B:436:THR:HG22	2:B:440:TYR:CE2	2.55	0.41
14:B:810:CLA:CBB	14:B:810:CLA:HHC	2.51	0.41
14:B:840:CLA:H18	17:I:101:BCR:H362	2.03	0.41
7:I:10:LEU:O	7:I:14:PHE:HD2	2.03	0.41
2:b:726:THR:HG23	14:b:803:CLA:O1D	2.19	0.41
6:f:42:LEU:HG	6:f:59:ARG:NH1	2.35	0.41
14:f:201:CLA:H101	8:j:14:LEU:HD11	2.02	0.41
1:1:596:PHE:CZ	1:1:728:ARG:HB3	2.55	0.41
2:2:468:ALA:HA	2:2:472:LYS:O	2.21	0.41
4:4:1:THR:C	4:4:2:THR:OG1	2.64	0.41
1:A:317:THR:HG21	14:A:813:CLA:CMA	2.51	0.41
2:B:314:VAL:O	2:B:319:ASN:HA	2.21	0.41
1:a:278:PHE:CD2	1:a:279:LEU:CD1	3.03	0.41
2:b:425:LEU:HG	14:b:840:CLA:CBB	2.51	0.41
2:b:500:LEU:N	2:b:501:PRO:CD	2.84	0.41
14:b:818:CLA:HBA1	14:b:818:CLA:H3A	1.89	0.41
14:b:838:CLA:C4	14:x:1701:CLA:HED1	2.50	0.41
1:1:278:PHE:CD2	1:1:279:LEU:CD1	3.03	0.41
1:1:359:ASN:O	1:1:363:MET:HG2	2.21	0.41
2:2:198:ILE:N	2:2:199:PRO:HD2	2.35	0.41
6:6:34:ARG:HD3	8:8:35:ASP:CG	2.46	0.41
1:A:70:ARG:NH2	1:A:185:PRO:O	2.51	0.41
1:A:74:SER:HB2	1:A:180:TYR:HB2	2.02	0.41
4:D:1:THR:C	4:D:2:THR:OG1	2.64	0.41
1:a:345:TYR:O	1:a:349:THR:HG23	2.20	0.41
2:b:37:THR:OG1	2:b:40:ASN:OD1	2.39	0.41
1:1:711:LEU:HD12	14:1:1642:CLA:HMA2	2.03	0.41
14:2:817:CLA:O2D	14:2:817:CLA:H2A	2.20	0.41
1:A:711:LEU:HD12	14:A:841:CLA:HMA2	2.03	0.41
12:X:18:LEU:C	12:X:18:LEU:HD23	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:41:ALA:HB3	6:f:49:PRO:HB3	2.01	0.41
10:l:131:SER:O	10:l:134:VAL:HG12	2.20	0.41
1:1:434:LEU:O	4:4:44:ALA:HB1	2.20	0.41
2:2:354:HIS:ND1	14:2:818:CLA:OBD	2.54	0.41
2:2:564:PRO:HA	2:2:712:ARG:HH22	1.85	0.41
14:2:817:CLA:H141	14:2:817:CLA:H161	1.85	0.41
6:6:34:ARG:NH1	8:8:35:ASP:OD2	2.44	0.41
12:z:18:LEU:C	12:z:18:LEU:HD23	2.46	0.41
1:A:29:ALA:HB2	8:J:3:HIS:HB3	2.03	0.41
1:A:355:GLN:NE2	21:A:902:HOH:O	2.51	0.41
1:A:359:ASN:O	1:A:363:MET:HG2	2.21	0.41
2:B:177:HIS:O	2:B:181:LEU:HB3	2.21	0.41
2:B:709:VAL:HG22	2:B:712:ARG:NH2	2.36	0.41
14:B:805:CLA:H8	14:B:824:CLA:O1A	2.21	0.41
14:B:837:CLA:H143	12:X:19:LEU:HB3	2.02	0.41
17:I:101:BCR:H20C	17:I:101:BCR:H361	1.95	0.41
10:L:24:SER:OG	10:L:25:GLY:N	2.54	0.41
1:a:74:SER:HB2	1:a:180:TYR:HB2	2.02	0.41
1:a:372:GLN:HG2	14:a:827:CLA:CED	2.51	0.41
2:b:468:ALA:HA	2:b:472:LYS:O	2.21	0.41
14:b:812:CLA:H2A	14:b:812:CLA:O1D	2.21	0.41
14:b:814:CLA:H2	14:b:814:CLA:H62	1.97	0.41
4:d:79:ASP:CG	4:d:79:ASP:O	2.64	0.41
1:1:106:ASP:HB3	1:1:110:ILE:HG12	2.03	0.41
1:1:117:VAL:CG1	1:1:123:GLN:HB3	2.51	0.41
1:1:300:HIS:HE2	14:1:1621:CLA:C2B	2.34	0.41
1:1:372:GLN:HG2	14:1:1628:CLA:CED	2.51	0.41
1:1:556:GLY:O	1:1:560:ALA:HB2	2.21	0.41
14:1:1617:CLA:C4	14:1:1617:CLA:O2A	2.69	0.41
14:1:1620:CLA:H62	14:1:1620:CLA:H41	1.91	0.41
14:1:1630:CLA:H2A	14:1:1630:CLA:O1D	2.20	0.41
2:2:500:LEU:N	2:2:501:PRO:CD	2.84	0.41
14:2:811:CLA:CBB	14:2:811:CLA:HHC	2.51	0.41
4:4:79:ASP:O	4:4:79:ASP:CG	2.64	0.41
1:A:117:VAL:CG1	1:A:123:GLN:HB3	2.51	0.41
1:A:300:HIS:HE2	14:A:820:CLA:C2B	2.34	0.41
14:A:804:CLA:H93	14:A:804:CLA:H62	1.93	0.41
6:F:54:ASP:OD2	6:F:54:ASP:N	2.54	0.41
10:L:68:LEU:HD11	10:l:148:ILE:HG22	2.02	0.41
2:b:95:PHE:HB2	7:i:1:FME:HE1	2.01	0.41
2:b:272:MET:O	2:b:275:HIS:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:354:HIS:ND1	14:b:818:CLA:OBD	2.54	0.41
14:b:811:CLA:CBB	14:b:811:CLA:HHC	2.51	0.41
12:x:18:LEU:HD23	12:x:18:LEU:C	2.46	0.41
1:1:279:LEU:HD21	1:1:302:LEU:HD22	2.02	0.41
1:1:317:THR:HG21	14:1:1614:CLA:CMA	2.51	0.41
2:2:180:GLY:O	2:2:181:LEU:C	2.64	0.41
2:2:709:VAL:HG22	2:2:712:ARG:NH2	2.36	0.41
17:0:201:BCR:H20C	17:0:201:BCR:H361	1.95	0.41
1:A:476:SER:C	1:A:478:THR:H	2.30	0.40
2:B:425:LEU:HG	14:B:839:CLA:CBB	2.51	0.40
2:B:500:LEU:N	2:B:501:PRO:CD	2.84	0.40
1:a:279:LEU:HD21	1:a:302:LEU:HD22	2.02	0.40
2:b:160:PHE:O	2:b:162:PRO:HD3	2.21	0.40
2:b:314:VAL:O	2:b:319:ASN:HA	2.21	0.40
4:d:1:THR:C	4:d:2:THR:OG1	2.64	0.40
7:i:10:LEU:O	7:i:14:PHE:HD2	2.03	0.40
10:l:24:SER:OG	10:l:25:GLY:N	2.54	0.40
1:1:26:GLU:HA	8:8:3:HIS:CD2	2.56	0.40
14:1:1604:CLA:HAC1	14:2:804:CLA:HMC3	2.04	0.40
2:2:177:HIS:O	2:2:181:LEU:HB3	2.21	0.40
2:2:436:THR:HG22	2:2:440:TYR:CE2	2.55	0.40
2:2:462:PHE:O	2:2:466:ILE:HG13	2.21	0.40
6:6:54:ASP:OD2	6:6:54:ASP:N	2.54	0.40
9:9:34:ILE:HD12	9:9:34:ILE:H	1.85	0.40
10:L:83:ILE:HA	10:L:129:MET:HE1	2.02	0.40
17:M:103:BCR:H20C	17:M:103:BCR:H361	1.93	0.40
1:a:117:VAL:CG1	1:a:123:GLN:HB3	2.51	0.40
1:a:433:VAL:HA	1:a:436:HIS:CE1	2.57	0.40
2:b:462:PHE:O	2:b:466:ILE:HG13	2.21	0.40
2:b:564:PRO:HA	2:b:712:ARG:HH22	1.85	0.40
8:j:2:LYS:HE2	8:j:2:LYS:HB2	1.80	0.40
6:6:57:LEU:O	6:6:58:SER:OG	2.37	0.40
12:z:26:VAL:HG23	14:z:102:CLA:CED	2.51	0.40
14:A:809:CLA:HBA2	14:A:809:CLA:H3A	1.93	0.40
2:B:354:HIS:ND1	14:B:817:CLA:OBD	2.54	0.40
14:B:811:CLA:O1D	14:B:811:CLA:H2A	2.21	0.40
10:L:6:LYS:HB2	10:L:7:PRO:CD	2.52	0.40
1:a:95:ALA:HB2	1:a:158:LEU:HB2	2.01	0.40
14:a:816:CLA:O2A	14:a:816:CLA:C4	2.69	0.40
2:b:177:HIS:O	2:b:181:LEU:HB3	2.21	0.40
2:b:709:VAL:HG22	2:b:712:ARG:NH2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:i:13:ILE:O	7:i:17:VAL:HG23	2.22	0.40
1:1:270:PHE:CD2	9:9:74:VAL:HG11	2.56	0.40
2:2:160:PHE:O	2:2:162:PRO:HD3	2.21	0.40
2:2:272:MET:O	2:2:275:HIS:HB3	2.20	0.40
2:2:504:LEU:HA	2:2:507:ILE:HG22	2.04	0.40
7:7:13:ILE:O	7:7:17:VAL:HG23	2.21	0.40
14:A:830:CLA:O1D	14:A:830:CLA:H2A	2.21	0.40
2:B:462:PHE:O	2:B:466:ILE:HG13	2.21	0.40
14:M:102:CLA:HHC	14:M:102:CLA:HBB1	2.02	0.40
1:a:317:THR:HG21	14:a:813:CLA:CMA	2.51	0.40
1:a:711:LEU:HD12	14:a:841:CLA:HMA2	2.03	0.40
2:b:286:ALA:HB2	14:b:820:CLA:HBC2	2.03	0.40
14:b:806:CLA:H8	14:b:825:CLA:O1A	2.21	0.40
5:e:8:LYS:HA	5:e:19:GLU:O	2.22	0.40
14:1:1611:CLA:HMA1	8:8:27:ILE:HD13	2.04	0.40
14:1:1624:CLA:O1D	14:1:1624:CLA:H2A	2.22	0.40
14:1:1624:CLA:HBA1	9:9:33:ALA:HA	2.04	0.40
14:2:815:CLA:H141	14:2:815:CLA:H161	1.86	0.40
3:3:60:ASP:CG	5:5:58:ASN:ND2	2.79	0.40
6:6:31:GLY:HA2	6:6:34:ARG:NH1	2.35	0.40
17:A:856:BCR:H313	8:J:31:ARG:HD3	2.03	0.40
2:B:14:ASP:HB3	2:B:19:ARG:HB2	2.04	0.40
2:B:160:PHE:O	2:B:162:PRO:HD3	2.21	0.40
2:B:468:ALA:HA	2:B:472:LYS:O	2.21	0.40
2:B:612:VAL:HG12	2:B:616:ASN:ND2	2.36	0.40
12:X:26:VAL:HG23	14:X:1701:CLA:CED	2.52	0.40
1:a:300:HIS:HE2	14:a:820:CLA:C2B	2.34	0.40
1:a:337:THR:O	1:a:337:THR:HG22	2.21	0.40
14:a:841:CLA:H192	6:f:110:MET:SD	2.61	0.40
2:b:14:ASP:HB3	2:b:19:ARG:HB2	2.04	0.40
2:b:110:ASN:OD1	2:b:110:ASN:N	2.52	0.40
2:b:157:GLN:O	2:b:158:PRO:C	2.65	0.40
10:l:6:LYS:HB2	10:l:7:PRO:CD	2.52	0.40
1:1:228:ASP:OD2	1:1:288:VAL:HG21	2.22	0.40
5:5:8:LYS:HA	5:5:19:GLU:O	2.22	0.40
6:6:48:LEU:O	6:6:50:HIS:ND1	2.53	0.40
10:0:6:LYS:HB2	10:0:7:PRO:CD	2.52	0.40
17:0:203:BCR:H24C	17:0:203:BCR:H371	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	744/755 (98%)	684 (92%)	60 (8%)	0	100	100
1	A	744/755 (98%)	684 (92%)	60 (8%)	0	100	100
1	a	744/755 (98%)	684 (92%)	60 (8%)	0	100	100
2	2	738/741 (100%)	679 (92%)	59 (8%)	0	100	100
2	B	738/741 (100%)	679 (92%)	59 (8%)	0	100	100
2	b	738/741 (100%)	679 (92%)	59 (8%)	0	100	100
3	3	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
3	C	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
3	c	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	4	136/139 (98%)	121 (89%)	15 (11%)	0	100	100
4	D	136/139 (98%)	121 (89%)	15 (11%)	0	100	100
4	d	136/139 (98%)	120 (88%)	16 (12%)	0	100	100
5	5	68/76 (90%)	62 (91%)	6 (9%)	0	100	100
5	E	68/76 (90%)	62 (91%)	6 (9%)	0	100	100
5	e	68/76 (90%)	62 (91%)	6 (9%)	0	100	100
6	6	139/141 (99%)	113 (81%)	26 (19%)	0	100	100
6	F	139/141 (99%)	112 (81%)	27 (19%)	0	100	100
6	f	139/141 (99%)	113 (81%)	26 (19%)	0	100	100
7	7	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
7	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
7	i	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	8	39/41 (95%)	35 (90%)	3 (8%)	1 (3%)	4	21
8	J	39/41 (95%)	35 (90%)	3 (8%)	1 (3%)	4	21
8	j	39/41 (95%)	35 (90%)	3 (8%)	1 (3%)	4	21
9	9	77/83 (93%)	68 (88%)	9 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	K	77/83 (93%)	68 (88%)	9 (12%)	0	100	100
9	k	77/83 (93%)	68 (88%)	9 (12%)	0	100	100
10	0	150/155 (97%)	143 (95%)	7 (5%)	0	100	100
10	L	150/155 (97%)	143 (95%)	7 (5%)	0	100	100
10	l	150/155 (97%)	143 (95%)	7 (5%)	0	100	100
11	M	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
11	m	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
11	y	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
12	X	25/36 (69%)	23 (92%)	2 (8%)	0	100	100
12	x	25/36 (69%)	23 (92%)	2 (8%)	0	100	100
12	z	25/36 (69%)	23 (92%)	2 (8%)	0	100	100
All	All	6777/6951 (98%)	6181 (91%)	593 (9%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	J	2	LYS
8	j	2	LYS
8	8	2	LYS

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	1	594/603 (98%)	567 (96%)	27 (4%)	24	53
1	A	594/603 (98%)	567 (96%)	27 (4%)	24	53
1	a	594/603 (98%)	567 (96%)	27 (4%)	24	53
2	2	597/598 (100%)	582 (98%)	15 (2%)	42	65
2	B	597/598 (100%)	582 (98%)	15 (2%)	42	65
2	b	597/598 (100%)	582 (98%)	15 (2%)	42	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	3	67/68 (98%)	67 (100%)	0	100	100
3	C	67/68 (98%)	67 (100%)	0	100	100
3	c	67/68 (98%)	67 (100%)	0	100	100
4	4	115/116 (99%)	109 (95%)	6 (5%)	21	49
4	D	115/116 (99%)	109 (95%)	6 (5%)	21	49
4	d	115/116 (99%)	109 (95%)	6 (5%)	21	49
5	5	60/65 (92%)	53 (88%)	7 (12%)	5	20
5	E	60/65 (92%)	53 (88%)	7 (12%)	5	20
5	e	60/65 (92%)	53 (88%)	7 (12%)	5	20
6	6	109/109 (100%)	96 (88%)	13 (12%)	5	20
6	F	109/109 (100%)	96 (88%)	13 (12%)	5	20
6	f	109/109 (100%)	96 (88%)	13 (12%)	5	20
7	7	31/31 (100%)	30 (97%)	1 (3%)	34	61
7	I	31/31 (100%)	30 (97%)	1 (3%)	34	61
7	i	31/31 (100%)	30 (97%)	1 (3%)	34	61
8	8	35/35 (100%)	33 (94%)	2 (6%)	18	47
8	J	35/35 (100%)	33 (94%)	2 (6%)	18	47
8	j	35/35 (100%)	33 (94%)	2 (6%)	18	47
9	9	58/61 (95%)	50 (86%)	8 (14%)	3	16
9	K	58/61 (95%)	50 (86%)	8 (14%)	3	16
9	k	58/61 (95%)	50 (86%)	8 (14%)	3	16
10	0	117/120 (98%)	115 (98%)	2 (2%)	53	70
10	L	117/120 (98%)	115 (98%)	2 (2%)	53	70
10	l	117/120 (98%)	115 (98%)	2 (2%)	53	70
11	M	26/26 (100%)	22 (85%)	4 (15%)	2	12
11	m	26/26 (100%)	22 (85%)	4 (15%)	2	12
11	y	26/26 (100%)	22 (85%)	4 (15%)	2	12
12	X	21/28 (75%)	19 (90%)	2 (10%)	8	29
12	x	21/28 (75%)	19 (90%)	2 (10%)	8	29
12	z	21/28 (75%)	19 (90%)	2 (10%)	8	29
All	All	5490/5580 (98%)	5229 (95%)	261 (5%)	24	52

All (261) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	21	VAL
1	A	36	ARG
1	A	43	GLN
1	A	63	SER
1	A	155	GLU
1	A	188	GLU
1	A	210	LEU
1	A	224	ASN
1	A	234	LYS
1	A	256	VAL
1	A	262	SER
1	A	307	LEU
1	A	327	GLU
1	A	351	SER
1	A	476	SER
1	A	478	THR
1	A	530	VAL
1	A	562	SER
1	A	625	VAL
1	A	628	ASP
1	A	630	THR
1	A	631	VAL
1	A	632	SER
1	A	659	SER
1	A	692	SER
1	A	705	VAL
2	B	32	SER
2	B	61	SER
2	B	97	LYS
2	B	136	GLN
2	B	165	SER
2	B	266	SER
2	B	269	LEU
2	B	302	GLU
2	B	304	MET
2	B	312	THR
2	B	327	GLU
2	B	398	VAL
2	B	405	GLN
2	B	485	ASP
2	B	672	SER

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Mol	Chain	Res	Type
4	D	2	THR
4	D	22	ASP
4	D	36	GLU
4	D	43	THR
4	D	92	VAL
4	D	133	LYS
5	E	19	GLU
5	E	25	SER
5	E	28	GLN
5	E	46	THR
5	E	51	SER
5	E	57	THR
5	E	67	GLU
6	F	15	GLN
6	F	16	LYS
6	F	36	GLU
6	F	39	SER
6	F	45	GLU
6	F	58	SER
6	F	65	ILE
6	F	88	VAL
6	F	107	ILE
6	F	112	THR
6	F	130	THR
6	F	135	GLU
6	F	137	THR
7	I	4	SER
8	J	2	LYS
8	J	17	ILE
9	K	5	THR
9	K	18	VAL
9	K	24	LEU
9	K	43	LEU
9	K	47	LEU
9	K	50	LEU
9	K	52	GLU
9	K	68	LEU
10	L	70	ASP
10	L	72	ASP
11	M	6	THR
11	M	16	LEU
11	M	26	SER

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Mol	Chain	Res	Type
11	M	27	THR
12	X	17	VAL
12	X	26	VAL
1	a	15	VAL
1	a	21	VAL
1	a	36	ARG
1	a	43	GLN
1	a	63	SER
1	a	155	GLU
1	a	188	GLU
1	a	210	LEU
1	a	224	ASN
1	a	234	LYS
1	a	256	VAL
1	a	262	SER
1	a	307	LEU
1	a	327	GLU
1	a	351	SER
1	a	476	SER
1	a	478	THR
1	a	530	VAL
1	a	562	SER
1	a	625	VAL
1	a	628	ASP
1	a	630	THR
1	a	631	VAL
1	a	632	SER
1	a	659	SER
1	a	692	SER
1	a	705	VAL
2	b	32	SER
2	b	61	SER
2	b	97	LYS
2	b	136	GLN
2	b	165	SER
2	b	266	SER
2	b	269	LEU
2	b	302	GLU
2	b	304	MET
2	b	312	THR
2	b	327	GLU
2	b	398	VAL

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Mol	Chain	Res	Type
2	b	405	GLN
2	b	485	ASP
2	b	672	SER
4	d	2	THR
4	d	22	ASP
4	d	36	GLU
4	d	43	THR
4	d	92	VAL
4	d	133	LYS
5	e	19	GLU
5	e	25	SER
5	e	28	GLN
5	e	46	THR
5	e	51	SER
5	e	57	THR
5	e	67	GLU
6	f	15	GLN
6	f	16	LYS
6	f	36	GLU
6	f	39	SER
6	f	45	GLU
6	f	58	SER
6	f	65	ILE
6	f	88	VAL
6	f	107	ILE
6	f	112	THR
6	f	130	THR
6	f	135	GLU
6	f	137	THR
7	i	4	SER
8	j	2	LYS
8	j	17	ILE
9	k	5	THR
9	k	18	VAL
9	k	24	LEU
9	k	43	LEU
9	k	47	LEU
9	k	50	LEU
9	k	52	GLU
9	k	68	LEU
10	l	70	ASP
10	l	72	ASP

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Mol	Chain	Res	Type
11	m	6	THR
11	m	16	LEU
11	m	26	SER
11	m	27	THR
12	x	17	VAL
12	x	26	VAL
1	1	15	VAL
1	1	21	VAL
1	1	36	ARG
1	1	43	GLN
1	1	63	SER
1	1	155	GLU
1	1	188	GLU
1	1	210	LEU
1	1	224	ASN
1	1	234	LYS
1	1	256	VAL
1	1	262	SER
1	1	307	LEU
1	1	327	GLU
1	1	351	SER
1	1	476	SER
1	1	478	THR
1	1	530	VAL
1	1	562	SER
1	1	625	VAL
1	1	628	ASP
1	1	630	THR
1	1	631	VAL
1	1	632	SER
1	1	659	SER
1	1	692	SER
1	1	705	VAL
2	2	32	SER
2	2	61	SER
2	2	97	LYS
2	2	136	GLN
2	2	165	SER
2	2	266	SER
2	2	269	LEU
2	2	302	GLU
2	2	304	MET

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Mol	Chain	Res	Type
2	2	312	THR
2	2	327	GLU
2	2	398	VAL
2	2	405	GLN
2	2	485	ASP
2	2	672	SER
4	4	2	THR
4	4	22	ASP
4	4	36	GLU
4	4	43	THR
4	4	92	VAL
4	4	133	LYS
5	5	19	GLU
5	5	25	SER
5	5	28	GLN
5	5	46	THR
5	5	51	SER
5	5	57	THR
5	5	67	GLU
6	6	15	GLN
6	6	16	LYS
6	6	36	GLU
6	6	39	SER
6	6	45	GLU
6	6	58	SER
6	6	65	ILE
6	6	88	VAL
6	6	107	ILE
6	6	112	THR
6	6	130	THR
6	6	135	GLU
6	6	137	THR
7	7	4	SER
8	8	2	LYS
8	8	17	ILE
9	9	5	THR
9	9	18	VAL
9	9	24	LEU
9	9	43	LEU
9	9	47	LEU
9	9	50	LEU
9	9	52	GLU

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Mol	Chain	Res	Type
9	9	68	LEU
10	0	70	ASP
10	0	72	ASP
11	y	6	THR
11	y	16	LEU
11	y	26	SER
11	y	27	THR
12	z	17	VAL
12	z	26	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	79	HIS
1	A	93	HIS
1	A	135	HIS
1	A	301	HIS
1	A	372	GLN
1	A	397	HIS
1	A	618	GLN
1	A	680	HIS
1	A	708	HIS
1	A	718	GLN
2	B	88	HIS
2	B	94	GLN
2	B	155	HIS
2	B	192	HIS
2	B	204	GLN
2	B	235	ASN
2	B	241	HIS
2	B	261	HIS
2	B	319	ASN
2	B	368	HIS
2	B	416	GLN
2	B	527	HIS
2	B	642	ASN
2	B	648	ASN
4	D	63	GLN
4	D	71	GLN
4	D	127	GLN
5	E	58	ASN

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Mol	Chain	Res	Type
8	J	39	HIS
9	K	23	ASN
9	K	78	GLN
10	L	75	ASN
10	L	102	GLN
1	a	56	HIS
1	a	79	HIS
1	a	93	HIS
1	a	135	HIS
1	a	301	HIS
1	a	372	GLN
1	a	397	HIS
1	a	618	GLN
1	a	680	HIS
1	a	708	HIS
2	b	33	HIS
2	b	88	HIS
2	b	94	GLN
2	b	155	HIS
2	b	192	HIS
2	b	204	GLN
2	b	235	ASN
2	b	241	HIS
2	b	261	HIS
2	b	293	GLN
2	b	319	ASN
2	b	368	HIS
2	b	416	GLN
2	b	527	HIS
2	b	642	ASN
2	b	648	ASN
4	d	63	GLN
4	d	71	GLN
4	d	127	GLN
9	k	23	ASN
9	k	78	GLN
10	l	75	ASN
1	1	56	HIS
1	1	79	HIS
1	1	93	HIS
1	1	135	HIS
1	1	301	HIS

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Mol	Chain	Res	Type
1	1	372	GLN
1	1	397	HIS
1	1	618	GLN
1	1	680	HIS
1	1	708	HIS
1	1	718	GLN
2	2	88	HIS
2	2	94	GLN
2	2	155	HIS
2	2	192	HIS
2	2	204	GLN
2	2	235	ASN
2	2	241	HIS
2	2	261	HIS
2	2	293	GLN
2	2	319	ASN
2	2	416	GLN
2	2	527	HIS
2	2	642	ASN
2	2	648	ASN
4	4	63	GLN
4	4	127	GLN
5	5	18	ASN
5	5	58	ASN
6	6	40	GLN
8	8	39	HIS
9	9	23	ASN
9	9	78	GLN
10	0	75	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	FME	i	1	7	8,9,10	1.00	0	7,9,11	0.82	0
7	FME	7	1	7	8,9,10	0.98	0	7,9,11	0.83	0
8	FME	j	1	8	8,9,10	1.01	0	7,9,11	1.37	2 (28%)
7	FME	I	1	7	8,9,10	0.98	0	7,9,11	0.83	0
8	FME	J	1	8	8,9,10	1.01	0	7,9,11	1.37	2 (28%)
8	FME	8	1	8	8,9,10	1.02	0	7,9,11	1.37	2 (28%)

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
7	FME	i	1	7	-	1/7/9/11	-
7	FME	7	1	7	-	1/7/9/11	-
8	FME	j	1	8	-	1/7/9/11	-
7	FME	I	1	7	-	1/7/9/11	-
8	FME	J	1	8	-	1/7/9/11	-
8	FME	8	1	8	-	1/7/9/11	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	j	1	FME	C-CA-N	2.57	114.36	109.73
8	8	1	FME	C-CA-N	2.56	114.36	109.73
8	J	1	FME	C-CA-N	2.56	114.34	109.73
8	j	1	FME	O-C-CA	-2.06	119.38	124.78
8	J	1	FME	O-C-CA	-2.06	119.38	124.78
8	8	1	FME	O-C-CA	-2.05	119.39	124.78

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	J	1	FME	CB-CA-N-CN
8	j	1	FME	CB-CA-N-CN

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Mol	Chain	Res	Type	Atoms
8	8	1	FME	CB-CA-N-CN
7	I	1	FME	N-CA-CB-CG
7	i	1	FME	N-CA-CB-CG
7	7	1	FME	N-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	i	1	FME	2	0
8	j	1	FME	1	0
7	I	1	FME	1	0
8	J	1	FME	1	0
8	8	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 402 ligands modelled in this entry, 6 are monoatomic - leaving 396 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	j	1303	-	42,45,73	1.59	9 (21%)	50,78,113	1.46	6 (12%)
14	CLA	b	832	2	53,57,73	1.41	9 (16%)	62,93,113	1.47	7 (11%)
14	CLA	b	818	2	69,73,73	1.26	9 (13%)	83,113,113	1.39	7 (8%)
14	CLA	2	835	2	69,73,73	1.25	9 (13%)	83,113,113	1.34	9 (10%)
14	CLA	A	830	-	69,73,73	1.24	10 (14%)	83,113,113	1.40	7 (8%)
14	CLA	a	827	21	69,73,73	1.26	9 (13%)	83,113,113	1.40	11 (13%)
14	CLA	a	834	1	69,73,73	1.26	11 (15%)	83,113,113	1.45	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	A	838	1	69,73,73	1.25	10 (14%)	83,113,113	1.43	7 (8%)
16	SF4	a	846	1,2	0,12,12	-	-	-		
17	BCR	f	204	-	41,41,41	1.19	2 (4%)	56,56,56	1.36	8 (14%)
14	CLA	b	806	2	69,73,73	1.26	9 (13%)	83,113,113	1.40	8 (9%)
14	CLA	B	838	2	69,73,73	1.27	9 (13%)	83,113,113	1.32	6 (7%)
17	BCR	A	847	-	41,41,41	1.15	2 (4%)	56,56,56	1.31	7 (12%)
17	BCR	B	843	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	4 (7%)
14	CLA	a	829	1	69,73,73	1.25	9 (13%)	83,113,113	1.31	8 (9%)
17	BCR	b	848	-	41,41,41	1.27	3 (7%)	56,56,56	1.31	9 (16%)
14	CLA	2	809	2	69,73,73	1.23	9 (13%)	83,113,113	1.46	8 (9%)
14	CLA	1	1635	1	69,73,73	1.26	11 (15%)	83,113,113	1.44	12 (14%)
14	CLA	2	812	2	69,73,73	1.25	9 (13%)	83,113,113	1.39	9 (10%)
14	CLA	B	837	2	64,68,73	1.31	10 (15%)	77,107,113	1.39	6 (7%)
14	CLA	j	1301	21	49,53,73	1.50	10 (20%)	59,89,113	1.45	8 (13%)
14	CLA	1	1608	1	69,73,73	1.27	10 (14%)	83,113,113	1.35	5 (6%)
14	CLA	a	844	18	49,53,73	1.47	9 (18%)	59,89,113	1.51	7 (11%)
14	CLA	k	101	9	50,54,73	1.46	9 (18%)	60,90,113	1.44	5 (8%)
14	CLA	a	842	1	69,73,73	1.27	10 (14%)	83,113,113	1.41	8 (9%)
14	CLA	a	815	1	69,73,73	1.26	10 (14%)	83,113,113	1.29	5 (6%)
14	CLA	z	102	12	49,53,73	1.49	9 (18%)	59,89,113	1.47	5 (8%)
14	CLA	A	825	1	69,73,73	1.26	10 (14%)	83,113,113	1.37	10 (12%)
14	CLA	b	822	2	49,53,73	1.48	10 (20%)	59,89,113	1.56	10 (16%)
14	CLA	j	1302	-	49,53,73	1.48	8 (16%)	59,89,113	1.46	6 (10%)
14	CLA	a	830	-	69,73,73	1.24	10 (14%)	83,113,113	1.39	7 (8%)
17	BCR	8	1306	-	41,41,41	1.21	2 (4%)	56,56,56	1.34	9 (16%)
15	PQN	2	843	-	34,34,34	0.45	0	42,45,45	0.38	0
14	CLA	1	1623	21	69,73,73	1.26	10 (14%)	83,113,113	1.34	8 (9%)
17	BCR	B	847	-	41,41,41	1.27	3 (7%)	56,56,56	1.31	9 (16%)
14	CLA	B	825	21	69,73,73	1.27	10 (14%)	83,113,113	1.43	9 (10%)
14	CLA	1	1634	1	69,73,73	1.27	11 (15%)	83,113,113	1.30	6 (7%)
14	CLA	a	813	1	49,53,73	1.50	10 (20%)	59,89,113	1.50	6 (10%)
17	BCR	6	202	-	41,41,41	1.25	3 (7%)	56,56,56	1.25	6 (10%)
14	CLA	A	816	1	69,73,73	1.25	8 (11%)	83,113,113	1.29	7 (8%)
14	CLA	1	1628	21	69,73,73	1.26	9 (13%)	83,113,113	1.40	11 (13%)
14	CLA	b	807	2	69,73,73	1.27	9 (13%)	83,113,113	1.32	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CL0	a	801	1	69,73,73	1.25	10 (14%)	83,113,113	1.37	6 (7%)
14	CLA	b	811	2	69,73,73	1.25	11 (15%)	83,113,113	1.41	6 (7%)
14	CLA	B	817	2	69,73,73	1.27	9 (13%)	83,113,113	1.39	7 (8%)
14	CLA	F	204	-	54,58,73	1.41	6 (11%)	65,95,113	1.37	6 (9%)
14	CLA	B	820	2	69,73,73	1.25	10 (14%)	83,113,113	1.22	5 (6%)
14	CLA	a	806	1	69,73,73	1.27	11 (15%)	83,113,113	1.47	12 (14%)
14	CLA	1	1615	1	69,73,73	1.26	9 (13%)	83,113,113	1.27	6 (7%)
14	CLA	A	823	1	49,53,73	1.48	9 (18%)	59,89,113	1.51	8 (13%)
14	CLA	A	840	1	69,73,73	1.26	10 (14%)	83,113,113	1.36	6 (7%)
14	CLA	b	841	21	69,73,73	1.26	9 (13%)	83,113,113	1.34	9 (10%)
18	LHG	a	853	-	48,48,48	0.74	1 (2%)	51,54,54	1.23	4 (7%)
14	CLA	a	831	1	69,73,73	1.28	11 (15%)	83,113,113	1.40	9 (10%)
17	BCR	A	848	-	41,41,41	1.18	3 (7%)	56,56,56	1.23	6 (10%)
17	BCR	1	1651	-	41,41,41	1.35	4 (9%)	56,56,56	1.28	7 (12%)
17	BCR	K	104	-	25,25,41	1.15	1 (4%)	33,33,56	1.15	4 (12%)
16	SF4	c	101	3	0,12,12	-	-	-		
14	CLA	1	1630	1	69,73,73	1.25	9 (13%)	83,113,113	1.31	8 (9%)
14	CLA	a	809	1	69,73,73	1.24	10 (14%)	83,113,113	1.39	9 (10%)
17	BCR	m	102	-	41,41,41	1.24	3 (7%)	56,56,56	1.22	5 (8%)
14	CLA	a	812	14,1	69,73,73	1.25	9 (13%)	83,113,113	1.27	5 (6%)
14	CLA	2	811	2	69,73,73	1.25	11 (15%)	83,113,113	1.41	7 (8%)
14	CLA	b	831	2	59,63,73	1.35	9 (15%)	71,101,113	1.42	8 (11%)
16	SF4	c	102	3	0,12,12	-	-	-		
14	CLA	B	823	2	49,53,73	1.48	10 (20%)	59,89,113	1.50	8 (13%)
17	BCR	B	848	-	41,41,41	1.39	4 (9%)	56,56,56	1.29	6 (10%)
14	CLA	a	824	1	69,73,73	1.27	8 (11%)	83,113,113	1.30	7 (8%)
17	BCR	8	1304	-	41,41,41	1.17	3 (7%)	56,56,56	1.20	7 (12%)
14	CLA	b	838	2	64,68,73	1.32	10 (15%)	77,107,113	1.39	6 (7%)
14	CLA	2	841	21	69,73,73	1.27	9 (13%)	83,113,113	1.34	9 (10%)
20	LMG	B	849	-	55,55,55	0.92	4 (7%)	63,63,63	1.35	10 (15%)
14	CLA	A	807	1	69,73,73	1.27	11 (15%)	83,113,113	1.35	6 (7%)
14	CLA	a	835	1	69,73,73	1.24	9 (13%)	83,113,113	1.38	5 (6%)
14	CLA	L	205	21	69,73,73	1.26	10 (14%)	83,113,113	1.36	11 (13%)
14	CLA	b	839	2	69,73,73	1.27	9 (13%)	83,113,113	1.31	5 (6%)
14	CLA	1	1632	1	69,73,73	1.28	11 (15%)	83,113,113	1.41	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	B	821	2	49,53,73	1.48	10 (20%)	59,89,113	1.56	10 (16%)
14	CLA	2	820	21	69,73,73	1.28	9 (13%)	83,113,113	1.26	8 (9%)
14	CLA	B	816	2	69,73,73	1.24	8 (11%)	83,113,113	1.37	7 (8%)
14	CLA	b	829	2	69,73,73	1.27	9 (13%)	83,113,113	1.20	4 (4%)
14	CLA	2	834	2	69,73,73	1.25	10 (14%)	83,113,113	1.35	5 (6%)
14	CLA	a	818	1	69,73,73	1.24	8 (11%)	83,113,113	1.34	5 (6%)
14	CLA	l	204	10	69,73,73	1.29	10 (14%)	83,113,113	1.31	7 (8%)
14	CLA	b	814	2	69,73,73	1.25	10 (14%)	83,113,113	1.34	9 (10%)
18	LHG	b	851	-	48,48,48	0.61	1 (2%)	51,54,54	1.20	5 (9%)
14	CLA	F	203	21	49,53,73	1.50	10 (20%)	59,89,113	1.45	8 (13%)
14	CLA	b	809	2	69,73,73	1.23	9 (13%)	83,113,113	1.45	8 (9%)
17	BCR	I	101	-	41,41,41	1.28	4 (9%)	56,56,56	1.25	3 (5%)
14	CLA	a	808	1	55,59,73	1.39	10 (18%)	66,96,113	1.43	6 (9%)
14	CLA	2	819	2	69,73,73	1.24	9 (13%)	83,113,113	1.39	10 (12%)
17	BCR	J	103	-	41,41,41	1.16	3 (7%)	56,56,56	1.19	6 (10%)
14	CLA	b	812	2	69,73,73	1.25	9 (13%)	83,113,113	1.38	10 (12%)
13	CL0	1	1602	1	69,73,73	1.26	10 (14%)	83,113,113	1.38	6 (7%)
14	CLA	A	841	1	69,73,73	1.24	9 (13%)	83,113,113	1.36	6 (7%)
16	SF4	C	102	3	0,12,12	-	-	-		
14	CLA	2	814	2	69,73,73	1.25	10 (14%)	83,113,113	1.35	9 (10%)
15	PQN	B	842	-	34,34,34	0.45	0	42,45,45	0.38	0
17	BCR	1	1652	-	41,41,41	1.27	2 (4%)	56,56,56	1.29	7 (12%)
17	BCR	f	202	-	41,41,41	1.24	3 (7%)	56,56,56	1.26	6 (10%)
18	LHG	z	101	-	48,48,48	0.61	1 (2%)	51,54,54	1.20	5 (9%)
14	CLA	a	832	1	64,68,73	1.31	11 (17%)	77,107,113	1.33	6 (7%)
17	BCR	F	202	-	41,41,41	1.25	3 (7%)	56,56,56	1.25	6 (10%)
14	CLA	a	807	1	69,73,73	1.27	11 (15%)	83,113,113	1.34	5 (6%)
14	CLA	b	837	21	49,53,73	1.51	8 (16%)	59,89,113	1.44	5 (8%)
14	CLA	a	821	1	69,73,73	1.26	7 (10%)	83,113,113	1.35	7 (8%)
17	BCR	a	851	-	41,41,41	1.27	3 (7%)	56,56,56	1.29	7 (12%)
14	CLA	A	857	-	40,44,73	1.59	9 (22%)	47,76,113	1.44	3 (6%)
16	SF4	C	101	3	0,12,12	-	-	-		
15	PQN	A	845	-	34,34,34	0.39	0	42,45,45	0.35	0
14	CLA	B	841	2	69,73,73	1.27	9 (13%)	83,113,113	1.41	6 (7%)
14	CLA	A	819	1	69,73,73	1.24	9 (13%)	83,113,113	1.34	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	2	815	2	69,73,73	1.25	10 (14%)	83,113,113	1.34	6 (7%)
14	CLA	B	840	21	69,73,73	1.27	9 (13%)	83,113,113	1.34	9 (10%)
14	CLA	2	828	2	69,73,73	1.28	10 (14%)	83,113,113	1.32	8 (9%)
17	BCR	b	852	-	41,41,41	1.21	2 (4%)	56,56,56	1.33	9 (16%)
14	CLA	B	836	21	49,53,73	1.51	8 (16%)	59,89,113	1.43	4 (6%)
14	CLA	A	839	1	69,73,73	1.25	9 (13%)	83,113,113	1.40	9 (10%)
14	CLA	1	1620	1	69,73,73	1.25	9 (13%)	83,113,113	1.34	8 (9%)
14	CLA	2	840	2	51,55,73	1.46	10 (19%)	61,91,113	1.37	7 (11%)
14	CLA	x	1701	12	49,53,73	1.49	8 (16%)	59,89,113	1.47	5 (8%)
14	CLA	a	823	1	49,53,73	1.48	9 (18%)	59,89,113	1.52	8 (13%)
14	CLA	l	206	21	69,73,73	1.26	11 (15%)	83,113,113	1.36	11 (13%)
17	BCR	A	850	-	41,41,41	1.33	3 (7%)	56,56,56	1.29	7 (12%)
14	CLA	b	802	21	69,73,73	1.24	10 (14%)	83,113,113	1.42	8 (9%)
14	CLA	B	831	2	53,57,73	1.41	10 (18%)	62,93,113	1.48	8 (12%)
14	CLA	a	814	1	69,73,73	1.27	10 (14%)	83,113,113	1.27	7 (8%)
14	CLA	1	1643	1	69,73,73	1.26	9 (13%)	83,113,113	1.41	8 (9%)
16	SF4	3	102	3	0,12,12	-	-	-		
14	CLA	B	819	21	69,73,73	1.28	9 (13%)	83,113,113	1.26	8 (9%)
14	CLA	A	833	1	69,73,73	1.26	11 (15%)	83,113,113	1.29	6 (7%)
14	CLA	b	820	21	69,73,73	1.27	9 (13%)	83,113,113	1.26	8 (9%)
14	CLA	a	816	1	69,73,73	1.26	8 (11%)	83,113,113	1.29	7 (8%)
14	CLA	1	1624	1	49,53,73	1.49	10 (20%)	59,89,113	1.51	8 (13%)
14	CLA	B	839	2	51,55,73	1.47	10 (19%)	61,91,113	1.38	7 (11%)
14	CLA	A	837	1	49,53,73	1.49	9 (18%)	59,89,113	1.42	7 (11%)
14	CLA	a	841	1	69,73,73	1.25	9 (13%)	83,113,113	1.35	7 (8%)
14	CLA	K	103	21	62,66,73	1.33	9 (14%)	74,104,113	1.35	10 (13%)
15	PQN	b	843	-	34,34,34	0.45	0	42,45,45	0.38	0
14	CLA	1	1607	1	69,73,73	1.26	11 (15%)	83,113,113	1.47	12 (14%)
18	LHG	L	208	-	38,38,48	0.73	0	41,44,54	1.26	3 (7%)
14	CLA	1	1625	1	69,73,73	1.26	8 (11%)	83,113,113	1.30	7 (8%)
14	CLA	2	807	2	69,73,73	1.27	9 (13%)	83,113,113	1.32	6 (7%)
18	LHG	a	854	14	40,40,48	0.77	1 (2%)	43,46,54	1.21	4 (9%)
14	CLA	B	814	2	69,73,73	1.24	9 (13%)	83,113,113	1.34	6 (7%)
14	CLA	1	1629	1	69,73,73	1.27	10 (14%)	83,113,113	1.30	8 (9%)
14	CLA	2	802	21	69,73,73	1.24	10 (14%)	83,113,113	1.42	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	6	201	21	62,66,73	1.33	10 (16%)	74,104,113	1.37	8 (10%)
14	CLA	2	806	2	69,73,73	1.25	10 (14%)	83,113,113	1.40	8 (9%)
14	CLA	a	828	1	69,73,73	1.27	10 (14%)	83,113,113	1.30	8 (9%)
14	CLA	a	840	1	69,73,73	1.26	10 (14%)	83,113,113	1.37	6 (7%)
17	BCR	a	848	-	41,41,41	1.19	3 (7%)	56,56,56	1.23	6 (10%)
14	CLA	2	827	2	69,73,73	1.28	10 (14%)	83,113,113	1.33	7 (8%)
14	CLA	a	819	1	69,73,73	1.24	9 (13%)	83,113,113	1.34	9 (10%)
16	SF4	1	1647	1,2	0,12,12	-	-	-		
14	CLA	a	811	1	53,57,73	1.42	9 (16%)	62,93,113	1.40	6 (9%)
14	CLA	k	103	21	62,66,73	1.33	9 (14%)	74,104,113	1.36	10 (13%)
14	CLA	b	821	2	69,73,73	1.25	10 (14%)	83,113,113	1.22	6 (7%)
14	CLA	b	817	2	69,73,73	1.24	8 (11%)	83,113,113	1.36	7 (8%)
14	CLA	b	816	2	69,73,73	1.24	9 (13%)	83,113,113	1.30	6 (7%)
14	CLA	2	831	2	59,63,73	1.36	9 (15%)	71,101,113	1.43	8 (11%)
14	CLA	J	102	-	42,45,73	1.58	10 (23%)	50,78,113	1.46	6 (12%)
17	BCR	A	852	-	25,25,41	1.13	1 (4%)	33,33,56	1.28	4 (12%)
14	CLA	b	823	21	59,63,73	1.36	10 (16%)	71,101,113	1.34	6 (8%)
18	LHG	y	101	-	48,48,48	0.71	2 (4%)	51,54,54	1.22	3 (5%)
14	CLA	B	813	2	69,73,73	1.26	10 (14%)	83,113,113	1.34	9 (10%)
14	CLA	1	1627	21	69,73,73	1.25	10 (14%)	83,113,113	1.39	9 (10%)
14	CLA	A	802	-	69,73,73	1.27	12 (17%)	83,113,113	1.39	9 (10%)
14	CLA	K	101	9	50,54,73	1.46	9 (18%)	60,90,113	1.44	5 (8%)
14	CLA	2	821	2	69,73,73	1.24	10 (14%)	83,113,113	1.21	5 (6%)
14	CLA	1	1613	14,1	69,73,73	1.25	9 (13%)	83,113,113	1.27	6 (7%)
14	CLA	A	827	21	69,73,73	1.26	10 (14%)	83,113,113	1.40	11 (13%)
14	CLA	A	834	1	69,73,73	1.26	11 (15%)	83,113,113	1.44	13 (15%)
17	BCR	A	851	-	41,41,41	1.27	2 (4%)	56,56,56	1.30	7 (12%)
14	CLA	B	804	2	69,73,73	1.26	10 (14%)	83,113,113	1.37	10 (12%)
14	CLA	A	836	1	69,73,73	1.25	9 (13%)	83,113,113	1.37	6 (7%)
14	CLA	B	802	2	69,73,73	1.25	10 (14%)	83,113,113	1.35	7 (8%)
14	CLA	A	828	1	69,73,73	1.27	10 (14%)	83,113,113	1.31	8 (9%)
14	CLA	1	1605	1	69,73,73	1.24	9 (13%)	83,113,113	1.36	6 (7%)
14	CLA	2	804	-	69,73,73	1.25	10 (14%)	83,113,113	1.39	6 (7%)
17	BCR	F	205	-	41,41,41	1.18	2 (4%)	56,56,56	1.36	8 (14%)
14	CLA	2	833	2	69,73,73	1.26	9 (13%)	83,113,113	1.36	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	B	806	2	69,73,73	1.28	9 (13%)	83,113,113	1.32	6 (7%)
14	CLA	1	1603	-	69,73,73	1.26	12 (17%)	83,113,113	1.39	9 (10%)
14	CLA	1	1604	21	69,73,73	1.29	10 (14%)	83,113,113	1.19	6 (7%)
14	CLA	L	204	10	69,73,73	1.26	10 (14%)	83,113,113	1.44	8 (9%)
14	CLA	A	831	1	69,73,73	1.28	11 (15%)	83,113,113	1.41	9 (10%)
14	CLA	A	829	1	69,73,73	1.25	9 (13%)	83,113,113	1.31	8 (9%)
14	CLA	1	1642	1	69,73,73	1.24	9 (13%)	83,113,113	1.36	7 (8%)
14	CLA	B	827	2	69,73,73	1.28	10 (14%)	83,113,113	1.32	8 (9%)
14	CLA	b	810	2	69,73,73	1.26	11 (15%)	83,113,113	1.48	9 (10%)
14	CLA	2	832	2	53,57,73	1.41	10 (18%)	62,93,113	1.47	7 (11%)
14	CLA	b	836	21	54,58,73	1.41	10 (18%)	65,95,113	1.43	7 (10%)
14	CLA	L	203	10	69,73,73	1.28	10 (14%)	83,113,113	1.32	7 (8%)
14	CLA	A	826	21	69,73,73	1.25	10 (14%)	83,113,113	1.38	9 (10%)
17	BCR	A	856	-	41,41,41	1.23	3 (7%)	56,56,56	1.28	8 (14%)
14	CLA	1	1631	-	69,73,73	1.24	10 (14%)	83,113,113	1.39	6 (7%)
14	CLA	1	1616	1	69,73,73	1.26	10 (14%)	83,113,113	1.29	5 (6%)
14	CLA	1	1619	1	69,73,73	1.24	8 (11%)	83,113,113	1.34	5 (6%)
14	CLA	A	815	1	69,73,73	1.26	10 (14%)	83,113,113	1.30	6 (7%)
14	CLA	2	818	2	69,73,73	1.26	9 (13%)	83,113,113	1.39	7 (8%)
14	CLA	a	843	21	69,73,73	1.28	10 (14%)	83,113,113	1.35	5 (6%)
18	LHG	M	101	-	48,48,48	0.70	2 (4%)	51,54,54	1.22	3 (5%)
14	CLA	A	805	14,1	63,67,73	1.29	10 (15%)	75,105,113	1.41	9 (12%)
14	CLA	A	803	21	69,73,73	1.29	10 (14%)	83,113,113	1.19	6 (7%)
14	CLA	1	1610	1	69,73,73	1.24	10 (14%)	83,113,113	1.39	9 (10%)
14	CLA	a	804	1	69,73,73	1.23	9 (13%)	83,113,113	1.36	6 (7%)
17	BCR	B	846	-	41,41,41	1.16	3 (7%)	56,56,56	1.24	7 (12%)
14	CLA	2	838	2	64,68,73	1.31	10 (15%)	77,107,113	1.39	6 (7%)
17	BCR	a	850	-	41,41,41	1.34	4 (9%)	56,56,56	1.29	7 (12%)
14	CLA	0	206	10	69,73,73	1.26	10 (14%)	83,113,113	1.44	8 (9%)
18	LHG	B	850	-	48,48,48	0.61	1 (2%)	51,54,54	1.20	5 (9%)
14	CLA	2	836	21	54,58,73	1.41	10 (18%)	65,95,113	1.43	7 (10%)
14	CLA	B	805	2	69,73,73	1.25	10 (14%)	83,113,113	1.39	8 (9%)
14	CLA	b	830	2	69,73,73	1.25	11 (15%)	83,113,113	1.45	7 (8%)
14	CLA	A	813	1	49,53,73	1.50	10 (20%)	59,89,113	1.50	7 (11%)
14	CLA	b	819	2	69,73,73	1.24	9 (13%)	83,113,113	1.38	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	8	1302	-	49,53,73	1.49	9 (18%)	59,89,113	1.45	6 (10%)
18	LHG	0	202	-	38,38,48	0.73	1 (2%)	41,44,54	1.26	3 (7%)
20	LMG	2	850	-	55,55,55	0.92	4 (7%)	63,63,63	1.35	9 (14%)
17	BCR	l	202	-	41,41,41	1.39	4 (9%)	56,56,56	1.32	7 (12%)
18	LHG	m	101	-	48,48,48	0.70	2 (4%)	51,54,54	1.22	3 (5%)
14	CLA	a	826	21	69,73,73	1.25	10 (14%)	83,113,113	1.38	9 (10%)
14	CLA	1	1606	14,1	63,67,73	1.29	10 (15%)	75,105,113	1.40	8 (10%)
14	CLA	2	813	2	49,53,73	1.48	9 (18%)	59,89,113	1.45	4 (6%)
14	CLA	B	826	2	69,73,73	1.28	10 (14%)	83,113,113	1.34	7 (8%)
14	CLA	B	832	2	69,73,73	1.26	9 (13%)	83,113,113	1.36	7 (8%)
14	CLA	A	842	1	69,73,73	1.26	11 (15%)	83,113,113	1.41	9 (10%)
15	PQN	a	845	-	34,34,34	0.40	0	42,45,45	0.35	0
14	CLA	a	838	1	69,73,73	1.25	10 (14%)	83,113,113	1.43	7 (8%)
20	LMG	b	850	-	55,55,55	0.92	4 (7%)	63,63,63	1.35	10 (15%)
14	CLA	a	833	1	69,73,73	1.26	11 (15%)	83,113,113	1.29	6 (7%)
17	BCR	j	1305	-	41,41,41	1.22	2 (4%)	56,56,56	1.28	8 (14%)
14	CLA	B	834	2	69,73,73	1.25	9 (13%)	83,113,113	1.34	9 (10%)
14	CLA	2	816	2	69,73,73	1.25	9 (13%)	83,113,113	1.30	6 (7%)
17	BCR	B	845	-	41,41,41	1.26	3 (7%)	56,56,56	1.24	6 (10%)
14	CLA	A	809	1	69,73,73	1.24	9 (13%)	83,113,113	1.39	8 (9%)
14	CLA	J	101	-	49,53,73	1.48	8 (16%)	59,89,113	1.45	6 (10%)
17	BCR	0	201	-	41,41,41	1.18	3 (7%)	56,56,56	1.28	7 (12%)
14	CLA	B	810	2	69,73,73	1.25	10 (14%)	83,113,113	1.41	7 (8%)
14	CLA	A	812	14,1	69,73,73	1.25	9 (13%)	83,113,113	1.26	6 (7%)
17	BCR	a	847	-	41,41,41	1.15	2 (4%)	56,56,56	1.30	7 (12%)
14	CLA	b	840	2	51,55,73	1.46	10 (19%)	61,91,113	1.37	6 (9%)
14	CLA	2	829	2	69,73,73	1.27	9 (13%)	83,113,113	1.21	5 (6%)
17	BCR	2	848	-	41,41,41	1.28	3 (7%)	56,56,56	1.31	8 (14%)
14	CLA	b	827	2	69,73,73	1.28	10 (14%)	83,113,113	1.34	7 (8%)
14	CLA	b	834	2	69,73,73	1.25	10 (14%)	83,113,113	1.35	5 (6%)
14	CLA	A	824	1	69,73,73	1.27	8 (11%)	83,113,113	1.29	7 (8%)
14	CLA	a	802	-	69,73,73	1.27	12 (17%)	83,113,113	1.39	9 (10%)
14	CLA	2	839	2	69,73,73	1.26	9 (13%)	83,113,113	1.31	6 (7%)
17	BCR	a	852	-	25,25,41	1.12	1 (4%)	33,33,56	1.29	4 (12%)
14	CLA	1	1644	21	69,73,73	1.28	10 (14%)	83,113,113	1.35	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	2	825	2	69,73,73	1.26	10 (14%)	83,113,113	1.35	6 (7%)
14	CLA	2	803	2	69,73,73	1.26	10 (14%)	83,113,113	1.36	7 (8%)
14	CLA	A	835	1	69,73,73	1.24	9 (13%)	83,113,113	1.37	4 (4%)
14	CLA	B	809	2	69,73,73	1.25	10 (14%)	83,113,113	1.48	9 (10%)
14	CLA	B	812	2	49,53,73	1.47	9 (18%)	59,89,113	1.46	4 (6%)
17	BCR	B	844	-	41,41,41	1.17	3 (7%)	56,56,56	1.19	3 (5%)
14	CLA	M	102	-	40,44,73	1.59	9 (22%)	47,76,113	1.43	3 (6%)
14	CLA	2	805	2	69,73,73	1.27	10 (14%)	83,113,113	1.36	10 (12%)
17	BCR	B	851	-	41,41,41	1.21	2 (4%)	56,56,56	1.34	9 (16%)
14	CLA	B	815	2	69,73,73	1.24	9 (13%)	83,113,113	1.30	6 (7%)
17	BCR	2	845	-	41,41,41	1.17	3 (7%)	56,56,56	1.19	3 (5%)
14	CLA	A	808	1	55,59,73	1.39	10 (18%)	66,96,113	1.43	6 (9%)
14	CLA	B	828	2	69,73,73	1.27	10 (14%)	83,113,113	1.20	5 (6%)
14	CLA	B	835	21	54,58,73	1.42	10 (18%)	65,95,113	1.44	7 (10%)
14	CLA	B	830	2	59,63,73	1.35	9 (15%)	71,101,113	1.42	8 (11%)
14	CLA	A	804	1	69,73,73	1.24	9 (13%)	83,113,113	1.36	6 (7%)
17	BCR	l	207	-	41,41,41	1.21	3 (7%)	56,56,56	1.34	7 (12%)
14	CLA	2	817	2	69,73,73	1.24	8 (11%)	83,113,113	1.36	7 (8%)
17	BCR	j	1304	-	41,41,41	1.17	3 (7%)	56,56,56	1.19	7 (12%)
17	BCR	7	101	-	41,41,41	1.29	4 (9%)	56,56,56	1.24	3 (5%)
14	CLA	1	1612	1	53,57,73	1.42	9 (16%)	62,93,113	1.40	6 (9%)
14	CLA	B	811	2	69,73,73	1.24	9 (13%)	83,113,113	1.39	9 (10%)
14	CLA	1	1640	1	69,73,73	1.25	9 (13%)	83,113,113	1.40	9 (10%)
17	BCR	9	102	-	41,41,41	1.18	2 (4%)	56,56,56	1.32	7 (12%)
14	CLA	b	808	2	69,73,73	1.26	9 (13%)	83,113,113	1.34	7 (8%)
14	CLA	a	803	21	69,73,73	1.29	10 (14%)	83,113,113	1.18	5 (6%)
14	CLA	A	832	1	64,68,73	1.32	11 (17%)	77,107,113	1.32	6 (7%)
14	CLA	1	1601	-	40,44,73	1.59	8 (20%)	47,76,113	1.43	3 (6%)
14	CLA	b	825	2	69,73,73	1.26	10 (14%)	83,113,113	1.36	6 (7%)
17	BCR	L	201	-	41,41,41	1.39	4 (9%)	56,56,56	1.33	7 (12%)
14	CLA	b	824	2	49,53,73	1.48	10 (20%)	59,89,113	1.50	8 (13%)
14	CLA	A	806	1	69,73,73	1.27	11 (15%)	83,113,113	1.47	12 (14%)
17	BCR	M	103	-	41,41,41	1.23	3 (7%)	56,56,56	1.22	5 (8%)
17	BCR	b	846	-	41,41,41	1.25	3 (7%)	56,56,56	1.24	6 (10%)
17	BCR	k	104	-	25,25,41	1.14	1 (4%)	33,33,56	1.15	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	a	825	1	69,73,73	1.26	10 (14%)	83,113,113	1.35	9 (10%)
14	CLA	2	830	2	69,73,73	1.24	11 (15%)	83,113,113	1.45	7 (8%)
14	CLA	2	824	2	49,53,73	1.48	10 (20%)	59,89,113	1.50	8 (13%)
14	CLA	b	803	2	69,73,73	1.25	10 (14%)	83,113,113	1.35	7 (8%)
14	CLA	0	207	21	69,73,73	1.26	11 (15%)	83,113,113	1.37	10 (12%)
14	CLA	1	1638	1	49,53,73	1.49	9 (18%)	59,89,113	1.42	7 (11%)
14	CLA	b	804	-	69,73,73	1.26	10 (14%)	83,113,113	1.39	6 (7%)
14	CLA	1	1639	1	69,73,73	1.25	11 (15%)	83,113,113	1.43	7 (8%)
17	BCR	2	847	-	41,41,41	1.16	3 (7%)	56,56,56	1.25	7 (12%)
14	CLA	2	810	2	69,73,73	1.26	11 (15%)	83,113,113	1.47	8 (9%)
14	CLA	a	839	1	69,73,73	1.25	9 (13%)	83,113,113	1.40	9 (10%)
17	BCR	1	1649	-	41,41,41	1.19	3 (7%)	56,56,56	1.22	6 (10%)
14	CLA	b	805	2	69,73,73	1.27	10 (14%)	83,113,113	1.37	11 (13%)
14	CLA	1	1618	21	69,73,73	1.24	10 (14%)	83,113,113	1.27	5 (6%)
17	BCR	0	208	-	41,41,41	1.22	3 (7%)	56,56,56	1.34	7 (12%)
18	LHG	A	854	14	40,40,48	0.77	1 (2%)	43,46,54	1.22	4 (9%)
17	BCR	b	845	-	41,41,41	1.17	3 (7%)	56,56,56	1.19	3 (5%)
14	CLA	b	842	2	69,73,73	1.26	9 (13%)	83,113,113	1.41	6 (7%)
14	CLA	2	808	2	69,73,73	1.27	9 (13%)	83,113,113	1.34	7 (8%)
14	CLA	l	205	10	69,73,73	1.26	10 (14%)	83,113,113	1.44	8 (9%)
14	CLA	A	820	1	69,73,73	1.25	10 (14%)	83,113,113	1.43	10 (12%)
14	CLA	a	810	1	69,73,73	1.27	9 (13%)	83,113,113	1.32	6 (7%)
14	CLA	b	826	21	69,73,73	1.27	10 (14%)	83,113,113	1.44	9 (10%)
14	CLA	X	1701	12	49,53,73	1.50	8 (16%)	59,89,113	1.46	5 (8%)
14	CLA	f	203	-	54,58,73	1.42	6 (11%)	65,95,113	1.38	6 (9%)
14	CLA	f	201	21	62,66,73	1.33	10 (16%)	74,104,113	1.37	8 (10%)
14	CLA	A	811	1	53,57,73	1.42	9 (16%)	62,93,113	1.39	6 (9%)
17	BCR	1	1653	-	25,25,41	1.13	1 (4%)	33,33,56	1.28	4 (12%)
14	CLA	A	817	21	69,73,73	1.25	10 (14%)	83,113,113	1.26	5 (6%)
14	CLA	6	203	-	54,58,73	1.42	5 (9%)	65,95,113	1.37	6 (9%)
14	CLA	9	101	-	50,54,73	1.45	9 (18%)	60,90,113	1.45	5 (8%)
14	CLA	B	808	2	69,73,73	1.23	9 (13%)	83,113,113	1.46	8 (9%)
17	BCR	2	849	-	41,41,41	1.39	4 (9%)	56,56,56	1.29	6 (10%)
14	CLA	8	1303	-	42,45,73	1.58	9 (21%)	50,78,113	1.45	6 (12%)
14	CLA	1	1617	1	69,73,73	1.25	8 (11%)	83,113,113	1.28	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	a	837	1	49,53,73	1.49	9 (18%)	59,89,113	1.43	7 (11%)
14	CLA	B	824	2	69,73,73	1.26	10 (14%)	83,113,113	1.35	6 (7%)
17	BCR	1	1648	-	41,41,41	1.15	2 (4%)	56,56,56	1.31	7 (12%)
14	CLA	A	818	1	69,73,73	1.24	8 (11%)	83,113,113	1.33	5 (6%)
14	CLA	1	1636	1	69,73,73	1.24	9 (13%)	83,113,113	1.37	4 (4%)
14	CLA	9	103	21	62,66,73	1.33	9 (14%)	74,104,113	1.35	10 (13%)
14	CLA	B	803	-	69,73,73	1.26	9 (13%)	83,113,113	1.40	6 (7%)
14	CLA	B	818	2	69,73,73	1.24	9 (13%)	83,113,113	1.38	9 (10%)
17	BCR	A	849	-	41,41,41	1.23	2 (4%)	56,56,56	1.20	6 (10%)
17	BCR	a	849	-	41,41,41	1.22	2 (4%)	56,56,56	1.20	6 (10%)
17	BCR	k	102	-	41,41,41	1.18	2 (4%)	56,56,56	1.31	7 (12%)
17	BCR	8	1305	-	41,41,41	1.22	2 (4%)	56,56,56	1.28	8 (14%)
17	BCR	K	102	-	41,41,41	1.18	2 (4%)	56,56,56	1.31	7 (12%)
17	BCR	b	844	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	4 (7%)
17	BCR	0	203	-	41,41,41	1.39	4 (9%)	56,56,56	1.33	7 (12%)
15	PQN	1	1646	-	34,34,34	0.40	0	42,45,45	0.36	0
14	CLA	2	837	21	49,53,73	1.50	8 (16%)	59,89,113	1.42	5 (8%)
16	SF4	3	101	3	0,12,12	-	-	-		
14	CLA	b	833	2	69,73,73	1.25	9 (13%)	83,113,113	1.36	7 (8%)
14	CLA	b	828	2	69,73,73	1.28	10 (14%)	83,113,113	1.32	8 (9%)
14	CLA	b	835	2	69,73,73	1.25	9 (13%)	83,113,113	1.34	9 (10%)
14	CLA	B	807	2	69,73,73	1.27	9 (13%)	83,113,113	1.33	8 (9%)
14	CLA	2	822	2	49,53,73	1.47	9 (18%)	59,89,113	1.56	10 (16%)
14	CLA	A	822	21	69,73,73	1.26	10 (14%)	83,113,113	1.34	8 (9%)
14	CLA	A	843	21	69,73,73	1.28	11 (15%)	83,113,113	1.35	5 (6%)
14	CLA	0	205	10	69,73,73	1.29	10 (14%)	83,113,113	1.31	7 (8%)
14	CLA	b	813	2	49,53,73	1.47	9 (18%)	59,89,113	1.45	4 (6%)
17	BCR	0	209	-	41,41,41	1.18	3 (7%)	56,56,56	1.28	7 (12%)
14	CLA	A	844	18	49,53,73	1.47	9 (18%)	59,89,113	1.50	7 (11%)
14	CLA	1	1622	1	69,73,73	1.26	7 (10%)	83,113,113	1.34	8 (9%)
14	CLA	1	1645	18	49,53,73	1.47	10 (20%)	59,89,113	1.50	7 (11%)
17	BCR	2	846	-	41,41,41	1.26	3 (7%)	56,56,56	1.25	6 (10%)
14	CLA	a	836	1	69,73,73	1.26	9 (13%)	83,113,113	1.37	6 (7%)
17	BCR	9	104	-	25,25,41	1.14	1 (4%)	33,33,56	1.15	4 (12%)
14	CLA	1	1637	1	69,73,73	1.26	9 (13%)	83,113,113	1.38	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	1	1621	1	69,73,73	1.25	10 (14%)	83,113,113	1.43	10 (12%)
14	CLA	B	822	21	59,63,73	1.37	10 (16%)	71,101,113	1.34	6 (8%)
14	CLA	2	823	21	59,63,73	1.36	10 (16%)	71,101,113	1.32	6 (8%)
14	CLA	1	1626	1	69,73,73	1.26	10 (14%)	83,113,113	1.35	10 (12%)
14	CLA	F	201	21	62,66,73	1.34	10 (16%)	74,104,113	1.36	8 (10%)
18	LHG	l	201	-	38,38,48	0.73	0	41,44,54	1.26	3 (7%)
14	CLA	b	815	2	69,73,73	1.24	10 (14%)	83,113,113	1.33	6 (7%)
14	CLA	1	1611	1	69,73,73	1.27	9 (13%)	83,113,113	1.31	6 (7%)
14	CLA	A	810	1	69,73,73	1.27	9 (13%)	83,113,113	1.33	6 (7%)
17	BCR	L	207	-	41,41,41	1.18	3 (7%)	56,56,56	1.28	7 (12%)
14	CLA	a	822	21	69,73,73	1.25	10 (14%)	83,113,113	1.34	8 (9%)
17	BCR	1	1650	-	41,41,41	1.22	2 (4%)	56,56,56	1.20	6 (10%)
14	CLA	A	814	1	69,73,73	1.27	9 (13%)	83,113,113	1.27	7 (8%)
18	LHG	A	853	-	48,48,48	0.75	2 (4%)	51,54,54	1.23	4 (7%)
14	CLA	8	1301	21	49,53,73	1.49	10 (20%)	59,89,113	1.45	8 (13%)
14	CLA	A	855	21	69,73,73	1.24	10 (14%)	83,113,113	1.42	8 (9%)
14	CLA	1	1609	1	55,59,73	1.40	10 (18%)	66,96,113	1.44	6 (9%)
14	CLA	2	826	21	69,73,73	1.27	10 (14%)	83,113,113	1.43	9 (10%)
18	LHG	1	1654	-	48,48,48	0.75	1 (2%)	51,54,54	1.23	4 (7%)
14	CLA	1	1614	1	49,53,73	1.49	10 (20%)	59,89,113	1.50	7 (11%)
17	BCR	L	206	-	41,41,41	1.21	3 (7%)	56,56,56	1.34	7 (12%)
14	CLA	1	1641	1	69,73,73	1.25	10 (14%)	83,113,113	1.37	6 (7%)
17	BCR	2	844	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	4 (7%)
14	CLA	2	842	2	69,73,73	1.26	9 (13%)	83,113,113	1.41	6 (7%)
14	CLA	B	833	2	69,73,73	1.25	10 (14%)	83,113,113	1.35	5 (6%)
18	LHG	1	1655	14	40,40,48	0.77	1 (2%)	43,46,54	1.21	4 (9%)
14	CLA	B	829	2	69,73,73	1.25	11 (15%)	83,113,113	1.45	7 (8%)
16	SF4	A	846	1,2	0,12,12	-	-	-		
17	BCR	i	101	-	41,41,41	1.29	4 (9%)	56,56,56	1.24	3 (5%)
17	BCR	6	204	-	41,41,41	1.18	2 (4%)	56,56,56	1.36	8 (14%)
14	CLA	1	1633	1	64,68,73	1.31	11 (17%)	77,107,113	1.33	6 (7%)
17	BCR	b	847	-	41,41,41	1.15	3 (7%)	56,56,56	1.25	8 (14%)
17	BCR	b	849	-	41,41,41	1.39	4 (9%)	56,56,56	1.29	6 (10%)
17	BCR	y	102	-	41,41,41	1.24	3 (7%)	56,56,56	1.22	5 (8%)
14	CLA	a	817	21	69,73,73	1.25	10 (14%)	83,113,113	1.26	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	a	820	1	69,73,73	1.25	10 (14%)	83,113,113	1.43	9 (10%)
14	CLA	A	821	1	69,73,73	1.25	7 (10%)	83,113,113	1.34	8 (9%)
13	CL0	A	801	1	69,73,73	1.26	10 (14%)	83,113,113	1.37	6 (7%)
14	CLA	a	805	14,1	63,67,73	1.29	10 (15%)	75,105,113	1.40	9 (12%)

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
14	CLA	j	1303	-	-	0/4/76/115	-
14	CLA	b	832	2	-	10/20/96/115	-
14	CLA	b	818	2	-	15/39/115/115	-
14	CLA	2	835	2	-	9/39/115/115	-
14	CLA	A	830	-	-	15/39/115/115	-
14	CLA	a	827	21	-	9/39/115/115	-
14	CLA	a	834	1	-	11/39/115/115	-
14	CLA	A	838	1	-	16/39/115/115	-
16	SF4	a	846	1,2	-	-	0/6/5/5
17	BCR	f	204	-	-	8/29/63/63	0/2/2/2
14	CLA	b	806	2	-	16/39/115/115	-
14	CLA	B	838	2	-	9/39/115/115	-
17	BCR	A	847	-	-	9/29/63/63	0/2/2/2
17	BCR	B	843	-	-	11/29/63/63	0/2/2/2
14	CLA	a	829	1	-	14/39/115/115	-
17	BCR	b	848	-	-	11/29/63/63	0/2/2/2
14	CLA	2	809	2	-	9/39/115/115	-
14	CLA	1	1635	1	-	11/39/115/115	-
14	CLA	2	812	2	-	10/39/115/115	-
14	CLA	B	837	2	-	5/33/109/115	-
14	CLA	j	1301	21	-	2/15/91/115	-
14	CLA	1	1608	1	-	15/39/115/115	-
14	CLA	a	844	18	-	5/15/91/115	-
14	CLA	k	101	9	-	12/17/93/115	-
14	CLA	a	842	1	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	815	1	-	14/39/115/115	-
14	CLA	z	102	12	-	7/15/91/115	-
14	CLA	A	825	1	-	14/39/115/115	-
14	CLA	b	822	2	-	5/15/91/115	-
14	CLA	j	1302	-	-	5/15/91/115	-
14	CLA	a	830	-	-	15/39/115/115	-
17	BCR	8	1306	-	-	15/29/63/63	0/2/2/2
15	PQN	2	843	-	-	1/23/43/43	0/2/2/2
14	CLA	1	1623	21	-	12/39/115/115	-
17	BCR	B	847	-	-	11/29/63/63	0/2/2/2
14	CLA	B	825	21	-	11/39/115/115	-
14	CLA	1	1634	1	-	12/39/115/115	-
14	CLA	a	813	1	-	4/15/91/115	-
17	BCR	6	202	-	-	12/29/63/63	0/2/2/2
14	CLA	A	816	1	-	19/39/115/115	-
14	CLA	1	1628	21	-	9/39/115/115	-
14	CLA	b	807	2	-	9/39/115/115	-
13	CL0	a	801	1	-	12/39/115/115	-
14	CLA	b	811	2	-	15/39/115/115	-
14	CLA	B	817	2	-	15/39/115/115	-
14	CLA	F	204	-	-	6/21/97/115	-
14	CLA	B	820	2	-	21/39/115/115	-
14	CLA	a	806	1	-	21/39/115/115	-
14	CLA	1	1615	1	-	17/39/115/115	-
14	CLA	A	823	1	-	8/15/91/115	-
14	CLA	A	840	1	-	18/39/115/115	-
14	CLA	b	841	21	-	9/39/115/115	-
18	LHG	a	853	-	-	21/53/53/53	-
14	CLA	a	831	1	-	7/39/115/115	-
17	BCR	A	848	-	-	15/29/63/63	0/2/2/2
17	BCR	1	1651	-	-	8/29/63/63	0/2/2/2
17	BCR	K	104	-	-	4/18/35/63	0/1/1/2
16	SF4	c	101	3	-	-	0/6/5/5
14	CLA	1	1630	1	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	809	1	-	11/39/115/115	-
17	BCR	m	102	-	-	9/29/63/63	0/2/2/2
14	CLA	a	812	14,1	-	13/39/115/115	-
14	CLA	2	811	2	-	15/39/115/115	-
14	CLA	b	831	2	-	13/27/103/115	-
16	SF4	c	102	3	-	-	0/6/5/5
14	CLA	B	823	2	-	5/15/91/115	-
17	BCR	B	848	-	-	5/29/63/63	0/2/2/2
14	CLA	a	824	1	-	12/39/115/115	-
17	BCR	8	1304	-	-	11/29/63/63	0/2/2/2
14	CLA	b	838	2	-	6/33/109/115	-
14	CLA	2	841	21	-	9/39/115/115	-
20	LMG	B	849	-	-	27/50/70/70	0/1/1/1
14	CLA	A	807	1	-	15/39/115/115	-
14	CLA	a	835	1	-	10/39/115/115	-
14	CLA	L	205	21	-	11/39/115/115	-
14	CLA	b	839	2	-	9/39/115/115	-
14	CLA	1	1632	1	-	7/39/115/115	-
14	CLA	B	821	2	-	5/15/91/115	-
14	CLA	2	820	21	-	17/39/115/115	-
14	CLA	B	816	2	-	12/39/115/115	-
14	CLA	b	829	2	-	11/39/115/115	-
14	CLA	2	834	2	-	11/39/115/115	-
14	CLA	a	818	1	-	10/39/115/115	-
14	CLA	l	204	10	-	17/39/115/115	-
14	CLA	b	814	2	-	16/39/115/115	-
18	LHG	b	851	-	-	18/53/53/53	-
14	CLA	F	203	21	-	2/15/91/115	-
14	CLA	b	809	2	-	9/39/115/115	-
17	BCR	I	101	-	-	7/29/63/63	0/2/2/2
14	CLA	a	808	1	-	6/23/99/115	-
14	CLA	2	819	2	-	17/39/115/115	-
17	BCR	J	103	-	-	11/29/63/63	0/2/2/2
14	CLA	b	812	2	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CL0	1	1602	1	-	12/39/115/115	-
14	CLA	A	841	1	-	14/39/115/115	-
16	SF4	C	102	3	-	-	0/6/5/5
14	CLA	2	814	2	-	16/39/115/115	-
15	PQN	B	842	-	-	1/23/43/43	0/2/2/2
17	BCR	1	1652	-	-	18/29/63/63	0/2/2/2
17	BCR	f	202	-	-	12/29/63/63	0/2/2/2
18	LHG	z	101	-	-	18/53/53/53	-
14	CLA	a	832	1	-	6/33/109/115	-
17	BCR	F	202	-	-	12/29/63/63	0/2/2/2
14	CLA	a	807	1	-	15/39/115/115	-
14	CLA	b	837	21	-	3/15/91/115	-
14	CLA	a	821	1	-	16/39/115/115	-
17	BCR	a	851	-	-	18/29/63/63	0/2/2/2
14	CLA	A	857	-	-	0/4/72/115	-
16	SF4	C	101	3	-	-	0/6/5/5
15	PQN	A	845	-	-	1/23/43/43	0/2/2/2
14	CLA	B	841	2	-	10/39/115/115	-
14	CLA	A	819	1	-	19/39/115/115	-
14	CLA	2	815	2	-	13/39/115/115	-
14	CLA	B	840	21	-	9/39/115/115	-
14	CLA	2	828	2	-	15/39/115/115	-
17	BCR	b	852	-	-	15/29/63/63	0/2/2/2
14	CLA	B	836	21	-	3/15/91/115	-
14	CLA	A	839	1	-	20/39/115/115	-
14	CLA	1	1620	1	-	19/39/115/115	-
14	CLA	2	840	2	-	2/18/94/115	-
14	CLA	x	1701	12	-	7/15/91/115	-
14	CLA	a	823	1	-	8/15/91/115	-
14	CLA	l	206	21	-	11/39/115/115	-
17	BCR	A	850	-	-	8/29/63/63	0/2/2/2
14	CLA	b	802	21	-	18/39/115/115	-
14	CLA	B	831	2	-	10/20/96/115	-
14	CLA	a	814	1	-	17/39/115/115	-
14	CLA	1	1643	1	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	SF4	3	102	3	-	-	0/6/5/5
14	CLA	B	819	21	-	17/39/115/115	-
14	CLA	A	833	1	-	12/39/115/115	-
14	CLA	b	820	21	-	17/39/115/115	-
14	CLA	a	816	1	-	19/39/115/115	-
14	CLA	1	1624	1	-	8/15/91/115	-
14	CLA	B	839	2	-	2/18/94/115	-
14	CLA	A	837	1	-	5/15/91/115	-
14	CLA	a	841	1	-	14/39/115/115	-
14	CLA	K	103	21	-	9/31/107/115	-
15	PQN	b	843	-	-	1/23/43/43	0/2/2/2
14	CLA	1	1607	1	-	21/39/115/115	-
18	LHG	L	208	-	-	27/43/43/53	-
14	CLA	1	1625	1	-	12/39/115/115	-
14	CLA	2	807	2	-	9/39/115/115	-
18	LHG	a	854	14	-	13/45/45/53	-
14	CLA	B	814	2	-	13/39/115/115	-
14	CLA	1	1629	1	-	7/39/115/115	-
14	CLA	2	802	21	-	18/39/115/115	-
14	CLA	6	201	21	-	6/31/107/115	-
14	CLA	2	806	2	-	16/39/115/115	-
14	CLA	a	828	1	-	7/39/115/115	-
14	CLA	a	840	1	-	18/39/115/115	-
17	BCR	a	848	-	-	15/29/63/63	0/2/2/2
14	CLA	2	827	2	-	6/39/115/115	-
14	CLA	a	819	1	-	19/39/115/115	-
16	SF4	1	1647	1,2	-	-	0/6/5/5
14	CLA	a	811	1	-	8/20/96/115	-
14	CLA	k	103	21	-	9/31/107/115	-
14	CLA	b	821	2	-	21/39/115/115	-
14	CLA	b	817	2	-	12/39/115/115	-
14	CLA	b	816	2	-	13/39/115/115	-
14	CLA	2	831	2	-	13/27/103/115	-
14	CLA	J	102	-	-	0/4/76/115	-
17	BCR	A	852	-	-	11/18/35/63	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	823	21	-	5/27/103/115	-
18	LHG	y	101	-	-	27/53/53/53	-
14	CLA	B	813	2	-	16/39/115/115	-
14	CLA	1	1627	21	-	13/39/115/115	-
14	CLA	A	802	-	-	15/39/115/115	-
14	CLA	K	101	9	-	12/17/93/115	-
14	CLA	2	821	2	-	21/39/115/115	-
14	CLA	1	1613	14,1	-	13/39/115/115	-
14	CLA	A	827	21	-	9/39/115/115	-
14	CLA	A	834	1	-	11/39/115/115	-
17	BCR	A	851	-	-	18/29/63/63	0/2/2/2
14	CLA	B	804	2	-	17/39/115/115	-
14	CLA	A	836	1	-	8/39/115/115	-
14	CLA	B	802	2	-	18/39/115/115	-
14	CLA	A	828	1	-	7/39/115/115	-
14	CLA	1	1605	1	-	16/39/115/115	-
14	CLA	2	804	-	-	12/39/115/115	-
17	BCR	F	205	-	-	8/29/63/63	0/2/2/2
14	CLA	2	833	2	-	16/39/115/115	-
14	CLA	B	806	2	-	9/39/115/115	-
14	CLA	1	1603	-	-	15/39/115/115	-
14	CLA	1	1604	21	-	6/39/115/115	-
14	CLA	L	204	10	-	11/39/115/115	-
14	CLA	A	831	1	-	7/39/115/115	-
14	CLA	A	829	1	-	14/39/115/115	-
14	CLA	1	1642	1	-	14/39/115/115	-
14	CLA	B	827	2	-	15/39/115/115	-
14	CLA	b	810	2	-	11/39/115/115	-
14	CLA	2	832	2	-	10/20/96/115	-
14	CLA	b	836	21	-	11/21/97/115	-
14	CLA	L	203	10	-	17/39/115/115	-
14	CLA	A	826	21	-	13/39/115/115	-
17	BCR	A	856	-	-	13/29/63/63	0/2/2/2
14	CLA	1	1631	-	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	1	1616	1	-	14/39/115/115	-
14	CLA	1	1619	1	-	10/39/115/115	-
14	CLA	A	815	1	-	14/39/115/115	-
14	CLA	2	818	2	-	15/39/115/115	-
14	CLA	a	843	21	-	16/39/115/115	-
18	LHG	M	101	-	-	27/53/53/53	-
14	CLA	A	805	14,1	-	10/32/108/115	-
14	CLA	A	803	21	-	6/39/115/115	-
14	CLA	1	1610	1	-	11/39/115/115	-
14	CLA	a	804	1	-	16/39/115/115	-
17	BCR	B	846	-	-	12/29/63/63	0/2/2/2
14	CLA	2	838	2	-	6/33/109/115	-
17	BCR	a	850	-	-	8/29/63/63	0/2/2/2
14	CLA	0	206	10	-	11/39/115/115	-
18	LHG	B	850	-	-	18/53/53/53	-
14	CLA	2	836	21	-	11/21/97/115	-
14	CLA	B	805	2	-	16/39/115/115	-
14	CLA	b	830	2	-	7/39/115/115	-
14	CLA	A	813	1	-	4/15/91/115	-
14	CLA	b	819	2	-	17/39/115/115	-
14	CLA	8	1302	-	-	5/15/91/115	-
18	LHG	0	202	-	-	27/43/43/53	-
20	LMG	2	850	-	-	27/50/70/70	0/1/1/1
17	BCR	l	202	-	-	8/29/63/63	0/2/2/2
18	LHG	m	101	-	-	27/53/53/53	-
14	CLA	a	826	21	-	13/39/115/115	-
14	CLA	1	1606	14,1	-	10/32/108/115	-
14	CLA	2	813	2	-	2/15/91/115	-
14	CLA	B	826	2	-	6/39/115/115	-
14	CLA	B	832	2	-	16/39/115/115	-
14	CLA	A	842	1	-	12/39/115/115	-
15	PQN	a	845	-	-	1/23/43/43	0/2/2/2
14	CLA	a	838	1	-	16/39/115/115	-
20	LMG	b	850	-	-	27/50/70/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	833	1	-	12/39/115/115	-
17	BCR	j	1305	-	-	13/29/63/63	0/2/2/2
14	CLA	B	834	2	-	9/39/115/115	-
14	CLA	2	816	2	-	13/39/115/115	-
17	BCR	B	845	-	-	11/29/63/63	0/2/2/2
14	CLA	A	809	1	-	11/39/115/115	-
14	CLA	J	101	-	-	5/15/91/115	-
17	BCR	0	201	-	-	5/29/63/63	0/2/2/2
14	CLA	B	810	2	-	15/39/115/115	-
14	CLA	A	812	14,1	-	13/39/115/115	-
17	BCR	a	847	-	-	9/29/63/63	0/2/2/2
14	CLA	b	840	2	-	2/18/94/115	-
14	CLA	2	829	2	-	11/39/115/115	-
17	BCR	2	848	-	-	11/29/63/63	0/2/2/2
14	CLA	b	827	2	-	6/39/115/115	-
14	CLA	b	834	2	-	11/39/115/115	-
14	CLA	A	824	1	-	12/39/115/115	-
14	CLA	a	802	-	-	15/39/115/115	-
14	CLA	2	839	2	-	9/39/115/115	-
17	BCR	a	852	-	-	11/18/35/63	0/1/1/2
14	CLA	1	1644	21	-	16/39/115/115	-
14	CLA	2	825	2	-	14/39/115/115	-
14	CLA	2	803	2	-	18/39/115/115	-
14	CLA	A	835	1	-	10/39/115/115	-
14	CLA	B	809	2	-	11/39/115/115	-
14	CLA	B	812	2	-	2/15/91/115	-
17	BCR	B	844	-	-	8/29/63/63	0/2/2/2
14	CLA	M	102	-	-	0/4/72/115	-
14	CLA	2	805	2	-	17/39/115/115	-
17	BCR	B	851	-	-	15/29/63/63	0/2/2/2
14	CLA	B	815	2	-	13/39/115/115	-
17	BCR	2	845	-	-	8/29/63/63	0/2/2/2
14	CLA	A	808	1	-	6/23/99/115	-
14	CLA	B	828	2	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	835	21	-	11/21/97/115	-
14	CLA	B	830	2	-	13/27/103/115	-
14	CLA	A	804	1	-	16/39/115/115	-
17	BCR	l	207	-	-	10/29/63/63	0/2/2/2
14	CLA	2	817	2	-	12/39/115/115	-
17	BCR	j	1304	-	-	11/29/63/63	0/2/2/2
17	BCR	7	101	-	-	7/29/63/63	0/2/2/2
14	CLA	1	1612	1	-	8/20/96/115	-
14	CLA	B	811	2	-	10/39/115/115	-
14	CLA	1	1640	1	-	20/39/115/115	-
17	BCR	9	102	-	-	6/29/63/63	0/2/2/2
14	CLA	b	808	2	-	8/39/115/115	-
14	CLA	a	803	21	-	6/39/115/115	-
14	CLA	A	832	1	-	6/33/109/115	-
14	CLA	1	1601	-	-	0/4/72/115	-
14	CLA	b	825	2	-	14/39/115/115	-
17	BCR	L	201	-	-	8/29/63/63	0/2/2/2
14	CLA	b	824	2	-	5/15/91/115	-
14	CLA	A	806	1	-	21/39/115/115	-
17	BCR	M	103	-	-	9/29/63/63	0/2/2/2
17	BCR	b	846	-	-	11/29/63/63	0/2/2/2
17	BCR	k	104	-	-	4/18/35/63	0/1/1/2
14	CLA	a	825	1	-	14/39/115/115	-
14	CLA	2	830	2	-	7/39/115/115	-
14	CLA	2	824	2	-	5/15/91/115	-
14	CLA	b	803	2	-	18/39/115/115	-
14	CLA	0	207	21	-	11/39/115/115	-
14	CLA	1	1638	1	-	5/15/91/115	-
14	CLA	b	804	-	-	12/39/115/115	-
14	CLA	1	1639	1	-	16/39/115/115	-
17	BCR	2	847	-	-	12/29/63/63	0/2/2/2
14	CLA	2	810	2	-	11/39/115/115	-
14	CLA	a	839	1	-	20/39/115/115	-
17	BCR	1	1649	-	-	15/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	805	2	-	17/39/115/115	-
14	CLA	1	1618	21	-	14/39/115/115	-
17	BCR	0	208	-	-	10/29/63/63	0/2/2/2
18	LHG	A	854	14	-	13/45/45/53	-
17	BCR	b	845	-	-	8/29/63/63	0/2/2/2
14	CLA	b	842	2	-	10/39/115/115	-
14	CLA	2	808	2	-	8/39/115/115	-
14	CLA	l	205	10	-	11/39/115/115	-
14	CLA	A	820	1	-	10/39/115/115	-
14	CLA	a	810	1	-	12/39/115/115	-
14	CLA	b	826	21	-	11/39/115/115	-
14	CLA	X	1701	12	-	7/15/91/115	-
14	CLA	f	203	-	-	6/21/97/115	-
14	CLA	f	201	21	-	6/31/107/115	-
14	CLA	A	811	1	-	8/20/96/115	-
17	BCR	1	1653	-	-	11/18/35/63	0/1/1/2
14	CLA	A	817	21	-	14/39/115/115	-
14	CLA	6	203	-	-	6/21/97/115	-
14	CLA	9	101	-	-	12/17/93/115	-
14	CLA	B	808	2	-	9/39/115/115	-
17	BCR	2	849	-	-	5/29/63/63	0/2/2/2
14	CLA	8	1303	-	-	0/4/76/115	-
14	CLA	1	1617	1	-	19/39/115/115	-
14	CLA	a	837	1	-	5/15/91/115	-
14	CLA	B	824	2	-	14/39/115/115	-
17	BCR	1	1648	-	-	9/29/63/63	0/2/2/2
14	CLA	A	818	1	-	10/39/115/115	-
14	CLA	1	1636	1	-	10/39/115/115	-
14	CLA	9	103	21	-	9/31/107/115	-
14	CLA	B	803	-	-	12/39/115/115	-
14	CLA	B	818	2	-	17/39/115/115	-
17	BCR	A	849	-	-	5/29/63/63	0/2/2/2
17	BCR	a	849	-	-	5/29/63/63	0/2/2/2
17	BCR	k	102	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	8	1305	-	-	13/29/63/63	0/2/2/2
17	BCR	K	102	-	-	6/29/63/63	0/2/2/2
17	BCR	b	844	-	-	11/29/63/63	0/2/2/2
17	BCR	0	203	-	-	8/29/63/63	0/2/2/2
15	PQN	1	1646	-	-	1/23/43/43	0/2/2/2
14	CLA	2	837	21	-	3/15/91/115	-
16	SF4	3	101	3	-	-	0/6/5/5
14	CLA	b	833	2	-	16/39/115/115	-
14	CLA	b	828	2	-	15/39/115/115	-
14	CLA	b	835	2	-	9/39/115/115	-
14	CLA	B	807	2	-	8/39/115/115	-
14	CLA	2	822	2	-	5/15/91/115	-
14	CLA	A	822	21	-	12/39/115/115	-
14	CLA	A	843	21	-	16/39/115/115	-
14	CLA	0	205	10	-	17/39/115/115	-
14	CLA	b	813	2	-	2/15/91/115	-
17	BCR	0	209	-	-	5/29/63/63	0/2/2/2
14	CLA	A	844	18	-	5/15/91/115	-
14	CLA	1	1622	1	-	16/39/115/115	-
14	CLA	1	1645	18	-	5/15/91/115	-
17	BCR	2	846	-	-	11/29/63/63	0/2/2/2
14	CLA	a	836	1	-	8/39/115/115	-
17	BCR	9	104	-	-	4/18/35/63	0/1/1/2
14	CLA	1	1637	1	-	8/39/115/115	-
14	CLA	1	1621	1	-	10/39/115/115	-
14	CLA	B	822	21	-	5/27/103/115	-
14	CLA	2	823	21	-	5/27/103/115	-
14	CLA	1	1626	1	-	14/39/115/115	-
14	CLA	F	201	21	-	6/31/107/115	-
18	LHG	l	201	-	-	27/43/43/53	-
14	CLA	b	815	2	-	13/39/115/115	-
14	CLA	1	1611	1	-	12/39/115/115	-
14	CLA	A	810	1	-	12/39/115/115	-
17	BCR	L	207	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	822	21	-	12/39/115/115	-
17	BCR	1	1650	-	-	5/29/63/63	0/2/2/2
14	CLA	A	814	1	-	17/39/115/115	-
18	LHG	A	853	-	-	21/53/53/53	-
14	CLA	8	1301	21	-	2/15/91/115	-
14	CLA	A	855	21	-	18/39/115/115	-
14	CLA	1	1609	1	-	6/23/99/115	-
14	CLA	2	826	21	-	11/39/115/115	-
18	LHG	1	1654	-	-	21/53/53/53	-
14	CLA	1	1614	1	-	4/15/91/115	-
17	BCR	L	206	-	-	10/29/63/63	0/2/2/2
14	CLA	1	1641	1	-	18/39/115/115	-
17	BCR	2	844	-	-	11/29/63/63	0/2/2/2
14	CLA	2	842	2	-	10/39/115/115	-
14	CLA	B	833	2	-	11/39/115/115	-
18	LHG	1	1655	14	-	13/45/45/53	-
14	CLA	B	829	2	-	7/39/115/115	-
17	BCR	i	101	-	-	7/29/63/63	0/2/2/2
16	SF4	A	846	1,2	-	-	0/6/5/5
17	BCR	6	204	-	-	8/29/63/63	0/2/2/2
14	CLA	1	1633	1	-	6/33/109/115	-
17	BCR	b	847	-	-	12/29/63/63	0/2/2/2
17	BCR	b	849	-	-	5/29/63/63	0/2/2/2
17	BCR	y	102	-	-	9/29/63/63	0/2/2/2
14	CLA	a	817	21	-	14/39/115/115	-
14	CLA	a	820	1	-	10/39/115/115	-
14	CLA	A	821	1	-	16/39/115/115	-
13	CL0	A	801	1	-	12/39/115/115	-
14	CLA	a	805	14,1	-	10/32/108/115	-

All (2998) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	845	BCR	C30-C25	-4.08	1.48	1.53
17	1	1651	BCR	C30-C25	-4.06	1.48	1.53
17	a	850	BCR	C30-C25	-4.02	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	846	BCR	C30-C25	-4.01	1.48	1.53
17	2	844	BCR	C1-C6	-4.01	1.48	1.53
17	B	848	BCR	C1-C6	-4.00	1.48	1.53
14	J	102	CLA	C1D-ND	3.99	1.42	1.37
14	j	1303	CLA	C1D-ND	3.99	1.42	1.37
17	2	846	BCR	C30-C25	-3.99	1.48	1.53
17	1	1650	BCR	C1-C6	-3.99	1.48	1.53
17	2	849	BCR	C1-C6	-3.98	1.48	1.53
17	B	843	BCR	C1-C6	-3.98	1.48	1.53
17	2	848	BCR	C30-C25	-3.97	1.48	1.53
17	A	850	BCR	C30-C25	-3.96	1.48	1.53
17	A	856	BCR	C1-C6	-3.96	1.48	1.53
17	b	849	BCR	C1-C6	-3.95	1.48	1.53
17	b	844	BCR	C1-C6	-3.95	1.48	1.53
17	j	1305	BCR	C1-C6	-3.94	1.48	1.53
17	A	849	BCR	C1-C6	-3.94	1.48	1.53
17	8	1305	BCR	C1-C6	-3.93	1.48	1.53
17	b	848	BCR	C30-C25	-3.93	1.48	1.53
17	B	847	BCR	C30-C25	-3.92	1.48	1.53
14	8	1303	CLA	C1D-ND	3.91	1.42	1.37
17	a	849	BCR	C1-C6	-3.91	1.48	1.53
17	m	102	BCR	C1-C6	-3.91	1.48	1.53
17	b	848	BCR	C1-C6	-3.90	1.48	1.53
17	7	101	BCR	C1-C6	-3.90	1.48	1.53
17	L	201	BCR	C1-C6	-3.89	1.48	1.53
17	I	101	BCR	C1-C6	-3.89	1.48	1.53
17	M	103	BCR	C1-C6	-3.88	1.48	1.53
17	2	849	BCR	C30-C25	-3.88	1.48	1.53
14	J	101	CLA	C1D-ND	3.88	1.42	1.37
14	8	1302	CLA	C1D-ND	3.87	1.42	1.37
14	K	103	CLA	C1D-ND	3.87	1.42	1.37
17	0	203	BCR	C1-C6	-3.87	1.48	1.53
14	k	103	CLA	C1D-ND	3.86	1.42	1.37
17	0	203	BCR	C30-C25	-3.86	1.48	1.53
17	1	1652	BCR	C1-C6	-3.85	1.48	1.53
17	i	101	BCR	C1-C6	-3.85	1.48	1.53
17	l	202	BCR	C30-C25	-3.85	1.48	1.53
17	F	202	BCR	C30-C25	-3.85	1.48	1.53
17	b	849	BCR	C30-C25	-3.85	1.48	1.53
14	j	1302	CLA	C1D-ND	3.85	1.42	1.37
14	a	816	CLA	C1D-ND	3.84	1.42	1.37
17	L	201	BCR	C30-C25	-3.84	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	851	BCR	C1-C6	-3.84	1.48	1.53
17	a	851	BCR	C1-C6	-3.84	1.48	1.53
17	l	202	BCR	C1-C6	-3.84	1.48	1.53
17	y	102	BCR	C1-C6	-3.84	1.48	1.53
17	6	202	BCR	C30-C25	-3.83	1.48	1.53
14	9	103	CLA	C1D-ND	3.83	1.42	1.37
17	2	848	BCR	C1-C6	-3.83	1.48	1.53
17	f	202	BCR	C30-C25	-3.83	1.48	1.53
17	a	848	BCR	C30-C25	-3.83	1.48	1.53
17	1	1649	BCR	C30-C25	-3.83	1.48	1.53
14	1	1618	CLA	C1D-ND	3.83	1.42	1.37
14	l	205	CLA	C4D-ND	-3.83	1.32	1.37
14	0	206	CLA	C4D-ND	-3.83	1.32	1.37
14	6	203	CLA	C1D-ND	3.82	1.42	1.37
14	B	819	CLA	C1D-ND	3.82	1.42	1.37
14	a	817	CLA	C1D-ND	3.82	1.42	1.37
14	1	1617	CLA	C1D-ND	3.82	1.42	1.37
14	A	816	CLA	C1D-ND	3.82	1.42	1.37
14	a	824	CLA	C1D-ND	3.82	1.42	1.37
14	a	821	CLA	C1D-ND	3.82	1.42	1.37
14	b	822	CLA	C1D-ND	3.81	1.42	1.37
14	A	817	CLA	C1D-ND	3.81	1.42	1.37
14	L	204	CLA	C4D-ND	-3.80	1.32	1.37
14	f	203	CLA	C1D-ND	3.80	1.42	1.37
14	1	1622	CLA	C1D-ND	3.80	1.42	1.37
17	B	847	BCR	C1-C6	-3.80	1.48	1.53
14	A	824	CLA	C1D-ND	3.79	1.42	1.37
14	B	821	CLA	C1D-ND	3.79	1.42	1.37
17	B	851	BCR	C1-C6	-3.78	1.48	1.53
14	A	821	CLA	C1D-ND	3.78	1.42	1.37
17	B	848	BCR	C30-C25	-3.77	1.48	1.53
14	1	1625	CLA	C1D-ND	3.77	1.42	1.37
14	2	820	CLA	C1D-ND	3.76	1.42	1.37
14	F	204	CLA	C1D-ND	3.76	1.42	1.37
14	A	815	CLA	C1D-ND	3.76	1.42	1.37
17	b	852	BCR	C1-C6	-3.75	1.48	1.53
17	8	1306	BCR	C1-C6	-3.75	1.48	1.53
17	B	845	BCR	C1-C6	-3.74	1.48	1.53
14	2	822	CLA	C1D-ND	3.74	1.42	1.37
17	2	846	BCR	C1-C6	-3.74	1.48	1.53
14	1	1616	CLA	C1D-ND	3.73	1.42	1.37
17	A	848	BCR	C30-C25	-3.72	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	846	BCR	C1-C6	-3.71	1.48	1.53
14	1	1601	CLA	C1D-ND	3.70	1.42	1.37
14	a	815	CLA	C1D-ND	3.70	1.42	1.37
14	1	1624	CLA	C1D-ND	3.69	1.42	1.37
14	b	820	CLA	C1D-ND	3.69	1.42	1.37
14	2	831	CLA	C1D-ND	3.68	1.42	1.37
14	2	840	CLA	C1D-ND	3.68	1.42	1.37
14	M	102	CLA	C1D-ND	3.68	1.42	1.37
14	A	857	CLA	C1D-ND	3.67	1.42	1.37
14	b	831	CLA	C1D-ND	3.67	1.42	1.37
14	B	824	CLA	C1D-ND	3.67	1.42	1.37
14	k	101	CLA	C1D-ND	3.66	1.42	1.37
14	B	817	CLA	C1D-ND	3.65	1.42	1.37
14	X	1701	CLA	C1D-ND	3.65	1.42	1.37
14	B	839	CLA	C1D-ND	3.65	1.42	1.37
14	2	827	CLA	C1D-ND	3.65	1.42	1.37
14	B	830	CLA	C1D-ND	3.65	1.42	1.37
14	K	101	CLA	C1D-ND	3.65	1.42	1.37
14	b	818	CLA	C1D-ND	3.64	1.42	1.37
17	1	1651	BCR	C1-C6	-3.64	1.48	1.53
14	a	823	CLA	C1D-ND	3.64	1.42	1.37
17	A	850	BCR	C1-C6	-3.63	1.48	1.53
17	f	204	BCR	C1-C6	-3.63	1.48	1.53
14	a	810	CLA	C1D-ND	3.63	1.42	1.37
14	x	1701	CLA	C1D-ND	3.63	1.42	1.37
14	1	1612	CLA	C1D-ND	3.62	1.42	1.37
14	9	101	CLA	C1D-ND	3.62	1.42	1.37
17	B	846	BCR	C30-C25	-3.62	1.48	1.53
17	F	205	BCR	C1-C6	-3.62	1.48	1.53
14	2	813	CLA	C1D-ND	3.62	1.42	1.37
14	2	818	CLA	C1D-ND	3.62	1.42	1.37
14	A	823	CLA	C1D-ND	3.62	1.42	1.37
14	B	836	CLA	C1D-ND	3.61	1.42	1.37
14	b	840	CLA	C1D-ND	3.61	1.42	1.37
14	a	820	CLA	C1D-ND	3.61	1.42	1.37
14	2	812	CLA	C1D-ND	3.61	1.42	1.37
14	1	1611	CLA	C1D-ND	3.60	1.42	1.37
14	b	827	CLA	C1D-ND	3.60	1.42	1.37
17	f	202	BCR	C1-C6	-3.60	1.48	1.53
14	B	826	CLA	C1D-ND	3.60	1.42	1.37
17	F	202	BCR	C1-C6	-3.60	1.48	1.53
14	b	825	CLA	C1D-ND	3.59	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	1645	CLA	C1D-ND	3.59	1.42	1.37
17	a	850	BCR	C1-C6	-3.59	1.48	1.53
14	b	812	CLA	C1D-ND	3.59	1.42	1.37
17	b	847	BCR	C30-C25	-3.59	1.48	1.53
17	2	847	BCR	C30-C25	-3.59	1.48	1.53
14	b	837	CLA	C1D-ND	3.59	1.42	1.37
14	A	844	CLA	C1D-ND	3.59	1.42	1.37
14	A	814	CLA	C1D-ND	3.58	1.42	1.37
14	A	820	CLA	C1D-ND	3.58	1.42	1.37
14	B	812	CLA	C1D-ND	3.58	1.42	1.37
14	b	813	CLA	C1D-ND	3.58	1.42	1.37
14	b	821	CLA	C1D-ND	3.58	1.42	1.37
14	f	203	CLA	C4B-NB	3.58	1.42	1.37
14	j	1301	CLA	C1D-ND	3.58	1.42	1.37
17	6	204	BCR	C1-C6	-3.58	1.48	1.53
14	B	816	CLA	C1D-ND	3.57	1.42	1.37
14	2	817	CLA	C1D-ND	3.57	1.42	1.37
14	B	820	CLA	C1D-ND	3.57	1.42	1.37
17	6	202	BCR	C1-C6	-3.57	1.48	1.53
14	2	825	CLA	C1D-ND	3.56	1.42	1.37
14	A	824	CLA	C4B-NB	3.56	1.42	1.37
14	F	203	CLA	C1D-ND	3.56	1.42	1.37
14	z	102	CLA	C1D-ND	3.56	1.42	1.37
14	A	813	CLA	C1D-ND	3.55	1.42	1.37
14	a	814	CLA	C1D-ND	3.55	1.42	1.37
14	1	1615	CLA	C1D-ND	3.55	1.42	1.37
14	2	837	CLA	C1D-ND	3.55	1.42	1.37
17	k	102	BCR	C1-C6	-3.55	1.48	1.53
14	B	813	CLA	C1D-ND	3.54	1.42	1.37
14	a	813	CLA	C1D-ND	3.54	1.42	1.37
14	A	810	CLA	C1D-ND	3.54	1.42	1.37
14	a	811	CLA	C1D-ND	3.54	1.42	1.37
14	B	811	CLA	C1D-ND	3.53	1.42	1.37
14	a	837	CLA	C1D-ND	3.53	1.42	1.37
14	2	824	CLA	C1D-ND	3.53	1.42	1.37
14	a	844	CLA	C1D-ND	3.53	1.42	1.37
14	1	1628	CLA	C4D-ND	-3.53	1.32	1.37
14	1	1621	CLA	C1D-ND	3.53	1.42	1.37
14	b	817	CLA	C1D-ND	3.53	1.42	1.37
14	F	204	CLA	C4B-NB	3.52	1.42	1.37
14	1	1625	CLA	C4B-NB	3.52	1.42	1.37
17	K	102	BCR	C1-C6	-3.52	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	811	CLA	C1D-ND	3.52	1.42	1.37
17	9	102	BCR	C1-C6	-3.51	1.48	1.53
14	6	203	CLA	C4B-NB	3.51	1.42	1.37
17	B	851	BCR	C30-C25	-3.50	1.49	1.53
14	2	814	CLA	C1D-ND	3.50	1.42	1.37
14	a	824	CLA	C4B-NB	3.50	1.42	1.37
14	A	837	CLA	C1D-ND	3.50	1.42	1.37
14	b	814	CLA	C1D-ND	3.50	1.42	1.37
14	A	827	CLA	C4D-ND	-3.49	1.32	1.37
14	8	1301	CLA	C1D-ND	3.49	1.42	1.37
14	A	818	CLA	C1D-ND	3.49	1.42	1.37
14	1	1614	CLA	C1D-ND	3.49	1.42	1.37
14	B	822	CLA	C1D-ND	3.49	1.42	1.37
14	B	823	CLA	C1D-ND	3.49	1.42	1.37
14	2	821	CLA	C1D-ND	3.49	1.42	1.37
14	M	102	CLA	C4B-NB	3.49	1.42	1.37
14	b	820	CLA	C4B-NB	3.48	1.42	1.37
14	B	836	CLA	C4B-NB	3.48	1.42	1.37
14	A	857	CLA	C4B-NB	3.48	1.42	1.37
14	a	821	CLA	C3B-C4B	3.48	1.50	1.42
17	K	104	BCR	C1-C6	-3.48	1.49	1.53
17	b	845	BCR	C1-C6	-3.48	1.49	1.53
14	B	831	CLA	C1D-ND	3.48	1.42	1.37
14	a	827	CLA	C4D-ND	-3.47	1.32	1.37
14	1	1634	CLA	C4D-ND	-3.47	1.32	1.37
17	i	101	BCR	C30-C25	-3.47	1.49	1.53
14	a	833	CLA	C4D-ND	-3.47	1.32	1.37
14	z	102	CLA	C4B-NB	3.47	1.42	1.37
14	b	824	CLA	C1D-ND	3.47	1.42	1.37
14	B	819	CLA	C4B-NB	3.47	1.42	1.37
14	2	823	CLA	C1D-ND	3.47	1.42	1.37
14	b	839	CLA	C1D-ND	3.47	1.42	1.37
14	1	1622	CLA	C3B-C4B	3.47	1.50	1.42
14	B	835	CLA	C1D-ND	3.46	1.42	1.37
14	1	1638	CLA	C1D-ND	3.46	1.42	1.37
14	2	836	CLA	C1D-ND	3.46	1.42	1.37
14	a	828	CLA	C4D-ND	-3.46	1.32	1.37
14	b	837	CLA	C4B-NB	3.46	1.42	1.37
17	8	1306	BCR	C30-C25	-3.46	1.49	1.53
14	b	808	CLA	C1D-ND	3.46	1.42	1.37
14	2	804	CLA	C4D-ND	-3.46	1.32	1.37
14	1	1630	CLA	C1D-ND	3.46	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	823	CLA	C1D-ND	3.46	1.42	1.37
14	b	832	CLA	C1D-ND	3.45	1.42	1.37
14	b	836	CLA	C1D-ND	3.45	1.42	1.37
14	A	822	CLA	C1D-ND	3.45	1.42	1.37
14	2	820	CLA	C4B-NB	3.45	1.42	1.37
14	X	1701	CLA	C4B-NB	3.45	1.42	1.37
14	b	835	CLA	C1D-ND	3.45	1.42	1.37
14	A	806	CLA	C4D-ND	-3.45	1.33	1.37
17	7	101	BCR	C30-C25	-3.45	1.49	1.53
17	9	102	BCR	C30-C25	-3.45	1.49	1.53
14	A	804	CLA	C1D-ND	3.45	1.42	1.37
14	2	837	CLA	C4B-NB	3.45	1.42	1.37
14	1	1619	CLA	C1D-ND	3.44	1.42	1.37
17	9	104	BCR	C1-C6	-3.44	1.49	1.53
14	1	1601	CLA	C4B-NB	3.44	1.42	1.37
14	A	821	CLA	C3B-C4B	3.44	1.50	1.42
14	A	832	CLA	C4D-ND	-3.44	1.33	1.37
14	b	828	CLA	C4D-ND	-3.44	1.33	1.37
17	b	852	BCR	C30-C25	-3.44	1.49	1.53
14	a	829	CLA	C1D-ND	3.44	1.42	1.37
14	A	833	CLA	C4D-ND	-3.44	1.33	1.37
14	1	1623	CLA	C1D-ND	3.44	1.42	1.37
14	1	1609	CLA	C1D-ND	3.44	1.42	1.37
17	B	844	BCR	C1-C6	-3.44	1.49	1.53
14	A	829	CLA	C1D-ND	3.43	1.42	1.37
14	2	832	CLA	C1D-ND	3.43	1.42	1.37
14	0	205	CLA	C4D-ND	-3.43	1.33	1.37
14	1	1629	CLA	C4D-ND	-3.43	1.33	1.37
14	2	808	CLA	C1D-ND	3.43	1.42	1.37
17	A	852	BCR	C1-C6	-3.43	1.49	1.53
14	B	814	CLA	C1D-ND	3.43	1.42	1.37
14	2	815	CLA	C1D-ND	3.43	1.42	1.37
14	b	815	CLA	C1D-ND	3.42	1.42	1.37
14	B	818	CLA	C4D-ND	-3.42	1.33	1.37
14	1	1605	CLA	C1D-ND	3.42	1.42	1.37
14	a	822	CLA	C1D-ND	3.42	1.42	1.37
14	2	842	CLA	C4D-ND	-3.42	1.33	1.37
14	a	802	CLA	C4D-ND	-3.41	1.33	1.37
14	a	806	CLA	C4D-ND	-3.41	1.33	1.37
14	b	804	CLA	C4D-ND	-3.41	1.33	1.37
17	y	102	BCR	C30-C25	-3.41	1.49	1.53
14	A	808	CLA	C1D-ND	3.41	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	839	CLA	C1D-ND	3.41	1.42	1.37
14	B	841	CLA	C4D-ND	-3.41	1.33	1.37
17	k	104	BCR	C1-C6	-3.41	1.49	1.53
14	B	840	CLA	C4D-ND	-3.41	1.33	1.37
14	b	816	CLA	C1D-ND	3.41	1.42	1.37
14	2	819	CLA	C4D-ND	-3.41	1.33	1.37
14	A	819	CLA	C1D-ND	3.41	1.42	1.37
17	1	1653	BCR	C1-C6	-3.40	1.49	1.53
14	B	805	CLA	C4D-ND	-3.40	1.33	1.37
17	K	102	BCR	C30-C25	-3.40	1.49	1.53
17	a	852	BCR	C1-C6	-3.40	1.49	1.53
14	B	827	CLA	C3B-C4B	3.40	1.50	1.42
14	a	818	CLA	C1D-ND	3.40	1.42	1.37
14	a	819	CLA	C1D-ND	3.40	1.42	1.37
14	A	828	CLA	C4D-ND	-3.40	1.33	1.37
14	1	1640	CLA	C1D-ND	3.40	1.42	1.37
14	a	808	CLA	C1D-ND	3.40	1.42	1.37
17	m	102	BCR	C30-C25	-3.40	1.49	1.53
14	A	802	CLA	C4D-ND	-3.40	1.33	1.37
14	1	1637	CLA	C1D-ND	3.40	1.42	1.37
14	2	816	CLA	C1D-ND	3.40	1.42	1.37
14	B	827	CLA	C4D-ND	-3.40	1.33	1.37
14	1	1607	CLA	C4D-ND	-3.40	1.33	1.37
14	2	841	CLA	C4D-ND	-3.40	1.33	1.37
17	2	845	BCR	C1-C6	-3.40	1.49	1.53
14	B	834	CLA	C1D-ND	3.40	1.42	1.37
14	B	832	CLA	C1D-ND	3.39	1.42	1.37
14	b	821	CLA	C4B-NB	3.39	1.42	1.37
14	B	838	CLA	C1D-ND	3.39	1.42	1.37
14	b	841	CLA	C4D-ND	-3.39	1.33	1.37
14	1	1644	CLA	C4D-ND	-3.39	1.33	1.37
14	B	803	CLA	C4D-ND	-3.39	1.33	1.37
17	F	205	BCR	C30-C25	-3.39	1.49	1.53
17	I	101	BCR	C30-C25	-3.39	1.49	1.53
14	B	815	CLA	C1D-ND	3.39	1.42	1.37
17	0	209	BCR	C1-C6	-3.39	1.49	1.53
14	a	812	CLA	C1D-ND	3.39	1.42	1.37
14	2	840	CLA	C4B-NB	3.39	1.41	1.37
14	a	842	CLA	C4D-ND	-3.39	1.33	1.37
14	a	825	CLA	C4D-ND	-3.38	1.33	1.37
14	A	812	CLA	C1D-ND	3.38	1.41	1.37
14	L	205	CLA	C4D-ND	-3.38	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	806	CLA	C4D-ND	-3.38	1.33	1.37
17	f	204	BCR	C30-C25	-3.38	1.49	1.53
14	A	839	CLA	C1D-ND	3.38	1.41	1.37
14	B	807	CLA	C1D-ND	3.38	1.41	1.37
14	A	842	CLA	C4D-ND	-3.38	1.33	1.37
14	2	839	CLA	C1D-ND	3.38	1.41	1.37
14	2	835	CLA	C1D-ND	3.38	1.41	1.37
14	b	805	CLA	C1D-ND	3.38	1.41	1.37
17	L	207	BCR	C1-C6	-3.38	1.49	1.53
14	b	828	CLA	C3B-C4B	3.38	1.50	1.42
17	0	201	BCR	C1-C6	-3.38	1.49	1.53
14	1	1620	CLA	C1D-ND	3.38	1.41	1.37
14	2	828	CLA	C3B-C4B	3.37	1.50	1.42
14	a	836	CLA	C1D-ND	3.37	1.41	1.37
14	b	819	CLA	C4D-ND	-3.37	1.33	1.37
17	6	204	BCR	C30-C25	-3.37	1.49	1.53
14	2	807	CLA	C4D-ND	-3.37	1.33	1.37
14	l	204	CLA	C4D-ND	-3.37	1.33	1.37
17	A	856	BCR	C30-C25	-3.37	1.49	1.53
14	B	839	CLA	C4B-NB	3.37	1.41	1.37
14	b	840	CLA	C4B-NB	3.37	1.41	1.37
14	a	841	CLA	C1D-ND	3.37	1.41	1.37
14	2	805	CLA	C1D-ND	3.37	1.41	1.37
17	k	102	BCR	C30-C25	-3.37	1.49	1.53
17	8	1305	BCR	C30-C25	-3.37	1.49	1.53
14	l	206	CLA	C1D-ND	3.37	1.41	1.37
14	1	1643	CLA	C4D-ND	-3.36	1.33	1.37
14	a	832	CLA	C4D-ND	-3.36	1.33	1.37
14	2	828	CLA	C4D-ND	-3.36	1.33	1.37
17	B	846	BCR	C1-C6	-3.36	1.49	1.53
14	1	1613	CLA	C1D-ND	3.36	1.41	1.37
14	A	803	CLA	C4D-ND	-3.36	1.33	1.37
14	l	206	CLA	C4D-ND	-3.36	1.33	1.37
17	A	849	BCR	C30-C25	-3.36	1.49	1.53
17	b	845	BCR	C30-C25	-3.36	1.49	1.53
14	A	836	CLA	C1D-ND	3.36	1.41	1.37
14	B	825	CLA	C4D-ND	-3.36	1.33	1.37
14	1	1633	CLA	C4D-ND	-3.36	1.33	1.37
14	0	207	CLA	C4D-ND	-3.36	1.33	1.37
17	j	1305	BCR	C30-C25	-3.35	1.49	1.53
14	x	1701	CLA	C4B-NB	3.35	1.41	1.37
14	2	828	CLA	C4B-NB	3.35	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	820	CLA	C4B-NB	3.35	1.41	1.37
14	a	826	CLA	C1D-ND	3.35	1.41	1.37
17	A	847	BCR	C30-C25	-3.35	1.49	1.53
14	A	834	CLA	C4D-ND	-3.35	1.33	1.37
17	a	847	BCR	C30-C25	-3.35	1.49	1.53
14	B	806	CLA	C4D-ND	-3.35	1.33	1.37
17	M	103	BCR	C30-C25	-3.35	1.49	1.53
14	b	842	CLA	C4D-ND	-3.35	1.33	1.37
14	A	826	CLA	C1D-ND	3.35	1.41	1.37
14	2	806	CLA	C4D-ND	-3.35	1.33	1.37
14	A	843	CLA	C4D-ND	-3.35	1.33	1.37
14	F	201	CLA	C1D-ND	3.35	1.41	1.37
14	A	825	CLA	C1D-ND	3.34	1.41	1.37
17	a	849	BCR	C30-C25	-3.34	1.49	1.53
14	2	826	CLA	C4D-ND	-3.34	1.33	1.37
14	1	1615	CLA	C4D-ND	-3.34	1.33	1.37
17	1	1648	BCR	C30-C25	-3.34	1.49	1.53
14	L	203	CLA	C4D-ND	-3.34	1.33	1.37
14	B	806	CLA	C1D-ND	3.34	1.41	1.37
17	B	844	BCR	C30-C25	-3.34	1.49	1.53
14	1	1603	CLA	C4D-ND	-3.33	1.33	1.37
14	1	1627	CLA	C1D-ND	3.33	1.41	1.37
14	b	826	CLA	C4D-ND	-3.33	1.33	1.37
17	2	847	BCR	C1-C6	-3.33	1.49	1.53
14	L	205	CLA	C1D-ND	3.33	1.41	1.37
14	2	803	CLA	C4D-ND	-3.33	1.33	1.37
14	a	804	CLA	C1D-ND	3.33	1.41	1.37
14	2	833	CLA	C1D-ND	3.33	1.41	1.37
14	1	1626	CLA	C1D-ND	3.33	1.41	1.37
14	1	1642	CLA	C1D-ND	3.33	1.41	1.37
17	b	847	BCR	C1-C6	-3.33	1.49	1.53
17	2	845	BCR	C30-C25	-3.33	1.49	1.53
17	J	103	BCR	C1-C6	-3.33	1.49	1.53
14	b	833	CLA	C1D-ND	3.33	1.41	1.37
14	A	825	CLA	C4D-ND	-3.32	1.33	1.37
17	A	848	BCR	C1-C6	-3.32	1.49	1.53
14	2	839	CLA	C4D-ND	-3.32	1.33	1.37
14	B	827	CLA	C4B-NB	3.32	1.41	1.37
17	A	847	BCR	C1-C6	-3.32	1.49	1.53
14	b	803	CLA	C4D-ND	-3.32	1.33	1.37
17	1	1649	BCR	C1-C6	-3.32	1.49	1.53
14	a	814	CLA	C4D-ND	-3.31	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	j	1304	BCR	C1-C6	-3.31	1.49	1.53
14	a	828	CLA	C1D-ND	3.31	1.41	1.37
14	B	838	CLA	C4D-ND	-3.31	1.33	1.37
14	b	813	CLA	C4B-NB	3.31	1.41	1.37
14	6	201	CLA	C1D-ND	3.31	1.41	1.37
14	2	821	CLA	C4B-NB	3.31	1.41	1.37
14	0	207	CLA	C1D-ND	3.31	1.41	1.37
14	b	834	CLA	C4D-ND	-3.31	1.33	1.37
14	A	814	CLA	C4D-ND	-3.31	1.33	1.37
14	b	827	CLA	C4D-ND	-3.31	1.33	1.37
14	b	833	CLA	C4B-NB	3.31	1.41	1.37
14	1	1635	CLA	C4D-ND	-3.30	1.33	1.37
17	a	848	BCR	C1-C6	-3.30	1.49	1.53
14	B	826	CLA	C4D-ND	-3.30	1.33	1.37
14	2	808	CLA	C4D-ND	-3.30	1.33	1.37
14	B	817	CLA	C4B-NB	3.30	1.41	1.37
14	B	807	CLA	C4D-ND	-3.30	1.33	1.37
14	A	830	CLA	C4D-ND	-3.30	1.33	1.37
14	B	829	CLA	C1D-ND	3.30	1.41	1.37
14	A	806	CLA	C1D-ND	3.30	1.41	1.37
14	a	805	CLA	C1D-ND	3.30	1.41	1.37
14	f	201	CLA	C1D-ND	3.30	1.41	1.37
14	a	843	CLA	C4D-ND	-3.30	1.33	1.37
17	1	1650	BCR	C30-C25	-3.30	1.49	1.53
14	b	830	CLA	C1D-ND	3.30	1.41	1.37
14	1	1606	CLA	C1D-ND	3.30	1.41	1.37
14	2	813	CLA	C4B-NB	3.30	1.41	1.37
14	a	834	CLA	C4D-ND	-3.29	1.33	1.37
14	B	818	CLA	C1D-ND	3.29	1.41	1.37
14	F	201	CLA	C4B-NB	3.29	1.41	1.37
14	b	823	CLA	C4B-NB	3.29	1.41	1.37
14	1	1626	CLA	C4D-ND	-3.29	1.33	1.37
14	1	1637	CLA	C4D-ND	-3.29	1.33	1.37
14	1	1604	CLA	C4D-ND	-3.29	1.33	1.37
14	A	841	CLA	C1D-ND	3.29	1.41	1.37
17	a	847	BCR	C1-C6	-3.29	1.49	1.53
14	B	832	CLA	C4B-NB	3.29	1.41	1.37
14	b	807	CLA	C1D-ND	3.29	1.41	1.37
14	b	828	CLA	C4B-NB	3.29	1.41	1.37
14	1	1629	CLA	C1D-ND	3.29	1.41	1.37
14	a	836	CLA	C4D-ND	-3.29	1.33	1.37
14	2	827	CLA	C4D-ND	-3.28	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	803	CLA	C4D-ND	-3.28	1.33	1.37
14	2	833	CLA	C4B-NB	3.28	1.41	1.37
17	8	1304	BCR	C1-C6	-3.28	1.49	1.53
14	B	822	CLA	C4B-NB	3.28	1.41	1.37
14	1	1616	CLA	C4B-NB	3.28	1.41	1.37
14	8	1303	CLA	C4B-NB	3.28	1.41	1.37
14	A	836	CLA	C4D-ND	-3.28	1.33	1.37
14	b	839	CLA	C4D-ND	-3.27	1.33	1.37
14	2	823	CLA	C4B-NB	3.27	1.41	1.37
14	J	102	CLA	C4B-NB	3.27	1.41	1.37
14	2	834	CLA	C4D-ND	-3.27	1.33	1.37
14	B	837	CLA	C1D-ND	3.27	1.41	1.37
14	j	1303	CLA	C4B-NB	3.27	1.41	1.37
14	b	826	CLA	C1D-ND	3.27	1.41	1.37
14	a	825	CLA	C1D-ND	3.27	1.41	1.37
14	b	818	CLA	C4B-NB	3.27	1.41	1.37
14	2	819	CLA	C1D-ND	3.27	1.41	1.37
14	B	835	CLA	C4B-NB	3.27	1.41	1.37
13	1	1602	CL0	C4D-ND	-3.27	1.33	1.37
14	f	201	CLA	C4D-ND	-3.27	1.33	1.37
14	a	809	CLA	C1D-ND	3.27	1.41	1.37
14	b	819	CLA	C1D-ND	3.27	1.41	1.37
14	B	804	CLA	C1D-ND	3.26	1.41	1.37
14	1	1620	CLA	C4B-NB	3.26	1.41	1.37
14	A	817	CLA	C4B-NB	3.26	1.41	1.37
14	B	825	CLA	C1D-ND	3.26	1.41	1.37
14	a	815	CLA	C4B-NB	3.26	1.41	1.37
14	A	837	CLA	C4B-NB	3.26	1.41	1.37
14	2	830	CLA	C1D-ND	3.26	1.41	1.37
14	6	201	CLA	C4B-NB	3.26	1.41	1.37
14	A	828	CLA	C1D-ND	3.26	1.41	1.37
14	2	807	CLA	C1D-ND	3.26	1.41	1.37
14	1	1639	CLA	C1D-ND	3.26	1.41	1.37
14	b	806	CLA	C1D-ND	3.26	1.41	1.37
14	b	809	CLA	C4D-ND	-3.26	1.33	1.37
14	b	807	CLA	C4D-ND	-3.26	1.33	1.37
14	a	837	CLA	C4B-NB	3.26	1.41	1.37
14	b	834	CLA	C1D-ND	3.26	1.41	1.37
14	2	838	CLA	C1D-ND	3.26	1.41	1.37
14	8	1302	CLA	C4B-NB	3.26	1.41	1.37
14	a	835	CLA	C4D-ND	-3.26	1.33	1.37
14	1	1608	CLA	C4D-ND	-3.25	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	838	CLA	C1D-ND	3.25	1.41	1.37
14	2	826	CLA	C1D-ND	3.25	1.41	1.37
14	0	205	CLA	C4B-NB	3.25	1.41	1.37
14	F	203	CLA	C4B-NB	3.25	1.41	1.37
14	8	1301	CLA	C4B-NB	3.25	1.41	1.37
17	1	1648	BCR	C1-C6	-3.25	1.49	1.53
13	A	801	CL0	C4D-ND	-3.24	1.33	1.37
14	B	833	CLA	C1D-ND	3.24	1.41	1.37
14	A	807	CLA	C4D-ND	-3.24	1.33	1.37
14	B	802	CLA	C4D-ND	-3.24	1.33	1.37
14	a	806	CLA	C1D-ND	3.24	1.41	1.37
14	A	819	CLA	C4B-NB	3.24	1.41	1.37
14	F	203	CLA	C4D-ND	-3.24	1.33	1.37
14	2	814	CLA	C4D-ND	-3.24	1.33	1.37
14	2	816	CLA	C4D-ND	-3.24	1.33	1.37
14	a	803	CLA	C4B-NB	3.24	1.41	1.37
14	B	830	CLA	C4D-ND	-3.24	1.33	1.37
14	A	838	CLA	C1D-ND	3.24	1.41	1.37
14	0	205	CLA	C1D-ND	3.24	1.41	1.37
14	2	831	CLA	C4D-ND	-3.23	1.33	1.37
17	8	1304	BCR	C30-C25	-3.23	1.49	1.53
14	B	833	CLA	C4D-ND	-3.23	1.33	1.37
14	2	836	CLA	C4B-NB	3.23	1.41	1.37
14	1	1604	CLA	C4B-NB	3.23	1.41	1.37
14	A	805	CLA	C1D-ND	3.23	1.41	1.37
14	a	812	CLA	C4D-ND	-3.23	1.33	1.37
17	j	1304	BCR	C30-C25	-3.23	1.49	1.53
14	a	819	CLA	C4B-NB	3.23	1.41	1.37
14	B	805	CLA	C1D-ND	3.23	1.41	1.37
14	B	809	CLA	C4D-ND	-3.23	1.33	1.37
17	l	207	BCR	C1-C6	-3.23	1.49	1.53
17	0	208	BCR	C1-C6	-3.23	1.49	1.53
14	B	813	CLA	C4D-ND	-3.23	1.33	1.37
14	A	840	CLA	C4D-ND	-3.23	1.33	1.37
14	1	1640	CLA	C4D-ND	-3.22	1.33	1.37
14	j	1301	CLA	C4B-NB	3.22	1.41	1.37
14	2	806	CLA	C1D-ND	3.22	1.41	1.37
14	l	204	CLA	C4B-NB	3.22	1.41	1.37
14	a	829	CLA	C4D-ND	-3.22	1.33	1.37
14	a	839	CLA	C4D-ND	-3.22	1.33	1.37
14	L	203	CLA	C3B-C4B	3.22	1.50	1.42
14	2	809	CLA	C4D-ND	-3.22	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	809	CLA	C1D-ND	3.22	1.41	1.37
14	8	1301	CLA	C4D-ND	-3.22	1.33	1.37
14	j	1302	CLA	C4B-NB	3.22	1.41	1.37
14	k	103	CLA	C4B-NB	3.22	1.41	1.37
14	f	201	CLA	C4B-NB	3.21	1.41	1.37
14	a	811	CLA	C4B-NB	3.21	1.41	1.37
14	b	838	CLA	C4D-ND	-3.21	1.33	1.37
14	j	1301	CLA	C4D-ND	-3.21	1.33	1.37
14	1	1636	CLA	C4D-ND	-3.21	1.33	1.37
14	1	1631	CLA	C4D-ND	-3.21	1.33	1.37
14	A	811	CLA	C4B-NB	3.21	1.41	1.37
14	l	204	CLA	C1D-ND	3.21	1.41	1.37
14	2	835	CLA	C4B-NB	3.21	1.41	1.37
14	b	808	CLA	C4D-ND	-3.21	1.33	1.37
14	B	812	CLA	C4B-NB	3.21	1.41	1.37
14	A	839	CLA	C4D-ND	-3.21	1.33	1.37
14	b	832	CLA	C4D-ND	-3.21	1.33	1.37
14	a	840	CLA	C4D-ND	-3.21	1.33	1.37
14	2	818	CLA	C4B-NB	3.21	1.41	1.37
14	1	1630	CLA	C4D-ND	-3.21	1.33	1.37
14	A	855	CLA	C4D-ND	-3.21	1.33	1.37
14	1	1638	CLA	C4B-NB	3.21	1.41	1.37
17	J	103	BCR	C30-C25	-3.20	1.49	1.53
14	B	810	CLA	C1D-ND	3.20	1.41	1.37
14	1	1620	CLA	C4D-ND	-3.20	1.33	1.37
14	B	808	CLA	C4D-ND	-3.20	1.33	1.37
14	l	204	CLA	C3B-C4B	3.20	1.50	1.42
14	a	818	CLA	C4B-NB	3.20	1.41	1.37
14	a	807	CLA	C4D-ND	-3.20	1.33	1.37
14	1	1607	CLA	C1D-ND	3.20	1.41	1.37
14	A	831	CLA	CMB-C2B	-3.20	1.44	1.50
14	A	835	CLA	C1D-ND	3.20	1.41	1.37
14	2	834	CLA	C1D-ND	3.20	1.41	1.37
14	A	822	CLA	C4D-ND	-3.20	1.33	1.37
14	1	1622	CLA	C4B-NB	3.20	1.41	1.37
14	A	815	CLA	C4B-NB	3.19	1.41	1.37
14	2	810	CLA	C4D-ND	-3.19	1.33	1.37
14	1	1632	CLA	CMB-C2B	-3.19	1.44	1.50
14	0	205	CLA	C3B-C4B	3.19	1.50	1.42
14	A	835	CLA	C4D-ND	-3.19	1.33	1.37
14	a	842	CLA	C1D-ND	3.19	1.41	1.37
14	a	830	CLA	C4D-ND	-3.19	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	801	CL0	C4D-ND	-3.19	1.33	1.37
14	F	201	CLA	C4D-ND	-3.19	1.33	1.37
14	A	821	CLA	C4B-NB	3.19	1.41	1.37
14	L	203	CLA	C4B-NB	3.19	1.41	1.37
14	1	1608	CLA	C1D-ND	3.19	1.41	1.37
17	L	206	BCR	C1-C6	-3.19	1.49	1.53
14	b	811	CLA	C1D-ND	3.19	1.41	1.37
14	2	832	CLA	C4D-ND	-3.19	1.33	1.37
14	a	817	CLA	C4B-NB	3.19	1.41	1.37
14	1	1612	CLA	C4B-NB	3.19	1.41	1.37
14	6	201	CLA	C4D-ND	-3.19	1.33	1.37
14	b	829	CLA	C4B-NB	3.19	1.41	1.37
14	9	103	CLA	C4B-NB	3.19	1.41	1.37
14	1	1610	CLA	C1D-ND	3.18	1.41	1.37
14	A	855	CLA	C1D-ND	3.18	1.41	1.37
14	a	838	CLA	C1D-ND	3.18	1.41	1.37
14	b	835	CLA	C4B-NB	3.18	1.41	1.37
14	2	829	CLA	C1D-ND	3.18	1.41	1.37
17	1	1652	BCR	C30-C25	-3.18	1.49	1.53
14	J	101	CLA	C4B-NB	3.18	1.41	1.37
17	0	209	BCR	C30-C25	-3.18	1.49	1.53
14	B	815	CLA	C4D-ND	-3.18	1.33	1.37
14	B	825	CLA	C4B-NB	3.18	1.41	1.37
14	2	809	CLA	C1D-ND	3.18	1.41	1.37
14	a	831	CLA	CMB-C2B	-3.18	1.44	1.50
14	b	810	CLA	C4D-ND	-3.17	1.33	1.37
14	1	1639	CLA	C4D-ND	-3.17	1.33	1.37
14	2	840	CLA	C4D-ND	-3.17	1.33	1.37
14	b	814	CLA	C4D-ND	-3.17	1.33	1.37
14	B	828	CLA	C1D-ND	3.17	1.41	1.37
14	B	839	CLA	C4D-ND	-3.17	1.33	1.37
14	a	831	CLA	C4D-ND	-3.17	1.33	1.37
14	B	837	CLA	C4D-ND	-3.17	1.33	1.37
14	B	834	CLA	C4B-NB	3.17	1.41	1.37
14	2	829	CLA	C4B-NB	3.17	1.41	1.37
14	A	829	CLA	C4D-ND	-3.16	1.33	1.37
14	2	838	CLA	C4D-ND	-3.16	1.33	1.37
14	A	834	CLA	C1D-ND	3.16	1.41	1.37
14	2	802	CLA	C4D-ND	-3.16	1.33	1.37
14	A	808	CLA	C4B-NB	3.16	1.41	1.37
14	B	831	CLA	C4D-ND	-3.16	1.33	1.37
14	A	803	CLA	C4B-NB	3.16	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	819	CLA	C4D-ND	-3.16	1.33	1.37
14	K	103	CLA	C4B-NB	3.16	1.41	1.37
14	b	840	CLA	C4D-ND	-3.15	1.33	1.37
14	b	836	CLA	C4B-NB	3.15	1.41	1.37
14	1	1632	CLA	C4D-ND	-3.15	1.33	1.37
17	a	851	BCR	C30-C25	-3.15	1.49	1.53
14	b	816	CLA	C4D-ND	-3.15	1.33	1.37
14	1	1613	CLA	C4D-ND	-3.15	1.33	1.37
14	B	808	CLA	C1D-ND	3.15	1.41	1.37
14	A	838	CLA	C4D-ND	-3.15	1.33	1.37
14	a	807	CLA	C1D-ND	3.15	1.41	1.37
14	a	840	CLA	C1D-ND	3.15	1.41	1.37
14	a	810	CLA	C4D-ND	-3.15	1.33	1.37
14	a	821	CLA	C4B-NB	3.15	1.41	1.37
14	a	808	CLA	C4D-ND	-3.15	1.33	1.37
14	B	828	CLA	C4B-NB	3.15	1.41	1.37
14	1	1618	CLA	C4B-NB	3.15	1.41	1.37
14	A	831	CLA	C4D-ND	-3.15	1.33	1.37
14	2	805	CLA	C4D-ND	-3.15	1.33	1.37
14	A	819	CLA	C4D-ND	-3.15	1.33	1.37
14	K	101	CLA	C4B-NB	3.14	1.41	1.37
14	1	1641	CLA	C4D-ND	-3.14	1.33	1.37
14	A	807	CLA	C1D-ND	3.14	1.41	1.37
14	A	842	CLA	C1D-ND	3.14	1.41	1.37
14	b	841	CLA	C1D-ND	3.14	1.41	1.37
14	2	811	CLA	C1D-ND	3.14	1.41	1.37
14	1	1623	CLA	C4D-ND	-3.14	1.33	1.37
14	1	1635	CLA	C1D-ND	3.14	1.41	1.37
14	1	1643	CLA	C1D-ND	3.14	1.41	1.37
14	b	805	CLA	C4D-ND	-3.14	1.33	1.37
14	B	837	CLA	C4B-NB	3.14	1.41	1.37
14	a	822	CLA	C4D-ND	-3.14	1.33	1.37
14	A	840	CLA	C1D-ND	3.14	1.41	1.37
14	a	811	CLA	C4D-ND	-3.14	1.33	1.37
14	a	826	CLA	C4D-ND	-3.14	1.33	1.37
14	1	1636	CLA	C1D-ND	3.14	1.41	1.37
14	B	810	CLA	C4D-ND	-3.14	1.33	1.37
14	2	833	CLA	C4D-ND	-3.14	1.33	1.37
14	B	823	CLA	C4B-NB	3.14	1.41	1.37
14	L	203	CLA	C1D-ND	3.14	1.41	1.37
14	a	813	CLA	C4D-ND	-3.14	1.33	1.37
14	b	802	CLA	C4D-ND	-3.14	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	829	CLA	C1D-ND	3.14	1.41	1.37
14	a	803	CLA	C1D-ND	3.13	1.41	1.37
14	2	826	CLA	C4B-NB	3.13	1.41	1.37
14	b	829	CLA	C4D-ND	-3.13	1.33	1.37
14	b	809	CLA	C1D-ND	3.13	1.41	1.37
14	2	811	CLA	C4D-ND	-3.13	1.33	1.37
14	b	838	CLA	C4B-NB	3.13	1.41	1.37
14	A	804	CLA	C4D-ND	-3.13	1.33	1.37
14	B	804	CLA	C4D-ND	-3.13	1.33	1.37
14	b	831	CLA	C4D-ND	-3.13	1.33	1.37
14	A	812	CLA	C4D-ND	-3.13	1.33	1.37
14	1	1605	CLA	C4D-ND	-3.13	1.33	1.37
17	A	851	BCR	C30-C25	-3.13	1.49	1.53
13	A	801	CL0	C1D-ND	3.13	1.41	1.37
14	b	826	CLA	C4B-NB	3.13	1.41	1.37
14	A	826	CLA	C4D-ND	-3.13	1.33	1.37
14	1	1614	CLA	C4B-NB	3.13	1.41	1.37
14	2	838	CLA	C4B-NB	3.12	1.41	1.37
14	1	1609	CLA	C4D-ND	-3.12	1.33	1.37
14	B	828	CLA	C4D-ND	-3.12	1.33	1.37
14	b	810	CLA	C1D-ND	3.12	1.41	1.37
17	0	201	BCR	C30-C25	-3.12	1.49	1.53
14	a	835	CLA	C1D-ND	3.12	1.41	1.37
14	a	812	CLA	C4B-NB	3.12	1.41	1.37
14	a	834	CLA	C1D-ND	3.12	1.41	1.37
17	L	207	BCR	C30-C25	-3.12	1.49	1.53
14	1	1609	CLA	C4B-NB	3.12	1.41	1.37
14	a	824	CLA	C3B-C4B	3.12	1.50	1.42
14	B	832	CLA	C4D-ND	-3.12	1.33	1.37
14	1	1624	CLA	C4D-ND	-3.11	1.33	1.37
13	1	1602	CL0	C1D-ND	3.11	1.41	1.37
14	A	813	CLA	C4B-NB	3.11	1.41	1.37
14	k	101	CLA	C4B-NB	3.11	1.41	1.37
14	A	823	CLA	C4D-ND	-3.11	1.33	1.37
14	A	818	CLA	C4B-NB	3.11	1.41	1.37
14	A	810	CLA	C4D-ND	-3.11	1.33	1.37
14	a	838	CLA	C4D-ND	-3.11	1.33	1.37
14	1	1611	CLA	C4D-ND	-3.11	1.33	1.37
14	1	1645	CLA	C4D-ND	-3.11	1.33	1.37
14	B	820	CLA	C4D-ND	-3.11	1.33	1.37
13	a	801	CL0	C1D-ND	3.10	1.41	1.37
14	B	840	CLA	C1D-ND	3.10	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	802	CLA	C1D-ND	3.10	1.41	1.37
14	2	802	CLA	C1D-ND	3.10	1.41	1.37
14	A	803	CLA	C1D-ND	3.10	1.41	1.37
14	B	833	CLA	C4B-NB	3.10	1.41	1.37
14	2	815	CLA	C4D-ND	-3.10	1.33	1.37
14	1	1644	CLA	C4B-NB	3.10	1.41	1.37
14	2	803	CLA	C1D-ND	3.10	1.41	1.37
14	2	829	CLA	C4D-ND	-3.10	1.33	1.37
14	1	1619	CLA	C4B-NB	3.10	1.41	1.37
14	1	1613	CLA	C4B-NB	3.10	1.41	1.37
14	1	1612	CLA	C4D-ND	-3.10	1.33	1.37
14	2	810	CLA	C1D-ND	3.10	1.41	1.37
14	A	808	CLA	C4D-ND	-3.10	1.33	1.37
14	a	843	CLA	C4B-NB	3.09	1.41	1.37
14	1	1610	CLA	C4D-ND	-3.09	1.33	1.37
14	A	813	CLA	C4D-ND	-3.09	1.33	1.37
14	a	808	CLA	C4B-NB	3.09	1.41	1.37
14	9	101	CLA	C4B-NB	3.09	1.41	1.37
14	1	1627	CLA	C4D-ND	-3.09	1.33	1.37
14	B	829	CLA	C4D-ND	-3.09	1.33	1.37
17	b	844	BCR	C30-C25	-3.09	1.49	1.53
14	1	1604	CLA	C1D-ND	3.09	1.41	1.37
14	a	815	CLA	C4D-ND	-3.09	1.33	1.37
14	k	101	CLA	C4D-ND	-3.09	1.33	1.37
14	A	812	CLA	C4B-NB	3.09	1.41	1.37
14	B	814	CLA	C4D-ND	-3.09	1.33	1.37
14	2	824	CLA	C4B-NB	3.09	1.41	1.37
14	A	816	CLA	C4D-ND	-3.09	1.33	1.37
14	1	1616	CLA	C4D-ND	-3.09	1.33	1.37
14	b	811	CLA	C4D-ND	-3.09	1.33	1.37
14	2	830	CLA	C4D-ND	-3.09	1.33	1.37
14	A	824	CLA	C3B-C4B	3.09	1.50	1.42
14	A	815	CLA	C4D-ND	-3.09	1.33	1.37
14	b	824	CLA	C4B-NB	3.08	1.41	1.37
14	a	809	CLA	C4D-ND	-3.08	1.33	1.37
14	a	814	CLA	C4B-NB	3.08	1.41	1.37
14	1	1641	CLA	C1D-ND	3.08	1.41	1.37
14	b	821	CLA	C4D-ND	-3.08	1.33	1.37
14	1	1614	CLA	C4D-ND	-3.08	1.33	1.37
17	2	844	BCR	C30-C25	-3.08	1.49	1.53
14	2	841	CLA	C1D-ND	3.08	1.41	1.37
14	A	805	CLA	C4D-ND	-3.08	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	813	CLA	C3B-C4B	3.08	1.50	1.42
14	a	816	CLA	C4B-NB	3.08	1.41	1.37
14	K	101	CLA	C4D-ND	-3.07	1.33	1.37
14	a	844	CLA	C4D-ND	-3.07	1.33	1.37
14	a	823	CLA	C4D-ND	-3.07	1.33	1.37
17	B	843	BCR	C30-C25	-3.07	1.49	1.53
14	B	822	CLA	C4D-ND	-3.07	1.33	1.37
14	A	816	CLA	C4B-NB	3.07	1.41	1.37
14	b	828	CLA	C1D-ND	3.07	1.41	1.37
14	A	813	CLA	C3B-C4B	3.07	1.49	1.42
14	1	1615	CLA	C4B-NB	3.07	1.41	1.37
14	A	844	CLA	C4D-ND	-3.07	1.33	1.37
14	b	830	CLA	C4D-ND	-3.07	1.33	1.37
14	B	835	CLA	C4D-ND	-3.07	1.33	1.37
14	1	1638	CLA	C4D-ND	-3.06	1.33	1.37
14	1	1606	CLA	C4D-ND	-3.06	1.33	1.37
14	9	101	CLA	C4D-ND	-3.06	1.33	1.37
14	1	1617	CLA	C4D-ND	-3.06	1.33	1.37
14	a	840	CLA	C4B-NB	3.06	1.41	1.37
14	1	1634	CLA	C1D-ND	3.06	1.41	1.37
14	a	804	CLA	C4D-ND	-3.06	1.33	1.37
14	a	816	CLA	C4D-ND	-3.06	1.33	1.37
14	A	809	CLA	C4D-ND	-3.06	1.33	1.37
14	A	837	CLA	C4D-ND	-3.06	1.33	1.37
14	B	827	CLA	C1D-ND	3.06	1.41	1.37
14	1	1632	CLA	C1D-ND	3.06	1.41	1.37
14	b	825	CLA	C4D-ND	-3.06	1.33	1.37
14	B	802	CLA	C1D-ND	3.06	1.41	1.37
14	b	803	CLA	C1D-ND	3.06	1.41	1.37
14	2	828	CLA	C1D-ND	3.06	1.41	1.37
14	a	841	CLA	C4D-ND	-3.06	1.33	1.37
14	a	813	CLA	C4B-NB	3.06	1.41	1.37
14	A	811	CLA	C4D-ND	-3.06	1.33	1.37
14	a	837	CLA	C4D-ND	-3.06	1.33	1.37
14	B	821	CLA	C4B-NB	3.06	1.41	1.37
14	1	1623	CLA	C4B-NB	3.06	1.41	1.37
14	B	832	CLA	C3B-C4B	3.05	1.49	1.42
14	b	812	CLA	C4D-ND	-3.05	1.33	1.37
14	1	1625	CLA	C3B-C4B	3.05	1.49	1.42
14	B	812	CLA	C4D-ND	-3.05	1.33	1.37
14	b	842	CLA	C1D-ND	3.05	1.41	1.37
14	b	822	CLA	C4B-NB	3.05	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	837	CLA	C4D-ND	-3.05	1.33	1.37
14	A	814	CLA	C4B-NB	3.05	1.41	1.37
14	A	841	CLA	C4D-ND	-3.05	1.33	1.37
14	1	1614	CLA	C3B-C4B	3.05	1.49	1.42
14	B	809	CLA	C1D-ND	3.05	1.41	1.37
14	b	817	CLA	C4B-NB	3.05	1.41	1.37
14	a	805	CLA	C4D-ND	-3.04	1.33	1.37
14	B	819	CLA	C4D-ND	-3.04	1.33	1.37
14	b	823	CLA	C4D-ND	-3.04	1.33	1.37
14	b	815	CLA	C4D-ND	-3.04	1.33	1.37
14	k	103	CLA	C4D-ND	-3.04	1.33	1.37
14	2	821	CLA	C4D-ND	-3.04	1.33	1.37
14	1	1643	CLA	C4B-NB	3.04	1.41	1.37
14	1	1617	CLA	C4B-NB	3.04	1.41	1.37
14	2	842	CLA	C1D-ND	3.04	1.41	1.37
14	A	832	CLA	C1D-ND	3.04	1.41	1.37
14	B	824	CLA	C4D-ND	-3.04	1.33	1.37
14	B	841	CLA	C1D-ND	3.03	1.41	1.37
14	a	831	CLA	C4B-NB	3.03	1.41	1.37
14	2	817	CLA	C4B-NB	3.03	1.41	1.37
14	B	817	CLA	C4D-ND	-3.03	1.33	1.37
14	1	1641	CLA	C4B-NB	3.03	1.41	1.37
14	K	103	CLA	C4D-ND	-3.03	1.33	1.37
14	1	1633	CLA	C1D-ND	3.03	1.41	1.37
14	b	820	CLA	C4D-ND	-3.03	1.33	1.37
14	1	1642	CLA	C4D-ND	-3.03	1.33	1.37
14	b	833	CLA	C4D-ND	-3.03	1.33	1.37
14	2	818	CLA	C4D-ND	-3.03	1.33	1.37
14	1	1624	CLA	C4B-NB	3.03	1.41	1.37
14	A	840	CLA	C4B-NB	3.03	1.41	1.37
14	2	834	CLA	C4B-NB	3.03	1.41	1.37
14	b	824	CLA	C3B-C4B	3.03	1.49	1.42
14	2	812	CLA	C4D-ND	-3.03	1.33	1.37
14	2	822	CLA	C4B-NB	3.03	1.41	1.37
14	2	813	CLA	C4D-ND	-3.03	1.33	1.37
14	a	828	CLA	C4B-NB	3.02	1.41	1.37
14	A	843	CLA	C4B-NB	3.02	1.41	1.37
14	B	811	CLA	C4D-ND	-3.02	1.33	1.37
14	2	820	CLA	C4D-ND	-3.02	1.33	1.37
14	A	823	CLA	C4B-NB	3.02	1.41	1.37
14	B	836	CLA	C4D-ND	-3.02	1.33	1.37
14	a	842	CLA	C4B-NB	3.01	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	837	CLA	C4D-ND	-3.01	1.33	1.37
14	A	831	CLA	C4B-NB	3.01	1.41	1.37
14	2	833	CLA	C3B-C4B	3.01	1.49	1.42
14	B	823	CLA	C3B-C4B	3.01	1.49	1.42
14	b	818	CLA	C4D-ND	-3.01	1.33	1.37
14	B	816	CLA	C4B-NB	3.01	1.41	1.37
14	b	804	CLA	C1D-ND	3.01	1.41	1.37
14	1	1617	CLA	C3B-C4B	3.01	1.49	1.42
14	9	103	CLA	C4D-ND	-3.00	1.33	1.37
14	b	833	CLA	C3B-C4B	3.00	1.49	1.42
14	2	824	CLA	C3B-C4B	3.00	1.49	1.42
14	b	834	CLA	C4B-NB	3.00	1.41	1.37
14	1	1611	CLA	C4B-NB	2.99	1.41	1.37
14	2	825	CLA	C4D-ND	-2.99	1.33	1.37
14	a	831	CLA	C1D-ND	2.99	1.41	1.37
14	A	811	CLA	C3B-C4B	2.99	1.49	1.42
14	2	805	CLA	C4B-NB	2.99	1.41	1.37
14	a	833	CLA	C1D-ND	2.99	1.41	1.37
14	2	836	CLA	C4D-ND	-2.99	1.33	1.37
14	A	820	CLA	C4D-ND	-2.99	1.33	1.37
14	2	823	CLA	C4D-ND	-2.99	1.33	1.37
14	A	810	CLA	C4B-NB	2.98	1.41	1.37
14	1	1629	CLA	C4B-NB	2.98	1.41	1.37
14	A	830	CLA	C1D-ND	2.98	1.41	1.37
14	2	816	CLA	C4B-NB	2.98	1.41	1.37
14	a	820	CLA	C4D-ND	-2.98	1.33	1.37
14	6	203	CLA	C4D-ND	-2.98	1.33	1.37
14	A	833	CLA	C1D-ND	2.98	1.41	1.37
14	a	829	CLA	C4B-NB	2.98	1.41	1.37
14	b	836	CLA	C4D-ND	-2.98	1.33	1.37
14	A	842	CLA	C3B-C4B	2.98	1.49	1.42
14	a	832	CLA	C1D-ND	2.98	1.41	1.37
14	M	102	CLA	C3B-C4B	2.98	1.49	1.42
14	F	204	CLA	C4D-ND	-2.98	1.33	1.37
14	A	822	CLA	C4B-NB	2.98	1.41	1.37
14	b	805	CLA	C4B-NB	2.98	1.41	1.37
14	a	842	CLA	C3B-C4B	2.98	1.49	1.42
14	1	1606	CLA	C4B-NB	2.97	1.41	1.37
14	1	1610	CLA	C4B-NB	2.97	1.41	1.37
14	1	1632	CLA	C4B-NB	2.97	1.41	1.37
14	a	816	CLA	C3B-C4B	2.97	1.49	1.42
14	a	829	CLA	C3B-C4B	2.97	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	1643	CLA	C3B-C4B	2.97	1.49	1.42
14	A	809	CLA	C4B-NB	2.97	1.41	1.37
14	a	805	CLA	C4B-NB	2.97	1.41	1.37
14	b	817	CLA	C4D-ND	-2.97	1.33	1.37
14	2	804	CLA	C1D-ND	2.97	1.41	1.37
14	2	822	CLA	C3B-C4B	2.97	1.49	1.42
14	a	830	CLA	C1D-ND	2.97	1.41	1.37
14	1	1644	CLA	CMD-C2D	-2.97	1.44	1.50
14	K	103	CLA	C3B-C4B	2.96	1.49	1.42
14	b	822	CLA	C3B-C4B	2.96	1.49	1.42
14	a	809	CLA	C4B-NB	2.96	1.41	1.37
14	f	203	CLA	C4D-ND	-2.96	1.33	1.37
14	1	1612	CLA	C3B-C4B	2.96	1.49	1.42
14	2	817	CLA	C4D-ND	-2.96	1.33	1.37
14	A	831	CLA	C1D-ND	2.96	1.41	1.37
14	a	843	CLA	CMD-C2D	-2.96	1.44	1.50
14	a	822	CLA	C4B-NB	2.96	1.41	1.37
14	a	823	CLA	C4B-NB	2.96	1.41	1.37
14	A	816	CLA	C3B-C4B	2.96	1.49	1.42
14	J	101	CLA	C4D-ND	-2.96	1.33	1.37
14	1	1621	CLA	C4D-ND	-2.95	1.33	1.37
20	B	849	LMG	O7-C8	-2.95	1.39	1.46
14	X	1701	CLA	C4D-ND	-2.95	1.33	1.37
14	A	805	CLA	C4B-NB	2.95	1.41	1.37
14	A	857	CLA	C3B-C4B	2.95	1.49	1.42
14	A	829	CLA	C3B-C4B	2.95	1.49	1.42
14	B	821	CLA	C3B-C4B	2.95	1.49	1.42
14	1	1601	CLA	C3B-C4B	2.95	1.49	1.42
14	a	811	CLA	C3B-C4B	2.95	1.49	1.42
14	A	842	CLA	C4B-NB	2.95	1.41	1.37
14	f	201	CLA	C3B-C4B	2.95	1.49	1.42
14	B	815	CLA	C4B-NB	2.95	1.41	1.37
14	b	813	CLA	C4D-ND	-2.95	1.33	1.37
14	a	810	CLA	C4B-NB	2.95	1.41	1.37
14	2	824	CLA	C4D-ND	-2.94	1.33	1.37
14	F	203	CLA	C3B-C4B	2.94	1.49	1.42
14	j	1301	CLA	C3B-C4B	2.94	1.49	1.42
14	9	103	CLA	C3B-C4B	2.94	1.49	1.42
14	F	201	CLA	C3B-C4B	2.94	1.49	1.42
14	B	816	CLA	C4D-ND	-2.94	1.33	1.37
14	B	804	CLA	C4B-NB	2.94	1.41	1.37
14	k	103	CLA	C3B-C4B	2.94	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	828	CLA	C4B-NB	2.94	1.41	1.37
14	B	831	CLA	C4B-NB	2.94	1.41	1.37
14	b	812	CLA	C4B-NB	2.94	1.41	1.37
14	1	1604	CLA	C3B-C4B	2.94	1.49	1.42
20	2	850	LMG	O7-C8	-2.94	1.39	1.46
20	b	850	LMG	O7-C8	-2.93	1.39	1.46
14	A	843	CLA	CMD-C2D	-2.93	1.44	1.50
14	1	1631	CLA	C1D-ND	2.93	1.41	1.37
14	1	1630	CLA	C4B-NB	2.93	1.41	1.37
14	a	824	CLA	C4D-ND	-2.93	1.33	1.37
14	a	836	CLA	C4B-NB	2.93	1.41	1.37
14	1	1608	CLA	C3B-C4B	2.93	1.49	1.42
14	1	1630	CLA	C3B-C4B	2.93	1.49	1.42
14	a	802	CLA	C3B-C4B	2.93	1.49	1.42
14	A	802	CLA	C3B-C4B	2.93	1.49	1.42
14	L	204	CLA	C1D-ND	2.92	1.41	1.37
14	a	841	CLA	C4B-NB	2.92	1.41	1.37
14	b	825	CLA	C4B-NB	2.92	1.41	1.37
14	1	1638	CLA	C3B-C4B	2.92	1.49	1.42
14	A	829	CLA	C4B-NB	2.92	1.41	1.37
14	6	201	CLA	C3B-C4B	2.92	1.49	1.42
14	B	821	CLA	C4D-ND	-2.92	1.33	1.37
14	A	837	CLA	C3B-C4B	2.92	1.49	1.42
14	2	825	CLA	C4B-NB	2.92	1.41	1.37
14	z	102	CLA	C3B-C4B	2.92	1.49	1.42
14	f	203	CLA	C3B-C4B	2.92	1.49	1.42
14	b	816	CLA	C4B-NB	2.92	1.41	1.37
14	B	836	CLA	C3B-C4B	2.92	1.49	1.42
14	A	821	CLA	C4D-ND	-2.92	1.33	1.37
14	F	204	CLA	C3B-C4B	2.92	1.49	1.42
14	1	1601	CLA	C4D-ND	-2.92	1.33	1.37
14	a	803	CLA	C3B-C4B	2.91	1.49	1.42
14	A	803	CLA	C3B-C4B	2.91	1.49	1.42
14	B	841	CLA	C4B-NB	2.91	1.41	1.37
14	b	824	CLA	C4D-ND	-2.91	1.33	1.37
14	1	1619	CLA	C3B-C4B	2.91	1.49	1.42
14	6	203	CLA	C3B-C4B	2.91	1.49	1.42
14	A	827	CLA	C1D-ND	2.91	1.41	1.37
14	1	1622	CLA	C4D-ND	-2.91	1.33	1.37
14	j	1302	CLA	C4D-ND	-2.91	1.33	1.37
14	B	823	CLA	C4D-ND	-2.91	1.33	1.37
14	2	842	CLA	C4B-NB	2.91	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	818	CLA	C3B-C4B	2.91	1.49	1.42
14	1	1603	CLA	C3B-C4B	2.91	1.49	1.42
14	8	1302	CLA	C4D-ND	-2.91	1.33	1.37
14	1	1635	CLA	C3B-C4B	2.90	1.49	1.42
14	B	803	CLA	C1D-ND	2.90	1.41	1.37
14	b	832	CLA	C4B-NB	2.90	1.41	1.37
14	A	857	CLA	C4D-ND	-2.90	1.33	1.37
14	1	1619	CLA	C4D-ND	-2.90	1.33	1.37
14	A	807	CLA	C3B-C4B	2.90	1.49	1.42
14	1	1625	CLA	C4D-ND	-2.90	1.33	1.37
14	A	834	CLA	C3B-C4B	2.90	1.49	1.42
14	A	818	CLA	C4D-ND	-2.90	1.33	1.37
14	A	824	CLA	C4D-ND	-2.90	1.33	1.37
14	8	1301	CLA	C3B-C4B	2.89	1.49	1.42
14	x	1701	CLA	C4D-ND	-2.89	1.33	1.37
14	A	818	CLA	C3B-C4B	2.89	1.49	1.42
14	a	827	CLA	C1D-ND	2.89	1.41	1.37
14	a	837	CLA	C3B-C4B	2.89	1.49	1.42
14	a	843	CLA	C1D-ND	2.89	1.41	1.37
14	b	842	CLA	C4B-NB	2.89	1.41	1.37
14	b	835	CLA	C4D-ND	-2.89	1.33	1.37
14	b	837	CLA	C3B-C4B	2.89	1.49	1.42
14	b	822	CLA	C4D-ND	-2.89	1.33	1.37
14	b	823	CLA	C3B-C4B	2.89	1.49	1.42
14	a	807	CLA	C3B-C4B	2.89	1.49	1.42
14	1	1637	CLA	C4B-NB	2.89	1.41	1.37
14	1	1628	CLA	C1D-ND	2.88	1.41	1.37
14	A	805	CLA	C3B-C4B	2.88	1.49	1.42
14	x	1701	CLA	C3B-C4B	2.88	1.49	1.42
14	2	823	CLA	C3B-C4B	2.88	1.49	1.42
14	1	1642	CLA	C4B-NB	2.88	1.41	1.37
14	2	812	CLA	C4B-NB	2.88	1.41	1.37
14	A	836	CLA	C4B-NB	2.88	1.41	1.37
18	A	853	LHG	O7-C5	-2.88	1.39	1.46
14	a	805	CLA	C3B-C4B	2.88	1.49	1.42
14	2	837	CLA	C3B-C4B	2.88	1.49	1.42
14	B	822	CLA	C3B-C4B	2.88	1.49	1.42
14	A	802	CLA	C1D-ND	2.88	1.41	1.37
14	a	818	CLA	C4D-ND	-2.88	1.33	1.37
14	b	827	CLA	C4B-NB	2.88	1.41	1.37
14	A	843	CLA	C3B-C4B	2.88	1.49	1.42
14	J	102	CLA	C3B-C4B	2.87	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	1606	CLA	C3B-C4B	2.87	1.49	1.42
14	z	102	CLA	C4D-ND	-2.87	1.33	1.37
14	1	1624	CLA	C3B-C4B	2.87	1.49	1.42
14	2	815	CLA	C4B-NB	2.87	1.41	1.37
14	j	1303	CLA	C3B-C4B	2.87	1.49	1.42
14	B	839	CLA	C3B-C4B	2.87	1.49	1.42
14	2	840	CLA	C3B-C4B	2.87	1.49	1.42
14	8	1303	CLA	C3B-C4B	2.87	1.49	1.42
14	M	102	CLA	C4D-ND	-2.86	1.33	1.37
14	B	824	CLA	C4B-NB	2.86	1.41	1.37
14	1	1603	CLA	C1D-ND	2.86	1.41	1.37
14	2	832	CLA	C4B-NB	2.86	1.41	1.37
14	2	822	CLA	C4D-ND	-2.86	1.33	1.37
14	B	810	CLA	C3B-C4B	2.86	1.49	1.42
14	2	811	CLA	C3B-C4B	2.86	1.49	1.42
14	b	811	CLA	C3B-C4B	2.86	1.49	1.42
14	b	836	CLA	C3B-C4B	2.86	1.49	1.42
14	2	827	CLA	C4B-NB	2.86	1.41	1.37
14	b	840	CLA	C3B-C4B	2.86	1.49	1.42
14	a	821	CLA	C4D-ND	-2.86	1.33	1.37
14	A	841	CLA	C4B-NB	2.86	1.41	1.37
14	b	815	CLA	C4B-NB	2.86	1.41	1.37
14	a	802	CLA	C1D-ND	2.86	1.41	1.37
14	X	1701	CLA	C3B-C4B	2.86	1.49	1.42
14	a	834	CLA	C3B-C4B	2.86	1.49	1.42
14	a	838	CLA	C3B-C4B	2.86	1.49	1.42
14	B	826	CLA	C4B-NB	2.85	1.41	1.37
14	a	826	CLA	C4B-NB	2.85	1.41	1.37
14	A	822	CLA	C3B-C4B	2.85	1.49	1.42
14	B	811	CLA	C4B-NB	2.85	1.41	1.37
14	B	805	CLA	C4B-NB	2.85	1.41	1.37
14	2	812	CLA	C3B-C4B	2.85	1.49	1.42
14	B	835	CLA	C3B-C4B	2.85	1.49	1.42
18	1	1654	LHG	O7-C5	-2.85	1.39	1.46
14	2	826	CLA	C3B-C4B	2.85	1.49	1.42
14	0	206	CLA	C1D-ND	2.85	1.41	1.37
14	a	844	CLA	C4B-NB	2.84	1.41	1.37
14	j	1303	CLA	C4D-ND	-2.84	1.33	1.37
14	2	806	CLA	C4B-NB	2.84	1.41	1.37
18	a	853	LHG	O7-C5	-2.84	1.39	1.46
14	B	811	CLA	C3B-C4B	2.84	1.49	1.42
14	2	841	CLA	CMD-C2D	-2.84	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	825	CLA	C3B-C4B	2.84	1.49	1.42
14	b	806	CLA	C3B-C4B	2.84	1.49	1.42
14	a	822	CLA	C3B-C4B	2.84	1.49	1.42
14	1	1644	CLA	C3B-C4B	2.84	1.49	1.42
14	2	835	CLA	C4D-ND	-2.84	1.33	1.37
14	b	826	CLA	C3B-C4B	2.84	1.49	1.42
14	A	826	CLA	C4B-NB	2.84	1.41	1.37
14	a	823	CLA	C3B-C4B	2.84	1.49	1.42
14	l	205	CLA	C1D-ND	2.84	1.41	1.37
14	2	832	CLA	C3B-C4B	2.84	1.49	1.42
14	1	1623	CLA	C3B-C4B	2.84	1.49	1.42
14	B	814	CLA	C4B-NB	2.83	1.41	1.37
14	a	820	CLA	C4B-NB	2.83	1.41	1.37
14	A	838	CLA	C3B-C4B	2.83	1.49	1.42
14	J	101	CLA	C3B-C4B	2.83	1.49	1.42
14	A	809	CLA	C3B-C4B	2.83	1.49	1.42
14	b	812	CLA	C3B-C4B	2.83	1.49	1.42
14	2	802	CLA	C3B-C4B	2.83	1.49	1.42
14	b	802	CLA	C3B-C4B	2.83	1.49	1.42
14	1	1613	CLA	C3B-C4B	2.83	1.49	1.42
14	2	836	CLA	C3B-C4B	2.83	1.49	1.42
14	A	825	CLA	C3B-C4B	2.83	1.49	1.42
14	2	838	CLA	C3B-C4B	2.83	1.49	1.42
14	a	820	CLA	C3B-C4B	2.82	1.49	1.42
14	2	807	CLA	C4B-NB	2.82	1.41	1.37
14	A	819	CLA	C3B-C4B	2.82	1.49	1.42
14	A	820	CLA	C3B-C4B	2.82	1.49	1.42
14	1	1620	CLA	C3B-C4B	2.82	1.49	1.42
14	1	1639	CLA	C3B-C4B	2.82	1.49	1.42
14	a	843	CLA	C3B-C4B	2.82	1.49	1.42
14	a	819	CLA	C3B-C4B	2.82	1.49	1.42
14	A	843	CLA	C1D-ND	2.82	1.41	1.37
14	B	834	CLA	C4D-ND	-2.82	1.33	1.37
14	1	1621	CLA	C4B-NB	2.82	1.41	1.37
14	B	840	CLA	CMD-C2D	-2.82	1.44	1.50
14	a	825	CLA	C3B-C4B	2.82	1.49	1.42
14	1	1627	CLA	C4B-NB	2.82	1.41	1.37
14	1	1621	CLA	C3B-C4B	2.81	1.49	1.42
14	A	820	CLA	C4B-NB	2.81	1.41	1.37
14	a	809	CLA	C3B-C4B	2.81	1.49	1.42
14	b	806	CLA	C4B-NB	2.81	1.41	1.37
14	1	1626	CLA	C3B-C4B	2.81	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	1645	CLA	C4B-NB	2.81	1.41	1.37
14	B	834	CLA	C3B-C4B	2.81	1.49	1.42
14	B	837	CLA	C3B-C4B	2.81	1.49	1.42
14	A	823	CLA	C3B-C4B	2.81	1.49	1.42
14	b	838	CLA	C3B-C4B	2.81	1.49	1.42
14	2	811	CLA	C4B-NB	2.80	1.41	1.37
14	b	811	CLA	C4B-NB	2.80	1.41	1.37
14	8	1302	CLA	C3B-C4B	2.80	1.49	1.42
14	8	1303	CLA	C4D-ND	-2.80	1.33	1.37
14	J	102	CLA	C4D-ND	-2.80	1.33	1.37
14	1	1618	CLA	C4D-ND	-2.80	1.33	1.37
14	2	806	CLA	C3B-C4B	2.80	1.49	1.42
14	a	812	CLA	C3B-C4B	2.80	1.49	1.42
14	b	807	CLA	C4B-NB	2.80	1.41	1.37
14	b	839	CLA	C4B-NB	2.80	1.41	1.37
14	B	818	CLA	C4B-NB	2.80	1.41	1.37
14	A	844	CLA	C4B-NB	2.80	1.41	1.37
14	A	812	CLA	C3B-C4B	2.79	1.49	1.42
14	b	832	CLA	C3B-C4B	2.79	1.49	1.42
14	j	1302	CLA	C3B-C4B	2.79	1.49	1.42
14	1	1631	CLA	CMD-C2D	-2.79	1.44	1.50
14	B	806	CLA	C4B-NB	2.79	1.41	1.37
14	2	839	CLA	C4B-NB	2.79	1.41	1.37
14	1	1641	CLA	C3B-C4B	2.79	1.49	1.42
14	B	810	CLA	C4B-NB	2.79	1.41	1.37
14	1	1644	CLA	C1D-ND	2.79	1.41	1.37
14	a	830	CLA	CMD-C2D	-2.79	1.44	1.50
14	A	825	CLA	C4B-NB	2.78	1.41	1.37
14	A	807	CLA	C4B-NB	2.78	1.41	1.37
14	A	855	CLA	C3B-C4B	2.78	1.49	1.42
14	b	835	CLA	C3B-C4B	2.78	1.49	1.42
14	b	841	CLA	CMD-C2D	-2.78	1.44	1.50
14	B	814	CLA	C3B-C4B	2.78	1.49	1.42
14	2	819	CLA	C4B-NB	2.78	1.41	1.37
14	a	840	CLA	C3B-C4B	2.78	1.49	1.42
14	2	835	CLA	C3B-C4B	2.78	1.49	1.42
14	a	817	CLA	C4D-ND	-2.78	1.33	1.37
14	1	1610	CLA	C3B-C4B	2.78	1.49	1.42
14	b	829	CLA	C3B-C4B	2.78	1.49	1.42
14	b	831	CLA	C4B-NB	2.78	1.41	1.37
14	B	805	CLA	C3B-C4B	2.78	1.49	1.42
14	A	817	CLA	C4D-ND	-2.77	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	827	CLA	C3B-C4B	2.77	1.49	1.42
14	B	831	CLA	C3B-C4B	2.77	1.49	1.42
14	B	813	CLA	C4B-NB	2.77	1.41	1.37
14	b	815	CLA	C3B-C4B	2.77	1.49	1.42
14	2	829	CLA	C3B-C4B	2.77	1.49	1.42
14	2	831	CLA	C4B-NB	2.77	1.41	1.37
14	B	807	CLA	C4B-NB	2.77	1.41	1.37
14	B	838	CLA	C4B-NB	2.76	1.41	1.37
14	a	802	CLA	CMD-C2D	-2.76	1.44	1.50
14	a	825	CLA	C4B-NB	2.76	1.41	1.37
14	b	814	CLA	C4B-NB	2.76	1.41	1.37
17	0	208	BCR	C30-C25	-2.76	1.50	1.53
14	2	820	CLA	C3B-C4B	2.76	1.49	1.42
14	a	807	CLA	C4B-NB	2.76	1.41	1.37
14	2	814	CLA	C4B-NB	2.76	1.41	1.37
14	A	840	CLA	C3B-C4B	2.76	1.49	1.42
14	2	825	CLA	C3B-C4B	2.75	1.49	1.42
14	2	841	CLA	C4B-NB	2.75	1.41	1.37
14	B	828	CLA	C3B-C4B	2.75	1.49	1.42
14	1	1611	CLA	C3B-C4B	2.75	1.49	1.42
14	B	819	CLA	C3B-C4B	2.75	1.49	1.42
14	b	805	CLA	C3B-C4B	2.75	1.49	1.42
14	2	808	CLA	C4B-NB	2.75	1.41	1.37
14	B	804	CLA	C3B-C4B	2.75	1.49	1.42
14	a	810	CLA	C3B-C4B	2.75	1.49	1.42
14	2	815	CLA	C3B-C4B	2.75	1.49	1.42
17	L	206	BCR	C30-C25	-2.74	1.50	1.53
14	a	832	CLA	CMB-C2B	-2.74	1.45	1.50
14	1	1628	CLA	C3B-C4B	2.74	1.49	1.42
14	B	820	CLA	C3B-C4B	2.74	1.49	1.42
14	B	840	CLA	C4B-NB	2.74	1.41	1.37
14	2	834	CLA	C3B-C4B	2.74	1.49	1.42
14	b	820	CLA	C3B-C4B	2.74	1.49	1.42
14	b	834	CLA	C3B-C4B	2.74	1.49	1.42
14	B	830	CLA	C4B-NB	2.74	1.41	1.37
14	b	810	CLA	CMB-C2B	-2.74	1.45	1.50
14	k	101	CLA	C1B-C2B	2.73	1.49	1.43
14	A	830	CLA	CMD-C2D	-2.73	1.45	1.50
14	B	809	CLA	CMB-C2B	-2.73	1.45	1.50
14	2	810	CLA	CMB-C2B	-2.73	1.45	1.50
14	1	1608	CLA	C4B-NB	2.73	1.41	1.37
14	A	828	CLA	C3B-C4B	2.73	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	1629	CLA	C3B-C4B	2.73	1.49	1.42
14	b	825	CLA	C3B-C4B	2.73	1.49	1.42
14	b	814	CLA	C3B-C4B	2.73	1.49	1.42
14	a	802	CLA	C4B-NB	2.73	1.41	1.37
14	A	810	CLA	C3B-C4B	2.73	1.49	1.42
14	K	101	CLA	C3B-C4B	2.73	1.49	1.42
14	a	830	CLA	C3B-C4B	2.73	1.49	1.42
14	b	808	CLA	C4B-NB	2.73	1.41	1.37
14	b	819	CLA	C4B-NB	2.73	1.41	1.37
14	a	834	CLA	C4B-NB	2.73	1.41	1.37
14	1	1639	CLA	C4B-NB	2.73	1.41	1.37
14	B	824	CLA	C3B-C4B	2.73	1.49	1.42
14	1	1603	CLA	C4B-NB	2.72	1.41	1.37
14	B	833	CLA	C3B-C4B	2.72	1.49	1.42
14	a	827	CLA	C3B-C4B	2.72	1.49	1.42
14	9	101	CLA	C3B-C4B	2.72	1.49	1.42
14	2	821	CLA	C3B-C4B	2.72	1.49	1.42
14	B	813	CLA	C3B-C4B	2.72	1.49	1.42
14	a	817	CLA	C3B-C4B	2.72	1.49	1.42
14	A	802	CLA	C4B-NB	2.71	1.41	1.37
14	A	802	CLA	CMD-C2D	-2.71	1.45	1.50
14	9	101	CLA	C1B-C2B	2.71	1.49	1.43
14	b	841	CLA	C4B-NB	2.71	1.41	1.37
14	2	805	CLA	C3B-C4B	2.71	1.49	1.42
14	A	827	CLA	C4B-NB	2.71	1.41	1.37
14	B	808	CLA	C4B-NB	2.71	1.41	1.37
14	2	829	CLA	CMD-C2D	-2.71	1.45	1.50
14	A	817	CLA	C3B-C4B	2.71	1.49	1.42
14	2	809	CLA	C4B-NB	2.71	1.41	1.37
14	b	842	CLA	C3B-C4B	2.71	1.49	1.42
14	b	821	CLA	C3B-C4B	2.71	1.49	1.42
14	1	1603	CLA	CMD-C2D	-2.71	1.45	1.50
14	2	819	CLA	C3B-C4B	2.71	1.49	1.42
14	1	1626	CLA	C4B-NB	2.71	1.41	1.37
14	A	808	CLA	C3B-C4B	2.70	1.49	1.42
14	K	101	CLA	C1B-C2B	2.70	1.49	1.43
14	B	817	CLA	C3B-C4B	2.70	1.49	1.42
14	A	857	CLA	C1B-C2B	2.70	1.49	1.43
14	A	804	CLA	C4B-NB	2.70	1.41	1.37
14	A	834	CLA	C4B-NB	2.70	1.41	1.37
14	A	855	CLA	C4B-NB	2.70	1.41	1.37
14	a	838	CLA	C4B-NB	2.70	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	828	CLA	C3B-C4B	2.70	1.49	1.42
14	k	101	CLA	C3B-C4B	2.70	1.49	1.42
14	1	1633	CLA	CMB-C2B	-2.70	1.45	1.50
14	1	1633	CLA	MG-NB	-2.70	2.00	2.05
14	A	832	CLA	CMB-C2B	-2.70	1.45	1.50
14	1	1609	CLA	C3B-C4B	2.70	1.49	1.42
14	b	819	CLA	C3B-C4B	2.70	1.49	1.42
14	B	841	CLA	C3B-C4B	2.69	1.49	1.42
14	1	1631	CLA	C3B-C4B	2.69	1.49	1.42
14	2	813	CLA	C3B-C4B	2.69	1.49	1.42
14	1	1601	CLA	C1B-C2B	2.69	1.49	1.43
14	2	814	CLA	C3B-C4B	2.69	1.49	1.42
17	l	207	BCR	C30-C25	-2.69	1.50	1.53
14	B	812	CLA	C3B-C4B	2.69	1.49	1.42
14	B	818	CLA	C3B-C4B	2.69	1.49	1.42
14	1	1635	CLA	C4B-NB	2.69	1.41	1.37
14	b	829	CLA	CMD-C2D	-2.69	1.45	1.50
20	b	850	LMG	O1-C7	-2.69	1.38	1.43
14	1	1618	CLA	C3B-C4B	2.69	1.49	1.42
14	a	832	CLA	MG-NB	-2.69	2.00	2.05
14	A	815	CLA	C3B-C4B	2.69	1.49	1.42
14	B	826	CLA	C3B-C4B	2.69	1.49	1.42
14	1	1636	CLA	C4B-NB	2.69	1.41	1.37
14	a	804	CLA	C4B-NB	2.69	1.41	1.37
14	A	830	CLA	C3B-C4B	2.69	1.49	1.42
14	a	808	CLA	C3B-C4B	2.68	1.49	1.42
14	B	828	CLA	CMD-C2D	-2.68	1.45	1.50
14	2	827	CLA	C3B-C4B	2.68	1.49	1.42
14	A	832	CLA	MG-NB	-2.68	2.00	2.05
14	a	835	CLA	C4B-NB	2.68	1.41	1.37
14	A	841	CLA	C3B-C4B	2.68	1.49	1.42
14	2	818	CLA	C3B-C4B	2.68	1.49	1.42
14	a	817	CLA	C1B-C2B	2.68	1.49	1.43
13	1	1602	CL0	C4B-NB	2.68	1.41	1.37
14	b	827	CLA	C3B-C4B	2.67	1.49	1.42
14	2	842	CLA	C3B-C4B	2.67	1.49	1.42
14	a	815	CLA	C3B-C4B	2.67	1.49	1.42
14	b	809	CLA	C4B-NB	2.67	1.41	1.37
14	A	835	CLA	C4B-NB	2.67	1.41	1.37
20	2	850	LMG	O1-C7	-2.67	1.38	1.43
14	8	1303	CLA	C1B-C2B	2.67	1.49	1.43
14	a	844	CLA	C3B-C4B	2.67	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	849	LMG	O1-C7	-2.67	1.38	1.43
14	a	841	CLA	C3B-C4B	2.66	1.49	1.42
14	b	802	CLA	C4B-NB	2.66	1.41	1.37
14	1	1605	CLA	C4B-NB	2.66	1.41	1.37
14	M	102	CLA	C1B-C2B	2.66	1.49	1.43
14	1	1642	CLA	C3B-C4B	2.66	1.49	1.42
14	A	817	CLA	C1B-C2B	2.66	1.49	1.43
14	a	833	CLA	C4B-NB	2.66	1.41	1.37
14	A	814	CLA	C3B-C4B	2.66	1.49	1.42
14	a	814	CLA	C3B-C4B	2.66	1.49	1.42
13	A	801	CL0	C4B-NB	2.66	1.41	1.37
14	a	833	CLA	MG-NB	-2.66	2.00	2.05
14	2	816	CLA	C3B-C4B	2.66	1.49	1.42
14	1	1628	CLA	C4B-NB	2.66	1.41	1.37
14	b	817	CLA	C3B-C4B	2.66	1.49	1.42
14	B	816	CLA	C1B-C2B	2.66	1.49	1.43
14	b	829	CLA	CMB-C2B	-2.66	1.45	1.50
14	1	1618	CLA	C1B-C2B	2.66	1.49	1.43
14	b	813	CLA	C3B-C4B	2.66	1.49	1.42
14	b	837	CLA	C1B-C2B	2.65	1.49	1.43
14	j	1303	CLA	C1B-C2B	2.65	1.49	1.43
14	A	838	CLA	C4B-NB	2.65	1.41	1.37
14	1	1616	CLA	C3B-C4B	2.65	1.49	1.42
14	b	817	CLA	C1B-C2B	2.65	1.49	1.43
14	B	816	CLA	C3B-C4B	2.65	1.49	1.42
14	A	832	CLA	C4B-NB	2.65	1.41	1.37
14	b	816	CLA	C3B-C4B	2.65	1.49	1.42
14	J	102	CLA	C1B-C2B	2.64	1.49	1.43
14	A	844	CLA	C3B-C4B	2.64	1.49	1.42
14	2	817	CLA	C3B-C4B	2.64	1.49	1.42
14	B	828	CLA	CMB-C2B	-2.64	1.45	1.50
14	A	840	CLA	CMD-C2D	-2.64	1.45	1.50
14	1	1634	CLA	MG-NB	-2.64	2.00	2.05
14	b	818	CLA	C3B-C4B	2.64	1.48	1.42
14	B	808	CLA	CMC-C2C	-2.64	1.45	1.50
14	1	1645	CLA	C3B-C4B	2.64	1.48	1.42
14	a	839	CLA	C4B-NB	2.64	1.41	1.37
13	1	1602	CL0	C1B-C2B	2.64	1.49	1.43
14	B	815	CLA	C3B-C4B	2.64	1.48	1.42
14	1	1633	CLA	C4B-NB	2.64	1.41	1.37
14	2	802	CLA	C4B-NB	2.64	1.41	1.37
14	2	817	CLA	C1B-C2B	2.64	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	829	CLA	CMB-C2B	-2.64	1.45	1.50
14	2	809	CLA	CMC-C2C	-2.64	1.45	1.50
13	a	801	CL0	C1B-C2B	2.64	1.49	1.43
14	B	836	CLA	C1B-C2B	2.63	1.49	1.43
14	2	810	CLA	C4B-NB	2.63	1.41	1.37
13	A	801	CL0	C1B-C2B	2.63	1.49	1.43
14	a	827	CLA	C4B-NB	2.63	1.41	1.37
14	2	837	CLA	C1B-C2B	2.63	1.49	1.43
14	b	810	CLA	C4B-NB	2.63	1.41	1.37
14	1	1634	CLA	C4B-NB	2.63	1.41	1.37
13	a	801	CL0	C4B-NB	2.63	1.41	1.37
14	f	203	CLA	C1B-C2B	2.63	1.49	1.43
14	l	206	CLA	C3B-C4B	2.63	1.48	1.42
14	1	1615	CLA	C3B-C4B	2.62	1.48	1.42
14	B	829	CLA	C4B-NB	2.62	1.41	1.37
14	0	207	CLA	C3B-C4B	2.62	1.48	1.42
14	L	205	CLA	C3B-C4B	2.62	1.48	1.42
14	F	204	CLA	C1B-C2B	2.62	1.49	1.43
14	b	809	CLA	CMC-C2C	-2.62	1.45	1.50
14	j	1302	CLA	C1B-C2B	2.62	1.49	1.43
14	0	207	CLA	C4B-NB	2.61	1.41	1.37
14	b	830	CLA	CMB-C2B	-2.61	1.45	1.50
14	A	833	CLA	C3B-C4B	2.61	1.48	1.42
14	z	102	CLA	C1B-C2B	2.61	1.49	1.43
14	a	832	CLA	C4B-NB	2.60	1.41	1.37
14	J	101	CLA	C1B-C2B	2.60	1.49	1.43
14	B	810	CLA	CMC-C2C	-2.60	1.45	1.50
14	A	833	CLA	MG-NB	-2.60	2.00	2.05
14	B	829	CLA	CMB-C2B	-2.60	1.45	1.50
14	6	203	CLA	C1B-C2B	2.60	1.49	1.43
14	A	833	CLA	C4B-NB	2.60	1.41	1.37
14	2	811	CLA	CMC-C2C	-2.60	1.45	1.50
14	X	1701	CLA	C1B-C2B	2.60	1.49	1.43
14	B	806	CLA	C3B-C4B	2.60	1.48	1.42
14	2	807	CLA	C3B-C4B	2.60	1.48	1.42
14	b	830	CLA	C4B-NB	2.60	1.41	1.37
14	B	807	CLA	CMD-C2D	-2.60	1.45	1.50
14	A	835	CLA	C3B-C4B	2.60	1.48	1.42
14	1	1641	CLA	CMD-C2D	-2.59	1.45	1.50
14	A	806	CLA	C4B-NB	2.59	1.41	1.37
14	L	205	CLA	C4B-NB	2.59	1.41	1.37
14	b	804	CLA	CMD-C2D	-2.59	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	835	CLA	C3B-C4B	2.59	1.48	1.42
14	2	808	CLA	CMD-C2D	-2.59	1.45	1.50
14	b	821	CLA	C1B-C2B	2.59	1.49	1.43
14	a	833	CLA	C3B-C4B	2.59	1.48	1.42
14	A	831	CLA	CMD-C2D	-2.59	1.45	1.50
14	L	204	CLA	C3B-C4B	2.59	1.48	1.42
14	1	1632	CLA	CMD-C2D	-2.59	1.45	1.50
14	a	840	CLA	CMD-C2D	-2.58	1.45	1.50
14	a	804	CLA	C3B-C4B	2.58	1.48	1.42
14	1	1605	CLA	C3B-C4B	2.58	1.48	1.42
14	1	1628	CLA	MG-NB	-2.58	2.00	2.05
14	a	831	CLA	CMD-C2D	-2.58	1.45	1.50
14	A	827	CLA	MG-NB	-2.58	2.00	2.05
14	b	811	CLA	CMC-C2C	-2.58	1.45	1.50
14	1	1633	CLA	CMD-C2D	-2.58	1.45	1.50
14	A	818	CLA	C1B-C2B	2.58	1.49	1.43
14	2	830	CLA	CMB-C2B	-2.58	1.45	1.50
14	A	804	CLA	C3B-C4B	2.58	1.48	1.42
14	A	808	CLA	C1B-C2B	2.58	1.49	1.43
14	1	1634	CLA	C3B-C4B	2.58	1.48	1.42
14	B	803	CLA	CMD-C2D	-2.58	1.45	1.50
14	b	830	CLA	C1B-C2B	2.58	1.49	1.43
14	x	1701	CLA	C1B-C2B	2.58	1.49	1.43
14	A	831	CLA	C3B-C4B	2.58	1.48	1.42
14	8	1302	CLA	C1B-C2B	2.57	1.49	1.43
14	a	831	CLA	C3B-C4B	2.57	1.48	1.42
14	2	834	CLA	CMC-C2C	-2.57	1.45	1.50
14	1	1632	CLA	C3B-C4B	2.57	1.48	1.42
14	2	830	CLA	C4B-NB	2.57	1.40	1.37
14	0	206	CLA	C3B-C4B	2.57	1.48	1.42
14	l	206	CLA	C4B-NB	2.57	1.40	1.37
14	1	1640	CLA	C4B-NB	2.57	1.40	1.37
14	a	827	CLA	MG-NB	-2.56	2.00	2.05
14	2	815	CLA	C1B-C2B	2.56	1.49	1.43
14	1	1636	CLA	C3B-C4B	2.56	1.48	1.42
14	1	1644	CLA	CMC-C2C	-2.56	1.45	1.50
14	b	807	CLA	C3B-C4B	2.56	1.48	1.42
14	A	811	CLA	C1B-C2B	2.56	1.49	1.43
14	A	835	CLA	C1B-C2B	2.56	1.49	1.43
14	1	1636	CLA	C1B-C2B	2.56	1.49	1.43
14	A	843	CLA	CMC-C2C	-2.56	1.45	1.50
14	b	834	CLA	CMC-C2C	-2.56	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	811	CLA	C1B-C2B	2.56	1.49	1.43
14	l	205	CLA	C3B-C4B	2.56	1.48	1.42
14	1	1609	CLA	C1B-C2B	2.56	1.49	1.43
14	1	1619	CLA	C1B-C2B	2.56	1.49	1.43
14	A	832	CLA	CMD-C2D	-2.56	1.45	1.50
14	b	815	CLA	C1B-C2B	2.55	1.49	1.43
14	a	832	CLA	CMD-C2D	-2.55	1.45	1.50
14	1	1640	CLA	CMD-C2D	-2.55	1.45	1.50
14	a	839	CLA	CMD-C2D	-2.55	1.45	1.50
14	2	830	CLA	C1B-C2B	2.55	1.49	1.43
14	A	814	CLA	C1B-C2B	2.55	1.49	1.43
14	a	806	CLA	C4B-NB	2.55	1.40	1.37
14	a	835	CLA	C1B-C2B	2.55	1.49	1.43
14	2	804	CLA	CMD-C2D	-2.55	1.45	1.50
14	K	103	CLA	C1B-C2B	2.55	1.49	1.43
14	2	809	CLA	C1B-C2B	2.55	1.49	1.43
14	b	809	CLA	C1B-C2B	2.55	1.49	1.43
14	2	841	CLA	C3B-C4B	2.55	1.48	1.42
14	b	808	CLA	CMD-C2D	-2.55	1.45	1.50
14	a	818	CLA	C1B-C2B	2.55	1.49	1.43
14	B	809	CLA	C4B-NB	2.55	1.40	1.37
14	1	1630	CLA	CMC-C2C	-2.54	1.45	1.50
14	b	841	CLA	C3B-C4B	2.54	1.48	1.42
13	A	801	CL0	CMD-C2D	-2.54	1.45	1.50
14	B	829	CLA	C1B-C2B	2.54	1.49	1.43
14	A	829	CLA	CMC-C2C	-2.54	1.45	1.50
14	B	808	CLA	C1B-C2B	2.54	1.49	1.43
14	B	840	CLA	C3B-C4B	2.54	1.48	1.42
13	1	1602	CL0	CMD-C2D	-2.54	1.45	1.50
14	a	843	CLA	CMB-C2B	-2.54	1.45	1.50
14	1	1612	CLA	C1B-C2B	2.54	1.49	1.43
14	1	1631	CLA	MG-NB	-2.54	2.00	2.05
14	a	806	CLA	C3B-C4B	2.54	1.48	1.42
14	a	814	CLA	C1B-C2B	2.54	1.49	1.43
13	a	801	CL0	CMD-C2D	-2.54	1.45	1.50
14	B	820	CLA	C1B-C2B	2.54	1.49	1.43
14	a	804	CLA	C1B-C2B	2.54	1.49	1.43
14	b	830	CLA	CMD-C2D	-2.54	1.45	1.50
14	B	803	CLA	C1B-C2B	2.54	1.49	1.43
14	2	805	CLA	CMD-C2D	-2.54	1.45	1.50
14	a	839	CLA	MG-NB	-2.54	2.00	2.05
14	1	1607	CLA	C4B-NB	2.54	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	814	CLA	C1B-C2B	2.53	1.49	1.43
14	2	810	CLA	CMC-C2C	-2.53	1.45	1.50
14	B	833	CLA	CMC-C2C	-2.53	1.45	1.50
14	a	830	CLA	MG-NB	-2.53	2.00	2.05
14	2	811	CLA	CMD-C2D	-2.53	1.45	1.50
14	A	804	CLA	C1B-C2B	2.53	1.49	1.43
14	1	1605	CLA	C1B-C2B	2.53	1.49	1.43
14	B	841	CLA	CMD-C2D	-2.53	1.45	1.50
14	a	808	CLA	C1B-C2B	2.53	1.49	1.43
14	2	821	CLA	C1B-C2B	2.53	1.49	1.43
14	1	1644	CLA	CMB-C2B	-2.53	1.45	1.50
14	b	804	CLA	C1B-C2B	2.53	1.49	1.43
14	B	810	CLA	CMD-C2D	-2.53	1.45	1.50
14	A	830	CLA	MG-NB	-2.53	2.00	2.05
14	a	843	CLA	CMC-C2C	-2.53	1.45	1.50
14	a	836	CLA	CMB-C2B	-2.53	1.45	1.50
18	y	101	LHG	O7-C5	-2.53	1.40	1.46
14	2	839	CLA	MG-NB	-2.53	2.00	2.05
14	9	103	CLA	C1B-C2B	2.53	1.49	1.43
14	b	810	CLA	CMC-C2C	-2.53	1.45	1.50
14	k	103	CLA	C1B-C2B	2.52	1.49	1.43
14	2	830	CLA	CMD-C2D	-2.52	1.45	1.50
14	A	839	CLA	CMD-C2D	-2.52	1.45	1.50
14	B	819	CLA	CMB-C2B	-2.52	1.45	1.50
14	a	821	CLA	CHC-C1C	2.52	1.43	1.38
14	b	805	CLA	CMD-C2D	-2.52	1.45	1.50
14	2	816	CLA	C1B-C2B	2.52	1.49	1.43
14	A	839	CLA	MG-NB	-2.52	2.00	2.05
14	B	829	CLA	CMD-C2D	-2.52	1.45	1.50
14	2	842	CLA	CMD-C2D	-2.52	1.45	1.50
14	A	839	CLA	C4B-NB	2.52	1.40	1.37
14	B	802	CLA	CMD-C2D	-2.52	1.45	1.50
14	1	1637	CLA	CMB-C2B	-2.52	1.45	1.50
18	m	101	LHG	O7-C5	-2.52	1.40	1.46
14	b	803	CLA	CMD-C2D	-2.52	1.45	1.50
14	a	829	CLA	CMC-C2C	-2.52	1.45	1.50
14	L	205	CLA	MG-NB	-2.51	2.00	2.05
14	2	803	CLA	MG-NB	-2.51	2.00	2.05
14	0	206	CLA	CMD-C2D	-2.51	1.45	1.50
14	A	843	CLA	CMB-C2B	-2.51	1.45	1.50
14	B	808	CLA	C3B-C4B	2.51	1.48	1.42
14	2	804	CLA	C1B-C2B	2.51	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	839	CLA	MG-NB	-2.51	2.00	2.05
14	b	818	CLA	CMB-C2B	-2.51	1.45	1.50
14	A	836	CLA	CMB-C2B	-2.51	1.45	1.50
14	1	1615	CLA	C1B-C2B	2.51	1.49	1.43
14	b	842	CLA	CMD-C2D	-2.51	1.45	1.50
14	b	809	CLA	C3B-C4B	2.51	1.48	1.42
14	1	1622	CLA	CHC-C1C	2.51	1.43	1.38
14	B	804	CLA	CMD-C2D	-2.51	1.45	1.50
14	2	803	CLA	CMB-C2B	-2.51	1.45	1.50
14	L	204	CLA	CMD-C2D	-2.51	1.45	1.50
14	b	820	CLA	CMB-C2B	-2.51	1.45	1.50
14	B	838	CLA	C3B-C4B	2.50	1.48	1.42
14	b	839	CLA	CMB-C2B	-2.50	1.45	1.50
14	b	816	CLA	C1B-C2B	2.50	1.49	1.43
14	2	803	CLA	C4B-NB	2.50	1.40	1.37
14	2	803	CLA	C1B-C2B	2.50	1.49	1.43
14	B	809	CLA	C3B-C4B	2.50	1.48	1.42
14	b	815	CLA	CMD-C2D	-2.50	1.45	1.50
14	A	812	CLA	C1B-C2B	2.50	1.49	1.43
14	B	817	CLA	C1B-C2B	2.50	1.49	1.43
14	B	817	CLA	CMB-C2B	-2.50	1.45	1.50
14	1	1627	CLA	C3B-C4B	2.50	1.48	1.42
14	2	809	CLA	C3B-C4B	2.50	1.48	1.42
14	2	803	CLA	CMD-C2D	-2.50	1.45	1.50
14	l	206	CLA	MG-NB	-2.50	2.00	2.05
14	a	828	CLA	MG-NB	-2.50	2.00	2.05
18	M	101	LHG	O7-C5	-2.50	1.40	1.46
14	B	841	CLA	C1B-C2B	2.50	1.49	1.43
14	B	802	CLA	MG-NB	-2.50	2.00	2.05
14	1	1625	CLA	C1B-C2B	2.50	1.49	1.43
14	A	806	CLA	C3B-C4B	2.50	1.48	1.42
14	2	815	CLA	CMD-C2D	-2.49	1.45	1.50
14	2	810	CLA	C3B-C4B	2.49	1.48	1.42
14	l	205	CLA	MG-NB	-2.49	2.00	2.05
14	1	1640	CLA	MG-NB	-2.49	2.00	2.05
14	B	835	CLA	C1B-C2B	2.49	1.49	1.43
14	2	842	CLA	C1B-C2B	2.49	1.49	1.43
14	a	842	CLA	CMD-C2D	-2.49	1.45	1.50
14	A	828	CLA	MG-NB	-2.49	2.00	2.05
14	B	814	CLA	CMD-C2D	-2.49	1.45	1.50
14	a	828	CLA	C1B-C2B	2.49	1.49	1.43
14	b	824	CLA	C1B-C2B	2.49	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	821	CLA	CHC-C1C	2.49	1.43	1.38
14	l	205	CLA	CMD-C2D	-2.49	1.45	1.50
14	b	810	CLA	C3B-C4B	2.49	1.48	1.42
13	a	801	CL0	CMB-C2B	-2.49	1.45	1.50
14	b	813	CLA	C1B-C2B	2.49	1.49	1.43
14	b	803	CLA	CMB-C2B	-2.49	1.45	1.50
14	B	809	CLA	CMC-C2C	-2.49	1.45	1.50
14	2	839	CLA	CMB-C2B	-2.49	1.45	1.50
14	2	820	CLA	CMB-C2B	-2.49	1.45	1.50
14	b	811	CLA	CMD-C2D	-2.49	1.45	1.50
14	B	812	CLA	C1B-C2B	2.49	1.49	1.43
14	1	1607	CLA	C3B-C4B	2.49	1.48	1.42
14	0	206	CLA	MG-NB	-2.49	2.00	2.05
13	A	801	CL0	CMB-C2B	-2.48	1.45	1.50
14	1	1637	CLA	CMC-C2C	-2.48	1.45	1.50
14	1	1634	CLA	CMB-C2B	-2.48	1.45	1.50
14	a	806	CLA	CMD-C2D	-2.48	1.45	1.50
14	a	803	CLA	CMD-C2D	-2.48	1.45	1.50
14	B	837	CLA	CMB-C2B	-2.48	1.45	1.50
14	2	822	CLA	C1B-C2B	2.48	1.49	1.43
14	A	842	CLA	CMC-C2C	-2.48	1.45	1.50
14	B	838	CLA	CMB-C2B	-2.48	1.45	1.50
14	B	802	CLA	CMB-C2B	-2.48	1.45	1.50
14	A	826	CLA	C3B-C4B	2.48	1.48	1.42
14	1	1604	CLA	CMD-C2D	-2.48	1.45	1.50
14	1	1613	CLA	C1B-C2B	2.48	1.49	1.43
14	B	806	CLA	C1B-C2B	2.48	1.49	1.43
14	a	824	CLA	C1B-C2B	2.48	1.49	1.43
14	2	838	CLA	CMB-C2B	-2.47	1.45	1.50
14	b	803	CLA	MG-NB	-2.47	2.00	2.05
14	1	1643	CLA	CMC-C2C	-2.47	1.45	1.50
14	a	826	CLA	C3B-C4B	2.47	1.48	1.42
14	A	836	CLA	CMC-C2C	-2.47	1.45	1.50
14	2	836	CLA	C1B-C2B	2.47	1.49	1.43
14	B	804	CLA	CMB-C2B	-2.47	1.45	1.50
14	b	805	CLA	CMB-C2B	-2.47	1.45	1.50
14	B	815	CLA	C1B-C2B	2.47	1.49	1.43
14	2	813	CLA	C1B-C2B	2.47	1.49	1.43
14	A	842	CLA	CMD-C2D	-2.47	1.45	1.50
14	1	1628	CLA	CMB-C2B	-2.47	1.45	1.50
14	A	827	CLA	CMB-C2B	-2.47	1.45	1.50
14	0	206	CLA	CMB-C2B	-2.47	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	816	CLA	C1B-C2B	2.47	1.49	1.43
14	2	805	CLA	CMB-C2B	-2.47	1.45	1.50
14	A	828	CLA	C1B-C2B	2.47	1.49	1.43
14	2	807	CLA	C1B-C2B	2.47	1.49	1.43
14	2	818	CLA	CMB-C2B	-2.47	1.45	1.50
14	B	802	CLA	C1B-C2B	2.47	1.49	1.43
14	B	821	CLA	C1B-C2B	2.47	1.49	1.43
14	A	841	CLA	CMD-C2D	-2.47	1.45	1.50
14	0	207	CLA	MG-NB	-2.47	2.00	2.05
14	l	206	CLA	CMB-C2B	-2.47	1.45	1.50
14	A	806	CLA	CMD-C2D	-2.47	1.45	1.50
14	a	827	CLA	CMB-C2B	-2.47	1.45	1.50
14	A	833	CLA	CMB-C2B	-2.47	1.45	1.50
14	a	842	CLA	CMC-C2C	-2.47	1.45	1.50
14	b	802	CLA	CMC-C2C	-2.47	1.45	1.50
14	a	812	CLA	C1B-C2B	2.46	1.49	1.43
14	b	831	CLA	C1B-C2B	2.46	1.49	1.43
14	1	1629	CLA	C1B-C2B	2.46	1.49	1.43
14	a	803	CLA	CMC-C2C	-2.46	1.45	1.50
14	a	836	CLA	CMC-C2C	-2.46	1.45	1.50
14	1	1637	CLA	C1B-C2B	2.46	1.49	1.43
14	A	803	CLA	CMD-C2D	-2.46	1.45	1.50
14	b	810	CLA	CMD-C2D	-2.46	1.45	1.50
14	A	832	CLA	C3B-C4B	2.46	1.48	1.42
13	1	1602	CL0	CMB-C2B	-2.46	1.45	1.50
14	b	803	CLA	C1B-C2B	2.46	1.49	1.43
14	a	841	CLA	CMD-C2D	-2.46	1.45	1.50
14	b	807	CLA	C1B-C2B	2.46	1.49	1.43
14	1	1642	CLA	C1B-C2B	2.46	1.49	1.43
14	1	1603	CLA	MG-NB	-2.46	2.00	2.05
14	B	838	CLA	MG-NB	-2.46	2.00	2.05
14	A	831	CLA	MG-NB	-2.46	2.00	2.05
14	2	824	CLA	C1B-C2B	2.46	1.49	1.43
14	a	807	CLA	CMD-C2D	-2.46	1.45	1.50
14	1	1603	CLA	CMC-C2C	-2.46	1.45	1.50
14	A	806	CLA	MG-NB	-2.46	2.00	2.05
14	A	826	CLA	MG-NB	-2.46	2.00	2.05
14	a	806	CLA	MG-NB	-2.46	2.00	2.05
14	A	836	CLA	C3B-C4B	2.45	1.48	1.42
14	A	836	CLA	C1B-C2B	2.45	1.49	1.43
14	2	818	CLA	C1B-C2B	2.45	1.49	1.43
14	L	205	CLA	CMD-C2D	-2.45	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	839	CLA	C3B-C4B	2.45	1.48	1.42
14	b	818	CLA	C1B-C2B	2.45	1.49	1.43
14	A	807	CLA	CMD-C2D	-2.45	1.45	1.50
14	b	805	CLA	CMC-C2C	-2.45	1.45	1.50
14	1	1622	CLA	C1B-C2B	2.45	1.49	1.43
14	2	802	CLA	CMC-C2C	-2.45	1.45	1.50
14	b	822	CLA	C1B-C2B	2.45	1.49	1.43
14	1	1626	CLA	MG-NB	-2.45	2.00	2.05
14	A	802	CLA	CMC-C2C	-2.45	1.45	1.50
14	A	855	CLA	CMC-C2C	-2.45	1.45	1.50
14	A	825	CLA	MG-NB	-2.45	2.00	2.05
14	L	204	CLA	MG-NB	-2.45	2.00	2.05
14	a	831	CLA	MG-NB	-2.45	2.00	2.05
14	a	841	CLA	C1B-C2B	2.45	1.49	1.43
14	a	821	CLA	C1B-C2B	2.45	1.49	1.43
14	l	205	CLA	CMB-C2B	-2.45	1.45	1.50
14	1	1607	CLA	CMD-C2D	-2.45	1.45	1.50
14	a	836	CLA	C1B-C2B	2.45	1.49	1.43
14	a	802	CLA	MG-NB	-2.45	2.00	2.05
14	A	803	CLA	CMC-C2C	-2.45	1.45	1.50
14	L	204	CLA	CMB-C2B	-2.45	1.45	1.50
14	1	1604	CLA	CMC-C2C	-2.45	1.45	1.50
14	1	1643	CLA	CMD-C2D	-2.45	1.45	1.50
14	b	836	CLA	C1B-C2B	2.45	1.49	1.43
14	a	816	CLA	C1B-C2B	2.45	1.49	1.43
14	B	823	CLA	C1B-C2B	2.45	1.49	1.43
14	b	842	CLA	C1B-C2B	2.45	1.49	1.43
14	b	806	CLA	CMB-C2B	-2.44	1.45	1.50
14	l	206	CLA	CMD-C2D	-2.44	1.45	1.50
14	b	839	CLA	C3B-C4B	2.44	1.48	1.42
14	1	1607	CLA	MG-NB	-2.44	2.00	2.05
14	2	808	CLA	C3B-C4B	2.44	1.48	1.42
14	1	1633	CLA	C3B-C4B	2.44	1.48	1.42
14	1	1623	CLA	CMB-C2B	-2.44	1.45	1.50
14	a	825	CLA	MG-NB	-2.44	2.01	2.05
14	2	812	CLA	C1B-C2B	2.44	1.49	1.43
14	2	805	CLA	CMC-C2C	-2.44	1.45	1.50
14	A	802	CLA	MG-NB	-2.44	2.01	2.05
14	1	1642	CLA	CMD-C2D	-2.44	1.45	1.50
14	1	1617	CLA	C1B-C2B	2.44	1.49	1.43
14	0	207	CLA	CMD-C2D	-2.44	1.45	1.50
14	2	808	CLA	MG-NB	-2.44	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	1608	CLA	CMD-C2D	-2.44	1.45	1.50
18	1	1655	LHG	O7-C5	-2.44	1.40	1.46
14	a	836	CLA	C3B-C4B	2.44	1.48	1.42
14	1	1632	CLA	MG-NB	-2.44	2.01	2.05
14	A	803	CLA	CMB-C2B	-2.44	1.45	1.50
14	a	832	CLA	C3B-C4B	2.43	1.48	1.42
14	2	831	CLA	C3B-C4B	2.43	1.48	1.42
14	l	205	CLA	CMC-C2C	-2.43	1.45	1.50
14	a	830	CLA	C4B-NB	2.43	1.40	1.37
14	6	201	CLA	CMD-C2D	-2.43	1.45	1.50
14	1	1634	CLA	CMD-C2D	-2.43	1.45	1.50
14	B	830	CLA	C1B-C2B	2.43	1.49	1.43
14	A	824	CLA	C1B-C2B	2.43	1.49	1.43
14	2	831	CLA	C1B-C2B	2.43	1.49	1.43
14	A	839	CLA	C3B-C4B	2.43	1.48	1.42
18	A	854	LHG	O7-C5	-2.43	1.40	1.46
14	a	822	CLA	CMB-C2B	-2.43	1.45	1.50
14	0	207	CLA	CMB-C2B	-2.43	1.45	1.50
14	A	826	CLA	CMD-C2D	-2.43	1.45	1.50
14	1	1637	CLA	C3B-C4B	2.43	1.48	1.42
18	a	854	LHG	O7-C5	-2.43	1.40	1.46
14	B	840	CLA	CMB-C2B	-2.43	1.45	1.50
14	B	804	CLA	CMC-C2C	-2.43	1.45	1.50
14	a	802	CLA	CMC-C2C	-2.43	1.45	1.50
14	b	808	CLA	MG-NB	-2.43	2.01	2.05
14	2	841	CLA	MG-NB	-2.43	2.01	2.05
14	B	809	CLA	CMD-C2D	-2.43	1.45	1.50
14	F	201	CLA	CMD-C2D	-2.43	1.45	1.50
14	1	1645	CLA	C1B-C2B	2.43	1.49	1.43
14	b	808	CLA	C3B-C4B	2.43	1.48	1.42
14	F	203	CLA	C1B-C2B	2.42	1.49	1.43
14	2	826	CLA	CMD-C2D	-2.42	1.45	1.50
14	A	839	CLA	C1B-C2B	2.42	1.49	1.43
14	1	1627	CLA	MG-NB	-2.42	2.01	2.05
14	B	830	CLA	MG-NB	-2.42	2.01	2.05
14	A	821	CLA	C1B-C2B	2.42	1.49	1.43
14	B	802	CLA	C4B-NB	2.42	1.40	1.37
14	b	831	CLA	C3B-C4B	2.42	1.48	1.42
14	1	1629	CLA	MG-NB	-2.42	2.01	2.05
14	1	1639	CLA	CMD-C2D	-2.42	1.45	1.50
14	b	841	CLA	MG-NB	-2.42	2.01	2.05
14	a	807	CLA	C1B-C2B	2.42	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	840	CLA	MG-NB	-2.42	2.01	2.05
14	a	839	CLA	C3B-C4B	2.42	1.48	1.42
14	b	841	CLA	CMB-C2B	-2.42	1.45	1.50
14	b	838	CLA	CMB-C2B	-2.42	1.45	1.50
14	A	822	CLA	CMB-C2B	-2.42	1.45	1.50
14	a	833	CLA	CMB-C2B	-2.42	1.45	1.50
14	1	1604	CLA	CMB-C2B	-2.42	1.45	1.50
14	1	1640	CLA	CMB-C2B	-2.42	1.45	1.50
14	a	803	CLA	CMB-C2B	-2.42	1.45	1.50
14	b	826	CLA	CMD-C2D	-2.42	1.45	1.50
14	A	844	CLA	C1B-C2B	2.42	1.48	1.43
14	a	826	CLA	MG-NB	-2.42	2.01	2.05
14	b	827	CLA	MG-NB	-2.42	2.01	2.05
14	b	839	CLA	C1B-C2B	2.42	1.48	1.43
14	B	811	CLA	C1B-C2B	2.42	1.48	1.43
14	L	205	CLA	CMB-C2B	-2.42	1.45	1.50
14	1	1627	CLA	CMD-C2D	-2.41	1.45	1.50
14	B	803	CLA	C3B-C4B	2.41	1.48	1.42
14	2	806	CLA	CMB-C2B	-2.41	1.45	1.50
13	A	801	CL0	MG-NB	-2.41	2.01	2.05
13	1	1602	CL0	MG-NB	-2.41	2.01	2.05
14	1	1640	CLA	C3B-C4B	2.41	1.48	1.42
14	a	844	CLA	C1B-C2B	2.41	1.48	1.43
14	0	206	CLA	C4B-NB	2.41	1.40	1.37
14	B	830	CLA	C3B-C4B	2.41	1.48	1.42
14	L	204	CLA	CMC-C2C	-2.41	1.45	1.50
14	B	807	CLA	MG-NB	-2.41	2.01	2.05
14	1	1640	CLA	C1B-C2B	2.41	1.48	1.43
14	2	806	CLA	CMC-C2C	-2.41	1.45	1.50
14	l	205	CLA	C4B-NB	2.41	1.40	1.37
14	2	810	CLA	CMD-C2D	-2.41	1.45	1.50
14	A	841	CLA	C1B-C2B	2.41	1.48	1.43
14	j	1301	CLA	C1B-C2B	2.41	1.48	1.43
14	8	1301	CLA	C1B-C2B	2.41	1.48	1.43
14	b	803	CLA	C4B-NB	2.41	1.40	1.37
14	B	807	CLA	C3B-C4B	2.41	1.48	1.42
14	1	1610	CLA	CMB-C2B	-2.41	1.45	1.50
14	1	1635	CLA	CMD-C2D	-2.41	1.45	1.50
14	A	838	CLA	CMD-C2D	-2.41	1.45	1.50
14	B	805	CLA	CMB-C2B	-2.41	1.45	1.50
14	a	826	CLA	CMD-C2D	-2.41	1.45	1.50
14	2	823	CLA	C1B-C2B	2.41	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	839	CLA	C1B-C2B	2.41	1.48	1.43
14	b	806	CLA	CMC-C2C	-2.40	1.45	1.50
14	B	822	CLA	C1B-C2B	2.40	1.48	1.43
14	1	1624	CLA	C1B-C2B	2.40	1.48	1.43
14	b	812	CLA	C1B-C2B	2.40	1.48	1.43
14	a	838	CLA	CMD-C2D	-2.40	1.45	1.50
14	A	830	CLA	C4B-NB	2.40	1.40	1.37
14	B	826	CLA	CMD-C2D	-2.40	1.45	1.50
14	b	814	CLA	MG-NB	-2.40	2.01	2.05
14	2	835	CLA	C1B-C2B	2.40	1.48	1.43
14	b	803	CLA	CMC-C2C	-2.40	1.45	1.50
14	1	1608	CLA	C1B-C2B	2.40	1.48	1.43
14	A	810	CLA	C1B-C2B	2.40	1.48	1.43
14	B	805	CLA	CMC-C2C	-2.40	1.45	1.50
14	B	841	CLA	CMC-C2C	-2.40	1.45	1.50
14	B	824	CLA	C1B-C2B	2.40	1.48	1.43
14	A	807	CLA	C1B-C2B	2.40	1.48	1.43
14	a	809	CLA	CMB-C2B	-2.40	1.45	1.50
14	a	827	CLA	CMD-C2D	-2.40	1.45	1.50
14	L	204	CLA	C4B-NB	2.40	1.40	1.37
14	b	808	CLA	C1B-C2B	2.40	1.48	1.43
14	A	836	CLA	MG-NB	-2.40	2.01	2.05
14	a	833	CLA	CMD-C2D	-2.40	1.45	1.50
14	1	1607	CLA	CMB-C2B	-2.40	1.45	1.50
14	1	1631	CLA	C4B-NB	2.40	1.40	1.37
14	b	823	CLA	C1B-C2B	2.40	1.48	1.43
14	a	837	CLA	CMB-C2B	-2.40	1.45	1.50
14	2	819	CLA	MG-NB	-2.40	2.01	2.05
14	a	834	CLA	CMD-C2D	-2.40	1.45	1.50
14	b	827	CLA	CMD-C2D	-2.40	1.45	1.50
14	0	206	CLA	CMC-C2C	-2.40	1.45	1.50
14	B	806	CLA	MG-NB	-2.40	2.01	2.05
14	a	820	CLA	CMD-C2D	-2.40	1.45	1.50
14	b	835	CLA	C1B-C2B	2.39	1.48	1.43
14	B	818	CLA	MG-NB	-2.39	2.01	2.05
14	A	809	CLA	CMB-C2B	-2.39	1.45	1.50
14	b	807	CLA	MG-NB	-2.39	2.01	2.05
14	b	804	CLA	C3B-C4B	2.39	1.48	1.42
14	a	823	CLA	C1B-C2B	2.39	1.48	1.43
14	b	835	CLA	CMB-C2B	-2.39	1.45	1.50
14	B	838	CLA	C1B-C2B	2.39	1.48	1.43
14	B	806	CLA	CMD-C2D	-2.39	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	825	CLA	CMD-C2D	-2.39	1.45	1.50
14	1	1636	CLA	CMD-C2D	-2.39	1.45	1.50
14	1	1638	CLA	CMB-C2B	-2.39	1.45	1.50
14	z	102	CLA	CHC-C1C	2.39	1.43	1.38
14	a	839	CLA	C1B-C2B	2.39	1.48	1.43
14	A	823	CLA	C1B-C2B	2.39	1.48	1.43
14	a	839	CLA	CMB-C2B	-2.39	1.45	1.50
14	a	806	CLA	CMB-C2B	-2.39	1.45	1.50
14	2	842	CLA	CMB-C2B	-2.39	1.45	1.50
14	f	201	CLA	CMD-C2D	-2.39	1.45	1.50
14	2	830	CLA	MG-NB	-2.39	2.01	2.05
14	2	838	CLA	CMD-C2D	-2.39	1.45	1.50
14	A	818	CLA	CMD-C2D	-2.39	1.45	1.50
14	A	833	CLA	CMD-C2D	-2.39	1.45	1.50
14	B	829	CLA	MG-NB	-2.39	2.01	2.05
14	a	829	CLA	CMD-C2D	-2.39	1.45	1.50
14	1	1628	CLA	CMD-C2D	-2.39	1.45	1.50
14	A	835	CLA	CMD-C2D	-2.39	1.45	1.50
14	b	834	CLA	CMD-C2D	-2.39	1.45	1.50
14	1	1643	CLA	MG-NB	-2.39	2.01	2.05
14	A	827	CLA	CMD-C2D	-2.39	1.45	1.50
14	B	841	CLA	CMB-C2B	-2.39	1.45	1.50
14	x	1701	CLA	CHC-C1C	2.38	1.43	1.38
14	A	839	CLA	CMB-C2B	-2.38	1.45	1.50
14	B	834	CLA	C1B-C2B	2.38	1.48	1.43
14	2	827	CLA	MG-NB	-2.38	2.01	2.05
14	a	842	CLA	MG-NB	-2.38	2.01	2.05
14	2	804	CLA	C3B-C4B	2.38	1.48	1.42
14	A	806	CLA	CMB-C2B	-2.38	1.45	1.50
14	2	841	CLA	CMB-C2B	-2.38	1.45	1.50
14	B	807	CLA	C1B-C2B	2.38	1.48	1.43
14	a	810	CLA	C1B-C2B	2.38	1.48	1.43
14	1	1611	CLA	C1B-C2B	2.38	1.48	1.43
14	2	831	CLA	CMB-C2B	-2.38	1.45	1.50
14	a	828	CLA	CMD-C2D	-2.38	1.45	1.50
14	2	827	CLA	CMD-C2D	-2.38	1.45	1.50
14	1	1630	CLA	C1B-C2B	2.38	1.48	1.43
14	2	834	CLA	C1B-C2B	2.38	1.48	1.43
14	B	826	CLA	MG-NB	-2.38	2.01	2.05
14	b	825	CLA	C1B-C2B	2.38	1.48	1.43
14	b	807	CLA	CMD-C2D	-2.38	1.45	1.50
14	B	803	CLA	MG-NB	-2.38	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	828	CLA	CMD-C2D	-2.38	1.45	1.50
14	b	828	CLA	CMC-C2C	-2.38	1.45	1.50
14	2	834	CLA	CMD-C2D	-2.38	1.45	1.50
14	A	813	CLA	CMD-C2D	-2.38	1.45	1.50
14	B	802	CLA	CMC-C2C	-2.38	1.45	1.50
14	a	837	CLA	C1B-C2B	2.37	1.48	1.43
14	A	815	CLA	C1B-C2B	2.37	1.48	1.43
14	b	826	CLA	CMB-C2B	-2.37	1.45	1.50
14	2	827	CLA	C1B-C2B	2.37	1.48	1.43
14	b	831	CLA	MG-NB	-2.37	2.01	2.05
13	a	801	CL0	MG-NB	-2.37	2.01	2.05
14	b	831	CLA	CMB-C2B	-2.37	1.45	1.50
14	a	836	CLA	MG-NB	-2.37	2.01	2.05
14	2	835	CLA	CMB-C2B	-2.37	1.45	1.50
14	X	1701	CLA	CHC-C1C	2.37	1.43	1.38
14	1	1621	CLA	CMD-C2D	-2.37	1.45	1.50
14	B	825	CLA	MG-NB	-2.37	2.01	2.05
14	A	842	CLA	CMB-C2B	-2.37	1.45	1.50
14	a	813	CLA	CMD-C2D	-2.37	1.45	1.50
14	B	830	CLA	CMB-C2B	-2.37	1.45	1.50
14	2	807	CLA	CMD-C2D	-2.37	1.45	1.50
14	B	826	CLA	C1B-C2B	2.37	1.48	1.43
14	2	808	CLA	C1B-C2B	2.37	1.48	1.43
14	b	842	CLA	CMC-C2C	-2.37	1.45	1.50
14	b	830	CLA	MG-NB	-2.37	2.01	2.05
14	B	833	CLA	CMD-C2D	-2.36	1.45	1.50
14	1	1638	CLA	C1B-C2B	2.36	1.48	1.43
14	B	819	CLA	C1B-C2B	2.36	1.48	1.43
14	2	823	CLA	CMD-C2D	-2.36	1.45	1.50
14	b	827	CLA	C1B-C2B	2.36	1.48	1.43
14	1	1616	CLA	C1B-C2B	2.36	1.48	1.43
14	A	837	CLA	C1B-C2B	2.36	1.48	1.43
14	B	833	CLA	C1B-C2B	2.36	1.48	1.43
14	B	841	CLA	MG-NB	-2.36	2.01	2.05
14	A	820	CLA	CMD-C2D	-2.36	1.45	1.50
14	2	825	CLA	C1B-C2B	2.36	1.48	1.43
14	a	815	CLA	C1B-C2B	2.36	1.48	1.43
14	A	837	CLA	CMB-C2B	-2.36	1.45	1.50
14	A	829	CLA	C1B-C2B	2.36	1.48	1.43
14	1	1635	CLA	MG-NB	-2.36	2.01	2.05
14	A	834	CLA	CMD-C2D	-2.36	1.45	1.50
14	1	1639	CLA	C1B-C2B	2.36	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	837	CLA	CMD-C2D	-2.36	1.45	1.50
14	a	805	CLA	C1B-C2B	2.36	1.48	1.43
14	1	1614	CLA	CMD-C2D	-2.36	1.45	1.50
14	2	842	CLA	CMC-C2C	-2.36	1.45	1.50
14	2	831	CLA	MG-NB	-2.36	2.01	2.05
14	B	831	CLA	C1B-C2B	2.36	1.48	1.43
14	1	1641	CLA	MG-NB	-2.36	2.01	2.05
14	b	819	CLA	MG-NB	-2.36	2.01	2.05
14	A	822	CLA	CMD-C2D	-2.36	1.45	1.50
14	B	834	CLA	CMD-C2D	-2.36	1.45	1.50
14	2	803	CLA	CMC-C2C	-2.35	1.45	1.50
14	B	827	CLA	CMC-C2C	-2.35	1.45	1.50
14	A	829	CLA	CMD-C2D	-2.35	1.45	1.50
14	a	829	CLA	C1B-C2B	2.35	1.48	1.43
14	1	1630	CLA	CMD-C2D	-2.35	1.45	1.50
14	a	822	CLA	CMD-C2D	-2.35	1.45	1.50
14	b	842	CLA	CMB-C2B	-2.35	1.45	1.50
14	B	818	CLA	CMD-C2D	-2.35	1.45	1.50
14	a	842	CLA	CMB-C2B	-2.35	1.45	1.50
14	2	807	CLA	CMB-C2B	-2.35	1.45	1.50
14	B	811	CLA	CMB-C2B	-2.35	1.45	1.50
14	B	813	CLA	MG-NB	-2.35	2.01	2.05
14	2	826	CLA	MG-NB	-2.35	2.01	2.05
14	1	1637	CLA	MG-NB	-2.35	2.01	2.05
14	b	834	CLA	C1B-C2B	2.35	1.48	1.43
14	B	822	CLA	CMD-C2D	-2.35	1.45	1.50
14	l	204	CLA	MG-NB	-2.35	2.01	2.05
14	l	204	CLA	CMD-C2D	-2.35	1.45	1.50
14	a	840	CLA	MG-NB	-2.35	2.01	2.05
14	1	1619	CLA	CMD-C2D	-2.35	1.45	1.50
14	B	834	CLA	CMB-C2B	-2.35	1.45	1.50
14	a	818	CLA	CMD-C2D	-2.35	1.45	1.50
14	b	838	CLA	CMD-C2D	-2.35	1.45	1.50
14	b	804	CLA	MG-NB	-2.35	2.01	2.05
14	2	804	CLA	CMC-C2C	-2.35	1.45	1.50
14	2	832	CLA	C1B-C2B	2.35	1.48	1.43
14	A	857	CLA	CMD-C2D	-2.34	1.45	1.50
14	L	203	CLA	CMD-C2D	-2.34	1.45	1.50
14	b	804	CLA	CMC-C2C	-2.34	1.45	1.50
14	B	832	CLA	C1B-C2B	2.34	1.48	1.43
14	L	203	CLA	MG-NB	-2.34	2.01	2.05
14	B	806	CLA	CMB-C2B	-2.34	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	809	CLA	CMD-C2D	-2.34	1.45	1.50
14	2	826	CLA	CMC-C2C	-2.34	1.45	1.50
14	2	828	CLA	CMC-C2C	-2.34	1.45	1.50
14	2	807	CLA	MG-NB	-2.34	2.01	2.05
14	1	1643	CLA	CMB-C2B	-2.34	1.45	1.50
14	B	810	CLA	C1B-C2B	2.34	1.48	1.43
14	A	826	CLA	C1B-C2B	2.34	1.48	1.43
14	2	814	CLA	MG-NB	-2.34	2.01	2.05
14	1	1611	CLA	CMD-C2D	-2.34	1.45	1.50
14	b	819	CLA	CMD-C2D	-2.34	1.45	1.50
14	b	823	CLA	CMD-C2D	-2.34	1.45	1.50
14	b	829	CLA	MG-NB	-2.34	2.01	2.05
14	b	833	CLA	C1B-C2B	2.34	1.48	1.43
14	b	810	CLA	MG-NB	-2.34	2.01	2.05
14	0	205	CLA	MG-NB	-2.34	2.01	2.05
14	a	835	CLA	CMD-C2D	-2.34	1.45	1.50
14	a	838	CLA	C1B-C2B	2.33	1.48	1.43
14	1	1629	CLA	CMD-C2D	-2.33	1.45	1.50
14	A	820	CLA	CMC-C2C	-2.33	1.45	1.50
14	B	815	CLA	MG-NB	-2.33	2.01	2.05
14	a	804	CLA	MG-NB	-2.33	2.01	2.05
14	b	826	CLA	MG-NB	-2.33	2.01	2.05
14	2	828	CLA	CMD-C2D	-2.33	1.45	1.50
14	b	842	CLA	MG-NB	-2.33	2.01	2.05
14	A	834	CLA	MG-NB	-2.33	2.01	2.05
14	b	832	CLA	MG-NB	-2.33	2.01	2.05
14	1	1615	CLA	CMC-C2C	-2.33	1.45	1.50
14	2	812	CLA	CMB-C2B	-2.33	1.45	1.50
14	b	820	CLA	C1B-C2B	2.33	1.48	1.43
14	A	822	CLA	MG-NB	-2.33	2.01	2.05
14	B	809	CLA	MG-NB	-2.33	2.01	2.05
14	2	833	CLA	C1B-C2B	2.33	1.48	1.43
14	2	820	CLA	C1B-C2B	2.33	1.48	1.43
14	A	804	CLA	MG-NB	-2.33	2.01	2.05
14	b	816	CLA	MG-NB	-2.33	2.01	2.05
14	2	829	CLA	MG-NB	-2.33	2.01	2.05
14	B	825	CLA	CMB-C2B	-2.33	1.45	1.50
14	1	1644	CLA	MG-NB	-2.33	2.01	2.05
14	B	805	CLA	C1B-C2B	2.33	1.48	1.43
14	a	826	CLA	C1B-C2B	2.33	1.48	1.43
14	A	810	CLA	CMB-C2B	-2.33	1.45	1.50
14	2	816	CLA	MG-NB	-2.33	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	832	CLA	MG-NB	-2.33	2.01	2.05
14	a	804	CLA	CMD-C2D	-2.33	1.45	1.50
14	B	838	CLA	CMD-C2D	-2.32	1.45	1.50
14	b	835	CLA	CMD-C2D	-2.32	1.45	1.50
14	B	827	CLA	CMD-C2D	-2.32	1.45	1.50
14	a	820	CLA	CMC-C2C	-2.32	1.45	1.50
14	2	840	CLA	CMD-C2D	-2.32	1.45	1.50
14	A	838	CLA	C1B-C2B	2.32	1.48	1.43
14	A	830	CLA	C1B-C2B	2.32	1.48	1.43
14	b	819	CLA	C1B-C2B	2.32	1.48	1.43
14	A	807	CLA	MG-NB	-2.32	2.01	2.05
14	2	810	CLA	MG-NB	-2.32	2.01	2.05
14	A	804	CLA	CMD-C2D	-2.32	1.45	1.50
14	1	1611	CLA	CMB-C2B	-2.32	1.45	1.50
14	2	839	CLA	CMD-C2D	-2.32	1.45	1.50
14	1	1606	CLA	MG-NB	-2.32	2.01	2.05
14	2	842	CLA	MG-NB	-2.32	2.01	2.05
14	A	805	CLA	MG-NB	-2.32	2.01	2.05
14	A	805	CLA	C1B-C2B	2.32	1.48	1.43
14	b	826	CLA	CMC-C2C	-2.32	1.45	1.50
14	2	819	CLA	CMD-C2D	-2.32	1.45	1.50
14	2	819	CLA	C1B-C2B	2.32	1.48	1.43
14	A	842	CLA	MG-NB	-2.32	2.01	2.05
14	a	809	CLA	CMD-C2D	-2.32	1.45	1.50
14	b	839	CLA	CMD-C2D	-2.32	1.45	1.50
14	a	843	CLA	C1B-C2B	2.32	1.48	1.43
14	M	102	CLA	CMD-C2D	-2.32	1.45	1.50
14	0	205	CLA	CMD-C2D	-2.32	1.45	1.50
14	b	811	CLA	C1B-C2B	2.32	1.48	1.43
14	A	837	CLA	MG-NB	-2.32	2.01	2.05
14	1	1606	CLA	C1B-C2B	2.32	1.48	1.43
14	2	835	CLA	CMD-C2D	-2.32	1.45	1.50
14	a	810	CLA	CMB-C2B	-2.31	1.45	1.50
14	a	805	CLA	MG-NB	-2.31	2.01	2.05
14	B	803	CLA	C4B-NB	2.31	1.40	1.37
14	a	810	CLA	CMD-C2D	-2.31	1.45	1.50
14	b	832	CLA	C1B-C2B	2.31	1.48	1.43
14	A	855	CLA	MG-NB	-2.31	2.01	2.05
14	1	1605	CLA	MG-NB	-2.31	2.01	2.05
14	A	826	CLA	CMB-C2B	-2.31	1.45	1.50
14	j	1301	CLA	MG-NB	-2.31	2.01	2.05
14	1	1621	CLA	CMC-C2C	-2.31	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	1610	CLA	CMD-C2D	-2.31	1.45	1.50
14	2	823	CLA	CMB-C2B	-2.31	1.45	1.50
14	b	840	CLA	CMD-C2D	-2.31	1.45	1.50
14	A	840	CLA	MG-NB	-2.31	2.01	2.05
14	B	839	CLA	CMD-C2D	-2.31	1.45	1.50
14	1	1608	CLA	MG-NB	-2.31	2.01	2.05
14	B	825	CLA	CMC-C2C	-2.31	1.45	1.50
17	b	849	BCR	C38-C26	-2.31	1.47	1.50
14	a	843	CLA	MG-NB	-2.31	2.01	2.05
14	A	843	CLA	C1B-C2B	2.31	1.48	1.43
14	b	806	CLA	C1B-C2B	2.31	1.48	1.43
14	a	826	CLA	CMB-C2B	-2.31	1.45	1.50
14	a	822	CLA	MG-NB	-2.31	2.01	2.05
14	2	804	CLA	MG-NB	-2.31	2.01	2.05
14	A	814	CLA	CMC-C2C	-2.31	1.45	1.50
14	B	828	CLA	MG-NB	-2.31	2.01	2.05
14	b	823	CLA	MG-NB	-2.31	2.01	2.05
14	1	1623	CLA	CMD-C2D	-2.30	1.45	1.50
14	b	835	CLA	MG-NB	-2.30	2.01	2.05
14	2	833	CLA	CMD-C2D	-2.30	1.45	1.50
14	F	203	CLA	MG-NB	-2.30	2.01	2.05
14	8	1301	CLA	MG-NB	-2.30	2.01	2.05
14	b	812	CLA	CMB-C2B	-2.30	1.45	1.50
14	b	837	CLA	CMB-C2B	-2.30	1.45	1.50
14	1	1627	CLA	C1B-C2B	2.30	1.48	1.43
14	b	802	CLA	MG-NB	-2.30	2.01	2.05
14	A	831	CLA	CMC-C2C	-2.30	1.45	1.50
14	a	814	CLA	CMC-C2C	-2.30	1.45	1.50
14	2	826	CLA	CMB-C2B	-2.30	1.45	1.50
14	A	816	CLA	CHC-C1C	2.30	1.43	1.38
14	a	838	CLA	C1B-NB	-2.30	1.35	1.37
20	b	850	LMG	O6-C5	-2.30	1.38	1.44
14	2	841	CLA	C1B-C2B	2.30	1.48	1.43
14	2	828	CLA	MG-NB	-2.30	2.01	2.05
14	a	819	CLA	CMB-C2B	-2.30	1.45	1.50
14	2	802	CLA	MG-NB	-2.30	2.01	2.05
17	B	848	BCR	C38-C26	-2.30	1.47	1.50
14	a	841	CLA	MG-NB	-2.30	2.01	2.05
14	1	1641	CLA	CMB-C2B	-2.30	1.45	1.50
14	B	803	CLA	CMC-C2C	-2.30	1.45	1.50
20	B	849	LMG	O8-C9	-2.30	1.39	1.45
14	b	807	CLA	CMB-C2B	-2.30	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	850	LMG	O8-C9	-2.29	1.39	1.45
14	A	843	CLA	MG-NB	-2.29	2.01	2.05
14	1	1613	CLA	CMD-C2D	-2.29	1.45	1.50
14	B	834	CLA	MG-NB	-2.29	2.01	2.05
14	2	837	CLA	CMB-C2B	-2.29	1.45	1.50
14	a	825	CLA	CMD-C2D	-2.29	1.45	1.50
14	b	823	CLA	CMB-C2B	-2.29	1.45	1.50
14	B	831	CLA	MG-NB	-2.29	2.01	2.05
14	1	1632	CLA	CMC-C2C	-2.29	1.45	1.50
14	1	1644	CLA	C1B-C2B	2.29	1.48	1.43
13	1	1602	CL0	C3B-C4B	2.29	1.48	1.42
14	A	810	CLA	CMD-C2D	-2.29	1.45	1.50
14	b	836	CLA	CMD-C2D	-2.29	1.45	1.50
14	1	1605	CLA	CMD-C2D	-2.29	1.45	1.50
14	b	810	CLA	C1B-NB	-2.29	1.35	1.37
14	B	815	CLA	CMD-C2D	-2.29	1.45	1.50
14	a	823	CLA	MG-NB	-2.29	2.01	2.05
14	1	1620	CLA	CMB-C2B	-2.29	1.45	1.50
14	b	804	CLA	C4B-NB	2.29	1.40	1.37
14	2	806	CLA	C1B-C2B	2.29	1.48	1.43
14	a	807	CLA	CMB-C2B	-2.29	1.45	1.50
14	a	841	CLA	CMB-C2B	-2.29	1.45	1.50
14	1	1601	CLA	CMD-C2D	-2.29	1.45	1.50
14	a	816	CLA	CHC-C1C	2.29	1.43	1.38
14	1	1642	CLA	MG-NB	-2.29	2.01	2.05
14	A	807	CLA	CMB-C2B	-2.29	1.46	1.50
14	1	1614	CLA	MG-NB	-2.29	2.01	2.05
14	j	1301	CLA	CMD-C2D	-2.29	1.46	1.50
14	1	1631	CLA	C1B-C2B	2.28	1.48	1.43
14	A	803	CLA	C1B-C2B	2.28	1.48	1.43
14	a	830	CLA	C1B-C2B	2.28	1.48	1.43
14	f	201	CLA	C1B-C2B	2.28	1.48	1.43
14	a	844	CLA	MG-NB	-2.28	2.01	2.05
14	b	840	CLA	MG-NB	-2.28	2.01	2.05
14	1	1638	CLA	MG-NB	-2.28	2.01	2.05
14	1	1604	CLA	C1B-C2B	2.28	1.48	1.43
14	A	823	CLA	CMD-C2D	-2.28	1.46	1.50
14	L	203	CLA	CMB-C2B	-2.28	1.46	1.50
14	1	1627	CLA	CMB-C2B	-2.28	1.46	1.50
14	A	841	CLA	MG-NB	-2.28	2.01	2.05
14	f	201	CLA	MG-NB	-2.28	2.01	2.05
14	B	836	CLA	CMB-C2B	-2.28	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	1639	CLA	MG-NB	-2.28	2.01	2.05
14	2	835	CLA	MG-NB	-2.28	2.01	2.05
14	2	811	CLA	C1B-C2B	2.28	1.48	1.43
14	B	832	CLA	CMD-C2D	-2.28	1.46	1.50
14	A	820	CLA	CMB-C2B	-2.28	1.46	1.50
14	A	840	CLA	CMB-C2B	-2.28	1.46	1.50
14	F	201	CLA	MG-NB	-2.28	2.01	2.05
20	B	849	LMG	O6-C5	-2.28	1.38	1.44
14	a	804	CLA	CMB-C2B	-2.28	1.46	1.50
14	a	837	CLA	MG-NB	-2.28	2.01	2.05
14	1	1620	CLA	CMD-C2D	-2.28	1.46	1.50
14	a	814	CLA	MG-NB	-2.28	2.01	2.05
14	A	855	CLA	C1B-C2B	2.28	1.48	1.43
14	B	822	CLA	CMB-C2B	-2.28	1.46	1.50
14	a	834	CLA	MG-NB	-2.28	2.01	2.05
20	2	850	LMG	O6-C5	-2.28	1.38	1.44
20	2	850	LMG	O8-C9	-2.28	1.40	1.45
14	b	838	CLA	MG-NB	-2.28	2.01	2.05
14	b	828	CLA	CMD-C2D	-2.28	1.46	1.50
14	6	201	CLA	MG-NB	-2.28	2.01	2.05
14	1	1608	CLA	CMB-C2B	-2.28	1.46	1.50
14	1	1614	CLA	C1B-C2B	2.27	1.48	1.43
14	1	1624	CLA	MG-NB	-2.27	2.01	2.05
14	1	1626	CLA	CMD-C2D	-2.27	1.46	1.50
14	2	825	CLA	CMC-C2C	-2.27	1.46	1.50
14	2	838	CLA	CMC-C2C	-2.27	1.46	1.50
14	A	844	CLA	MG-NB	-2.27	2.01	2.05
14	1	1615	CLA	MG-NB	-2.27	2.01	2.05
14	A	812	CLA	CMD-C2D	-2.27	1.46	1.50
14	a	840	CLA	CMB-C2B	-2.27	1.46	1.50
14	a	802	CLA	CMB-C2B	-2.27	1.46	1.50
14	j	1301	CLA	CMC-C2C	-2.27	1.46	1.50
14	a	807	CLA	MG-NB	-2.27	2.01	2.05
14	b	805	CLA	MG-NB	-2.27	2.01	2.05
14	1	1645	CLA	MG-NB	-2.27	2.01	2.05
14	A	802	CLA	CMB-C2B	-2.27	1.46	1.50
14	B	839	CLA	MG-NB	-2.27	2.01	2.05
14	2	838	CLA	MG-NB	-2.27	2.01	2.05
14	2	804	CLA	C4B-NB	2.27	1.40	1.37
14	a	819	CLA	CMD-C2D	-2.27	1.46	1.50
14	a	807	CLA	C1B-NB	-2.27	1.35	1.37
14	B	840	CLA	C1B-C2B	2.27	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	838	CLA	C1B-C2B	2.27	1.48	1.43
14	l	204	CLA	CMC-C2C	-2.27	1.46	1.50
14	1	1623	CLA	MG-NB	-2.27	2.01	2.05
14	a	819	CLA	C1B-C2B	2.27	1.48	1.43
14	b	832	CLA	CMD-C2D	-2.27	1.46	1.50
14	2	834	CLA	MG-NB	-2.27	2.01	2.05
14	2	838	CLA	C1B-C2B	2.27	1.48	1.43
14	a	812	CLA	MG-NB	-2.27	2.01	2.05
14	k	101	CLA	CMD-C2D	-2.27	1.46	1.50
14	a	831	CLA	CMC-C2C	-2.27	1.46	1.50
14	a	803	CLA	C1B-C2B	2.27	1.48	1.43
14	B	807	CLA	CMB-C2B	-2.27	1.46	1.50
14	2	816	CLA	CMD-C2D	-2.27	1.46	1.50
14	A	820	CLA	C1B-NB	-2.27	1.35	1.37
13	A	801	CL0	C3B-C4B	2.27	1.48	1.42
13	a	801	CL0	C3B-C4B	2.27	1.48	1.42
14	B	818	CLA	C1B-C2B	2.27	1.48	1.43
14	A	810	CLA	MG-NB	-2.27	2.01	2.05
14	B	837	CLA	CMC-C2C	-2.27	1.46	1.50
14	B	839	CLA	CMB-C2B	-2.26	1.46	1.50
14	B	813	CLA	C1B-C2B	2.26	1.48	1.43
14	a	824	CLA	CMB-C2B	-2.26	1.46	1.50
14	b	838	CLA	CMC-C2C	-2.26	1.46	1.50
14	b	840	CLA	CMB-C2B	-2.26	1.46	1.50
14	1	1607	CLA	CMC-C2C	-2.26	1.46	1.50
14	A	825	CLA	CMD-C2D	-2.26	1.46	1.50
14	8	1301	CLA	CMC-C2C	-2.26	1.46	1.50
14	2	805	CLA	MG-NB	-2.26	2.01	2.05
14	A	819	CLA	CMD-C2D	-2.26	1.46	1.50
14	a	812	CLA	CMD-C2D	-2.26	1.46	1.50
14	a	813	CLA	C1B-C2B	2.26	1.48	1.43
14	b	806	CLA	CMD-C2D	-2.26	1.46	1.50
14	1	1612	CLA	CHC-C1C	2.26	1.43	1.38
14	A	812	CLA	MG-NB	-2.26	2.01	2.05
14	B	837	CLA	MG-NB	-2.26	2.01	2.05
14	b	806	CLA	MG-NB	-2.26	2.01	2.05
14	b	816	CLA	CMD-C2D	-2.26	1.46	1.50
14	A	838	CLA	MG-NB	-2.26	2.01	2.05
14	B	837	CLA	C1B-C2B	2.26	1.48	1.43
14	b	841	CLA	C1B-C2B	2.26	1.48	1.43
14	b	808	CLA	CMB-C2B	-2.26	1.46	1.50
14	2	808	CLA	CMB-C2B	-2.26	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	805	CLA	MG-NB	-2.26	2.01	2.05
14	B	816	CLA	MG-NB	-2.26	2.01	2.05
14	a	838	CLA	MG-NB	-2.26	2.01	2.05
14	B	805	CLA	CMD-C2D	-2.26	1.46	1.50
14	l	204	CLA	CMB-C2B	-2.26	1.46	1.50
14	b	817	CLA	MG-NB	-2.26	2.01	2.05
14	2	806	CLA	MG-NB	-2.26	2.01	2.05
14	2	832	CLA	CMD-C2D	-2.26	1.46	1.50
14	2	806	CLA	CMD-C2D	-2.26	1.46	1.50
14	A	822	CLA	C1B-C2B	2.26	1.48	1.43
14	2	836	CLA	CMD-C2D	-2.26	1.46	1.50
14	a	820	CLA	MG-NB	-2.26	2.01	2.05
14	2	840	CLA	MG-NB	-2.26	2.01	2.05
14	b	828	CLA	CMB-C2B	-2.26	1.46	1.50
14	1	1624	CLA	CMD-C2D	-2.26	1.46	1.50
14	1	1621	CLA	C1B-C2B	2.26	1.48	1.43
14	A	813	CLA	CMB-C2B	-2.26	1.46	1.50
14	0	207	CLA	CMC-C2C	-2.26	1.46	1.50
14	B	824	CLA	CMC-C2C	-2.26	1.46	1.50
14	b	828	CLA	MG-NB	-2.26	2.01	2.05
14	B	822	CLA	MG-NB	-2.25	2.01	2.05
14	2	823	CLA	MG-NB	-2.25	2.01	2.05
14	b	814	CLA	CMD-C2D	-2.25	1.46	1.50
14	0	205	CLA	CMC-C2C	-2.25	1.46	1.50
14	1	1617	CLA	CHC-C1C	2.25	1.43	1.38
14	A	833	CLA	CMC-C2C	-2.25	1.46	1.50
14	B	813	CLA	CMD-C2D	-2.25	1.46	1.50
14	B	835	CLA	CMD-C2D	-2.25	1.46	1.50
14	A	841	CLA	CMB-C2B	-2.25	1.46	1.50
14	a	824	CLA	CMD-C2D	-2.25	1.46	1.50
14	1	1603	CLA	CMB-C2B	-2.25	1.46	1.50
14	A	820	CLA	C1B-C2B	2.25	1.48	1.43
14	2	817	CLA	MG-NB	-2.25	2.01	2.05
14	A	824	CLA	CMD-C2D	-2.25	1.46	1.50
14	b	833	CLA	CMD-C2D	-2.25	1.46	1.50
14	B	809	CLA	C1B-NB	-2.25	1.35	1.37
14	6	201	CLA	C1B-C2B	2.25	1.48	1.43
14	B	804	CLA	MG-NB	-2.25	2.01	2.05
14	a	808	CLA	MG-NB	-2.25	2.01	2.05
14	B	831	CLA	CMD-C2D	-2.25	1.46	1.50
14	8	1301	CLA	CMD-C2D	-2.25	1.46	1.50
14	B	833	CLA	CMB-C2B	-2.25	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	0	205	CLA	CMB-C2B	-2.25	1.46	1.50
14	a	831	CLA	C1B-NB	-2.25	1.35	1.37
14	b	812	CLA	MG-NB	-2.25	2.01	2.05
14	b	834	CLA	MG-NB	-2.25	2.01	2.05
14	A	813	CLA	C1B-C2B	2.25	1.48	1.43
14	B	829	CLA	CMC-C2C	-2.25	1.46	1.50
14	1	1621	CLA	CMB-C2B	-2.25	1.46	1.50
14	B	810	CLA	MG-NB	-2.25	2.01	2.05
14	A	807	CLA	C1B-NB	-2.25	1.35	1.37
14	a	805	CLA	CMD-C2D	-2.25	1.46	1.50
14	1	1604	CLA	MG-NB	-2.25	2.01	2.05
14	1	1611	CLA	MG-NB	-2.25	2.01	2.05
14	a	834	CLA	CMC-C2C	-2.25	1.46	1.50
14	1	1605	CLA	CMB-C2B	-2.25	1.46	1.50
14	A	804	CLA	CMB-C2B	-2.25	1.46	1.50
17	2	849	BCR	C38-C26	-2.25	1.47	1.50
14	A	808	CLA	MG-NB	-2.25	2.01	2.05
14	l	204	CLA	CHC-C1C	2.25	1.43	1.38
14	a	820	CLA	C1B-C2B	2.25	1.48	1.43
14	A	855	CLA	CMB-C2B	-2.25	1.46	1.50
14	2	830	CLA	CMC-C2C	-2.25	1.46	1.50
14	A	811	CLA	CHC-C1C	2.25	1.43	1.38
14	b	836	CLA	MG-NB	-2.25	2.01	2.05
14	B	835	CLA	MG-NB	-2.24	2.01	2.05
14	K	101	CLA	CMD-C2D	-2.24	1.46	1.50
14	1	1623	CLA	C1B-C2B	2.24	1.48	1.43
14	B	827	CLA	MG-NB	-2.24	2.01	2.05
14	B	833	CLA	MG-NB	-2.24	2.01	2.05
14	A	838	CLA	C1B-NB	-2.24	1.35	1.37
14	1	1625	CLA	CMD-C2D	-2.24	1.46	1.50
14	9	101	CLA	CMD-C2D	-2.24	1.46	1.50
14	A	823	CLA	MG-NB	-2.24	2.01	2.05
14	b	802	CLA	C1B-C2B	2.24	1.48	1.43
14	B	822	CLA	CHC-C1C	2.24	1.43	1.38
14	a	840	CLA	C1B-C2B	2.24	1.48	1.43
14	1	1606	CLA	CMD-C2D	-2.24	1.46	1.50
14	F	201	CLA	C1B-C2B	2.24	1.48	1.43
14	B	811	CLA	MG-NB	-2.24	2.01	2.05
14	2	823	CLA	CHC-C1C	2.24	1.43	1.38
14	A	815	CLA	CMB-C2B	-2.24	1.46	1.50
14	1	1620	CLA	MG-NB	-2.24	2.01	2.05
14	1	1620	CLA	C1B-C2B	2.24	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	8	1303	CLA	CHC-C1C	2.24	1.43	1.38
14	a	820	CLA	CMB-C2B	-2.24	1.46	1.50
14	b	825	CLA	MG-NB	-2.24	2.01	2.05
14	F	203	CLA	CMC-C2C	-2.24	1.46	1.50
14	a	806	CLA	CMC-C2C	-2.24	1.46	1.50
14	1	1635	CLA	CMC-C2C	-2.24	1.46	1.50
14	a	815	CLA	CMB-C2B	-2.24	1.46	1.50
14	1	1636	CLA	CMB-C2B	-2.24	1.46	1.50
14	2	814	CLA	CMD-C2D	-2.24	1.46	1.50
14	l	206	CLA	CMC-C2C	-2.24	1.46	1.50
14	b	826	CLA	C1B-C2B	2.24	1.48	1.43
14	1	1608	CLA	C1B-NB	-2.24	1.35	1.37
14	1	1641	CLA	CMC-C2C	-2.24	1.46	1.50
14	b	814	CLA	C1B-C2B	2.23	1.48	1.43
14	A	835	CLA	MG-NB	-2.23	2.01	2.05
14	a	823	CLA	CMD-C2D	-2.23	1.46	1.50
14	A	840	CLA	C1B-C2B	2.23	1.48	1.43
14	2	814	CLA	C1B-C2B	2.23	1.48	1.43
14	b	825	CLA	CMC-C2C	-2.23	1.46	1.50
14	1	1616	CLA	CMB-C2B	-2.23	1.46	1.50
14	2	802	CLA	C1B-C2B	2.23	1.48	1.43
14	A	819	CLA	CMB-C2B	-2.23	1.46	1.50
14	b	830	CLA	CMC-C2C	-2.23	1.46	1.50
14	1	1642	CLA	CMB-C2B	-2.23	1.46	1.50
14	1	1610	CLA	C1B-C2B	2.23	1.48	1.43
14	a	830	CLA	MG-ND	-2.23	2.01	2.05
14	B	808	CLA	CMD-C2D	-2.23	1.46	1.50
14	2	834	CLA	CMB-C2B	-2.23	1.46	1.50
14	a	835	CLA	CMB-C2B	-2.23	1.46	1.50
14	L	203	CLA	CMC-C2C	-2.23	1.46	1.50
14	A	834	CLA	CMC-C2C	-2.23	1.46	1.50
14	F	203	CLA	CMD-C2D	-2.23	1.46	1.50
14	b	832	CLA	CMB-C2B	-2.23	1.46	1.50
14	1	1625	CLA	CMB-C2B	-2.23	1.46	1.50
14	B	824	CLA	MG-NB	-2.23	2.01	2.05
14	1	1609	CLA	CMC-C2C	-2.23	1.46	1.50
14	b	811	CLA	MG-NB	-2.23	2.01	2.05
14	A	805	CLA	CMD-C2D	-2.23	1.46	1.50
14	A	840	CLA	CMC-C2C	-2.23	1.46	1.50
14	A	830	CLA	MG-ND	-2.23	2.01	2.05
14	b	834	CLA	CMB-C2B	-2.23	1.46	1.50
14	A	803	CLA	MG-NB	-2.23	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	1613	CLA	MG-NB	-2.23	2.01	2.05
14	A	809	CLA	MG-NB	-2.23	2.01	2.05
14	A	819	CLA	MG-NB	-2.23	2.01	2.05
14	2	821	CLA	CMD-C2D	-2.23	1.46	1.50
14	1	1626	CLA	CMB-C2B	-2.23	1.46	1.50
14	b	821	CLA	CMD-C2D	-2.23	1.46	1.50
14	1	1632	CLA	C1B-NB	-2.23	1.35	1.37
14	a	835	CLA	MG-NB	-2.23	2.01	2.05
14	2	836	CLA	MG-NB	-2.23	2.01	2.05
14	a	822	CLA	C1B-C2B	2.23	1.48	1.43
14	a	819	CLA	MG-NB	-2.23	2.01	2.05
14	a	803	CLA	MG-NB	-2.22	2.01	2.05
14	2	811	CLA	MG-NB	-2.22	2.01	2.05
14	0	205	CLA	CHC-C1C	2.22	1.43	1.38
14	L	205	CLA	CMC-C2C	-2.22	1.46	1.50
14	b	814	CLA	CMB-C2B	-2.22	1.46	1.50
14	a	815	CLA	MG-NB	-2.22	2.01	2.05
14	B	835	CLA	CMB-C2B	-2.22	1.46	1.50
14	1	1631	CLA	MG-ND	-2.22	2.01	2.05
14	B	820	CLA	CMD-C2D	-2.22	1.46	1.50
14	2	840	CLA	CMB-C2B	-2.22	1.46	1.50
14	2	815	CLA	MG-NB	-2.22	2.01	2.05
14	b	802	CLA	CMB-C2B	-2.22	1.46	1.50
14	2	810	CLA	C1B-NB	-2.22	1.35	1.37
14	a	809	CLA	C1B-C2B	2.22	1.48	1.43
14	B	832	CLA	CMB-C2B	-2.22	1.46	1.50
14	a	813	CLA	CMB-C2B	-2.22	1.46	1.50
14	2	820	CLA	CMD-C2D	-2.22	1.46	1.50
14	a	810	CLA	MG-NB	-2.22	2.01	2.05
17	B	845	BCR	C38-C26	-2.22	1.47	1.50
14	A	806	CLA	CMC-C2C	-2.22	1.46	1.50
14	a	808	CLA	CMC-C2C	-2.22	1.46	1.50
14	A	844	CLA	CMB-C2B	-2.22	1.46	1.50
14	a	825	CLA	CMB-C2B	-2.22	1.46	1.50
14	b	802	CLA	CMD-C2D	-2.22	1.46	1.50
14	b	805	CLA	C1B-C2B	2.22	1.48	1.43
17	2	846	BCR	C38-C26	-2.22	1.47	1.50
14	2	832	CLA	CMB-C2B	-2.22	1.46	1.50
14	A	835	CLA	CMB-C2B	-2.22	1.46	1.50
14	2	802	CLA	CMD-C2D	-2.22	1.46	1.50
14	1	1639	CLA	C1B-NB	-2.22	1.35	1.37
14	A	834	CLA	CMB-C2B	-2.22	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	819	CLA	CMD-C2D	-2.22	1.46	1.50
14	2	826	CLA	C1B-C2B	2.22	1.48	1.43
14	1	1621	CLA	C1B-NB	-2.22	1.35	1.37
14	1	1641	CLA	C1B-C2B	2.22	1.48	1.43
14	B	813	CLA	CMB-C2B	-2.22	1.46	1.50
14	B	831	CLA	CMB-C2B	-2.22	1.46	1.50
14	2	824	CLA	CHC-C1C	2.22	1.43	1.38
14	2	805	CLA	C1B-C2B	2.21	1.48	1.43
14	A	819	CLA	C1B-C2B	2.21	1.48	1.43
14	A	809	CLA	C1B-C2B	2.21	1.48	1.43
17	l	202	BCR	C33-C5	-2.21	1.47	1.50
14	1	1616	CLA	MG-NB	-2.21	2.01	2.05
14	b	809	CLA	CMD-C2D	-2.21	1.46	1.50
14	2	836	CLA	CMB-C2B	-2.21	1.46	1.50
14	a	813	CLA	MG-NB	-2.21	2.01	2.05
14	2	812	CLA	MG-NB	-2.21	2.01	2.05
14	A	814	CLA	MG-NB	-2.21	2.01	2.05
14	b	823	CLA	CHC-C1C	2.21	1.43	1.38
17	0	203	BCR	C33-C5	-2.21	1.47	1.50
14	2	830	CLA	C3B-C4B	2.21	1.47	1.42
14	1	1634	CLA	CMC-C2C	-2.21	1.46	1.50
14	B	806	CLA	CMC-C2C	-2.21	1.46	1.50
14	b	841	CLA	CMC-C2C	-2.21	1.46	1.50
14	A	815	CLA	MG-NB	-2.21	2.01	2.05
17	B	848	BCR	C33-C5	-2.21	1.47	1.50
14	f	201	CLA	CMB-C2B	-2.21	1.46	1.50
14	a	809	CLA	MG-NB	-2.21	2.01	2.05
14	1	1609	CLA	MG-NB	-2.21	2.01	2.05
14	a	820	CLA	C1B-NB	-2.21	1.35	1.37
14	1	1621	CLA	MG-NB	-2.21	2.01	2.05
14	j	1303	CLA	CHC-C1C	2.21	1.43	1.38
14	2	809	CLA	CMD-C2D	-2.21	1.46	1.50
14	b	829	CLA	C1B-C2B	2.21	1.48	1.43
14	B	827	CLA	CMB-C2B	-2.21	1.46	1.50
14	B	804	CLA	C1B-C2B	2.20	1.48	1.43
14	1	1645	CLA	CMB-C2B	-2.20	1.46	1.50
14	b	815	CLA	MG-NB	-2.20	2.01	2.05
14	b	837	CLA	MG-NB	-2.20	2.01	2.05
14	2	804	CLA	CMB-C2B	-2.20	1.46	1.50
14	a	833	CLA	CMC-C2C	-2.20	1.46	1.50
14	A	824	CLA	CMB-C2B	-2.20	1.46	1.50
14	b	833	CLA	CMB-C2B	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	844	CLA	CMB-C2B	-2.20	1.46	1.50
14	B	825	CLA	C1B-C2B	2.20	1.48	1.43
14	A	808	CLA	CMC-C2C	-2.20	1.46	1.50
14	B	812	CLA	CMB-C2B	-2.20	1.46	1.50
14	a	812	CLA	CMB-C2B	-2.20	1.46	1.50
14	b	820	CLA	CMD-C2D	-2.20	1.46	1.50
14	X	1701	CLA	CMD-C2D	-2.20	1.46	1.50
14	b	811	CLA	CMB-C2B	-2.20	1.46	1.50
14	1	1636	CLA	MG-NB	-2.20	2.01	2.05
17	b	846	BCR	C38-C26	-2.20	1.47	1.50
14	A	855	CLA	CMD-C2D	-2.20	1.46	1.50
14	B	813	CLA	CMC-C2C	-2.20	1.46	1.50
14	F	201	CLA	CMB-C2B	-2.20	1.46	1.50
14	J	102	CLA	CHC-C1C	2.20	1.43	1.38
14	A	820	CLA	MG-NB	-2.20	2.01	2.05
14	b	807	CLA	CMC-C2C	-2.20	1.46	1.50
14	B	814	CLA	MG-NB	-2.20	2.01	2.05
14	b	808	CLA	CMC-C2C	-2.20	1.46	1.50
14	a	840	CLA	CMC-C2C	-2.20	1.46	1.50
14	2	812	CLA	CMD-C2D	-2.20	1.46	1.50
14	L	203	CLA	CHC-C1C	2.20	1.43	1.38
14	B	803	CLA	CMB-C2B	-2.20	1.46	1.50
14	b	817	CLA	CMD-C2D	-2.20	1.46	1.50
14	b	836	CLA	CMB-C2B	-2.20	1.46	1.50
14	2	828	CLA	CMB-C2B	-2.20	1.46	1.50
14	B	828	CLA	C1B-C2B	2.20	1.48	1.43
14	1	1635	CLA	CMB-C2B	-2.20	1.46	1.50
14	2	802	CLA	CMB-C2B	-2.20	1.46	1.50
14	b	830	CLA	C3B-C4B	2.20	1.47	1.42
14	B	816	CLA	CMD-C2D	-2.19	1.46	1.50
14	1	1607	CLA	C1B-C2B	2.19	1.48	1.43
14	6	201	CLA	CMB-C2B	-2.19	1.46	1.50
14	2	814	CLA	CMC-C2C	-2.19	1.46	1.50
14	A	813	CLA	MG-NB	-2.19	2.01	2.05
14	B	839	CLA	CHC-C1C	2.19	1.43	1.38
17	b	849	BCR	C33-C5	-2.19	1.47	1.50
14	b	804	CLA	CMB-C2B	-2.19	1.46	1.50
17	7	101	BCR	C38-C26	-2.19	1.47	1.50
14	9	101	CLA	MG-NB	-2.19	2.01	2.05
14	b	819	CLA	CMB-C2B	-2.19	1.46	1.50
14	2	833	CLA	CMB-C2B	-2.19	1.46	1.50
14	K	101	CLA	MG-NB	-2.19	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	1614	CLA	CMB-C2B	-2.19	1.46	1.50
14	B	808	CLA	MG-NB	-2.19	2.01	2.05
14	a	811	CLA	CHC-C1C	2.19	1.43	1.38
14	b	840	CLA	CHC-C1C	2.19	1.43	1.38
14	B	836	CLA	CMD-C2D	-2.19	1.46	1.50
14	1	1613	CLA	CMB-C2B	-2.19	1.46	1.50
17	2	849	BCR	C33-C5	-2.19	1.47	1.50
14	B	817	CLA	CMC-C2C	-2.19	1.46	1.50
14	2	816	CLA	CMB-C2B	-2.19	1.46	1.50
17	1	1649	BCR	C38-C26	-2.19	1.47	1.50
14	a	824	CLA	CMC-C2C	-2.19	1.46	1.50
14	8	1301	CLA	CHC-C1C	2.19	1.43	1.38
14	b	820	CLA	MG-NB	-2.19	2.01	2.05
14	b	817	CLA	CMB-C2B	-2.19	1.46	1.50
14	2	825	CLA	CMD-C2D	-2.19	1.46	1.50
14	1	1610	CLA	MG-NB	-2.19	2.01	2.05
14	a	834	CLA	C1B-NB	-2.19	1.35	1.37
14	A	825	CLA	CMB-C2B	-2.19	1.46	1.50
14	b	814	CLA	CMC-C2C	-2.19	1.46	1.50
14	B	807	CLA	CMC-C2C	-2.18	1.46	1.50
14	2	818	CLA	CMC-C2C	-2.18	1.46	1.50
14	F	203	CLA	CHC-C1C	2.18	1.43	1.38
14	b	810	CLA	C1B-C2B	2.18	1.48	1.43
14	B	810	CLA	CMB-C2B	-2.18	1.46	1.50
14	b	824	CLA	CHC-C1C	2.18	1.43	1.38
14	a	825	CLA	CMC-C2C	-2.18	1.46	1.50
14	2	813	CLA	CMD-C2D	-2.18	1.46	1.50
14	B	809	CLA	C1B-C2B	2.18	1.48	1.43
14	B	817	CLA	MG-NB	-2.18	2.01	2.05
14	B	811	CLA	CMD-C2D	-2.18	1.46	1.50
14	B	815	CLA	CMB-C2B	-2.18	1.46	1.50
14	a	811	CLA	CMD-C2D	-2.18	1.46	1.50
14	A	812	CLA	CMC-C2C	-2.18	1.46	1.50
14	A	806	CLA	C1B-C2B	2.18	1.48	1.43
14	1	1612	CLA	CMD-C2D	-2.18	1.46	1.50
14	2	814	CLA	CMB-C2B	-2.18	1.46	1.50
14	2	841	CLA	CMC-C2C	-2.18	1.46	1.50
14	B	832	CLA	MG-NB	-2.18	2.01	2.05
14	B	816	CLA	CMB-C2B	-2.18	1.46	1.50
14	2	817	CLA	CMB-C2B	-2.18	1.46	1.50
14	2	831	CLA	CMD-C2D	-2.18	1.46	1.50
14	a	838	CLA	CMB-C2B	-2.18	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	825	CLA	CMD-C2D	-2.18	1.46	1.50
14	a	843	CLA	MG-ND	-2.18	2.01	2.05
14	2	820	CLA	MG-NB	-2.18	2.01	2.05
14	A	828	CLA	CMC-C2C	-2.18	1.46	1.50
14	1	1625	CLA	CMC-C2C	-2.18	1.46	1.50
14	1	1629	CLA	CMB-C2B	-2.18	1.46	1.50
14	1	1636	CLA	CMC-C2C	-2.18	1.46	1.50
17	M	103	BCR	C33-C5	-2.17	1.47	1.50
14	A	828	CLA	CMB-C2B	-2.17	1.46	1.50
14	a	834	CLA	CMB-C2B	-2.17	1.46	1.50
14	X	1701	CLA	MG-NB	-2.17	2.01	2.05
14	2	833	CLA	MG-NB	-2.17	2.01	2.05
14	k	103	CLA	CHC-C1C	2.17	1.42	1.38
14	b	813	CLA	MG-NB	-2.17	2.01	2.05
14	A	825	CLA	CMC-C2C	-2.17	1.46	1.50
14	b	812	CLA	CMD-C2D	-2.17	1.46	1.50
14	2	819	CLA	CMB-C2B	-2.17	1.46	1.50
14	2	825	CLA	MG-NB	-2.17	2.01	2.05
14	a	835	CLA	CMC-C2C	-2.17	1.46	1.50
14	A	831	CLA	C1B-NB	-2.17	1.35	1.37
14	1	1617	CLA	MG-NB	-2.17	2.01	2.05
14	B	823	CLA	CHC-C1C	2.17	1.42	1.38
14	B	820	CLA	CMB-C2B	-2.17	1.46	1.50
14	a	828	CLA	CMB-C2B	-2.17	1.46	1.50
14	A	835	CLA	CMC-C2C	-2.17	1.46	1.50
14	2	808	CLA	CMC-C2C	-2.17	1.46	1.50
14	2	811	CLA	CMB-C2B	-2.17	1.46	1.50
14	b	833	CLA	MG-NB	-2.17	2.01	2.05
14	F	201	CLA	CHC-C1C	2.17	1.42	1.38
14	a	814	CLA	CMB-C2B	-2.17	1.46	1.50
14	2	837	CLA	MG-NB	-2.17	2.01	2.05
14	1	1619	CLA	CHC-C1C	2.17	1.42	1.38
14	B	829	CLA	C3B-C4B	2.17	1.47	1.42
17	L	206	BCR	C38-C26	-2.17	1.47	1.50
14	b	813	CLA	CMD-C2D	-2.17	1.46	1.50
14	b	831	CLA	CMD-C2D	-2.17	1.46	1.50
14	1	1620	CLA	CMC-C2C	-2.17	1.46	1.50
14	j	1303	CLA	CBD-CAD	2.17	1.56	1.51
14	A	819	CLA	CMC-C2C	-2.17	1.46	1.50
14	2	807	CLA	CMC-C2C	-2.17	1.46	1.50
14	a	808	CLA	CMD-C2D	-2.17	1.46	1.50
17	l	207	BCR	C38-C26	-2.17	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	806	CLA	C1B-C2B	2.17	1.48	1.43
14	x	1701	CLA	CMD-C2D	-2.17	1.46	1.50
14	1	1613	CLA	CMC-C2C	-2.17	1.46	1.50
14	1	1615	CLA	CMB-C2B	-2.17	1.46	1.50
14	A	802	CLA	CHC-C1C	2.17	1.42	1.38
14	2	810	CLA	C1B-C2B	2.17	1.48	1.43
14	z	102	CLA	CMD-C2D	-2.17	1.46	1.50
14	A	839	CLA	CMC-C2C	-2.16	1.46	1.50
14	j	1301	CLA	CHC-C1C	2.16	1.42	1.38
14	A	832	CLA	CMC-C2C	-2.16	1.46	1.50
14	B	820	CLA	CHC-C1C	2.16	1.42	1.38
14	B	824	CLA	CMD-C2D	-2.16	1.46	1.50
14	1	1637	CLA	CMD-C2D	-2.16	1.46	1.50
14	A	804	CLA	CMC-C2C	-2.16	1.46	1.50
14	B	808	CLA	CMB-C2B	-2.16	1.46	1.50
14	1	1640	CLA	CMC-C2C	-2.16	1.46	1.50
14	9	103	CLA	CHC-C1C	2.16	1.42	1.38
14	A	812	CLA	CMB-C2B	-2.16	1.46	1.50
14	B	836	CLA	MG-NB	-2.16	2.01	2.05
14	a	812	CLA	CMC-C2C	-2.16	1.46	1.50
14	a	819	CLA	CMC-C2C	-2.16	1.46	1.50
14	f	201	CLA	CHC-C1C	2.16	1.42	1.38
14	z	102	CLA	MG-NB	-2.16	2.01	2.05
14	1	1618	CLA	CHC-C1C	2.16	1.42	1.38
14	1	1629	CLA	CMC-C2C	-2.16	1.46	1.50
14	2	829	CLA	C1B-C2B	2.16	1.48	1.43
14	K	103	CLA	CHC-C1C	2.16	1.42	1.38
14	1	1645	CLA	CMC-C2C	-2.16	1.46	1.50
14	B	812	CLA	MG-NB	-2.16	2.01	2.05
14	1	1626	CLA	CMC-C2C	-2.16	1.46	1.50
14	2	817	CLA	CMD-C2D	-2.16	1.46	1.50
14	A	833	CLA	MG-ND	-2.16	2.01	2.05
14	a	818	CLA	MG-NB	-2.16	2.01	2.05
14	k	101	CLA	MG-NB	-2.16	2.01	2.05
14	8	1303	CLA	CBD-CAD	2.16	1.56	1.51
14	2	819	CLA	CMC-C2C	-2.16	1.46	1.50
14	a	827	CLA	C1B-NB	-2.16	1.35	1.37
14	1	1619	CLA	MG-NB	-2.16	2.01	2.05
14	a	844	CLA	CMC-C2C	-2.16	1.46	1.50
14	A	806	CLA	C1B-NB	-2.16	1.35	1.37
14	2	821	CLA	CMB-C2B	-2.16	1.46	1.50
14	L	205	CLA	C1B-C2B	2.16	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	F	202	BCR	C38-C26	-2.16	1.47	1.50
13	a	801	CL0	MG-ND	-2.16	2.01	2.05
14	b	809	CLA	MG-NB	-2.16	2.01	2.05
14	1	1605	CLA	CMC-C2C	-2.16	1.46	1.50
14	a	806	CLA	C1B-NB	-2.16	1.35	1.37
14	2	821	CLA	CHC-C1C	2.16	1.42	1.38
14	A	811	CLA	CMD-C2D	-2.16	1.46	1.50
14	l	206	CLA	C1B-C2B	2.15	1.48	1.43
14	a	807	CLA	CMC-C2C	-2.15	1.46	1.50
14	B	840	CLA	CMC-C2C	-2.15	1.46	1.50
14	A	817	CLA	CHC-C1C	2.15	1.42	1.38
14	A	808	CLA	CMB-C2B	-2.15	1.46	1.50
14	1	1606	CLA	CMB-C2B	-2.15	1.46	1.50
18	y	101	LHG	P-O6	2.15	1.68	1.59
14	A	836	CLA	CMD-C2D	-2.15	1.46	1.50
14	a	836	CLA	CMD-C2D	-2.15	1.46	1.50
14	b	821	CLA	CMB-C2B	-2.15	1.46	1.50
14	2	840	CLA	CHC-C1C	2.15	1.42	1.38
14	1	1634	CLA	C1B-NB	-2.15	1.35	1.37
14	B	819	CLA	MG-NB	-2.15	2.01	2.05
14	a	842	CLA	C1B-C2B	2.15	1.48	1.43
14	B	830	CLA	CMD-C2D	-2.15	1.46	1.50
17	L	201	BCR	C33-C5	-2.15	1.47	1.50
14	B	802	CLA	C3B-C4B	2.15	1.47	1.42
14	B	818	CLA	CMC-C2C	-2.15	1.46	1.50
14	a	810	CLA	CMC-C2C	-2.15	1.46	1.50
14	b	816	CLA	CMB-C2B	-2.15	1.46	1.50
14	b	821	CLA	CHC-C1C	2.15	1.42	1.38
14	a	804	CLA	CMC-C2C	-2.15	1.46	1.50
14	A	818	CLA	CHC-C1C	2.15	1.42	1.38
14	A	833	CLA	C1B-NB	-2.15	1.35	1.37
14	b	824	CLA	CMD-C2D	-2.15	1.46	1.50
14	a	829	CLA	MG-NB	-2.15	2.01	2.05
14	2	824	CLA	CMB-C2B	-2.15	1.46	1.50
14	a	828	CLA	CMC-C2C	-2.15	1.46	1.50
14	a	841	CLA	CMC-C2C	-2.15	1.46	1.50
14	b	803	CLA	C3B-C4B	2.15	1.47	1.42
14	2	840	CLA	C1B-C2B	2.15	1.48	1.43
14	A	841	CLA	CMC-C2C	-2.15	1.46	1.50
14	8	1303	CLA	CMD-C2D	-2.15	1.46	1.50
14	J	102	CLA	CBD-CAD	2.15	1.56	1.51
14	b	818	CLA	MG-NB	-2.15	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	1632	CLA	MG-ND	-2.15	2.01	2.05
14	B	812	CLA	CMD-C2D	-2.15	1.46	1.50
14	b	840	CLA	C1B-C2B	2.15	1.48	1.43
14	0	207	CLA	C1B-C2B	2.14	1.48	1.43
14	A	838	CLA	CMB-C2B	-2.14	1.46	1.50
14	1	1642	CLA	CMC-C2C	-2.14	1.46	1.50
14	A	813	CLA	CMC-C2C	-2.14	1.46	1.50
14	a	817	CLA	CHC-C1C	2.14	1.42	1.38
14	6	201	CLA	CHC-C1C	2.14	1.42	1.38
14	j	1303	CLA	CMD-C2D	-2.14	1.46	1.50
14	k	101	CLA	CMB-C2B	-2.14	1.46	1.50
14	1	1639	CLA	CMB-C2B	-2.14	1.46	1.50
14	2	813	CLA	CMB-C2B	-2.14	1.46	1.50
14	1	1643	CLA	C1B-C2B	2.14	1.48	1.43
14	2	803	CLA	C3B-C4B	2.14	1.47	1.42
14	2	827	CLA	CMC-C2C	-2.14	1.46	1.50
14	1	1603	CLA	C1B-C2B	2.14	1.48	1.43
14	A	814	CLA	CMB-C2B	-2.14	1.46	1.50
14	a	805	CLA	CMB-C2B	-2.14	1.46	1.50
14	B	824	CLA	CMB-C2B	-2.14	1.46	1.50
14	b	813	CLA	CMB-C2B	-2.14	1.46	1.50
14	K	103	CLA	MG-NB	-2.14	2.01	2.05
14	b	809	CLA	CMB-C2B	-2.14	1.46	1.50
14	b	818	CLA	CMC-C2C	-2.14	1.46	1.50
18	M	101	LHG	P-O6	2.14	1.68	1.59
17	i	101	BCR	C38-C26	-2.14	1.47	1.50
14	2	829	CLA	CMC-C2C	-2.14	1.46	1.50
14	a	837	CLA	CMD-C2D	-2.14	1.46	1.50
17	f	202	BCR	C38-C26	-2.14	1.47	1.50
14	A	818	CLA	MG-NB	-2.14	2.01	2.05
14	2	818	CLA	MG-NB	-2.14	2.01	2.05
14	a	839	CLA	CMC-C2C	-2.14	1.46	1.50
18	m	101	LHG	P-O6	2.14	1.67	1.59
14	A	802	CLA	C1B-C2B	2.14	1.48	1.43
14	B	812	CLA	CMC-C2C	-2.13	1.46	1.50
14	2	837	CLA	CMD-C2D	-2.13	1.46	1.50
17	l	202	BCR	C38-C26	-2.13	1.47	1.50
14	B	821	CLA	CMD-C2D	-2.13	1.46	1.50
14	2	830	CLA	CAC-C3C	-2.13	1.45	1.51
14	A	837	CLA	CHC-C1C	2.13	1.42	1.38
14	B	839	CLA	C1B-C2B	2.13	1.48	1.43
14	A	805	CLA	CMB-C2B	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	810	CLA	CMC-C2C	-2.13	1.46	1.50
14	b	837	CLA	CMD-C2D	-2.13	1.46	1.50
14	2	827	CLA	CMB-C2B	-2.13	1.46	1.50
14	1	1614	CLA	CMC-C2C	-2.13	1.46	1.50
17	y	102	BCR	C33-C5	-2.13	1.47	1.50
14	b	818	CLA	CMD-C2D	-2.13	1.46	1.50
14	b	827	CLA	CMB-C2B	-2.13	1.46	1.50
14	A	805	CLA	CMC-C2C	-2.13	1.46	1.50
13	A	801	CL0	CMC-C2C	-2.13	1.46	1.50
14	2	813	CLA	MG-NB	-2.13	2.01	2.05
14	1	1609	CLA	CMD-C2D	-2.13	1.46	1.50
14	A	830	CLA	CMC-C2C	-2.13	1.46	1.50
14	b	813	CLA	CMC-C2C	-2.13	1.46	1.50
14	2	809	CLA	MG-NB	-2.13	2.01	2.05
14	a	818	CLA	CHC-C1C	2.13	1.42	1.38
14	1	1638	CLA	CHC-C1C	2.13	1.42	1.38
14	A	824	CLA	CMC-C2C	-2.13	1.46	1.50
14	A	843	CLA	MG-ND	-2.13	2.01	2.05
14	A	827	CLA	C1B-NB	-2.13	1.35	1.37
14	a	833	CLA	C1B-NB	-2.13	1.35	1.37
14	L	204	CLA	MG-ND	-2.13	2.01	2.05
14	k	103	CLA	MG-NB	-2.13	2.01	2.05
14	b	833	CLA	CMC-C2C	-2.13	1.46	1.50
14	1	1611	CLA	CMC-C2C	-2.13	1.46	1.50
14	2	836	CLA	CMC-C2C	-2.13	1.46	1.50
17	I	101	BCR	C38-C26	-2.13	1.47	1.50
17	6	202	BCR	C38-C26	-2.13	1.47	1.50
14	A	833	CLA	C1B-C2B	2.13	1.48	1.43
14	a	831	CLA	MG-ND	-2.13	2.01	2.05
14	x	1701	CLA	MG-NB	-2.13	2.01	2.05
14	A	817	CLA	CMD-C2D	-2.13	1.46	1.50
14	a	832	CLA	CMC-C2C	-2.13	1.46	1.50
14	B	829	CLA	CAC-C3C	-2.13	1.45	1.51
14	2	809	CLA	CMB-C2B	-2.13	1.46	1.50
14	a	816	CLA	MG-NB	-2.13	2.01	2.05
14	1	1612	CLA	MG-NB	-2.13	2.01	2.05
14	A	832	CLA	MG-ND	-2.13	2.01	2.05
14	b	822	CLA	CMD-C2D	-2.13	1.46	1.50
17	2	848	BCR	C38-C26	-2.12	1.47	1.50
14	B	835	CLA	CHC-C1C	2.12	1.42	1.38
14	j	1302	CLA	CHC-C1C	2.12	1.42	1.38
14	A	816	CLA	MG-NB	-2.12	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	808	CLA	CMD-C2D	-2.12	1.46	1.50
14	1	1630	CLA	MG-NB	-2.12	2.01	2.05
14	b	824	CLA	CMB-C2B	-2.12	1.46	1.50
14	A	842	CLA	C1B-C2B	2.12	1.48	1.43
14	1	1626	CLA	C1B-C2B	2.12	1.48	1.43
14	b	838	CLA	CHC-C1C	2.12	1.42	1.38
14	A	827	CLA	CMC-C2C	-2.12	1.46	1.50
14	1	1633	CLA	MG-ND	-2.12	2.01	2.05
14	b	830	CLA	CAC-C3C	-2.12	1.45	1.51
14	b	836	CLA	CHC-C1C	2.12	1.42	1.38
14	2	818	CLA	CMD-C2D	-2.12	1.46	1.50
14	a	802	CLA	CHC-C1C	2.12	1.42	1.38
14	J	102	CLA	CMD-C2D	-2.12	1.46	1.50
14	B	826	CLA	CMC-C2C	-2.12	1.46	1.50
14	1	1634	CLA	C1B-C2B	2.12	1.48	1.43
14	A	844	CLA	CMC-C2C	-2.12	1.46	1.50
14	9	101	CLA	CMB-C2B	-2.12	1.46	1.50
14	a	811	CLA	MG-NB	-2.12	2.01	2.05
14	b	803	CLA	MG-ND	-2.12	2.01	2.05
14	B	828	CLA	CMC-C2C	-2.12	1.46	1.50
14	1	1632	CLA	C1B-C2B	2.12	1.48	1.43
14	1	1606	CLA	CMC-C2C	-2.12	1.46	1.50
17	A	848	BCR	C38-C26	-2.12	1.47	1.50
14	B	817	CLA	CMD-C2D	-2.12	1.46	1.50
14	1	1603	CLA	CHC-C1C	2.12	1.42	1.38
14	9	103	CLA	MG-NB	-2.12	2.01	2.05
14	A	828	CLA	CHC-C1C	2.12	1.42	1.38
14	A	837	CLA	CMD-C2D	-2.12	1.46	1.50
14	a	808	CLA	CMB-C2B	-2.12	1.46	1.50
14	1	1618	CLA	CMD-C2D	-2.12	1.46	1.50
14	B	818	CLA	CMB-C2B	-2.11	1.46	1.50
14	b	819	CLA	CMC-C2C	-2.11	1.46	1.50
14	1	1608	CLA	CMC-C2C	-2.11	1.46	1.50
14	A	831	CLA	MG-ND	-2.11	2.01	2.05
17	b	845	BCR	C38-C26	-2.11	1.47	1.50
14	A	829	CLA	MG-NB	-2.11	2.01	2.05
14	a	802	CLA	C1B-C2B	2.11	1.48	1.43
14	1	1607	CLA	C1B-NB	-2.11	1.35	1.37
17	b	848	BCR	C38-C26	-2.11	1.47	1.50
14	a	830	CLA	CMB-C2B	-2.11	1.46	1.50
14	1	1631	CLA	CMB-C2B	-2.11	1.46	1.50
17	B	844	BCR	C38-C26	-2.11	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	m	102	BCR	C33-C5	-2.11	1.47	1.50
14	a	832	CLA	MG-ND	-2.11	2.01	2.05
14	2	805	CLA	CHC-C1C	2.11	1.42	1.38
14	B	823	CLA	CMB-C2B	-2.11	1.46	1.50
14	2	836	CLA	CHC-C1C	2.11	1.42	1.38
14	b	828	CLA	C1B-NB	-2.11	1.35	1.37
14	A	826	CLA	CMC-C2C	-2.11	1.46	1.50
14	B	823	CLA	CMD-C2D	-2.11	1.46	1.50
14	a	830	CLA	CMC-C2C	-2.11	1.46	1.50
14	B	802	CLA	MG-ND	-2.11	2.01	2.05
14	0	207	CLA	MG-ND	-2.11	2.01	2.05
14	A	832	CLA	C1B-C2B	2.11	1.48	1.43
14	B	821	CLA	MG-NB	-2.11	2.01	2.05
14	1	1634	CLA	MG-ND	-2.11	2.01	2.05
14	1	1644	CLA	MG-ND	-2.11	2.01	2.05
14	1	1624	CLA	CMB-C2B	-2.11	1.46	1.50
14	A	844	CLA	CMD-C2D	-2.11	1.46	1.50
14	1	1616	CLA	CHC-C1C	2.11	1.42	1.38
14	b	836	CLA	CMC-C2C	-2.11	1.46	1.50
14	A	815	CLA	CMD-C2D	-2.11	1.46	1.50
14	A	832	CLA	C1B-NB	-2.11	1.35	1.37
14	a	832	CLA	C1B-C2B	2.11	1.48	1.43
14	F	203	CLA	CMB-C2B	-2.11	1.46	1.50
14	B	823	CLA	MG-NB	-2.11	2.01	2.05
14	b	822	CLA	MG-NB	-2.11	2.01	2.05
14	a	831	CLA	C1B-C2B	2.11	1.48	1.43
14	A	830	CLA	CMB-C2B	-2.11	1.46	1.50
14	b	816	CLA	CMC-C2C	-2.11	1.46	1.50
14	2	833	CLA	CMC-C2C	-2.11	1.46	1.50
13	A	801	CL0	MG-ND	-2.11	2.01	2.05
14	B	830	CLA	CMC-C2C	-2.11	1.46	1.50
14	1	1628	CLA	CMC-C2C	-2.11	1.46	1.50
14	2	825	CLA	CMB-C2B	-2.11	1.46	1.50
14	B	813	CLA	CHC-C1C	2.11	1.42	1.38
14	2	824	CLA	CMD-C2D	-2.11	1.46	1.50
14	a	828	CLA	CHC-C1C	2.11	1.42	1.38
14	a	805	CLA	CMC-C2C	-2.11	1.46	1.50
14	1	1612	CLA	CMC-C2C	-2.11	1.46	1.50
14	9	101	CLA	CMC-C2C	-2.11	1.46	1.50
14	8	1302	CLA	CHC-C1C	2.11	1.42	1.38
17	L	201	BCR	C38-C26	-2.10	1.47	1.50
14	b	820	CLA	CHC-C1C	2.10	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	838	CLA	CHC-C1C	2.10	1.42	1.38
14	K	101	CLA	CMB-C2B	-2.10	1.46	1.50
14	A	813	CLA	CHC-C1C	2.10	1.42	1.38
14	a	823	CLA	CMB-C2B	-2.10	1.46	1.50
14	B	827	CLA	CHC-C1C	2.10	1.42	1.38
17	a	850	BCR	C38-C26	-2.10	1.47	1.50
17	2	845	BCR	C38-C26	-2.10	1.47	1.50
17	0	208	BCR	C38-C26	-2.10	1.47	1.50
14	1	1633	CLA	CMC-C2C	-2.10	1.46	1.50
14	1	1638	CLA	CMD-C2D	-2.10	1.46	1.50
14	a	833	CLA	C1B-C2B	2.10	1.48	1.43
14	8	1302	CLA	MG-NB	-2.10	2.01	2.05
14	B	835	CLA	CMC-C2C	-2.10	1.46	1.50
14	1	1627	CLA	CMC-C2C	-2.10	1.46	1.50
17	B	847	BCR	C38-C26	-2.10	1.47	1.50
17	a	848	BCR	C38-C26	-2.10	1.47	1.50
14	B	826	CLA	CMB-C2B	-2.10	1.46	1.50
14	2	822	CLA	MG-NB	-2.10	2.01	2.05
14	b	835	CLA	CHC-C1C	2.10	1.42	1.38
14	2	803	CLA	MG-ND	-2.10	2.01	2.05
14	B	837	CLA	CHC-C1C	2.10	1.42	1.38
14	A	821	CLA	CMD-C2D	-2.10	1.46	1.50
14	1	1631	CLA	CMC-C2C	-2.10	1.46	1.50
14	A	831	CLA	C1B-C2B	2.10	1.48	1.43
14	2	822	CLA	CMD-C2D	-2.10	1.46	1.50
14	A	834	CLA	C1B-NB	-2.10	1.35	1.37
14	A	811	CLA	MG-NB	-2.10	2.01	2.05
14	2	835	CLA	CHC-C1C	2.10	1.42	1.38
14	B	815	CLA	CMC-C2C	-2.10	1.46	1.50
14	a	826	CLA	CMC-C2C	-2.10	1.46	1.50
14	L	205	CLA	MG-ND	-2.10	2.01	2.05
14	1	1627	CLA	MG-ND	-2.10	2.01	2.05
14	a	837	CLA	CHC-C1C	2.10	1.42	1.38
14	2	828	CLA	CHC-C1C	2.10	1.42	1.38
17	1	1651	BCR	C38-C26	-2.10	1.47	1.50
17	0	209	BCR	C38-C26	-2.10	1.47	1.50
14	a	813	CLA	CMC-C2C	-2.09	1.46	1.50
14	2	816	CLA	CMC-C2C	-2.09	1.46	1.50
14	a	815	CLA	CMD-C2D	-2.09	1.46	1.50
17	0	203	BCR	C38-C26	-2.09	1.47	1.50
14	B	832	CLA	CMC-C2C	-2.09	1.46	1.50
14	b	829	CLA	CMC-C2C	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	1	1602	CL0	MG-ND	-2.09	2.01	2.05
14	A	811	CLA	CMC-C2C	-2.09	1.46	1.50
14	a	822	CLA	CMC-C2C	-2.09	1.46	1.50
14	b	831	CLA	CMC-C2C	-2.09	1.46	1.50
14	b	824	CLA	MG-NB	-2.09	2.01	2.05
14	A	823	CLA	CMB-C2B	-2.09	1.46	1.50
14	b	825	CLA	CMB-C2B	-2.09	1.46	1.50
14	2	815	CLA	CHC-C1C	2.09	1.42	1.38
14	B	839	CLA	CMC-C2C	-2.09	1.46	1.50
14	a	827	CLA	CMC-C2C	-2.09	1.46	1.50
14	1	1645	CLA	CMD-C2D	-2.09	1.46	1.50
17	L	207	BCR	C38-C26	-2.09	1.47	1.50
14	A	815	CLA	CHC-C1C	2.09	1.42	1.38
14	K	101	CLA	CMC-C2C	-2.09	1.46	1.50
14	1	1609	CLA	CMB-C2B	-2.09	1.46	1.50
14	1	1603	CLA	C1B-NB	-2.09	1.35	1.37
14	1	1633	CLA	C1B-C2B	2.09	1.48	1.43
14	2	820	CLA	CHC-C1C	2.09	1.42	1.38
14	J	102	CLA	CMC-C2C	-2.09	1.46	1.50
14	K	103	CLA	CMC-C2C	-2.09	1.46	1.50
17	0	201	BCR	C38-C26	-2.09	1.47	1.50
14	b	814	CLA	CHC-C1C	2.09	1.42	1.38
14	b	815	CLA	CHC-C1C	2.09	1.42	1.38
14	k	101	CLA	CMC-C2C	-2.09	1.46	1.50
14	2	831	CLA	CMC-C2C	-2.09	1.46	1.50
14	A	807	CLA	CMC-C2C	-2.08	1.46	1.50
14	a	813	CLA	CHC-C1C	2.08	1.42	1.38
14	b	805	CLA	CHC-C1C	2.08	1.42	1.38
14	J	101	CLA	CHC-C1C	2.08	1.42	1.38
14	2	813	CLA	CMC-C2C	-2.08	1.46	1.50
14	A	825	CLA	C1B-C2B	2.08	1.48	1.43
14	A	814	CLA	CMD-C2D	-2.08	1.46	1.50
14	1	1609	CLA	CHC-C1C	2.08	1.42	1.38
14	l	206	CLA	MG-ND	-2.08	2.01	2.05
14	2	824	CLA	MG-NB	-2.08	2.01	2.05
14	0	207	CLA	C1B-NB	-2.08	1.35	1.37
14	j	1303	CLA	CMC-C2C	-2.08	1.46	1.50
14	a	816	CLA	CMC-C2C	-2.08	1.46	1.50
14	a	817	CLA	CMD-C2D	-2.08	1.46	1.50
14	a	815	CLA	CHC-C1C	2.08	1.42	1.38
14	a	821	CLA	CMD-C2D	-2.08	1.46	1.50
14	a	844	CLA	CMD-C2D	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	1610	CLA	CMC-C2C	-2.08	1.46	1.50
14	b	830	CLA	MG-ND	-2.08	2.01	2.05
14	1	1614	CLA	CHC-C1C	2.08	1.42	1.38
14	a	833	CLA	MG-ND	-2.08	2.01	2.05
14	1	1626	CLA	CHC-C1C	2.08	1.42	1.38
14	B	838	CLA	CMC-C2C	-2.08	1.46	1.50
14	l	205	CLA	MG-ND	-2.08	2.01	2.05
14	k	103	CLA	CMC-C2C	-2.08	1.46	1.50
14	b	802	CLA	C1B-NB	-2.07	1.35	1.37
14	1	1623	CLA	CMC-C2C	-2.07	1.46	1.50
14	j	1301	CLA	CMB-C2B	-2.07	1.46	1.50
14	a	825	CLA	CHC-C1C	2.07	1.42	1.38
14	a	834	CLA	C1B-C2B	2.07	1.48	1.43
14	j	1302	CLA	MG-NB	-2.07	2.01	2.05
14	j	1302	CLA	CMB-C2B	-2.07	1.46	1.50
14	a	825	CLA	C1B-C2B	2.07	1.48	1.43
14	a	826	CLA	MG-ND	-2.07	2.01	2.05
14	2	811	CLA	MG-ND	-2.07	2.01	2.05
13	1	1602	CL0	CMC-C2C	-2.07	1.46	1.50
14	2	840	CLA	CMC-C2C	-2.07	1.46	1.50
17	j	1304	BCR	C38-C26	-2.07	1.47	1.50
14	b	826	CLA	CHC-C1C	2.07	1.42	1.38
14	b	828	CLA	CHC-C1C	2.07	1.42	1.38
14	J	101	CLA	CMB-C2B	-2.07	1.46	1.50
14	A	817	CLA	MG-NB	-2.07	2.01	2.05
14	1	1616	CLA	CMD-C2D	-2.07	1.46	1.50
14	B	825	CLA	CHC-C1C	2.07	1.42	1.38
14	8	1302	CLA	CMB-C2B	-2.07	1.46	1.50
14	0	206	CLA	MG-ND	-2.07	2.01	2.05
14	L	204	CLA	C1B-C2B	2.07	1.48	1.43
14	A	834	CLA	C1B-C2B	2.07	1.48	1.43
17	B	846	BCR	C38-C26	-2.07	1.47	1.50
14	l	205	CLA	C1B-C2B	2.07	1.48	1.43
14	B	829	CLA	MG-ND	-2.07	2.01	2.05
14	A	803	CLA	CHC-C1C	2.07	1.42	1.38
14	J	101	CLA	MG-NB	-2.07	2.01	2.05
14	a	817	CLA	MG-NB	-2.07	2.01	2.05
14	b	832	CLA	CMC-C2C	-2.06	1.46	1.50
14	a	807	CLA	MG-ND	-2.06	2.01	2.05
14	1	1622	CLA	CMD-C2D	-2.06	1.46	1.50
14	A	855	CLA	C1B-NB	-2.06	1.35	1.37
14	2	828	CLA	C1B-NB	-2.06	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	822	CLA	CMC-C2C	-2.06	1.46	1.50
14	1	1629	CLA	CHC-C1C	2.06	1.42	1.38
13	a	801	CL0	CMC-C2C	-2.06	1.46	1.50
14	A	826	CLA	MG-ND	-2.06	2.01	2.05
14	B	831	CLA	CMC-C2C	-2.06	1.46	1.50
14	9	103	CLA	CMC-C2C	-2.06	1.46	1.50
14	A	802	CLA	C1B-NB	-2.06	1.35	1.37
14	1	1628	CLA	C1B-NB	-2.06	1.35	1.37
14	a	809	CLA	CHC-C1C	2.06	1.42	1.38
14	2	832	CLA	CMC-C2C	-2.06	1.46	1.50
14	B	827	CLA	C1B-NB	-2.06	1.35	1.37
14	2	826	CLA	CHC-C1C	2.06	1.42	1.38
14	A	825	CLA	CHC-C1C	2.06	1.42	1.38
14	A	809	CLA	CMC-C2C	-2.06	1.46	1.50
14	6	201	CLA	CMC-C2C	-2.06	1.46	1.50
14	A	840	CLA	CHC-C1C	2.06	1.42	1.38
14	B	834	CLA	CHC-C1C	2.06	1.42	1.38
14	a	822	CLA	CHC-C1C	2.06	1.42	1.38
14	2	814	CLA	CHC-C1C	2.06	1.42	1.38
14	B	833	CLA	CHC-C1C	2.06	1.42	1.38
14	b	825	CLA	CHC-C1C	2.06	1.42	1.38
14	A	823	CLA	CHC-C1C	2.06	1.42	1.38
14	b	804	CLA	MG-ND	-2.06	2.01	2.05
17	2	847	BCR	C38-C26	-2.06	1.47	1.50
14	A	815	CLA	CMC-C2C	-2.06	1.46	1.50
14	b	827	CLA	CMC-C2C	-2.06	1.46	1.50
14	B	810	CLA	MG-ND	-2.06	2.01	2.05
14	2	806	CLA	C1B-NB	-2.06	1.35	1.37
18	B	850	LHG	O7-C5	-2.06	1.41	1.46
14	8	1301	CLA	CMB-C2B	-2.06	1.46	1.50
14	0	206	CLA	C1B-C2B	2.06	1.48	1.43
14	B	804	CLA	CHC-C1C	2.05	1.42	1.38
14	K	103	CLA	CMD-C2D	-2.05	1.46	1.50
14	B	821	CLA	CMB-C2B	-2.05	1.46	1.50
14	B	819	CLA	CHC-C1C	2.05	1.42	1.38
14	1	1604	CLA	CHC-C1C	2.05	1.42	1.38
14	A	842	CLA	CHC-C1C	2.05	1.42	1.38
14	a	811	CLA	CMC-C2C	-2.05	1.46	1.50
14	8	1303	CLA	CMC-C2C	-2.05	1.46	1.50
14	A	806	CLA	MG-ND	-2.05	2.01	2.05
14	A	834	CLA	CHC-C1C	2.05	1.42	1.38
14	1	1624	CLA	CHC-C1C	2.05	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	8	1304	BCR	C38-C26	-2.05	1.47	1.50
14	2	823	CLA	CMC-C2C	-2.05	1.46	1.50
14	M	102	CLA	CBD-CAD	2.05	1.56	1.51
14	B	821	CLA	CMC-C2C	-2.05	1.46	1.50
14	b	821	CLA	CMC-C2C	-2.05	1.46	1.50
14	2	812	CLA	CMC-C2C	-2.05	1.46	1.50
14	B	814	CLA	CHC-C1C	2.05	1.42	1.38
14	B	822	CLA	CMC-C2C	-2.05	1.46	1.50
14	A	822	CLA	CHC-C1C	2.05	1.42	1.38
14	M	102	CLA	CMB-C2B	-2.05	1.46	1.50
17	7	101	BCR	C33-C5	-2.05	1.47	1.50
14	A	857	CLA	CMB-C2B	-2.05	1.46	1.50
14	1	1616	CLA	CMC-C2C	-2.05	1.46	1.50
14	b	834	CLA	CHC-C1C	2.05	1.42	1.38
14	1	1617	CLA	CMC-C2C	-2.05	1.46	1.50
14	b	821	CLA	MG-NB	-2.05	2.01	2.05
14	2	804	CLA	MG-ND	-2.05	2.01	2.05
14	A	802	CLA	MG-ND	-2.05	2.01	2.05
14	L	203	CLA	C1B-C2B	2.04	1.48	1.43
14	1	1635	CLA	C1B-NB	-2.04	1.35	1.37
14	a	814	CLA	CMD-C2D	-2.04	1.46	1.50
14	b	840	CLA	CMC-C2C	-2.04	1.46	1.50
14	B	824	CLA	CHC-C1C	2.04	1.42	1.38
14	1	1623	CLA	CHC-C1C	2.04	1.42	1.38
14	a	832	CLA	C1B-NB	-2.04	1.35	1.37
14	b	811	CLA	MG-ND	-2.04	2.01	2.05
14	a	815	CLA	CMC-C2C	-2.04	1.46	1.50
17	A	850	BCR	C38-C26	-2.04	1.47	1.50
14	1	1618	CLA	MG-NB	-2.04	2.01	2.05
14	f	203	CLA	CMB-C2B	-2.04	1.46	1.50
14	1	1601	CLA	CBD-CAD	2.04	1.56	1.51
14	2	834	CLA	CHC-C1C	2.04	1.42	1.38
14	a	802	CLA	MG-ND	-2.04	2.01	2.05
14	a	817	CLA	CMC-C2C	-2.04	1.46	1.50
14	b	827	CLA	CHC-C1C	2.04	1.42	1.38
14	A	857	CLA	CBD-CAD	2.04	1.56	1.51
17	a	850	BCR	C33-C5	-2.04	1.47	1.50
14	B	826	CLA	CHC-C1C	2.04	1.42	1.38
14	1	1603	CLA	MG-ND	-2.04	2.01	2.05
14	l	204	CLA	C1B-C2B	2.04	1.48	1.43
17	b	847	BCR	C38-C26	-2.04	1.47	1.50
14	B	820	CLA	MG-NB	-2.04	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	1641	CLA	CHC-C1C	2.04	1.42	1.38
14	1	1607	CLA	MG-ND	-2.04	2.01	2.05
14	a	802	CLA	C1B-NB	-2.04	1.35	1.37
14	a	834	CLA	CHC-C1C	2.04	1.42	1.38
14	2	839	CLA	CMC-C2C	-2.04	1.46	1.50
17	i	101	BCR	C33-C5	-2.04	1.47	1.50
14	B	820	CLA	CMC-C2C	-2.03	1.46	1.50
14	B	823	CLA	CMC-C2C	-2.03	1.46	1.50
14	2	822	CLA	CMC-C2C	-2.03	1.46	1.50
14	a	840	CLA	CHC-C1C	2.03	1.42	1.38
14	J	102	CLA	MG-NB	-2.03	2.01	2.05
14	2	825	CLA	CHC-C1C	2.03	1.42	1.38
14	B	828	CLA	CHC-C1C	2.03	1.42	1.38
14	1	1615	CLA	CMD-C2D	-2.03	1.46	1.50
14	2	830	CLA	MG-ND	-2.03	2.01	2.05
14	A	817	CLA	CMC-C2C	-2.03	1.46	1.50
14	l	206	CLA	C1B-NB	-2.03	1.35	1.37
14	1	1635	CLA	C1B-C2B	2.03	1.48	1.43
14	b	812	CLA	CMC-C2C	-2.03	1.46	1.50
14	a	823	CLA	CHC-C1C	2.03	1.42	1.38
14	1	1635	CLA	CHC-C1C	2.03	1.42	1.38
14	2	824	CLA	CMC-C2C	-2.03	1.46	1.50
14	b	822	CLA	CMC-C2C	-2.03	1.46	1.50
14	A	808	CLA	CHC-C1C	2.03	1.42	1.38
14	a	806	CLA	MG-ND	-2.03	2.01	2.05
14	F	201	CLA	CMC-C2C	-2.03	1.46	1.50
14	a	809	CLA	CMC-C2C	-2.03	1.46	1.50
14	f	201	CLA	CMC-C2C	-2.03	1.46	1.50
14	b	822	CLA	CHC-C1C	2.03	1.42	1.38
14	b	823	CLA	CMC-C2C	-2.03	1.46	1.50
14	b	824	CLA	CMC-C2C	-2.03	1.46	1.50
14	1	1606	CLA	CHC-C1C	2.03	1.42	1.38
14	B	805	CLA	C1B-NB	-2.03	1.35	1.37
14	A	805	CLA	CHC-C1C	2.03	1.42	1.38
14	2	827	CLA	CHC-C1C	2.03	1.42	1.38
14	k	103	CLA	CMD-C2D	-2.03	1.46	1.50
14	b	811	CLA	C1B-NB	-2.02	1.35	1.37
14	1	1601	CLA	CMB-C2B	-2.02	1.46	1.50
14	0	205	CLA	C1B-C2B	2.02	1.48	1.43
14	A	817	CLA	CMB-C2B	-2.02	1.46	1.50
14	a	805	CLA	CHC-C1C	2.02	1.42	1.38
14	A	838	CLA	MG-ND	-2.02	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	204	CLA	CMB-C2B	-2.02	1.46	1.50
14	2	821	CLA	CMC-C2C	-2.02	1.46	1.50
14	1	1618	CLA	CMB-C2B	-2.02	1.46	1.50
14	9	103	CLA	CMD-C2D	-2.02	1.46	1.50
14	a	838	CLA	MG-ND	-2.02	2.01	2.05
14	2	811	CLA	C1B-NB	-2.02	1.35	1.37
14	a	814	CLA	CHC-C1C	2.02	1.42	1.38
14	A	816	CLA	CMC-C2C	-2.02	1.46	1.50
14	a	808	CLA	CHC-C1C	2.02	1.42	1.38
14	a	842	CLA	CHC-C1C	2.02	1.42	1.38
18	b	851	LHG	O7-C5	-2.02	1.41	1.46
17	a	851	BCR	C38-C26	-2.02	1.47	1.50
17	1	1651	BCR	C33-C5	-2.02	1.47	1.50
14	a	829	CLA	CMB-C2B	-2.02	1.46	1.50
14	1	1630	CLA	CMB-C2B	-2.02	1.46	1.50
14	B	821	CLA	CHC-C1C	2.02	1.42	1.38
14	A	842	CLA	MG-ND	-2.02	2.01	2.05
18	z	101	LHG	O7-C5	-2.01	1.41	1.46
14	2	822	CLA	CMB-C2B	-2.01	1.46	1.50
14	1	1610	CLA	CHC-C1C	2.01	1.42	1.38
18	A	853	LHG	O8-C6	-2.01	1.40	1.45
14	1	1645	CLA	CHC-C1C	2.01	1.42	1.38
14	1	1633	CLA	C1B-NB	-2.01	1.35	1.37
14	b	839	CLA	CMC-C2C	-2.01	1.46	1.50
14	A	857	CLA	MG-NB	-2.01	2.01	2.05
14	a	817	CLA	CMB-C2B	-2.01	1.46	1.50
18	0	202	LHG	O7-C5	-2.01	1.41	1.46
17	J	103	BCR	C38-C26	-2.01	1.47	1.50
14	a	803	CLA	CHC-C1C	2.01	1.42	1.38
14	2	815	CLA	CMB-C2B	-2.01	1.46	1.50
14	8	1302	CLA	CMC-C2C	-2.01	1.46	1.50
14	B	811	CLA	CMC-C2C	-2.01	1.46	1.50
14	2	815	CLA	CMC-C2C	-2.01	1.46	1.50
14	1	1639	CLA	CMC-C2C	-2.01	1.46	1.50
14	B	831	CLA	CHC-C1C	2.01	1.42	1.38
17	A	856	BCR	C38-C26	-2.01	1.47	1.50
17	I	101	BCR	C33-C5	-2.01	1.47	1.50
14	A	807	CLA	MG-ND	-2.01	2.01	2.05
14	1	1639	CLA	MG-ND	-2.01	2.01	2.05
14	z	102	CLA	CMB-C2B	-2.01	1.46	1.50
14	1	1624	CLA	CMC-C2C	-2.01	1.46	1.50
14	A	843	CLA	C1B-NB	-2.01	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	822	CLA	CMB-C2B	-2.01	1.46	1.50
14	M	102	CLA	MG-NB	-2.00	2.01	2.05
14	2	821	CLA	MG-NB	-2.00	2.01	2.05
14	A	827	CLA	MG-ND	-2.00	2.01	2.05
14	2	802	CLA	MG-ND	-2.00	2.01	2.05
14	1	1618	CLA	CMC-C2C	-2.00	1.46	1.50
14	b	815	CLA	CMC-C2C	-2.00	1.46	1.50
14	B	814	CLA	CMB-C2B	-2.00	1.46	1.50
14	b	810	CLA	CAC-C3C	-2.00	1.46	1.51
14	2	832	CLA	CHC-C1C	2.00	1.42	1.38
14	A	829	CLA	CMB-C2B	-2.00	1.46	1.50
14	2	810	CLA	CAC-C3C	-2.00	1.46	1.51
14	b	815	CLA	CMB-C2B	-2.00	1.46	1.50

All (2628) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	808	CLA	C4A-NA-C1A	8.39	110.48	106.71
14	2	809	CLA	C4A-NA-C1A	8.34	110.46	106.71
14	b	809	CLA	C4A-NA-C1A	8.29	110.43	106.71
14	B	803	CLA	C4A-NA-C1A	8.28	110.43	106.71
14	a	835	CLA	C4A-NA-C1A	8.24	110.41	106.71
14	1	1636	CLA	C4A-NA-C1A	8.24	110.41	106.71
14	A	835	CLA	C4A-NA-C1A	8.20	110.39	106.71
14	b	804	CLA	C4A-NA-C1A	8.17	110.38	106.71
14	2	804	CLA	C4A-NA-C1A	8.10	110.35	106.71
14	B	809	CLA	C4A-NA-C1A	8.06	110.33	106.71
14	b	810	CLA	C4A-NA-C1A	8.06	110.33	106.71
14	2	810	CLA	C4A-NA-C1A	8.04	110.32	106.71
14	b	842	CLA	C4A-NA-C1A	7.94	110.28	106.71
14	B	841	CLA	C4A-NA-C1A	7.87	110.24	106.71
13	1	1602	CL0	C4A-NA-C1A	7.87	110.24	106.71
14	2	842	CLA	C4A-NA-C1A	7.81	110.22	106.71
13	A	801	CL0	C4A-NA-C1A	7.80	110.21	106.71
13	a	801	CL0	C4A-NA-C1A	7.77	110.20	106.71
14	B	829	CLA	C4A-NA-C1A	7.75	110.19	106.71
14	b	830	CLA	C4A-NA-C1A	7.73	110.18	106.71
14	2	830	CLA	C4A-NA-C1A	7.71	110.17	106.71
14	2	811	CLA	C4A-NA-C1A	7.68	110.16	106.71
14	B	810	CLA	C4A-NA-C1A	7.68	110.16	106.71
14	b	811	CLA	C4A-NA-C1A	7.62	110.13	106.71
14	1	1632	CLA	C4A-NA-C1A	7.57	110.11	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	804	CLA	C4A-NA-C1A	7.56	110.10	106.71
14	A	831	CLA	C4A-NA-C1A	7.51	110.08	106.71
14	a	829	CLA	C4A-NA-C1A	7.49	110.07	106.71
14	b	841	CLA	C4A-NA-C1A	7.48	110.07	106.71
14	2	841	CLA	C4A-NA-C1A	7.47	110.06	106.71
14	A	804	CLA	C4A-NA-C1A	7.47	110.06	106.71
14	A	841	CLA	C4A-NA-C1A	7.46	110.06	106.71
14	a	831	CLA	C4A-NA-C1A	7.46	110.06	106.71
14	1	1630	CLA	C4A-NA-C1A	7.46	110.06	106.71
14	B	840	CLA	C4A-NA-C1A	7.45	110.06	106.71
14	A	829	CLA	C4A-NA-C1A	7.43	110.05	106.71
14	A	843	CLA	C4A-NA-C1A	7.42	110.04	106.71
14	1	1605	CLA	C4A-NA-C1A	7.40	110.03	106.71
14	a	843	CLA	C4A-NA-C1A	7.40	110.03	106.71
14	a	841	CLA	C4A-NA-C1A	7.39	110.03	106.71
14	1	1644	CLA	C4A-NA-C1A	7.39	110.03	106.71
14	1	1642	CLA	C4A-NA-C1A	7.38	110.03	106.71
14	1	1637	CLA	C4A-NA-C1A	7.36	110.02	106.71
14	a	820	CLA	C4A-NA-C1A	7.36	110.01	106.71
14	b	834	CLA	C4A-NA-C1A	7.35	110.01	106.71
14	2	806	CLA	C4A-NA-C1A	7.34	110.01	106.71
14	A	805	CLA	C4A-NA-C1A	7.33	110.00	106.71
14	A	836	CLA	C4A-NA-C1A	7.32	110.00	106.71
14	1	1641	CLA	C4A-NA-C1A	7.31	109.99	106.71
14	A	820	CLA	C4A-NA-C1A	7.30	109.99	106.71
14	a	840	CLA	C4A-NA-C1A	7.30	109.99	106.71
14	B	816	CLA	C4A-NA-C1A	7.29	109.98	106.71
14	a	836	CLA	C4A-NA-C1A	7.28	109.98	106.71
14	1	1621	CLA	C4A-NA-C1A	7.27	109.98	106.71
14	1	1627	CLA	C4A-NA-C1A	7.27	109.97	106.71
14	2	834	CLA	C4A-NA-C1A	7.27	109.97	106.71
14	B	833	CLA	C4A-NA-C1A	7.26	109.97	106.71
14	b	806	CLA	C4A-NA-C1A	7.25	109.97	106.71
14	a	805	CLA	C4A-NA-C1A	7.25	109.96	106.71
14	b	807	CLA	C4A-NA-C1A	7.25	109.96	106.71
14	b	825	CLA	C4A-NA-C1A	7.24	109.96	106.71
14	B	806	CLA	C4A-NA-C1A	7.23	109.96	106.71
14	A	809	CLA	C4A-NA-C1A	7.22	109.95	106.71
14	a	809	CLA	C4A-NA-C1A	7.22	109.95	106.71
14	2	817	CLA	C4A-NA-C1A	7.22	109.95	106.71
14	A	807	CLA	C4A-NA-C1A	7.22	109.95	106.71
14	a	826	CLA	C4A-NA-C1A	7.21	109.95	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1	1606	CLA	C4A-NA-C1A	7.21	109.95	106.71
14	1	1610	CLA	C4A-NA-C1A	7.20	109.94	106.71
14	B	805	CLA	C4A-NA-C1A	7.19	109.94	106.71
14	b	817	CLA	C4A-NA-C1A	7.18	109.94	106.71
14	2	838	CLA	C4A-NA-C1A	7.18	109.94	106.71
14	2	807	CLA	C4A-NA-C1A	7.18	109.93	106.71
14	A	840	CLA	C4A-NA-C1A	7.17	109.93	106.71
14	1	1608	CLA	C4A-NA-C1A	7.17	109.93	106.71
14	b	838	CLA	C4A-NA-C1A	7.17	109.93	106.71
14	A	826	CLA	C4A-NA-C1A	7.16	109.93	106.71
14	B	832	CLA	C4A-NA-C1A	7.15	109.92	106.71
14	2	825	CLA	C4A-NA-C1A	7.14	109.92	106.71
14	B	837	CLA	C4A-NA-C1A	7.14	109.92	106.71
14	a	818	CLA	C4A-NA-C1A	7.13	109.91	106.71
14	1	1631	CLA	C4A-NA-C1A	7.13	109.91	106.71
14	B	824	CLA	C4A-NA-C1A	7.12	109.91	106.71
14	2	803	CLA	C4A-NA-C1A	7.12	109.91	106.71
14	2	833	CLA	C4A-NA-C1A	7.12	109.91	106.71
14	1	1619	CLA	C4A-NA-C1A	7.11	109.90	106.71
14	b	803	CLA	C4A-NA-C1A	7.10	109.90	106.71
14	l	205	CLA	C4A-NA-C1A	7.08	109.89	106.71
14	b	833	CLA	C4A-NA-C1A	7.08	109.89	106.71
14	0	206	CLA	C4A-NA-C1A	7.08	109.89	106.71
14	L	204	CLA	C4A-NA-C1A	7.07	109.89	106.71
14	A	830	CLA	C4A-NA-C1A	7.07	109.89	106.71
14	a	807	CLA	C4A-NA-C1A	7.06	109.88	106.71
14	A	818	CLA	C4A-NA-C1A	7.05	109.88	106.71
14	a	830	CLA	C4A-NA-C1A	7.04	109.87	106.71
14	b	805	CLA	C4A-NA-C1A	7.03	109.86	106.71
14	B	802	CLA	C4A-NA-C1A	7.02	109.86	106.71
14	B	804	CLA	C4A-NA-C1A	7.02	109.86	106.71
14	B	830	CLA	C4A-NA-C1A	7.02	109.86	106.71
14	2	831	CLA	C4A-NA-C1A	7.02	109.86	106.71
14	1	1625	CLA	C4A-NA-C1A	7.01	109.86	106.71
14	A	810	CLA	C4A-NA-C1A	7.00	109.85	106.71
14	2	815	CLA	C4A-NA-C1A	6.99	109.85	106.71
14	1	1603	CLA	C4A-NA-C1A	6.99	109.85	106.71
14	j	1302	CLA	C4A-NA-C1A	6.98	109.85	106.71
14	2	805	CLA	C4A-NA-C1A	6.98	109.84	106.71
14	B	821	CLA	C4A-NA-C1A	6.98	109.84	106.71
14	b	808	CLA	C4A-NA-C1A	6.97	109.84	106.71
14	a	824	CLA	C4A-NA-C1A	6.97	109.84	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1	1623	CLA	C4A-NA-C1A	6.97	109.84	106.71
14	A	822	CLA	C4A-NA-C1A	6.96	109.84	106.71
14	A	838	CLA	C4A-NA-C1A	6.96	109.84	106.71
14	1	1609	CLA	C4A-NA-C1A	6.96	109.83	106.71
14	a	834	CLA	C4A-NA-C1A	6.95	109.83	106.71
14	a	806	CLA	C4A-NA-C1A	6.94	109.83	106.71
14	b	831	CLA	C4A-NA-C1A	6.94	109.83	106.71
14	A	808	CLA	C4A-NA-C1A	6.93	109.82	106.71
14	9	101	CLA	C4A-NA-C1A	6.93	109.82	106.71
14	B	831	CLA	C4A-NA-C1A	6.93	109.82	106.71
14	b	822	CLA	C4A-NA-C1A	6.93	109.82	106.71
14	1	1639	CLA	C4A-NA-C1A	6.93	109.82	106.71
14	J	101	CLA	C4A-NA-C1A	6.92	109.82	106.71
14	a	822	CLA	C4A-NA-C1A	6.92	109.82	106.71
14	a	838	CLA	C4A-NA-C1A	6.92	109.82	106.71
14	2	822	CLA	C4A-NA-C1A	6.91	109.81	106.71
14	B	815	CLA	C4A-NA-C1A	6.91	109.81	106.71
14	2	808	CLA	C4A-NA-C1A	6.90	109.81	106.71
14	b	815	CLA	C4A-NA-C1A	6.90	109.81	106.71
14	A	802	CLA	C4A-NA-C1A	6.90	109.81	106.71
14	8	1302	CLA	C4A-NA-C1A	6.89	109.81	106.71
14	1	1607	CLA	C4A-NA-C1A	6.89	109.80	106.71
14	b	816	CLA	C4A-NA-C1A	6.89	109.80	106.71
14	1	1635	CLA	C4A-NA-C1A	6.89	109.80	106.71
14	2	812	CLA	C4A-NA-C1A	6.88	109.80	106.71
14	a	802	CLA	C4A-NA-C1A	6.88	109.80	106.71
14	B	814	CLA	C4A-NA-C1A	6.88	109.80	106.71
14	A	824	CLA	C4A-NA-C1A	6.87	109.80	106.71
14	B	838	CLA	C4A-NA-C1A	6.87	109.79	106.71
14	2	832	CLA	C4A-NA-C1A	6.86	109.79	106.71
14	B	811	CLA	C4A-NA-C1A	6.86	109.79	106.71
14	a	844	CLA	C4A-NA-C1A	6.86	109.79	106.71
14	B	807	CLA	C4A-NA-C1A	6.85	109.78	106.71
14	a	810	CLA	C4A-NA-C1A	6.85	109.78	106.71
14	K	101	CLA	C4A-NA-C1A	6.84	109.78	106.71
14	a	808	CLA	C4A-NA-C1A	6.84	109.78	106.71
14	2	816	CLA	C4A-NA-C1A	6.83	109.78	106.71
14	2	839	CLA	C4A-NA-C1A	6.83	109.78	106.71
14	k	101	CLA	C4A-NA-C1A	6.82	109.77	106.71
14	A	834	CLA	C4A-NA-C1A	6.81	109.77	106.71
14	A	806	CLA	C4A-NA-C1A	6.81	109.77	106.71
14	A	844	CLA	C4A-NA-C1A	6.79	109.76	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1	1611	CLA	C4A-NA-C1A	6.79	109.76	106.71
14	b	832	CLA	C4A-NA-C1A	6.78	109.75	106.71
14	b	812	CLA	C4A-NA-C1A	6.77	109.75	106.71
14	b	839	CLA	C4A-NA-C1A	6.75	109.74	106.71
14	1	1618	CLA	C4A-NA-C1A	6.74	109.73	106.71
14	A	823	CLA	C4A-NA-C1A	6.73	109.73	106.71
14	a	823	CLA	C4A-NA-C1A	6.73	109.73	106.71
14	1	1645	CLA	C4A-NA-C1A	6.72	109.72	106.71
14	A	842	CLA	C4A-NA-C1A	6.71	109.72	106.71
14	B	834	CLA	C4A-NA-C1A	6.71	109.72	106.71
14	1	1624	CLA	C4A-NA-C1A	6.71	109.72	106.71
14	b	837	CLA	C4A-NA-C1A	6.70	109.72	106.71
14	b	821	CLA	C4A-NA-C1A	6.70	109.72	106.71
14	6	201	CLA	C4A-NA-C1A	6.70	109.72	106.71
14	B	836	CLA	C4A-NA-C1A	6.69	109.71	106.71
14	A	815	CLA	C4A-NA-C1A	6.68	109.71	106.71
14	A	857	CLA	C4A-NA-C1A	6.68	109.71	106.71
14	A	817	CLA	C4A-NA-C1A	6.66	109.70	106.71
14	1	1643	CLA	C4A-NA-C1A	6.66	109.70	106.71
14	2	835	CLA	C4A-NA-C1A	6.66	109.70	106.71
14	a	842	CLA	C4A-NA-C1A	6.65	109.70	106.71
14	B	820	CLA	C4A-NA-C1A	6.65	109.69	106.71
14	a	839	CLA	C4A-NA-C1A	6.65	109.69	106.71
14	1	1612	CLA	C4A-NA-C1A	6.65	109.69	106.71
14	a	817	CLA	C4A-NA-C1A	6.64	109.69	106.71
14	f	201	CLA	C4A-NA-C1A	6.64	109.69	106.71
14	1	1616	CLA	C4A-NA-C1A	6.64	109.69	106.71
14	a	812	CLA	C4A-NA-C1A	6.63	109.69	106.71
14	b	835	CLA	C4A-NA-C1A	6.62	109.68	106.71
14	A	839	CLA	C4A-NA-C1A	6.61	109.68	106.71
14	a	811	CLA	C4A-NA-C1A	6.61	109.68	106.71
14	b	823	CLA	C4A-NA-C1A	6.61	109.68	106.71
14	M	102	CLA	C4A-NA-C1A	6.60	109.67	106.71
14	1	1640	CLA	C4A-NA-C1A	6.60	109.67	106.71
14	1	1633	CLA	C4A-NA-C1A	6.60	109.67	106.71
14	a	816	CLA	C4A-NA-C1A	6.59	109.67	106.71
14	a	828	CLA	C4A-NA-C1A	6.58	109.67	106.71
14	A	825	CLA	C4A-NA-C1A	6.58	109.66	106.71
14	a	815	CLA	C4A-NA-C1A	6.58	109.66	106.71
14	F	201	CLA	C4A-NA-C1A	6.57	109.66	106.71
14	b	813	CLA	C4A-NA-C1A	6.57	109.66	106.71
14	A	811	CLA	C4A-NA-C1A	6.57	109.66	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	812	CLA	C4A-NA-C1A	6.57	109.66	106.71
14	a	832	CLA	C4A-NA-C1A	6.57	109.66	106.71
14	A	828	CLA	C4A-NA-C1A	6.56	109.66	106.71
14	2	837	CLA	C4A-NA-C1A	6.56	109.66	106.71
14	B	835	CLA	C4A-NA-C1A	6.56	109.66	106.71
14	2	819	CLA	C4A-NA-C1A	6.56	109.65	106.71
14	2	813	CLA	C4A-NA-C1A	6.56	109.65	106.71
14	1	1601	CLA	C4A-NA-C1A	6.55	109.65	106.71
14	a	827	CLA	C4A-NA-C1A	6.54	109.65	106.71
14	A	827	CLA	C4A-NA-C1A	6.54	109.65	106.71
14	x	1701	CLA	C4A-NA-C1A	6.54	109.65	106.71
14	B	822	CLA	C4A-NA-C1A	6.53	109.64	106.71
14	1	1613	CLA	C4A-NA-C1A	6.53	109.64	106.71
14	2	836	CLA	C4A-NA-C1A	6.52	109.64	106.71
14	f	203	CLA	C4A-NA-C1A	6.52	109.64	106.71
14	1	1629	CLA	C4A-NA-C1A	6.51	109.63	106.71
14	2	821	CLA	C4A-NA-C1A	6.50	109.63	106.71
14	z	102	CLA	C4A-NA-C1A	6.50	109.63	106.71
14	B	818	CLA	C4A-NA-C1A	6.48	109.62	106.71
14	1	1628	CLA	C4A-NA-C1A	6.48	109.62	106.71
14	b	819	CLA	C4A-NA-C1A	6.48	109.62	106.71
14	a	825	CLA	C4A-NA-C1A	6.47	109.62	106.71
14	A	812	CLA	C4A-NA-C1A	6.47	109.62	106.71
14	b	836	CLA	C4A-NA-C1A	6.47	109.61	106.71
14	A	816	CLA	C4A-NA-C1A	6.46	109.61	106.71
14	L	203	CLA	C4A-NA-C1A	6.46	109.61	106.71
14	1	1604	CLA	C4A-NA-C1A	6.45	109.61	106.71
14	A	803	CLA	C4A-NA-C1A	6.43	109.60	106.71
14	F	204	CLA	C4A-NA-C1A	6.42	109.59	106.71
14	l	204	CLA	C4A-NA-C1A	6.42	109.59	106.71
14	A	821	CLA	C4A-NA-C1A	6.41	109.59	106.71
14	b	826	CLA	C4A-NA-C1A	6.41	109.59	106.71
14	b	827	CLA	C4A-NA-C1A	6.41	109.59	106.71
14	6	203	CLA	C4A-NA-C1A	6.41	109.59	106.71
14	k	103	CLA	C4A-NA-C1A	6.41	109.59	106.71
14	1	1617	CLA	C4A-NA-C1A	6.40	109.58	106.71
14	A	832	CLA	C4A-NA-C1A	6.40	109.58	106.71
14	a	803	CLA	C4A-NA-C1A	6.39	109.58	106.71
14	B	826	CLA	C4A-NA-C1A	6.39	109.58	106.71
14	1	1622	CLA	C4A-NA-C1A	6.38	109.58	106.71
14	X	1701	CLA	C4A-NA-C1A	6.38	109.57	106.71
14	2	823	CLA	C4A-NA-C1A	6.37	109.57	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1	1626	CLA	C4A-NA-C1A	6.37	109.57	106.71
14	2	826	CLA	C4A-NA-C1A	6.37	109.57	106.71
14	a	821	CLA	C4A-NA-C1A	6.36	109.57	106.71
14	8	1301	CLA	C4A-NA-C1A	6.36	109.56	106.71
14	j	1301	CLA	C4A-NA-C1A	6.35	109.56	106.71
14	1	1614	CLA	C4A-NA-C1A	6.35	109.56	106.71
14	2	827	CLA	C4A-NA-C1A	6.34	109.56	106.71
14	B	817	CLA	C4A-NA-C1A	6.32	109.55	106.71
14	B	825	CLA	C4A-NA-C1A	6.31	109.54	106.71
14	F	203	CLA	C4A-NA-C1A	6.31	109.54	106.71
14	b	818	CLA	C4A-NA-C1A	6.29	109.53	106.71
14	0	205	CLA	C4A-NA-C1A	6.28	109.53	106.71
14	9	103	CLA	C4A-NA-C1A	6.27	109.53	106.71
14	K	103	CLA	C4A-NA-C1A	6.27	109.53	106.71
14	2	814	CLA	C4A-NA-C1A	6.27	109.52	106.71
14	b	824	CLA	C4A-NA-C1A	6.25	109.52	106.71
14	a	813	CLA	C4A-NA-C1A	6.24	109.51	106.71
14	B	823	CLA	C4A-NA-C1A	6.23	109.50	106.71
14	0	207	CLA	C4A-NA-C1A	6.23	109.50	106.71
14	2	818	CLA	C4A-NA-C1A	6.22	109.50	106.71
14	A	813	CLA	C4A-NA-C1A	6.21	109.50	106.71
14	L	205	CLA	C4A-NA-C1A	6.21	109.50	106.71
14	a	814	CLA	C4A-NA-C1A	6.21	109.50	106.71
14	b	814	CLA	C4A-NA-C1A	6.21	109.50	106.71
14	l	206	CLA	C4A-NA-C1A	6.19	109.49	106.71
14	1	1615	CLA	C4A-NA-C1A	6.19	109.49	106.71
14	A	814	CLA	C4A-NA-C1A	6.19	109.49	106.71
14	J	102	CLA	C4A-NA-C1A	6.19	109.49	106.71
14	1	1634	CLA	C4A-NA-C1A	6.19	109.49	106.71
14	B	819	CLA	C4A-NA-C1A	6.18	109.48	106.71
14	2	820	CLA	C4A-NA-C1A	6.18	109.48	106.71
14	2	824	CLA	C4A-NA-C1A	6.16	109.48	106.71
14	a	833	CLA	C4A-NA-C1A	6.15	109.47	106.71
14	8	1303	CLA	C4A-NA-C1A	6.15	109.47	106.71
14	b	820	CLA	C4A-NA-C1A	6.14	109.47	106.71
14	j	1303	CLA	C4A-NA-C1A	6.14	109.47	106.71
14	2	829	CLA	C4A-NA-C1A	6.09	109.44	106.71
14	B	813	CLA	C4A-NA-C1A	6.06	109.43	106.71
14	A	833	CLA	C4A-NA-C1A	6.02	109.41	106.71
14	b	829	CLA	C4A-NA-C1A	6.00	109.41	106.71
14	a	837	CLA	C4A-NA-C1A	6.00	109.40	106.71
14	B	828	CLA	C4A-NA-C1A	5.98	109.39	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	837	CLA	C4A-NA-C1A	5.97	109.39	106.71
14	b	802	CLA	C4A-NA-C1A	5.95	109.38	106.71
14	2	802	CLA	C4A-NA-C1A	5.94	109.38	106.71
14	1	1638	CLA	C4A-NA-C1A	5.91	109.36	106.71
14	A	855	CLA	C4A-NA-C1A	5.88	109.35	106.71
14	B	839	CLA	C4A-NA-C1A	5.81	109.32	106.71
14	2	828	CLA	C4A-NA-C1A	5.80	109.31	106.71
14	b	840	CLA	C4A-NA-C1A	5.78	109.31	106.71
14	B	827	CLA	C4A-NA-C1A	5.75	109.29	106.71
14	2	840	CLA	C4A-NA-C1A	5.73	109.28	106.71
14	b	828	CLA	C4A-NA-C1A	5.70	109.27	106.71
14	1	1620	CLA	C4A-NA-C1A	5.69	109.27	106.71
14	a	819	CLA	C4A-NA-C1A	5.64	109.24	106.71
14	A	819	CLA	C4A-NA-C1A	5.63	109.23	106.71
18	a	854	LHG	O4-P-O5	4.30	133.51	112.24
18	A	854	LHG	O4-P-O5	4.30	133.50	112.24
18	1	1655	LHG	O4-P-O5	4.30	133.49	112.24
18	A	853	LHG	O4-P-O5	4.29	133.46	112.24
18	1	1654	LHG	O4-P-O5	4.29	133.45	112.24
18	a	853	LHG	O4-P-O5	4.28	133.41	112.24
18	L	208	LHG	O4-P-O5	4.23	133.16	112.24
18	0	202	LHG	O4-P-O5	4.23	133.13	112.24
18	l	201	LHG	O4-P-O5	4.22	133.12	112.24
18	M	101	LHG	O4-P-O5	4.20	133.00	112.24
18	m	101	LHG	O4-P-O5	4.19	132.96	112.24
18	y	101	LHG	O4-P-O5	4.19	132.95	112.24
18	z	101	LHG	O4-P-O5	4.17	132.86	112.24
18	b	851	LHG	O4-P-O5	4.17	132.84	112.24
18	B	850	LHG	O4-P-O5	4.16	132.82	112.24
17	B	843	BCR	C15-C16-C17	-4.03	115.22	123.47
14	1	1639	CLA	CMB-C2B-C1B	-4.03	119.23	125.37
17	2	844	BCR	C15-C16-C17	-4.03	115.23	123.47
17	b	844	BCR	C15-C16-C17	-4.02	115.23	123.47
14	A	838	CLA	CMB-C2B-C1B	-3.99	119.29	125.37
14	a	838	CLA	CMB-C2B-C1B	-3.96	119.33	125.37
14	b	826	CLA	O2D-CGD-O1D	-3.95	116.11	123.84
17	A	847	BCR	C2-C1-C6	3.95	116.57	110.48
14	2	802	CLA	C4-C3-C5	3.95	121.92	115.27
14	b	802	CLA	C4-C3-C5	3.95	121.91	115.27
14	2	826	CLA	O2D-CGD-O1D	-3.94	116.12	123.84
14	A	855	CLA	C4-C3-C5	3.94	121.91	115.27
14	B	825	CLA	O2D-CGD-O1D	-3.94	116.13	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	a	847	BCR	C2-C1-C6	3.93	116.53	110.48
17	1	1648	BCR	C2-C1-C6	3.92	116.51	110.48
14	0	205	CLA	C3B-C4B-NB	-3.88	106.91	110.52
14	0	206	CLA	O2D-CGD-O1D	-3.88	116.26	123.84
14	l	205	CLA	O2D-CGD-O1D	-3.88	116.26	123.84
14	L	204	CLA	O2D-CGD-O1D	-3.88	116.26	123.84
14	L	203	CLA	C3B-C4B-NB	-3.85	106.94	110.52
14	a	839	CLA	O2D-CGD-O1D	-3.82	116.36	123.84
14	A	839	CLA	O2D-CGD-O1D	-3.82	116.37	123.84
14	l	204	CLA	C3B-C4B-NB	-3.81	106.98	110.52
14	1	1640	CLA	O2D-CGD-O1D	-3.80	116.42	123.84
14	1	1608	CLA	CMB-C2B-C1B	-3.75	119.66	125.37
14	a	821	CLA	CMB-C2B-C1B	-3.74	119.67	125.37
14	a	807	CLA	CMB-C2B-C1B	-3.74	119.68	125.37
14	1	1622	CLA	CMB-C2B-C1B	-3.73	119.69	125.37
14	A	807	CLA	CMB-C2B-C1B	-3.73	119.69	125.37
14	A	821	CLA	CMB-C2B-C1B	-3.71	119.71	125.37
17	l	207	BCR	C2-C1-C6	3.68	116.14	110.48
17	L	206	BCR	C2-C1-C6	3.68	116.14	110.48
17	0	208	BCR	C2-C1-C6	3.66	116.12	110.48
14	1	1620	CLA	C4-C3-C5	3.59	121.32	115.27
14	a	819	CLA	C4-C3-C5	3.59	121.30	115.27
14	A	819	CLA	C4-C3-C5	3.58	121.29	115.27
14	B	805	CLA	CMB-C2B-C1B	-3.57	119.94	125.37
17	B	851	BCR	C7-C8-C9	-3.56	120.85	126.23
14	2	806	CLA	CMB-C2B-C1B	-3.56	119.95	125.37
17	8	1306	BCR	C7-C8-C9	-3.55	120.87	126.23
17	b	852	BCR	C7-C8-C9	-3.54	120.88	126.23
14	b	806	CLA	CMB-C2B-C1B	-3.53	119.99	125.37
14	b	818	CLA	C4-C3-C5	3.49	121.15	115.27
14	B	817	CLA	C4-C3-C5	3.49	121.15	115.27
14	2	818	CLA	C4-C3-C5	3.49	121.15	115.27
14	A	855	CLA	O2D-CGD-O1D	-3.49	117.01	123.84
14	B	829	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
14	b	802	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
14	2	802	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
14	2	830	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
14	b	830	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
14	F	203	CLA	CMB-C2B-C1B	-3.47	120.08	125.37
17	F	205	BCR	C35-C13-C14	-3.47	118.06	122.92
17	M	103	BCR	C24-C23-C22	-3.47	121.00	126.23
17	y	102	BCR	C24-C23-C22	-3.46	121.00	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	825	CLA	CHB-C4A-NA	3.46	129.30	124.51
17	6	204	BCR	C35-C13-C14	-3.46	118.08	122.92
14	b	802	CLA	CMB-C2B-C1B	-3.46	120.11	125.37
14	j	1301	CLA	CMB-C2B-C1B	-3.45	120.11	125.37
14	2	802	CLA	CMB-C2B-C1B	-3.45	120.11	125.37
14	8	1301	CLA	CMB-C2B-C1B	-3.45	120.11	125.37
14	A	855	CLA	CMB-C2B-C1B	-3.45	120.11	125.37
14	B	824	CLA	CHB-C4A-NA	3.45	129.28	124.51
14	1	1603	CLA	CMB-C2B-C1B	-3.45	120.12	125.37
14	a	802	CLA	CMB-C2B-C1B	-3.45	120.12	125.37
14	1	1609	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
14	2	825	CLA	CHB-C4A-NA	3.44	129.27	124.51
17	f	204	BCR	C35-C13-C14	-3.43	118.11	122.92
14	A	802	CLA	CMB-C2B-C1B	-3.43	120.14	125.37
17	m	102	BCR	C24-C23-C22	-3.43	121.06	126.23
14	A	840	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
17	a	849	BCR	C15-C16-C17	-3.42	116.47	123.47
14	B	825	CLA	C1-C2-C3	-3.40	120.16	126.04
14	l	206	CLA	O2D-CGD-O1D	-3.40	117.20	123.84
14	a	808	CLA	O2D-CGD-O1D	-3.39	117.20	123.84
14	A	808	CLA	O2D-CGD-O1D	-3.39	117.20	123.84
14	1	1641	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
14	0	207	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
14	a	840	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
14	X	1701	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
14	2	826	CLA	C1-C2-C3	-3.38	120.19	126.04
17	1	1650	BCR	C15-C16-C17	-3.38	116.55	123.47
14	x	1701	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
17	A	849	BCR	C15-C16-C17	-3.38	116.55	123.47
14	z	102	CLA	O2D-CGD-O1D	-3.38	117.24	123.84
14	b	826	CLA	C1-C2-C3	-3.37	120.21	126.04
13	a	801	CL0	O2D-CGD-O1D	-3.37	117.25	123.84
14	B	809	CLA	C1-C2-C3	-3.36	120.23	126.04
14	L	205	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
13	1	1602	CL0	O2D-CGD-O1D	-3.35	117.29	123.84
14	2	812	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
14	b	808	CLA	O2D-CGD-O1D	-3.35	117.30	123.84
14	1	1614	CLA	O2D-CGD-O1D	-3.35	117.30	123.84
14	A	813	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
14	B	807	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
14	b	812	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
14	2	810	CLA	C1-C2-C3	-3.34	120.27	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	813	CLA	O2D-CGD-O1D	-3.34	117.32	123.84
14	B	811	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
14	2	808	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
14	A	825	CLA	C3B-C4B-NB	-3.33	107.43	110.52
14	b	810	CLA	C1-C2-C3	-3.33	120.29	126.04
13	A	801	CL0	O2D-CGD-O1D	-3.32	117.34	123.84
14	A	830	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
14	2	838	CLA	O2D-CGD-O1D	-3.31	117.38	123.84
14	A	834	CLA	C1-C2-C3	-3.30	120.33	126.04
14	1	1631	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
14	B	812	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
17	b	848	BCR	C15-C16-C17	-3.29	116.72	123.47
17	2	848	BCR	C15-C16-C17	-3.29	116.73	123.47
14	B	837	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
14	B	841	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
14	a	834	CLA	C1-C2-C3	-3.28	120.37	126.04
14	1	1635	CLA	C1-C2-C3	-3.28	120.37	126.04
14	a	830	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
14	2	842	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
14	a	825	CLA	C3B-C4B-NB	-3.28	107.47	110.52
14	2	813	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
14	2	842	CLA	C1-C2-C3	-3.27	120.38	126.04
17	B	847	BCR	C15-C16-C17	-3.27	116.77	123.47
14	a	829	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
14	1	1626	CLA	C3B-C4B-NB	-3.27	107.48	110.52
14	B	841	CLA	C1-C2-C3	-3.27	120.39	126.04
14	b	842	CLA	C1-C2-C3	-3.26	120.40	126.04
14	1	1643	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
14	A	842	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
14	b	838	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
14	A	829	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
14	1	1643	CLA	C4-C3-C5	3.26	120.75	115.27
14	1	1630	CLA	O2D-CGD-O1D	-3.25	117.47	123.84
14	b	842	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
14	A	842	CLA	C4-C3-C5	3.25	120.74	115.27
14	6	201	CLA	C3B-C4B-NB	-3.25	107.50	110.52
14	b	813	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
14	1	1632	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
14	a	842	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
14	a	831	CLA	O2D-CGD-O1D	-3.23	117.51	123.84
17	J	103	BCR	C2-C1-C6	3.23	115.46	110.48
14	B	808	CLA	O2D-CGD-O1D	-3.23	117.53	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	8	1304	BCR	C2-C1-C6	3.22	115.44	110.48
14	a	842	CLA	C4-C3-C5	3.22	120.69	115.27
14	A	831	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
14	l	205	CLA	C3B-C4B-NB	-3.21	107.54	110.52
14	b	833	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
14	b	809	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
14	2	809	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
17	A	848	BCR	C37-C22-C21	-3.21	118.43	122.92
14	2	833	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
14	L	204	CLA	C3B-C4B-NB	-3.21	107.54	110.52
17	a	848	BCR	C37-C22-C21	-3.21	118.43	122.92
14	0	206	CLA	C3B-C4B-NB	-3.20	107.54	110.52
17	j	1304	BCR	C2-C1-C6	3.20	115.41	110.48
14	1	1607	CLA	C4-C3-C5	3.20	120.65	115.27
14	2	822	CLA	CMB-C2B-C1B	-3.20	120.50	125.37
14	B	832	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
14	1	1621	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
14	A	820	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
14	B	809	CLA	CHB-C4A-NA	3.19	128.93	124.51
14	a	820	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
17	1	1649	BCR	C37-C22-C21	-3.19	118.46	122.92
14	B	821	CLA	CMB-C2B-C1B	-3.19	120.52	125.37
14	F	201	CLA	C3B-C4B-NB	-3.18	107.56	110.52
14	A	806	CLA	C4-C3-C5	3.18	120.62	115.27
14	f	201	CLA	C3B-C4B-NB	-3.18	107.57	110.52
14	2	819	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
14	b	822	CLA	CMB-C2B-C1B	-3.17	120.54	125.37
14	a	806	CLA	C4-C3-C5	3.17	120.60	115.27
14	B	818	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
14	b	810	CLA	CHB-C4A-NA	3.17	128.89	124.51
14	2	810	CLA	CHB-C4A-NA	3.17	128.89	124.51
14	A	805	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
14	1	1606	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
14	a	835	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
14	b	812	CLA	CMB-C2B-C1B	-3.15	120.57	125.37
14	a	805	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
14	b	819	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
14	A	833	CLA	C3B-C4B-NB	-3.14	107.60	110.52
14	1	1636	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
14	2	812	CLA	CMB-C2B-C1B	-3.14	120.59	125.37
14	1	1610	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
14	2	836	CLA	C3B-C4B-NB	-3.14	107.60	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	806	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
14	b	838	CLA	C3B-C4B-NB	-3.14	107.61	110.52
14	A	804	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
14	b	817	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
14	a	809	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
14	B	811	CLA	CMB-C2B-C1B	-3.13	120.61	125.37
14	1	1634	CLA	C3B-C4B-NB	-3.13	107.61	110.52
14	A	835	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
14	2	838	CLA	C3B-C4B-NB	-3.12	107.62	110.52
14	B	805	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
14	b	835	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
14	1	1643	CLA	C3B-C4B-NB	-3.12	107.62	110.52
14	a	811	CLA	C3B-C4B-NB	-3.12	107.62	110.52
14	2	817	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
14	B	837	CLA	C3B-C4B-NB	-3.11	107.63	110.52
14	B	835	CLA	C3B-C4B-NB	-3.11	107.63	110.52
14	a	842	CLA	C3B-C4B-NB	-3.11	107.63	110.52
14	B	816	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
14	2	806	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
14	b	836	CLA	C3B-C4B-NB	-3.11	107.63	110.52
14	2	835	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
14	A	809	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
14	1	1605	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
14	a	804	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
14	B	834	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
14	2	826	CLA	O2D-CGD-CBD	3.10	116.78	111.27
14	b	826	CLA	O2D-CGD-CBD	3.10	116.78	111.27
14	A	811	CLA	C3B-C4B-NB	-3.10	107.64	110.52
14	B	825	CLA	O2D-CGD-CBD	3.10	116.77	111.27
14	a	809	CLA	CHB-C4A-NA	3.10	128.79	124.51
14	b	831	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
14	a	833	CLA	C3B-C4B-NB	-3.09	107.65	110.52
14	2	831	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
14	A	805	CLA	CHB-C4A-NA	3.09	128.79	124.51
14	a	805	CLA	CHB-C4A-NA	3.09	128.78	124.51
14	B	832	CLA	C3B-C4B-NB	-3.09	107.65	110.52
14	A	816	CLA	C3B-C4B-NB	-3.08	107.66	110.52
14	1	1612	CLA	C3B-C4B-NB	-3.08	107.66	110.52
14	A	809	CLA	CHB-C4A-NA	3.08	128.77	124.51
14	A	802	CLA	C3B-C4B-NB	-3.08	107.66	110.52
14	1	1610	CLA	CHB-C4A-NA	3.08	128.77	124.51
14	1	1629	CLA	C3B-C4B-NB	-3.08	107.66	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	842	CLA	C3B-C4B-NB	-3.07	107.66	110.52
14	a	802	CLA	C3B-C4B-NB	-3.07	107.67	110.52
14	B	830	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
14	a	816	CLA	C3B-C4B-NB	-3.07	107.67	110.52
14	B	823	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
14	1	1603	CLA	C3B-C4B-NB	-3.07	107.67	110.52
14	A	813	CLA	C3B-C4B-NB	-3.07	107.67	110.52
14	b	833	CLA	C3B-C4B-NB	-3.06	107.67	110.52
14	b	840	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
14	B	839	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
14	a	837	CLA	C3B-C4B-NB	-3.05	107.68	110.52
14	2	840	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
14	A	844	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
17	B	847	BCR	C37-C22-C21	-3.05	118.65	122.92
14	A	828	CLA	C3B-C4B-NB	-3.05	107.69	110.52
14	1	1645	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
14	0	205	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
17	b	848	BCR	C37-C22-C21	-3.04	118.66	122.92
14	a	828	CLA	C3B-C4B-NB	-3.04	107.69	110.52
17	2	848	BCR	C37-C22-C21	-3.04	118.67	122.92
14	2	824	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
14	1	1606	CLA	CHB-C4A-NA	3.04	128.71	124.51
14	2	833	CLA	C3B-C4B-NB	-3.04	107.70	110.52
14	1	1635	CLA	CHB-C4A-NA	3.04	128.71	124.51
14	A	824	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
17	A	851	BCR	C24-C23-C22	-3.04	121.65	126.23
14	a	813	CLA	C3B-C4B-NB	-3.03	107.70	110.52
14	a	834	CLA	CHB-C4A-NA	3.03	128.70	124.51
14	b	811	CLA	CHB-C4A-NA	3.03	128.70	124.51
14	1	1625	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
14	2	822	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
14	l	204	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
14	a	844	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
14	B	810	CLA	CHB-C4A-NA	3.03	128.70	124.51
14	1	1641	CLA	C3B-C4B-NB	-3.02	107.71	110.52
14	a	824	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
17	1	1652	BCR	C24-C23-C22	-3.02	121.67	126.23
14	1	1639	CLA	CMB-C2B-C3B	3.02	133.91	126.59
14	A	837	CLA	C3B-C4B-NB	-3.02	107.71	110.52
14	b	824	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
17	f	204	BCR	C2-C1-C6	3.02	115.13	110.48
14	1	1617	CLA	C3B-C4B-NB	-3.01	107.72	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1	1638	CLA	C3B-C4B-NB	-3.01	107.72	110.52
14	L	203	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
14	2	811	CLA	CHB-C4A-NA	3.01	128.67	124.51
14	a	838	CLA	CMB-C2B-C3B	3.01	133.87	126.59
14	A	838	CLA	CMB-C2B-C3B	3.00	133.87	126.59
14	b	824	CLA	CMB-C2B-C1B	-3.00	120.79	125.37
14	A	834	CLA	CHB-C4A-NA	3.00	128.66	124.51
14	A	828	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
14	1	1628	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
17	1	1651	BCR	C15-C16-C17	-3.00	117.33	123.47
14	A	827	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
14	a	827	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
17	a	850	BCR	C15-C16-C17	-3.00	117.33	123.47
14	a	830	CLA	C3B-C4B-NB	-3.00	107.73	110.52
14	b	822	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
14	A	843	CLA	C3B-C4B-NB	-2.99	107.74	110.52
14	1	1644	CLA	C3B-C4B-NB	-2.99	107.74	110.52
14	A	840	CLA	C3B-C4B-NB	-2.99	107.74	110.52
17	a	851	BCR	C24-C23-C22	-2.99	121.71	126.23
14	B	821	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
14	a	843	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
14	f	203	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
14	a	840	CLA	C3B-C4B-NB	-2.99	107.74	110.52
14	A	830	CLA	C3B-C4B-NB	-2.98	107.75	110.52
14	B	822	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
14	b	823	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
14	1	1636	CLA	CHB-C4A-NA	2.98	128.64	124.51
17	A	850	BCR	C15-C16-C17	-2.98	117.36	123.47
14	a	828	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
17	F	205	BCR	C2-C1-C6	2.98	115.07	110.48
14	a	821	CLA	CMB-C2B-C3B	2.98	133.80	126.59
14	A	827	CLA	C3B-C4B-NB	-2.98	107.75	110.52
14	a	843	CLA	C3B-C4B-NB	-2.98	107.75	110.52
14	b	831	CLA	C3B-C4B-NB	-2.98	107.75	110.52
14	2	819	CLA	C4-C3-C5	2.98	120.28	115.27
14	L	204	CLA	O2D-CGD-CBD	2.98	116.56	111.27
14	1	1629	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
14	A	830	CLA	CMB-C2B-C1B	-2.98	120.84	125.37
14	1	1614	CLA	C3B-C4B-NB	-2.98	107.75	110.52
14	b	819	CLA	C4-C3-C5	2.97	120.27	115.27
17	6	204	BCR	C2-C1-C6	2.97	115.06	110.48
14	A	843	CLA	O2D-CGD-O1D	-2.97	118.02	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	830	CLA	CHB-C4A-NA	2.97	128.62	124.51
14	b	839	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
14	B	826	CLA	C3B-C4B-NB	-2.97	107.76	110.52
14	F	204	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
14	2	823	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
14	1	1631	CLA	C3B-C4B-NB	-2.97	107.76	110.52
14	A	806	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
14	2	824	CLA	CMB-C2B-C1B	-2.97	120.85	125.37
14	a	827	CLA	C3B-C4B-NB	-2.97	107.76	110.52
14	a	806	CLA	CHB-C4A-NA	2.97	128.61	124.51
14	B	838	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
14	a	835	CLA	CHB-C4A-NA	2.96	128.61	124.51
14	0	206	CLA	O2D-CGD-CBD	2.96	116.54	111.27
14	A	819	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
14	a	830	CLA	CMB-C2B-C1B	-2.96	120.86	125.37
14	a	806	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
14	B	818	CLA	C4-C3-C5	2.96	120.26	115.27
14	B	823	CLA	CMB-C2B-C1B	-2.96	120.86	125.37
14	1	1622	CLA	CMB-C2B-C3B	2.96	133.76	126.59
14	b	821	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
14	6	203	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
14	2	832	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
14	a	820	CLA	CMB-C2B-C1B	-2.96	120.87	125.37
14	2	821	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
14	A	821	CLA	CMB-C2B-C3B	2.96	133.75	126.59
14	A	835	CLA	CHB-C4A-NA	2.95	128.60	124.51
14	a	830	CLA	CHB-C4A-NA	2.95	128.60	124.51
17	a	852	BCR	C15-C16-C17	-2.95	117.42	123.47
14	1	1634	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
14	1	1644	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
17	K	102	BCR	C7-C8-C9	-2.95	121.77	126.23
14	1	1621	CLA	CMB-C2B-C1B	-2.95	120.87	125.37
14	2	831	CLA	C3B-C4B-NB	-2.95	107.78	110.52
14	b	832	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
14	2	820	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
14	B	830	CLA	C3B-C4B-NB	-2.95	107.78	110.52
14	b	820	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
14	1	1631	CLA	CHB-C4A-NA	2.95	128.59	124.51
14	2	827	CLA	C3B-C4B-NB	-2.94	107.78	110.52
14	1	1628	CLA	C3B-C4B-NB	-2.94	107.78	110.52
14	B	820	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
14	B	831	CLA	O2D-CGD-O1D	-2.94	118.09	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	819	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
17	1	1653	BCR	C15-C16-C17	-2.94	117.45	123.47
14	1	1607	CLA	CHB-C4A-NA	2.94	128.58	124.51
14	1	1631	CLA	CMB-C2B-C1B	-2.94	120.89	125.37
14	A	833	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
17	A	852	BCR	C15-C16-C17	-2.94	117.46	123.47
14	l	205	CLA	O2D-CGD-CBD	2.94	116.48	111.27
14	1	1620	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
17	k	102	BCR	C7-C8-C9	-2.93	121.80	126.23
14	2	839	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
14	1	1607	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
14	1	1628	CLA	CMB-C2B-C1B	-2.93	120.91	125.37
17	9	102	BCR	C7-C8-C9	-2.93	121.81	126.23
17	L	207	BCR	C36-C18-C17	-2.93	118.82	122.92
14	B	819	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
17	L	201	BCR	C15-C16-C17	-2.93	117.48	123.47
14	A	806	CLA	CHB-C4A-NA	2.93	128.56	124.51
14	B	828	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
14	b	829	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
17	0	209	BCR	C36-C18-C17	-2.92	118.83	122.92
14	B	840	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
14	b	827	CLA	C3B-C4B-NB	-2.92	107.81	110.52
17	l	202	BCR	C15-C16-C17	-2.91	117.50	123.47
14	A	820	CLA	CMB-C2B-C1B	-2.91	120.93	125.37
14	A	827	CLA	CMB-C2B-C1B	-2.91	120.93	125.37
14	1	1642	CLA	C3B-C4B-NB	-2.91	107.81	110.52
14	L	203	CLA	CHB-C4A-NA	2.91	128.53	124.51
14	2	841	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
14	a	833	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
14	a	827	CLA	CMB-C2B-C1B	-2.90	120.94	125.37
17	0	203	BCR	C15-C16-C17	-2.90	117.53	123.47
14	2	826	CLA	CAA-C2A-C1A	-2.90	102.46	111.97
14	B	824	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
14	2	816	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
14	2	837	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
14	B	813	CLA	C3B-C4B-NB	-2.90	107.83	110.52
14	B	827	CLA	C3B-C4B-NB	-2.90	107.83	110.52
14	b	805	CLA	C3B-C4B-NB	-2.90	107.83	110.52
14	B	827	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
14	2	814	CLA	C3B-C4B-NB	-2.89	107.83	110.52
18	y	101	LHG	O8-C23-C24	2.89	120.98	111.91
14	b	841	CLA	O2D-CGD-O1D	-2.89	118.18	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	826	CLA	CAA-C2A-C1A	-2.89	102.50	111.97
14	B	841	CLA	C3B-C4B-NB	-2.89	107.83	110.52
14	b	842	CLA	C3B-C4B-NB	-2.89	107.83	110.52
14	k	103	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
14	9	103	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
14	2	828	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
14	2	834	CLA	C4-C3-C5	2.89	120.13	115.27
14	2	828	CLA	CHB-C1B-NB	2.89	127.31	124.26
14	b	834	CLA	C4-C3-C5	2.89	120.13	115.27
17	0	201	BCR	C36-C18-C17	-2.89	118.88	122.92
14	2	842	CLA	C3B-C4B-NB	-2.89	107.84	110.52
14	2	829	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
14	B	836	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
14	b	837	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
14	2	840	CLA	C3B-C4B-NB	-2.88	107.84	110.52
14	2	815	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
14	B	825	CLA	CAA-C2A-C1A	-2.88	102.53	111.97
18	M	101	LHG	O8-C23-C24	2.88	120.95	111.91
14	b	818	CLA	CHB-C4A-NA	2.88	128.49	124.51
14	a	818	CLA	CHB-C4A-NA	2.88	128.49	124.51
14	b	816	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
14	K	103	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
14	a	823	CLA	C3B-C4B-NB	-2.88	107.85	110.52
14	b	828	CLA	C3B-C4B-NB	-2.88	107.85	110.52
14	2	805	CLA	C3B-C4B-NB	-2.88	107.85	110.52
14	1	1619	CLA	CHB-C4A-NA	2.88	128.49	124.51
14	B	815	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
14	A	825	CLA	C1-C2-C3	-2.87	121.07	126.04
14	b	828	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
14	l	204	CLA	CHB-C4A-NA	2.87	128.48	124.51
14	B	833	CLA	C4-C3-C5	2.87	120.10	115.27
14	A	823	CLA	C3B-C4B-NB	-2.87	107.85	110.52
14	B	817	CLA	CHB-C4A-NA	2.87	128.48	124.51
14	A	841	CLA	C3B-C4B-NB	-2.87	107.86	110.52
14	b	825	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
18	m	101	LHG	O8-C23-C24	2.87	120.90	111.91
14	2	826	CLA	C3B-C4B-NB	-2.87	107.86	110.52
17	B	845	BCR	C24-C23-C22	-2.86	121.91	126.23
14	1	1633	CLA	C3B-C4B-NB	-2.86	107.86	110.52
14	2	825	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
14	B	804	CLA	C3B-C4B-NB	-2.86	107.86	110.52
14	b	842	CLA	CHB-C4A-NA	2.86	128.47	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	b	846	BCR	C24-C23-C22	-2.86	121.92	126.23
14	a	825	CLA	C1-C2-C3	-2.86	121.10	126.04
14	B	835	CLA	C1-C2-C3	-2.86	122.13	126.75
14	b	828	CLA	CHB-C1B-NB	2.86	127.28	124.26
17	2	844	BCR	C24-C23-C22	-2.85	121.92	126.23
14	2	842	CLA	CHB-C4A-NA	2.85	128.46	124.51
17	2	846	BCR	C24-C23-C22	-2.85	121.92	126.23
14	2	818	CLA	CHB-C4A-NA	2.85	128.46	124.51
14	1	1604	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
14	B	827	CLA	CHB-C1B-NB	2.85	127.28	124.26
14	1	1606	CLA	C3B-C4B-NB	-2.85	107.87	110.52
14	b	815	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
14	1	1623	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
14	B	814	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
17	b	844	BCR	C24-C23-C22	-2.85	121.93	126.23
14	B	825	CLA	C3B-C4B-NB	-2.85	107.88	110.52
14	1	1613	CLA	C3B-C4B-NB	-2.85	107.88	110.52
14	1	1624	CLA	C3B-C4B-NB	-2.85	107.88	110.52
14	a	826	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
13	1	1602	CL0	CHB-C4A-NA	2.84	128.45	124.51
14	B	827	CLA	CMB-C2B-C1B	-2.84	121.04	125.37
17	B	843	BCR	C24-C23-C22	-2.84	121.94	126.23
14	2	828	CLA	C3B-C4B-NB	-2.84	107.88	110.52
14	b	827	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
14	J	101	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
14	A	832	CLA	C3B-C4B-NB	-2.84	107.88	110.52
17	B	847	BCR	C27-C26-C25	2.84	126.85	122.73
14	1	1626	CLA	C1-C2-C3	-2.84	121.13	126.04
17	A	847	BCR	C15-C16-C17	-2.84	117.66	123.47
14	B	839	CLA	C3B-C4B-NB	-2.84	107.88	110.52
14	1	1627	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
14	b	826	CLA	C3B-C4B-NB	-2.83	107.89	110.52
14	A	802	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
14	A	822	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
14	8	1302	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
14	a	839	CLA	C3B-C4B-NB	-2.83	107.89	110.52
14	b	814	CLA	C3B-C4B-NB	-2.83	107.89	110.52
14	A	836	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
17	f	204	BCR	C16-C15-C14	-2.83	117.67	123.47
14	A	826	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
14	z	102	CLA	C3B-C4B-NB	-2.83	107.89	110.52
14	B	826	CLA	O2D-CGD-O1D	-2.83	118.30	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	841	CLA	CHB-C4A-NA	2.83	128.43	124.51
14	1	1637	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
14	a	836	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
14	a	821	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
14	a	818	CLA	C3B-C4B-NB	-2.83	107.89	110.52
13	a	801	CL0	CHB-C4A-NA	2.83	128.42	124.51
14	0	205	CLA	CHB-C4A-NA	2.83	128.42	124.51
14	a	840	CLA	CHB-C4A-NA	2.82	128.42	124.51
14	a	802	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
14	a	841	CLA	C3B-C4B-NB	-2.82	107.89	110.52
13	A	801	CL0	CHB-C4A-NA	2.82	128.42	124.51
14	1	1618	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
14	b	828	CLA	CMB-C2B-C1B	-2.82	121.07	125.37
14	a	822	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
17	a	847	BCR	C15-C16-C17	-2.82	117.69	123.47
14	j	1302	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
17	F	205	BCR	C16-C15-C14	-2.82	117.69	123.47
14	1	1641	CLA	CHB-C4A-NA	2.82	128.41	124.51
14	2	828	CLA	CMB-C2B-C1B	-2.82	121.07	125.37
14	A	814	CLA	C3B-C4B-NB	-2.82	107.90	110.52
14	2	841	CLA	C3B-C4B-NB	-2.82	107.90	110.52
17	1	1648	BCR	C15-C16-C17	-2.82	117.70	123.47
14	1	1622	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
14	A	807	CLA	CHB-C4A-NA	2.82	128.41	124.51
14	2	836	CLA	C1-C2-C3	-2.82	122.19	126.75
14	A	818	CLA	CHB-C4A-NA	2.82	128.41	124.51
14	2	838	CLA	CHB-C4A-NA	2.82	128.41	124.51
14	a	817	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
14	A	834	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
14	A	805	CLA	C3B-C4B-NB	-2.81	107.90	110.52
14	a	812	CLA	C3B-C4B-NB	-2.81	107.90	110.52
17	2	848	BCR	C27-C26-C25	2.81	126.82	122.73
14	x	1701	CLA	C3B-C4B-NB	-2.81	107.91	110.52
14	2	827	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
14	B	837	CLA	CHB-C4A-NA	2.81	128.40	124.51
14	a	807	CLA	CHB-C4A-NA	2.81	128.40	124.51
14	1	1608	CLA	CHB-C4A-NA	2.81	128.40	124.51
14	b	840	CLA	C3B-C4B-NB	-2.81	107.91	110.52
14	1	1640	CLA	C3B-C4B-NB	-2.81	107.91	110.52
17	0	203	BCR	C37-C22-C21	-2.81	118.99	122.92
14	a	832	CLA	C3B-C4B-NB	-2.81	107.91	110.52
14	B	810	CLA	O2D-CGD-O1D	-2.81	118.35	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	851	BCR	C15-C16-C17	-2.81	117.72	123.47
14	A	818	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
14	A	817	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
14	A	804	CLA	CHB-C4A-NA	2.81	128.39	124.51
14	B	814	CLA	C3B-C4B-NB	-2.81	107.91	110.52
14	a	804	CLA	CHB-C4A-NA	2.80	128.39	124.51
14	a	818	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
14	A	803	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
17	8	1306	BCR	C15-C16-C17	-2.80	117.73	123.47
14	1	1603	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
17	b	848	BCR	C27-C26-C25	2.80	126.80	122.73
14	b	838	CLA	CHB-C4A-NA	2.80	128.38	124.51
14	B	803	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
14	a	834	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
14	a	805	CLA	C3B-C4B-NB	-2.80	107.92	110.52
14	1	1612	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
14	b	836	CLA	C1-C2-C3	-2.80	122.22	126.75
14	A	812	CLA	C3B-C4B-NB	-2.80	107.92	110.52
14	A	821	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
14	a	803	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
17	6	204	BCR	C16-C15-C14	-2.79	117.75	123.47
14	2	811	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
17	L	201	BCR	C37-C22-C21	-2.79	119.01	122.92
14	a	814	CLA	C3B-C4B-NB	-2.79	107.92	110.52
14	1	1619	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
14	a	836	CLA	C3B-C4B-NB	-2.79	107.93	110.52
14	1	1619	CLA	C3B-C4B-NB	-2.79	107.93	110.52
14	1	1621	CLA	CHB-C4A-NA	2.79	128.37	124.51
14	b	815	CLA	C3B-C4B-NB	-2.79	107.93	110.52
14	b	811	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
17	f	202	BCR	C15-C16-C17	-2.79	117.76	123.47
14	A	840	CLA	CHB-C4A-NA	2.79	128.37	124.51
17	b	852	BCR	C15-C16-C17	-2.79	117.77	123.47
14	2	804	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
17	F	202	BCR	C15-C16-C17	-2.78	117.78	123.47
17	6	202	BCR	C15-C16-C17	-2.78	117.78	123.47
14	1	1635	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
14	A	839	CLA	C3B-C4B-NB	-2.78	107.94	110.52
14	B	840	CLA	C3B-C4B-NB	-2.77	107.94	110.52
17	L	201	BCR	C2-C1-C6	2.77	114.75	110.48
14	1	1605	CLA	CHB-C4A-NA	2.77	128.35	124.51
14	b	804	CLA	O2D-CGD-O1D	-2.77	118.42	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	811	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
14	a	811	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
14	A	820	CLA	CHB-C4A-NA	2.77	128.34	124.51
14	a	820	CLA	CHB-C4A-NA	2.77	128.34	124.51
14	2	807	CLA	C3B-C4B-NB	-2.77	107.94	110.52
14	2	807	CLA	CHB-C4A-NA	2.77	128.34	124.51
14	L	203	CLA	CHB-C1B-NB	2.77	127.19	124.26
14	1	1626	CLA	CHB-C1B-NB	2.77	127.19	124.26
14	a	814	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
14	A	823	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
14	A	855	CLA	CMB-C2B-C3B	2.77	133.29	126.59
14	b	807	CLA	CHB-C4A-NA	2.77	128.34	124.51
17	l	202	BCR	C37-C22-C21	-2.77	119.05	122.92
14	a	823	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
14	2	814	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
14	A	825	CLA	CHB-C1B-NB	2.76	127.18	124.26
17	0	203	BCR	C2-C1-C6	2.76	114.74	110.48
14	1	1615	CLA	C3B-C4B-NB	-2.76	107.95	110.52
14	b	810	CLA	C4-C3-C5	2.76	119.92	115.27
14	X	1701	CLA	C3B-C4B-NB	-2.76	107.95	110.52
14	A	818	CLA	C3B-C4B-NB	-2.76	107.95	110.52
14	B	834	CLA	C3B-C4B-NB	-2.76	107.95	110.52
17	b	847	BCR	C27-C26-C25	2.76	126.74	122.73
14	a	825	CLA	CHB-C1B-NB	2.76	127.18	124.26
14	2	815	CLA	C3B-C4B-NB	-2.76	107.96	110.52
14	b	802	CLA	CMB-C2B-C3B	2.76	133.27	126.59
14	b	841	CLA	C3B-C4B-NB	-2.75	107.96	110.52
14	B	806	CLA	CHB-C4A-NA	2.75	128.32	124.51
17	6	202	BCR	C2-C1-C6	2.75	114.72	110.48
14	1	1613	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
14	2	836	CLA	CHB-C4A-NA	2.75	128.31	124.51
17	F	202	BCR	C2-C1-C6	2.75	114.71	110.48
17	f	202	BCR	C2-C1-C6	2.75	114.71	110.48
14	B	815	CLA	C3B-C4B-NB	-2.75	107.97	110.52
14	1	1637	CLA	C3B-C4B-NB	-2.75	107.97	110.52
14	B	809	CLA	C4-C3-C5	2.75	119.89	115.27
14	a	807	CLA	CMB-C2B-C3B	2.75	133.24	126.59
14	A	814	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
14	A	836	CLA	C3B-C4B-NB	-2.74	107.97	110.52
14	1	1624	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
14	B	808	CLA	O2A-CGA-O1A	-2.74	116.67	123.59
14	2	809	CLA	O2A-CGA-O1A	-2.74	116.67	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1	1609	CLA	O2D-CGD-CBD	2.74	116.14	111.27
14	B	809	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
14	1	1615	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
14	b	836	CLA	CHB-C4A-NA	2.74	128.30	124.51
14	a	838	CLA	O2A-CGA-O1A	-2.74	116.68	123.59
14	b	814	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
14	A	808	CLA	O2D-CGD-CBD	2.74	116.13	111.27
14	2	835	CLA	C3B-C4B-NB	-2.73	107.98	110.52
14	A	812	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
14	b	816	CLA	C3B-C4B-NB	-2.73	107.98	110.52
14	1	1623	CLA	C3B-C4B-NB	-2.73	107.98	110.52
14	B	835	CLA	CHB-C4A-NA	2.73	128.29	124.51
17	l	202	BCR	C2-C1-C6	2.73	114.69	110.48
14	2	802	CLA	CMB-C2B-C3B	2.73	133.21	126.59
14	b	809	CLA	O2A-CGA-O1A	-2.73	116.70	123.59
14	B	814	CLA	CHB-C4A-NA	2.73	128.29	124.51
17	B	846	BCR	C27-C26-C25	2.73	126.69	122.73
14	1	1608	CLA	CMB-C2B-C3B	2.73	133.19	126.59
14	1	1639	CLA	O2A-CGA-O1A	-2.73	116.71	123.59
14	2	810	CLA	C4-C3-C5	2.73	119.86	115.27
14	2	803	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
17	i	101	BCR	C15-C16-C17	-2.72	117.89	123.47
14	B	813	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
14	2	816	CLA	C3B-C4B-NB	-2.72	107.99	110.52
14	k	101	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
14	l	204	CLA	CHB-C1B-NB	2.72	127.14	124.26
14	9	101	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
14	a	832	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
14	b	810	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
14	1	1624	CLA	CHB-C4A-NA	2.72	128.27	124.51
14	K	101	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
14	a	812	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
17	I	101	BCR	C15-C16-C17	-2.72	117.91	123.47
17	0	201	BCR	C15-C16-C17	-2.72	117.91	123.47
14	B	833	CLA	C3B-C4B-NB	-2.72	108.00	110.52
14	1	1609	CLA	C3B-C4B-NB	-2.72	108.00	110.52
14	A	807	CLA	CMB-C2B-C3B	2.71	133.16	126.59
17	7	101	BCR	C15-C16-C17	-2.71	117.92	123.47
14	B	802	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
17	L	207	BCR	C15-C16-C17	-2.71	117.92	123.47
14	b	835	CLA	C3B-C4B-NB	-2.71	108.00	110.52
17	2	847	BCR	C27-C26-C25	2.71	126.67	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	0	209	BCR	C15-C16-C17	-2.71	117.92	123.47
14	a	823	CLA	CHB-C4A-NA	2.71	128.26	124.51
14	b	805	CLA	CHB-C4A-NA	2.71	128.26	124.51
14	2	815	CLA	CHB-C4A-NA	2.71	128.26	124.51
14	A	838	CLA	O2A-CGA-O1A	-2.71	116.76	123.59
14	b	803	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
14	A	822	CLA	C3B-C4B-NB	-2.71	108.00	110.52
14	a	808	CLA	O2D-CGD-CBD	2.70	116.07	111.27
14	0	205	CLA	CHB-C1B-NB	2.70	127.12	124.26
14	B	806	CLA	C3B-C4B-NB	-2.70	108.01	110.52
14	b	831	CLA	CHD-C1D-ND	-2.70	121.97	124.45
17	2	849	BCR	C15-C16-C17	-2.70	117.94	123.47
14	A	823	CLA	CHB-C4A-NA	2.70	128.24	124.51
14	B	836	CLA	C3B-C4B-NB	-2.70	108.01	110.52
14	A	832	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
14	b	815	CLA	CHB-C4A-NA	2.70	128.24	124.51
14	b	811	CLA	C3B-C4B-NB	-2.69	108.02	110.52
14	2	810	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
20	B	849	LMG	O6-C1-O1	-2.69	103.60	109.97
14	2	837	CLA	C3B-C4B-NB	-2.69	108.02	110.52
14	B	804	CLA	CHB-C4A-NA	2.69	128.23	124.51
14	A	821	CLA	CHB-C4A-NA	2.69	128.23	124.51
14	1	1642	CLA	CHB-C4A-NA	2.69	128.23	124.51
14	2	805	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
14	a	821	CLA	CHB-C4A-NA	2.69	128.23	124.51
14	b	805	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
20	2	850	LMG	O6-C1-O1	-2.69	103.61	109.97
14	A	808	CLA	C3B-C4B-NB	-2.69	108.02	110.52
14	A	841	CLA	CHB-C4A-NA	2.69	128.23	124.51
14	B	803	CLA	CHB-C4A-NA	2.69	128.23	124.51
14	a	822	CLA	C3B-C4B-NB	-2.69	108.02	110.52
14	A	840	CLA	O2D-CGD-CBD	2.68	116.04	111.27
14	2	805	CLA	CHB-C4A-NA	2.68	128.22	124.51
14	a	808	CLA	C3B-C4B-NB	-2.68	108.03	110.52
17	B	848	BCR	C15-C16-C17	-2.68	117.98	123.47
14	1	1633	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
14	b	822	CLA	CHB-C4A-NA	2.68	128.22	124.51
14	B	804	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
17	b	849	BCR	C15-C16-C17	-2.68	117.98	123.47
14	b	834	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
14	B	833	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
14	A	830	CLA	CMB-C2B-C3B	2.68	133.07	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	841	CLA	CHB-C4A-NA	2.68	128.22	124.51
14	B	821	CLA	CHB-C4A-NA	2.68	128.21	124.51
14	A	806	CLA	C3B-C4B-NB	-2.68	108.03	110.52
14	2	811	CLA	C3B-C4B-NB	-2.68	108.03	110.52
14	1	1632	CLA	CHB-C4A-NA	2.68	128.21	124.51
17	2	846	BCR	C37-C22-C21	-2.68	119.17	122.92
20	b	850	LMG	O6-C1-O1	-2.68	103.64	109.97
14	a	806	CLA	C3B-C4B-NB	-2.68	108.03	110.52
14	1	1622	CLA	CHB-C4A-NA	2.67	128.21	124.51
14	b	807	CLA	C3B-C4B-NB	-2.67	108.04	110.52
14	2	831	CLA	CHD-C1D-ND	-2.67	122.00	124.45
14	b	837	CLA	C3B-C4B-NB	-2.67	108.04	110.52
14	2	825	CLA	C3B-C4B-NB	-2.67	108.04	110.52
14	b	809	CLA	C3A-C2A-C1A	2.67	105.34	101.34
14	2	834	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
17	K	104	BCR	C15-C16-C17	-2.67	118.01	123.47
18	0	202	LHG	O8-C23-C24	2.66	120.27	111.91
17	9	102	BCR	C15-C16-C17	-2.66	118.02	123.47
14	2	833	CLA	CHB-C4A-NA	2.66	128.19	124.51
14	1	1621	CLA	O2D-CGD-CBD	2.66	116.00	111.27
14	B	832	CLA	CHB-C4A-NA	2.66	128.19	124.51
14	A	831	CLA	CHB-C4A-NA	2.66	128.19	124.51
14	a	830	CLA	CMB-C2B-C3B	2.66	133.03	126.59
17	K	102	BCR	C15-C16-C17	-2.66	118.03	123.47
14	0	207	CLA	CHB-C4A-NA	2.66	128.19	124.51
14	A	809	CLA	C3B-C4B-NB	-2.66	108.05	110.52
14	b	833	CLA	CHB-C4A-NA	2.66	128.19	124.51
14	a	842	CLA	CHB-C1B-NB	2.66	127.07	124.26
17	B	845	BCR	C37-C22-C21	-2.66	119.20	122.92
14	B	831	CLA	CMB-C2B-C1B	-2.65	121.33	125.37
17	a	852	BCR	C15-C14-C13	-2.65	123.52	127.31
14	A	842	CLA	CHB-C1B-NB	2.65	127.07	124.26
17	9	104	BCR	C15-C16-C17	-2.65	118.04	123.47
14	B	823	CLA	CHB-C4A-NA	2.65	128.18	124.51
14	2	822	CLA	CHB-C4A-NA	2.65	128.18	124.51
14	b	825	CLA	C3B-C4B-NB	-2.65	108.06	110.52
17	k	102	BCR	C15-C16-C17	-2.65	118.05	123.47
14	b	824	CLA	CHB-C4A-NA	2.65	128.18	124.51
17	k	104	BCR	C15-C16-C17	-2.65	118.05	123.47
14	A	820	CLA	O2D-CGD-CBD	2.65	115.97	111.27
18	L	208	LHG	O8-C23-C24	2.65	120.22	111.91
14	a	827	CLA	CHB-C1B-NB	2.65	127.06	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	802	CLA	CMB-C2B-C3B	2.65	133.00	126.59
18	A	853	LHG	C20-C19-C18	-2.65	100.98	114.42
17	b	846	BCR	C37-C22-C21	-2.65	119.21	122.92
14	k	103	CLA	C3B-C4B-NB	-2.65	108.06	110.52
14	1	1641	CLA	O2D-CGD-CBD	2.65	115.97	111.27
14	a	840	CLA	O2D-CGD-CBD	2.65	115.97	111.27
14	B	810	CLA	C3B-C4B-NB	-2.65	108.06	110.52
14	a	831	CLA	CHB-C4A-NA	2.65	128.17	124.51
14	1	1603	CLA	CMB-C2B-C3B	2.65	133.00	126.59
18	l	201	LHG	O8-C23-C24	2.64	120.21	111.91
14	1	1631	CLA	CMB-C2B-C3B	2.64	132.99	126.59
14	1	1628	CLA	CHB-C1B-NB	2.64	127.06	124.26
14	a	834	CLA	CMB-C2B-C1B	-2.64	121.34	125.37
14	l	206	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	a	853	LHG	C20-C19-C18	-2.64	101.02	114.42
14	K	103	CLA	C3B-C4B-NB	-2.64	108.07	110.52
14	b	834	CLA	C3B-C4B-NB	-2.64	108.07	110.52
17	1	1653	BCR	C15-C14-C13	-2.64	123.54	127.31
14	2	834	CLA	C3B-C4B-NB	-2.64	108.07	110.52
14	A	802	CLA	CMB-C2B-C3B	2.64	132.98	126.59
14	A	825	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
14	b	804	CLA	CHB-C4A-NA	2.64	128.16	124.51
14	1	1639	CLA	CHB-C4A-NA	2.64	128.16	124.51
14	9	103	CLA	C3B-C4B-NB	-2.64	108.07	110.52
14	B	816	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	1	1654	LHG	C20-C19-C18	-2.64	101.05	114.42
14	2	817	CLA	CHB-C4A-NA	2.64	128.16	124.51
14	2	832	CLA	CMB-C2B-C1B	-2.63	121.36	125.37
14	b	817	CLA	CHB-C4A-NA	2.63	128.16	124.51
14	2	831	CLA	CHB-C4A-NA	2.63	128.16	124.51
14	L	205	CLA	CHB-C4A-NA	2.63	128.15	124.51
14	a	820	CLA	O2D-CGD-CBD	2.63	115.95	111.27
14	2	819	CLA	C3B-C4B-NB	-2.63	108.07	110.52
14	a	838	CLA	CHB-C4A-NA	2.63	128.15	124.51
14	B	838	CLA	C3B-C4B-NB	-2.63	108.07	110.52
14	2	809	CLA	C3A-C2A-C1A	2.63	105.28	101.34
14	A	834	CLA	CMB-C2B-C1B	-2.63	121.36	125.37
14	b	831	CLA	CHB-C4A-NA	2.63	128.15	124.51
14	b	823	CLA	C3B-C4B-NB	-2.63	108.08	110.52
14	2	809	CLA	C1-C2-C3	-2.63	121.50	126.04
14	A	827	CLA	CHB-C1B-NB	2.63	127.04	124.26
14	a	825	CLA	O2D-CGD-O1D	-2.63	118.70	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	824	CLA	CHB-C4A-NA	2.63	128.15	124.51
14	1	1635	CLA	CMB-C2B-C1B	-2.63	121.37	125.37
14	2	830	CLA	C2D-C1D-ND	-2.62	108.17	110.10
14	L	205	CLA	CMB-C2B-C1B	-2.62	121.37	125.37
17	A	852	BCR	C15-C14-C13	-2.62	123.57	127.31
14	A	838	CLA	CHB-C4A-NA	2.62	128.14	124.51
14	1	1626	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
17	1	1652	BCR	C2-C1-C6	2.62	114.52	110.48
14	L	204	CLA	CHB-C4A-NA	2.62	128.14	124.51
17	A	851	BCR	C15-C16-C17	-2.62	118.11	123.47
18	z	101	LHG	O8-C23-C24	2.62	120.13	111.91
17	A	851	BCR	C16-C15-C14	-2.62	118.11	123.47
17	a	851	BCR	C2-C1-C6	2.62	114.51	110.48
14	a	841	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
18	B	850	LHG	O8-C23-C24	2.62	120.12	111.91
14	1	1607	CLA	C3B-C4B-NB	-2.62	108.09	110.52
17	A	851	BCR	C2-C1-C6	2.61	114.51	110.48
18	b	851	LHG	O8-C23-C24	2.61	120.11	111.91
14	0	206	CLA	CHB-C4A-NA	2.61	128.13	124.51
17	2	846	BCR	C27-C26-C25	2.61	126.53	122.73
14	b	819	CLA	C3B-C4B-NB	-2.61	108.09	110.52
14	2	823	CLA	C3B-C4B-NB	-2.61	108.09	110.52
14	1	1643	CLA	CHB-C1B-NB	2.61	127.02	124.26
14	B	822	CLA	C3B-C4B-NB	-2.61	108.09	110.52
14	2	804	CLA	CHB-C4A-NA	2.61	128.12	124.51
14	l	206	CLA	CMB-C2B-C1B	-2.61	121.39	125.37
14	a	843	CLA	CHB-C4A-NA	2.61	128.12	124.51
14	1	1644	CLA	CHB-C4A-NA	2.61	128.12	124.51
14	F	203	CLA	CMB-C2B-C3B	2.61	132.91	126.59
14	1	1642	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
14	A	822	CLA	CMB-C2B-C1B	-2.61	121.40	125.37
17	b	846	BCR	C27-C26-C25	2.61	126.52	122.73
14	A	815	CLA	CHB-C4A-NA	2.61	128.12	124.51
14	a	838	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
14	1	1612	CLA	CHB-C4A-NA	2.60	128.11	124.51
14	l	205	CLA	CHB-C4A-NA	2.60	128.11	124.51
14	b	832	CLA	CMB-C2B-C1B	-2.60	121.40	125.37
14	1	1610	CLA	C3B-C4B-NB	-2.60	108.10	110.52
14	B	808	CLA	C3A-C2A-C1A	2.60	105.24	101.34
14	B	805	CLA	CMB-C2B-C3B	2.60	132.89	126.59
14	B	830	CLA	CHB-C4A-NA	2.60	128.11	124.51
14	A	834	CLA	C3B-C4B-NB	-2.60	108.10	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	1	1652	BCR	C16-C15-C14	-2.60	118.14	123.47
14	A	802	CLA	C1-C2-C3	-2.60	121.54	126.04
14	B	824	CLA	C3B-C4B-NB	-2.60	108.10	110.52
14	B	827	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
14	1	1623	CLA	CMB-C2B-C1B	-2.60	121.41	125.37
14	0	207	CLA	CMB-C2B-C1B	-2.60	121.41	125.37
14	b	826	CLA	CHD-C1D-ND	-2.60	122.06	124.45
14	A	807	CLA	O1D-CGD-CBD	2.60	129.81	124.48
17	a	851	BCR	C16-C15-C14	-2.60	118.15	123.47
14	a	807	CLA	O1D-CGD-CBD	2.60	129.80	124.48
14	j	1301	CLA	CMB-C2B-C3B	2.60	132.88	126.59
14	2	828	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
14	B	817	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
14	1	1617	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
14	A	816	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
14	A	841	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
14	B	818	CLA	C3B-C4B-NB	-2.60	108.11	110.52
14	a	834	CLA	C3B-C4B-NB	-2.60	108.11	110.52
17	2	849	BCR	C16-C15-C14	-2.60	118.16	123.47
14	b	809	CLA	C1-C2-C3	-2.59	121.56	126.04
14	2	818	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
14	a	839	CLA	O2D-CGD-CBD	2.59	115.88	111.27
17	j	1305	BCR	C15-C16-C17	-2.59	118.16	123.47
17	8	1305	BCR	C15-C16-C17	-2.59	118.16	123.47
14	A	838	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
17	A	856	BCR	C15-C16-C17	-2.59	118.17	123.47
14	A	811	CLA	CHB-C4A-NA	2.59	128.09	124.51
14	1	1603	CLA	C1-C2-C3	-2.59	121.56	126.04
14	a	835	CLA	C3B-C4B-NB	-2.59	108.11	110.52
17	2	846	BCR	C15-C16-C17	-2.59	118.17	123.47
14	A	802	CLA	CHB-C4A-NA	2.59	128.09	124.51
14	b	806	CLA	CMB-C2B-C3B	2.59	132.86	126.59
14	8	1301	CLA	CMB-C2B-C3B	2.59	132.86	126.59
14	A	843	CLA	CHB-C4A-NA	2.59	128.09	124.51
14	1	1623	CLA	CHB-C4A-NA	2.59	128.09	124.51
17	1	1652	BCR	C15-C16-C17	-2.59	118.17	123.47
14	a	822	CLA	CMB-C2B-C1B	-2.59	121.43	125.37
14	b	839	CLA	C3B-C4B-NB	-2.59	108.11	110.52
14	b	828	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
14	A	817	CLA	C3B-C4B-NB	-2.59	108.12	110.52
14	B	830	CLA	CHD-C1D-ND	-2.59	122.08	124.45
14	a	811	CLA	CHB-C4A-NA	2.59	128.09	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1	1603	CLA	CHB-C4A-NA	2.59	128.09	124.51
14	A	813	CLA	CHB-C4A-NA	2.58	128.09	124.51
14	B	811	CLA	CHB-C4A-NA	2.58	128.09	124.51
14	2	839	CLA	C3B-C4B-NB	-2.58	108.12	110.52
14	A	827	CLA	C1-C2-C3	-2.58	121.58	126.04
14	1	1614	CLA	CHB-C4A-NA	2.58	128.08	124.51
14	a	802	CLA	C1-C2-C3	-2.58	121.58	126.04
14	A	822	CLA	CHB-C4A-NA	2.58	128.08	124.51
17	L	206	BCR	C15-C16-C17	-2.58	118.19	123.47
17	b	849	BCR	C16-C15-C14	-2.58	118.19	123.47
14	a	822	CLA	CHB-C4A-NA	2.58	128.08	124.51
14	B	808	CLA	C1-C2-C3	-2.58	121.58	126.04
14	a	839	CLA	C1-C2-C3	-2.58	121.58	126.04
14	a	809	CLA	C3B-C4B-NB	-2.58	108.12	110.52
14	2	806	CLA	CMB-C2B-C3B	2.58	132.83	126.59
17	a	851	BCR	C15-C16-C17	-2.58	118.20	123.47
14	a	815	CLA	CHB-C4A-NA	2.58	128.07	124.51
14	2	819	CLA	CHB-C4A-NA	2.58	128.07	124.51
17	B	845	BCR	C27-C26-C25	2.57	126.47	122.73
14	B	829	CLA	C2D-C1D-ND	-2.57	108.21	110.10
17	B	848	BCR	C16-C15-C14	-2.57	118.20	123.47
17	a	847	BCR	C27-C26-C25	2.57	126.47	122.73
14	1	1616	CLA	CHB-C4A-NA	2.57	128.07	124.51
14	1	1608	CLA	O1D-CGD-CBD	2.57	129.75	124.48
14	1	1616	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
14	a	815	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
17	A	847	BCR	C27-C26-C25	2.57	126.46	122.73
14	A	839	CLA	C1-C2-C3	-2.57	121.60	126.04
14	b	818	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
17	B	845	BCR	C15-C16-C17	-2.57	118.22	123.47
14	a	816	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
14	A	821	CLA	C3B-C4B-NB	-2.57	108.14	110.52
14	A	815	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
14	a	802	CLA	CHB-C4A-NA	2.56	128.06	124.51
17	0	208	BCR	C15-C16-C17	-2.56	118.22	123.47
14	a	817	CLA	C3B-C4B-NB	-2.56	108.14	110.52
14	1	1640	CLA	C1-C2-C3	-2.56	121.61	126.04
17	1	1648	BCR	C27-C26-C25	2.56	126.45	122.73
17	b	846	BCR	C15-C16-C17	-2.56	118.23	123.47
17	l	207	BCR	C15-C16-C17	-2.56	118.23	123.47
14	a	821	CLA	C3B-C4B-NB	-2.56	108.14	110.52
14	1	1640	CLA	O2D-CGD-CBD	2.56	115.82	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	816	CLA	CHB-C4A-NA	2.56	128.05	124.51
14	1	1609	CLA	CHB-C4A-NA	2.55	128.04	124.51
14	1	1628	CLA	C1-C2-C3	-2.55	121.62	126.04
17	A	848	BCR	C27-C26-C25	2.55	126.44	122.73
14	B	825	CLA	CHD-C1D-ND	-2.55	122.11	124.45
14	a	827	CLA	C1-C2-C3	-2.55	121.63	126.04
14	2	812	CLA	CHB-C4A-NA	2.55	128.04	124.51
17	0	201	BCR	C27-C26-C25	2.55	126.44	122.73
14	j	1302	CLA	C3B-C4B-NB	-2.55	108.15	110.52
14	1	1628	CLA	CAA-C2A-C1A	-2.55	103.61	111.97
17	a	848	BCR	C27-C26-C25	2.55	126.44	122.73
14	A	839	CLA	O2D-CGD-CBD	2.55	115.80	111.27
17	0	209	BCR	C27-C26-C25	2.55	126.44	122.73
14	b	836	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
14	1	1639	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
14	a	808	CLA	CHB-C4A-NA	2.55	128.04	124.51
14	a	827	CLA	CAA-C2A-C1A	-2.55	103.62	111.97
14	2	832	CLA	CHB-C4A-NA	2.55	128.03	124.51
14	j	1302	CLA	CHB-C4A-NA	2.55	128.03	124.51
14	a	826	CLA	C3B-C4B-NB	-2.55	108.15	110.52
14	1	1638	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
14	A	827	CLA	CAA-C2A-C1A	-2.54	103.64	111.97
14	b	830	CLA	C2D-C1D-ND	-2.54	108.23	110.10
14	2	829	CLA	C3B-C4B-NB	-2.54	108.16	110.52
14	B	831	CLA	CHB-C4A-NA	2.54	128.03	124.51
14	a	813	CLA	CHB-C4A-NA	2.54	128.03	124.51
14	2	811	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
14	A	810	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
14	B	810	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
17	l	207	BCR	C7-C8-C9	-2.54	122.40	126.23
14	b	830	CLA	O2D-CGD-CBD	2.54	115.78	111.27
14	J	101	CLA	CHB-C4A-NA	2.54	128.02	124.51
14	A	837	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
14	9	101	CLA	CHB-C4A-NA	2.54	128.02	124.51
14	A	808	CLA	CHB-C4A-NA	2.54	128.02	124.51
14	B	835	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
14	b	812	CLA	CHB-C4A-NA	2.53	128.02	124.51
14	2	836	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
14	B	818	CLA	CHB-C4A-NA	2.53	128.01	124.51
14	b	829	CLA	C3B-C4B-NB	-2.53	108.17	110.52
14	0	207	CLA	C3B-C4B-NB	-2.53	108.17	110.52
14	1	1635	CLA	C3B-C4B-NB	-2.53	108.17	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	836	CLA	CHB-C4A-NA	2.53	128.01	124.51
14	a	837	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
17	f	202	BCR	C27-C26-C25	2.53	126.40	122.73
14	b	811	CLA	O2A-CGA-O1A	-2.53	117.21	123.59
14	8	1302	CLA	CHB-C4A-NA	2.53	128.01	124.51
14	1	1636	CLA	C3B-C4B-NB	-2.53	108.17	110.52
17	F	202	BCR	C27-C26-C25	2.53	126.40	122.73
14	B	829	CLA	O2D-CGD-CBD	2.52	115.75	111.27
14	J	101	CLA	C3B-C4B-NB	-2.52	108.17	110.52
14	B	831	CLA	C3B-C4B-NB	-2.52	108.17	110.52
14	b	832	CLA	CHB-C4A-NA	2.52	128.00	124.51
14	1	1625	CLA	CHB-C4A-NA	2.52	128.00	124.51
14	1	1627	CLA	C3B-C4B-NB	-2.52	108.18	110.52
14	8	1302	CLA	C3B-C4B-NB	-2.52	108.18	110.52
14	2	826	CLA	CHD-C1D-ND	-2.52	122.14	124.45
14	b	819	CLA	CHB-C4A-NA	2.52	128.00	124.51
14	A	810	CLA	CMB-C2B-C1B	-2.52	121.53	125.37
14	l	206	CLA	C3B-C4B-NB	-2.52	108.18	110.52
14	1	1622	CLA	C3B-C4B-NB	-2.52	108.18	110.52
17	0	208	BCR	C29-C30-C25	2.52	114.36	110.48
17	L	206	BCR	C7-C8-C9	-2.52	122.43	126.23
17	1	1649	BCR	C27-C26-C25	2.52	126.39	122.73
14	b	830	CLA	CHB-C4A-NA	2.52	127.99	124.51
14	A	835	CLA	C3B-C4B-NB	-2.52	108.18	110.52
14	a	810	CLA	CMB-C2B-C1B	-2.52	121.54	125.37
14	1	1645	CLA	CMB-C2B-C1B	-2.52	121.54	125.37
14	2	835	CLA	CHB-C4A-NA	2.52	127.99	124.51
14	A	826	CLA	C3B-C4B-NB	-2.51	108.18	110.52
14	2	830	CLA	CHB-C4A-NA	2.51	127.99	124.51
14	K	103	CLA	CMB-C2B-C1B	-2.51	121.54	125.37
14	2	817	CLA	O2D-CGD-CBD	2.51	115.73	111.27
14	2	830	CLA	O2D-CGD-CBD	2.51	115.73	111.27
14	1	1637	CLA	CHB-C4A-NA	2.51	127.99	124.51
14	B	823	CLA	C3B-C4B-NB	-2.51	108.19	110.52
14	b	832	CLA	C3B-C4B-NB	-2.51	108.19	110.52
14	A	827	CLA	CHB-C4A-NA	2.51	127.98	124.51
17	L	207	BCR	C27-C26-C25	2.51	126.37	122.73
14	B	829	CLA	CHB-C4A-NA	2.51	127.98	124.51
17	6	202	BCR	C27-C26-C25	2.51	126.37	122.73
14	f	201	CLA	CHB-C1B-NB	2.51	126.91	124.26
14	1	1618	CLA	C3B-C4B-NB	-2.51	108.19	110.52
14	2	806	CLA	CHB-C4A-NA	2.51	127.98	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	828	CLA	C3B-C4B-NB	-2.51	108.19	110.52
14	K	101	CLA	CHB-C4A-NA	2.51	127.98	124.51
14	a	844	CLA	CMB-C2B-C1B	-2.50	121.56	125.37
14	b	817	CLA	O2D-CGD-CBD	2.50	115.72	111.27
17	B	848	BCR	C27-C26-C25	2.50	126.37	122.73
17	b	849	BCR	C27-C26-C25	2.50	126.36	122.73
17	1	1649	BCR	C15-C14-C13	-2.50	123.74	127.31
14	9	103	CLA	CMB-C2B-C1B	-2.50	121.56	125.37
14	a	837	CLA	CHB-C1B-NB	2.50	126.91	124.26
14	b	835	CLA	CHB-C4A-NA	2.50	127.97	124.51
17	A	848	BCR	C15-C14-C13	-2.50	123.74	127.31
14	a	836	CLA	CHB-C4A-NA	2.50	127.96	124.51
17	a	848	BCR	C15-C14-C13	-2.50	123.75	127.31
14	B	816	CLA	O2D-CGD-CBD	2.49	115.70	111.27
14	B	834	CLA	CHB-C4A-NA	2.49	127.96	124.51
14	a	824	CLA	CHB-C4A-NA	2.49	127.96	124.51
14	A	844	CLA	CMB-C2B-C1B	-2.49	121.58	125.37
14	1	1638	CLA	CHB-C1B-NB	2.49	126.89	124.26
14	1	1611	CLA	CMB-C2B-C1B	-2.49	121.58	125.37
14	a	810	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
17	b	847	BCR	C38-C26-C25	-2.49	121.73	124.53
14	A	816	CLA	CHB-C4A-NA	2.49	127.95	124.51
17	0	208	BCR	C7-C8-C9	-2.49	122.47	126.23
14	1	1607	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
14	a	827	CLA	CHB-C4A-NA	2.49	127.95	124.51
14	A	825	CLA	CMB-C2B-C1B	-2.49	121.58	125.37
14	1	1611	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
14	k	101	CLA	CHB-C4A-NA	2.48	127.95	124.51
17	2	846	BCR	C38-C26-C25	-2.48	121.74	124.53
17	2	849	BCR	C27-C26-C25	2.48	126.33	122.73
14	b	808	CLA	CHB-C4A-NA	2.48	127.94	124.51
14	1	1626	CLA	CMB-C2B-C1B	-2.48	121.59	125.37
14	b	806	CLA	CHB-C4A-NA	2.48	127.94	124.51
14	1	1617	CLA	CHB-C4A-NA	2.48	127.94	124.51
14	2	832	CLA	C3B-C4B-NB	-2.47	108.22	110.52
14	b	827	CLA	CHB-C4A-NA	2.47	127.93	124.51
17	6	204	BCR	C38-C26-C25	-2.47	121.75	124.53
14	2	822	CLA	CMB-C2B-C3B	2.47	132.58	126.59
14	a	813	CLA	CHB-C1B-NB	2.47	126.88	124.26
14	k	103	CLA	CMB-C2B-C1B	-2.47	121.60	125.37
17	L	206	BCR	C29-C30-C25	2.47	114.28	110.48
18	A	853	LHG	O8-C23-C24	2.47	119.66	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	b	846	BCR	C38-C26-C25	-2.47	121.75	124.53
17	y	102	BCR	C27-C26-C25	2.47	126.32	122.73
14	a	817	CLA	CHB-C4A-NA	2.47	127.93	124.51
14	1	1628	CLA	CHB-C4A-NA	2.47	127.92	124.51
14	B	821	CLA	CMB-C2B-C3B	2.47	132.56	126.59
17	f	202	BCR	C38-C26-C25	-2.47	121.76	124.53
14	b	824	CLA	C3B-C4B-NB	-2.47	108.23	110.52
14	2	803	CLA	C3B-C4B-NB	-2.47	108.23	110.52
14	B	826	CLA	C1-C2-C3	-2.47	121.78	126.04
14	1	1618	CLA	CHB-C4A-NA	2.47	127.92	124.51
14	2	820	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
14	B	805	CLA	CHB-C4A-NA	2.46	127.92	124.51
17	l	207	BCR	C29-C30-C25	2.46	114.27	110.48
14	K	101	CLA	C3B-C4B-NB	-2.46	108.23	110.52
17	m	102	BCR	C15-C16-C17	-2.46	118.43	123.47
14	b	803	CLA	CHC-C4B-NB	2.46	126.86	124.26
14	6	201	CLA	CHB-C1B-NB	2.46	126.86	124.26
17	m	102	BCR	C27-C26-C25	2.46	126.30	122.73
14	b	822	CLA	CMB-C2B-C3B	2.46	132.54	126.59
14	1	1644	CLA	C4-C3-C5	2.46	119.41	115.27
18	a	853	LHG	O8-C23-C24	2.46	119.61	111.91
14	b	803	CLA	C3B-C4B-NB	-2.46	108.24	110.52
14	A	806	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
14	A	813	CLA	CHB-C1B-NB	2.46	126.86	124.26
14	B	802	CLA	C3B-C4B-NB	-2.45	108.24	110.52
14	2	814	CLA	CHB-C1B-NB	2.45	126.86	124.26
14	a	844	CLA	CHB-C4A-NA	2.45	127.91	124.51
17	F	202	BCR	C38-C26-C25	-2.45	121.77	124.53
17	I	101	BCR	C27-C26-C25	2.45	126.29	122.73
14	A	824	CLA	CHB-C4A-NA	2.45	127.90	124.51
14	2	803	CLA	CHC-C4B-NB	2.45	126.85	124.26
14	A	837	CLA	CHB-C1B-NB	2.45	126.85	124.26
14	B	807	CLA	C3B-C4B-NB	-2.45	108.24	110.52
14	2	824	CLA	C3B-C4B-NB	-2.45	108.24	110.52
14	a	806	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
14	B	808	CLA	CHB-C4A-NA	2.45	127.90	124.51
14	B	802	CLA	CHC-C4B-NB	2.45	126.85	124.26
14	1	1614	CLA	CHB-C1B-NB	2.45	126.85	124.26
17	f	204	BCR	C38-C26-C25	-2.45	121.78	124.53
17	M	103	BCR	C27-C26-C25	2.45	126.29	122.73
14	B	809	CLA	O1D-CGD-CBD	2.45	129.49	124.48
14	B	819	CLA	C3B-C4B-NB	-2.45	108.24	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	809	CLA	C3B-C4B-NB	-2.45	108.24	110.52
14	2	820	CLA	C3B-C4B-NB	-2.45	108.24	110.52
17	0	203	BCR	C8-C7-C6	-2.45	120.33	127.20
14	B	813	CLA	CHB-C1B-NB	2.45	126.85	124.26
14	b	820	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
14	b	810	CLA	O1D-CGD-CBD	2.45	129.49	124.48
14	A	833	CLA	CHB-C1B-NB	2.45	126.85	124.26
14	k	101	CLA	C3B-C4B-NB	-2.44	108.25	110.52
14	1	1634	CLA	CHB-C1B-NB	2.44	126.84	124.26
14	B	807	CLA	CHB-C4A-NA	2.44	127.89	124.51
17	L	201	BCR	C8-C7-C6	-2.44	120.34	127.20
18	1	1654	LHG	O8-C23-C24	2.44	119.58	111.91
14	a	829	CLA	CMB-C2B-C1B	-2.44	121.65	125.37
14	1	1632	CLA	CHB-C1B-NB	2.44	126.84	124.26
14	2	825	CLA	C2A-C1A-CHA	2.44	128.13	123.86
14	1	1630	CLA	CMB-C2B-C1B	-2.44	121.65	125.37
17	B	851	BCR	C11-C10-C9	-2.44	123.83	127.31
14	L	205	CLA	C3B-C4B-NB	-2.44	108.25	110.52
17	2	847	BCR	C38-C26-C25	-2.44	121.79	124.53
14	2	808	CLA	CHB-C4A-NA	2.44	127.89	124.51
14	2	827	CLA	C1-C2-C3	-2.44	121.82	126.04
17	y	102	BCR	C15-C16-C17	-2.44	118.48	123.47
14	b	820	CLA	C3B-C4B-NB	-2.44	108.25	110.52
14	2	809	CLA	CHB-C4A-NA	2.44	127.89	124.51
14	A	817	CLA	CHB-C4A-NA	2.44	127.88	124.51
14	A	843	CLA	C4-C3-C5	2.44	119.37	115.27
17	M	103	BCR	C15-C16-C17	-2.44	118.48	123.47
14	1	1622	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
14	a	825	CLA	CMB-C2B-C1B	-2.44	121.66	125.37
14	a	818	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
14	A	831	CLA	CHB-C1B-NB	2.44	126.83	124.26
14	1	1619	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
14	B	840	CLA	CHB-C4A-NA	2.43	127.88	124.51
14	A	829	CLA	CMB-C2B-C1B	-2.43	121.66	125.37
14	A	822	CLA	CHB-C1B-NB	2.43	126.83	124.26
17	6	202	BCR	C38-C26-C25	-2.43	121.80	124.53
14	1	1645	CLA	CHB-C4A-NA	2.43	127.88	124.51
14	9	101	CLA	C3B-C4B-NB	-2.43	108.26	110.52
14	B	824	CLA	C2A-C1A-CHA	2.43	128.11	123.86
14	2	808	CLA	C3B-C4B-NB	-2.43	108.26	110.52
14	2	841	CLA	CHB-C4A-NA	2.43	127.87	124.51
17	y	102	BCR	C37-C22-C21	-2.43	119.52	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	821	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
14	B	819	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
17	B	845	BCR	C38-C26-C25	-2.43	121.80	124.53
14	a	821	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
17	8	1306	BCR	C11-C10-C9	-2.43	123.85	127.31
14	a	810	CLA	C3B-C4B-NB	-2.43	108.26	110.52
17	7	101	BCR	C27-C26-C25	2.43	126.25	122.73
17	l	202	BCR	C8-C7-C6	-2.43	120.39	127.20
17	9	102	BCR	C36-C18-C19	2.42	121.90	118.08
14	A	832	CLA	CHB-C1B-NB	2.42	126.82	124.26
17	0	208	BCR	C24-C23-C22	-2.42	122.57	126.23
14	A	810	CLA	CHB-C4A-NA	2.42	127.86	124.51
14	k	103	CLA	CHB-C4A-NA	2.42	127.86	124.51
17	B	846	BCR	C38-C26-C25	-2.42	121.81	124.53
14	b	814	CLA	CHB-C1B-NB	2.42	126.82	124.26
14	b	827	CLA	C1-C2-C3	-2.42	121.85	126.04
14	a	843	CLA	C4-C3-C5	2.42	119.34	115.27
17	6	204	BCR	C27-C26-C25	2.42	126.25	122.73
14	a	810	CLA	CHB-C4A-NA	2.42	127.86	124.51
14	f	201	CLA	CHB-C4A-NA	2.42	127.86	124.51
14	A	844	CLA	CHB-C4A-NA	2.42	127.86	124.51
17	F	205	BCR	C38-C26-C25	-2.42	121.81	124.53
14	a	842	CLA	C1-C2-C3	-2.42	121.86	126.04
14	1	1623	CLA	CHB-C1B-NB	2.42	126.82	124.26
14	A	842	CLA	C1-C2-C3	-2.42	121.86	126.04
14	A	818	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
20	B	849	LMG	C1-O6-C5	-2.42	108.94	113.69
17	i	101	BCR	C27-C26-C25	2.42	126.24	122.73
14	A	825	CLA	CHB-C4A-NA	2.42	127.85	124.51
14	F	201	CLA	CHB-C1B-NB	2.42	126.81	124.26
14	B	826	CLA	CHB-C4A-NA	2.42	127.85	124.51
14	6	201	CLA	CHB-C4A-NA	2.41	127.85	124.51
14	B	808	CLA	C3B-C4B-NB	-2.41	108.28	110.52
14	b	841	CLA	CHB-C4A-NA	2.41	127.85	124.51
17	k	102	BCR	C36-C18-C19	2.41	121.88	118.08
14	a	809	CLA	CMB-C2B-C1B	-2.41	121.69	125.37
20	2	850	LMG	C1-O6-C5	-2.41	108.95	113.69
14	1	1633	CLA	CHB-C4A-NA	2.41	127.85	124.51
14	b	825	CLA	C2A-C1A-CHA	2.41	128.08	123.86
14	B	814	CLA	CHD-C1D-ND	-2.41	122.24	124.45
17	f	204	BCR	C27-C26-C25	2.41	126.23	122.73
14	9	103	CLA	CHB-C4A-NA	2.41	127.84	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	809	CLA	C3B-C4B-NB	-2.41	108.28	110.52
14	1	1611	CLA	C3B-C4B-NB	-2.41	108.28	110.52
14	1	1643	CLA	C1-C2-C3	-2.40	121.89	126.04
17	F	205	BCR	C27-C26-C25	2.40	126.22	122.73
14	a	836	CLA	C4-C3-C5	2.40	119.31	115.27
14	b	808	CLA	C3B-C4B-NB	-2.40	108.29	110.52
14	2	810	CLA	O1D-CGD-CBD	2.40	129.40	124.48
17	k	102	BCR	C38-C26-C25	-2.40	121.83	124.53
14	a	805	CLA	CMB-C2B-C1B	-2.40	121.71	125.37
14	A	842	CLA	CHB-C4A-NA	2.40	127.83	124.51
14	2	827	CLA	CHB-C4A-NA	2.40	127.83	124.51
14	1	1610	CLA	CMB-C2B-C1B	-2.40	121.72	125.37
14	a	824	CLA	C3B-C4B-NB	-2.40	108.29	110.52
14	a	833	CLA	CHB-C1B-NB	2.40	126.80	124.26
14	K	103	CLA	CHB-C4A-NA	2.40	127.83	124.51
17	m	102	BCR	C37-C22-C21	-2.40	119.56	122.92
14	1	1605	CLA	CMB-C2B-C1B	-2.40	121.72	125.37
14	a	832	CLA	CHB-C4A-NA	2.40	127.83	124.51
17	L	206	BCR	C24-C23-C22	-2.40	122.61	126.23
14	A	809	CLA	CMB-C2B-C1B	-2.40	121.72	125.37
17	K	102	BCR	C38-C26-C25	-2.40	121.84	124.53
17	K	102	BCR	C36-C18-C19	2.40	121.85	118.08
14	1	1606	CLA	CMB-C2B-C1B	-2.40	121.72	125.37
14	1	1616	CLA	C3B-C4B-NB	-2.40	108.29	110.52
14	F	201	CLA	CHB-C4A-NA	2.39	127.82	124.51
14	a	815	CLA	C3B-C4B-NB	-2.39	108.30	110.52
20	b	850	LMG	C1-O6-C5	-2.39	109.00	113.69
14	b	809	CLA	CHB-C4A-NA	2.39	127.82	124.51
14	A	816	CLA	CHB-C1B-NB	2.39	126.78	124.26
14	a	825	CLA	CHB-C4A-NA	2.39	127.81	124.51
14	b	815	CLA	CHD-C1D-ND	-2.39	122.26	124.45
17	l	207	BCR	C24-C23-C22	-2.39	122.63	126.23
14	A	827	CLA	CMB-C2B-C3B	2.39	132.37	126.59
14	a	833	CLA	CMB-C2B-C1B	-2.39	121.74	125.37
14	1	1628	CLA	CMB-C2B-C3B	2.38	132.36	126.59
14	2	812	CLA	CMB-C2B-C3B	2.38	132.36	126.59
14	2	815	CLA	CHD-C1D-ND	-2.38	122.26	124.45
17	9	102	BCR	C38-C26-C25	-2.38	121.86	124.53
14	B	811	CLA	CMB-C2B-C3B	2.38	132.35	126.59
14	a	822	CLA	CHB-C1B-NB	2.38	126.78	124.26
14	a	831	CLA	CHB-C1B-NB	2.38	126.78	124.26
14	1	1611	CLA	CHB-C4A-NA	2.38	127.80	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	812	CLA	CMB-C2B-C3B	2.38	132.35	126.59
14	A	810	CLA	C3B-C4B-NB	-2.38	108.31	110.52
14	A	831	CLA	C3B-C4B-NB	-2.38	108.31	110.52
14	1	1637	CLA	C4-C3-C5	2.38	119.27	115.27
14	A	805	CLA	CMB-C2B-C1B	-2.38	121.75	125.37
14	a	827	CLA	CMB-C2B-C3B	2.38	132.35	126.59
17	2	848	BCR	C38-C26-C25	-2.38	121.86	124.53
17	1	1649	BCR	C15-C16-C17	-2.38	118.61	123.47
14	1	1627	CLA	CHB-C4A-NA	2.38	127.80	124.51
17	b	852	BCR	C11-C10-C9	-2.38	123.92	127.31
14	x	1701	CLA	CHB-C4A-NA	2.37	127.80	124.51
14	A	824	CLA	C3B-C4B-NB	-2.37	108.31	110.52
17	B	847	BCR	C38-C26-C25	-2.37	121.86	124.53
17	A	848	BCR	C15-C16-C17	-2.37	118.61	123.47
17	K	104	BCR	C2-C1-C6	2.37	114.13	110.48
14	a	816	CLA	CHB-C1B-NB	2.37	126.77	124.26
17	k	104	BCR	C2-C1-C6	2.37	114.13	110.48
14	A	833	CLA	CMB-C2B-C1B	-2.37	121.76	125.37
14	a	826	CLA	CHB-C4A-NA	2.37	127.79	124.51
14	1	1626	CLA	CHB-C4A-NA	2.37	127.79	124.51
14	1	1630	CLA	CHB-C4A-NA	2.37	127.78	124.51
17	M	103	BCR	C37-C22-C21	-2.36	119.61	122.92
14	A	836	CLA	C4-C3-C5	2.36	119.25	115.27
14	B	820	CLA	CHB-C4A-NA	2.36	127.78	124.51
14	1	1634	CLA	CMB-C2B-C1B	-2.36	121.77	125.37
14	a	829	CLA	C3B-C4B-NB	-2.36	108.32	110.52
14	1	1632	CLA	C3B-C4B-NB	-2.36	108.32	110.52
14	1	1634	CLA	CHB-C4A-NA	2.36	127.78	124.51
14	a	834	CLA	CHD-C1D-ND	-2.36	122.28	124.45
14	2	819	CLA	CMB-C2B-C1B	-2.36	121.78	125.37
14	a	820	CLA	CMB-C2B-C3B	2.36	132.30	126.59
14	b	821	CLA	CHB-C4A-NA	2.36	127.77	124.51
14	2	840	CLA	CHB-C1B-NB	2.36	126.75	124.26
14	J	102	CLA	CHB-C4A-NA	2.36	127.77	124.51
14	a	804	CLA	CMB-C2B-C1B	-2.36	121.78	125.37
14	b	813	CLA	CHB-C4A-NA	2.36	127.77	124.51
17	2	845	BCR	C15-C16-C17	-2.36	118.64	123.47
14	B	812	CLA	CHB-C4A-NA	2.36	127.77	124.51
14	1	1604	CLA	C3B-C4B-NB	-2.36	108.33	110.52
14	2	802	CLA	O2D-CGD-CBD	2.36	115.45	111.27
14	2	814	CLA	CHB-C4A-NA	2.35	127.77	124.51
17	a	850	BCR	C16-C15-C14	-2.35	118.65	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	806	CLA	CHD-C1D-ND	-2.35	122.29	124.45
14	a	842	CLA	CHB-C4A-NA	2.35	127.77	124.51
14	a	829	CLA	CHB-C4A-NA	2.35	127.77	124.51
14	l	205	CLA	CHB-C1B-NB	2.35	126.75	124.26
17	a	848	BCR	C15-C16-C17	-2.35	118.66	123.47
14	B	818	CLA	CMB-C2B-C1B	-2.35	121.79	125.37
14	A	832	CLA	CHB-C4A-NA	2.35	127.76	124.51
18	A	854	LHG	O8-C23-C24	2.35	119.28	111.91
14	b	819	CLA	CMB-C2B-C1B	-2.35	121.79	125.37
14	a	806	CLA	CHD-C1D-ND	-2.35	122.29	124.45
14	A	826	CLA	CHB-C4A-NA	2.35	127.76	124.51
17	9	104	BCR	C2-C1-C6	2.35	114.10	110.48
14	1	1621	CLA	CMB-C2B-C3B	2.35	132.28	126.59
14	1	1633	CLA	CHB-C1B-NB	2.35	126.74	124.26
14	b	840	CLA	CHD-C1D-ND	-2.35	122.30	124.45
14	B	819	CLA	C1-O2A-CGA	2.35	122.60	116.44
14	b	820	CLA	C1-O2A-CGA	2.35	122.60	116.44
14	2	820	CLA	C1-O2A-CGA	2.35	122.60	116.44
14	1	1643	CLA	CHB-C4A-NA	2.35	127.76	124.51
14	a	832	CLA	CHB-C1B-NB	2.35	126.74	124.26
14	a	811	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
14	1	1607	CLA	CHD-C1D-ND	-2.35	122.30	124.45
17	6	204	BCR	C24-C23-C22	-2.35	122.69	126.23
14	A	811	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
14	b	824	CLA	CMB-C2B-C3B	2.35	132.27	126.59
14	x	1701	CLA	CHB-C1B-NB	2.35	126.74	124.26
14	2	842	CLA	CHD-C1D-ND	-2.35	122.30	124.45
14	A	855	CLA	O2D-CGD-CBD	2.35	115.44	111.27
14	L	204	CLA	CHB-C1B-NB	2.35	126.74	124.26
17	F	205	BCR	C24-C23-C22	-2.35	122.69	126.23
14	A	815	CLA	C3B-C4B-NB	-2.34	108.34	110.52
14	f	201	CLA	O2D-CGD-O1D	-2.34	119.25	123.84
14	A	834	CLA	CHD-C1D-ND	-2.34	122.30	124.45
17	b	845	BCR	C15-C16-C17	-2.34	118.67	123.47
17	1	1651	BCR	C16-C15-C14	-2.34	118.67	123.47
14	A	802	CLA	CHB-C1B-NB	2.34	126.74	124.26
14	a	831	CLA	C3B-C4B-NB	-2.34	108.34	110.52
14	a	844	CLA	C3B-C4B-NB	-2.34	108.34	110.52
17	b	848	BCR	C38-C26-C25	-2.34	121.90	124.53
17	A	850	BCR	C16-C15-C14	-2.34	118.67	123.47
14	b	840	CLA	CHB-C1B-NB	2.34	126.74	124.26
14	A	820	CLA	CMB-C2B-C3B	2.34	132.26	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1	1612	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
14	j	1303	CLA	CHB-C4A-NA	2.34	127.75	124.51
14	2	840	CLA	CHD-C1D-ND	-2.34	122.30	124.45
14	b	802	CLA	O2D-CGD-CBD	2.34	115.42	111.27
14	B	841	CLA	CHD-C1D-ND	-2.34	122.31	124.45
14	1	1625	CLA	C3B-C4B-NB	-2.34	108.35	110.52
14	A	829	CLA	CHB-C4A-NA	2.34	127.75	124.51
14	1	1603	CLA	CHB-C1B-NB	2.34	126.73	124.26
17	1	1649	BCR	C8-C7-C6	-2.34	120.64	127.20
17	B	844	BCR	C15-C16-C17	-2.34	118.69	123.47
14	2	824	CLA	CMB-C2B-C3B	2.34	132.25	126.59
14	A	804	CLA	CMB-C2B-C1B	-2.34	121.81	125.37
14	8	1303	CLA	CHB-C4A-NA	2.34	127.74	124.51
14	1	1635	CLA	CHD-C1D-ND	-2.34	122.31	124.45
14	6	201	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
17	A	847	BCR	C38-C26-C25	-2.34	121.91	124.53
14	a	833	CLA	CHB-C4A-NA	2.34	127.74	124.51
17	9	102	BCR	C24-C23-C22	-2.34	122.71	126.23
17	A	848	BCR	C8-C7-C6	-2.33	120.65	127.20
14	A	820	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
14	F	204	CLA	C1-C2-C3	-2.33	122.98	126.75
14	a	803	CLA	C3B-C4B-NB	-2.33	108.35	110.52
18	a	854	LHG	O8-C23-C24	2.33	119.22	111.91
14	1	1630	CLA	C3B-C4B-NB	-2.33	108.35	110.52
14	F	201	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
14	B	839	CLA	CHD-C1D-ND	-2.33	122.31	124.45
17	1	1648	BCR	C37-C22-C21	-2.33	119.66	122.92
14	A	824	CLA	O2D-CGD-CBD	2.33	115.41	111.27
14	b	814	CLA	CHB-C4A-NA	2.33	127.73	124.51
14	f	203	CLA	CHB-C4A-NA	2.33	127.73	124.51
14	2	821	CLA	CHB-C4A-NA	2.33	127.73	124.51
14	B	823	CLA	CMB-C2B-C3B	2.33	132.23	126.59
17	A	850	BCR	C38-C26-C25	-2.33	121.91	124.53
17	a	850	BCR	C8-C7-C6	-2.33	120.67	127.20
17	a	848	BCR	C8-C7-C6	-2.33	120.67	127.20
14	1	1621	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
14	a	820	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
14	f	203	CLA	C1-C2-C3	-2.33	122.99	126.75
14	b	842	CLA	CHD-C1D-ND	-2.32	122.32	124.45
17	a	847	BCR	C37-C22-C21	-2.32	119.67	122.92
14	A	828	CLA	CHB-C4A-NA	2.32	127.72	124.51
14	2	813	CLA	CHB-C4A-NA	2.32	127.72	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	827	CLA	CHD-C1D-ND	-2.32	122.32	124.45
14	a	824	CLA	O2D-CGD-CBD	2.32	115.39	111.27
17	A	850	BCR	C8-C7-C6	-2.32	120.69	127.20
14	z	102	CLA	CHB-C4A-NA	2.32	127.72	124.51
14	B	822	CLA	CMB-C2B-C1B	-2.32	121.84	125.37
14	a	802	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
14	1	1603	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
17	6	202	BCR	C8-C7-C6	-2.32	120.69	127.20
14	0	206	CLA	CHB-C1B-NB	2.32	126.71	124.26
18	1	1655	LHG	O8-C23-C24	2.32	119.18	111.91
14	1	1625	CLA	O2D-CGD-CBD	2.32	115.39	111.27
17	b	847	BCR	C35-C13-C14	-2.32	119.68	122.92
17	k	102	BCR	C24-C23-C22	-2.32	122.74	126.23
17	1	1651	BCR	C8-C7-C6	-2.31	120.70	127.20
14	A	826	CLA	CMB-C2B-C1B	-2.31	121.84	125.37
14	1	1617	CLA	CHB-C1B-NB	2.31	126.71	124.26
14	b	826	CLA	CHB-C4A-NA	2.31	127.71	124.51
17	f	204	BCR	C24-C23-C22	-2.31	122.74	126.23
14	1	1633	CLA	CMB-C2B-C1B	-2.31	121.85	125.37
14	B	839	CLA	CHB-C1B-NB	2.31	126.70	124.26
14	1	1645	CLA	C3B-C4B-NB	-2.31	108.37	110.52
18	B	850	LHG	C11-C10-C9	-2.31	102.69	114.42
14	B	813	CLA	CHB-C4A-NA	2.31	127.71	124.51
14	A	829	CLA	C3B-C4B-NB	-2.31	108.37	110.52
17	a	850	BCR	C38-C26-C25	-2.31	121.93	124.53
14	B	834	CLA	CMB-C2B-C1B	-2.31	121.85	125.37
14	1	1627	CLA	C6-C5-C3	2.31	119.51	113.45
14	k	103	CLA	CHD-C1D-ND	-2.31	122.33	124.45
17	A	850	BCR	C2-C1-C6	2.31	114.04	110.48
14	X	1701	CLA	CHB-C4A-NA	2.31	127.71	124.51
14	2	814	CLA	C5-C3-C2	2.31	125.79	121.12
14	2	834	CLA	CHB-C4A-NA	2.31	127.70	124.51
14	B	804	CLA	CHB-C1B-NB	2.31	126.70	124.26
20	2	850	LMG	O3-C3-C2	-2.31	105.01	110.35
14	b	834	CLA	CHB-C4A-NA	2.31	127.70	124.51
18	b	851	LHG	C11-C10-C9	-2.31	102.71	114.42
14	2	805	CLA	CHB-C1B-NB	2.31	126.70	124.26
14	F	204	CLA	CHB-C4A-NA	2.31	127.70	124.51
14	A	802	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
14	b	805	CLA	CHB-C1B-NB	2.31	126.70	124.26
18	z	101	LHG	C11-C10-C9	-2.31	102.72	114.42
14	A	829	CLA	O1D-CGD-CBD	2.31	129.20	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	I	101	BCR	C8-C7-C6	-2.30	120.73	127.20
14	A	833	CLA	CHB-C4A-NA	2.30	127.70	124.51
14	6	203	CLA	C1-C2-C3	-2.30	123.03	126.75
17	F	202	BCR	C8-C7-C6	-2.30	120.73	127.20
17	1	1651	BCR	C38-C26-C25	-2.30	121.94	124.53
14	l	206	CLA	O2D-CGD-CBD	2.30	115.36	111.27
14	b	824	CLA	CHD-C1D-ND	-2.30	122.34	124.45
14	1	1628	CLA	CHD-C1D-ND	-2.30	122.34	124.45
14	6	203	CLA	CHB-C4A-NA	2.30	127.70	124.51
14	A	826	CLA	C6-C5-C3	2.30	119.49	113.45
20	2	850	LMG	C40-C39-C38	-2.30	102.74	114.42
14	B	806	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
17	1	1651	BCR	C2-C1-C6	2.30	114.02	110.48
14	b	803	CLA	C11-C10-C8	-2.30	108.48	115.92
14	2	803	CLA	C11-C10-C8	-2.30	108.48	115.92
20	b	850	LMG	C40-C39-C38	-2.30	102.75	114.42
14	2	826	CLA	CHB-C4A-NA	2.30	127.69	124.51
14	b	823	CLA	CMB-C2B-C1B	-2.30	121.87	125.37
14	B	813	CLA	C5-C3-C2	2.30	125.77	121.12
17	A	856	BCR	C38-C26-C25	-2.30	121.95	124.53
17	i	101	BCR	C8-C7-C6	-2.30	120.75	127.20
14	2	823	CLA	CMB-C2B-C1B	-2.30	121.87	125.37
14	b	807	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
14	j	1301	CLA	O1D-CGD-CBD	2.30	129.19	124.48
14	B	807	CLA	C1-C2-C3	-2.30	122.07	126.04
20	B	849	LMG	C40-C39-C38	-2.30	102.77	114.42
14	2	838	CLA	CHB-C1B-NB	2.30	126.69	124.26
14	b	830	CLA	C3C-C4C-NC	-2.30	108.00	110.57
17	7	101	BCR	C8-C7-C6	-2.30	120.75	127.20
20	B	849	LMG	O3-C3-C2	-2.30	105.04	110.35
17	f	202	BCR	C8-C7-C6	-2.30	120.75	127.20
14	A	832	CLA	CMB-C2B-C1B	-2.30	121.87	125.37
14	a	826	CLA	CMB-C2B-C1B	-2.30	121.87	125.37
17	A	847	BCR	C37-C22-C21	-2.30	119.71	122.92
14	a	829	CLA	O1D-CGD-CBD	2.30	129.18	124.48
17	1	1648	BCR	C38-C26-C25	-2.29	121.95	124.53
20	b	850	LMG	O3-C3-C2	-2.29	105.04	110.35
14	B	802	CLA	C11-C10-C8	-2.29	108.50	115.92
14	B	825	CLA	CHB-C4A-NA	2.29	127.68	124.51
14	A	803	CLA	C3B-C4B-NB	-2.29	108.39	110.52
14	j	1303	CLA	C3B-C4B-NB	-2.29	108.39	110.52
17	a	850	BCR	C2-C1-C6	2.29	114.01	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	F	203	CLA	O1D-CGD-CBD	2.29	129.17	124.48
14	B	833	CLA	CHB-C4A-NA	2.29	127.68	124.51
14	B	811	CLA	CHD-C1D-ND	-2.29	122.35	124.45
14	0	207	CLA	O2D-CGD-CBD	2.29	115.34	111.27
14	B	837	CLA	CHB-C1B-NB	2.29	126.68	124.26
17	B	846	BCR	C35-C13-C14	-2.29	119.72	122.92
14	A	839	CLA	CHB-C1B-NB	2.29	126.68	124.26
14	8	1301	CLA	O1D-CGD-CBD	2.29	129.17	124.48
14	a	826	CLA	C6-C5-C3	2.29	119.46	113.45
14	b	814	CLA	C5-C3-C2	2.29	125.75	121.12
14	a	834	CLA	CMB-C2B-C3B	2.29	132.13	126.59
17	a	851	BCR	C38-C26-C25	-2.29	121.96	124.53
17	K	102	BCR	C24-C23-C22	-2.29	122.78	126.23
14	a	844	CLA	CHD-C1D-ND	-2.29	122.35	124.45
17	a	847	BCR	C38-C26-C25	-2.28	121.96	124.53
14	a	827	CLA	CHD-C1D-ND	-2.28	122.36	124.45
14	9	103	CLA	CHD-C1D-ND	-2.28	122.36	124.45
14	X	1701	CLA	CHB-C1B-NB	2.28	126.67	124.26
14	a	832	CLA	CMB-C2B-C1B	-2.28	121.89	125.37
14	a	820	CLA	C3B-C4B-NB	-2.28	108.40	110.52
17	k	102	BCR	C27-C26-C25	2.28	126.04	122.73
17	2	847	BCR	C35-C13-C14	-2.28	119.73	122.92
14	B	829	CLA	C3C-C4C-NC	-2.28	108.01	110.57
17	j	1304	BCR	C24-C23-C22	-2.28	122.79	126.23
14	A	844	CLA	C3B-C4B-NB	-2.28	108.40	110.52
14	a	805	CLA	O2D-CGD-CBD	2.28	115.32	111.27
14	b	838	CLA	CHB-C1B-NB	2.28	126.67	124.26
14	1	1630	CLA	O1D-CGD-CBD	2.28	129.15	124.48
14	1	1621	CLA	C3B-C4B-NB	-2.28	108.40	110.52
20	2	850	LMG	O2-C2-C1	-2.28	104.51	110.05
14	K	103	CLA	CHD-C1D-ND	-2.28	122.36	124.45
14	a	803	CLA	CHD-C1D-ND	-2.28	122.36	124.45
14	a	802	CLA	CHB-C1B-NB	2.28	126.67	124.26
14	b	823	CLA	CHB-C1B-NB	2.28	126.67	124.26
14	2	820	CLA	CHB-C1B-NB	2.28	126.67	124.26
14	L	205	CLA	O2D-CGD-CBD	2.28	115.31	111.27
14	A	834	CLA	CMB-C2B-C3B	2.28	132.10	126.59
17	a	852	BCR	C8-C7-C6	-2.28	120.81	127.20
14	B	819	CLA	CHB-C1B-NB	2.28	126.67	124.26
14	z	102	CLA	CHB-C1B-NB	2.28	126.67	124.26
17	8	1305	BCR	C38-C26-C25	-2.28	121.97	124.53
14	2	824	CLA	CHD-C1D-ND	-2.27	122.36	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	808	CLA	C1-C2-C3	-2.27	122.11	126.04
14	6	201	CLA	C1-C2-C3	-2.27	122.11	126.04
14	b	811	CLA	C2A-C1A-CHA	2.27	127.83	123.86
14	b	812	CLA	CHD-C1D-ND	-2.27	122.36	124.45
14	1	1627	CLA	CMB-C2B-C1B	-2.27	121.91	125.37
14	1	1606	CLA	O2D-CGD-CBD	2.27	115.31	111.27
14	B	822	CLA	CHB-C1B-NB	2.27	126.66	124.26
14	2	804	CLA	C3B-C4B-NB	-2.27	108.41	110.52
17	B	848	BCR	C24-C23-C22	-2.27	122.80	126.23
17	A	851	BCR	C38-C26-C25	-2.27	121.98	124.53
14	1	1635	CLA	CMB-C2B-C3B	2.27	132.09	126.59
17	b	848	BCR	C15-C14-C13	-2.27	124.07	127.31
14	B	810	CLA	C2A-C1A-CHA	2.27	127.83	123.86
17	8	1304	BCR	C24-C23-C22	-2.27	122.80	126.23
14	1	1642	CLA	C1-C2-C3	-2.27	122.12	126.04
14	b	827	CLA	CHB-C1B-NB	2.27	126.66	124.26
14	8	1301	CLA	CHB-C1B-NB	2.27	126.66	124.26
14	2	811	CLA	C2A-C1A-CHA	2.27	127.83	123.86
14	2	808	CLA	C1-C2-C3	-2.27	122.12	126.04
14	A	803	CLA	CHD-C1D-ND	-2.27	122.37	124.45
14	2	812	CLA	CHD-C1D-ND	-2.27	122.37	124.45
17	M	103	BCR	C8-C7-C6	-2.27	120.83	127.20
14	b	804	CLA	C3B-C4B-NB	-2.27	108.41	110.52
14	2	814	CLA	CMB-C2B-C1B	-2.27	121.92	125.37
14	F	201	CLA	C1-C2-C3	-2.27	122.12	126.04
14	2	823	CLA	CHB-C1B-NB	2.27	126.66	124.26
14	2	835	CLA	CMB-C2B-C1B	-2.27	121.92	125.37
14	B	815	CLA	CHB-C4A-NA	2.27	127.64	124.51
14	b	816	CLA	CHB-C4A-NA	2.27	127.64	124.51
14	b	823	CLA	CHB-C4A-NA	2.27	127.64	124.51
14	f	201	CLA	C1-C2-C3	-2.27	122.12	126.04
14	b	835	CLA	CMB-C2B-C1B	-2.27	121.92	125.37
17	j	1305	BCR	C36-C18-C17	-2.27	119.75	122.92
14	A	820	CLA	C3B-C4B-NB	-2.26	108.41	110.52
17	K	102	BCR	C27-C26-C25	2.26	126.02	122.73
14	b	820	CLA	CHD-C1D-ND	-2.26	122.37	124.45
17	j	1305	BCR	C38-C26-C25	-2.26	121.99	124.53
17	1	1653	BCR	C8-C7-C6	-2.26	120.85	127.20
14	B	826	CLA	CHB-C1B-NB	2.26	126.65	124.26
20	B	849	LMG	O2-C2-C1	-2.26	104.55	110.05
17	A	852	BCR	C8-C7-C6	-2.26	120.85	127.20
14	8	1303	CLA	C3B-C4B-NB	-2.26	108.42	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	841	CLA	C1-C2-C3	-2.26	122.13	126.04
14	B	819	CLA	CHD-C1D-ND	-2.26	122.38	124.45
14	b	820	CLA	CHB-C1B-NB	2.26	126.65	124.26
14	2	807	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
14	1	1601	CLA	CHB-C4A-NA	2.26	127.64	124.51
17	9	102	BCR	C27-C26-C25	2.26	126.01	122.73
14	L	203	CLA	C1-C2-C3	-2.26	122.14	126.04
14	2	841	CLA	CHB-C1B-NB	2.26	126.65	124.26
17	m	102	BCR	C8-C7-C6	-2.26	120.86	127.20
14	M	102	CLA	CHB-C4A-NA	2.26	127.63	124.51
14	F	203	CLA	CHB-C1B-NB	2.26	126.65	124.26
17	y	102	BCR	C8-C7-C6	-2.26	120.86	127.20
20	b	850	LMG	O2-C2-C1	-2.26	104.56	110.05
14	2	820	CLA	CHB-C4A-NA	2.26	127.63	124.51
14	B	804	CLA	C1-C2-C3	-2.26	122.14	126.04
20	B	849	LMG	O1-C1-C2	-2.26	104.78	108.30
14	2	816	CLA	CHB-C4A-NA	2.25	127.63	124.51
17	b	847	BCR	C7-C8-C9	-2.25	122.83	126.23
14	B	819	CLA	CHB-C4A-NA	2.25	127.63	124.51
14	b	817	CLA	C3B-C4B-NB	-2.25	108.42	110.52
14	l	204	CLA	C1-C2-C3	-2.25	122.14	126.04
14	A	844	CLA	CHD-C1D-ND	-2.25	122.38	124.45
14	B	813	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
14	a	828	CLA	CHB-C4A-NA	2.25	127.63	124.51
14	A	819	CLA	C3B-C4B-NB	-2.25	108.42	110.52
14	a	819	CLA	C3B-C4B-NB	-2.25	108.42	110.52
14	A	805	CLA	O2D-CGD-CBD	2.25	115.27	111.27
17	J	103	BCR	C24-C23-C22	-2.25	122.83	126.23
14	j	1302	CLA	O2A-CGA-O1A	-2.25	117.69	123.30
18	z	101	LHG	C27-C26-C25	-2.25	102.99	114.42
17	b	849	BCR	C36-C18-C17	-2.25	119.77	122.92
14	b	814	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
14	1	1604	CLA	CHD-C1D-ND	-2.25	122.39	124.45
17	A	856	BCR	C8-C7-C6	-2.25	120.88	127.20
14	1	1640	CLA	CHB-C1B-NB	2.25	126.64	124.26
20	b	850	LMG	O1-C1-C2	-2.25	104.79	108.30
18	B	850	LHG	C27-C26-C25	-2.25	103.01	114.42
14	8	1302	CLA	O2A-CGA-O1A	-2.25	117.69	123.30
14	1	1629	CLA	CHB-C4A-NA	2.25	127.62	124.51
14	a	823	CLA	CHD-C1D-ND	-2.25	122.39	124.45
14	2	830	CLA	C3C-C4C-NC	-2.25	108.05	110.57
17	0	203	BCR	C15-C14-C13	-2.25	124.10	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	805	CLA	C1-C2-C3	-2.25	122.16	126.04
14	J	102	CLA	C3B-C4B-NB	-2.25	108.43	110.52
18	b	851	LHG	C20-C19-C18	-2.25	103.02	114.42
17	l	202	BCR	C15-C14-C13	-2.25	124.11	127.31
14	B	803	CLA	C3B-C4B-NB	-2.25	108.43	110.52
18	b	851	LHG	C27-C26-C25	-2.24	103.03	114.42
17	2	847	BCR	C7-C8-C9	-2.24	122.85	126.23
14	A	808	CLA	CHD-C1D-ND	-2.24	122.39	124.45
14	a	812	CLA	CHB-C4A-NA	2.24	127.61	124.51
14	A	841	CLA	C1-C2-C3	-2.24	122.17	126.04
17	b	849	BCR	C24-C23-C22	-2.24	122.85	126.23
14	B	816	CLA	C3B-C4B-NB	-2.24	108.44	110.52
14	1	1607	CLA	C2D-C1D-ND	-2.24	108.45	110.10
18	B	850	LHG	C20-C19-C18	-2.24	103.05	114.42
14	2	805	CLA	CHD-C1D-ND	-2.24	122.39	124.45
14	2	820	CLA	CHD-C1D-ND	-2.24	122.39	124.45
14	A	806	CLA	C2D-C1D-ND	-2.24	108.45	110.10
14	1	1632	CLA	C2D-C1D-ND	-2.24	108.45	110.10
14	A	812	CLA	CHB-C4A-NA	2.24	127.61	124.51
18	z	101	LHG	C20-C19-C18	-2.24	103.05	114.42
14	B	823	CLA	CHD-C1D-ND	-2.24	122.40	124.45
14	B	809	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
17	8	1304	BCR	C15-C16-C17	-2.24	118.89	123.47
17	B	847	BCR	C15-C14-C13	-2.24	124.12	127.31
14	B	840	CLA	CHB-C1B-NB	2.24	126.62	124.26
17	f	204	BCR	C15-C16-C17	-2.24	118.89	123.47
14	2	805	CLA	C1-C2-C3	-2.24	122.17	126.04
14	1	1632	CLA	O2D-CGD-CBD	2.24	115.24	111.27
14	A	857	CLA	CHB-C4A-NA	2.24	127.60	124.51
14	b	810	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
14	1	1624	CLA	CHD-C1D-ND	-2.24	122.40	124.45
14	1	1620	CLA	C3B-C4B-NB	-2.23	108.44	110.52
14	J	101	CLA	O2A-CGA-O1A	-2.23	117.73	123.30
14	B	805	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
17	J	103	BCR	C38-C26-C25	-2.23	122.02	124.53
14	b	806	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
17	b	849	BCR	C8-C7-C6	-2.23	120.93	127.20
17	b	847	BCR	C15-C14-C13	-2.23	124.12	127.31
14	a	839	CLA	CHB-C1B-NB	2.23	126.62	124.26
14	1	1609	CLA	CHD-C1D-ND	-2.23	122.40	124.45
17	1	1652	BCR	C38-C26-C25	-2.23	122.02	124.53
17	8	1305	BCR	C8-C7-C6	-2.23	120.93	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	f	203	CLA	C3B-C4B-NB	-2.23	108.44	110.52
14	B	840	CLA	C3A-C2A-C1A	2.23	104.68	101.34
17	j	1305	BCR	C8-C7-C6	-2.23	120.94	127.20
17	2	849	BCR	C36-C18-C17	-2.23	119.80	122.92
13	A	801	CL0	C2A-C1A-CHA	2.23	127.76	123.86
17	B	846	BCR	C15-C14-C13	-2.23	124.13	127.31
17	9	102	BCR	C15-C14-C13	-2.23	124.13	127.31
14	j	1301	CLA	CHB-C1B-NB	2.23	126.62	124.26
14	b	833	CLA	CHD-C1D-ND	-2.23	122.41	124.45
17	B	848	BCR	C8-C7-C6	-2.23	120.94	127.20
17	2	848	BCR	C15-C14-C13	-2.23	124.13	127.31
17	A	856	BCR	C36-C18-C17	-2.23	119.80	122.92
14	b	814	CLA	C6-C5-C3	2.23	119.30	113.45
17	2	849	BCR	C8-C7-C6	-2.23	120.94	127.20
14	2	827	CLA	CHB-C1B-NB	2.23	126.62	124.26
14	a	831	CLA	C2D-C1D-ND	-2.23	108.46	110.10
17	B	846	BCR	C7-C8-C9	-2.23	122.87	126.23
14	B	804	CLA	CHD-C1D-ND	-2.23	122.41	124.45
14	1	1626	CLA	CHD-C1D-ND	-2.23	122.41	124.45
14	b	826	CLA	CHB-C1B-NB	2.23	126.61	124.26
14	2	813	CLA	O2D-CGD-CBD	2.23	115.22	111.27
14	B	813	CLA	C6-C5-C3	2.23	119.29	113.45
14	2	833	CLA	CHB-C1B-NB	2.23	126.61	124.26
20	2	850	LMG	O1-C1-C2	-2.23	104.83	108.30
17	F	205	BCR	C15-C16-C17	-2.23	118.92	123.47
14	a	837	CLA	CHB-C4A-NA	2.22	127.59	124.51
17	2	849	BCR	C24-C23-C22	-2.22	122.87	126.23
14	A	806	CLA	CMB-C2B-C1B	-2.22	121.98	125.37
14	b	841	CLA	C3A-C2A-C1A	2.22	104.67	101.34
14	2	806	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
17	B	848	BCR	C36-C18-C17	-2.22	119.81	122.92
17	8	1305	BCR	C36-C18-C17	-2.22	119.81	122.92
14	B	839	CLA	CHB-C4A-NA	2.22	127.58	124.51
14	1	1613	CLA	CHB-C4A-NA	2.22	127.58	124.51
14	a	834	CLA	C6-C5-C3	2.22	119.28	113.45
14	1	1635	CLA	C6-C5-C3	2.22	119.28	113.45
14	B	832	CLA	CHB-C1B-NB	2.22	126.61	124.26
14	A	834	CLA	C6-C5-C3	2.22	119.27	113.45
14	b	820	CLA	CHB-C4A-NA	2.22	127.58	124.51
14	0	205	CLA	C1-C2-C3	-2.22	122.21	126.04
14	B	822	CLA	CHB-C4A-NA	2.22	127.58	124.51
14	A	823	CLA	CHD-C1D-ND	-2.22	122.42	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	812	CLA	O2D-CGD-CBD	2.22	115.21	111.27
14	a	806	CLA	C2D-C1D-ND	-2.22	108.47	110.10
17	8	1306	BCR	C33-C5-C6	-2.22	122.04	124.53
14	6	201	CLA	CHD-C1D-ND	-2.22	122.42	124.45
17	j	1304	BCR	C15-C16-C17	-2.22	118.94	123.47
14	B	807	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
14	a	831	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
14	b	841	CLA	CHB-C1B-NB	2.22	126.60	124.26
14	2	814	CLA	C6-C5-C3	2.21	119.26	113.45
17	L	201	BCR	C15-C14-C13	-2.21	124.15	127.31
14	b	833	CLA	CHB-C1B-NB	2.21	126.60	124.26
17	1	1650	BCR	C38-C26-C25	-2.21	122.04	124.53
14	L	205	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
14	l	206	CLA	CMB-C2B-C3B	2.21	131.95	126.59
17	8	1304	BCR	C38-C26-C25	-2.21	122.04	124.53
17	L	207	BCR	C24-C23-C22	-2.21	122.89	126.23
14	0	207	CLA	C1-C2-C3	-2.21	122.22	126.04
14	b	828	CLA	CHB-C4A-NA	2.21	127.57	124.51
14	a	810	CLA	CHD-C1D-ND	-2.21	122.42	124.45
14	f	201	CLA	CHD-C1D-ND	-2.21	122.42	124.45
14	A	837	CLA	CHB-C4A-NA	2.21	127.57	124.51
14	b	813	CLA	O2D-CGD-CBD	2.21	115.19	111.27
14	A	828	CLA	C1-C2-C3	-2.21	122.22	126.04
14	B	835	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
14	2	810	CLA	CMB-C2B-C1B	-2.21	122.00	125.37
14	B	816	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
17	A	851	BCR	C8-C7-C6	-2.21	121.00	127.20
14	A	809	CLA	CHD-C1D-ND	-2.21	122.42	124.45
14	l	206	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
14	1	1629	CLA	C1-C2-C3	-2.21	122.22	126.04
17	2	847	BCR	C15-C14-C13	-2.21	124.16	127.31
14	a	840	CLA	C5-C3-C2	2.21	125.58	121.12
14	b	833	CLA	C1-C2-C3	-2.21	122.23	126.04
14	L	205	CLA	CMB-C2B-C3B	2.21	131.93	126.59
14	B	832	CLA	C1-C2-C3	-2.21	122.23	126.04
14	2	808	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
14	2	836	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
17	j	1305	BCR	C28-C27-C26	-2.20	110.14	114.08
14	b	805	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
14	b	808	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
14	A	840	CLA	C5-C3-C2	2.20	125.58	121.12
17	B	844	BCR	C28-C27-C26	-2.20	110.14	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	836	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
14	1	1632	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
14	1	1630	CLA	CMB-C2B-C3B	2.20	131.92	126.59
14	b	805	CLA	CHD-C1D-ND	-2.20	122.43	124.45
14	1	1645	CLA	CHD-C1D-ND	-2.20	122.43	124.45
14	a	809	CLA	CHB-C1B-NB	2.20	126.59	124.26
17	K	102	BCR	C15-C14-C13	-2.20	124.17	127.31
14	a	814	CLA	CHB-C4A-NA	2.20	127.56	124.51
14	B	804	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
14	2	805	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
13	a	801	CL0	C2A-C1A-CHA	2.20	127.71	123.86
18	1	1654	LHG	C18-C17-C16	-2.20	103.26	114.42
14	l	206	CLA	C1-C2-C3	-2.20	122.24	126.04
14	2	833	CLA	C1-C2-C3	-2.20	122.24	126.04
14	A	831	CLA	O2D-CGD-CBD	2.20	115.18	111.27
13	1	1602	CL0	C2A-C1A-CHA	2.20	127.70	123.86
14	F	201	CLA	CHD-C1D-ND	-2.20	122.43	124.45
14	A	831	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
14	1	1610	CLA	CHB-C1B-NB	2.20	126.58	124.26
14	6	203	CLA	C3B-C4B-NB	-2.20	108.47	110.52
14	a	831	CLA	O2D-CGD-CBD	2.20	115.17	111.27
18	a	853	LHG	C18-C17-C16	-2.20	103.27	114.42
14	A	810	CLA	CHD-C1D-ND	-2.20	122.44	124.45
14	A	814	CLA	CHB-C4A-NA	2.20	127.55	124.51
17	b	845	BCR	C28-C27-C26	-2.20	110.16	114.08
14	2	817	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
14	a	808	CLA	CHD-C1D-ND	-2.20	122.44	124.45
14	b	807	CLA	CHD-C1D-ND	-2.20	122.44	124.45
14	1	1624	CLA	CMB-C2B-C1B	-2.20	122.03	125.37
14	1	1615	CLA	CHB-C4A-NA	2.20	127.55	124.51
17	a	851	BCR	C8-C7-C6	-2.20	121.04	127.20
14	a	823	CLA	CMB-C2B-C1B	-2.19	122.03	125.37
14	1	1607	CLA	CMB-C2B-C1B	-2.19	122.03	125.37
14	2	833	CLA	CHD-C1D-ND	-2.19	122.44	124.45
14	8	1301	CLA	CHB-C4A-NA	2.19	127.55	124.51
17	1	1652	BCR	C8-C7-C6	-2.19	121.04	127.20
14	2	826	CLA	CHB-C1B-NB	2.19	126.58	124.26
14	1	1641	CLA	C5-C3-C2	2.19	125.56	121.12
14	a	842	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
14	2	841	CLA	C3A-C2A-C1A	2.19	104.62	101.34
14	0	207	CLA	CMB-C2B-C3B	2.19	131.90	126.59
14	2	823	CLA	CHB-C4A-NA	2.19	127.54	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	828	CLA	C1-C2-C3	-2.19	122.25	126.04
17	B	851	BCR	C33-C5-C6	-2.19	122.07	124.53
14	2	835	CLA	CHB-C1B-NB	2.19	126.58	124.26
14	b	816	CLA	CHB-C1B-NB	2.19	126.58	124.26
14	0	207	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
14	b	822	CLA	C3B-C4B-NB	-2.19	108.48	110.52
18	A	853	LHG	C18-C17-C16	-2.19	103.31	114.42
17	J	103	BCR	C15-C16-C17	-2.19	118.99	123.47
14	A	809	CLA	CHB-C1B-NB	2.19	126.58	124.26
14	B	803	CLA	O1D-CGD-CBD	2.19	128.96	124.48
17	2	845	BCR	C28-C27-C26	-2.19	110.17	114.08
14	B	827	CLA	CHB-C4A-NA	2.19	127.54	124.51
14	j	1301	CLA	CHB-C4A-NA	2.19	127.54	124.51
17	a	849	BCR	C38-C26-C25	-2.19	122.07	124.53
14	1	1628	CLA	O2D-CGD-CBD	2.19	115.16	111.27
14	A	825	CLA	CHD-C1D-ND	-2.19	122.44	124.45
14	F	204	CLA	C3B-C4B-NB	-2.19	108.48	110.52
14	2	822	CLA	C3B-C4B-NB	-2.19	108.48	110.52
14	a	834	CLA	C5-C3-C2	2.19	125.54	121.12
17	b	852	BCR	C33-C5-C6	-2.19	122.07	124.53
14	a	829	CLA	CMB-C2B-C3B	2.19	131.88	126.59
14	1	1611	CLA	CHD-C1D-ND	-2.19	122.44	124.45
14	1	1638	CLA	CHB-C4A-NA	2.19	127.53	124.51
14	2	816	CLA	CHB-C1B-NB	2.19	126.57	124.26
17	B	851	BCR	C20-C21-C22	-2.18	124.19	127.31
17	8	1305	BCR	C28-C27-C26	-2.18	110.18	114.08
17	6	204	BCR	C15-C16-C17	-2.18	119.00	123.47
14	2	828	CLA	CHB-C4A-NA	2.18	127.53	124.51
14	B	815	CLA	CHB-C1B-NB	2.18	126.57	124.26
14	B	834	CLA	CHB-C1B-NB	2.18	126.57	124.26
14	b	817	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
17	A	856	BCR	C28-C27-C26	-2.18	110.18	114.08
17	B	847	BCR	C8-C7-C6	-2.18	121.07	127.20
17	B	851	BCR	C27-C26-C25	2.18	125.90	122.73
14	a	806	CLA	CMB-C2B-C1B	-2.18	122.05	125.37
17	b	848	BCR	C8-C7-C6	-2.18	121.07	127.20
14	A	831	CLA	C2D-C1D-ND	-2.18	108.50	110.10
17	b	848	BCR	C2-C1-C6	2.18	113.84	110.48
14	b	840	CLA	CHB-C4A-NA	2.18	127.53	124.51
14	L	205	CLA	C1-C2-C3	-2.18	122.27	126.04
14	a	809	CLA	CHD-C1D-ND	-2.18	122.45	124.45
18	y	101	LHG	C20-C19-C18	-2.18	103.36	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	848	BCR	C8-C7-C6	-2.18	121.08	127.20
18	m	101	LHG	C20-C19-C18	-2.18	103.36	114.42
14	1	1638	CLA	O2A-CGA-O1A	-2.18	117.87	123.30
17	A	849	BCR	C38-C26-C25	-2.18	122.08	124.53
17	1	1648	BCR	C24-C23-C22	-2.18	122.94	126.23
14	b	828	CLA	CMB-C2B-C3B	2.18	131.86	126.59
14	2	803	CLA	CHB-C4A-NA	2.18	127.52	124.51
14	A	823	CLA	CMB-C2B-C1B	-2.18	122.05	125.37
17	B	845	BCR	C8-C7-C6	-2.18	121.09	127.20
17	1	1650	BCR	C27-C26-C25	2.18	125.89	122.73
14	b	804	CLA	O1D-CGD-CBD	2.18	128.94	124.48
14	a	827	CLA	O2D-CGD-CBD	2.17	115.13	111.27
14	2	817	CLA	C3B-C4B-NB	-2.17	108.50	110.52
14	b	835	CLA	CHB-C1B-NB	2.17	126.56	124.26
14	2	825	CLA	CHA-C1A-NA	-2.17	121.42	126.40
14	1	1627	CLA	CAA-CBA-CGA	-2.17	106.91	113.25
14	b	809	CLA	O2D-CGD-CBD	2.17	115.13	111.27
17	0	201	BCR	C24-C23-C22	-2.17	122.95	126.23
14	A	834	CLA	C5-C3-C2	2.17	125.51	121.12
14	1	1635	CLA	C5-C3-C2	2.17	125.51	121.12
14	b	824	CLA	CHB-C1B-NB	2.17	126.56	124.26
18	M	101	LHG	C20-C19-C18	-2.17	103.40	114.42
14	0	206	CLA	C1-C2-C3	-2.17	122.29	126.04
14	j	1303	CLA	C2D-C1D-ND	-2.17	108.50	110.10
14	A	842	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
17	B	847	BCR	C2-C1-C6	2.17	113.82	110.48
14	2	840	CLA	CHB-C4A-NA	2.17	127.51	124.51
14	l	205	CLA	C1-C2-C3	-2.17	122.29	126.04
14	B	808	CLA	O2D-CGD-CBD	2.17	115.12	111.27
14	a	822	CLA	CHD-C1D-ND	-2.17	122.46	124.45
14	1	1643	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
17	0	209	BCR	C24-C23-C22	-2.17	122.96	126.23
17	b	846	BCR	C8-C7-C6	-2.17	121.11	127.20
14	B	832	CLA	CHD-C1D-ND	-2.17	122.46	124.45
14	2	806	CLA	CHD-C1D-ND	-2.17	122.46	124.45
14	a	826	CLA	CAA-CBA-CGA	-2.17	106.92	113.25
14	8	1303	CLA	CMB-C2B-C1B	-2.17	122.07	125.37
14	A	837	CLA	O2A-CGA-O1A	-2.17	117.90	123.30
14	F	203	CLA	CHB-C4A-NA	2.17	127.51	124.51
14	L	204	CLA	C1-C2-C3	-2.17	122.30	126.04
14	A	812	CLA	CHB-C1B-NB	2.17	126.55	124.26
14	B	830	CLA	CHC-C4B-NB	2.17	126.55	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	829	CLA	CMB-C2B-C3B	2.17	131.84	126.59
14	2	804	CLA	O1D-CGD-CBD	2.17	128.92	124.48
17	A	849	BCR	C24-C23-C22	-2.17	122.96	126.23
14	A	826	CLA	CAA-CBA-CGA	-2.17	106.92	113.25
14	B	824	CLA	CHA-C1A-NA	-2.17	121.44	126.40
17	0	208	BCR	C28-C27-C26	-2.16	110.21	114.08
17	j	1304	BCR	C38-C26-C25	-2.16	122.10	124.53
17	2	848	BCR	C2-C1-C6	2.16	113.81	110.48
17	1	1650	BCR	C24-C23-C22	-2.16	122.97	126.23
17	2	846	BCR	C8-C7-C6	-2.16	121.13	127.20
14	2	809	CLA	O2D-CGD-CBD	2.16	115.11	111.27
14	2	816	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
14	b	831	CLA	CHC-C4B-NB	2.16	126.54	124.26
14	B	831	CLA	CMB-C2B-C3B	2.16	131.82	126.59
14	B	802	CLA	CHB-C4A-NA	2.16	127.50	124.51
14	l	205	CLA	CHD-C1D-ND	-2.16	122.47	124.45
17	k	102	BCR	C15-C14-C13	-2.16	124.23	127.31
14	b	803	CLA	CHB-C4A-NA	2.16	127.50	124.51
14	A	827	CLA	O2D-CGD-CBD	2.16	115.10	111.27
14	2	812	CLA	C3B-C4B-NB	-2.16	108.51	110.52
14	2	829	CLA	C2D-C1D-ND	-2.16	108.52	110.10
14	B	827	CLA	CMB-C2B-C3B	2.16	131.81	126.59
14	A	828	CLA	CHB-C1B-NB	2.16	126.54	124.26
17	B	851	BCR	C38-C26-C25	-2.16	122.11	124.53
14	8	1303	CLA	C2D-C1D-ND	-2.15	108.52	110.10
14	1	1610	CLA	CHD-C1D-ND	-2.15	122.47	124.45
17	k	104	BCR	C8-C7-C6	-2.15	121.16	127.20
17	6	202	BCR	C37-C22-C21	-2.15	119.91	122.92
17	b	847	BCR	C36-C18-C19	2.15	121.47	118.08
14	j	1301	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
17	1	1648	BCR	C8-C7-C6	-2.15	121.16	127.20
14	K	101	CLA	CHD-C1D-ND	-2.15	122.48	124.45
17	a	849	BCR	C27-C26-C25	2.15	125.85	122.73
14	J	102	CLA	C2D-C1D-ND	-2.15	108.52	110.10
14	a	837	CLA	O2A-CGA-O1A	-2.15	117.94	123.30
14	B	811	CLA	C3B-C4B-NB	-2.15	108.52	110.52
14	1	1617	CLA	CHD-C1D-ND	-2.15	122.48	124.45
14	a	824	CLA	C1-C2-C3	-2.15	122.33	126.04
17	A	847	BCR	C8-C7-C6	-2.15	121.17	127.20
17	2	847	BCR	C36-C18-C19	2.15	121.46	118.08
14	J	102	CLA	CMB-C2B-C1B	-2.15	122.10	125.37
14	B	840	CLA	C2D-C1D-ND	-2.15	108.52	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	a	847	BCR	C8-C7-C6	-2.15	121.17	127.20
14	b	807	CLA	O1D-CGD-CBD	2.15	128.88	124.48
14	b	841	CLA	C2D-C1D-ND	-2.15	108.52	110.10
17	8	1306	BCR	C37-C22-C21	-2.15	119.92	122.92
14	a	825	CLA	CHD-C1D-ND	-2.15	122.48	124.45
14	A	824	CLA	C1-C2-C3	-2.15	122.33	126.04
14	1	1638	CLA	O1A-CGA-CBA	2.15	129.97	123.08
17	K	104	BCR	C8-C7-C6	-2.15	121.18	127.20
14	8	1301	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
14	A	837	CLA	O1A-CGA-CBA	2.14	129.97	123.08
14	B	825	CLA	CHB-C1B-NB	2.14	126.53	124.26
14	2	824	CLA	CHB-C1B-NB	2.14	126.53	124.26
14	2	832	CLA	CMB-C2B-C3B	2.14	131.78	126.59
14	b	816	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
17	B	844	BCR	C38-C26-C25	-2.14	122.12	124.53
17	8	1306	BCR	C38-C26-C25	-2.14	122.12	124.53
17	8	1306	BCR	C37-C22-C23	2.14	121.45	118.08
14	B	838	CLA	CHB-C1B-NB	2.14	126.53	124.26
17	9	104	BCR	C8-C7-C6	-2.14	121.18	127.20
18	A	854	LHG	C11-C10-C9	-2.14	103.55	114.42
17	0	201	BCR	C8-C7-C6	-2.14	121.19	127.20
14	2	828	CLA	CMB-C2B-C3B	2.14	131.78	126.59
14	A	814	CLA	CHB-C1B-NB	2.14	126.52	124.26
14	B	815	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
18	1	1655	LHG	C11-C10-C9	-2.14	103.56	114.42
14	1	1629	CLA	CHB-C1B-NB	2.14	126.52	124.26
14	1	1613	CLA	CHB-C1B-NB	2.14	126.52	124.26
17	F	202	BCR	C37-C22-C21	-2.14	119.93	122.92
14	J	102	CLA	CHD-C1D-ND	-2.14	122.49	124.45
17	8	1306	BCR	C27-C26-C25	2.14	125.84	122.73
14	2	841	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
14	A	857	CLA	C3B-C4B-NB	-2.14	108.53	110.52
14	2	819	CLA	CMB-C2B-C3B	2.14	131.77	126.59
14	B	806	CLA	CHD-C1D-ND	-2.14	122.49	124.45
17	L	206	BCR	C28-C27-C26	-2.14	110.26	114.08
14	b	825	CLA	CHA-C1A-NA	-2.14	121.50	126.40
14	B	823	CLA	CHB-C1B-NB	2.14	126.52	124.26
17	b	844	BCR	C8-C7-C6	-2.14	121.20	127.20
17	f	202	BCR	C37-C22-C21	-2.14	119.93	122.92
17	b	845	BCR	C38-C26-C25	-2.14	122.13	124.53
20	b	850	LMG	C38-C37-C36	-2.14	103.58	114.42
14	A	823	CLA	CHB-C1B-NB	2.14	126.52	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	j	1303	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
17	b	852	BCR	C20-C21-C22	-2.14	124.26	127.31
14	a	806	CLA	C1-O2A-CGA	2.14	122.05	116.44
14	B	828	CLA	C2D-C1D-ND	-2.14	108.53	110.10
14	B	817	CLA	C3B-C4B-NB	-2.14	108.53	110.52
14	B	821	CLA	C3B-C4B-NB	-2.14	108.53	110.52
14	F	203	CLA	O2D-CGD-O1D	-2.13	119.66	123.84
17	L	207	BCR	C8-C7-C6	-2.13	121.21	127.20
14	b	806	CLA	C3B-C4B-NB	-2.13	108.53	110.52
18	A	854	LHG	O8-C23-O10	-2.13	118.21	123.59
18	a	854	LHG	C11-C10-C9	-2.13	103.59	114.42
14	b	832	CLA	CMB-C2B-C3B	2.13	131.75	126.59
14	M	102	CLA	C3B-C4B-NB	-2.13	108.54	110.52
20	B	849	LMG	C38-C37-C36	-2.13	103.60	114.42
14	1	1626	CLA	CMB-C2B-C3B	2.13	131.75	126.59
18	a	854	LHG	O8-C23-O10	-2.13	118.21	123.59
18	l	201	LHG	C20-C19-C18	-2.13	103.60	114.42
17	b	852	BCR	C37-C22-C23	2.13	121.44	118.08
17	A	849	BCR	C27-C26-C25	2.13	125.83	122.73
17	A	847	BCR	C24-C23-C22	-2.13	123.01	126.23
14	A	806	CLA	C1-O2A-CGA	2.13	122.04	116.44
14	k	101	CLA	CHD-C1D-ND	-2.13	122.50	124.45
17	l	207	BCR	C28-C27-C26	-2.13	110.27	114.08
17	0	209	BCR	C8-C7-C6	-2.13	121.22	127.20
14	b	819	CLA	CMB-C2B-C3B	2.13	131.75	126.59
14	b	839	CLA	CHB-C1B-NB	2.13	126.51	124.26
18	L	208	LHG	C20-C19-C18	-2.13	103.61	114.42
20	2	850	LMG	C38-C37-C36	-2.13	103.62	114.42
14	a	828	CLA	CHB-C1B-NB	2.13	126.51	124.26
14	0	207	CLA	CHB-C1B-NB	2.13	126.51	124.26
18	0	202	LHG	C20-C19-C18	-2.13	103.63	114.42
17	a	849	BCR	C24-C23-C22	-2.13	123.02	126.23
14	2	831	CLA	CHC-C4B-NB	2.13	126.51	124.26
17	8	1306	BCR	C20-C21-C22	-2.13	124.28	127.31
14	b	835	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
14	b	812	CLA	C3B-C4B-NB	-2.12	108.54	110.52
14	2	818	CLA	C3B-C4B-NB	-2.12	108.54	110.52
14	a	837	CLA	O1A-CGA-CBA	2.12	129.91	123.08
14	A	825	CLA	CMB-C2B-C3B	2.12	131.73	126.59
14	1	1607	CLA	C1-O2A-CGA	2.12	122.02	116.44
14	L	204	CLA	CHD-C1D-ND	-2.12	122.50	124.45
14	2	822	CLA	CHD-C1D-ND	-2.12	122.50	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	1	1655	LHG	O8-C23-O10	-2.12	118.23	123.59
17	b	852	BCR	C27-C26-C25	2.12	125.81	122.73
14	b	831	CLA	O2D-CGD-CBD	2.12	115.04	111.27
14	B	806	CLA	O1D-CGD-CBD	2.12	128.82	124.48
17	2	844	BCR	C8-C7-C6	-2.12	121.25	127.20
14	K	103	CLA	CMB-C2B-C3B	2.12	131.72	126.59
17	B	846	BCR	C36-C18-C19	2.12	121.42	118.08
14	A	809	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
17	a	849	BCR	C8-C7-C6	-2.12	121.25	127.20
14	B	834	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
14	B	826	CLA	C2D-C1D-ND	-2.12	108.54	110.10
17	0	203	BCR	C27-C26-C25	2.12	125.81	122.73
17	a	847	BCR	C24-C23-C22	-2.12	123.03	126.23
14	b	806	CLA	CHD-C1D-ND	-2.12	122.51	124.45
17	8	1305	BCR	C29-C30-C25	2.12	113.74	110.48
17	B	851	BCR	C37-C22-C23	2.12	121.41	118.08
14	1	1640	CLA	CHB-C4A-NA	2.12	127.44	124.51
14	1	1625	CLA	C1-C2-C3	-2.12	122.39	126.04
17	A	849	BCR	C8-C7-C6	-2.11	121.26	127.20
14	9	103	CLA	CMB-C2B-C3B	2.11	131.71	126.59
14	a	809	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
14	A	839	CLA	CHC-C4B-NB	2.11	126.49	124.26
14	b	829	CLA	C2D-C1D-ND	-2.11	108.55	110.10
17	B	843	BCR	C8-C7-C6	-2.11	121.27	127.20
14	A	819	CLA	CHB-C4A-NA	2.11	127.43	124.51
14	a	803	CLA	CHB-C4A-NA	2.11	127.43	124.51
17	b	852	BCR	C38-C26-C25	-2.11	122.16	124.53
17	1	1652	BCR	C7-C8-C9	-2.11	123.05	126.23
14	B	818	CLA	CMB-C2B-C3B	2.11	131.70	126.59
14	2	831	CLA	O2D-CGD-CBD	2.11	115.02	111.27
14	k	103	CLA	CMB-C2B-C3B	2.11	131.70	126.59
13	1	1602	CL0	CHC-C4B-NB	2.11	126.49	124.26
14	1	1620	CLA	CHB-C4A-NA	2.11	127.43	124.51
14	2	807	CLA	CHD-C1D-ND	-2.11	122.52	124.45
14	9	101	CLA	CHD-C1D-ND	-2.11	122.52	124.45
14	a	839	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
14	1	1640	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
14	a	823	CLA	CHB-C1B-NB	2.11	126.49	124.26
14	a	816	CLA	CHD-C1D-ND	-2.11	122.52	124.45
14	A	803	CLA	CHB-C4A-NA	2.11	127.43	124.51
17	0	201	BCR	C7-C8-C9	-2.11	123.05	126.23
14	9	103	CLA	CHB-C1B-NB	2.11	126.49	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	850	BCR	C27-C26-C25	2.11	125.79	122.73
14	1	1629	CLA	CHD-C1D-ND	-2.11	122.52	124.45
14	B	840	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
17	1	1650	BCR	C8-C7-C6	-2.11	121.28	127.20
17	0	209	BCR	C20-C21-C22	-2.11	124.30	127.31
14	b	841	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
14	0	206	CLA	CHD-C1D-ND	-2.11	122.52	124.45
17	0	201	BCR	C20-C21-C22	-2.11	124.30	127.31
17	l	202	BCR	C27-C26-C25	2.11	125.79	122.73
14	b	818	CLA	C3B-C4B-NB	-2.11	108.56	110.52
20	B	849	LMG	C42-C41-C40	-2.10	103.74	114.42
14	A	816	CLA	CHD-C1D-ND	-2.10	122.52	124.45
14	1	1645	CLA	CMB-C2B-C3B	2.10	131.68	126.59
14	1	1624	CLA	CHB-C1B-NB	2.10	126.48	124.26
17	L	201	BCR	C27-C26-C25	2.10	125.78	122.73
14	j	1303	CLA	CHD-C1D-ND	-2.10	122.52	124.45
14	2	835	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
20	b	850	LMG	C42-C41-C40	-2.10	103.75	114.42
14	2	822	CLA	CHB-C1B-NB	2.10	126.48	124.26
14	B	805	CLA	CHD-C1D-ND	-2.10	122.52	124.45
17	A	851	BCR	C7-C8-C9	-2.10	123.06	126.23
17	6	204	BCR	C37-C22-C21	-2.10	119.98	122.92
14	a	817	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
14	A	811	CLA	CHD-C1D-ND	-2.10	122.52	124.45
14	1	1610	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
20	2	850	LMG	C42-C41-C40	-2.10	103.77	114.42
14	1	1607	CLA	CHB-C1B-NB	2.10	126.48	124.26
14	2	839	CLA	CHB-C1B-NB	2.10	126.48	124.26
14	1	1601	CLA	C3B-C4B-NB	-2.10	108.57	110.52
14	a	825	CLA	CMB-C2B-C3B	2.10	131.67	126.59
14	b	802	CLA	CHB-C4A-NA	2.10	127.41	124.51
17	2	845	BCR	C38-C26-C25	-2.10	122.17	124.53
14	b	822	CLA	CHD-C1D-ND	-2.10	122.53	124.45
14	A	855	CLA	CHB-C4A-NA	2.10	127.41	124.51
14	2	808	CLA	C2D-C1D-ND	-2.10	108.56	110.10
17	a	849	BCR	C7-C8-C9	-2.10	123.07	126.23
14	K	103	CLA	CHB-C1B-NB	2.10	126.48	124.26
14	0	205	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
14	A	844	CLA	CMB-C2B-C3B	2.10	131.67	126.59
14	B	820	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
14	1	1635	CLA	C16-C15-C13	-2.10	109.14	115.92
14	a	819	CLA	CHB-C4A-NA	2.10	127.41	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	j	1305	BCR	C16-C15-C14	-2.10	119.18	123.47
14	a	812	CLA	CHB-C1B-NB	2.10	126.47	124.26
14	1	1614	CLA	O2D-CGD-CBD	2.09	114.99	111.27
14	A	828	CLA	CHD-C1D-ND	-2.09	122.53	124.45
14	a	828	CLA	CHD-C1D-ND	-2.09	122.53	124.45
14	b	841	CLA	CHD-C1D-ND	-2.09	122.53	124.45
14	8	1303	CLA	CHD-C1D-ND	-2.09	122.53	124.45
14	A	817	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
17	1	1651	BCR	C27-C26-C25	2.09	125.77	122.73
17	1	1650	BCR	C7-C8-C9	-2.09	123.07	126.23
14	2	822	CLA	O2D-CGD-CBD	2.09	114.98	111.27
14	a	819	CLA	C1-C2-C3	-2.09	122.43	126.04
17	A	856	BCR	C29-C30-C25	2.09	113.70	110.48
14	A	813	CLA	O2D-CGD-CBD	2.09	114.98	111.27
17	a	851	BCR	C7-C8-C9	-2.09	123.08	126.23
14	A	839	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
14	l	204	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
14	a	844	CLA	CMB-C2B-C3B	2.09	131.65	126.59
14	B	821	CLA	CHD-C1D-ND	-2.09	122.53	124.45
14	2	841	CLA	CHD-C1D-ND	-2.09	122.53	124.45
14	1	1604	CLA	CHB-C4A-NA	2.09	127.40	124.51
14	2	802	CLA	CHB-C4A-NA	2.09	127.40	124.51
17	8	1305	BCR	C16-C15-C14	-2.09	119.19	123.47
17	A	856	BCR	C24-C23-C22	-2.09	123.08	126.23
14	1	1640	CLA	CHC-C4B-NB	2.09	126.47	124.26
14	2	827	CLA	C2D-C1D-ND	-2.09	108.56	110.10
17	b	852	BCR	C37-C22-C21	-2.09	120.00	122.92
17	A	849	BCR	C7-C8-C9	-2.09	123.08	126.23
14	A	822	CLA	CHD-C1D-ND	-2.09	122.54	124.45
14	B	830	CLA	O2D-CGD-CBD	2.09	114.98	111.27
14	2	838	CLA	O2D-CGD-CBD	2.09	114.98	111.27
17	a	850	BCR	C27-C26-C25	2.09	125.76	122.73
14	b	822	CLA	O2D-CGD-CBD	2.09	114.97	111.27
14	A	804	CLA	C3B-C4B-NB	-2.09	108.58	110.52
14	l	206	CLA	CHB-C1B-NB	2.09	126.47	124.26
14	1	1615	CLA	CHB-C1B-NB	2.09	126.47	124.26
14	1	1620	CLA	C1-C2-C3	-2.09	122.44	126.04
14	1	1606	CLA	CMB-C2B-C3B	2.09	131.64	126.59
14	B	831	CLA	CHB-C1B-NB	2.08	126.46	124.26
14	B	809	CLA	C3B-C4B-NB	-2.08	108.58	110.52
14	2	841	CLA	C2D-C1D-ND	-2.08	108.57	110.10
14	A	806	CLA	C3C-C4C-NC	-2.08	108.23	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	844	BCR	C27-C26-C25	2.08	125.76	122.73
14	b	837	CLA	CHB-C4A-NA	2.08	127.39	124.51
14	A	841	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
14	1	1618	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
13	A	801	CL0	CHC-C4B-NB	2.08	126.46	124.26
14	a	839	CLA	CHC-C4B-NB	2.08	126.46	124.26
14	b	822	CLA	CHB-C1B-NB	2.08	126.46	124.26
14	k	103	CLA	CHB-C1B-NB	2.08	126.46	124.26
17	L	207	BCR	C7-C8-C9	-2.08	123.09	126.23
17	8	1305	BCR	C24-C23-C22	-2.08	123.09	126.23
14	2	807	CLA	O1D-CGD-CBD	2.08	128.74	124.48
14	A	836	CLA	CHB-C1B-NB	2.08	126.46	124.26
17	b	848	BCR	C36-C18-C19	2.08	121.36	118.08
17	L	207	BCR	C20-C21-C22	-2.08	124.34	127.31
17	f	204	BCR	C37-C22-C21	-2.08	120.01	122.92
14	B	817	CLA	C2D-C1D-ND	-2.08	108.57	110.10
14	A	819	CLA	CMB-C2B-C1B	-2.08	122.20	125.37
17	b	847	BCR	C8-C7-C6	-2.08	121.36	127.20
14	B	805	CLA	C3B-C4B-NB	-2.08	108.58	110.52
17	0	209	BCR	C7-C8-C9	-2.08	123.09	126.23
14	a	839	CLA	CHB-C4A-NA	2.08	127.39	124.51
17	A	850	BCR	C33-C5-C6	-2.08	122.19	124.53
17	L	206	BCR	C8-C7-C6	-2.08	121.36	127.20
14	1	1642	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
17	a	850	BCR	C33-C5-C6	-2.08	122.19	124.53
14	j	1302	CLA	CHD-C1D-ND	-2.08	122.54	124.45
14	B	821	CLA	O2D-CGD-CBD	2.08	114.96	111.27
14	b	810	CLA	C3B-C4B-NB	-2.08	108.59	110.52
17	B	851	BCR	C37-C22-C21	-2.08	120.01	122.92
17	2	848	BCR	C36-C18-C19	2.08	121.35	118.08
17	l	207	BCR	C8-C7-C6	-2.08	121.37	127.20
14	b	821	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
14	F	204	CLA	CHD-C1D-ND	-2.08	122.55	124.45
14	1	1623	CLA	CHD-C1D-ND	-2.08	122.55	124.45
14	2	832	CLA	CHB-C1B-NB	2.08	126.46	124.26
14	B	836	CLA	CHB-C4A-NA	2.08	127.38	124.51
14	a	841	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
14	L	203	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
14	b	812	CLA	C1-C2-C3	-2.08	122.45	126.04
14	a	805	CLA	CMB-C2B-C3B	2.08	131.61	126.59
14	2	819	CLA	CHD-C1D-ND	-2.08	122.55	124.45
14	2	810	CLA	C3B-C4B-NB	-2.08	108.59	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	806	CLA	C3C-C4C-NC	-2.07	108.24	110.57
14	B	814	CLA	C2D-C1D-ND	-2.07	108.58	110.10
14	2	818	CLA	C2D-C1D-ND	-2.07	108.58	110.10
14	A	834	CLA	C16-C15-C13	-2.07	109.21	115.92
14	a	819	CLA	CMB-C2B-C1B	-2.07	122.21	125.37
14	2	806	CLA	C3B-C4B-NB	-2.07	108.59	110.52
14	f	203	CLA	CHD-C1D-ND	-2.07	122.55	124.45
14	B	838	CLA	CHC-C4B-NB	2.07	126.45	124.26
14	A	813	CLA	C2D-C1D-ND	-2.07	108.58	110.10
14	l	206	CLA	C2D-C1D-ND	-2.07	108.58	110.10
14	L	205	CLA	CHB-C1B-NB	2.07	126.45	124.26
14	b	805	CLA	O1D-CGD-CBD	2.07	128.72	124.48
17	l	202	BCR	C37-C22-C23	2.07	121.34	118.08
14	a	813	CLA	O2D-CGD-CBD	2.07	114.95	111.27
14	B	835	CLA	CHB-C1B-NB	2.07	126.45	124.26
14	1	1627	CLA	CHC-C4B-NB	2.07	126.45	124.26
14	F	203	CLA	C3B-C4B-NB	-2.07	108.59	110.52
17	1	1651	BCR	C33-C5-C6	-2.07	122.20	124.53
14	b	818	CLA	C2D-C1D-ND	-2.07	108.58	110.10
14	b	835	CLA	C2D-C1D-ND	-2.07	108.58	110.10
17	0	203	BCR	C37-C22-C23	2.07	121.34	118.08
14	a	814	CLA	CHB-C1B-NB	2.07	126.45	124.26
14	a	815	CLA	CHD-C1D-ND	-2.07	122.55	124.45
14	A	819	CLA	C1-C2-C3	-2.07	122.47	126.04
14	a	838	CLA	C3B-C4B-NB	-2.07	108.60	110.52
14	a	834	CLA	C16-C15-C13	-2.07	109.24	115.92
17	B	847	BCR	C36-C18-C19	2.07	121.33	118.08
14	2	821	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
17	F	205	BCR	C37-C22-C21	-2.07	120.03	122.92
14	1	1605	CLA	C3B-C4B-NB	-2.07	108.60	110.52
17	b	844	BCR	C27-C26-C25	2.07	125.73	122.73
17	2	847	BCR	C8-C7-C6	-2.07	121.40	127.20
14	2	837	CLA	CHB-C4A-NA	2.07	127.37	124.51
14	a	811	CLA	CHD-C1D-ND	-2.07	122.56	124.45
14	b	827	CLA	C2D-C1D-ND	-2.07	108.58	110.10
14	1	1642	CLA	CHB-C1B-NB	2.06	126.44	124.26
14	A	839	CLA	CHB-C4A-NA	2.06	127.37	124.51
17	j	1305	BCR	C24-C23-C22	-2.06	123.12	126.23
14	2	836	CLA	CHB-C1B-NB	2.06	126.44	124.26
14	B	817	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
17	L	201	BCR	C37-C22-C23	2.06	121.33	118.08
14	b	835	CLA	CAA-CBA-CGA	-2.06	107.22	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1	1616	CLA	CHD-C1D-ND	-2.06	122.56	124.45
14	A	826	CLA	CHC-C4B-NB	2.06	126.44	124.26
14	B	821	CLA	CHB-C1B-NB	2.06	126.44	124.26
14	2	805	CLA	O1D-CGD-CBD	2.06	128.71	124.48
17	A	856	BCR	C16-C15-C14	-2.06	119.25	123.47
14	2	830	CLA	CAC-C3C-C4C	2.06	127.49	124.81
14	B	811	CLA	C1-C2-C3	-2.06	122.48	126.04
14	B	837	CLA	O2D-CGD-CBD	2.06	114.93	111.27
14	A	828	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
14	1	1637	CLA	CHB-C1B-NB	2.06	126.44	124.26
14	a	804	CLA	C3B-C4B-NB	-2.06	108.60	110.52
14	1	1612	CLA	CHD-C1D-ND	-2.06	122.56	124.45
17	0	208	BCR	C8-C7-C6	-2.06	121.41	127.20
14	2	812	CLA	C1-C2-C3	-2.06	122.48	126.04
17	a	852	BCR	C36-C18-C19	2.06	119.15	114.60
14	A	826	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
14	2	815	CLA	C2D-C1D-ND	-2.06	108.59	110.10
14	b	818	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
14	A	804	CLA	O2D-CGD-CBD	2.06	114.93	111.27
14	b	822	CLA	O2A-CGA-O1A	-2.06	118.17	123.30
17	B	843	BCR	C27-C26-C25	2.06	125.72	122.73
14	A	815	CLA	CHD-C1D-ND	-2.06	122.56	124.45
14	b	836	CLA	CHB-C1B-NB	2.06	126.43	124.26
14	j	1301	CLA	C3B-C4B-NB	-2.06	108.61	110.52
14	A	806	CLA	CHB-C1B-NB	2.06	126.43	124.26
14	2	818	CLA	O2A-CGA-O1A	-2.06	118.41	123.59
14	b	832	CLA	CHB-C1B-NB	2.05	126.43	124.26
17	B	846	BCR	C8-C7-C6	-2.05	121.43	127.20
14	B	818	CLA	CHD-C1D-ND	-2.05	122.57	124.45
17	1	1653	BCR	C36-C18-C19	2.05	119.14	114.60
14	A	805	CLA	CMB-C2B-C3B	2.05	131.56	126.59
14	B	818	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
17	j	1305	BCR	C29-C30-C25	2.05	113.64	110.48
14	b	819	CLA	CHD-C1D-ND	-2.05	122.57	124.45
14	A	816	CLA	CMB-C2B-C1B	-2.05	122.24	125.37
14	a	804	CLA	O2D-CGD-CBD	2.05	114.91	111.27
13	a	801	CL0	CHC-C4B-NB	2.05	126.43	124.26
14	a	826	CLA	CHC-C4B-NB	2.05	126.43	124.26
14	2	835	CLA	CAA-CBA-CGA	-2.05	107.26	113.25
14	B	807	CLA	C2D-C1D-ND	-2.05	108.59	110.10
14	B	834	CLA	CAA-CBA-CGA	-2.05	107.26	113.25
14	1	1617	CLA	CMB-C2B-C1B	-2.05	122.25	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	826	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
14	A	812	CLA	CHD-C1D-ND	-2.05	122.57	124.45
14	1	1625	CLA	CHD-C1D-ND	-2.05	122.57	124.45
14	6	203	CLA	CHD-C1D-ND	-2.05	122.57	124.45
14	1	1627	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
14	F	201	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
14	a	828	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
14	J	101	CLA	CHD-C1D-ND	-2.05	122.57	124.45
14	b	808	CLA	C2D-C1D-ND	-2.05	108.59	110.10
14	2	835	CLA	C2D-C1D-ND	-2.05	108.59	110.10
14	L	205	CLA	C2D-C1D-ND	-2.05	108.60	110.10
14	A	831	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
14	A	834	CLA	O1D-CGD-CBD	2.05	128.67	124.48
14	1	1607	CLA	C3C-C4C-NC	-2.05	108.28	110.57
14	b	830	CLA	CAC-C3C-C4C	2.05	127.46	124.81
14	a	829	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
14	a	806	CLA	CHB-C1B-NB	2.05	126.42	124.26
14	1	1635	CLA	O1D-CGD-CBD	2.04	128.67	124.48
14	2	839	CLA	CHB-C4A-NA	2.04	127.34	124.51
17	8	1304	BCR	C16-C15-C14	-2.04	119.29	123.47
14	1	1622	CLA	CHB-C1B-NB	2.04	126.42	124.26
14	B	820	CLA	C3B-C4B-NB	-2.04	108.62	110.52
20	B	849	LMG	O1-C7-C8	-2.04	105.97	110.90
14	2	822	CLA	O2A-CGA-O1A	-2.04	118.21	123.30
20	b	850	LMG	O1-C7-C8	-2.04	105.97	110.90
14	a	836	CLA	CHB-C1B-NB	2.04	126.42	124.26
14	2	814	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
17	A	852	BCR	C36-C18-C19	2.04	119.11	114.60
14	a	823	CLA	O2A-CGA-O1A	-2.04	118.21	123.30
14	b	815	CLA	C2D-C1D-ND	-2.04	108.60	110.10
14	2	819	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
14	a	816	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
14	B	804	CLA	O1D-CGD-CBD	2.04	128.66	124.48
14	a	805	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
14	f	201	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
14	B	821	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
14	2	817	CLA	CMB-C2B-C1B	-2.04	122.27	125.37
14	1	1620	CLA	CMB-C2B-C1B	-2.04	122.27	125.37
14	a	824	CLA	CHD-C1D-ND	-2.04	122.58	124.45
14	a	834	CLA	O1D-CGD-CBD	2.04	128.65	124.48
14	b	819	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
14	1	1621	CLA	CHB-C1B-NB	2.04	126.41	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	850	LMG	O1-C7-C8	-2.04	105.99	110.90
17	j	1304	BCR	C16-C15-C14	-2.04	119.30	123.47
14	B	813	CLA	O2A-CGA-O1A	-2.04	118.46	123.59
14	b	814	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
17	b	848	BCR	C36-C18-C17	-2.03	120.07	122.92
14	1	1605	CLA	O2D-CGD-CBD	2.03	114.88	111.27
14	A	823	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
14	6	201	CLA	CMB-C2B-C1B	-2.03	122.27	125.37
14	b	805	CLA	C2D-C1D-ND	-2.03	108.61	110.10
14	a	814	CLA	CHD-C1D-ND	-2.03	122.59	124.45
14	2	811	CLA	CAC-C3C-C4C	2.03	127.45	124.81
14	B	831	CLA	CHD-C1D-ND	-2.03	122.59	124.45
14	1	1610	CLA	O2D-CGD-CBD	2.03	114.88	111.27
17	K	104	BCR	C16-C15-C14	-2.03	119.31	123.47
14	A	805	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
14	B	834	CLA	C2D-C1D-ND	-2.03	108.61	110.10
14	A	838	CLA	C3B-C4B-NB	-2.03	108.63	110.52
14	1	1613	CLA	CHD-C1D-ND	-2.03	122.59	124.45
14	a	841	CLA	CHB-C1B-NB	2.03	126.41	124.26
14	a	835	CLA	O2D-CGD-CBD	2.03	114.87	111.27
14	1	1639	CLA	C3B-C4B-NB	-2.03	108.63	110.52
14	B	829	CLA	CAC-C3C-C4C	2.03	127.44	124.81
14	8	1301	CLA	C3B-C4B-NB	-2.03	108.64	110.52
14	B	810	CLA	CAC-C3C-C4C	2.03	127.44	124.81
14	A	814	CLA	CHD-C1D-ND	-2.03	122.59	124.45
14	1	1629	CLA	CMB-C2B-C1B	-2.02	122.28	125.37
14	9	103	CLA	C1-C2-C3	-2.02	122.54	126.04
14	b	805	CLA	C4-C3-C5	2.02	118.68	115.27
14	8	1302	CLA	CHD-C1D-ND	-2.02	122.59	124.45
14	a	820	CLA	C1-C2-C3	-2.02	122.54	126.04
14	B	830	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
14	b	838	CLA	O2D-CGD-CBD	2.02	114.86	111.27
13	a	801	CL0	O2A-CGA-O1A	-2.02	118.49	123.59
17	J	103	BCR	C16-C15-C14	-2.02	119.33	123.47
14	B	809	CLA	C3C-C4C-NC	-2.02	108.30	110.57
14	a	809	CLA	O2D-CGD-CBD	2.02	114.86	111.27
17	b	847	BCR	C37-C22-C21	-2.02	120.09	122.92
14	K	103	CLA	C1-C2-C3	-2.02	122.55	126.04
13	1	1602	CL0	O2A-CGA-O1A	-2.02	118.49	123.59
14	b	812	CLA	C4-C3-C5	2.02	118.67	115.27
14	A	834	CLA	C2D-C1D-ND	-2.02	108.61	110.10
14	A	803	CLA	O2A-CGA-O1A	-2.02	118.49	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	840	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
14	1	1621	CLA	C1-C2-C3	-2.02	122.55	126.04
13	A	801	CL0	O2A-CGA-O1A	-2.02	118.50	123.59
14	1	1606	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
14	a	831	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
14	2	839	CLA	CHC-C4B-NB	2.02	126.39	124.26
14	b	821	CLA	CHD-C1D-ND	-2.02	122.60	124.45
14	1	1626	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
14	2	831	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
17	a	848	BCR	C36-C18-C17	-2.02	120.10	122.92
14	A	820	CLA	C1-C2-C3	-2.02	122.55	126.04
17	1	1649	BCR	C36-C18-C17	-2.02	120.10	122.92
14	B	803	CLA	CAC-C3C-C4C	2.02	127.43	124.81
14	B	802	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
14	k	103	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
14	B	807	CLA	O2D-CGD-CBD	2.02	114.85	111.27
14	1	1630	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
14	B	816	CLA	CMB-C2B-C1B	-2.02	122.30	125.37
14	b	804	CLA	CAC-C3C-C4C	2.01	127.42	124.81
14	2	804	CLA	CAC-C3C-C4C	2.01	127.42	124.81
14	1	1632	CLA	CMB-C2B-C1B	-2.01	122.30	125.37
14	B	839	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
14	B	804	CLA	C4-C3-C5	2.01	118.66	115.27
14	B	811	CLA	C4-C3-C5	2.01	118.66	115.27
17	A	848	BCR	C36-C18-C17	-2.01	120.10	122.92
14	1	1604	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
14	A	819	CLA	C6-C5-C3	2.01	118.73	113.45
14	1	1615	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
14	1	1624	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
14	A	822	CLA	CMB-C2B-C3B	2.01	131.46	126.59
17	B	847	BCR	C36-C18-C17	-2.01	120.10	122.92
17	8	1304	BCR	C29-C30-C25	2.01	113.58	110.48
14	A	830	CLA	O1D-CGD-CBD	2.01	128.60	124.48
14	A	821	CLA	CHB-C1B-NB	2.01	126.39	124.26
14	b	803	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
14	A	855	CLA	C3B-C4B-NB	-2.01	108.65	110.52
14	1	1620	CLA	C6-C5-C3	2.01	118.73	113.45
14	B	840	CLA	CHD-C1D-ND	-2.01	122.61	124.45
14	A	825	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
14	k	103	CLA	C1-C2-C3	-2.01	122.57	126.04
14	2	829	CLA	CHB-C4A-NA	2.01	127.29	124.51
14	b	821	CLA	C3B-C4B-NB	-2.01	108.65	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	821	CLA	C3B-C4B-NB	-2.01	108.65	110.52
17	j	1304	BCR	C8-C7-C6	-2.01	121.56	127.20
14	A	842	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
17	k	104	BCR	C16-C15-C14	-2.01	119.36	123.47
14	a	819	CLA	C6-C5-C3	2.01	118.72	113.45
14	2	803	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
14	2	805	CLA	C4-C3-C5	2.01	118.65	115.27
14	A	820	CLA	CHB-C1B-NB	2.01	126.38	124.26
14	b	837	CLA	CHB-C1B-NB	2.01	126.38	124.26
14	2	837	CLA	CHB-C1B-NB	2.01	126.38	124.26
14	b	810	CLA	C3C-C4C-NC	-2.01	108.32	110.57
14	1	1623	CLA	CMB-C2B-C3B	2.01	131.45	126.59
17	j	1304	BCR	C29-C30-C25	2.01	113.57	110.48
20	B	849	LMG	O7-C10-O9	-2.01	118.85	123.70
14	A	805	CLA	CHB-C1B-NB	2.01	126.38	124.26
14	a	805	CLA	CHB-C1B-NB	2.01	126.38	124.26
14	A	807	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
14	K	103	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
14	b	802	CLA	C3B-C4B-NB	-2.01	108.65	110.52
14	1	1614	CLA	C2D-C1D-ND	-2.01	108.62	110.10
14	A	829	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
14	9	103	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
14	b	812	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
14	2	812	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
17	J	103	BCR	C8-C7-C6	-2.01	121.57	127.20
14	A	814	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
14	a	819	CLA	O2D-CGD-CBD	2.01	114.83	111.27
17	9	104	BCR	C16-C15-C14	-2.00	119.37	123.47
14	a	822	CLA	CMB-C2B-C3B	2.00	131.44	126.59
14	A	815	CLA	CHB-C1B-NB	2.00	126.38	124.26
17	8	1304	BCR	C8-C7-C6	-2.00	121.57	127.20
14	B	838	CLA	CHB-C4A-NA	2.00	127.28	124.51
14	B	828	CLA	CHD-C1D-ND	-2.00	122.61	124.45
14	a	830	CLA	O1D-CGD-CBD	2.00	128.58	124.48
20	b	850	LMG	O7-C10-O9	-2.00	118.86	123.70
14	b	817	CLA	CMB-C2B-C1B	-2.00	122.32	125.37
14	a	814	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
14	2	819	CLA	O1D-CGD-CBD	2.00	128.58	124.48
14	b	839	CLA	CHC-C4B-NB	2.00	126.38	124.26
14	b	831	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
14	A	824	CLA	CHD-C1D-ND	-2.00	122.62	124.45

There are no chirality outliers.

All (4325) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	802	CLA	CBD-CGD-O2D-CED
14	A	803	CLA	C6-C7-C8-C9
14	A	804	CLA	CHA-CBD-CGD-O1D
14	A	804	CLA	CHA-CBD-CGD-O2D
14	A	805	CLA	C1A-C2A-CAA-CBA
14	A	805	CLA	C3A-C2A-CAA-CBA
14	A	805	CLA	CHA-CBD-CGD-O1D
14	A	805	CLA	CHA-CBD-CGD-O2D
14	A	806	CLA	C1A-C2A-CAA-CBA
14	A	806	CLA	CHA-CBD-CGD-O1D
14	A	806	CLA	CHA-CBD-CGD-O2D
14	A	806	CLA	CAD-CBD-CGD-O1D
14	A	806	CLA	CAD-CBD-CGD-O2D
14	A	806	CLA	O2A-C1-C2-C3
14	A	807	CLA	C1A-C2A-CAA-CBA
14	A	807	CLA	C3A-C2A-CAA-CBA
14	A	809	CLA	C3A-C2A-CAA-CBA
14	A	809	CLA	CHA-CBD-CGD-O1D
14	A	809	CLA	CHA-CBD-CGD-O2D
14	A	812	CLA	CHA-CBD-CGD-O1D
14	A	812	CLA	CHA-CBD-CGD-O2D
14	A	812	CLA	CBD-CGD-O2D-CED
14	A	814	CLA	CHA-CBD-CGD-O1D
14	A	814	CLA	CHA-CBD-CGD-O2D
14	A	814	CLA	CAD-CBD-CGD-O1D
14	A	814	CLA	CAD-CBD-CGD-O2D
14	A	815	CLA	C1A-C2A-CAA-CBA
14	A	815	CLA	C2B-C3B-CAB-CBB
14	A	815	CLA	C4B-C3B-CAB-CBB
14	A	816	CLA	CHA-CBD-CGD-O1D
14	A	816	CLA	CHA-CBD-CGD-O2D
14	A	816	CLA	CAD-CBD-CGD-O1D
14	A	816	CLA	CAD-CBD-CGD-O2D
14	A	816	CLA	O2A-C1-C2-C3
14	A	817	CLA	CBD-CGD-O2D-CED
14	A	819	CLA	C2B-C3B-CAB-CBB
14	A	819	CLA	C4B-C3B-CAB-CBB
14	A	819	CLA	C2-C3-C5-C6
14	A	819	CLA	C4-C3-C5-C6
14	A	820	CLA	C1A-C2A-CAA-CBA
14	A	820	CLA	C3A-C2A-CAA-CBA
14	A	821	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	A	823	CLA	CAD-CBD-CGD-O1D
14	A	823	CLA	CAD-CBD-CGD-O2D
14	A	823	CLA	CBD-CGD-O2D-CED
14	A	824	CLA	C1A-C2A-CAA-CBA
14	A	824	CLA	CAD-CBD-CGD-O2D
14	A	825	CLA	CHA-CBD-CGD-O1D
14	A	825	CLA	CHA-CBD-CGD-O2D
14	A	829	CLA	CBD-CGD-O2D-CED
14	A	829	CLA	O2A-C1-C2-C3
14	A	830	CLA	C1A-C2A-CAA-CBA
14	A	831	CLA	CHA-CBD-CGD-O2D
14	A	835	CLA	CHA-CBD-CGD-O1D
14	A	835	CLA	CHA-CBD-CGD-O2D
14	A	836	CLA	C2-C3-C5-C6
14	A	836	CLA	C4-C3-C5-C6
14	A	837	CLA	CHA-CBD-CGD-O1D
14	A	837	CLA	CHA-CBD-CGD-O2D
14	A	839	CLA	CAD-CBD-CGD-O1D
14	A	839	CLA	CAD-CBD-CGD-O2D
14	A	842	CLA	C2-C3-C5-C6
14	A	842	CLA	C4-C3-C5-C6
14	A	844	CLA	CHA-CBD-CGD-O1D
14	A	844	CLA	CHA-CBD-CGD-O2D
14	A	855	CLA	CHA-CBD-CGD-O1D
14	A	855	CLA	CHA-CBD-CGD-O2D
14	A	855	CLA	CAD-CBD-CGD-O1D
14	B	803	CLA	CBD-CGD-O2D-CED
14	B	804	CLA	C11-C12-C13-C14
14	B	805	CLA	C3A-C2A-CAA-CBA
14	B	805	CLA	CHA-CBD-CGD-O1D
14	B	805	CLA	CHA-CBD-CGD-O2D
14	B	805	CLA	CAD-CBD-CGD-O1D
14	B	805	CLA	CAD-CBD-CGD-O2D
14	B	809	CLA	C2-C3-C5-C6
14	B	809	CLA	C4-C3-C5-C6
14	B	817	CLA	C1A-C2A-CAA-CBA
14	B	817	CLA	C3A-C2A-CAA-CBA
14	B	817	CLA	C4B-C3B-CAB-CBB
14	B	818	CLA	C3A-C2A-CAA-CBA
14	B	818	CLA	CAD-CBD-CGD-O1D
14	B	818	CLA	CAD-CBD-CGD-O2D
14	B	819	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	B	819	CLA	C4B-C3B-CAB-CBB
14	B	819	CLA	CBD-CGD-O2D-CED
14	B	820	CLA	C1A-C2A-CAA-CBA
14	B	820	CLA	C3A-C2A-CAA-CBA
14	B	822	CLA	CBD-CGD-O2D-CED
14	B	824	CLA	C1A-C2A-CAA-CBA
14	B	824	CLA	C3A-C2A-CAA-CBA
14	B	824	CLA	C2A-CAA-CBA-CGA
14	B	825	CLA	C1A-C2A-CAA-CBA
14	B	825	CLA	C11-C10-C8-C7
14	B	826	CLA	CHA-CBD-CGD-O1D
14	B	826	CLA	CHA-CBD-CGD-O2D
14	B	827	CLA	C1A-C2A-CAA-CBA
14	B	827	CLA	C3A-C2A-CAA-CBA
14	B	829	CLA	CHA-CBD-CGD-O1D
14	B	829	CLA	CHA-CBD-CGD-O2D
14	B	830	CLA	C1A-C2A-CAA-CBA
14	B	830	CLA	C3A-C2A-CAA-CBA
14	B	831	CLA	C1A-C2A-CAA-CBA
14	B	832	CLA	CAD-CBD-CGD-O1D
14	B	832	CLA	CAD-CBD-CGD-O2D
14	B	834	CLA	C1A-C2A-CAA-CBA
14	B	834	CLA	CBD-CGD-O2D-CED
14	B	841	CLA	CAD-CBD-CGD-O1D
14	B	841	CLA	CAD-CBD-CGD-O2D
14	F	201	CLA	CHA-CBD-CGD-O1D
14	F	201	CLA	CBD-CGD-O2D-CED
14	F	204	CLA	C1A-C2A-CAA-CBA
14	F	204	CLA	C3A-C2A-CAA-CBA
14	K	101	CLA	C3A-C2A-CAA-CBA
14	K	101	CLA	CHA-CBD-CGD-O1D
14	K	101	CLA	CHA-CBD-CGD-O2D
14	K	101	CLA	CAD-CBD-CGD-O1D
14	K	103	CLA	CAD-CBD-CGD-O1D
14	K	103	CLA	CAD-CBD-CGD-O2D
14	L	203	CLA	C1A-C2A-CAA-CBA
14	L	203	CLA	C3A-C2A-CAA-CBA
14	X	1701	CLA	CAD-CBD-CGD-O1D
14	X	1701	CLA	CAD-CBD-CGD-O2D
14	a	802	CLA	CBD-CGD-O2D-CED
14	a	803	CLA	C6-C7-C8-C9
14	a	804	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	a	804	CLA	CHA-CBD-CGD-O2D
14	a	805	CLA	C1A-C2A-CAA-CBA
14	a	805	CLA	C3A-C2A-CAA-CBA
14	a	805	CLA	CHA-CBD-CGD-O1D
14	a	805	CLA	CHA-CBD-CGD-O2D
14	a	806	CLA	C1A-C2A-CAA-CBA
14	a	806	CLA	CHA-CBD-CGD-O1D
14	a	806	CLA	CHA-CBD-CGD-O2D
14	a	806	CLA	CAD-CBD-CGD-O1D
14	a	806	CLA	CAD-CBD-CGD-O2D
14	a	806	CLA	O2A-C1-C2-C3
14	a	807	CLA	C1A-C2A-CAA-CBA
14	a	807	CLA	C3A-C2A-CAA-CBA
14	a	809	CLA	C3A-C2A-CAA-CBA
14	a	809	CLA	CHA-CBD-CGD-O1D
14	a	809	CLA	CHA-CBD-CGD-O2D
14	a	812	CLA	CHA-CBD-CGD-O1D
14	a	812	CLA	CHA-CBD-CGD-O2D
14	a	812	CLA	CBD-CGD-O2D-CED
14	a	814	CLA	CHA-CBD-CGD-O1D
14	a	814	CLA	CHA-CBD-CGD-O2D
14	a	814	CLA	CAD-CBD-CGD-O1D
14	a	814	CLA	CAD-CBD-CGD-O2D
14	a	815	CLA	C1A-C2A-CAA-CBA
14	a	815	CLA	C2B-C3B-CAB-CBB
14	a	815	CLA	C4B-C3B-CAB-CBB
14	a	816	CLA	CHA-CBD-CGD-O1D
14	a	816	CLA	CHA-CBD-CGD-O2D
14	a	816	CLA	CAD-CBD-CGD-O1D
14	a	816	CLA	CAD-CBD-CGD-O2D
14	a	816	CLA	O2A-C1-C2-C3
14	a	817	CLA	CBD-CGD-O2D-CED
14	a	819	CLA	C2B-C3B-CAB-CBB
14	a	819	CLA	C4B-C3B-CAB-CBB
14	a	819	CLA	C2-C3-C5-C6
14	a	819	CLA	C4-C3-C5-C6
14	a	820	CLA	C1A-C2A-CAA-CBA
14	a	820	CLA	C3A-C2A-CAA-CBA
14	a	821	CLA	CBD-CGD-O2D-CED
14	a	823	CLA	CAD-CBD-CGD-O1D
14	a	823	CLA	CAD-CBD-CGD-O2D
14	a	823	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	a	824	CLA	C1A-C2A-CAA-CBA
14	a	824	CLA	CAD-CBD-CGD-O2D
14	a	825	CLA	CHA-CBD-CGD-O1D
14	a	825	CLA	CHA-CBD-CGD-O2D
14	a	829	CLA	CBD-CGD-O2D-CED
14	a	829	CLA	O2A-C1-C2-C3
14	a	830	CLA	C1A-C2A-CAA-CBA
14	a	831	CLA	CHA-CBD-CGD-O2D
14	a	835	CLA	CHA-CBD-CGD-O1D
14	a	835	CLA	CHA-CBD-CGD-O2D
14	a	836	CLA	C2-C3-C5-C6
14	a	836	CLA	C4-C3-C5-C6
14	a	837	CLA	CHA-CBD-CGD-O1D
14	a	837	CLA	CHA-CBD-CGD-O2D
14	a	839	CLA	CAD-CBD-CGD-O1D
14	a	839	CLA	CAD-CBD-CGD-O2D
14	a	842	CLA	C2-C3-C5-C6
14	a	842	CLA	C4-C3-C5-C6
14	a	844	CLA	CHA-CBD-CGD-O1D
14	a	844	CLA	CHA-CBD-CGD-O2D
14	b	802	CLA	CHA-CBD-CGD-O1D
14	b	802	CLA	CHA-CBD-CGD-O2D
14	b	802	CLA	CAD-CBD-CGD-O1D
14	b	804	CLA	CBD-CGD-O2D-CED
14	b	805	CLA	C11-C12-C13-C14
14	b	806	CLA	C3A-C2A-CAA-CBA
14	b	806	CLA	CHA-CBD-CGD-O1D
14	b	806	CLA	CHA-CBD-CGD-O2D
14	b	806	CLA	CAD-CBD-CGD-O1D
14	b	806	CLA	CAD-CBD-CGD-O2D
14	b	810	CLA	C2-C3-C5-C6
14	b	810	CLA	C4-C3-C5-C6
14	b	818	CLA	C1A-C2A-CAA-CBA
14	b	818	CLA	C3A-C2A-CAA-CBA
14	b	818	CLA	C4B-C3B-CAB-CBB
14	b	819	CLA	C3A-C2A-CAA-CBA
14	b	819	CLA	CAD-CBD-CGD-O1D
14	b	819	CLA	CAD-CBD-CGD-O2D
14	b	820	CLA	C2B-C3B-CAB-CBB
14	b	820	CLA	C4B-C3B-CAB-CBB
14	b	820	CLA	CBD-CGD-O2D-CED
14	b	821	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	b	821	CLA	C3A-C2A-CAA-CBA
14	b	823	CLA	CBD-CGD-O2D-CED
14	b	825	CLA	C1A-C2A-CAA-CBA
14	b	825	CLA	C3A-C2A-CAA-CBA
14	b	825	CLA	C2A-CAA-CBA-CGA
14	b	826	CLA	C1A-C2A-CAA-CBA
14	b	826	CLA	C11-C10-C8-C7
14	b	827	CLA	CHA-CBD-CGD-O1D
14	b	827	CLA	CHA-CBD-CGD-O2D
14	b	828	CLA	C1A-C2A-CAA-CBA
14	b	828	CLA	C3A-C2A-CAA-CBA
14	b	830	CLA	CHA-CBD-CGD-O1D
14	b	830	CLA	CHA-CBD-CGD-O2D
14	b	831	CLA	C1A-C2A-CAA-CBA
14	b	831	CLA	C3A-C2A-CAA-CBA
14	b	832	CLA	C1A-C2A-CAA-CBA
14	b	833	CLA	CAD-CBD-CGD-O1D
14	b	833	CLA	CAD-CBD-CGD-O2D
14	b	835	CLA	C1A-C2A-CAA-CBA
14	b	835	CLA	CBD-CGD-O2D-CED
14	b	842	CLA	CAD-CBD-CGD-O1D
14	b	842	CLA	CAD-CBD-CGD-O2D
14	f	201	CLA	CHA-CBD-CGD-O1D
14	f	201	CLA	CBD-CGD-O2D-CED
14	f	203	CLA	C1A-C2A-CAA-CBA
14	f	203	CLA	C3A-C2A-CAA-CBA
14	k	101	CLA	C3A-C2A-CAA-CBA
14	k	101	CLA	CHA-CBD-CGD-O1D
14	k	101	CLA	CHA-CBD-CGD-O2D
14	k	101	CLA	CAD-CBD-CGD-O1D
14	k	103	CLA	CAD-CBD-CGD-O1D
14	k	103	CLA	CAD-CBD-CGD-O2D
14	l	204	CLA	C1A-C2A-CAA-CBA
14	l	204	CLA	C3A-C2A-CAA-CBA
14	x	1701	CLA	CAD-CBD-CGD-O1D
14	x	1701	CLA	CAD-CBD-CGD-O2D
14	1	1603	CLA	CBD-CGD-O2D-CED
14	1	1605	CLA	CHA-CBD-CGD-O1D
14	1	1605	CLA	CHA-CBD-CGD-O2D
14	1	1606	CLA	C1A-C2A-CAA-CBA
14	1	1606	CLA	C3A-C2A-CAA-CBA
14	1	1606	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	1	1606	CLA	CHA-CBD-CGD-O2D
14	1	1607	CLA	C1A-C2A-CAA-CBA
14	1	1607	CLA	CHA-CBD-CGD-O1D
14	1	1607	CLA	CHA-CBD-CGD-O2D
14	1	1607	CLA	CAD-CBD-CGD-O1D
14	1	1607	CLA	CAD-CBD-CGD-O2D
14	1	1607	CLA	O2A-C1-C2-C3
14	1	1608	CLA	C1A-C2A-CAA-CBA
14	1	1608	CLA	C3A-C2A-CAA-CBA
14	1	1610	CLA	C3A-C2A-CAA-CBA
14	1	1610	CLA	CHA-CBD-CGD-O1D
14	1	1610	CLA	CHA-CBD-CGD-O2D
14	1	1613	CLA	CHA-CBD-CGD-O1D
14	1	1613	CLA	CHA-CBD-CGD-O2D
14	1	1613	CLA	CBD-CGD-O2D-CED
14	1	1615	CLA	CHA-CBD-CGD-O1D
14	1	1615	CLA	CHA-CBD-CGD-O2D
14	1	1615	CLA	CAD-CBD-CGD-O1D
14	1	1615	CLA	CAD-CBD-CGD-O2D
14	1	1616	CLA	C1A-C2A-CAA-CBA
14	1	1616	CLA	C2B-C3B-CAB-CBB
14	1	1616	CLA	C4B-C3B-CAB-CBB
14	1	1617	CLA	CHA-CBD-CGD-O1D
14	1	1617	CLA	CHA-CBD-CGD-O2D
14	1	1617	CLA	CAD-CBD-CGD-O1D
14	1	1617	CLA	CAD-CBD-CGD-O2D
14	1	1617	CLA	O2A-C1-C2-C3
14	1	1618	CLA	CBD-CGD-O2D-CED
14	1	1620	CLA	C2B-C3B-CAB-CBB
14	1	1620	CLA	C4B-C3B-CAB-CBB
14	1	1620	CLA	C2-C3-C5-C6
14	1	1620	CLA	C4-C3-C5-C6
14	1	1621	CLA	C1A-C2A-CAA-CBA
14	1	1621	CLA	C3A-C2A-CAA-CBA
14	1	1622	CLA	CBD-CGD-O2D-CED
14	1	1624	CLA	CAD-CBD-CGD-O1D
14	1	1624	CLA	CAD-CBD-CGD-O2D
14	1	1624	CLA	CBD-CGD-O2D-CED
14	1	1625	CLA	C1A-C2A-CAA-CBA
14	1	1625	CLA	CAD-CBD-CGD-O2D
14	1	1626	CLA	CHA-CBD-CGD-O1D
14	1	1626	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	1	1630	CLA	CBD-CGD-O2D-CED
14	1	1630	CLA	O2A-C1-C2-C3
14	1	1631	CLA	C1A-C2A-CAA-CBA
14	1	1632	CLA	CHA-CBD-CGD-O2D
14	1	1636	CLA	CHA-CBD-CGD-O1D
14	1	1636	CLA	CHA-CBD-CGD-O2D
14	1	1637	CLA	C2-C3-C5-C6
14	1	1637	CLA	C4-C3-C5-C6
14	1	1638	CLA	CHA-CBD-CGD-O1D
14	1	1638	CLA	CHA-CBD-CGD-O2D
14	1	1640	CLA	CAD-CBD-CGD-O1D
14	1	1640	CLA	CAD-CBD-CGD-O2D
14	1	1643	CLA	C2-C3-C5-C6
14	1	1643	CLA	C4-C3-C5-C6
14	1	1645	CLA	CHA-CBD-CGD-O1D
14	1	1645	CLA	CHA-CBD-CGD-O2D
14	2	802	CLA	CHA-CBD-CGD-O1D
14	2	802	CLA	CHA-CBD-CGD-O2D
14	2	802	CLA	CAD-CBD-CGD-O1D
14	2	804	CLA	CBD-CGD-O2D-CED
14	2	805	CLA	C11-C12-C13-C14
14	2	806	CLA	C3A-C2A-CAA-CBA
14	2	806	CLA	CHA-CBD-CGD-O1D
14	2	806	CLA	CHA-CBD-CGD-O2D
14	2	806	CLA	CAD-CBD-CGD-O1D
14	2	806	CLA	CAD-CBD-CGD-O2D
14	2	810	CLA	C2-C3-C5-C6
14	2	810	CLA	C4-C3-C5-C6
14	2	818	CLA	C1A-C2A-CAA-CBA
14	2	818	CLA	C3A-C2A-CAA-CBA
14	2	818	CLA	C4B-C3B-CAB-CBB
14	2	819	CLA	C3A-C2A-CAA-CBA
14	2	819	CLA	CAD-CBD-CGD-O1D
14	2	819	CLA	CAD-CBD-CGD-O2D
14	2	820	CLA	C2B-C3B-CAB-CBB
14	2	820	CLA	C4B-C3B-CAB-CBB
14	2	820	CLA	CBD-CGD-O2D-CED
14	2	821	CLA	C1A-C2A-CAA-CBA
14	2	821	CLA	C3A-C2A-CAA-CBA
14	2	823	CLA	CBD-CGD-O2D-CED
14	2	825	CLA	C1A-C2A-CAA-CBA
14	2	825	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	2	825	CLA	C2A-CAA-CBA-CGA
14	2	826	CLA	C1A-C2A-CAA-CBA
14	2	826	CLA	C11-C10-C8-C7
14	2	827	CLA	CHA-CBD-CGD-O1D
14	2	827	CLA	CHA-CBD-CGD-O2D
14	2	828	CLA	C1A-C2A-CAA-CBA
14	2	828	CLA	C3A-C2A-CAA-CBA
14	2	830	CLA	CHA-CBD-CGD-O1D
14	2	830	CLA	CHA-CBD-CGD-O2D
14	2	831	CLA	C1A-C2A-CAA-CBA
14	2	831	CLA	C3A-C2A-CAA-CBA
14	2	832	CLA	C1A-C2A-CAA-CBA
14	2	833	CLA	CAD-CBD-CGD-O1D
14	2	833	CLA	CAD-CBD-CGD-O2D
14	2	835	CLA	C1A-C2A-CAA-CBA
14	2	835	CLA	CBD-CGD-O2D-CED
14	2	842	CLA	CAD-CBD-CGD-O1D
14	2	842	CLA	CAD-CBD-CGD-O2D
14	6	201	CLA	CHA-CBD-CGD-O1D
14	6	201	CLA	CBD-CGD-O2D-CED
14	6	203	CLA	C1A-C2A-CAA-CBA
14	6	203	CLA	C3A-C2A-CAA-CBA
14	9	101	CLA	C3A-C2A-CAA-CBA
14	9	101	CLA	CHA-CBD-CGD-O1D
14	9	101	CLA	CHA-CBD-CGD-O2D
14	9	101	CLA	CAD-CBD-CGD-O1D
14	9	103	CLA	CAD-CBD-CGD-O1D
14	9	103	CLA	CAD-CBD-CGD-O2D
14	0	205	CLA	C1A-C2A-CAA-CBA
14	0	205	CLA	C3A-C2A-CAA-CBA
14	z	102	CLA	CAD-CBD-CGD-O1D
14	z	102	CLA	CAD-CBD-CGD-O2D
17	A	847	BCR	C7-C8-C9-C34
17	A	847	BCR	C11-C12-C13-C35
17	A	847	BCR	C36-C18-C19-C20
17	A	847	BCR	C22-C23-C24-C25
17	A	847	BCR	C23-C24-C25-C30
17	A	848	BCR	C7-C8-C9-C34
17	A	848	BCR	C12-C13-C14-C15
17	A	848	BCR	C35-C13-C14-C15
17	A	848	BCR	C13-C14-C15-C16
17	A	848	BCR	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
17	A	848	BCR	C16-C17-C18-C19
17	A	848	BCR	C16-C17-C18-C36
17	A	848	BCR	C20-C21-C22-C37
17	A	849	BCR	C20-C21-C22-C37
17	A	850	BCR	C36-C18-C19-C20
17	A	850	BCR	C20-C21-C22-C37
17	A	850	BCR	C21-C22-C23-C24
17	A	851	BCR	C1-C6-C7-C8
17	A	851	BCR	C7-C8-C9-C34
17	A	851	BCR	C16-C17-C18-C36
17	A	851	BCR	C18-C19-C20-C21
17	A	851	BCR	C20-C21-C22-C23
17	A	851	BCR	C20-C21-C22-C37
17	A	851	BCR	C21-C22-C23-C24
17	A	851	BCR	C37-C22-C23-C24
17	A	851	BCR	C23-C24-C25-C26
17	A	851	BCR	C23-C24-C25-C30
17	A	852	BCR	C7-C8-C9-C10
17	A	852	BCR	C7-C8-C9-C34
17	A	852	BCR	C16-C17-C18-C36
17	A	856	BCR	C7-C8-C9-C34
17	A	856	BCR	C14-C15-C16-C17
17	A	856	BCR	C21-C22-C23-C24
17	B	843	BCR	C7-C8-C9-C10
17	B	843	BCR	C16-C17-C18-C36
17	B	843	BCR	C17-C18-C19-C20
17	B	843	BCR	C21-C22-C23-C24
17	B	843	BCR	C22-C23-C24-C25
17	B	844	BCR	C1-C6-C7-C8
17	B	844	BCR	C6-C7-C8-C9
17	B	844	BCR	C7-C8-C9-C10
17	B	844	BCR	C7-C8-C9-C34
17	B	844	BCR	C21-C22-C23-C24
17	B	845	BCR	C7-C8-C9-C34
17	B	845	BCR	C20-C21-C22-C23
17	B	845	BCR	C20-C21-C22-C37
17	B	845	BCR	C37-C22-C23-C24
17	B	846	BCR	C6-C7-C8-C9
17	B	846	BCR	C7-C8-C9-C34
17	B	846	BCR	C14-C15-C16-C17
17	B	846	BCR	C20-C21-C22-C37
17	B	846	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
17	B	847	BCR	C6-C7-C8-C9
17	B	847	BCR	C11-C12-C13-C14
17	B	847	BCR	C11-C12-C13-C35
17	B	847	BCR	C37-C22-C23-C24
17	B	851	BCR	C36-C18-C19-C20
17	B	851	BCR	C18-C19-C20-C21
17	B	851	BCR	C20-C21-C22-C37
17	B	851	BCR	C22-C23-C24-C25
17	F	202	BCR	C7-C8-C9-C34
17	F	202	BCR	C37-C22-C23-C24
17	F	205	BCR	C12-C13-C14-C15
17	F	205	BCR	C37-C22-C23-C24
17	F	205	BCR	C23-C24-C25-C30
17	I	101	BCR	C7-C8-C9-C34
17	J	103	BCR	C1-C6-C7-C8
17	J	103	BCR	C6-C7-C8-C9
17	J	103	BCR	C7-C8-C9-C10
17	J	103	BCR	C7-C8-C9-C34
17	J	103	BCR	C36-C18-C19-C20
17	J	103	BCR	C37-C22-C23-C24
17	K	102	BCR	C6-C7-C8-C9
17	K	102	BCR	C7-C8-C9-C34
17	L	201	BCR	C7-C8-C9-C34
17	L	201	BCR	C20-C21-C22-C23
17	L	201	BCR	C20-C21-C22-C37
17	L	206	BCR	C7-C8-C9-C10
17	L	206	BCR	C7-C8-C9-C34
17	L	206	BCR	C21-C22-C23-C24
17	L	207	BCR	C11-C12-C13-C35
17	M	103	BCR	C7-C8-C9-C34
17	M	103	BCR	C21-C22-C23-C24
17	a	847	BCR	C7-C8-C9-C34
17	a	847	BCR	C11-C12-C13-C35
17	a	847	BCR	C36-C18-C19-C20
17	a	847	BCR	C22-C23-C24-C25
17	a	847	BCR	C23-C24-C25-C30
17	a	848	BCR	C7-C8-C9-C34
17	a	848	BCR	C12-C13-C14-C15
17	a	848	BCR	C35-C13-C14-C15
17	a	848	BCR	C13-C14-C15-C16
17	a	848	BCR	C14-C15-C16-C17
17	a	848	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
17	a	848	BCR	C16-C17-C18-C36
17	a	848	BCR	C20-C21-C22-C37
17	a	849	BCR	C20-C21-C22-C37
17	a	850	BCR	C36-C18-C19-C20
17	a	850	BCR	C20-C21-C22-C37
17	a	850	BCR	C21-C22-C23-C24
17	a	851	BCR	C1-C6-C7-C8
17	a	851	BCR	C7-C8-C9-C34
17	a	851	BCR	C16-C17-C18-C36
17	a	851	BCR	C18-C19-C20-C21
17	a	851	BCR	C20-C21-C22-C23
17	a	851	BCR	C20-C21-C22-C37
17	a	851	BCR	C21-C22-C23-C24
17	a	851	BCR	C37-C22-C23-C24
17	a	851	BCR	C23-C24-C25-C26
17	a	851	BCR	C23-C24-C25-C30
17	a	852	BCR	C7-C8-C9-C10
17	a	852	BCR	C7-C8-C9-C34
17	a	852	BCR	C16-C17-C18-C36
17	b	844	BCR	C7-C8-C9-C10
17	b	844	BCR	C16-C17-C18-C36
17	b	844	BCR	C17-C18-C19-C20
17	b	844	BCR	C21-C22-C23-C24
17	b	844	BCR	C22-C23-C24-C25
17	b	845	BCR	C1-C6-C7-C8
17	b	845	BCR	C6-C7-C8-C9
17	b	845	BCR	C7-C8-C9-C10
17	b	845	BCR	C7-C8-C9-C34
17	b	845	BCR	C21-C22-C23-C24
17	b	846	BCR	C7-C8-C9-C34
17	b	846	BCR	C20-C21-C22-C23
17	b	846	BCR	C20-C21-C22-C37
17	b	846	BCR	C37-C22-C23-C24
17	b	847	BCR	C6-C7-C8-C9
17	b	847	BCR	C7-C8-C9-C34
17	b	847	BCR	C14-C15-C16-C17
17	b	847	BCR	C20-C21-C22-C37
17	b	847	BCR	C23-C24-C25-C30
17	b	848	BCR	C6-C7-C8-C9
17	b	848	BCR	C11-C12-C13-C14
17	b	848	BCR	C11-C12-C13-C35
17	b	848	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
17	b	852	BCR	C36-C18-C19-C20
17	b	852	BCR	C18-C19-C20-C21
17	b	852	BCR	C20-C21-C22-C37
17	b	852	BCR	C22-C23-C24-C25
17	f	202	BCR	C7-C8-C9-C34
17	f	202	BCR	C37-C22-C23-C24
17	f	204	BCR	C12-C13-C14-C15
17	f	204	BCR	C37-C22-C23-C24
17	f	204	BCR	C23-C24-C25-C30
17	i	101	BCR	C7-C8-C9-C34
17	j	1304	BCR	C1-C6-C7-C8
17	j	1304	BCR	C6-C7-C8-C9
17	j	1304	BCR	C7-C8-C9-C10
17	j	1304	BCR	C7-C8-C9-C34
17	j	1304	BCR	C36-C18-C19-C20
17	j	1304	BCR	C37-C22-C23-C24
17	j	1305	BCR	C7-C8-C9-C34
17	j	1305	BCR	C14-C15-C16-C17
17	j	1305	BCR	C21-C22-C23-C24
17	k	102	BCR	C6-C7-C8-C9
17	k	102	BCR	C7-C8-C9-C34
17	l	202	BCR	C7-C8-C9-C34
17	l	202	BCR	C20-C21-C22-C23
17	l	202	BCR	C20-C21-C22-C37
17	l	207	BCR	C7-C8-C9-C10
17	l	207	BCR	C7-C8-C9-C34
17	l	207	BCR	C21-C22-C23-C24
17	m	102	BCR	C7-C8-C9-C34
17	m	102	BCR	C21-C22-C23-C24
17	1	1648	BCR	C7-C8-C9-C34
17	1	1648	BCR	C36-C18-C19-C20
17	1	1648	BCR	C22-C23-C24-C25
17	1	1648	BCR	C23-C24-C25-C30
17	1	1649	BCR	C7-C8-C9-C34
17	1	1649	BCR	C12-C13-C14-C15
17	1	1649	BCR	C35-C13-C14-C15
17	1	1649	BCR	C13-C14-C15-C16
17	1	1649	BCR	C14-C15-C16-C17
17	1	1649	BCR	C16-C17-C18-C19
17	1	1649	BCR	C16-C17-C18-C36
17	1	1649	BCR	C20-C21-C22-C37
17	1	1650	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
17	1	1651	BCR	C36-C18-C19-C20
17	1	1651	BCR	C20-C21-C22-C37
17	1	1651	BCR	C21-C22-C23-C24
17	1	1652	BCR	C7-C8-C9-C34
17	1	1652	BCR	C16-C17-C18-C36
17	1	1652	BCR	C18-C19-C20-C21
17	1	1652	BCR	C20-C21-C22-C23
17	1	1652	BCR	C20-C21-C22-C37
17	1	1652	BCR	C21-C22-C23-C24
17	1	1652	BCR	C37-C22-C23-C24
17	1	1652	BCR	C23-C24-C25-C26
17	1	1652	BCR	C23-C24-C25-C30
17	1	1653	BCR	C7-C8-C9-C10
17	1	1653	BCR	C7-C8-C9-C34
17	1	1653	BCR	C16-C17-C18-C36
17	2	844	BCR	C7-C8-C9-C10
17	2	844	BCR	C16-C17-C18-C36
17	2	844	BCR	C17-C18-C19-C20
17	2	844	BCR	C21-C22-C23-C24
17	2	844	BCR	C22-C23-C24-C25
17	2	845	BCR	C1-C6-C7-C8
17	2	845	BCR	C6-C7-C8-C9
17	2	845	BCR	C7-C8-C9-C10
17	2	845	BCR	C7-C8-C9-C34
17	2	845	BCR	C21-C22-C23-C24
17	2	846	BCR	C7-C8-C9-C34
17	2	846	BCR	C20-C21-C22-C23
17	2	846	BCR	C20-C21-C22-C37
17	2	846	BCR	C37-C22-C23-C24
17	2	847	BCR	C6-C7-C8-C9
17	2	847	BCR	C7-C8-C9-C34
17	2	847	BCR	C14-C15-C16-C17
17	2	847	BCR	C20-C21-C22-C37
17	2	847	BCR	C23-C24-C25-C30
17	2	848	BCR	C6-C7-C8-C9
17	2	848	BCR	C11-C12-C13-C14
17	2	848	BCR	C11-C12-C13-C35
17	2	848	BCR	C37-C22-C23-C24
17	6	202	BCR	C7-C8-C9-C34
17	6	202	BCR	C37-C22-C23-C24
17	6	204	BCR	C12-C13-C14-C15
17	6	204	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
17	6	204	BCR	C23-C24-C25-C30
17	7	101	BCR	C7-C8-C9-C34
17	8	1304	BCR	C1-C6-C7-C8
17	8	1304	BCR	C6-C7-C8-C9
17	8	1304	BCR	C7-C8-C9-C10
17	8	1304	BCR	C7-C8-C9-C34
17	8	1304	BCR	C36-C18-C19-C20
17	8	1304	BCR	C37-C22-C23-C24
17	8	1305	BCR	C7-C8-C9-C34
17	8	1305	BCR	C14-C15-C16-C17
17	8	1305	BCR	C21-C22-C23-C24
17	8	1306	BCR	C36-C18-C19-C20
17	8	1306	BCR	C18-C19-C20-C21
17	8	1306	BCR	C20-C21-C22-C37
17	8	1306	BCR	C22-C23-C24-C25
17	9	102	BCR	C6-C7-C8-C9
17	9	102	BCR	C7-C8-C9-C34
17	0	201	BCR	C11-C12-C13-C35
17	0	203	BCR	C7-C8-C9-C34
17	0	203	BCR	C20-C21-C22-C23
17	0	203	BCR	C20-C21-C22-C37
17	0	208	BCR	C7-C8-C9-C10
17	0	208	BCR	C7-C8-C9-C34
17	0	208	BCR	C21-C22-C23-C24
17	0	209	BCR	C11-C12-C13-C35
17	y	102	BCR	C7-C8-C9-C34
17	y	102	BCR	C21-C22-C23-C24
18	A	854	LHG	C4-O6-P-O5
18	B	850	LHG	C3-O3-P-O5
18	B	850	LHG	C4-O6-P-O5
18	B	850	LHG	C8-C7-O7-C5
18	L	208	LHG	O1-C1-C2-C3
18	L	208	LHG	C1-C2-C3-O3
18	L	208	LHG	C2-C3-O3-P
18	L	208	LHG	C4-O6-P-O4
18	M	101	LHG	C3-O3-P-O4
18	M	101	LHG	C3-O3-P-O5
18	M	101	LHG	C3-O3-P-O6
18	M	101	LHG	C4-O6-P-O5
18	M	101	LHG	O10-C23-O8-C6
18	M	101	LHG	C24-C23-O8-C6
18	a	854	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
18	b	851	LHG	C3-O3-P-O5
18	b	851	LHG	C4-O6-P-O5
18	b	851	LHG	C8-C7-O7-C5
18	l	201	LHG	O1-C1-C2-C3
18	l	201	LHG	C1-C2-C3-O3
18	l	201	LHG	C2-C3-O3-P
18	l	201	LHG	C4-O6-P-O4
18	m	101	LHG	C3-O3-P-O4
18	m	101	LHG	C3-O3-P-O5
18	m	101	LHG	C3-O3-P-O6
18	m	101	LHG	C4-O6-P-O5
18	m	101	LHG	O10-C23-O8-C6
18	m	101	LHG	C24-C23-O8-C6
18	1	1655	LHG	C4-O6-P-O5
18	0	202	LHG	O1-C1-C2-C3
18	0	202	LHG	C1-C2-C3-O3
18	0	202	LHG	C2-C3-O3-P
18	0	202	LHG	C4-O6-P-O4
18	y	101	LHG	C3-O3-P-O4
18	y	101	LHG	C3-O3-P-O5
18	y	101	LHG	C3-O3-P-O6
18	y	101	LHG	C4-O6-P-O5
18	y	101	LHG	O10-C23-O8-C6
18	y	101	LHG	C24-C23-O8-C6
18	z	101	LHG	C3-O3-P-O5
18	z	101	LHG	C4-O6-P-O5
18	z	101	LHG	C8-C7-O7-C5
14	A	817	CLA	O1D-CGD-O2D-CED
14	A	824	CLA	O1D-CGD-O2D-CED
14	B	823	CLA	O1D-CGD-O2D-CED
14	B	835	CLA	O1D-CGD-O2D-CED
14	F	201	CLA	O1D-CGD-O2D-CED
14	K	101	CLA	O1D-CGD-O2D-CED
14	a	817	CLA	O1D-CGD-O2D-CED
14	a	824	CLA	O1D-CGD-O2D-CED
14	b	824	CLA	O1D-CGD-O2D-CED
14	b	836	CLA	O1D-CGD-O2D-CED
14	f	201	CLA	O1D-CGD-O2D-CED
14	k	101	CLA	O1D-CGD-O2D-CED
14	1	1618	CLA	O1D-CGD-O2D-CED
14	1	1625	CLA	O1D-CGD-O2D-CED
14	2	824	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	2	836	CLA	O1D-CGD-O2D-CED
14	6	201	CLA	O1D-CGD-O2D-CED
14	9	101	CLA	O1D-CGD-O2D-CED
14	A	812	CLA	O1D-CGD-O2D-CED
14	B	822	CLA	O1D-CGD-O2D-CED
14	B	834	CLA	O1D-CGD-O2D-CED
14	a	812	CLA	O1D-CGD-O2D-CED
14	b	823	CLA	O1D-CGD-O2D-CED
14	b	835	CLA	O1D-CGD-O2D-CED
14	1	1613	CLA	O1D-CGD-O2D-CED
14	2	823	CLA	O1D-CGD-O2D-CED
14	2	835	CLA	O1D-CGD-O2D-CED
14	A	810	CLA	CBD-CGD-O2D-CED
14	A	811	CLA	CBD-CGD-O2D-CED
14	A	818	CLA	CBD-CGD-O2D-CED
14	A	822	CLA	CBD-CGD-O2D-CED
14	A	824	CLA	CBD-CGD-O2D-CED
14	A	830	CLA	CBD-CGD-O2D-CED
14	B	802	CLA	CBD-CGD-O2D-CED
14	B	809	CLA	CBD-CGD-O2D-CED
14	B	823	CLA	CBD-CGD-O2D-CED
14	B	835	CLA	CBD-CGD-O2D-CED
14	F	204	CLA	CBD-CGD-O2D-CED
14	J	101	CLA	CBD-CGD-O2D-CED
14	K	101	CLA	CBD-CGD-O2D-CED
14	a	810	CLA	CBD-CGD-O2D-CED
14	a	811	CLA	CBD-CGD-O2D-CED
14	a	818	CLA	CBD-CGD-O2D-CED
14	a	822	CLA	CBD-CGD-O2D-CED
14	a	824	CLA	CBD-CGD-O2D-CED
14	a	830	CLA	CBD-CGD-O2D-CED
14	b	803	CLA	CBD-CGD-O2D-CED
14	b	810	CLA	CBD-CGD-O2D-CED
14	b	824	CLA	CBD-CGD-O2D-CED
14	b	836	CLA	CBD-CGD-O2D-CED
14	f	203	CLA	CBD-CGD-O2D-CED
14	j	1302	CLA	CBD-CGD-O2D-CED
14	k	101	CLA	CBD-CGD-O2D-CED
14	1	1611	CLA	CBD-CGD-O2D-CED
14	1	1612	CLA	CBD-CGD-O2D-CED
14	1	1619	CLA	CBD-CGD-O2D-CED
14	1	1623	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	1	1625	CLA	CBD-CGD-O2D-CED
14	1	1631	CLA	CBD-CGD-O2D-CED
14	2	803	CLA	CBD-CGD-O2D-CED
14	2	810	CLA	CBD-CGD-O2D-CED
14	2	824	CLA	CBD-CGD-O2D-CED
14	2	836	CLA	CBD-CGD-O2D-CED
14	6	203	CLA	CBD-CGD-O2D-CED
14	8	1302	CLA	CBD-CGD-O2D-CED
14	9	101	CLA	CBD-CGD-O2D-CED
14	A	806	CLA	O1A-CGA-O2A-C1
14	A	838	CLA	O1A-CGA-O2A-C1
14	B	820	CLA	O1A-CGA-O2A-C1
14	a	806	CLA	O1A-CGA-O2A-C1
14	a	838	CLA	O1A-CGA-O2A-C1
14	b	821	CLA	O1A-CGA-O2A-C1
14	1	1607	CLA	O1A-CGA-O2A-C1
14	1	1639	CLA	O1A-CGA-O2A-C1
14	2	821	CLA	O1A-CGA-O2A-C1
14	A	821	CLA	O1D-CGD-O2D-CED
14	F	204	CLA	O1D-CGD-O2D-CED
14	J	101	CLA	O1D-CGD-O2D-CED
14	a	821	CLA	O1D-CGD-O2D-CED
14	f	203	CLA	O1D-CGD-O2D-CED
14	j	1302	CLA	O1D-CGD-O2D-CED
14	1	1622	CLA	O1D-CGD-O2D-CED
14	6	203	CLA	O1D-CGD-O2D-CED
14	8	1302	CLA	O1D-CGD-O2D-CED
14	A	810	CLA	O1D-CGD-O2D-CED
14	B	803	CLA	O1D-CGD-O2D-CED
14	a	810	CLA	O1D-CGD-O2D-CED
14	a	823	CLA	O1D-CGD-O2D-CED
14	b	804	CLA	O1D-CGD-O2D-CED
14	1	1611	CLA	O1D-CGD-O2D-CED
14	1	1624	CLA	O1D-CGD-O2D-CED
14	2	804	CLA	O1D-CGD-O2D-CED
14	A	806	CLA	CBA-CGA-O2A-C1
14	A	838	CLA	CBA-CGA-O2A-C1
14	a	806	CLA	CBA-CGA-O2A-C1
14	a	838	CLA	CBA-CGA-O2A-C1
14	1	1607	CLA	CBA-CGA-O2A-C1
14	1	1639	CLA	CBA-CGA-O2A-C1
14	A	834	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	B	813	CLA	CBD-CGD-O2D-CED
14	B	816	CLA	CBD-CGD-O2D-CED
14	B	821	CLA	CBD-CGD-O2D-CED
14	B	827	CLA	CBD-CGD-O2D-CED
14	B	841	CLA	CBD-CGD-O2D-CED
14	X	1701	CLA	CBD-CGD-O2D-CED
14	a	834	CLA	CBD-CGD-O2D-CED
14	b	814	CLA	CBD-CGD-O2D-CED
14	b	817	CLA	CBD-CGD-O2D-CED
14	b	822	CLA	CBD-CGD-O2D-CED
14	b	828	CLA	CBD-CGD-O2D-CED
14	b	842	CLA	CBD-CGD-O2D-CED
14	x	1701	CLA	CBD-CGD-O2D-CED
14	1	1635	CLA	CBD-CGD-O2D-CED
14	2	814	CLA	CBD-CGD-O2D-CED
14	2	817	CLA	CBD-CGD-O2D-CED
14	2	822	CLA	CBD-CGD-O2D-CED
14	2	828	CLA	CBD-CGD-O2D-CED
14	2	842	CLA	CBD-CGD-O2D-CED
14	z	102	CLA	CBD-CGD-O2D-CED
14	A	802	CLA	O1A-CGA-O2A-C1
14	A	811	CLA	O1A-CGA-O2A-C1
14	A	817	CLA	O1A-CGA-O2A-C1
14	A	818	CLA	O1A-CGA-O2A-C1
14	A	833	CLA	O1A-CGA-O2A-C1
14	B	819	CLA	O1A-CGA-O2A-C1
14	B	830	CLA	O1A-CGA-O2A-C1
14	a	802	CLA	O1A-CGA-O2A-C1
14	a	811	CLA	O1A-CGA-O2A-C1
14	a	817	CLA	O1A-CGA-O2A-C1
14	a	818	CLA	O1A-CGA-O2A-C1
14	a	833	CLA	O1A-CGA-O2A-C1
14	b	820	CLA	O1A-CGA-O2A-C1
14	b	831	CLA	O1A-CGA-O2A-C1
14	1	1603	CLA	O1A-CGA-O2A-C1
14	1	1612	CLA	O1A-CGA-O2A-C1
14	1	1618	CLA	O1A-CGA-O2A-C1
14	1	1619	CLA	O1A-CGA-O2A-C1
14	1	1634	CLA	O1A-CGA-O2A-C1
14	2	820	CLA	O1A-CGA-O2A-C1
14	2	831	CLA	O1A-CGA-O2A-C1
14	A	823	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	A	829	CLA	O1D-CGD-O2D-CED
14	B	819	CLA	O1D-CGD-O2D-CED
14	a	829	CLA	O1D-CGD-O2D-CED
14	b	820	CLA	O1D-CGD-O2D-CED
14	1	1630	CLA	O1D-CGD-O2D-CED
14	2	820	CLA	O1D-CGD-O2D-CED
14	A	802	CLA	O1D-CGD-O2D-CED
14	a	802	CLA	O1D-CGD-O2D-CED
14	1	1603	CLA	O1D-CGD-O2D-CED
18	B	850	LHG	O9-C7-O7-C5
18	b	851	LHG	O9-C7-O7-C5
18	z	101	LHG	O9-C7-O7-C5
14	A	809	CLA	C3-C5-C6-C7
14	A	827	CLA	C3-C5-C6-C7
14	A	834	CLA	C3-C5-C6-C7
14	B	804	CLA	C3-C5-C6-C7
14	B	813	CLA	C3-C5-C6-C7
14	B	814	CLA	C3-C5-C6-C7
14	B	840	CLA	C3-C5-C6-C7
14	L	205	CLA	C3-C5-C6-C7
14	a	809	CLA	C3-C5-C6-C7
14	a	827	CLA	C3-C5-C6-C7
14	a	834	CLA	C3-C5-C6-C7
14	a	838	CLA	C3-C5-C6-C7
14	b	805	CLA	C3-C5-C6-C7
14	b	814	CLA	C3-C5-C6-C7
14	b	815	CLA	C3-C5-C6-C7
14	b	841	CLA	C3-C5-C6-C7
14	l	206	CLA	C3-C5-C6-C7
14	1	1610	CLA	C3-C5-C6-C7
14	1	1628	CLA	C3-C5-C6-C7
14	1	1635	CLA	C3-C5-C6-C7
14	2	805	CLA	C3-C5-C6-C7
14	2	814	CLA	C3-C5-C6-C7
14	2	815	CLA	C3-C5-C6-C7
14	2	841	CLA	C3-C5-C6-C7
14	0	207	CLA	C3-C5-C6-C7
14	A	802	CLA	CBA-CGA-O2A-C1
14	A	818	CLA	CBA-CGA-O2A-C1
14	B	819	CLA	CBA-CGA-O2A-C1
14	B	820	CLA	CBA-CGA-O2A-C1
14	a	802	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	a	818	CLA	CBA-CGA-O2A-C1
14	b	820	CLA	CBA-CGA-O2A-C1
14	b	821	CLA	CBA-CGA-O2A-C1
14	1	1603	CLA	CBA-CGA-O2A-C1
14	1	1619	CLA	CBA-CGA-O2A-C1
14	2	820	CLA	CBA-CGA-O2A-C1
14	2	821	CLA	CBA-CGA-O2A-C1
18	L	208	LHG	C24-C23-O8-C6
18	l	201	LHG	C24-C23-O8-C6
18	0	202	LHG	C24-C23-O8-C6
14	A	806	CLA	C4-C3-C5-C6
14	A	833	CLA	C4-C3-C5-C6
14	B	817	CLA	C4-C3-C5-C6
14	a	806	CLA	C4-C3-C5-C6
14	a	833	CLA	C4-C3-C5-C6
14	b	818	CLA	C4-C3-C5-C6
14	1	1607	CLA	C4-C3-C5-C6
14	1	1634	CLA	C4-C3-C5-C6
14	2	818	CLA	C4-C3-C5-C6
14	A	806	CLA	C2-C3-C5-C6
14	B	817	CLA	C2-C3-C5-C6
14	a	806	CLA	C2-C3-C5-C6
14	b	818	CLA	C2-C3-C5-C6
14	1	1607	CLA	C2-C3-C5-C6
14	2	818	CLA	C2-C3-C5-C6
14	B	811	CLA	CBD-CGD-O2D-CED
14	b	812	CLA	CBD-CGD-O2D-CED
14	2	812	CLA	CBD-CGD-O2D-CED
14	A	813	CLA	C2A-CAA-CBA-CGA
14	A	818	CLA	C2A-CAA-CBA-CGA
14	A	830	CLA	C2A-CAA-CBA-CGA
14	A	835	CLA	C2A-CAA-CBA-CGA
14	A	855	CLA	C2A-CAA-CBA-CGA
14	B	840	CLA	C2A-CAA-CBA-CGA
14	a	813	CLA	C2A-CAA-CBA-CGA
14	a	818	CLA	C2A-CAA-CBA-CGA
14	a	830	CLA	C2A-CAA-CBA-CGA
14	a	835	CLA	C2A-CAA-CBA-CGA
14	b	802	CLA	C2A-CAA-CBA-CGA
14	b	841	CLA	C2A-CAA-CBA-CGA
14	1	1614	CLA	C2A-CAA-CBA-CGA
14	1	1619	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	1	1631	CLA	C2A-CAA-CBA-CGA
14	1	1636	CLA	C2A-CAA-CBA-CGA
14	2	802	CLA	C2A-CAA-CBA-CGA
14	2	841	CLA	C2A-CAA-CBA-CGA
14	B	810	CLA	O1A-CGA-O2A-C1
14	b	811	CLA	O1A-CGA-O2A-C1
14	2	811	CLA	O1A-CGA-O2A-C1
14	A	819	CLA	C3-C5-C6-C7
14	A	838	CLA	C3-C5-C6-C7
14	B	811	CLA	C3-C5-C6-C7
14	B	820	CLA	C3-C5-C6-C7
14	B	822	CLA	C3-C5-C6-C7
14	F	201	CLA	C3-C5-C6-C7
14	a	819	CLA	C3-C5-C6-C7
14	a	833	CLA	C3-C5-C6-C7
14	b	812	CLA	C3-C5-C6-C7
14	b	821	CLA	C3-C5-C6-C7
14	b	823	CLA	C3-C5-C6-C7
14	f	201	CLA	C3-C5-C6-C7
14	1	1620	CLA	C3-C5-C6-C7
14	1	1634	CLA	C3-C5-C6-C7
14	1	1639	CLA	C3-C5-C6-C7
14	2	812	CLA	C3-C5-C6-C7
14	2	821	CLA	C3-C5-C6-C7
14	2	823	CLA	C3-C5-C6-C7
14	6	201	CLA	C3-C5-C6-C7
14	A	805	CLA	CBA-CGA-O2A-C1
14	A	811	CLA	CBA-CGA-O2A-C1
14	A	817	CLA	CBA-CGA-O2A-C1
14	A	820	CLA	CBA-CGA-O2A-C1
14	A	833	CLA	CBA-CGA-O2A-C1
14	B	815	CLA	CBA-CGA-O2A-C1
14	B	818	CLA	CBA-CGA-O2A-C1
14	B	824	CLA	CBA-CGA-O2A-C1
14	B	830	CLA	CBA-CGA-O2A-C1
14	a	805	CLA	CBA-CGA-O2A-C1
14	a	811	CLA	CBA-CGA-O2A-C1
14	a	817	CLA	CBA-CGA-O2A-C1
14	a	820	CLA	CBA-CGA-O2A-C1
14	a	833	CLA	CBA-CGA-O2A-C1
14	b	816	CLA	CBA-CGA-O2A-C1
14	b	819	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	b	825	CLA	CBA-CGA-O2A-C1
14	b	831	CLA	CBA-CGA-O2A-C1
14	1	1606	CLA	CBA-CGA-O2A-C1
14	1	1612	CLA	CBA-CGA-O2A-C1
14	1	1618	CLA	CBA-CGA-O2A-C1
14	1	1621	CLA	CBA-CGA-O2A-C1
14	1	1634	CLA	CBA-CGA-O2A-C1
14	2	816	CLA	CBA-CGA-O2A-C1
14	2	819	CLA	CBA-CGA-O2A-C1
14	2	825	CLA	CBA-CGA-O2A-C1
14	2	831	CLA	CBA-CGA-O2A-C1
14	B	803	CLA	C2C-C3C-CAC-CBC
14	b	804	CLA	C2C-C3C-CAC-CBC
14	2	804	CLA	C2C-C3C-CAC-CBC
14	B	802	CLA	O1D-CGD-O2D-CED
14	b	803	CLA	O1D-CGD-O2D-CED
14	2	803	CLA	O1D-CGD-O2D-CED
14	A	820	CLA	O1A-CGA-O2A-C1
14	B	815	CLA	O1A-CGA-O2A-C1
14	B	817	CLA	O1A-CGA-O2A-C1
14	B	818	CLA	O1A-CGA-O2A-C1
14	B	824	CLA	O1A-CGA-O2A-C1
14	B	825	CLA	O1A-CGA-O2A-C1
14	a	820	CLA	O1A-CGA-O2A-C1
14	b	816	CLA	O1A-CGA-O2A-C1
14	b	818	CLA	O1A-CGA-O2A-C1
14	b	819	CLA	O1A-CGA-O2A-C1
14	b	825	CLA	O1A-CGA-O2A-C1
14	b	826	CLA	O1A-CGA-O2A-C1
14	1	1621	CLA	O1A-CGA-O2A-C1
14	2	816	CLA	O1A-CGA-O2A-C1
14	2	818	CLA	O1A-CGA-O2A-C1
14	2	819	CLA	O1A-CGA-O2A-C1
14	2	825	CLA	O1A-CGA-O2A-C1
18	L	208	LHG	O10-C23-O8-C6
18	l	201	LHG	O10-C23-O8-C6
18	0	202	LHG	O10-C23-O8-C6
14	A	811	CLA	O1D-CGD-O2D-CED
14	a	811	CLA	O1D-CGD-O2D-CED
14	1	1612	CLA	O1D-CGD-O2D-CED
14	B	830	CLA	CBD-CGD-O2D-CED
14	b	831	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	2	831	CLA	CBD-CGD-O2D-CED
14	A	818	CLA	O1D-CGD-O2D-CED
14	A	830	CLA	O1D-CGD-O2D-CED
14	a	818	CLA	O1D-CGD-O2D-CED
14	a	830	CLA	O1D-CGD-O2D-CED
14	1	1619	CLA	O1D-CGD-O2D-CED
14	1	1631	CLA	O1D-CGD-O2D-CED
18	L	208	LHG	O2-C2-C3-O3
18	l	201	LHG	O2-C2-C3-O3
18	0	202	LHG	O2-C2-C3-O3
14	A	833	CLA	C3-C5-C6-C7
14	B	808	CLA	C3-C5-C6-C7
14	b	809	CLA	C3-C5-C6-C7
14	2	809	CLA	C3-C5-C6-C7
14	A	809	CLA	CBA-CGA-O2A-C1
14	B	809	CLA	CBA-CGA-O2A-C1
14	B	810	CLA	CBA-CGA-O2A-C1
14	L	205	CLA	CBA-CGA-O2A-C1
14	a	809	CLA	CBA-CGA-O2A-C1
14	b	810	CLA	CBA-CGA-O2A-C1
14	b	811	CLA	CBA-CGA-O2A-C1
14	l	206	CLA	CBA-CGA-O2A-C1
14	1	1610	CLA	CBA-CGA-O2A-C1
14	2	810	CLA	CBA-CGA-O2A-C1
14	2	811	CLA	CBA-CGA-O2A-C1
14	0	207	CLA	CBA-CGA-O2A-C1
14	2	826	CLA	O1A-CGA-O2A-C1
14	B	809	CLA	O1D-CGD-O2D-CED
14	b	810	CLA	O1D-CGD-O2D-CED
14	2	810	CLA	O1D-CGD-O2D-CED
14	A	837	CLA	CBD-CGD-O2D-CED
14	A	841	CLA	CBD-CGD-O2D-CED
14	B	831	CLA	CBD-CGD-O2D-CED
14	a	837	CLA	CBD-CGD-O2D-CED
14	a	841	CLA	CBD-CGD-O2D-CED
14	b	832	CLA	CBD-CGD-O2D-CED
14	1	1638	CLA	CBD-CGD-O2D-CED
14	1	1642	CLA	CBD-CGD-O2D-CED
14	2	832	CLA	CBD-CGD-O2D-CED
14	A	805	CLA	O1A-CGA-O2A-C1
14	a	805	CLA	O1A-CGA-O2A-C1
14	1	1606	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	A	840	CLA	C3-C5-C6-C7
14	A	841	CLA	C3-C5-C6-C7
14	a	840	CLA	C3-C5-C6-C7
14	a	841	CLA	C3-C5-C6-C7
14	1	1641	CLA	C3-C5-C6-C7
14	1	1642	CLA	C3-C5-C6-C7
14	B	817	CLA	CBA-CGA-O2A-C1
14	B	825	CLA	CBA-CGA-O2A-C1
14	b	818	CLA	CBA-CGA-O2A-C1
14	b	826	CLA	CBA-CGA-O2A-C1
14	2	818	CLA	CBA-CGA-O2A-C1
14	2	826	CLA	CBA-CGA-O2A-C1
20	B	849	LMG	O6-C5-C6-O5
20	b	850	LMG	O6-C5-C6-O5
20	2	850	LMG	O6-C5-C6-O5
14	A	855	CLA	C4-C3-C5-C6
14	B	818	CLA	C4-C3-C5-C6
14	b	802	CLA	C4-C3-C5-C6
14	b	819	CLA	C4-C3-C5-C6
14	2	802	CLA	C4-C3-C5-C6
14	2	819	CLA	C4-C3-C5-C6
14	A	833	CLA	C2-C3-C5-C6
14	A	855	CLA	C2-C3-C5-C6
14	B	818	CLA	C2-C3-C5-C6
14	a	833	CLA	C2-C3-C5-C6
14	b	802	CLA	C2-C3-C5-C6
14	b	819	CLA	C2-C3-C5-C6
14	1	1634	CLA	C2-C3-C5-C6
14	2	802	CLA	C2-C3-C5-C6
14	2	819	CLA	C2-C3-C5-C6
14	A	802	CLA	C2A-CAA-CBA-CGA
14	B	814	CLA	C2A-CAA-CBA-CGA
14	a	802	CLA	C2A-CAA-CBA-CGA
14	b	815	CLA	C2A-CAA-CBA-CGA
14	1	1603	CLA	C2A-CAA-CBA-CGA
14	2	815	CLA	C2A-CAA-CBA-CGA
14	A	809	CLA	O1A-CGA-O2A-C1
14	B	809	CLA	O1A-CGA-O2A-C1
14	L	205	CLA	O1A-CGA-O2A-C1
14	a	809	CLA	O1A-CGA-O2A-C1
14	b	810	CLA	O1A-CGA-O2A-C1
14	l	206	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	1	1610	CLA	O1A-CGA-O2A-C1
14	2	810	CLA	O1A-CGA-O2A-C1
14	0	207	CLA	O1A-CGA-O2A-C1
14	A	822	CLA	O1D-CGD-O2D-CED
14	a	822	CLA	O1D-CGD-O2D-CED
14	1	1623	CLA	O1D-CGD-O2D-CED
14	B	821	CLA	O1D-CGD-O2D-CED
14	b	822	CLA	O1D-CGD-O2D-CED
14	2	822	CLA	O1D-CGD-O2D-CED
14	X	1701	CLA	O1D-CGD-O2D-CED
14	x	1701	CLA	O1D-CGD-O2D-CED
14	z	102	CLA	O1D-CGD-O2D-CED
14	L	204	CLA	C3-C5-C6-C7
14	l	205	CLA	C3-C5-C6-C7
14	0	206	CLA	C3-C5-C6-C7
14	B	841	CLA	O1D-CGD-O2D-CED
14	b	842	CLA	O1D-CGD-O2D-CED
14	2	842	CLA	O1D-CGD-O2D-CED
14	A	812	CLA	CBA-CGA-O2A-C1
14	A	825	CLA	CBA-CGA-O2A-C1
14	B	805	CLA	CBA-CGA-O2A-C1
14	B	816	CLA	CBA-CGA-O2A-C1
14	B	835	CLA	CBA-CGA-O2A-C1
14	L	203	CLA	CBA-CGA-O2A-C1
14	a	812	CLA	CBA-CGA-O2A-C1
14	a	825	CLA	CBA-CGA-O2A-C1
14	b	806	CLA	CBA-CGA-O2A-C1
14	b	817	CLA	CBA-CGA-O2A-C1
14	b	836	CLA	CBA-CGA-O2A-C1
14	l	204	CLA	CBA-CGA-O2A-C1
14	1	1613	CLA	CBA-CGA-O2A-C1
14	1	1626	CLA	CBA-CGA-O2A-C1
14	2	806	CLA	CBA-CGA-O2A-C1
14	2	817	CLA	CBA-CGA-O2A-C1
14	2	836	CLA	CBA-CGA-O2A-C1
14	0	205	CLA	CBA-CGA-O2A-C1
18	m	101	LHG	C28-C29-C30-C31
14	B	828	CLA	C13-C15-C16-C17
14	B	838	CLA	C5-C6-C7-C8
14	b	839	CLA	C5-C6-C7-C8
14	2	839	CLA	C5-C6-C7-C8
18	A	853	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
18	a	853	LHG	O2-C2-C3-O3
18	1	1654	LHG	O2-C2-C3-O3
18	M	101	LHG	C28-C29-C30-C31
18	y	101	LHG	C28-C29-C30-C31
14	A	805	CLA	C6-C7-C8-C9
14	A	806	CLA	C14-C13-C15-C16
14	A	817	CLA	C14-C13-C15-C16
14	A	833	CLA	C11-C12-C13-C14
14	A	834	CLA	C11-C12-C13-C14
14	A	839	CLA	C6-C7-C8-C9
14	B	803	CLA	C11-C12-C13-C14
14	B	807	CLA	C11-C12-C13-C14
14	B	813	CLA	C11-C12-C13-C14
14	B	816	CLA	C14-C13-C15-C16
14	L	204	CLA	C6-C7-C8-C9
14	a	805	CLA	C6-C7-C8-C9
14	a	806	CLA	C14-C13-C15-C16
14	a	817	CLA	C14-C13-C15-C16
14	a	833	CLA	C11-C12-C13-C14
14	a	834	CLA	C11-C12-C13-C14
14	a	839	CLA	C6-C7-C8-C9
14	b	804	CLA	C11-C12-C13-C14
14	b	808	CLA	C11-C12-C13-C14
14	b	814	CLA	C11-C12-C13-C14
14	b	817	CLA	C14-C13-C15-C16
14	l	205	CLA	C6-C7-C8-C9
14	1	1604	CLA	C6-C7-C8-C9
14	1	1606	CLA	C6-C7-C8-C9
14	1	1607	CLA	C14-C13-C15-C16
14	1	1618	CLA	C14-C13-C15-C16
14	1	1634	CLA	C11-C12-C13-C14
14	1	1635	CLA	C11-C12-C13-C14
14	1	1640	CLA	C6-C7-C8-C9
14	2	804	CLA	C11-C12-C13-C14
14	2	808	CLA	C11-C12-C13-C14
14	2	814	CLA	C11-C12-C13-C14
14	2	817	CLA	C14-C13-C15-C16
14	0	206	CLA	C6-C7-C8-C9
14	A	834	CLA	O1D-CGD-O2D-CED
14	B	816	CLA	O1D-CGD-O2D-CED
14	a	834	CLA	O1D-CGD-O2D-CED
14	b	817	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	1	1635	CLA	O1D-CGD-O2D-CED
14	2	817	CLA	O1D-CGD-O2D-CED
14	B	807	CLA	C15-C16-C17-C18
14	b	808	CLA	C15-C16-C17-C18
14	b	829	CLA	C13-C15-C16-C17
14	2	808	CLA	C15-C16-C17-C18
14	2	829	CLA	C13-C15-C16-C17
14	A	843	CLA	C2A-CAA-CBA-CGA
14	a	843	CLA	C2A-CAA-CBA-CGA
14	1	1644	CLA	C2A-CAA-CBA-CGA
17	A	848	BCR	C37-C22-C23-C24
17	B	843	BCR	C7-C8-C9-C34
17	B	846	BCR	C11-C12-C13-C35
17	B	847	BCR	C7-C8-C9-C34
17	L	201	BCR	C11-C12-C13-C35
17	M	103	BCR	C37-C22-C23-C24
17	a	848	BCR	C37-C22-C23-C24
17	b	844	BCR	C7-C8-C9-C34
17	b	847	BCR	C11-C12-C13-C35
17	b	848	BCR	C7-C8-C9-C34
17	m	102	BCR	C37-C22-C23-C24
17	1	1648	BCR	C11-C12-C13-C35
17	1	1649	BCR	C37-C22-C23-C24
17	2	844	BCR	C7-C8-C9-C34
17	2	847	BCR	C11-C12-C13-C35
17	2	848	BCR	C7-C8-C9-C34
17	y	102	BCR	C37-C22-C23-C24
14	B	805	CLA	O1A-CGA-O2A-C1
14	B	835	CLA	O1A-CGA-O2A-C1
14	b	806	CLA	O1A-CGA-O2A-C1
14	b	836	CLA	O1A-CGA-O2A-C1
14	2	806	CLA	O1A-CGA-O2A-C1
14	2	836	CLA	O1A-CGA-O2A-C1
14	B	802	CLA	C15-C16-C17-C18
14	B	826	CLA	C13-C15-C16-C17
14	B	840	CLA	C8-C10-C11-C12
14	a	807	CLA	C8-C10-C11-C12
14	b	803	CLA	C15-C16-C17-C18
14	b	827	CLA	C13-C15-C16-C17
14	b	841	CLA	C8-C10-C11-C12
14	1	1608	CLA	C8-C10-C11-C12
14	2	803	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
14	2	827	CLA	C13-C15-C16-C17
14	2	841	CLA	C8-C10-C11-C12
14	A	842	CLA	CBD-CGD-O2D-CED
14	a	842	CLA	CBD-CGD-O2D-CED
14	1	1643	CLA	CBD-CGD-O2D-CED
20	B	849	LMG	C4-C5-C6-O5
20	b	850	LMG	C4-C5-C6-O5
20	2	850	LMG	C4-C5-C6-O5
18	A	854	LHG	C29-C30-C31-C32
14	B	825	CLA	C3-C5-C6-C7
14	b	826	CLA	C3-C5-C6-C7
14	2	826	CLA	C3-C5-C6-C7
14	B	802	CLA	CBA-CGA-O2A-C1
14	B	828	CLA	CBA-CGA-O2A-C1
14	B	831	CLA	CBA-CGA-O2A-C1
14	b	803	CLA	CBA-CGA-O2A-C1
14	b	829	CLA	CBA-CGA-O2A-C1
14	b	832	CLA	CBA-CGA-O2A-C1
14	2	803	CLA	CBA-CGA-O2A-C1
14	2	829	CLA	CBA-CGA-O2A-C1
14	2	832	CLA	CBA-CGA-O2A-C1
14	A	807	CLA	C5-C6-C7-C8
14	A	807	CLA	C8-C10-C11-C12
14	A	841	CLA	C8-C10-C11-C12
14	B	808	CLA	C13-C15-C16-C17
14	B	813	CLA	C15-C16-C17-C18
14	B	824	CLA	C15-C16-C17-C18
14	L	205	CLA	C5-C6-C7-C8
14	a	807	CLA	C5-C6-C7-C8
14	a	841	CLA	C8-C10-C11-C12
14	b	809	CLA	C13-C15-C16-C17
14	b	814	CLA	C15-C16-C17-C18
14	b	825	CLA	C15-C16-C17-C18
14	l	206	CLA	C5-C6-C7-C8
14	1	1608	CLA	C5-C6-C7-C8
14	1	1642	CLA	C8-C10-C11-C12
14	2	809	CLA	C13-C15-C16-C17
14	2	814	CLA	C15-C16-C17-C18
14	2	825	CLA	C15-C16-C17-C18
14	0	207	CLA	C5-C6-C7-C8
18	a	854	LHG	C29-C30-C31-C32
18	1	1655	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
14	F	203	CLA	CBD-CGD-O2D-CED
14	j	1301	CLA	CBD-CGD-O2D-CED
14	8	1301	CLA	CBD-CGD-O2D-CED
14	A	807	CLA	C13-C15-C16-C17
14	A	828	CLA	C15-C16-C17-C18
14	A	839	CLA	C15-C16-C17-C18
14	A	855	CLA	C15-C16-C17-C18
14	B	814	CLA	C10-C11-C12-C13
14	B	817	CLA	C5-C6-C7-C8
14	B	834	CLA	C8-C10-C11-C12
14	a	807	CLA	C13-C15-C16-C17
14	a	828	CLA	C15-C16-C17-C18
14	a	839	CLA	C15-C16-C17-C18
14	b	802	CLA	C15-C16-C17-C18
14	b	815	CLA	C10-C11-C12-C13
14	b	818	CLA	C5-C6-C7-C8
14	b	835	CLA	C8-C10-C11-C12
14	1	1608	CLA	C13-C15-C16-C17
14	1	1629	CLA	C15-C16-C17-C18
14	1	1640	CLA	C15-C16-C17-C18
14	2	802	CLA	C15-C16-C17-C18
14	2	815	CLA	C10-C11-C12-C13
14	2	818	CLA	C5-C6-C7-C8
14	2	835	CLA	C8-C10-C11-C12
18	A	853	LHG	O1-C1-C2-O2
18	B	850	LHG	O1-C1-C2-O2
18	L	208	LHG	O1-C1-C2-O2
18	a	853	LHG	O1-C1-C2-O2
18	b	851	LHG	O1-C1-C2-O2
18	l	201	LHG	O1-C1-C2-O2
18	1	1654	LHG	O1-C1-C2-O2
18	0	202	LHG	O1-C1-C2-O2
18	z	101	LHG	O1-C1-C2-O2
14	L	203	CLA	O1A-CGA-O2A-C1
14	l	204	CLA	O1A-CGA-O2A-C1
14	2	817	CLA	O1A-CGA-O2A-C1
14	0	205	CLA	O1A-CGA-O2A-C1
13	A	801	CL0	C8-C10-C11-C12
13	a	801	CL0	C8-C10-C11-C12
13	1	1602	CL0	C8-C10-C11-C12
14	A	810	CLA	C8-C10-C11-C12
14	A	818	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	A	828	CLA	C5-C6-C7-C8
14	A	836	CLA	C15-C16-C17-C18
14	B	829	CLA	C13-C15-C16-C17
14	B	833	CLA	C13-C15-C16-C17
14	a	810	CLA	C8-C10-C11-C12
14	a	818	CLA	C5-C6-C7-C8
14	a	828	CLA	C5-C6-C7-C8
14	a	836	CLA	C15-C16-C17-C18
14	b	830	CLA	C13-C15-C16-C17
14	b	834	CLA	C13-C15-C16-C17
14	1	1611	CLA	C8-C10-C11-C12
14	1	1619	CLA	C5-C6-C7-C8
14	1	1629	CLA	C5-C6-C7-C8
14	1	1637	CLA	C15-C16-C17-C18
14	2	830	CLA	C13-C15-C16-C17
14	2	834	CLA	C13-C15-C16-C17
14	A	829	CLA	CBA-CGA-O2A-C1
14	a	829	CLA	CBA-CGA-O2A-C1
14	1	1630	CLA	CBA-CGA-O2A-C1
14	B	813	CLA	O1D-CGD-O2D-CED
14	B	827	CLA	O1D-CGD-O2D-CED
14	b	828	CLA	O1D-CGD-O2D-CED
14	2	828	CLA	O1D-CGD-O2D-CED
14	A	825	CLA	C13-C15-C16-C17
14	a	825	CLA	C13-C15-C16-C17
14	1	1626	CLA	C13-C15-C16-C17
14	b	817	CLA	O1A-CGA-O2A-C1
14	A	804	CLA	C5-C6-C7-C8
14	a	804	CLA	C5-C6-C7-C8
14	1	1605	CLA	C5-C6-C7-C8
13	A	801	CL0	C11-C12-C13-C15
13	a	801	CL0	C11-C12-C13-C15
13	1	1602	CL0	C11-C12-C13-C15
14	A	822	CLA	C6-C7-C8-C10
14	A	840	CLA	C6-C7-C8-C10
14	B	810	CLA	C6-C7-C8-C10
14	a	822	CLA	C6-C7-C8-C10
14	a	840	CLA	C6-C7-C8-C10
14	b	811	CLA	C6-C7-C8-C10
14	1	1623	CLA	C6-C7-C8-C10
14	1	1641	CLA	C6-C7-C8-C10
14	2	811	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
14	A	825	CLA	O1A-CGA-O2A-C1
14	B	816	CLA	O1A-CGA-O2A-C1
14	a	825	CLA	O1A-CGA-O2A-C1
14	1	1626	CLA	O1A-CGA-O2A-C1
17	A	848	BCR	C15-C16-C17-C18
17	a	848	BCR	C15-C16-C17-C18
17	1	1649	BCR	C15-C16-C17-C18
14	A	803	CLA	C2A-CAA-CBA-CGA
14	A	822	CLA	C2A-CAA-CBA-CGA
14	A	825	CLA	C2A-CAA-CBA-CGA
14	B	827	CLA	C2A-CAA-CBA-CGA
14	a	822	CLA	C2A-CAA-CBA-CGA
14	a	825	CLA	C2A-CAA-CBA-CGA
14	b	828	CLA	C2A-CAA-CBA-CGA
14	1	1604	CLA	C2A-CAA-CBA-CGA
14	1	1623	CLA	C2A-CAA-CBA-CGA
14	1	1626	CLA	C2A-CAA-CBA-CGA
14	2	828	CLA	C2A-CAA-CBA-CGA
14	b	814	CLA	O1D-CGD-O2D-CED
14	2	814	CLA	O1D-CGD-O2D-CED
14	A	812	CLA	C10-C11-C12-C13
14	A	828	CLA	C8-C10-C11-C12
14	a	812	CLA	C10-C11-C12-C13
14	a	828	CLA	C8-C10-C11-C12
14	1	1613	CLA	C10-C11-C12-C13
14	1	1629	CLA	C8-C10-C11-C12
14	B	803	CLA	C4C-C3C-CAC-CBC
14	b	804	CLA	C4C-C3C-CAC-CBC
14	2	804	CLA	C4C-C3C-CAC-CBC
17	L	206	BCR	C22-C23-C24-C25
17	M	103	BCR	C22-C23-C24-C25
17	l	207	BCR	C22-C23-C24-C25
17	m	102	BCR	C22-C23-C24-C25
17	0	208	BCR	C22-C23-C24-C25
17	y	102	BCR	C22-C23-C24-C25
14	A	812	CLA	O1A-CGA-O2A-C1
14	a	812	CLA	O1A-CGA-O2A-C1
14	1	1613	CLA	O1A-CGA-O2A-C1
20	B	849	LMG	O6-C1-O1-C7
20	b	850	LMG	O6-C1-O1-C7
20	2	850	LMG	O6-C1-O1-C7
17	B	845	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
17	B	847	BCR	C10-C11-C12-C13
17	K	102	BCR	C10-C11-C12-C13
17	M	103	BCR	C18-C19-C20-C21
17	b	846	BCR	C18-C19-C20-C21
17	b	848	BCR	C10-C11-C12-C13
17	k	102	BCR	C10-C11-C12-C13
17	m	102	BCR	C18-C19-C20-C21
17	2	846	BCR	C18-C19-C20-C21
17	2	848	BCR	C10-C11-C12-C13
17	9	102	BCR	C10-C11-C12-C13
17	y	102	BCR	C18-C19-C20-C21
14	A	843	CLA	C3-C5-C6-C7
14	a	843	CLA	C3-C5-C6-C7
14	1	1644	CLA	C3-C5-C6-C7
14	A	841	CLA	C5-C6-C7-C8
14	B	804	CLA	C15-C16-C17-C18
14	B	810	CLA	C15-C16-C17-C18
14	B	824	CLA	C13-C15-C16-C17
14	B	834	CLA	C15-C16-C17-C18
14	a	841	CLA	C5-C6-C7-C8
14	b	805	CLA	C15-C16-C17-C18
14	b	811	CLA	C15-C16-C17-C18
14	b	825	CLA	C13-C15-C16-C17
14	b	835	CLA	C15-C16-C17-C18
14	1	1642	CLA	C5-C6-C7-C8
14	2	805	CLA	C15-C16-C17-C18
14	2	811	CLA	C15-C16-C17-C18
14	2	825	CLA	C13-C15-C16-C17
14	2	835	CLA	C15-C16-C17-C18
14	B	831	CLA	O1A-CGA-O2A-C1
14	2	832	CLA	O1A-CGA-O2A-C1
14	A	802	CLA	C15-C16-C17-C18
14	A	818	CLA	C15-C16-C17-C18
14	A	829	CLA	C10-C11-C12-C13
14	A	840	CLA	C13-C15-C16-C17
14	B	811	CLA	C15-C16-C17-C18
14	B	816	CLA	C13-C15-C16-C17
14	B	819	CLA	C8-C10-C11-C12
14	B	825	CLA	C8-C10-C11-C12
14	a	802	CLA	C15-C16-C17-C18
14	a	818	CLA	C15-C16-C17-C18
14	a	829	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	a	840	CLA	C13-C15-C16-C17
14	b	812	CLA	C15-C16-C17-C18
14	b	817	CLA	C13-C15-C16-C17
14	b	820	CLA	C8-C10-C11-C12
14	b	826	CLA	C8-C10-C11-C12
14	1	1603	CLA	C15-C16-C17-C18
14	1	1619	CLA	C15-C16-C17-C18
14	1	1630	CLA	C10-C11-C12-C13
14	1	1641	CLA	C13-C15-C16-C17
14	2	812	CLA	C15-C16-C17-C18
14	2	817	CLA	C13-C15-C16-C17
14	2	820	CLA	C8-C10-C11-C12
14	2	826	CLA	C8-C10-C11-C12
14	B	802	CLA	O1A-CGA-O2A-C1
14	a	829	CLA	O1A-CGA-O2A-C1
14	b	803	CLA	O1A-CGA-O2A-C1
14	b	832	CLA	O1A-CGA-O2A-C1
14	2	803	CLA	O1A-CGA-O2A-C1
18	M	101	LHG	C32-C33-C34-C35
18	m	101	LHG	C32-C33-C34-C35
18	y	101	LHG	C32-C33-C34-C35
14	A	824	CLA	C13-C15-C16-C17
14	B	805	CLA	C13-C15-C16-C17
14	B	805	CLA	C15-C16-C17-C18
14	a	824	CLA	C13-C15-C16-C17
14	b	806	CLA	C13-C15-C16-C17
14	b	806	CLA	C15-C16-C17-C18
14	1	1625	CLA	C13-C15-C16-C17
14	2	806	CLA	C13-C15-C16-C17
14	2	806	CLA	C15-C16-C17-C18
18	A	853	LHG	C3-O3-P-O6
18	L	208	LHG	C3-O3-P-O6
18	L	208	LHG	C4-O6-P-O3
18	M	101	LHG	C4-O6-P-O3
18	a	853	LHG	C3-O3-P-O6
18	l	201	LHG	C3-O3-P-O6
18	l	201	LHG	C4-O6-P-O3
18	m	101	LHG	C4-O6-P-O3
18	1	1654	LHG	C3-O3-P-O6
18	0	202	LHG	C3-O3-P-O6
18	0	202	LHG	C4-O6-P-O3
18	y	101	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
14	B	834	CLA	CBA-CGA-O2A-C1
14	b	835	CLA	CBA-CGA-O2A-C1
14	2	835	CLA	CBA-CGA-O2A-C1
14	A	829	CLA	O1A-CGA-O2A-C1
14	1	1630	CLA	O1A-CGA-O2A-C1
14	B	811	CLA	O1D-CGD-O2D-CED
14	b	812	CLA	O1D-CGD-O2D-CED
14	2	812	CLA	O1D-CGD-O2D-CED
14	b	829	CLA	O1A-CGA-O2A-C1
14	2	829	CLA	O1A-CGA-O2A-C1
14	A	814	CLA	C2A-CAA-CBA-CGA
14	A	823	CLA	C2A-CAA-CBA-CGA
14	B	821	CLA	C2A-CAA-CBA-CGA
14	X	1701	CLA	C2A-CAA-CBA-CGA
14	a	803	CLA	C2A-CAA-CBA-CGA
14	a	814	CLA	C2A-CAA-CBA-CGA
14	a	823	CLA	C2A-CAA-CBA-CGA
14	x	1701	CLA	C2A-CAA-CBA-CGA
14	1	1615	CLA	C2A-CAA-CBA-CGA
14	1	1624	CLA	C2A-CAA-CBA-CGA
14	2	822	CLA	C2A-CAA-CBA-CGA
14	z	102	CLA	C2A-CAA-CBA-CGA
14	K	103	CLA	CBA-CGA-O2A-C1
14	k	103	CLA	CBA-CGA-O2A-C1
14	9	103	CLA	CBA-CGA-O2A-C1
14	B	827	CLA	C10-C11-C12-C13
14	b	828	CLA	C10-C11-C12-C13
14	2	828	CLA	C10-C11-C12-C13
17	A	852	BCR	C9-C10-C11-C12
17	B	843	BCR	C15-C16-C17-C18
17	a	852	BCR	C9-C10-C11-C12
17	1	1653	BCR	C9-C10-C11-C12
18	b	851	LHG	C32-C33-C34-C35
17	A	847	BCR	C20-C21-C22-C37
17	A	850	BCR	C16-C17-C18-C36
17	A	851	BCR	C35-C13-C14-C15
17	A	856	BCR	C35-C13-C14-C15
17	A	856	BCR	C20-C21-C22-C37
17	B	846	BCR	C16-C17-C18-C36
17	B	851	BCR	C16-C17-C18-C36
17	F	202	BCR	C11-C10-C9-C34
17	F	202	BCR	C35-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
17	F	202	BCR	C20-C21-C22-C37
17	F	205	BCR	C35-C13-C14-C15
17	I	101	BCR	C35-C13-C14-C15
17	L	201	BCR	C35-C13-C14-C15
17	L	206	BCR	C20-C21-C22-C37
17	M	103	BCR	C35-C13-C14-C15
17	M	103	BCR	C20-C21-C22-C37
17	a	847	BCR	C20-C21-C22-C37
17	a	850	BCR	C16-C17-C18-C36
17	a	851	BCR	C35-C13-C14-C15
17	b	847	BCR	C16-C17-C18-C36
17	b	852	BCR	C16-C17-C18-C36
17	f	202	BCR	C11-C10-C9-C34
17	f	202	BCR	C35-C13-C14-C15
17	f	202	BCR	C20-C21-C22-C37
17	f	204	BCR	C35-C13-C14-C15
17	i	101	BCR	C35-C13-C14-C15
17	j	1305	BCR	C35-C13-C14-C15
17	j	1305	BCR	C20-C21-C22-C37
17	l	202	BCR	C35-C13-C14-C15
17	l	207	BCR	C20-C21-C22-C37
17	m	102	BCR	C35-C13-C14-C15
17	m	102	BCR	C20-C21-C22-C37
17	1	1648	BCR	C20-C21-C22-C37
17	1	1651	BCR	C16-C17-C18-C36
17	1	1652	BCR	C35-C13-C14-C15
17	2	847	BCR	C16-C17-C18-C36
17	6	202	BCR	C11-C10-C9-C34
17	6	202	BCR	C35-C13-C14-C15
17	6	202	BCR	C20-C21-C22-C37
17	6	204	BCR	C35-C13-C14-C15
17	7	101	BCR	C35-C13-C14-C15
17	8	1305	BCR	C35-C13-C14-C15
17	8	1305	BCR	C20-C21-C22-C37
17	0	203	BCR	C35-C13-C14-C15
17	0	208	BCR	C20-C21-C22-C37
17	y	102	BCR	C35-C13-C14-C15
17	y	102	BCR	C20-C21-C22-C37
18	B	850	LHG	C32-C33-C34-C35
18	L	208	LHG	C15-C16-C17-C18
18	l	201	LHG	C15-C16-C17-C18
18	0	202	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
18	z	101	LHG	C32-C33-C34-C35
14	B	828	CLA	O1A-CGA-O2A-C1
14	A	819	CLA	C16-C17-C18-C20
14	A	821	CLA	C16-C17-C18-C19
14	B	824	CLA	C16-C17-C18-C20
14	a	819	CLA	C16-C17-C18-C20
14	a	821	CLA	C16-C17-C18-C19
14	b	825	CLA	C16-C17-C18-C20
14	1	1620	CLA	C16-C17-C18-C20
14	1	1622	CLA	C16-C17-C18-C19
14	2	825	CLA	C16-C17-C18-C20
14	b	805	CLA	CBA-CGA-O2A-C1
14	A	819	CLA	C8-C10-C11-C12
14	B	833	CLA	C10-C11-C12-C13
14	a	819	CLA	C8-C10-C11-C12
14	1	1620	CLA	C8-C10-C11-C12
14	2	834	CLA	C10-C11-C12-C13
18	B	850	LHG	C11-C10-C9-C8
18	b	851	LHG	C11-C10-C9-C8
18	M	101	LHG	C30-C31-C32-C33
18	m	101	LHG	C30-C31-C32-C33
18	y	101	LHG	C30-C31-C32-C33
18	z	101	LHG	C11-C10-C9-C8
20	B	849	LMG	C18-C19-C20-C21
20	b	850	LMG	C18-C19-C20-C21
20	2	850	LMG	C18-C19-C20-C21
14	b	834	CLA	C10-C11-C12-C13
18	A	853	LHG	C24-C25-C26-C27
18	a	853	LHG	C24-C25-C26-C27
18	1	1654	LHG	C24-C25-C26-C27
14	B	824	CLA	C3-C5-C6-C7
14	b	825	CLA	C3-C5-C6-C7
14	2	825	CLA	C3-C5-C6-C7
17	A	848	BCR	C20-C21-C22-C23
17	A	850	BCR	C20-C21-C22-C23
17	A	851	BCR	C11-C10-C9-C8
17	A	851	BCR	C16-C17-C18-C19
17	B	843	BCR	C16-C17-C18-C19
17	B	845	BCR	C11-C10-C9-C8
17	B	851	BCR	C20-C21-C22-C23
17	K	104	BCR	C11-C10-C9-C8
17	a	848	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
17	a	850	BCR	C20-C21-C22-C23
17	a	851	BCR	C11-C10-C9-C8
17	a	851	BCR	C16-C17-C18-C19
17	b	844	BCR	C16-C17-C18-C19
17	b	846	BCR	C11-C10-C9-C8
17	b	852	BCR	C20-C21-C22-C23
17	k	104	BCR	C11-C10-C9-C8
17	1	1649	BCR	C20-C21-C22-C23
17	1	1651	BCR	C20-C21-C22-C23
17	1	1652	BCR	C11-C10-C9-C8
17	1	1652	BCR	C16-C17-C18-C19
17	2	844	BCR	C16-C17-C18-C19
17	2	846	BCR	C11-C10-C9-C8
17	8	1306	BCR	C20-C21-C22-C23
17	9	104	BCR	C11-C10-C9-C8
20	B	849	LMG	C2-C1-O1-C7
20	b	850	LMG	C2-C1-O1-C7
20	2	850	LMG	C2-C1-O1-C7
14	B	804	CLA	CBA-CGA-O2A-C1
14	2	805	CLA	CBA-CGA-O2A-C1
18	A	853	LHG	C11-C10-C9-C8
18	B	850	LHG	C15-C16-C17-C18
18	L	208	LHG	C12-C13-C14-C15
18	a	853	LHG	C11-C10-C9-C8
18	l	201	LHG	C12-C13-C14-C15
18	1	1654	LHG	C11-C10-C9-C8
14	A	831	CLA	C5-C6-C7-C8
14	a	831	CLA	C5-C6-C7-C8
14	1	1632	CLA	C5-C6-C7-C8
14	B	834	CLA	O1A-CGA-O2A-C1
14	b	835	CLA	O1A-CGA-O2A-C1
14	2	835	CLA	O1A-CGA-O2A-C1
14	B	810	CLA	C16-C17-C18-C19
14	B	810	CLA	C16-C17-C18-C20
14	B	818	CLA	C16-C17-C18-C20
14	B	824	CLA	C16-C17-C18-C19
14	b	811	CLA	C16-C17-C18-C19
14	b	811	CLA	C16-C17-C18-C20
14	b	819	CLA	C16-C17-C18-C20
14	b	825	CLA	C16-C17-C18-C19
14	2	811	CLA	C16-C17-C18-C20
14	2	819	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
14	b	831	CLA	O1D-CGD-O2D-CED
14	A	820	CLA	C4-C3-C5-C6
14	A	822	CLA	C4-C3-C5-C6
14	a	820	CLA	C4-C3-C5-C6
14	a	822	CLA	C4-C3-C5-C6
14	1	1621	CLA	C4-C3-C5-C6
14	1	1623	CLA	C4-C3-C5-C6
18	a	853	LHG	C32-C33-C34-C35
18	b	851	LHG	C15-C16-C17-C18
18	0	202	LHG	C12-C13-C14-C15
18	z	101	LHG	C15-C16-C17-C18
14	A	812	CLA	C2-C3-C5-C6
14	A	822	CLA	C2-C3-C5-C6
14	B	814	CLA	C2-C3-C5-C6
14	a	812	CLA	C2-C3-C5-C6
14	a	822	CLA	C2-C3-C5-C6
14	b	815	CLA	C2-C3-C5-C6
14	1	1613	CLA	C2-C3-C5-C6
14	1	1623	CLA	C2-C3-C5-C6
14	2	815	CLA	C2-C3-C5-C6
14	A	804	CLA	C6-C7-C8-C9
14	A	816	CLA	C11-C12-C13-C14
14	A	830	CLA	C11-C12-C13-C14
14	B	810	CLA	C11-C12-C13-C14
14	a	804	CLA	C6-C7-C8-C9
14	a	816	CLA	C11-C12-C13-C14
14	a	830	CLA	C11-C12-C13-C14
14	b	811	CLA	C11-C12-C13-C14
14	1	1605	CLA	C6-C7-C8-C9
14	1	1617	CLA	C11-C12-C13-C14
14	1	1631	CLA	C11-C12-C13-C14
14	2	811	CLA	C11-C12-C13-C14
14	B	830	CLA	O1D-CGD-O2D-CED
14	2	831	CLA	O1D-CGD-O2D-CED
18	A	853	LHG	C32-C33-C34-C35
18	1	1654	LHG	C32-C33-C34-C35
20	B	849	LMG	C12-C13-C14-C15
20	b	850	LMG	C12-C13-C14-C15
20	2	850	LMG	C12-C13-C14-C15
14	A	834	CLA	C2A-CAA-CBA-CGA
14	B	809	CLA	C2A-CAA-CBA-CGA
14	B	823	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	a	834	CLA	C2A-CAA-CBA-CGA
14	b	810	CLA	C2A-CAA-CBA-CGA
14	b	822	CLA	C2A-CAA-CBA-CGA
14	b	824	CLA	C2A-CAA-CBA-CGA
14	1	1635	CLA	C2A-CAA-CBA-CGA
14	2	810	CLA	C2A-CAA-CBA-CGA
14	2	824	CLA	C2A-CAA-CBA-CGA
17	B	843	BCR	C37-C22-C23-C24
17	b	844	BCR	C37-C22-C23-C24
17	l	202	BCR	C11-C12-C13-C35
17	2	844	BCR	C37-C22-C23-C24
17	0	203	BCR	C11-C12-C13-C35
18	A	853	LHG	O1-C1-C2-C3
18	B	850	LHG	O1-C1-C2-C3
18	M	101	LHG	O1-C1-C2-C3
18	a	853	LHG	O1-C1-C2-C3
18	b	851	LHG	O1-C1-C2-C3
18	m	101	LHG	O1-C1-C2-C3
18	1	1654	LHG	O1-C1-C2-C3
18	y	101	LHG	O1-C1-C2-C3
18	z	101	LHG	O1-C1-C2-C3
14	B	814	CLA	CBD-CGD-O2D-CED
20	B	849	LMG	C35-C36-C37-C38
20	2	850	LMG	C35-C36-C37-C38
14	A	835	CLA	C4B-C3B-CAB-CBB
14	B	812	CLA	C4B-C3B-CAB-CBB
14	B	820	CLA	C4B-C3B-CAB-CBB
14	a	835	CLA	C4B-C3B-CAB-CBB
14	b	813	CLA	C4B-C3B-CAB-CBB
14	b	821	CLA	C4B-C3B-CAB-CBB
14	1	1636	CLA	C4B-C3B-CAB-CBB
14	2	813	CLA	C4B-C3B-CAB-CBB
14	2	821	CLA	C4B-C3B-CAB-CBB
14	A	816	CLA	C16-C17-C18-C19
14	B	828	CLA	C16-C17-C18-C19
14	B	830	CLA	C6-C7-C8-C10
14	a	816	CLA	C16-C17-C18-C19
14	a	816	CLA	C16-C17-C18-C20
14	b	829	CLA	C16-C17-C18-C19
14	b	831	CLA	C6-C7-C8-C10
14	1	1617	CLA	C16-C17-C18-C19
14	2	811	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
14	2	825	CLA	C16-C17-C18-C19
14	2	829	CLA	C16-C17-C18-C19
14	2	831	CLA	C6-C7-C8-C10
14	A	804	CLA	C10-C11-C12-C13
14	a	804	CLA	C10-C11-C12-C13
14	1	1605	CLA	C10-C11-C12-C13
18	A	853	LHG	C10-C11-C12-C13
18	M	101	LHG	C34-C35-C36-C37
18	a	853	LHG	C10-C11-C12-C13
18	m	101	LHG	C34-C35-C36-C37
18	1	1654	LHG	C10-C11-C12-C13
18	y	101	LHG	C34-C35-C36-C37
20	b	850	LMG	C35-C36-C37-C38
14	a	820	CLA	CBD-CGD-O2D-CED
14	b	815	CLA	CBD-CGD-O2D-CED
14	2	815	CLA	CBD-CGD-O2D-CED
20	B	849	LMG	O10-C28-O8-C9
20	b	850	LMG	O10-C28-O8-C9
20	2	850	LMG	O10-C28-O8-C9
18	A	854	LHG	C24-C25-C26-C27
18	a	854	LHG	C24-C25-C26-C27
18	1	1655	LHG	C24-C25-C26-C27
13	A	801	CL0	C3-C5-C6-C7
13	a	801	CL0	C3-C5-C6-C7
13	1	1602	CL0	C3-C5-C6-C7
14	A	832	CLA	C3-C5-C6-C7
14	a	832	CLA	C3-C5-C6-C7
14	1	1633	CLA	C3-C5-C6-C7
18	A	853	LHG	C9-C10-C11-C12
18	a	853	LHG	C9-C10-C11-C12
18	1	1654	LHG	C9-C10-C11-C12
14	A	804	CLA	C3A-C2A-CAA-CBA
14	A	806	CLA	C3A-C2A-CAA-CBA
14	B	813	CLA	C3A-C2A-CAA-CBA
14	B	825	CLA	C3A-C2A-CAA-CBA
14	B	836	CLA	C3A-C2A-CAA-CBA
14	a	804	CLA	C3A-C2A-CAA-CBA
14	a	806	CLA	C3A-C2A-CAA-CBA
14	b	814	CLA	C3A-C2A-CAA-CBA
14	b	826	CLA	C3A-C2A-CAA-CBA
14	b	837	CLA	C3A-C2A-CAA-CBA
14	1	1605	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	1	1607	CLA	C3A-C2A-CAA-CBA
14	2	814	CLA	C3A-C2A-CAA-CBA
14	2	826	CLA	C3A-C2A-CAA-CBA
14	2	837	CLA	C3A-C2A-CAA-CBA
14	B	838	CLA	C13-C15-C16-C17
14	b	839	CLA	C13-C15-C16-C17
14	2	839	CLA	C13-C15-C16-C17
17	b	844	BCR	C15-C16-C17-C18
17	2	844	BCR	C15-C16-C17-C18
18	M	101	LHG	C11-C10-C9-C8
18	m	101	LHG	C11-C10-C9-C8
14	A	816	CLA	C16-C17-C18-C20
14	A	821	CLA	C16-C17-C18-C20
14	A	839	CLA	C16-C17-C18-C20
14	B	828	CLA	C16-C17-C18-C20
14	a	821	CLA	C16-C17-C18-C20
14	a	839	CLA	C16-C17-C18-C20
14	b	829	CLA	C16-C17-C18-C20
14	1	1617	CLA	C16-C17-C18-C20
14	1	1622	CLA	C16-C17-C18-C20
14	1	1640	CLA	C16-C17-C18-C20
14	2	829	CLA	C16-C17-C18-C20
14	2	831	CLA	C6-C7-C8-C9
18	y	101	LHG	C11-C10-C9-C8
14	A	820	CLA	CBD-CGD-O2D-CED
14	b	840	CLA	CBD-CGD-O2D-CED
14	1	1621	CLA	CBD-CGD-O2D-CED
14	2	840	CLA	CBD-CGD-O2D-CED
17	6	202	BCR	C14-C15-C16-C17
14	A	812	CLA	C3-C5-C6-C7
14	A	826	CLA	C3-C5-C6-C7
14	a	826	CLA	C3-C5-C6-C7
14	1	1627	CLA	C3-C5-C6-C7
18	M	101	LHG	C7-C8-C9-C10
18	m	101	LHG	C7-C8-C9-C10
18	y	101	LHG	C7-C8-C9-C10
14	A	804	CLA	C8-C10-C11-C12
14	a	804	CLA	C8-C10-C11-C12
14	1	1605	CLA	C8-C10-C11-C12
14	A	812	CLA	C4-C3-C5-C6
14	A	825	CLA	C4-C3-C5-C6
14	B	814	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	a	812	CLA	C4-C3-C5-C6
14	a	825	CLA	C4-C3-C5-C6
14	b	815	CLA	C4-C3-C5-C6
14	1	1613	CLA	C4-C3-C5-C6
14	1	1626	CLA	C4-C3-C5-C6
14	2	815	CLA	C4-C3-C5-C6
14	a	825	CLA	C2-C3-C5-C6
14	1	1626	CLA	C2-C3-C5-C6
14	B	839	CLA	CBD-CGD-O2D-CED
14	B	835	CLA	C2A-CAA-CBA-CGA
14	b	836	CLA	C2A-CAA-CBA-CGA
14	2	836	CLA	C2A-CAA-CBA-CGA
14	K	103	CLA	O1A-CGA-O2A-C1
14	k	103	CLA	O1A-CGA-O2A-C1
14	9	103	CLA	O1A-CGA-O2A-C1
14	B	830	CLA	C6-C7-C8-C9
14	b	831	CLA	C6-C7-C8-C9
14	A	835	CLA	C2B-C3B-CAB-CBB
14	B	812	CLA	C2B-C3B-CAB-CBB
14	B	817	CLA	C2B-C3B-CAB-CBB
14	B	820	CLA	C2B-C3B-CAB-CBB
14	a	835	CLA	C2B-C3B-CAB-CBB
14	b	813	CLA	C2B-C3B-CAB-CBB
14	b	818	CLA	C2B-C3B-CAB-CBB
14	b	821	CLA	C2B-C3B-CAB-CBB
14	1	1636	CLA	C2B-C3B-CAB-CBB
14	2	813	CLA	C2B-C3B-CAB-CBB
14	2	818	CLA	C2B-C3B-CAB-CBB
14	2	821	CLA	C2B-C3B-CAB-CBB
14	A	812	CLA	C8-C10-C11-C12
14	A	832	CLA	C5-C6-C7-C8
14	a	812	CLA	C8-C10-C11-C12
14	a	832	CLA	C5-C6-C7-C8
14	1	1613	CLA	C8-C10-C11-C12
14	a	812	CLA	C3-C5-C6-C7
14	1	1613	CLA	C3-C5-C6-C7
14	A	819	CLA	C2-C1-O2A-CGA
14	B	819	CLA	C2-C1-O2A-CGA
14	a	819	CLA	C2-C1-O2A-CGA
14	b	820	CLA	C2-C1-O2A-CGA
14	1	1620	CLA	C2-C1-O2A-CGA
14	2	820	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
14	A	838	CLA	C2C-C3C-CAC-CBC
14	a	838	CLA	C2C-C3C-CAC-CBC
14	1	1639	CLA	C2C-C3C-CAC-CBC
18	L	208	LHG	C14-C15-C16-C17
18	l	201	LHG	C14-C15-C16-C17
18	0	202	LHG	C14-C15-C16-C17
14	A	816	CLA	C8-C10-C11-C12
14	A	825	CLA	C15-C16-C17-C18
14	a	816	CLA	C8-C10-C11-C12
14	a	825	CLA	C15-C16-C17-C18
14	1	1617	CLA	C8-C10-C11-C12
14	1	1626	CLA	C15-C16-C17-C18
14	1	1633	CLA	C5-C6-C7-C8
14	B	804	CLA	O1A-CGA-O2A-C1
14	b	805	CLA	O1A-CGA-O2A-C1
14	2	805	CLA	O1A-CGA-O2A-C1
18	A	853	LHG	C27-C28-C29-C30
18	A	854	LHG	C32-C33-C34-C35
18	a	853	LHG	C27-C28-C29-C30
18	a	854	LHG	C32-C33-C34-C35
18	1	1654	LHG	C27-C28-C29-C30
17	A	847	BCR	C23-C24-C25-C26
17	A	849	BCR	C23-C24-C25-C26
17	A	849	BCR	C23-C24-C25-C30
17	A	851	BCR	C5-C6-C7-C8
17	A	856	BCR	C1-C6-C7-C8
17	A	856	BCR	C5-C6-C7-C8
17	A	856	BCR	C23-C24-C25-C26
17	A	856	BCR	C23-C24-C25-C30
17	B	844	BCR	C5-C6-C7-C8
17	B	845	BCR	C1-C6-C7-C8
17	B	847	BCR	C23-C24-C25-C26
17	B	847	BCR	C23-C24-C25-C30
17	B	851	BCR	C1-C6-C7-C8
17	B	851	BCR	C5-C6-C7-C8
17	F	205	BCR	C5-C6-C7-C8
17	F	205	BCR	C23-C24-C25-C26
17	J	103	BCR	C5-C6-C7-C8
17	L	206	BCR	C23-C24-C25-C26
17	L	206	BCR	C23-C24-C25-C30
17	M	103	BCR	C1-C6-C7-C8
17	M	103	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
17	a	847	BCR	C23-C24-C25-C26
17	a	849	BCR	C23-C24-C25-C26
17	a	849	BCR	C23-C24-C25-C30
17	a	851	BCR	C5-C6-C7-C8
17	b	845	BCR	C5-C6-C7-C8
17	b	846	BCR	C1-C6-C7-C8
17	b	848	BCR	C23-C24-C25-C26
17	b	848	BCR	C23-C24-C25-C30
17	b	852	BCR	C1-C6-C7-C8
17	b	852	BCR	C5-C6-C7-C8
17	f	204	BCR	C5-C6-C7-C8
17	f	204	BCR	C23-C24-C25-C26
17	j	1304	BCR	C5-C6-C7-C8
17	j	1305	BCR	C1-C6-C7-C8
17	j	1305	BCR	C5-C6-C7-C8
17	j	1305	BCR	C23-C24-C25-C26
17	j	1305	BCR	C23-C24-C25-C30
17	l	207	BCR	C23-C24-C25-C26
17	l	207	BCR	C23-C24-C25-C30
17	m	102	BCR	C1-C6-C7-C8
17	m	102	BCR	C5-C6-C7-C8
17	1	1648	BCR	C23-C24-C25-C26
17	1	1650	BCR	C23-C24-C25-C26
17	1	1650	BCR	C23-C24-C25-C30
17	1	1652	BCR	C1-C6-C7-C8
17	1	1652	BCR	C5-C6-C7-C8
17	2	845	BCR	C5-C6-C7-C8
17	2	846	BCR	C1-C6-C7-C8
17	2	848	BCR	C23-C24-C25-C26
17	2	848	BCR	C23-C24-C25-C30
17	6	204	BCR	C5-C6-C7-C8
17	6	204	BCR	C23-C24-C25-C26
17	8	1304	BCR	C5-C6-C7-C8
17	8	1305	BCR	C1-C6-C7-C8
17	8	1305	BCR	C5-C6-C7-C8
17	8	1305	BCR	C23-C24-C25-C26
17	8	1305	BCR	C23-C24-C25-C30
17	8	1306	BCR	C1-C6-C7-C8
17	8	1306	BCR	C5-C6-C7-C8
17	0	208	BCR	C23-C24-C25-C26
17	0	208	BCR	C23-C24-C25-C30
17	y	102	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
17	y	102	BCR	C5-C6-C7-C8
18	a	853	LHG	C15-C16-C17-C18
18	1	1654	LHG	C15-C16-C17-C18
18	1	1655	LHG	C32-C33-C34-C35
14	B	831	CLA	O1D-CGD-O2D-CED
14	A	843	CLA	CBA-CGA-O2A-C1
14	a	843	CLA	CBA-CGA-O2A-C1
14	1	1644	CLA	CBA-CGA-O2A-C1
18	L	208	LHG	C8-C7-O7-C5
18	l	201	LHG	C8-C7-O7-C5
18	0	202	LHG	C8-C7-O7-C5
20	B	849	LMG	C11-C10-O7-C8
18	A	853	LHG	C15-C16-C17-C18
14	b	832	CLA	O1D-CGD-O2D-CED
18	A	853	LHG	C29-C30-C31-C32
18	a	853	LHG	C29-C30-C31-C32
18	1	1654	LHG	C29-C30-C31-C32
14	A	839	CLA	C5-C6-C7-C8
14	2	832	CLA	O1D-CGD-O2D-CED
18	M	101	LHG	C16-C17-C18-C19
18	m	101	LHG	C16-C17-C18-C19
18	y	101	LHG	C16-C17-C18-C19
14	A	803	CLA	C4-C3-C5-C6
14	a	803	CLA	C4-C3-C5-C6
14	1	1604	CLA	C4-C3-C5-C6
14	a	841	CLA	O1D-CGD-O2D-CED
14	A	804	CLA	C11-C10-C8-C7
14	A	805	CLA	C6-C7-C8-C10
14	A	806	CLA	C12-C13-C15-C16
14	A	820	CLA	C2-C3-C5-C6
14	A	825	CLA	C2-C3-C5-C6
14	A	830	CLA	C11-C12-C13-C15
14	A	833	CLA	C11-C12-C13-C15
14	A	834	CLA	C11-C10-C8-C7
14	A	834	CLA	C11-C12-C13-C15
14	A	836	CLA	C11-C10-C8-C7
14	B	802	CLA	C11-C12-C13-C15
14	B	805	CLA	C11-C10-C8-C7
14	B	810	CLA	C11-C12-C13-C15
14	B	827	CLA	C11-C12-C13-C15
14	B	838	CLA	C12-C13-C15-C16
14	a	804	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
14	a	805	CLA	C6-C7-C8-C10
14	a	806	CLA	C12-C13-C15-C16
14	a	820	CLA	C2-C3-C5-C6
14	a	830	CLA	C11-C12-C13-C15
14	a	833	CLA	C11-C12-C13-C15
14	a	834	CLA	C11-C10-C8-C7
14	a	834	CLA	C11-C12-C13-C15
14	a	836	CLA	C11-C10-C8-C7
14	b	803	CLA	C11-C12-C13-C15
14	b	806	CLA	C11-C10-C8-C7
14	b	811	CLA	C11-C12-C13-C15
14	b	828	CLA	C11-C12-C13-C15
14	b	839	CLA	C12-C13-C15-C16
14	1	1605	CLA	C11-C10-C8-C7
14	1	1606	CLA	C6-C7-C8-C10
14	1	1607	CLA	C12-C13-C15-C16
14	1	1621	CLA	C2-C3-C5-C6
14	1	1631	CLA	C11-C12-C13-C15
14	1	1634	CLA	C11-C12-C13-C15
14	1	1635	CLA	C11-C10-C8-C7
14	1	1635	CLA	C11-C12-C13-C15
14	1	1637	CLA	C11-C10-C8-C7
14	2	803	CLA	C11-C12-C13-C15
14	2	806	CLA	C11-C10-C8-C7
14	2	811	CLA	C11-C12-C13-C15
14	2	828	CLA	C11-C12-C13-C15
14	2	839	CLA	C12-C13-C15-C16
14	A	821	CLA	C3-C5-C6-C7
14	a	821	CLA	C3-C5-C6-C7
14	1	1622	CLA	C3-C5-C6-C7
14	A	828	CLA	C10-C11-C12-C13
14	A	838	CLA	C13-C15-C16-C17
14	B	825	CLA	C10-C11-C12-C13
14	a	828	CLA	C10-C11-C12-C13
14	a	838	CLA	C13-C15-C16-C17
14	a	839	CLA	C5-C6-C7-C8
14	b	826	CLA	C10-C11-C12-C13
14	1	1629	CLA	C10-C11-C12-C13
14	1	1639	CLA	C13-C15-C16-C17
14	1	1640	CLA	C5-C6-C7-C8
14	2	826	CLA	C10-C11-C12-C13
14	A	843	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	a	843	CLA	CBD-CGD-O2D-CED
14	1	1644	CLA	CBD-CGD-O2D-CED
14	B	815	CLA	C16-C17-C18-C20
14	b	816	CLA	C16-C17-C18-C20
14	2	816	CLA	C16-C17-C18-C20
14	A	837	CLA	O1D-CGD-O2D-CED
14	A	841	CLA	O1D-CGD-O2D-CED
14	a	837	CLA	O1D-CGD-O2D-CED
14	1	1638	CLA	O1D-CGD-O2D-CED
14	A	814	CLA	CBA-CGA-O2A-C1
14	B	832	CLA	CBA-CGA-O2A-C1
14	a	814	CLA	CBA-CGA-O2A-C1
14	b	833	CLA	CBA-CGA-O2A-C1
14	1	1615	CLA	CBA-CGA-O2A-C1
14	2	833	CLA	CBA-CGA-O2A-C1
18	A	854	LHG	C24-C23-O8-C6
18	a	854	LHG	C24-C23-O8-C6
18	1	1655	LHG	C24-C23-O8-C6
14	A	816	CLA	C2A-CAA-CBA-CGA
14	B	807	CLA	C2A-CAA-CBA-CGA
14	B	819	CLA	C2A-CAA-CBA-CGA
14	B	828	CLA	C2A-CAA-CBA-CGA
14	J	101	CLA	C2A-CAA-CBA-CGA
14	a	816	CLA	C2A-CAA-CBA-CGA
14	b	808	CLA	C2A-CAA-CBA-CGA
14	b	820	CLA	C2A-CAA-CBA-CGA
14	b	829	CLA	C2A-CAA-CBA-CGA
14	j	1302	CLA	C2A-CAA-CBA-CGA
14	1	1617	CLA	C2A-CAA-CBA-CGA
14	2	808	CLA	C2A-CAA-CBA-CGA
14	2	820	CLA	C2A-CAA-CBA-CGA
14	2	829	CLA	C2A-CAA-CBA-CGA
14	8	1302	CLA	C2A-CAA-CBA-CGA
14	1	1642	CLA	O1D-CGD-O2D-CED
14	A	819	CLA	C15-C16-C17-C18
14	A	826	CLA	C5-C6-C7-C8
14	a	819	CLA	C15-C16-C17-C18
14	a	826	CLA	C5-C6-C7-C8
14	1	1620	CLA	C15-C16-C17-C18
14	1	1627	CLA	C5-C6-C7-C8
14	b	819	CLA	C5-C6-C7-C8
14	2	819	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
17	A	848	BCR	C6-C7-C8-C9
17	B	848	BCR	C22-C23-C24-C25
17	I	101	BCR	C22-C23-C24-C25
17	a	848	BCR	C6-C7-C8-C9
17	b	849	BCR	C22-C23-C24-C25
17	i	101	BCR	C22-C23-C24-C25
17	1	1649	BCR	C6-C7-C8-C9
17	2	849	BCR	C22-C23-C24-C25
17	7	101	BCR	C22-C23-C24-C25
14	B	811	CLA	C5-C6-C7-C8
14	B	818	CLA	C5-C6-C7-C8
14	B	825	CLA	C5-C6-C7-C8
14	L	203	CLA	C8-C10-C11-C12
14	b	812	CLA	C5-C6-C7-C8
14	b	826	CLA	C5-C6-C7-C8
14	l	204	CLA	C8-C10-C11-C12
14	2	812	CLA	C5-C6-C7-C8
14	2	826	CLA	C5-C6-C7-C8
14	0	205	CLA	C8-C10-C11-C12
18	A	853	LHG	C8-C7-O7-C5
18	a	853	LHG	C8-C7-O7-C5
18	1	1654	LHG	C8-C7-O7-C5
20	b	850	LMG	C11-C10-O7-C8
20	2	850	LMG	C11-C10-O7-C8
17	B	848	BCR	C18-C19-C20-C21
17	L	206	BCR	C18-C19-C20-C21
17	b	849	BCR	C18-C19-C20-C21
17	l	207	BCR	C18-C19-C20-C21
17	2	849	BCR	C18-C19-C20-C21
17	0	208	BCR	C18-C19-C20-C21
17	F	202	BCR	C14-C15-C16-C17
17	L	206	BCR	C14-C15-C16-C17
17	f	202	BCR	C14-C15-C16-C17
17	l	207	BCR	C14-C15-C16-C17
17	0	208	BCR	C14-C15-C16-C17
14	B	816	CLA	C5-C6-C7-C8
14	b	817	CLA	C5-C6-C7-C8
14	1	1631	CLA	C5-C6-C7-C8
14	2	817	CLA	C5-C6-C7-C8
14	A	806	CLA	CBD-CGD-O2D-CED
14	a	806	CLA	CBD-CGD-O2D-CED
14	1	1607	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	A	854	LHG	C27-C28-C29-C30
18	a	854	LHG	C27-C28-C29-C30
18	1	1655	LHG	C27-C28-C29-C30
14	A	807	CLA	C3-C5-C6-C7
14	a	807	CLA	C3-C5-C6-C7
14	1	1608	CLA	C3-C5-C6-C7
18	A	854	LHG	O7-C5-C6-O8
18	a	854	LHG	O7-C5-C6-O8
18	1	1655	LHG	O7-C5-C6-O8
14	a	843	CLA	O1A-CGA-O2A-C1
14	1	1644	CLA	O1A-CGA-O2A-C1
14	B	818	CLA	C16-C17-C18-C19
14	b	819	CLA	C16-C17-C18-C19
14	2	819	CLA	C16-C17-C18-C19
14	A	830	CLA	C5-C6-C7-C8
14	a	830	CLA	C5-C6-C7-C8
18	z	101	LHG	C7-C8-C9-C10
14	A	803	CLA	C2-C3-C5-C6
14	L	205	CLA	C2-C3-C5-C6
14	a	803	CLA	C2-C3-C5-C6
14	l	206	CLA	C2-C3-C5-C6
14	1	1604	CLA	C2-C3-C5-C6
14	0	207	CLA	C2-C3-C5-C6
13	A	801	CL0	C11-C12-C13-C14
13	a	801	CL0	C11-C12-C13-C14
13	1	1602	CL0	C11-C12-C13-C14
14	A	804	CLA	C11-C10-C8-C9
14	A	824	CLA	C11-C10-C8-C9
14	A	827	CLA	C14-C13-C15-C16
14	A	834	CLA	C14-C13-C15-C16
14	B	805	CLA	C11-C10-C8-C9
14	B	810	CLA	C6-C7-C8-C9
14	B	827	CLA	C11-C12-C13-C14
14	B	838	CLA	C14-C13-C15-C16
14	L	203	CLA	C11-C10-C8-C9
14	L	203	CLA	C14-C13-C15-C16
14	a	804	CLA	C11-C10-C8-C9
14	a	824	CLA	C11-C10-C8-C9
14	a	827	CLA	C14-C13-C15-C16
14	a	834	CLA	C14-C13-C15-C16
14	b	806	CLA	C11-C10-C8-C9
14	b	811	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	b	828	CLA	C11-C12-C13-C14
14	b	839	CLA	C14-C13-C15-C16
14	l	204	CLA	C11-C10-C8-C9
14	l	204	CLA	C14-C13-C15-C16
14	1	1605	CLA	C11-C10-C8-C9
14	1	1625	CLA	C11-C10-C8-C9
14	1	1628	CLA	C14-C13-C15-C16
14	1	1635	CLA	C14-C13-C15-C16
14	2	806	CLA	C11-C10-C8-C9
14	2	811	CLA	C6-C7-C8-C9
14	2	828	CLA	C11-C12-C13-C14
14	2	839	CLA	C14-C13-C15-C16
14	0	205	CLA	C11-C10-C8-C9
14	0	205	CLA	C14-C13-C15-C16
14	B	818	CLA	CBD-CGD-O2D-CED
14	2	819	CLA	CBD-CGD-O2D-CED
14	A	843	CLA	O1A-CGA-O2A-C1
18	b	851	LHG	C7-C8-C9-C10
14	A	804	CLA	C1A-C2A-CAA-CBA
14	A	809	CLA	C1A-C2A-CAA-CBA
14	A	819	CLA	C1A-C2A-CAA-CBA
14	A	827	CLA	C1A-C2A-CAA-CBA
14	B	805	CLA	C1A-C2A-CAA-CBA
14	B	813	CLA	C1A-C2A-CAA-CBA
14	B	818	CLA	C1A-C2A-CAA-CBA
14	B	832	CLA	C1A-C2A-CAA-CBA
14	B	835	CLA	C1A-C2A-CAA-CBA
14	B	836	CLA	C1A-C2A-CAA-CBA
14	K	101	CLA	C1A-C2A-CAA-CBA
14	a	804	CLA	C1A-C2A-CAA-CBA
14	a	809	CLA	C1A-C2A-CAA-CBA
14	a	819	CLA	C1A-C2A-CAA-CBA
14	a	827	CLA	C1A-C2A-CAA-CBA
14	b	806	CLA	C1A-C2A-CAA-CBA
14	b	814	CLA	C1A-C2A-CAA-CBA
14	b	819	CLA	C1A-C2A-CAA-CBA
14	b	833	CLA	C1A-C2A-CAA-CBA
14	b	836	CLA	C1A-C2A-CAA-CBA
14	b	837	CLA	C1A-C2A-CAA-CBA
14	k	101	CLA	C1A-C2A-CAA-CBA
14	1	1605	CLA	C1A-C2A-CAA-CBA
14	1	1610	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	1	1620	CLA	C1A-C2A-CAA-CBA
14	1	1628	CLA	C1A-C2A-CAA-CBA
14	2	806	CLA	C1A-C2A-CAA-CBA
14	2	814	CLA	C1A-C2A-CAA-CBA
14	2	819	CLA	C1A-C2A-CAA-CBA
14	2	833	CLA	C1A-C2A-CAA-CBA
14	2	836	CLA	C1A-C2A-CAA-CBA
14	2	837	CLA	C1A-C2A-CAA-CBA
14	9	101	CLA	C1A-C2A-CAA-CBA
14	B	815	CLA	C16-C17-C18-C19
14	b	816	CLA	C16-C17-C18-C19
14	2	816	CLA	C16-C17-C18-C19
18	B	850	LHG	C4-O6-P-O3
18	b	851	LHG	C4-O6-P-O3
18	z	101	LHG	C4-O6-P-O3
18	B	850	LHG	C7-C8-C9-C10
18	l	201	LHG	C23-C24-C25-C26
14	b	819	CLA	CBD-CGD-O2D-CED
14	A	812	CLA	C5-C6-C7-C8
14	a	812	CLA	C5-C6-C7-C8
14	b	802	CLA	C8-C10-C11-C12
14	1	1613	CLA	C5-C6-C7-C8
18	L	208	LHG	C23-C24-C25-C26
18	0	202	LHG	C23-C24-C25-C26
14	A	855	CLA	C8-C10-C11-C12
14	2	802	CLA	C8-C10-C11-C12
14	A	819	CLA	C16-C17-C18-C19
14	a	819	CLA	C16-C17-C18-C19
14	1	1620	CLA	C16-C17-C18-C19
14	A	829	CLA	C3-C5-C6-C7
14	a	829	CLA	C3-C5-C6-C7
14	1	1630	CLA	C3-C5-C6-C7
14	A	838	CLA	C5-C6-C7-C8
14	a	838	CLA	C5-C6-C7-C8
14	1	1639	CLA	C5-C6-C7-C8
14	a	839	CLA	CBD-CGD-O2D-CED
18	1	1655	LHG	C10-C11-C12-C13
14	B	808	CLA	C8-C10-C11-C12
14	b	809	CLA	C8-C10-C11-C12
14	2	809	CLA	C8-C10-C11-C12
18	A	854	LHG	C10-C11-C12-C13
18	a	854	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
18	1	1655	LHG	C23-C24-C25-C26
14	A	814	CLA	O1A-CGA-O2A-C1
14	a	814	CLA	O1A-CGA-O2A-C1
14	1	1615	CLA	O1A-CGA-O2A-C1
14	j	1301	CLA	O1D-CGD-O2D-CED
18	A	854	LHG	C4-C5-C6-O8
18	B	850	LHG	C4-C5-C6-O8
18	M	101	LHG	C4-C5-C6-O8
18	a	854	LHG	C4-C5-C6-O8
18	b	851	LHG	C4-C5-C6-O8
18	m	101	LHG	C4-C5-C6-O8
18	1	1655	LHG	C4-C5-C6-O8
18	y	101	LHG	C4-C5-C6-O8
18	z	101	LHG	C4-C5-C6-O8
14	l	205	CLA	C2C-C3C-CAC-CBC
18	L	208	LHG	C25-C26-C27-C28
18	l	201	LHG	C25-C26-C27-C28
18	0	202	LHG	C25-C26-C27-C28
14	F	203	CLA	O1D-CGD-O2D-CED
14	8	1301	CLA	O1D-CGD-O2D-CED
14	A	839	CLA	CBD-CGD-O2D-CED
14	1	1640	CLA	CBD-CGD-O2D-CED
18	A	854	LHG	C11-C10-C9-C8
18	a	854	LHG	C11-C10-C9-C8
18	1	1655	LHG	C11-C10-C9-C8
18	A	854	LHG	C23-C24-C25-C26
18	a	854	LHG	C23-C24-C25-C26
14	2	833	CLA	O1A-CGA-O2A-C1
18	M	101	LHG	C31-C32-C33-C34
18	M	101	LHG	O1-C1-C2-O2
18	m	101	LHG	O1-C1-C2-O2
18	y	101	LHG	O1-C1-C2-O2
14	L	204	CLA	C2C-C3C-CAC-CBC
18	m	101	LHG	C31-C32-C33-C34
18	y	101	LHG	C31-C32-C33-C34
14	B	832	CLA	O1A-CGA-O2A-C1
18	M	101	LHG	C17-C18-C19-C20
18	m	101	LHG	C17-C18-C19-C20
18	y	101	LHG	C17-C18-C19-C20
14	0	206	CLA	C2C-C3C-CAC-CBC
17	B	851	BCR	C11-C10-C9-C34
17	L	207	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
17	b	852	BCR	C11-C10-C9-C34
17	8	1306	BCR	C11-C10-C9-C34
17	8	1306	BCR	C16-C17-C18-C36
17	0	201	BCR	C16-C17-C18-C36
17	0	209	BCR	C16-C17-C18-C36
14	B	808	CLA	C4-C3-C5-C6
14	L	205	CLA	C4-C3-C5-C6
14	b	809	CLA	C4-C3-C5-C6
14	l	206	CLA	C4-C3-C5-C6
14	2	809	CLA	C4-C3-C5-C6
14	0	207	CLA	C4-C3-C5-C6
14	b	833	CLA	O1A-CGA-O2A-C1
20	B	849	LMG	C29-C28-O8-C9
20	b	850	LMG	C29-C28-O8-C9
20	2	850	LMG	C29-C28-O8-C9
18	l	201	LHG	C19-C20-C21-C22
14	b	833	CLA	C15-C16-C17-C18
14	2	833	CLA	C15-C16-C17-C18
14	A	816	CLA	C2-C1-O2A-CGA
14	a	816	CLA	C2-C1-O2A-CGA
14	1	1617	CLA	C2-C1-O2A-CGA
18	L	208	LHG	C19-C20-C21-C22
18	0	202	LHG	C19-C20-C21-C22
14	A	842	CLA	O1D-CGD-O2D-CED
14	a	842	CLA	O1D-CGD-O2D-CED
14	1	1643	CLA	O1D-CGD-O2D-CED
14	B	832	CLA	C15-C16-C17-C18
14	A	840	CLA	CBA-CGA-O2A-C1
14	a	840	CLA	CBA-CGA-O2A-C1
14	1	1641	CLA	CBA-CGA-O2A-C1
18	L	208	LHG	O6-C4-C5-O7
18	l	201	LHG	O6-C4-C5-O7
18	0	202	LHG	O6-C4-C5-O7
14	A	824	CLA	C10-C11-C12-C13
14	a	824	CLA	C10-C11-C12-C13
14	1	1625	CLA	C10-C11-C12-C13
17	A	852	BCR	C12-C13-C14-C15
17	B	846	BCR	C16-C17-C18-C19
17	a	852	BCR	C12-C13-C14-C15
17	b	847	BCR	C16-C17-C18-C19
17	1	1653	BCR	C12-C13-C14-C15
17	2	847	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
18	A	853	LHG	O7-C5-C6-O8
18	B	850	LHG	O7-C5-C6-O8
18	a	853	LHG	O7-C5-C6-O8
18	1	1654	LHG	O7-C5-C6-O8
18	z	101	LHG	O7-C5-C6-O8
14	A	839	CLA	C16-C17-C18-C19
14	a	839	CLA	C16-C17-C18-C19
14	1	1640	CLA	C16-C17-C18-C19
18	A	853	LHG	C30-C31-C32-C33
18	a	853	LHG	C30-C31-C32-C33
18	1	1654	LHG	C30-C31-C32-C33
13	A	801	CL0	C12-C13-C15-C16
13	a	801	CL0	C12-C13-C15-C16
13	1	1602	CL0	C12-C13-C15-C16
14	A	807	CLA	C11-C12-C13-C15
14	A	821	CLA	C6-C7-C8-C10
14	A	821	CLA	C11-C12-C13-C15
14	A	824	CLA	C11-C10-C8-C7
14	A	827	CLA	C11-C10-C8-C7
14	A	827	CLA	C12-C13-C15-C16
14	A	832	CLA	C11-C10-C8-C7
14	A	833	CLA	C6-C7-C8-C10
14	A	834	CLA	C12-C13-C15-C16
14	A	839	CLA	C12-C13-C15-C16
14	A	840	CLA	C12-C13-C15-C16
14	A	841	CLA	C11-C12-C13-C15
14	B	802	CLA	C11-C10-C8-C7
14	B	803	CLA	C11-C12-C13-C15
14	B	804	CLA	C11-C12-C13-C15
14	B	804	CLA	C12-C13-C15-C16
14	B	806	CLA	C12-C13-C15-C16
14	B	810	CLA	C12-C13-C15-C16
14	B	819	CLA	C11-C12-C13-C15
14	B	820	CLA	C11-C10-C8-C7
14	B	833	CLA	C6-C7-C8-C10
14	B	833	CLA	C11-C10-C8-C7
14	B	841	CLA	C11-C12-C13-C15
14	L	203	CLA	C11-C10-C8-C7
14	L	203	CLA	C12-C13-C15-C16
14	a	807	CLA	C11-C12-C13-C15
14	a	821	CLA	C6-C7-C8-C10
14	a	821	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
14	a	824	CLA	C11-C10-C8-C7
14	a	827	CLA	C11-C10-C8-C7
14	a	827	CLA	C12-C13-C15-C16
14	a	832	CLA	C11-C10-C8-C7
14	a	833	CLA	C6-C7-C8-C10
14	a	834	CLA	C12-C13-C15-C16
14	a	839	CLA	C12-C13-C15-C16
14	a	840	CLA	C12-C13-C15-C16
14	a	841	CLA	C11-C12-C13-C15
14	b	803	CLA	C11-C10-C8-C7
14	b	804	CLA	C11-C12-C13-C15
14	b	805	CLA	C11-C12-C13-C15
14	b	805	CLA	C12-C13-C15-C16
14	b	807	CLA	C12-C13-C15-C16
14	b	811	CLA	C12-C13-C15-C16
14	b	820	CLA	C11-C12-C13-C15
14	b	821	CLA	C11-C10-C8-C7
14	b	834	CLA	C6-C7-C8-C10
14	b	834	CLA	C11-C10-C8-C7
14	b	842	CLA	C11-C12-C13-C15
14	l	204	CLA	C11-C10-C8-C7
14	l	204	CLA	C12-C13-C15-C16
14	1	1608	CLA	C11-C12-C13-C15
14	1	1622	CLA	C6-C7-C8-C10
14	1	1622	CLA	C11-C12-C13-C15
14	1	1625	CLA	C11-C10-C8-C7
14	1	1628	CLA	C11-C10-C8-C7
14	1	1628	CLA	C12-C13-C15-C16
14	1	1633	CLA	C11-C10-C8-C7
14	1	1634	CLA	C6-C7-C8-C10
14	1	1635	CLA	C12-C13-C15-C16
14	1	1640	CLA	C12-C13-C15-C16
14	1	1641	CLA	C12-C13-C15-C16
14	1	1642	CLA	C11-C12-C13-C15
14	2	803	CLA	C11-C10-C8-C7
14	2	804	CLA	C11-C12-C13-C15
14	2	805	CLA	C11-C12-C13-C15
14	2	805	CLA	C12-C13-C15-C16
14	2	807	CLA	C12-C13-C15-C16
14	2	811	CLA	C12-C13-C15-C16
14	2	820	CLA	C11-C12-C13-C15
14	2	821	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
14	2	834	CLA	C6-C7-C8-C10
14	2	834	CLA	C11-C10-C8-C7
14	2	842	CLA	C11-C12-C13-C15
14	0	205	CLA	C11-C10-C8-C7
14	0	205	CLA	C12-C13-C15-C16
18	B	850	LHG	C10-C11-C12-C13
14	A	802	CLA	C14-C13-C15-C16
14	A	806	CLA	C6-C7-C8-C9
14	A	806	CLA	C11-C12-C13-C14
14	A	807	CLA	C11-C12-C13-C14
14	A	821	CLA	C11-C12-C13-C14
14	A	822	CLA	C6-C7-C8-C9
14	A	825	CLA	C11-C10-C8-C9
14	A	827	CLA	C11-C10-C8-C9
14	A	830	CLA	C14-C13-C15-C16
14	A	832	CLA	C11-C10-C8-C9
14	A	833	CLA	C6-C7-C8-C9
14	A	835	CLA	C14-C13-C15-C16
14	A	839	CLA	C11-C12-C13-C14
14	A	840	CLA	C6-C7-C8-C9
14	A	841	CLA	C11-C12-C13-C14
14	A	841	CLA	C14-C13-C15-C16
14	A	843	CLA	C6-C7-C8-C9
14	A	843	CLA	C14-C13-C15-C16
14	B	802	CLA	C11-C10-C8-C9
14	B	804	CLA	C6-C7-C8-C9
14	B	804	CLA	C14-C13-C15-C16
14	B	806	CLA	C14-C13-C15-C16
14	B	811	CLA	C11-C12-C13-C14
14	B	816	CLA	C11-C12-C13-C14
14	B	817	CLA	C11-C12-C13-C14
14	B	819	CLA	C11-C12-C13-C14
14	B	832	CLA	C14-C13-C15-C16
14	B	833	CLA	C6-C7-C8-C9
14	B	833	CLA	C11-C10-C8-C9
14	B	840	CLA	C11-C12-C13-C14
14	B	841	CLA	C11-C12-C13-C14
14	L	205	CLA	C6-C7-C8-C9
14	a	802	CLA	C14-C13-C15-C16
14	a	806	CLA	C6-C7-C8-C9
14	a	806	CLA	C11-C12-C13-C14
14	a	807	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
14	a	821	CLA	C11-C12-C13-C14
14	a	822	CLA	C6-C7-C8-C9
14	a	825	CLA	C11-C10-C8-C9
14	a	827	CLA	C11-C10-C8-C9
14	a	830	CLA	C14-C13-C15-C16
14	a	832	CLA	C11-C10-C8-C9
14	a	833	CLA	C6-C7-C8-C9
14	a	835	CLA	C14-C13-C15-C16
14	a	839	CLA	C11-C12-C13-C14
14	a	840	CLA	C6-C7-C8-C9
14	a	841	CLA	C11-C12-C13-C14
14	a	841	CLA	C14-C13-C15-C16
14	a	843	CLA	C6-C7-C8-C9
14	a	843	CLA	C14-C13-C15-C16
14	b	803	CLA	C11-C10-C8-C9
14	b	805	CLA	C6-C7-C8-C9
14	b	805	CLA	C14-C13-C15-C16
14	b	807	CLA	C14-C13-C15-C16
14	b	812	CLA	C11-C12-C13-C14
14	b	817	CLA	C11-C12-C13-C14
14	b	818	CLA	C11-C12-C13-C14
14	b	820	CLA	C11-C12-C13-C14
14	b	833	CLA	C14-C13-C15-C16
14	b	834	CLA	C6-C7-C8-C9
14	b	834	CLA	C11-C10-C8-C9
14	b	841	CLA	C11-C12-C13-C14
14	b	842	CLA	C11-C12-C13-C14
14	l	206	CLA	C6-C7-C8-C9
14	1	1603	CLA	C14-C13-C15-C16
14	1	1607	CLA	C6-C7-C8-C9
14	1	1607	CLA	C11-C12-C13-C14
14	1	1608	CLA	C11-C12-C13-C14
14	1	1622	CLA	C11-C12-C13-C14
14	1	1623	CLA	C6-C7-C8-C9
14	1	1626	CLA	C11-C10-C8-C9
14	1	1628	CLA	C11-C10-C8-C9
14	1	1631	CLA	C14-C13-C15-C16
14	1	1633	CLA	C11-C10-C8-C9
14	1	1634	CLA	C6-C7-C8-C9
14	1	1636	CLA	C14-C13-C15-C16
14	1	1640	CLA	C11-C12-C13-C14
14	1	1641	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	1	1642	CLA	C11-C12-C13-C14
14	1	1642	CLA	C14-C13-C15-C16
14	1	1644	CLA	C6-C7-C8-C9
14	1	1644	CLA	C14-C13-C15-C16
14	2	803	CLA	C11-C10-C8-C9
14	2	805	CLA	C6-C7-C8-C9
14	2	805	CLA	C14-C13-C15-C16
14	2	807	CLA	C14-C13-C15-C16
14	2	812	CLA	C11-C12-C13-C14
14	2	817	CLA	C11-C12-C13-C14
14	2	818	CLA	C11-C12-C13-C14
14	2	820	CLA	C11-C12-C13-C14
14	2	833	CLA	C14-C13-C15-C16
14	2	834	CLA	C6-C7-C8-C9
14	2	834	CLA	C11-C10-C8-C9
14	2	841	CLA	C11-C12-C13-C14
14	2	842	CLA	C11-C12-C13-C14
14	0	206	CLA	C14-C13-C15-C16
14	0	207	CLA	C6-C7-C8-C9
18	b	851	LHG	C10-C11-C12-C13
18	z	101	LHG	C10-C11-C12-C13
14	A	832	CLA	CBA-CGA-O2A-C1
14	a	832	CLA	CBA-CGA-O2A-C1
14	1	1633	CLA	CBA-CGA-O2A-C1
14	A	817	CLA	C5-C6-C7-C8
14	a	817	CLA	C5-C6-C7-C8
14	1	1618	CLA	C5-C6-C7-C8
17	A	849	BCR	C36-C18-C19-C20
17	B	844	BCR	C37-C22-C23-C24
17	a	849	BCR	C36-C18-C19-C20
17	b	845	BCR	C37-C22-C23-C24
17	1	1650	BCR	C36-C18-C19-C20
17	2	845	BCR	C37-C22-C23-C24
14	A	855	CLA	C3-C5-C6-C7
14	b	802	CLA	C3-C5-C6-C7
14	2	802	CLA	C3-C5-C6-C7
14	B	829	CLA	C10-C11-C12-C13
14	b	830	CLA	C10-C11-C12-C13
14	2	830	CLA	C10-C11-C12-C13
14	B	841	CLA	CBA-CGA-O2A-C1
14	b	842	CLA	CBA-CGA-O2A-C1
14	2	842	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	A	826	CLA	C13-C15-C16-C17
14	a	826	CLA	C13-C15-C16-C17
14	1	1627	CLA	C13-C15-C16-C17
17	B	845	BCR	C22-C23-C24-C25
17	b	846	BCR	C22-C23-C24-C25
17	2	846	BCR	C22-C23-C24-C25
13	A	801	CL0	C4B-C3B-CAB-CBB
13	a	801	CL0	C4B-C3B-CAB-CBB
13	1	1602	CL0	C4B-C3B-CAB-CBB
14	A	814	CLA	C4B-C3B-CAB-CBB
14	B	807	CLA	C4B-C3B-CAB-CBB
14	B	835	CLA	C4B-C3B-CAB-CBB
14	B	840	CLA	C4B-C3B-CAB-CBB
14	a	814	CLA	C4B-C3B-CAB-CBB
14	b	808	CLA	C4B-C3B-CAB-CBB
14	b	836	CLA	C4B-C3B-CAB-CBB
14	b	841	CLA	C4B-C3B-CAB-CBB
14	1	1615	CLA	C4B-C3B-CAB-CBB
14	2	808	CLA	C4B-C3B-CAB-CBB
14	2	836	CLA	C4B-C3B-CAB-CBB
14	2	841	CLA	C4B-C3B-CAB-CBB
14	A	838	CLA	C15-C16-C17-C18
15	B	842	PQN	C18-C20-C21-C22
15	b	843	PQN	C18-C20-C21-C22
15	2	843	PQN	C18-C20-C21-C22
14	B	808	CLA	C2-C3-C5-C6
14	b	809	CLA	C2-C3-C5-C6
14	2	809	CLA	C2-C3-C5-C6
14	B	838	CLA	C8-C10-C11-C12
14	a	838	CLA	C15-C16-C17-C18
14	1	1639	CLA	C15-C16-C17-C18
14	2	839	CLA	C8-C10-C11-C12
14	b	839	CLA	C8-C10-C11-C12
14	F	204	CLA	CBA-CGA-O2A-C1
14	f	203	CLA	CBA-CGA-O2A-C1
14	6	203	CLA	CBA-CGA-O2A-C1
14	B	802	CLA	CAA-CBA-CGA-O2A
14	b	803	CLA	CAA-CBA-CGA-O2A
14	2	803	CLA	CAA-CBA-CGA-O2A
18	z	101	LHG	C29-C30-C31-C32
14	b	815	CLA	O1D-CGD-O2D-CED
14	A	815	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	A	819	CLA	C3A-C2A-CAA-CBA
14	A	824	CLA	C3A-C2A-CAA-CBA
14	A	827	CLA	C3A-C2A-CAA-CBA
14	A	830	CLA	C3A-C2A-CAA-CBA
14	B	809	CLA	C3A-C2A-CAA-CBA
14	B	831	CLA	C3A-C2A-CAA-CBA
14	B	834	CLA	C3A-C2A-CAA-CBA
14	a	815	CLA	C3A-C2A-CAA-CBA
14	a	819	CLA	C3A-C2A-CAA-CBA
14	a	824	CLA	C3A-C2A-CAA-CBA
14	a	827	CLA	C3A-C2A-CAA-CBA
14	a	830	CLA	C3A-C2A-CAA-CBA
14	b	810	CLA	C3A-C2A-CAA-CBA
14	b	832	CLA	C3A-C2A-CAA-CBA
14	b	835	CLA	C3A-C2A-CAA-CBA
14	1	1616	CLA	C3A-C2A-CAA-CBA
14	1	1620	CLA	C3A-C2A-CAA-CBA
14	1	1625	CLA	C3A-C2A-CAA-CBA
14	1	1628	CLA	C3A-C2A-CAA-CBA
14	1	1631	CLA	C3A-C2A-CAA-CBA
14	2	810	CLA	C3A-C2A-CAA-CBA
14	2	832	CLA	C3A-C2A-CAA-CBA
14	2	835	CLA	C3A-C2A-CAA-CBA
18	b	851	LHG	C29-C30-C31-C32
18	B	850	LHG	C29-C30-C31-C32
14	2	815	CLA	O1D-CGD-O2D-CED
14	A	822	CLA	CBA-CGA-O2A-C1
14	a	822	CLA	CBA-CGA-O2A-C1
14	1	1623	CLA	CBA-CGA-O2A-C1
18	L	208	LHG	C4-C5-C6-O8
18	l	201	LHG	C4-C5-C6-O8
18	0	202	LHG	C4-C5-C6-O8
14	L	205	CLA	O2A-C1-C2-C3
14	l	206	CLA	O2A-C1-C2-C3
14	0	207	CLA	O2A-C1-C2-C3
14	B	814	CLA	O1D-CGD-O2D-CED
14	A	843	CLA	C4-C3-C5-C6
14	a	843	CLA	C4-C3-C5-C6
14	1	1644	CLA	C4-C3-C5-C6
18	y	101	LHG	C10-C11-C12-C13
18	M	101	LHG	C10-C11-C12-C13
18	m	101	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	A	827	CLA	CBA-CGA-O2A-C1
14	a	827	CLA	CBA-CGA-O2A-C1
14	1	1628	CLA	CBA-CGA-O2A-C1
14	A	820	CLA	O1D-CGD-O2D-CED
14	A	843	CLA	O1D-CGD-O2D-CED
14	A	840	CLA	O1A-CGA-O2A-C1
14	a	840	CLA	O1A-CGA-O2A-C1
14	1	1641	CLA	O1A-CGA-O2A-C1
14	1	1644	CLA	O1D-CGD-O2D-CED
14	B	835	CLA	C2B-C3B-CAB-CBB
14	B	840	CLA	C2B-C3B-CAB-CBB
14	b	836	CLA	C2B-C3B-CAB-CBB
14	b	841	CLA	C2B-C3B-CAB-CBB
14	2	836	CLA	C2B-C3B-CAB-CBB
14	2	841	CLA	C2B-C3B-CAB-CBB
14	a	843	CLA	O1D-CGD-O2D-CED
14	B	814	CLA	C13-C15-C16-C17
14	b	815	CLA	C13-C15-C16-C17
14	2	815	CLA	C13-C15-C16-C17
18	M	101	LHG	O7-C5-C6-O8
18	b	851	LHG	O7-C5-C6-O8
18	m	101	LHG	O7-C5-C6-O8
18	y	101	LHG	O7-C5-C6-O8
14	1	1621	CLA	O1D-CGD-O2D-CED
18	L	208	LHG	C18-C19-C20-C21
18	0	202	LHG	C18-C19-C20-C21
14	A	829	CLA	C16-C17-C18-C20
14	a	829	CLA	C16-C17-C18-C20
14	1	1630	CLA	C16-C17-C18-C20
18	l	201	LHG	C18-C19-C20-C21
14	B	804	CLA	C13-C15-C16-C17
14	A	810	CLA	C4-C3-C5-C6
14	a	810	CLA	C4-C3-C5-C6
14	1	1611	CLA	C4-C3-C5-C6
14	A	817	CLA	C2-C1-O2A-CGA
14	A	843	CLA	C2-C1-O2A-CGA
14	A	855	CLA	C2-C1-O2A-CGA
14	B	820	CLA	C2-C1-O2A-CGA
14	a	817	CLA	C2-C1-O2A-CGA
14	a	843	CLA	C2-C1-O2A-CGA
14	b	802	CLA	C2-C1-O2A-CGA
14	b	821	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
14	1	1618	CLA	C2-C1-O2A-CGA
14	1	1644	CLA	C2-C1-O2A-CGA
14	2	802	CLA	C2-C1-O2A-CGA
14	2	821	CLA	C2-C1-O2A-CGA
14	a	820	CLA	O1D-CGD-O2D-CED
14	B	802	CLA	C13-C15-C16-C17
14	b	803	CLA	C13-C15-C16-C17
14	2	803	CLA	C13-C15-C16-C17
14	2	805	CLA	C13-C15-C16-C17
14	A	815	CLA	C14-C13-C15-C16
14	A	819	CLA	C14-C13-C15-C16
14	A	836	CLA	C11-C12-C13-C14
14	A	839	CLA	C14-C13-C15-C16
14	A	841	CLA	C11-C10-C8-C9
14	A	855	CLA	C6-C7-C8-C9
14	B	814	CLA	C11-C10-C8-C9
14	B	820	CLA	C11-C10-C8-C9
14	B	828	CLA	C11-C12-C13-C14
14	L	204	CLA	C14-C13-C15-C16
14	a	815	CLA	C14-C13-C15-C16
14	a	819	CLA	C14-C13-C15-C16
14	a	836	CLA	C11-C12-C13-C14
14	a	839	CLA	C14-C13-C15-C16
14	a	841	CLA	C11-C10-C8-C9
14	b	802	CLA	C6-C7-C8-C9
14	b	821	CLA	C11-C10-C8-C9
14	b	829	CLA	C11-C12-C13-C14
14	l	205	CLA	C14-C13-C15-C16
14	1	1616	CLA	C14-C13-C15-C16
14	1	1620	CLA	C14-C13-C15-C16
14	1	1637	CLA	C11-C12-C13-C14
14	1	1640	CLA	C14-C13-C15-C16
14	1	1642	CLA	C11-C10-C8-C9
14	2	802	CLA	C6-C7-C8-C9
14	2	815	CLA	C11-C10-C8-C9
14	2	821	CLA	C11-C10-C8-C9
14	2	826	CLA	C11-C10-C8-C9
14	2	829	CLA	C11-C12-C13-C14
18	L	208	LHG	C16-C17-C18-C19
18	l	201	LHG	C16-C17-C18-C19
18	0	202	LHG	C16-C17-C18-C19
20	B	849	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
20	b	850	LMG	C38-C39-C40-C41
20	2	850	LMG	C38-C39-C40-C41
14	A	814	CLA	C10-C11-C12-C13
14	B	806	CLA	C15-C16-C17-C18
14	B	820	CLA	C15-C16-C17-C18
14	b	805	CLA	C13-C15-C16-C17
14	b	807	CLA	C15-C16-C17-C18
14	b	821	CLA	C15-C16-C17-C18
14	2	807	CLA	C15-C16-C17-C18
14	2	821	CLA	C15-C16-C17-C18
18	L	208	LHG	C5-C4-O6-P
18	l	201	LHG	C5-C4-O6-P
18	0	202	LHG	C5-C4-O6-P
14	A	829	CLA	C2A-CAA-CBA-CGA
14	a	829	CLA	C2A-CAA-CBA-CGA
14	1	1630	CLA	C2A-CAA-CBA-CGA
14	L	204	CLA	C16-C17-C18-C20
14	l	205	CLA	C16-C17-C18-C20
14	0	206	CLA	C16-C17-C18-C20
17	A	852	BCR	C1-C6-C7-C8
17	A	852	BCR	C5-C6-C7-C8
17	B	846	BCR	C23-C24-C25-C26
17	B	848	BCR	C1-C6-C7-C8
17	B	848	BCR	C5-C6-C7-C8
17	B	851	BCR	C23-C24-C25-C26
17	B	851	BCR	C23-C24-C25-C30
17	F	202	BCR	C23-C24-C25-C26
17	F	202	BCR	C23-C24-C25-C30
17	F	205	BCR	C1-C6-C7-C8
17	L	201	BCR	C23-C24-C25-C26
17	L	207	BCR	C1-C6-C7-C8
17	L	207	BCR	C5-C6-C7-C8
17	a	852	BCR	C1-C6-C7-C8
17	a	852	BCR	C5-C6-C7-C8
17	b	847	BCR	C23-C24-C25-C26
17	b	849	BCR	C1-C6-C7-C8
17	b	849	BCR	C5-C6-C7-C8
17	b	852	BCR	C23-C24-C25-C26
17	b	852	BCR	C23-C24-C25-C30
17	f	202	BCR	C23-C24-C25-C26
17	f	202	BCR	C23-C24-C25-C30
17	f	204	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
17	l	202	BCR	C23-C24-C25-C26
17	1	1653	BCR	C1-C6-C7-C8
17	1	1653	BCR	C5-C6-C7-C8
17	2	847	BCR	C23-C24-C25-C26
17	2	849	BCR	C1-C6-C7-C8
17	2	849	BCR	C5-C6-C7-C8
17	6	202	BCR	C23-C24-C25-C26
17	6	202	BCR	C23-C24-C25-C30
17	6	204	BCR	C1-C6-C7-C8
17	8	1306	BCR	C23-C24-C25-C26
17	8	1306	BCR	C23-C24-C25-C30
17	0	201	BCR	C1-C6-C7-C8
17	0	201	BCR	C5-C6-C7-C8
17	0	203	BCR	C23-C24-C25-C26
17	0	209	BCR	C1-C6-C7-C8
17	0	209	BCR	C5-C6-C7-C8
14	a	814	CLA	C10-C11-C12-C13
17	L	207	BCR	C37-C22-C23-C24
17	0	201	BCR	C37-C22-C23-C24
17	0	209	BCR	C37-C22-C23-C24
17	A	851	BCR	C7-C8-C9-C10
17	A	852	BCR	C16-C17-C18-C19
17	A	856	BCR	C7-C8-C9-C10
17	B	851	BCR	C7-C8-C9-C10
17	K	104	BCR	C16-C17-C18-C36
17	a	851	BCR	C7-C8-C9-C10
17	a	852	BCR	C16-C17-C18-C19
17	b	852	BCR	C7-C8-C9-C10
17	j	1305	BCR	C7-C8-C9-C10
17	k	104	BCR	C16-C17-C18-C36
17	1	1652	BCR	C7-C8-C9-C10
17	1	1653	BCR	C16-C17-C18-C19
17	8	1305	BCR	C7-C8-C9-C10
17	8	1306	BCR	C7-C8-C9-C10
17	9	104	BCR	C16-C17-C18-C36
14	1	1615	CLA	C10-C11-C12-C13
18	L	208	LHG	C11-C12-C13-C14
18	l	201	LHG	C11-C12-C13-C14
18	0	202	LHG	C11-C12-C13-C14
14	A	832	CLA	O1A-CGA-O2A-C1
14	A	840	CLA	C16-C17-C18-C20
14	B	804	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
14	a	840	CLA	C16-C17-C18-C20
14	b	805	CLA	C16-C17-C18-C20
14	1	1641	CLA	C16-C17-C18-C20
14	2	805	CLA	C16-C17-C18-C20
14	a	832	CLA	O1A-CGA-O2A-C1
14	1	1633	CLA	O1A-CGA-O2A-C1
14	B	839	CLA	O1D-CGD-O2D-CED
14	b	840	CLA	O1D-CGD-O2D-CED
14	2	840	CLA	O1D-CGD-O2D-CED
18	L	208	LHG	O6-C4-C5-C6
18	l	201	LHG	O6-C4-C5-C6
18	0	202	LHG	O6-C4-C5-C6
14	A	804	CLA	C6-C7-C8-C10
14	A	806	CLA	C11-C10-C8-C7
14	A	806	CLA	C11-C12-C13-C15
14	A	810	CLA	C2-C3-C5-C6
14	A	810	CLA	C11-C12-C13-C15
14	A	815	CLA	C12-C13-C15-C16
14	A	819	CLA	C12-C13-C15-C16
14	A	825	CLA	C11-C10-C8-C7
14	A	825	CLA	C12-C13-C15-C16
14	A	826	CLA	C12-C13-C15-C16
14	A	830	CLA	C12-C13-C15-C16
14	A	833	CLA	C12-C13-C15-C16
14	A	835	CLA	C12-C13-C15-C16
14	A	836	CLA	C11-C12-C13-C15
14	A	839	CLA	C11-C12-C13-C15
14	A	840	CLA	C11-C12-C13-C15
14	A	841	CLA	C11-C10-C8-C7
14	A	842	CLA	C11-C10-C8-C7
14	A	843	CLA	C6-C7-C8-C10
14	A	843	CLA	C12-C13-C15-C16
14	B	803	CLA	C6-C7-C8-C10
14	B	804	CLA	C6-C7-C8-C10
14	B	811	CLA	C11-C12-C13-C15
14	B	813	CLA	C11-C10-C8-C7
14	B	814	CLA	C6-C7-C8-C10
14	B	817	CLA	C11-C12-C13-C15
14	B	819	CLA	C6-C7-C8-C10
14	B	832	CLA	C12-C13-C15-C16
14	B	837	CLA	C11-C10-C8-C7
14	B	840	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
14	L	204	CLA	C12-C13-C15-C16
14	a	804	CLA	C6-C7-C8-C10
14	a	806	CLA	C11-C10-C8-C7
14	a	806	CLA	C11-C12-C13-C15
14	a	810	CLA	C2-C3-C5-C6
14	a	810	CLA	C11-C12-C13-C15
14	a	815	CLA	C12-C13-C15-C16
14	a	819	CLA	C12-C13-C15-C16
14	a	825	CLA	C11-C10-C8-C7
14	a	825	CLA	C12-C13-C15-C16
14	a	826	CLA	C12-C13-C15-C16
14	a	830	CLA	C12-C13-C15-C16
14	a	833	CLA	C12-C13-C15-C16
14	a	835	CLA	C12-C13-C15-C16
14	a	836	CLA	C11-C12-C13-C15
14	a	839	CLA	C11-C12-C13-C15
14	a	840	CLA	C11-C12-C13-C15
14	a	841	CLA	C11-C10-C8-C7
14	a	842	CLA	C11-C10-C8-C7
14	a	843	CLA	C6-C7-C8-C10
14	a	843	CLA	C12-C13-C15-C16
14	b	804	CLA	C6-C7-C8-C10
14	b	805	CLA	C6-C7-C8-C10
14	b	812	CLA	C11-C12-C13-C15
14	b	814	CLA	C11-C10-C8-C7
14	b	815	CLA	C6-C7-C8-C10
14	b	818	CLA	C11-C12-C13-C15
14	b	820	CLA	C6-C7-C8-C10
14	b	833	CLA	C12-C13-C15-C16
14	b	838	CLA	C11-C10-C8-C7
14	b	841	CLA	C11-C12-C13-C15
14	l	205	CLA	C12-C13-C15-C16
14	1	1605	CLA	C6-C7-C8-C10
14	1	1607	CLA	C11-C10-C8-C7
14	1	1607	CLA	C11-C12-C13-C15
14	1	1611	CLA	C2-C3-C5-C6
14	1	1611	CLA	C11-C12-C13-C15
14	1	1616	CLA	C12-C13-C15-C16
14	1	1620	CLA	C12-C13-C15-C16
14	1	1626	CLA	C11-C10-C8-C7
14	1	1626	CLA	C12-C13-C15-C16
14	1	1627	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	1	1631	CLA	C12-C13-C15-C16
14	1	1634	CLA	C12-C13-C15-C16
14	1	1636	CLA	C12-C13-C15-C16
14	1	1637	CLA	C11-C12-C13-C15
14	1	1640	CLA	C11-C12-C13-C15
14	1	1641	CLA	C11-C12-C13-C15
14	1	1642	CLA	C11-C10-C8-C7
14	1	1643	CLA	C11-C10-C8-C7
14	1	1644	CLA	C6-C7-C8-C10
14	1	1644	CLA	C12-C13-C15-C16
14	2	804	CLA	C6-C7-C8-C10
14	2	805	CLA	C6-C7-C8-C10
14	2	812	CLA	C11-C12-C13-C15
14	2	814	CLA	C11-C10-C8-C7
14	2	815	CLA	C6-C7-C8-C10
14	2	818	CLA	C11-C12-C13-C15
14	2	820	CLA	C6-C7-C8-C10
14	2	833	CLA	C12-C13-C15-C16
14	2	838	CLA	C11-C10-C8-C7
14	2	841	CLA	C11-C12-C13-C15
14	0	206	CLA	C12-C13-C15-C16
14	1	1623	CLA	O1A-CGA-O2A-C1
14	A	822	CLA	C15-C16-C17-C18
14	a	822	CLA	C15-C16-C17-C18
17	A	852	BCR	C13-C14-C15-C16
17	B	851	BCR	C9-C10-C11-C12
17	K	102	BCR	C9-C10-C11-C12
17	a	852	BCR	C13-C14-C15-C16
17	b	852	BCR	C9-C10-C11-C12
17	k	102	BCR	C9-C10-C11-C12
17	1	1653	BCR	C13-C14-C15-C16
17	8	1306	BCR	C9-C10-C11-C12
17	9	102	BCR	C9-C10-C11-C12
14	A	831	CLA	CBA-CGA-O2A-C1
14	a	831	CLA	CBA-CGA-O2A-C1
14	1	1632	CLA	CBA-CGA-O2A-C1
14	1	1623	CLA	C15-C16-C17-C18
13	a	801	CL0	CAA-CBA-CGA-O2A
13	1	1602	CL0	CAA-CBA-CGA-O2A
14	A	822	CLA	O1A-CGA-O2A-C1
14	B	841	CLA	O1A-CGA-O2A-C1
14	a	822	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	b	842	CLA	O1A-CGA-O2A-C1
14	A	811	CLA	C2A-CAA-CBA-CGA
14	B	831	CLA	C2A-CAA-CBA-CGA
14	a	811	CLA	C2A-CAA-CBA-CGA
14	1	1612	CLA	C2A-CAA-CBA-CGA
17	A	852	BCR	C11-C10-C9-C34
17	A	852	BCR	C35-C13-C14-C15
17	A	856	BCR	C11-C10-C9-C34
17	B	844	BCR	C20-C21-C22-C37
17	B	848	BCR	C20-C21-C22-C37
17	K	104	BCR	C11-C10-C9-C34
17	a	852	BCR	C11-C10-C9-C34
17	a	852	BCR	C35-C13-C14-C15
17	b	845	BCR	C20-C21-C22-C37
17	b	849	BCR	C20-C21-C22-C37
17	j	1305	BCR	C11-C10-C9-C34
17	k	104	BCR	C11-C10-C9-C34
17	1	1653	BCR	C11-C10-C9-C34
17	1	1653	BCR	C35-C13-C14-C15
17	2	845	BCR	C20-C21-C22-C37
17	2	849	BCR	C20-C21-C22-C37
17	8	1305	BCR	C11-C10-C9-C34
17	9	104	BCR	C11-C10-C9-C34
18	a	854	LHG	C31-C32-C33-C34
18	1	1655	LHG	C31-C32-C33-C34
20	B	849	LMG	C30-C31-C32-C33
20	b	850	LMG	C30-C31-C32-C33
20	2	850	LMG	C30-C31-C32-C33
14	2	842	CLA	O1A-CGA-O2A-C1
14	A	807	CLA	C16-C17-C18-C19
14	A	807	CLA	C16-C17-C18-C20
14	A	842	CLA	C16-C17-C18-C20
14	a	807	CLA	C16-C17-C18-C19
14	a	807	CLA	C16-C17-C18-C20
14	a	842	CLA	C16-C17-C18-C20
14	1	1608	CLA	C16-C17-C18-C19
14	1	1608	CLA	C16-C17-C18-C20
14	1	1643	CLA	C16-C17-C18-C20
14	A	818	CLA	C8-C10-C11-C12
14	B	834	CLA	C5-C6-C7-C8
14	a	818	CLA	C8-C10-C11-C12
14	b	835	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	1	1619	CLA	C8-C10-C11-C12
14	2	835	CLA	C5-C6-C7-C8
13	A	801	CL0	CAA-CBA-CGA-O2A
18	A	854	LHG	C31-C32-C33-C34
14	B	827	CLA	C8-C10-C11-C12
14	a	839	CLA	C8-C10-C11-C12
14	b	828	CLA	C8-C10-C11-C12
14	1	1640	CLA	C8-C10-C11-C12
14	2	828	CLA	C8-C10-C11-C12
14	A	855	CLA	CBD-CGD-O2D-CED
14	2	802	CLA	CBD-CGD-O2D-CED
14	A	815	CLA	CAD-CBD-CGD-O2D
14	A	840	CLA	CAD-CBD-CGD-O2D
14	A	855	CLA	CAD-CBD-CGD-O2D
14	B	806	CLA	CAD-CBD-CGD-O2D
14	K	101	CLA	CAD-CBD-CGD-O2D
14	a	815	CLA	CAD-CBD-CGD-O2D
14	a	840	CLA	CAD-CBD-CGD-O2D
14	b	802	CLA	CAD-CBD-CGD-O2D
14	b	807	CLA	CAD-CBD-CGD-O2D
14	k	101	CLA	CAD-CBD-CGD-O2D
14	1	1616	CLA	CAD-CBD-CGD-O2D
14	1	1641	CLA	CAD-CBD-CGD-O2D
14	2	802	CLA	CAD-CBD-CGD-O2D
14	2	807	CLA	CAD-CBD-CGD-O2D
14	9	101	CLA	CAD-CBD-CGD-O2D
14	A	839	CLA	C8-C10-C11-C12
17	I	101	BCR	C6-C7-C8-C9
17	K	104	BCR	C6-C7-C8-C9
17	i	101	BCR	C6-C7-C8-C9
17	k	104	BCR	C6-C7-C8-C9
17	7	101	BCR	C6-C7-C8-C9
17	9	104	BCR	C6-C7-C8-C9
14	B	804	CLA	C10-C11-C12-C13
14	b	805	CLA	C10-C11-C12-C13
14	2	805	CLA	C10-C11-C12-C13
14	b	802	CLA	CBD-CGD-O2D-CED
14	B	827	CLA	C5-C6-C7-C8
14	L	203	CLA	C5-C6-C7-C8
14	b	828	CLA	C5-C6-C7-C8
14	l	204	CLA	C5-C6-C7-C8
14	1	1616	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	2	828	CLA	C5-C6-C7-C8
14	0	205	CLA	C5-C6-C7-C8
14	B	831	CLA	O2A-C1-C2-C3
14	b	832	CLA	O2A-C1-C2-C3
14	2	832	CLA	O2A-C1-C2-C3
20	b	850	LMG	C17-C18-C19-C20
14	b	832	CLA	C2A-CAA-CBA-CGA
14	2	832	CLA	C2A-CAA-CBA-CGA
17	B	843	BCR	C14-C15-C16-C17
17	b	844	BCR	C14-C15-C16-C17
17	2	844	BCR	C14-C15-C16-C17
14	A	815	CLA	C10-C11-C12-C13
20	2	850	LMG	C17-C18-C19-C20
20	B	849	LMG	C17-C18-C19-C20
14	A	806	CLA	O1D-CGD-O2D-CED
14	A	811	CLA	CHA-CBD-CGD-O1D
14	A	831	CLA	CHA-CBD-CGD-O1D
14	A	841	CLA	CHA-CBD-CGD-O1D
14	A	841	CLA	CHA-CBD-CGD-O2D
14	B	802	CLA	CHA-CBD-CGD-O1D
14	B	802	CLA	CHA-CBD-CGD-O2D
14	B	803	CLA	CHA-CBD-CGD-O1D
14	B	803	CLA	CHA-CBD-CGD-O2D
14	B	808	CLA	CHA-CBD-CGD-O1D
14	B	808	CLA	CHA-CBD-CGD-O2D
14	B	813	CLA	CHA-CBD-CGD-O1D
14	B	813	CLA	CHA-CBD-CGD-O2D
14	B	814	CLA	CHA-CBD-CGD-O1D
14	B	814	CLA	CHA-CBD-CGD-O2D
14	B	815	CLA	CHA-CBD-CGD-O1D
14	B	815	CLA	CHA-CBD-CGD-O2D
14	B	816	CLA	CHA-CBD-CGD-O1D
14	B	816	CLA	CHA-CBD-CGD-O2D
14	B	821	CLA	CHA-CBD-CGD-O1D
14	B	821	CLA	CHA-CBD-CGD-O2D
14	B	830	CLA	CHA-CBD-CGD-O1D
14	B	830	CLA	CHA-CBD-CGD-O2D
14	B	833	CLA	CHA-CBD-CGD-O1D
14	B	833	CLA	CHA-CBD-CGD-O2D
14	B	837	CLA	CHA-CBD-CGD-O1D
14	B	837	CLA	CHA-CBD-CGD-O2D
14	F	201	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	L	203	CLA	CHA-CBD-CGD-O1D
14	a	811	CLA	CHA-CBD-CGD-O1D
14	a	831	CLA	CHA-CBD-CGD-O1D
14	a	841	CLA	CHA-CBD-CGD-O1D
14	a	841	CLA	CHA-CBD-CGD-O2D
14	b	803	CLA	CHA-CBD-CGD-O1D
14	b	803	CLA	CHA-CBD-CGD-O2D
14	b	804	CLA	CHA-CBD-CGD-O1D
14	b	804	CLA	CHA-CBD-CGD-O2D
14	b	809	CLA	CHA-CBD-CGD-O1D
14	b	809	CLA	CHA-CBD-CGD-O2D
14	b	814	CLA	CHA-CBD-CGD-O1D
14	b	814	CLA	CHA-CBD-CGD-O2D
14	b	815	CLA	CHA-CBD-CGD-O1D
14	b	815	CLA	CHA-CBD-CGD-O2D
14	b	816	CLA	CHA-CBD-CGD-O1D
14	b	816	CLA	CHA-CBD-CGD-O2D
14	b	817	CLA	CHA-CBD-CGD-O1D
14	b	817	CLA	CHA-CBD-CGD-O2D
14	b	822	CLA	CHA-CBD-CGD-O1D
14	b	822	CLA	CHA-CBD-CGD-O2D
14	b	831	CLA	CHA-CBD-CGD-O1D
14	b	831	CLA	CHA-CBD-CGD-O2D
14	b	834	CLA	CHA-CBD-CGD-O1D
14	b	834	CLA	CHA-CBD-CGD-O2D
14	b	838	CLA	CHA-CBD-CGD-O1D
14	b	838	CLA	CHA-CBD-CGD-O2D
14	f	201	CLA	CHA-CBD-CGD-O2D
14	l	204	CLA	CHA-CBD-CGD-O1D
14	1	1612	CLA	CHA-CBD-CGD-O1D
14	1	1632	CLA	CHA-CBD-CGD-O1D
14	1	1642	CLA	CHA-CBD-CGD-O1D
14	1	1642	CLA	CHA-CBD-CGD-O2D
14	2	803	CLA	CHA-CBD-CGD-O1D
14	2	803	CLA	CHA-CBD-CGD-O2D
14	2	804	CLA	CHA-CBD-CGD-O1D
14	2	804	CLA	CHA-CBD-CGD-O2D
14	2	809	CLA	CHA-CBD-CGD-O1D
14	2	809	CLA	CHA-CBD-CGD-O2D
14	2	814	CLA	CHA-CBD-CGD-O1D
14	2	814	CLA	CHA-CBD-CGD-O2D
14	2	815	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	2	815	CLA	CHA-CBD-CGD-O2D
14	2	816	CLA	CHA-CBD-CGD-O1D
14	2	816	CLA	CHA-CBD-CGD-O2D
14	2	817	CLA	CHA-CBD-CGD-O1D
14	2	817	CLA	CHA-CBD-CGD-O2D
14	2	822	CLA	CHA-CBD-CGD-O1D
14	2	822	CLA	CHA-CBD-CGD-O2D
14	2	831	CLA	CHA-CBD-CGD-O1D
14	2	831	CLA	CHA-CBD-CGD-O2D
14	2	834	CLA	CHA-CBD-CGD-O1D
14	2	834	CLA	CHA-CBD-CGD-O2D
14	2	838	CLA	CHA-CBD-CGD-O1D
14	2	838	CLA	CHA-CBD-CGD-O2D
14	6	201	CLA	CHA-CBD-CGD-O2D
14	0	205	CLA	CHA-CBD-CGD-O1D
14	a	815	CLA	C10-C11-C12-C13
20	B	849	LMG	C11-C12-C13-C14
20	b	850	LMG	C11-C12-C13-C14
14	F	204	CLA	O1A-CGA-O2A-C1
20	2	850	LMG	C11-C12-C13-C14
14	b	819	CLA	O1D-CGD-O2D-CED
14	1	1607	CLA	O1D-CGD-O2D-CED
17	J	103	BCR	C11-C10-C9-C8
17	j	1304	BCR	C11-C10-C9-C8
17	8	1304	BCR	C11-C10-C9-C8
14	a	806	CLA	O1D-CGD-O2D-CED
14	A	827	CLA	O1A-CGA-O2A-C1
14	a	827	CLA	O1A-CGA-O2A-C1
14	f	203	CLA	O1A-CGA-O2A-C1
14	6	203	CLA	O1A-CGA-O2A-C1
14	l	205	CLA	C16-C17-C18-C19
14	B	818	CLA	O1D-CGD-O2D-CED
14	2	819	CLA	O1D-CGD-O2D-CED
14	A	810	CLA	C11-C12-C13-C14
14	A	840	CLA	C11-C12-C13-C14
14	B	814	CLA	C6-C7-C8-C9
14	B	825	CLA	C11-C10-C8-C9
14	B	837	CLA	C11-C10-C8-C9
14	a	810	CLA	C11-C12-C13-C14
14	a	840	CLA	C11-C12-C13-C14
14	b	815	CLA	C6-C7-C8-C9
14	b	815	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
14	b	826	CLA	C11-C10-C8-C9
14	b	838	CLA	C11-C10-C8-C9
14	1	1611	CLA	C11-C12-C13-C14
14	1	1641	CLA	C11-C12-C13-C14
14	2	815	CLA	C6-C7-C8-C9
14	2	838	CLA	C11-C10-C8-C9
14	A	831	CLA	O1A-CGA-O2A-C1
14	a	831	CLA	O1A-CGA-O2A-C1
14	1	1628	CLA	O1A-CGA-O2A-C1
14	1	1632	CLA	O1A-CGA-O2A-C1
18	M	101	LHG	C33-C34-C35-C36
18	y	101	LHG	C33-C34-C35-C36
14	L	204	CLA	C16-C17-C18-C19
14	0	206	CLA	C16-C17-C18-C19
18	m	101	LHG	C33-C34-C35-C36
14	A	819	CLA	C2A-CAA-CBA-CGA
14	A	821	CLA	C2A-CAA-CBA-CGA
14	a	819	CLA	C2A-CAA-CBA-CGA
14	a	821	CLA	C2A-CAA-CBA-CGA
14	1	1620	CLA	C2A-CAA-CBA-CGA
14	1	1622	CLA	C2A-CAA-CBA-CGA
17	F	202	BCR	C11-C12-C13-C35
17	f	202	BCR	C11-C12-C13-C35
17	6	202	BCR	C11-C12-C13-C35
18	M	101	LHG	C24-C25-C26-C27
18	m	101	LHG	C24-C25-C26-C27
17	F	205	BCR	C21-C22-C23-C24
17	J	103	BCR	C21-C22-C23-C24
17	f	204	BCR	C21-C22-C23-C24
17	j	1304	BCR	C21-C22-C23-C24
17	6	204	BCR	C21-C22-C23-C24
17	8	1304	BCR	C21-C22-C23-C24
18	M	101	LHG	C27-C28-C29-C30
18	m	101	LHG	C27-C28-C29-C30
18	y	101	LHG	C24-C25-C26-C27
18	y	101	LHG	C27-C28-C29-C30
14	A	855	CLA	C16-C17-C18-C20
14	b	802	CLA	C16-C17-C18-C20
14	2	802	CLA	C16-C17-C18-C20
14	a	819	CLA	CBA-CGA-O2A-C1
20	b	850	LMG	C15-C16-C17-C18
17	B	847	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
18	B	850	LHG	C3-O3-P-O6
18	b	851	LHG	C3-O3-P-O6
18	z	101	LHG	C3-O3-P-O6
20	B	849	LMG	C15-C16-C17-C18
20	2	850	LMG	C15-C16-C17-C18
14	A	817	CLA	C4B-C3B-CAB-CBB
14	A	836	CLA	C4B-C3B-CAB-CBB
14	a	817	CLA	C4B-C3B-CAB-CBB
14	a	836	CLA	C4B-C3B-CAB-CBB
14	1	1618	CLA	C4B-C3B-CAB-CBB
14	1	1637	CLA	C4B-C3B-CAB-CBB
18	A	853	LHG	C3-O3-P-O5
18	L	208	LHG	C3-O3-P-O5
18	L	208	LHG	C4-O6-P-O5
18	M	101	LHG	C4-O6-P-O4
18	a	853	LHG	C3-O3-P-O5
18	l	201	LHG	C3-O3-P-O5
18	l	201	LHG	C4-O6-P-O5
18	m	101	LHG	C4-O6-P-O4
18	1	1654	LHG	C3-O3-P-O5
18	0	202	LHG	C3-O3-P-O5
18	0	202	LHG	C4-O6-P-O5
18	y	101	LHG	C4-O6-P-O4
14	A	814	CLA	C16-C17-C18-C20
14	A	829	CLA	C16-C17-C18-C19
14	a	814	CLA	C16-C17-C18-C20
14	1	1615	CLA	C16-C17-C18-C20
14	a	842	CLA	C5-C6-C7-C8
14	1	1643	CLA	C5-C6-C7-C8
14	A	807	CLA	CBA-CGA-O2A-C1
14	A	819	CLA	CBA-CGA-O2A-C1
14	A	855	CLA	CBA-CGA-O2A-C1
14	a	807	CLA	CBA-CGA-O2A-C1
14	b	802	CLA	CBA-CGA-O2A-C1
14	1	1608	CLA	CBA-CGA-O2A-C1
14	1	1620	CLA	CBA-CGA-O2A-C1
14	2	802	CLA	CBA-CGA-O2A-C1
14	A	855	CLA	O1A-CGA-O2A-C1
14	A	842	CLA	C5-C6-C7-C8
14	A	810	CLA	C2A-CAA-CBA-CGA
14	a	810	CLA	C2A-CAA-CBA-CGA
14	1	1611	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	A	810	CLA	C3-C5-C6-C7
14	B	806	CLA	C3-C5-C6-C7
14	a	810	CLA	C3-C5-C6-C7
14	b	807	CLA	C3-C5-C6-C7
14	1	1611	CLA	C3-C5-C6-C7
14	2	807	CLA	C3-C5-C6-C7
14	2	802	CLA	O1A-CGA-O2A-C1
14	B	813	CLA	C16-C17-C18-C20
14	L	203	CLA	C16-C17-C18-C20
14	a	829	CLA	C16-C17-C18-C19
14	b	814	CLA	C16-C17-C18-C20
14	l	204	CLA	C16-C17-C18-C20
14	1	1630	CLA	C16-C17-C18-C19
14	2	814	CLA	C16-C17-C18-C20
14	0	205	CLA	C16-C17-C18-C20
14	A	810	CLA	CAD-CBD-CGD-O1D
14	A	829	CLA	CAD-CBD-CGD-O1D
14	A	844	CLA	CAD-CBD-CGD-O1D
14	B	811	CLA	CAD-CBD-CGD-O1D
14	B	813	CLA	CAD-CBD-CGD-O1D
14	B	815	CLA	CAD-CBD-CGD-O1D
14	B	822	CLA	CAD-CBD-CGD-O1D
14	B	826	CLA	CAD-CBD-CGD-O1D
14	L	203	CLA	CAD-CBD-CGD-O1D
14	a	810	CLA	CAD-CBD-CGD-O1D
14	a	829	CLA	CAD-CBD-CGD-O1D
14	a	844	CLA	CAD-CBD-CGD-O1D
14	b	812	CLA	CAD-CBD-CGD-O1D
14	b	814	CLA	CAD-CBD-CGD-O1D
14	b	816	CLA	CAD-CBD-CGD-O1D
14	b	823	CLA	CAD-CBD-CGD-O1D
14	b	827	CLA	CAD-CBD-CGD-O1D
14	l	204	CLA	CAD-CBD-CGD-O1D
14	1	1611	CLA	CAD-CBD-CGD-O1D
14	1	1630	CLA	CAD-CBD-CGD-O1D
14	1	1645	CLA	CAD-CBD-CGD-O1D
14	2	812	CLA	CAD-CBD-CGD-O1D
14	2	814	CLA	CAD-CBD-CGD-O1D
14	2	816	CLA	CAD-CBD-CGD-O1D
14	2	823	CLA	CAD-CBD-CGD-O1D
14	2	827	CLA	CAD-CBD-CGD-O1D
14	0	205	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	K	101	CLA	CBA-CGA-O2A-C1
14	b	802	CLA	O1A-CGA-O2A-C1
14	A	833	CLA	C15-C16-C17-C18
14	a	833	CLA	C15-C16-C17-C18
14	A	804	CLA	CBA-CGA-O2A-C1
14	1	1634	CLA	C15-C16-C17-C18
14	k	101	CLA	CBA-CGA-O2A-C1
14	9	101	CLA	CBA-CGA-O2A-C1
14	A	807	CLA	C11-C10-C8-C7
14	A	817	CLA	C12-C13-C15-C16
14	A	824	CLA	C12-C13-C15-C16
14	A	829	CLA	C11-C12-C13-C15
14	A	831	CLA	C11-C10-C8-C7
14	B	802	CLA	C12-C13-C15-C16
14	B	805	CLA	C12-C13-C15-C16
14	B	820	CLA	C6-C7-C8-C10
14	B	820	CLA	C11-C12-C13-C15
14	B	826	CLA	C6-C7-C8-C10
14	B	838	CLA	C6-C7-C8-C10
14	L	204	CLA	C6-C7-C8-C10
14	a	807	CLA	C11-C10-C8-C7
14	a	817	CLA	C12-C13-C15-C16
14	a	824	CLA	C12-C13-C15-C16
14	a	829	CLA	C11-C12-C13-C15
14	a	831	CLA	C11-C10-C8-C7
14	b	803	CLA	C12-C13-C15-C16
14	b	806	CLA	C12-C13-C15-C16
14	b	821	CLA	C6-C7-C8-C10
14	b	821	CLA	C11-C12-C13-C15
14	b	827	CLA	C6-C7-C8-C10
14	b	839	CLA	C6-C7-C8-C10
14	l	205	CLA	C6-C7-C8-C10
14	1	1608	CLA	C11-C10-C8-C7
14	1	1618	CLA	C12-C13-C15-C16
14	1	1625	CLA	C12-C13-C15-C16
14	1	1630	CLA	C11-C12-C13-C15
14	1	1632	CLA	C11-C10-C8-C7
14	2	803	CLA	C12-C13-C15-C16
14	2	806	CLA	C12-C13-C15-C16
14	2	821	CLA	C6-C7-C8-C10
14	2	821	CLA	C11-C12-C13-C15
14	2	827	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
14	2	839	CLA	C6-C7-C8-C10
14	0	206	CLA	C6-C7-C8-C10
14	A	816	CLA	C3-C5-C6-C7
14	a	816	CLA	C3-C5-C6-C7
14	1	1617	CLA	C3-C5-C6-C7
17	b	848	BCR	C15-C16-C17-C18
17	2	848	BCR	C15-C16-C17-C18
14	B	802	CLA	C10-C11-C12-C13
14	b	803	CLA	C10-C11-C12-C13
14	2	803	CLA	C10-C11-C12-C13
20	B	849	LMG	C31-C32-C33-C34
20	b	850	LMG	C31-C32-C33-C34
20	2	850	LMG	C31-C32-C33-C34
14	A	807	CLA	O1A-CGA-O2A-C1
14	a	807	CLA	O1A-CGA-O2A-C1
14	1	1608	CLA	O1A-CGA-O2A-C1
14	2	809	CLA	C5-C6-C7-C8
14	A	841	CLA	C2A-CAA-CBA-CGA
14	a	841	CLA	C2A-CAA-CBA-CGA
14	a	842	CLA	C2A-CAA-CBA-CGA
14	1	1642	CLA	C2A-CAA-CBA-CGA
14	1	1643	CLA	C2A-CAA-CBA-CGA
14	B	804	CLA	C16-C17-C18-C19
14	b	805	CLA	C16-C17-C18-C19
14	2	805	CLA	C16-C17-C18-C19
14	A	843	CLA	C5-C6-C7-C8
14	B	808	CLA	C5-C6-C7-C8
14	a	843	CLA	C5-C6-C7-C8
14	b	809	CLA	C5-C6-C7-C8
18	L	208	LHG	O7-C5-C6-O8
18	l	201	LHG	O7-C5-C6-O8
18	0	202	LHG	O7-C5-C6-O8
14	a	804	CLA	CBA-CGA-O2A-C1
14	B	818	CLA	O2A-C1-C2-C3
14	b	819	CLA	O2A-C1-C2-C3
14	2	819	CLA	O2A-C1-C2-C3
14	A	819	CLA	C13-C15-C16-C17
14	a	819	CLA	C13-C15-C16-C17
14	1	1620	CLA	C13-C15-C16-C17
14	1	1644	CLA	C5-C6-C7-C8
14	B	806	CLA	C8-C10-C11-C12
14	b	807	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
14	2	807	CLA	C8-C10-C11-C12
14	1	1605	CLA	CBA-CGA-O2A-C1
14	A	822	CLA	C11-C10-C8-C9
14	A	826	CLA	C11-C12-C13-C14
14	A	833	CLA	C14-C13-C15-C16
14	B	803	CLA	C6-C7-C8-C9
14	B	813	CLA	C11-C10-C8-C9
14	B	819	CLA	C6-C7-C8-C9
14	a	822	CLA	C11-C10-C8-C9
14	a	826	CLA	C11-C12-C13-C14
14	a	833	CLA	C14-C13-C15-C16
14	b	804	CLA	C6-C7-C8-C9
14	b	814	CLA	C11-C10-C8-C9
14	b	820	CLA	C6-C7-C8-C9
14	1	1607	CLA	C11-C10-C8-C9
14	1	1623	CLA	C11-C10-C8-C9
14	1	1627	CLA	C11-C12-C13-C14
14	1	1634	CLA	C14-C13-C15-C16
14	2	804	CLA	C6-C7-C8-C9
14	2	814	CLA	C11-C10-C8-C9
14	2	820	CLA	C6-C7-C8-C9
17	A	848	BCR	C22-C23-C24-C25
17	a	848	BCR	C22-C23-C24-C25
17	1	1649	BCR	C22-C23-C24-C25
14	A	842	CLA	C2A-CAA-CBA-CGA
14	B	827	CLA	CAA-CBA-CGA-O2A
14	b	828	CLA	CAA-CBA-CGA-O2A
14	2	828	CLA	CAA-CBA-CGA-O2A
14	a	804	CLA	O1A-CGA-O2A-C1
20	B	849	LMG	C32-C33-C34-C35
20	b	850	LMG	C32-C33-C34-C35
20	2	850	LMG	C32-C33-C34-C35
13	A	801	CL0	C2B-C3B-CAB-CBB
13	a	801	CL0	C2B-C3B-CAB-CBB
13	1	1602	CL0	C2B-C3B-CAB-CBB
14	A	814	CLA	C2B-C3B-CAB-CBB
14	A	817	CLA	C2B-C3B-CAB-CBB
14	A	836	CLA	C2B-C3B-CAB-CBB
14	B	807	CLA	C2B-C3B-CAB-CBB
14	a	814	CLA	C2B-C3B-CAB-CBB
14	a	817	CLA	C2B-C3B-CAB-CBB
14	a	836	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	b	808	CLA	C2B-C3B-CAB-CBB
14	1	1615	CLA	C2B-C3B-CAB-CBB
14	1	1618	CLA	C2B-C3B-CAB-CBB
14	1	1637	CLA	C2B-C3B-CAB-CBB
14	2	808	CLA	C2B-C3B-CAB-CBB
14	A	804	CLA	O1A-CGA-O2A-C1
14	B	838	CLA	C15-C16-C17-C18
14	b	839	CLA	C15-C16-C17-C18
14	1	1605	CLA	O1A-CGA-O2A-C1
14	B	813	CLA	C16-C17-C18-C19
14	B	827	CLA	C16-C17-C18-C20
14	b	814	CLA	C16-C17-C18-C19
14	b	828	CLA	C16-C17-C18-C20
14	2	814	CLA	C16-C17-C18-C19
14	2	828	CLA	C16-C17-C18-C20
14	2	839	CLA	C15-C16-C17-C18
14	B	831	CLA	C1-C2-C3-C4
14	b	832	CLA	C1-C2-C3-C4
14	2	832	CLA	C1-C2-C3-C4
14	B	803	CLA	C2A-CAA-CBA-CGA
14	b	804	CLA	C2A-CAA-CBA-CGA
14	2	804	CLA	C2A-CAA-CBA-CGA
14	A	807	CLA	C2-C1-O2A-CGA
14	B	828	CLA	C2-C1-O2A-CGA
14	a	807	CLA	C2-C1-O2A-CGA
14	b	829	CLA	C2-C1-O2A-CGA
14	1	1608	CLA	C2-C1-O2A-CGA
14	2	829	CLA	C2-C1-O2A-CGA
14	1	1616	CLA	O1A-CGA-O2A-C1
14	A	815	CLA	O1A-CGA-O2A-C1
14	A	819	CLA	O1A-CGA-O2A-C1
14	a	815	CLA	O1A-CGA-O2A-C1
14	1	1620	CLA	O1A-CGA-O2A-C1
14	B	819	CLA	C16-C17-C18-C20
14	b	820	CLA	C16-C17-C18-C20
14	2	820	CLA	C16-C17-C18-C20
14	A	821	CLA	C4-C3-C5-C6
14	a	821	CLA	C4-C3-C5-C6
14	1	1622	CLA	C4-C3-C5-C6
17	A	847	BCR	C1-C6-C7-C8
17	B	845	BCR	C5-C6-C7-C8
17	L	201	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
17	a	847	BCR	C1-C6-C7-C8
17	b	846	BCR	C5-C6-C7-C8
17	l	202	BCR	C23-C24-C25-C30
17	1	1648	BCR	C1-C6-C7-C8
17	2	846	BCR	C5-C6-C7-C8
17	0	203	BCR	C23-C24-C25-C30
14	a	819	CLA	O1A-CGA-O2A-C1
14	b	830	CLA	O1A-CGA-O2A-C1
14	A	840	CLA	C10-C11-C12-C13
14	1	1641	CLA	C10-C11-C12-C13
14	b	830	CLA	CBA-CGA-O2A-C1
14	B	822	CLA	C5-C6-C7-C8
14	a	840	CLA	C10-C11-C12-C13
14	b	823	CLA	C5-C6-C7-C8
14	2	823	CLA	C5-C6-C7-C8
17	B	846	BCR	C12-C13-C14-C15
17	b	847	BCR	C12-C13-C14-C15
17	2	847	BCR	C12-C13-C14-C15
14	L	204	CLA	C4C-C3C-CAC-CBC
14	l	205	CLA	C4C-C3C-CAC-CBC
14	0	206	CLA	C4C-C3C-CAC-CBC
20	B	849	LMG	C24-C25-C26-C27
20	2	850	LMG	C24-C25-C26-C27
14	B	829	CLA	CBA-CGA-O2A-C1
14	2	830	CLA	CBA-CGA-O2A-C1
14	1	1640	CLA	O1D-CGD-O2D-CED
20	b	850	LMG	C24-C25-C26-C27
20	2	850	LMG	C16-C17-C18-C19
20	B	849	LMG	C16-C17-C18-C19
20	b	850	LMG	C16-C17-C18-C19
14	A	839	CLA	O1D-CGD-O2D-CED
14	a	839	CLA	O1D-CGD-O2D-CED
18	A	853	LHG	C4-C5-C6-O8
18	a	853	LHG	C4-C5-C6-O8
18	1	1654	LHG	C4-C5-C6-O8
14	A	838	CLA	C4-C3-C5-C6
14	a	838	CLA	C4-C3-C5-C6
14	1	1639	CLA	C4-C3-C5-C6
14	A	802	CLA	C12-C13-C15-C16
14	A	828	CLA	C6-C7-C8-C10
14	A	838	CLA	C12-C13-C15-C16
14	A	843	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	B	817	CLA	C6-C7-C8-C10
14	a	802	CLA	C12-C13-C15-C16
14	a	828	CLA	C6-C7-C8-C10
14	a	838	CLA	C12-C13-C15-C16
14	a	843	CLA	C2-C3-C5-C6
14	b	818	CLA	C6-C7-C8-C10
14	1	1603	CLA	C12-C13-C15-C16
14	1	1629	CLA	C6-C7-C8-C10
14	1	1639	CLA	C12-C13-C15-C16
14	1	1644	CLA	C2-C3-C5-C6
14	2	818	CLA	C6-C7-C8-C10
14	2	830	CLA	O1A-CGA-O2A-C1
14	A	804	CLA	C14-C13-C15-C16
14	A	806	CLA	C11-C10-C8-C9
14	A	826	CLA	C14-C13-C15-C16
14	A	831	CLA	C11-C10-C8-C9
14	A	842	CLA	C11-C10-C8-C9
14	B	802	CLA	C14-C13-C15-C16
14	B	810	CLA	C14-C13-C15-C16
14	B	820	CLA	C6-C7-C8-C9
14	B	826	CLA	C6-C7-C8-C9
14	B	838	CLA	C6-C7-C8-C9
14	a	804	CLA	C14-C13-C15-C16
14	a	806	CLA	C11-C10-C8-C9
14	a	826	CLA	C14-C13-C15-C16
14	a	831	CLA	C11-C10-C8-C9
14	a	842	CLA	C11-C10-C8-C9
14	b	803	CLA	C14-C13-C15-C16
14	b	811	CLA	C14-C13-C15-C16
14	b	821	CLA	C6-C7-C8-C9
14	b	827	CLA	C6-C7-C8-C9
14	b	839	CLA	C6-C7-C8-C9
14	1	1605	CLA	C14-C13-C15-C16
14	1	1627	CLA	C14-C13-C15-C16
14	1	1632	CLA	C11-C10-C8-C9
14	1	1643	CLA	C11-C10-C8-C9
14	2	803	CLA	C14-C13-C15-C16
14	2	811	CLA	C14-C13-C15-C16
14	2	821	CLA	C6-C7-C8-C9
14	2	827	CLA	C6-C7-C8-C9
14	2	839	CLA	C6-C7-C8-C9
17	B	845	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
17	b	846	BCR	C15-C16-C17-C18
17	2	846	BCR	C15-C16-C17-C18
14	A	838	CLA	C16-C17-C18-C20
14	a	838	CLA	C16-C17-C18-C20
14	1	1639	CLA	C16-C17-C18-C20
18	M	101	LHG	C14-C15-C16-C17
18	m	101	LHG	C14-C15-C16-C17
18	y	101	LHG	C14-C15-C16-C17
14	B	829	CLA	O1A-CGA-O2A-C1
20	B	849	LMG	C34-C35-C36-C37
20	b	850	LMG	C34-C35-C36-C37
20	2	850	LMG	C34-C35-C36-C37
14	A	808	CLA	C2A-CAA-CBA-CGA
14	a	808	CLA	C2A-CAA-CBA-CGA
14	1	1609	CLA	C2A-CAA-CBA-CGA
14	2	816	CLA	C15-C16-C17-C18
14	B	815	CLA	C15-C16-C17-C18
14	b	816	CLA	C15-C16-C17-C18
14	A	814	CLA	C16-C17-C18-C19
14	a	814	CLA	C16-C17-C18-C19
14	1	1615	CLA	C16-C17-C18-C19
14	2	812	CLA	C16-C17-C18-C20
20	B	849	LMG	C42-C43-C44-C45
20	2	850	LMG	C42-C43-C44-C45
17	F	202	BCR	C7-C8-C9-C10
17	f	202	BCR	C7-C8-C9-C10
17	6	202	BCR	C7-C8-C9-C10
20	b	850	LMG	C42-C43-C44-C45
14	1	1627	CLA	CBD-CGD-O2D-CED
14	B	811	CLA	C16-C17-C18-C20
14	b	812	CLA	C16-C17-C18-C20
14	A	815	CLA	CBA-CGA-O2A-C1
14	A	839	CLA	CBA-CGA-O2A-C1
14	a	815	CLA	CBA-CGA-O2A-C1
14	1	1616	CLA	CBA-CGA-O2A-C1
14	1	1640	CLA	CBA-CGA-O2A-C1
14	A	826	CLA	CBD-CGD-O2D-CED
14	a	826	CLA	CBD-CGD-O2D-CED
15	A	845	PQN	C23-C25-C26-C27
15	a	845	PQN	C23-C25-C26-C27
15	1	1646	PQN	C23-C25-C26-C27
14	a	839	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	A	834	CLA	C4B-C3B-CAB-CBB
14	B	808	CLA	C4B-C3B-CAB-CBB
14	K	101	CLA	C4B-C3B-CAB-CBB
14	a	808	CLA	C4B-C3B-CAB-CBB
14	a	834	CLA	C4B-C3B-CAB-CBB
14	b	809	CLA	C4B-C3B-CAB-CBB
14	k	101	CLA	C4B-C3B-CAB-CBB
14	1	1635	CLA	C4B-C3B-CAB-CBB
14	2	809	CLA	C4B-C3B-CAB-CBB
14	9	101	CLA	C4B-C3B-CAB-CBB
14	A	838	CLA	C16-C17-C18-C19
14	a	838	CLA	C16-C17-C18-C19
14	1	1639	CLA	C16-C17-C18-C19
17	B	851	BCR	C19-C20-C21-C22
17	b	852	BCR	C19-C20-C21-C22
17	8	1306	BCR	C19-C20-C21-C22
14	A	839	CLA	O1A-CGA-O2A-C1
14	a	839	CLA	O1A-CGA-O2A-C1
14	1	1640	CLA	O1A-CGA-O2A-C1
17	A	856	BCR	C10-C11-C12-C13
17	B	847	BCR	C18-C19-C20-C21
17	b	848	BCR	C18-C19-C20-C21
17	j	1305	BCR	C10-C11-C12-C13
17	2	848	BCR	C18-C19-C20-C21
17	8	1305	BCR	C10-C11-C12-C13
14	a	826	CLA	O1D-CGD-O2D-CED
14	A	802	CLA	C3-C5-C6-C7
14	a	802	CLA	C3-C5-C6-C7
14	1	1603	CLA	C3-C5-C6-C7
14	B	833	CLA	C4-C3-C5-C6
14	L	203	CLA	C4-C3-C5-C6
14	b	834	CLA	C4-C3-C5-C6
14	l	204	CLA	C4-C3-C5-C6
14	2	834	CLA	C4-C3-C5-C6
14	0	205	CLA	C4-C3-C5-C6
14	a	815	CLA	CBD-CGD-O2D-CED
14	1	1616	CLA	CBD-CGD-O2D-CED
14	L	203	CLA	C2-C3-C5-C6
14	l	204	CLA	C2-C3-C5-C6
14	0	205	CLA	C2-C3-C5-C6
14	A	826	CLA	O1D-CGD-O2D-CED
14	L	203	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	l	204	CLA	C13-C15-C16-C17
14	0	205	CLA	C13-C15-C16-C17
14	1	1627	CLA	O1D-CGD-O2D-CED
14	A	814	CLA	C2-C1-O2A-CGA
14	B	804	CLA	C2-C1-O2A-CGA
14	B	805	CLA	C2-C1-O2A-CGA
14	B	818	CLA	C2-C1-O2A-CGA
14	B	824	CLA	C2-C1-O2A-CGA
14	B	833	CLA	C2-C1-O2A-CGA
14	B	838	CLA	C2-C1-O2A-CGA
14	a	814	CLA	C2-C1-O2A-CGA
14	b	805	CLA	C2-C1-O2A-CGA
14	b	806	CLA	C2-C1-O2A-CGA
14	b	819	CLA	C2-C1-O2A-CGA
14	b	825	CLA	C2-C1-O2A-CGA
14	b	834	CLA	C2-C1-O2A-CGA
14	b	839	CLA	C2-C1-O2A-CGA
14	1	1615	CLA	C2-C1-O2A-CGA
14	2	805	CLA	C2-C1-O2A-CGA
14	2	806	CLA	C2-C1-O2A-CGA
14	2	819	CLA	C2-C1-O2A-CGA
14	2	834	CLA	C2-C1-O2A-CGA
14	2	839	CLA	C2-C1-O2A-CGA
14	A	815	CLA	CBD-CGD-O2D-CED
14	b	842	CLA	C2C-C3C-CAC-CBC
14	B	841	CLA	C2C-C3C-CAC-CBC
14	2	842	CLA	C2C-C3C-CAC-CBC
14	A	812	CLA	C14-C13-C15-C16
14	B	809	CLA	C14-C13-C15-C16
14	B	819	CLA	C14-C13-C15-C16
14	a	812	CLA	C14-C13-C15-C16
14	b	810	CLA	C14-C13-C15-C16
14	b	820	CLA	C14-C13-C15-C16
14	1	1613	CLA	C14-C13-C15-C16
14	2	810	CLA	C14-C13-C15-C16
14	2	820	CLA	C14-C13-C15-C16
14	B	823	CLA	CAA-CBA-CGA-O2A
14	b	824	CLA	CAA-CBA-CGA-O2A
14	2	824	CLA	CAA-CBA-CGA-O2A
14	A	816	CLA	C5-C6-C7-C8
14	a	816	CLA	C5-C6-C7-C8
14	1	1617	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	1	1622	CLA	O1A-CGA-O2A-C1
20	b	850	LMG	C20-C21-C22-C23
17	A	851	BCR	C11-C10-C9-C34
17	B	846	BCR	C35-C13-C14-C15
17	a	851	BCR	C11-C10-C9-C34
17	b	847	BCR	C35-C13-C14-C15
17	1	1652	BCR	C11-C10-C9-C34
17	2	847	BCR	C35-C13-C14-C15
14	B	815	CLA	C2A-CAA-CBA-CGA
14	L	204	CLA	C2A-CAA-CBA-CGA
14	b	816	CLA	C2A-CAA-CBA-CGA
14	l	205	CLA	C2A-CAA-CBA-CGA
14	0	206	CLA	C2A-CAA-CBA-CGA
13	A	801	CL0	C5-C6-C7-C8
13	a	801	CL0	C5-C6-C7-C8
13	1	1602	CL0	C5-C6-C7-C8
20	B	849	LMG	C20-C21-C22-C23
20	2	850	LMG	C20-C21-C22-C23
14	A	821	CLA	O1A-CGA-O2A-C1
14	a	821	CLA	O1A-CGA-O2A-C1
14	A	802	CLA	C16-C17-C18-C19
14	a	802	CLA	C16-C17-C18-C19
14	1	1603	CLA	C16-C17-C18-C19
14	B	816	CLA	O2A-C1-C2-C3
14	B	830	CLA	O2A-C1-C2-C3
14	b	817	CLA	O2A-C1-C2-C3
14	b	831	CLA	O2A-C1-C2-C3
14	2	817	CLA	O2A-C1-C2-C3
14	2	831	CLA	O2A-C1-C2-C3
14	a	842	CLA	CBA-CGA-O2A-C1
14	1	1643	CLA	CBA-CGA-O2A-C1
20	B	849	LMG	C14-C15-C16-C17
20	2	850	LMG	C14-C15-C16-C17
17	A	856	BCR	C36-C18-C19-C20
17	j	1305	BCR	C36-C18-C19-C20
17	1	1652	BCR	C11-C12-C13-C35
17	8	1305	BCR	C36-C18-C19-C20
20	b	850	LMG	C14-C15-C16-C17
14	a	804	CLA	C13-C15-C16-C17
14	1	1605	CLA	C13-C15-C16-C17
14	B	823	CLA	CAA-CBA-CGA-O1A
14	b	824	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
14	2	824	CLA	CAA-CBA-CGA-O1A
14	A	804	CLA	C13-C15-C16-C17
14	A	809	CLA	C8-C10-C11-C12
14	a	809	CLA	C8-C10-C11-C12
14	1	1610	CLA	C8-C10-C11-C12
14	A	814	CLA	C1A-C2A-CAA-CBA
14	A	838	CLA	C1A-C2A-CAA-CBA
14	B	810	CLA	C1A-C2A-CAA-CBA
14	B	816	CLA	C1A-C2A-CAA-CBA
14	a	814	CLA	C1A-C2A-CAA-CBA
14	a	838	CLA	C1A-C2A-CAA-CBA
14	b	811	CLA	C1A-C2A-CAA-CBA
14	b	817	CLA	C1A-C2A-CAA-CBA
14	1	1615	CLA	C1A-C2A-CAA-CBA
14	1	1639	CLA	C1A-C2A-CAA-CBA
14	2	811	CLA	C1A-C2A-CAA-CBA
14	2	817	CLA	C1A-C2A-CAA-CBA
14	A	842	CLA	CBA-CGA-O2A-C1
14	A	803	CLA	C6-C7-C8-C10
14	A	814	CLA	C11-C10-C8-C7
14	A	816	CLA	C11-C12-C13-C15
14	B	815	CLA	C11-C10-C8-C7
14	B	832	CLA	C11-C10-C8-C7
14	a	803	CLA	C6-C7-C8-C10
14	a	814	CLA	C11-C10-C8-C7
14	a	816	CLA	C11-C12-C13-C15
14	b	816	CLA	C11-C10-C8-C7
14	b	833	CLA	C11-C10-C8-C7
14	1	1604	CLA	C6-C7-C8-C10
14	1	1615	CLA	C11-C10-C8-C7
14	1	1617	CLA	C11-C12-C13-C15
14	2	816	CLA	C11-C10-C8-C7
14	2	833	CLA	C11-C10-C8-C7
14	B	820	CLA	C16-C17-C18-C20
14	A	839	CLA	C2A-CAA-CBA-CGA
14	a	839	CLA	C2A-CAA-CBA-CGA
14	l	206	CLA	C2A-CAA-CBA-CGA
14	1	1640	CLA	C2A-CAA-CBA-CGA
14	2	816	CLA	C2A-CAA-CBA-CGA
14	0	207	CLA	C2A-CAA-CBA-CGA
14	A	810	CLA	C10-C11-C12-C13
14	a	810	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	b	816	CLA	C5-C6-C7-C8
14	1	1611	CLA	C10-C11-C12-C13
14	2	816	CLA	C5-C6-C7-C8
14	B	815	CLA	C5-C6-C7-C8
14	A	821	CLA	CBA-CGA-O2A-C1
14	a	821	CLA	CBA-CGA-O2A-C1
14	1	1622	CLA	CBA-CGA-O2A-C1
14	A	842	CLA	C16-C17-C18-C19
14	B	809	CLA	C16-C17-C18-C19
14	a	802	CLA	C16-C17-C18-C20
14	a	842	CLA	C16-C17-C18-C19
14	b	810	CLA	C16-C17-C18-C19
14	b	821	CLA	C16-C17-C18-C20
14	1	1643	CLA	C16-C17-C18-C19
14	2	810	CLA	C16-C17-C18-C19
14	2	821	CLA	C16-C17-C18-C20
14	B	806	CLA	C5-C6-C7-C8
14	a	826	CLA	C8-C10-C11-C12
14	2	807	CLA	C5-C6-C7-C8
14	B	841	CLA	C4C-C3C-CAC-CBC
14	2	802	CLA	O1D-CGD-O2D-CED
14	A	816	CLA	C4-C3-C5-C6
14	A	830	CLA	C4-C3-C5-C6
14	B	827	CLA	C4-C3-C5-C6
14	B	830	CLA	C4-C3-C5-C6
14	a	816	CLA	C4-C3-C5-C6
14	a	830	CLA	C4-C3-C5-C6
14	b	828	CLA	C4-C3-C5-C6
14	b	831	CLA	C4-C3-C5-C6
14	1	1617	CLA	C4-C3-C5-C6
14	1	1631	CLA	C4-C3-C5-C6
14	2	828	CLA	C4-C3-C5-C6
14	2	831	CLA	C4-C3-C5-C6
14	A	826	CLA	C8-C10-C11-C12
14	K	103	CLA	C5-C6-C7-C8
14	b	807	CLA	C5-C6-C7-C8
14	k	103	CLA	C5-C6-C7-C8
14	1	1627	CLA	C8-C10-C11-C12
14	9	103	CLA	C5-C6-C7-C8
14	A	808	CLA	C2B-C3B-CAB-CBB
14	A	825	CLA	C2B-C3B-CAB-CBB
14	K	101	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	a	808	CLA	C2B-C3B-CAB-CBB
14	a	825	CLA	C2B-C3B-CAB-CBB
14	k	101	CLA	C2B-C3B-CAB-CBB
14	1	1609	CLA	C2B-C3B-CAB-CBB
14	1	1626	CLA	C2B-C3B-CAB-CBB
14	9	101	CLA	C2B-C3B-CAB-CBB
14	A	842	CLA	O1A-CGA-O2A-C1
14	a	842	CLA	O1A-CGA-O2A-C1
20	B	849	LMG	C13-C14-C15-C16
20	b	850	LMG	C13-C14-C15-C16
14	A	802	CLA	C16-C17-C18-C20
14	A	840	CLA	C16-C17-C18-C19
14	a	840	CLA	C16-C17-C18-C19
14	1	1603	CLA	C16-C17-C18-C20
14	1	1641	CLA	C16-C17-C18-C19
14	2	842	CLA	C4C-C3C-CAC-CBC
20	2	850	LMG	C13-C14-C15-C16
14	b	842	CLA	C4C-C3C-CAC-CBC
17	A	851	BCR	C22-C23-C24-C25
17	B	851	BCR	C6-C7-C8-C9
17	F	202	BCR	C6-C7-C8-C9
17	a	851	BCR	C22-C23-C24-C25
17	b	852	BCR	C6-C7-C8-C9
17	f	202	BCR	C6-C7-C8-C9
17	1	1652	BCR	C22-C23-C24-C25
17	6	202	BCR	C6-C7-C8-C9
17	8	1306	BCR	C6-C7-C8-C9
14	1	1643	CLA	O1A-CGA-O2A-C1
14	A	855	CLA	O1D-CGD-O2D-CED
14	1	1639	CLA	C4C-C3C-CAC-CBC
14	A	818	CLA	C2-C1-O2A-CGA
14	F	201	CLA	C2-C1-O2A-CGA
14	a	818	CLA	C2-C1-O2A-CGA
14	f	201	CLA	C2-C1-O2A-CGA
14	1	1619	CLA	C2-C1-O2A-CGA
14	6	201	CLA	C2-C1-O2A-CGA
14	b	802	CLA	O1D-CGD-O2D-CED
14	A	838	CLA	C2-C3-C5-C6
14	a	838	CLA	C2-C3-C5-C6
14	1	1639	CLA	C2-C3-C5-C6
14	A	838	CLA	C4C-C3C-CAC-CBC
14	a	838	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
14	B	815	CLA	C6-C7-C8-C9
14	b	816	CLA	C6-C7-C8-C9
14	2	816	CLA	C6-C7-C8-C9
14	L	205	CLA	C2A-CAA-CBA-CGA
18	A	854	LHG	C9-C10-C11-C12
17	A	848	BCR	C1-C6-C7-C8
17	A	850	BCR	C1-C6-C7-C8
17	A	850	BCR	C5-C6-C7-C8
17	B	843	BCR	C1-C6-C7-C8
17	B	846	BCR	C1-C6-C7-C8
17	B	847	BCR	C1-C6-C7-C8
17	I	101	BCR	C1-C6-C7-C8
17	J	103	BCR	C23-C24-C25-C30
17	K	102	BCR	C23-C24-C25-C30
17	a	848	BCR	C1-C6-C7-C8
17	a	850	BCR	C1-C6-C7-C8
17	a	850	BCR	C5-C6-C7-C8
17	b	844	BCR	C1-C6-C7-C8
17	b	847	BCR	C1-C6-C7-C8
17	b	848	BCR	C1-C6-C7-C8
17	i	101	BCR	C1-C6-C7-C8
17	j	1304	BCR	C23-C24-C25-C30
17	k	102	BCR	C23-C24-C25-C30
17	1	1649	BCR	C1-C6-C7-C8
17	1	1651	BCR	C1-C6-C7-C8
17	1	1651	BCR	C5-C6-C7-C8
17	2	844	BCR	C1-C6-C7-C8
17	2	847	BCR	C1-C6-C7-C8
17	2	848	BCR	C1-C6-C7-C8
17	7	101	BCR	C1-C6-C7-C8
17	8	1304	BCR	C23-C24-C25-C30
17	9	102	BCR	C23-C24-C25-C30
14	A	815	CLA	O1D-CGD-O2D-CED
18	a	854	LHG	C9-C10-C11-C12
18	1	1655	LHG	C9-C10-C11-C12
14	B	810	CLA	C4-C3-C5-C6
14	b	811	CLA	C4-C3-C5-C6
14	2	811	CLA	C4-C3-C5-C6
17	L	201	BCR	C7-C8-C9-C10
17	l	202	BCR	C7-C8-C9-C10
17	0	203	BCR	C7-C8-C9-C10
14	A	819	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	1	1620	CLA	C10-C11-C12-C13
14	A	821	CLA	C2-C3-C5-C6
14	a	821	CLA	C2-C3-C5-C6
14	b	828	CLA	C2-C3-C5-C6
14	1	1622	CLA	C2-C3-C5-C6
14	2	828	CLA	C2-C3-C5-C6
14	a	819	CLA	C10-C11-C12-C13
14	a	815	CLA	O1D-CGD-O2D-CED
14	B	832	CLA	C2A-CAA-CBA-CGA
14	b	833	CLA	C2A-CAA-CBA-CGA
14	2	833	CLA	C2A-CAA-CBA-CGA
14	A	808	CLA	C4B-C3B-CAB-CBB
14	A	825	CLA	C4B-C3B-CAB-CBB
14	a	825	CLA	C4B-C3B-CAB-CBB
14	1	1609	CLA	C4B-C3B-CAB-CBB
14	1	1626	CLA	C4B-C3B-CAB-CBB
14	a	821	CLA	CAA-CBA-CGA-O2A
14	1	1622	CLA	CAA-CBA-CGA-O2A
14	B	807	CLA	O1A-CGA-O2A-C1
14	b	808	CLA	O1A-CGA-O2A-C1
14	2	808	CLA	O1A-CGA-O2A-C1
14	B	830	CLA	C2-C3-C5-C6
14	b	831	CLA	C2-C3-C5-C6
14	2	831	CLA	C2-C3-C5-C6
14	2	808	CLA	CBA-CGA-O2A-C1
14	A	821	CLA	CAA-CBA-CGA-O2A
14	B	811	CLA	C16-C17-C18-C19
14	b	812	CLA	C16-C17-C18-C19
14	2	812	CLA	C16-C17-C18-C19
18	A	853	LHG	C1-C2-C3-O3
18	a	853	LHG	C1-C2-C3-O3
18	1	1654	LHG	C1-C2-C3-O3
14	B	807	CLA	CBA-CGA-O2A-C1
14	b	808	CLA	CBA-CGA-O2A-C1
14	B	802	CLA	CAA-CBA-CGA-O1A
14	b	803	CLA	CAA-CBA-CGA-O1A
14	2	803	CLA	CAA-CBA-CGA-O1A
14	B	835	CLA	CAA-CBA-CGA-O2A
14	L	205	CLA	CAA-CBA-CGA-O2A
14	l	206	CLA	CAA-CBA-CGA-O2A
14	0	207	CLA	CAA-CBA-CGA-O2A
14	a	811	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
14	1	1612	CLA	C2C-C3C-CAC-CBC
17	B	845	BCR	C11-C10-C9-C34
17	L	206	BCR	C35-C13-C14-C15
17	b	846	BCR	C11-C10-C9-C34
17	l	207	BCR	C35-C13-C14-C15
17	2	846	BCR	C11-C10-C9-C34
17	0	208	BCR	C35-C13-C14-C15
14	b	836	CLA	CAA-CBA-CGA-O2A
14	A	811	CLA	C2C-C3C-CAC-CBC
14	1	1616	CLA	O1D-CGD-O2D-CED
14	B	828	CLA	C10-C11-C12-C13
14	b	829	CLA	C10-C11-C12-C13
14	2	829	CLA	C10-C11-C12-C13
14	A	805	CLA	C2-C3-C5-C6
14	B	810	CLA	C2-C3-C5-C6
14	B	827	CLA	C2-C3-C5-C6
14	B	832	CLA	C2-C3-C5-C6
14	B	833	CLA	C2-C3-C5-C6
14	a	805	CLA	C2-C3-C5-C6
14	b	811	CLA	C2-C3-C5-C6
14	b	833	CLA	C2-C3-C5-C6
14	b	834	CLA	C2-C3-C5-C6
14	2	811	CLA	C2-C3-C5-C6
14	2	833	CLA	C2-C3-C5-C6
14	2	834	CLA	C2-C3-C5-C6
14	2	836	CLA	CAA-CBA-CGA-O2A
14	A	807	CLA	C11-C10-C8-C9
14	A	815	CLA	C11-C12-C13-C14
14	A	824	CLA	C14-C13-C15-C16
14	A	828	CLA	C6-C7-C8-C9
14	A	829	CLA	C11-C12-C13-C14
14	A	838	CLA	C14-C13-C15-C16
14	A	840	CLA	C14-C13-C15-C16
14	B	805	CLA	C6-C7-C8-C9
14	B	805	CLA	C14-C13-C15-C16
14	B	820	CLA	C11-C12-C13-C14
14	B	824	CLA	C6-C7-C8-C9
14	B	832	CLA	C11-C10-C8-C9
14	a	807	CLA	C11-C10-C8-C9
14	a	815	CLA	C11-C12-C13-C14
14	a	824	CLA	C14-C13-C15-C16
14	a	828	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	a	829	CLA	C11-C12-C13-C14
14	a	838	CLA	C14-C13-C15-C16
14	a	840	CLA	C14-C13-C15-C16
14	b	806	CLA	C6-C7-C8-C9
14	b	806	CLA	C14-C13-C15-C16
14	b	821	CLA	C11-C12-C13-C14
14	b	825	CLA	C6-C7-C8-C9
14	b	833	CLA	C11-C10-C8-C9
14	1	1608	CLA	C11-C10-C8-C9
14	1	1616	CLA	C11-C12-C13-C14
14	1	1625	CLA	C14-C13-C15-C16
14	1	1629	CLA	C6-C7-C8-C9
14	1	1630	CLA	C11-C12-C13-C14
14	1	1639	CLA	C14-C13-C15-C16
14	1	1641	CLA	C14-C13-C15-C16
14	2	806	CLA	C6-C7-C8-C9
14	2	806	CLA	C14-C13-C15-C16
14	2	821	CLA	C11-C12-C13-C14
14	2	825	CLA	C6-C7-C8-C9
14	2	833	CLA	C11-C10-C8-C9
18	b	851	LHG	C27-C28-C29-C30
18	z	101	LHG	C27-C28-C29-C30
14	A	823	CLA	CAA-CBA-CGA-O2A
14	a	823	CLA	CAA-CBA-CGA-O2A
14	1	1624	CLA	CAA-CBA-CGA-O2A
14	A	814	CLA	C3A-C2A-CAA-CBA
14	a	814	CLA	C3A-C2A-CAA-CBA
14	1	1615	CLA	C3A-C2A-CAA-CBA
18	B	850	LHG	C27-C28-C29-C30
14	A	808	CLA	CAD-CBD-CGD-O2D
14	A	813	CLA	CAD-CBD-CGD-O2D
14	A	818	CLA	CAD-CBD-CGD-O2D
14	A	822	CLA	CAD-CBD-CGD-O2D
14	A	828	CLA	CAD-CBD-CGD-O2D
14	A	834	CLA	CAD-CBD-CGD-O2D
14	B	820	CLA	CAD-CBD-CGD-O2D
14	B	836	CLA	CAD-CBD-CGD-O2D
14	B	840	CLA	CAD-CBD-CGD-O2D
14	L	205	CLA	CAD-CBD-CGD-O2D
14	a	808	CLA	CAD-CBD-CGD-O2D
14	a	813	CLA	CAD-CBD-CGD-O2D
14	a	818	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	a	822	CLA	CAD-CBD-CGD-O2D
14	a	828	CLA	CAD-CBD-CGD-O2D
14	a	834	CLA	CAD-CBD-CGD-O2D
14	b	821	CLA	CAD-CBD-CGD-O2D
14	b	837	CLA	CAD-CBD-CGD-O2D
14	b	841	CLA	CAD-CBD-CGD-O2D
14	l	206	CLA	CAD-CBD-CGD-O2D
14	1	1609	CLA	CAD-CBD-CGD-O2D
14	1	1614	CLA	CAD-CBD-CGD-O2D
14	1	1619	CLA	CAD-CBD-CGD-O2D
14	1	1623	CLA	CAD-CBD-CGD-O2D
14	1	1629	CLA	CAD-CBD-CGD-O2D
14	1	1635	CLA	CAD-CBD-CGD-O2D
14	2	821	CLA	CAD-CBD-CGD-O2D
14	2	837	CLA	CAD-CBD-CGD-O2D
14	2	841	CLA	CAD-CBD-CGD-O2D
14	0	207	CLA	CAD-CBD-CGD-O2D
14	A	803	CLA	C13-C15-C16-C17
14	a	803	CLA	C13-C15-C16-C17
14	A	802	CLA	C2-C1-O2A-CGA
14	a	802	CLA	C2-C1-O2A-CGA
14	1	1603	CLA	C2-C1-O2A-CGA
14	2	825	CLA	C2-C1-O2A-CGA
14	B	813	CLA	CAA-CBA-CGA-O2A
14	K	103	CLA	CAA-CBA-CGA-O2A
14	b	814	CLA	CAA-CBA-CGA-O2A
14	b	820	CLA	CAA-CBA-CGA-O2A
14	2	814	CLA	CAA-CBA-CGA-O2A
14	1	1604	CLA	C13-C15-C16-C17
14	A	816	CLA	C2-C3-C5-C6
14	A	830	CLA	C2-C3-C5-C6
14	a	816	CLA	C2-C3-C5-C6
14	a	830	CLA	C2-C3-C5-C6
14	1	1606	CLA	C2-C3-C5-C6
14	1	1617	CLA	C2-C3-C5-C6
14	1	1631	CLA	C2-C3-C5-C6
14	B	806	CLA	CAA-CBA-CGA-O2A
14	B	819	CLA	CAA-CBA-CGA-O2A
14	b	807	CLA	CAA-CBA-CGA-O2A
14	k	103	CLA	CAA-CBA-CGA-O2A
14	2	807	CLA	CAA-CBA-CGA-O2A
14	2	820	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
14	9	103	CLA	CAA-CBA-CGA-O2A
17	A	849	BCR	C21-C22-C23-C24
17	F	202	BCR	C21-C22-C23-C24
17	I	101	BCR	C7-C8-C9-C10
17	K	102	BCR	C7-C8-C9-C10
17	a	849	BCR	C21-C22-C23-C24
17	f	202	BCR	C21-C22-C23-C24
17	i	101	BCR	C7-C8-C9-C10
17	k	102	BCR	C7-C8-C9-C10
17	1	1650	BCR	C21-C22-C23-C24
17	6	202	BCR	C21-C22-C23-C24
17	7	101	BCR	C7-C8-C9-C10
17	9	102	BCR	C7-C8-C9-C10
14	X	1701	CLA	CAA-CBA-CGA-O2A
14	x	1701	CLA	CAA-CBA-CGA-O2A
14	z	102	CLA	CAA-CBA-CGA-O2A
14	A	802	CLA	O2A-C1-C2-C3
14	A	826	CLA	O2A-C1-C2-C3
14	A	838	CLA	O2A-C1-C2-C3
14	B	804	CLA	O2A-C1-C2-C3
14	B	825	CLA	O2A-C1-C2-C3
14	a	802	CLA	O2A-C1-C2-C3
14	a	826	CLA	O2A-C1-C2-C3
14	a	838	CLA	O2A-C1-C2-C3
14	b	805	CLA	O2A-C1-C2-C3
14	b	826	CLA	O2A-C1-C2-C3
14	1	1603	CLA	O2A-C1-C2-C3
14	1	1627	CLA	O2A-C1-C2-C3
14	1	1639	CLA	O2A-C1-C2-C3
14	2	805	CLA	O2A-C1-C2-C3
14	2	826	CLA	O2A-C1-C2-C3
14	A	844	CLA	CAA-CBA-CGA-O2A
14	a	823	CLA	CAA-CBA-CGA-O1A
14	a	844	CLA	CAA-CBA-CGA-O2A
14	1	1624	CLA	CAA-CBA-CGA-O1A
14	1	1645	CLA	CAA-CBA-CGA-O1A
14	1	1645	CLA	CAA-CBA-CGA-O2A
14	K	101	CLA	O1A-CGA-O2A-C1
14	k	101	CLA	O1A-CGA-O2A-C1
14	9	101	CLA	O1A-CGA-O2A-C1
14	A	811	CLA	CHA-CBD-CGD-O2D
14	A	815	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	A	817	CLA	CHA-CBD-CGD-O1D
14	A	817	CLA	CHA-CBD-CGD-O2D
14	A	820	CLA	CHA-CBD-CGD-O1D
14	A	820	CLA	CHA-CBD-CGD-O2D
14	A	826	CLA	CHA-CBD-CGD-O1D
14	A	839	CLA	CHA-CBD-CGD-O1D
14	A	839	CLA	CHA-CBD-CGD-O2D
14	A	840	CLA	CHA-CBD-CGD-O2D
14	B	804	CLA	CHA-CBD-CGD-O1D
14	B	818	CLA	CHA-CBD-CGD-O1D
14	B	818	CLA	CHA-CBD-CGD-O2D
14	B	824	CLA	CHA-CBD-CGD-O1D
14	B	832	CLA	CHA-CBD-CGD-O1D
14	B	832	CLA	CHA-CBD-CGD-O2D
14	B	835	CLA	CHA-CBD-CGD-O2D
14	K	103	CLA	CHA-CBD-CGD-O1D
14	K	103	CLA	CHA-CBD-CGD-O2D
14	L	203	CLA	CHA-CBD-CGD-O2D
14	a	811	CLA	CHA-CBD-CGD-O2D
14	a	815	CLA	CHA-CBD-CGD-O2D
14	a	817	CLA	CHA-CBD-CGD-O1D
14	a	817	CLA	CHA-CBD-CGD-O2D
14	a	820	CLA	CHA-CBD-CGD-O1D
14	a	820	CLA	CHA-CBD-CGD-O2D
14	a	826	CLA	CHA-CBD-CGD-O1D
14	a	839	CLA	CHA-CBD-CGD-O1D
14	a	839	CLA	CHA-CBD-CGD-O2D
14	a	840	CLA	CHA-CBD-CGD-O2D
14	b	805	CLA	CHA-CBD-CGD-O1D
14	b	819	CLA	CHA-CBD-CGD-O1D
14	b	819	CLA	CHA-CBD-CGD-O2D
14	b	825	CLA	CHA-CBD-CGD-O1D
14	b	833	CLA	CHA-CBD-CGD-O1D
14	b	833	CLA	CHA-CBD-CGD-O2D
14	b	836	CLA	CHA-CBD-CGD-O2D
14	k	103	CLA	CHA-CBD-CGD-O1D
14	k	103	CLA	CHA-CBD-CGD-O2D
14	l	204	CLA	CHA-CBD-CGD-O2D
14	1	1612	CLA	CHA-CBD-CGD-O2D
14	1	1616	CLA	CHA-CBD-CGD-O2D
14	1	1618	CLA	CHA-CBD-CGD-O1D
14	1	1618	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	1	1621	CLA	CHA-CBD-CGD-O1D
14	1	1621	CLA	CHA-CBD-CGD-O2D
14	1	1627	CLA	CHA-CBD-CGD-O1D
14	1	1640	CLA	CHA-CBD-CGD-O1D
14	1	1640	CLA	CHA-CBD-CGD-O2D
14	1	1641	CLA	CHA-CBD-CGD-O2D
14	2	805	CLA	CHA-CBD-CGD-O1D
14	2	819	CLA	CHA-CBD-CGD-O1D
14	2	819	CLA	CHA-CBD-CGD-O2D
14	2	825	CLA	CHA-CBD-CGD-O1D
14	2	833	CLA	CHA-CBD-CGD-O1D
14	2	833	CLA	CHA-CBD-CGD-O2D
14	2	836	CLA	CHA-CBD-CGD-O2D
14	9	103	CLA	CHA-CBD-CGD-O1D
14	9	103	CLA	CHA-CBD-CGD-O2D
14	0	205	CLA	CHA-CBD-CGD-O2D
14	A	823	CLA	CAA-CBA-CGA-O1A
14	X	1701	CLA	CAA-CBA-CGA-O1A
14	x	1701	CLA	CAA-CBA-CGA-O1A
14	z	102	CLA	CAA-CBA-CGA-O1A
14	A	844	CLA	CAA-CBA-CGA-O1A
14	b	803	CLA	C16-C17-C18-C20
14	A	802	CLA	CAA-CBA-CGA-O2A
14	A	809	CLA	CAA-CBA-CGA-O2A
14	a	802	CLA	CAA-CBA-CGA-O2A
14	a	809	CLA	CAA-CBA-CGA-O2A
14	1	1603	CLA	CAA-CBA-CGA-O2A
14	1	1610	CLA	CAA-CBA-CGA-O2A
14	a	844	CLA	CAA-CBA-CGA-O1A
20	b	850	LMG	C19-C20-C21-C22
14	B	802	CLA	C16-C17-C18-C20
20	2	850	LMG	C19-C20-C21-C22
14	A	826	CLA	CAA-CBA-CGA-O2A
20	B	849	LMG	C19-C20-C21-C22
14	A	839	CLA	C6-C7-C8-C10
14	a	839	CLA	C6-C7-C8-C10
14	1	1640	CLA	C6-C7-C8-C10
14	A	843	CLA	CAA-CBA-CGA-O2A
14	a	826	CLA	CAA-CBA-CGA-O2A
14	1	1627	CLA	CAA-CBA-CGA-O2A
14	1	1644	CLA	CAA-CBA-CGA-O2A
13	A	801	CL0	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
13	a	801	CL0	C14-C13-C15-C16
13	1	1602	CL0	C14-C13-C15-C16
14	A	814	CLA	C11-C10-C8-C9
14	A	821	CLA	C6-C7-C8-C9
14	B	802	CLA	C11-C12-C13-C14
14	a	814	CLA	C11-C10-C8-C9
14	a	821	CLA	C6-C7-C8-C9
14	b	803	CLA	C11-C12-C13-C14
14	1	1615	CLA	C11-C10-C8-C9
14	1	1622	CLA	C6-C7-C8-C9
14	2	803	CLA	C11-C12-C13-C14
17	A	847	BCR	C14-C15-C16-C17
17	a	847	BCR	C14-C15-C16-C17
17	1	1648	BCR	C14-C15-C16-C17
14	a	843	CLA	CAA-CBA-CGA-O2A
14	A	835	CLA	C16-C17-C18-C20
14	a	835	CLA	C16-C17-C18-C20
14	1	1636	CLA	C16-C17-C18-C20
14	2	803	CLA	C16-C17-C18-C20
17	A	851	BCR	C11-C12-C13-C35
17	a	851	BCR	C11-C12-C13-C35
14	B	820	CLA	C16-C17-C18-C19
14	b	821	CLA	C16-C17-C18-C19
14	2	821	CLA	C16-C17-C18-C19
17	j	1304	BCR	C17-C18-C19-C20
14	A	835	CLA	C5-C6-C7-C8
14	A	821	CLA	C1A-C2A-CAA-CBA
14	A	823	CLA	C1A-C2A-CAA-CBA
14	A	837	CLA	C1A-C2A-CAA-CBA
14	A	855	CLA	C1A-C2A-CAA-CBA
14	B	809	CLA	C1A-C2A-CAA-CBA
14	J	101	CLA	C1A-C2A-CAA-CBA
14	a	821	CLA	C1A-C2A-CAA-CBA
14	a	823	CLA	C1A-C2A-CAA-CBA
14	a	837	CLA	C1A-C2A-CAA-CBA
14	b	802	CLA	C1A-C2A-CAA-CBA
14	b	810	CLA	C1A-C2A-CAA-CBA
14	j	1302	CLA	C1A-C2A-CAA-CBA
14	1	1622	CLA	C1A-C2A-CAA-CBA
14	1	1624	CLA	C1A-C2A-CAA-CBA
14	1	1638	CLA	C1A-C2A-CAA-CBA
14	2	802	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	2	810	CLA	C1A-C2A-CAA-CBA
14	8	1302	CLA	C1A-C2A-CAA-CBA
14	a	835	CLA	C5-C6-C7-C8
14	1	1636	CLA	C5-C6-C7-C8
14	B	813	CLA	CAA-CBA-CGA-O1A
14	B	835	CLA	CAA-CBA-CGA-O1A
14	b	836	CLA	CAA-CBA-CGA-O1A
14	2	836	CLA	CAA-CBA-CGA-O1A
14	A	813	CLA	CAA-CBA-CGA-O2A
14	a	813	CLA	CAA-CBA-CGA-O2A
14	1	1614	CLA	CAA-CBA-CGA-O2A
14	A	808	CLA	CAA-CBA-CGA-O2A
14	a	808	CLA	CAA-CBA-CGA-O2A
14	1	1609	CLA	CAA-CBA-CGA-O2A
14	2	821	CLA	C13-C15-C16-C17
14	b	814	CLA	CAA-CBA-CGA-O1A
14	2	814	CLA	CAA-CBA-CGA-O1A
14	B	820	CLA	C13-C15-C16-C17
14	b	821	CLA	C13-C15-C16-C17
14	A	805	CLA	C4-C3-C5-C6
14	a	805	CLA	C4-C3-C5-C6
14	B	810	CLA	C5-C6-C7-C8
14	B	829	CLA	C8-C10-C11-C12
14	b	811	CLA	C5-C6-C7-C8
14	b	830	CLA	C8-C10-C11-C12
14	2	811	CLA	C5-C6-C7-C8
14	2	830	CLA	C8-C10-C11-C12
14	A	840	CLA	C4B-C3B-CAB-CBB
14	B	837	CLA	C4B-C3B-CAB-CBB
14	a	840	CLA	C4B-C3B-CAB-CBB
14	b	838	CLA	C4B-C3B-CAB-CBB
14	1	1641	CLA	C4B-C3B-CAB-CBB
14	2	838	CLA	C4B-C3B-CAB-CBB
18	A	853	LHG	C4-O6-P-O5
18	a	853	LHG	C4-O6-P-O5
18	1	1654	LHG	C4-O6-P-O5
14	B	806	CLA	CAA-CBA-CGA-O1A
14	k	103	CLA	CAA-CBA-CGA-O1A
14	9	103	CLA	CAA-CBA-CGA-O1A
18	A	853	LHG	O9-C7-C8-C9
18	a	853	LHG	O9-C7-C8-C9
18	1	1654	LHG	O9-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
18	M	101	LHG	O6-C4-C5-C6
18	m	101	LHG	O6-C4-C5-C6
18	y	101	LHG	O6-C4-C5-C6
17	A	848	BCR	C5-C6-C7-C8
17	I	101	BCR	C5-C6-C7-C8
17	a	848	BCR	C5-C6-C7-C8
17	i	101	BCR	C5-C6-C7-C8
17	1	1649	BCR	C5-C6-C7-C8
17	7	101	BCR	C5-C6-C7-C8
14	K	103	CLA	CAA-CBA-CGA-O1A
13	A	801	CL0	CAA-CBA-CGA-O1A
13	a	801	CL0	CAA-CBA-CGA-O1A
13	1	1602	CL0	CAA-CBA-CGA-O1A
14	A	802	CLA	CAA-CBA-CGA-O1A
14	B	819	CLA	CAA-CBA-CGA-O1A
14	a	802	CLA	CAA-CBA-CGA-O1A
14	b	807	CLA	CAA-CBA-CGA-O1A
14	b	820	CLA	CAA-CBA-CGA-O1A
14	1	1603	CLA	CAA-CBA-CGA-O1A
14	2	807	CLA	CAA-CBA-CGA-O1A
14	2	821	CLA	C10-C11-C12-C13
14	A	810	CLA	CAA-CBA-CGA-O2A
14	a	810	CLA	CAA-CBA-CGA-O2A
14	1	1611	CLA	CAA-CBA-CGA-O2A
14	B	820	CLA	C10-C11-C12-C13
14	b	821	CLA	C10-C11-C12-C13
14	2	820	CLA	CAA-CBA-CGA-O1A
14	1	1606	CLA	C4-C3-C5-C6
17	A	850	BCR	C19-C20-C21-C22
13	A	801	CL0	CAD-CBD-CGD-O1D
13	a	801	CL0	CAD-CBD-CGD-O1D
13	1	1602	CL0	CAD-CBD-CGD-O1D
14	A	824	CLA	CAD-CBD-CGD-O1D
14	A	830	CLA	CAD-CBD-CGD-O1D
14	B	807	CLA	CAD-CBD-CGD-O1D
14	B	828	CLA	CAD-CBD-CGD-O1D
14	B	831	CLA	CAD-CBD-CGD-O1D
14	J	101	CLA	CAD-CBD-CGD-O1D
14	a	824	CLA	CAD-CBD-CGD-O1D
14	a	830	CLA	CAD-CBD-CGD-O1D
14	b	808	CLA	CAD-CBD-CGD-O1D
14	b	829	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	b	832	CLA	CAD-CBD-CGD-O1D
14	b	838	CLA	CAD-CBD-CGD-O1D
14	j	1302	CLA	CAD-CBD-CGD-O1D
14	1	1625	CLA	CAD-CBD-CGD-O1D
14	1	1631	CLA	CAD-CBD-CGD-O1D
14	2	808	CLA	CAD-CBD-CGD-O1D
14	2	829	CLA	CAD-CBD-CGD-O1D
14	2	832	CLA	CAD-CBD-CGD-O1D
14	2	838	CLA	CAD-CBD-CGD-O1D
14	8	1302	CLA	CAD-CBD-CGD-O1D
20	B	849	LMG	O9-C10-C11-C12
20	b	850	LMG	O9-C10-C11-C12
20	2	850	LMG	O9-C10-C11-C12
14	A	830	CLA	C13-C15-C16-C17
14	a	830	CLA	C13-C15-C16-C17
14	1	1631	CLA	C13-C15-C16-C17
14	A	816	CLA	C11-C10-C8-C9
14	B	832	CLA	C6-C7-C8-C9
14	B	840	CLA	C14-C13-C15-C16
14	a	816	CLA	C11-C10-C8-C9
14	b	833	CLA	C6-C7-C8-C9
14	b	841	CLA	C14-C13-C15-C16
14	1	1617	CLA	C11-C10-C8-C9
14	2	833	CLA	C6-C7-C8-C9
14	2	841	CLA	C14-C13-C15-C16
18	a	853	LHG	C14-C15-C16-C17
14	0	206	CLA	C13-C15-C16-C17
18	1	1654	LHG	C14-C15-C16-C17
18	A	853	LHG	C14-C15-C16-C17
14	L	204	CLA	C13-C15-C16-C17
14	l	205	CLA	C13-C15-C16-C17
14	B	827	CLA	C2C-C3C-CAC-CBC
18	B	850	LHG	C17-C18-C19-C20
18	z	101	LHG	C17-C18-C19-C20
14	A	816	CLA	CAA-CBA-CGA-O2A
14	A	840	CLA	CAA-CBA-CGA-O2A
14	a	840	CLA	CAA-CBA-CGA-O2A
14	b	829	CLA	CAA-CBA-CGA-O2A
14	1	1641	CLA	CAA-CBA-CGA-O2A
14	2	829	CLA	CAA-CBA-CGA-O2A
14	A	830	CLA	C8-C10-C11-C12
14	a	830	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
18	b	851	LHG	C17-C18-C19-C20
14	B	832	CLA	C4-C3-C5-C6
14	b	833	CLA	C4-C3-C5-C6
14	2	833	CLA	C4-C3-C5-C6
14	1	1631	CLA	C8-C10-C11-C12
14	A	804	CLA	C12-C13-C15-C16
14	A	809	CLA	C6-C7-C8-C10
14	A	829	CLA	C6-C7-C8-C10
14	B	815	CLA	C6-C7-C8-C10
14	B	817	CLA	C12-C13-C15-C16
14	B	824	CLA	C11-C10-C8-C7
14	a	804	CLA	C12-C13-C15-C16
14	a	809	CLA	C6-C7-C8-C10
14	a	829	CLA	C6-C7-C8-C10
14	b	816	CLA	C6-C7-C8-C10
14	b	818	CLA	C12-C13-C15-C16
14	b	825	CLA	C11-C10-C8-C7
14	1	1605	CLA	C12-C13-C15-C16
14	1	1610	CLA	C6-C7-C8-C10
14	1	1630	CLA	C6-C7-C8-C10
14	2	816	CLA	C6-C7-C8-C10
14	2	818	CLA	C12-C13-C15-C16
14	2	825	CLA	C11-C10-C8-C7
14	A	809	CLA	CAA-CBA-CGA-O1A
14	A	843	CLA	CAA-CBA-CGA-O1A
14	B	817	CLA	CAA-CBA-CGA-O1A
14	a	809	CLA	CAA-CBA-CGA-O1A
14	a	843	CLA	CAA-CBA-CGA-O1A
14	b	828	CLA	C2C-C3C-CAC-CBC
14	B	803	CLA	CAA-CBA-CGA-O2A
14	B	817	CLA	CAA-CBA-CGA-O2A
14	B	828	CLA	CAA-CBA-CGA-O2A
14	a	816	CLA	CAA-CBA-CGA-O2A
14	b	804	CLA	CAA-CBA-CGA-O2A
14	b	818	CLA	CAA-CBA-CGA-O2A
14	1	1617	CLA	CAA-CBA-CGA-O2A
14	2	804	CLA	CAA-CBA-CGA-O2A
14	2	818	CLA	CAA-CBA-CGA-O2A
20	B	849	LMG	C33-C34-C35-C36
20	b	850	LMG	C33-C34-C35-C36
20	2	850	LMG	C33-C34-C35-C36
17	J	103	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
17	8	1304	BCR	C17-C18-C19-C20
14	b	818	CLA	CAA-CBA-CGA-O1A
14	1	1610	CLA	CAA-CBA-CGA-O1A
14	2	818	CLA	CAA-CBA-CGA-O1A
14	A	813	CLA	CAA-CBA-CGA-O1A
14	a	813	CLA	CAA-CBA-CGA-O1A
14	1	1614	CLA	CAA-CBA-CGA-O1A
17	a	850	BCR	C19-C20-C21-C22
17	1	1651	BCR	C19-C20-C21-C22
14	A	835	CLA	C16-C17-C18-C19
14	a	835	CLA	C16-C17-C18-C19
14	1	1636	CLA	C16-C17-C18-C19
14	a	841	CLA	CAA-CBA-CGA-O2A
14	2	828	CLA	C2C-C3C-CAC-CBC
14	A	817	CLA	C10-C11-C12-C13
14	a	817	CLA	C10-C11-C12-C13
14	1	1618	CLA	C10-C11-C12-C13
14	A	808	CLA	CAA-CBA-CGA-O1A
14	A	816	CLA	CAA-CBA-CGA-O1A
14	A	840	CLA	CAA-CBA-CGA-O1A
14	a	808	CLA	CAA-CBA-CGA-O1A
14	1	1609	CLA	CAA-CBA-CGA-O1A
14	1	1617	CLA	CAA-CBA-CGA-O1A
14	1	1644	CLA	CAA-CBA-CGA-O1A
14	A	841	CLA	CAA-CBA-CGA-O2A
14	1	1642	CLA	CAA-CBA-CGA-O2A
14	A	826	CLA	CAA-CBA-CGA-O1A
14	a	816	CLA	CAA-CBA-CGA-O1A
14	a	826	CLA	CAA-CBA-CGA-O1A
14	a	840	CLA	CAA-CBA-CGA-O1A
14	1	1627	CLA	CAA-CBA-CGA-O1A
14	1	1641	CLA	CAA-CBA-CGA-O1A
14	B	820	CLA	C2A-CAA-CBA-CGA
14	b	821	CLA	C2A-CAA-CBA-CGA
14	2	821	CLA	C2A-CAA-CBA-CGA
14	A	806	CLA	C15-C16-C17-C18
14	A	817	CLA	C8-C10-C11-C12
14	a	806	CLA	C15-C16-C17-C18
14	a	817	CLA	C8-C10-C11-C12
14	1	1607	CLA	C15-C16-C17-C18
14	1	1618	CLA	C8-C10-C11-C12

There are no ring outliers.

221 monomers are involved in 322 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b	818	CLA	4	0
14	2	835	CLA	2	0
14	A	830	CLA	2	0
14	a	827	CLA	2	0
14	b	806	CLA	1	0
14	a	829	CLA	2	0
14	2	809	CLA	1	0
14	1	1635	CLA	2	0
14	2	812	CLA	2	0
14	B	837	CLA	1	0
14	j	1301	CLA	1	0
14	1	1608	CLA	1	0
14	a	815	CLA	2	0
14	z	102	CLA	3	0
14	A	825	CLA	1	0
14	j	1302	CLA	1	0
14	a	830	CLA	1	0
14	1	1634	CLA	2	0
14	a	813	CLA	1	0
14	A	816	CLA	1	0
14	1	1628	CLA	2	0
13	a	801	CL0	2	0
14	b	811	CLA	4	0
14	B	817	CLA	3	0
14	a	806	CLA	1	0
14	1	1615	CLA	2	0
14	A	840	CLA	1	0
18	a	853	LHG	1	0
14	a	831	CLA	1	0
14	1	1630	CLA	2	0
17	m	102	BCR	2	0
14	a	812	CLA	1	0
14	2	811	CLA	2	0
14	a	824	CLA	2	0
14	b	838	CLA	2	0
14	A	807	CLA	1	0
14	a	835	CLA	1	0
14	L	205	CLA	2	0
14	b	839	CLA	1	0
14	1	1632	CLA	1	0
14	B	816	CLA	1	0
14	a	818	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	l	204	CLA	1	0
14	b	814	CLA	1	0
18	b	851	LHG	3	0
14	F	203	CLA	2	0
14	b	809	CLA	1	0
17	I	101	BCR	3	0
14	b	812	CLA	3	0
14	A	841	CLA	3	0
17	1	1652	BCR	3	0
17	f	202	BCR	1	0
18	z	101	LHG	13	0
14	a	832	CLA	1	0
17	F	202	BCR	1	0
14	a	807	CLA	1	0
14	a	821	CLA	2	0
17	a	851	BCR	4	0
14	A	857	CLA	1	0
15	A	845	PQN	1	0
14	B	841	CLA	1	0
14	A	819	CLA	3	0
14	2	815	CLA	2	0
14	B	840	CLA	1	0
14	2	828	CLA	1	0
17	b	852	BCR	1	0
14	A	839	CLA	1	0
14	1	1620	CLA	5	0
14	x	1701	CLA	4	0
14	a	823	CLA	1	0
14	l	206	CLA	2	0
14	b	802	CLA	4	0
14	B	831	CLA	3	0
14	a	814	CLA	2	0
14	B	819	CLA	1	0
14	A	833	CLA	1	0
14	b	820	CLA	1	0
14	a	816	CLA	1	0
14	1	1624	CLA	3	0
14	B	839	CLA	1	0
14	a	841	CLA	3	0
14	1	1607	CLA	1	0
18	L	208	LHG	1	0
14	1	1625	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	814	CLA	2	0
14	1	1629	CLA	1	0
14	2	802	CLA	2	0
14	6	201	CLA	2	0
14	a	828	CLA	1	0
14	a	840	CLA	1	0
14	a	819	CLA	3	0
14	b	817	CLA	1	0
14	b	823	CLA	1	0
18	y	101	LHG	2	0
14	A	802	CLA	2	0
14	K	101	CLA	1	0
14	1	1613	CLA	1	0
14	A	827	CLA	2	0
14	A	834	CLA	1	0
17	A	851	BCR	4	0
14	B	804	CLA	1	0
14	B	802	CLA	1	0
14	A	828	CLA	1	0
14	1	1605	CLA	1	0
14	2	804	CLA	2	0
14	2	833	CLA	1	0
14	1	1603	CLA	2	0
14	1	1604	CLA	1	0
14	L	204	CLA	1	0
14	A	831	CLA	1	0
14	A	829	CLA	2	0
14	1	1642	CLA	3	0
14	B	827	CLA	1	0
14	2	832	CLA	2	0
14	b	836	CLA	3	0
14	L	203	CLA	1	0
17	A	856	BCR	2	0
14	1	1616	CLA	2	0
14	1	1619	CLA	3	0
14	A	815	CLA	2	0
14	2	818	CLA	3	0
14	a	843	CLA	2	0
18	M	101	LHG	1	0
14	a	804	CLA	1	0
17	B	846	BCR	1	0
14	0	206	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	850	LHG	3	0
14	2	836	CLA	1	0
14	B	805	CLA	1	0
14	A	813	CLA	1	0
14	8	1302	CLA	1	0
18	0	202	LHG	1	0
18	m	101	LHG	1	0
14	B	832	CLA	2	0
15	a	845	PQN	1	0
14	a	833	CLA	2	0
14	B	834	CLA	2	0
14	A	809	CLA	1	0
14	J	101	CLA	1	0
17	0	201	BCR	1	0
14	B	810	CLA	2	0
14	A	812	CLA	1	0
14	b	840	CLA	1	0
14	b	834	CLA	2	0
14	A	824	CLA	2	0
14	2	839	CLA	2	0
14	1	1644	CLA	1	0
14	2	825	CLA	1	0
14	2	803	CLA	1	0
14	A	835	CLA	1	0
14	M	102	CLA	1	0
14	2	805	CLA	1	0
14	B	835	CLA	1	0
14	A	804	CLA	2	0
17	l	207	BCR	1	0
14	2	817	CLA	2	0
14	B	811	CLA	3	0
14	1	1640	CLA	1	0
17	9	102	BCR	1	0
14	b	808	CLA	1	0
14	1	1601	CLA	1	0
14	b	825	CLA	2	0
14	A	806	CLA	1	0
17	M	103	BCR	4	0
14	a	825	CLA	1	0
14	b	803	CLA	1	0
14	0	207	CLA	2	0
14	b	804	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	2	847	BCR	1	0
14	a	839	CLA	1	0
14	b	805	CLA	1	0
17	0	208	BCR	1	0
14	2	808	CLA	2	0
14	l	205	CLA	1	0
14	A	820	CLA	1	0
14	a	810	CLA	1	0
14	X	1701	CLA	3	0
14	f	201	CLA	3	0
17	1	1653	BCR	1	0
14	B	808	CLA	1	0
14	1	1617	CLA	1	0
14	B	824	CLA	2	0
14	A	818	CLA	3	0
14	1	1636	CLA	1	0
14	9	103	CLA	1	0
14	B	803	CLA	1	0
17	A	849	BCR	1	0
17	a	849	BCR	1	0
17	8	1305	BCR	2	0
17	0	203	BCR	2	0
15	1	1646	PQN	1	0
14	b	833	CLA	2	0
14	b	828	CLA	1	0
14	b	835	CLA	2	0
14	A	843	CLA	1	0
14	0	205	CLA	1	0
14	1	1622	CLA	2	0
14	1	1621	CLA	1	0
14	B	822	CLA	1	0
14	2	823	CLA	1	0
14	1	1626	CLA	1	0
14	F	201	CLA	2	0
18	l	201	LHG	1	0
14	b	815	CLA	1	0
14	1	1611	CLA	2	0
14	A	810	CLA	1	0
17	1	1650	BCR	1	0
14	A	814	CLA	2	0
18	A	853	LHG	1	0
14	8	1301	CLA	1	0

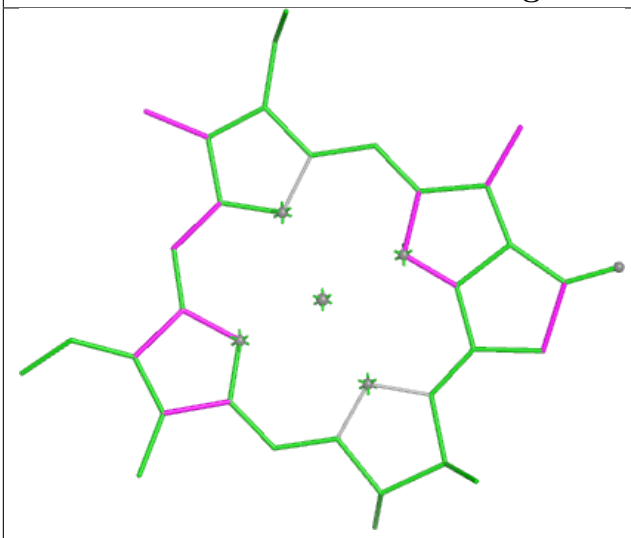
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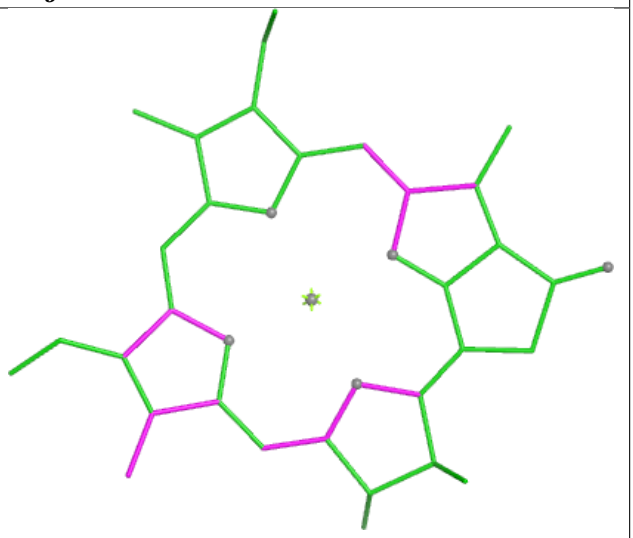
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	855	CLA	2	0
18	1	1654	LHG	1	0
14	1	1614	CLA	1	0
17	L	206	BCR	1	0
14	1	1641	CLA	1	0
14	B	833	CLA	2	0
17	6	204	BCR	2	0
17	b	847	BCR	1	0
17	y	102	BCR	2	0
14	a	820	CLA	1	0
14	A	821	CLA	2	0

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.

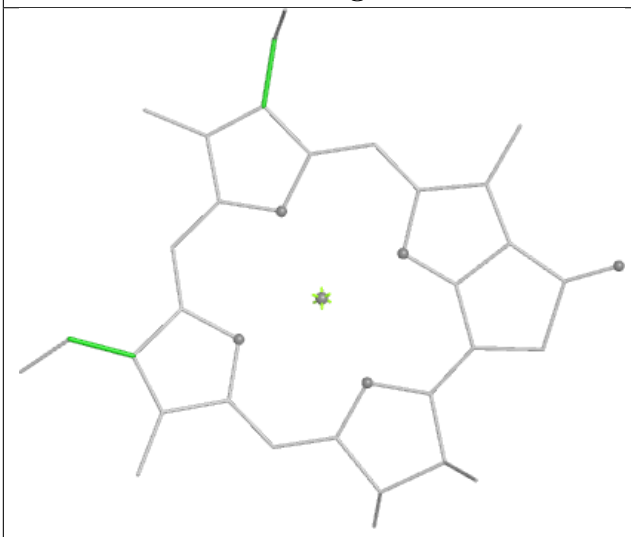
Ligand CLA j 1303



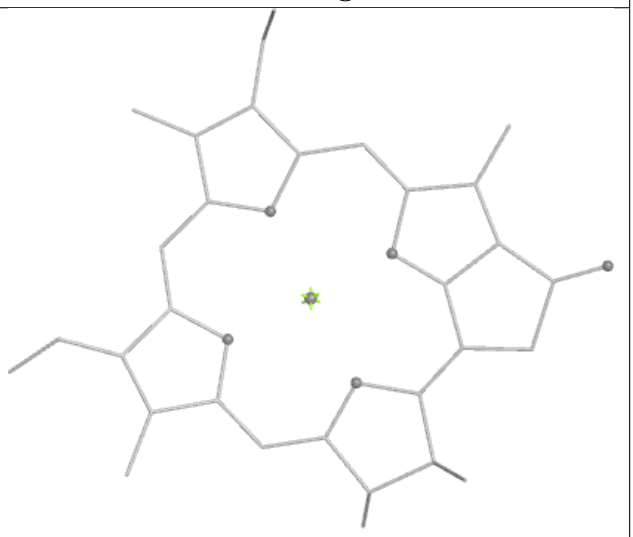
Bond lengths



Bond angles

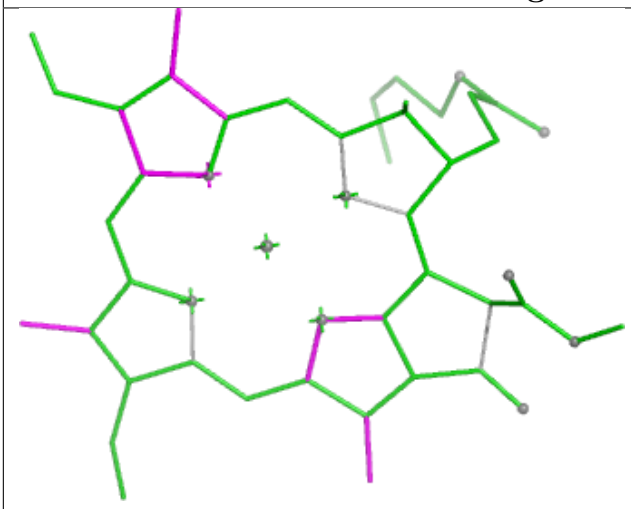


Torsions



Rings

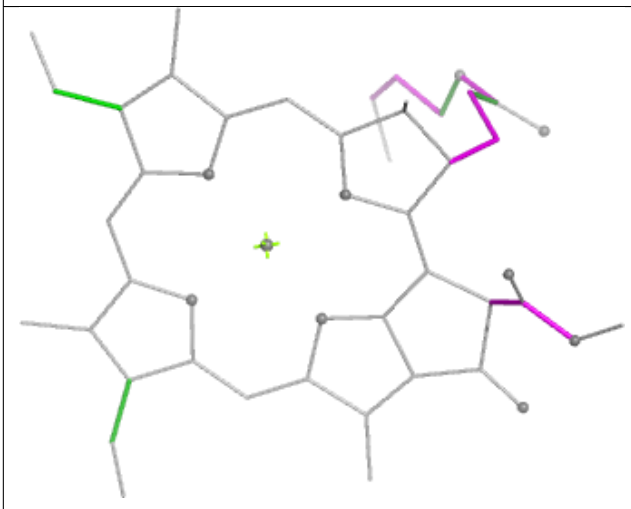
Ligand CLA b 832



Bond lengths



Bond angles

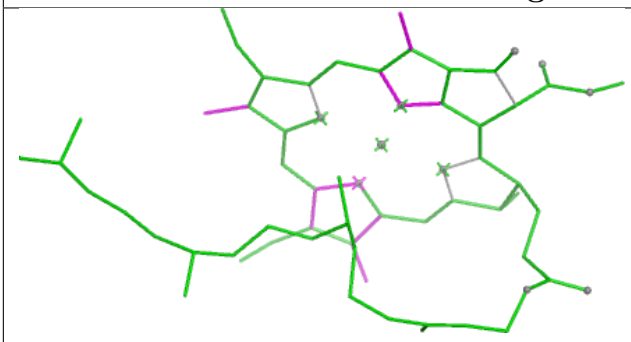


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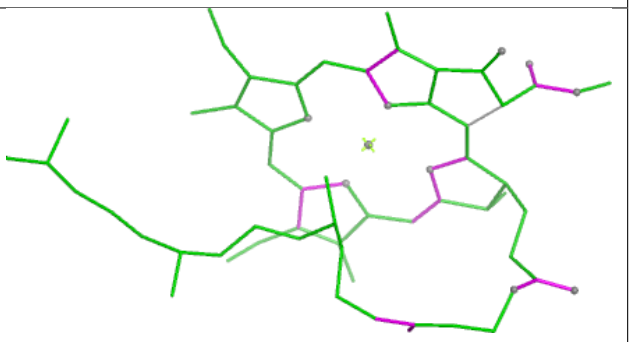


Rings

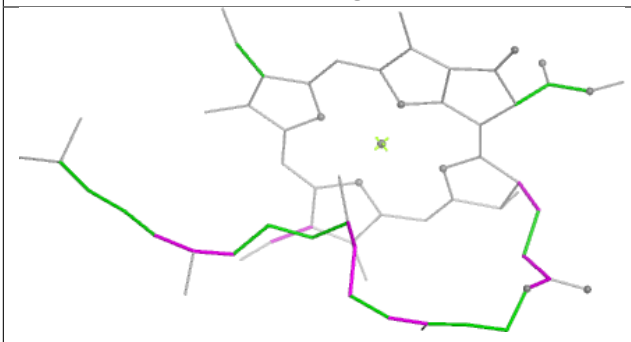
Ligand CLA b 818



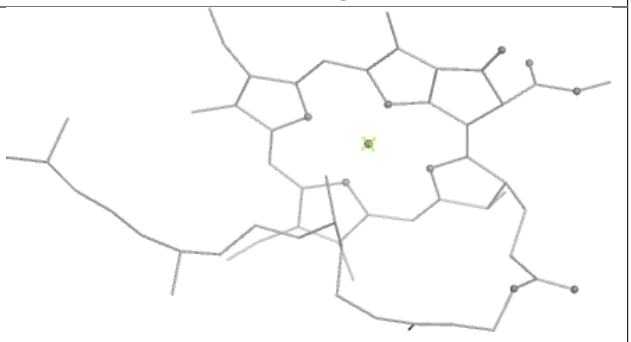
Bond lengths



Bond angles

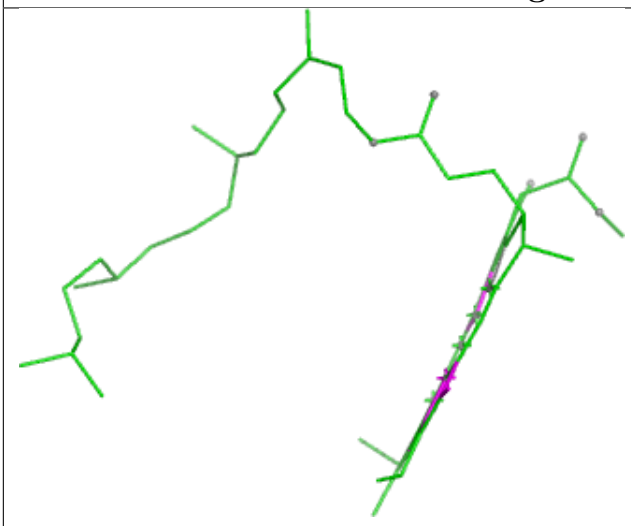


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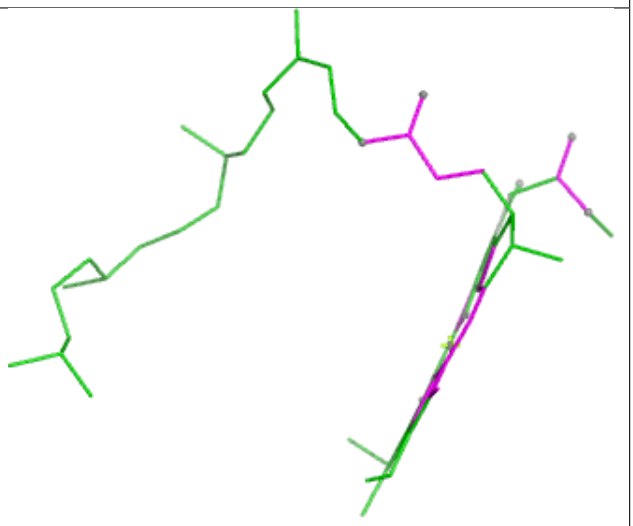


Rings

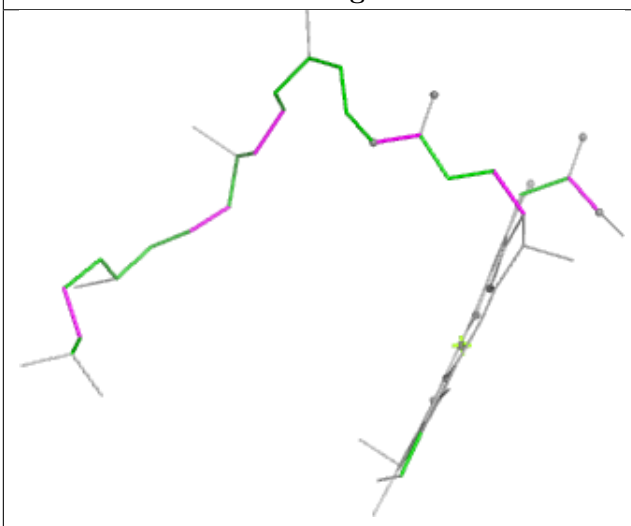
Ligand CLA 2 835



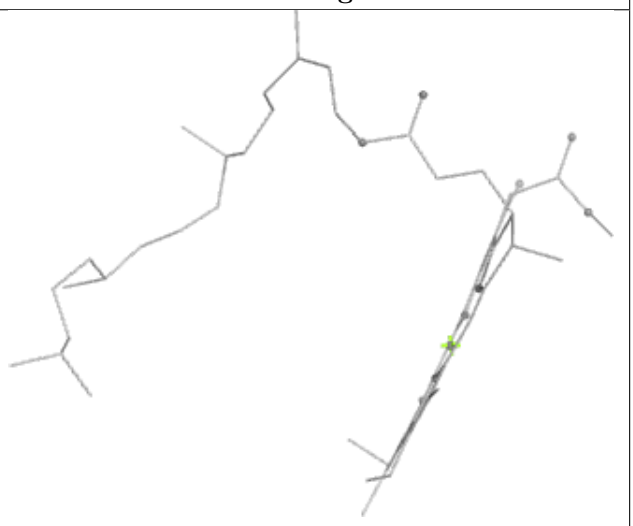
Bond lengths



Bond angles

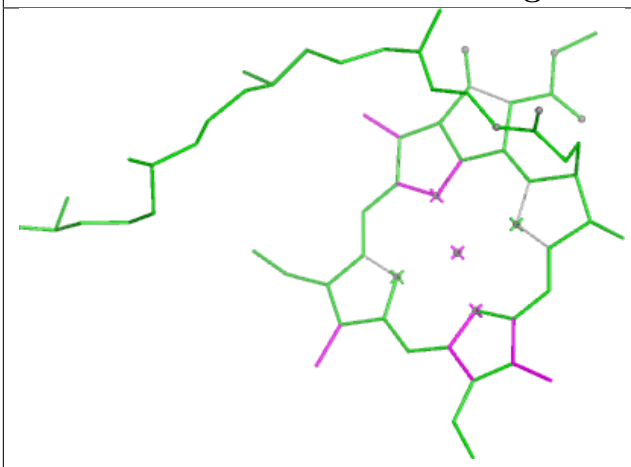


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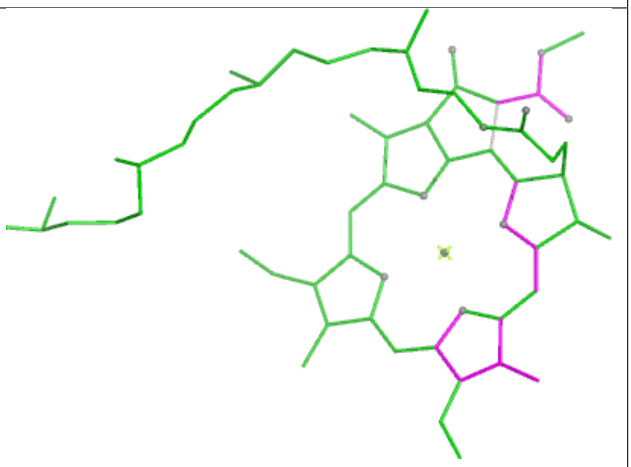


Rings

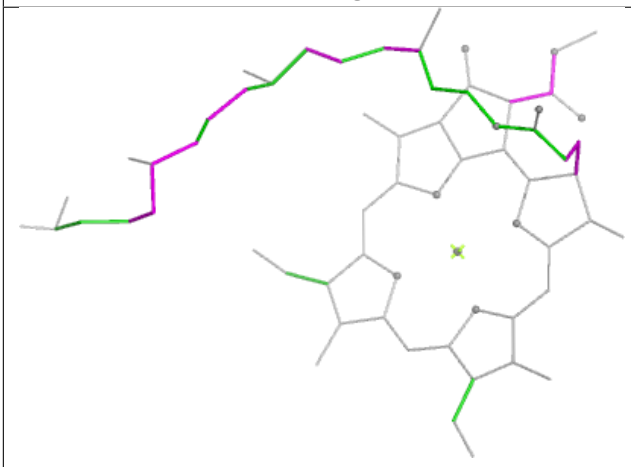
Ligand CLA A 830



Bond lengths



Bond angles

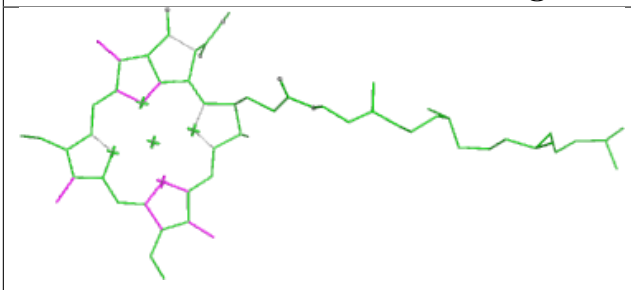


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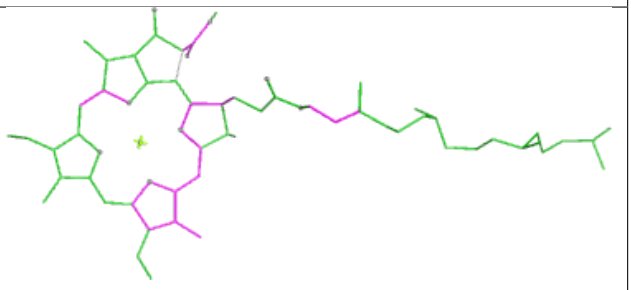


Rings

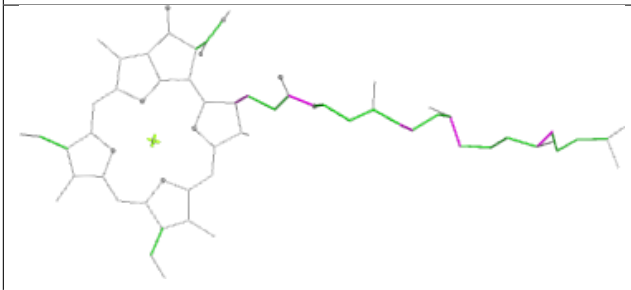
Ligand CLA a 827



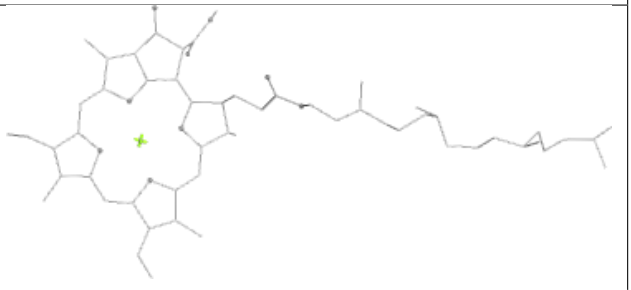
Bond lengths



Bond angles

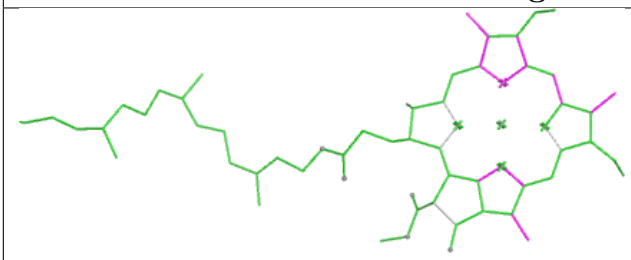


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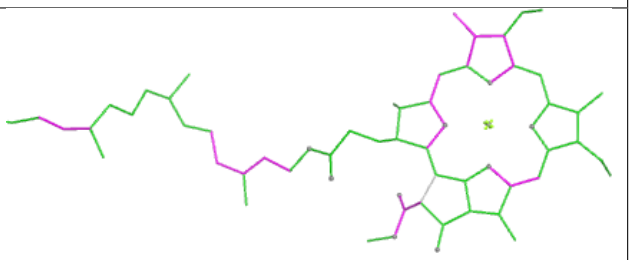


Rings

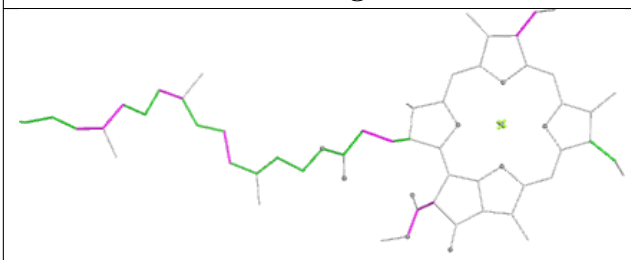
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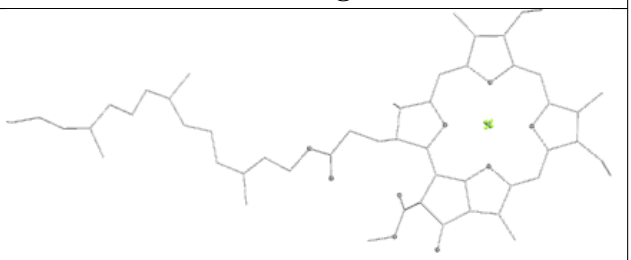
Bond lengths



Bond angles

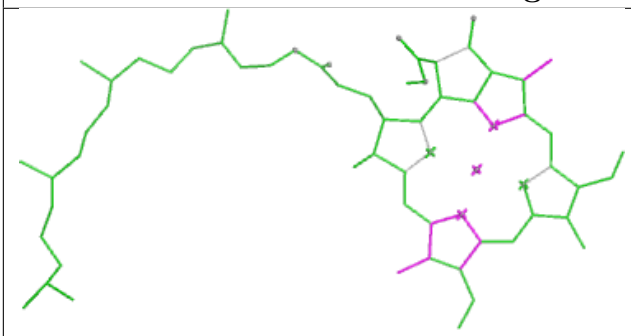


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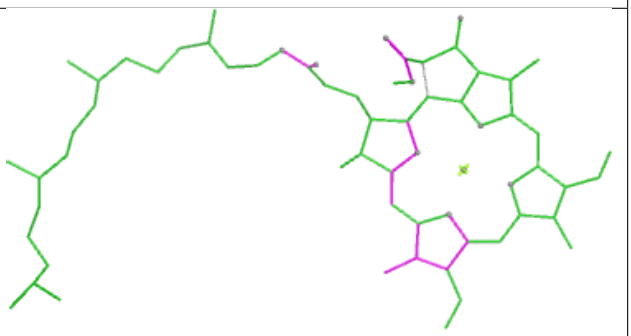


Rings

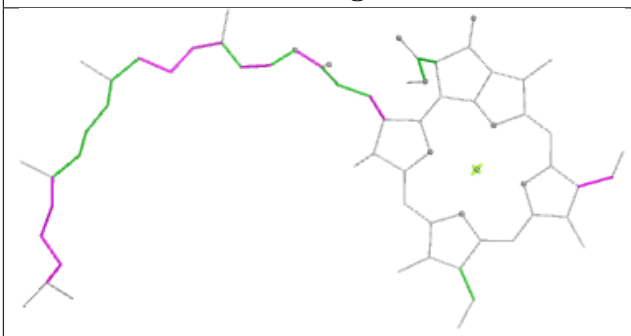
Ligand CLA A 838



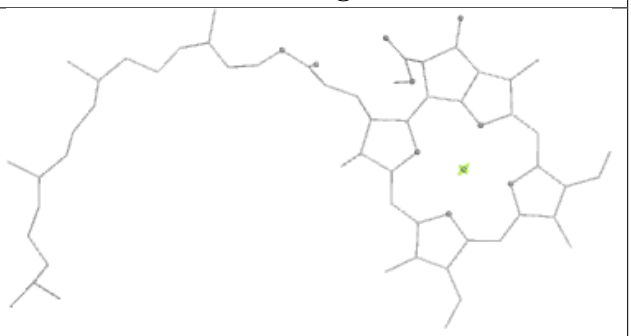
Bond lengths



Bond angles

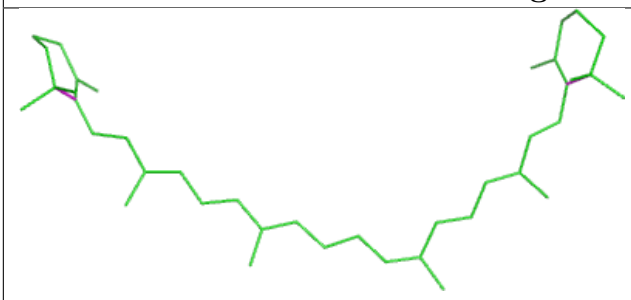


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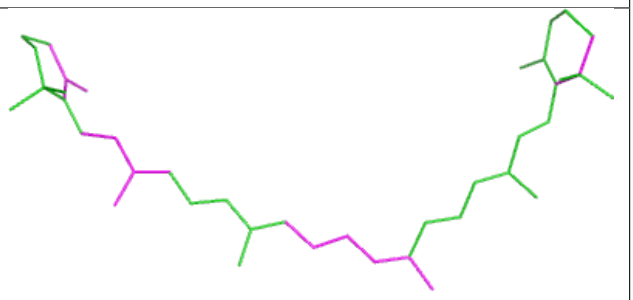


Rings

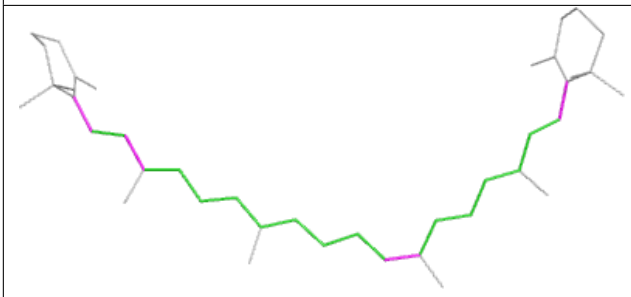
Ligand BCR f 204



Bond lengths



Bond angles

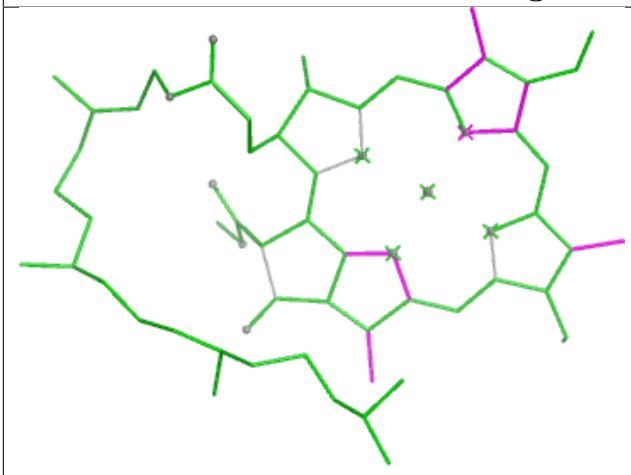


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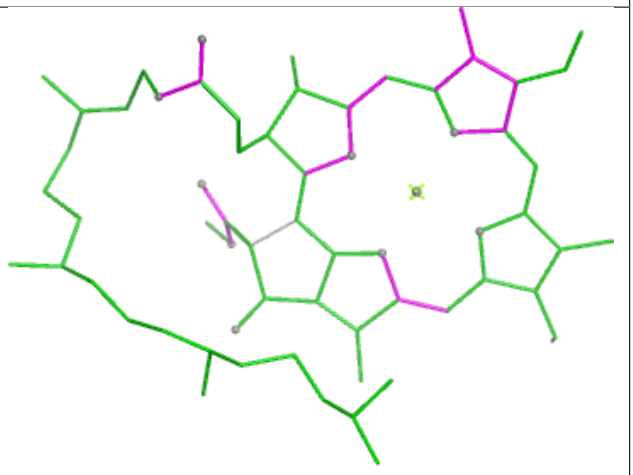


Rings

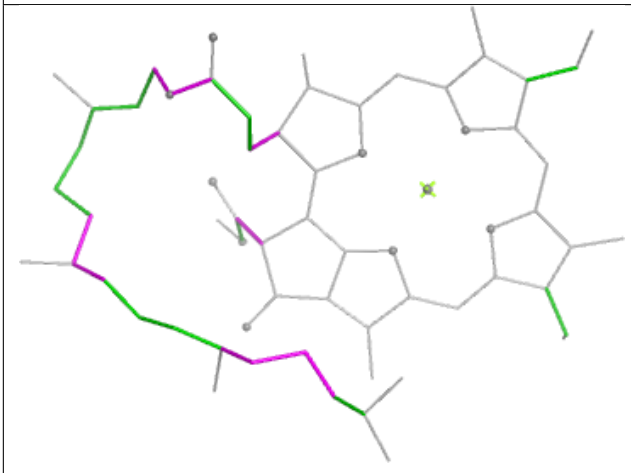
Ligand CLA b 806



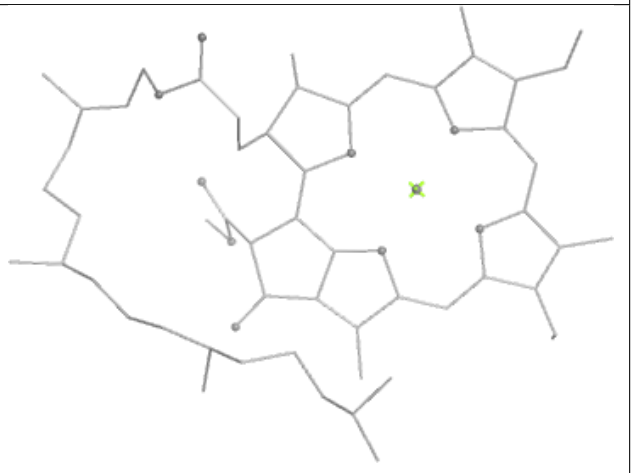
Bond lengths



Bond angles

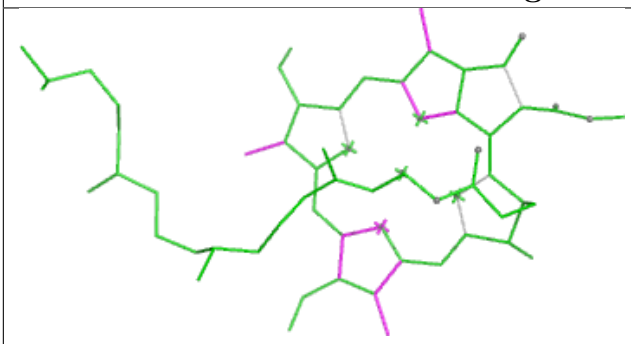


Torsions

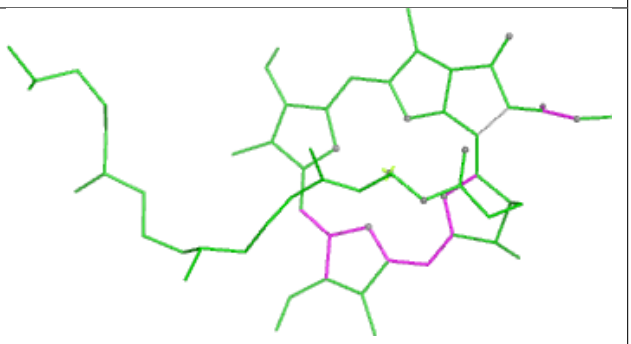


Rings

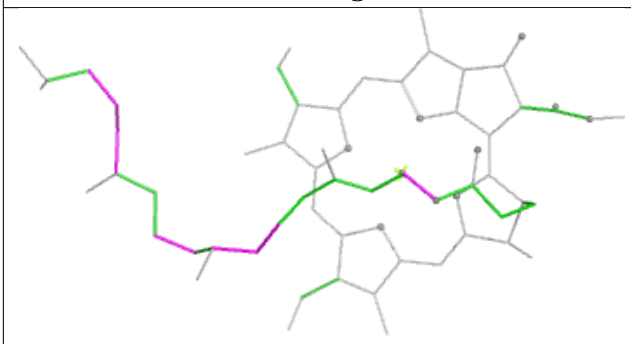
Ligand CLA B 838



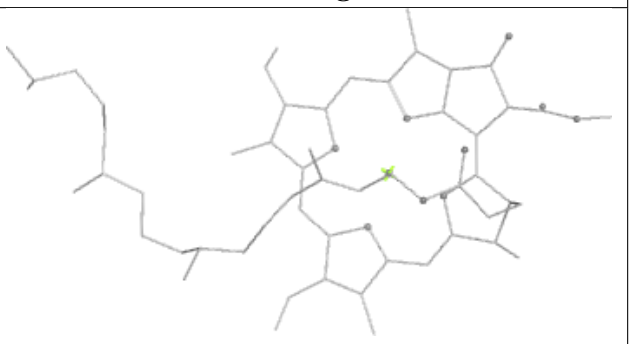
Bond lengths



Bond angles



Torsions

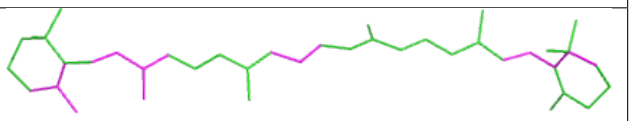


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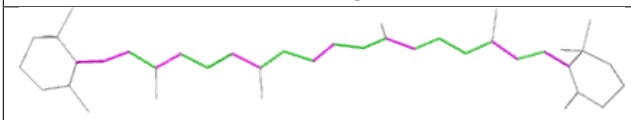
Ligand BCR A 847



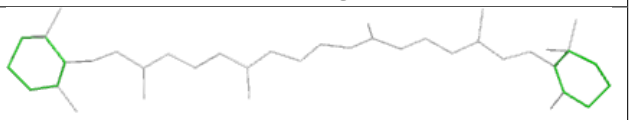
Bond lengths



Bond angles

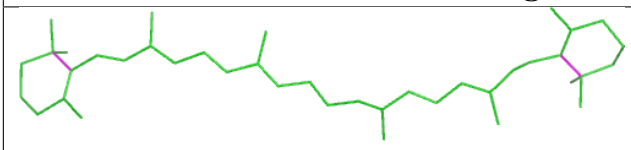


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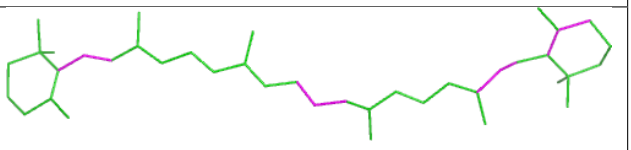


Rings

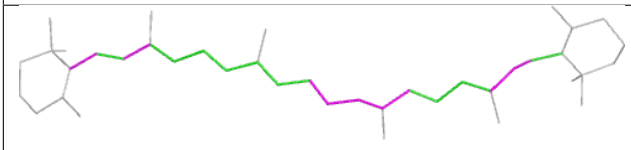
Ligand BCR B 843



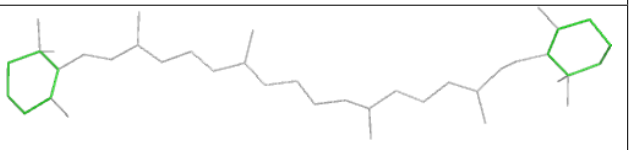
Bond lengths



Bond angles

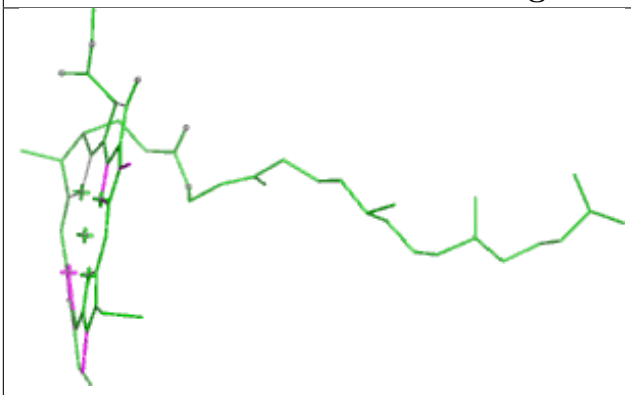


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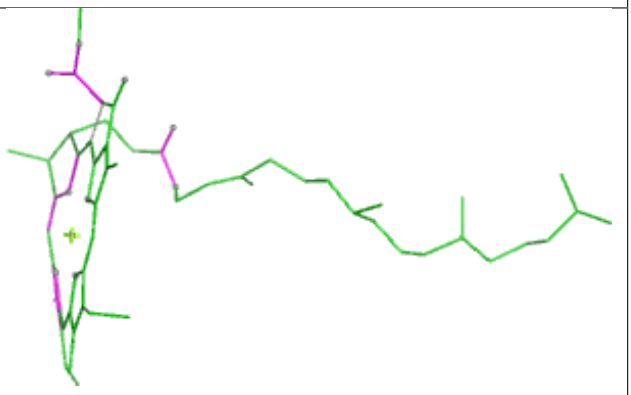


Rings

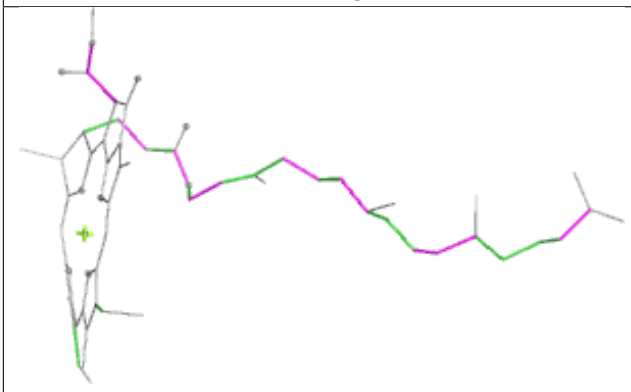
Ligand CLA a 829



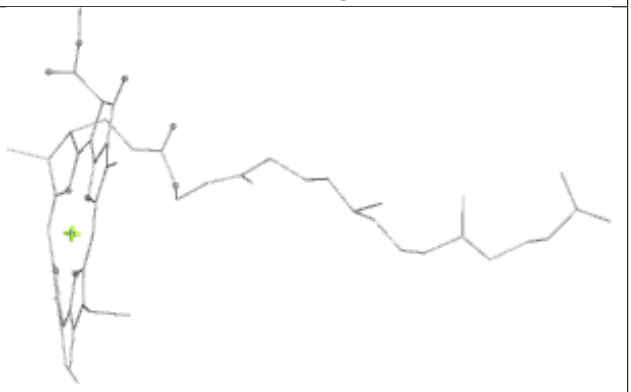
Bond lengths



Bond angles



Torsions



Rings

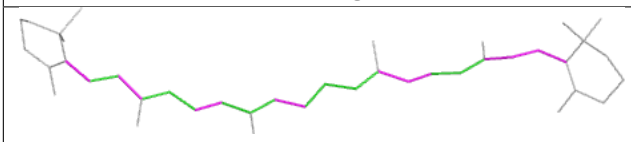
Ligand BCR b 848



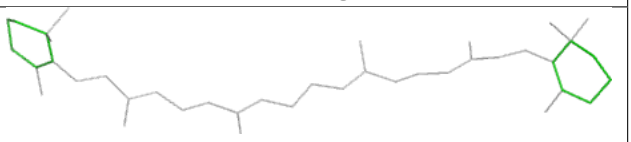
Bond lengths



Bond angles

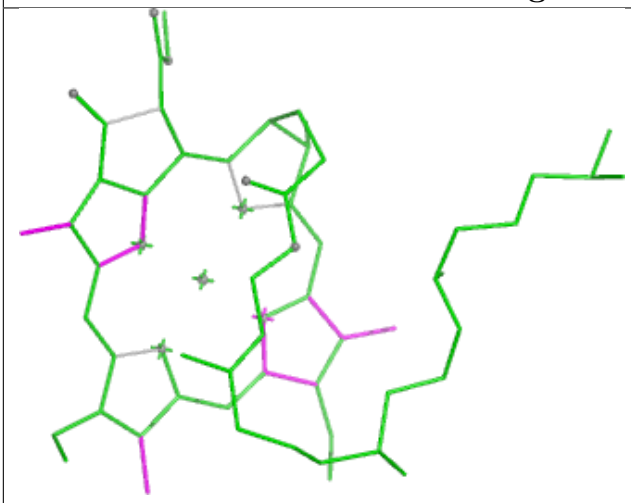


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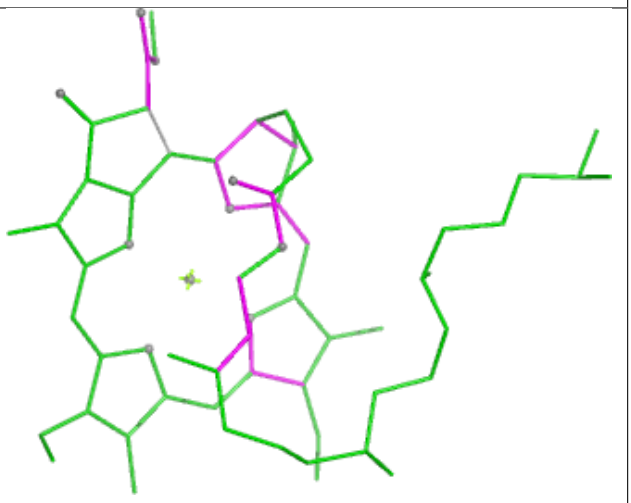


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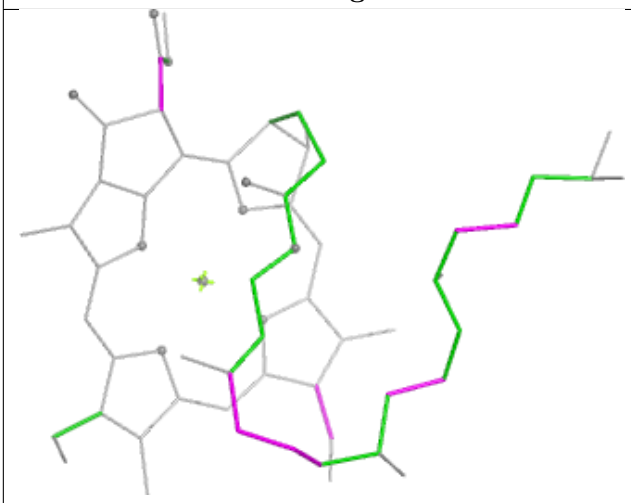
Ligand CLA 2 809



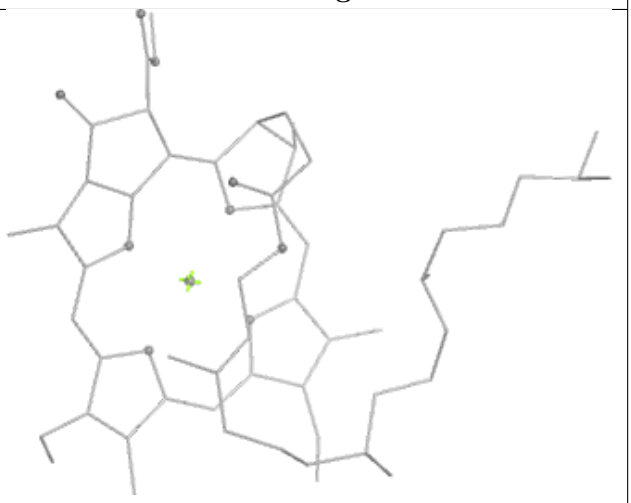
Bond lengths



Bond angles

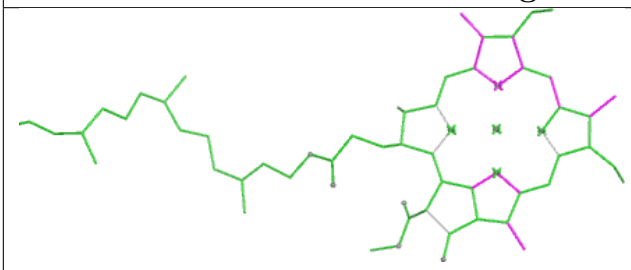


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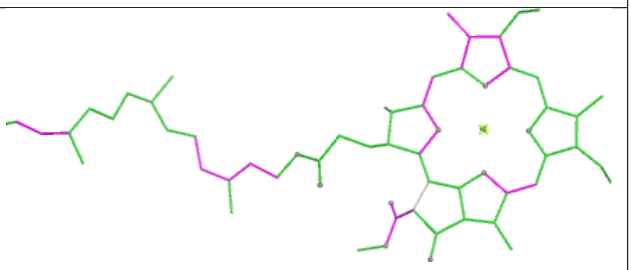


Rings

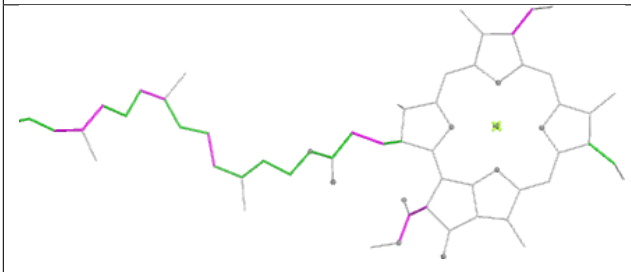
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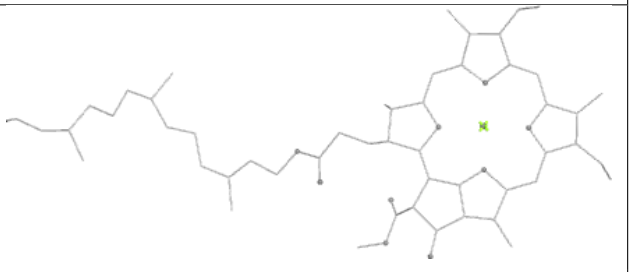
Bond lengths



Bond angles



Torsions



Rings

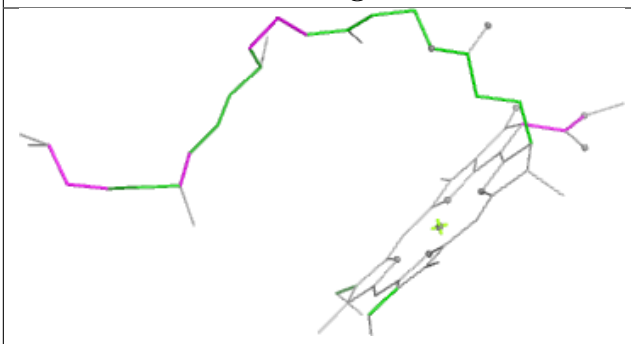
Ligand CLA 2 812



Bond lengths



Bond angles

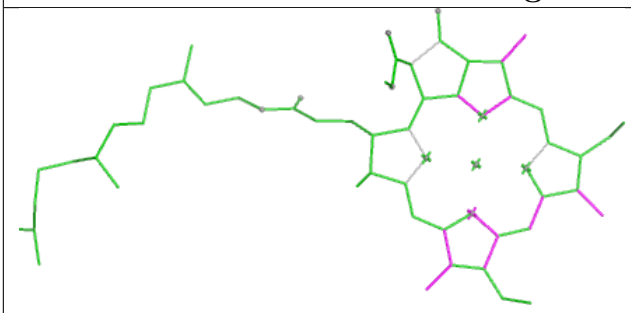


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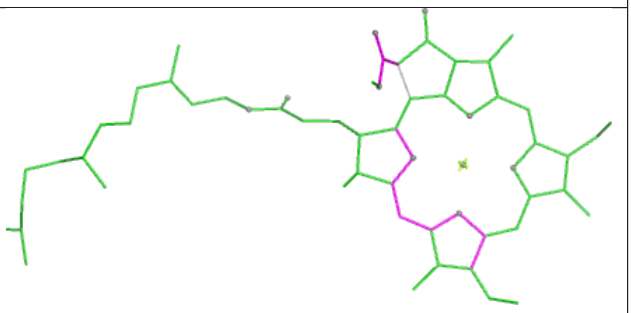


Rings

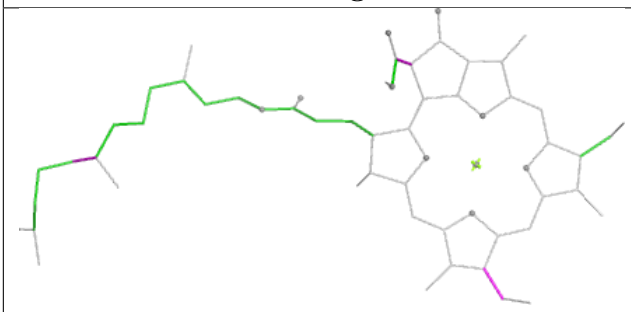
Ligand CLA B 837



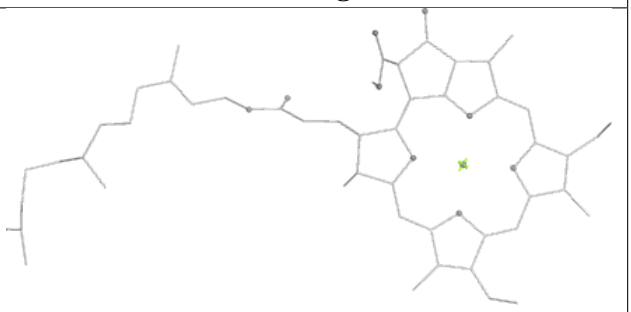
Bond lengths



Bond angles

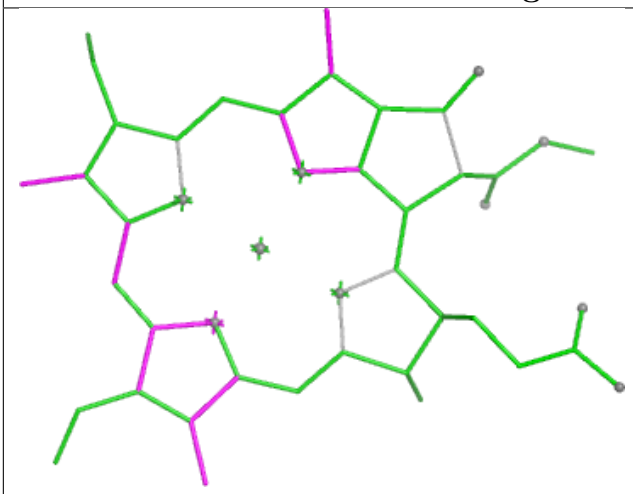


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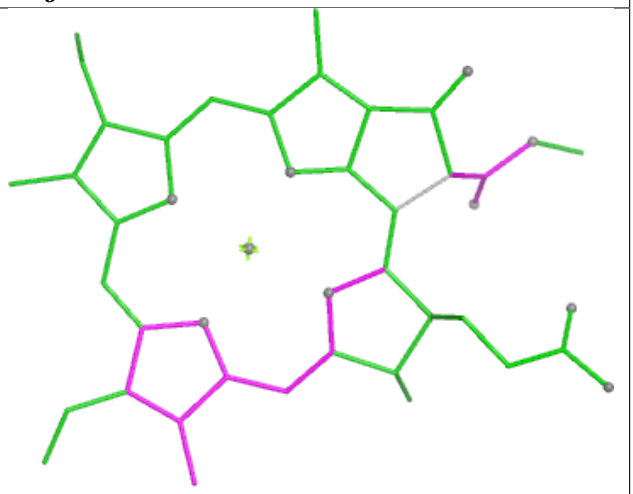


Rings

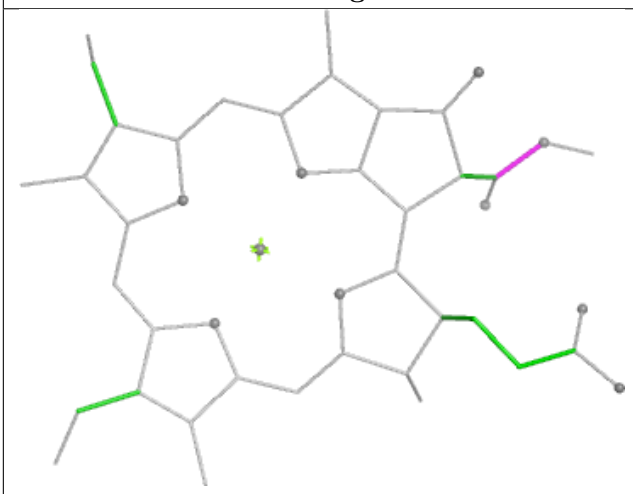
Ligand CLA j 1301



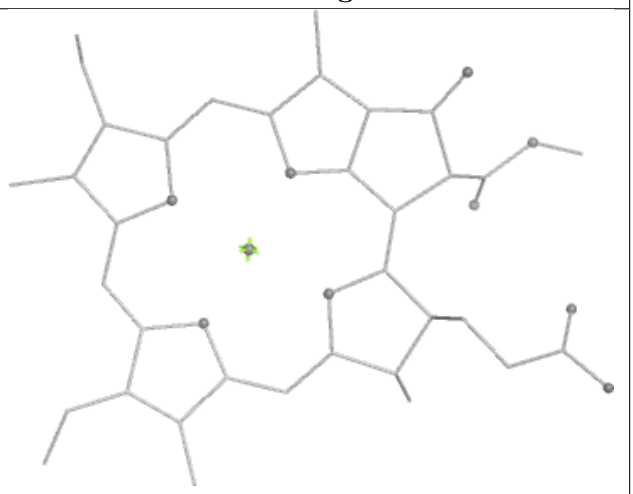
Bond lengths



Bond angles

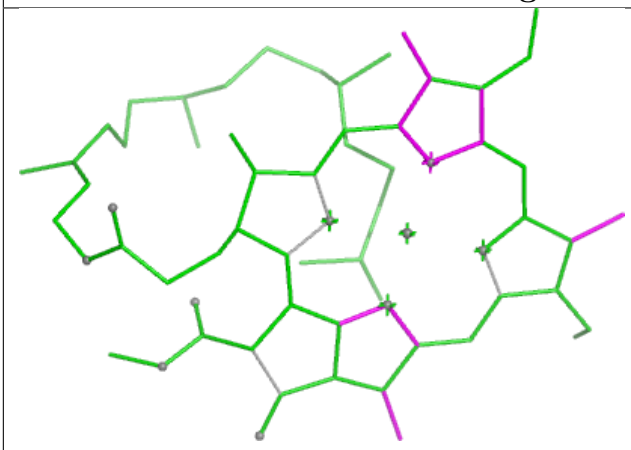


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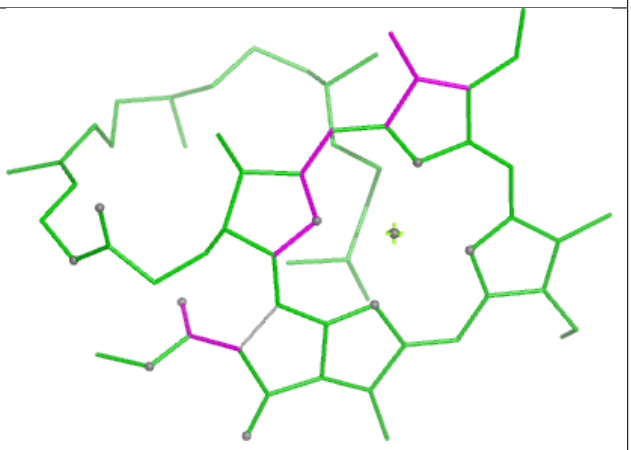


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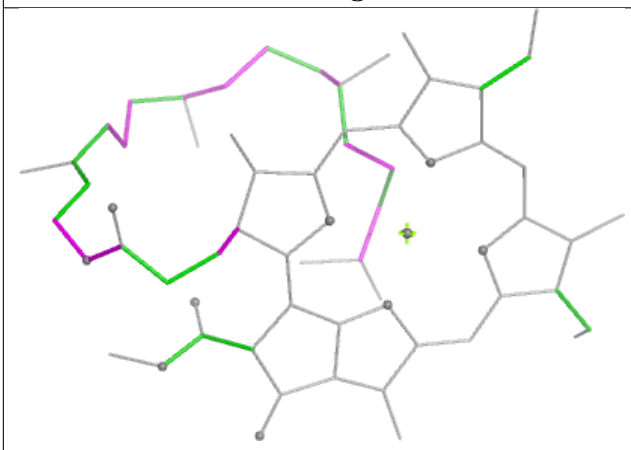
Ligand CLA 1 1608



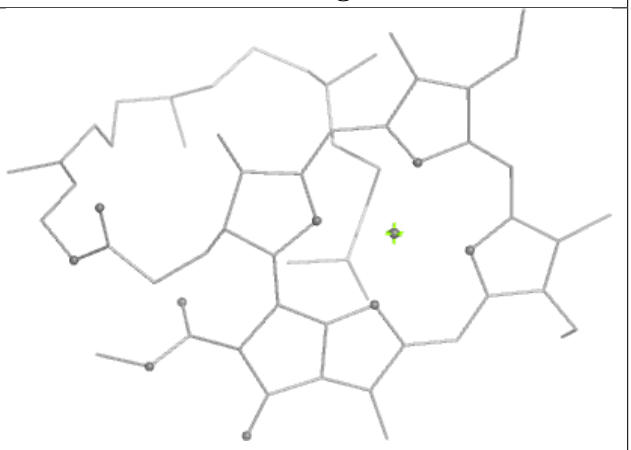
Bond lengths



Bond angles

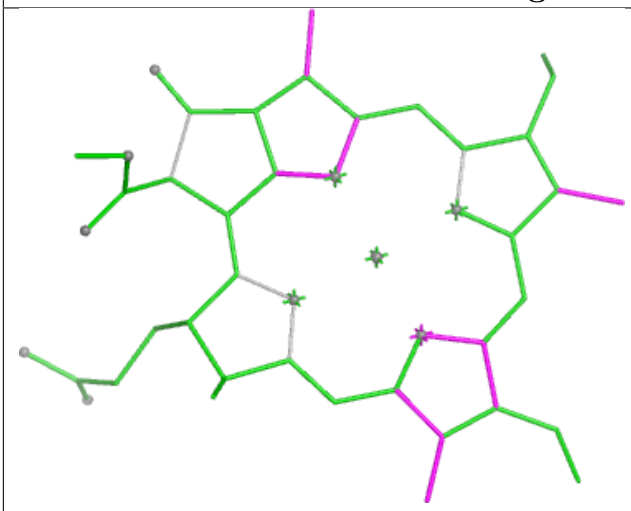


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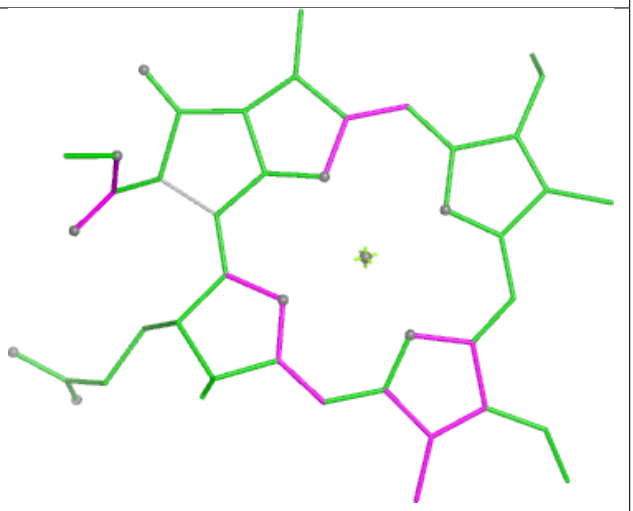


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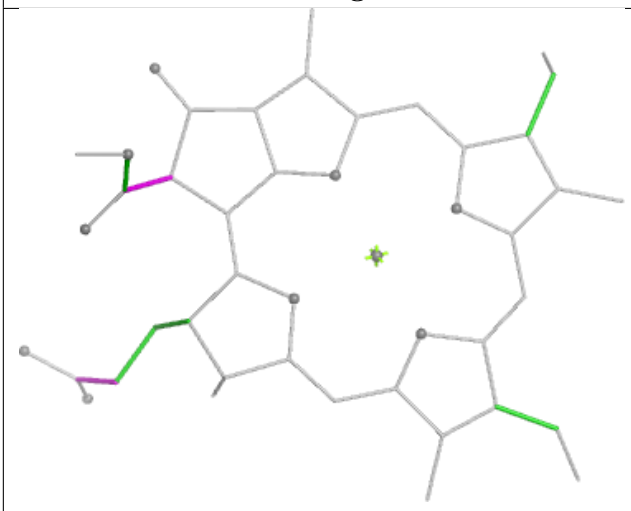
Ligand CLA a 844



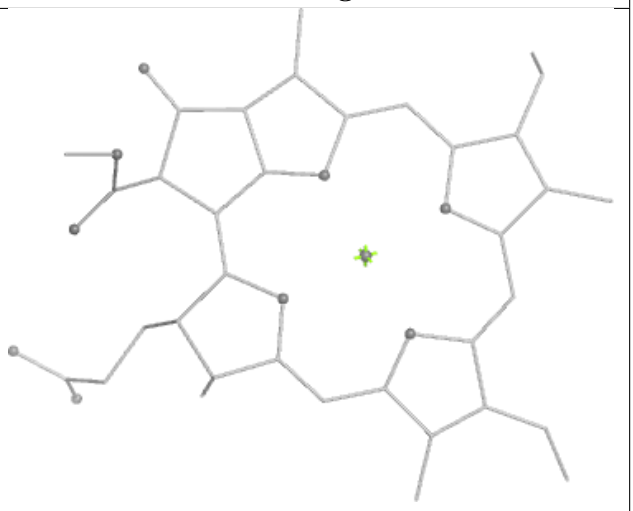
Bond lengths



Bond angles

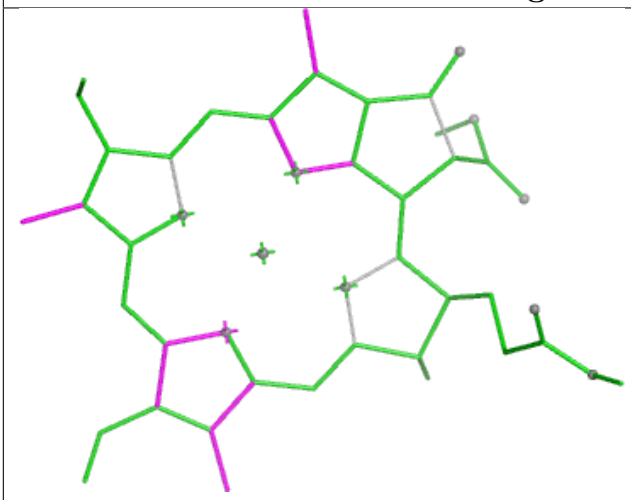


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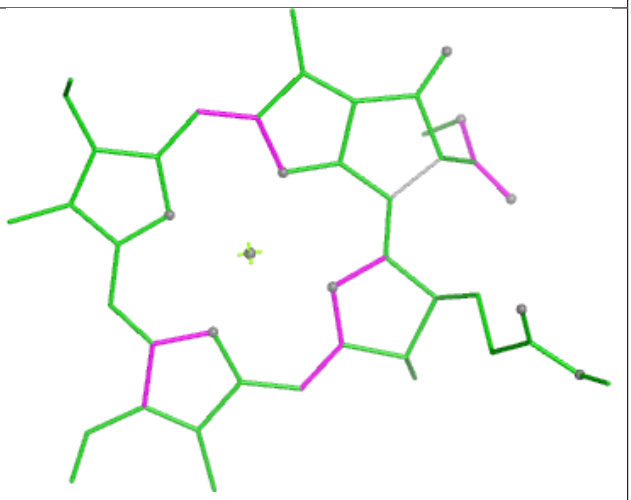


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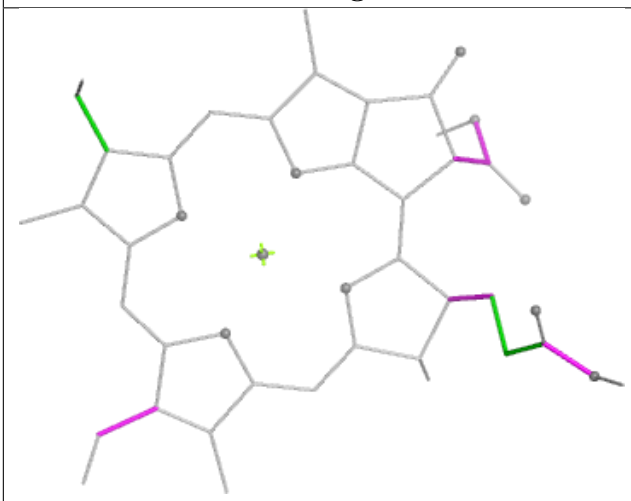
Ligand CLA k 101



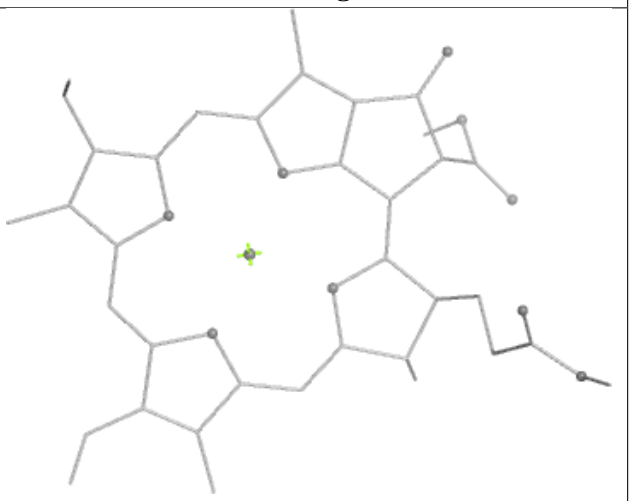
Bond lengths



Bond angles

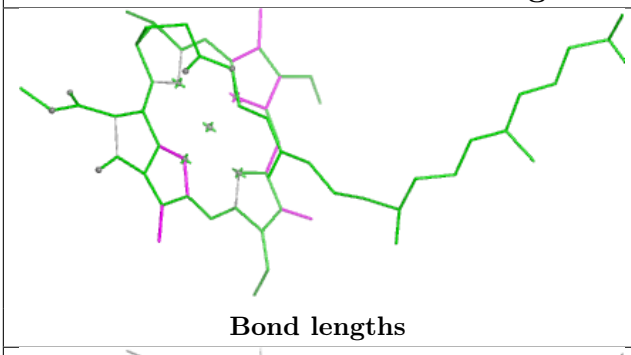


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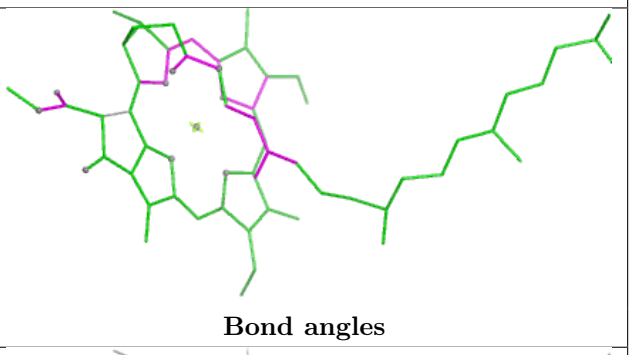


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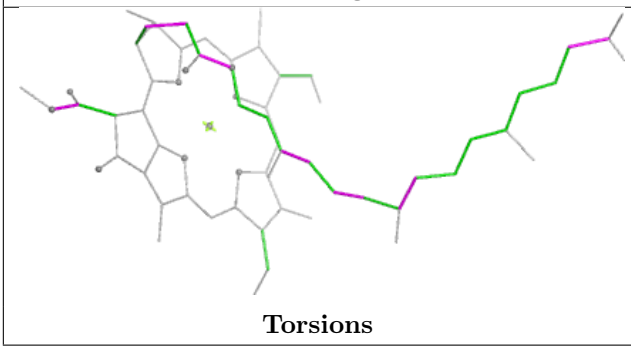
Ligand CLA a 842



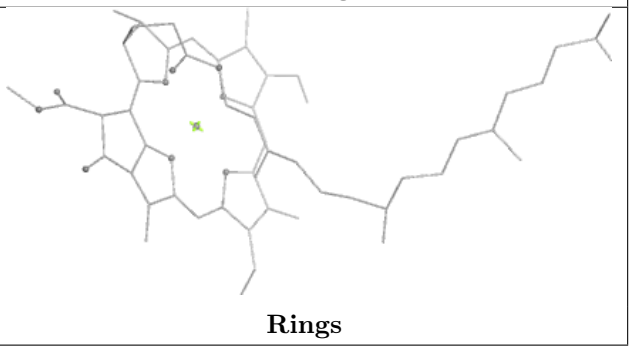
Bond lengths



Bond angles

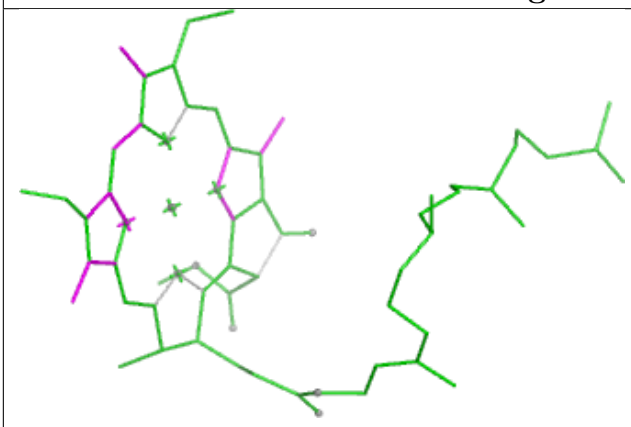


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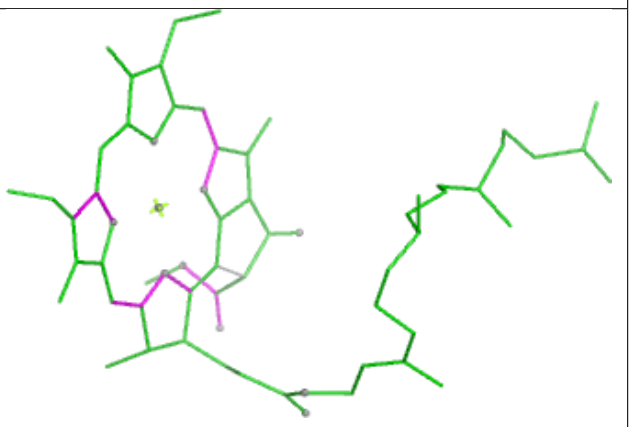


Rings

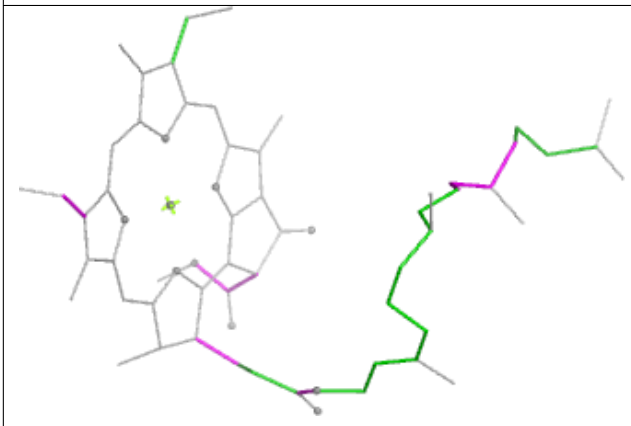
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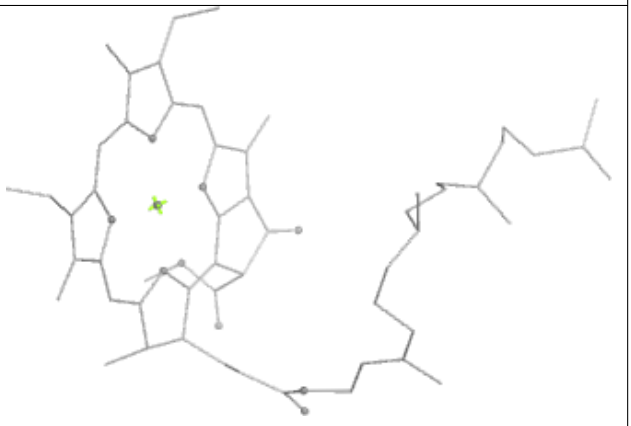
Bond lengths



Bond angles

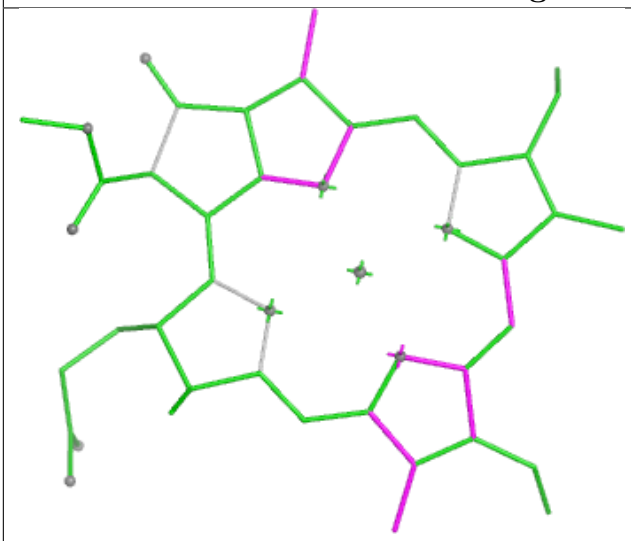


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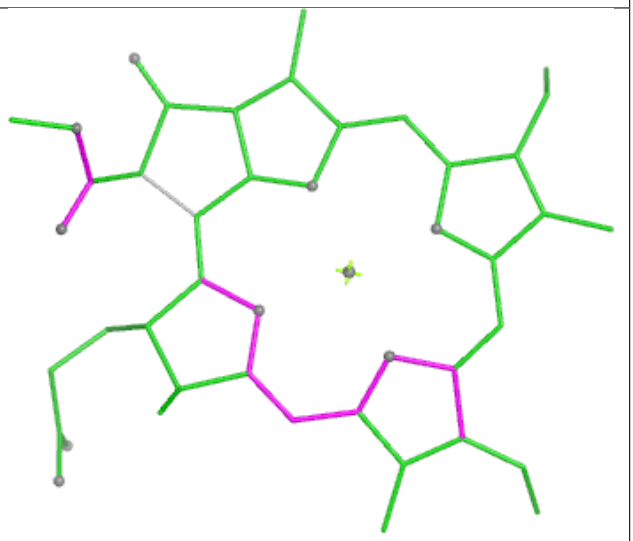


Rings

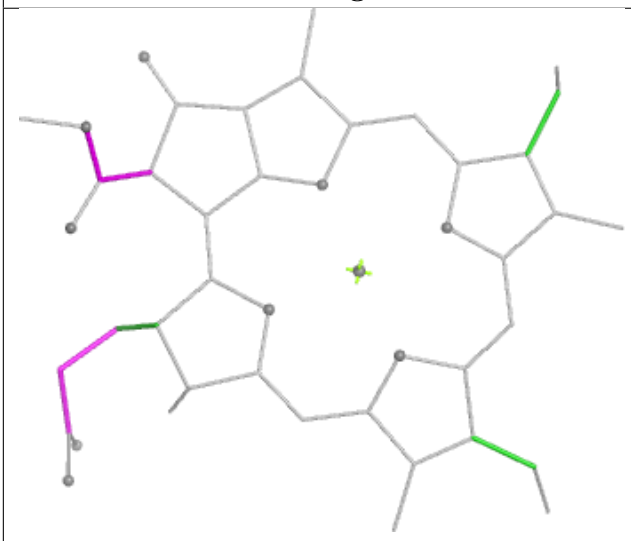
Ligand CLA z 102



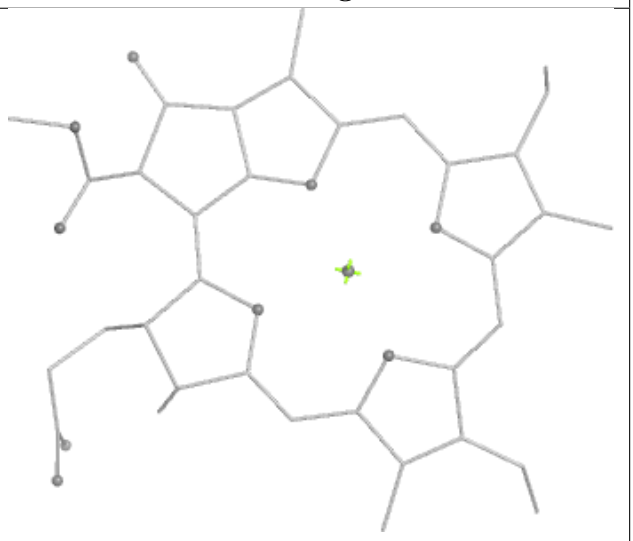
Bond lengths



Bond angles

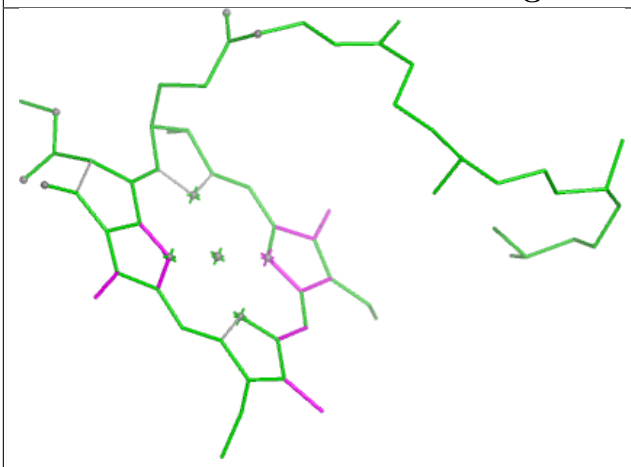


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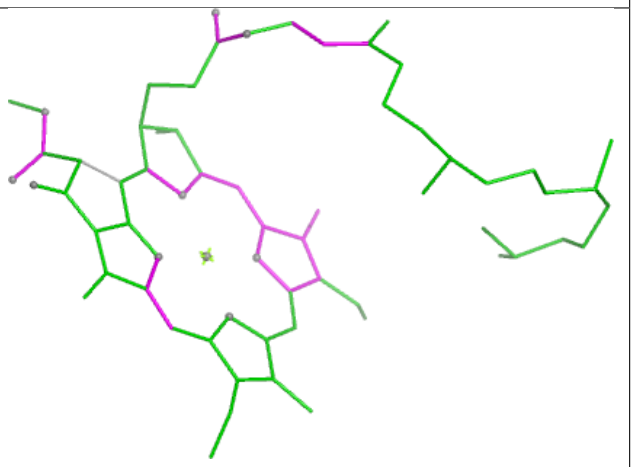


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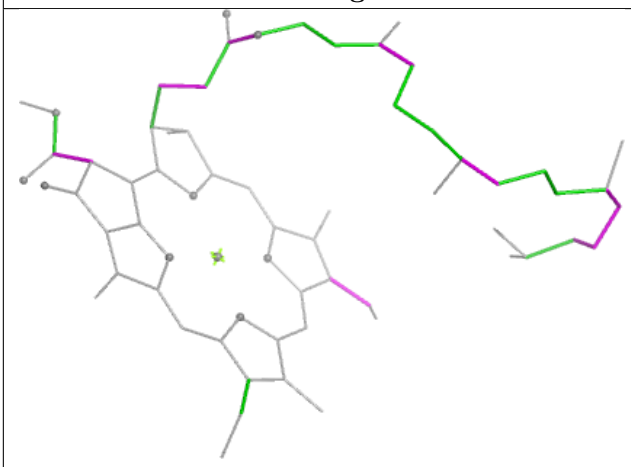
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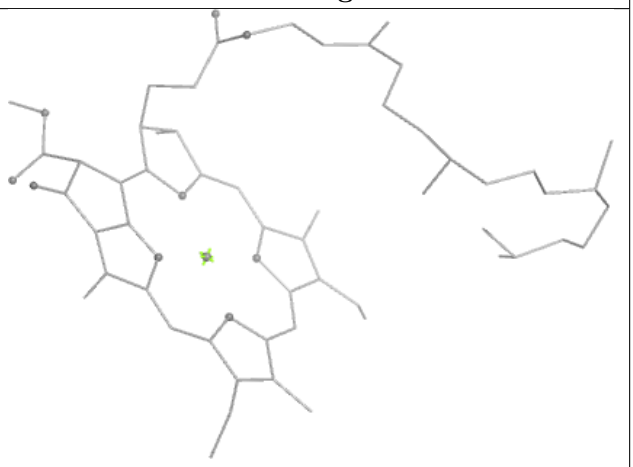
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Bond angles

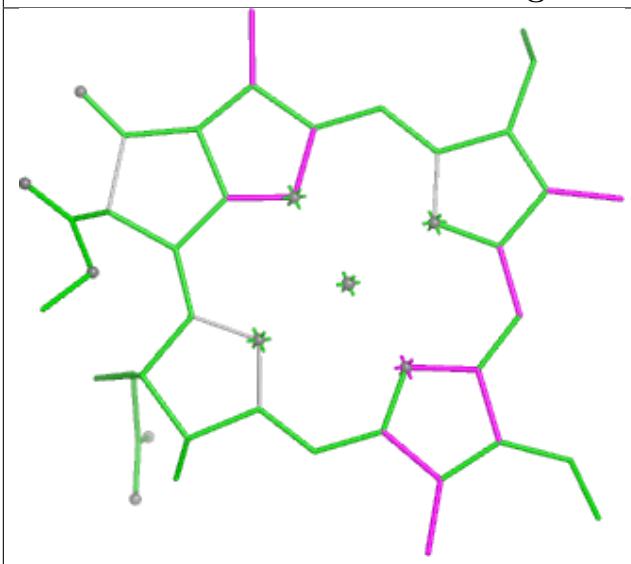


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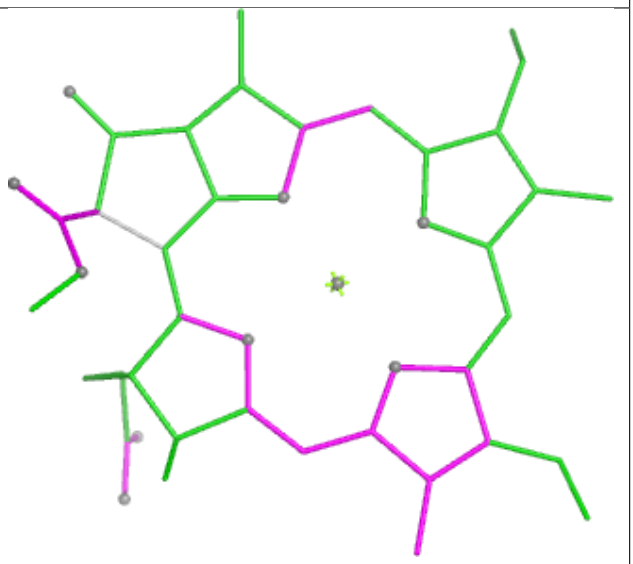


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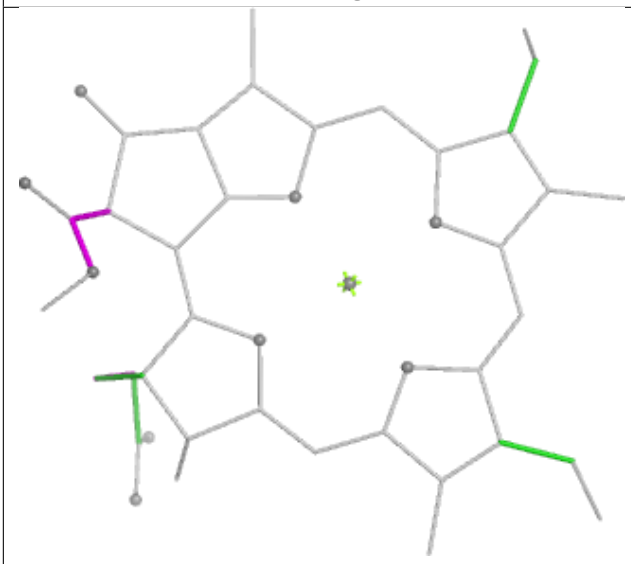
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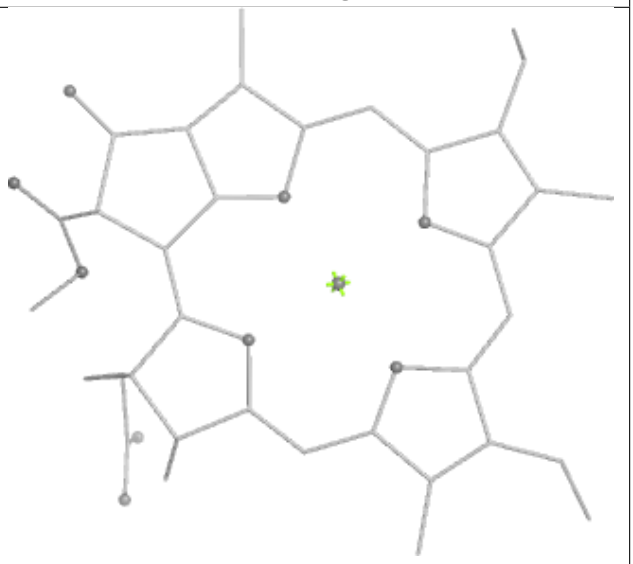
Bond lengths



Bond angles

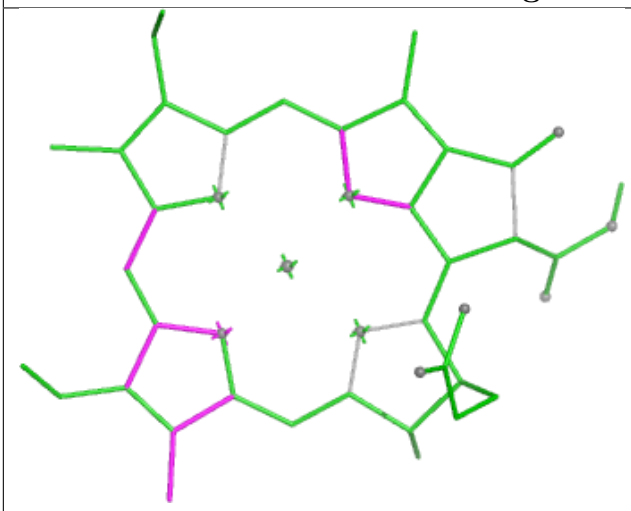


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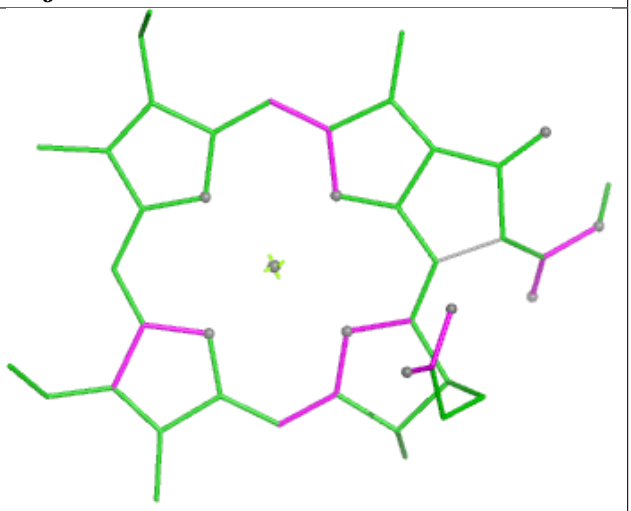


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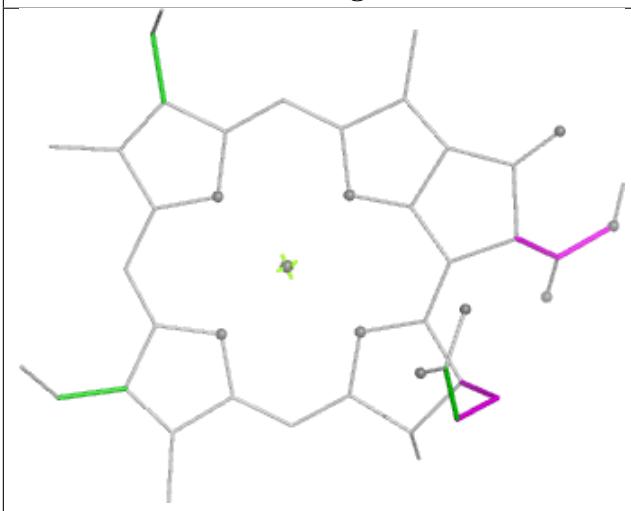
Ligand CLA j 1302



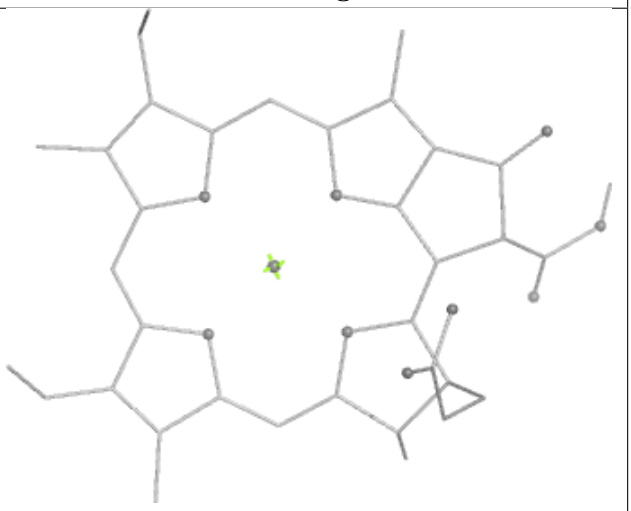
Bond lengths



Bond angles

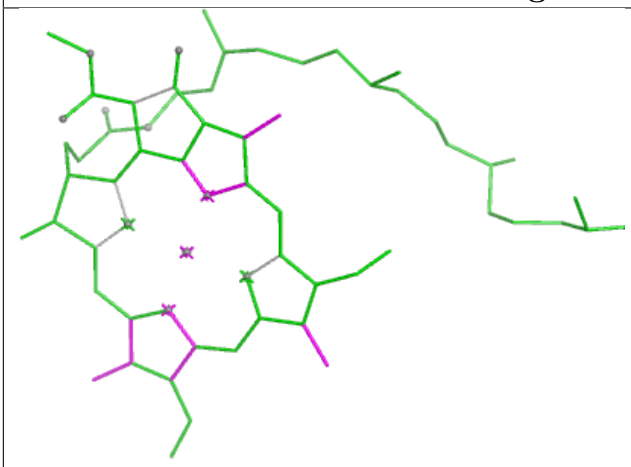


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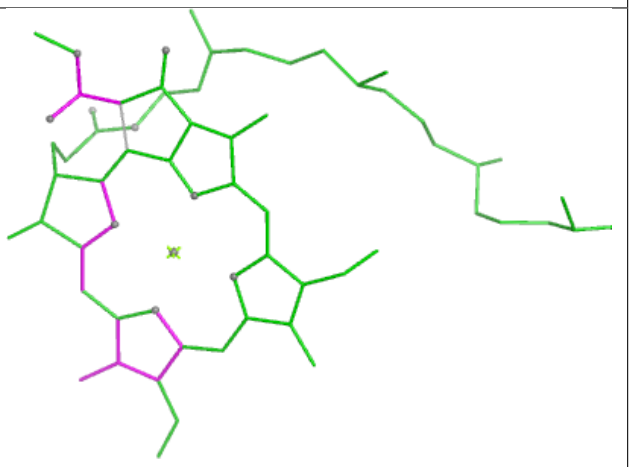


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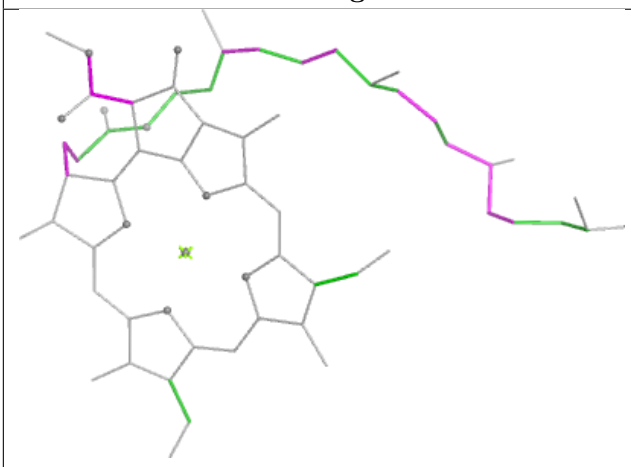
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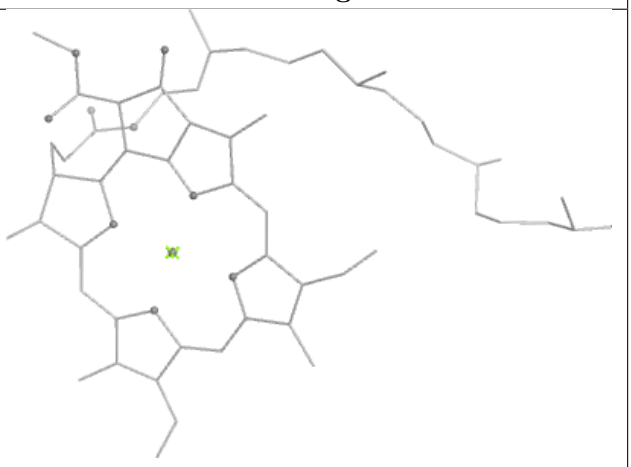
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Bond angles

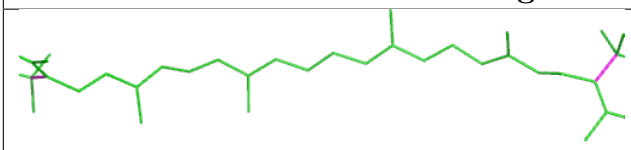


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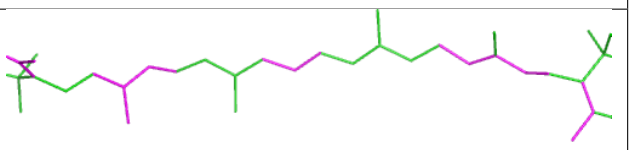


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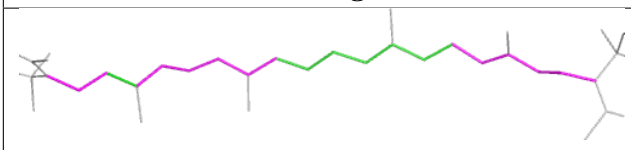
Ligand BCR 8 1306



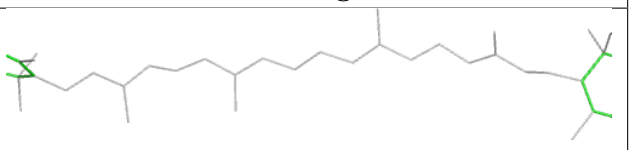
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Bond angles

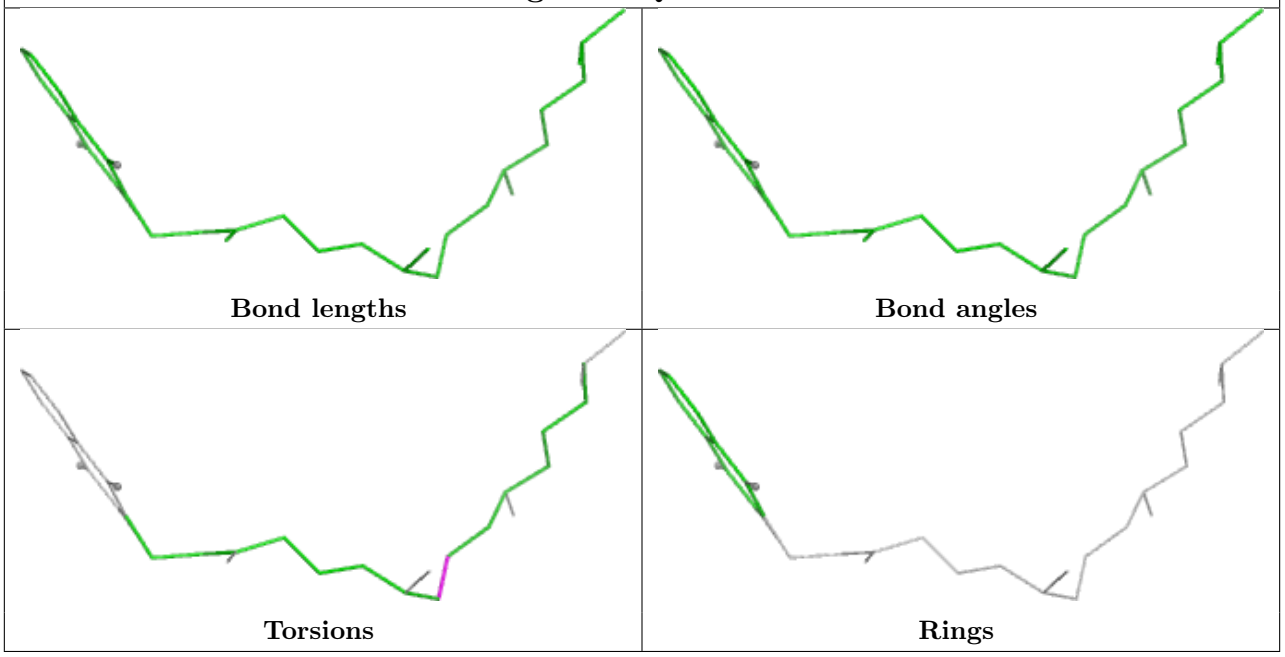


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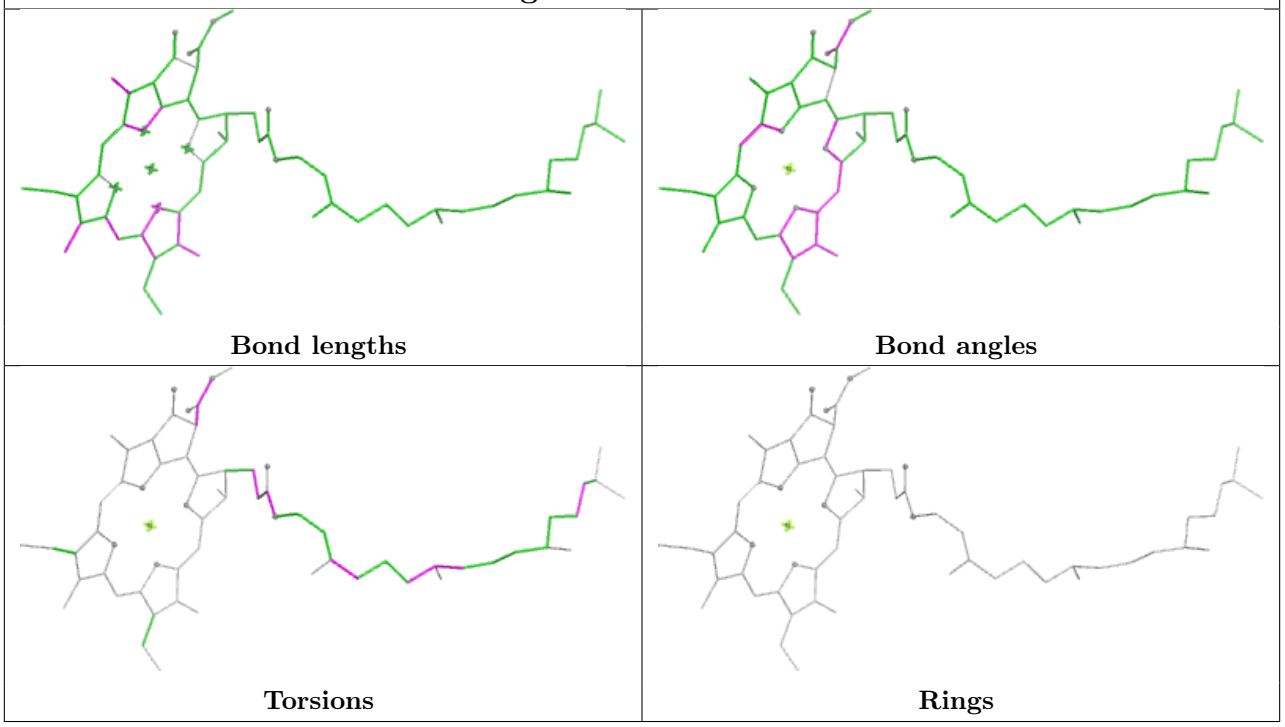


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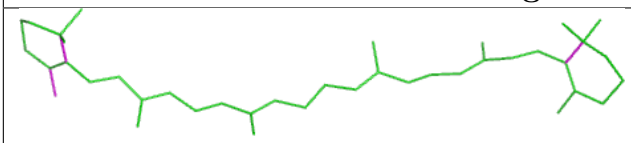
Ligand PQN 2 843



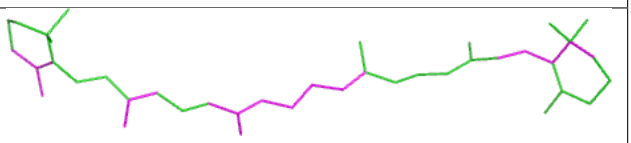
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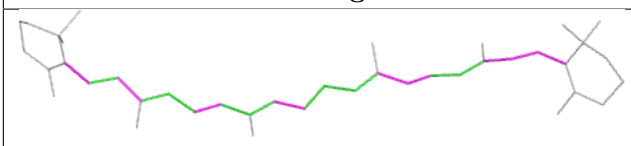
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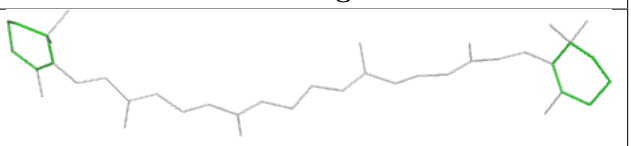
Bond lengths



Bond angles

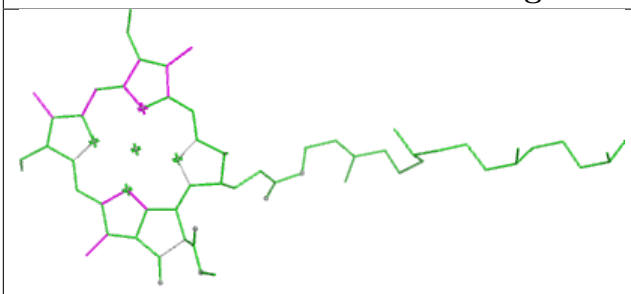


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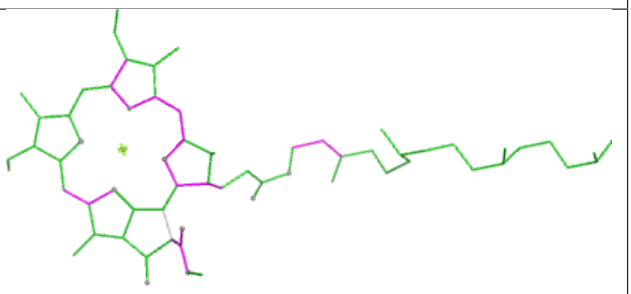


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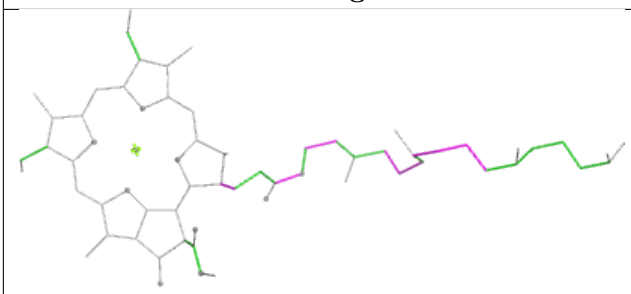
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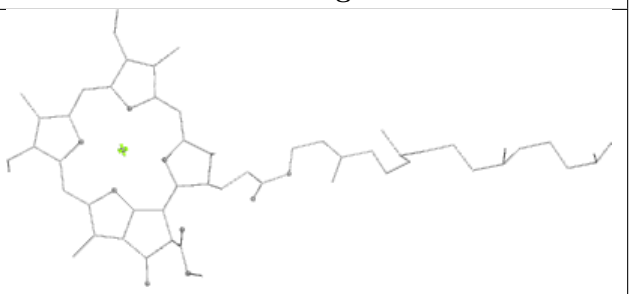
Bond lengths



Bond angles

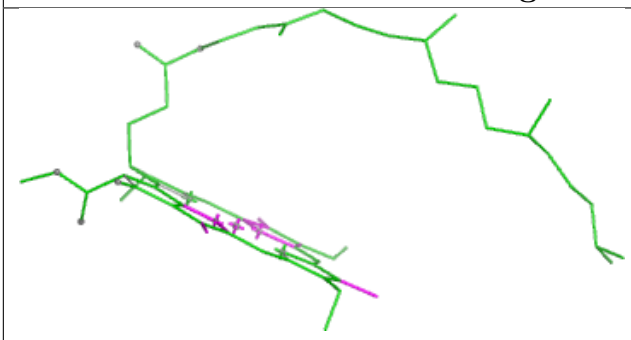


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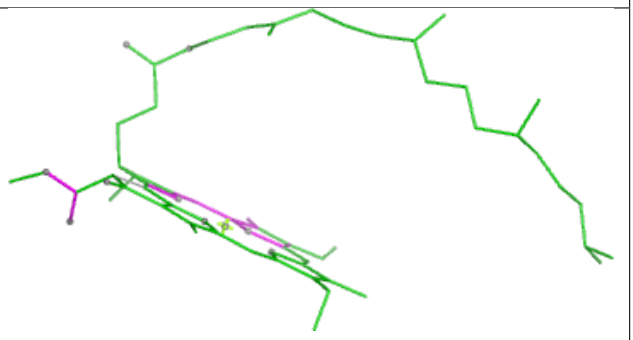


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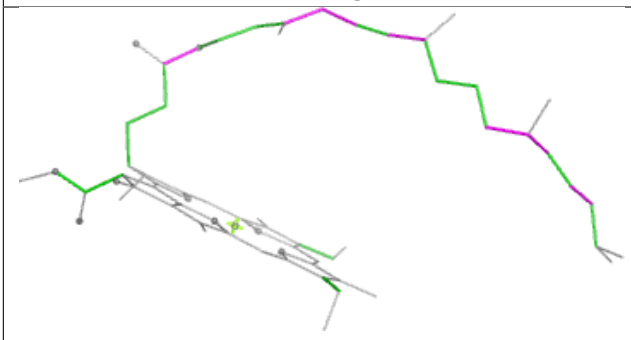
Ligand CLA 1 1634



Bond lengths



Bond angles

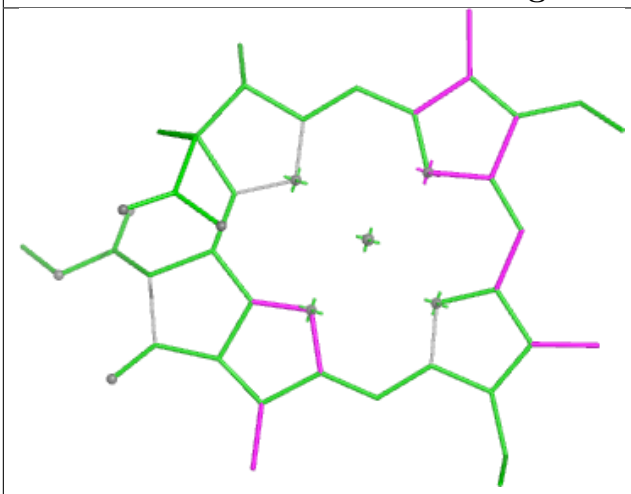


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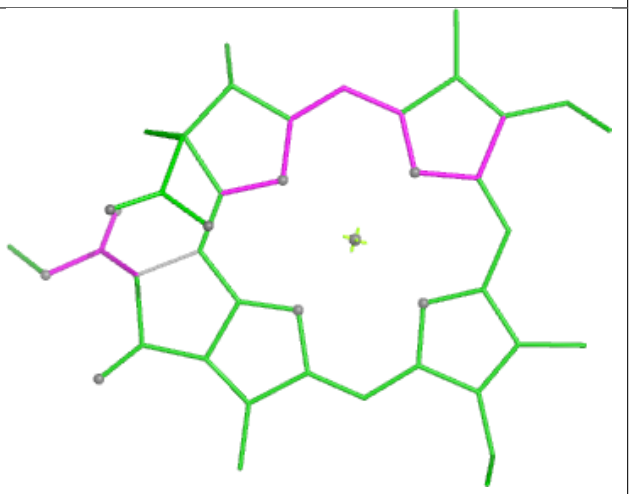


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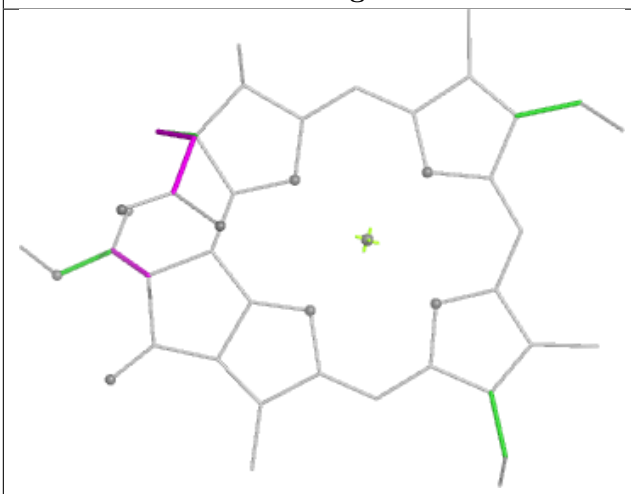
Ligand CLA a 813



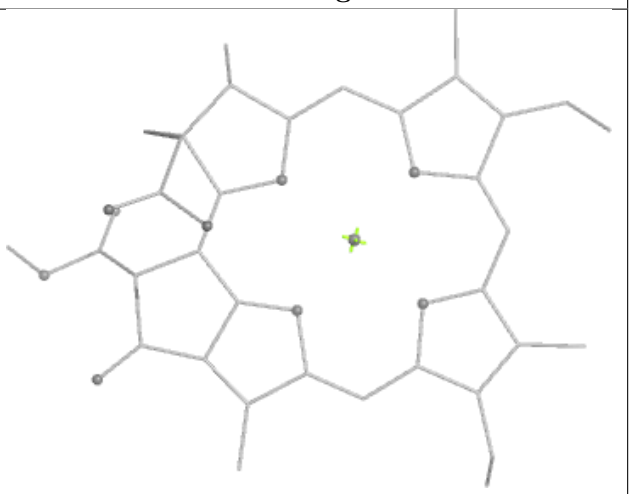
Bond lengths



Bond angles

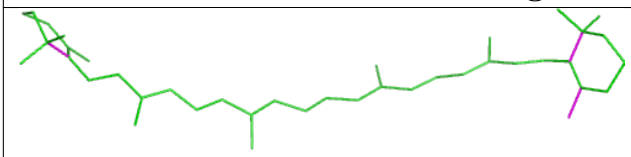


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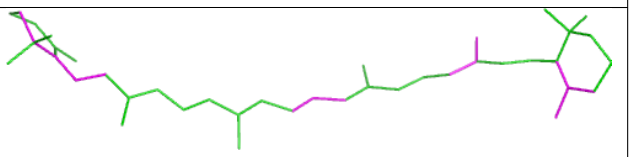


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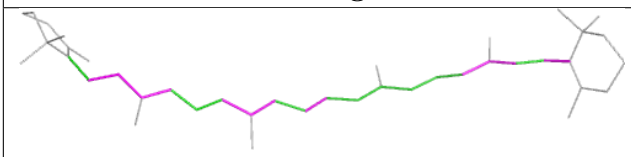
Ligand BCR 6 202



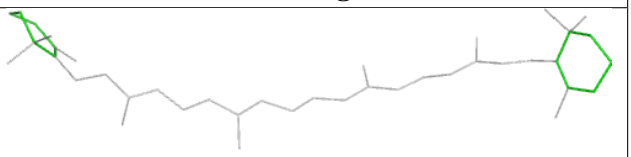
Bond lengths



Bond angles

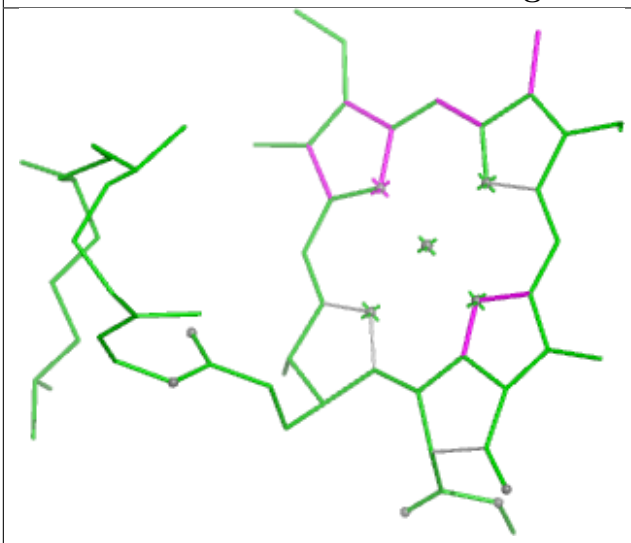


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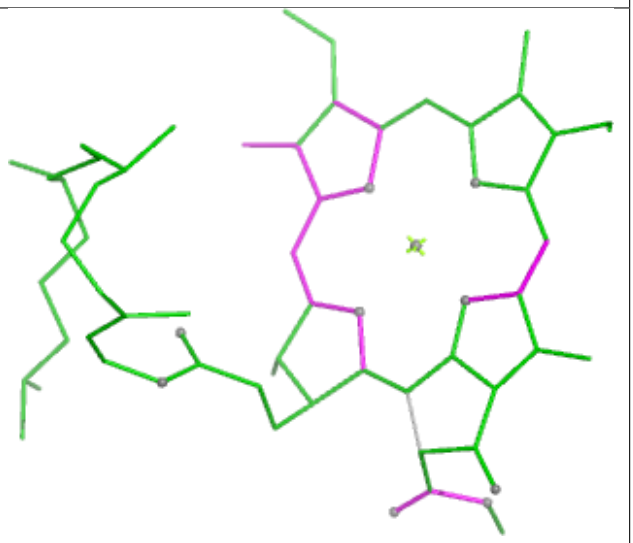


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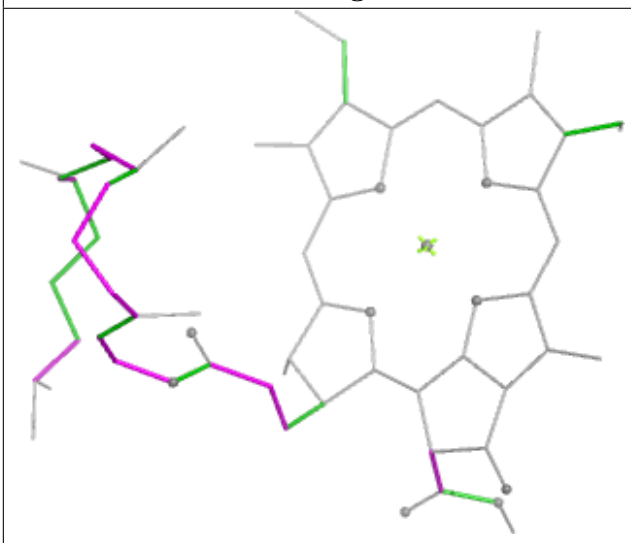
Ligand CLA A 816



Bond lengths



Bond angles

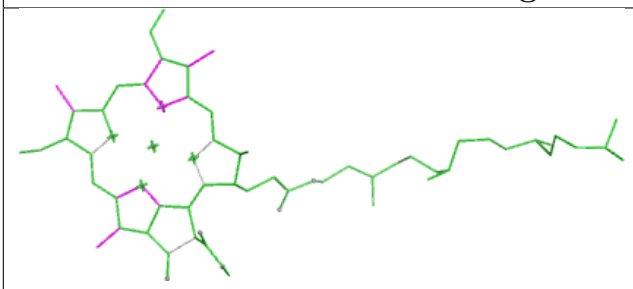


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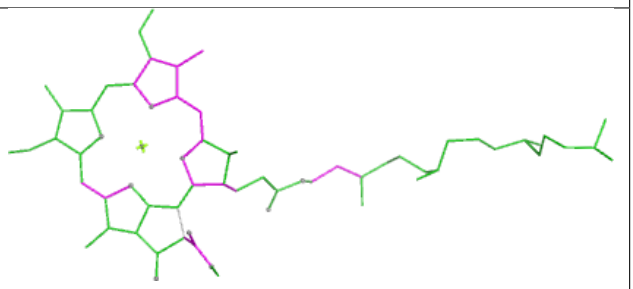


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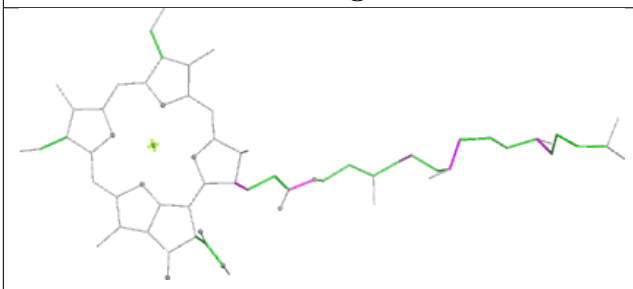
Ligand CLA 1 1628



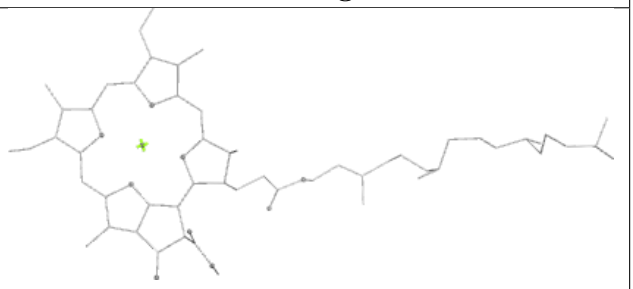
Bond lengths



Bond angles

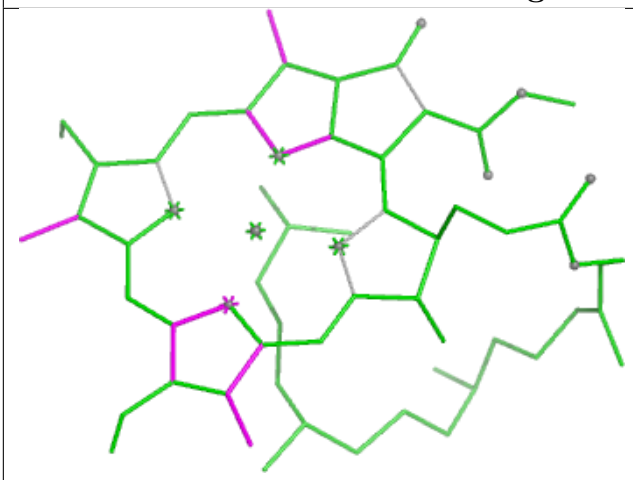


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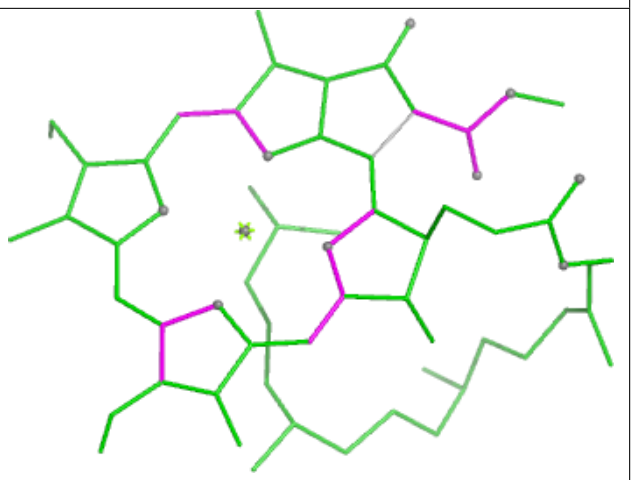


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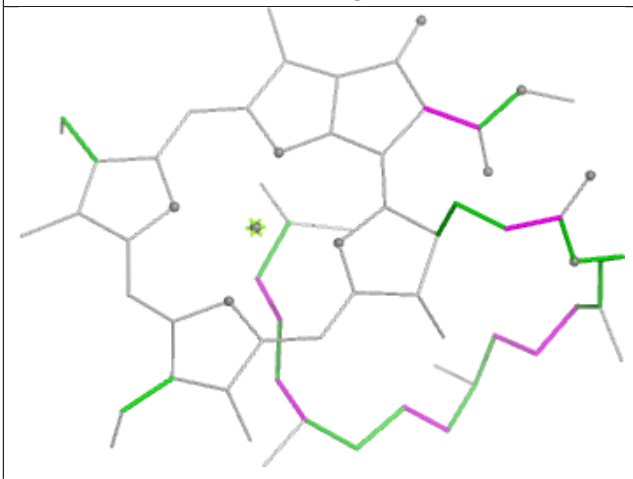
Ligand CLA b 807



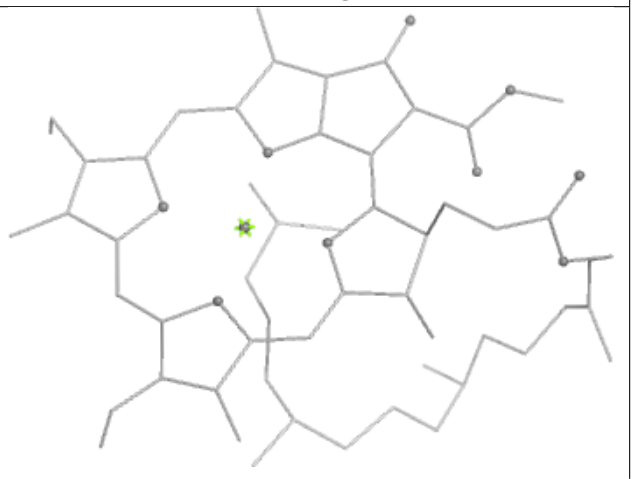
Bond lengths



Bond angles

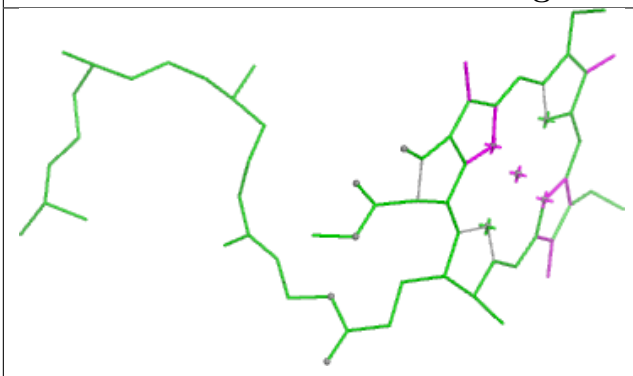


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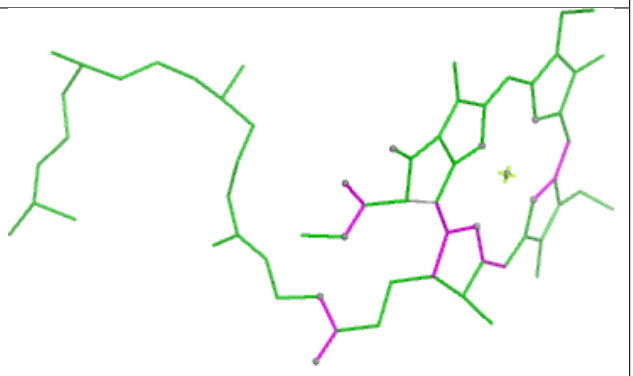


Rings

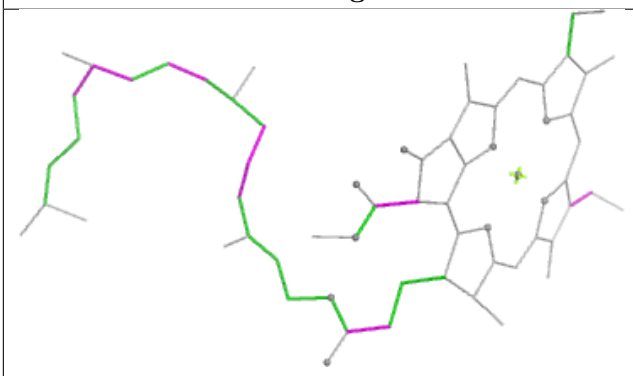
Ligand CL0 a 801



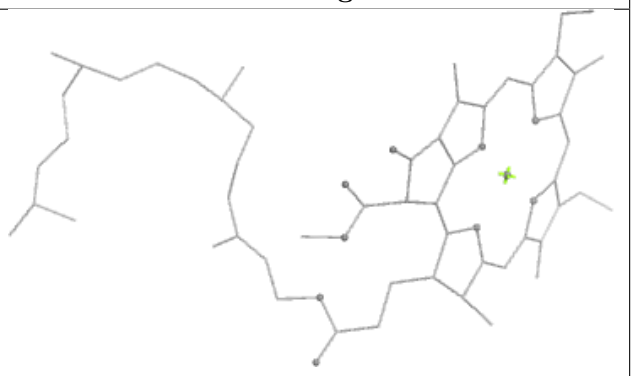
Bond lengths



Bond angles

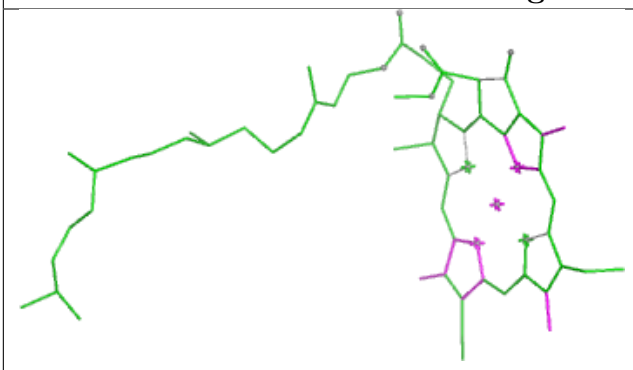


Torsions

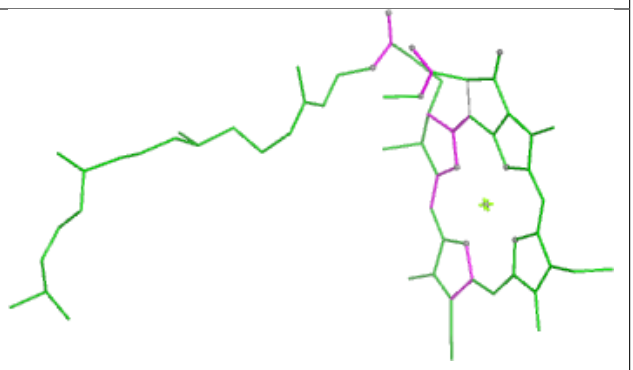


Rings

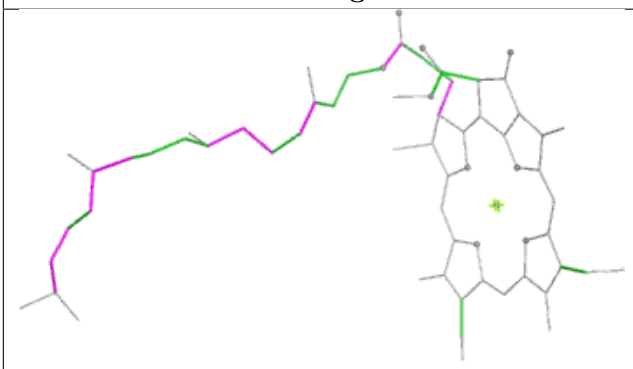
Ligand CLA b 811



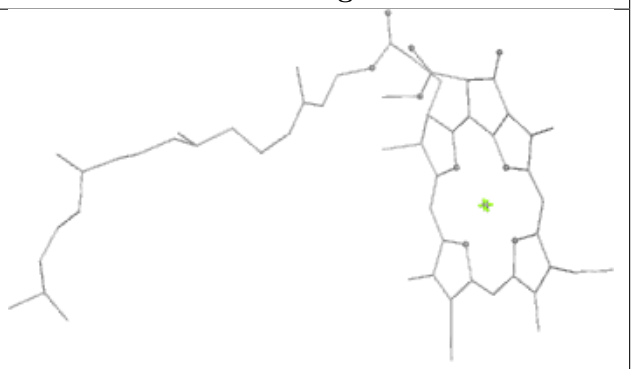
Bond lengths



Bond angles

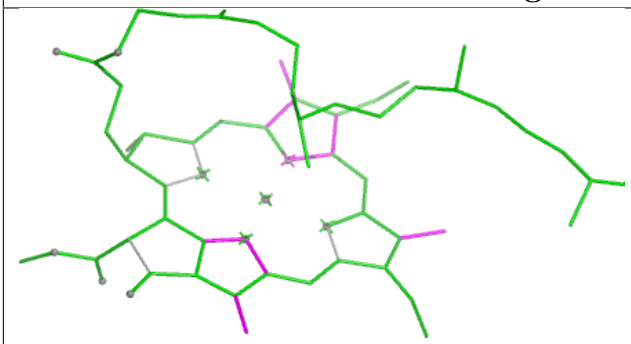


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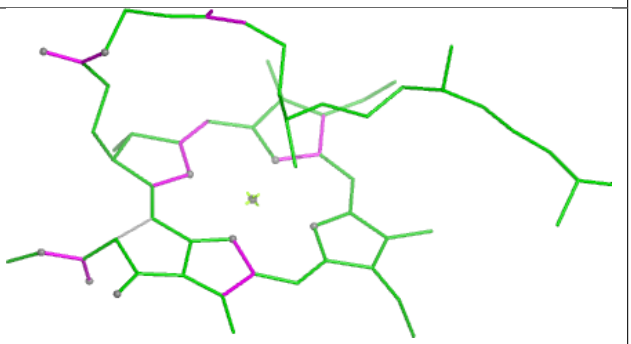


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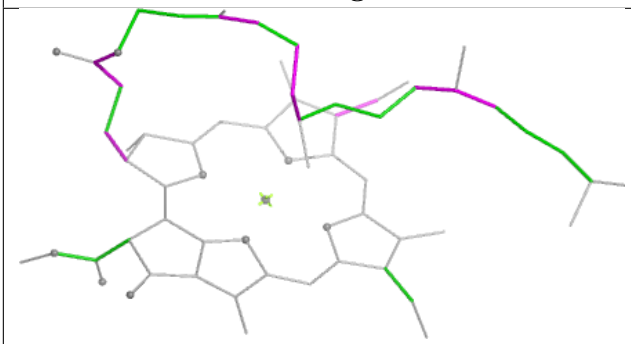
Ligand CLA B 817



Bond lengths



Bond angles

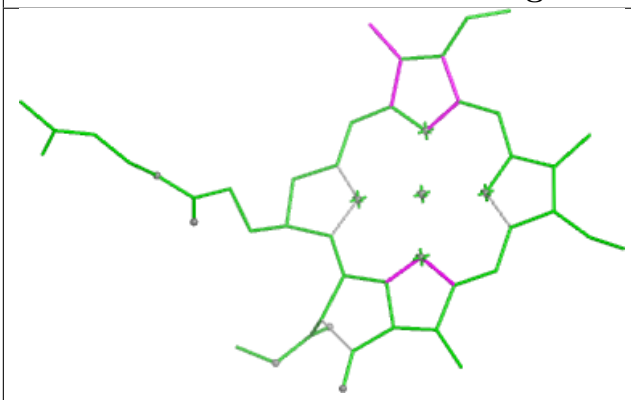


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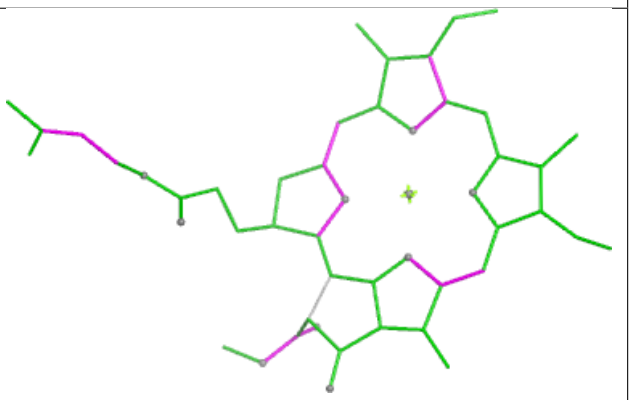


Rings

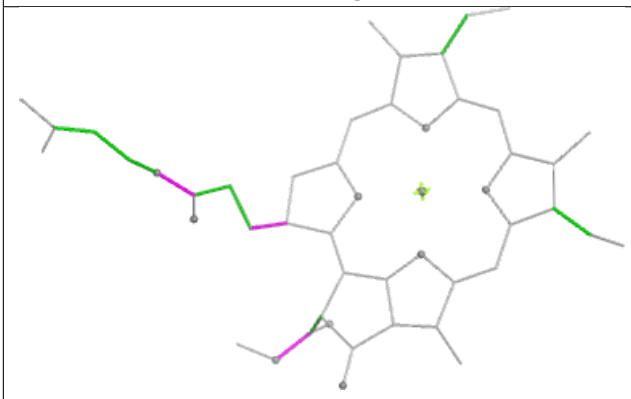
Ligand CLA F 204



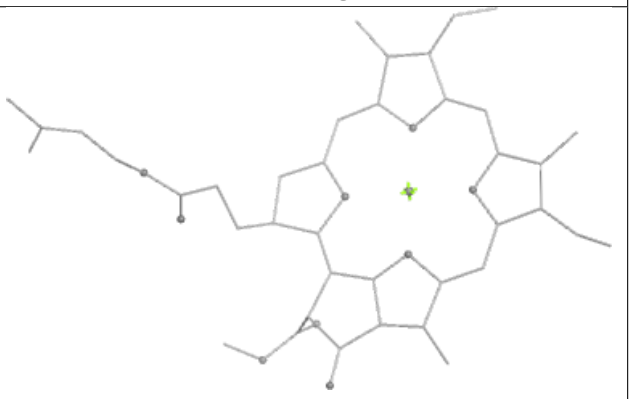
Bond lengths



Bond angles

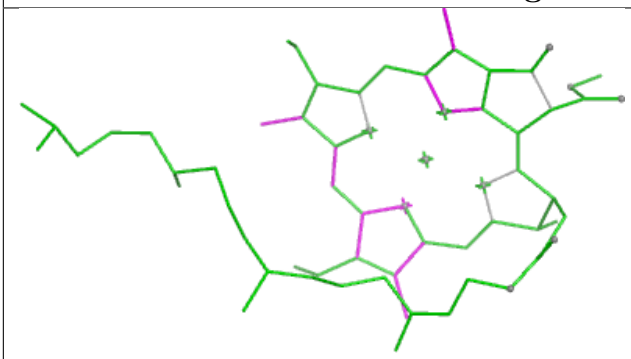


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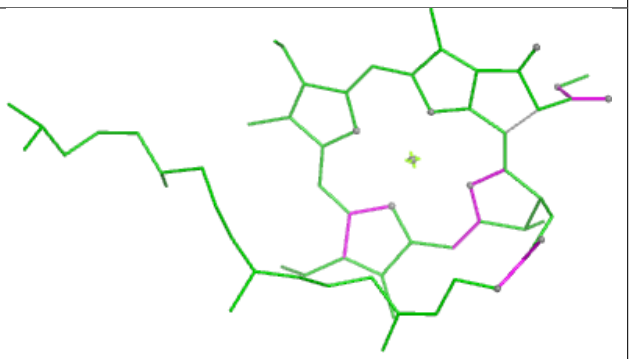


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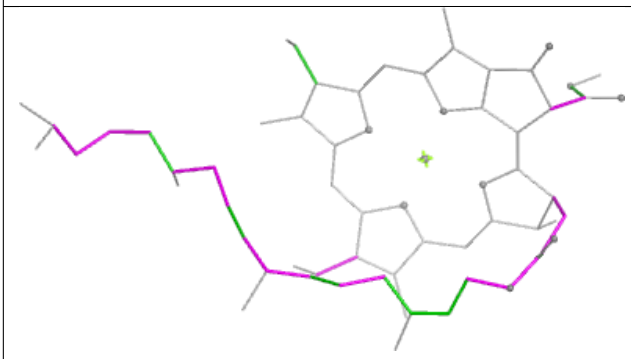
Ligand CLA B 820



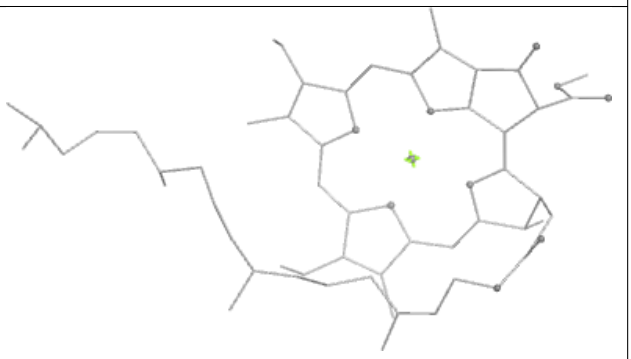
Bond lengths



Bond angles

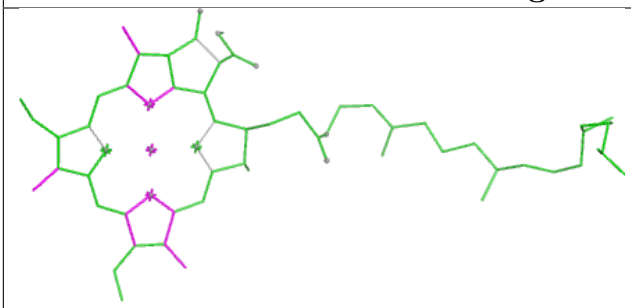


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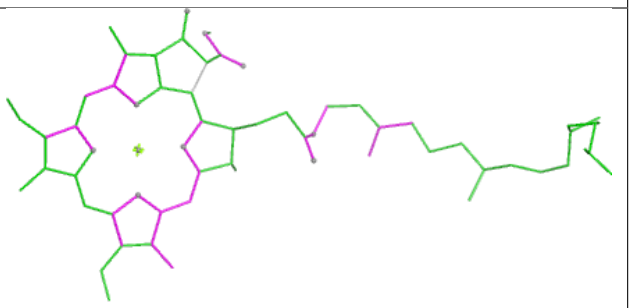


Rings

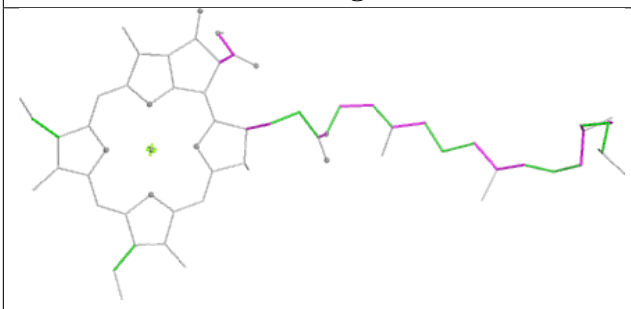
Ligand CLA a 806



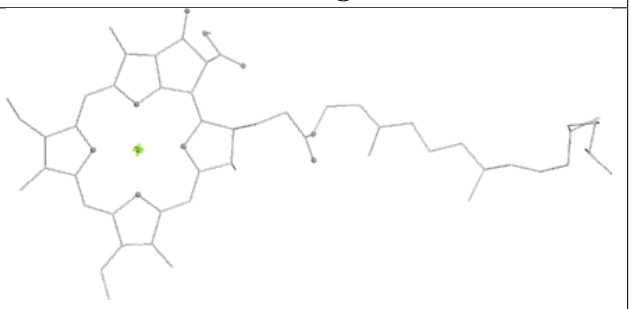
Bond lengths



Bond angles

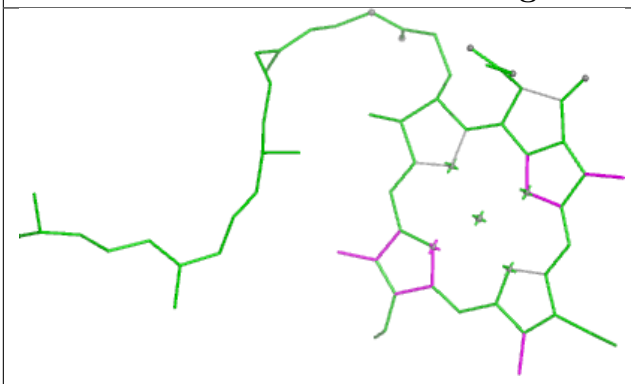


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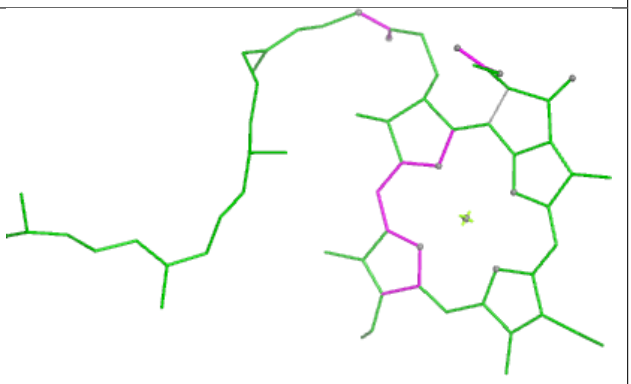


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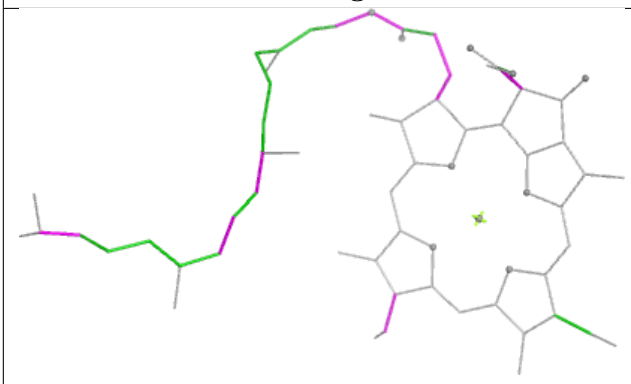
Ligand CLA 1 1615



Bond lengths



Bond angles

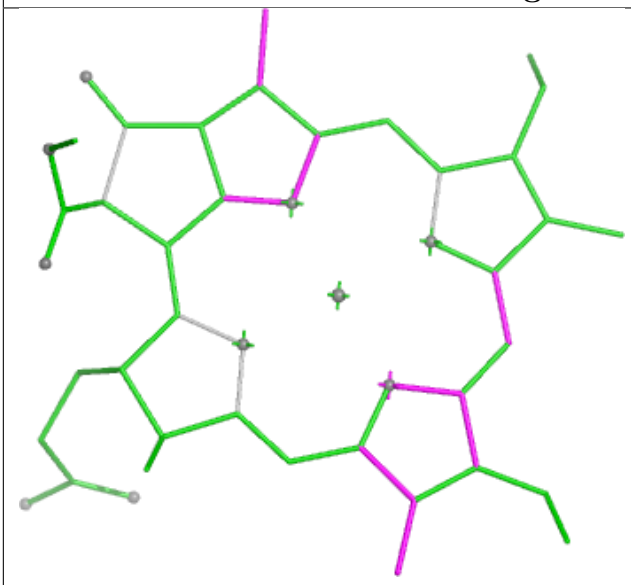


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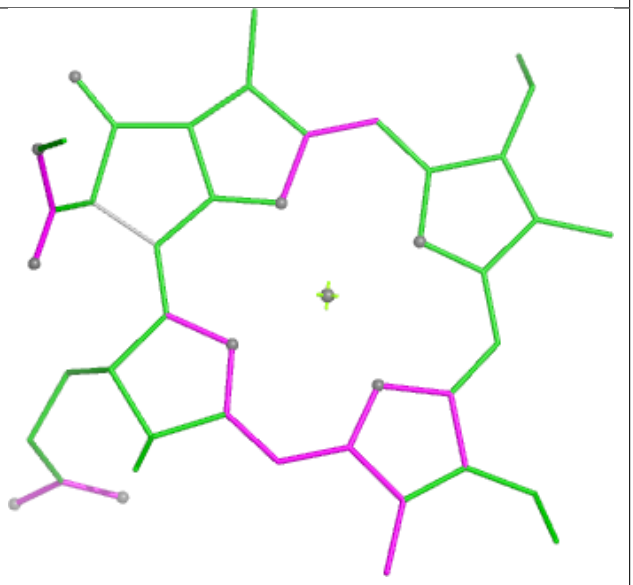


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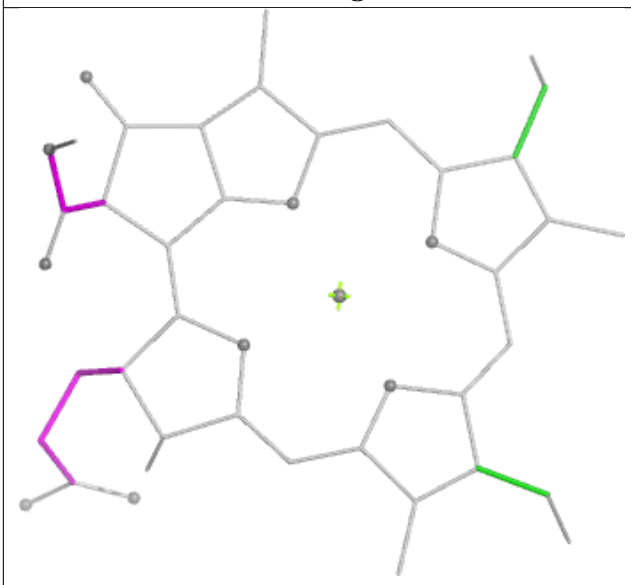
Ligand CLA A 823



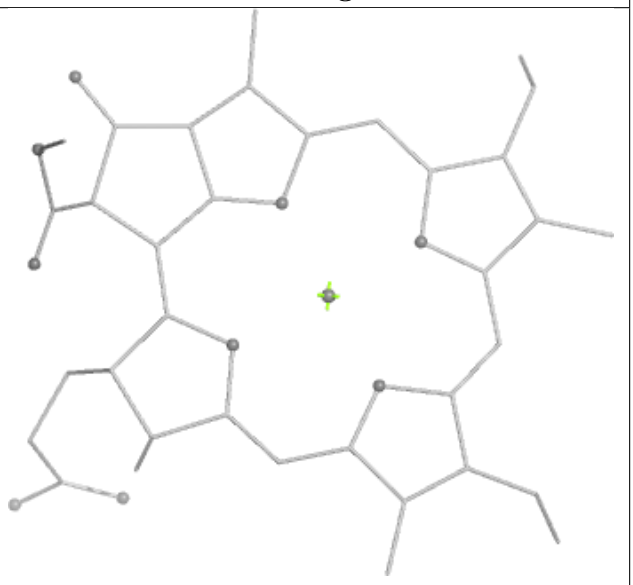
Bond lengths



Bond angles

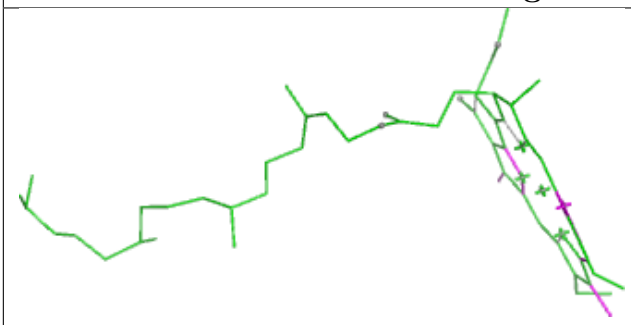


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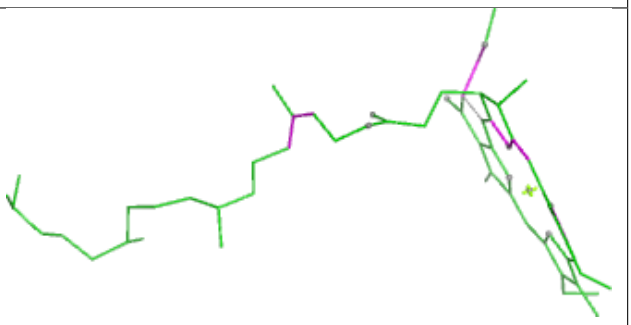


Rings

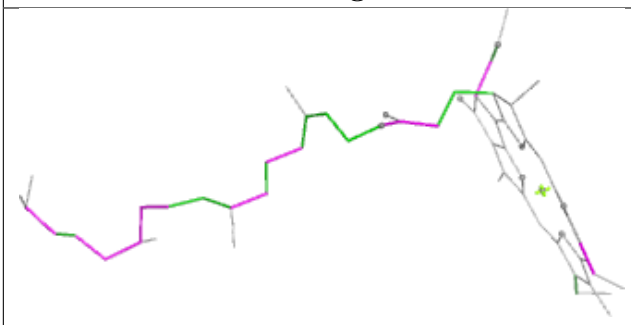
Ligand CLA A 840



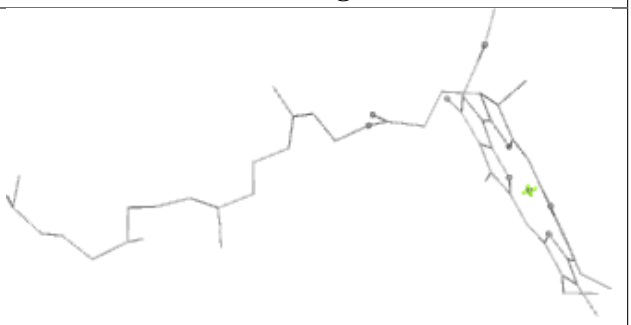
Bond lengths



Bond angles

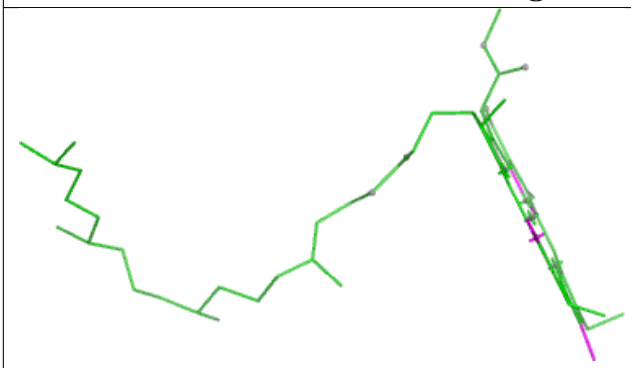


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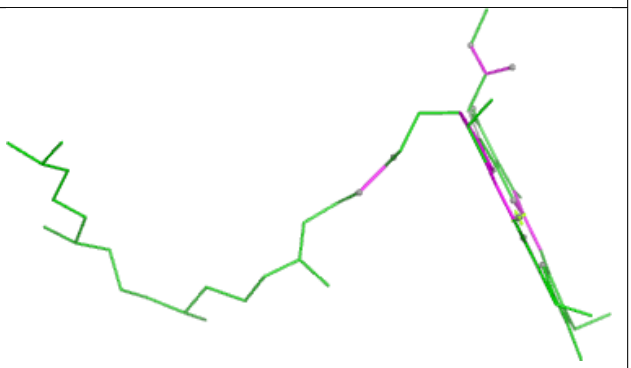


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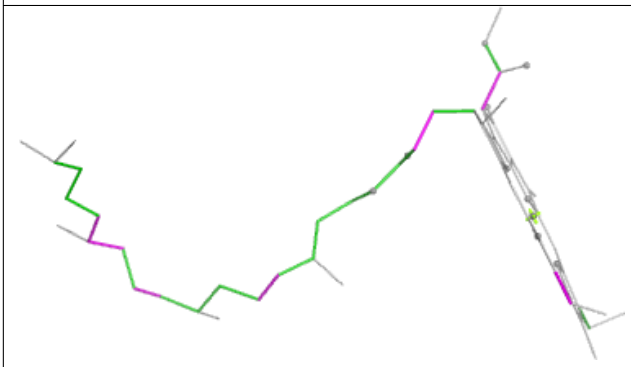
Ligand CLA b 841



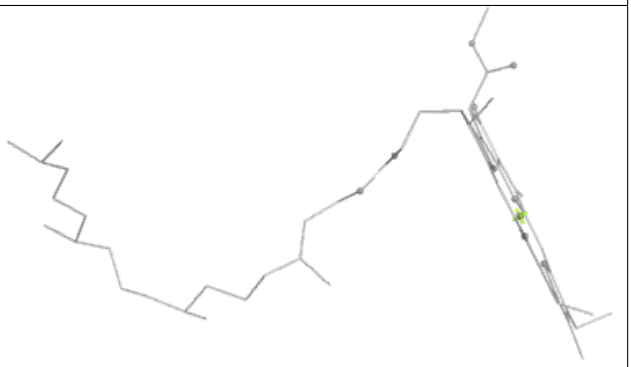
Bond lengths



Bond angles

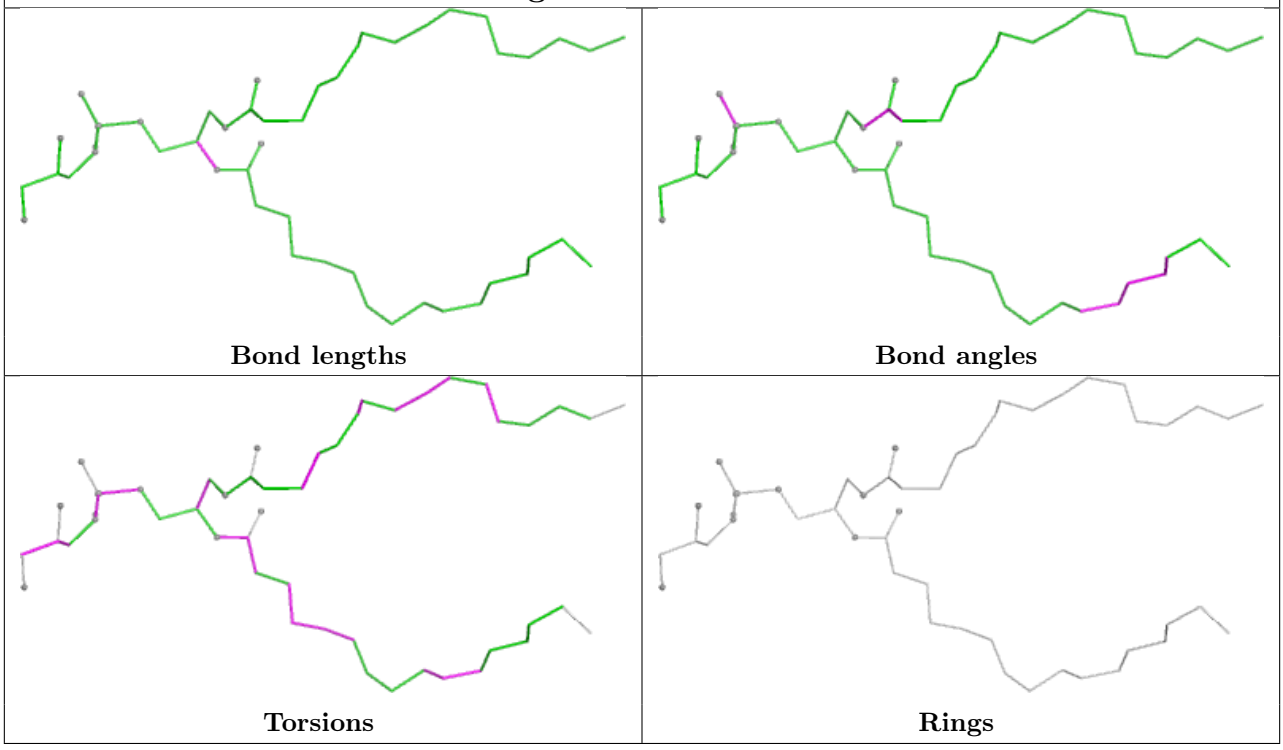


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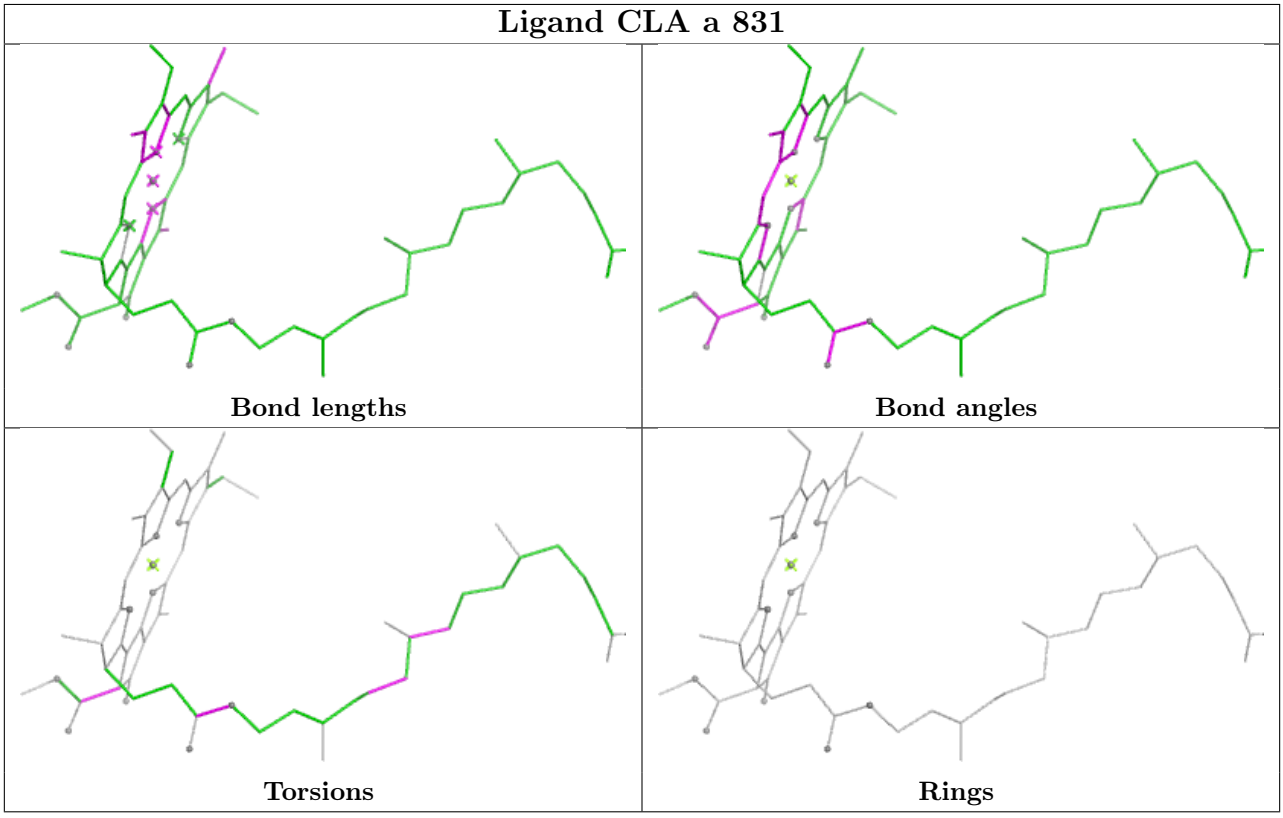


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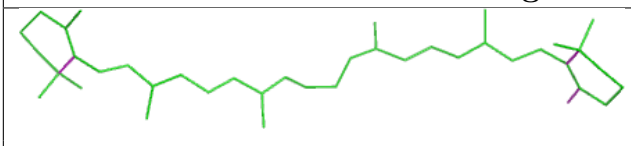
Ligand LHG a 853



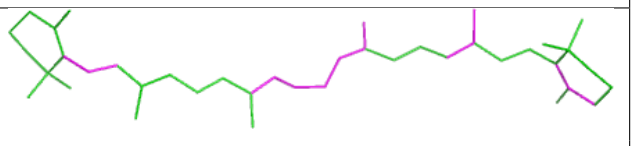
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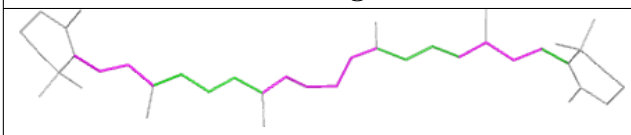
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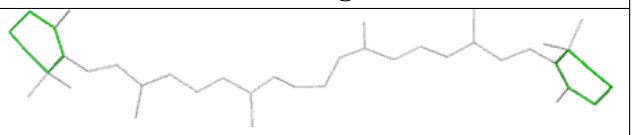
Bond lengths



Bond angles



Torsions

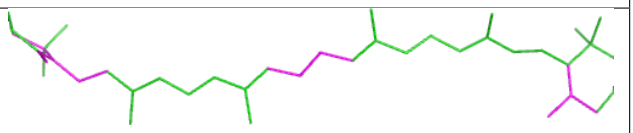


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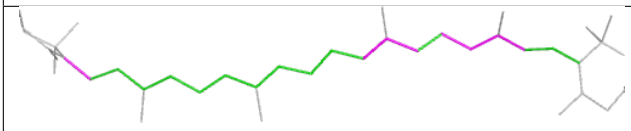
Ligand BCR 1 1651



Bond lengths



Bond angles

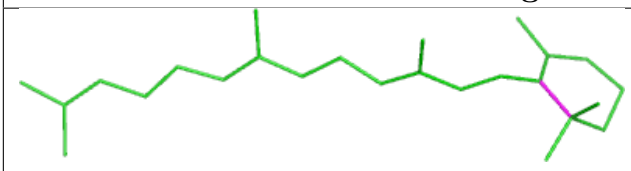


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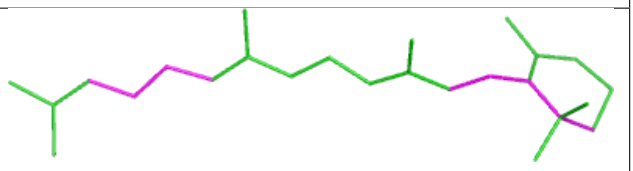


Rings

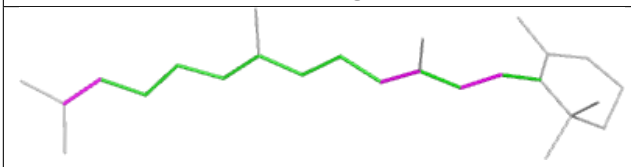
Ligand BCR K 104



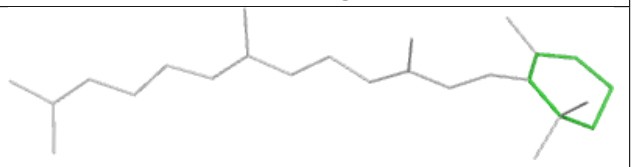
Bond lengths



Bond angles

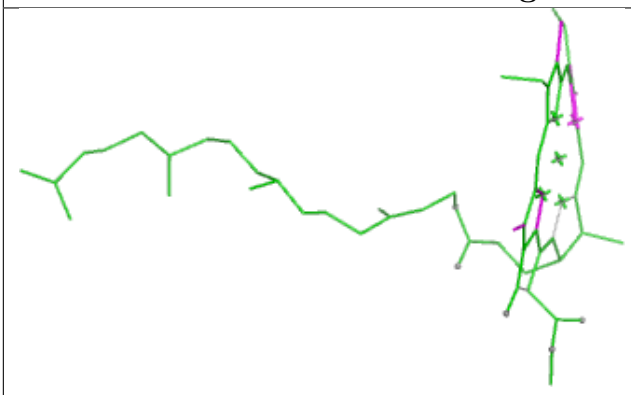


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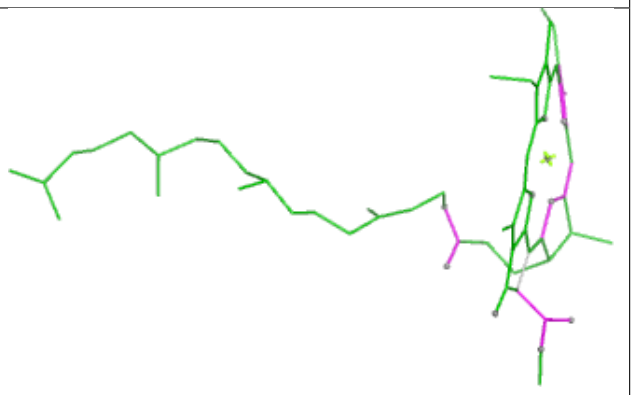


Rings

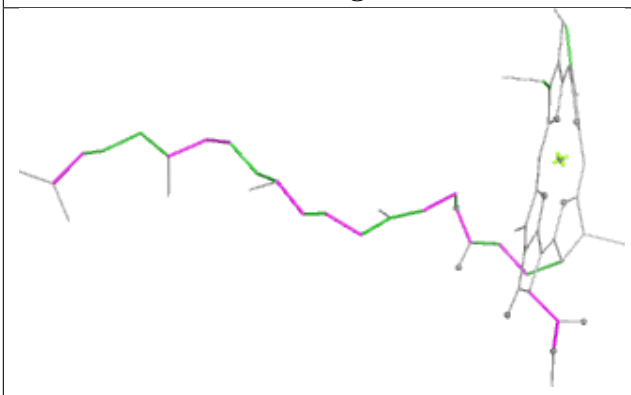
Ligand CLA 1 1630



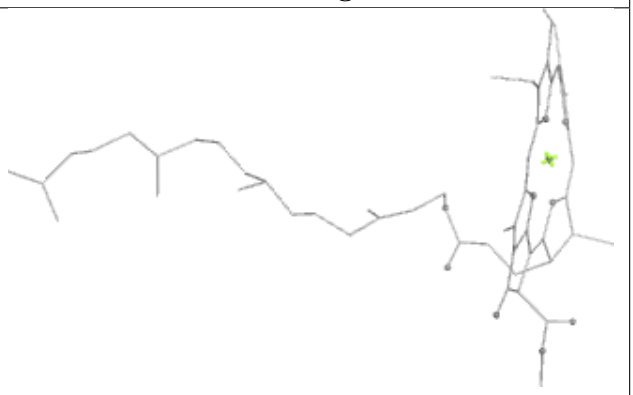
Bond lengths



Bond angles

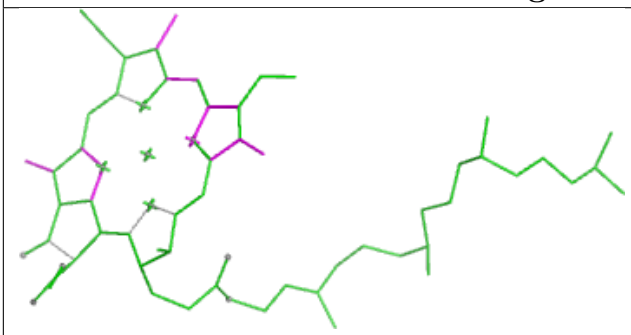


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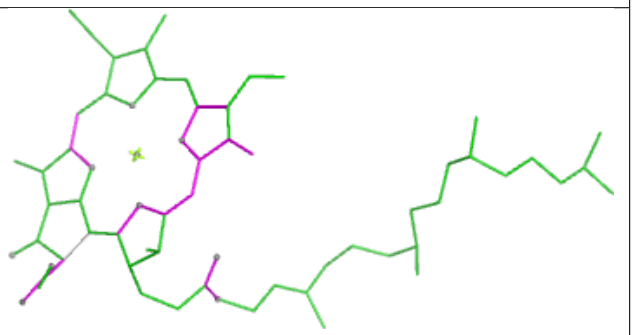


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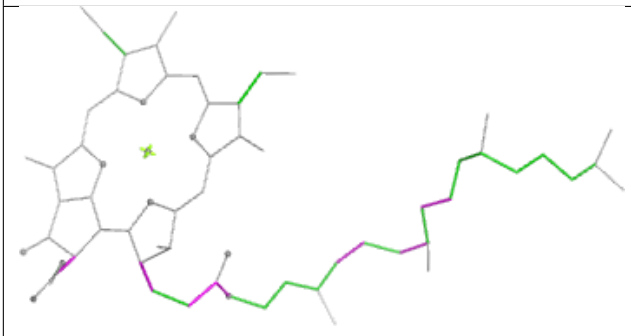
Ligand CLA a 809



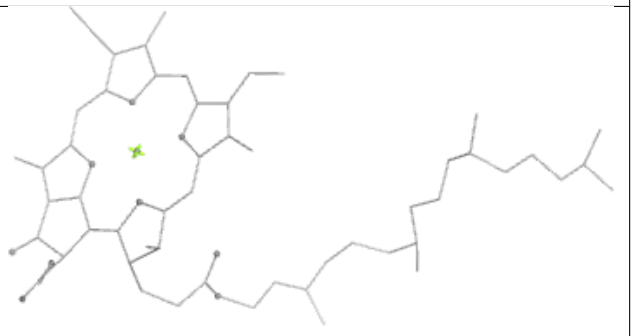
Bond lengths



Bond angles

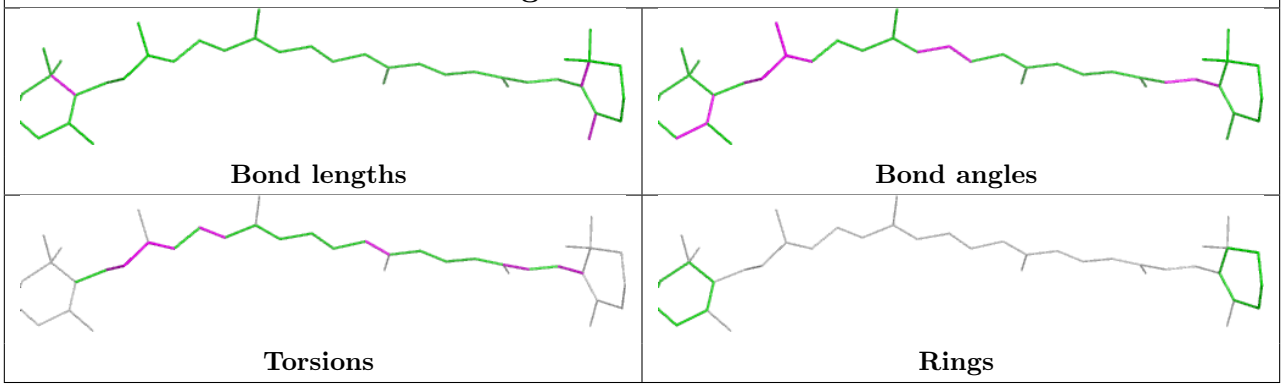


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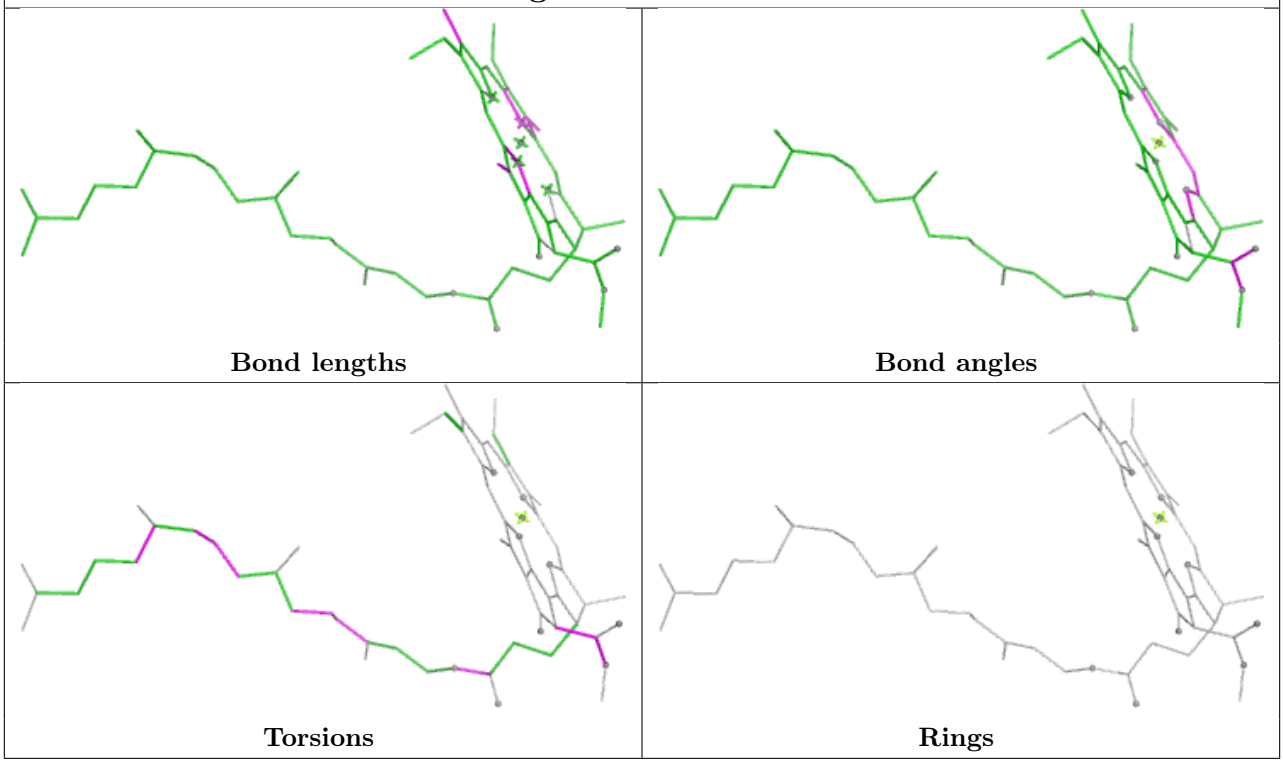


Rings

Ligand BCR m 102



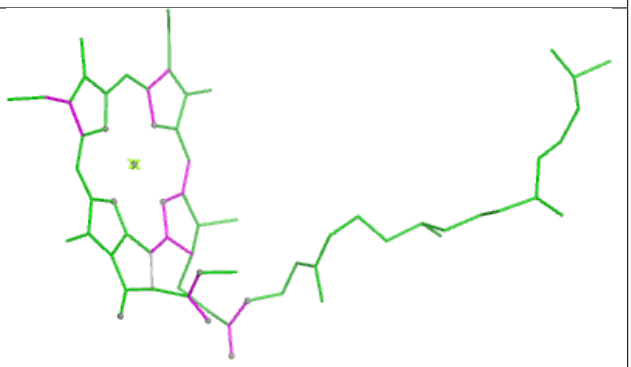
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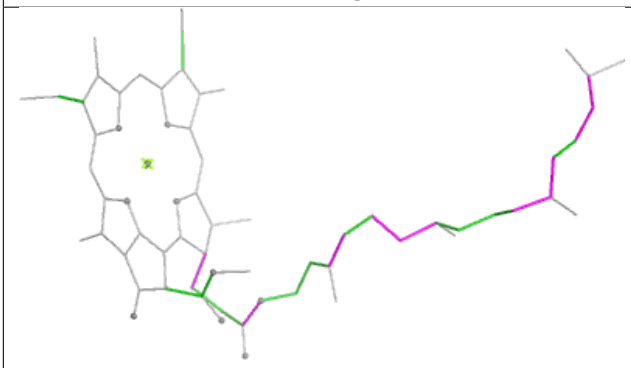
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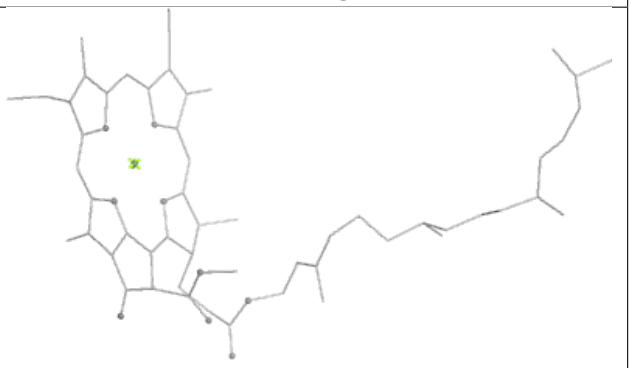
Bond lengths



Bond angles

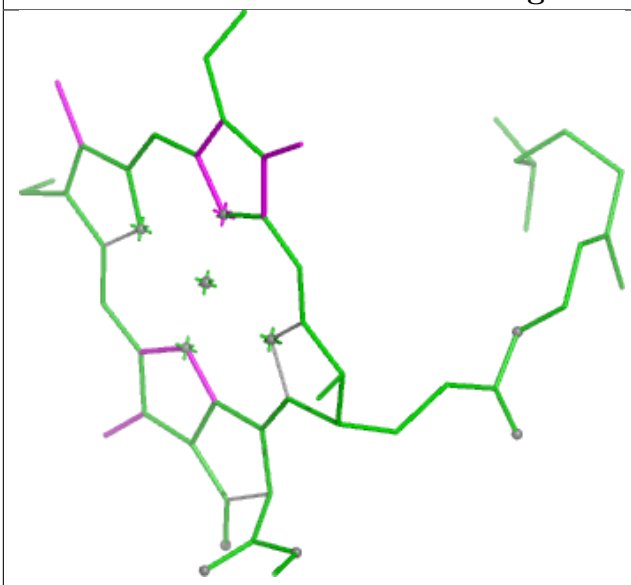


Torsions

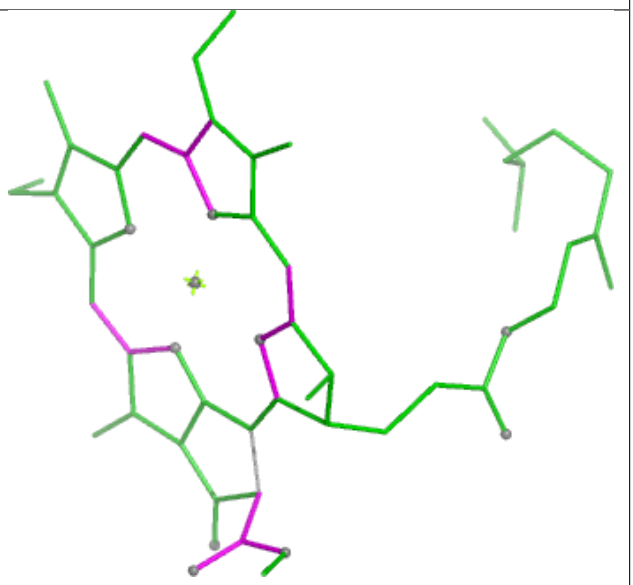


Rings

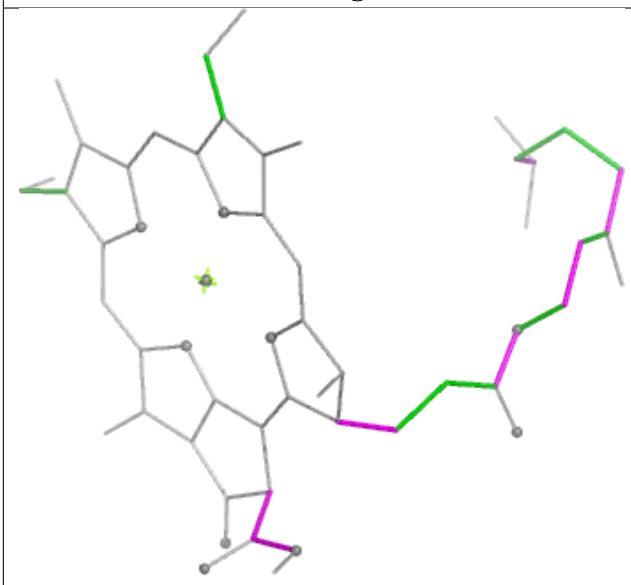
Ligand CLA b 831



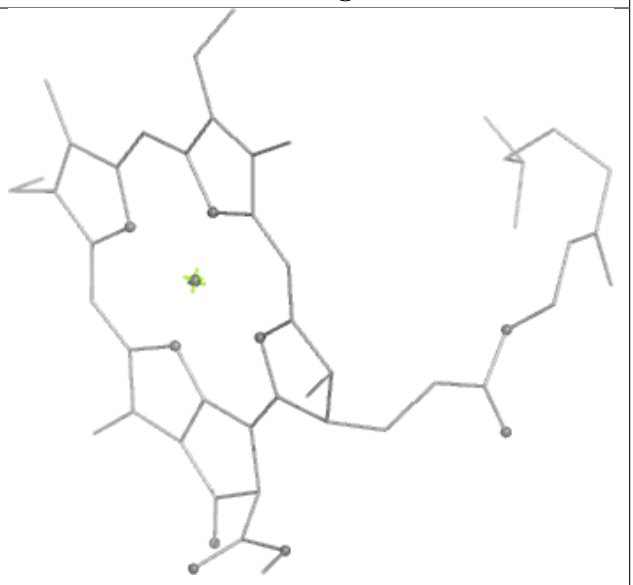
Bond lengths



Bond angles

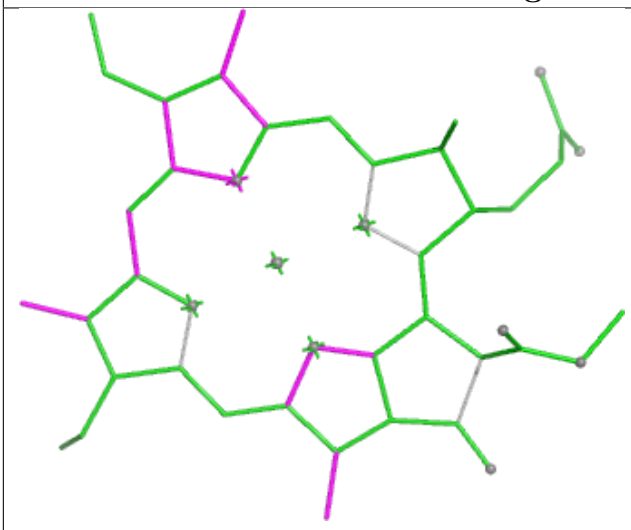


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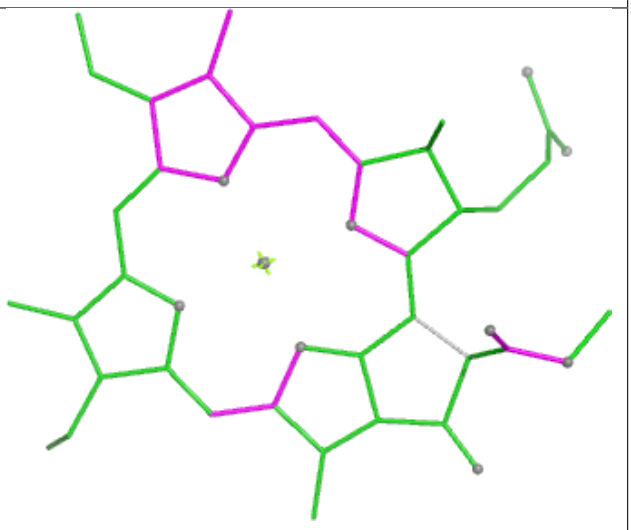


Rings

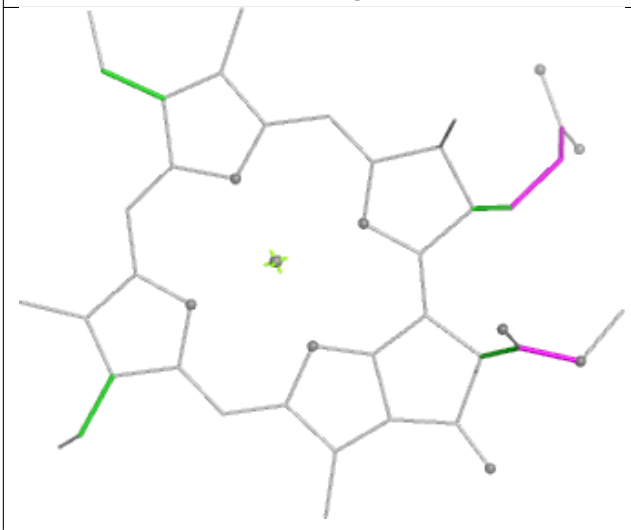
Ligand CLA B 823



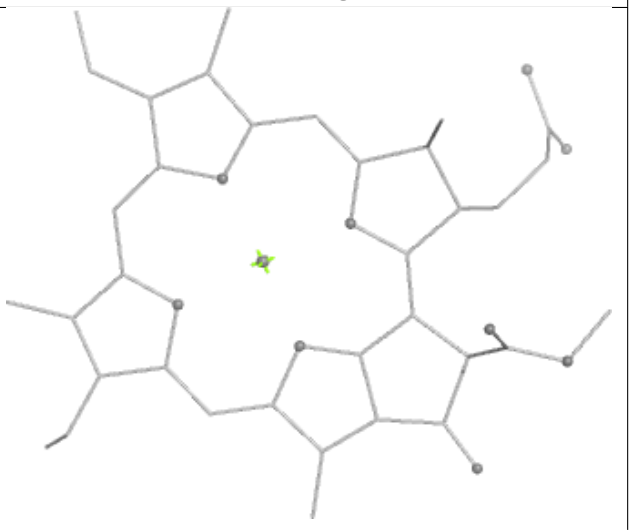
Bond lengths



Bond angles

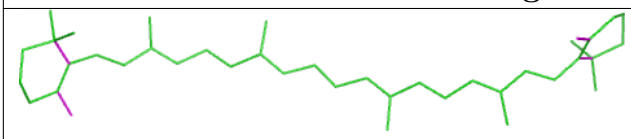


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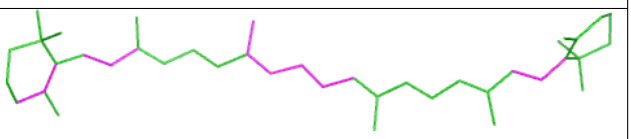


Rings

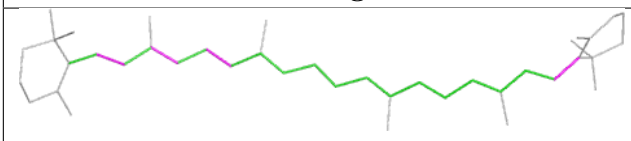
Ligand BCR B 848



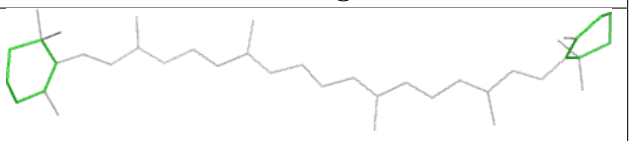
Bond lengths



Bond angles

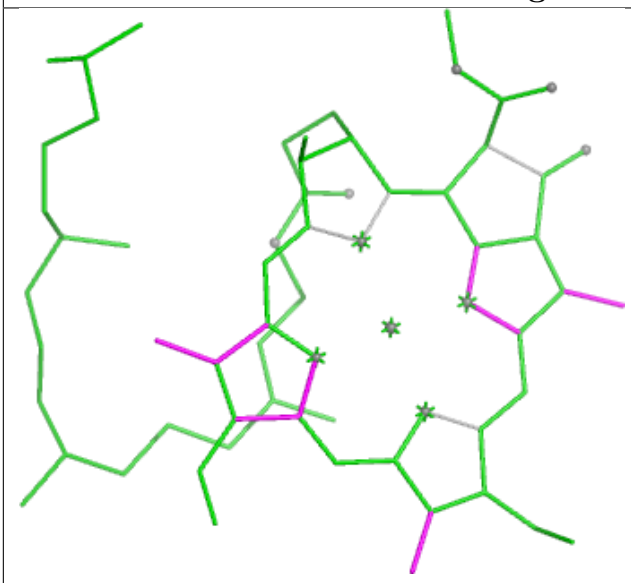


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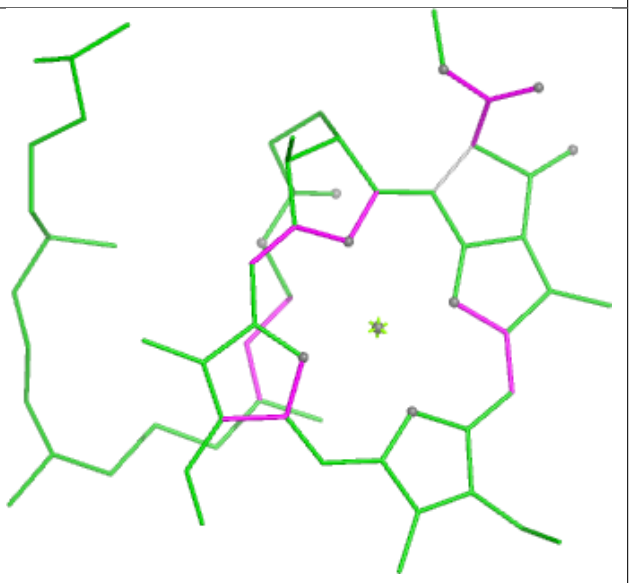


Rings

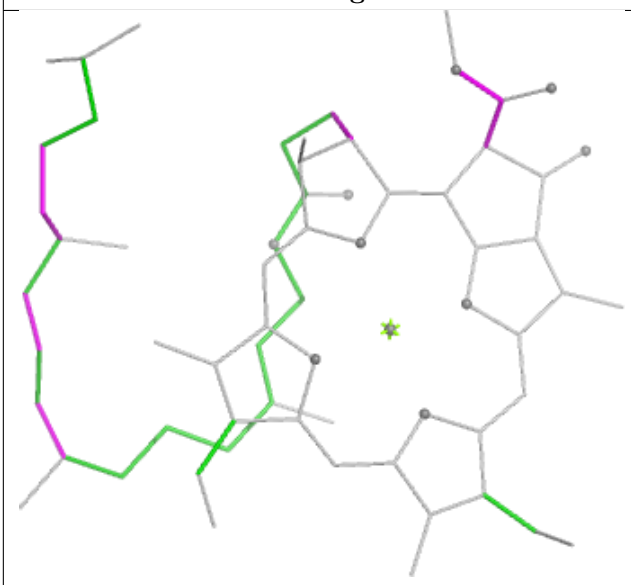
Ligand CLA a 824



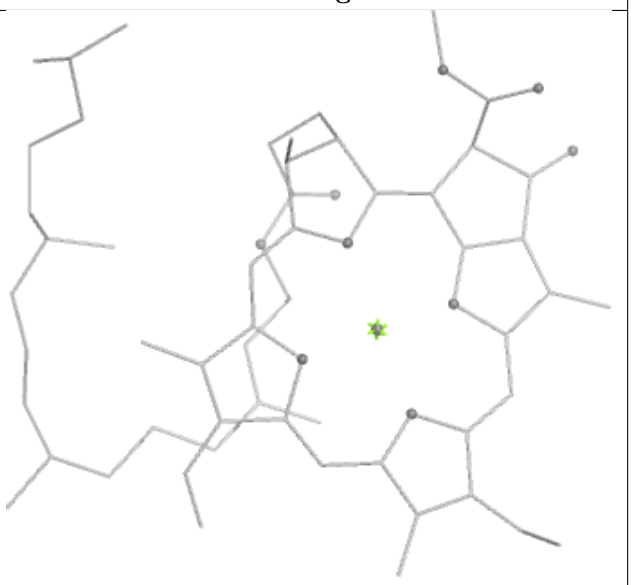
Bond lengths



Bond angles



Torsions

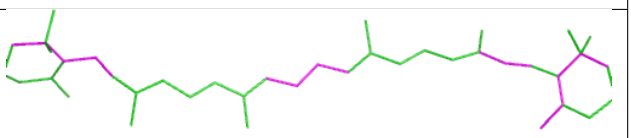


Rings

Ligand BCR 8 1304



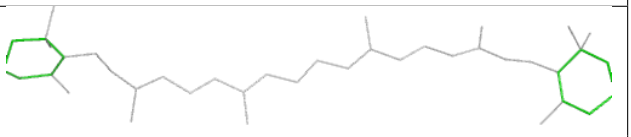
Bond lengths



Bond angles

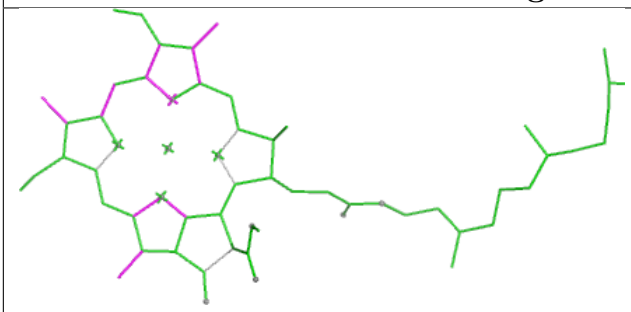


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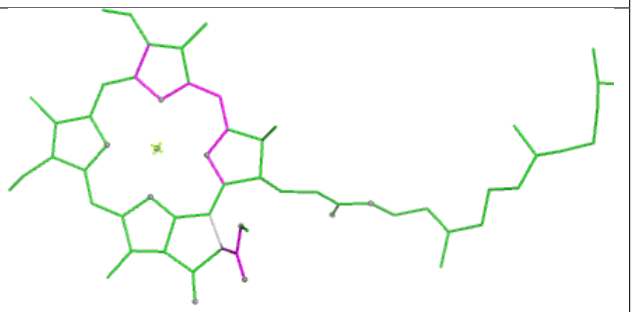


Rings

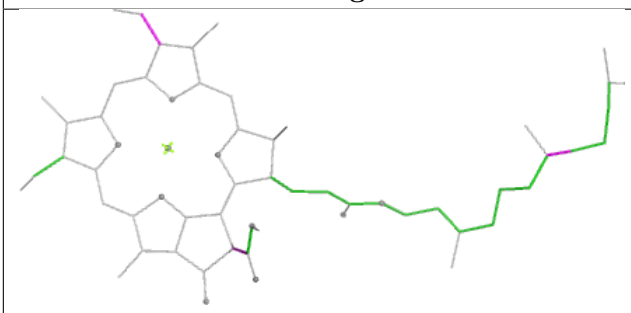
Ligand CLA b 838



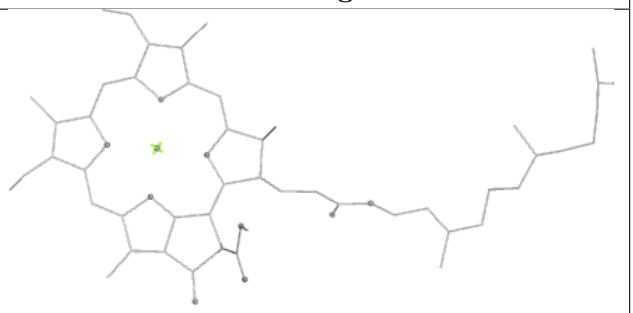
Bond lengths



Bond angles

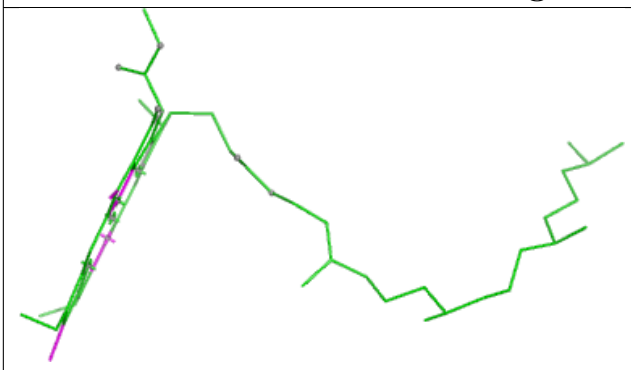


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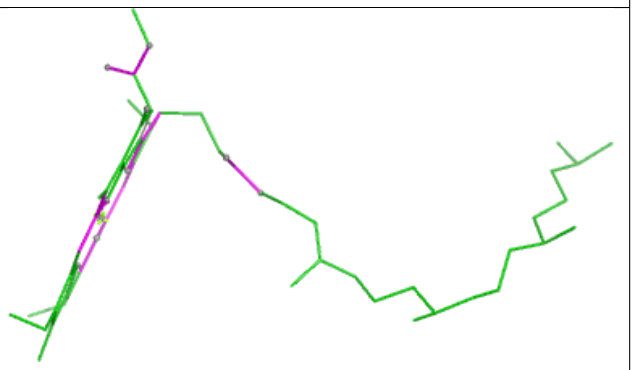


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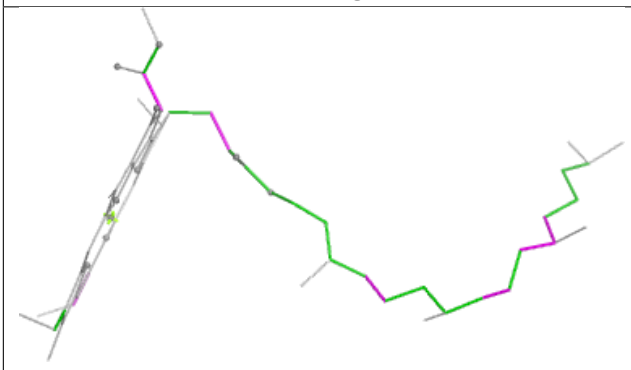
Ligand CLA 2 841



Bond lengths



Bond angles

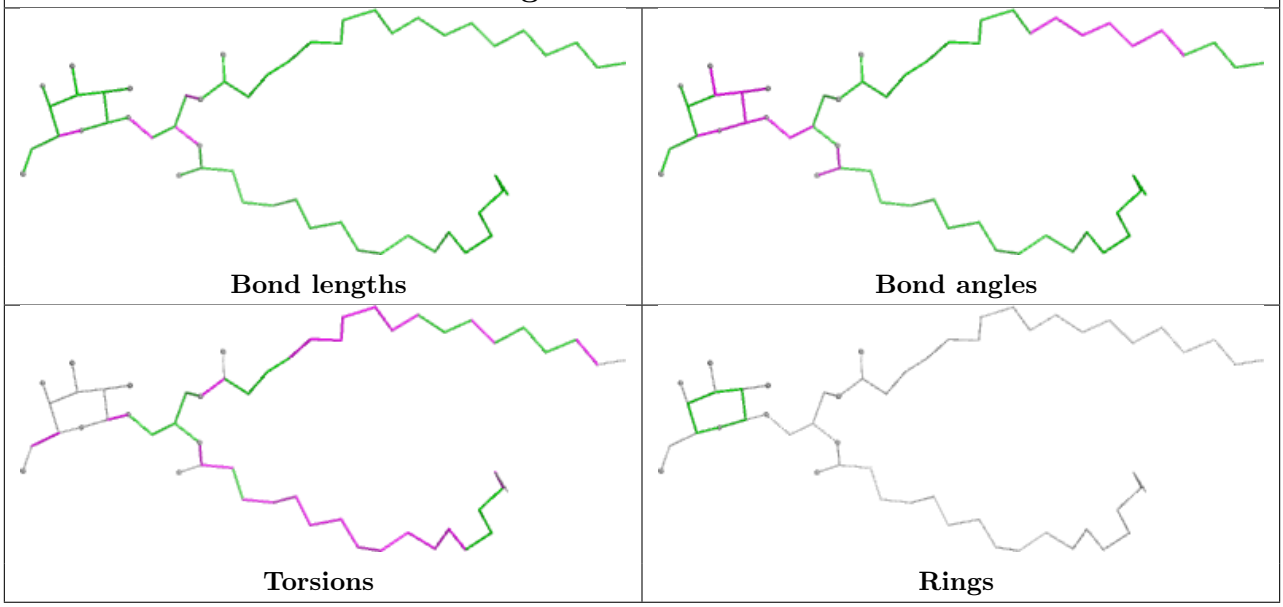


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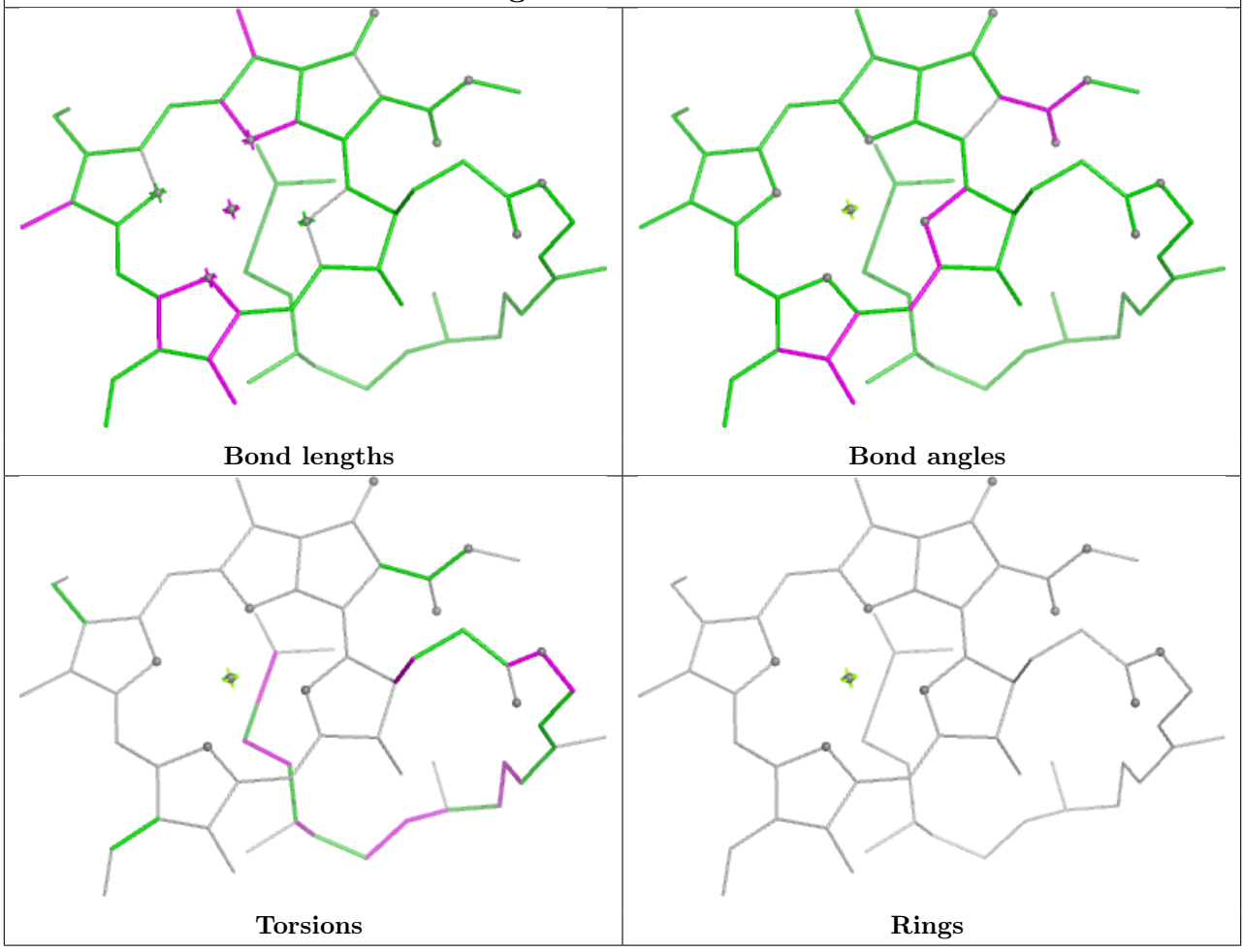


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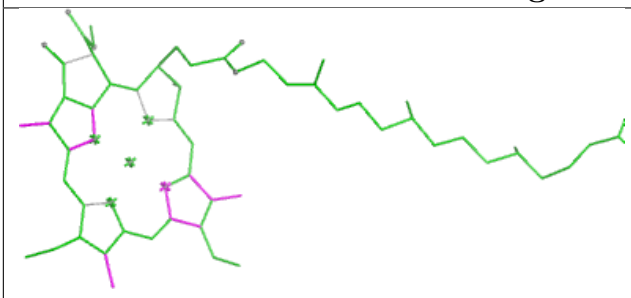
Ligand LMG B 849



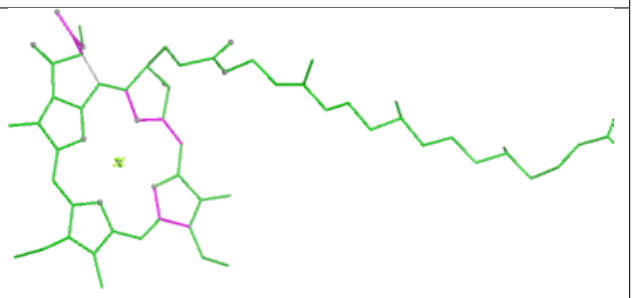
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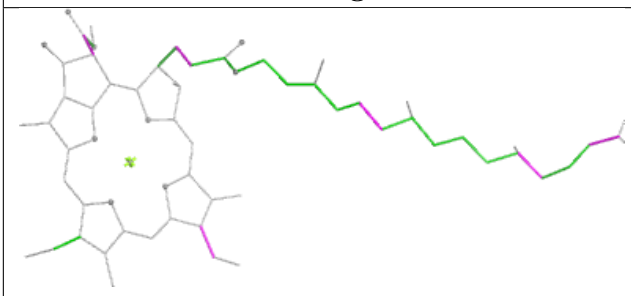
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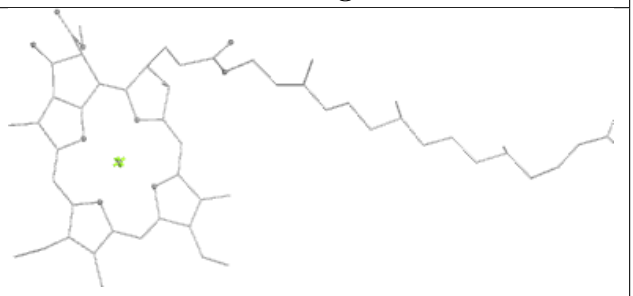
Bond lengths



Bond angles

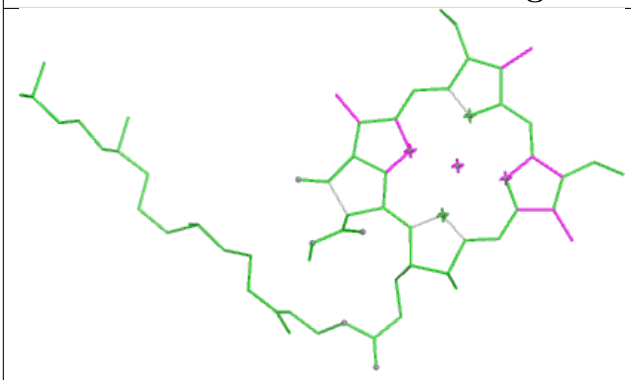


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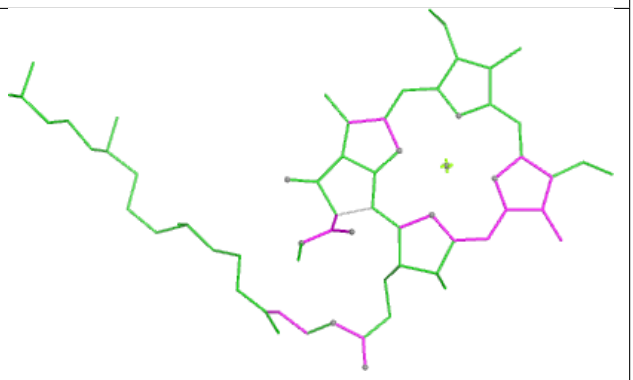


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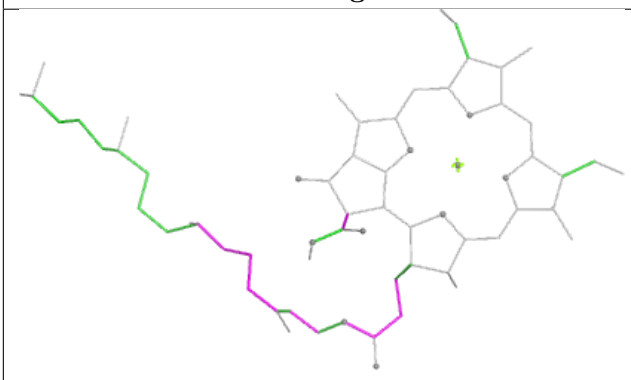
Ligand CLA L 205



Bond lengths



Bond angles

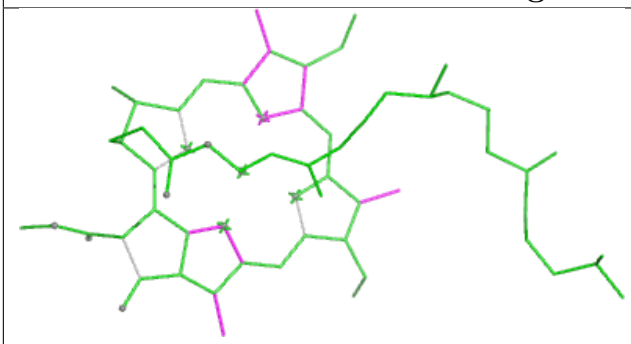


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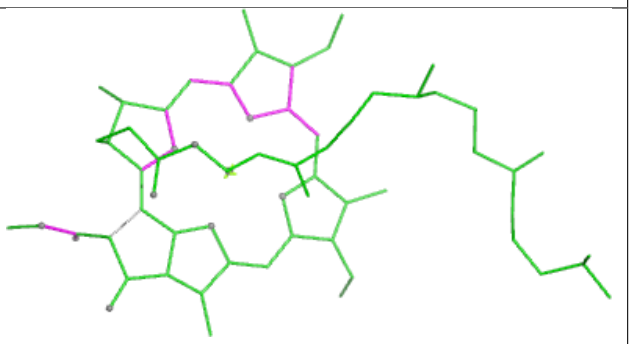


Rings

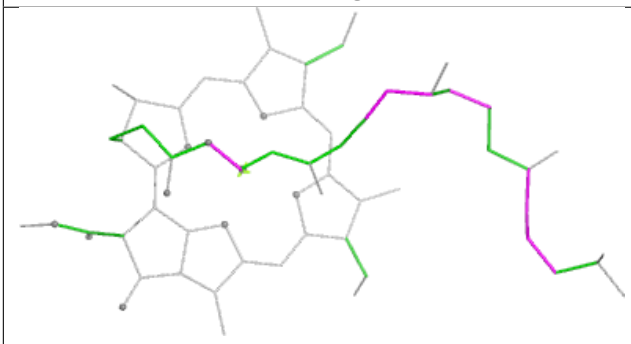
Ligand CLA b 839



Bond lengths



Bond angles

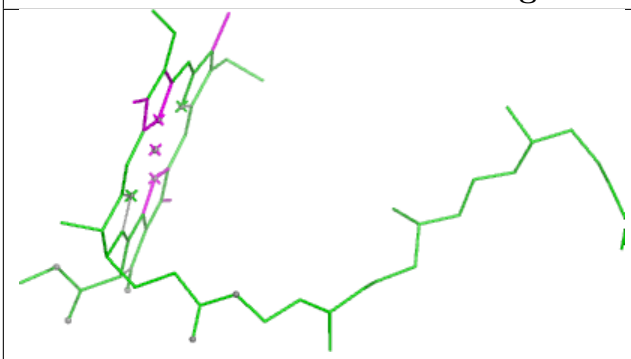


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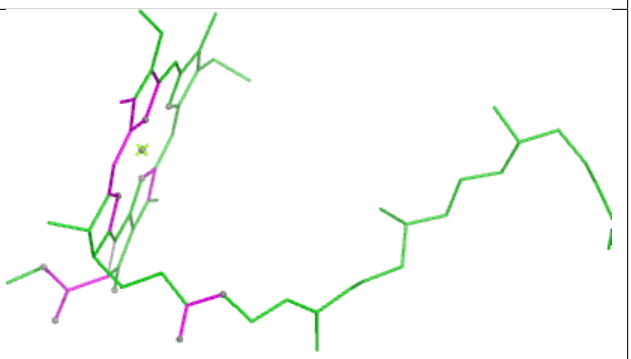


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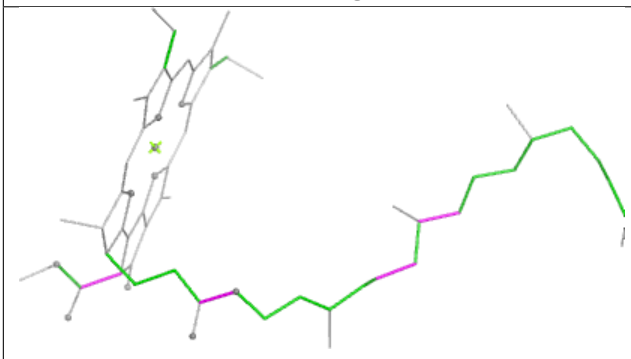
Ligand CLA 1 1632



Bond lengths



Bond angles

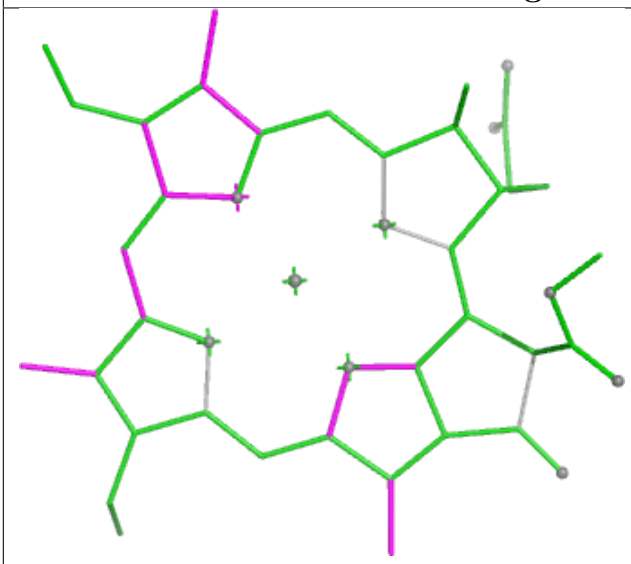


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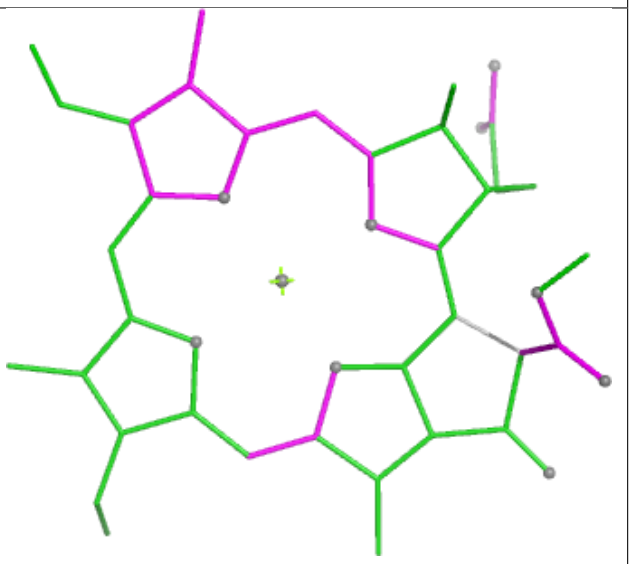


Rings

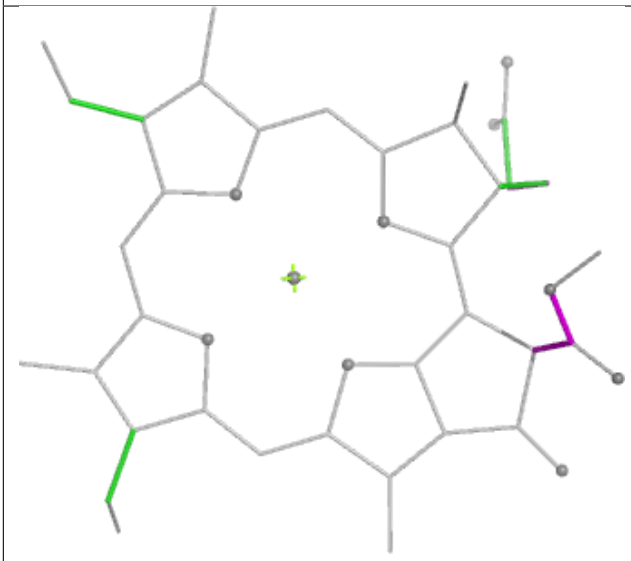
Ligand CLA B 821



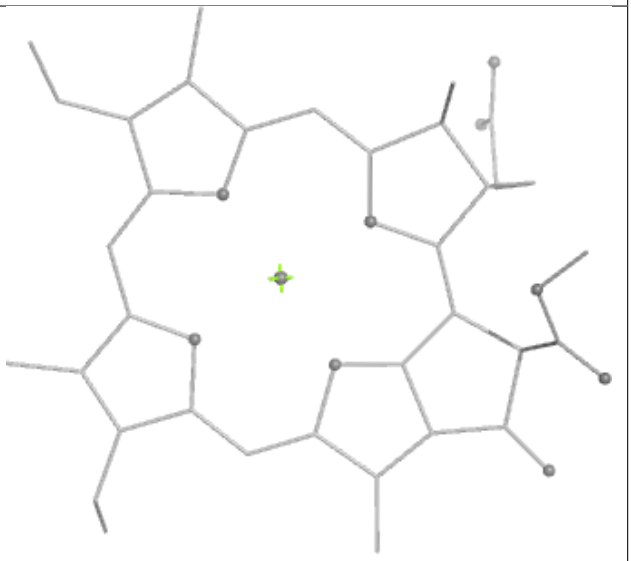
Bond lengths



Bond angles

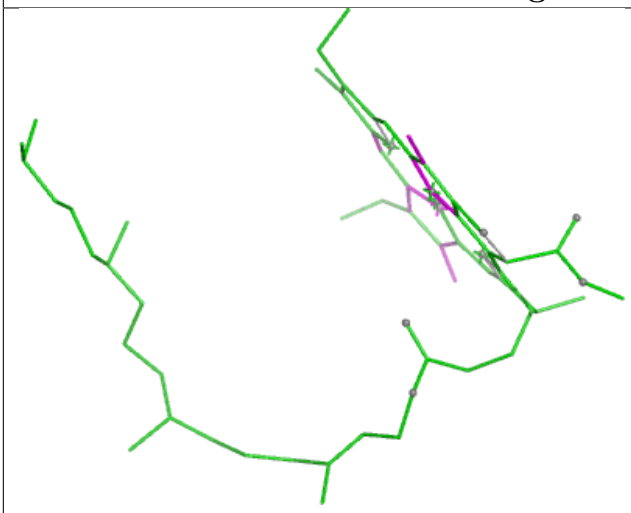


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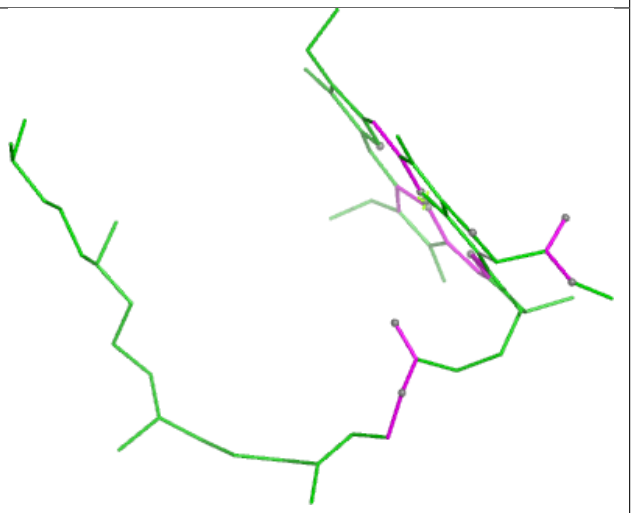


Rings

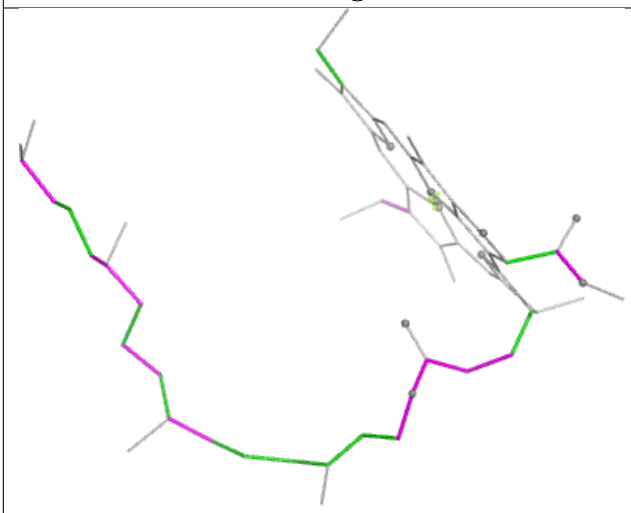
Ligand CLA 2 820



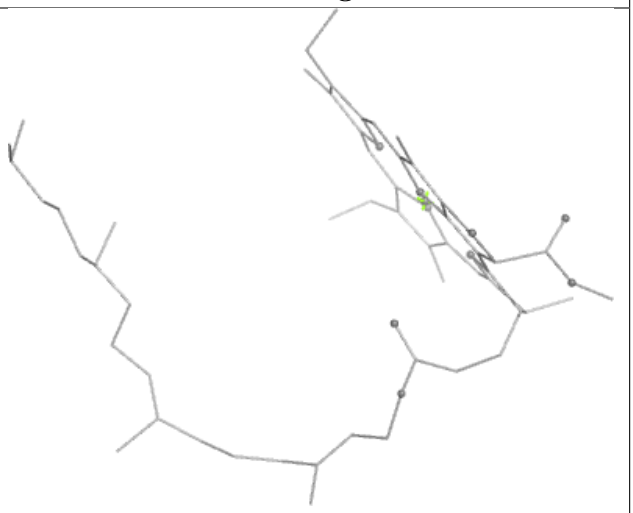
Bond lengths



Bond angles

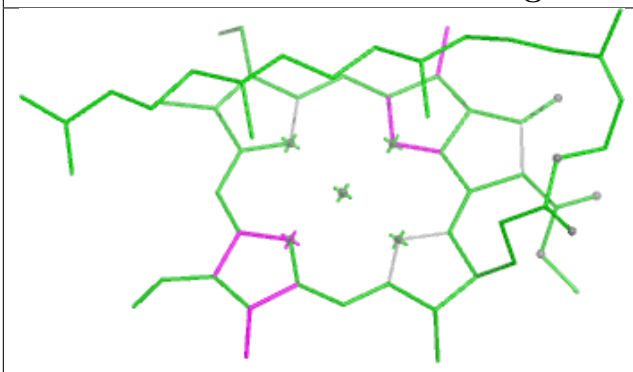


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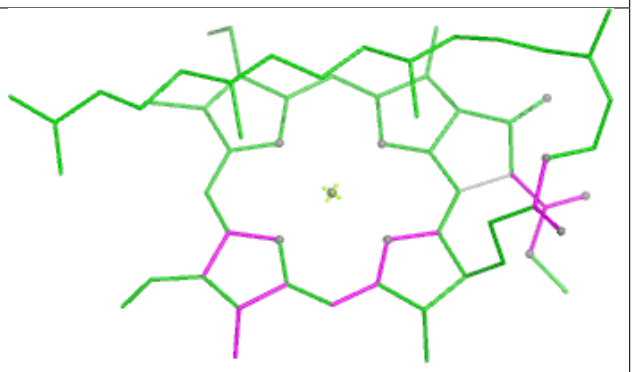


Rings

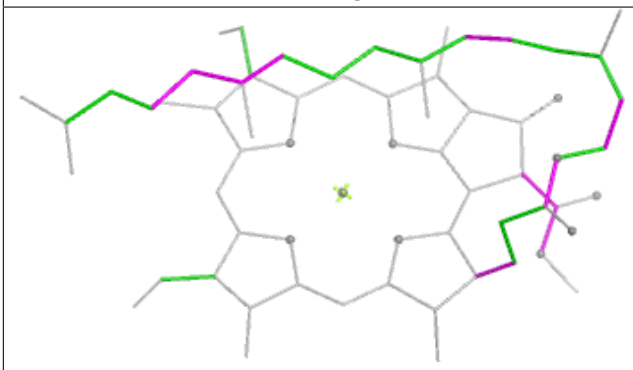
Ligand CLA B 816



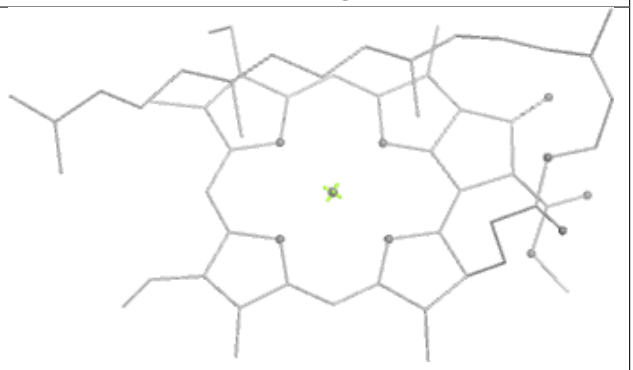
Bond lengths



Bond angles



Torsions

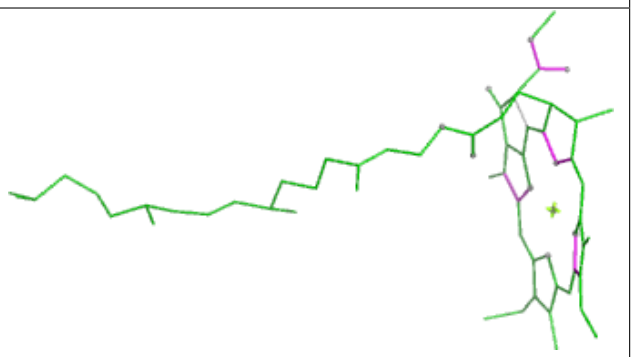


Rings

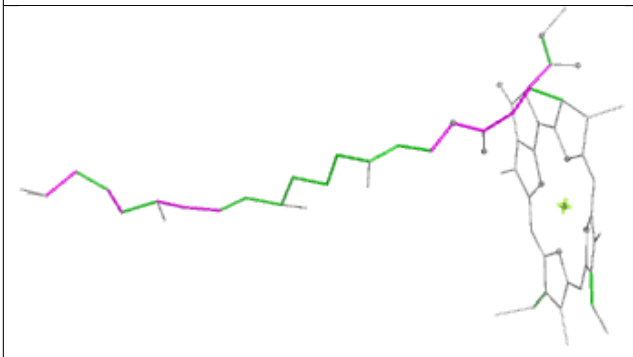
Ligand CLA b 829



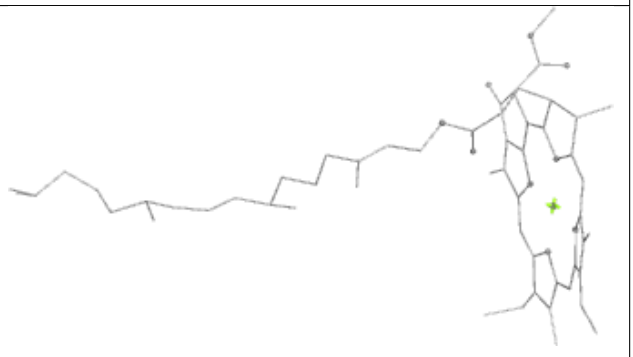
Bond lengths



Bond angles

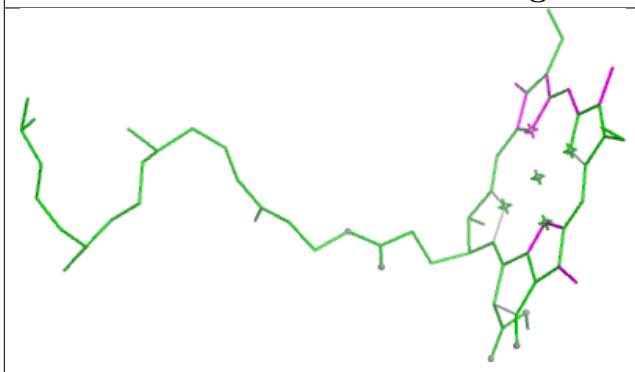


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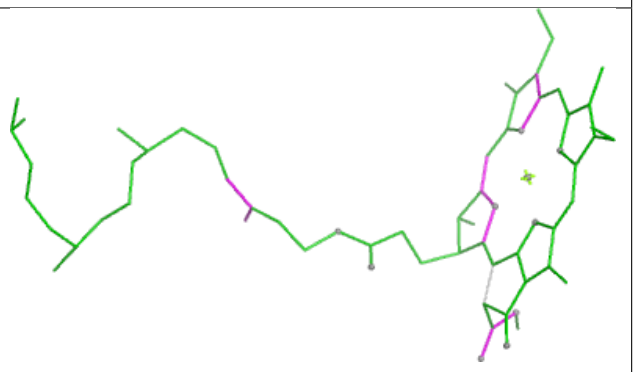


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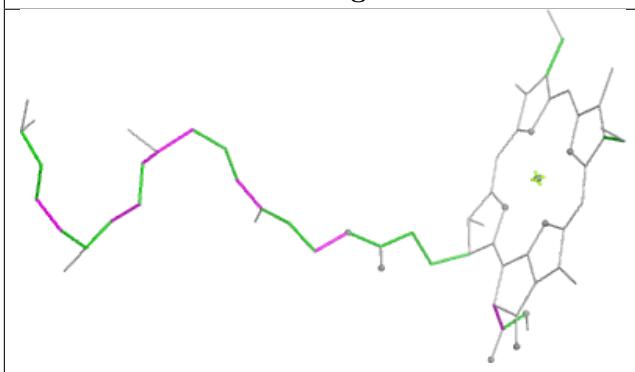
Ligand CLA 2 834



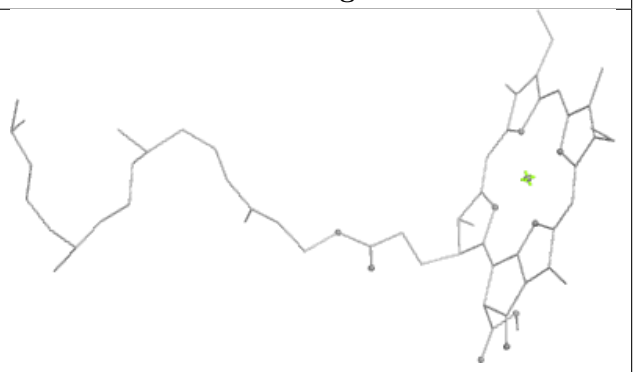
Bond lengths



Bond angles

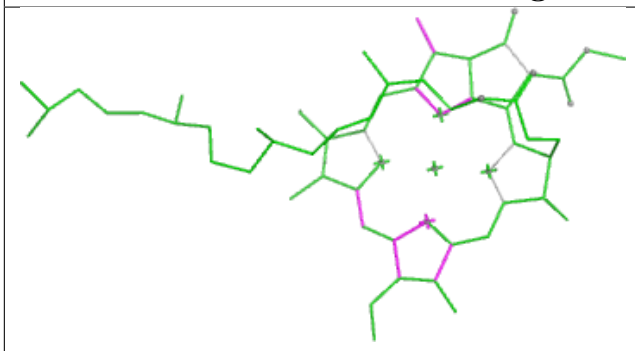


Torsions

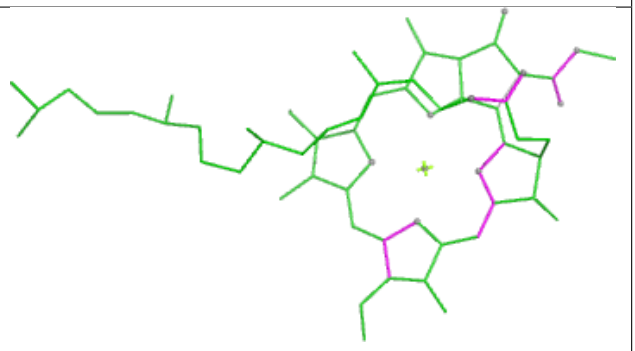


Rings

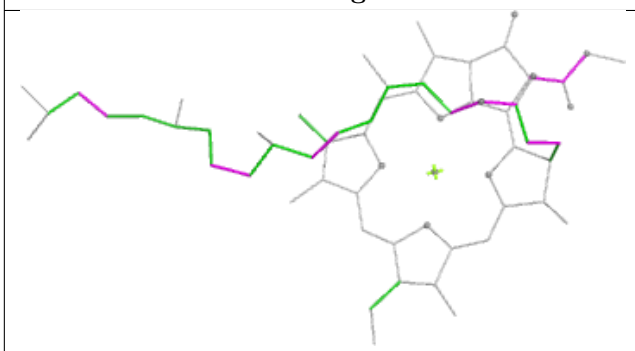
Ligand CLA a 818



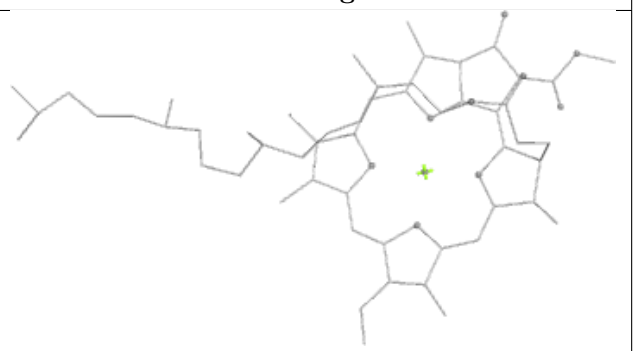
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Bond angles

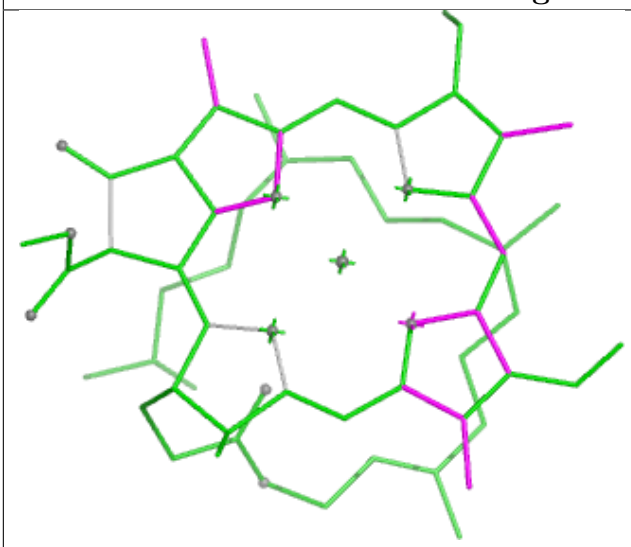


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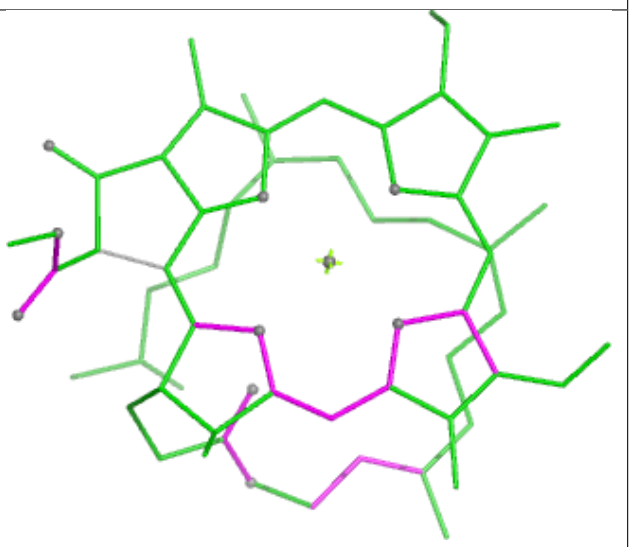


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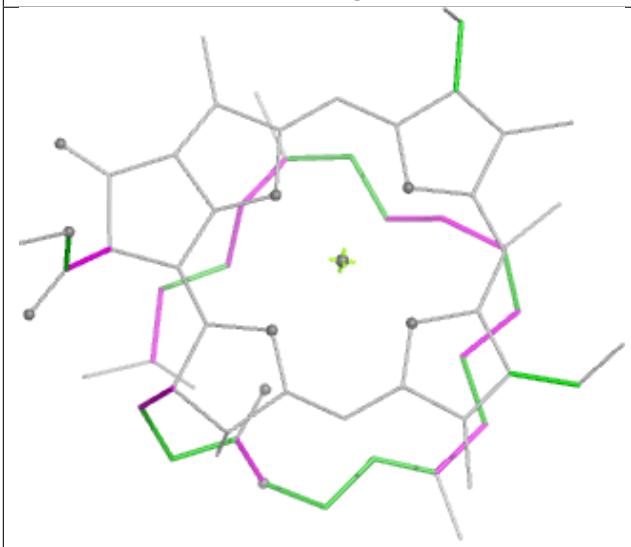
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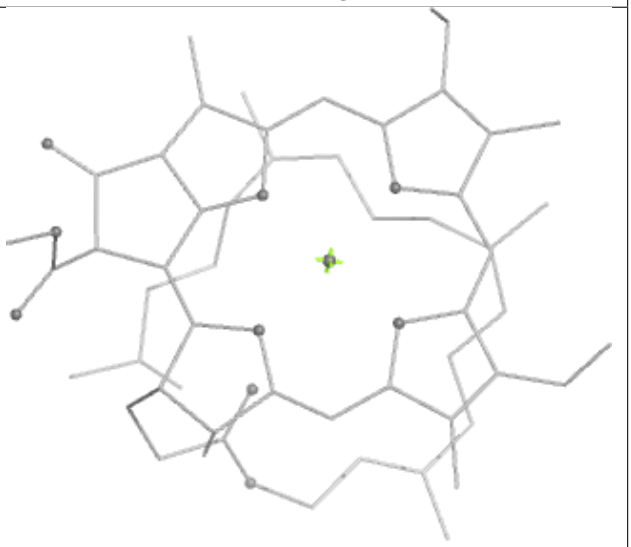
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Bond angles

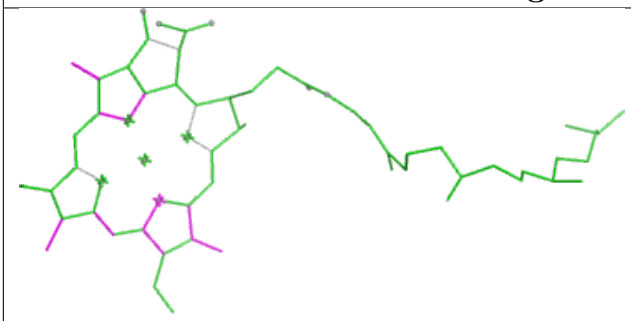


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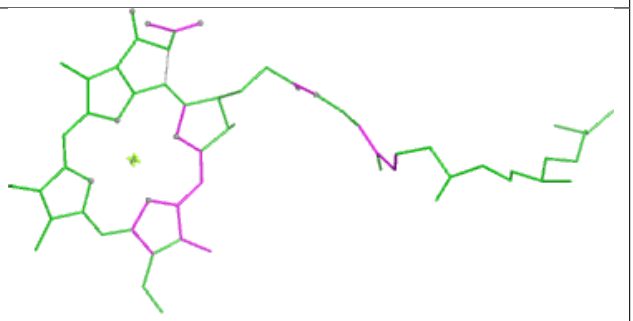


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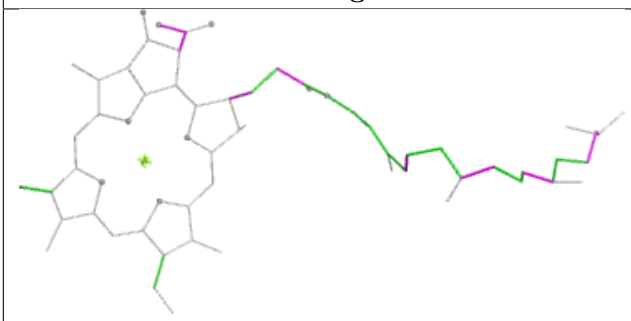
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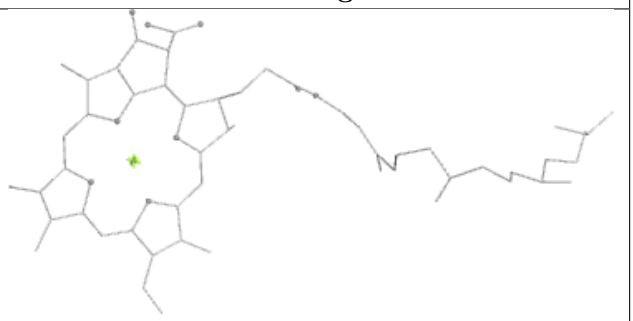
Bond lengths



Bond angles

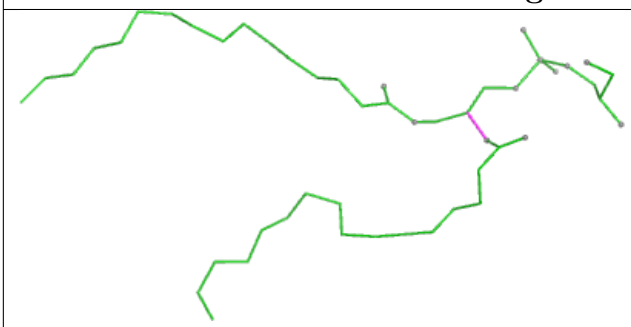


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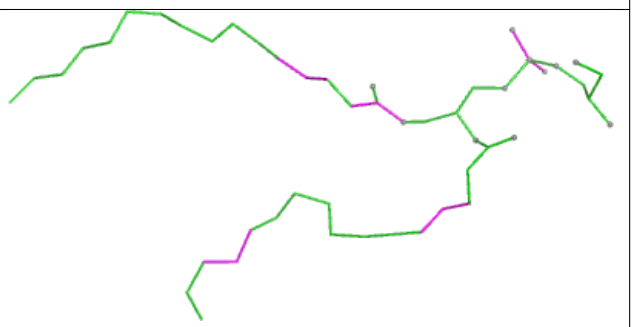


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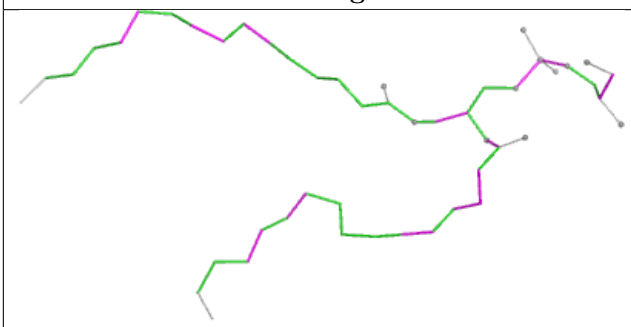
Ligand LHG b 851



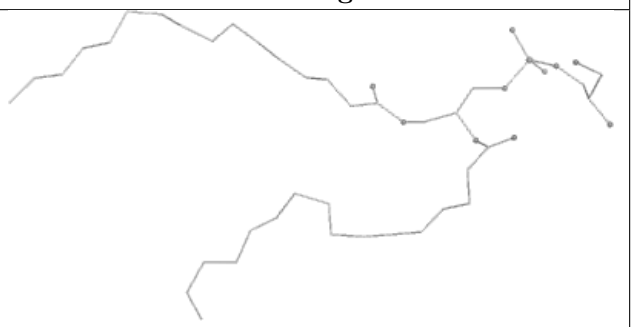
Bond lengths



Bond angles

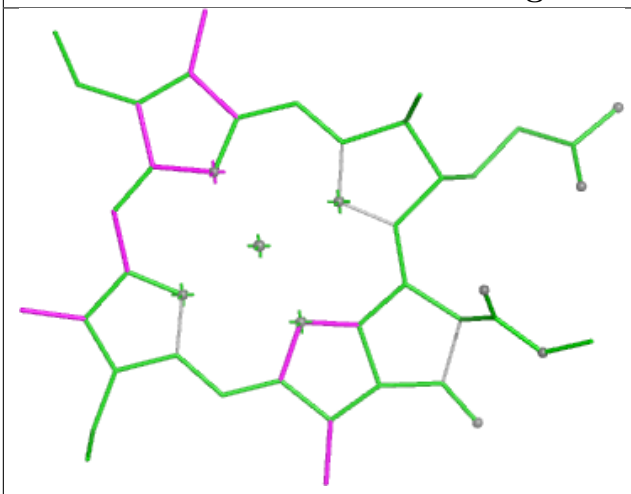


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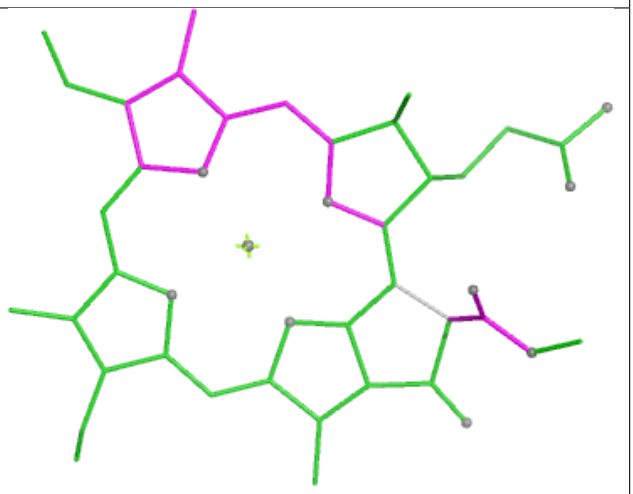


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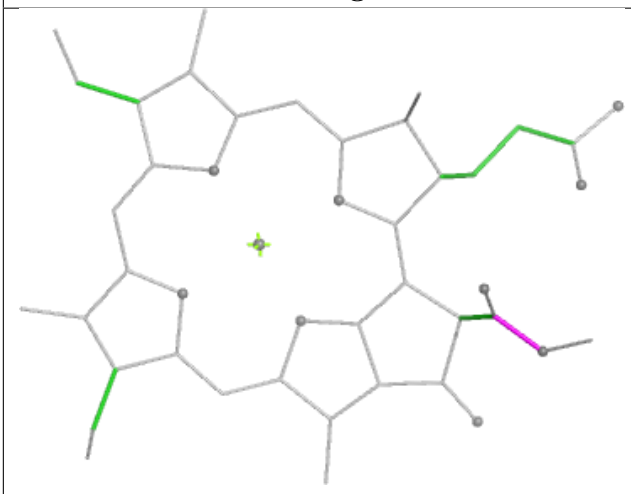
Ligand CLA F 203



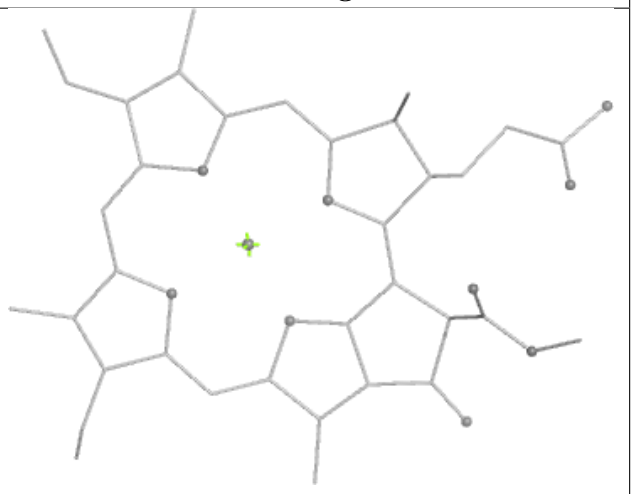
Bond lengths



Bond angles

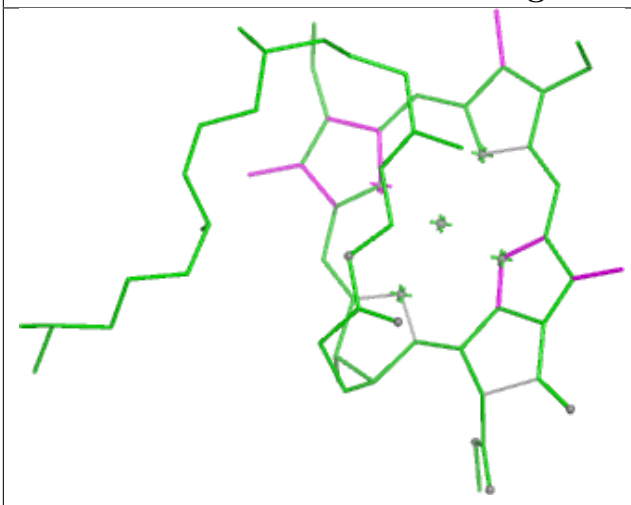


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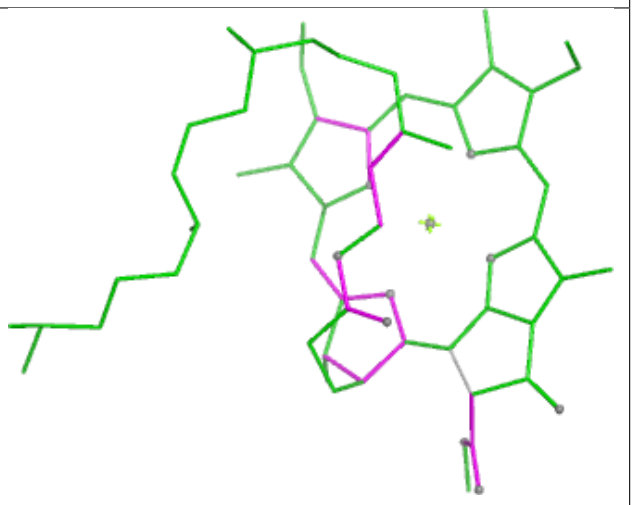


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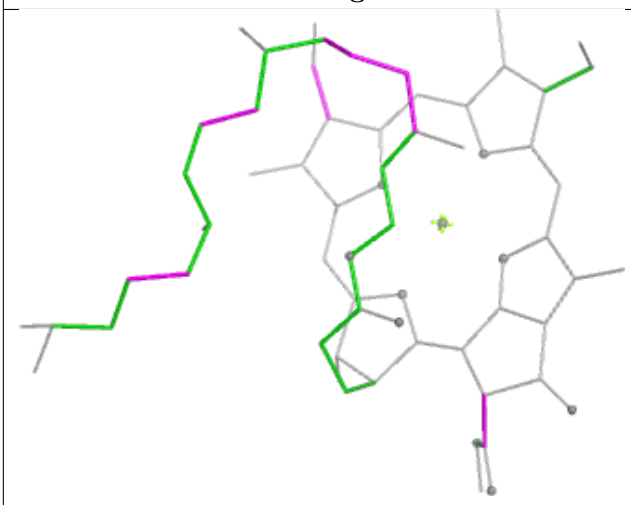
Ligand CLA b 809



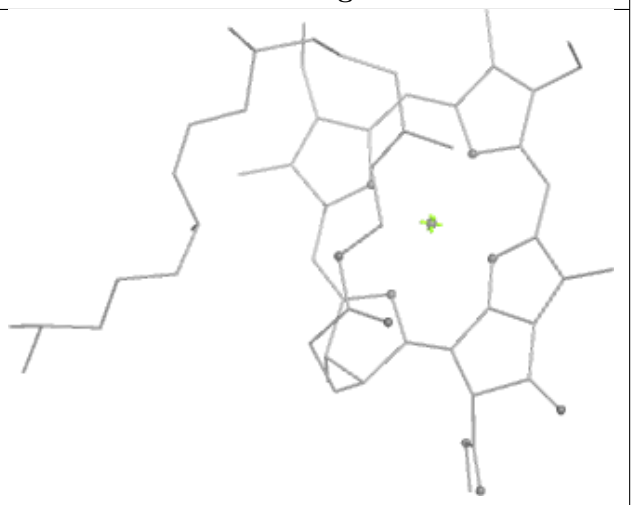
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Bond angles

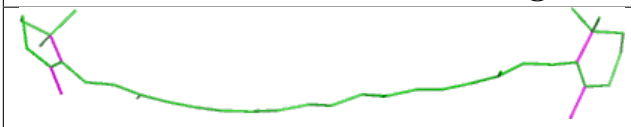


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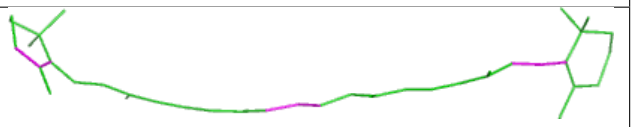


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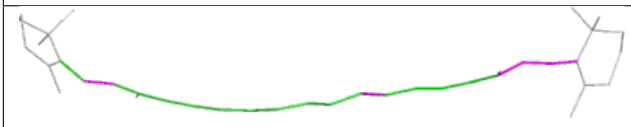
Ligand BCR I 101



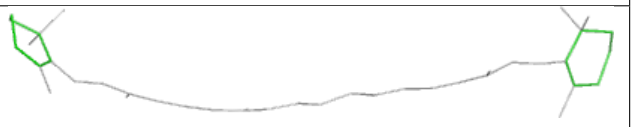
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Bond angles

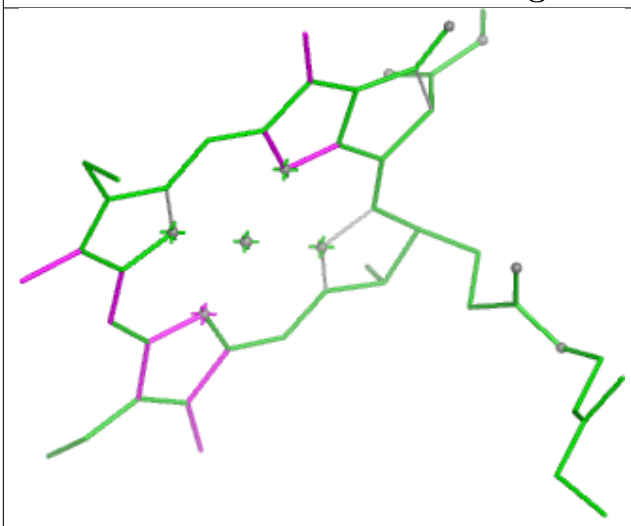


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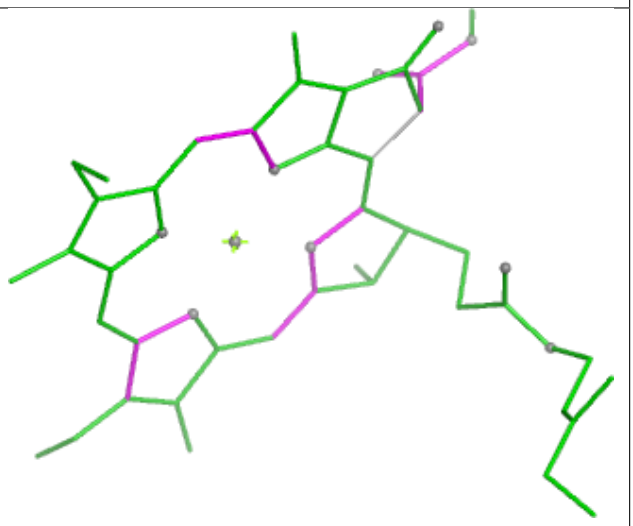


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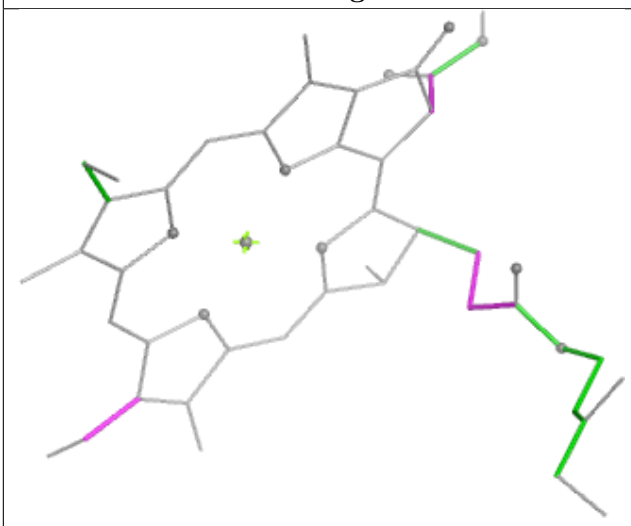
Ligand CLA a 808



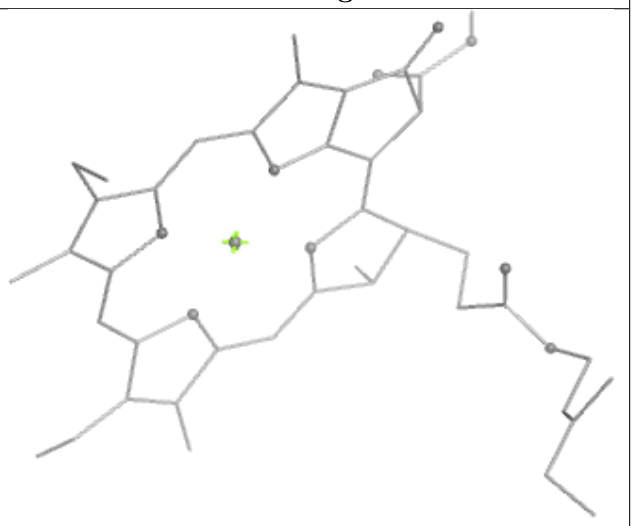
Bond lengths



Bond angles

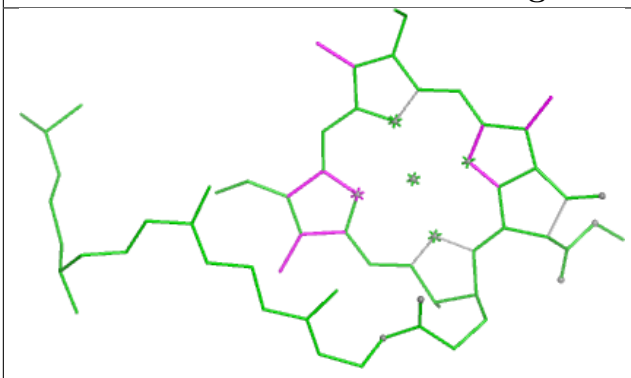


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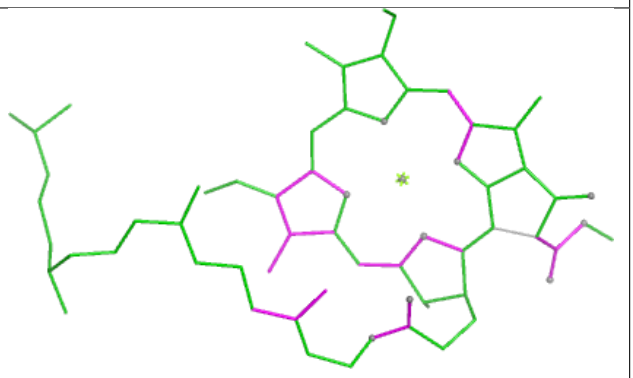


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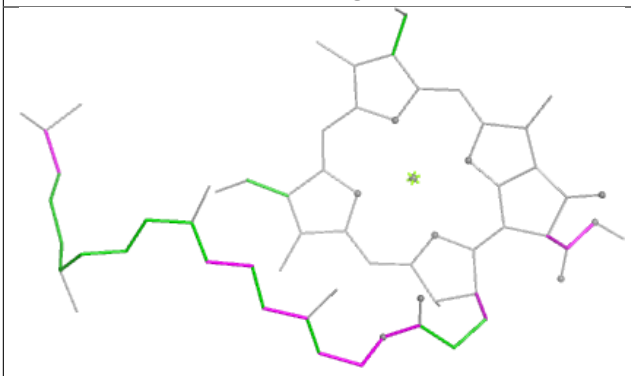
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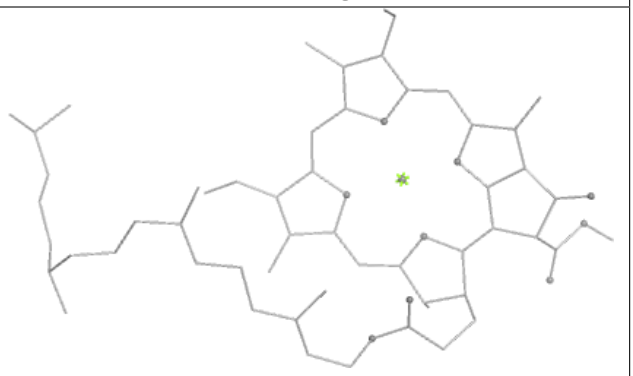
Bond lengths



Bond angles

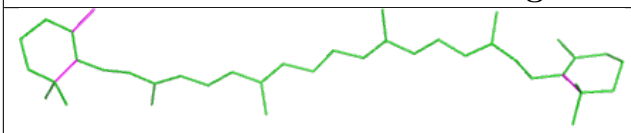


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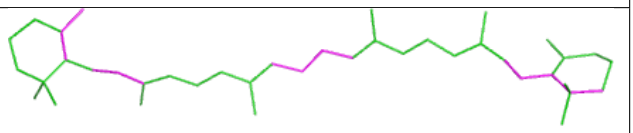


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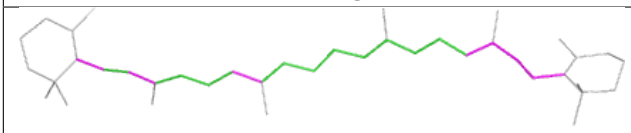
Ligand BCR J 103



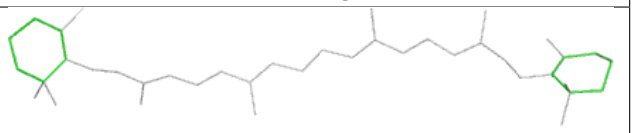
Bond lengths



Bond angles

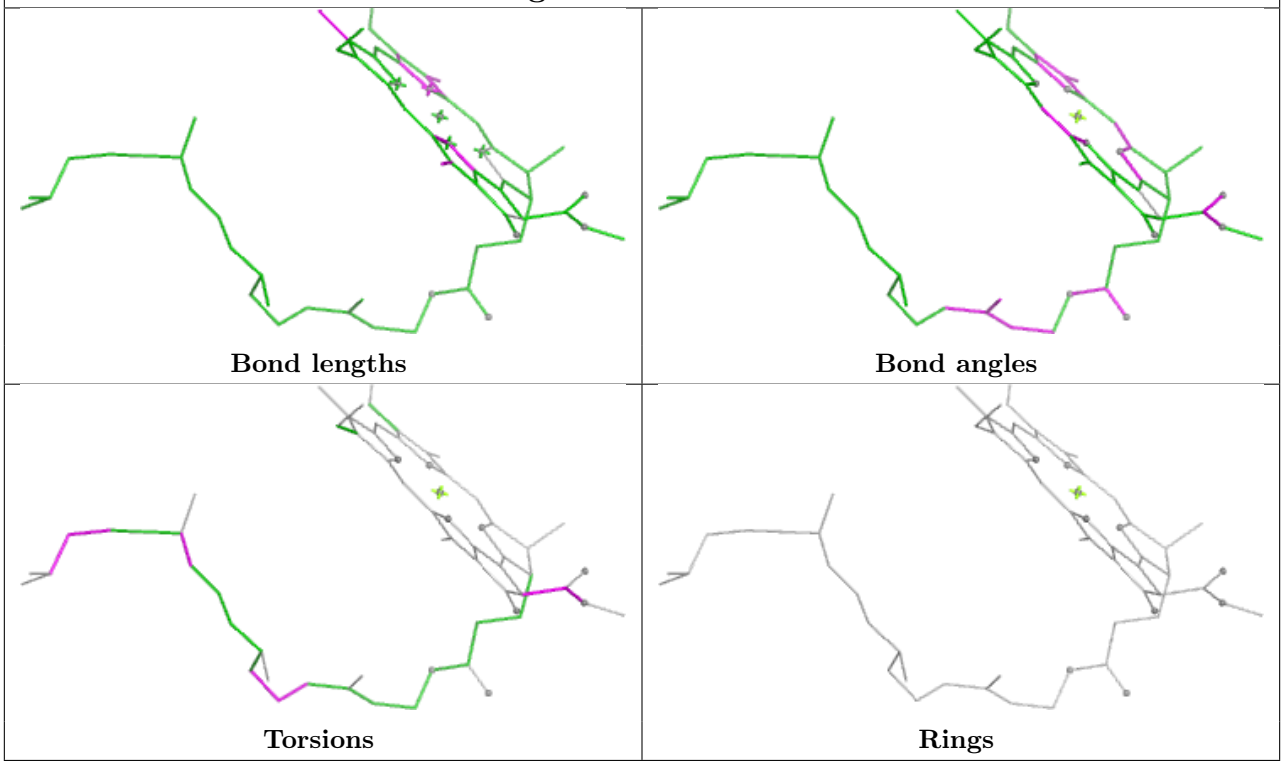


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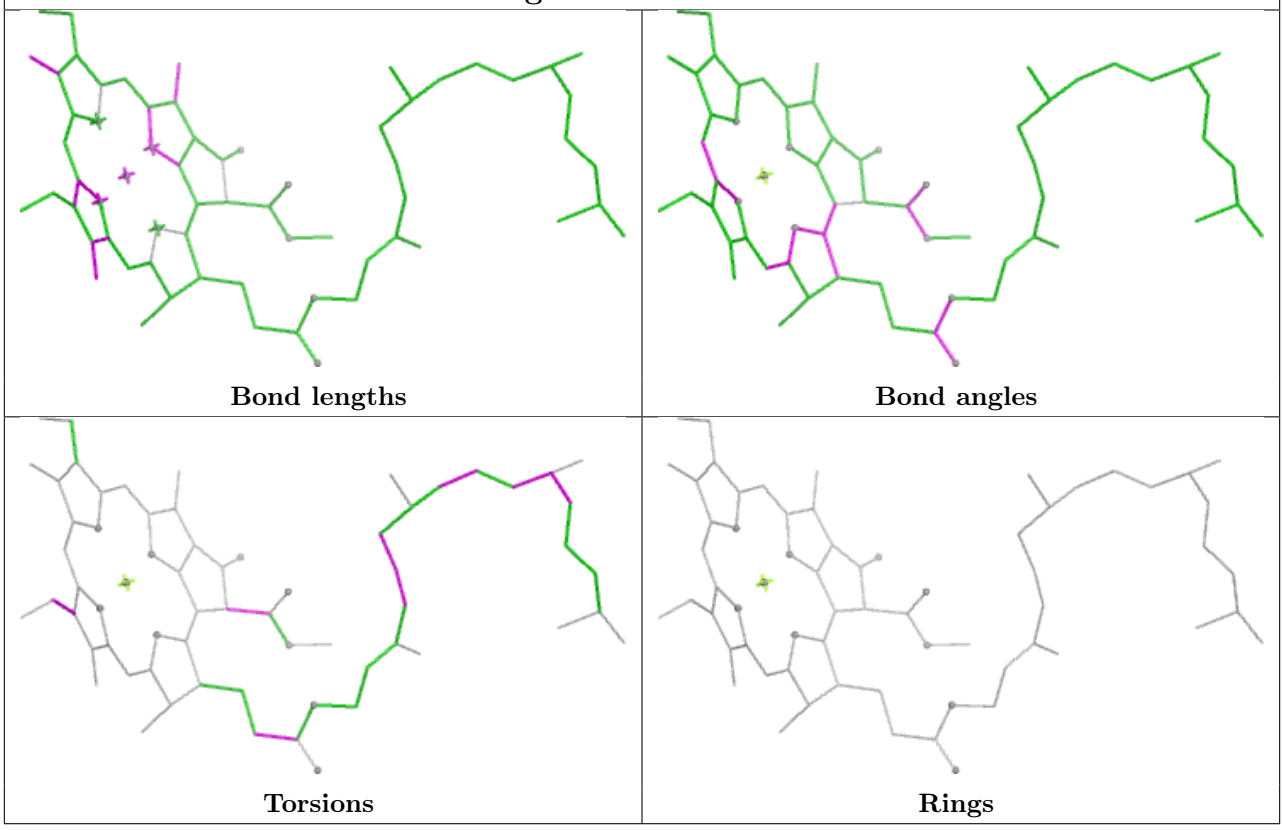


Rings

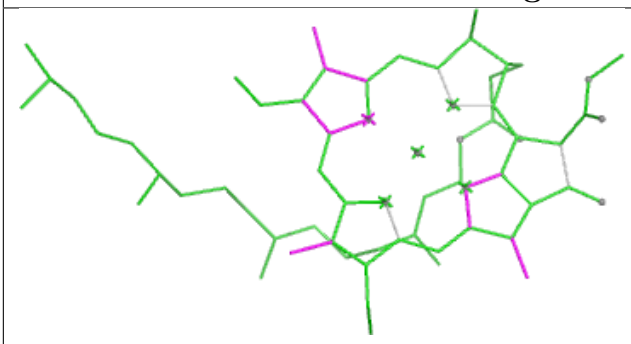
Ligand CLA b 812



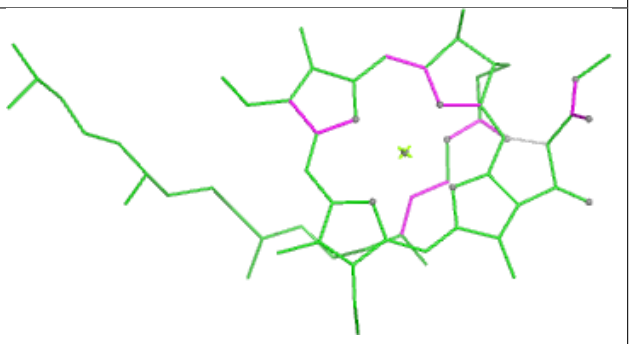
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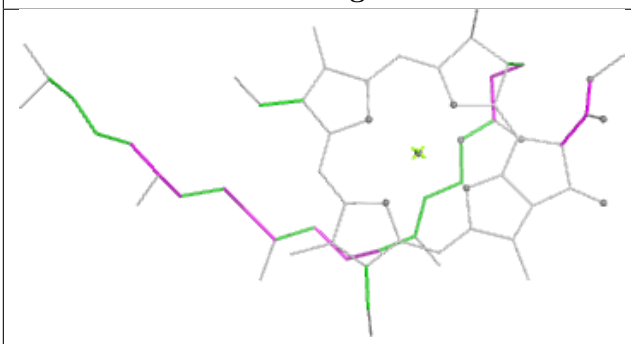
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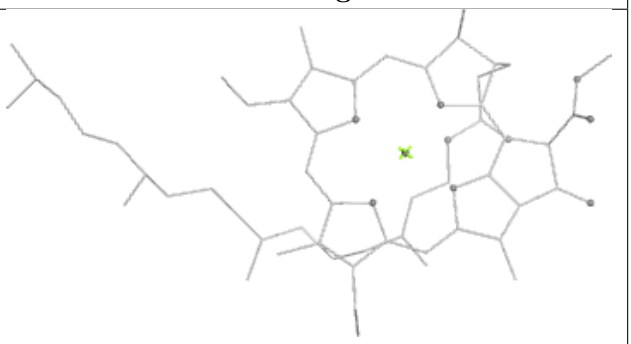
Bond lengths



Bond angles

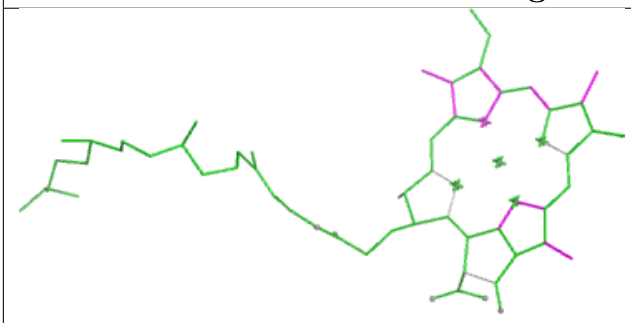


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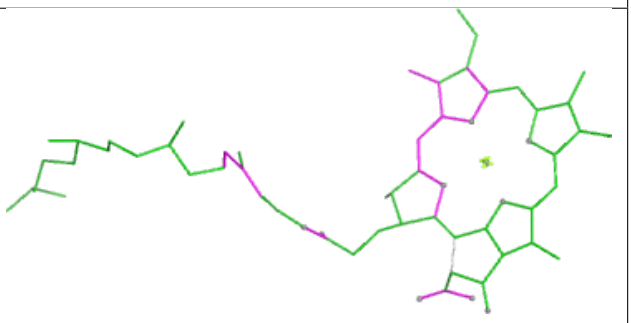


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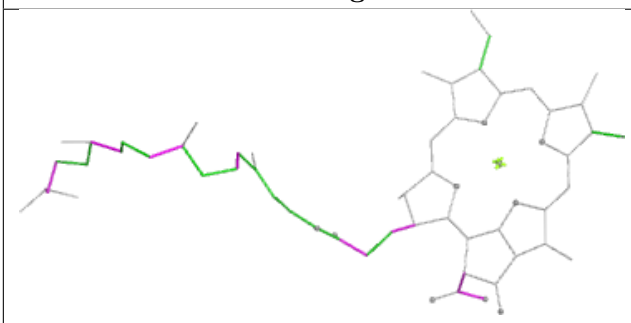
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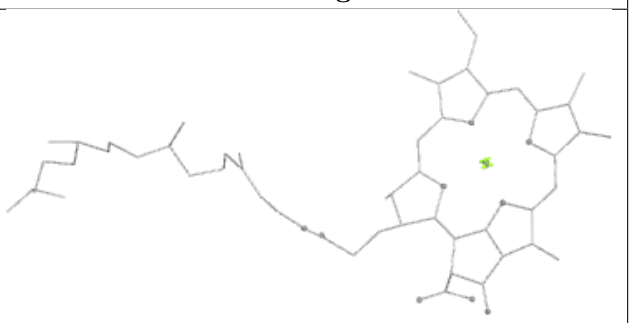
Bond lengths



Bond angles

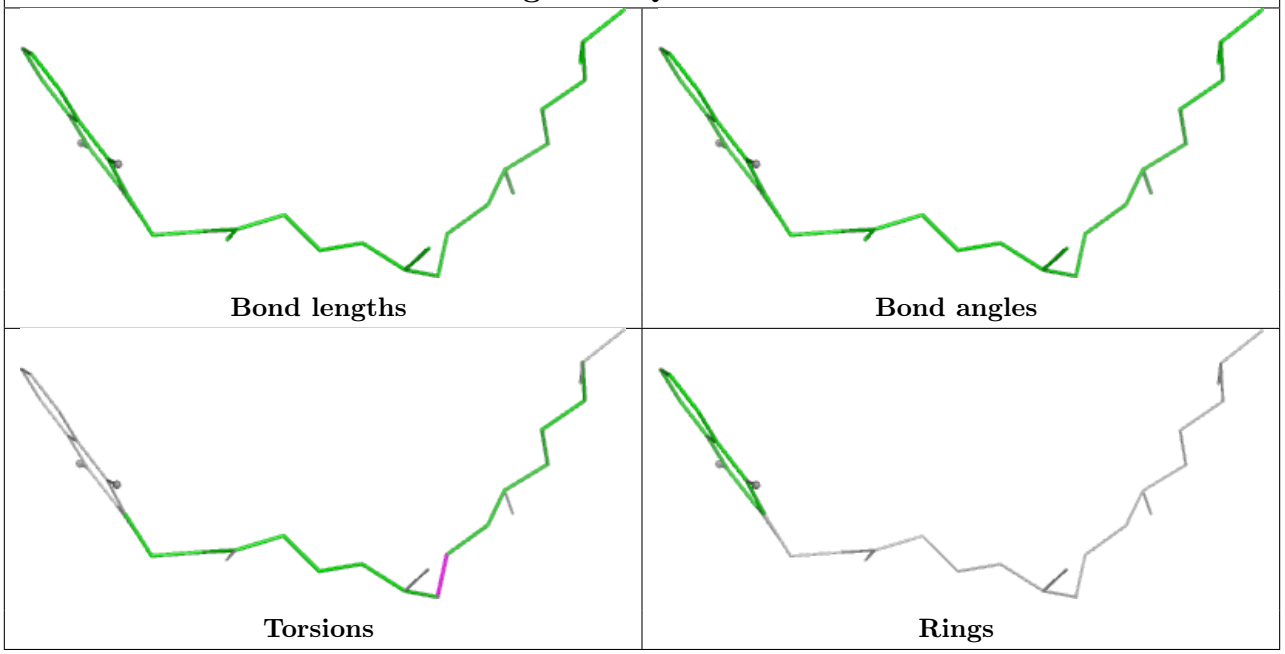


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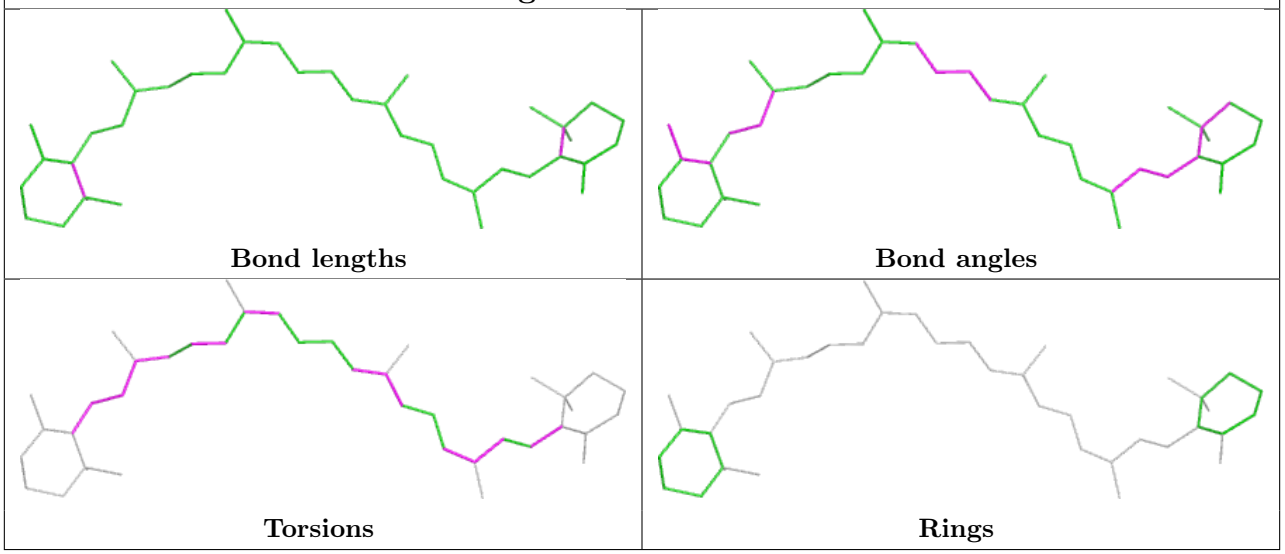


Rings

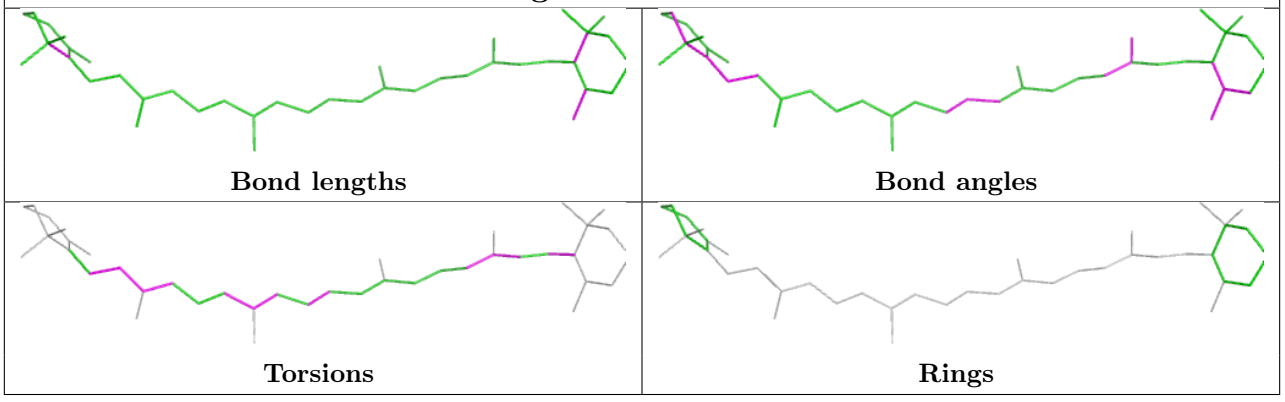
Ligand PQN B 842



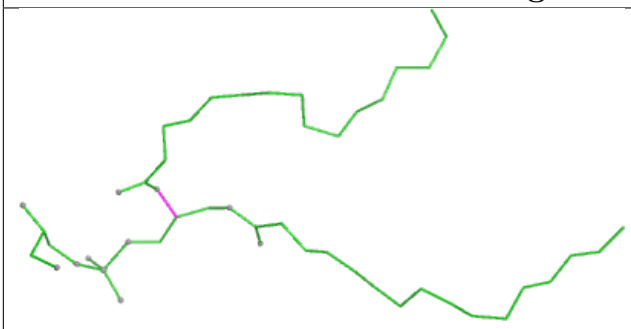
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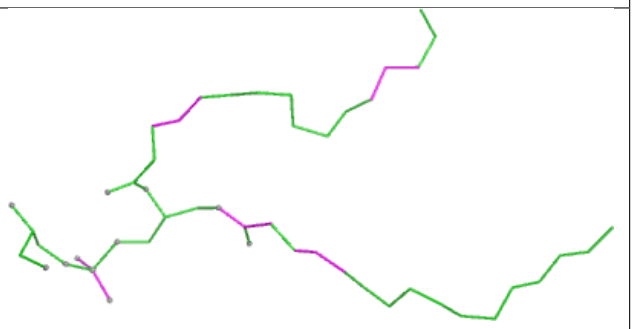
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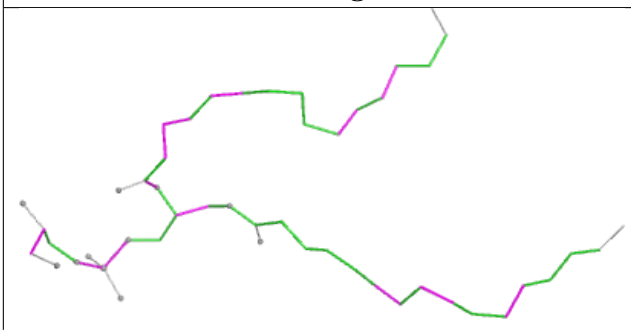
Ligand LHG z 101



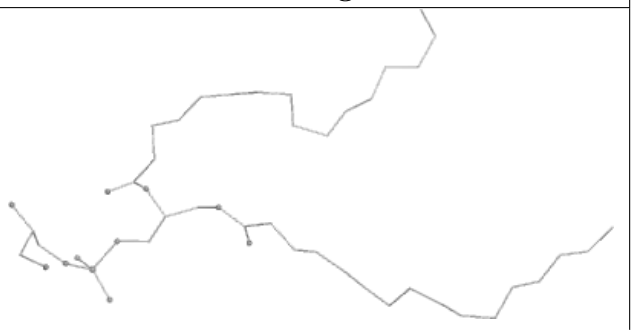
Bond lengths



Bond angles

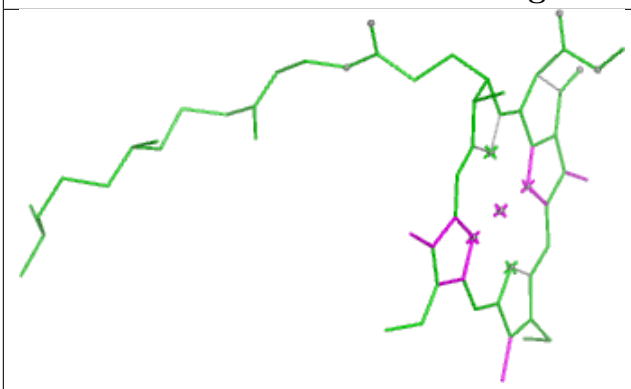


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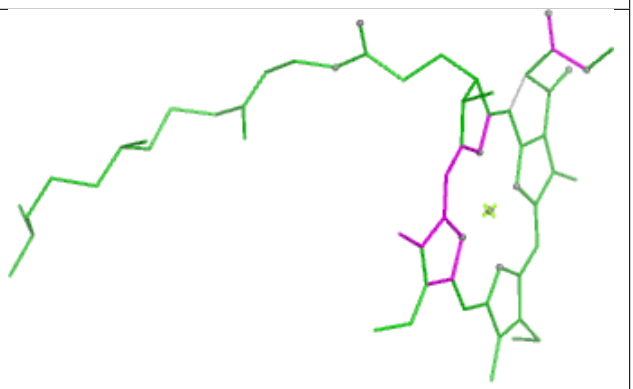


Rings

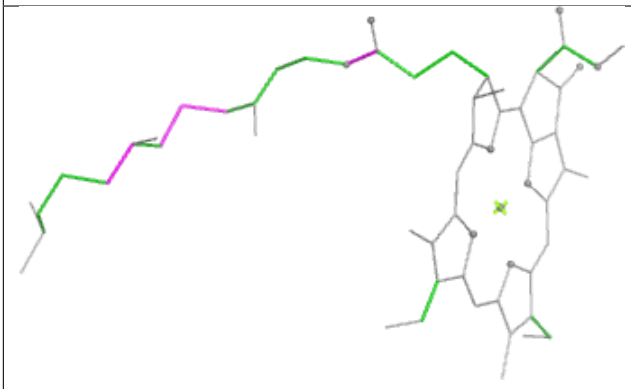
Ligand CLA a 832



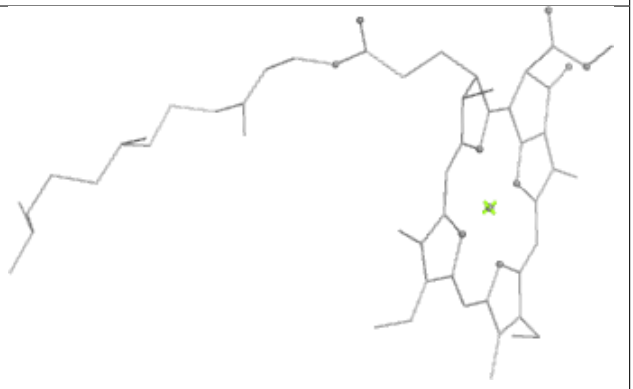
Bond lengths



Bond angles

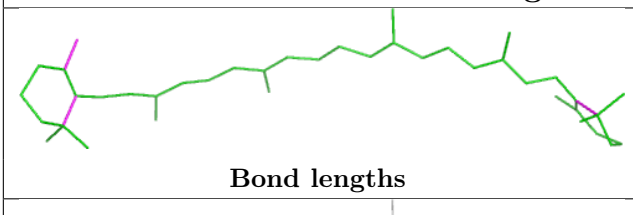


Torsions

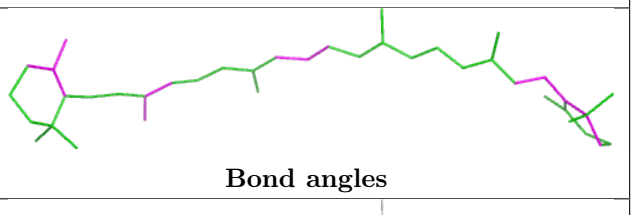


Rings

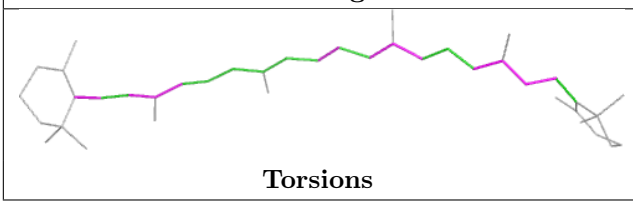
Ligand BCR F 202



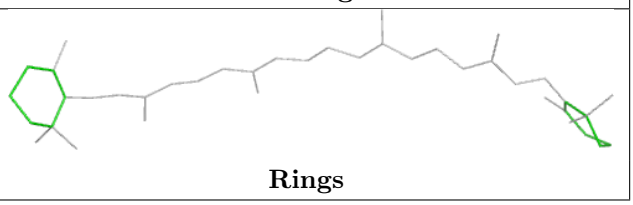
Bond lengths



Bond angles

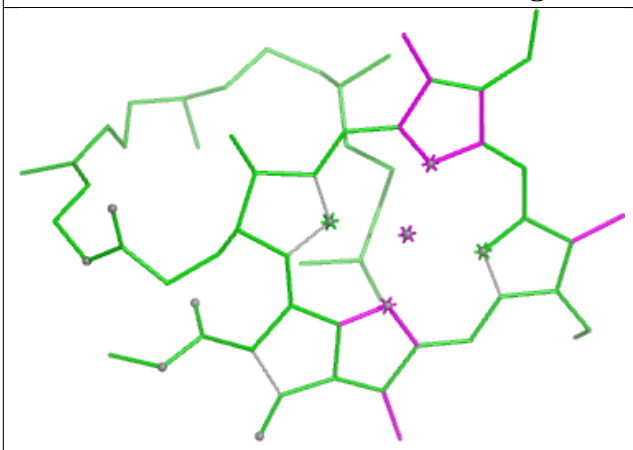


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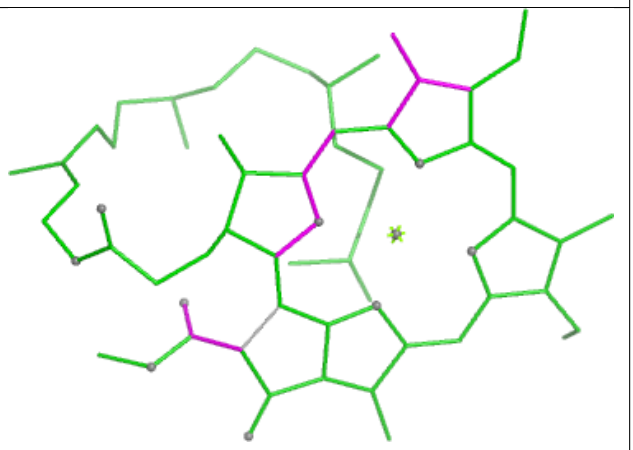


Rings

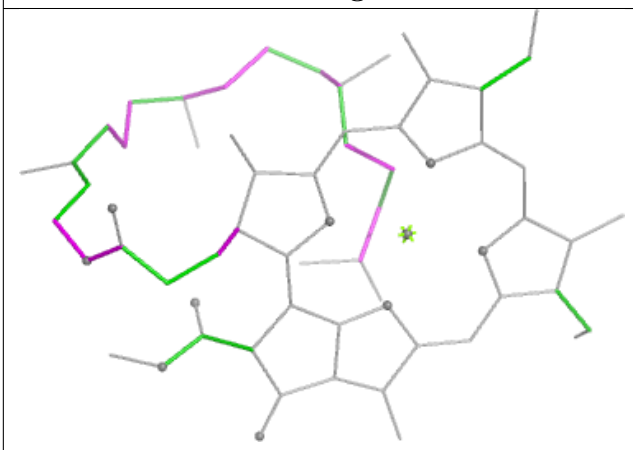
Ligand CLA a 807



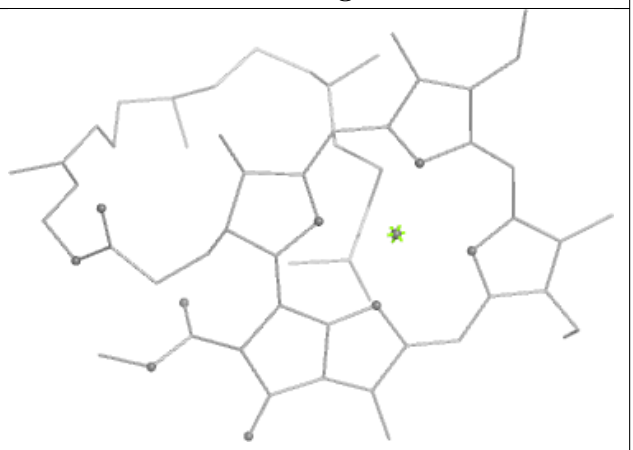
Bond lengths



Bond angles

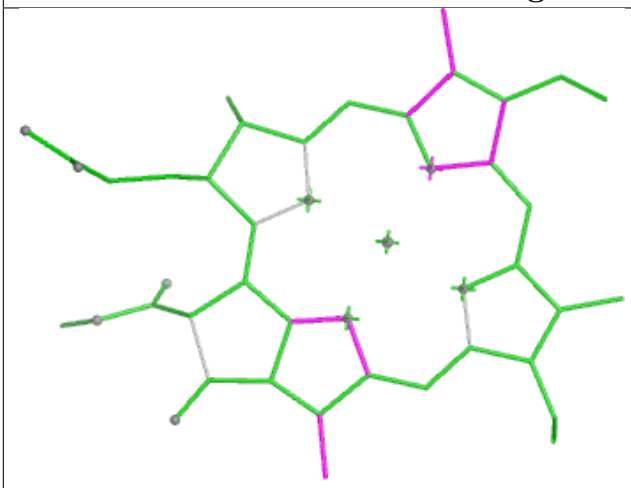


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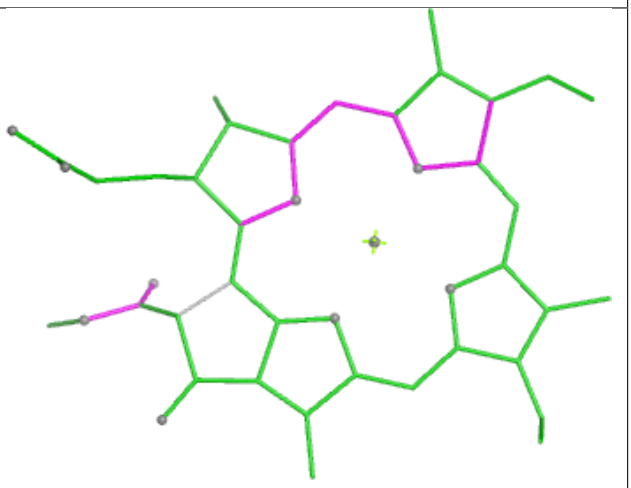


Rings

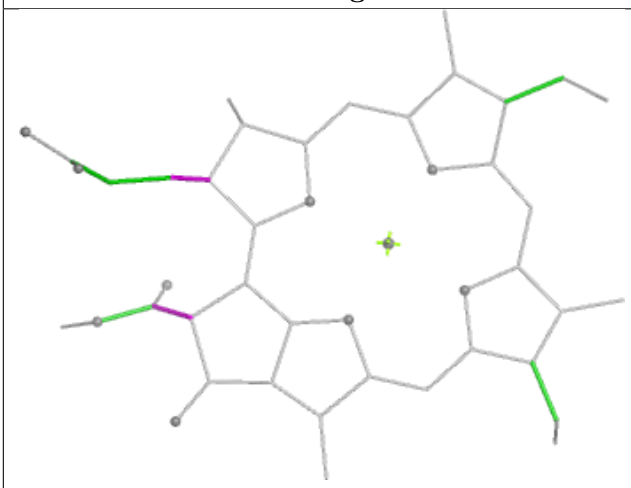
Ligand CLA b 837



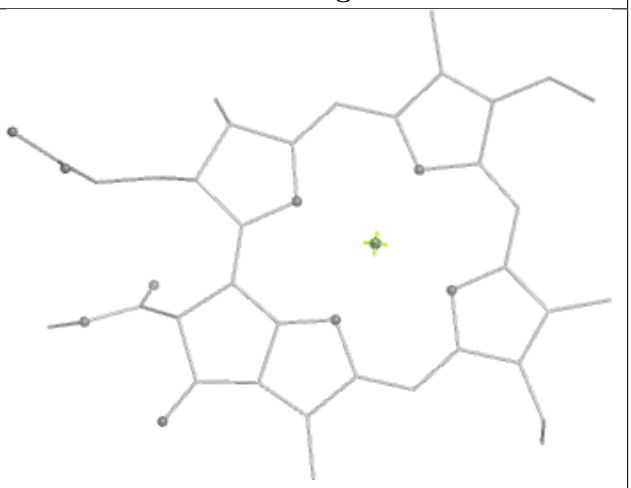
Bond lengths



Bond angles

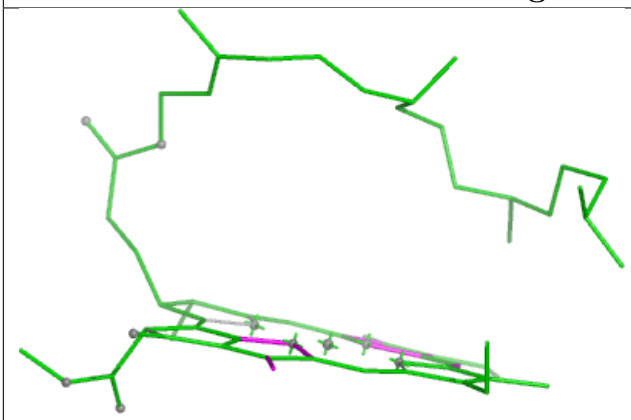


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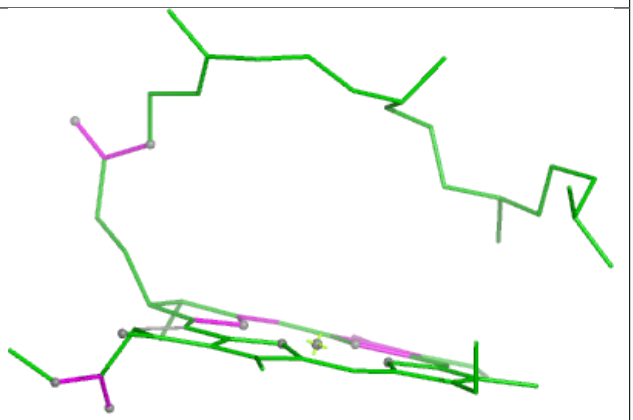


Rings

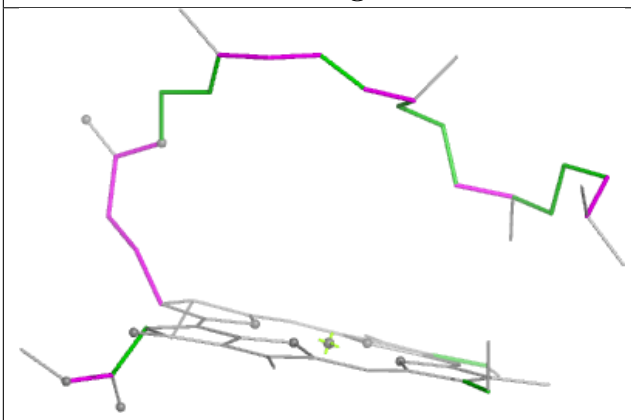
Ligand CLA a 821



Bond lengths



Bond angles

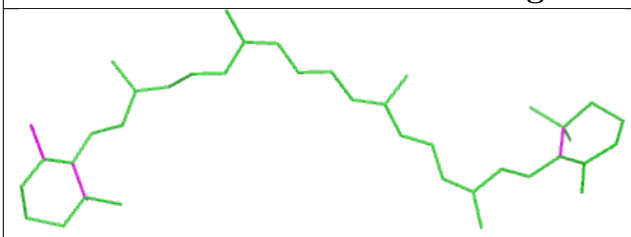


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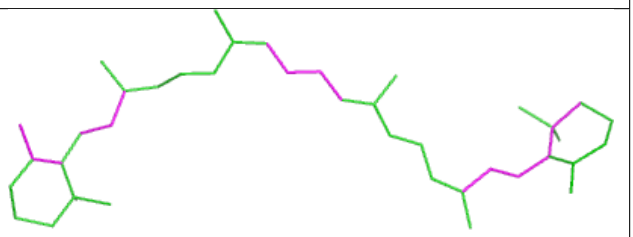


Rings

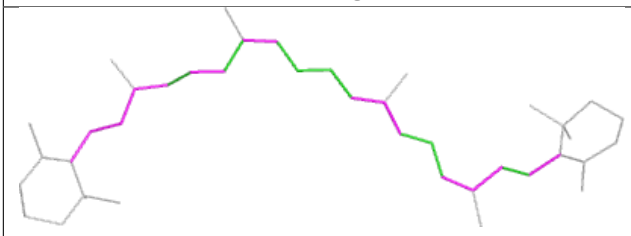
Ligand BCR a 851



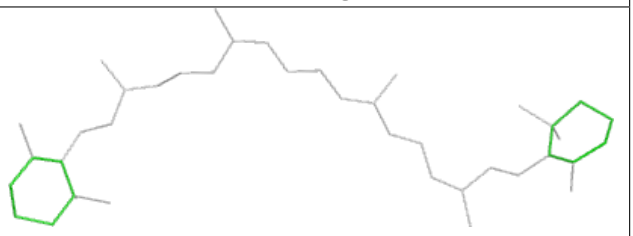
Bond lengths



Bond angles

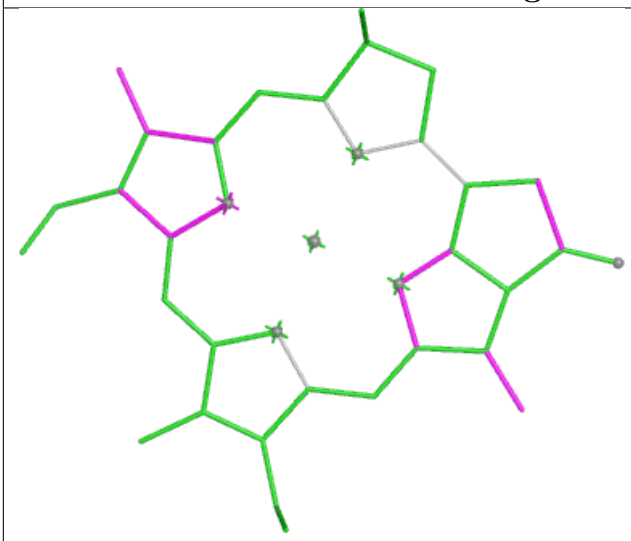


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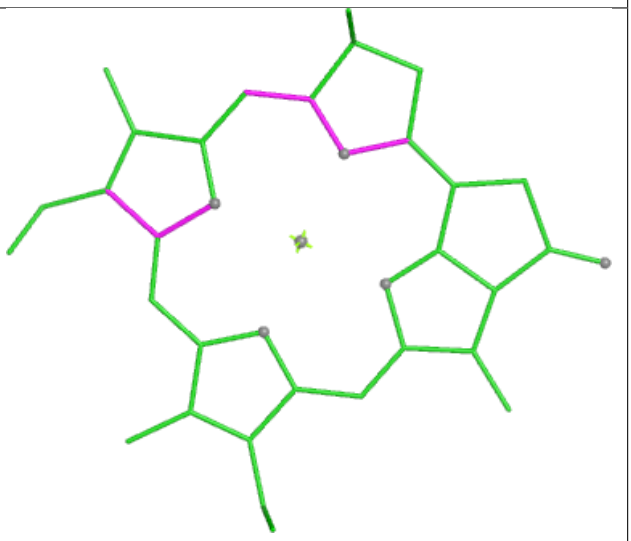


Rings

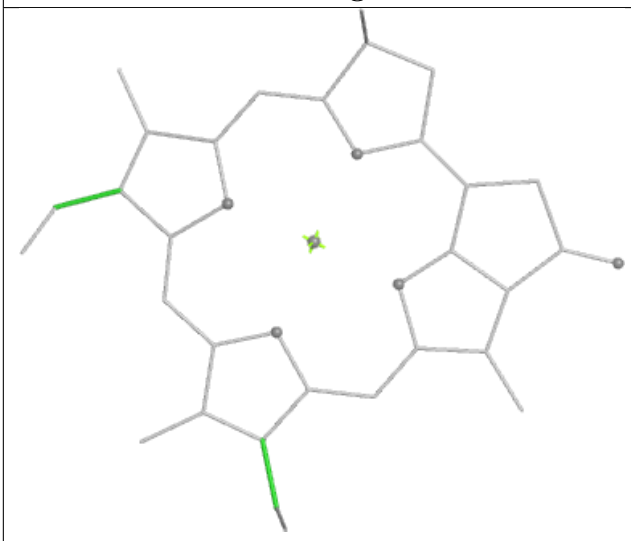
Ligand CLA A 857



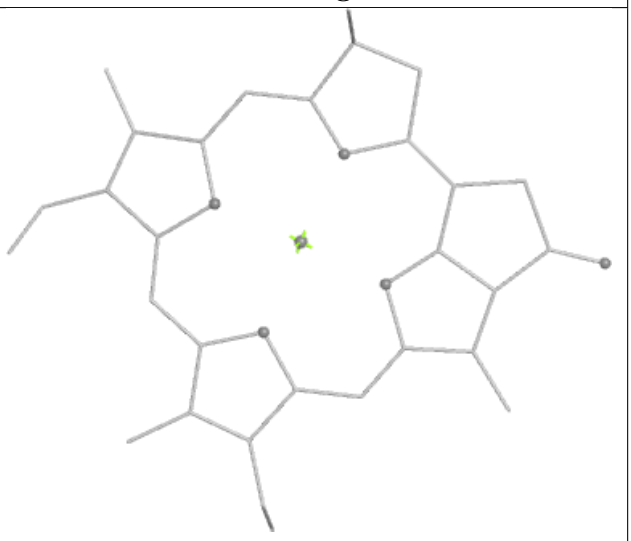
Bond lengths



Bond angles



Torsions

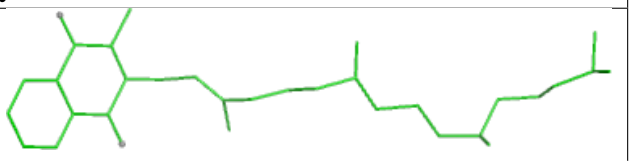


Rings

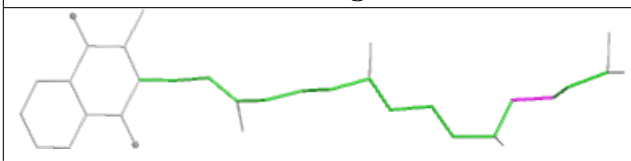
Ligand PQN A 845



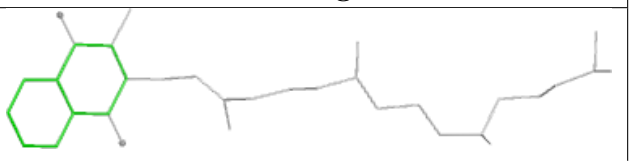
Bond lengths



Bond angles

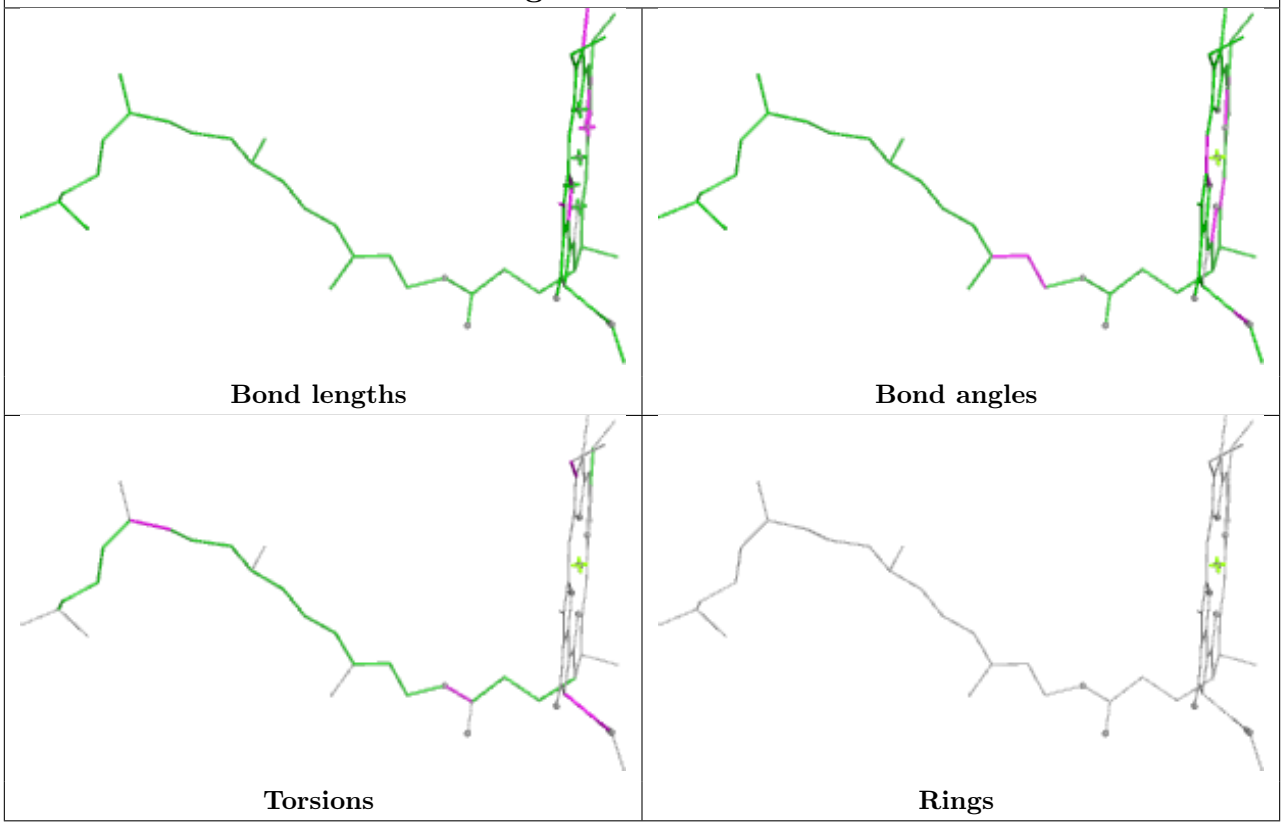


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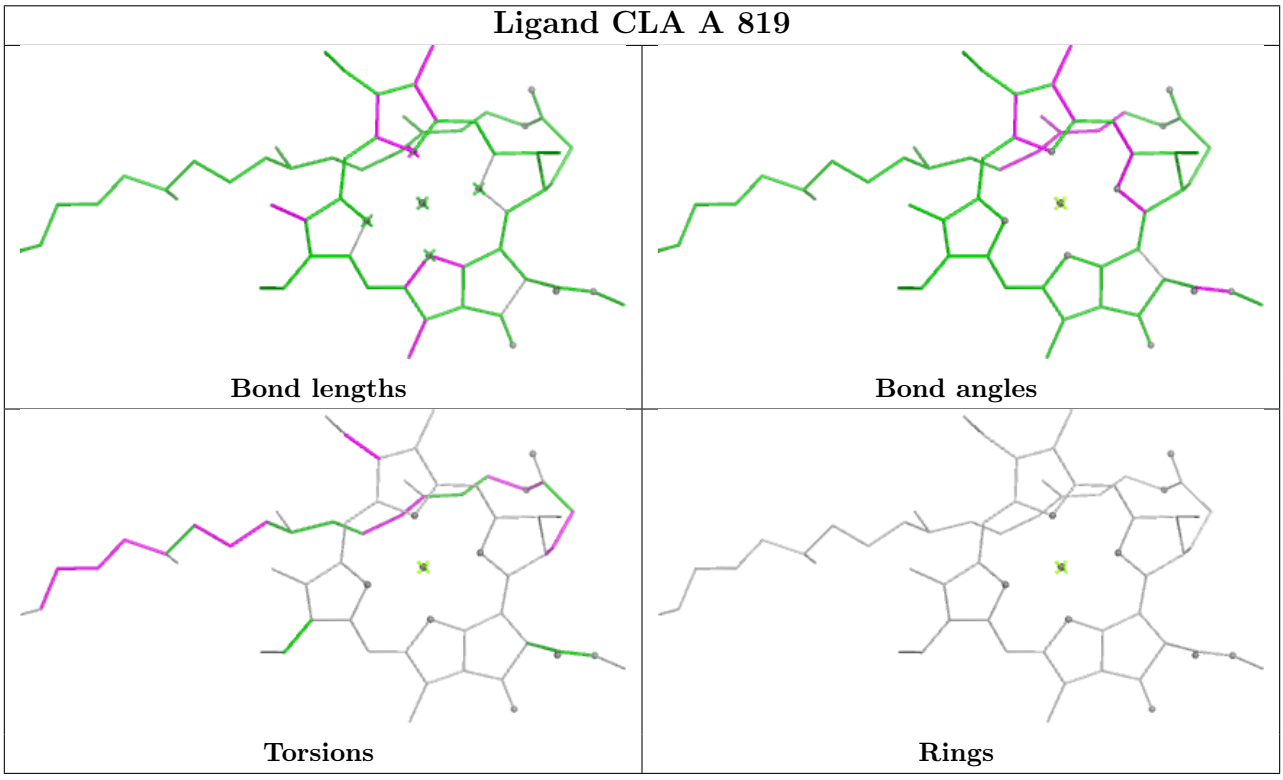


Rings

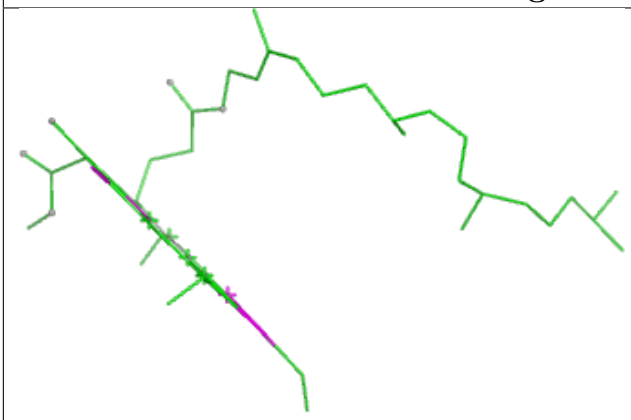
Ligand CLA B 841



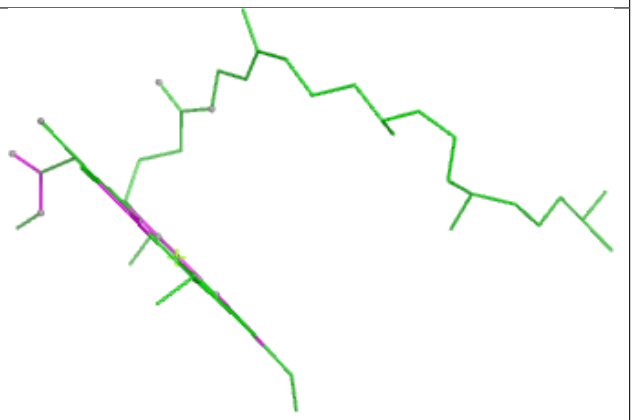
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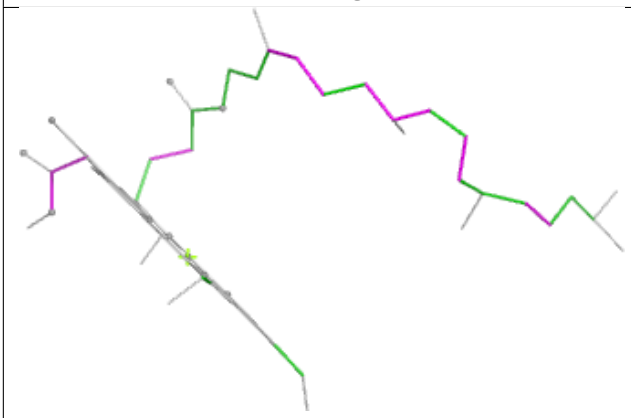
Ligand CLA 2 815



Bond lengths



Bond angles

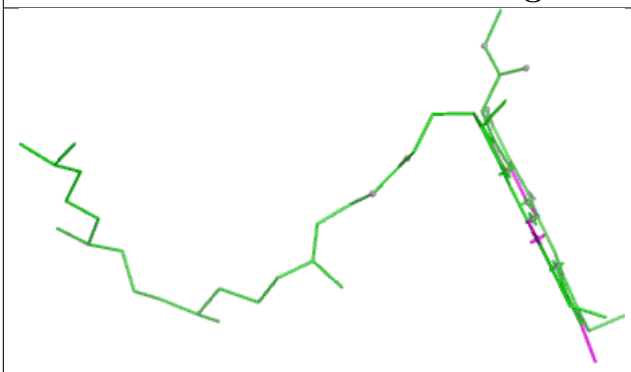


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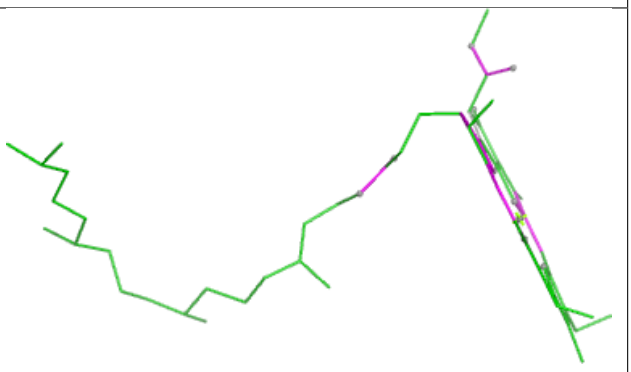


Rings

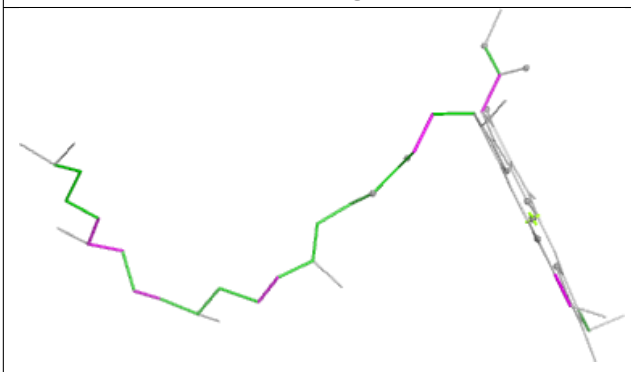
Ligand CLA B 840



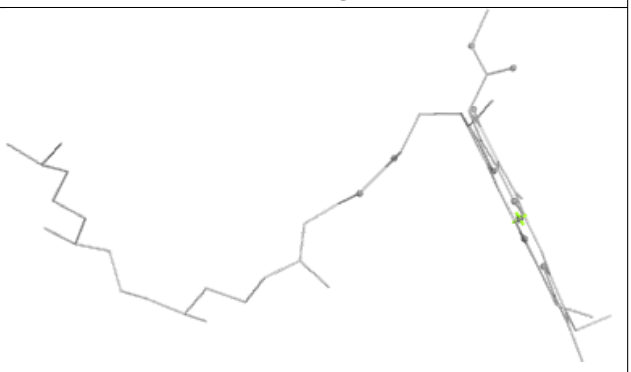
Bond lengths



Bond angles

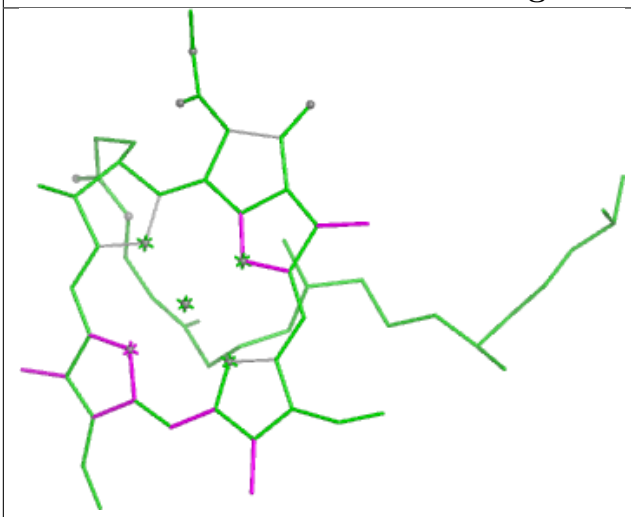


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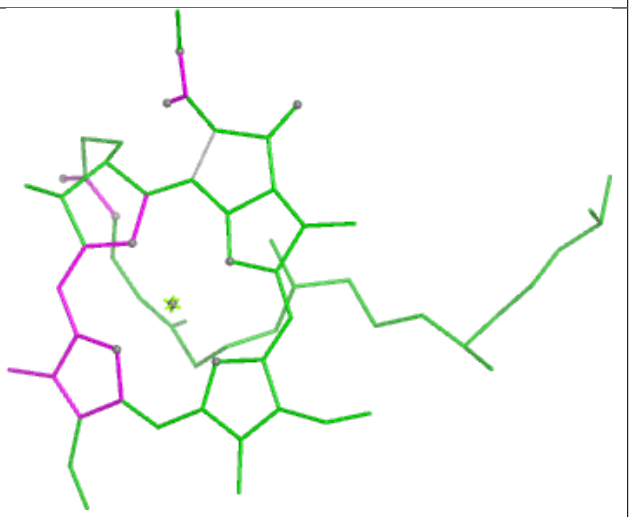


Rings

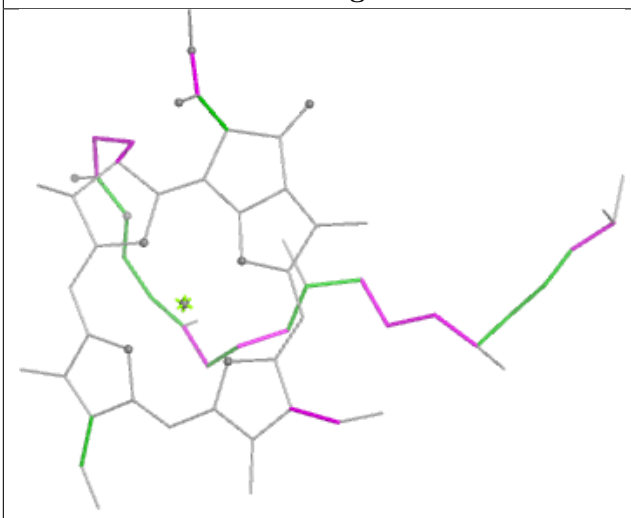
Ligand CLA 2 828



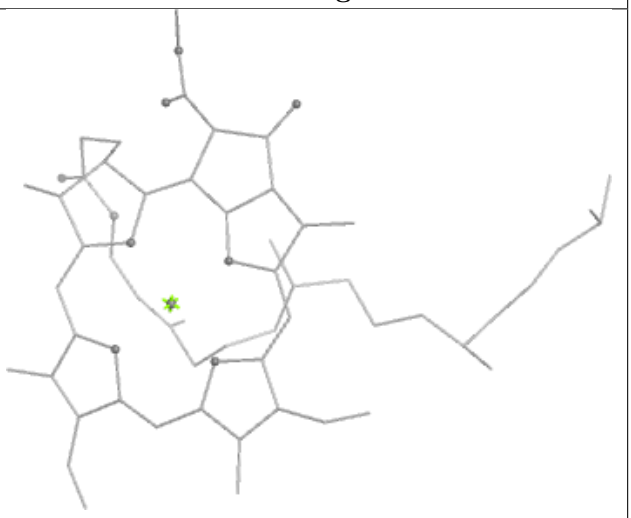
Bond lengths



Bond angles

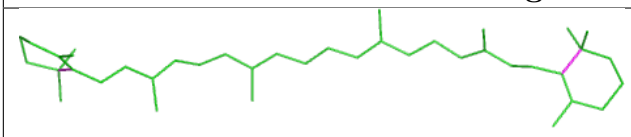


Torsions

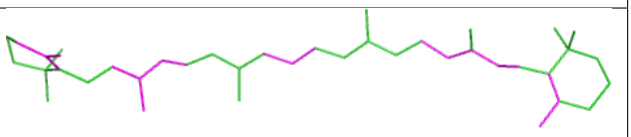


Rings

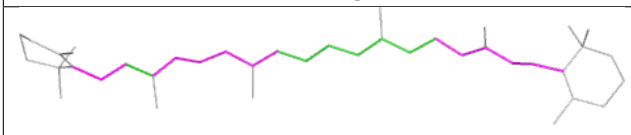
Ligand BCR b 852



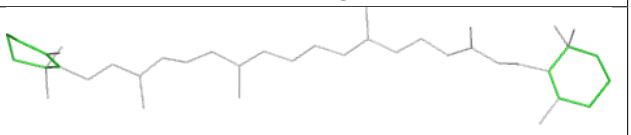
Bond lengths



Bond angles

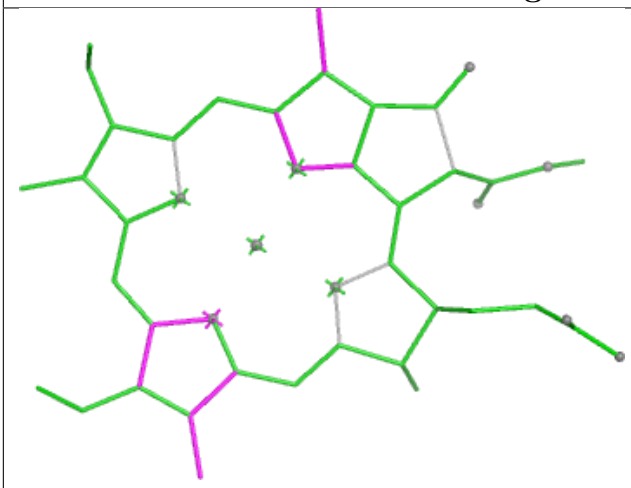


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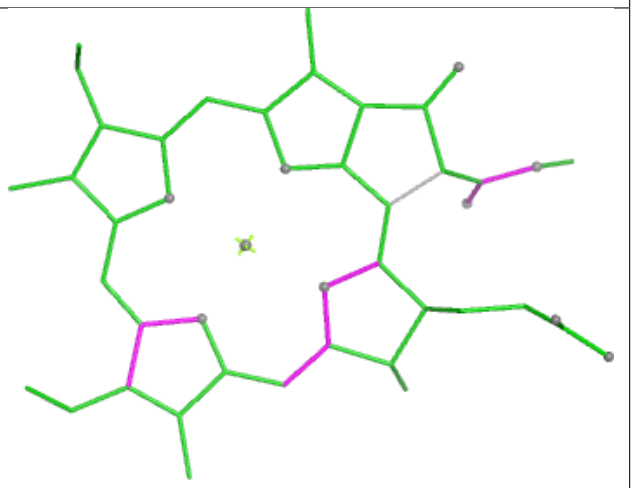


Rings

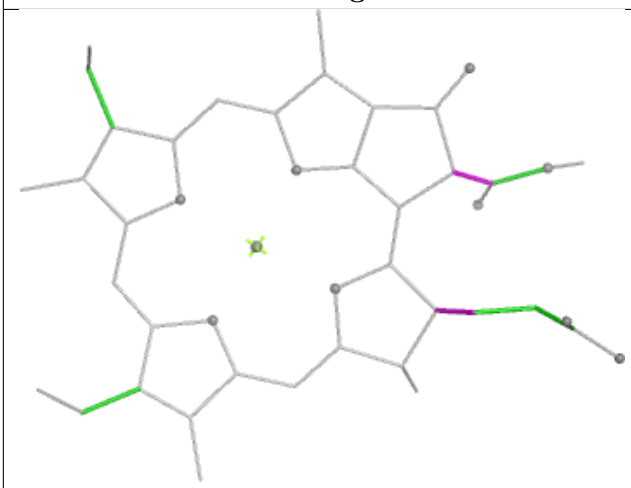
Ligand CLA B 836



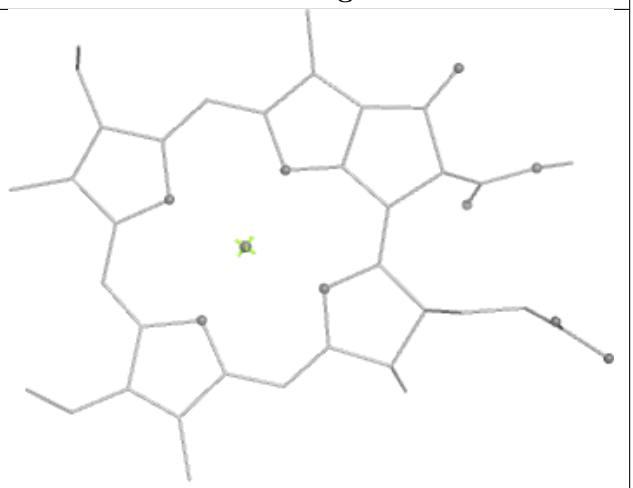
Bond lengths



Bond angles

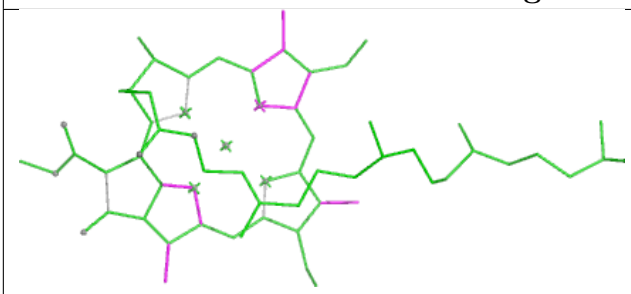


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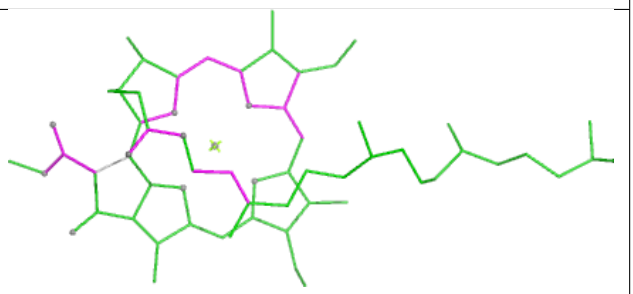


Rings

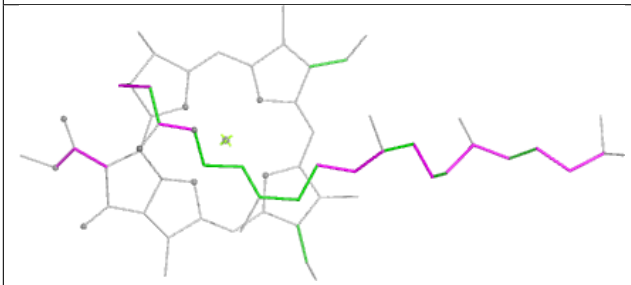
Ligand CLA A 839



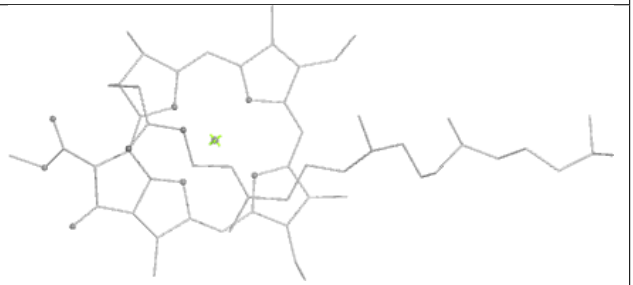
Bond lengths



Bond angles

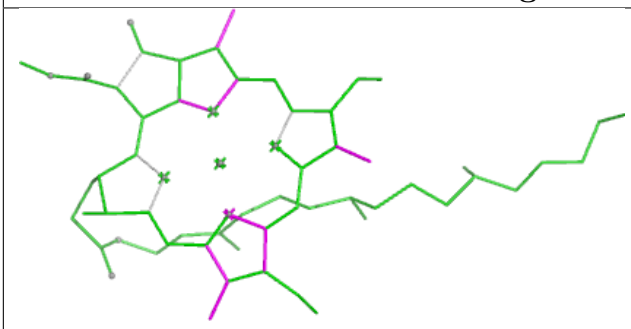


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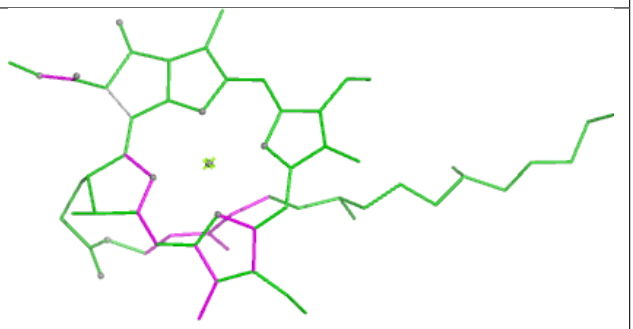


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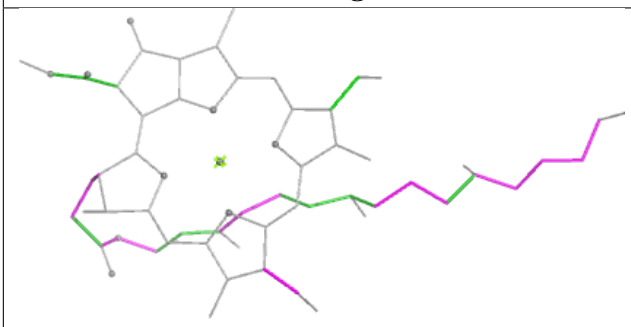
Ligand CLA 1 1620



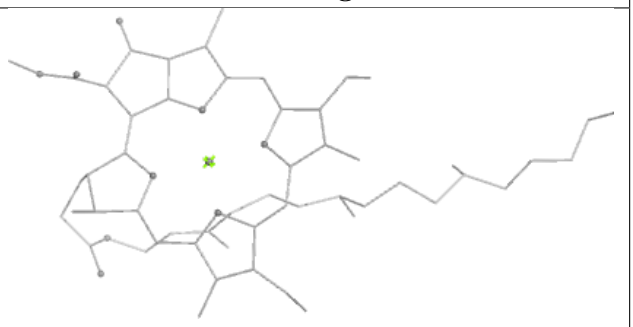
Bond lengths



Bond angles

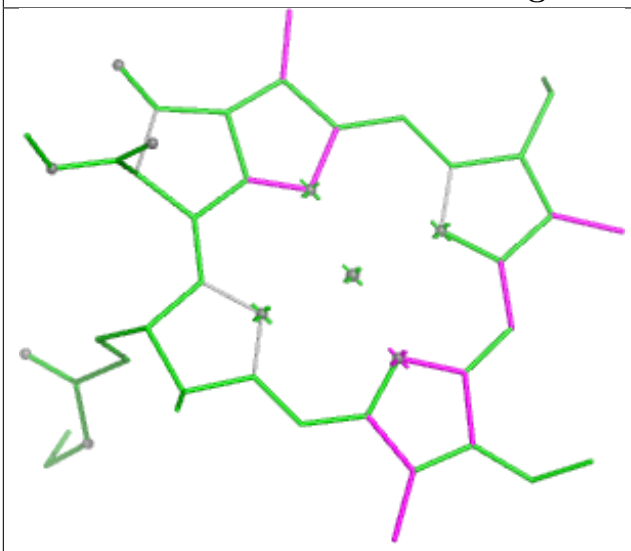


Torsions

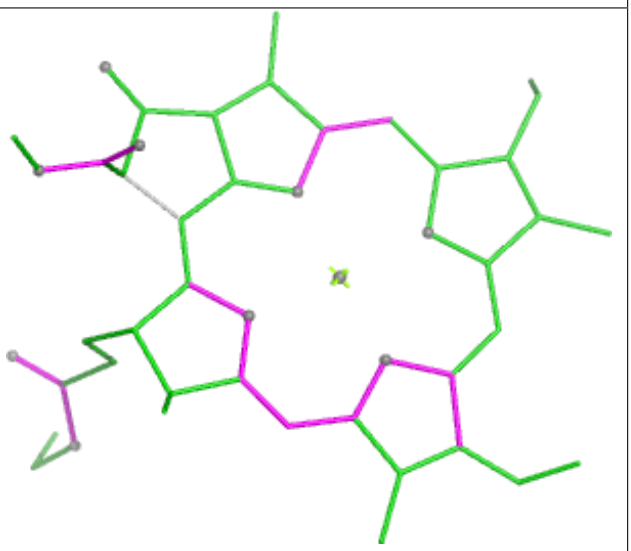


Rings

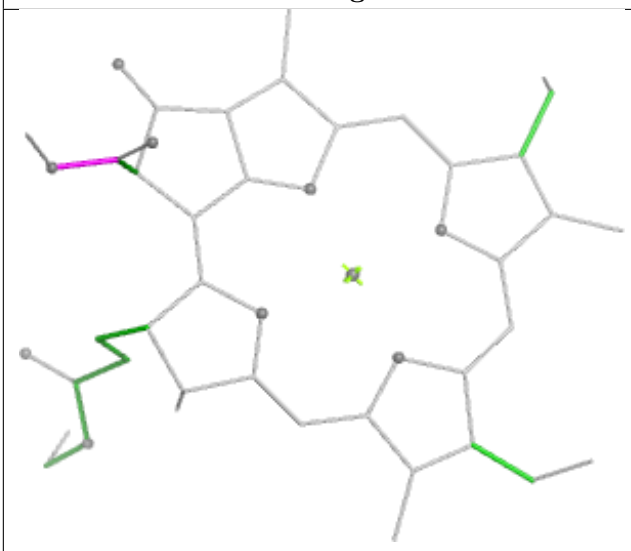
Ligand CLA 2 840



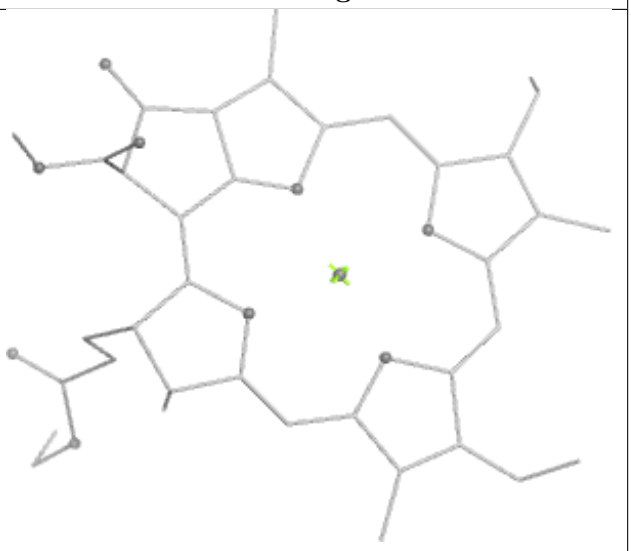
Bond lengths



Bond angles

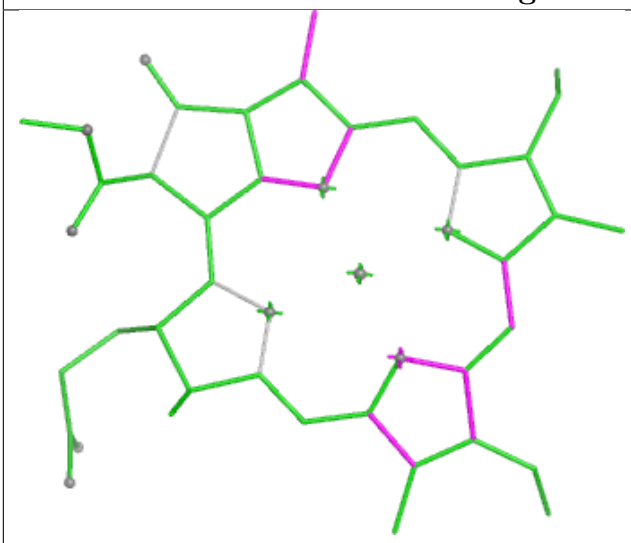


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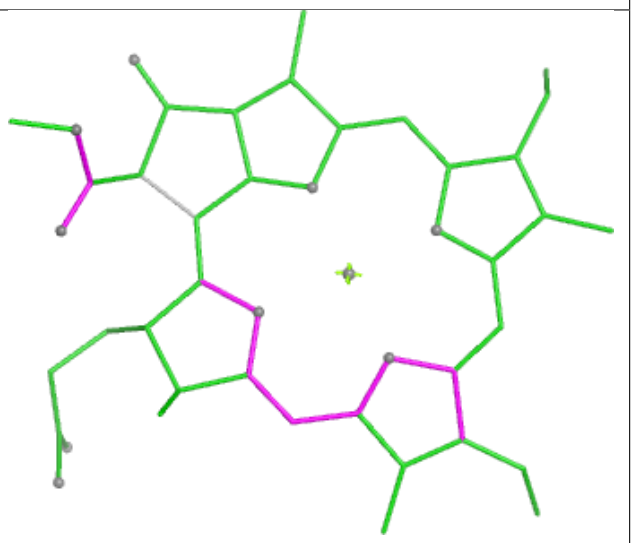


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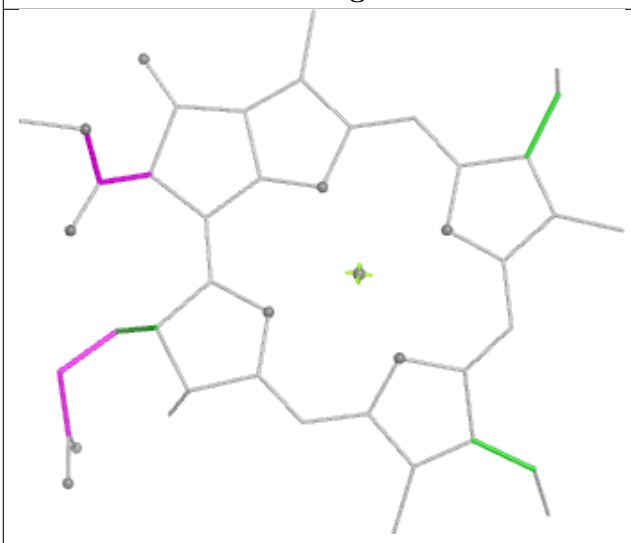
Ligand CLA x 1701



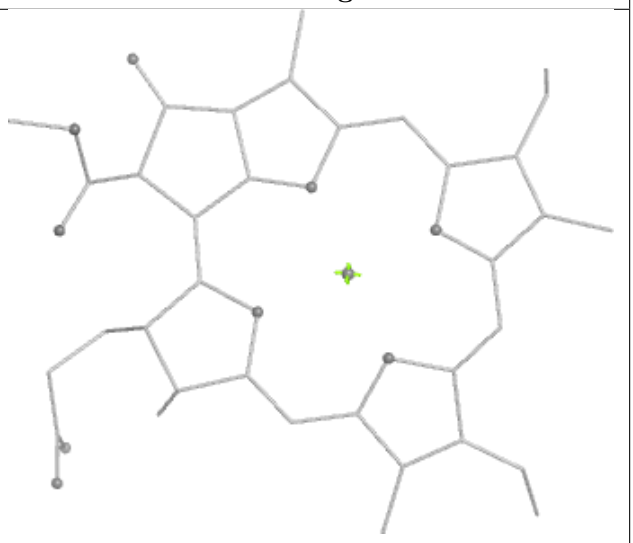
Bond lengths



Bond angles

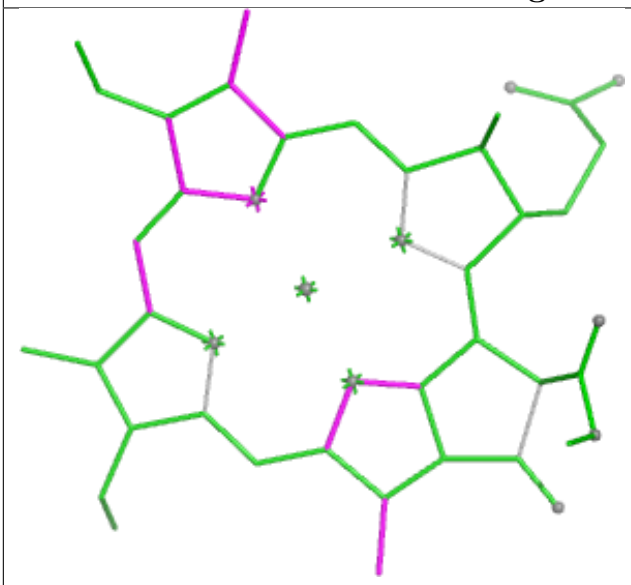


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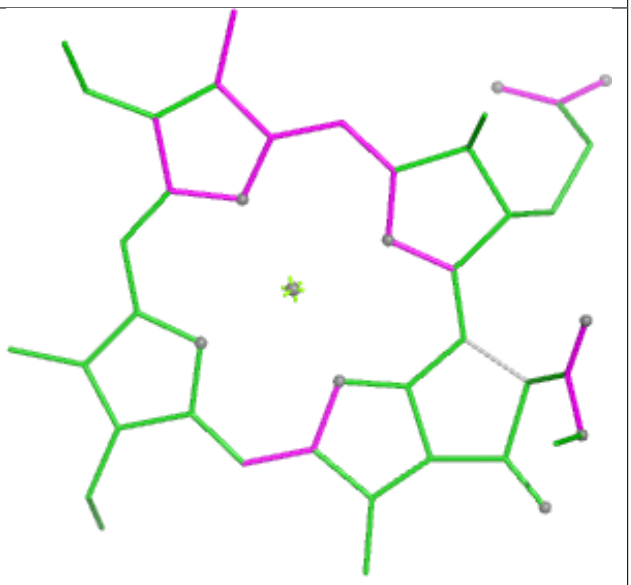


Rings

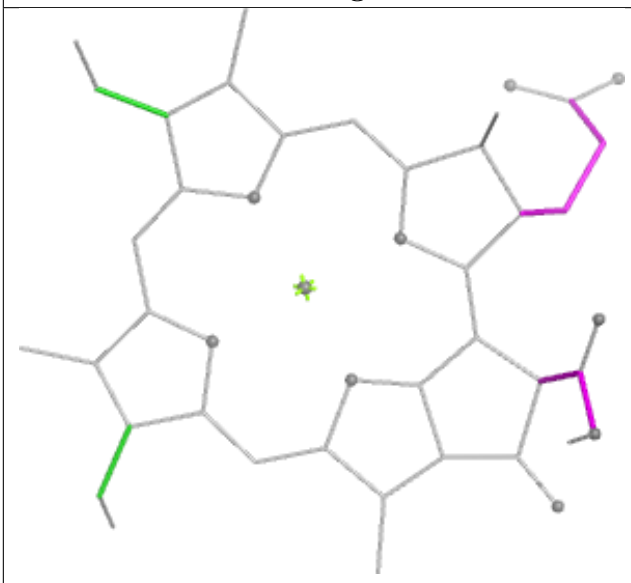
Ligand CLA a 823



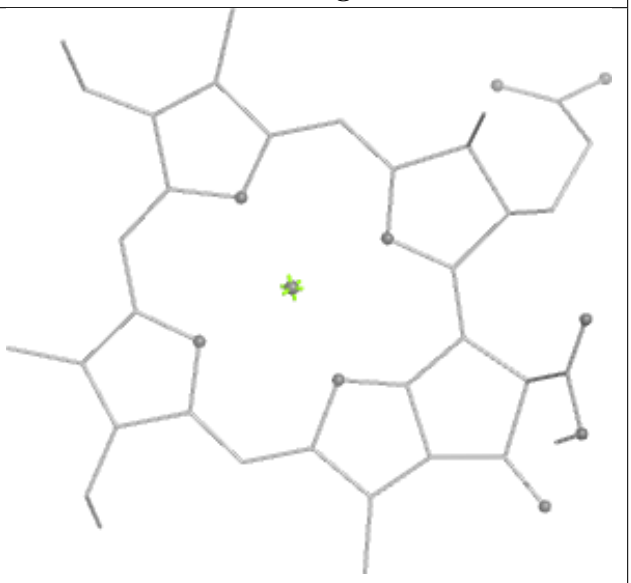
Bond lengths



Bond angles

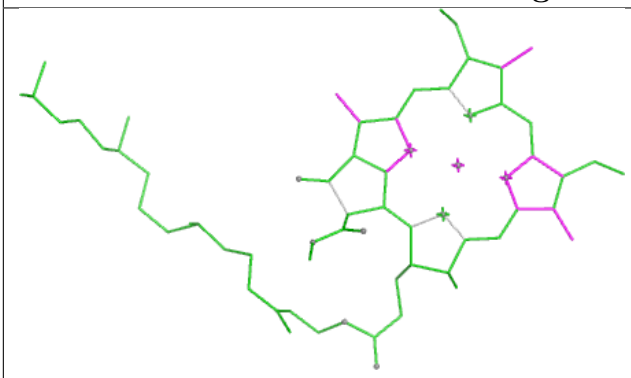


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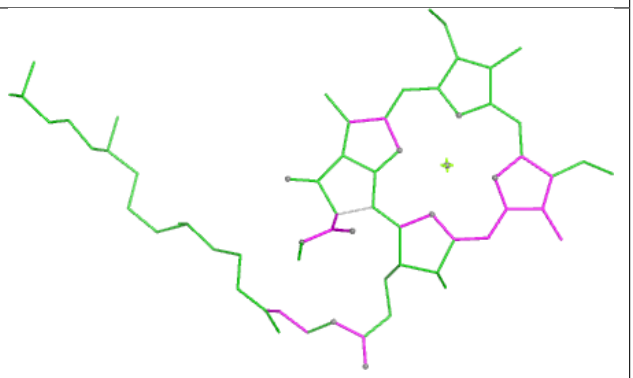


Rings

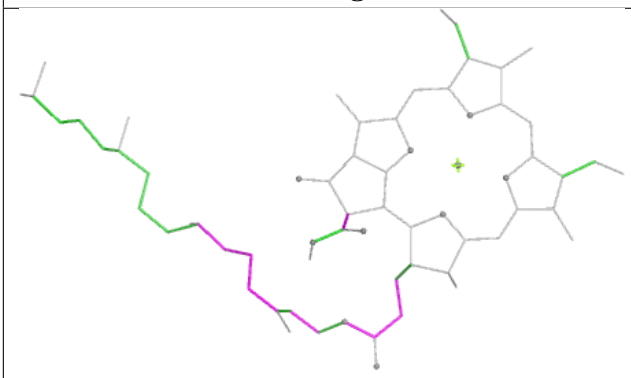
Ligand CLA l 206



Bond lengths



Bond angles



Torsions

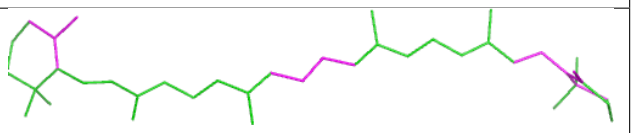


Rings

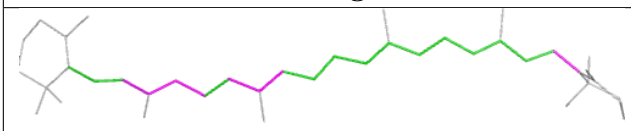
Ligand BCR A 850



Bond lengths



Bond angles

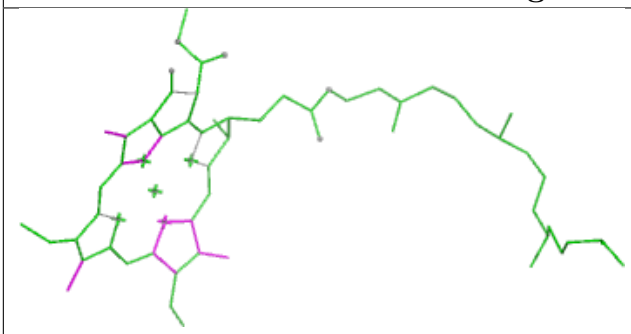


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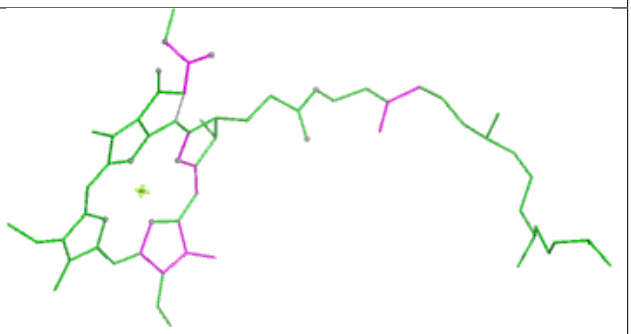


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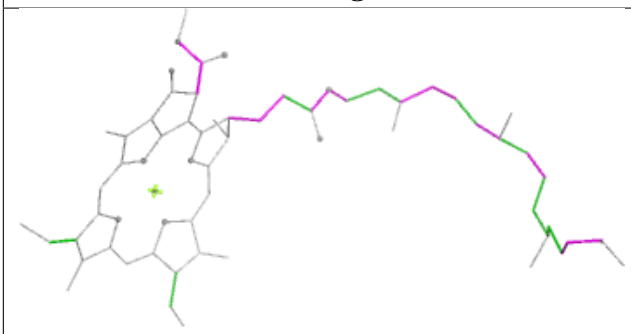
Ligand CLA b 802



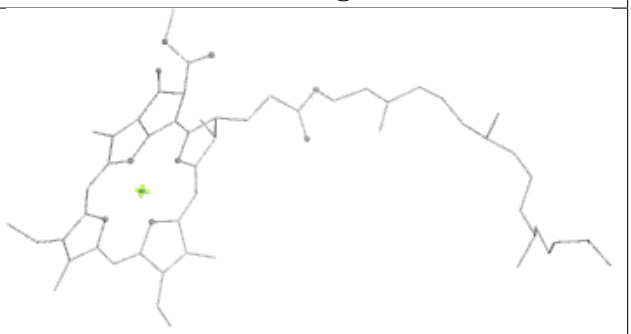
Bond lengths



Bond angles

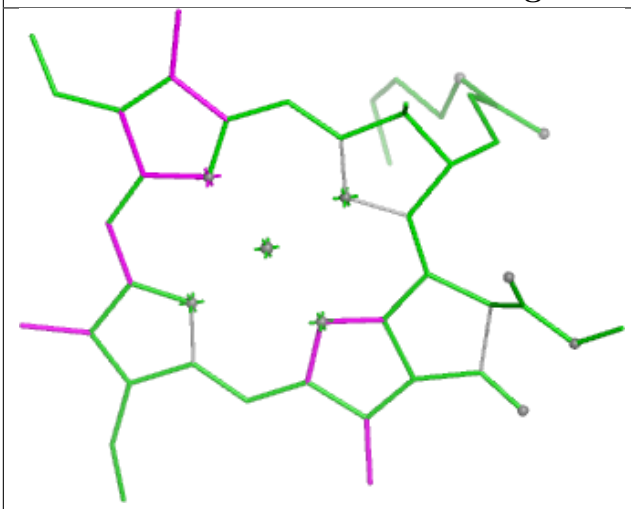


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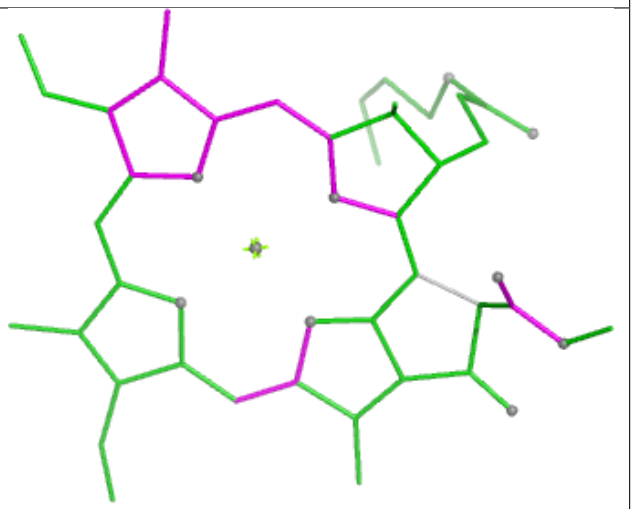


Rings

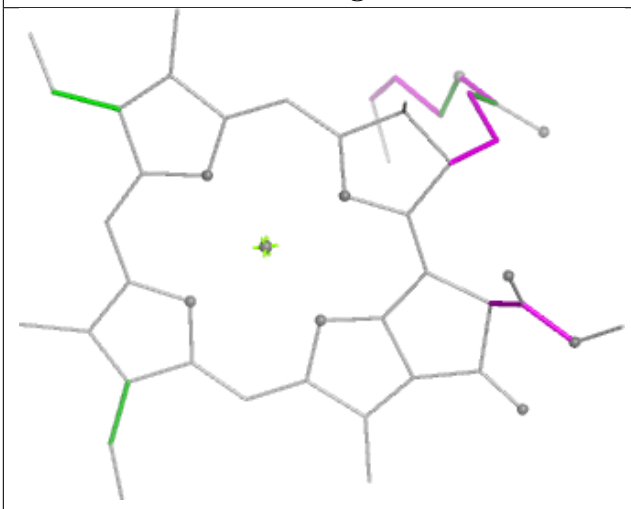
Ligand CLA B 831



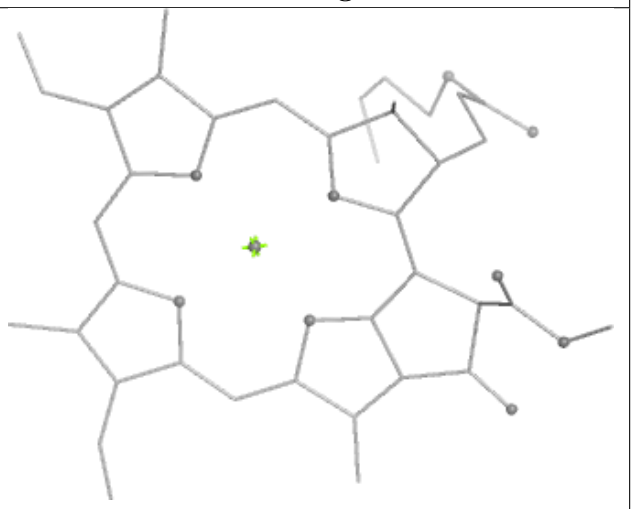
Bond lengths



Bond angles

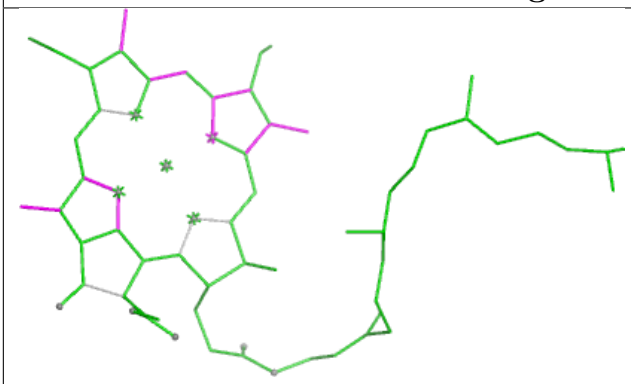


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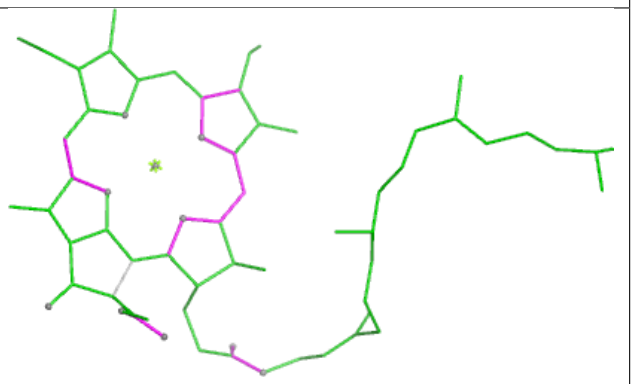


Rings

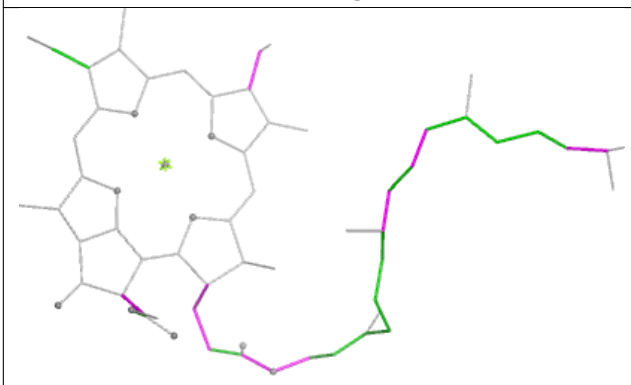
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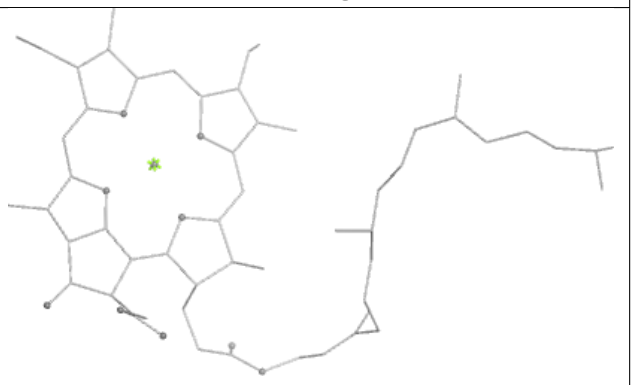
Bond lengths



Bond angles

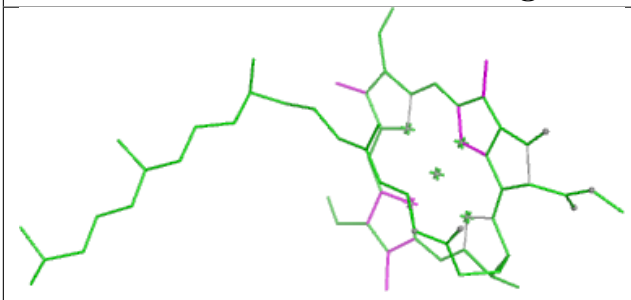


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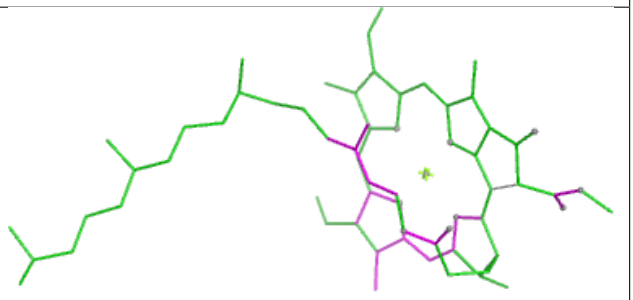


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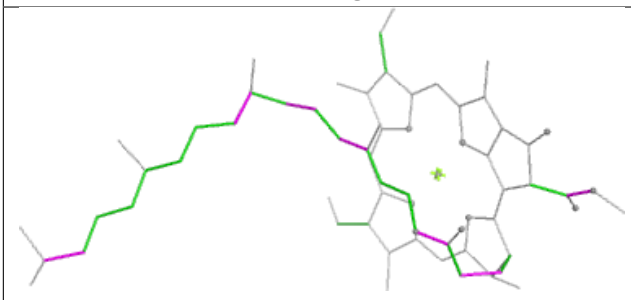
Ligand CLA 1 1643



Bond lengths



Bond angles



Torsions

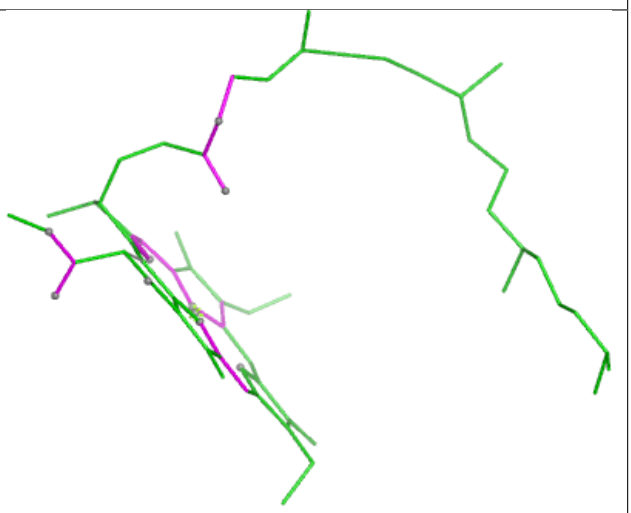


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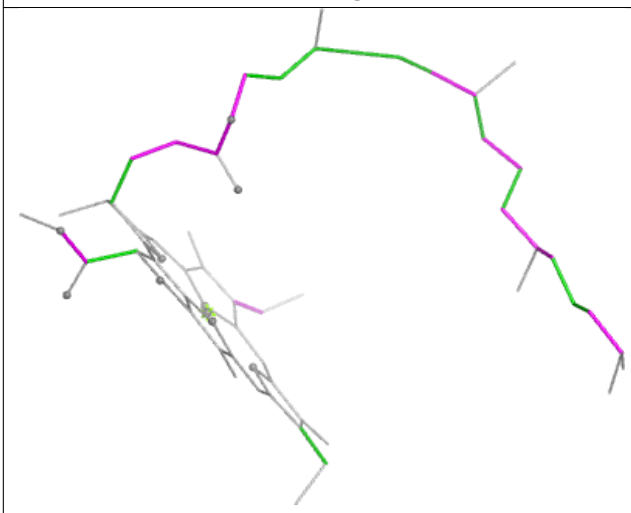
Ligand CLA B 819



Bond lengths



Bond angles

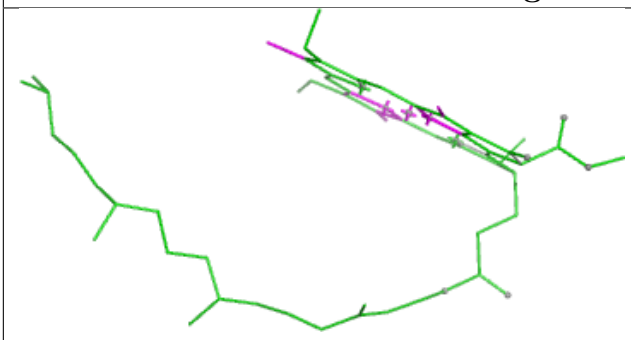


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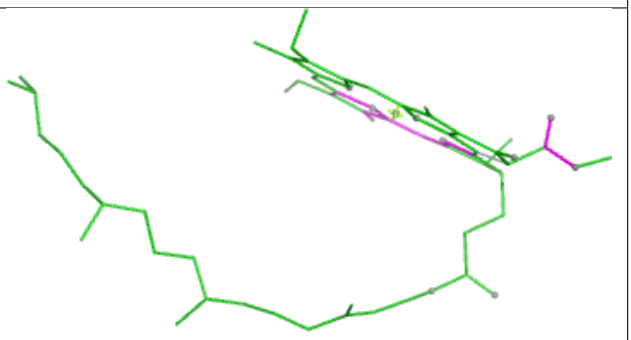


Rings

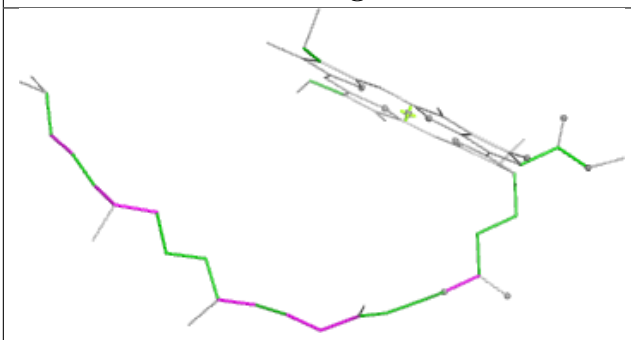
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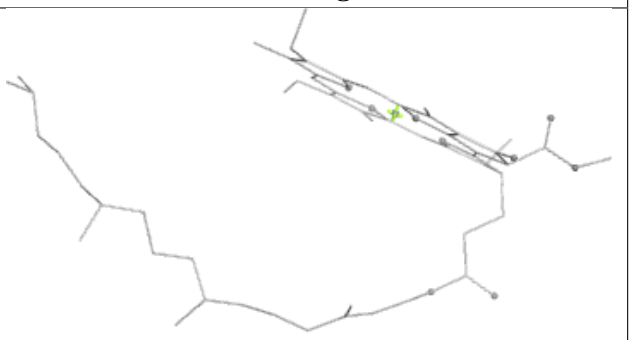
Bond lengths



Bond angles

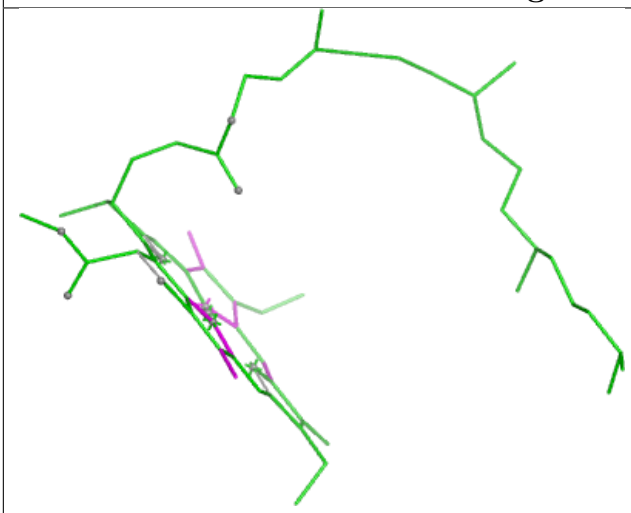


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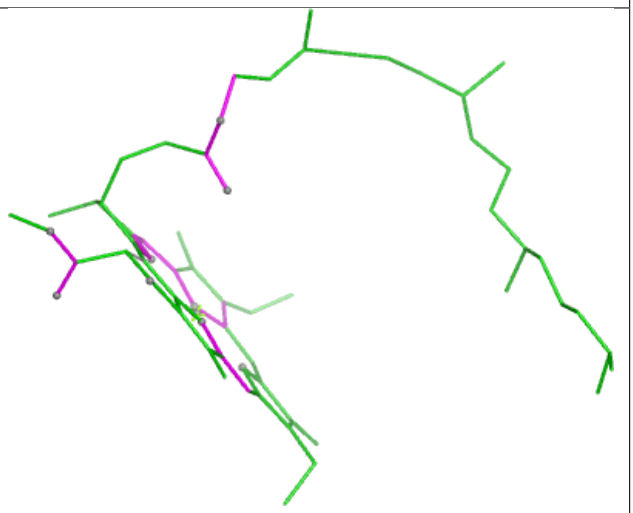


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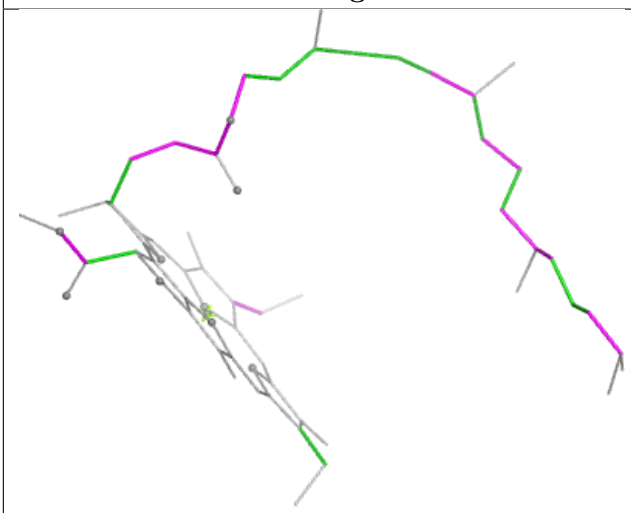
Ligand CLA b 820



Bond lengths



Bond angles



Torsions

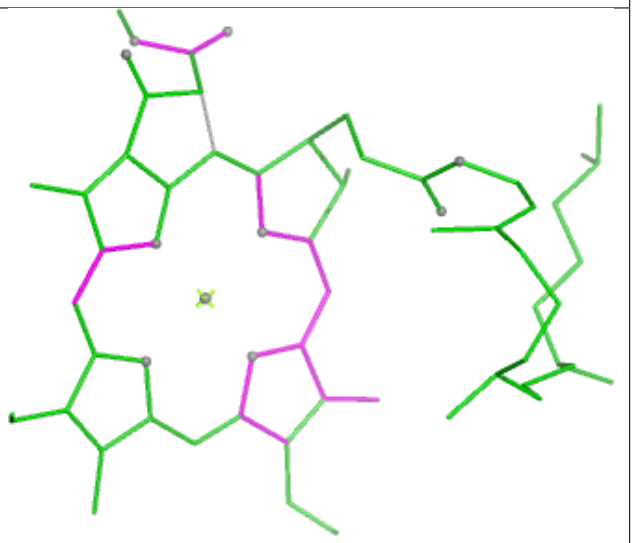


Rings

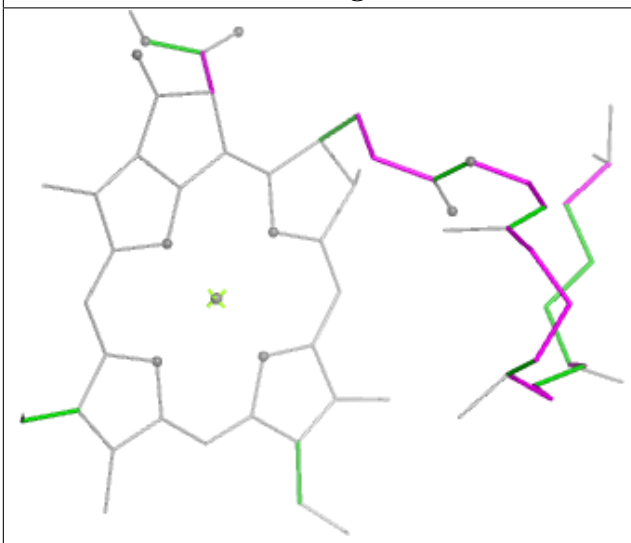
Ligand CLA a 816



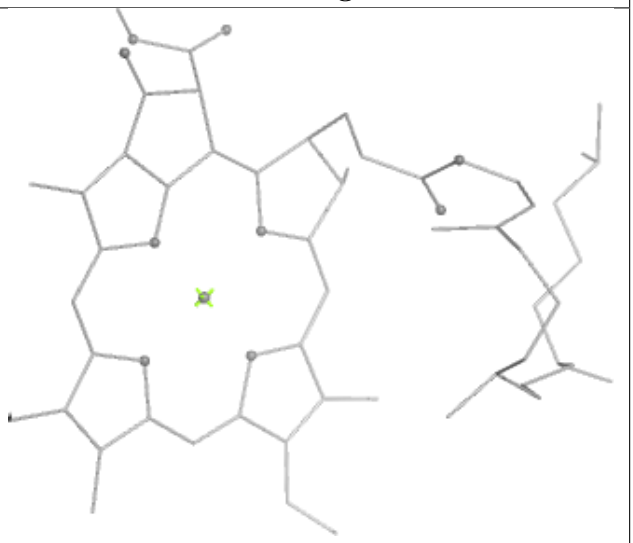
Bond lengths



Bond angles

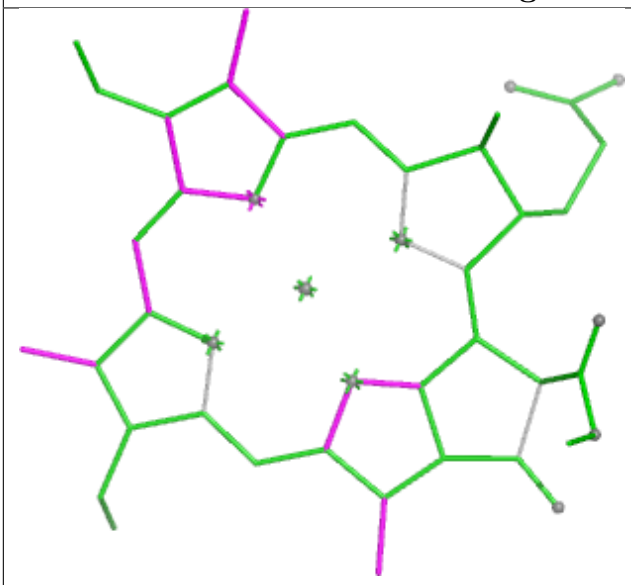


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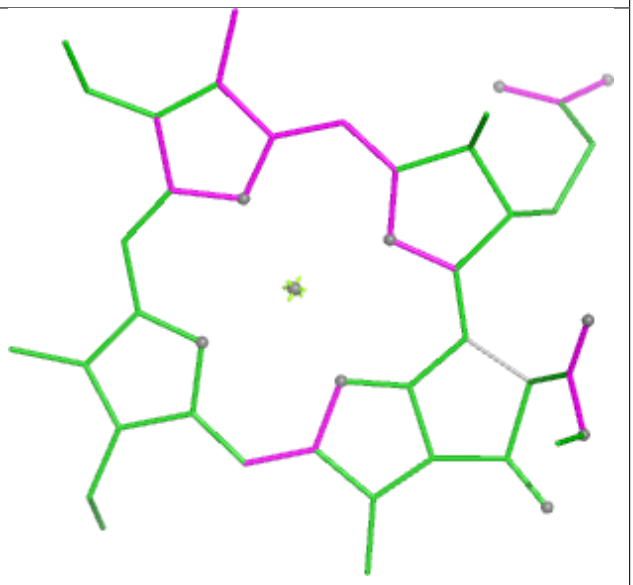


Rings

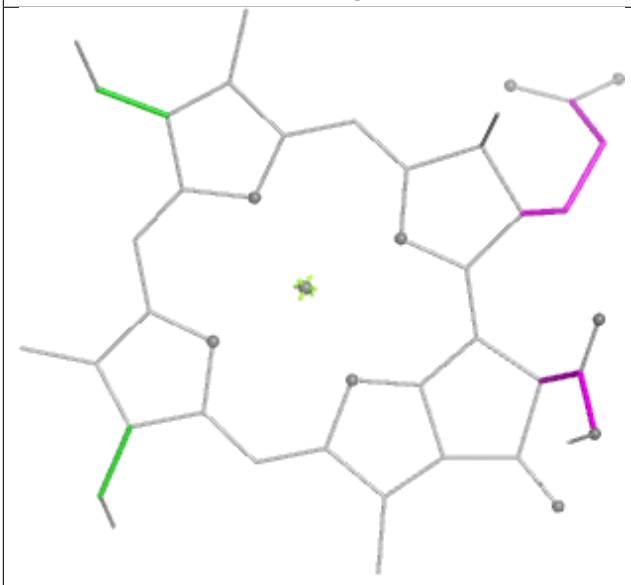
Ligand CLA 1 1624



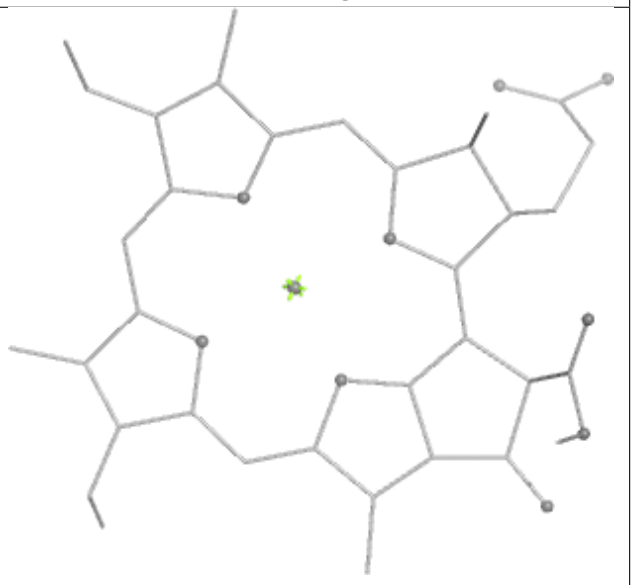
Bond lengths



Bond angles

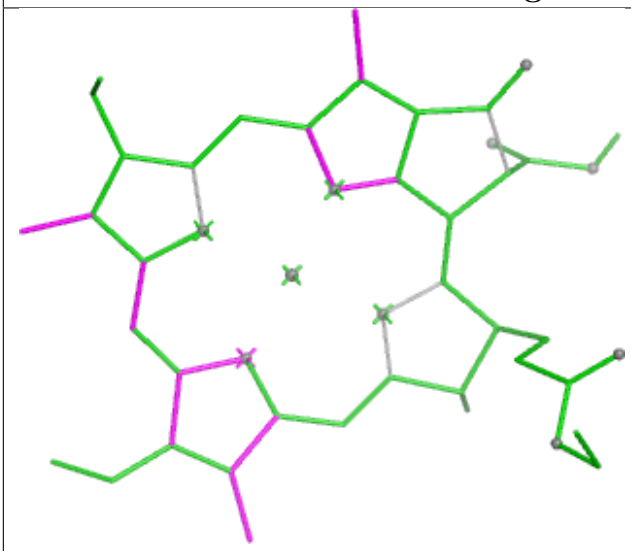


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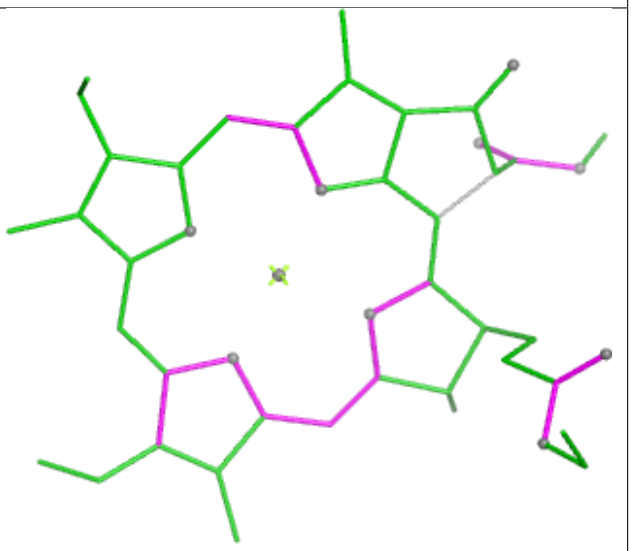


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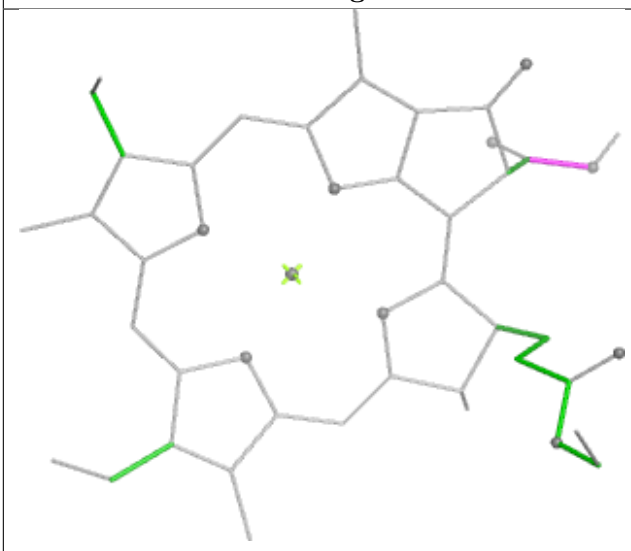
Ligand CLA B 839



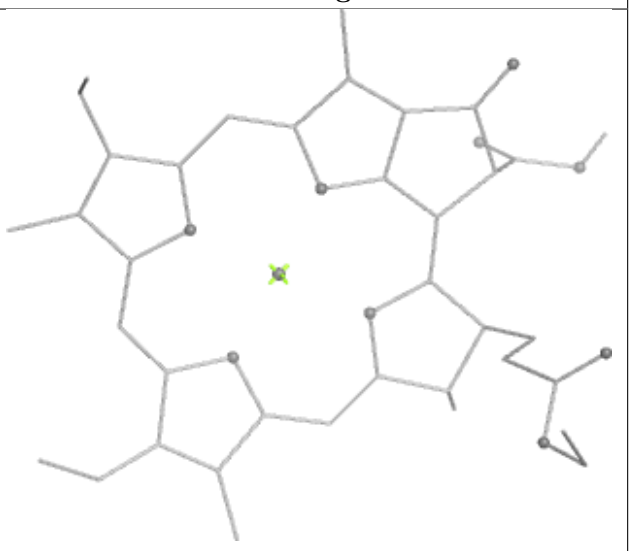
Bond lengths



Bond angles

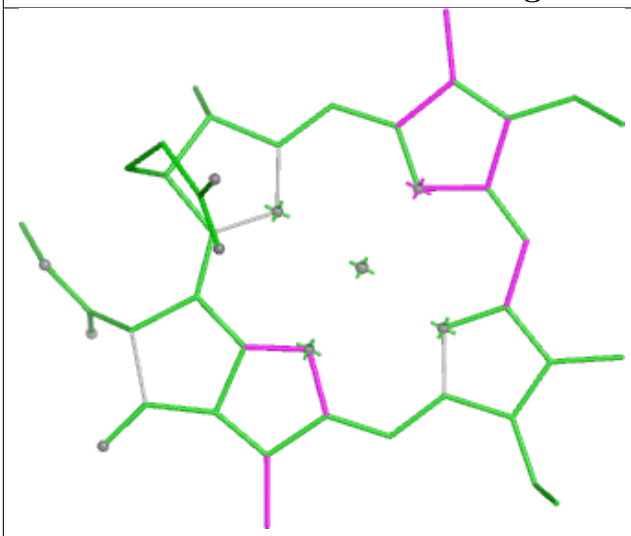


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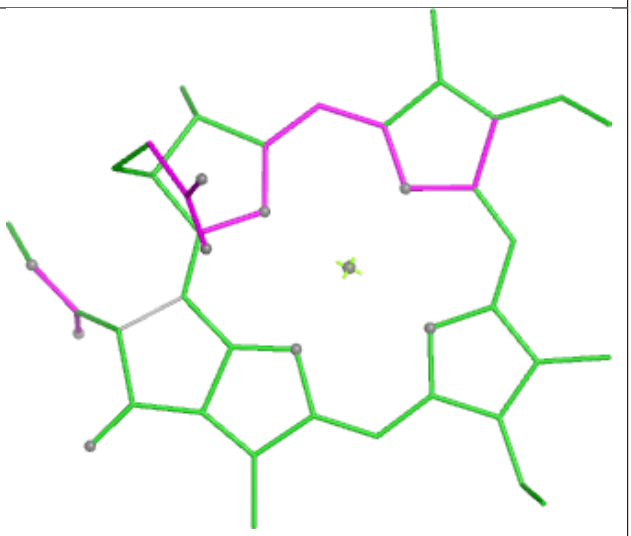


Rings

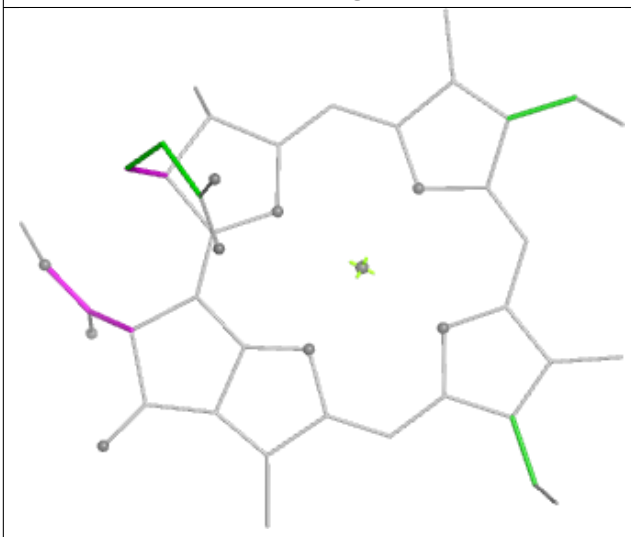
Ligand CLA A 837



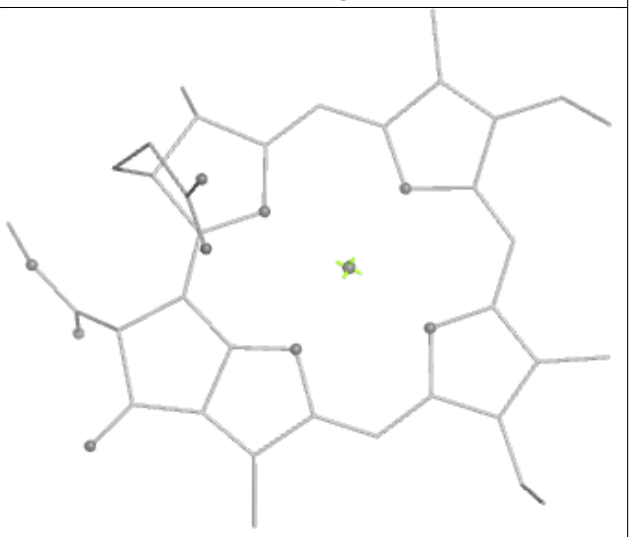
Bond lengths



Bond angles

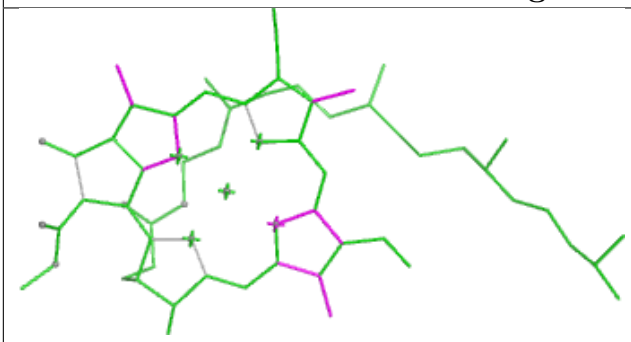


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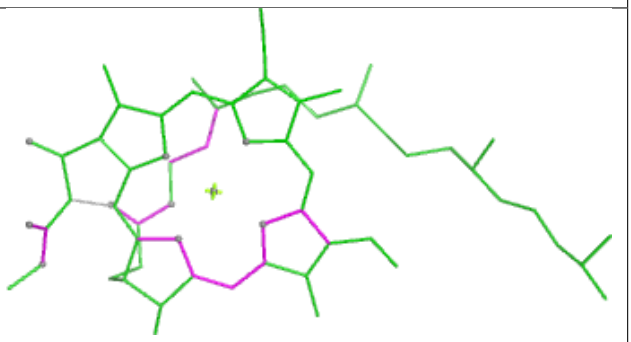


Rings

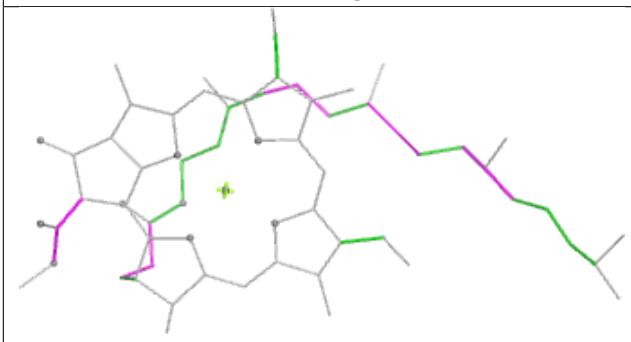
Ligand CLA a 841



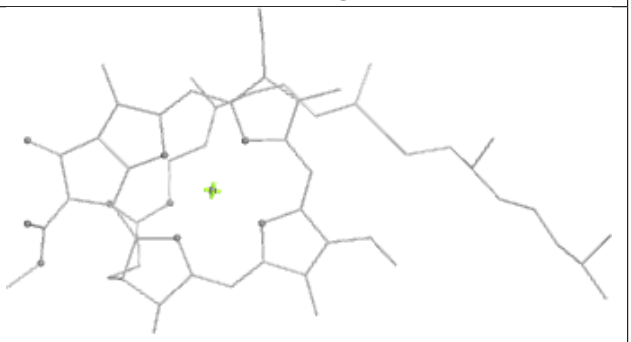
Bond lengths



Bond angles

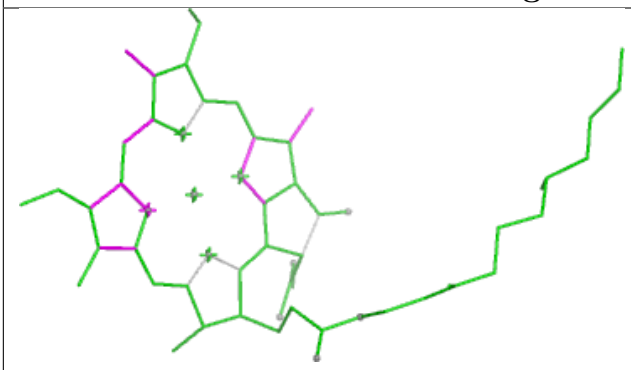


Torsions

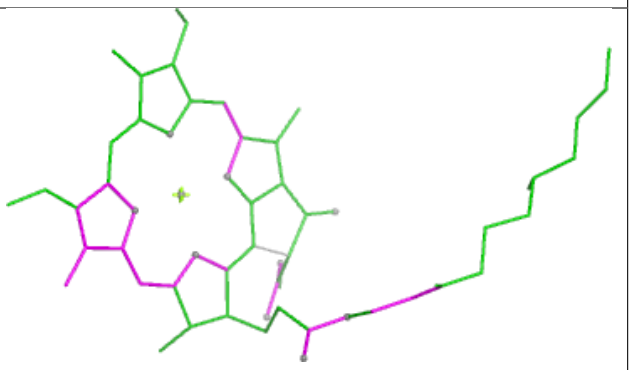


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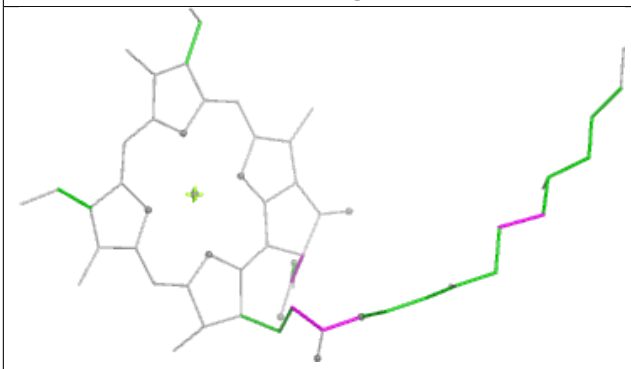
Ligand CLA K 103



Bond lengths



Bond angles

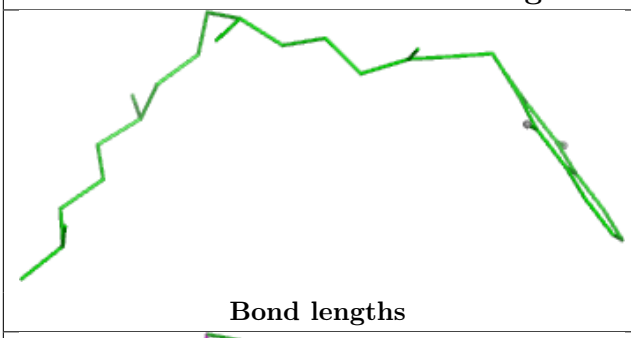


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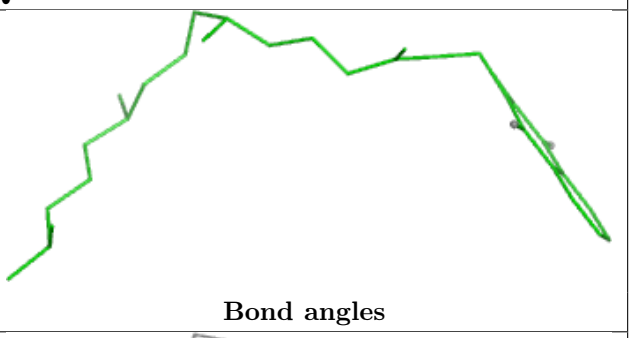


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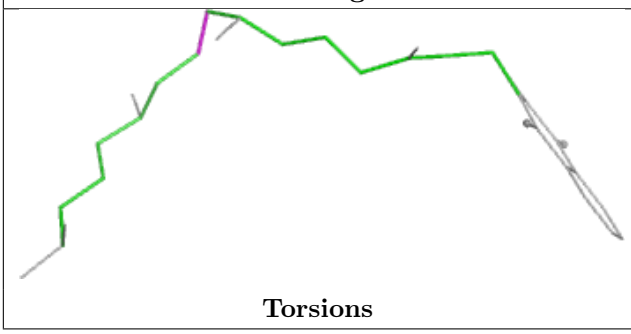
Ligand PQN b 843



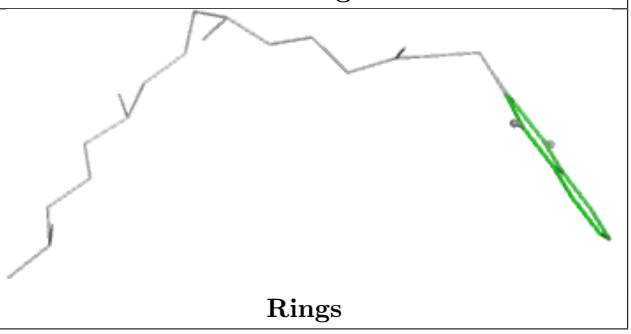
Bond lengths



Bond angles

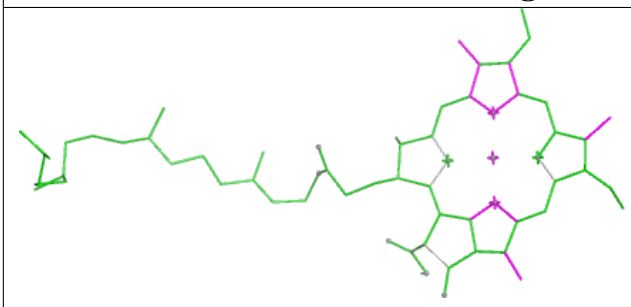


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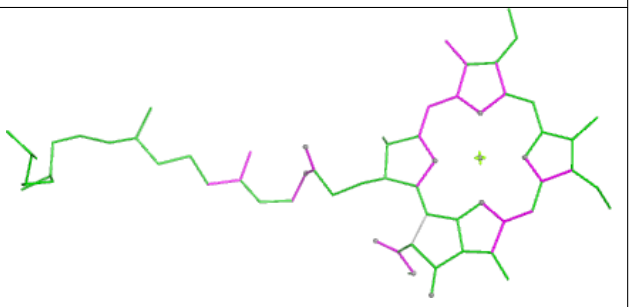


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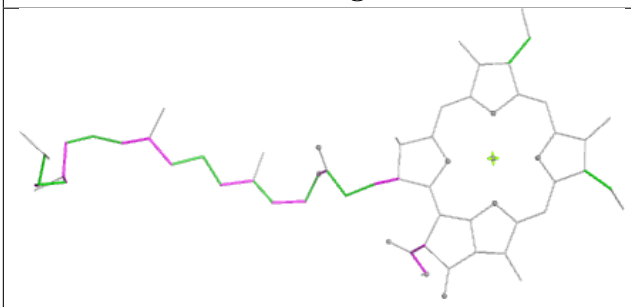
Ligand CLA 1 1607



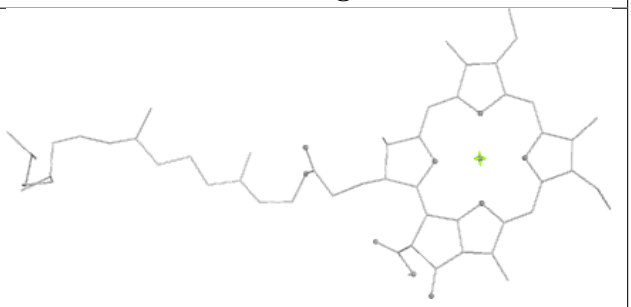
Bond lengths



Bond angles

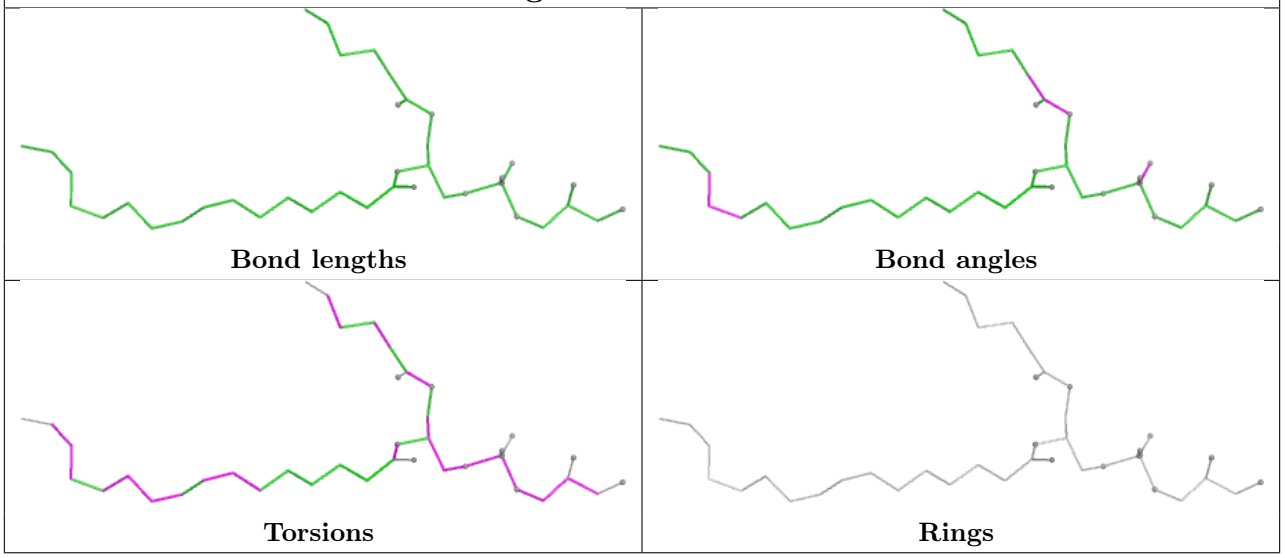


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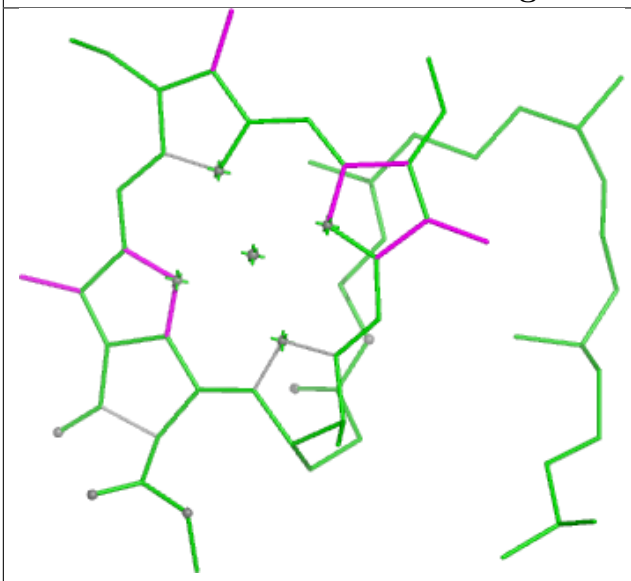


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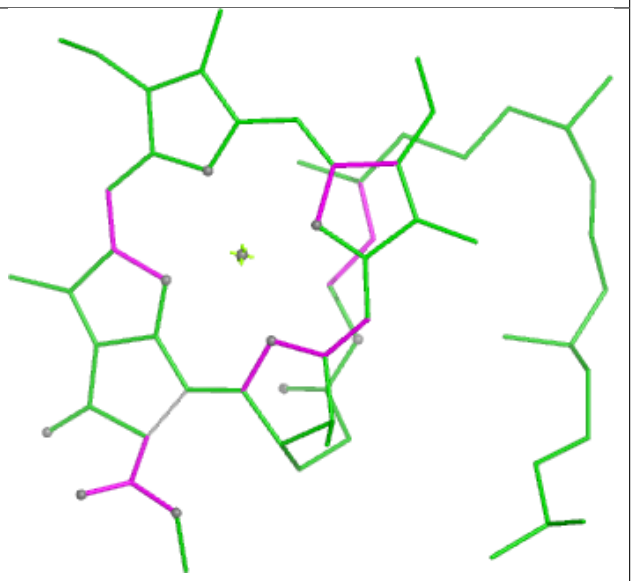
Ligand LHG L 208



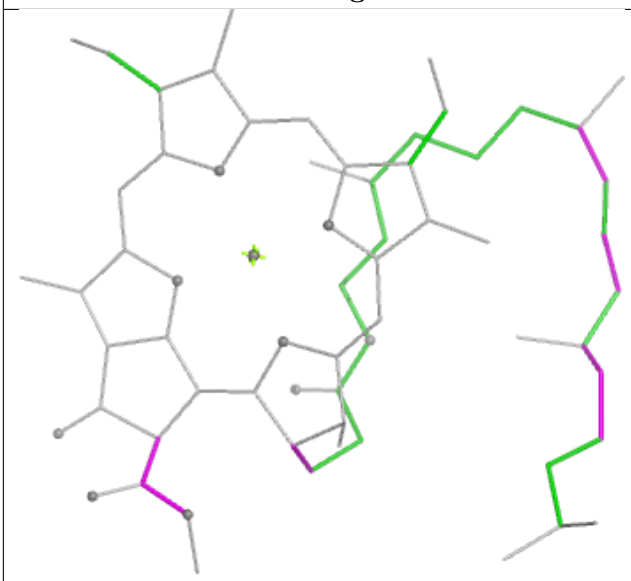
Ligand CLA 1 1625



Bond lengths



Bond angles

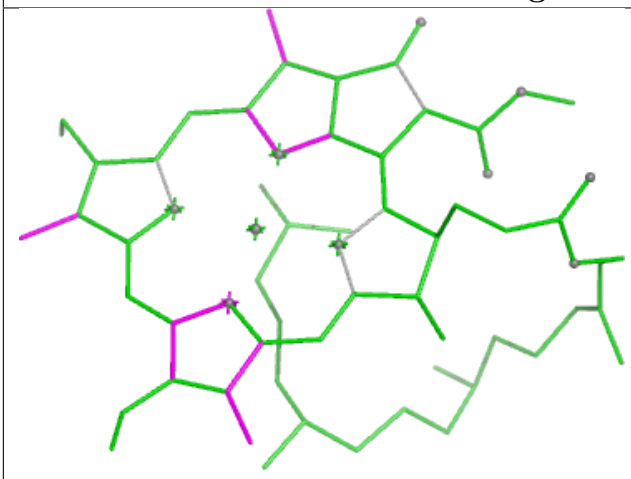


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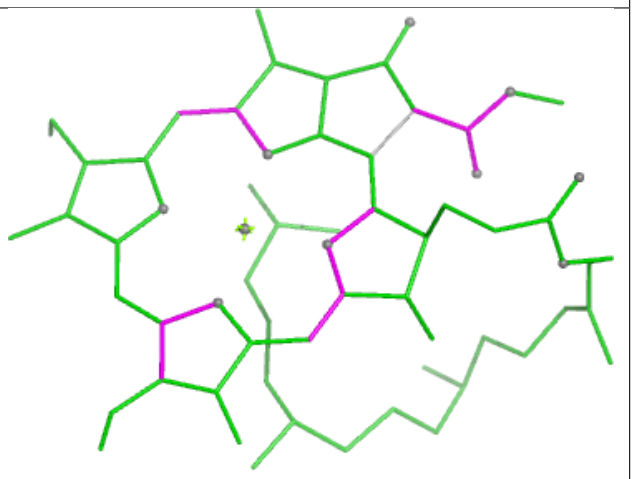


Rings

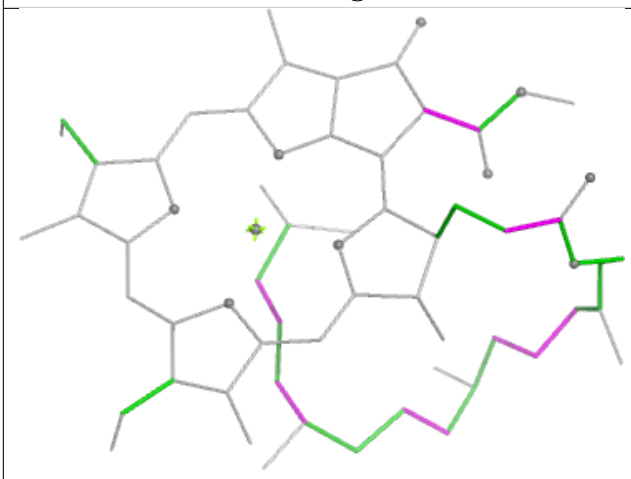
Ligand CLA 2 807



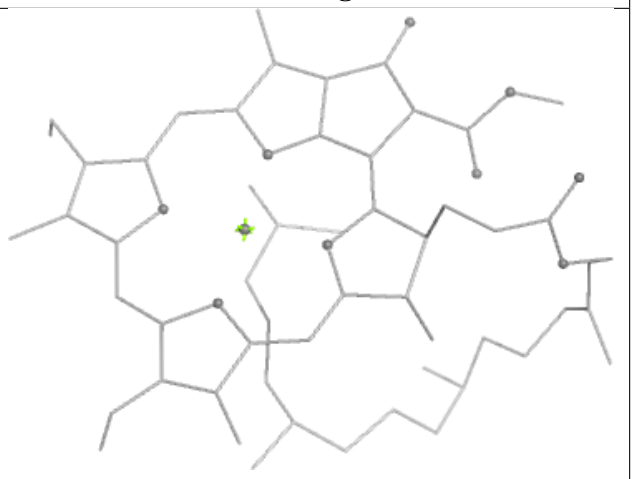
Bond lengths



Bond angles

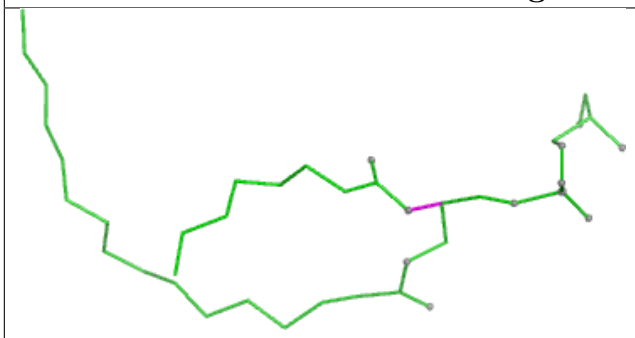


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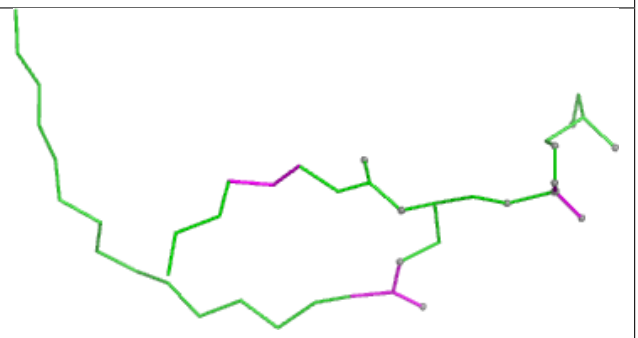


Rings

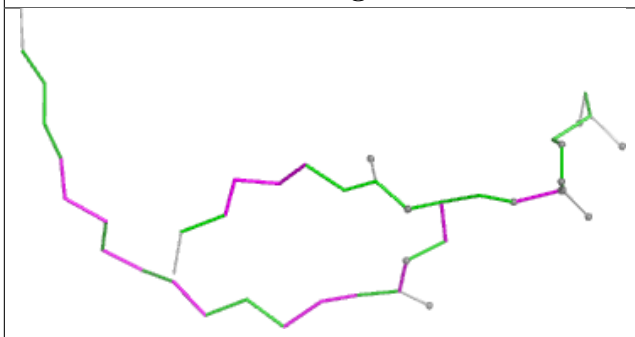
Ligand LHG a 854



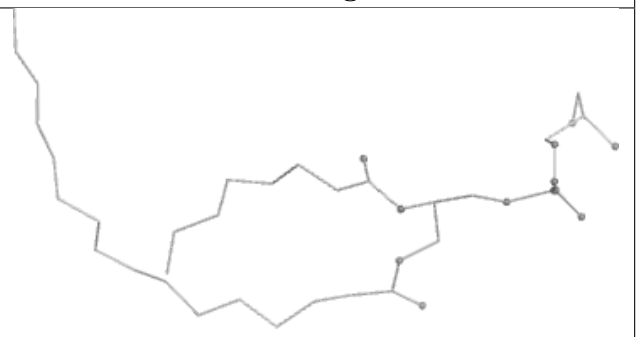
Bond lengths



Bond angles

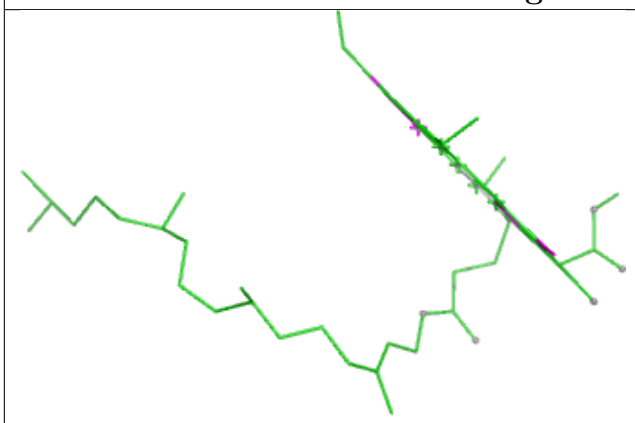


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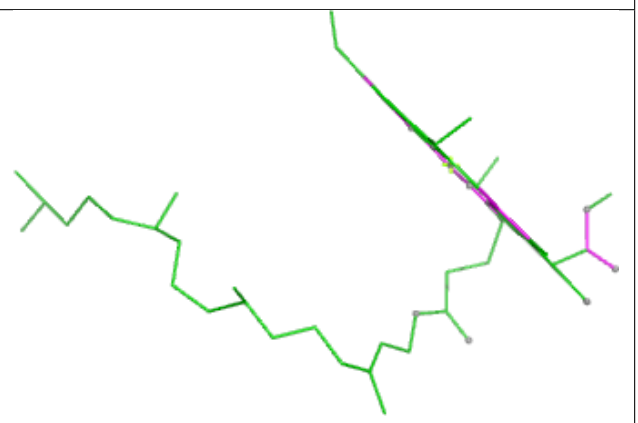


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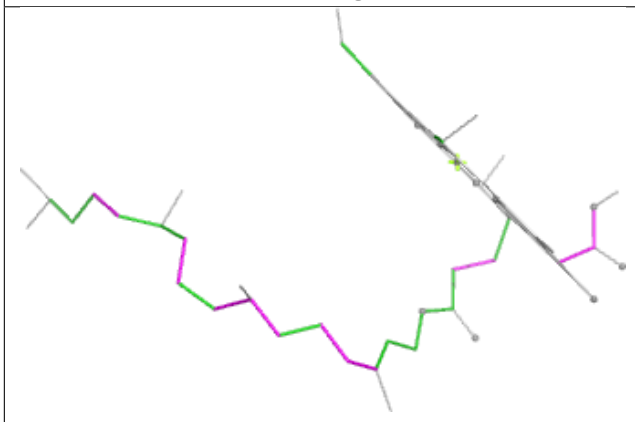
Ligand CLA B 814



Bond lengths



Bond angles

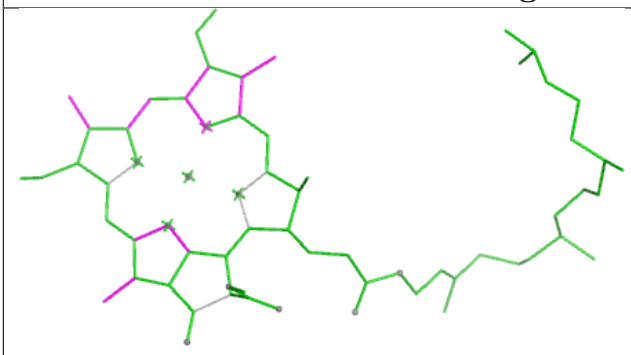


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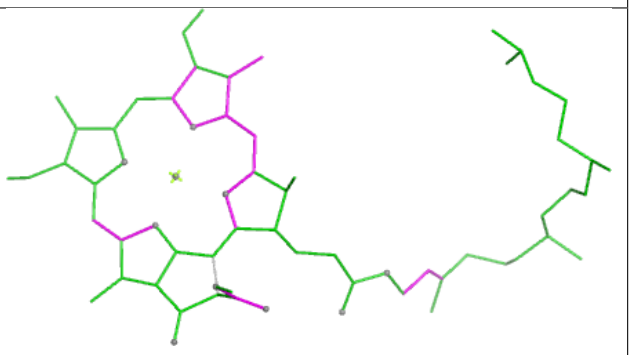


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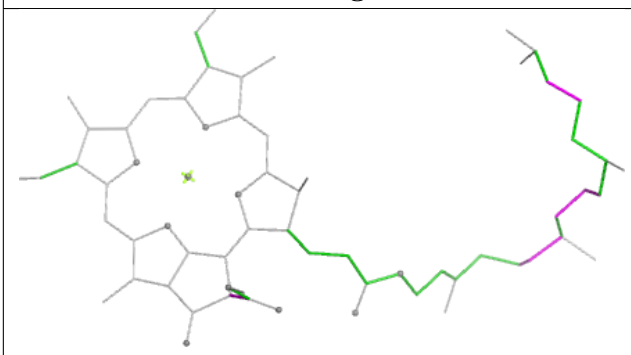
Ligand CLA 1 1629



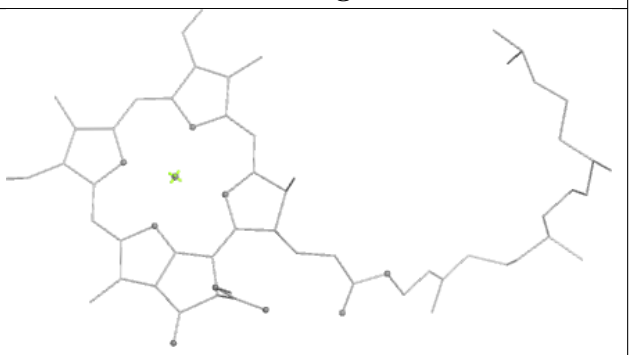
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Bond angles

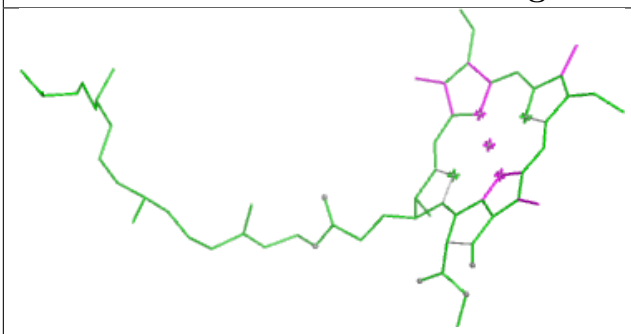


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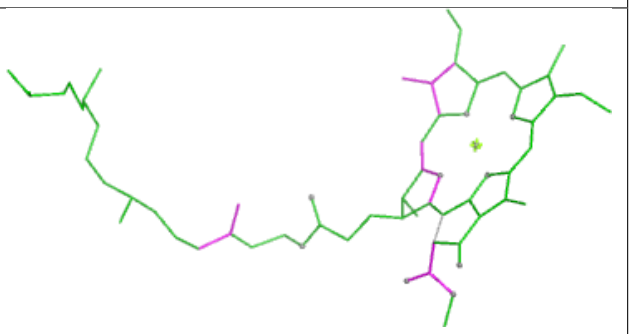


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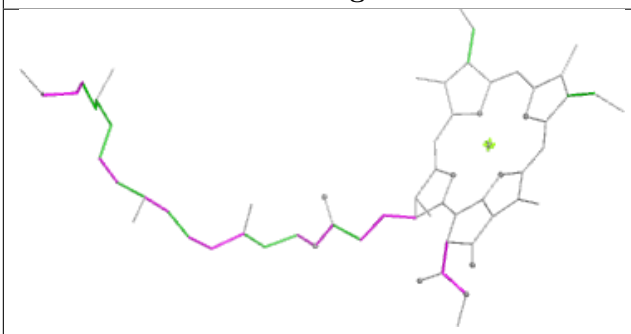
Ligand CLA 2 802



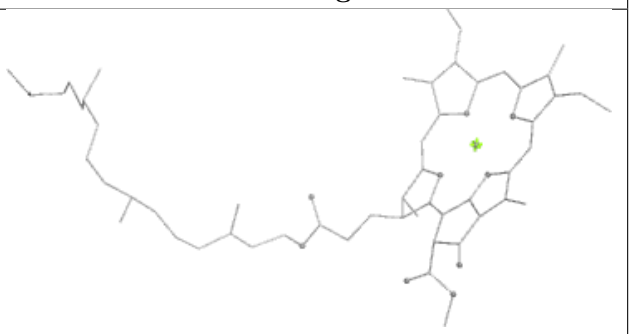
Bond lengths



Bond angles

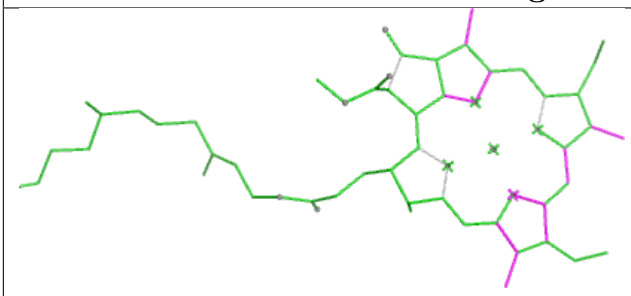


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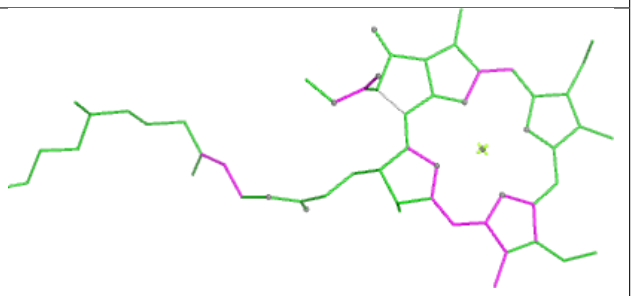


Rings

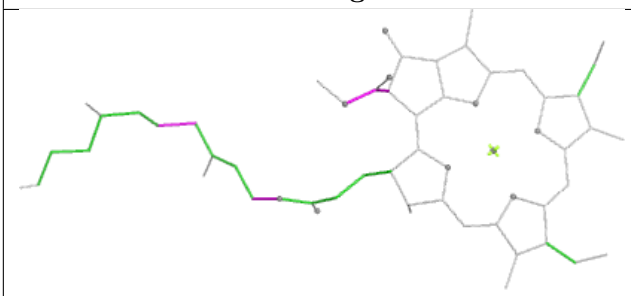
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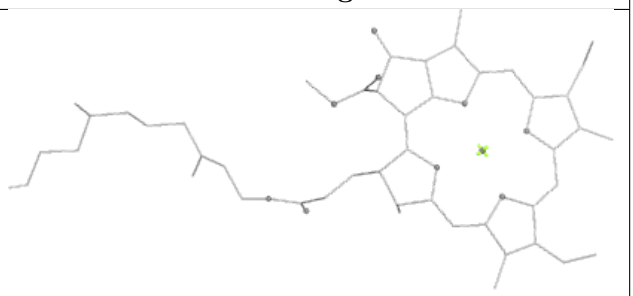
Bond lengths



Bond angles

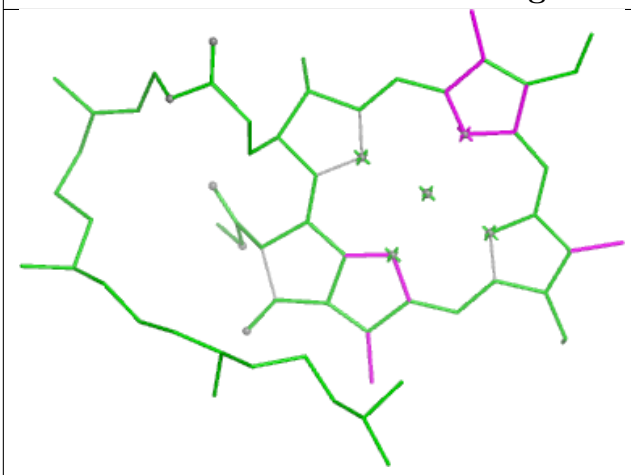


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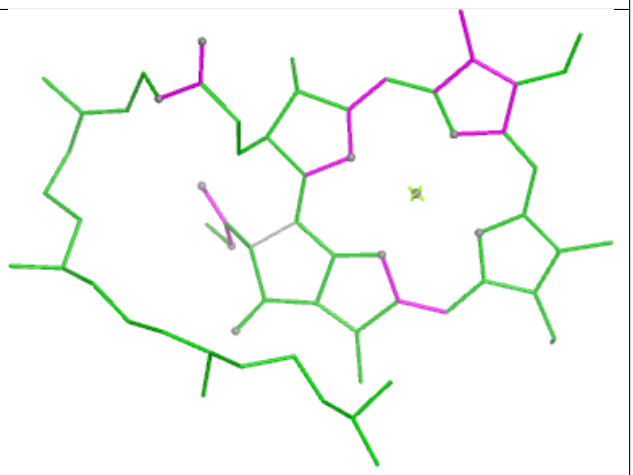


Rings

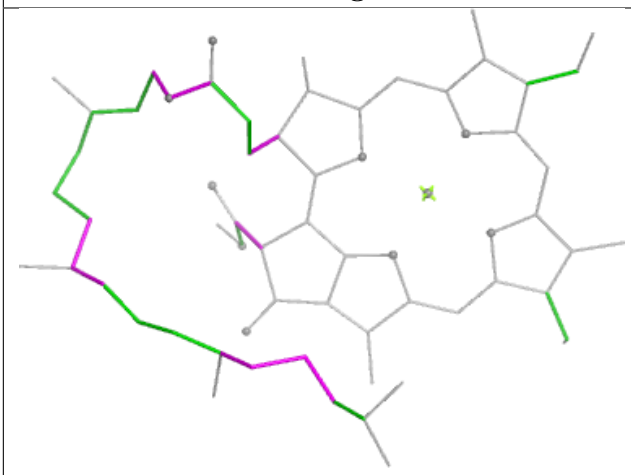
Ligand CLA 2 806



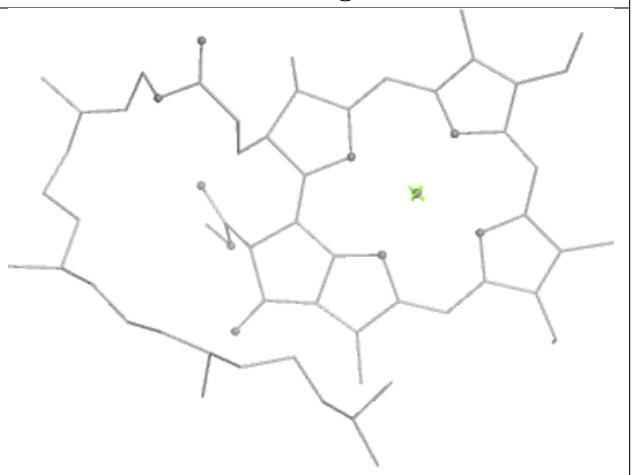
Bond lengths



Bond angles

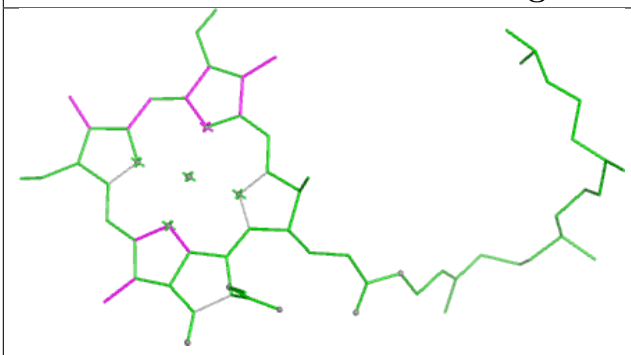


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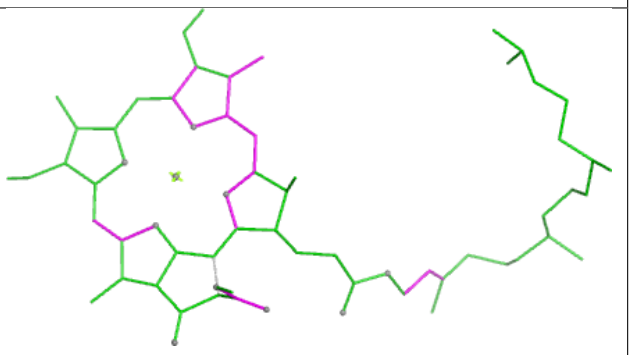


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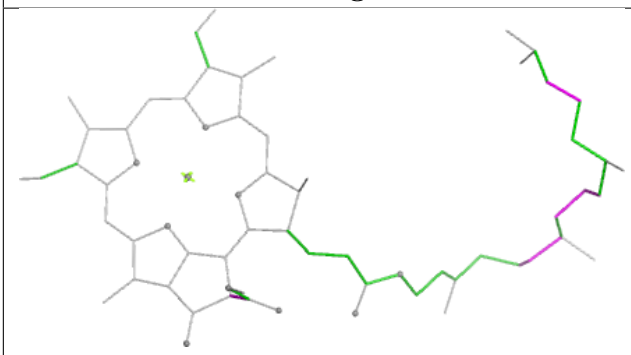
Ligand CLA a 828



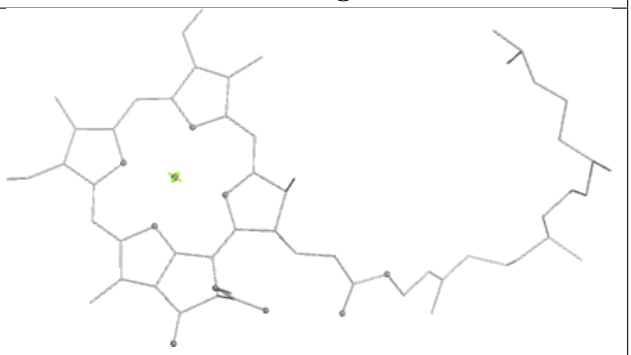
Bond lengths



Bond angles

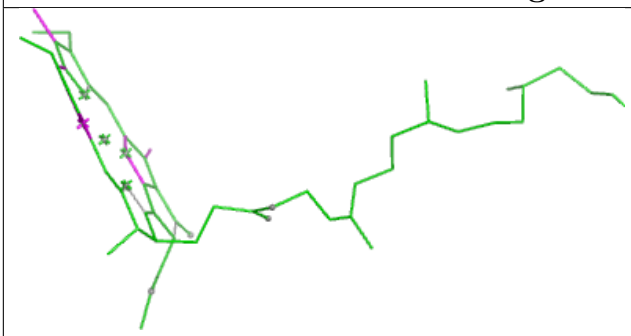


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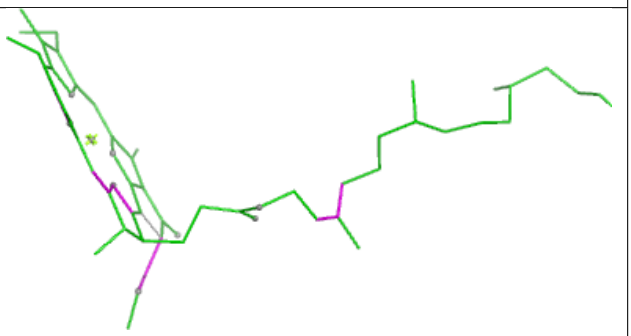


Rings

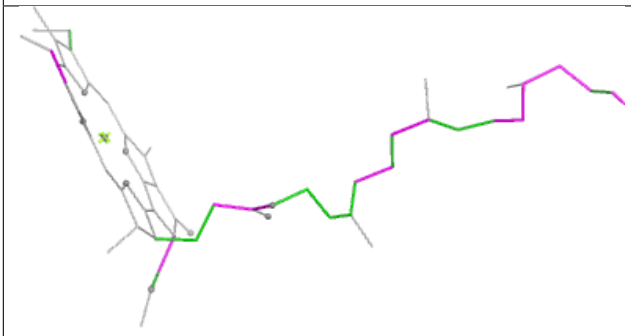
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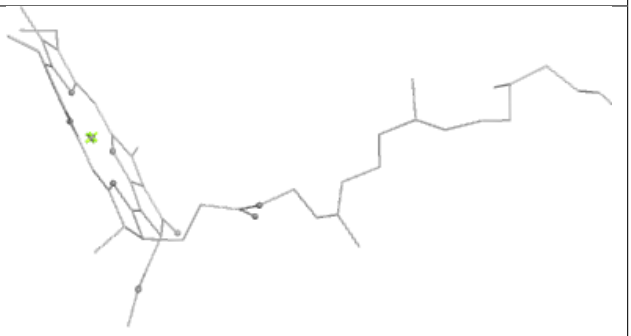
Bond lengths



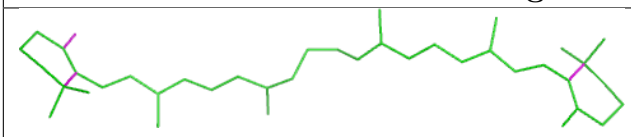
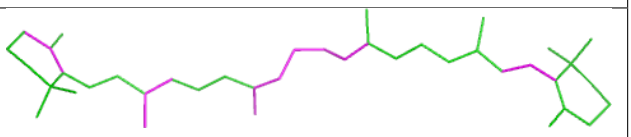
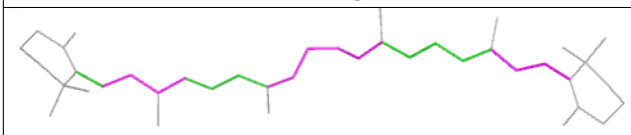
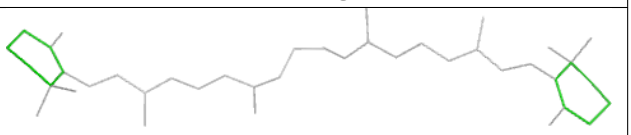
Bond angles

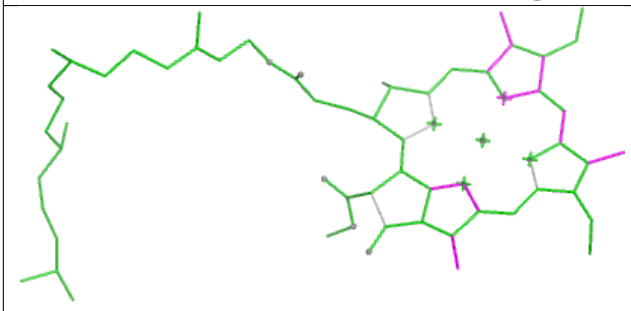
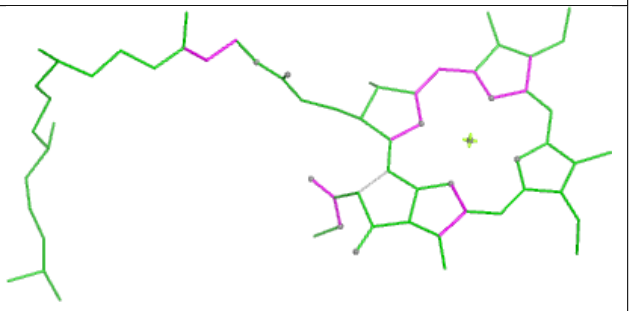
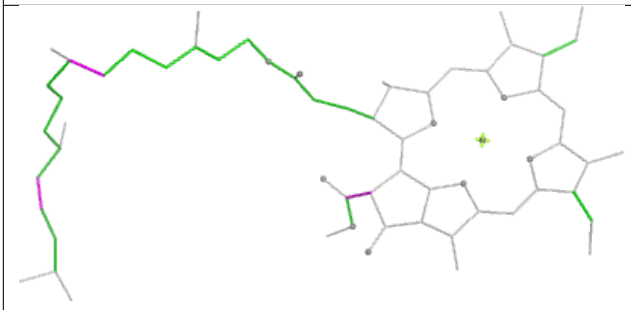
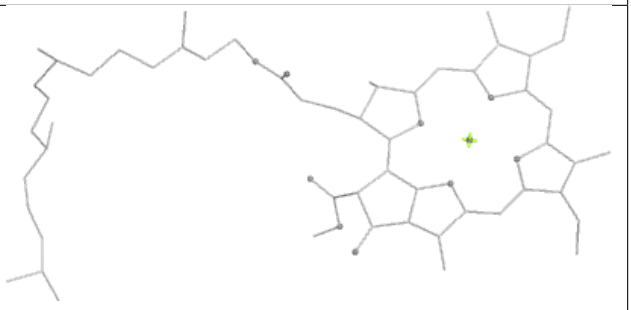


Torsions

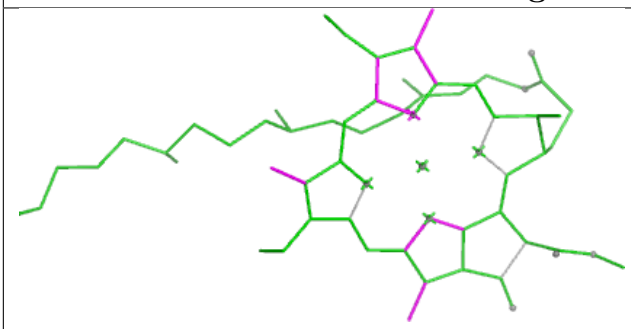


Rings

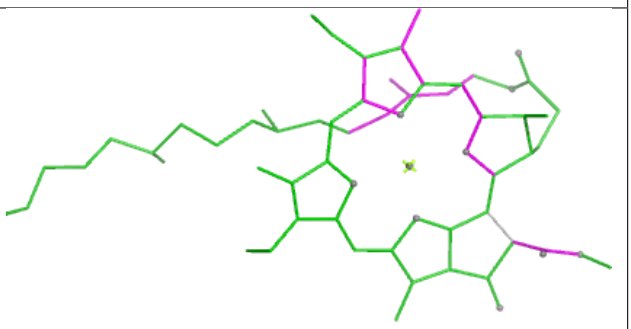
Ligand BCR a 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 827	
 Bond lengths	 Bond angles
 Torsions	 Rings

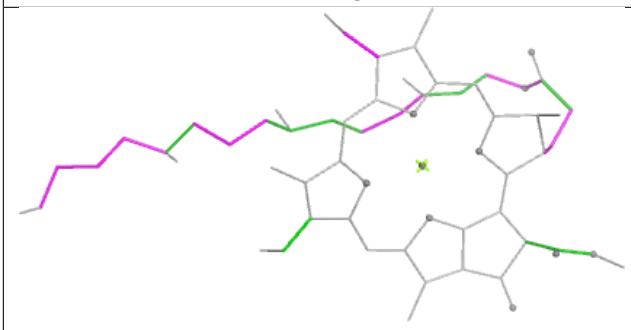
Ligand CLA a 819



Bond lengths



Bond angles

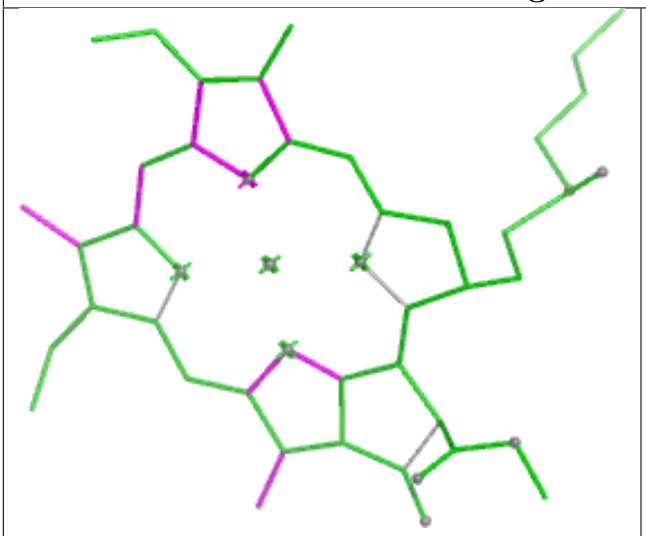


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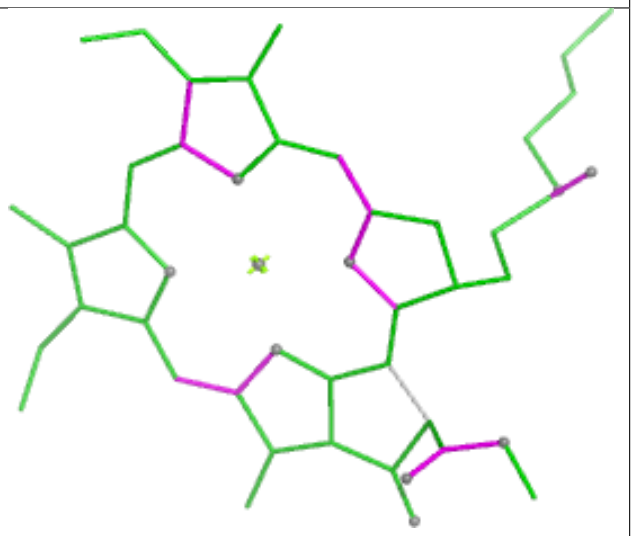


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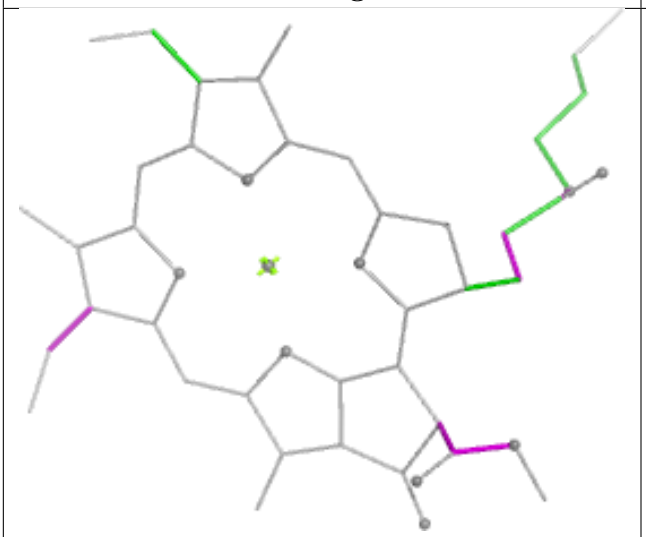
Ligand CLA a 811



Bond lengths



Bond angles

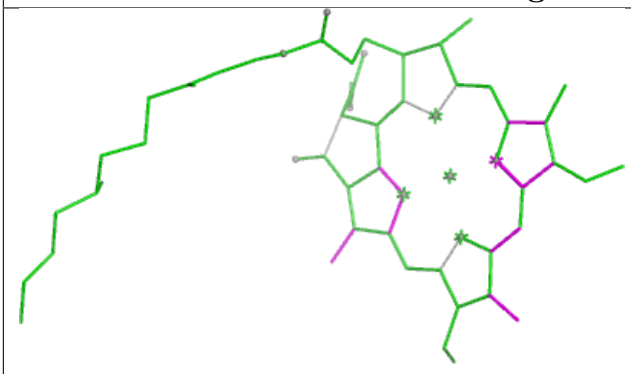


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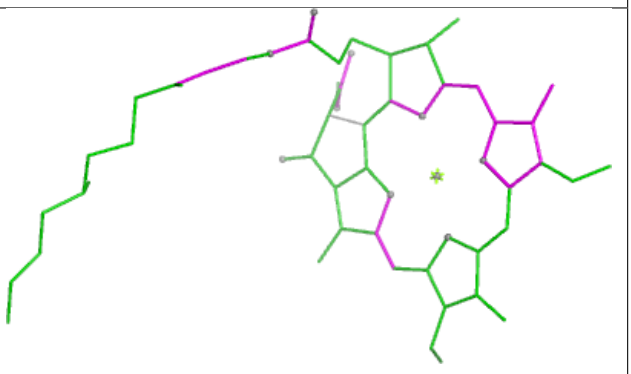


Rings

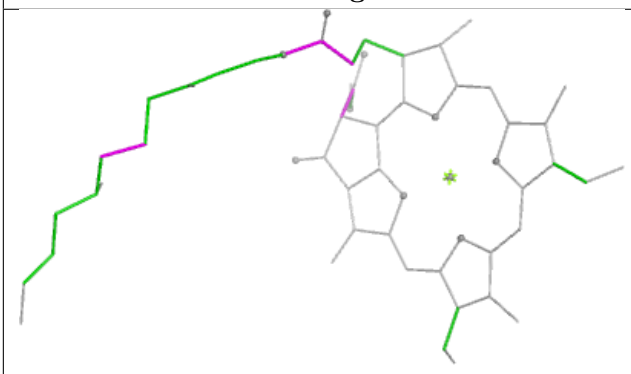
Ligand CLA k 103



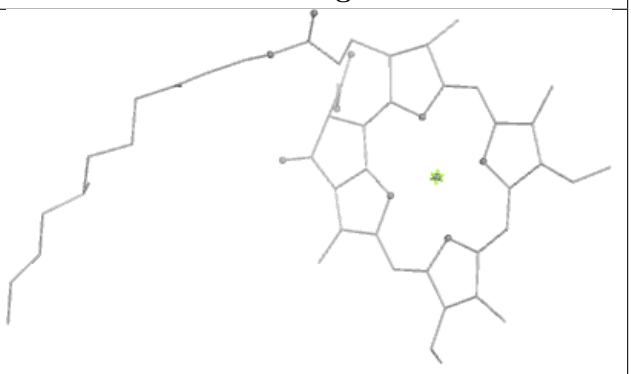
Bond lengths



Bond angles

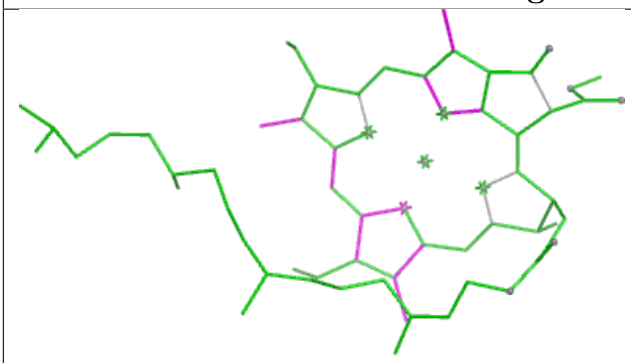


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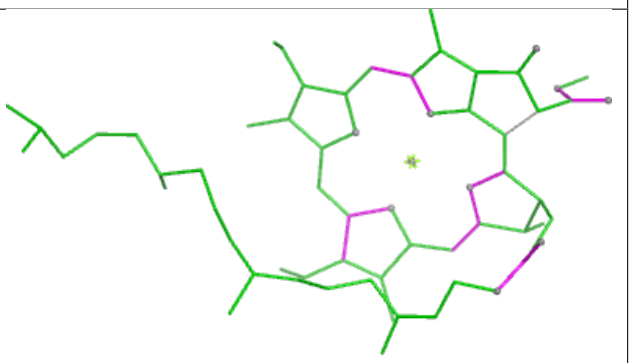


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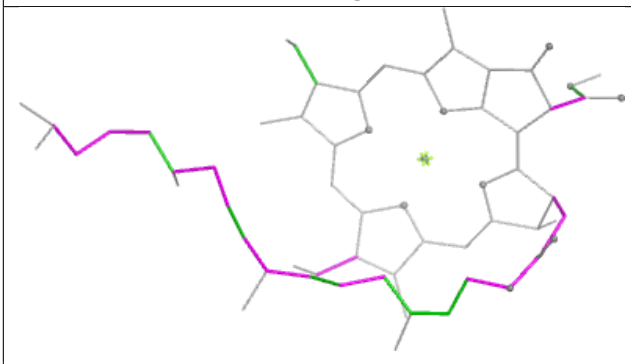
Ligand CLA b 821



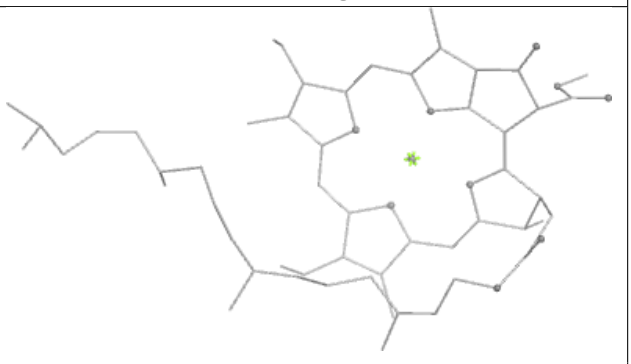
Bond lengths



Bond angles

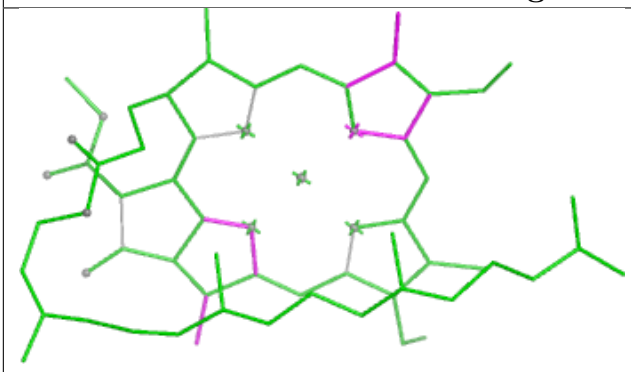


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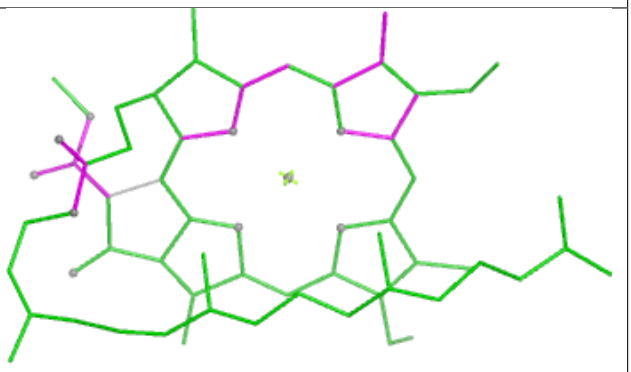


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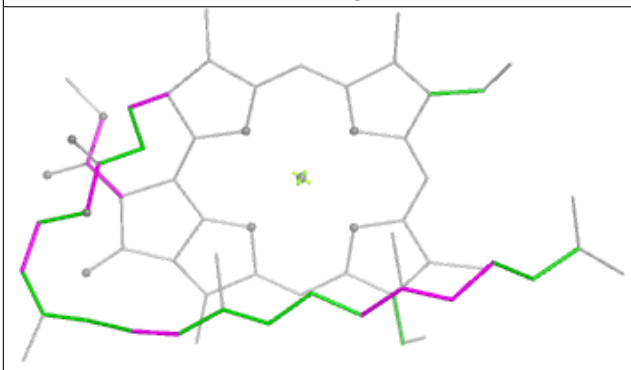
Ligand CLA b 817



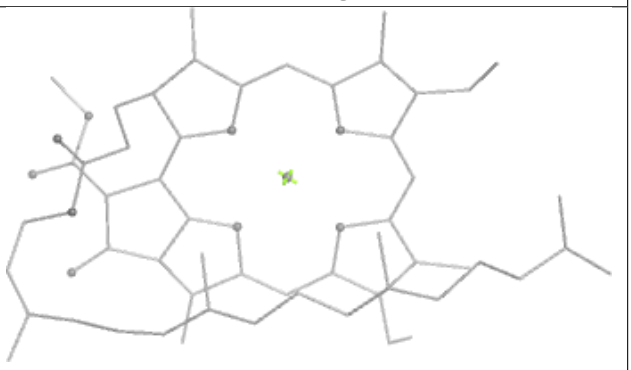
Bond lengths



Bond angles

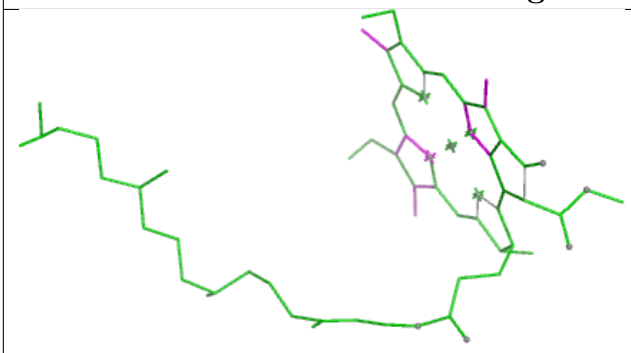


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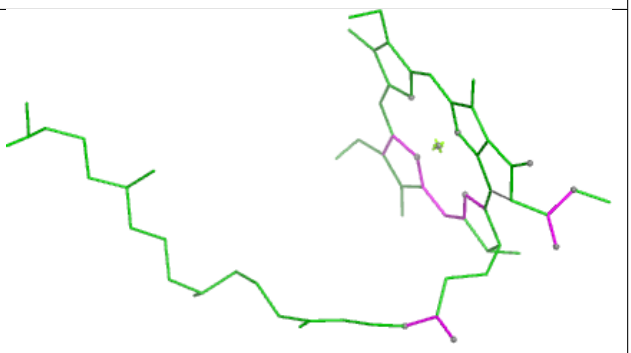


Rings

Ligand CLA b 816



Bond lengths



Bond angles

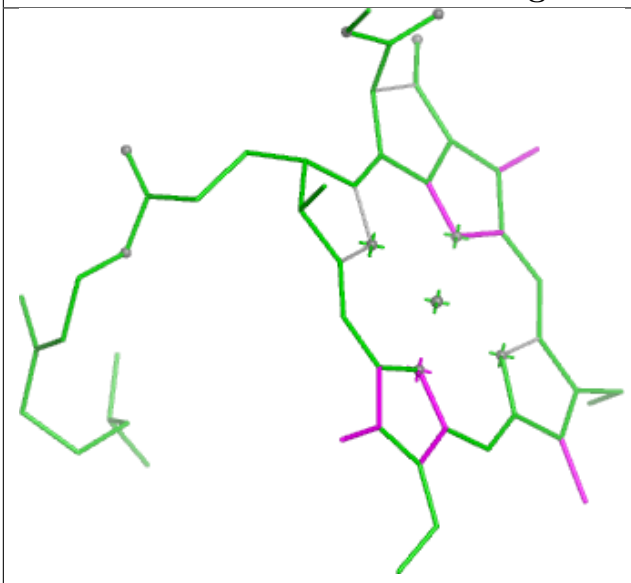


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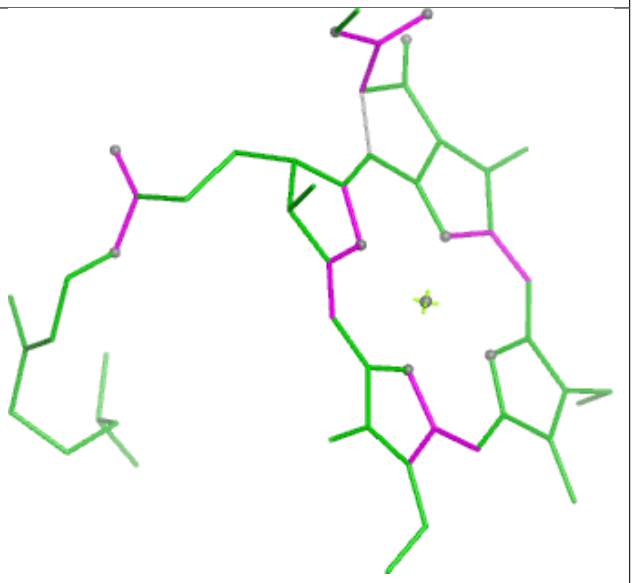


Rings

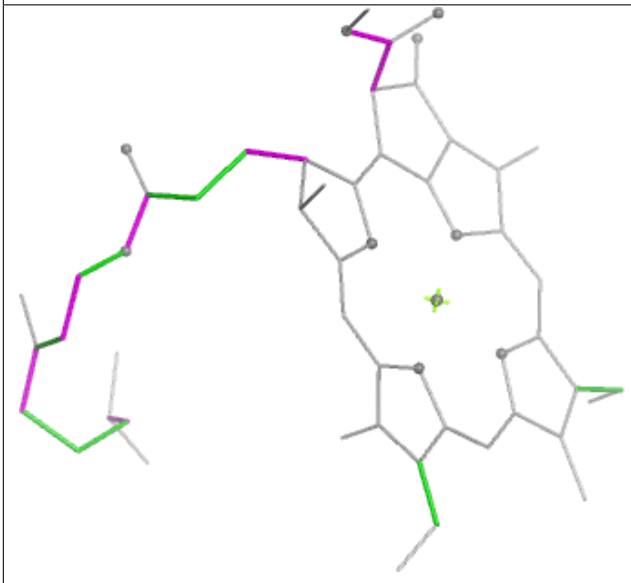
Ligand CLA 2 831



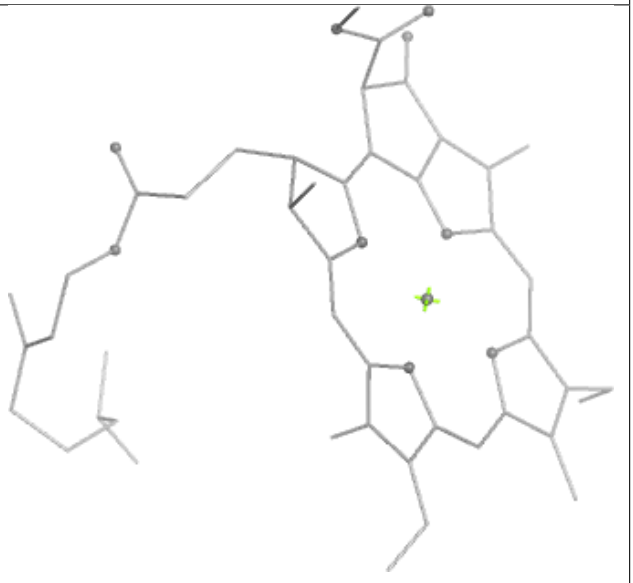
Bond lengths



Bond angles

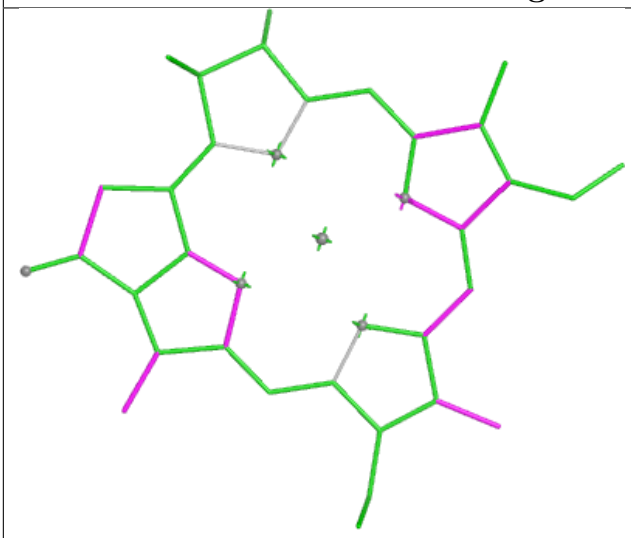


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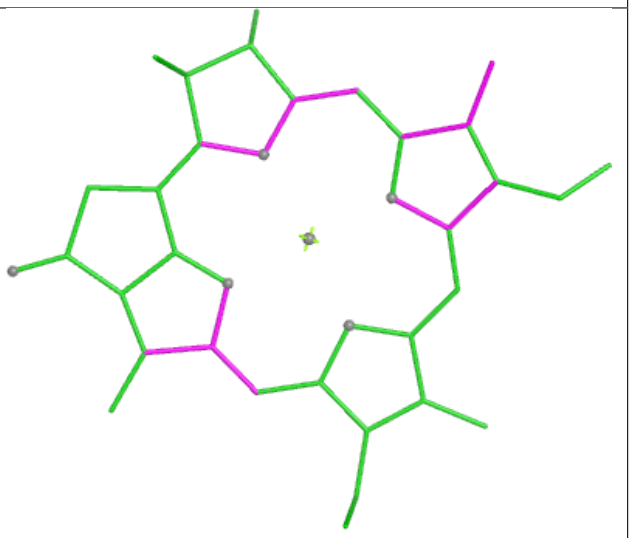


Rings

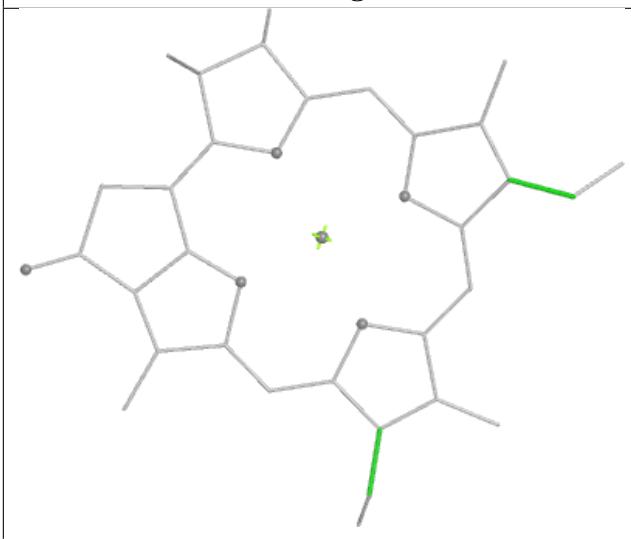
Ligand CLA J 102



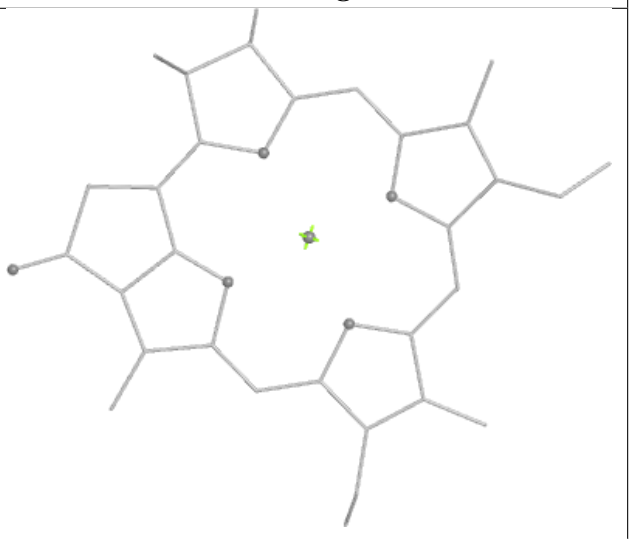
Bond lengths



Bond angles

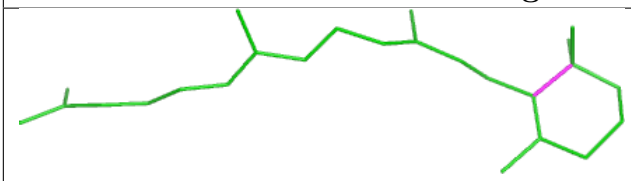


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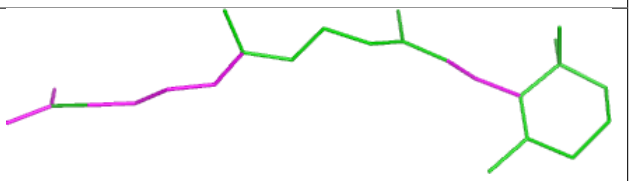


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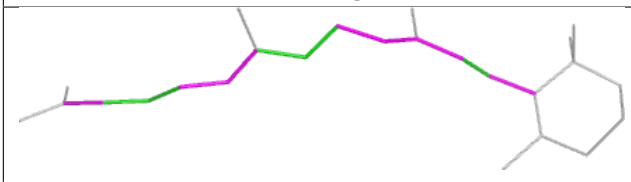
Ligand BCR A 852



Bond lengths



Bond angles

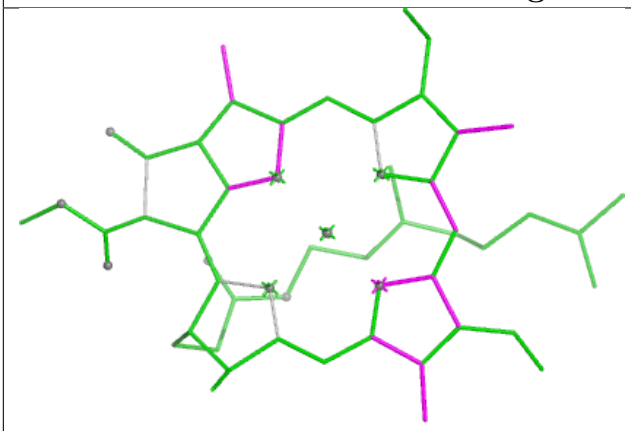


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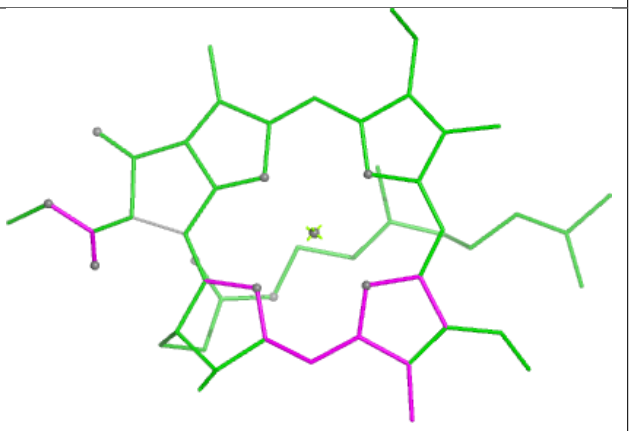


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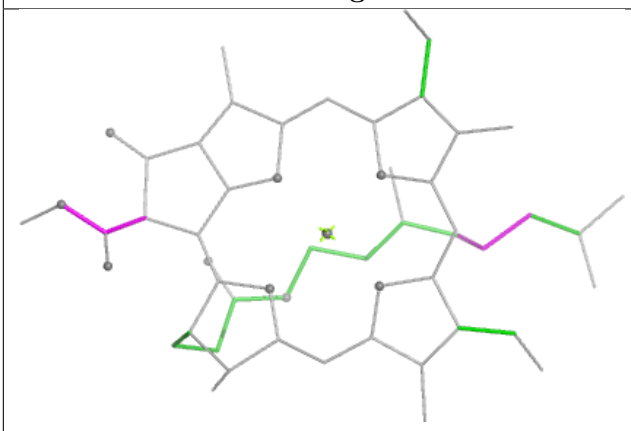
Ligand CLA b 823



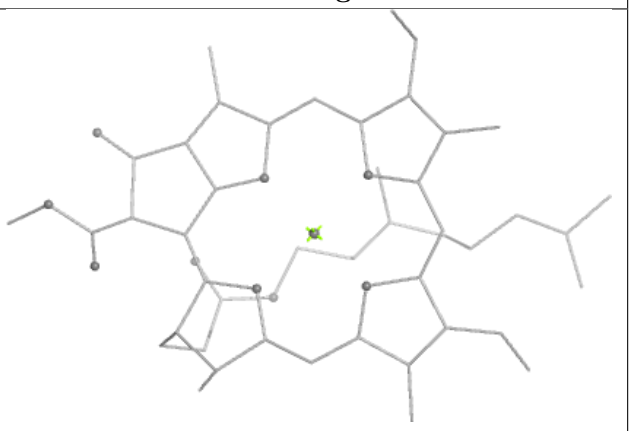
Bond lengths



Bond angles

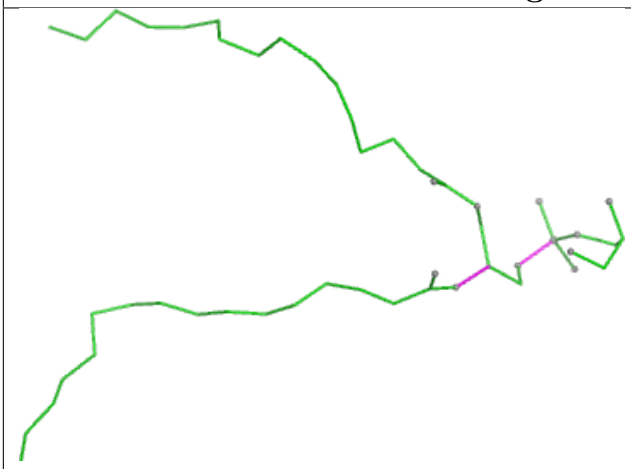


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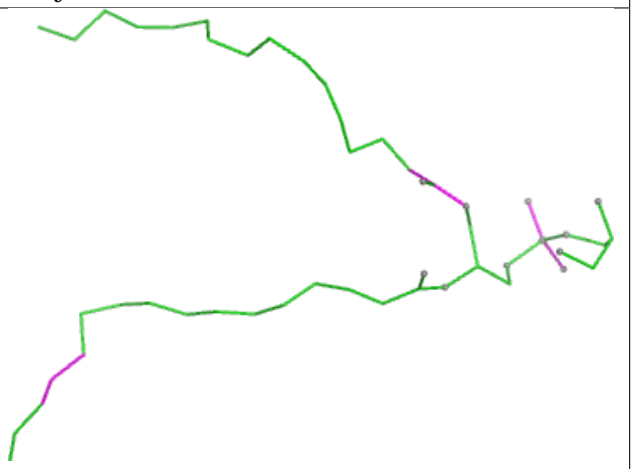


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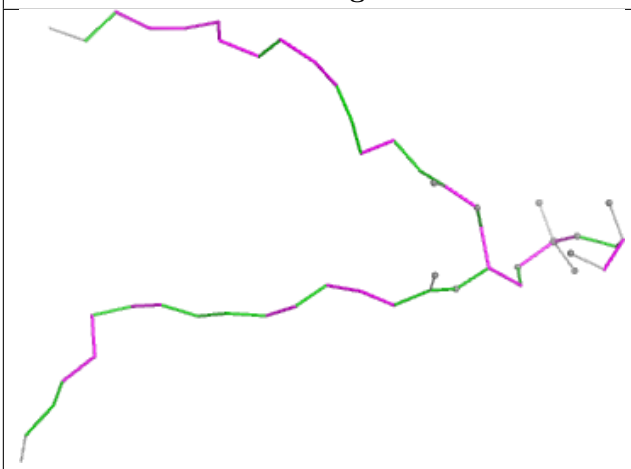
Ligand LHG y 101



Bond lengths



Bond angles

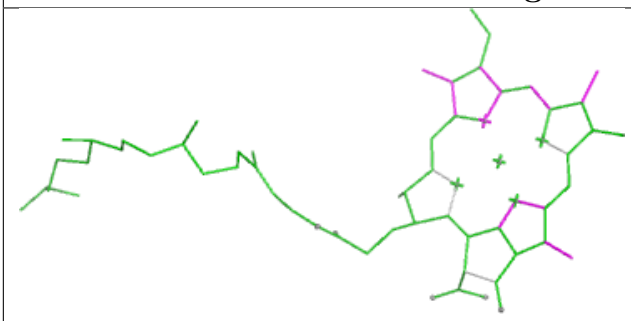


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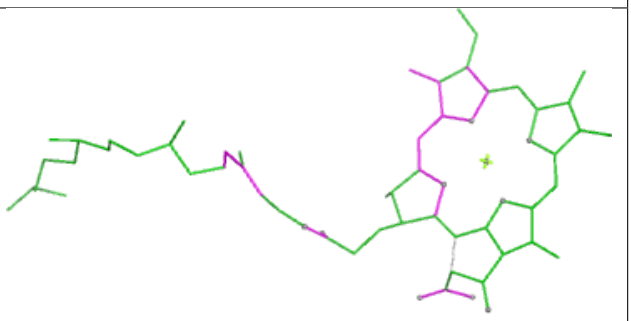


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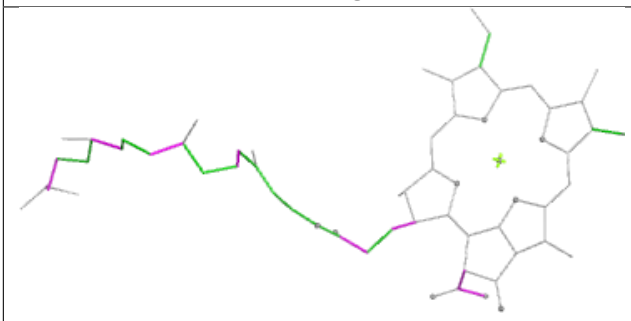
Ligand CLA B 813



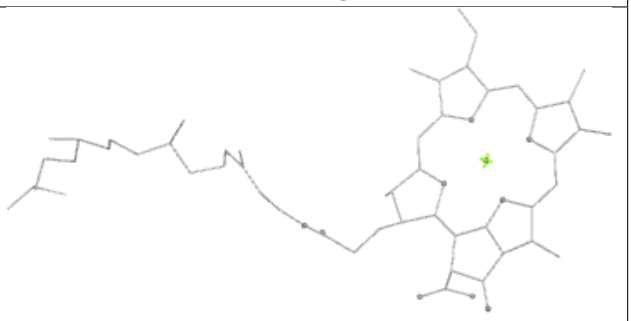
Bond lengths



Bond angles

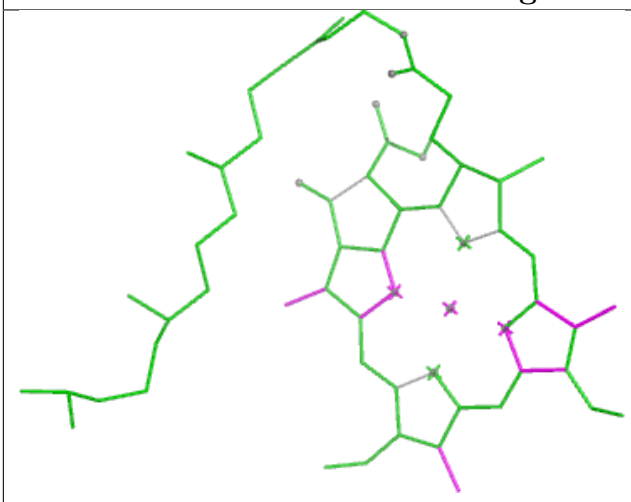


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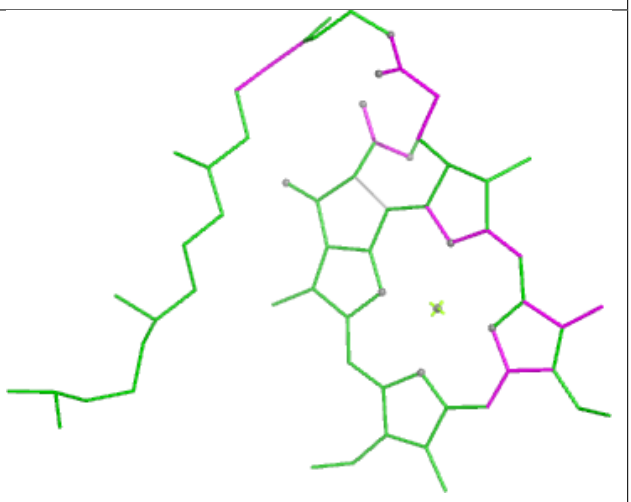


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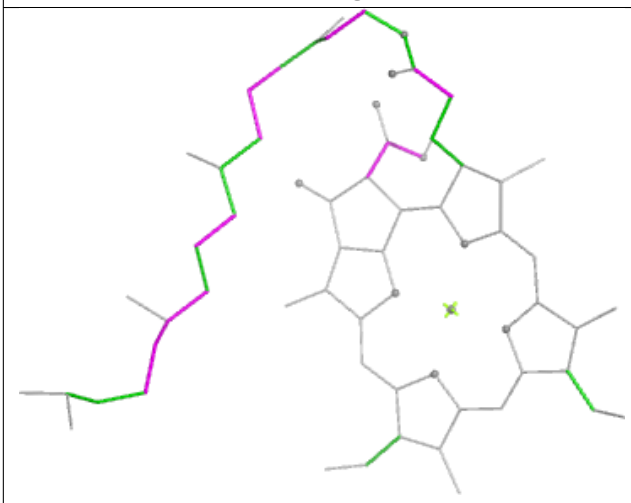
Ligand CLA 1 1627



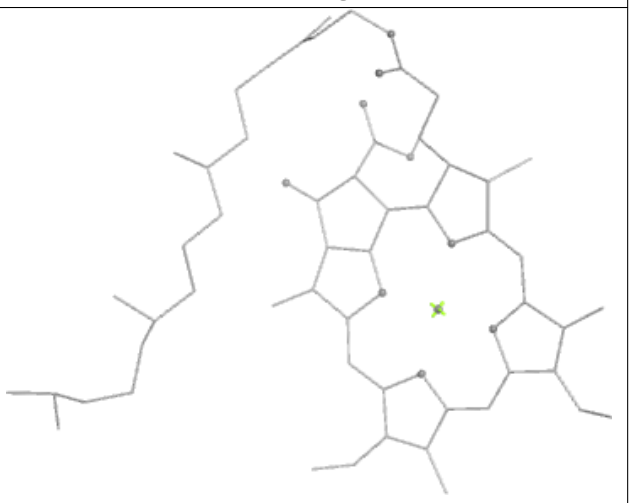
Bond lengths



Bond angles

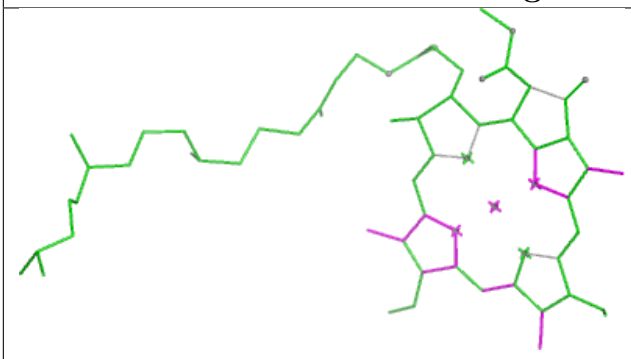


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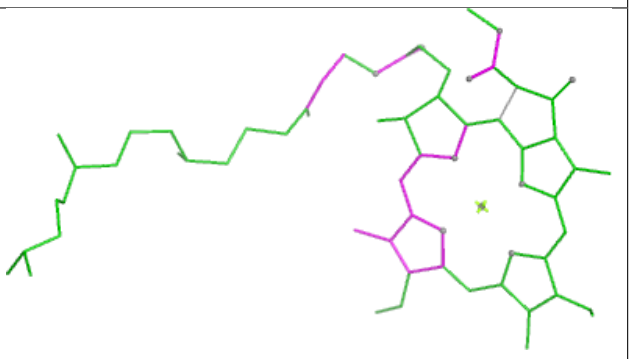


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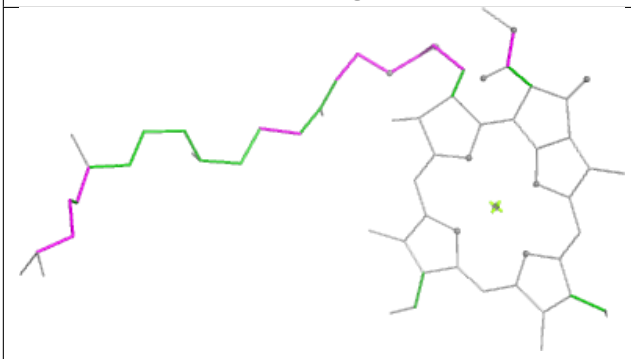
Ligand CLA A 802



Bond lengths



Bond angles

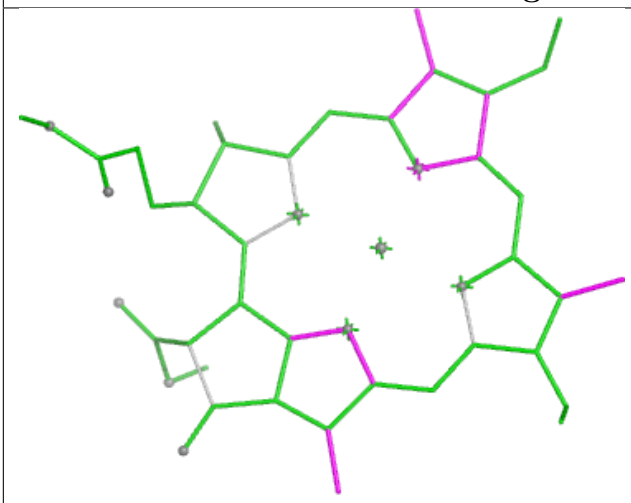


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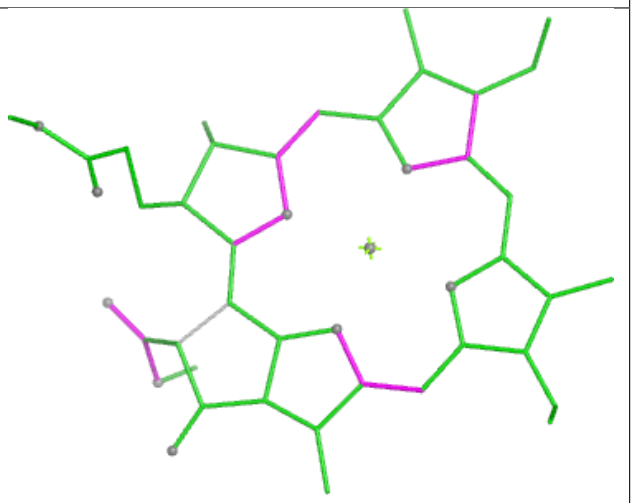


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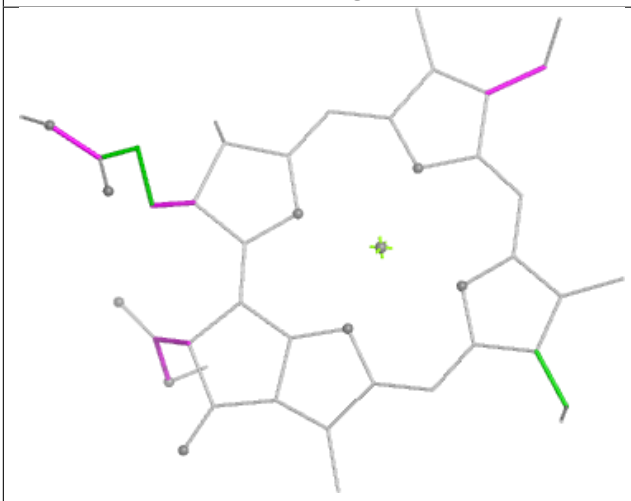
Ligand CLA K 101



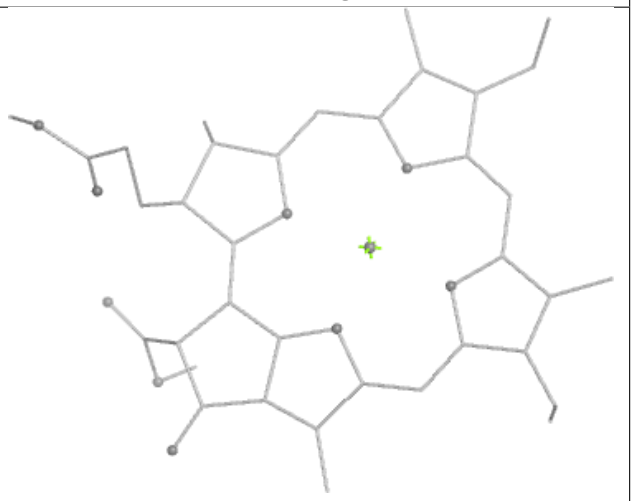
Bond lengths



Bond angles

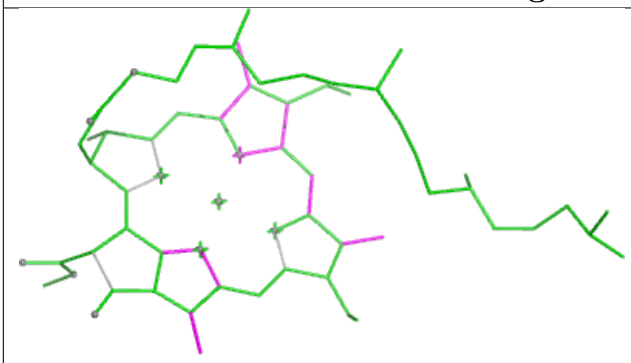


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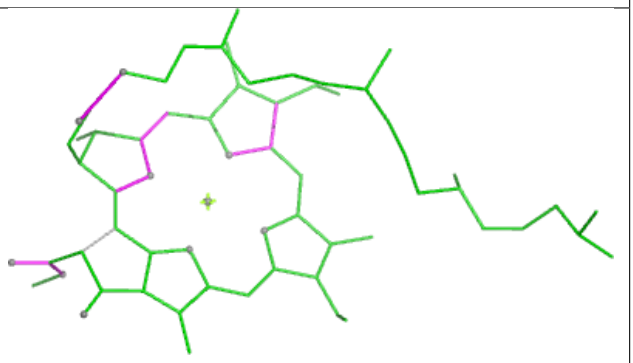


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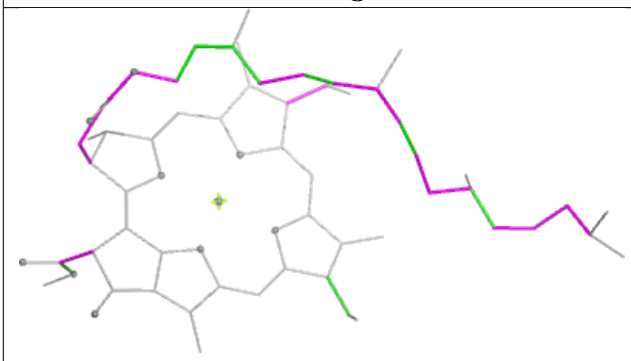
Ligand CLA 2 821



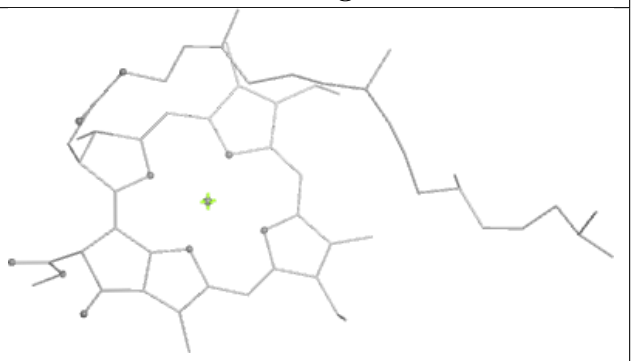
Bond lengths



Bond angles

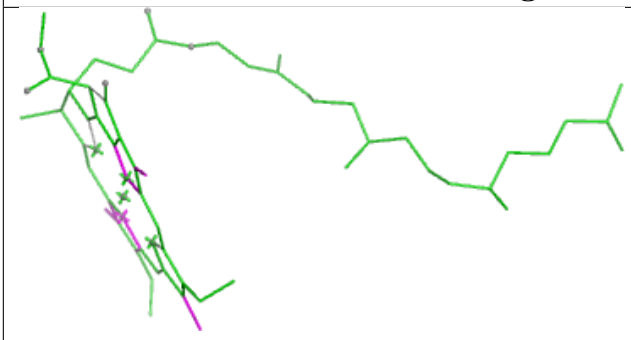


Torsions

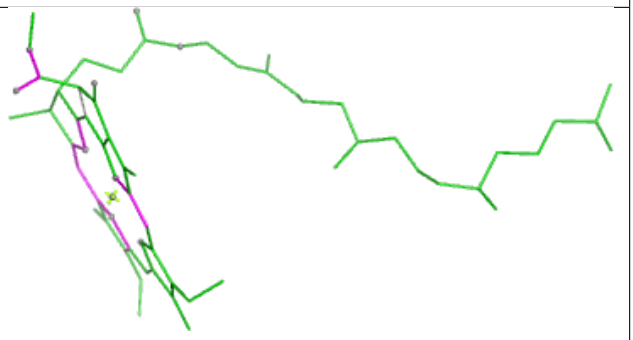


Rings

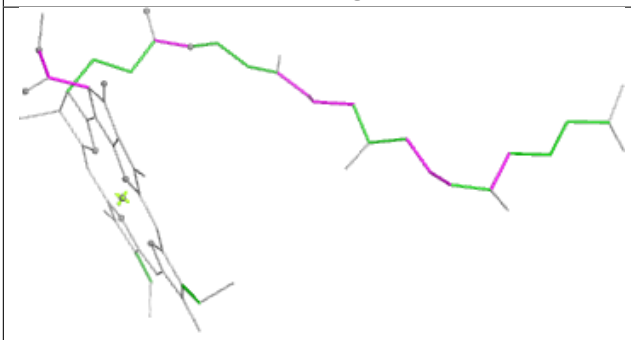
Ligand CLA 1 1613



Bond lengths



Bond angles

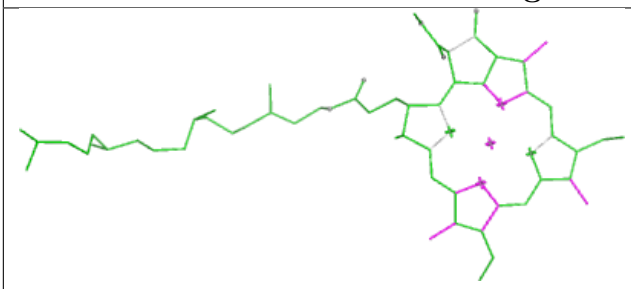


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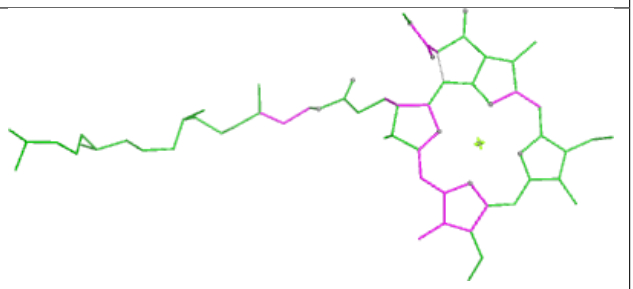


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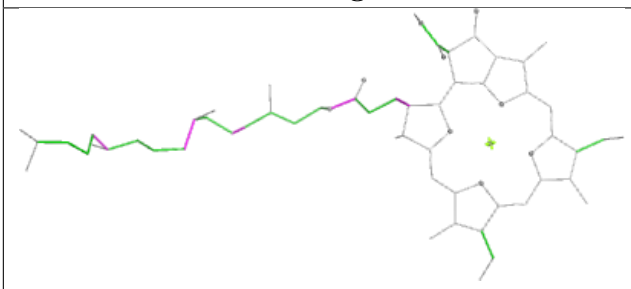
Ligand CLA A 827



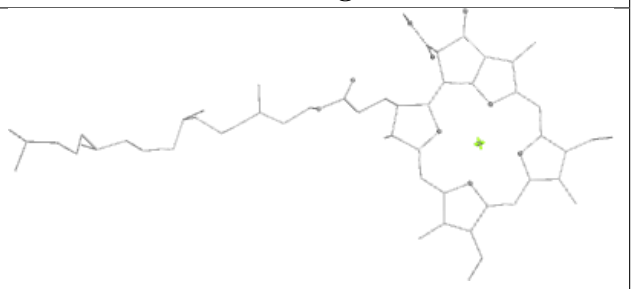
Bond lengths



Bond angles

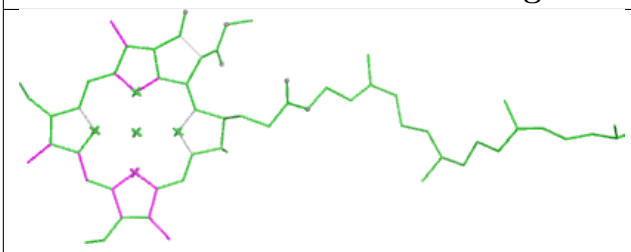


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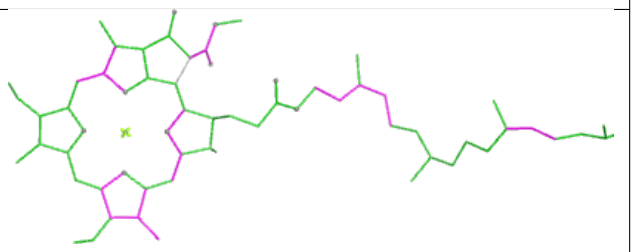


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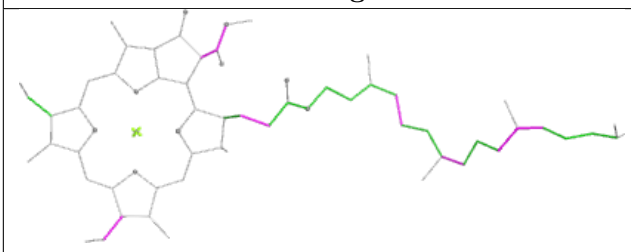
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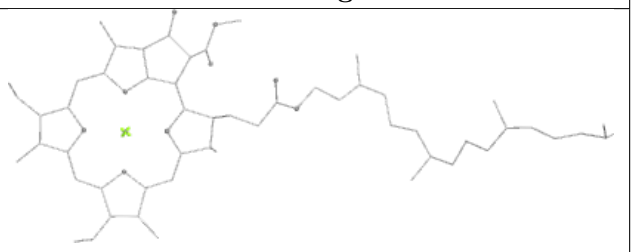
Bond lengths



Bond angles

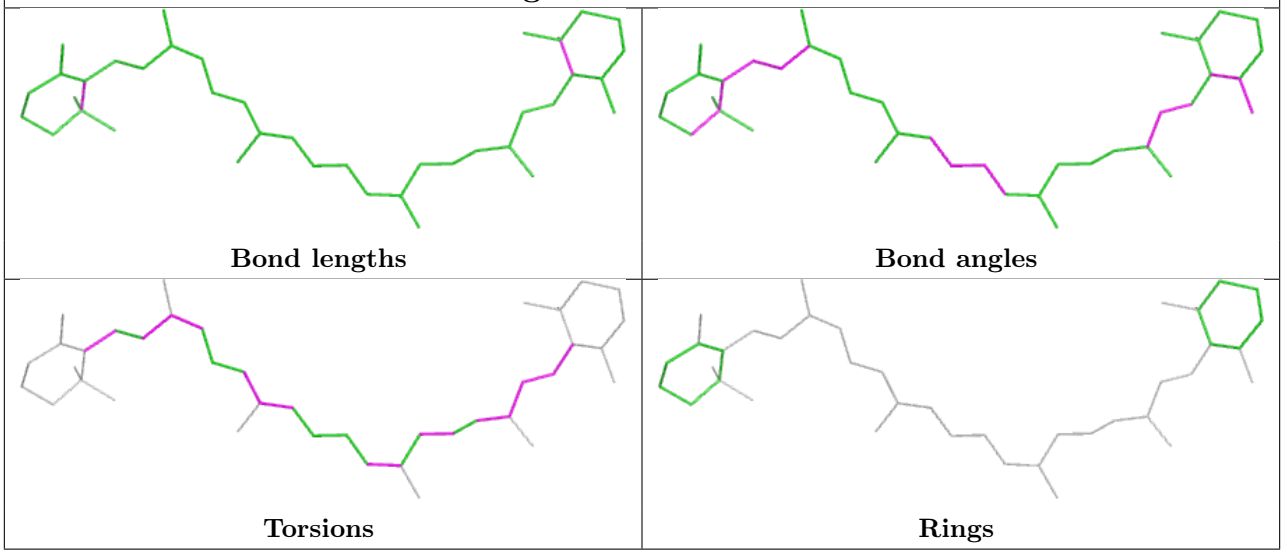


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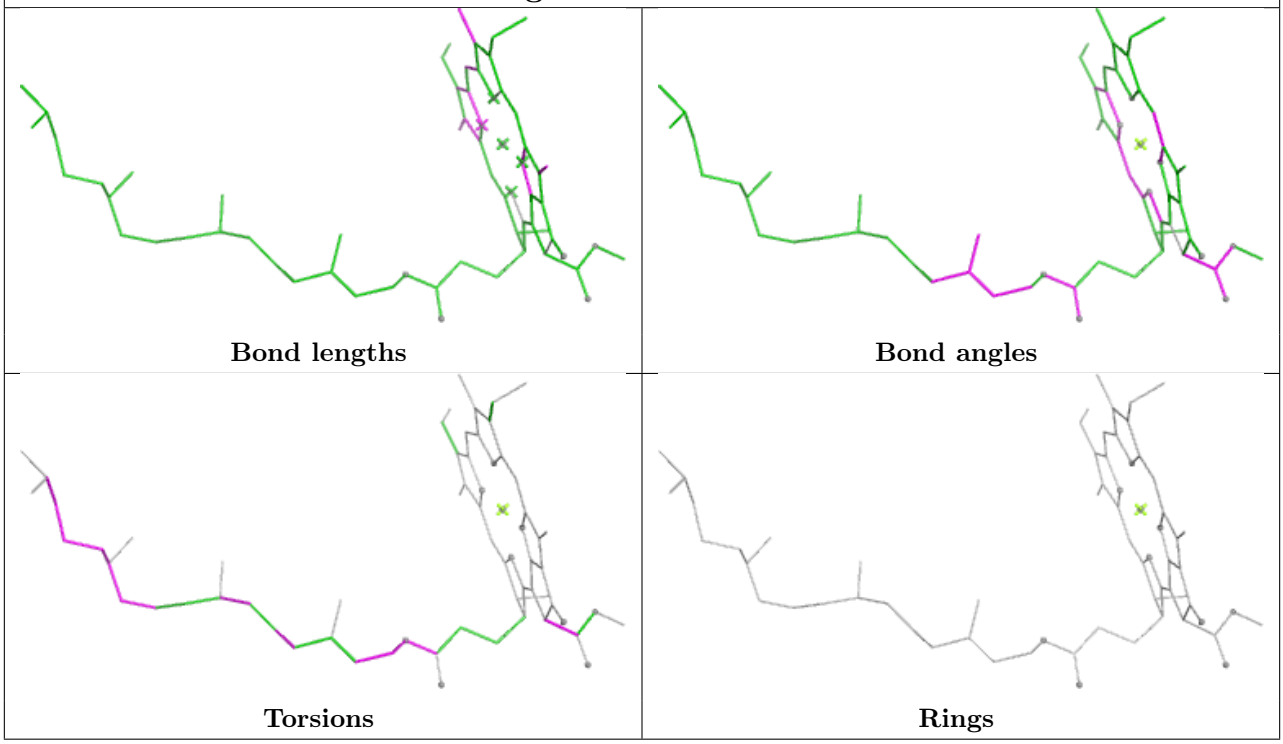


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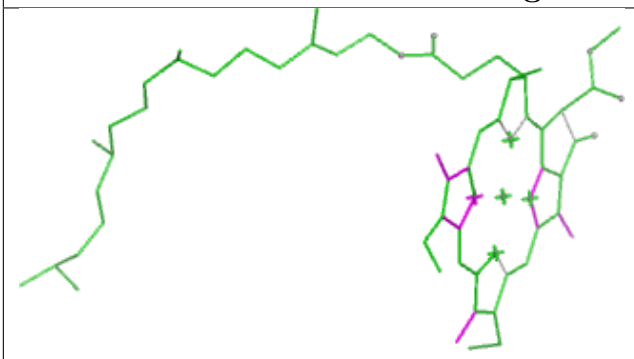
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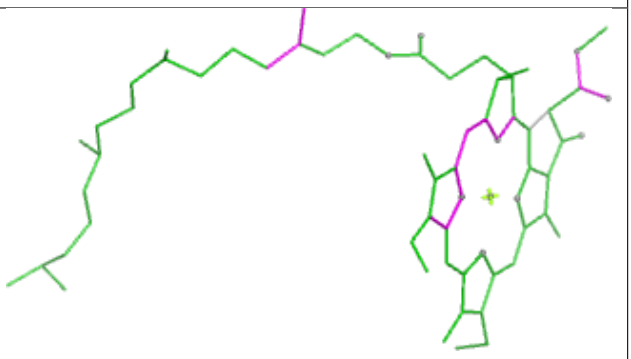
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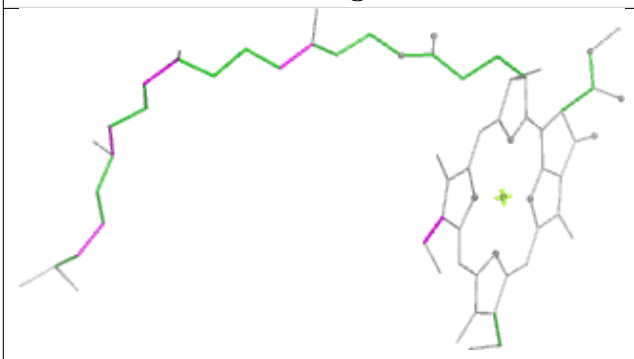
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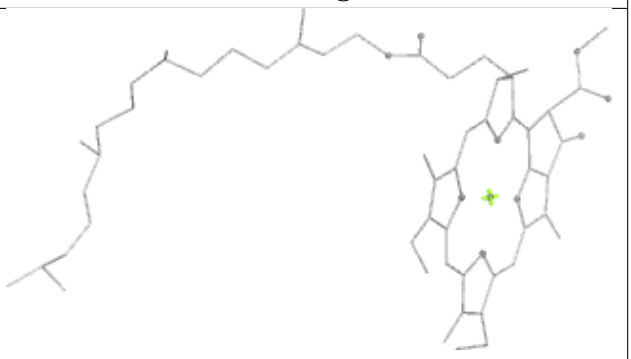
Bond lengths



Bond angles

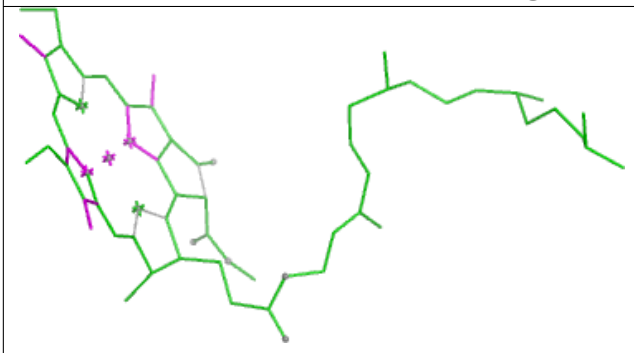


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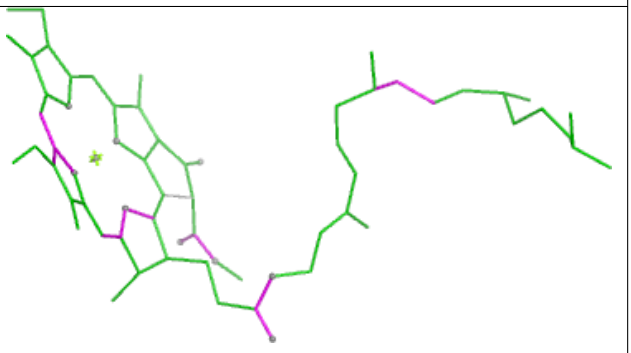


Rings

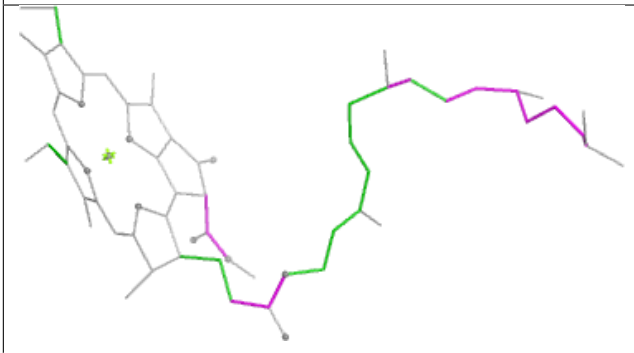
Ligand CLA B 802



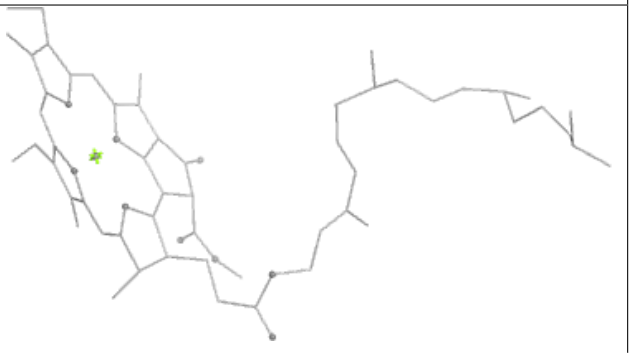
Bond lengths



Bond angles

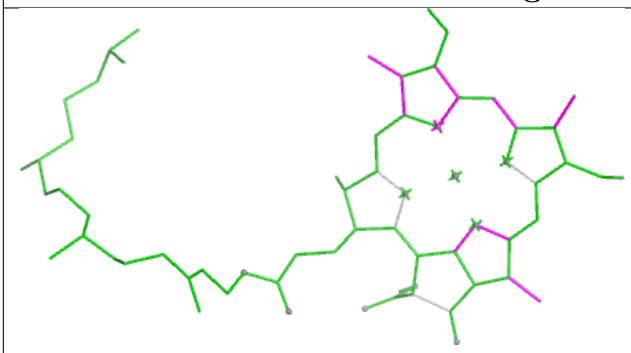


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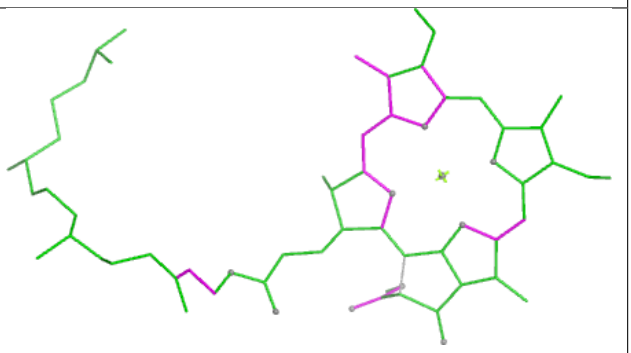


Rings

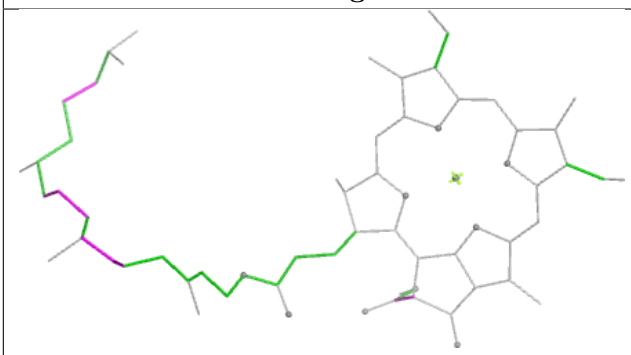
Ligand CLA A 828



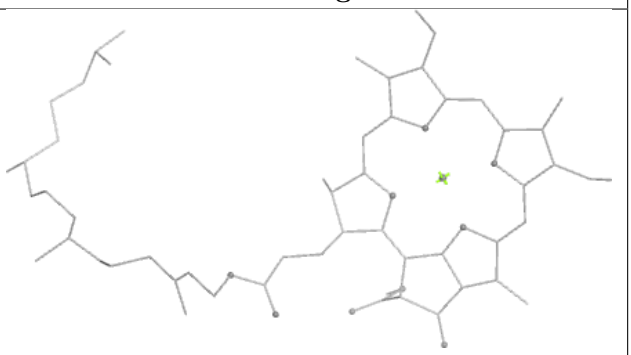
Bond lengths



Bond angles

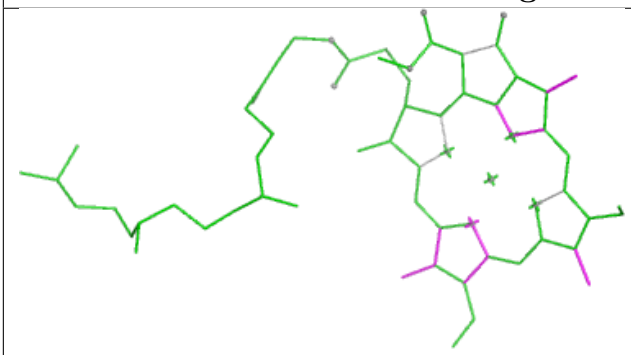


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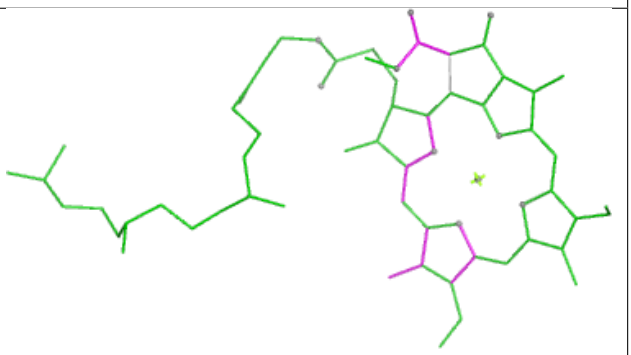


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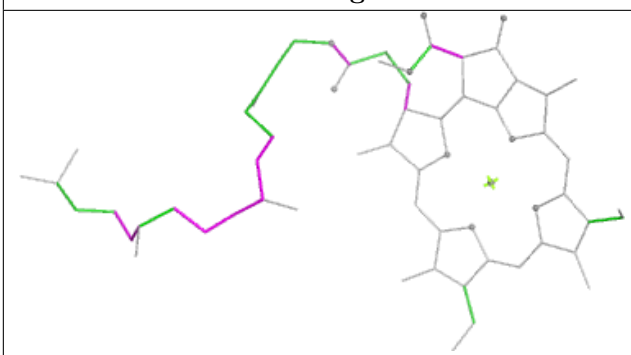
Ligand CLA 1 1605



Bond lengths



Bond angles



Torsions

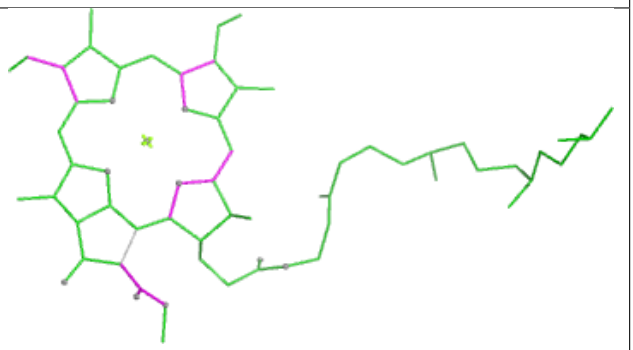


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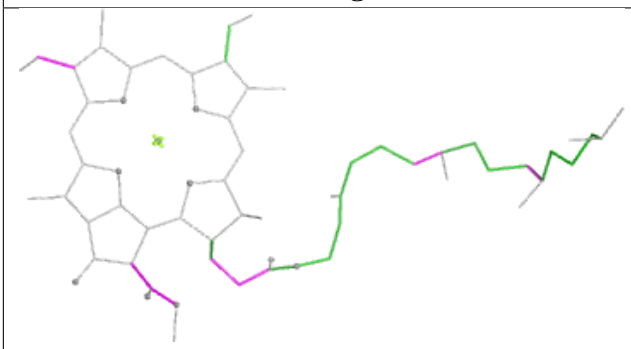
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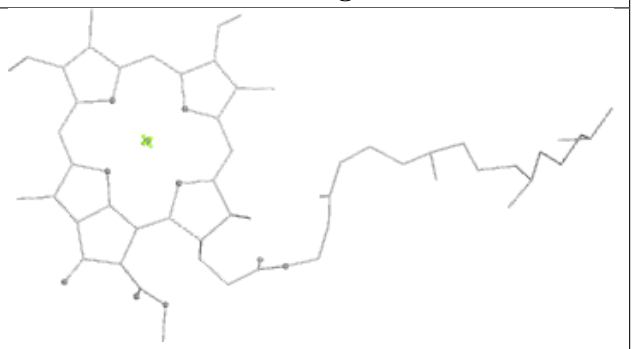
Bond lengths



Bond angles

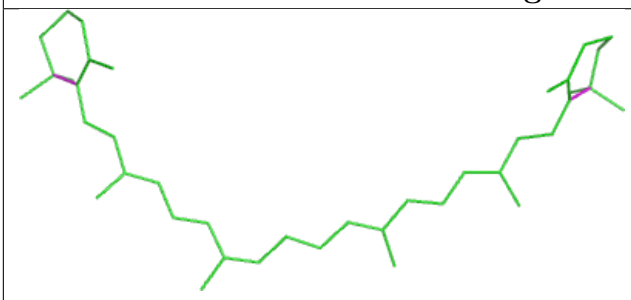


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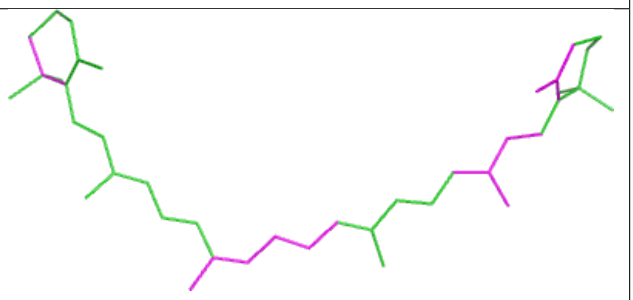


Rings

Ligand BCR F 205



Bond lengths



Bond angles

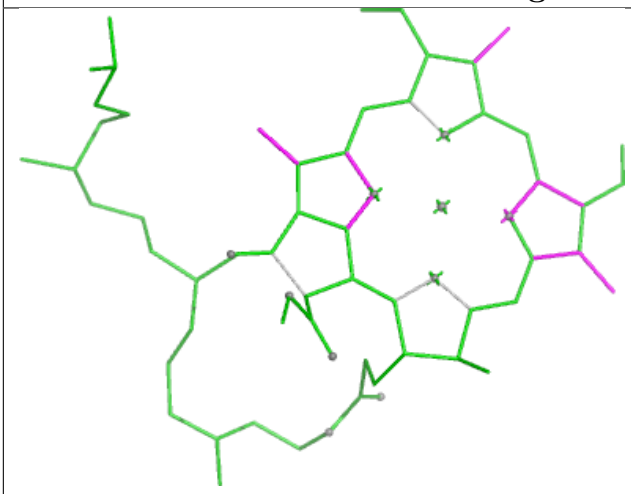


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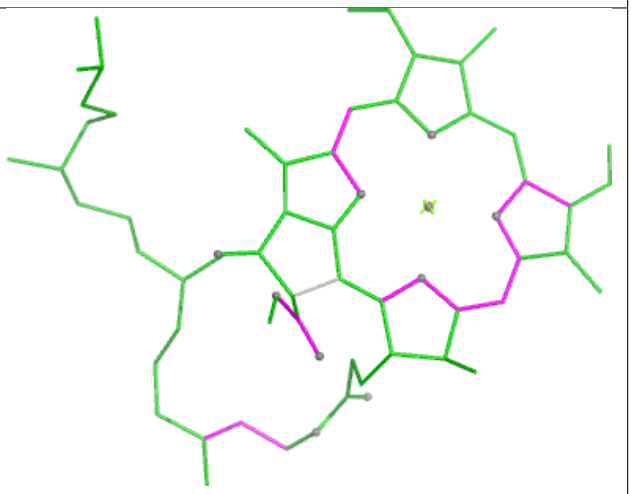


Rings

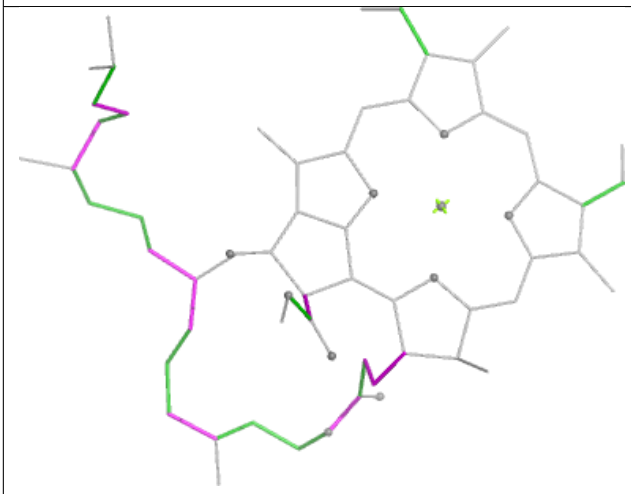
Ligand CLA 2 833



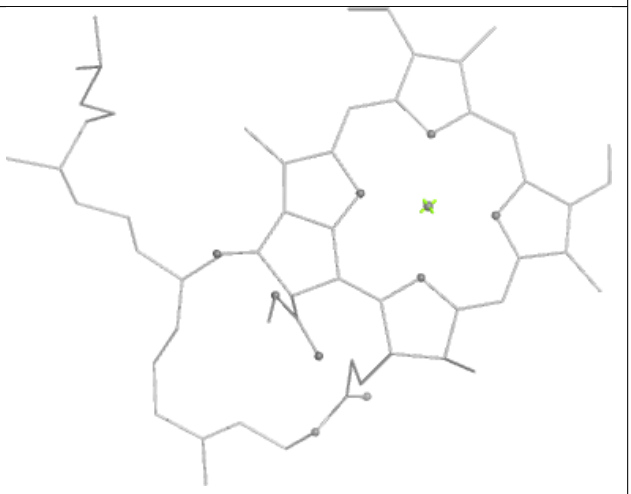
Bond lengths



Bond angles

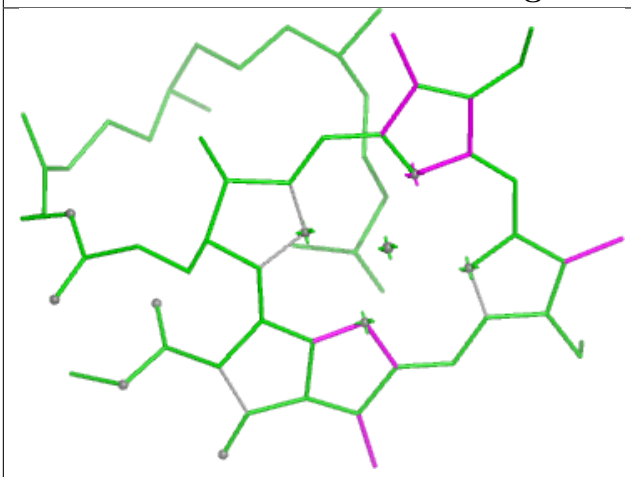


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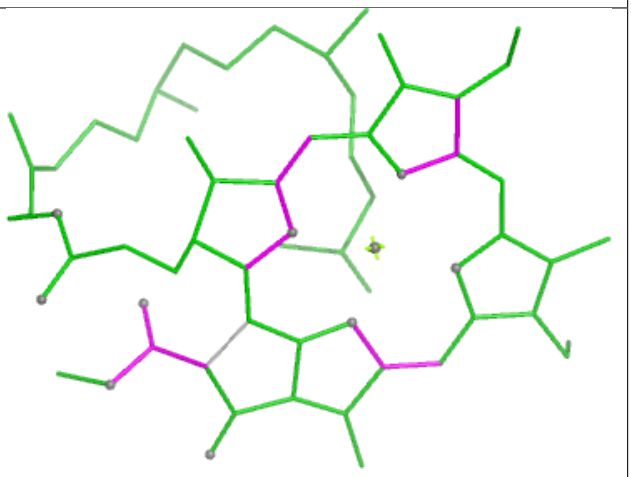


Rings

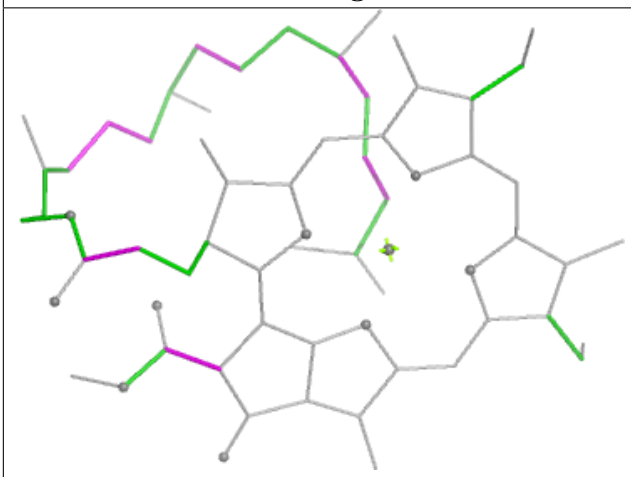
Ligand CLA B 806



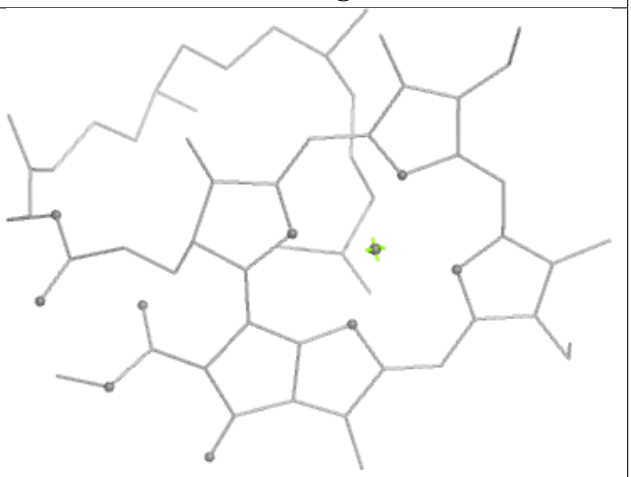
Bond lengths



Bond angles

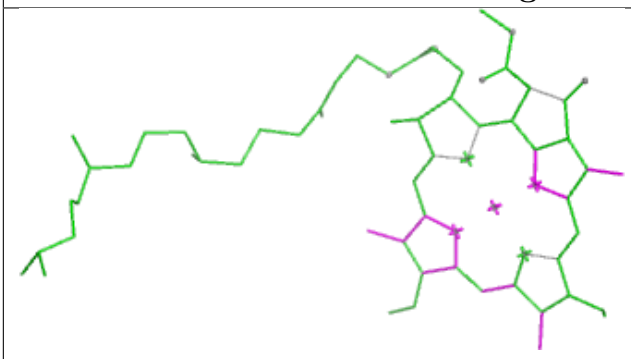


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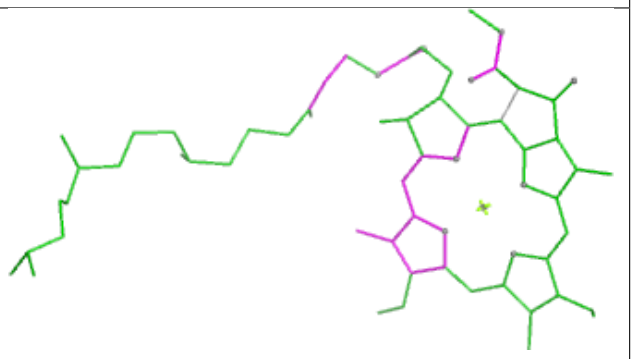


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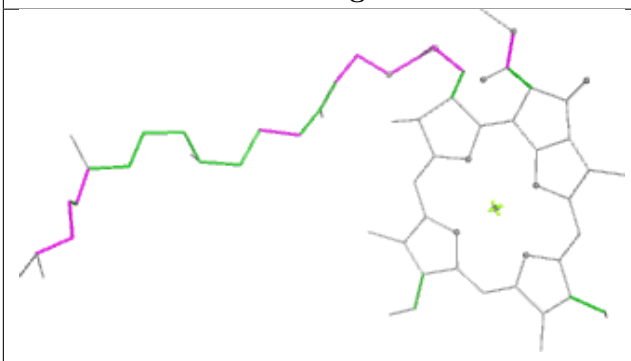
Ligand CLA 1 1603



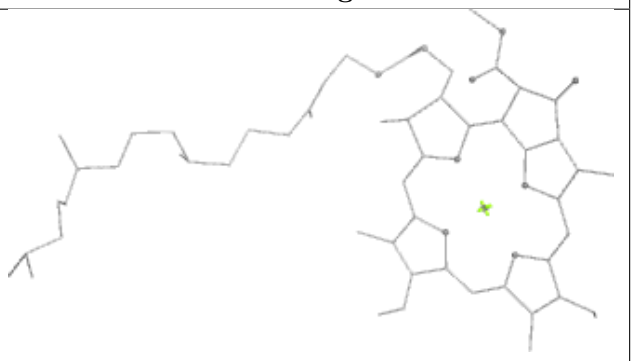
Bond lengths



Bond angles

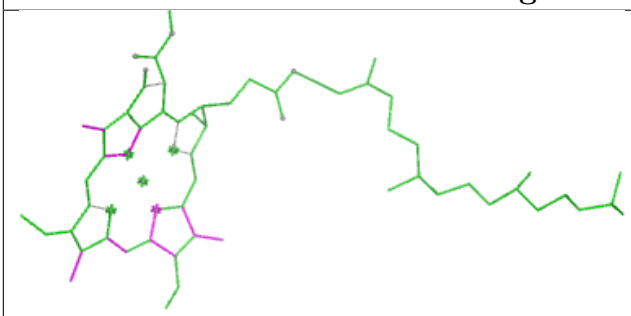


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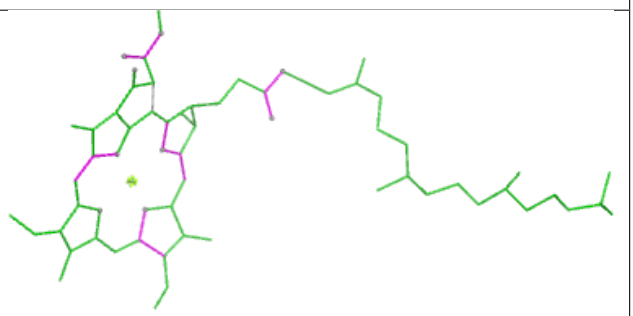


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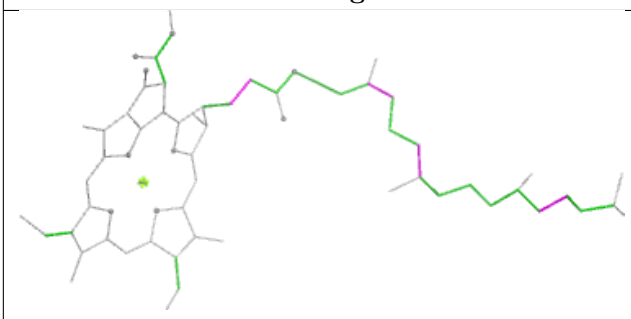
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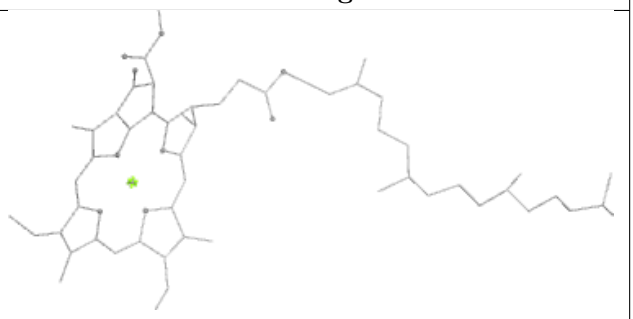
Bond lengths



Bond angles

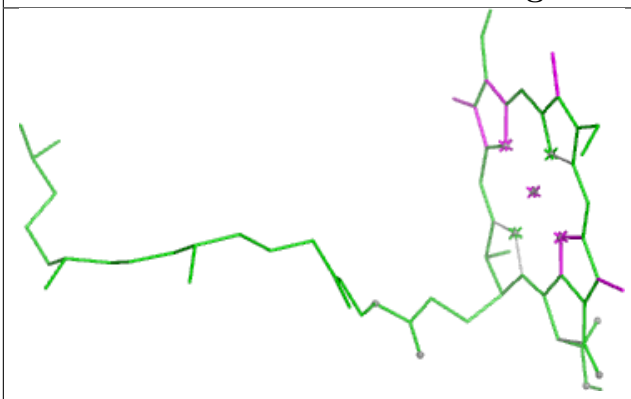


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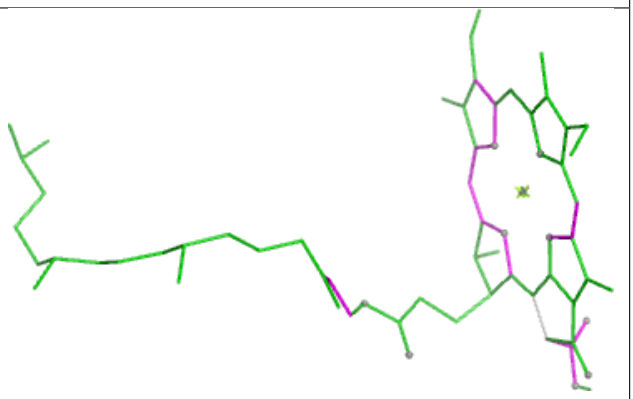


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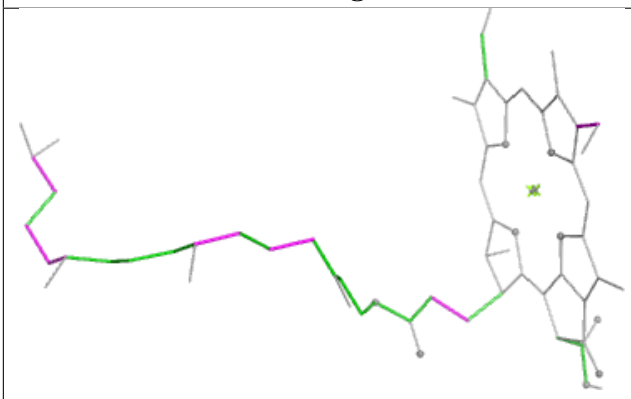
Ligand CLA L 204



Bond lengths



Bond angles

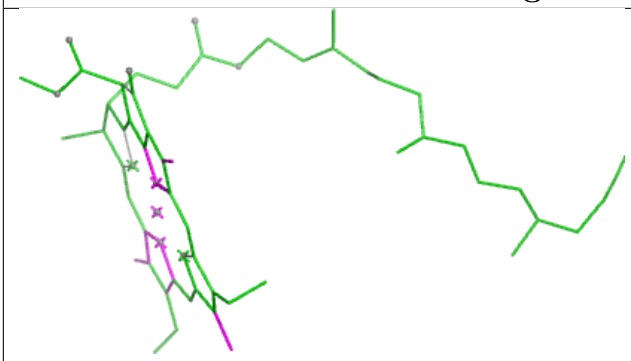


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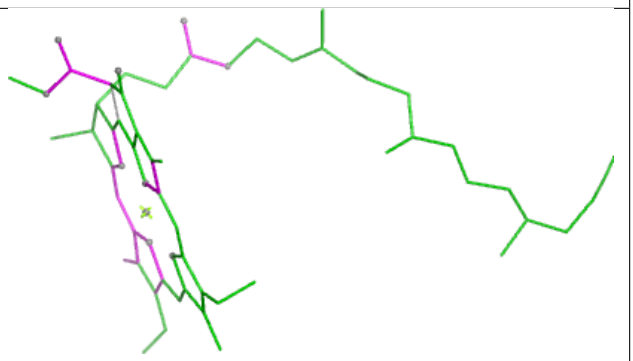


Rings

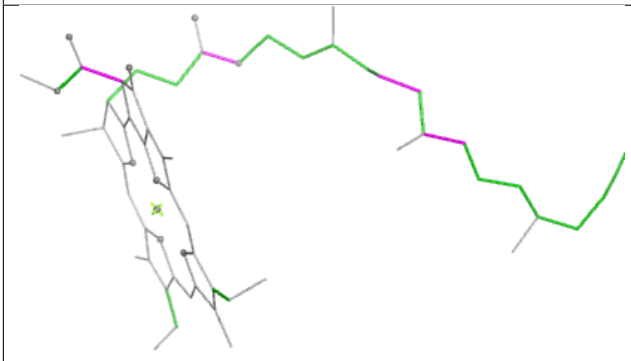
Ligand CLA A 831



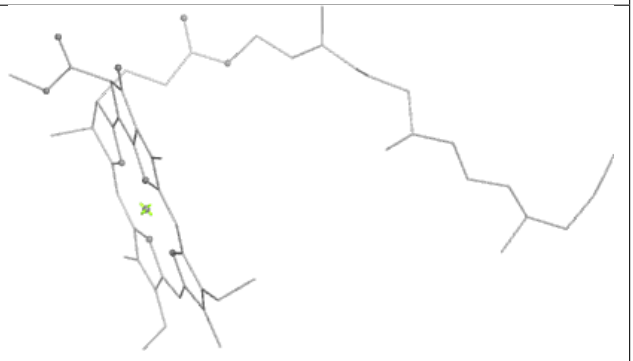
Bond lengths



Bond angles

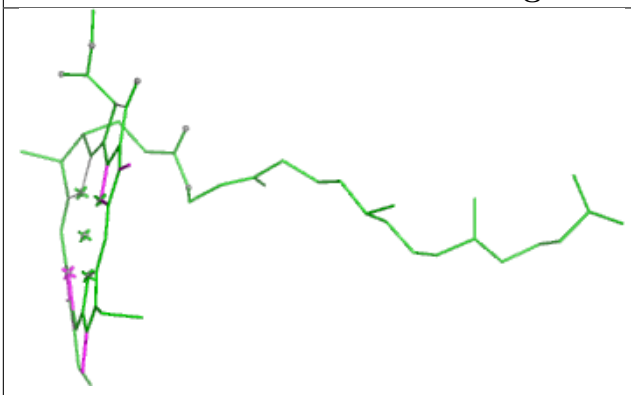


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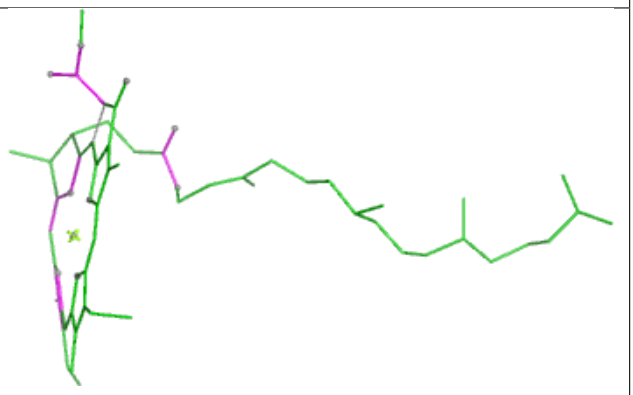


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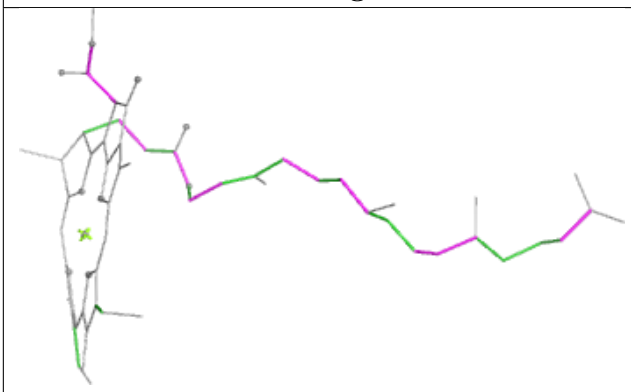
Ligand CLA A 829



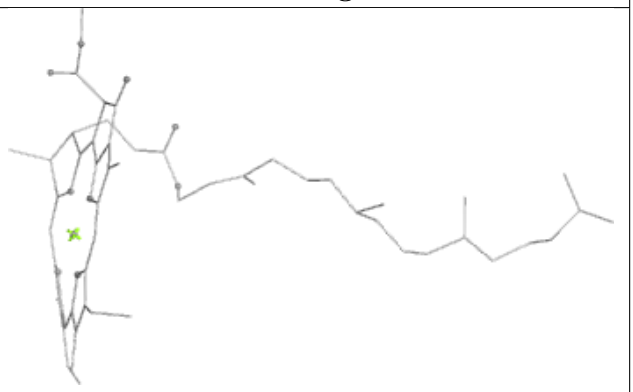
Bond lengths



Bond angles

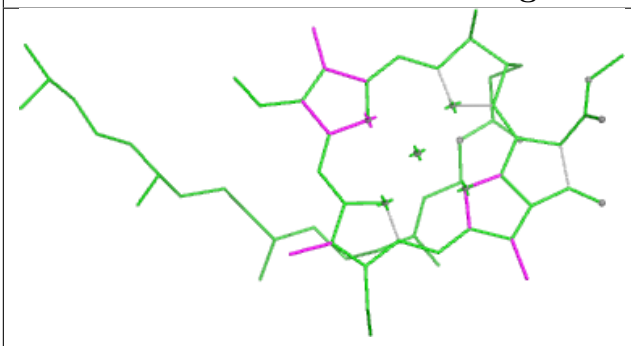


Torsions

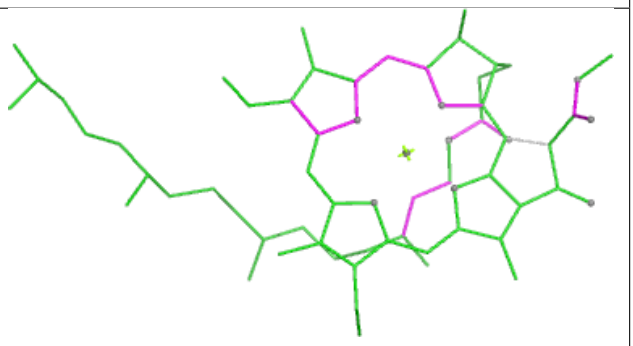


Rings

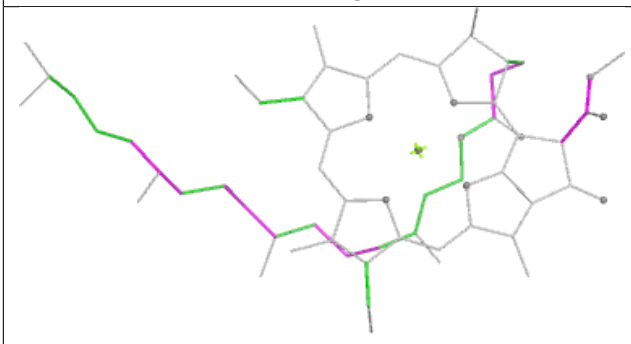
Ligand CLA 1 1642



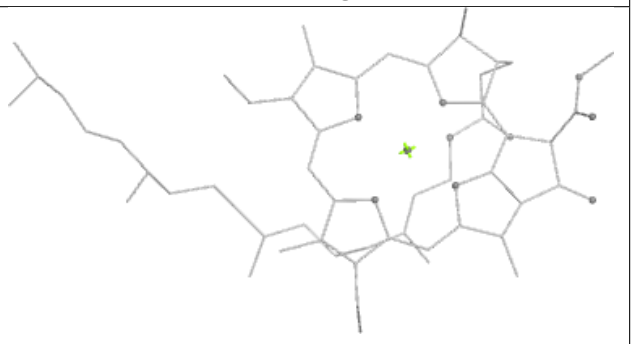
Bond lengths



Bond angles

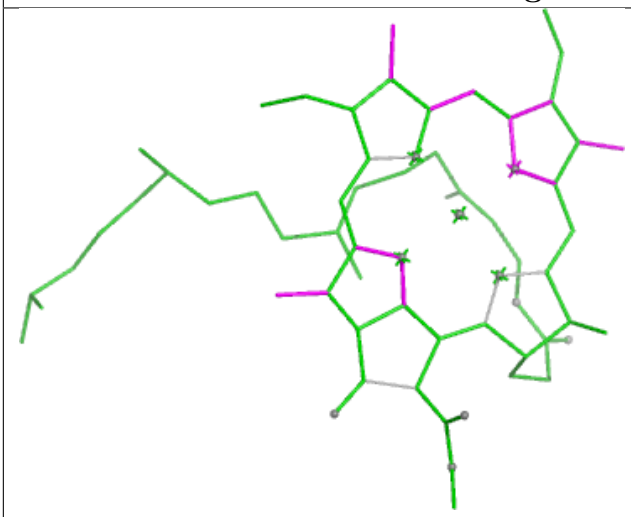


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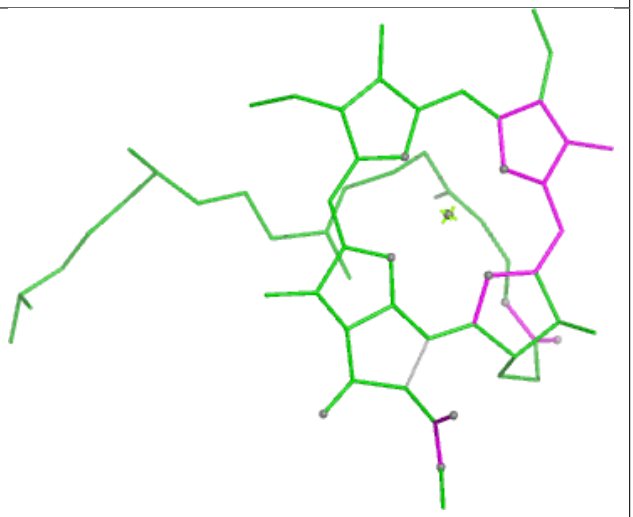


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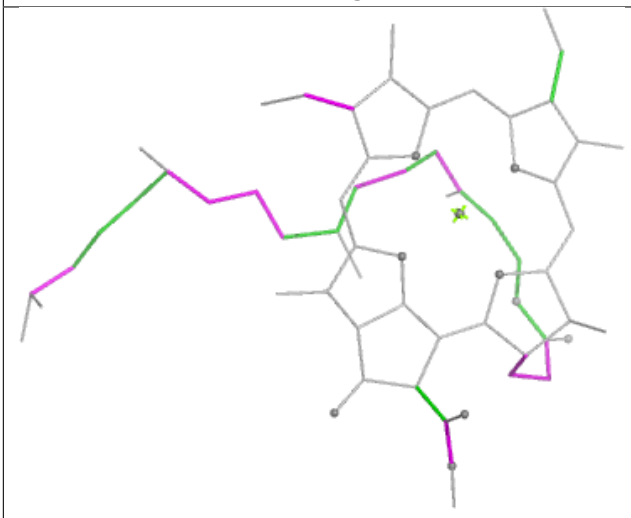
Ligand CLA B 827



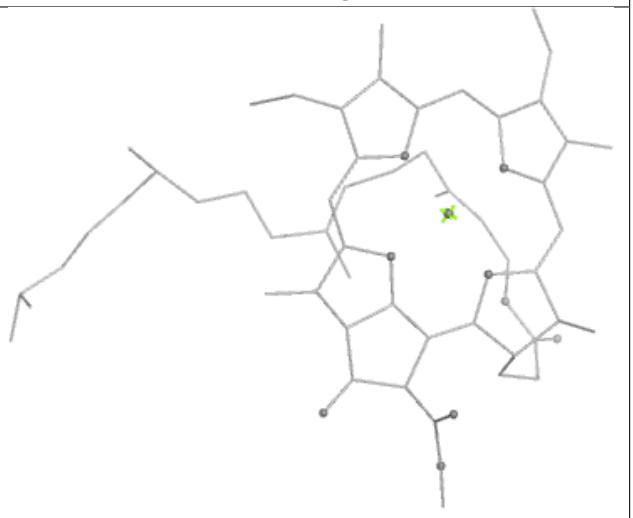
Bond lengths



Bond angles

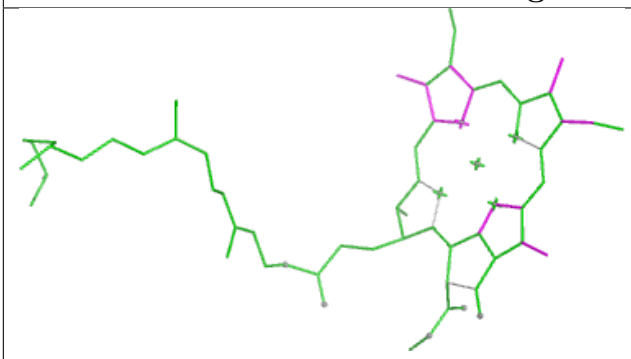


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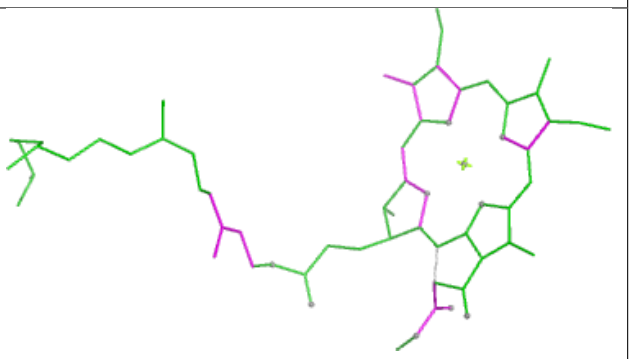


Rings

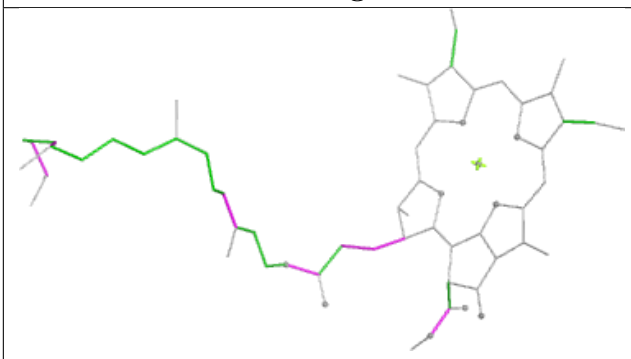
Ligand CLA b 810



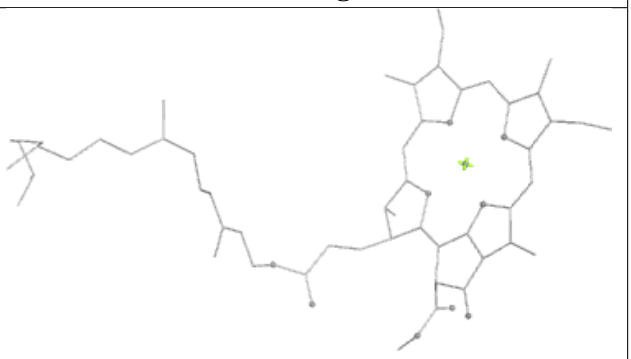
Bond lengths



Bond angles

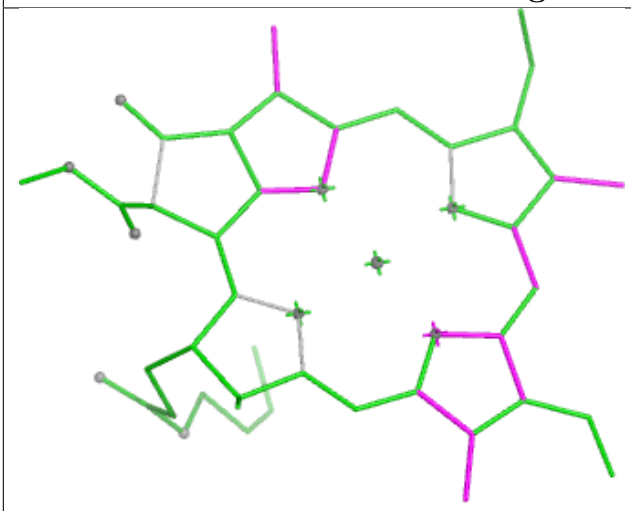


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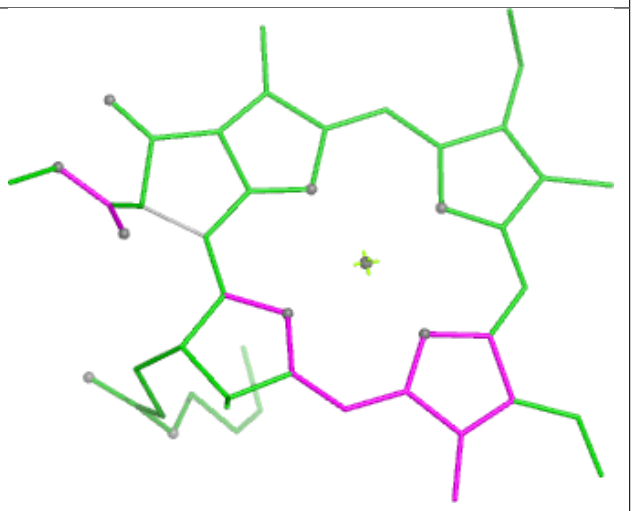


Rings

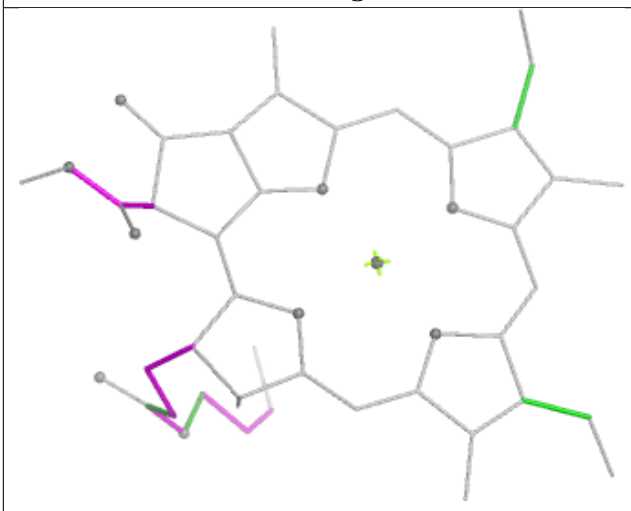
Ligand CLA 2 832



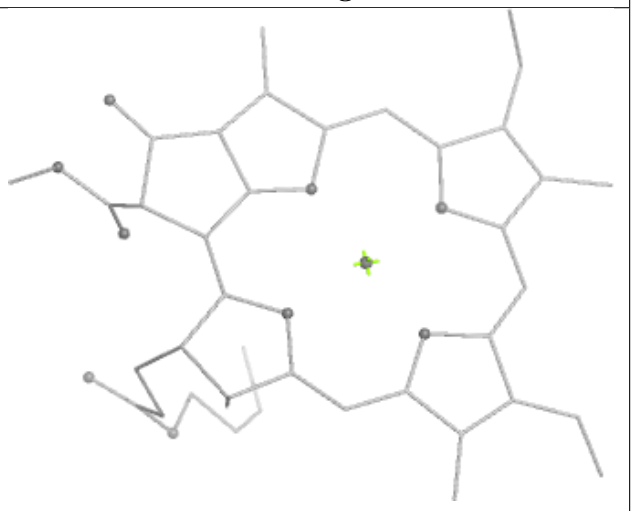
Bond lengths



Bond angles

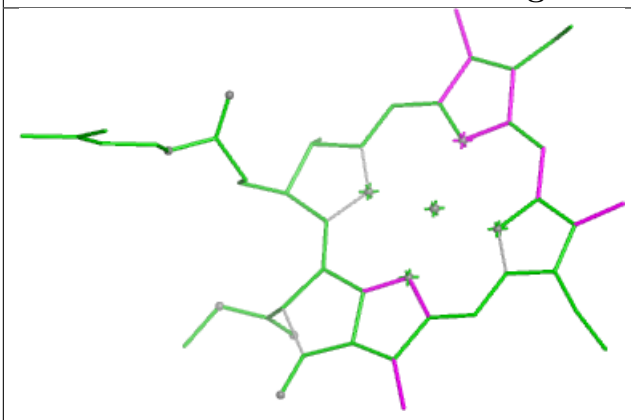


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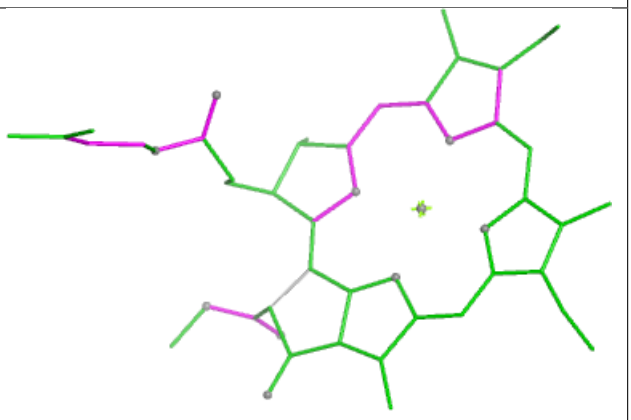


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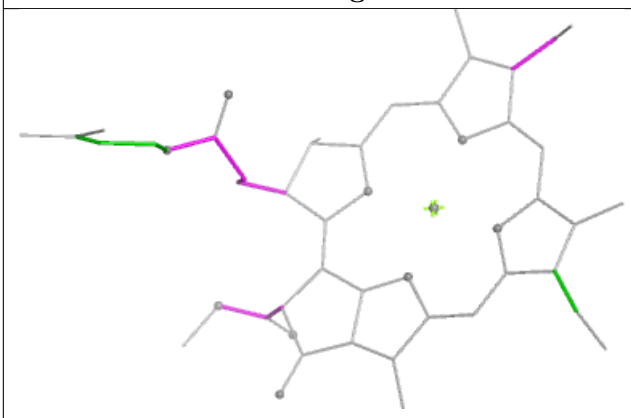
Ligand CLA b 836



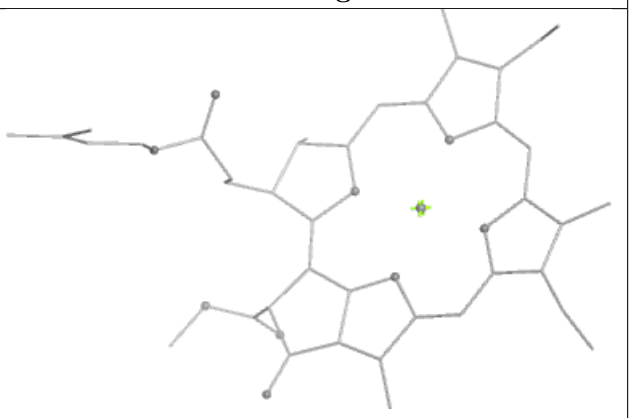
Bond lengths



Bond angles

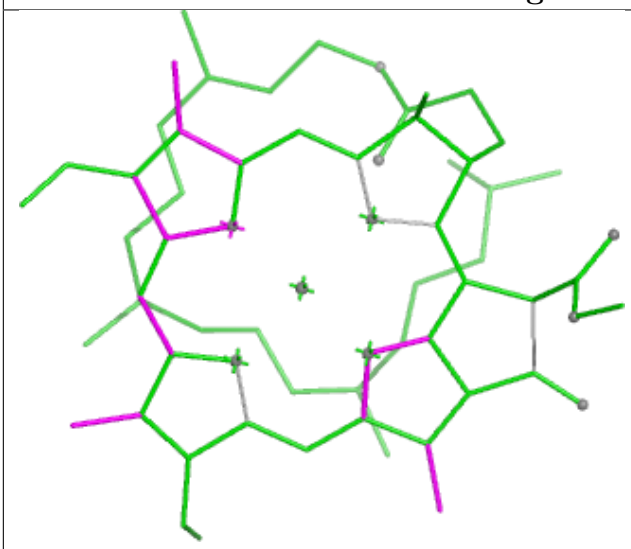


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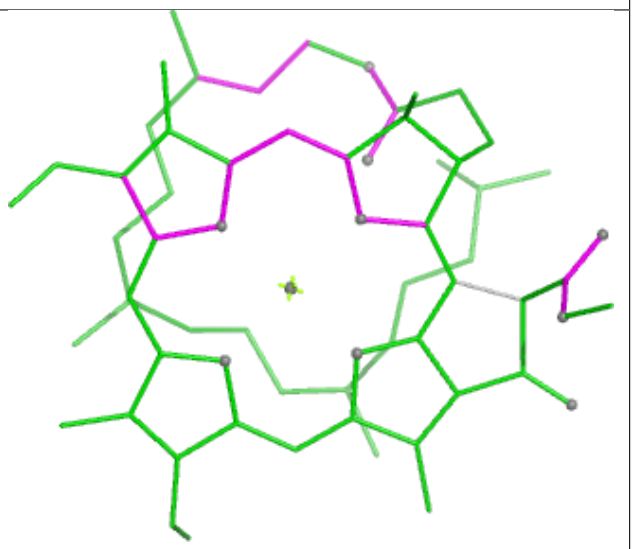


Rings

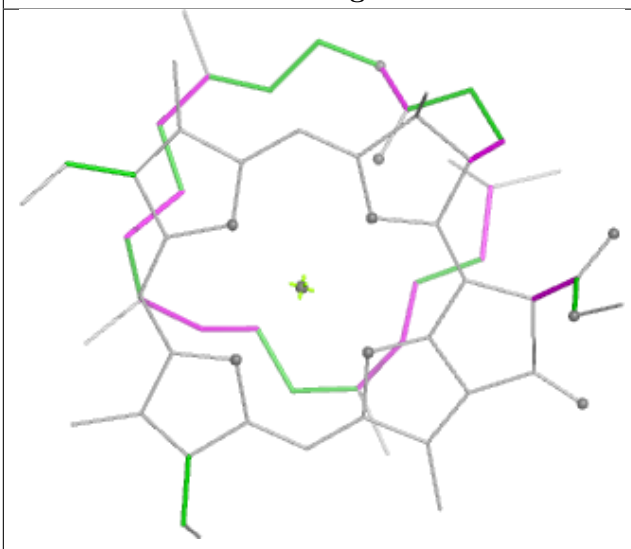
Ligand CLA L 203



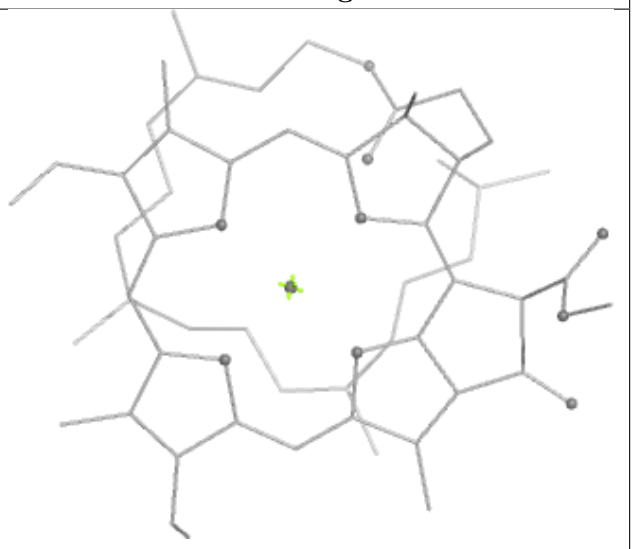
Bond lengths



Bond angles

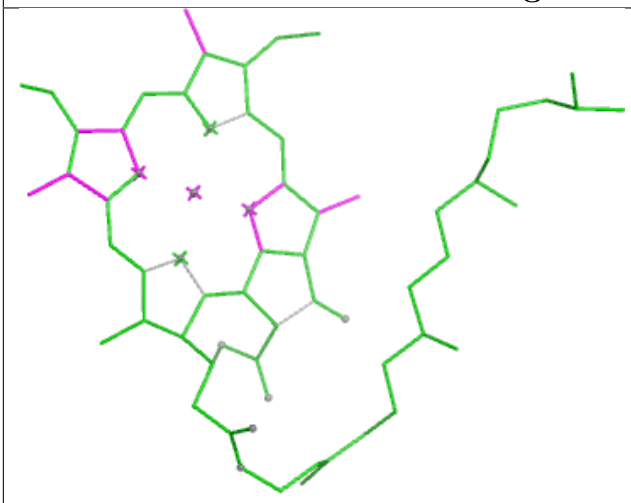


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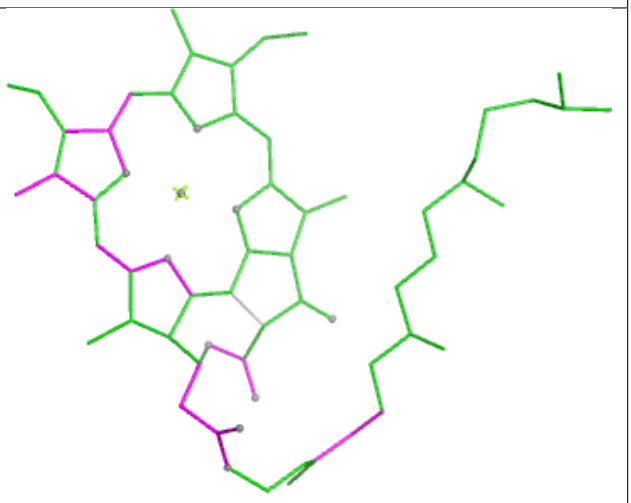


Rings

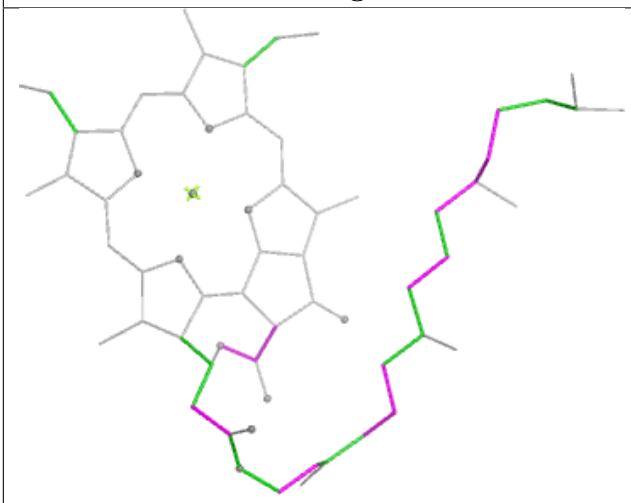
Ligand CLA A 826



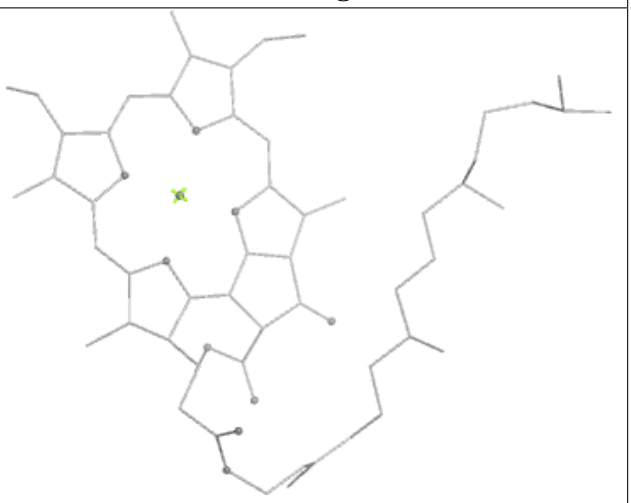
Bond lengths



Bond angles

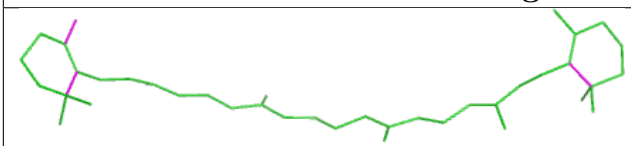


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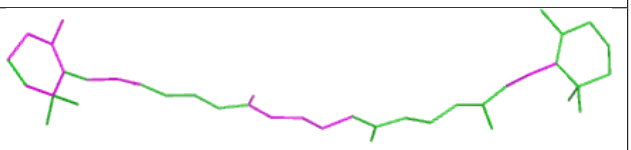


Rings

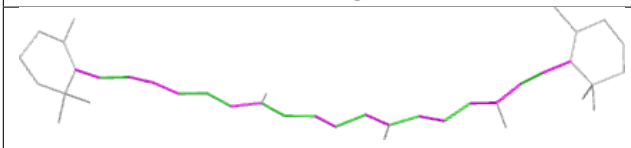
Ligand BCR A 856



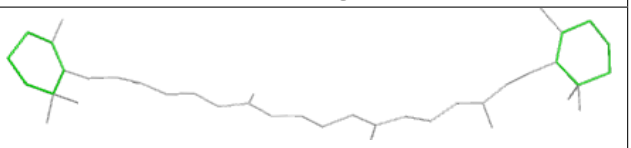
Bond lengths



Bond angles

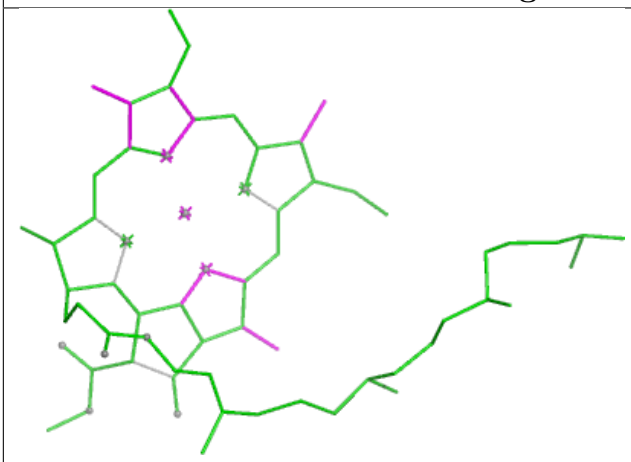


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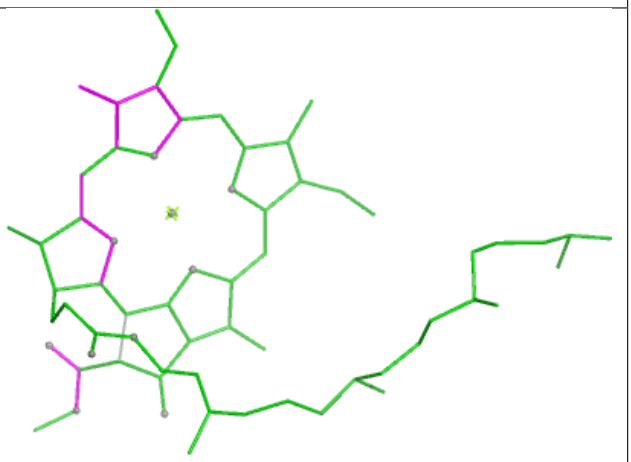


Rings

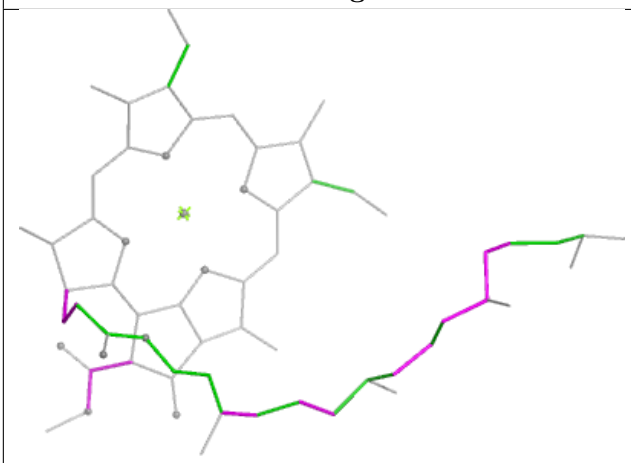
Ligand CLA 1 1631



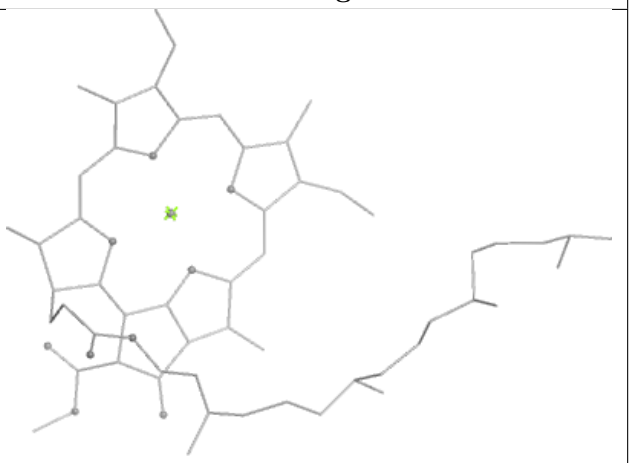
Bond lengths



Bond angles

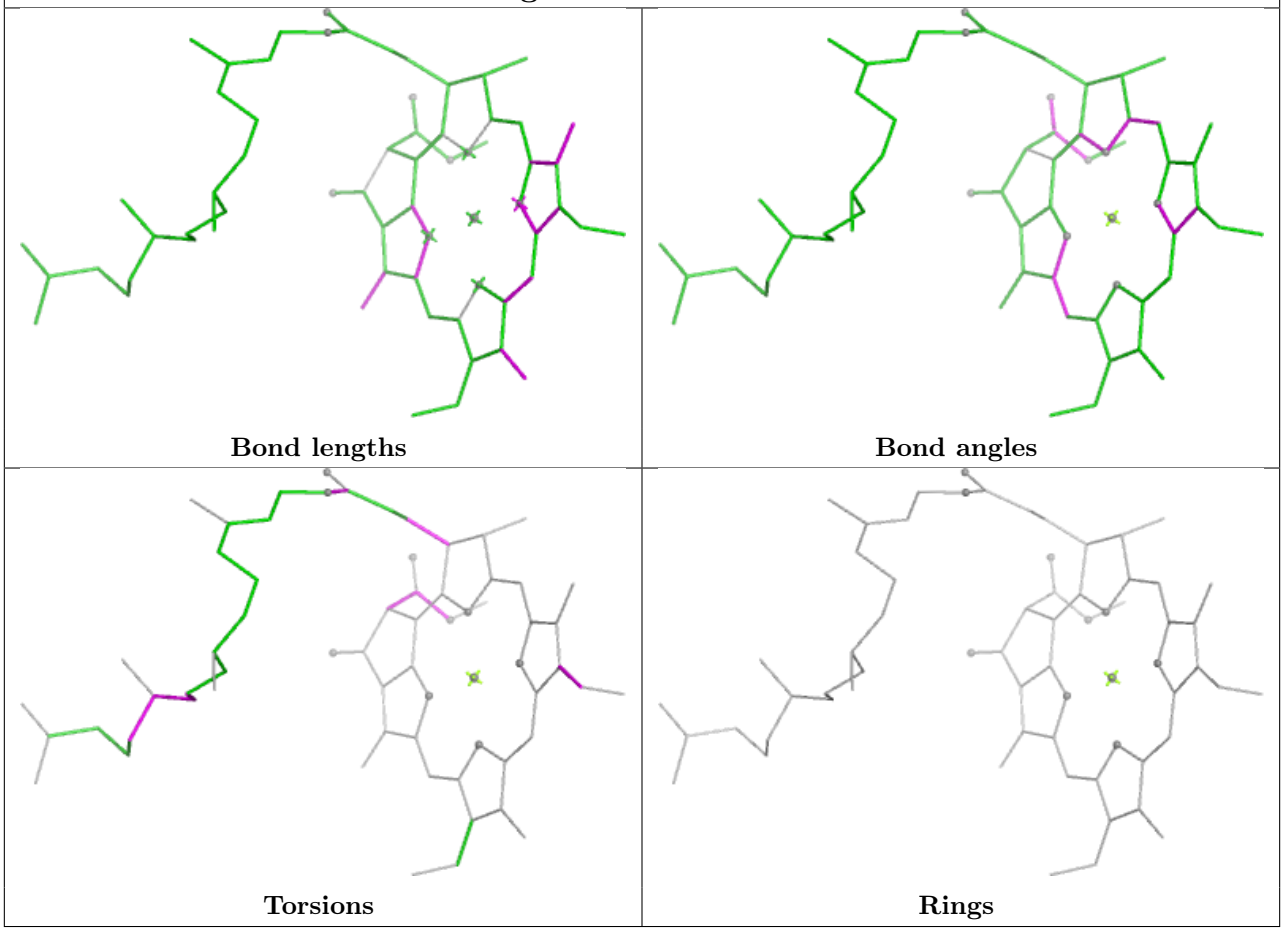


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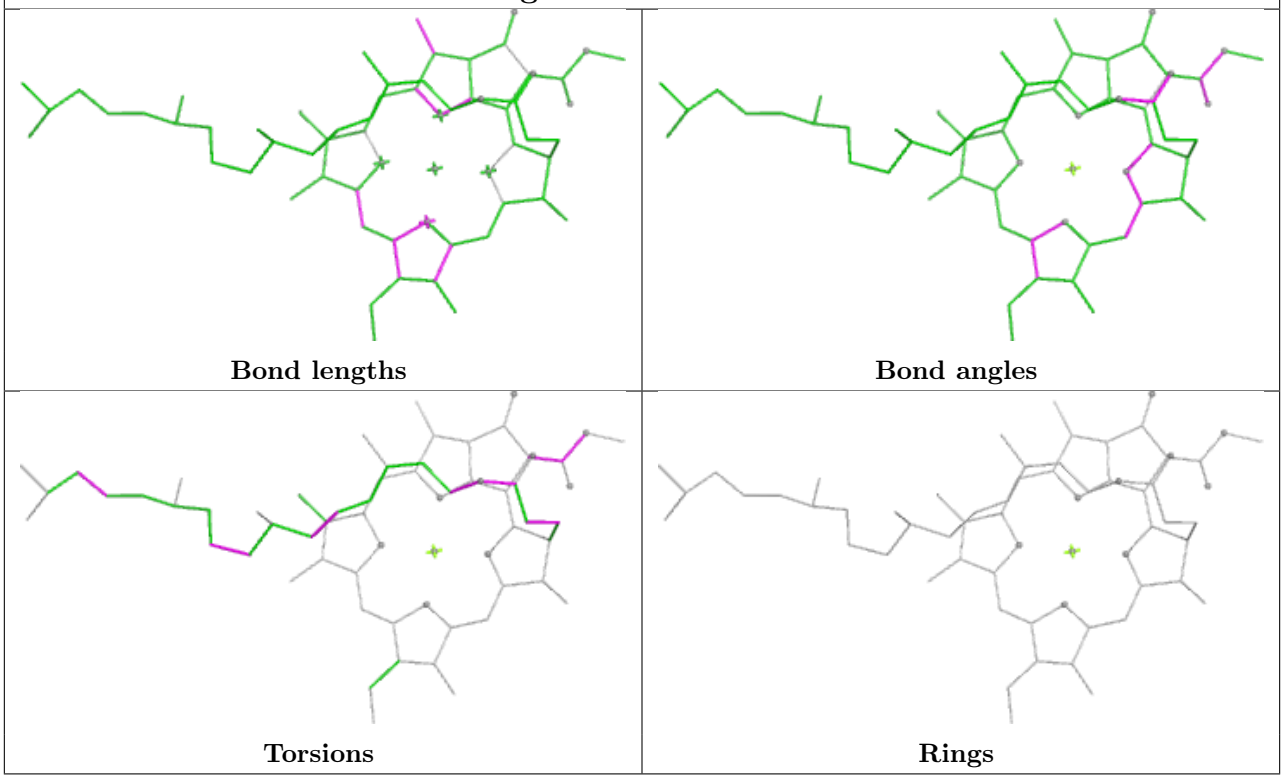


Rings

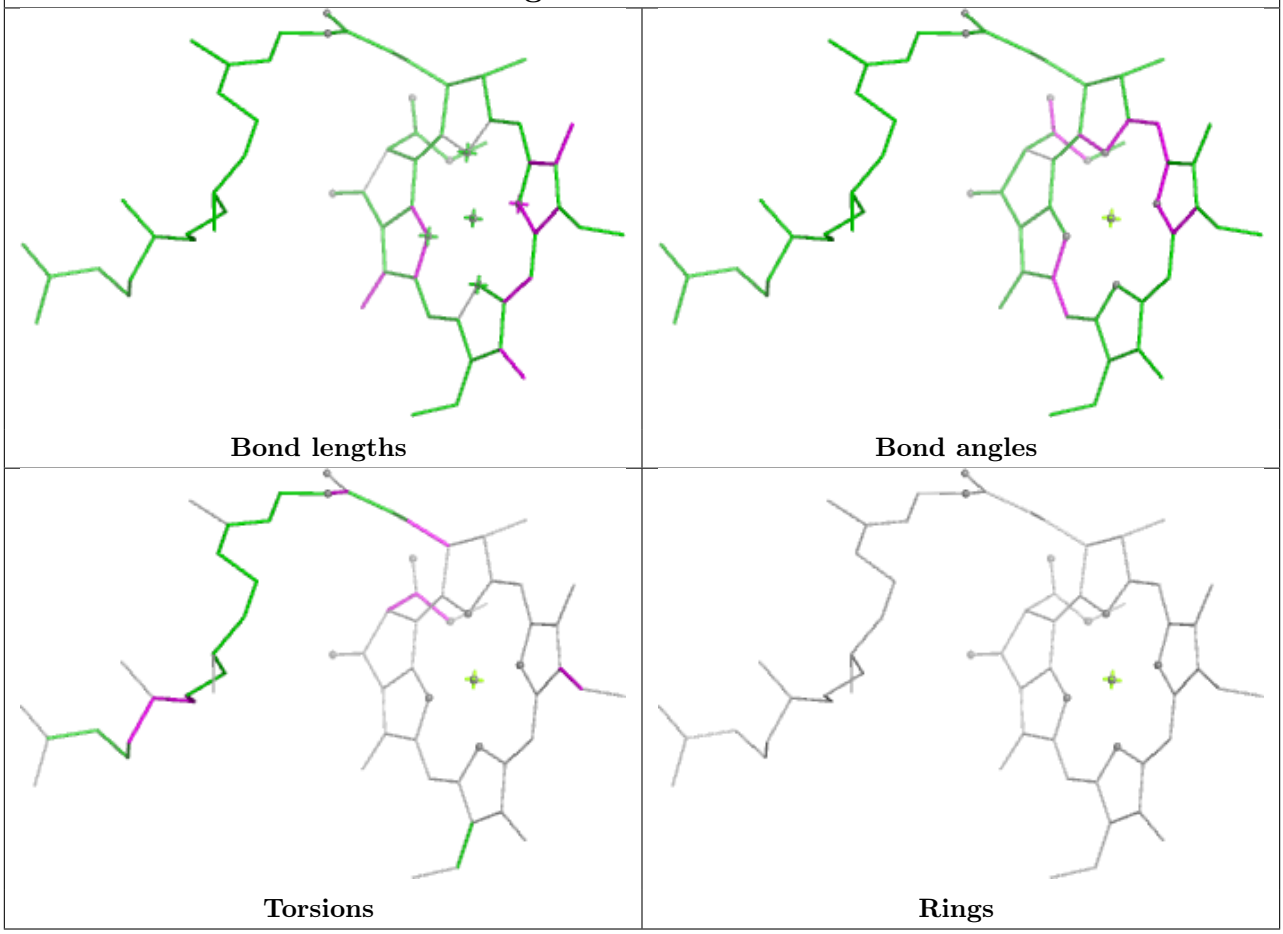
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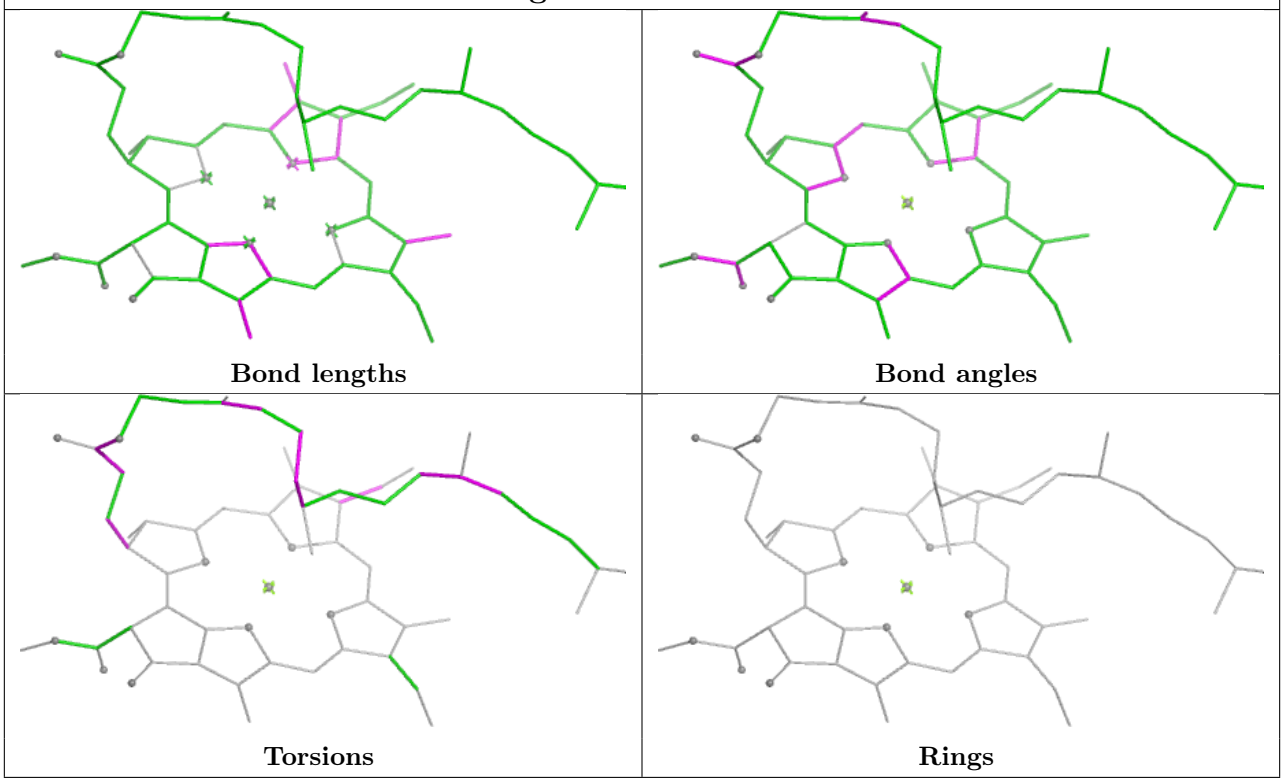
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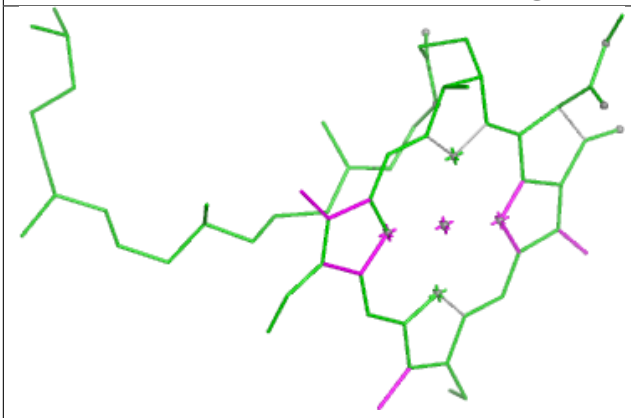
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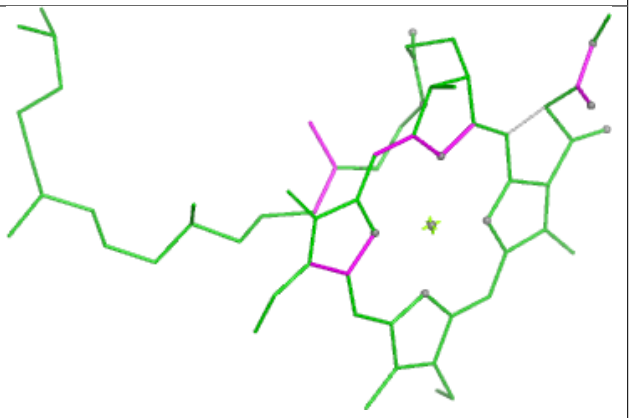
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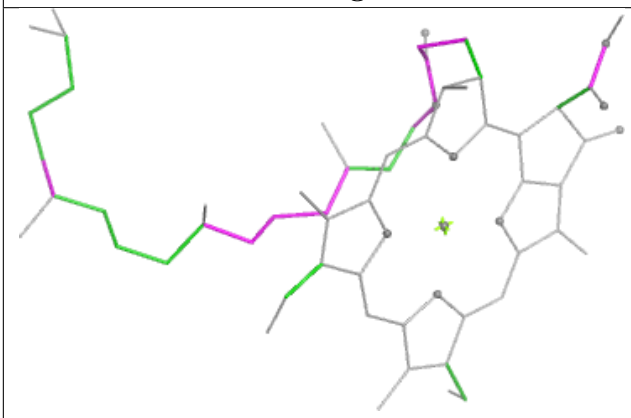
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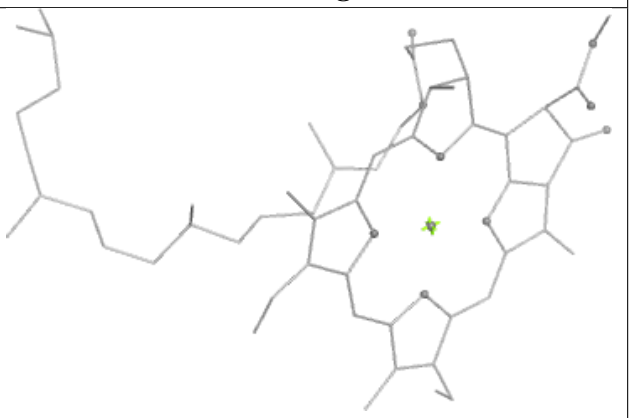
Bond lengths



Bond angles

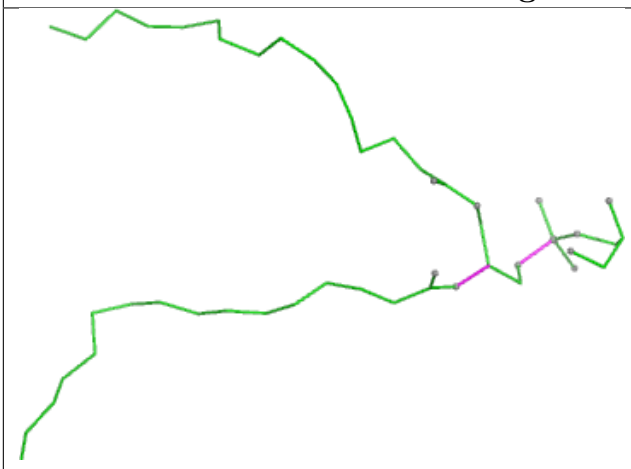


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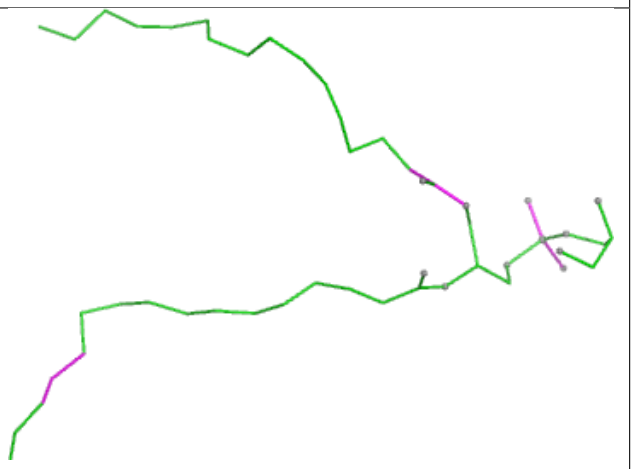


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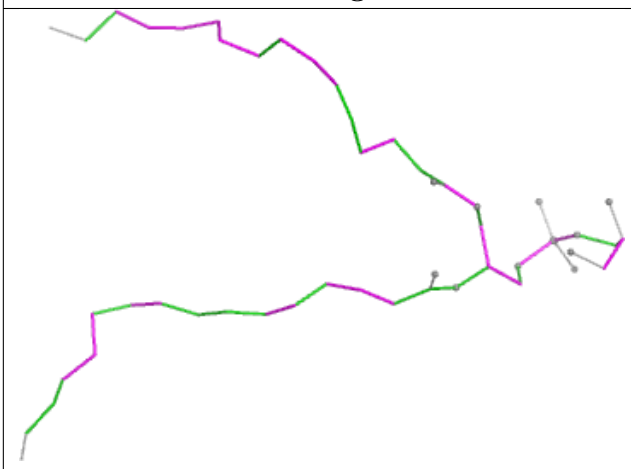
Ligand LHG M 101



Bond lengths



Bond angles

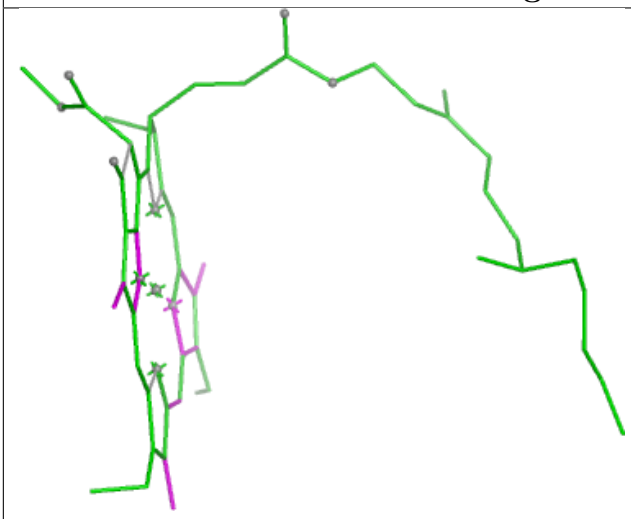


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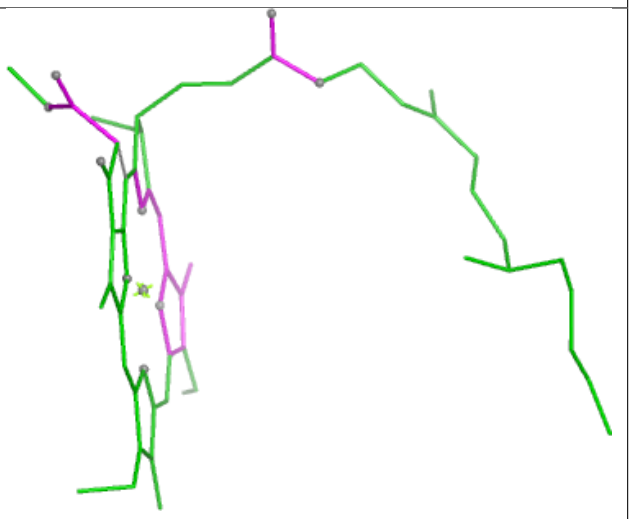


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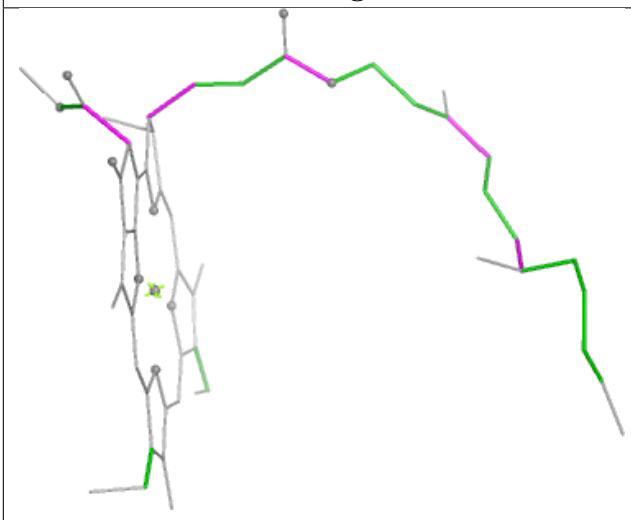
Ligand CLA A 805



Bond lengths



Bond angles

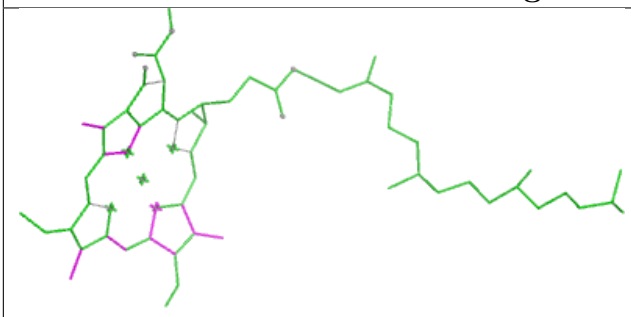


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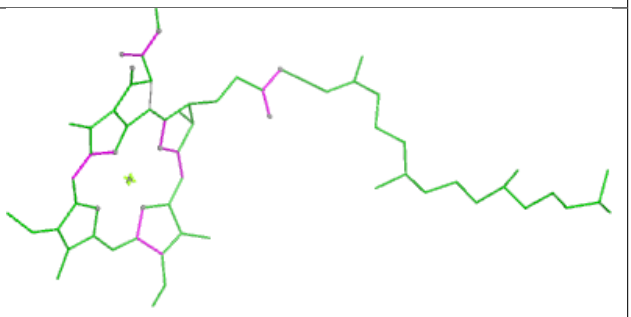


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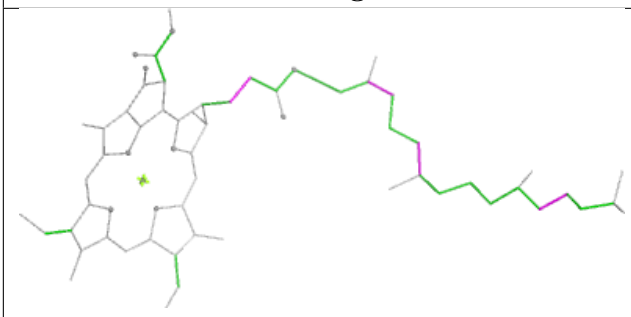
Ligand CLA A 803



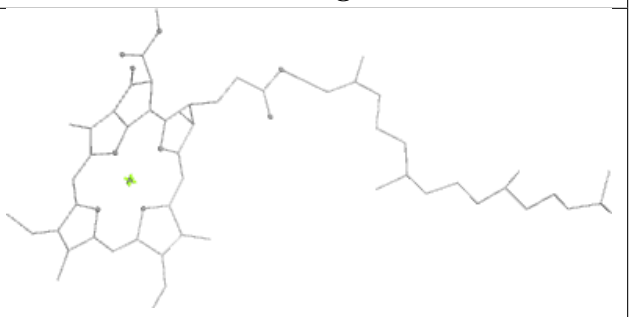
Bond lengths



Bond angles

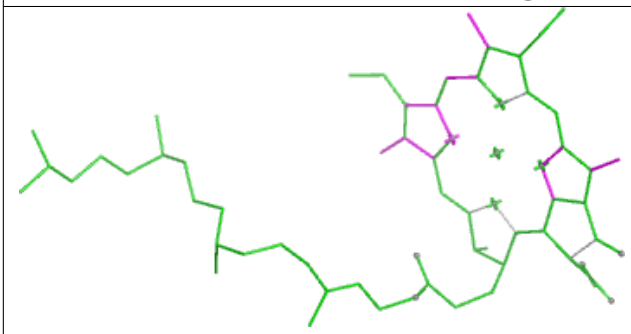


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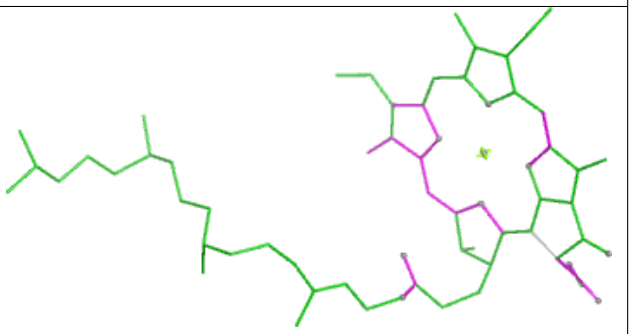


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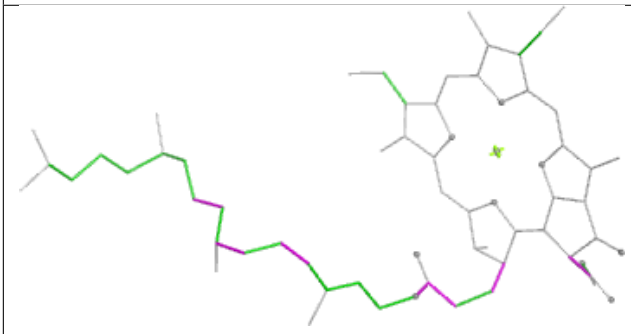
Ligand CLA 1 1610



Bond lengths



Bond angles

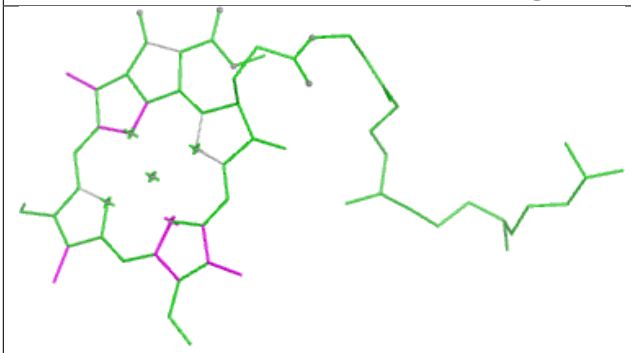


Torsions

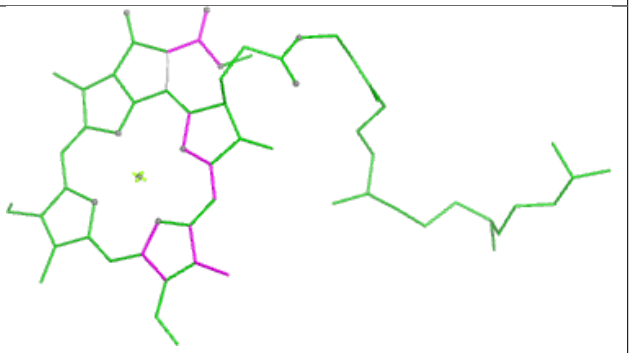


Rings

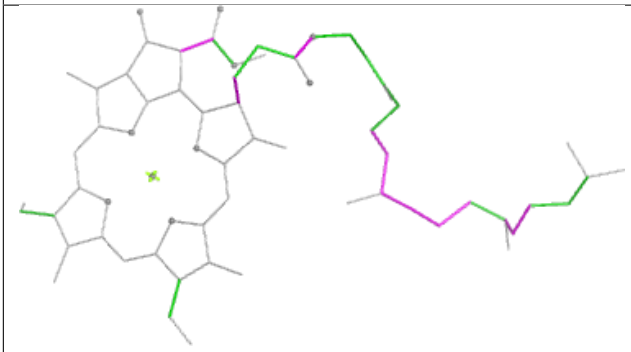
Ligand CLA a 804



Bond lengths



Bond angles

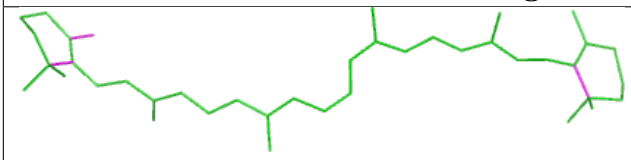


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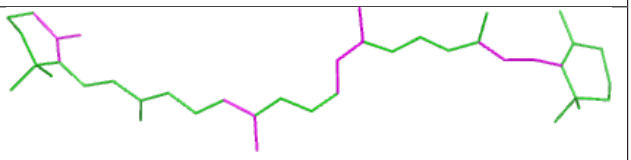


Rings

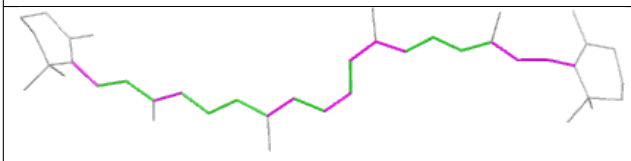
Ligand BCR B 846



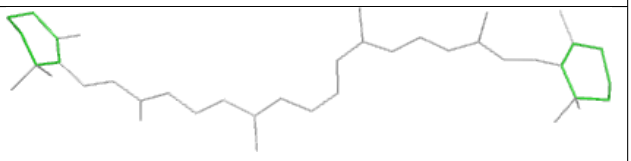
Bond lengths



Bond angles

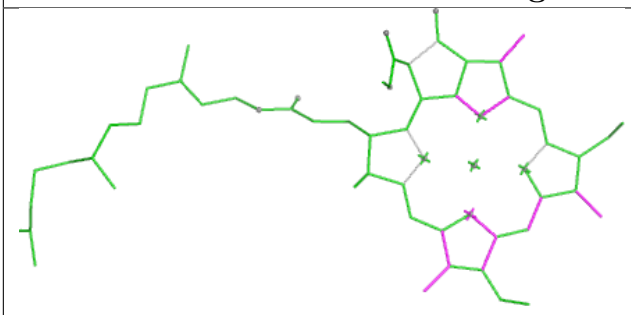


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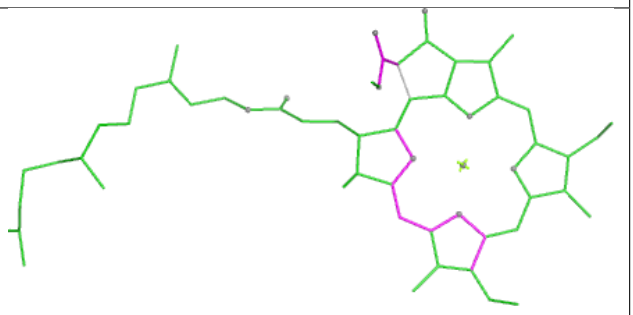


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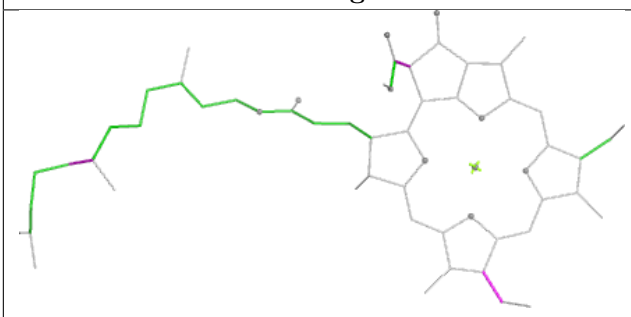
Ligand CLA 2 838



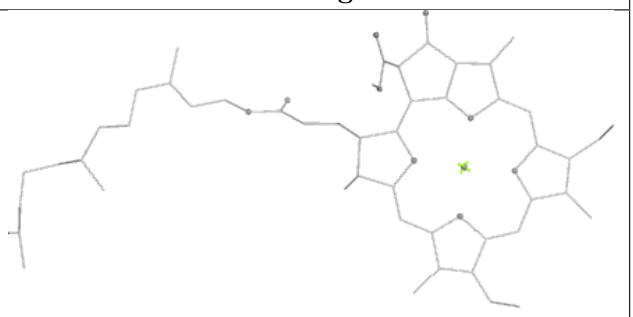
Bond lengths



Bond angles



Torsions

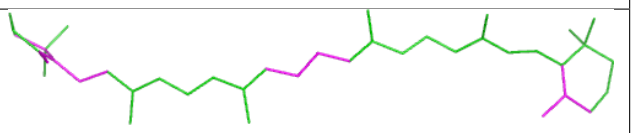


Rings

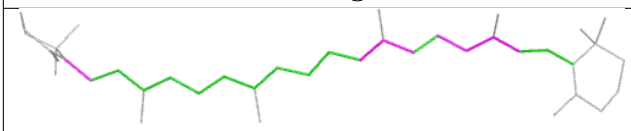
Ligand BCR a 850



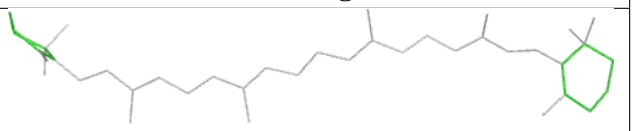
Bond lengths



Bond angles

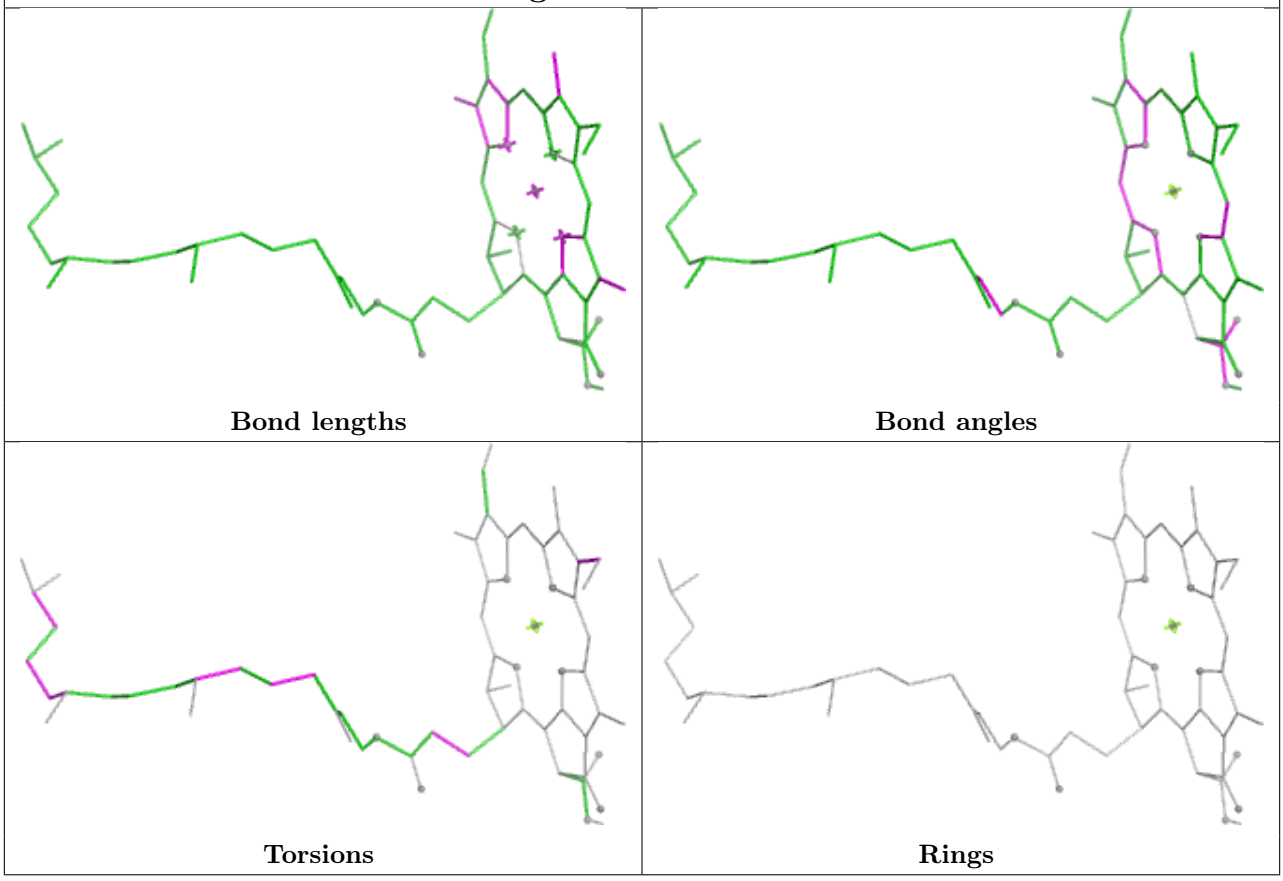


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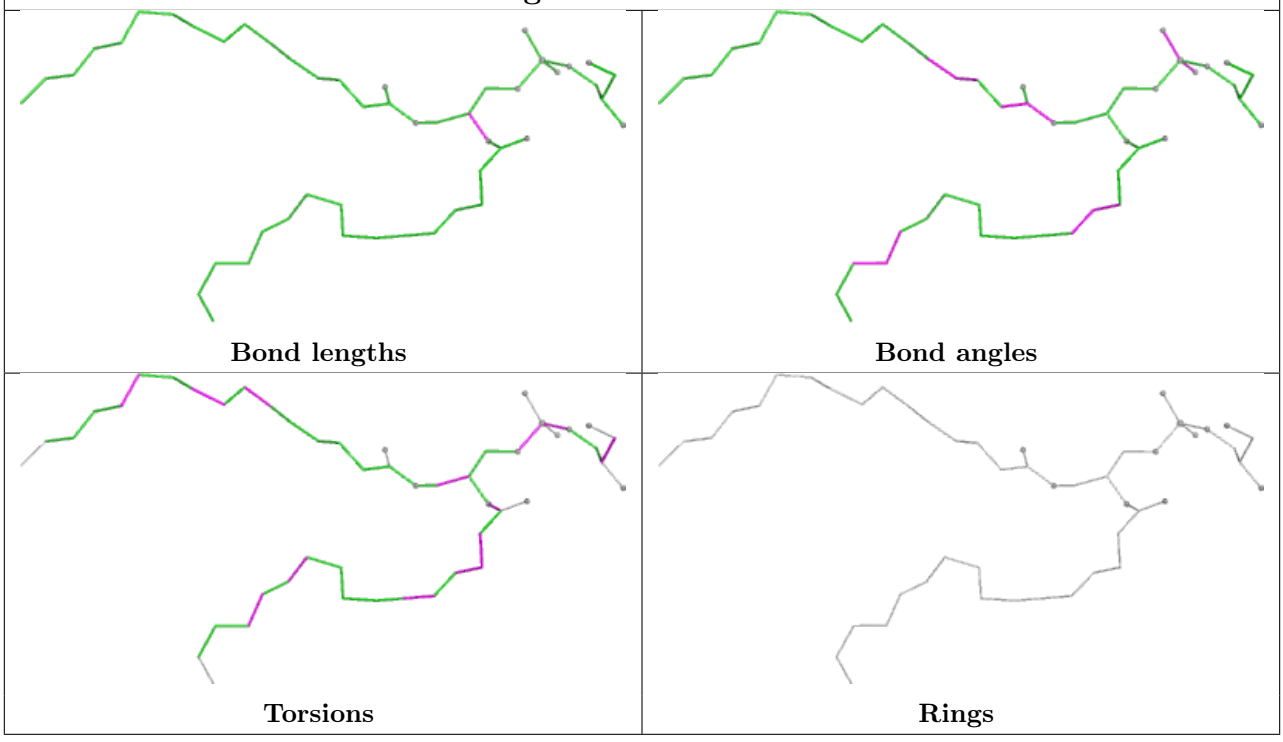


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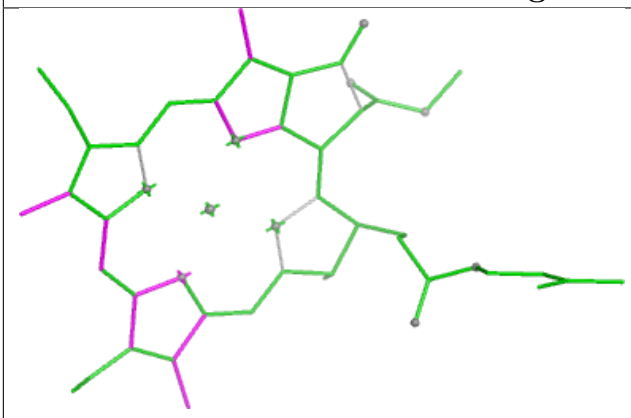
Ligand CLA 0 206



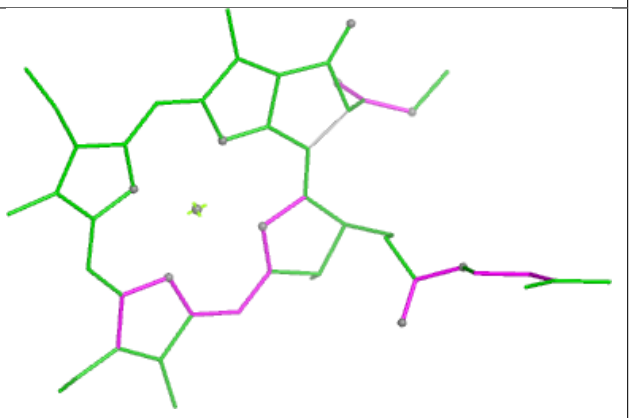
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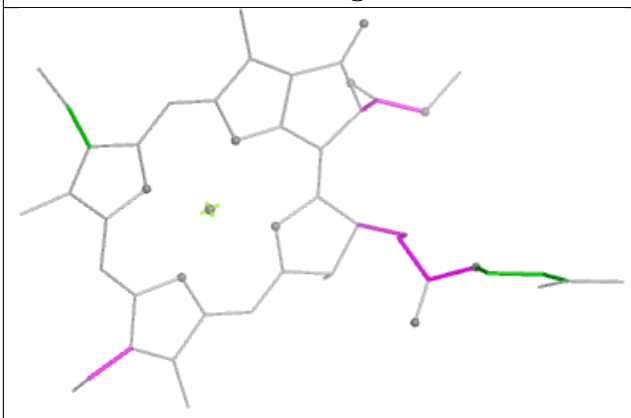
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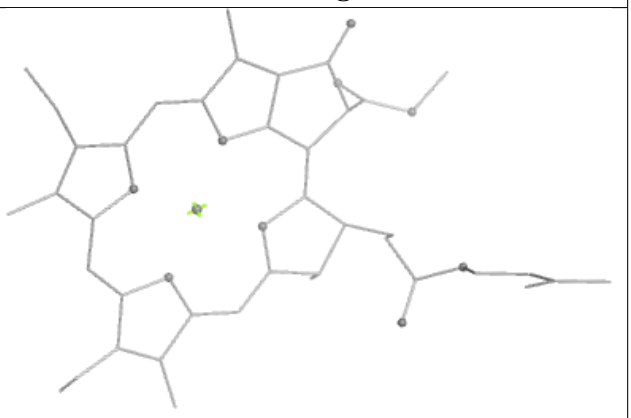
Bond lengths



Bond angles

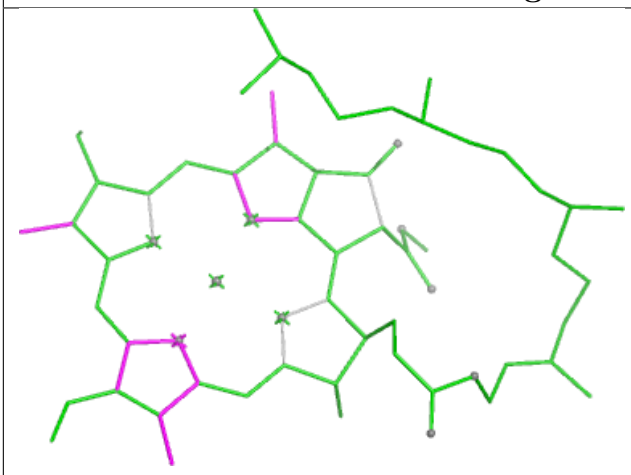


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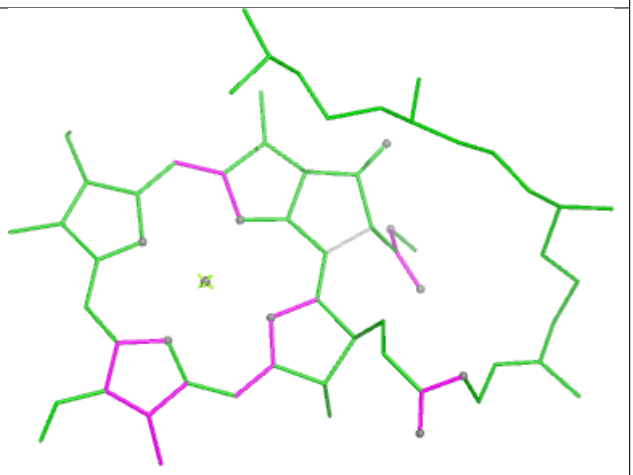


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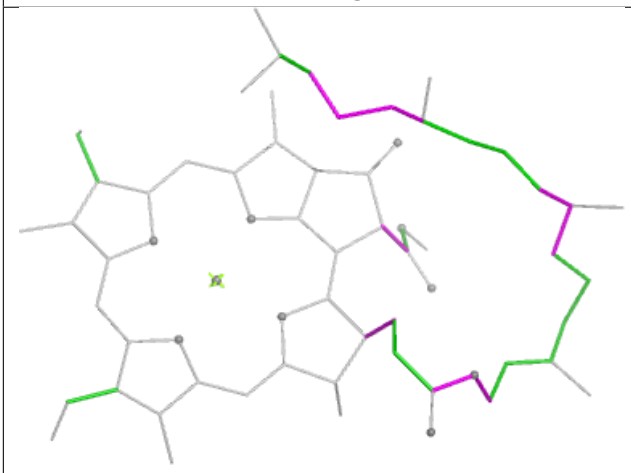
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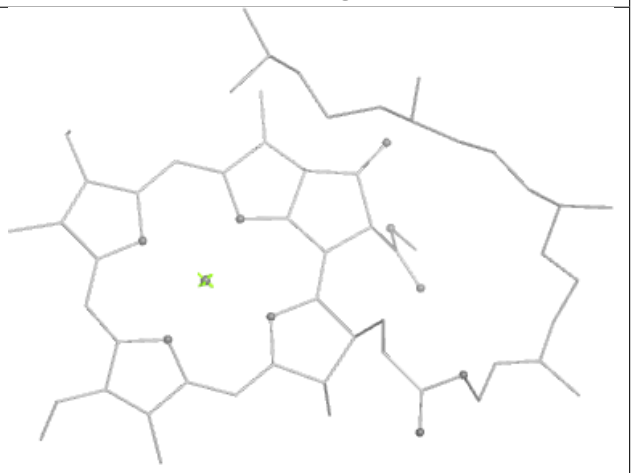
Bond lengths



Bond angles

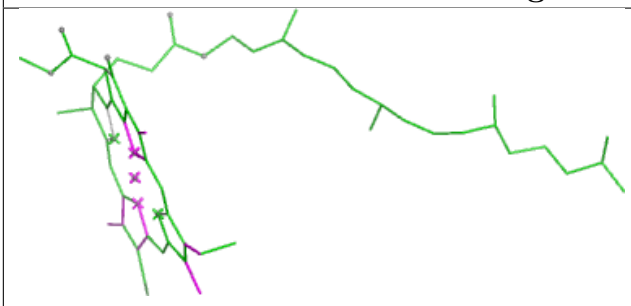


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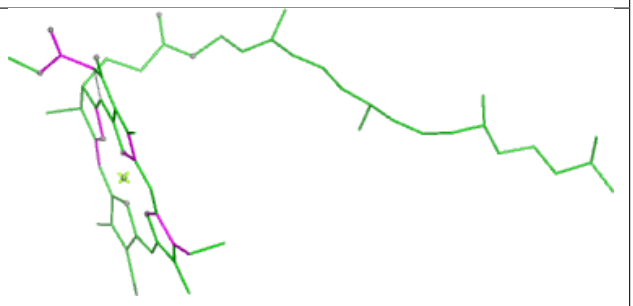


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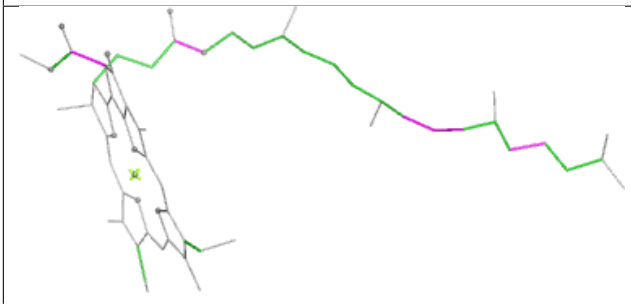
Ligand CLA b 830



Bond lengths



Bond angles

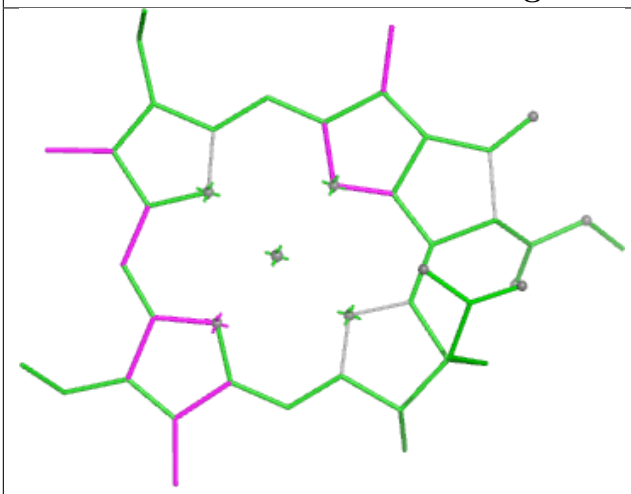


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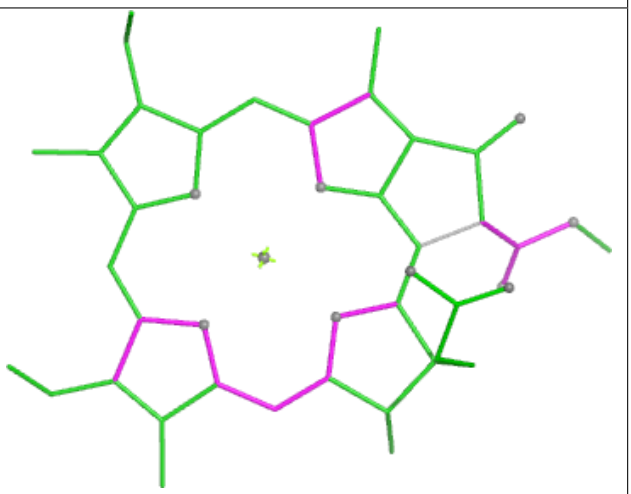


Rings

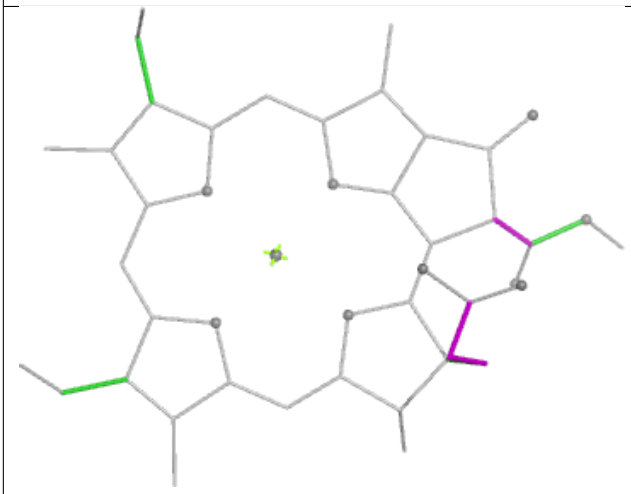
Ligand CLA A 813



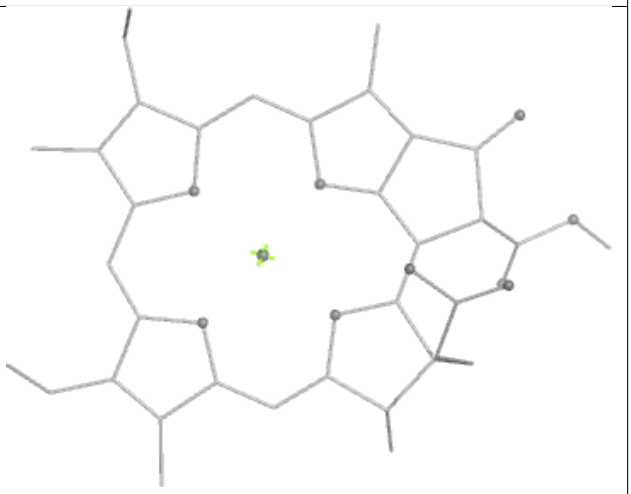
Bond lengths



Bond angles

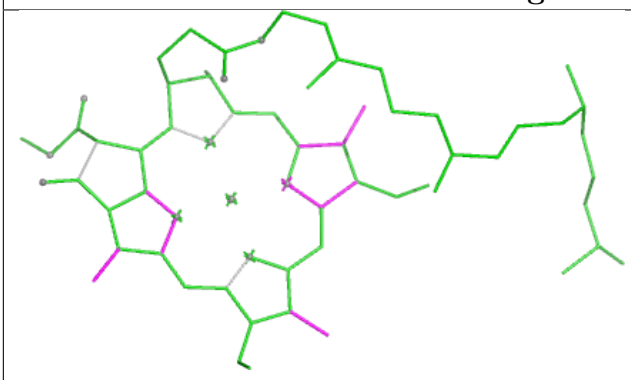


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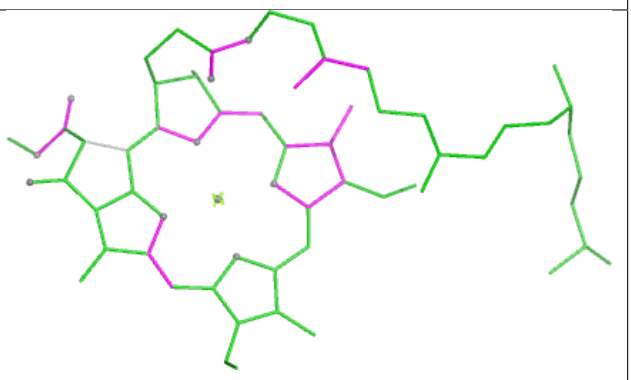


Rings

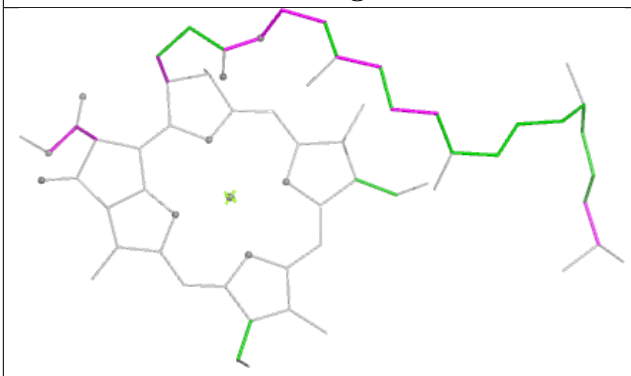
Ligand CLA b 819



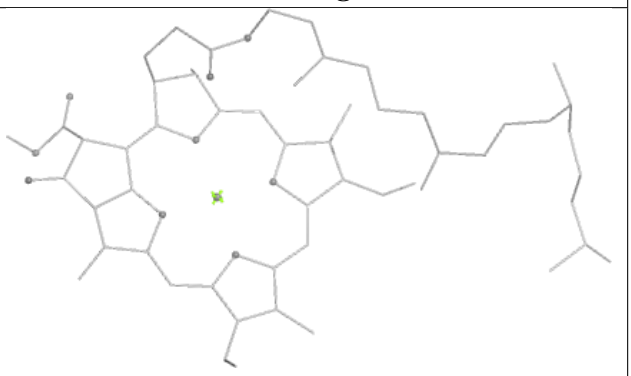
Bond lengths



Bond angles

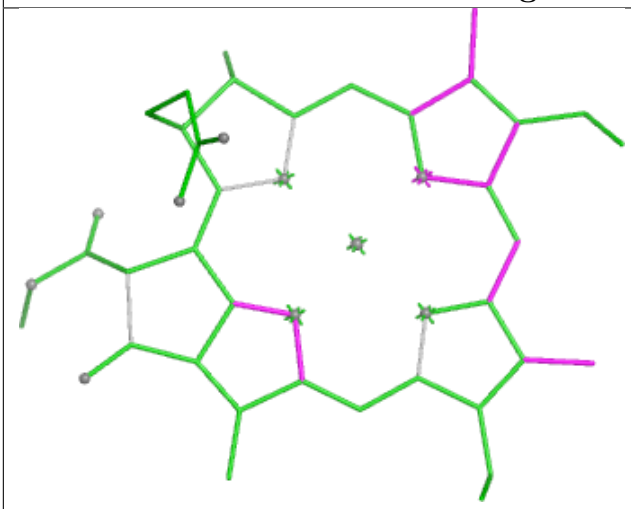


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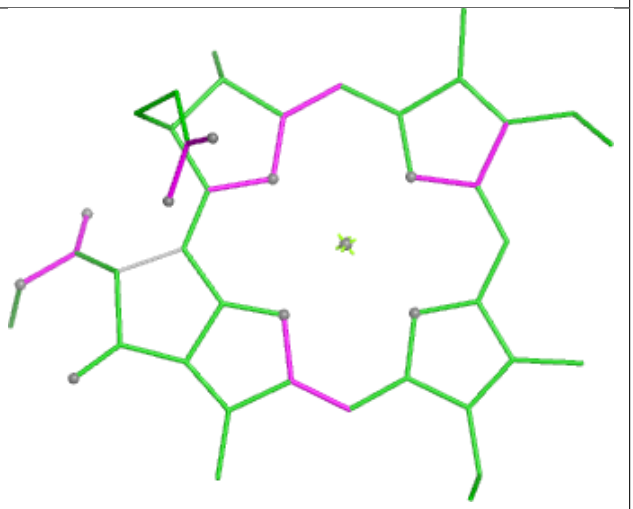


Rings

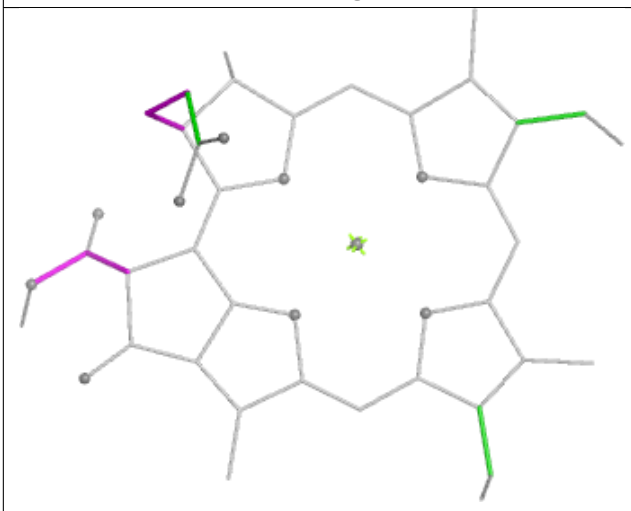
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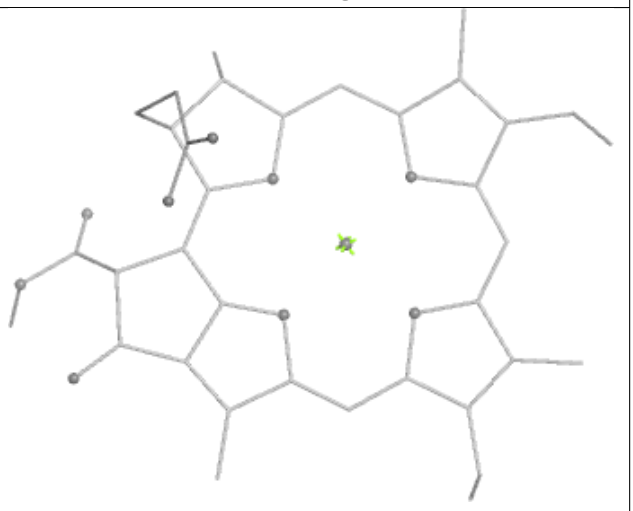
Bond lengths



Bond angles

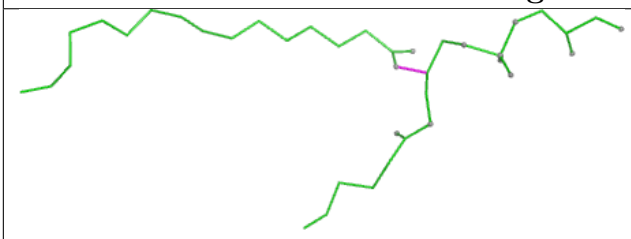


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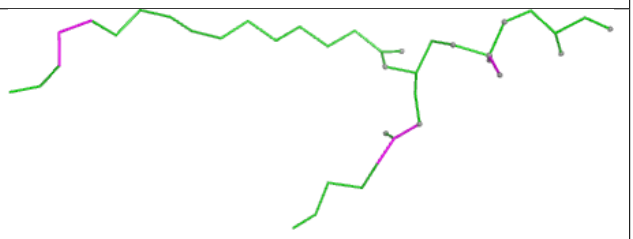


Rings

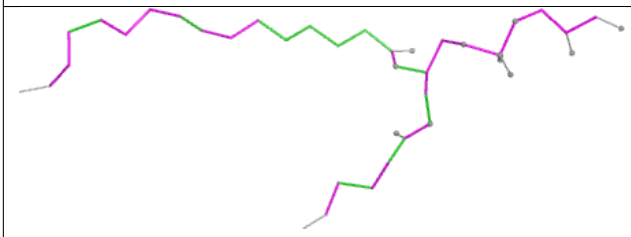
Ligand LHG 0 202



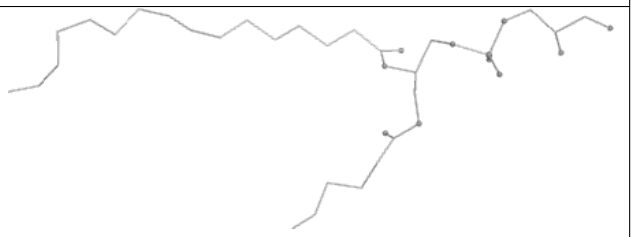
Bond lengths



Bond angles

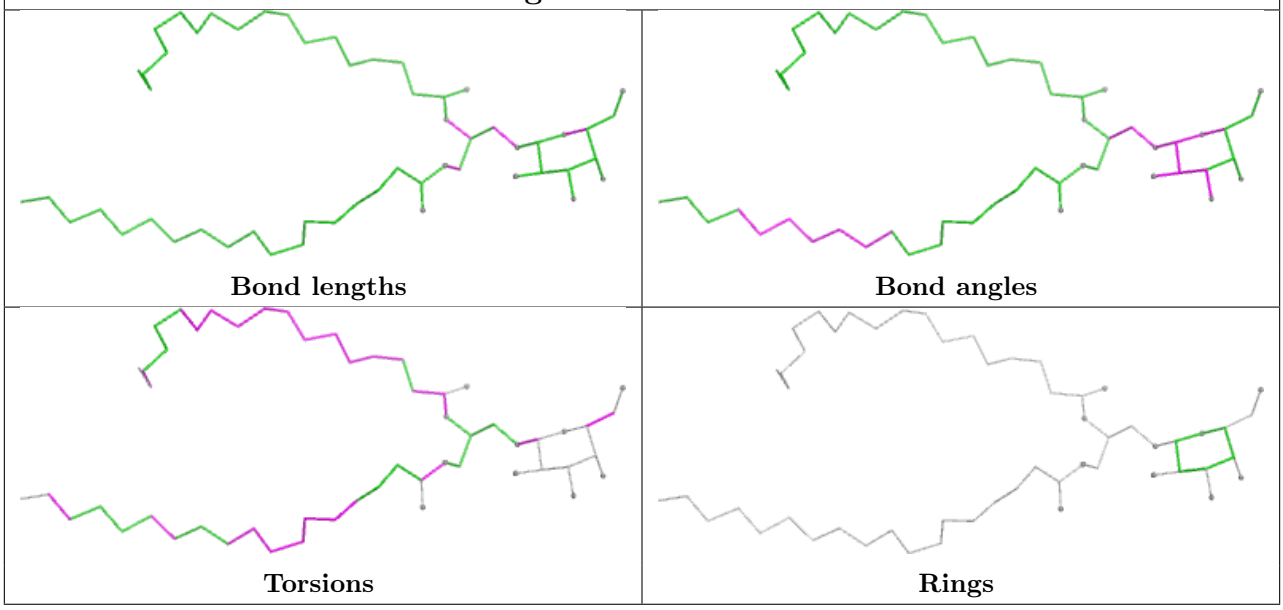


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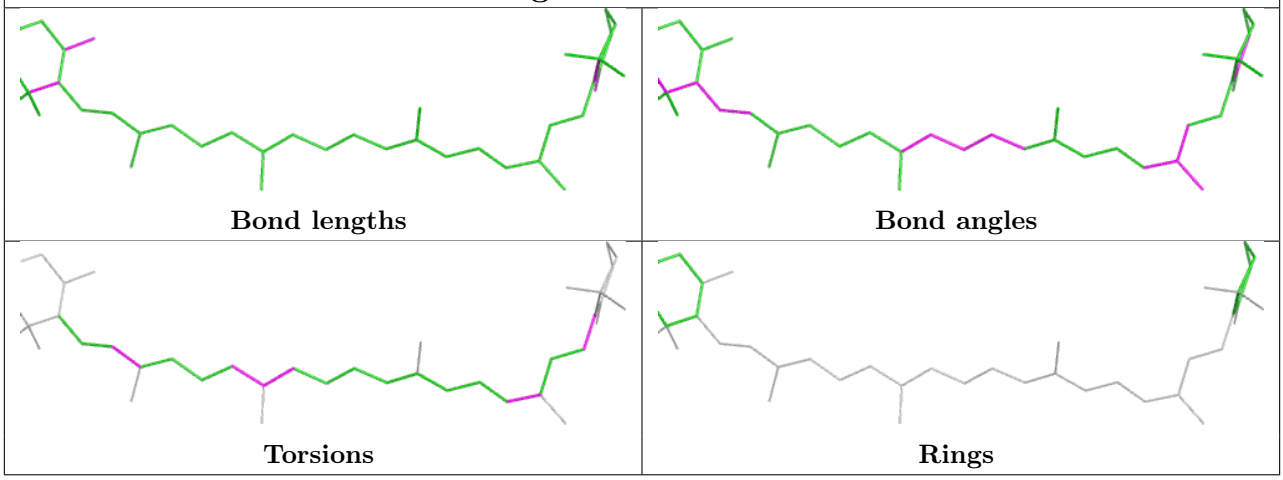


Rings

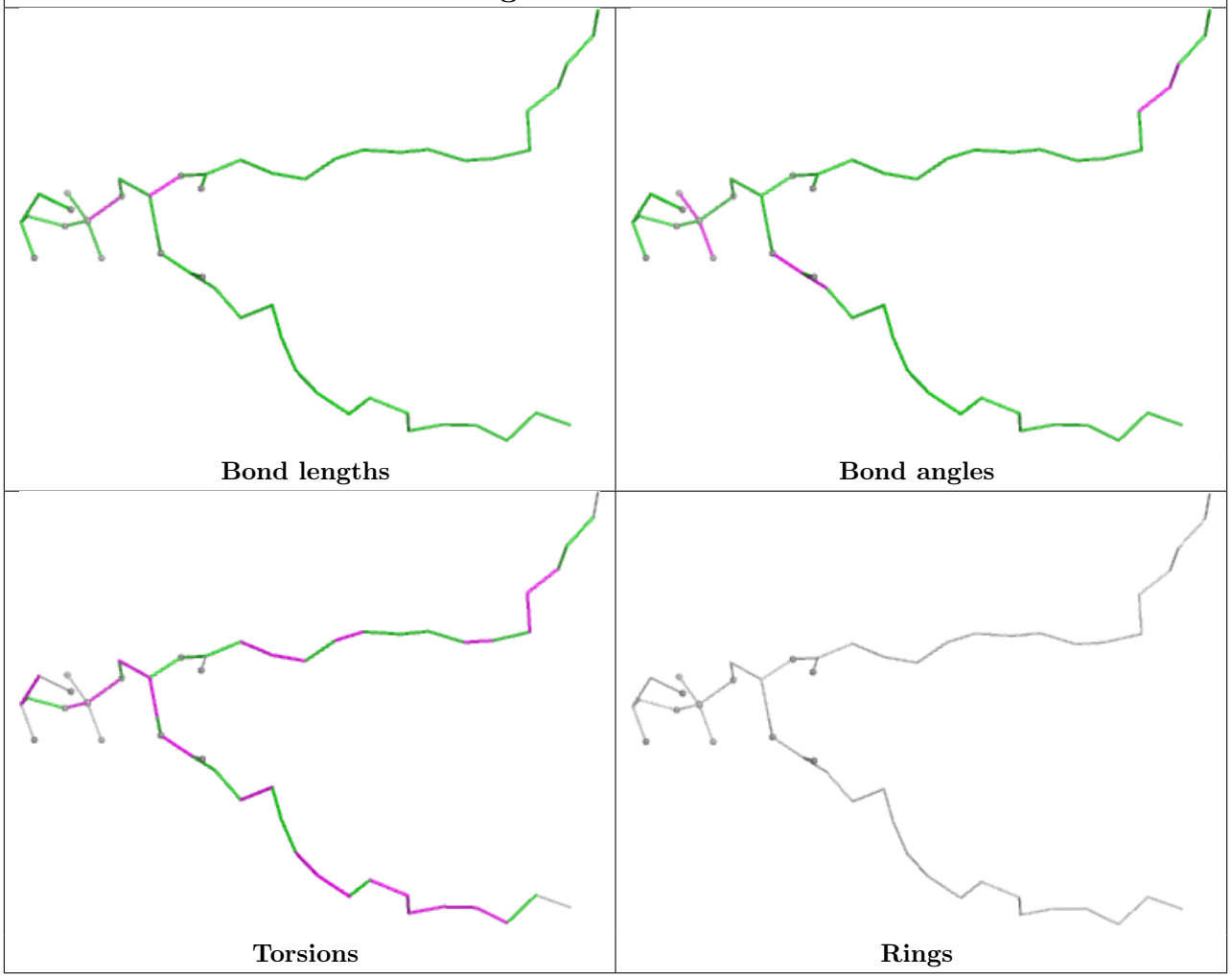
Ligand LMG 2 850



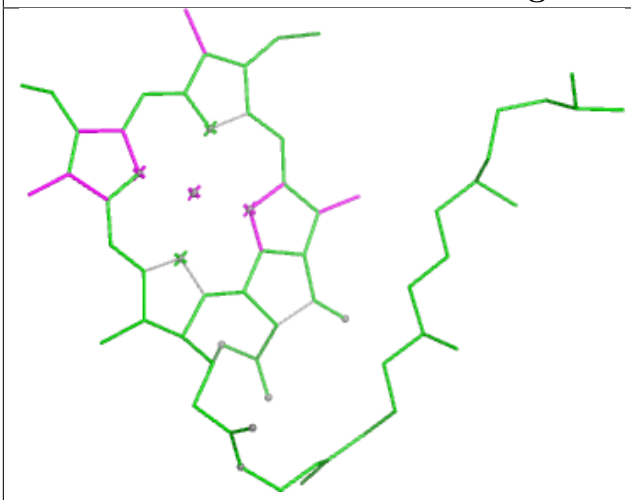
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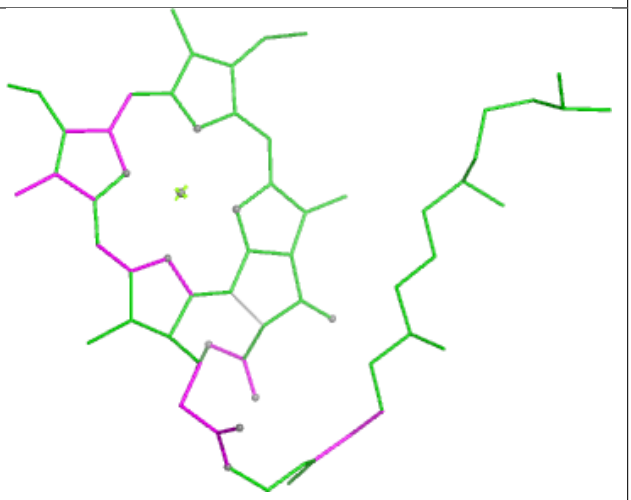
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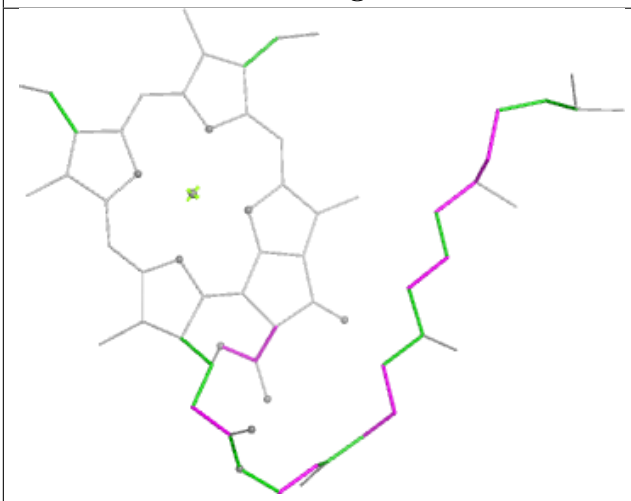
Ligand CLA a 826



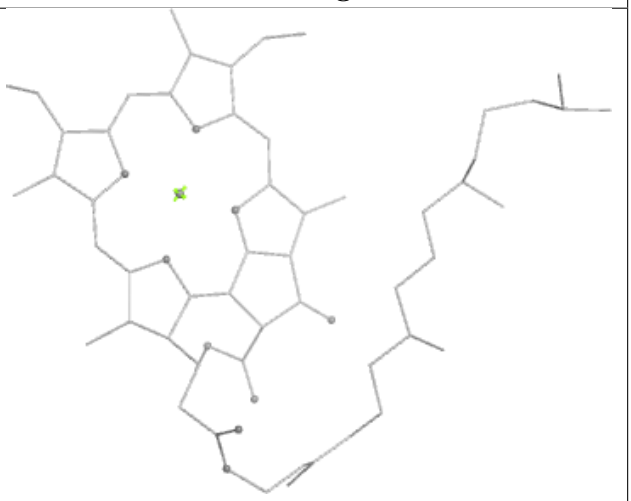
Bond lengths



Bond angles

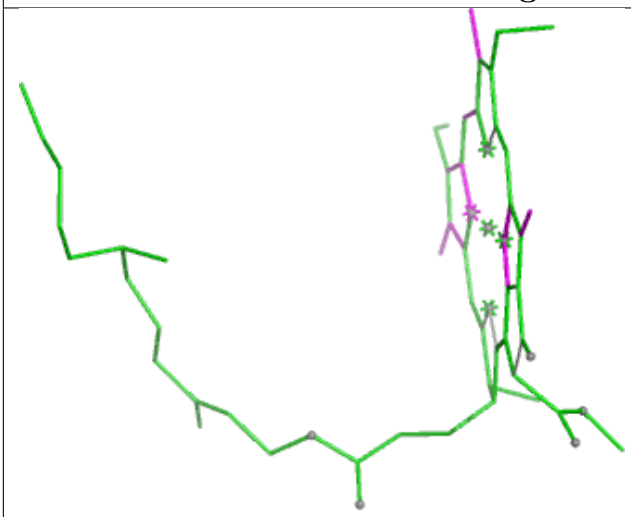


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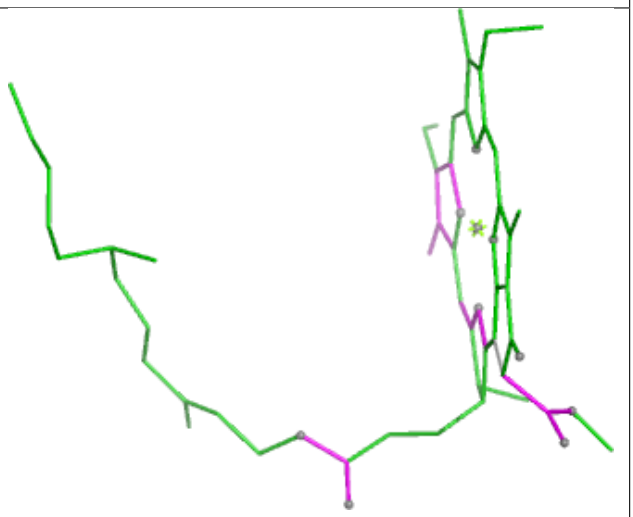


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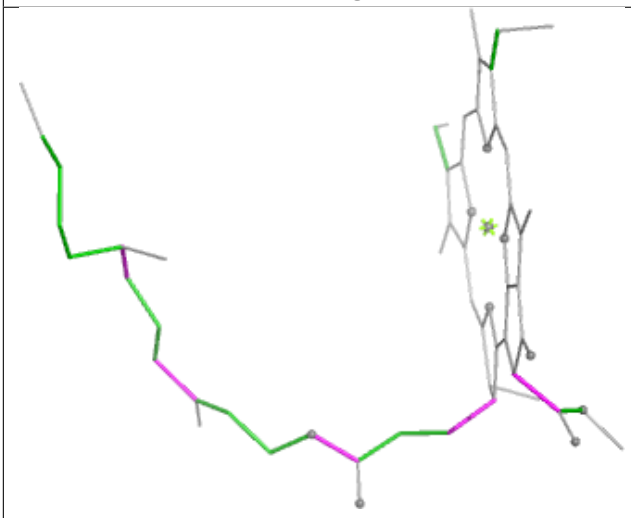
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Bond lengths



Bond angles

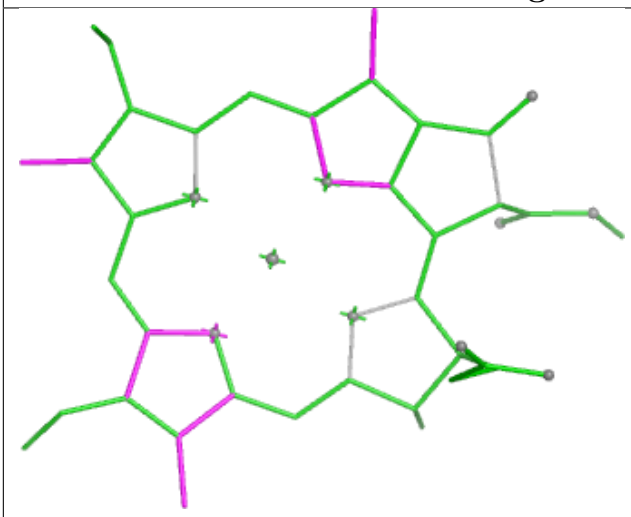


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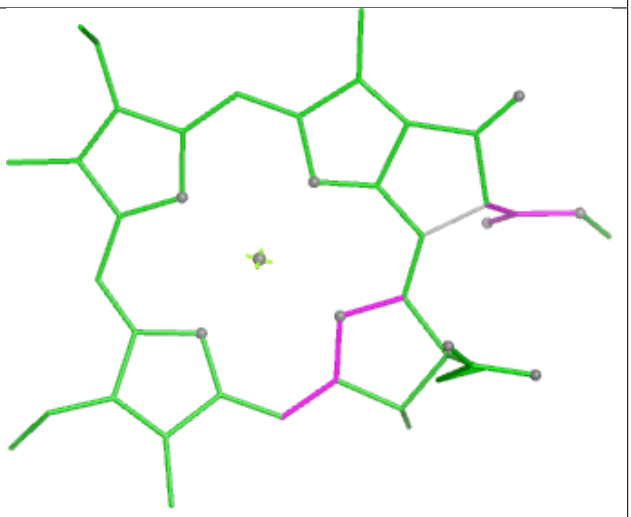


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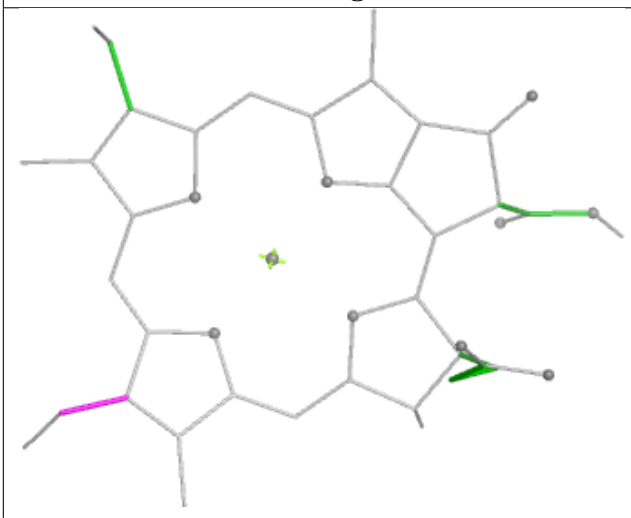
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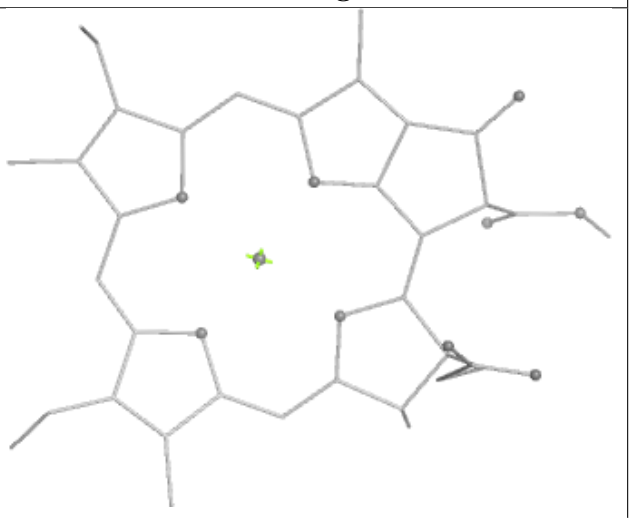
Bond lengths



Bond angles

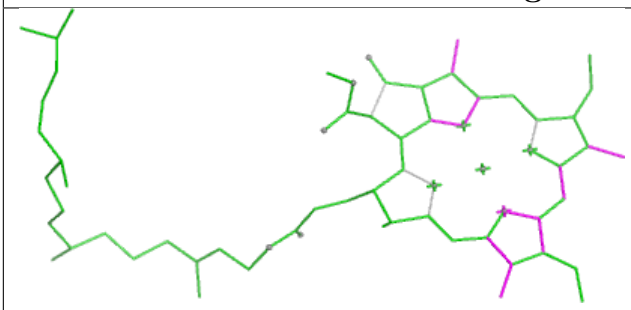


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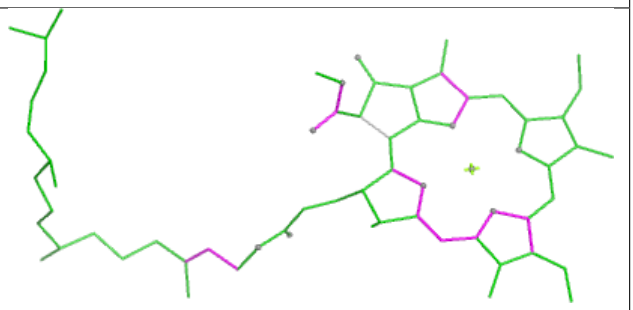


Rings

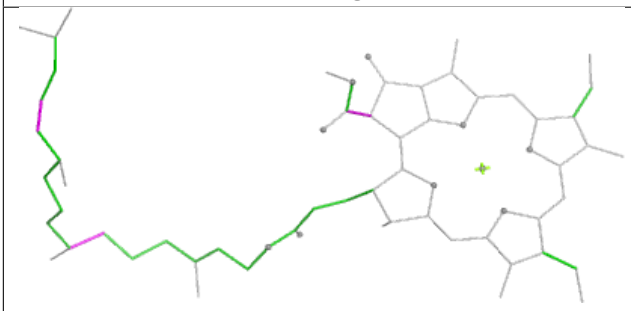
Ligand CLA B 826



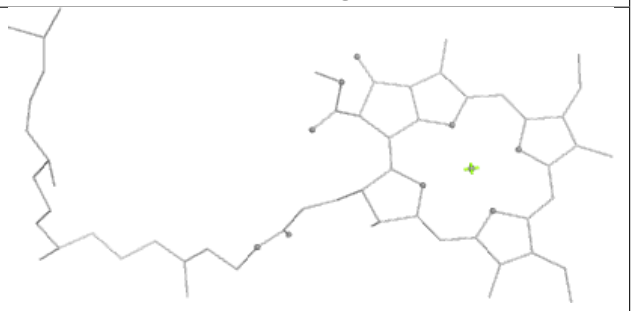
Bond lengths



Bond angles

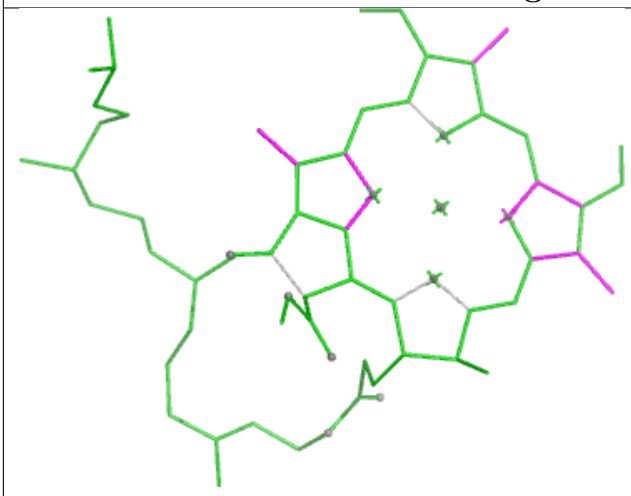


Torsions

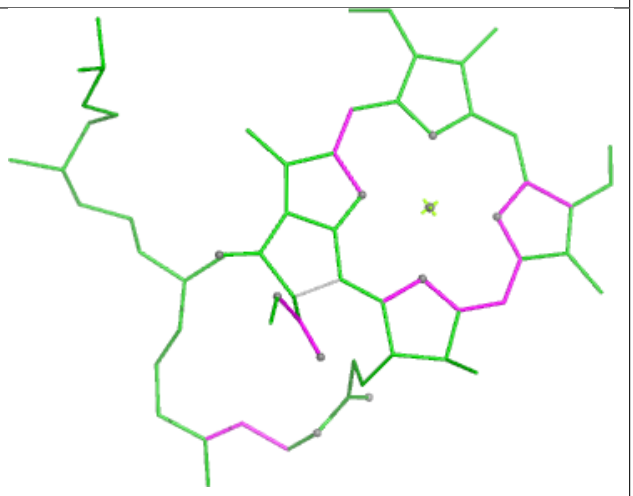


Rings

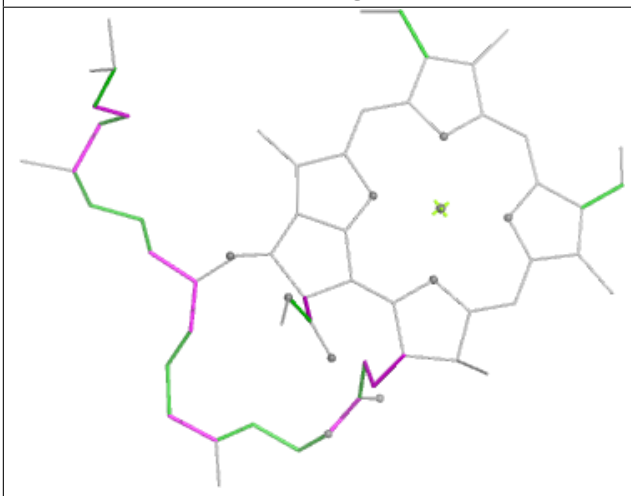
Ligand CLA B 832



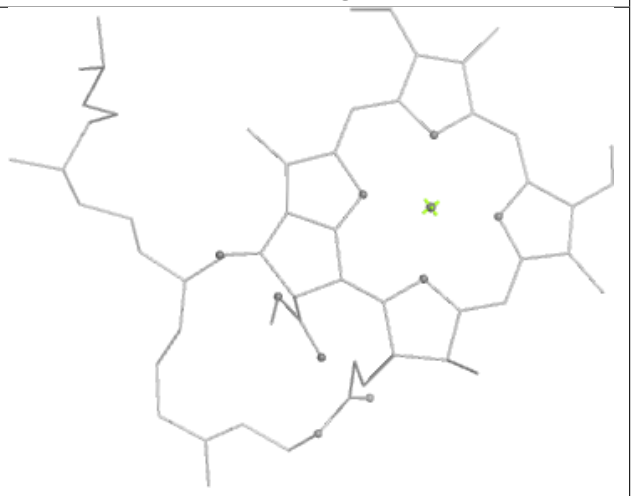
Bond lengths



Bond angles

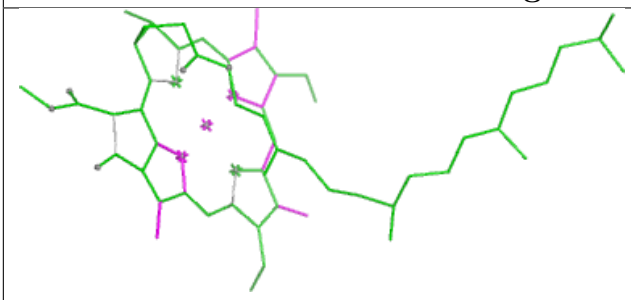


Torsions



Rings

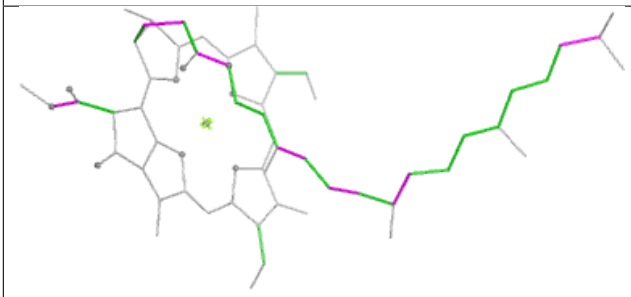
Ligand CLA A 842



Bond lengths



Bond angles



Torsions

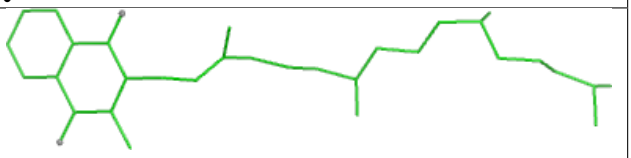


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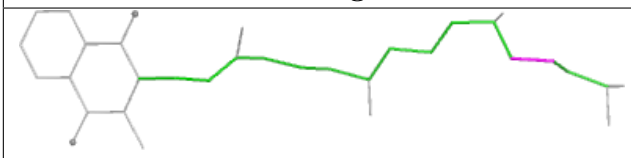
Ligand PQN a 845



Bond lengths



Bond angles

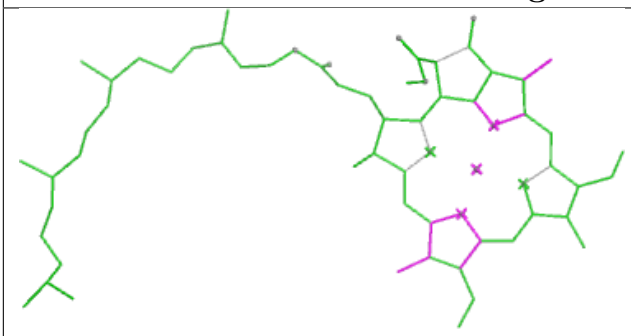


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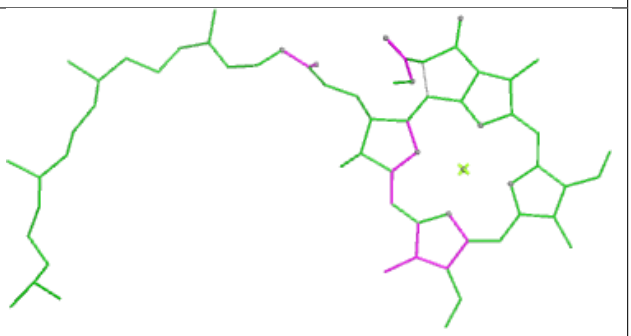


Rings

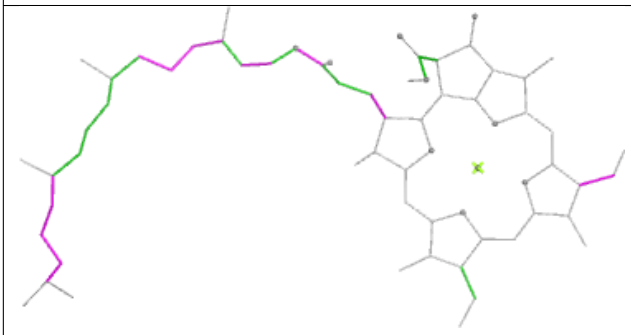
Ligand CLA a 838



Bond lengths



Bond angles

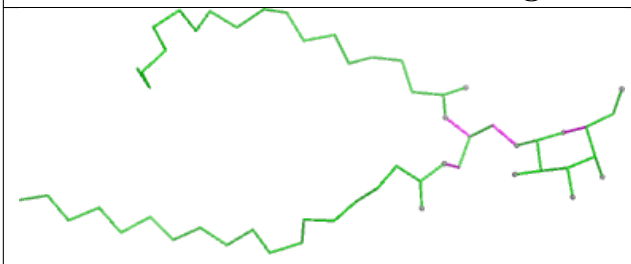


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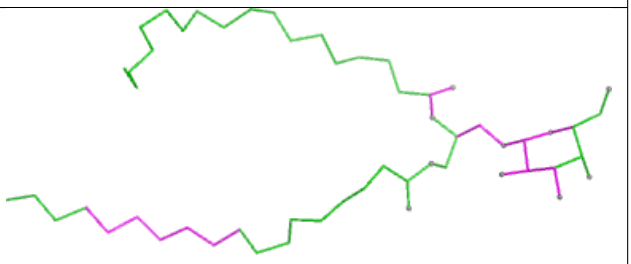


Rings

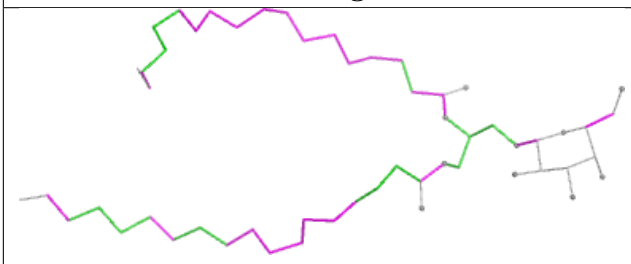
Ligand LMG b 850



Bond lengths



Bond angles

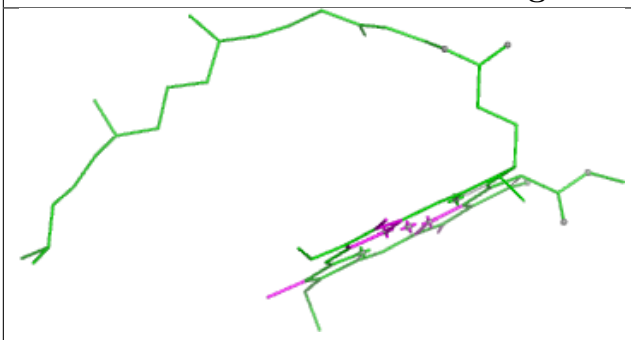


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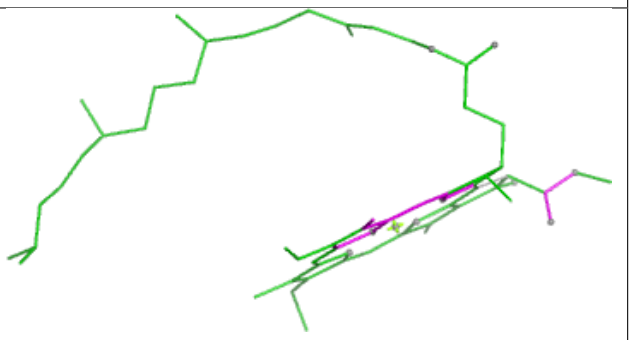


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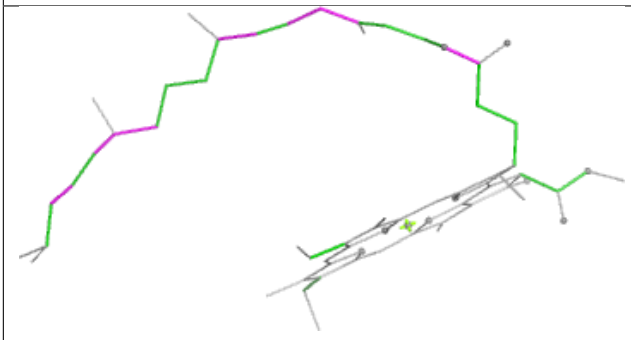
Ligand CLA a 833



Bond lengths



Bond angles



Torsions

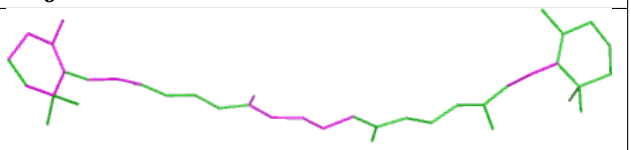


Rings

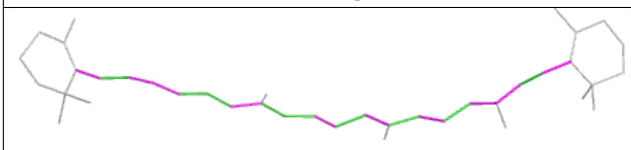
Ligand BCR j 1305



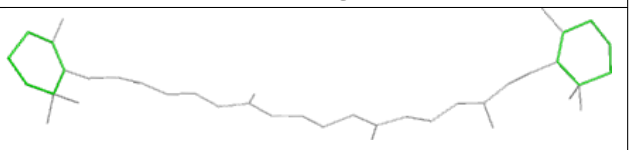
Bond lengths



Bond angles

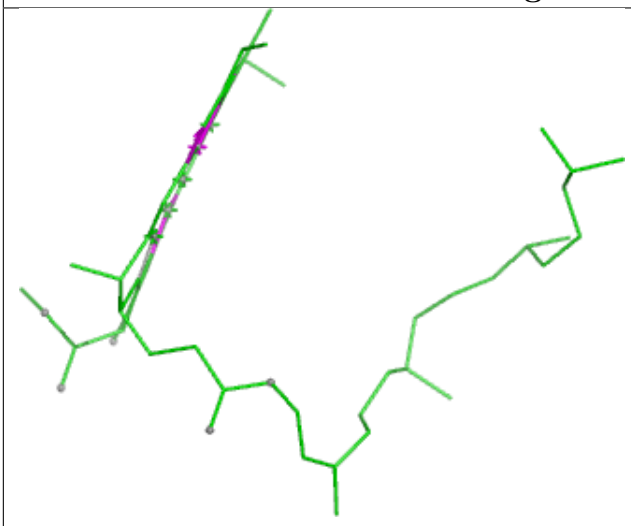


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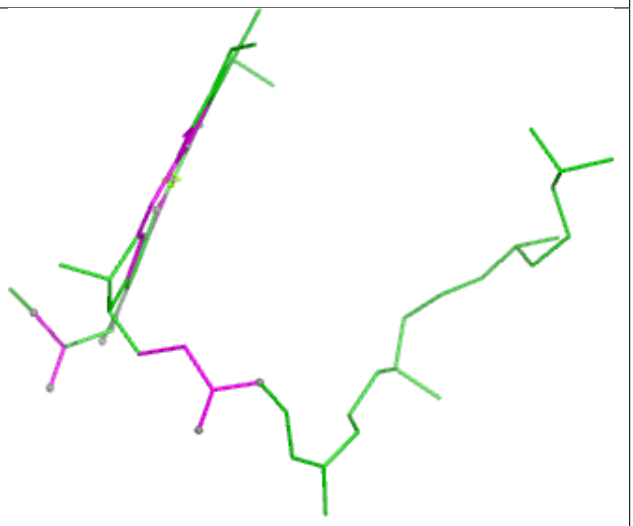


Rings

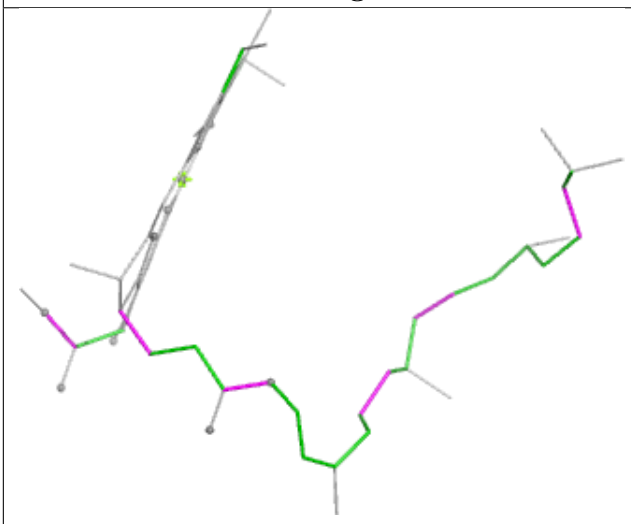
Ligand CLA B 834



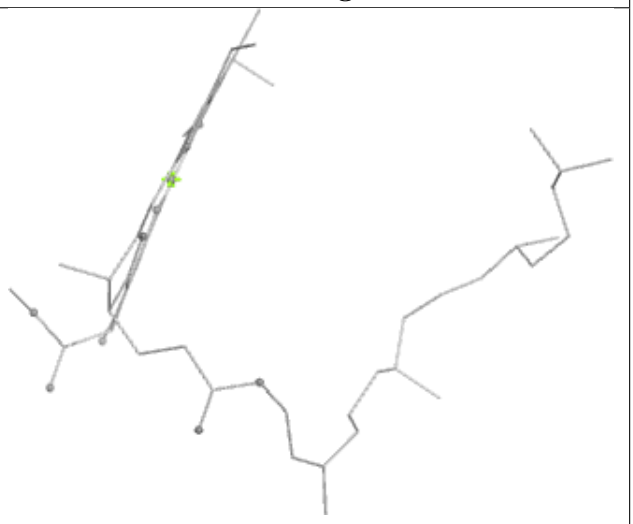
Bond lengths



Bond angles

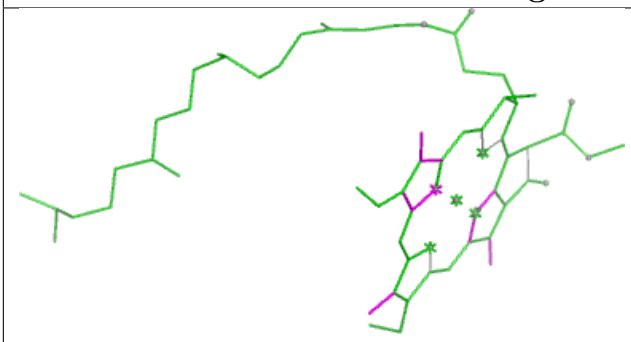


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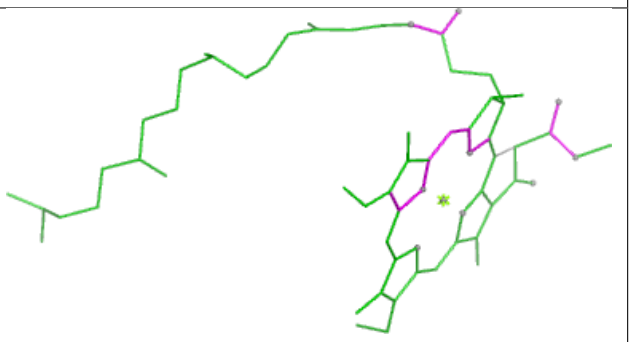


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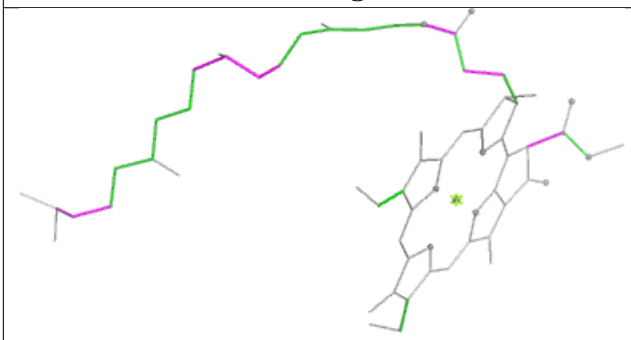
Ligand CLA 2 816



Bond lengths



Bond angles

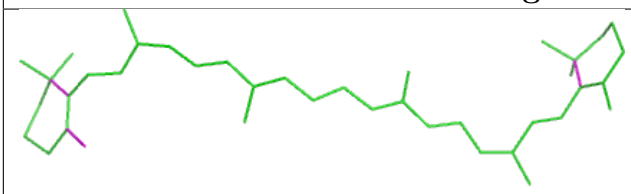


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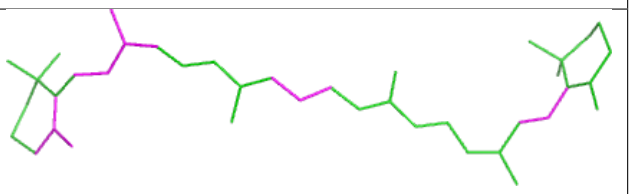


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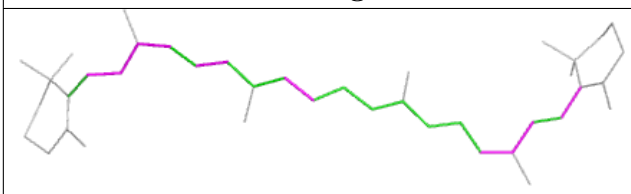
Ligand BCR B 845



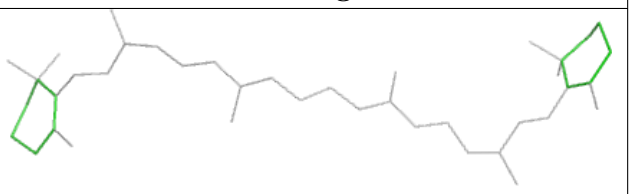
Bond lengths



Bond angles

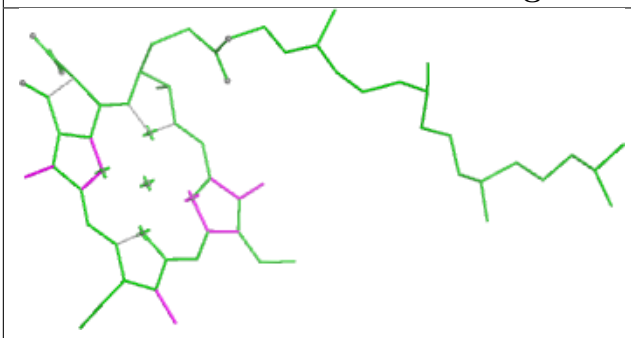


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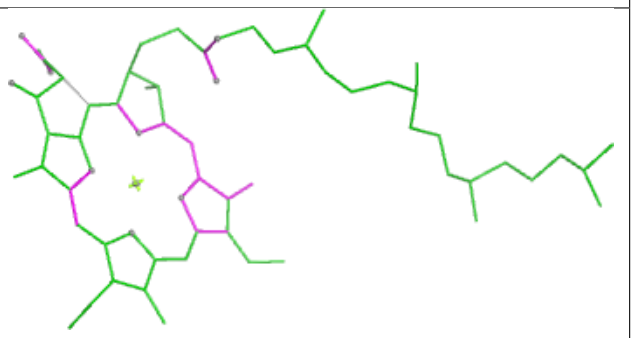


Rings

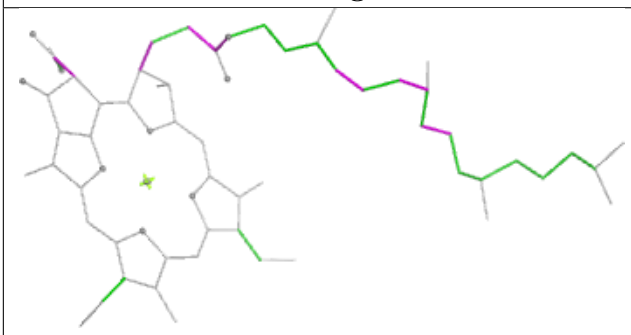
Ligand CLA A 809



Bond lengths



Bond angles

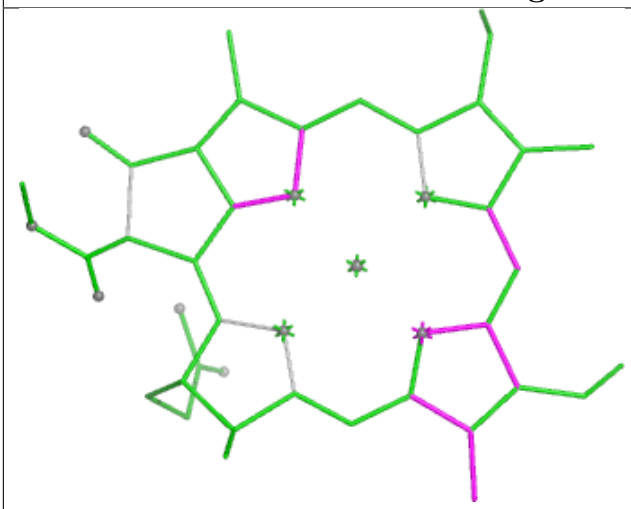


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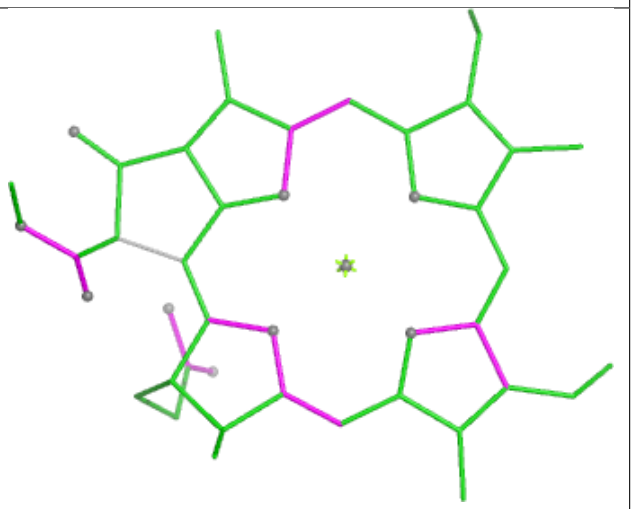


Rings

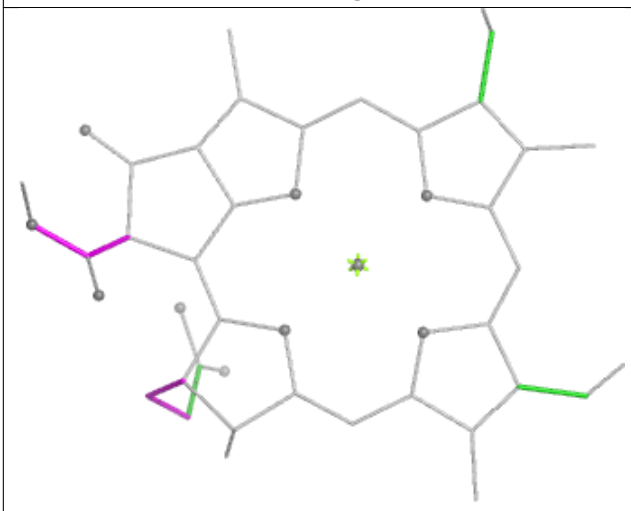
Ligand CLA J 101



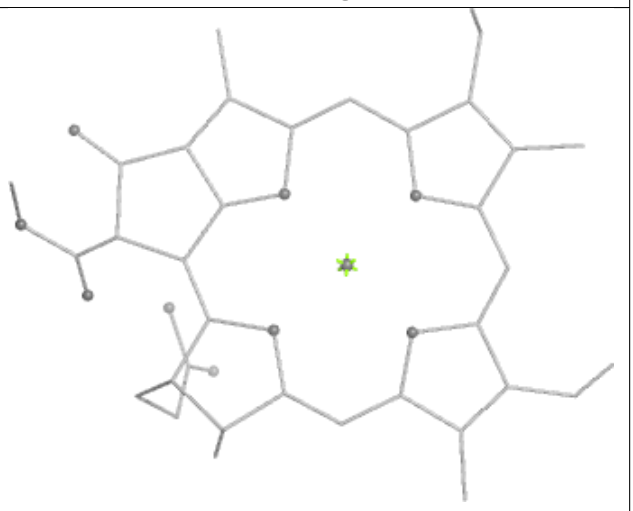
Bond lengths



Bond angles

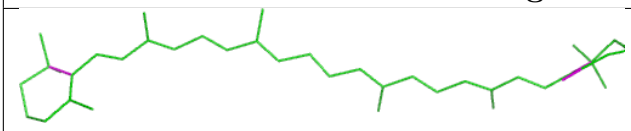


Torsions



Rings

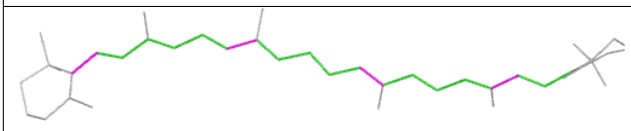
Ligand BCR 0 201



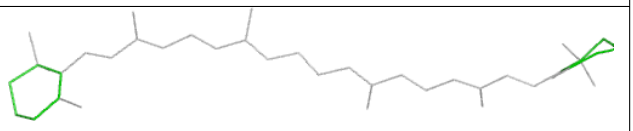
Bond lengths



Bond angles

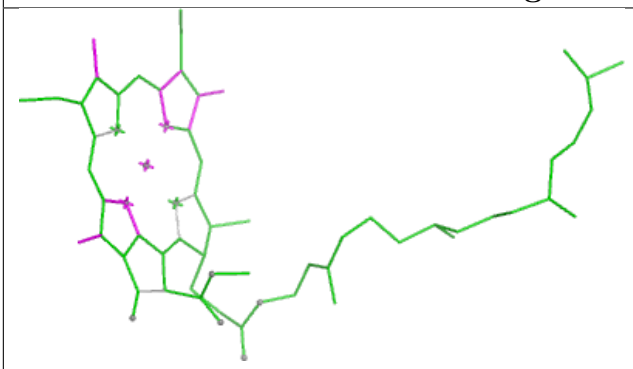


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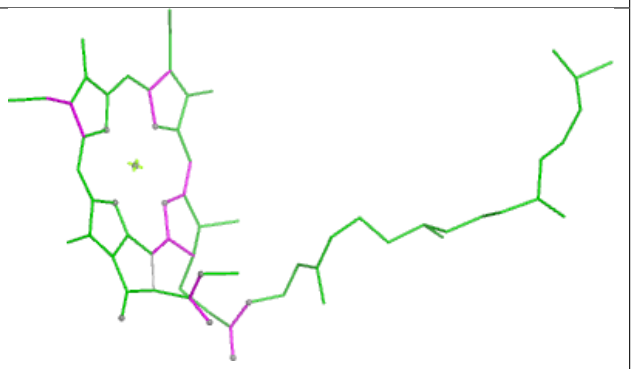


Rings

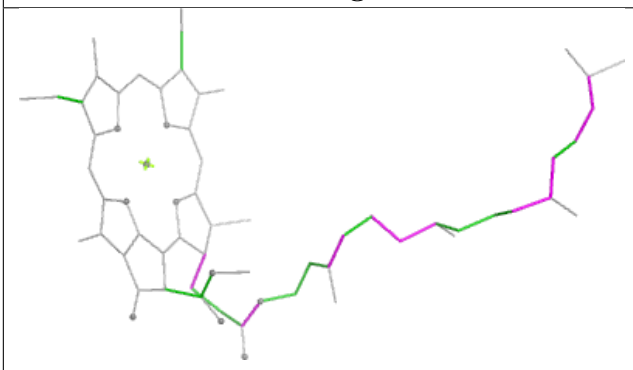
Ligand CLA B 810



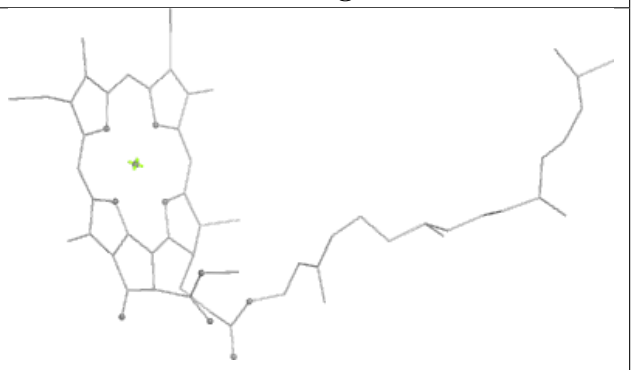
Bond lengths



Bond angles

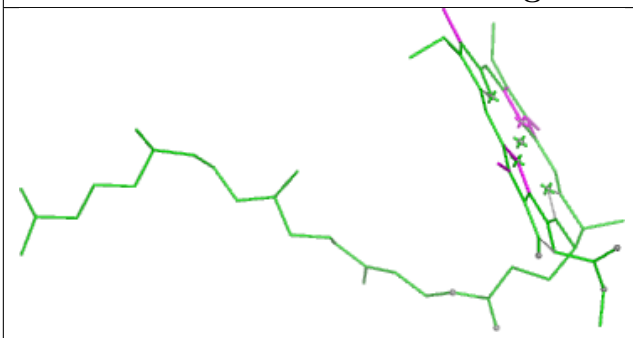


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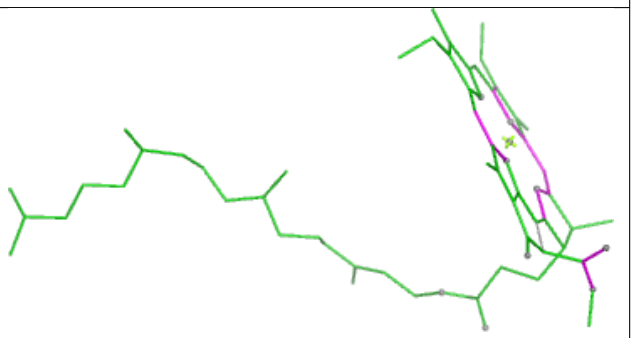


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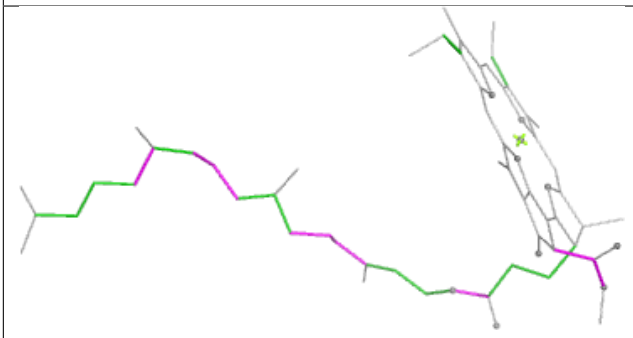
Ligand CLA A 812



Bond lengths



Bond angles

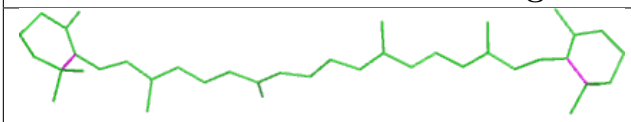


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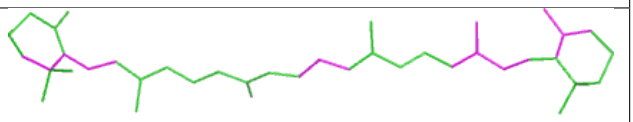


Rings

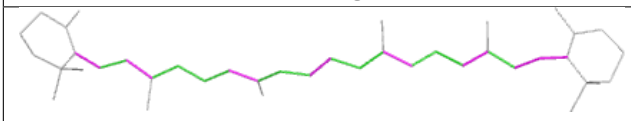
Ligand BCR a 847



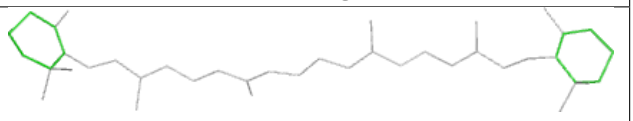
Bond lengths



Bond angles

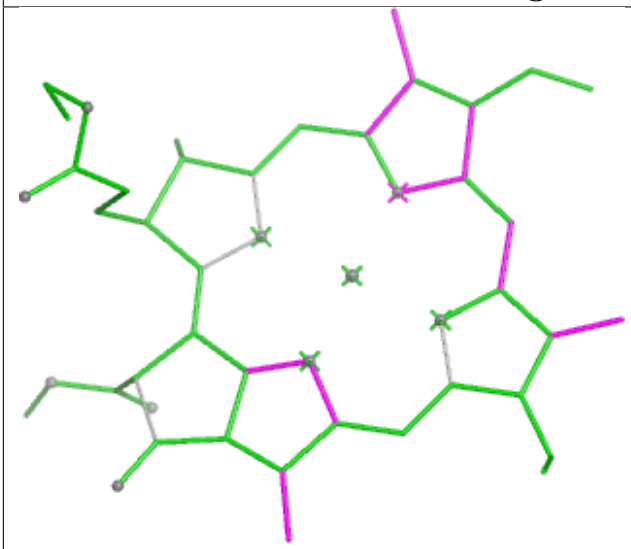


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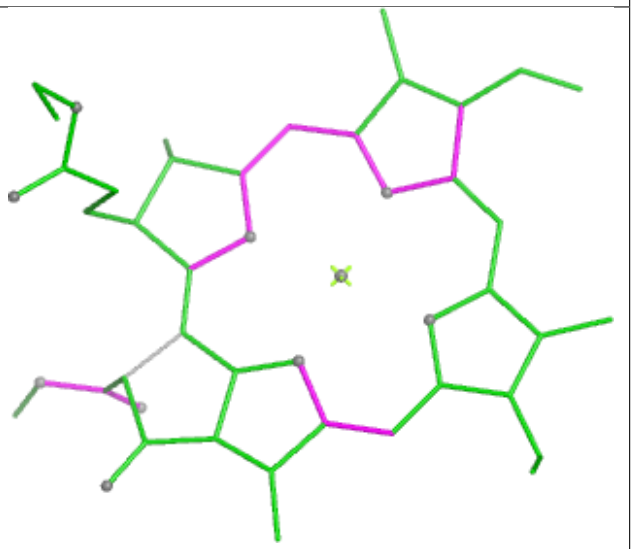


Rings

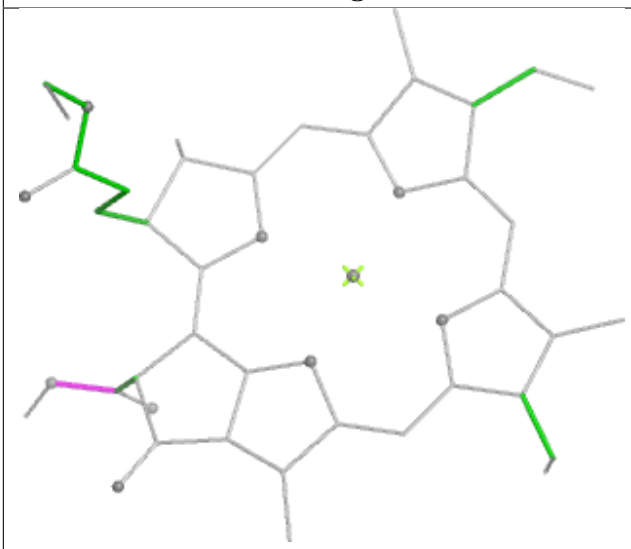
Ligand CLA b 840



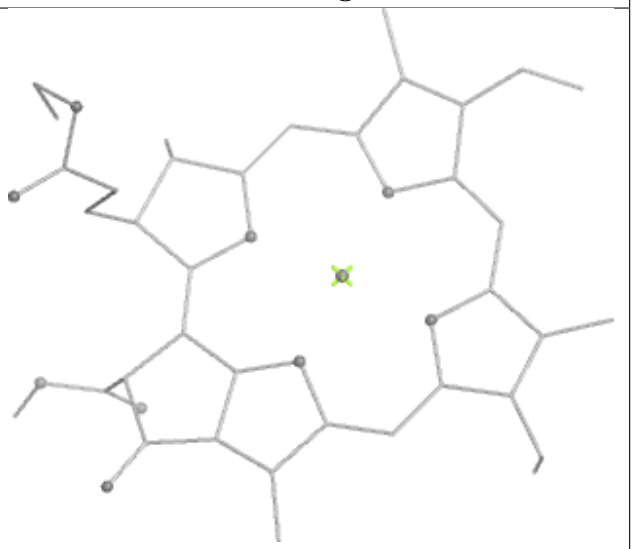
Bond lengths



Bond angles

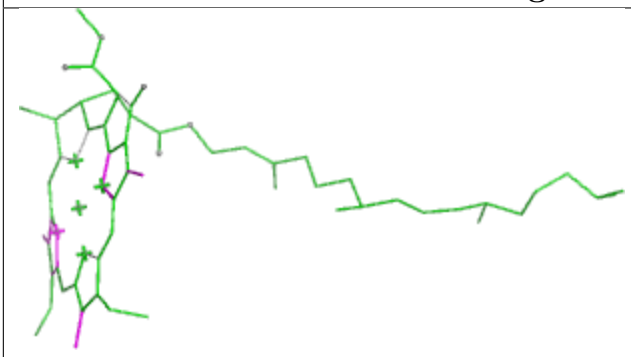


Torsions

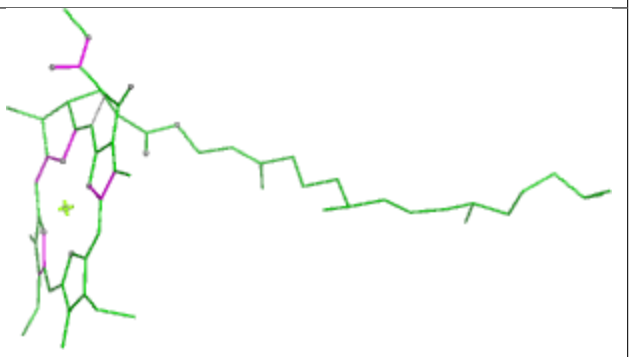


Rings

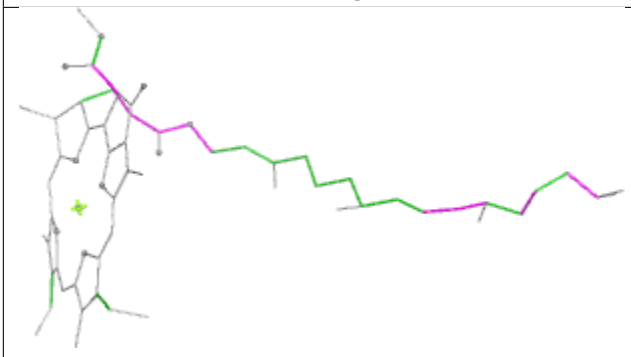
Ligand CLA 2 829



Bond lengths



Bond angles

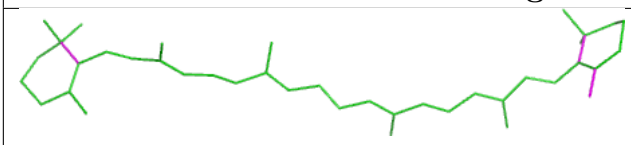


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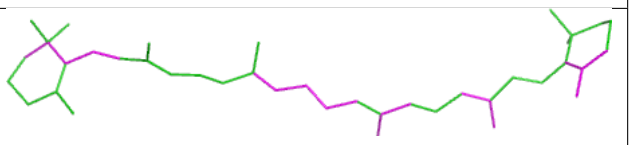


Rings

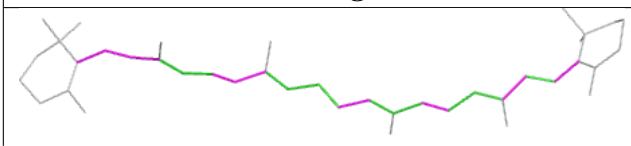
Ligand BCR 2 848



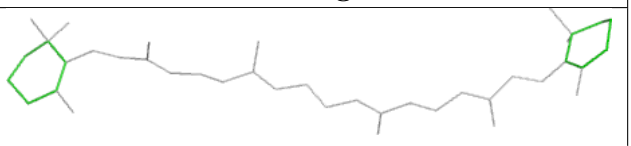
Bond lengths



Bond angles

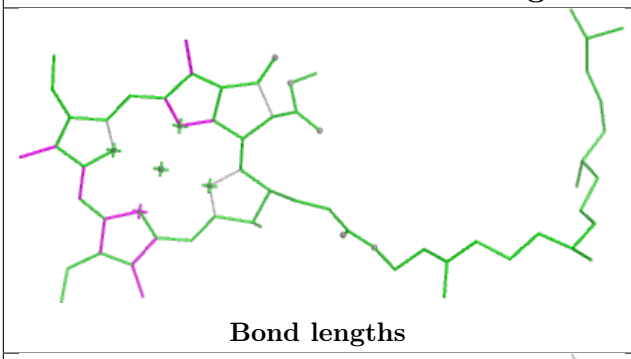


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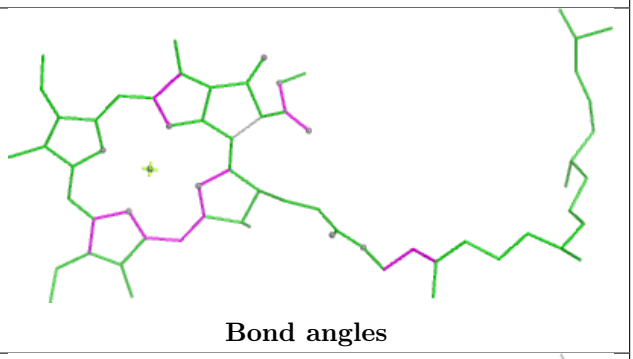


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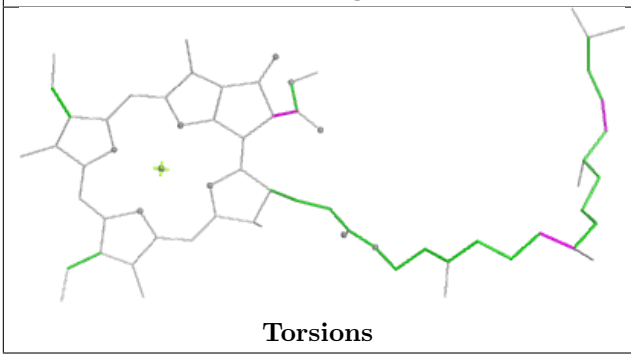
Ligand CLA b 827



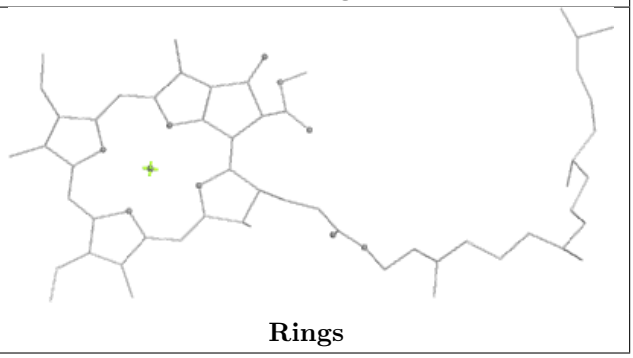
Bond lengths



Bond angles

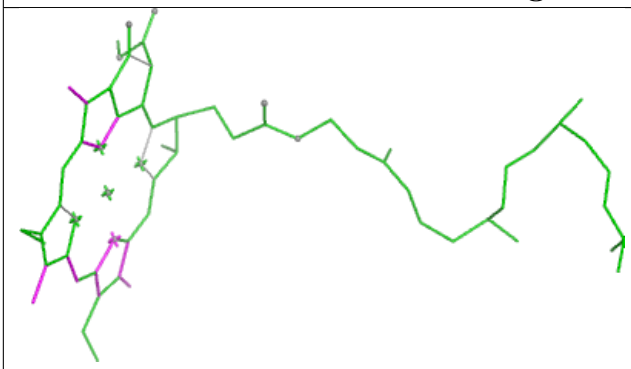


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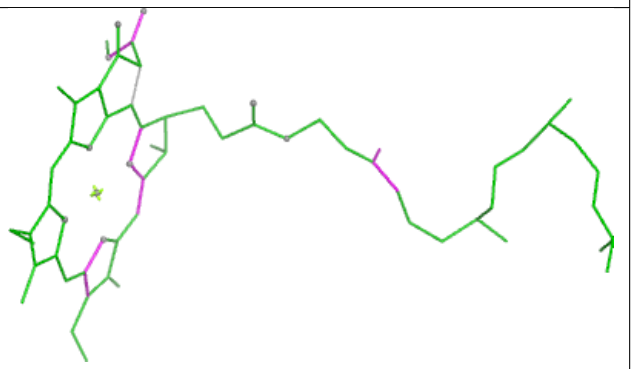


Rings

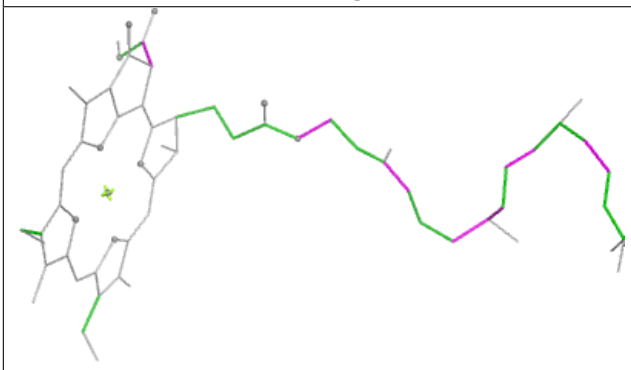
Ligand CLA b 834



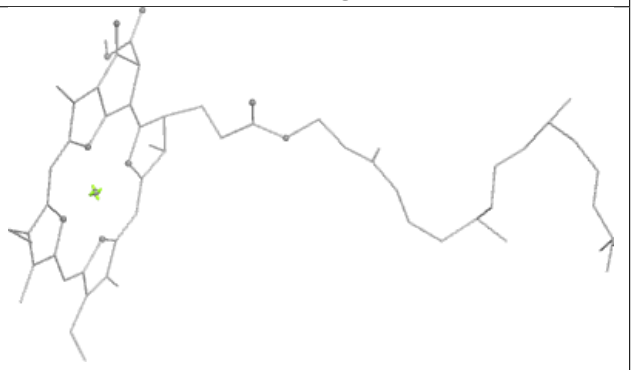
Bond lengths



Bond angles

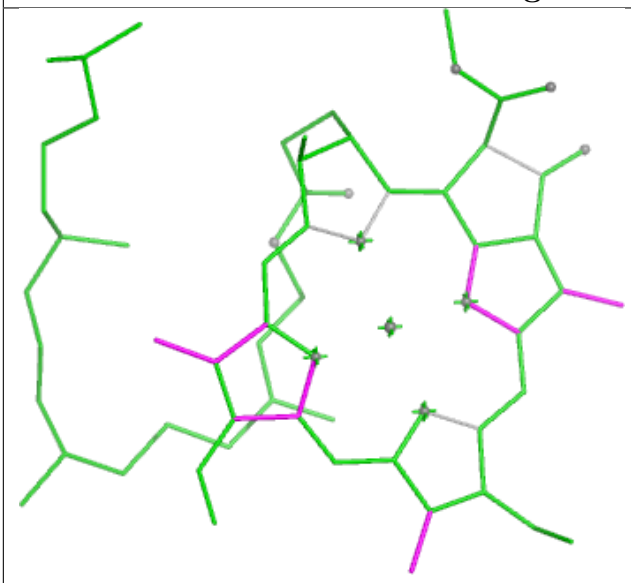


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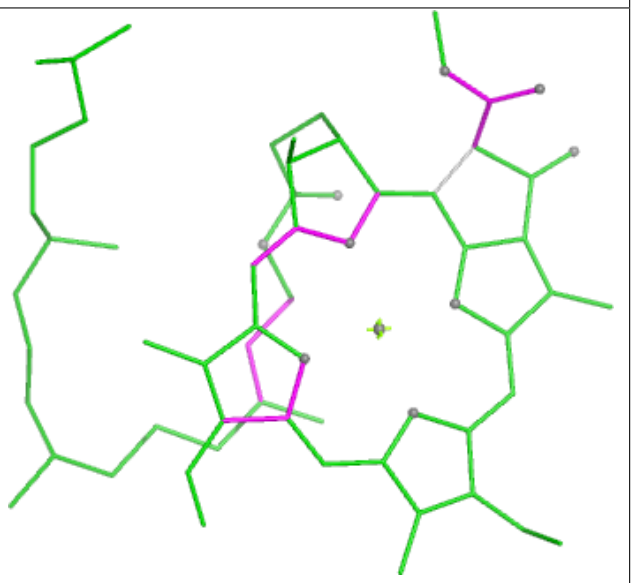


Rings

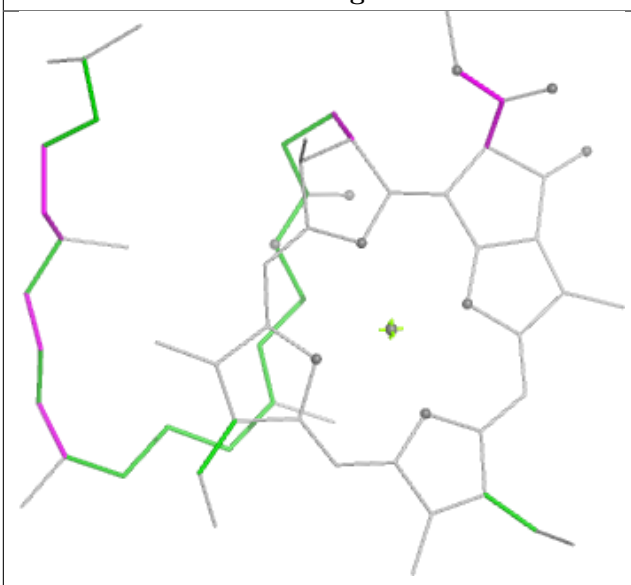
Ligand CLA A 824



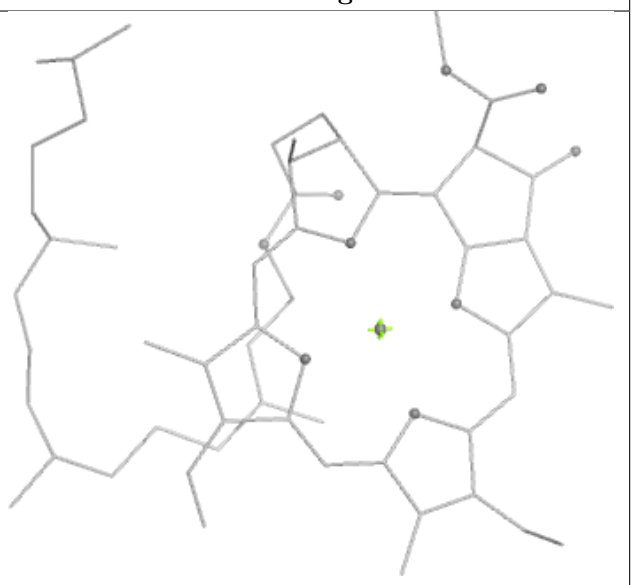
Bond lengths



Bond angles

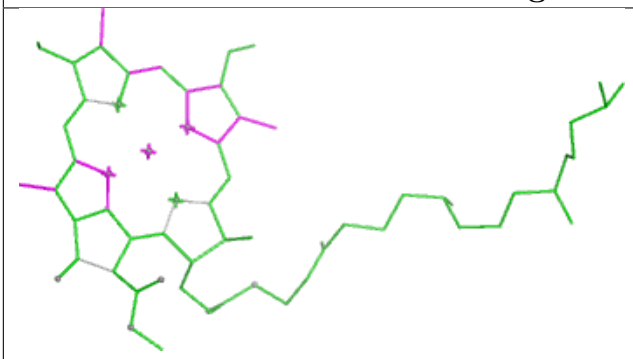


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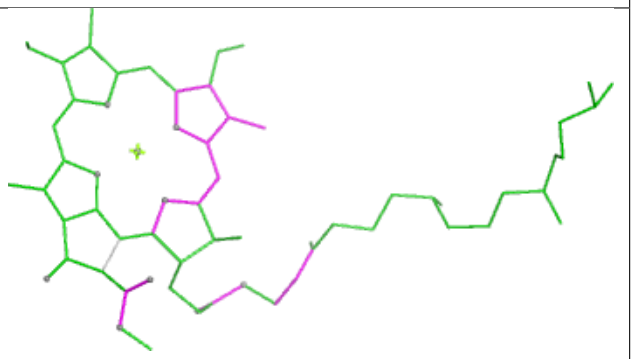


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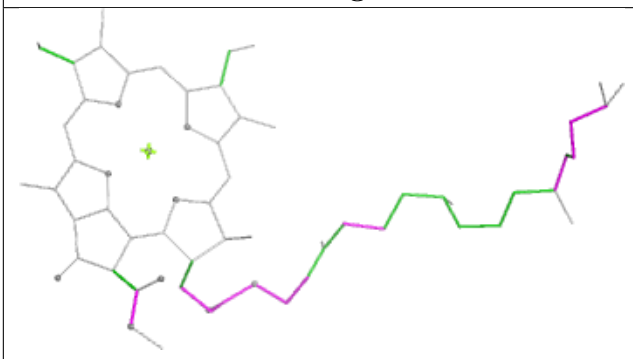
Ligand CLA a 802



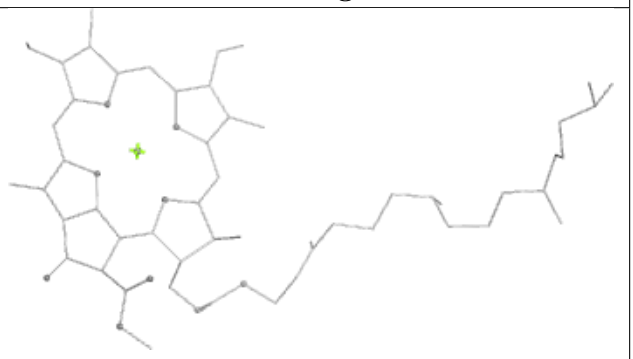
Bond lengths



Bond angles

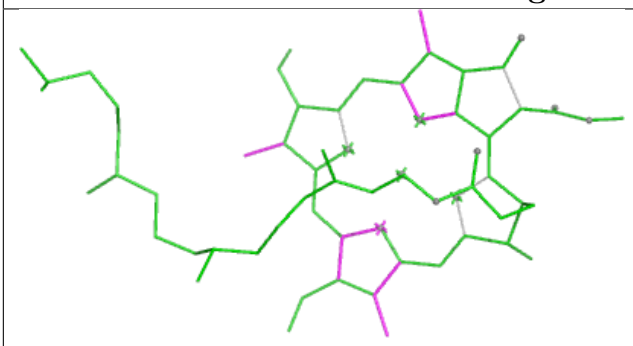


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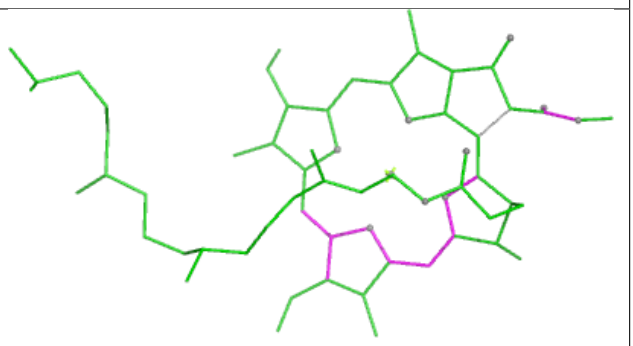


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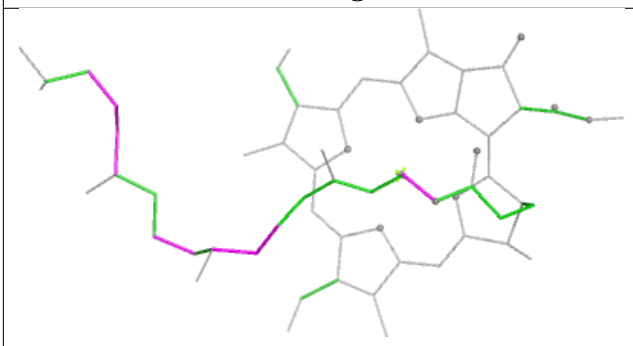
Ligand CLA 2 839



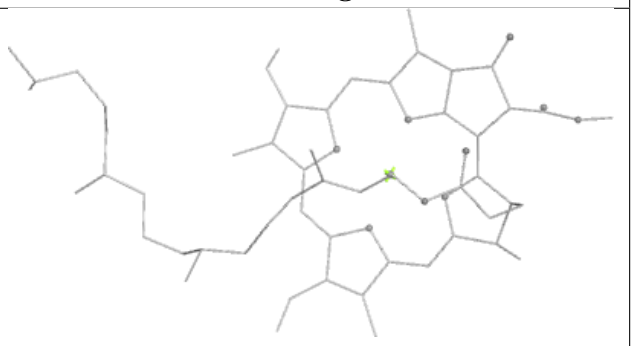
Bond lengths



Bond angles

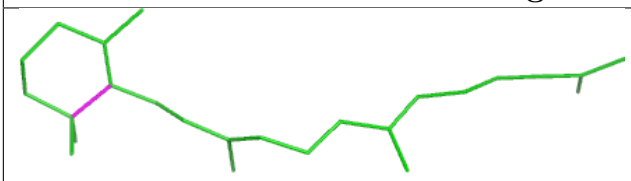


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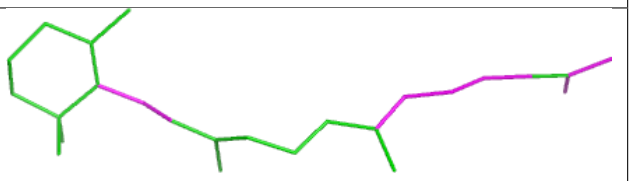


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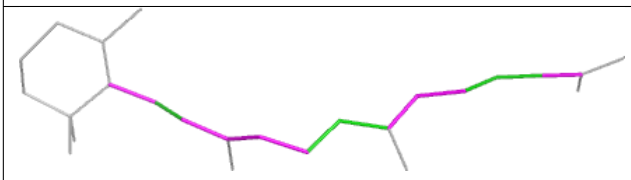
Ligand BCR a 852



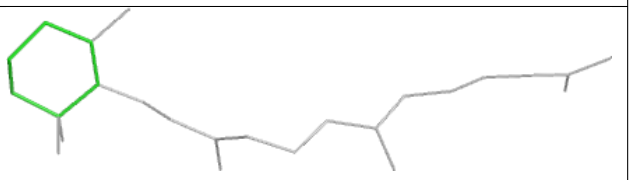
Bond lengths



Bond angles

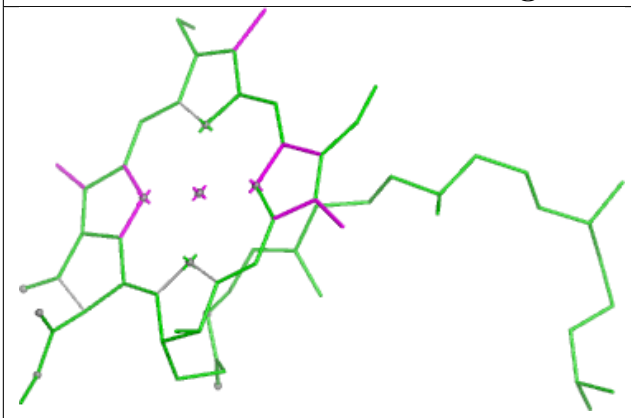


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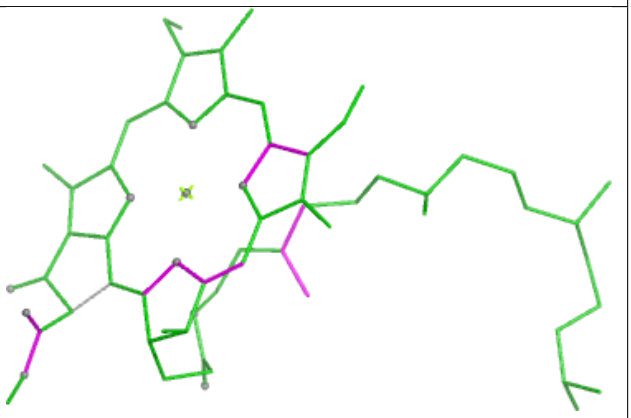


Rings

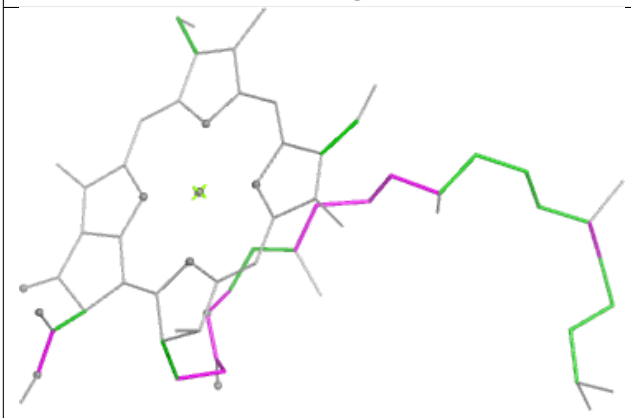
Ligand CLA 1 1644



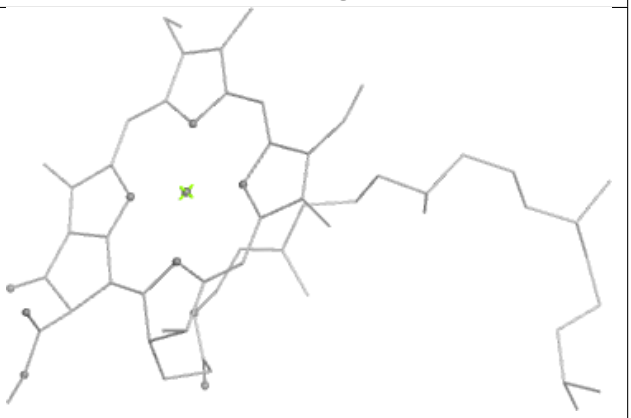
Bond lengths



Bond angles

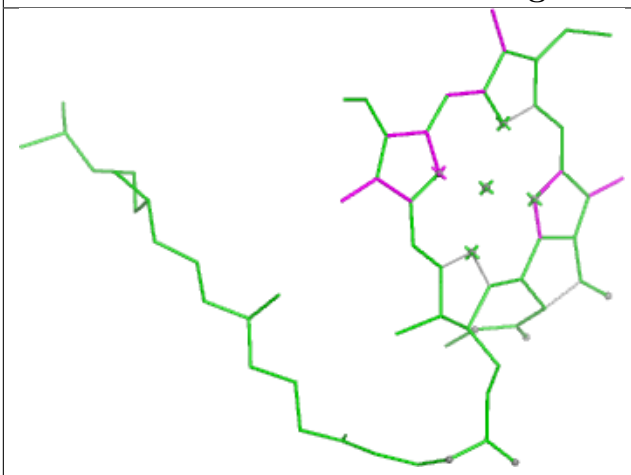


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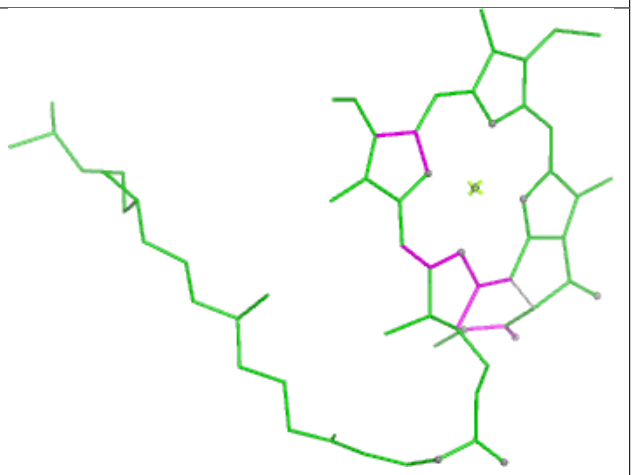


Rings

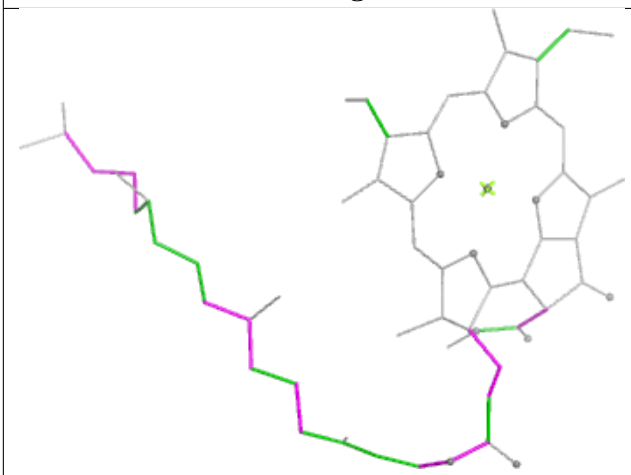
Ligand CLA 2 825



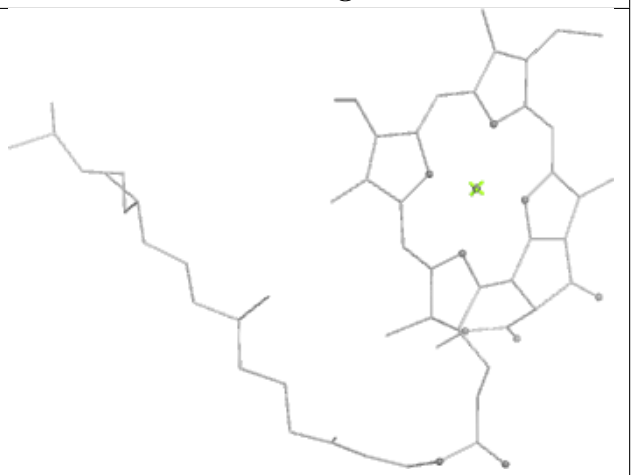
Bond lengths



Bond angles

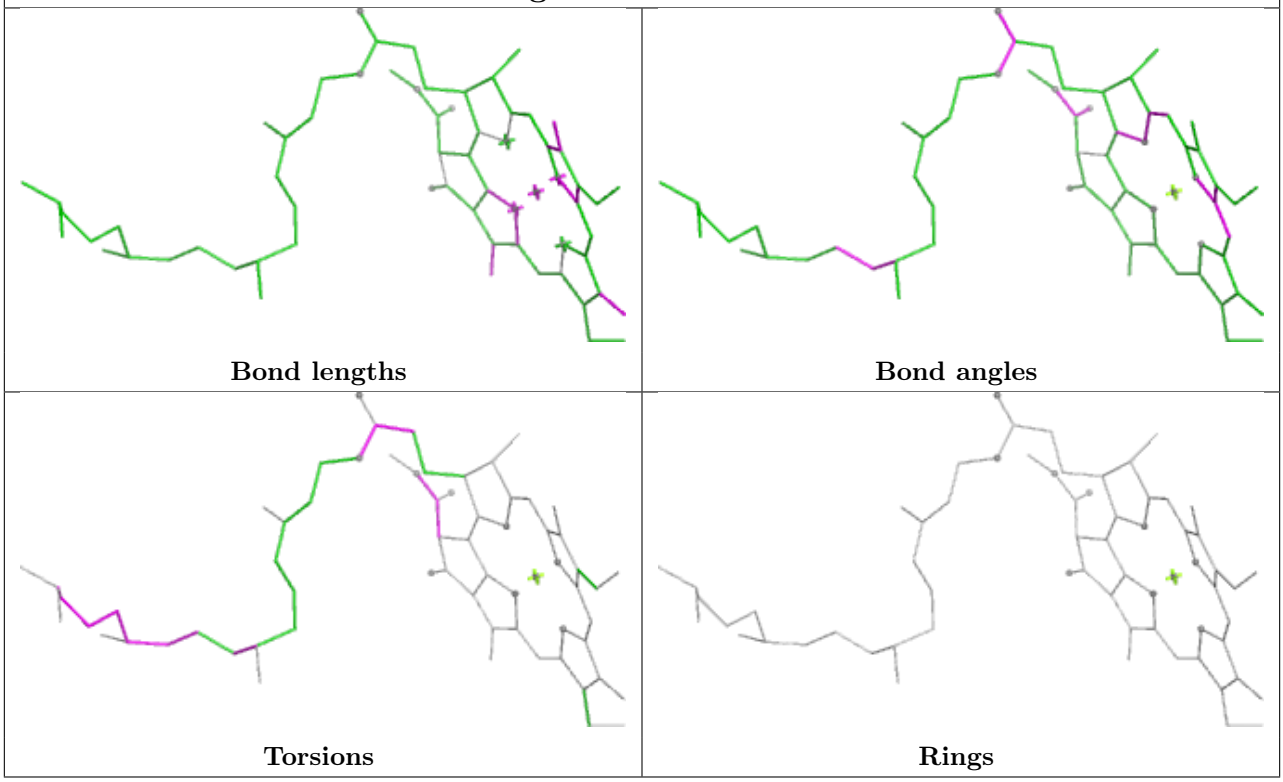


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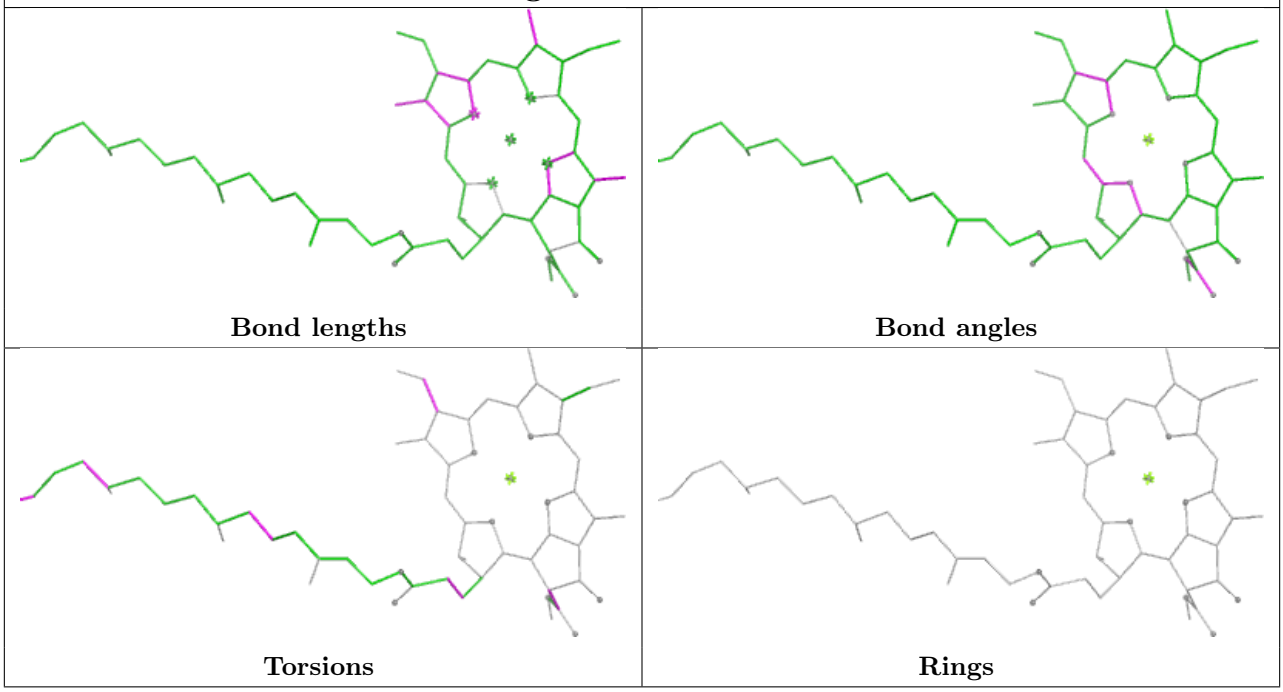


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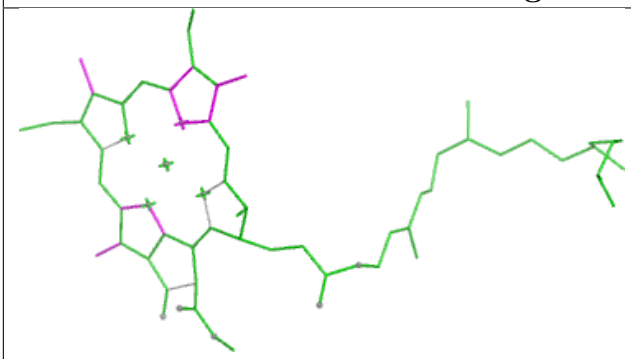
Ligand CLA 2 803



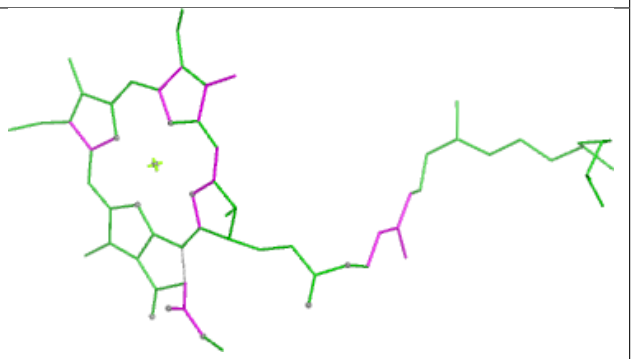
Ligand CLA A 835



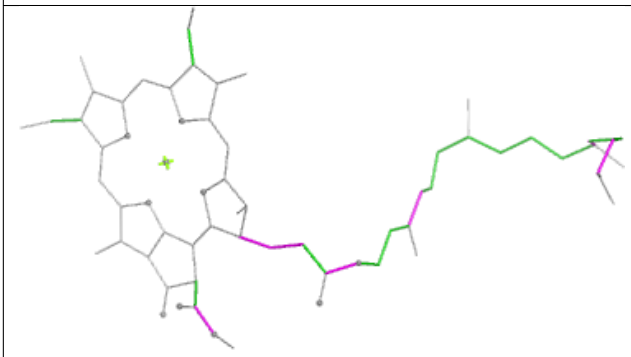
Ligand CLA B 809



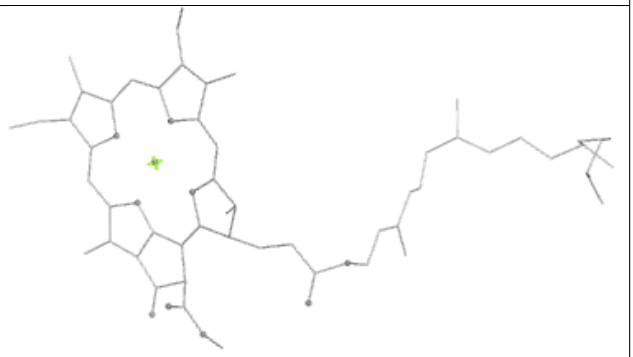
Bond lengths



Bond angles

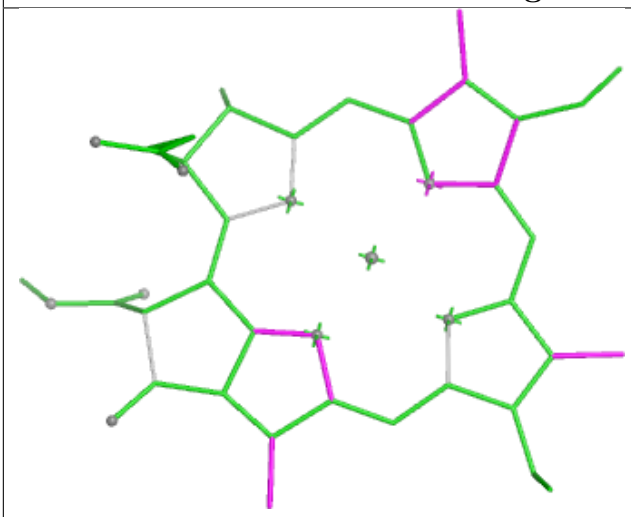


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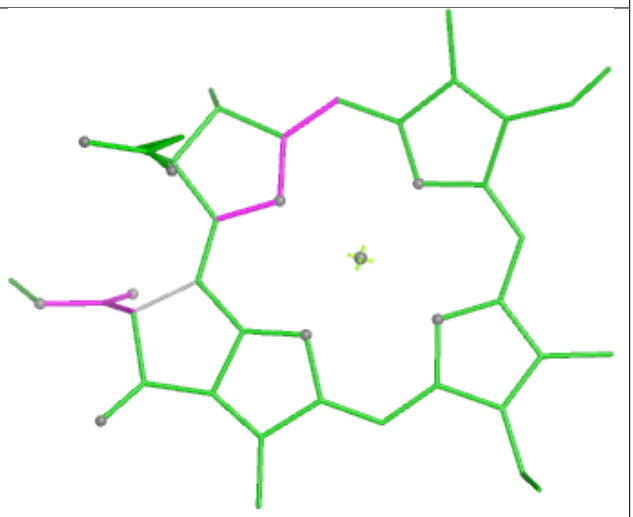


Rings

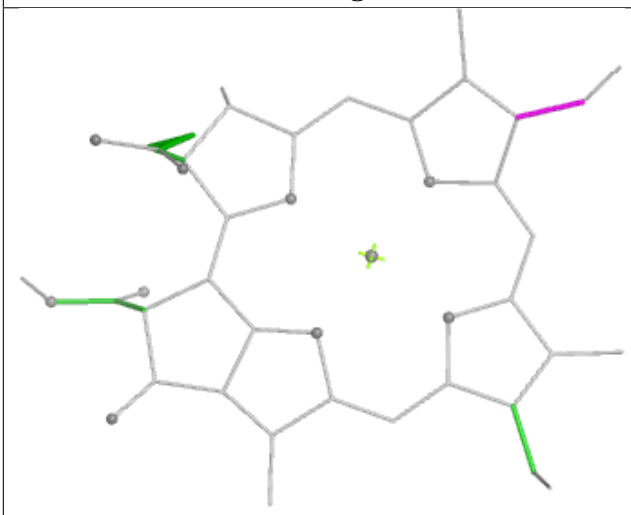
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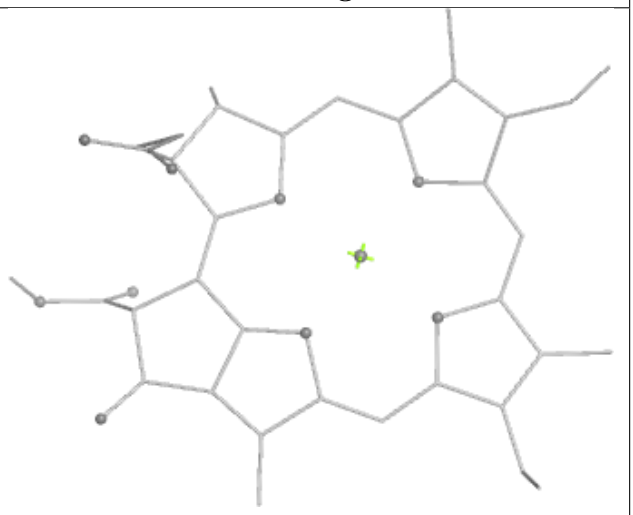
Bond lengths



Bond angles



Torsions



Rings

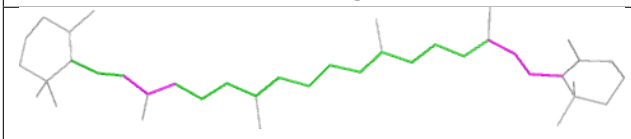
Ligand BCR B 844



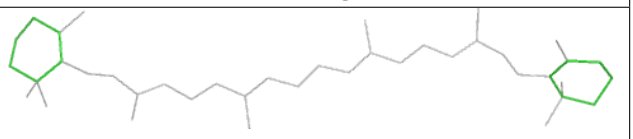
Bond lengths



Bond angles



Torsions



Rings

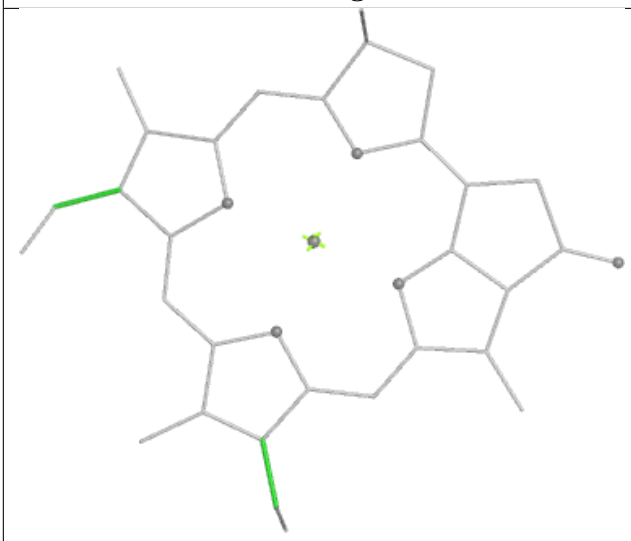
Ligand CLA M 102



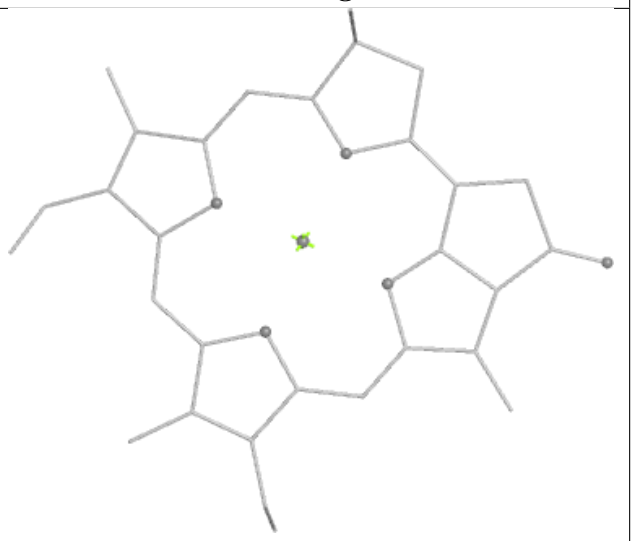
Bond lengths



Bond angles

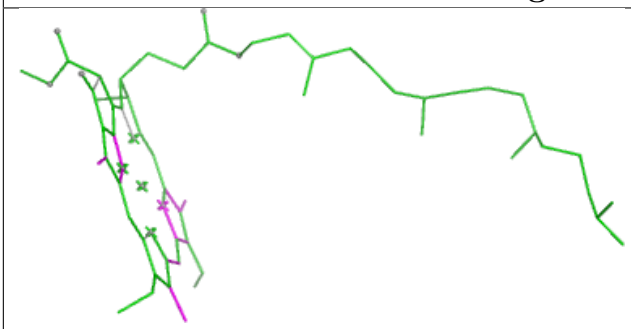


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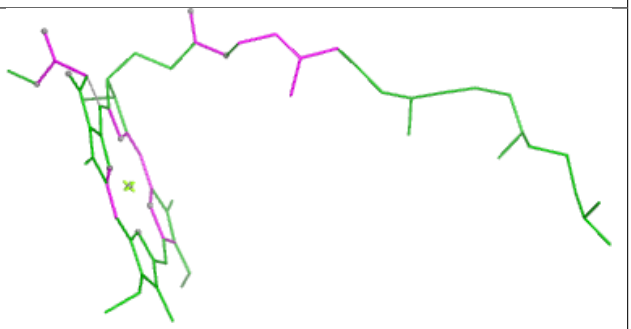


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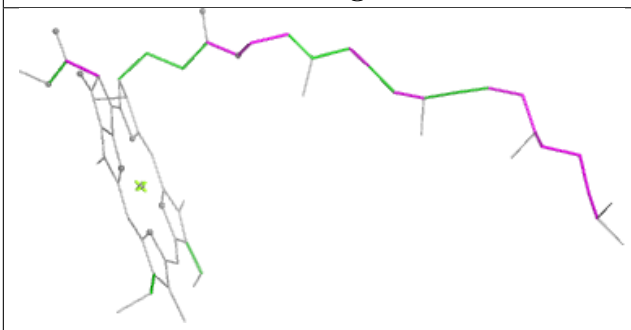
Ligand CLA 2 805



Bond lengths



Bond angles

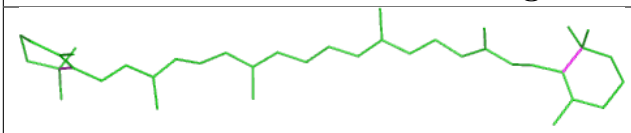


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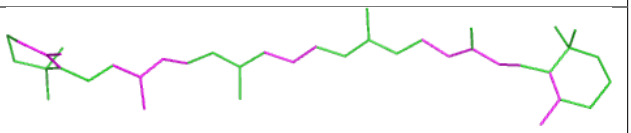


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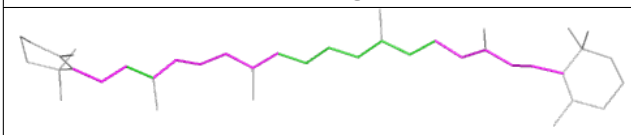
Ligand BCR B 851



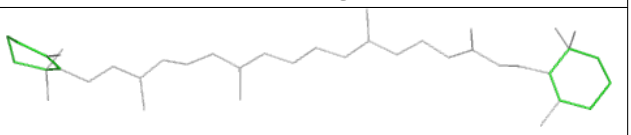
Bond lengths



Bond angles

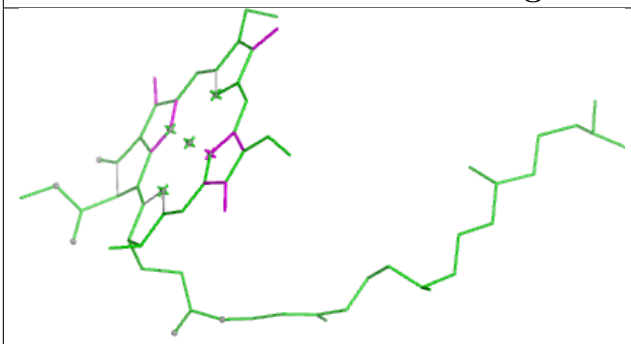


Torsions

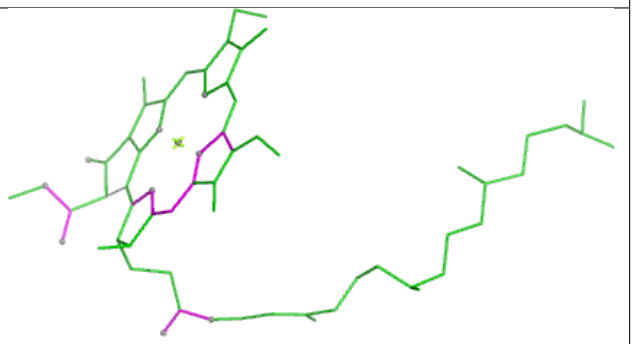


Rings

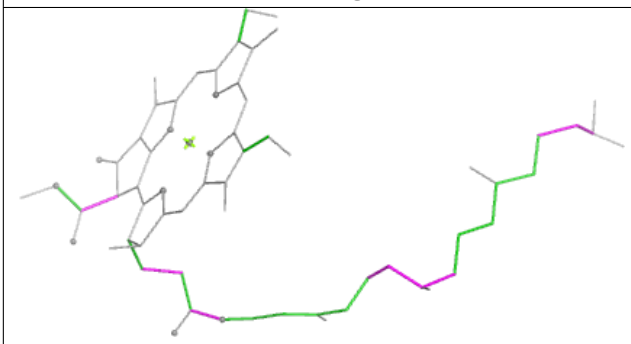
Ligand CLA B 815



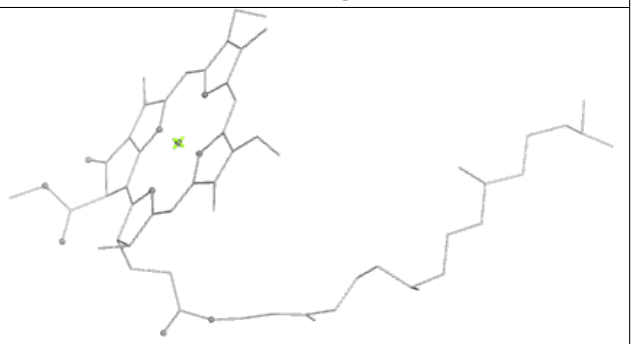
Bond lengths



Bond angles



Torsions

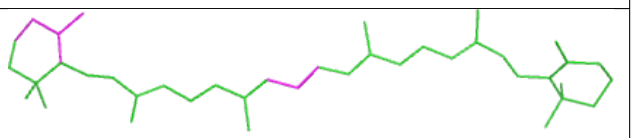


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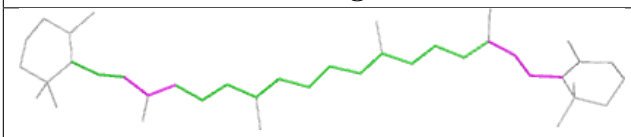
Ligand BCR 2 845



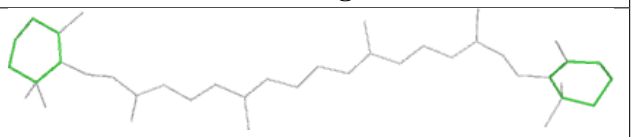
Bond lengths



Bond angles

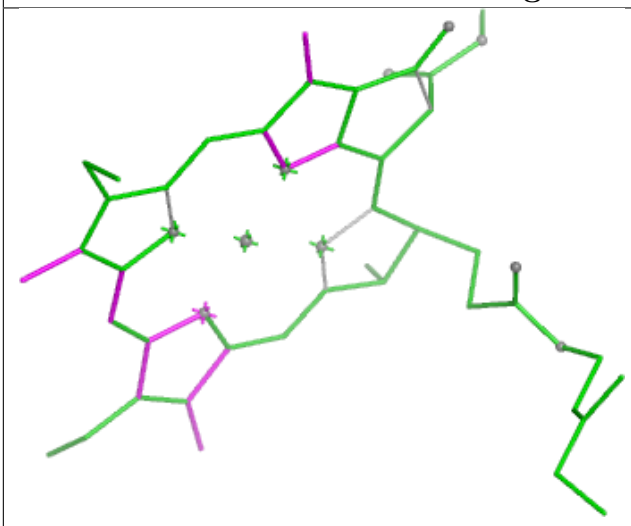


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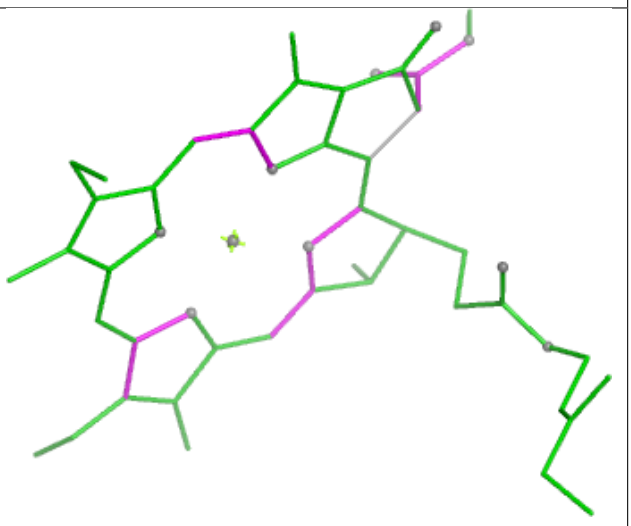


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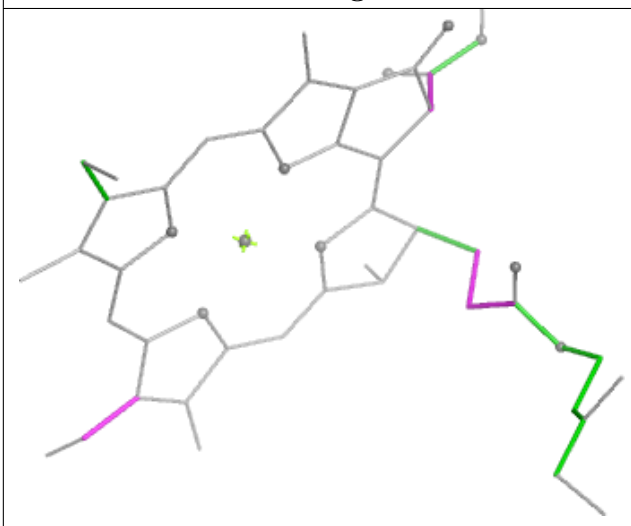
Ligand CLA A 808



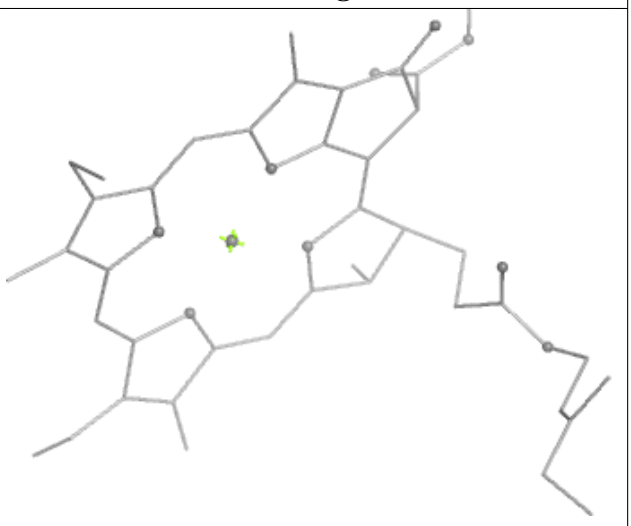
Bond lengths



Bond angles

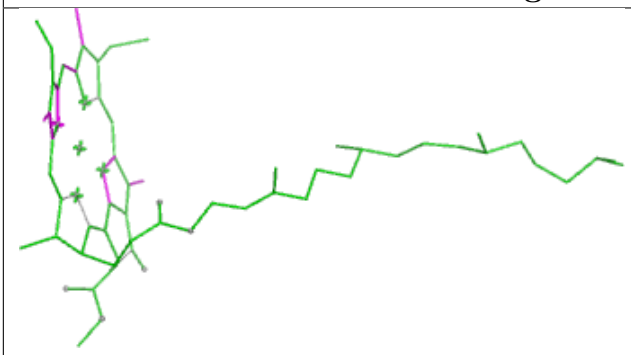


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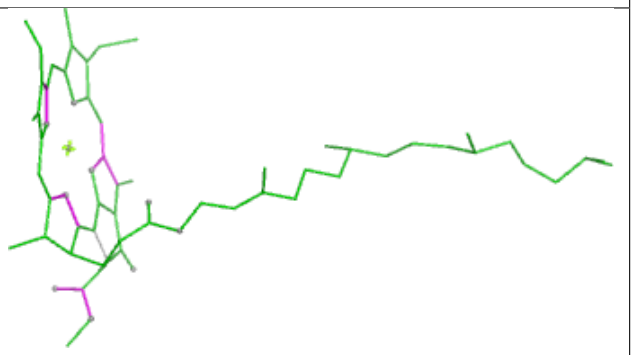


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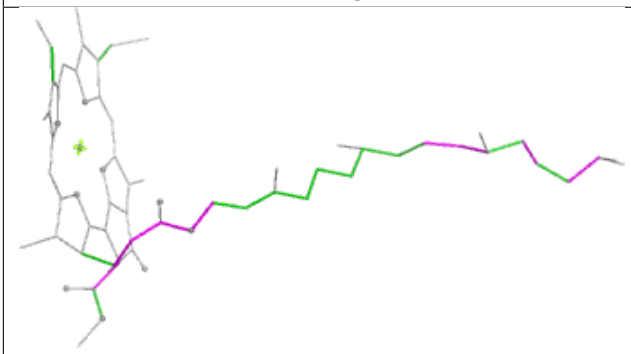
Ligand CLA B 828



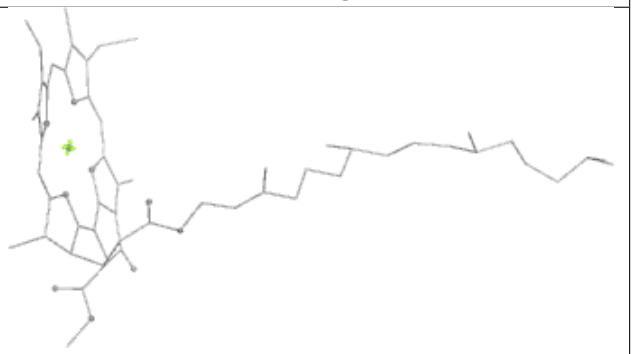
Bond lengths



Bond angles

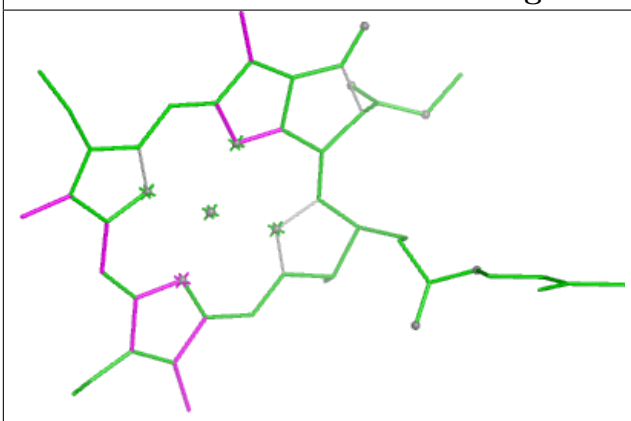


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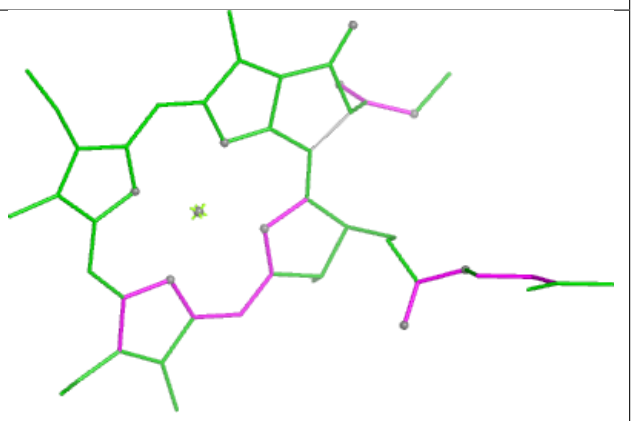


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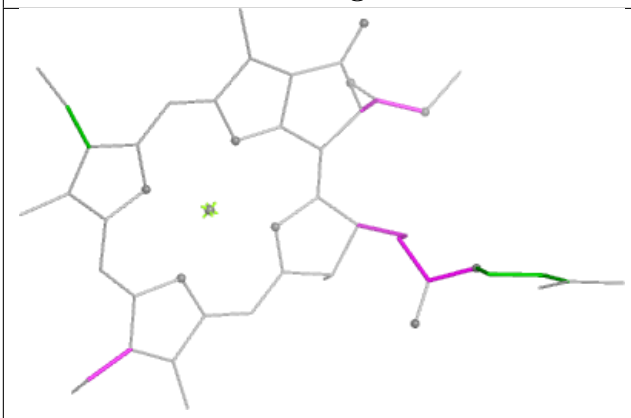
Ligand CLA B 835



Bond lengths



Bond angles

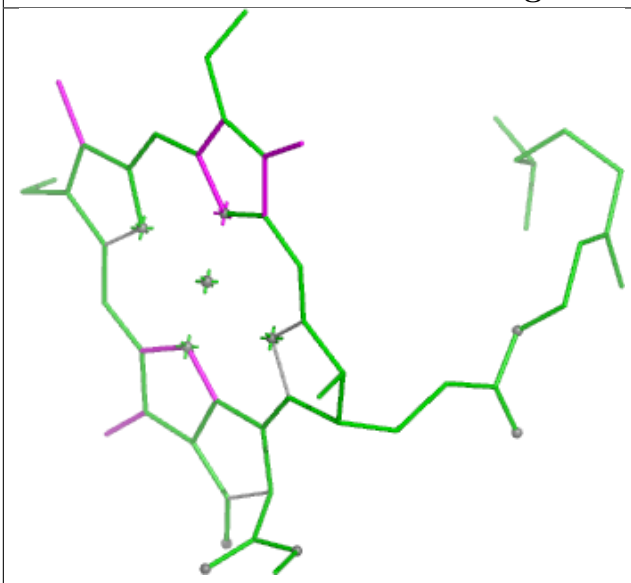


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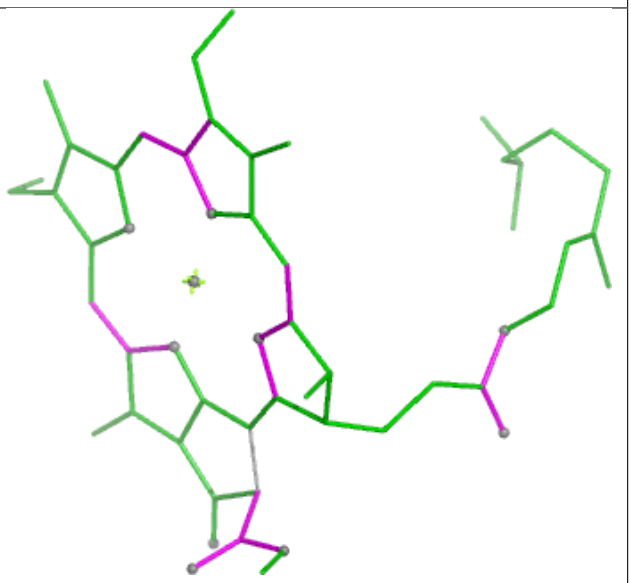


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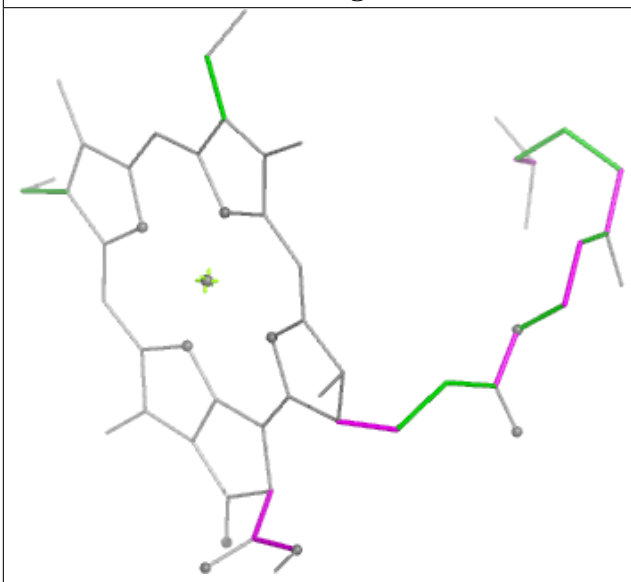
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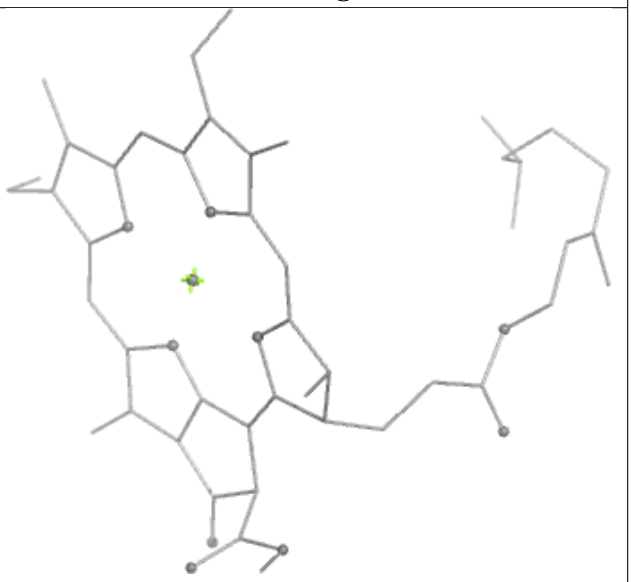
Bond lengths



Bond angles

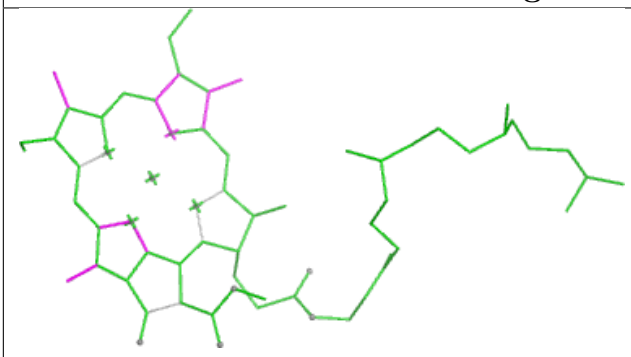


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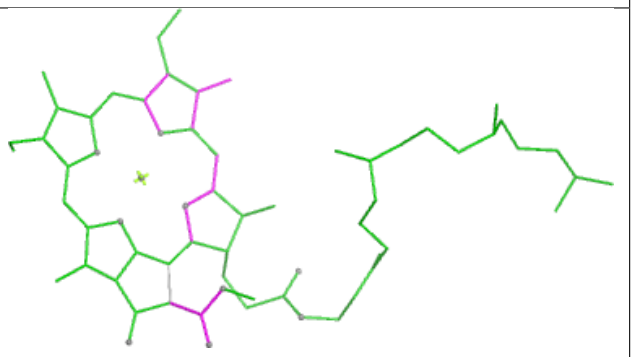


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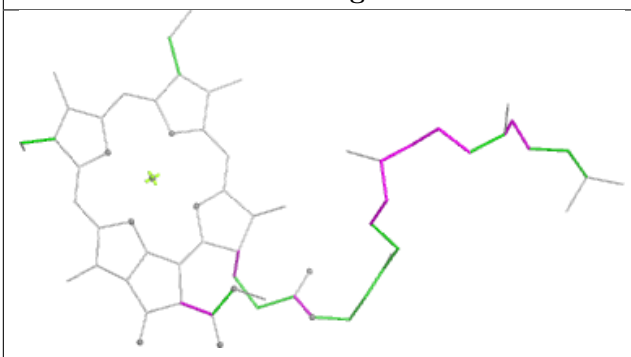
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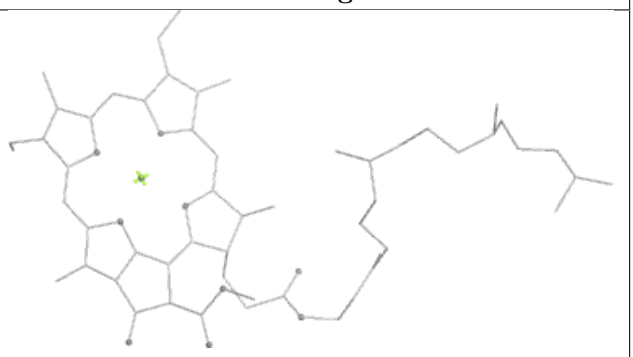
Bond lengths



Bond angles

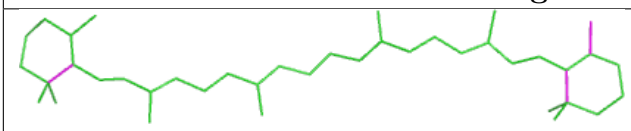


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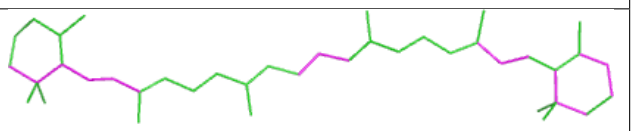


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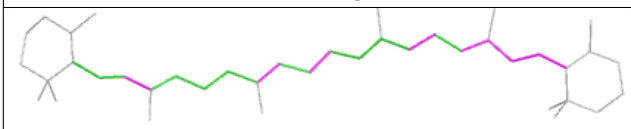
Ligand BCR l 207



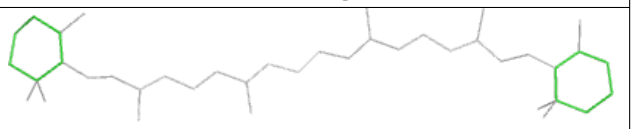
Bond lengths



Bond angles

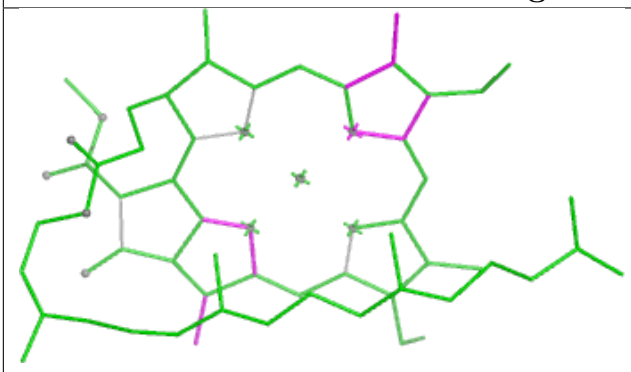


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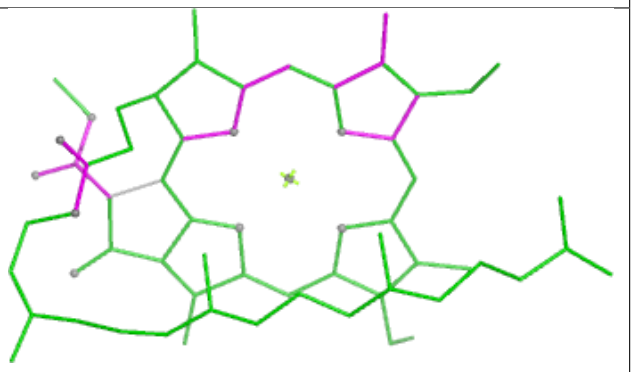


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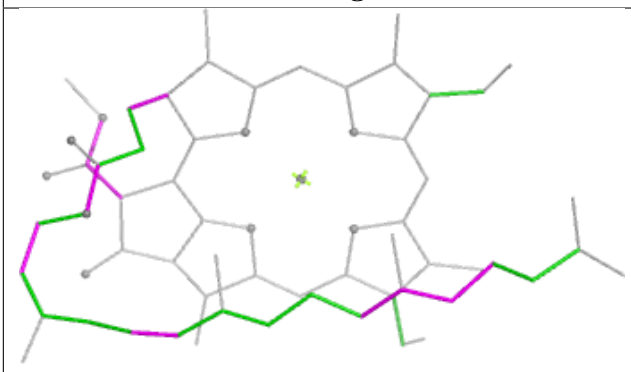
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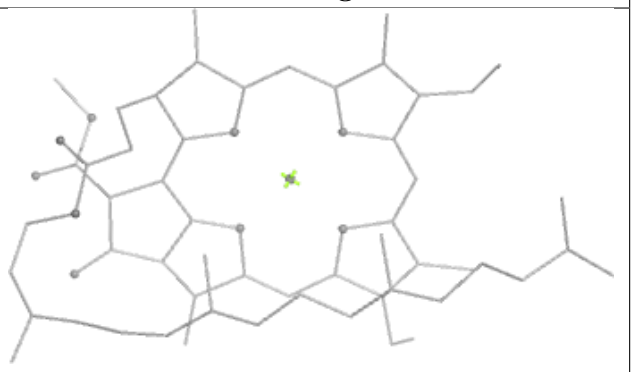
Bond lengths



Bond angles



Torsions

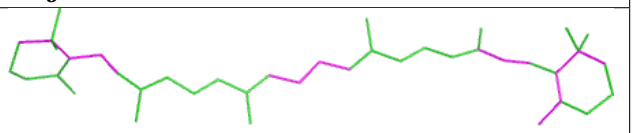


Rings

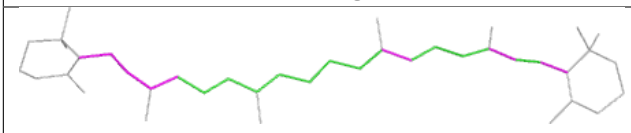
Ligand BCR j 1304



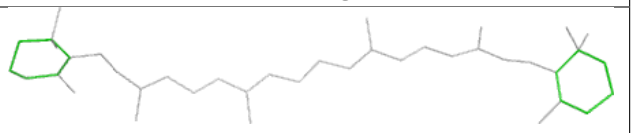
Bond lengths



Bond angles

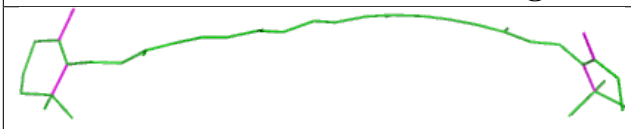


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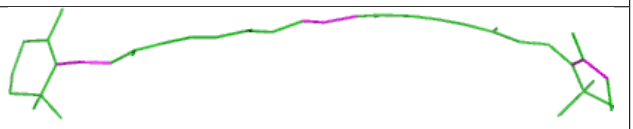


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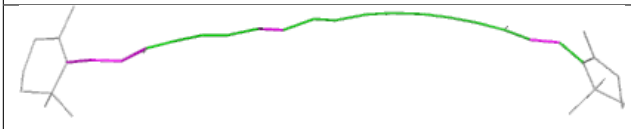
Ligand BCR 7 101



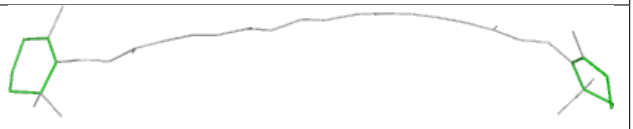
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Bond angles

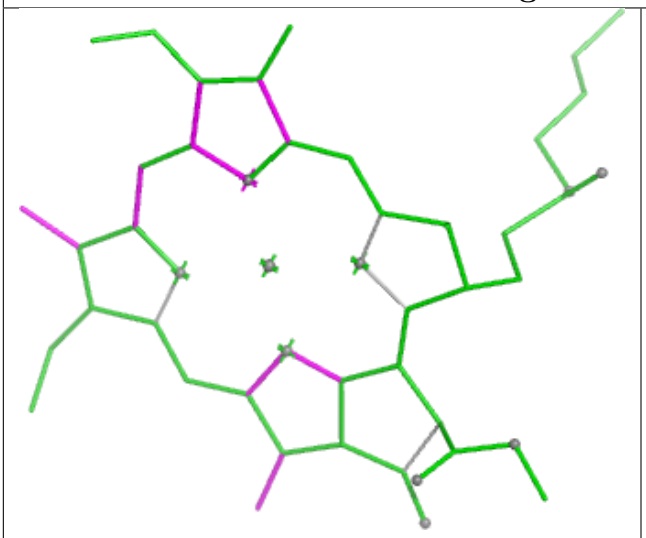


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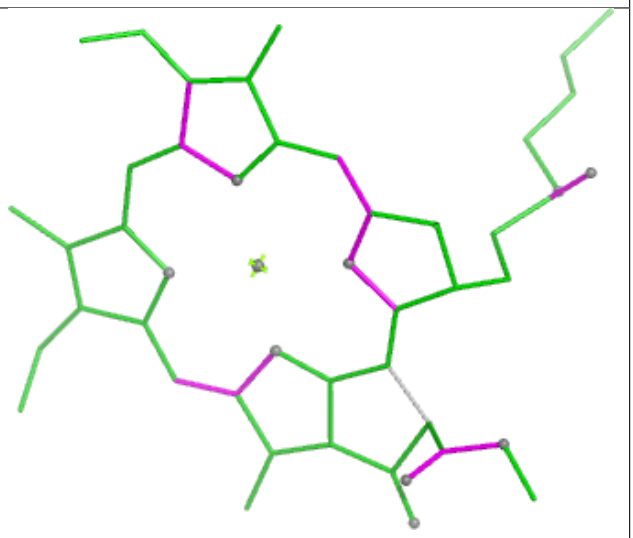


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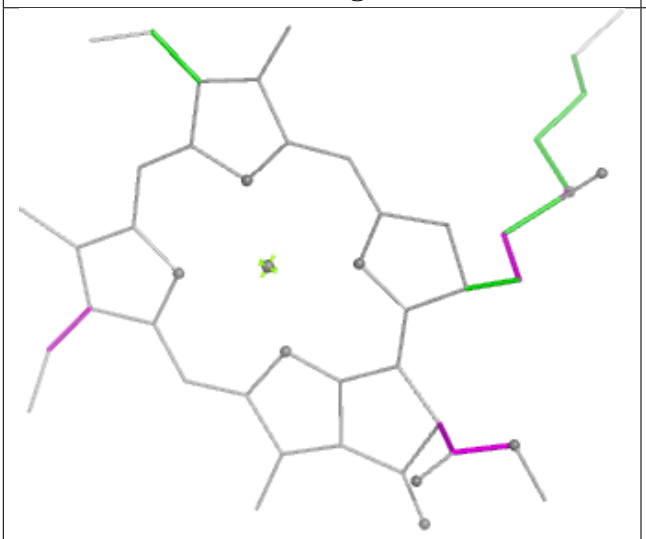
Ligand CLA 1 1612



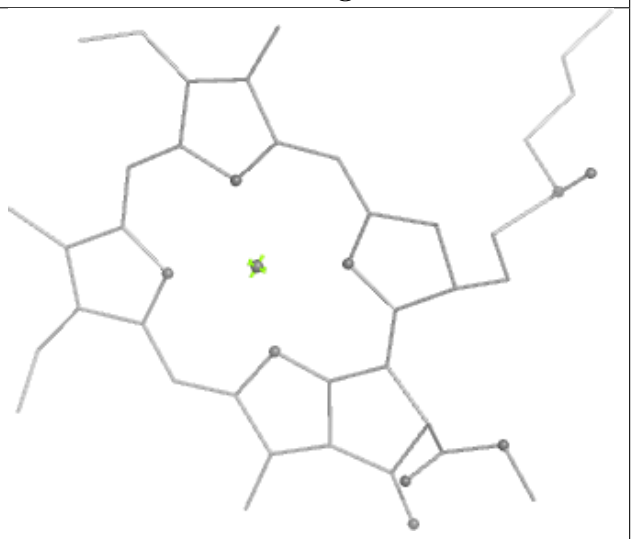
Bond lengths



Bond angles

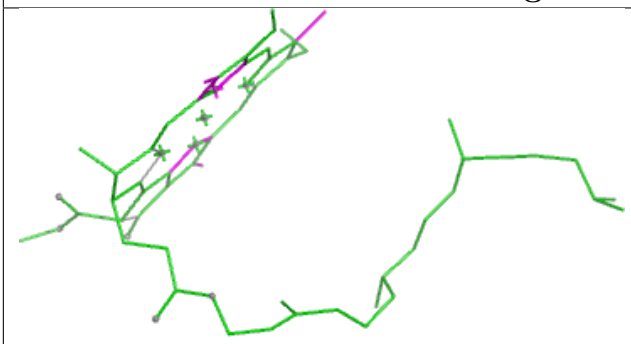


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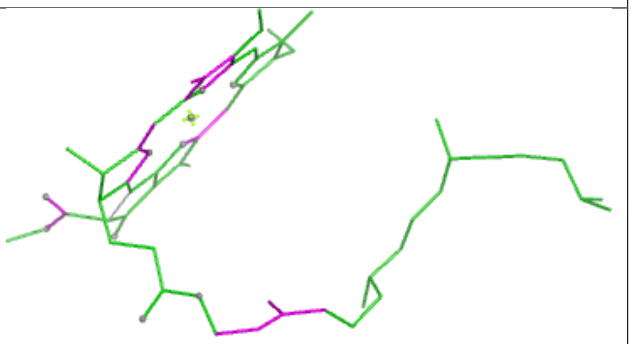


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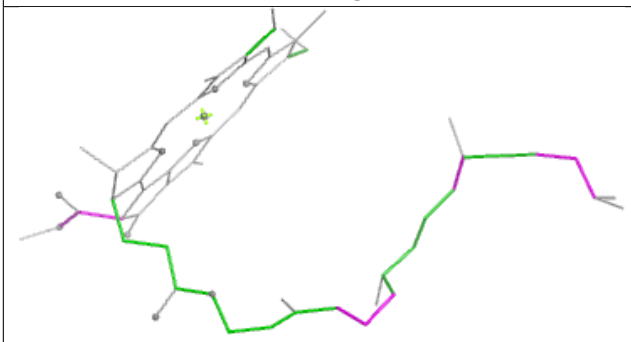
Ligand CLA B 811



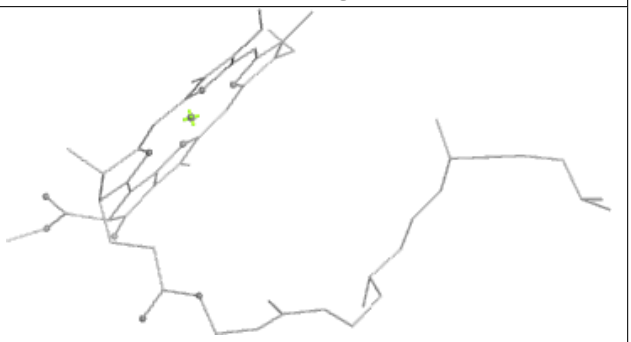
Bond lengths



Bond angles

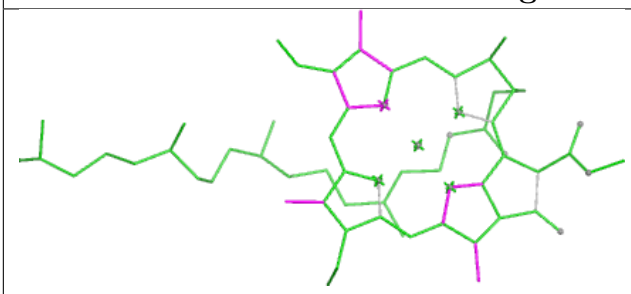


Torsions



Rings

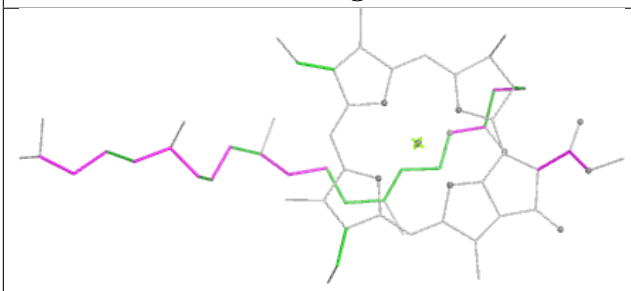
Ligand CLA 1 1640



Bond lengths



Bond angles

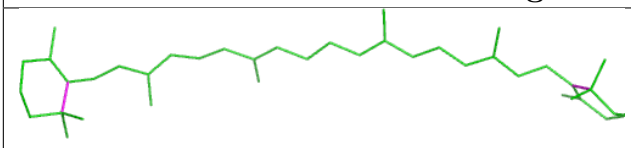


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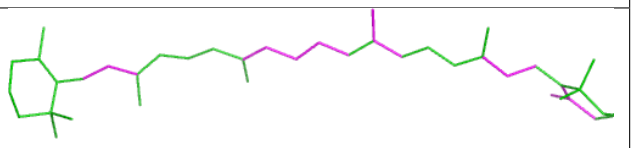


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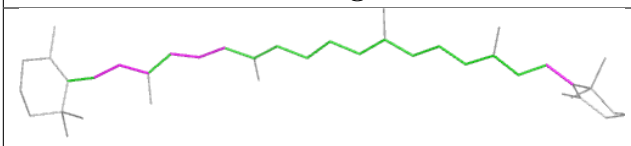
Ligand BCR 9 102



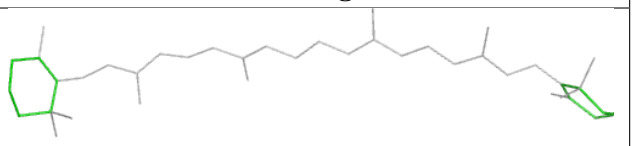
Bond lengths



Bond angles

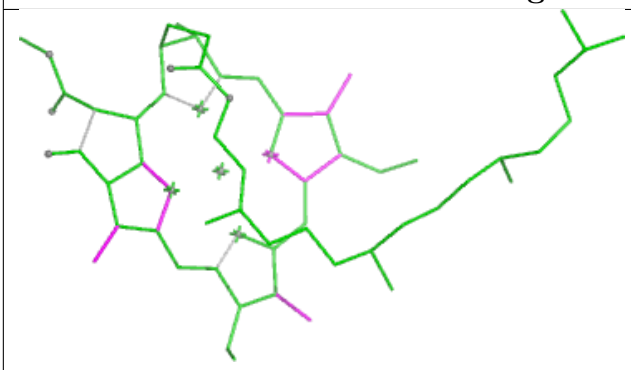


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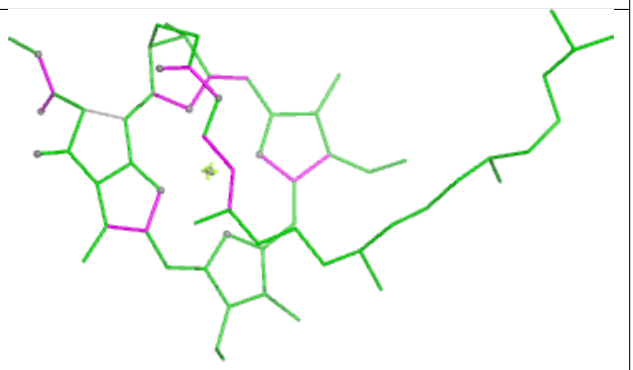


Rings

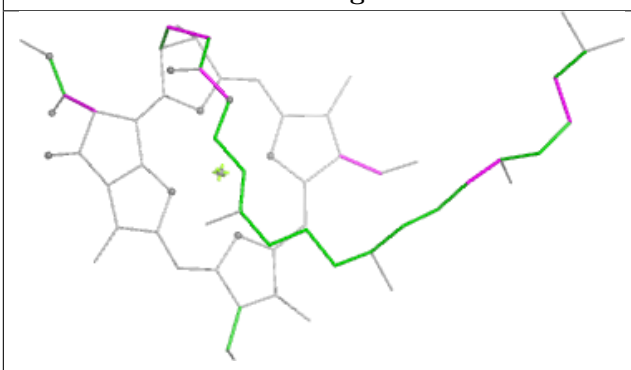
Ligand CLA b 808



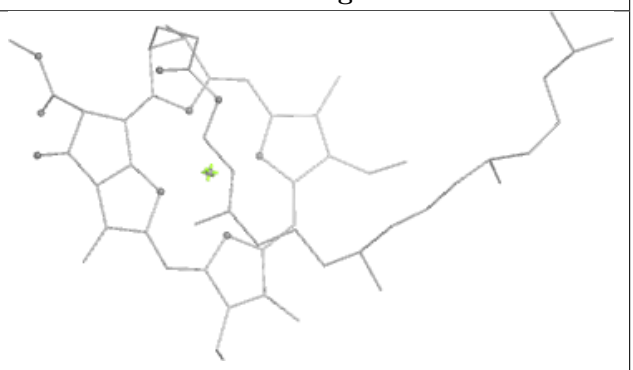
Bond lengths



Bond angles

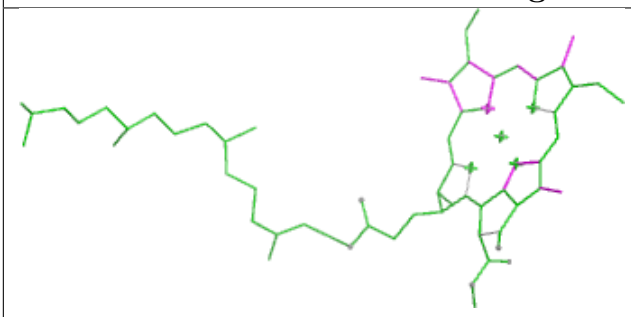


Torsions

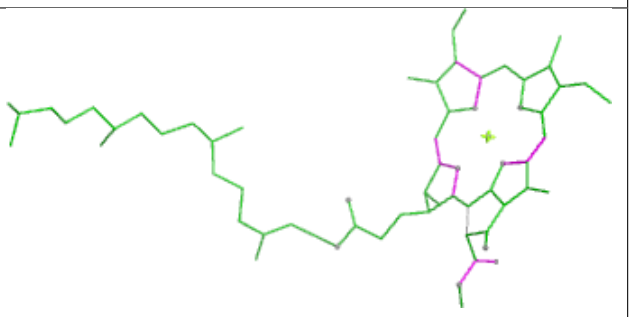


Rings

Ligand CLA a 803



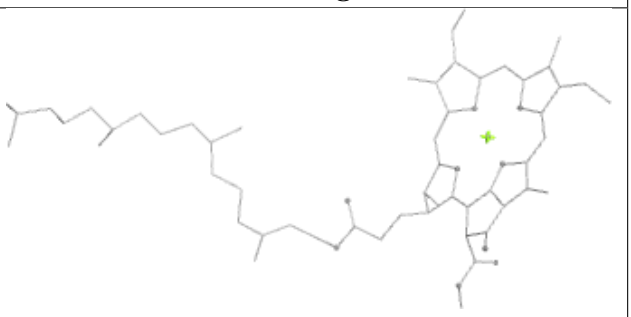
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Bond angles

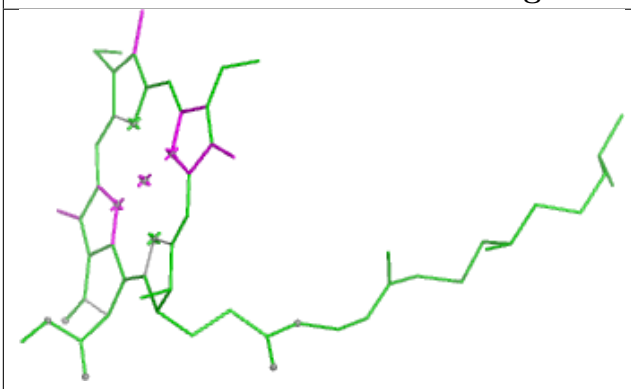


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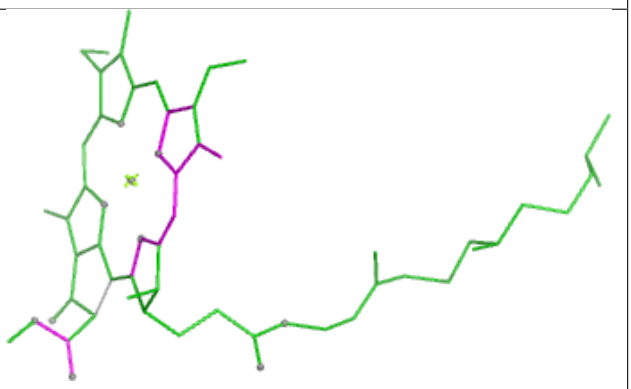


Rings

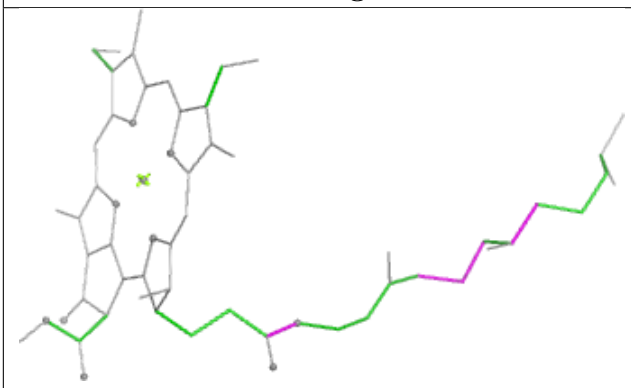
Ligand CLA A 832



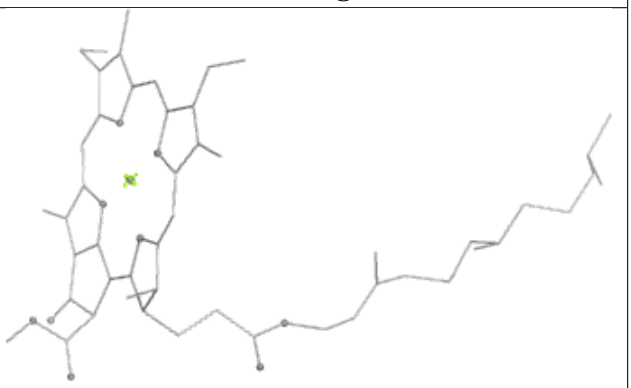
Bond lengths



Bond angles

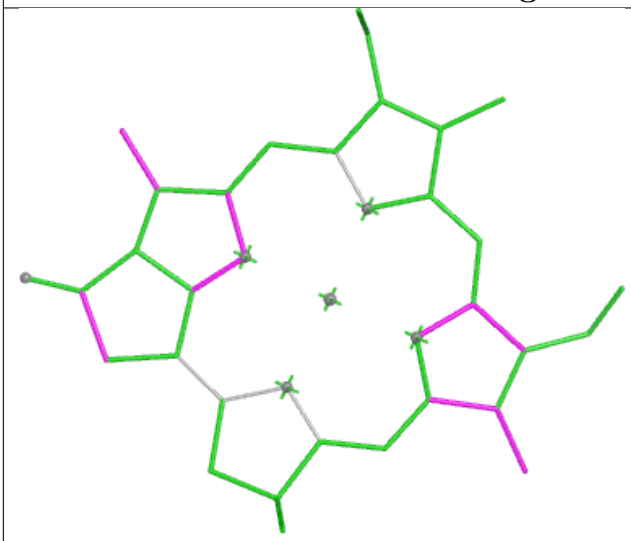


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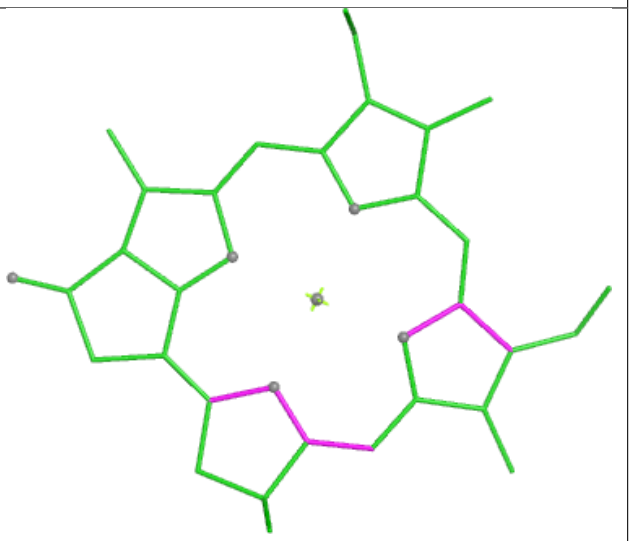


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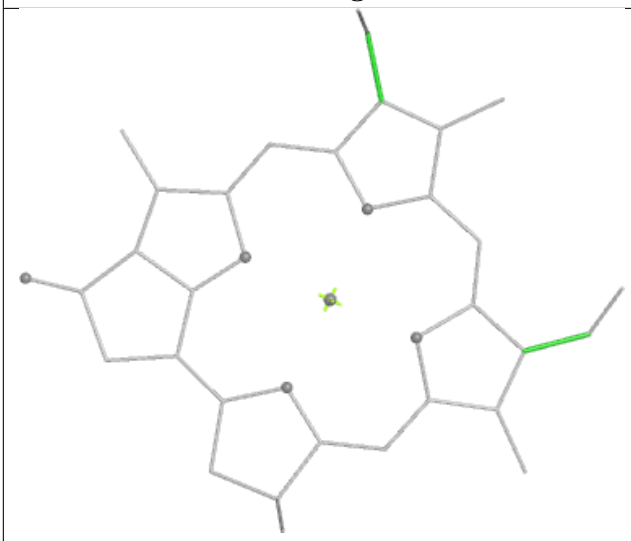
Ligand CLA 1 1601



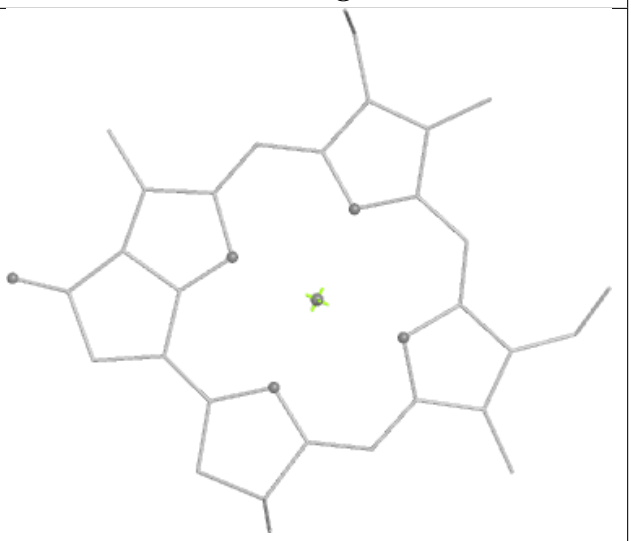
Bond lengths



Bond angles

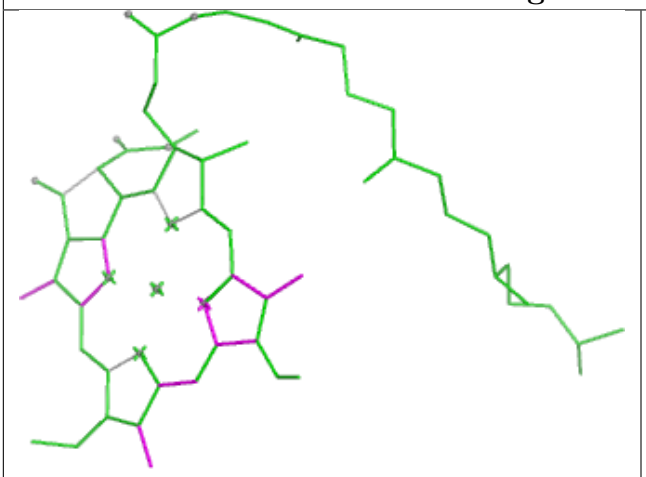


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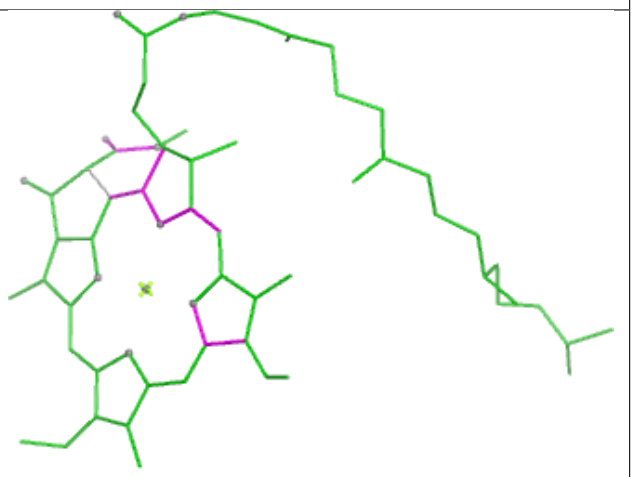


Rings

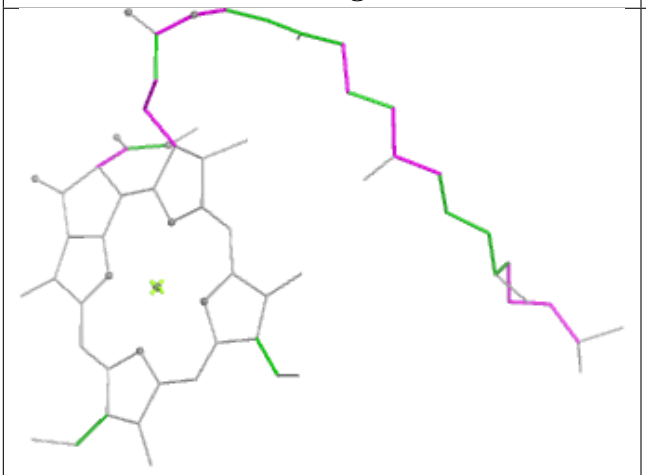
Ligand CLA b 825



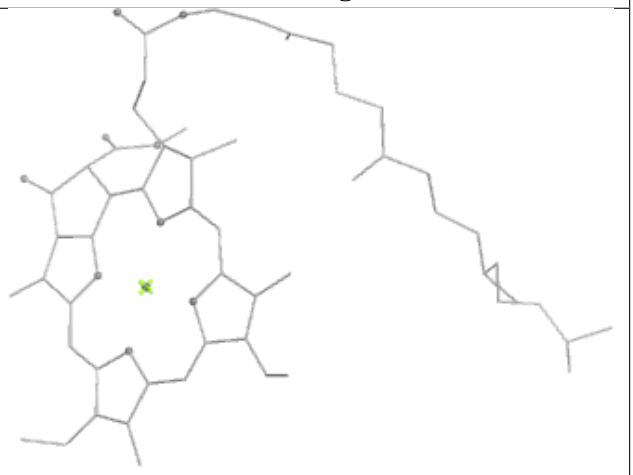
Bond lengths



Bond angles

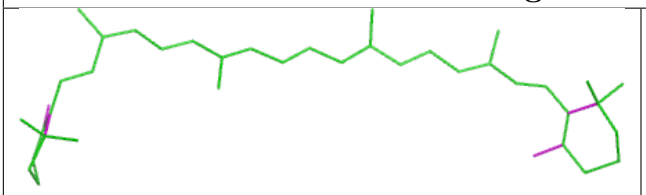


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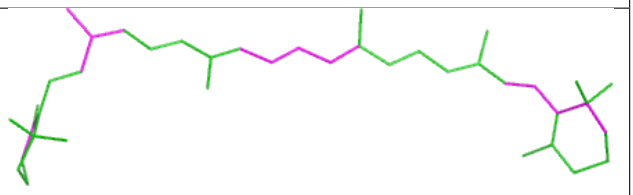


Rings

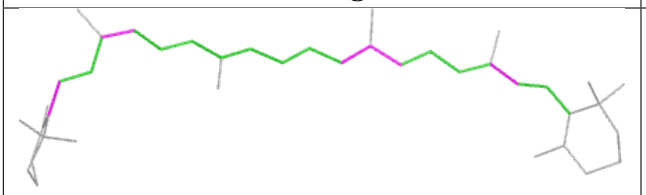
Ligand BCR L 201



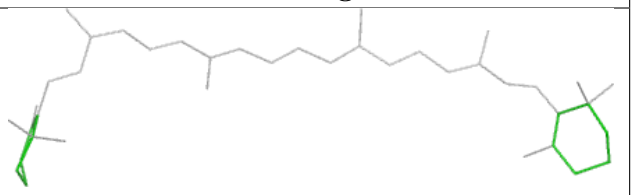
Bond lengths



Bond angles

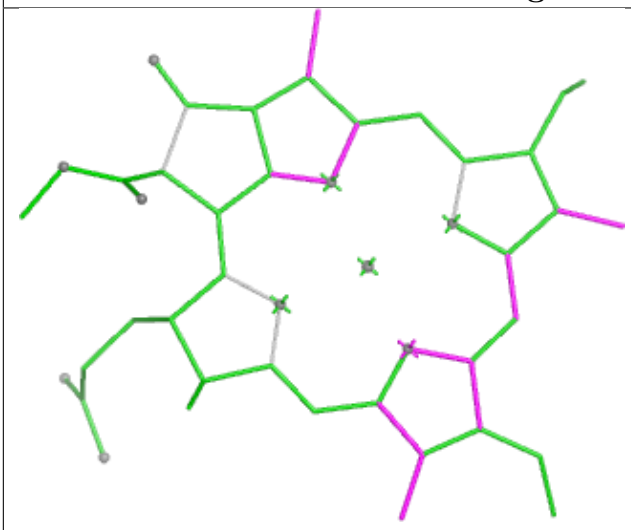


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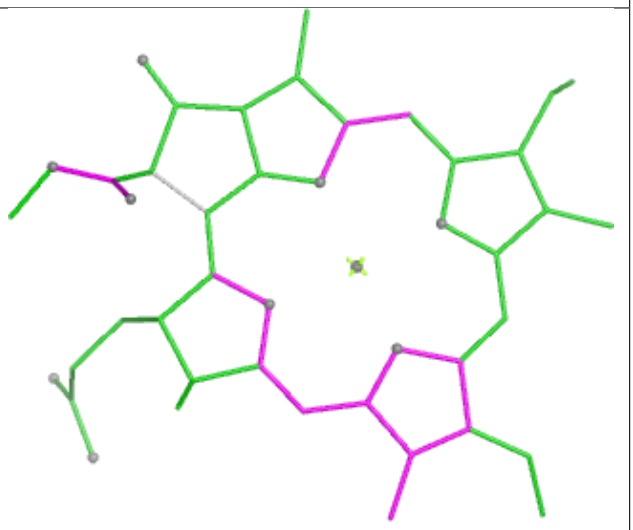


Rings

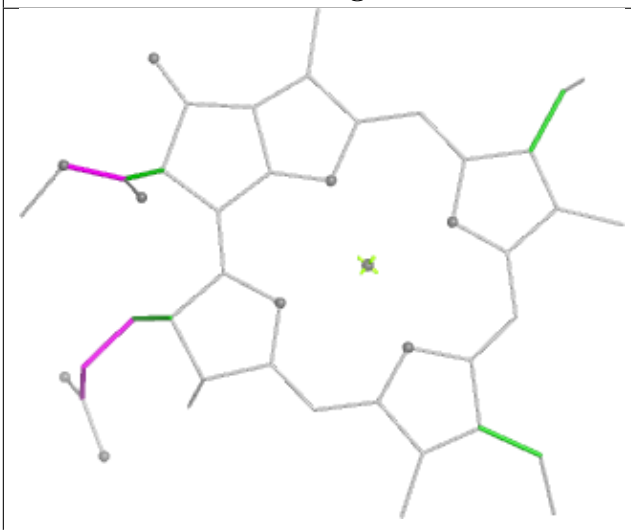
Ligand CLA b 824



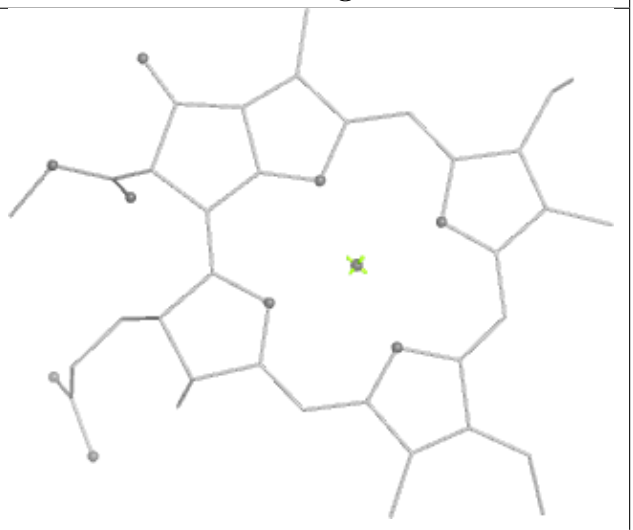
Bond lengths



Bond angles

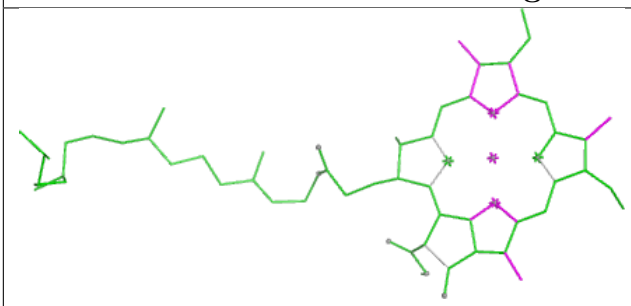


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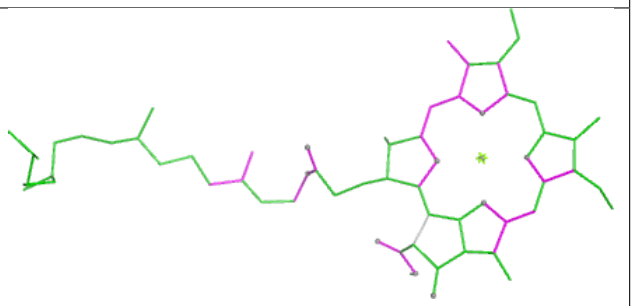


Rings

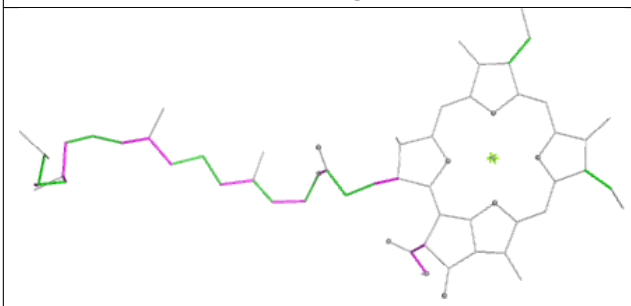
Ligand CLA A 806



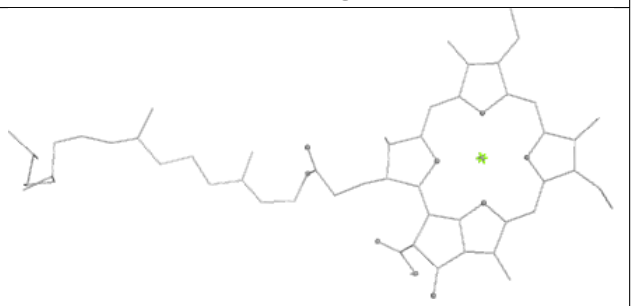
Bond lengths



Bond angles

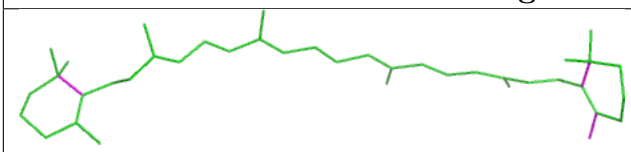


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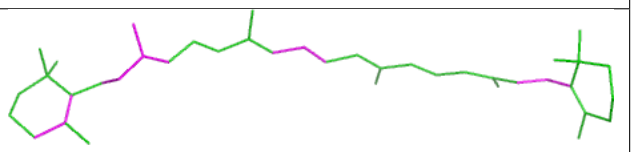


Rings

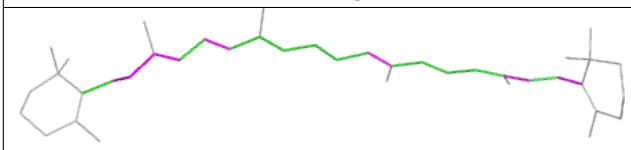
Ligand BCR M 103



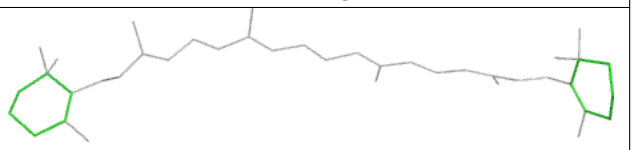
Bond lengths



Bond angles

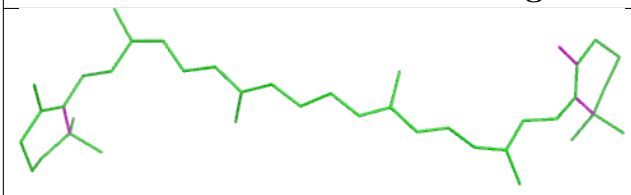


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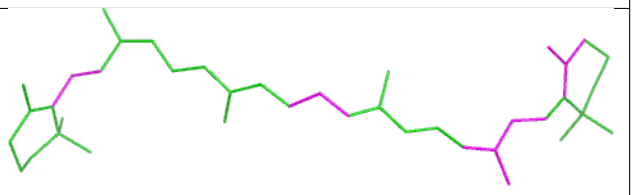


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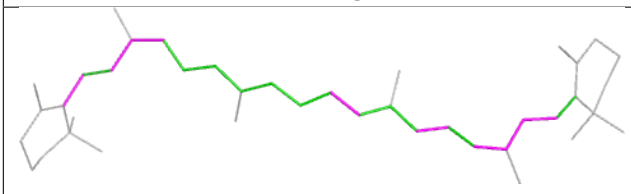
Ligand BCR b 846



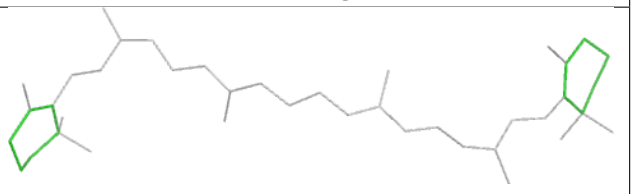
Bond lengths



Bond angles

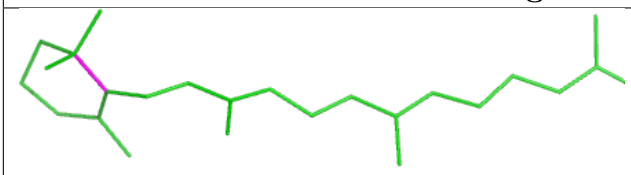


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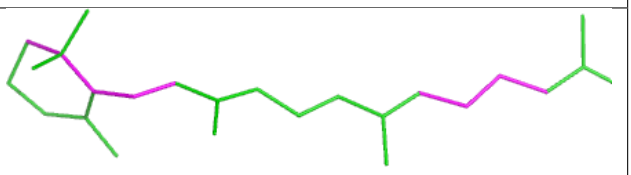


Rings

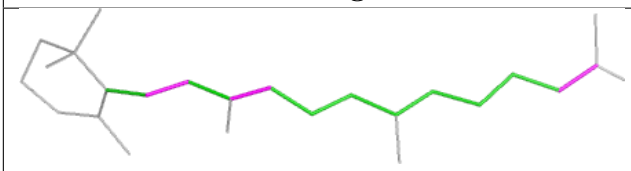
Ligand BCR k 104



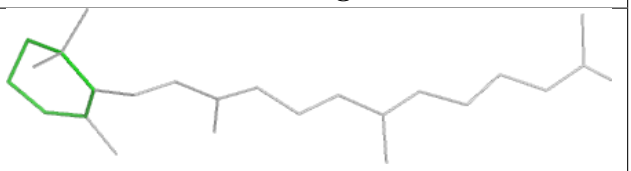
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Bond angles

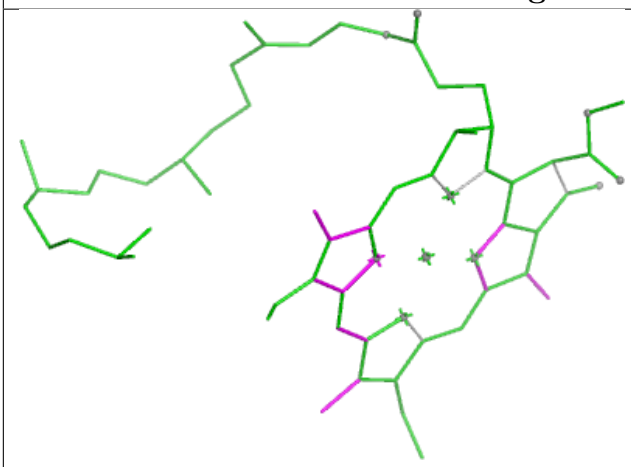


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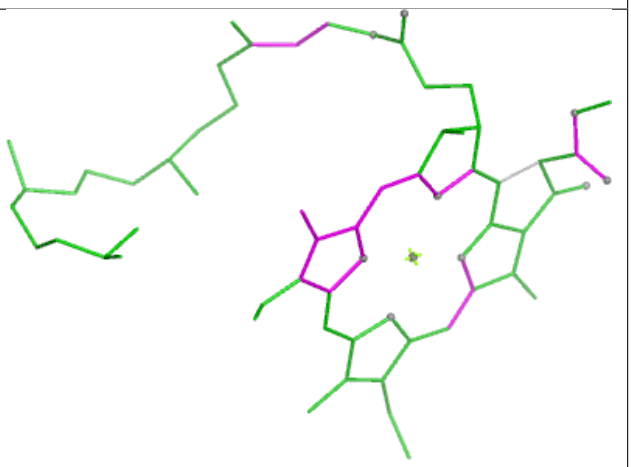


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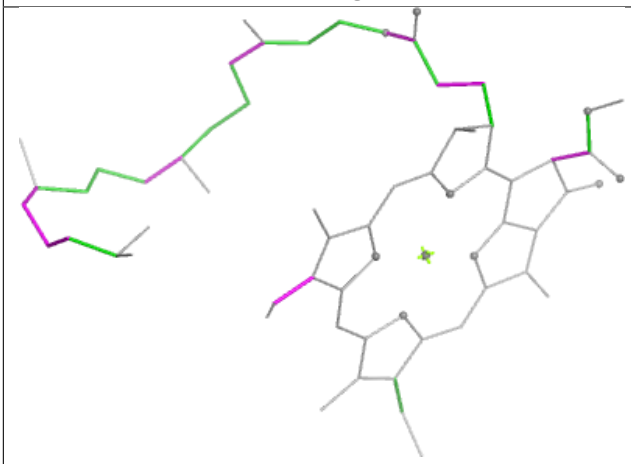
Ligand CLA a 825



Bond lengths



Bond angles

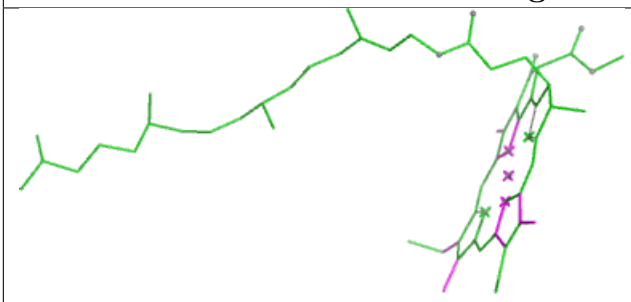


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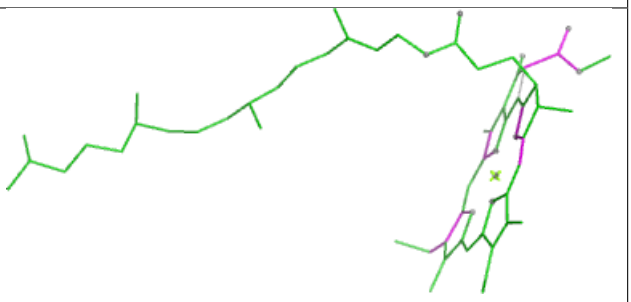


Rings

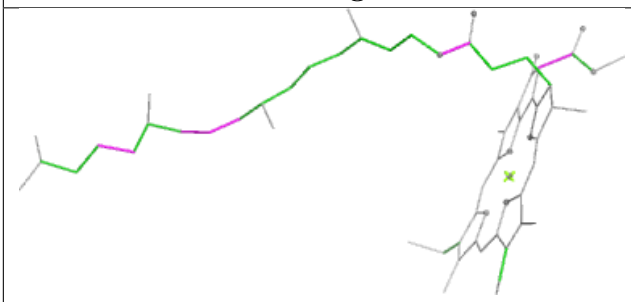
Ligand CLA 2 830



Bond lengths



Bond angles

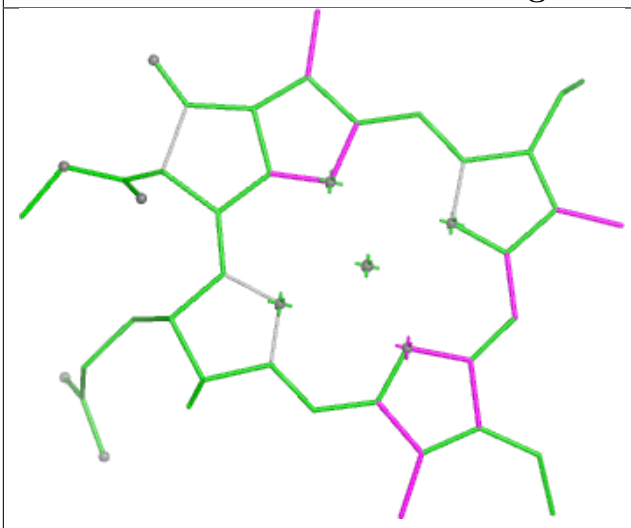


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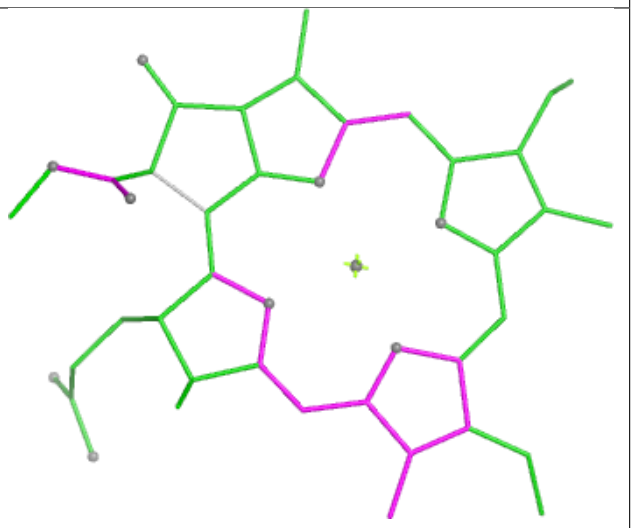


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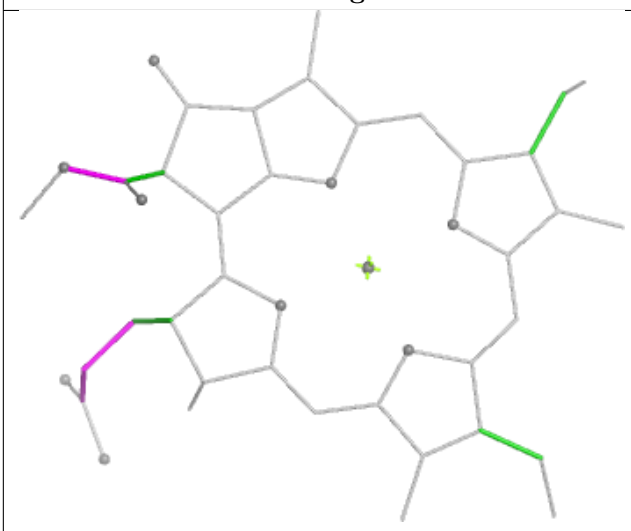
Ligand CLA 2 824



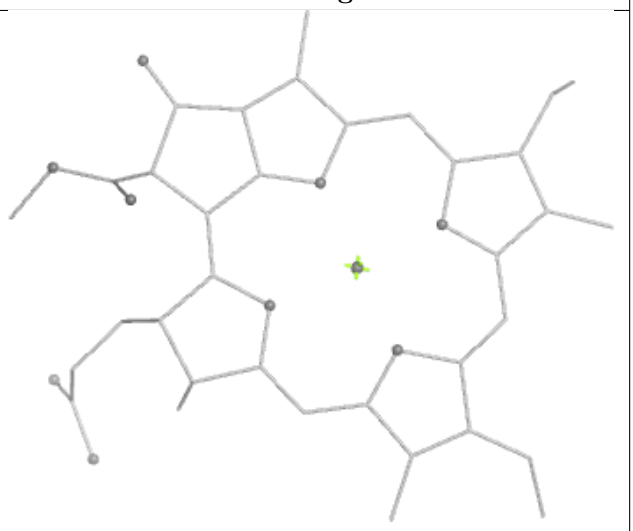
Bond lengths



Bond angles

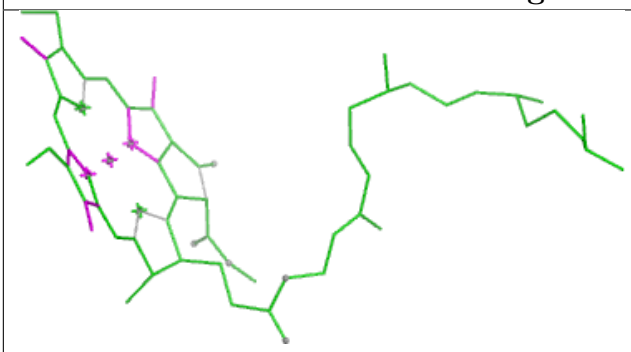


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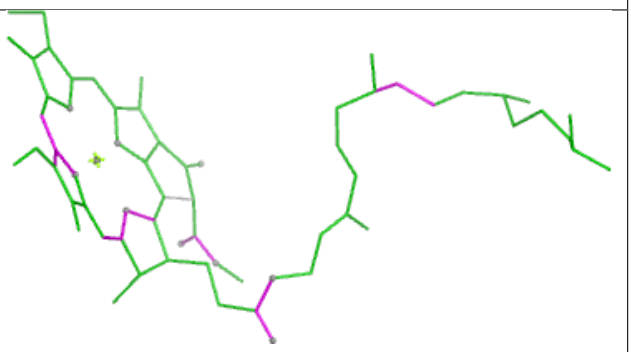


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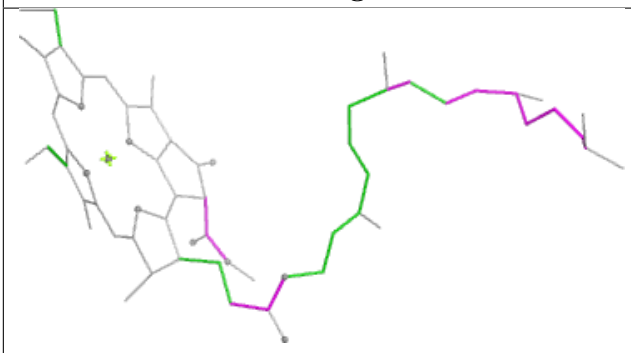
Ligand CLA b 803



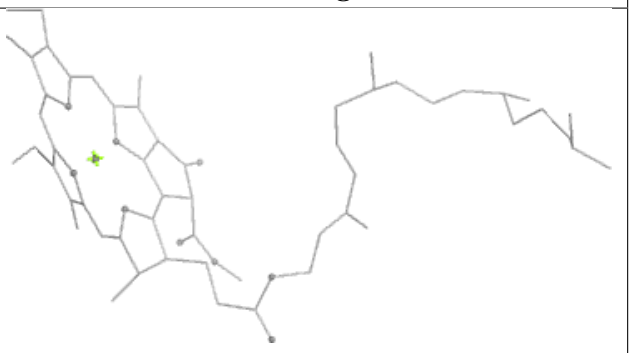
Bond lengths



Bond angles

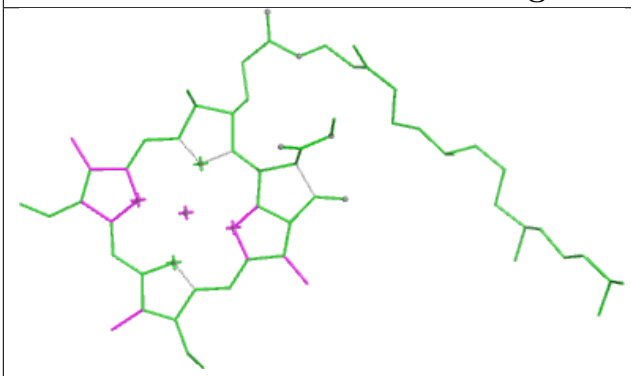


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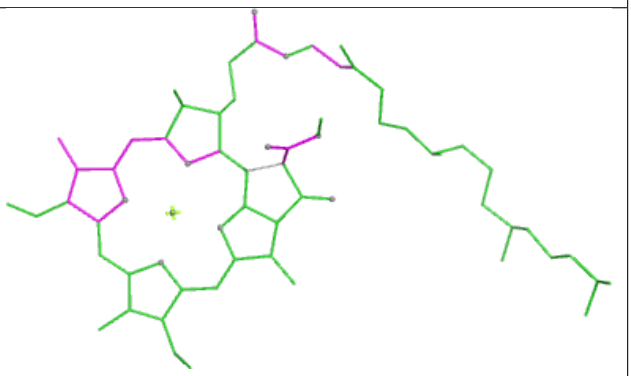


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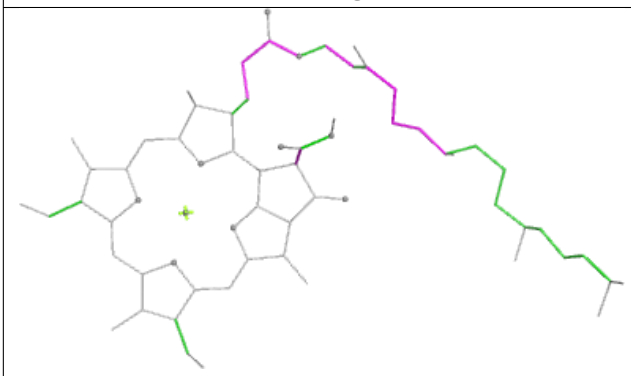
Ligand CLA 0 207



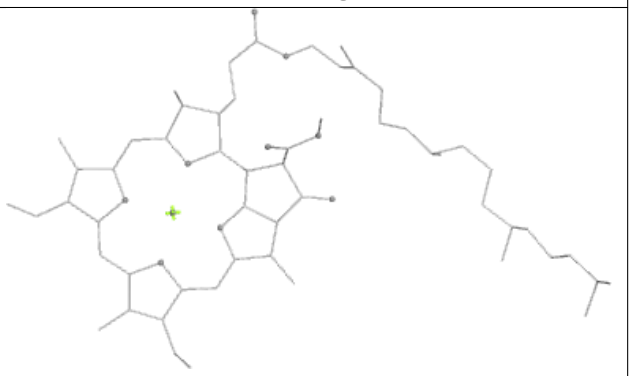
Bond lengths



Bond angles

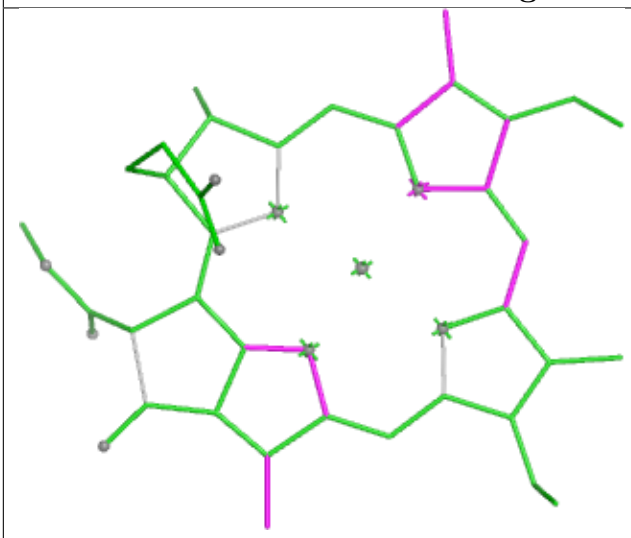


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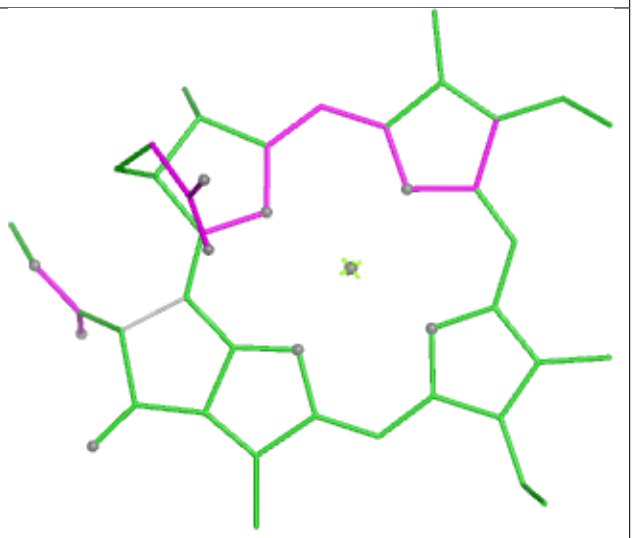


Rings

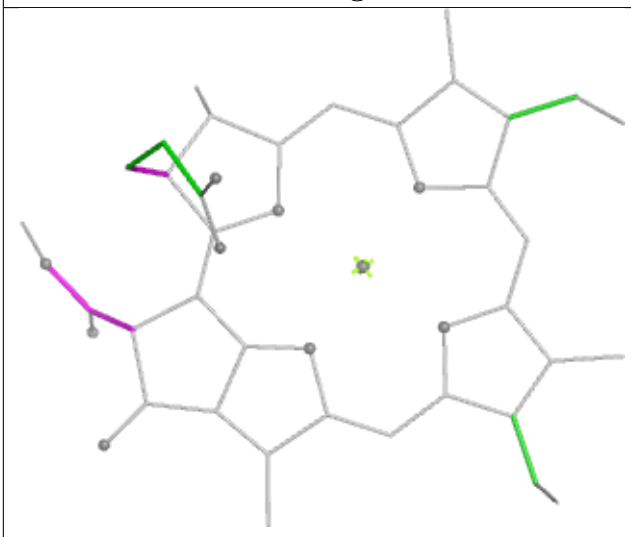
Ligand CLA 1 1638



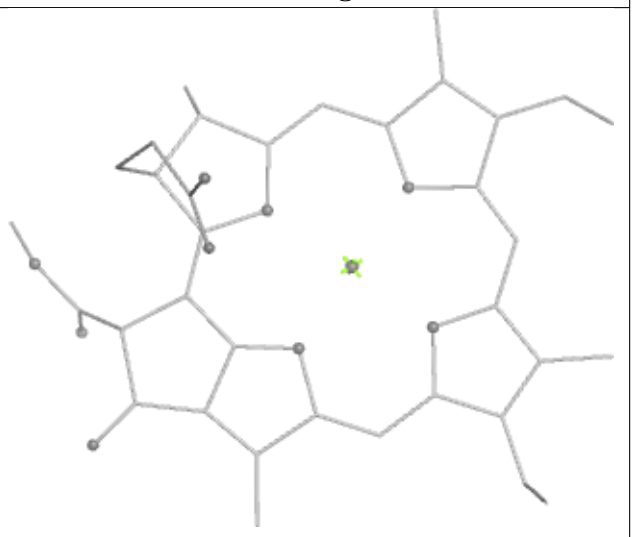
Bond lengths



Bond angles



Torsions

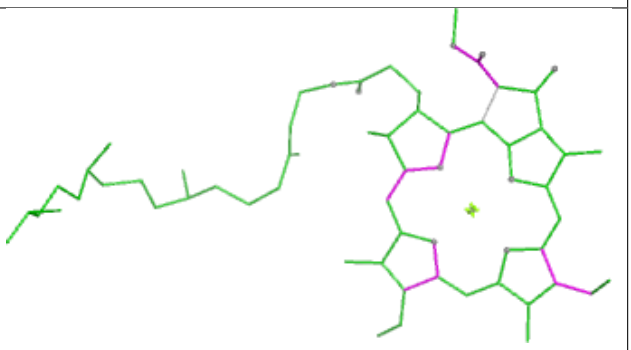


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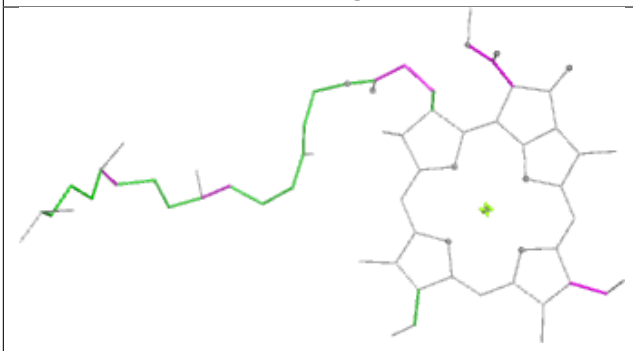
Ligand CLA b 804



Bond lengths



Bond angles

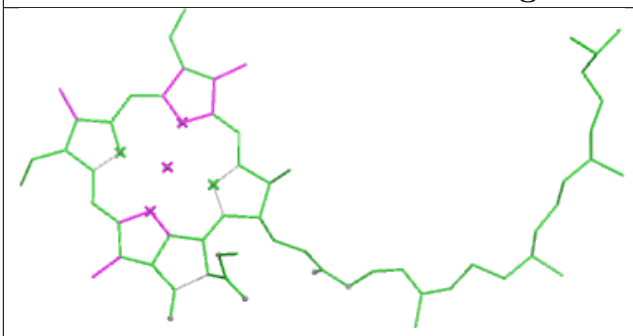


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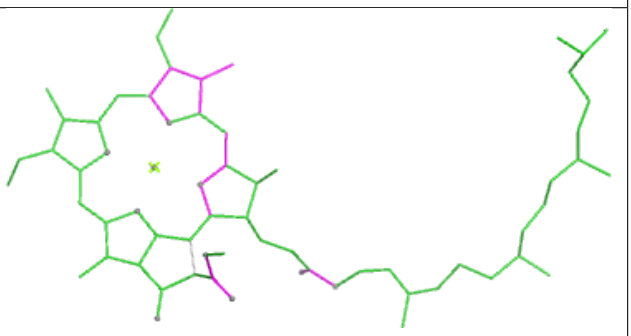


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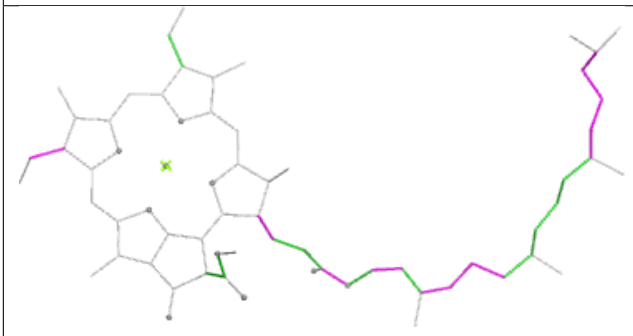
Ligand CLA 1 1639



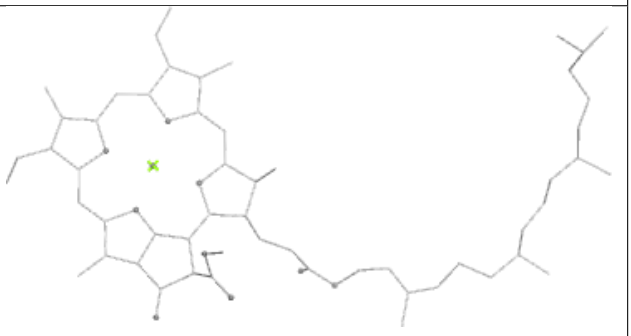
Bond lengths



Bond angles

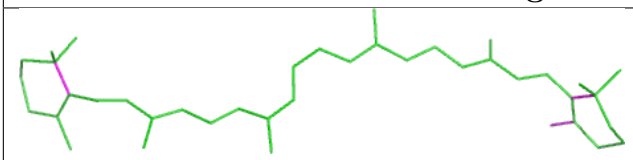


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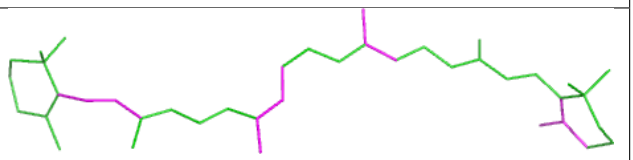


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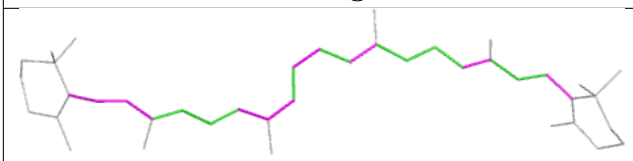
Ligand BCR 2 847



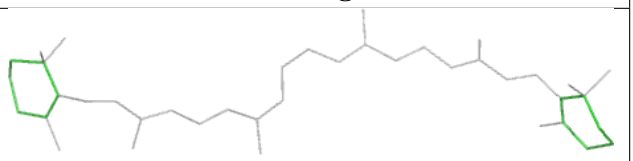
Bond lengths



Bond angles

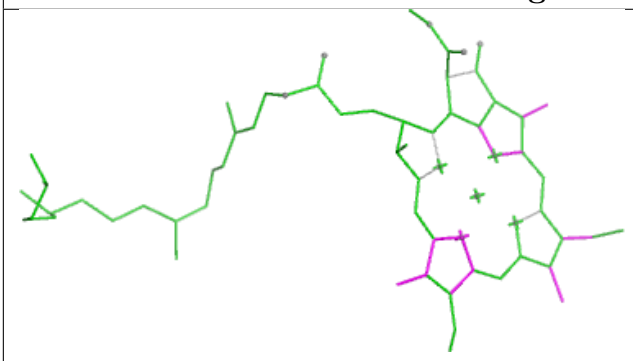


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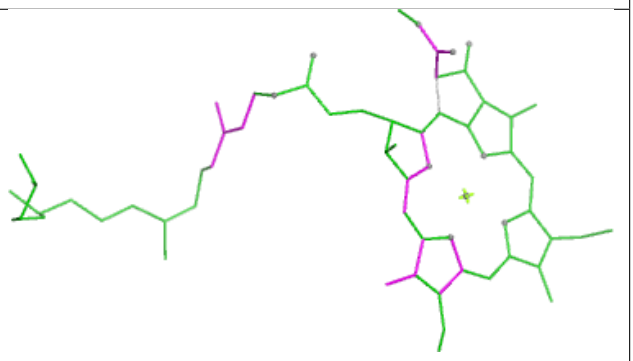


Rings

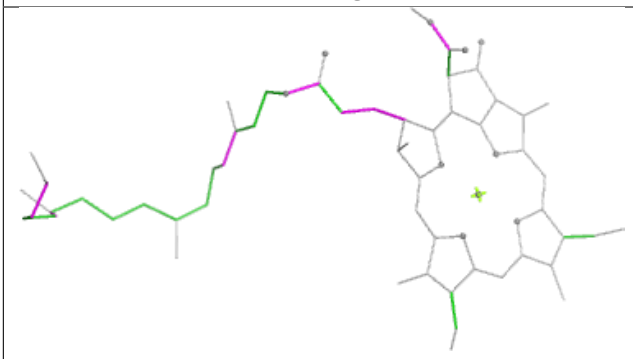
Ligand CLA 2 810



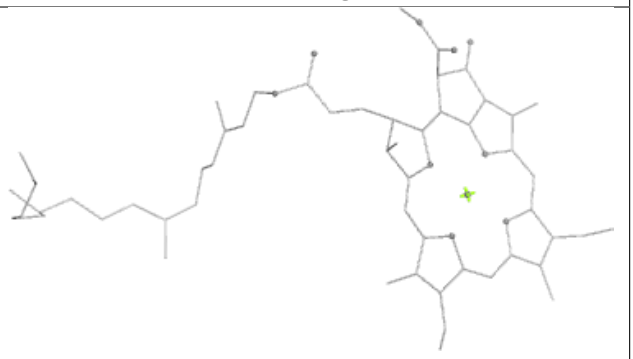
Bond lengths



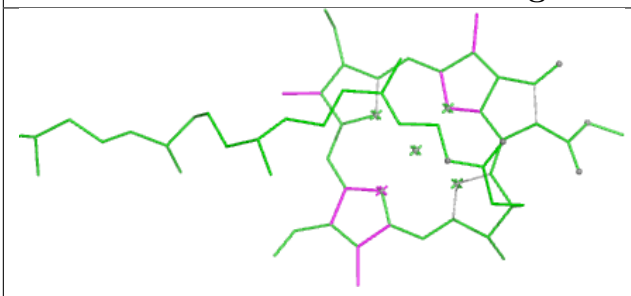
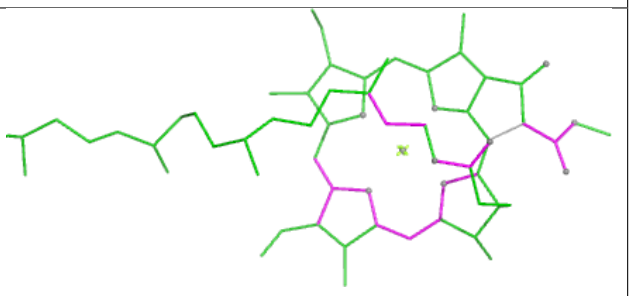
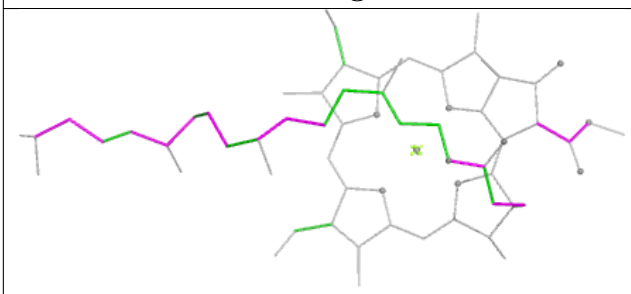
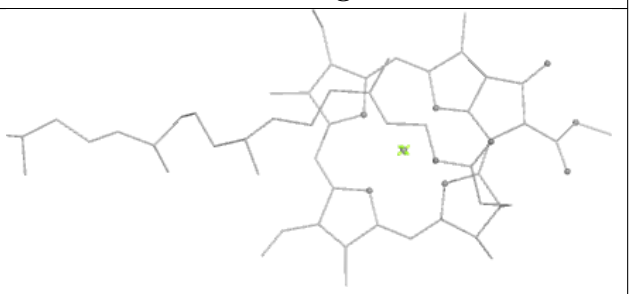
Bond angles

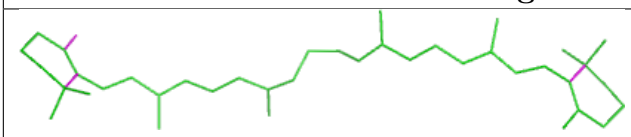
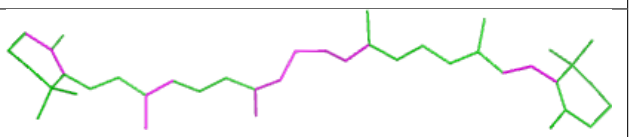
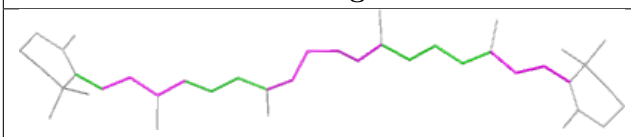
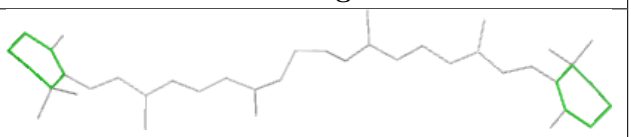


Torsions

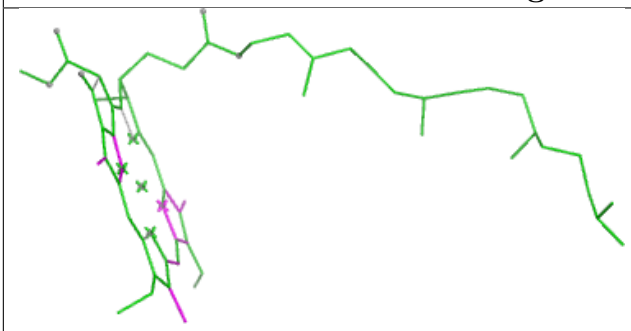


Rings

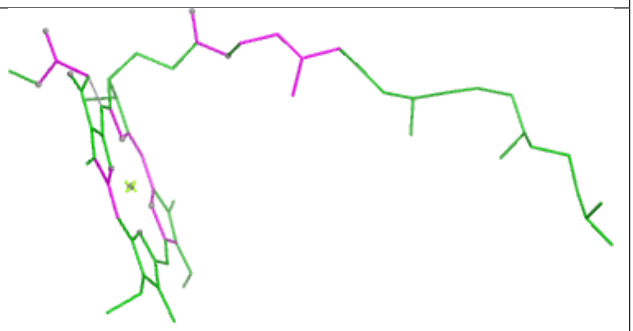
Ligand CLA a 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR 1 1649	
 Bond lengths	 Bond angles
 Torsions	 Rings

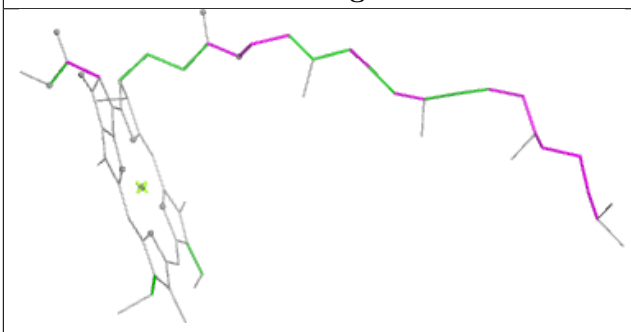
Ligand CLA b 805



Bond lengths



Bond angles

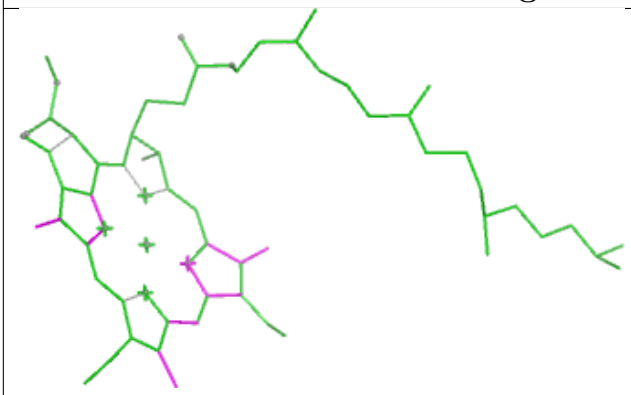


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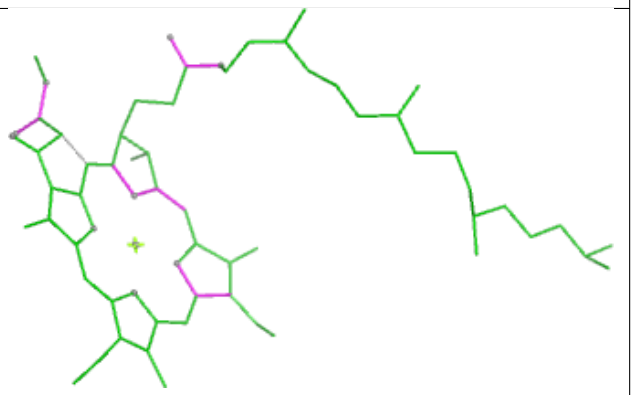


Rings

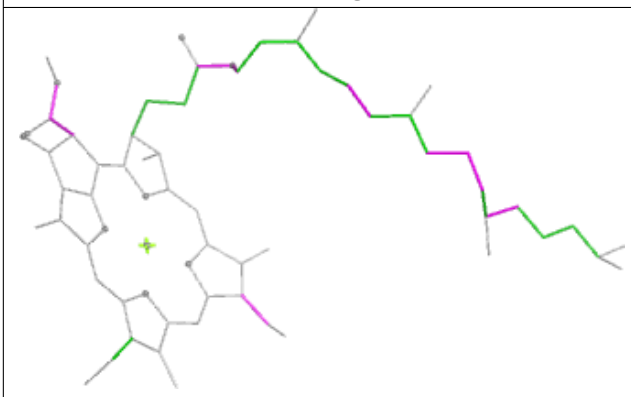
Ligand CLA 1 1618



Bond lengths



Bond angles

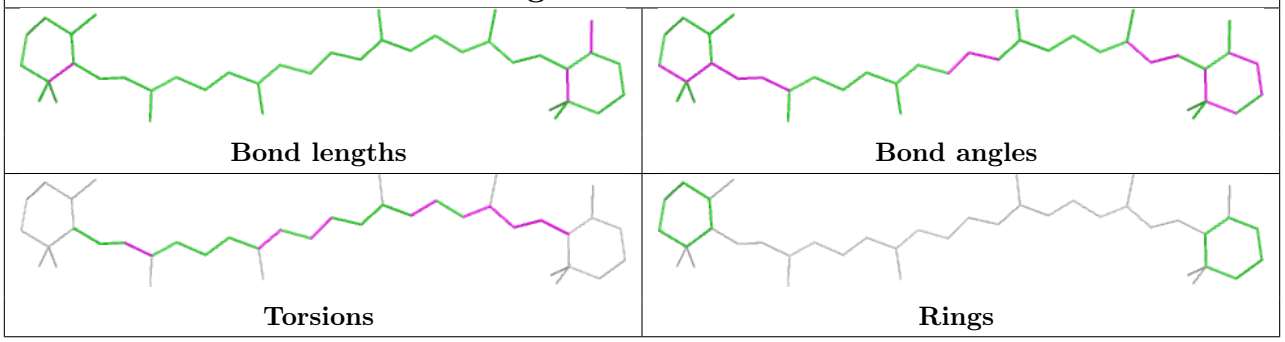


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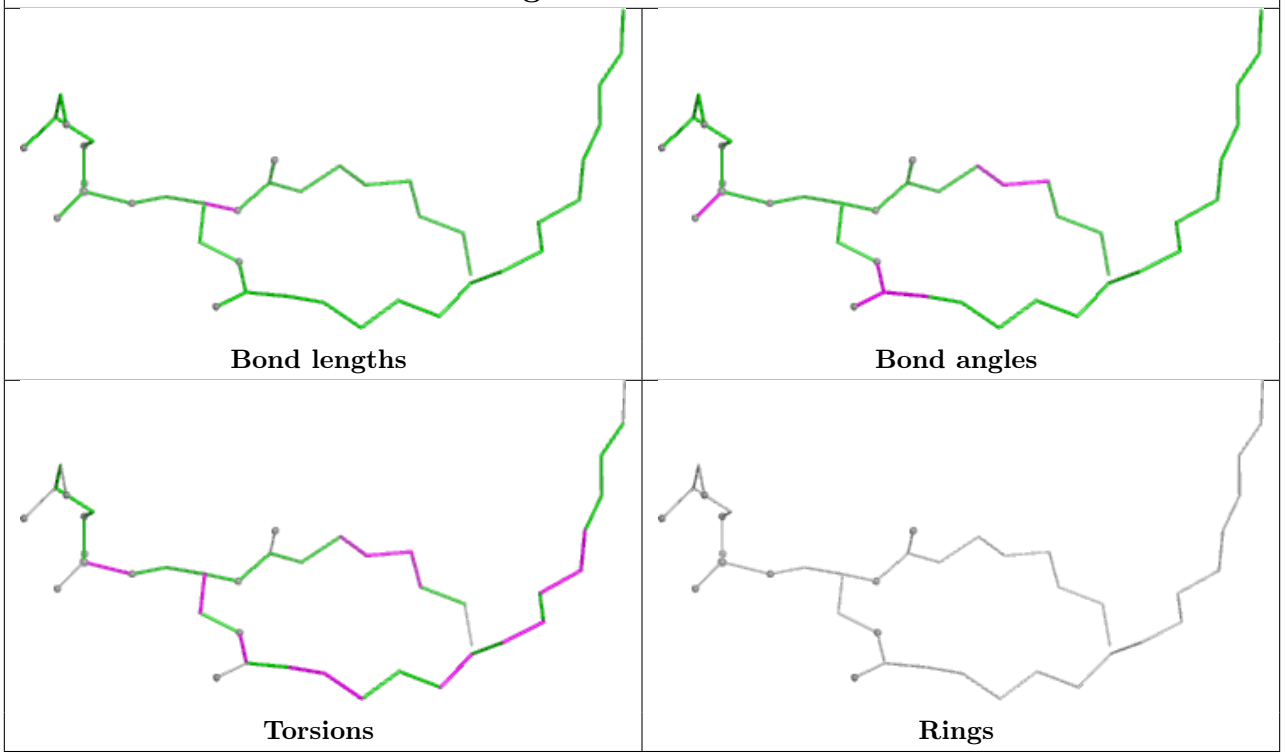


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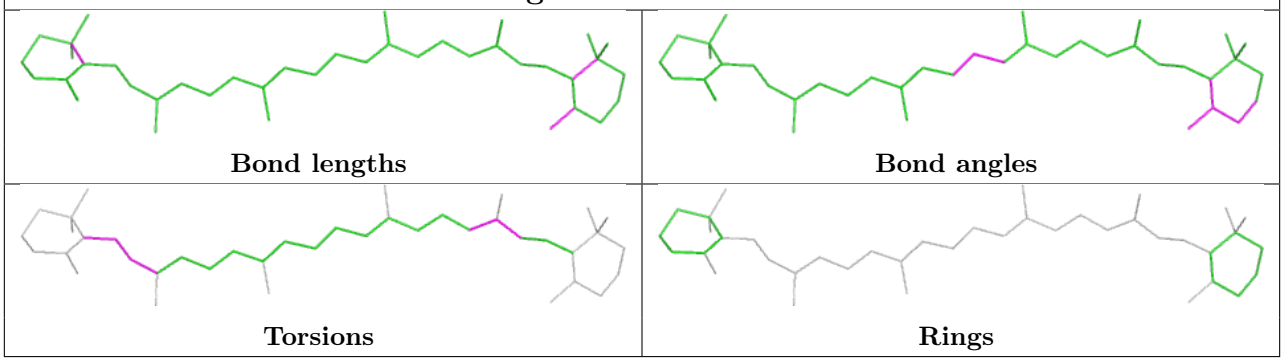
Ligand BCR 0 208



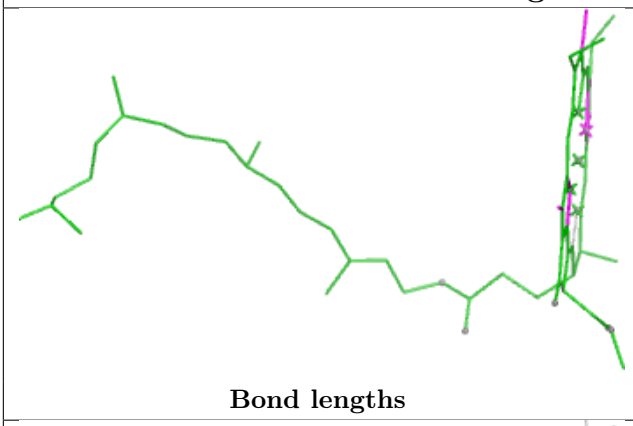
Ligand LHG A 854



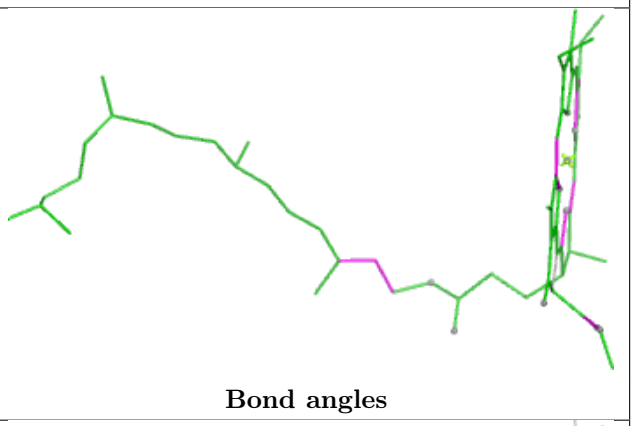
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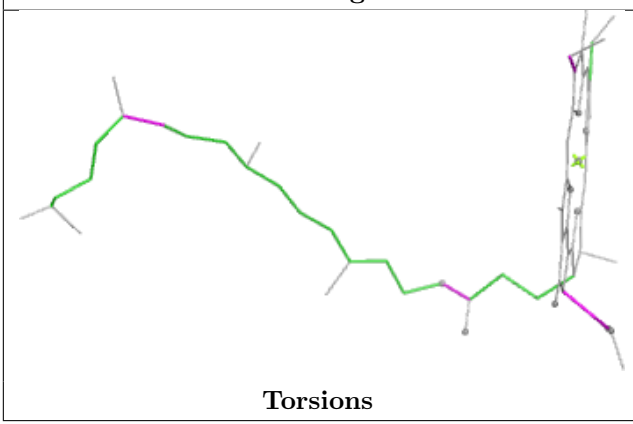
Ligand CLA b 842



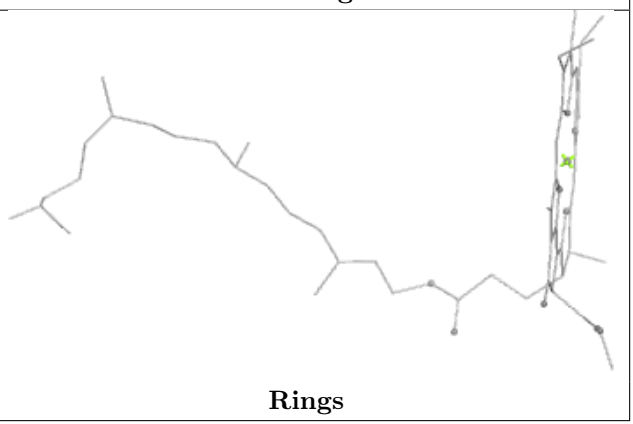
Bond lengths



Bond angles

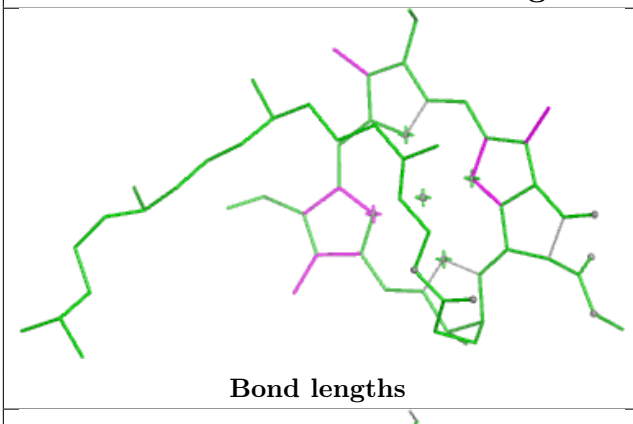


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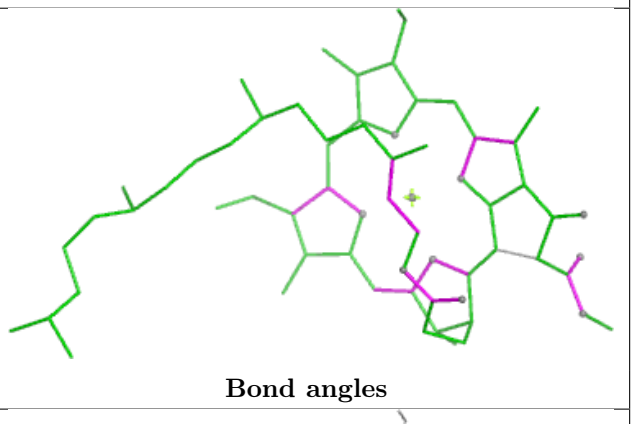


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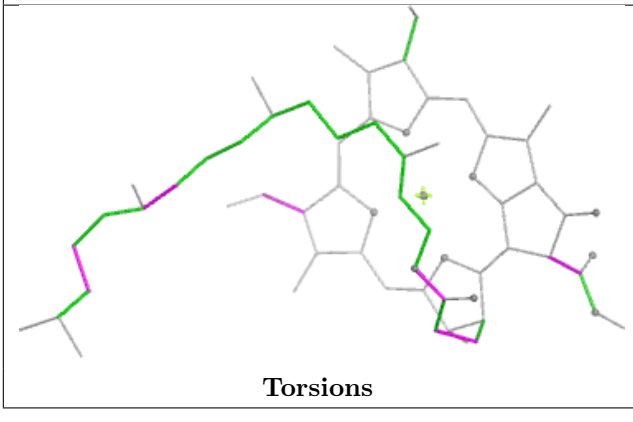
Ligand CLA 2 808



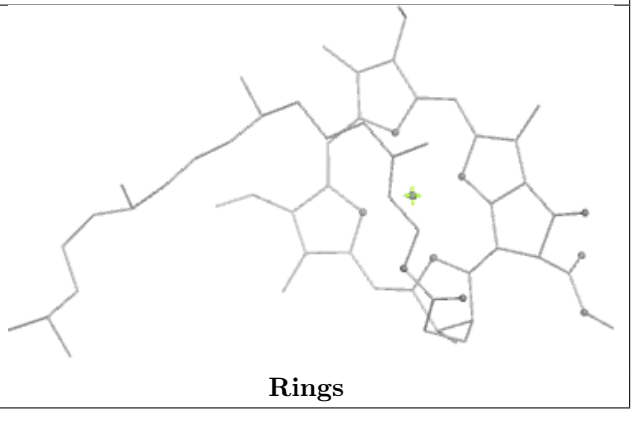
Bond lengths



Bond angles

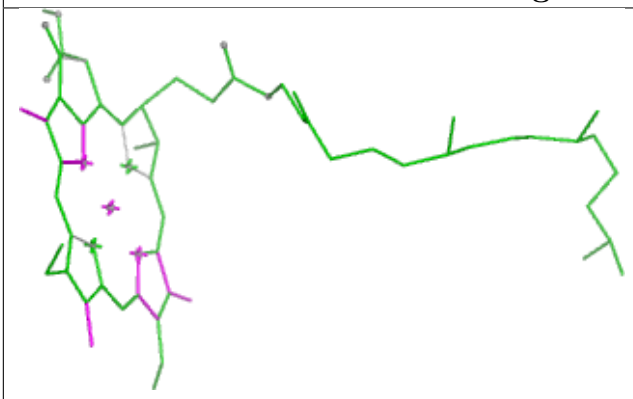


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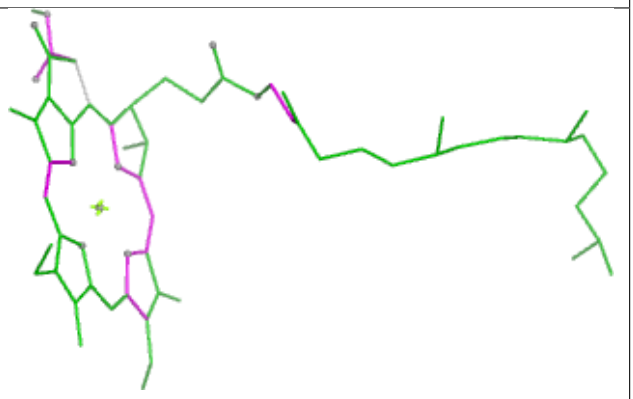


Rings

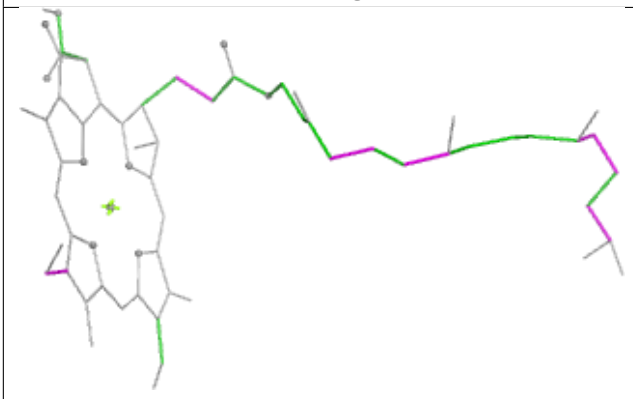
Ligand CLA l 205



Bond lengths



Bond angles

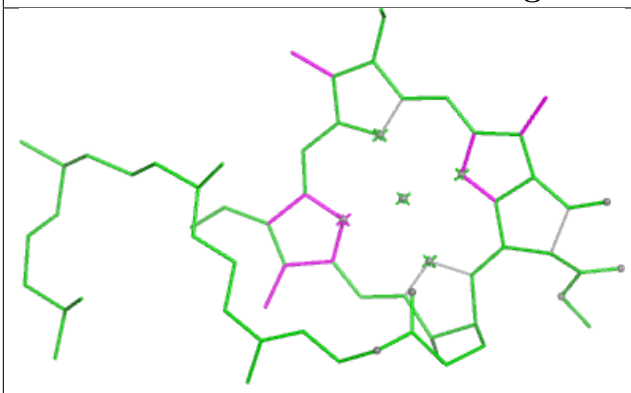


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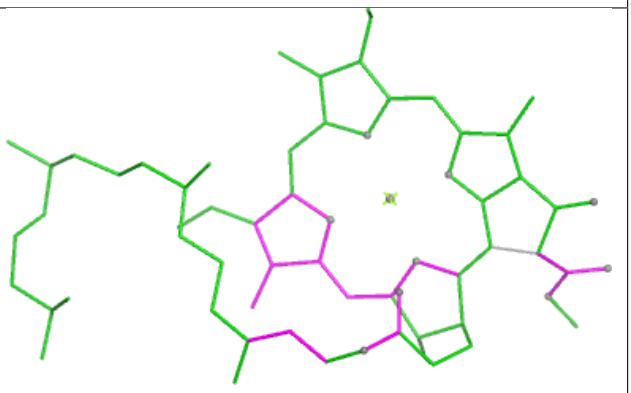


Rings

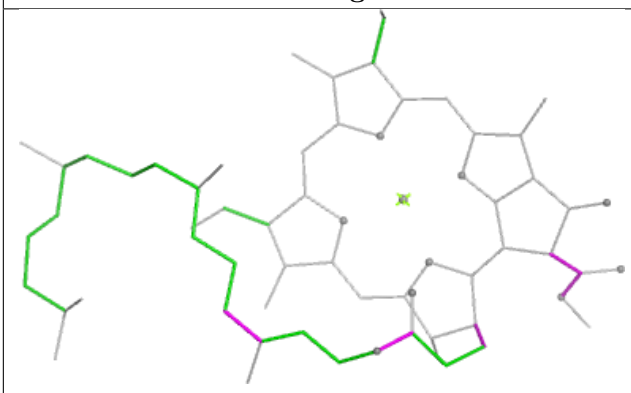
Ligand CLA A 820



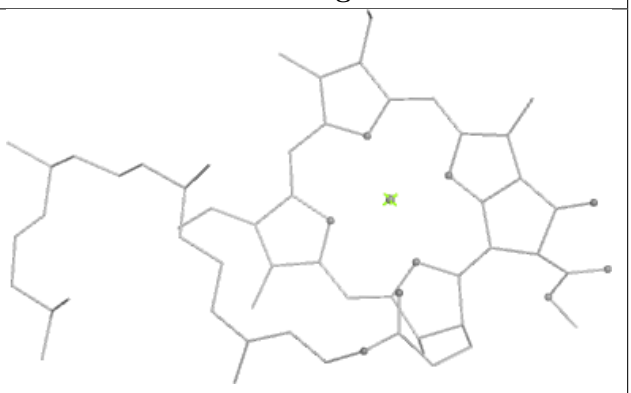
Bond lengths



Bond angles

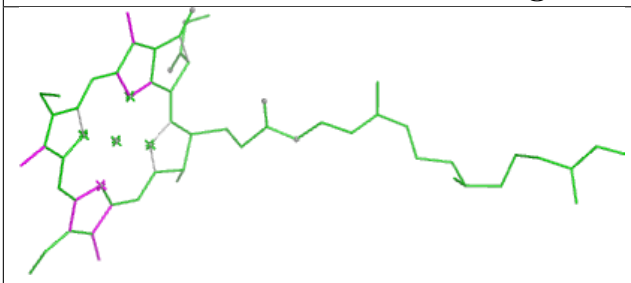


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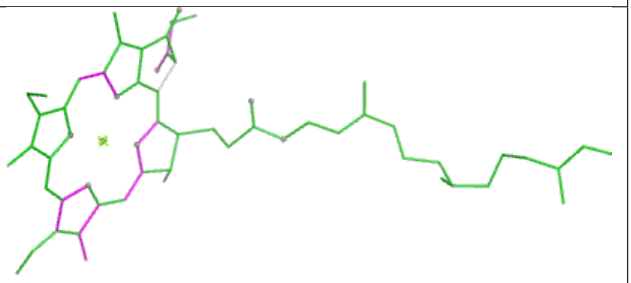


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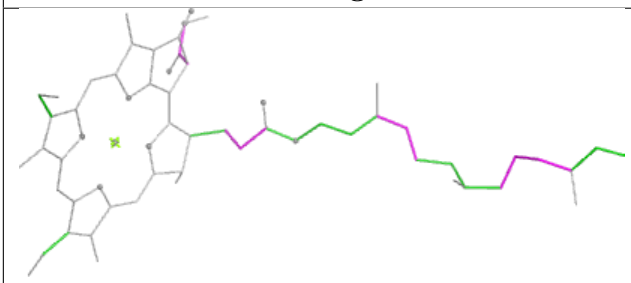
Ligand CLA a 810



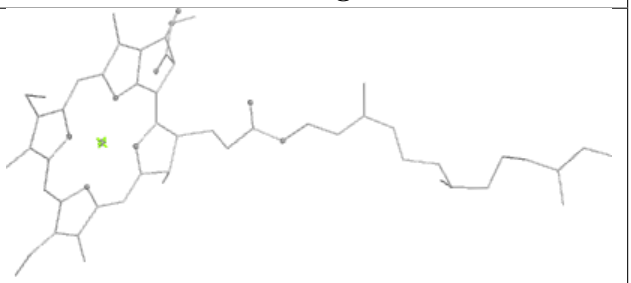
Bond lengths



Bond angles

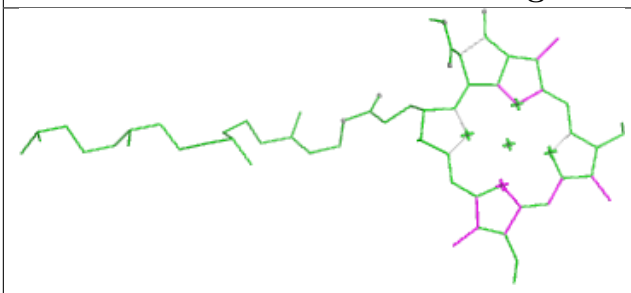


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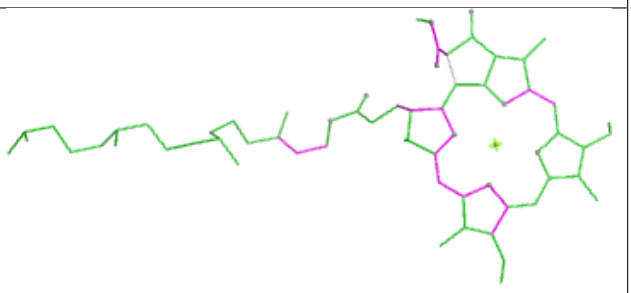


Rings

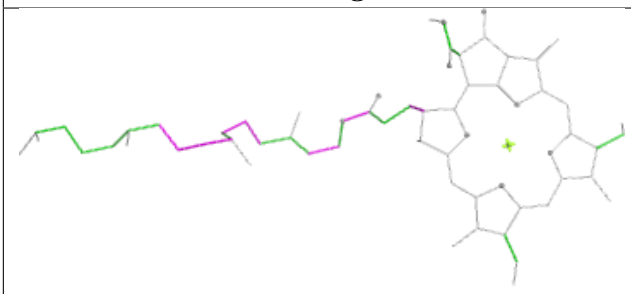
Ligand CLA b 826



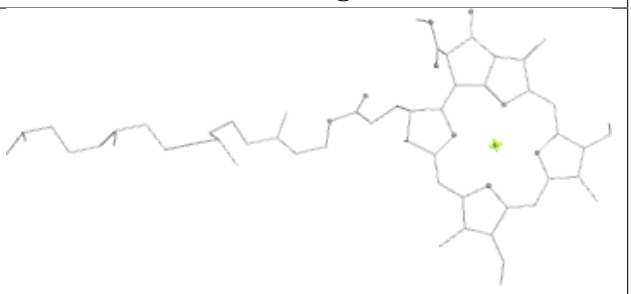
Bond lengths



Bond angles

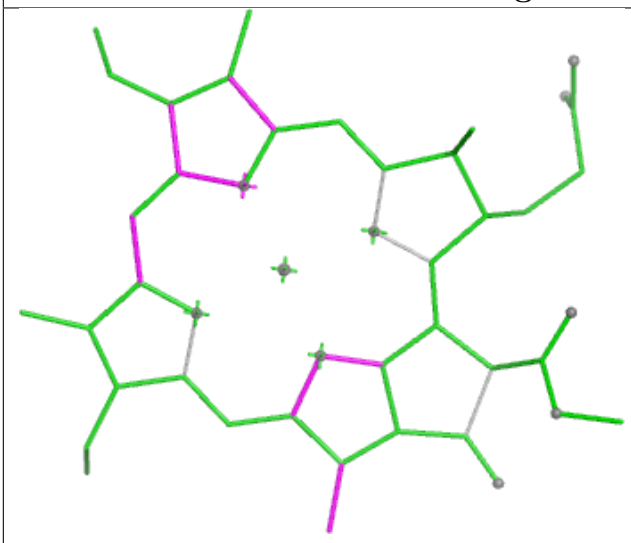


Torsions

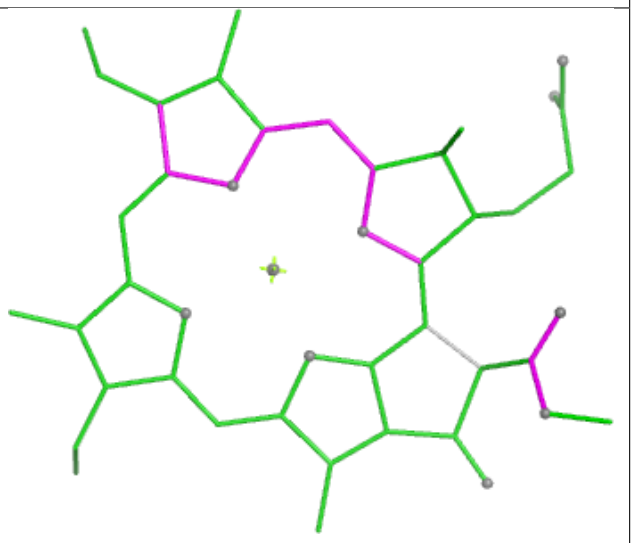


Rings

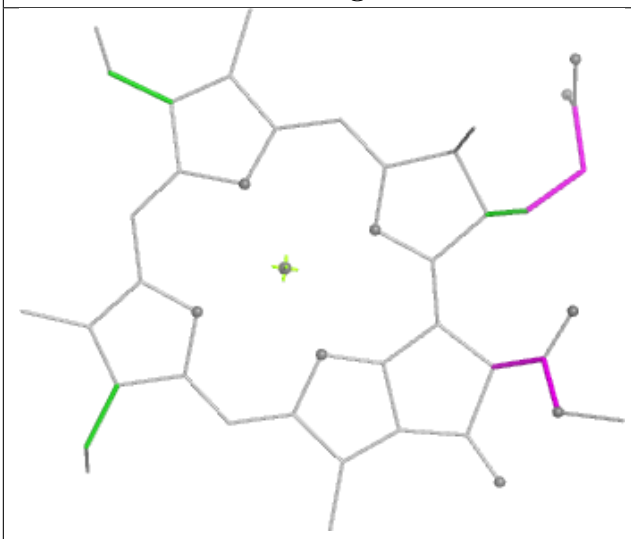
Ligand CLA X 1701



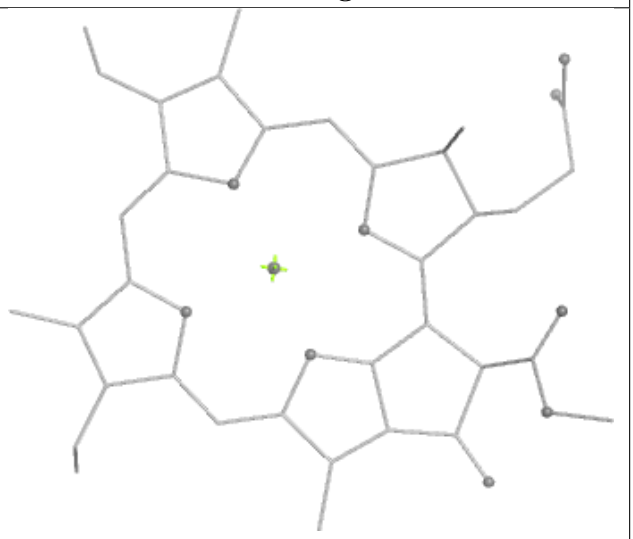
Bond lengths



Bond angles

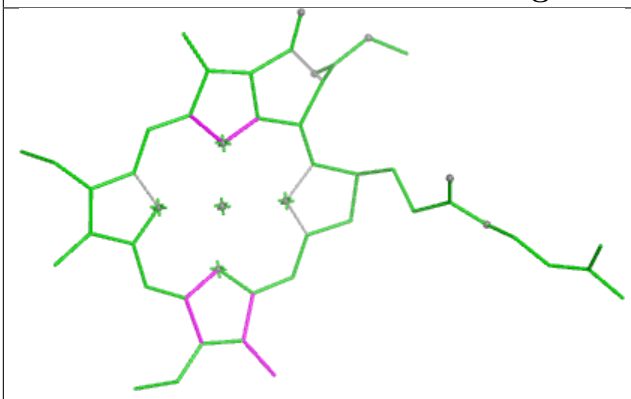


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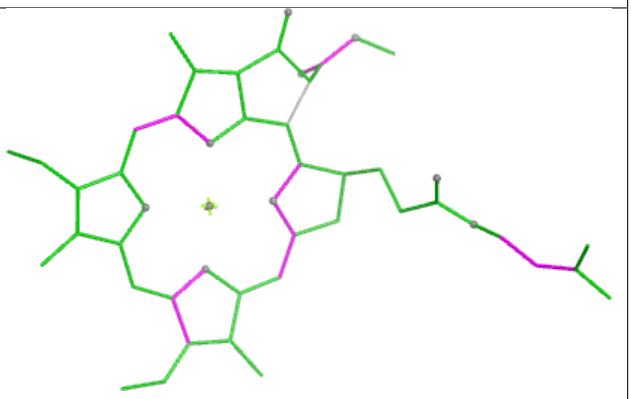


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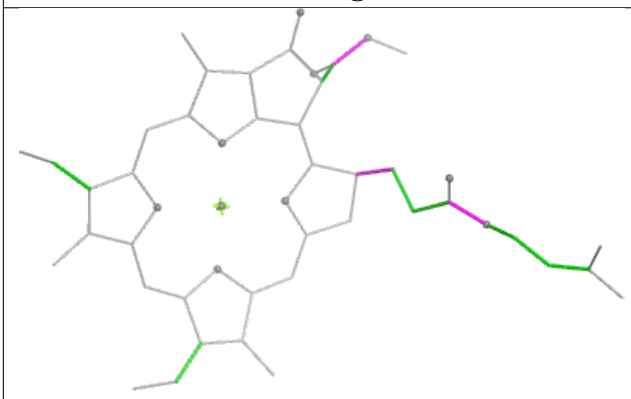
Ligand CLA f 203



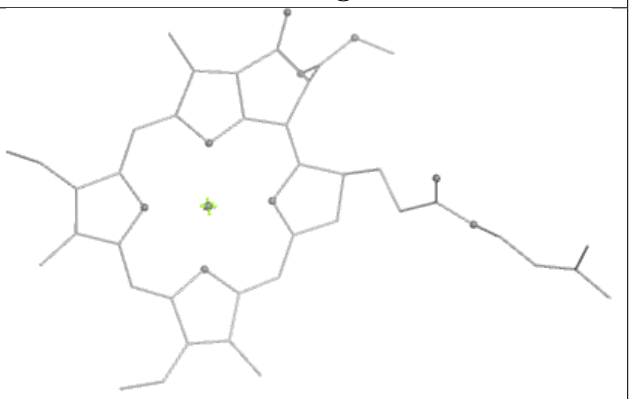
Bond lengths



Bond angles

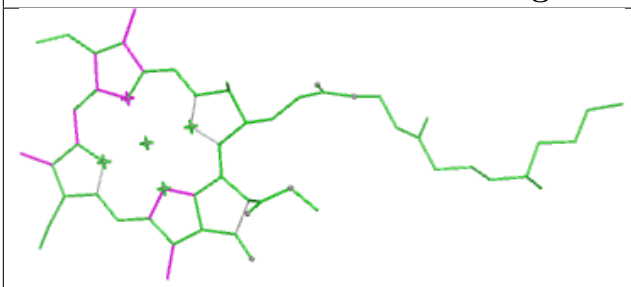


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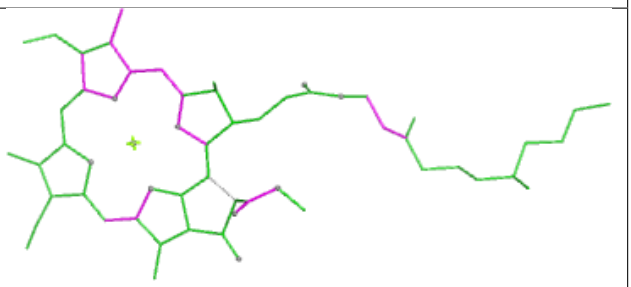


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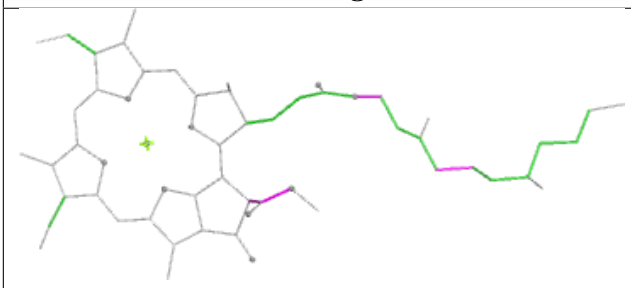
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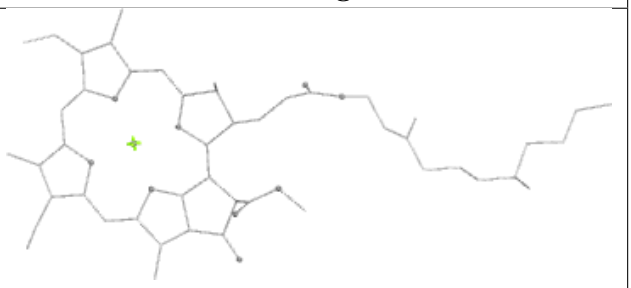
Bond lengths



Bond angles

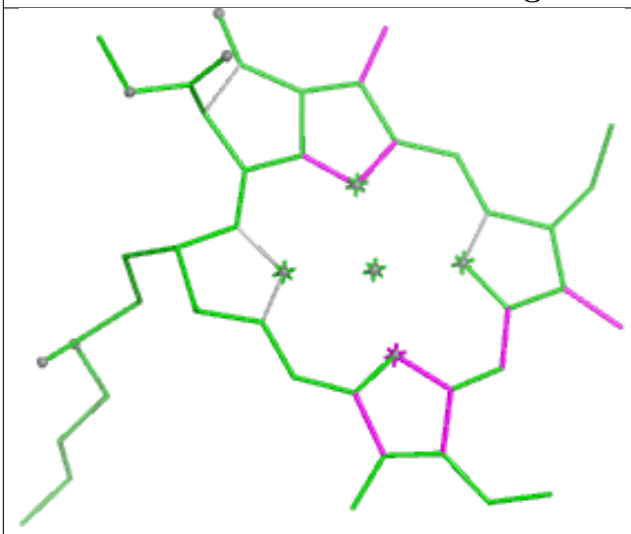


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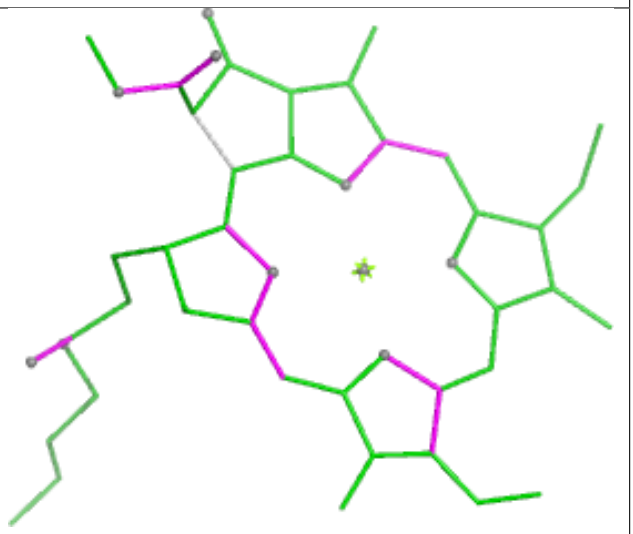


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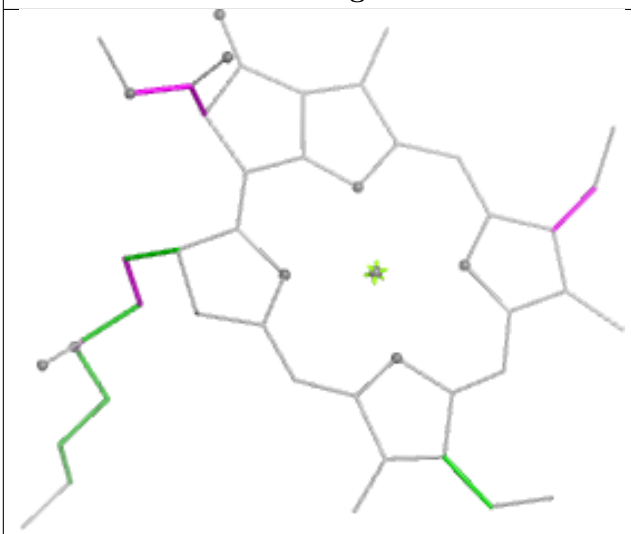
Ligand CLA A 811



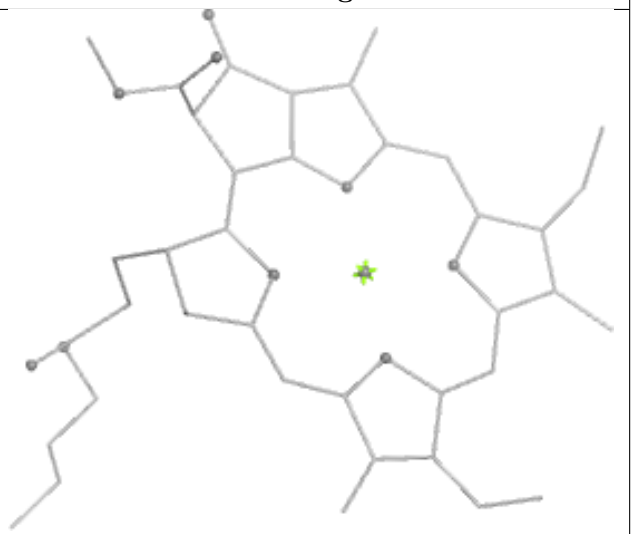
Bond lengths



Bond angles



Torsions



Rings

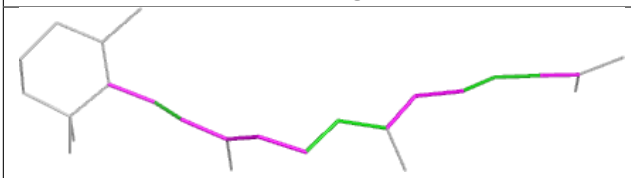
Ligand BCR 1 1653



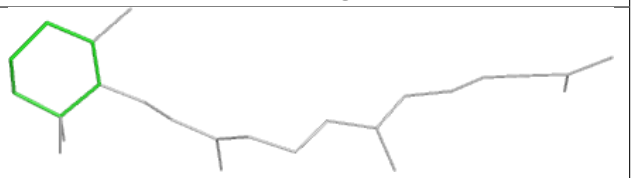
Bond lengths



Bond angles

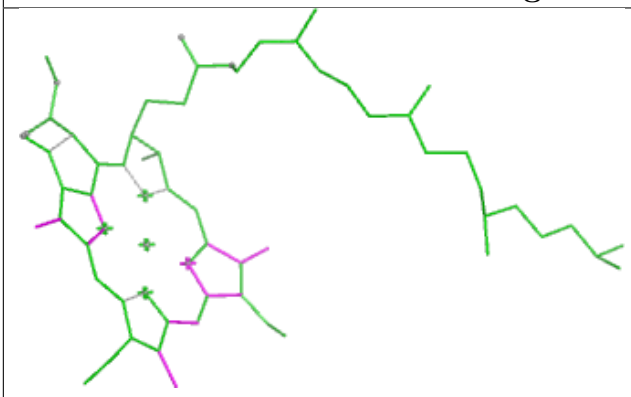


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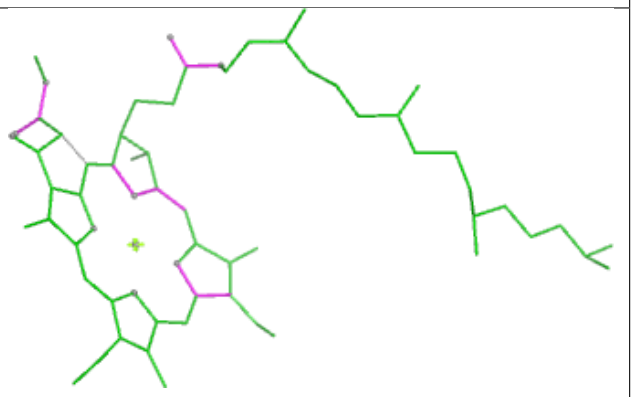


Rings

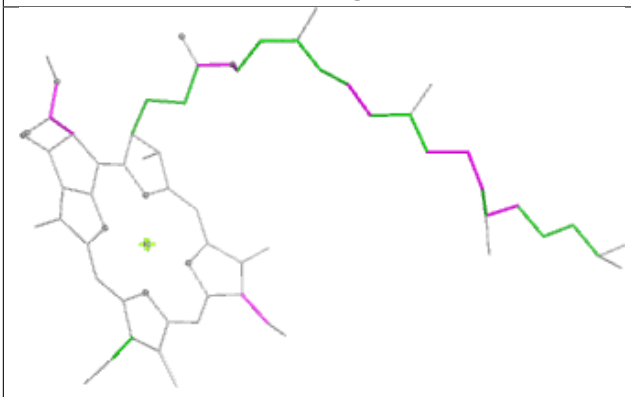
Ligand CLA A 817



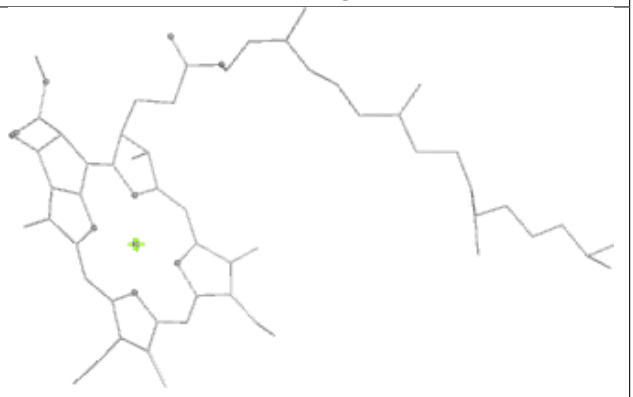
Bond lengths



Bond angles

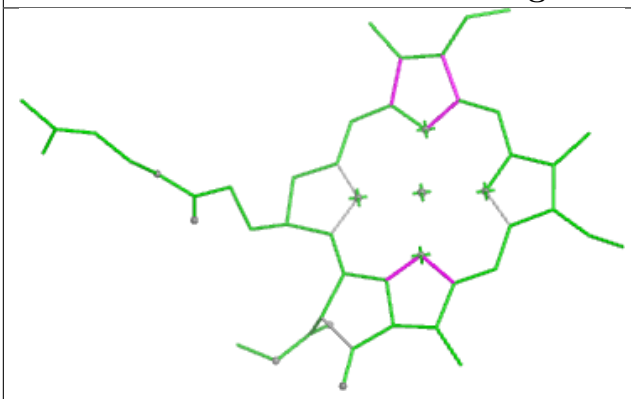


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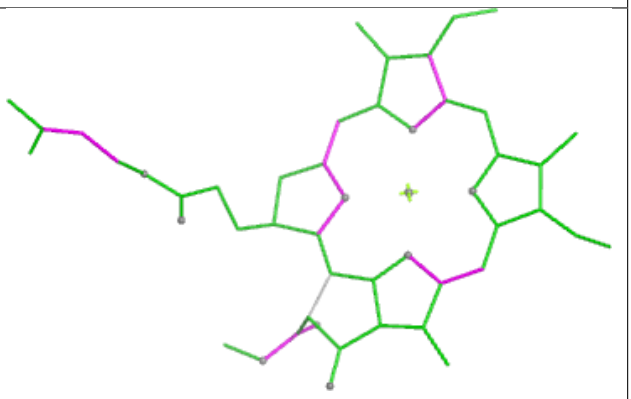


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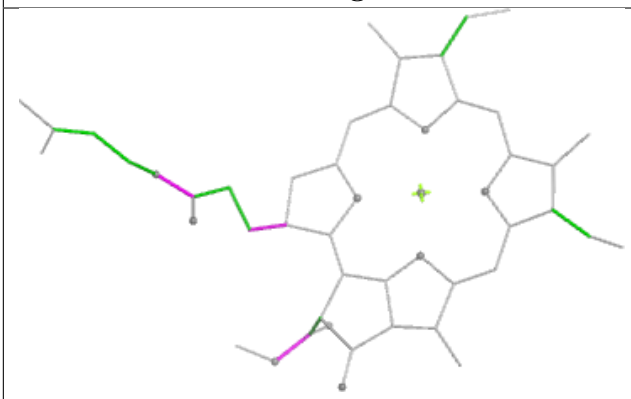
Ligand CLA 6 203



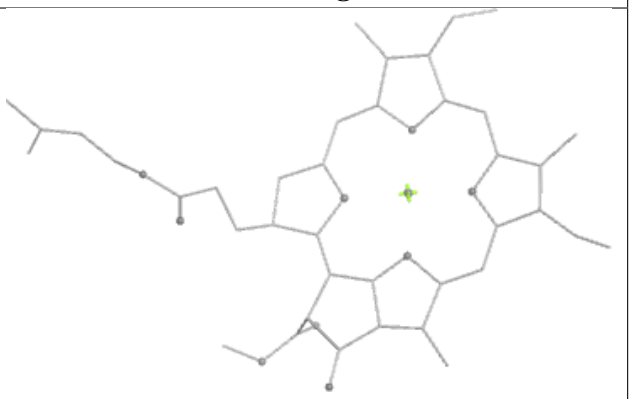
Bond lengths



Bond angles

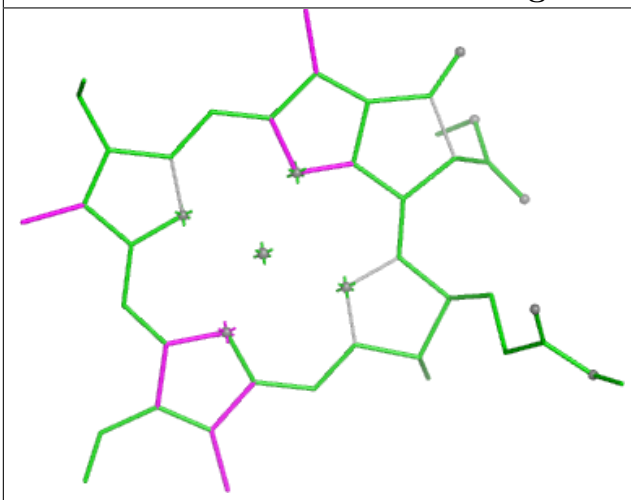


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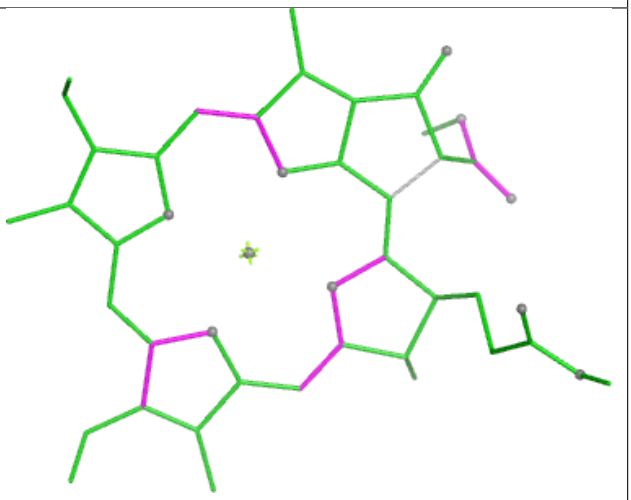


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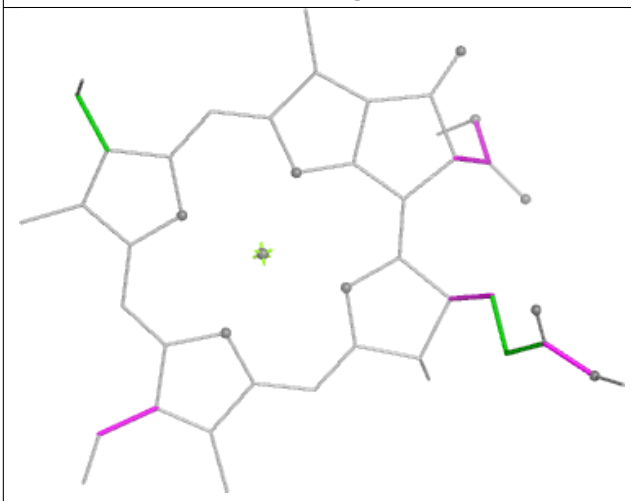
Ligand CLA 9 101



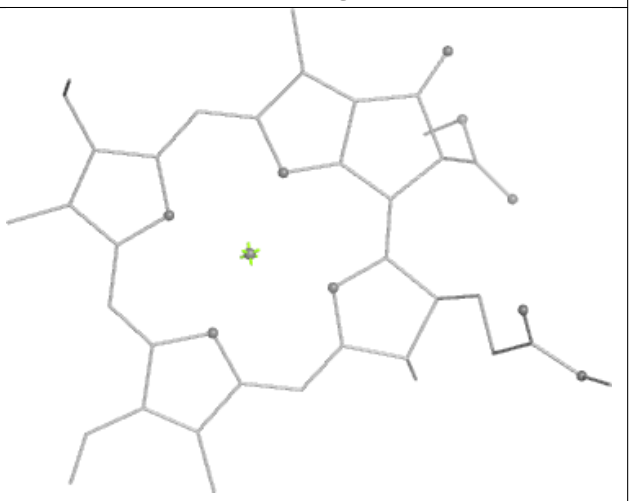
Bond lengths



Bond angles

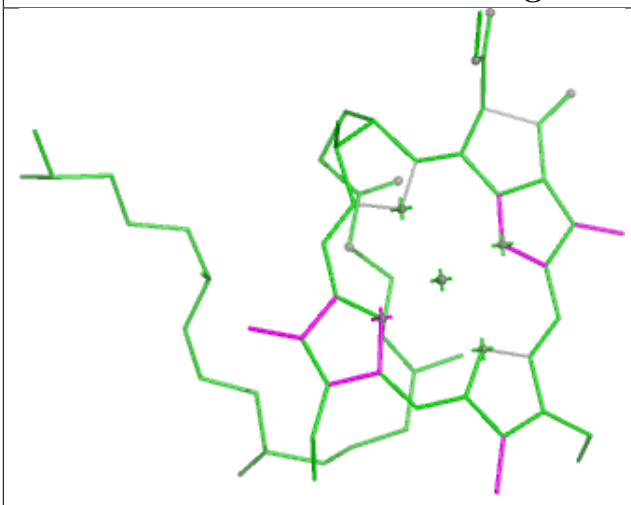


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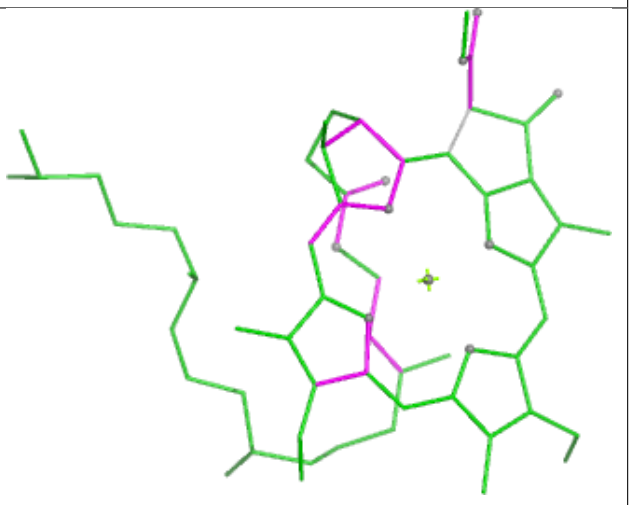


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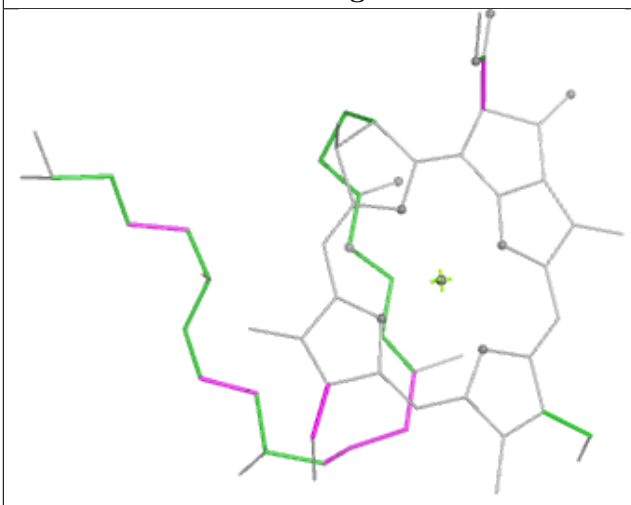
Ligand CLA B 808



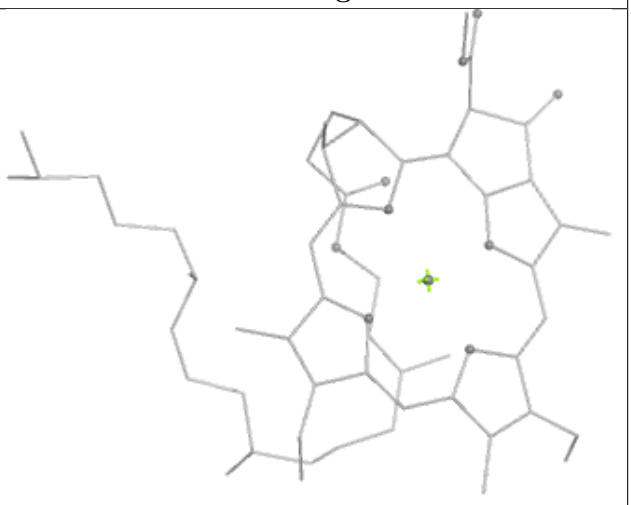
Bond lengths



Bond angles

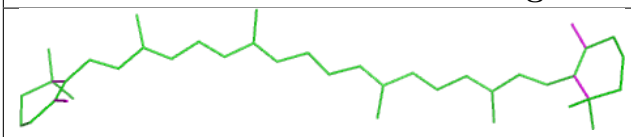


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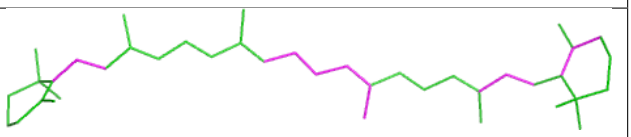


Rings

Ligand BCR 2 849



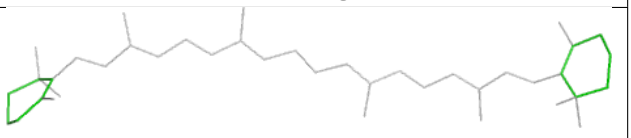
Bond lengths



Bond angles

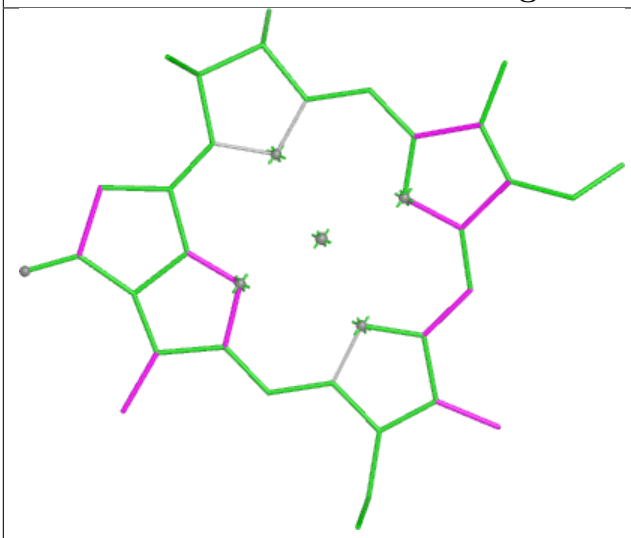


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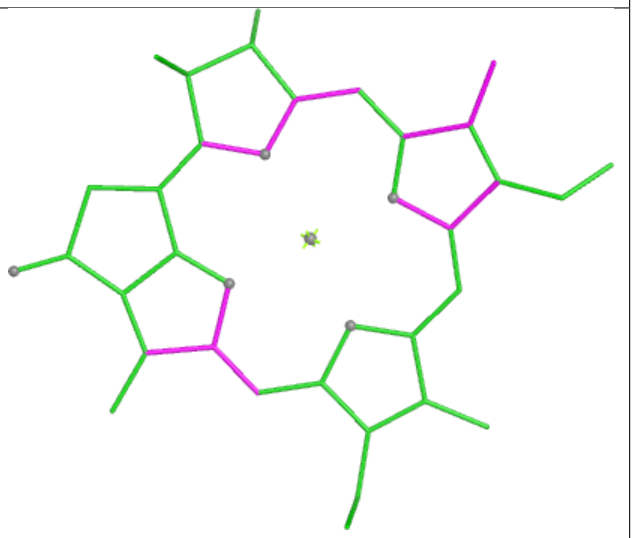


Rings

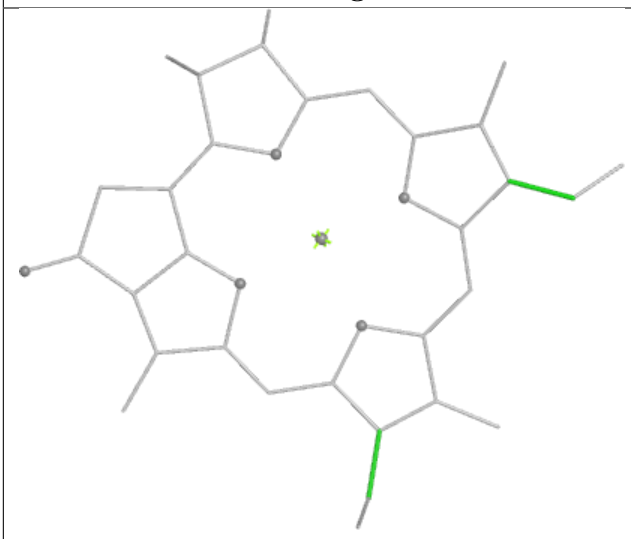
Ligand CLA 8 1303



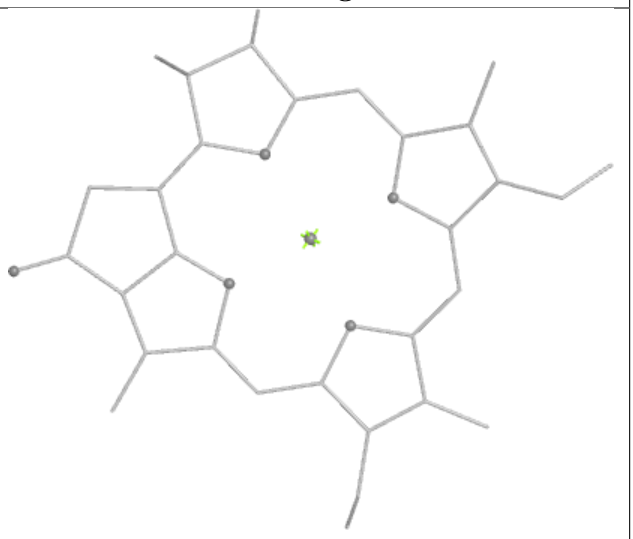
Bond lengths



Bond angles

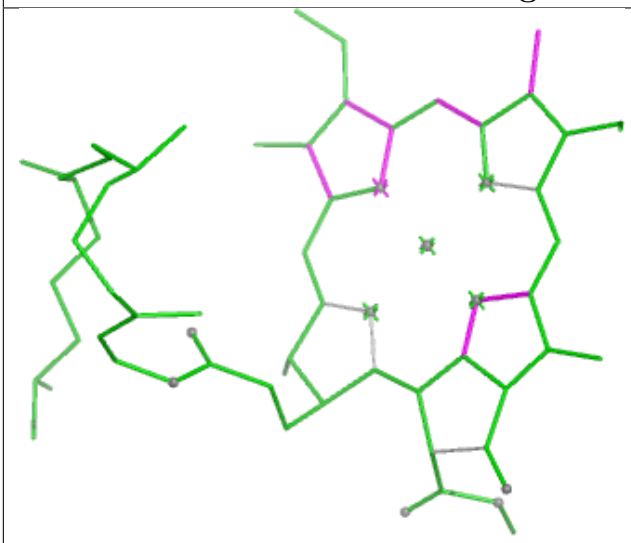


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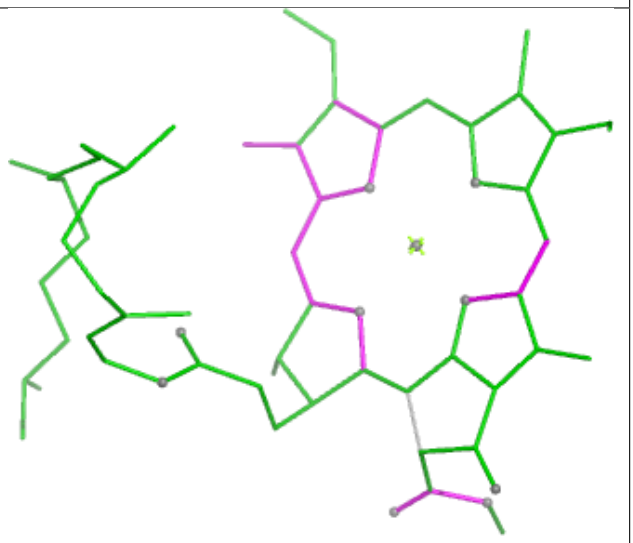


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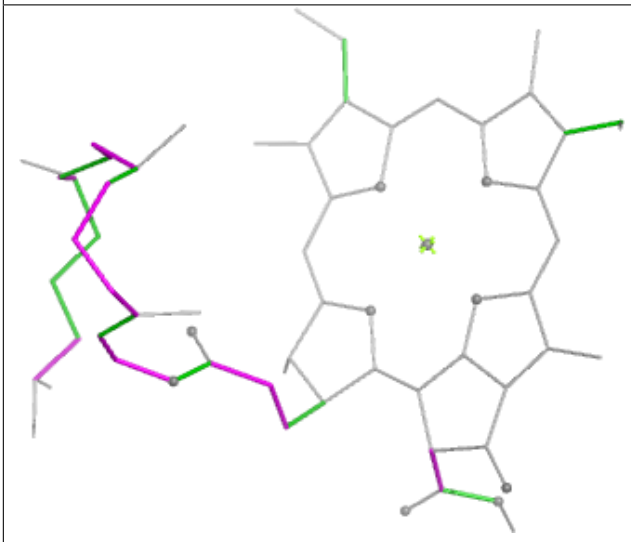
Ligand CLA 1 1617



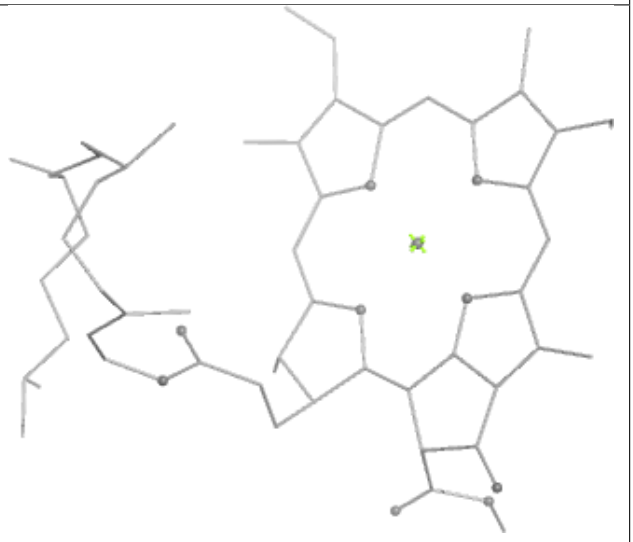
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Bond angles

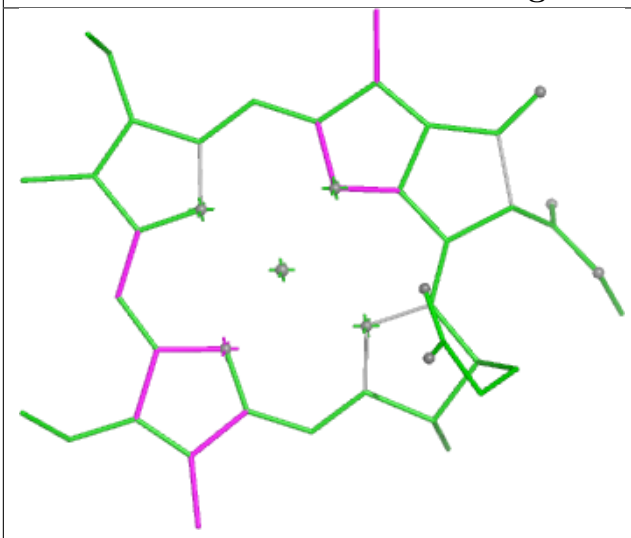


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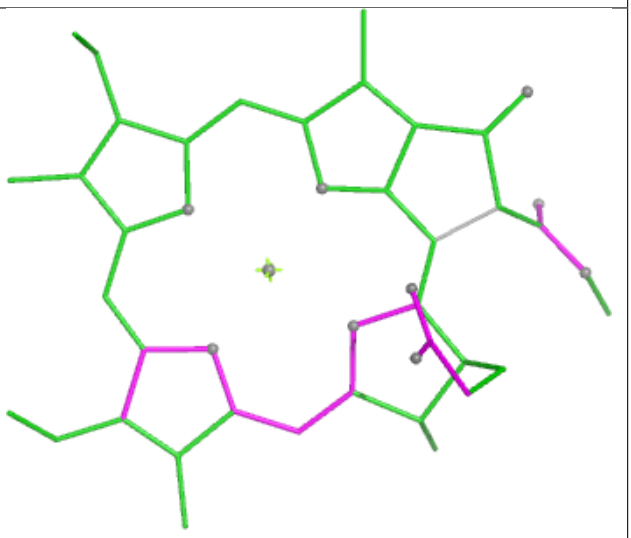


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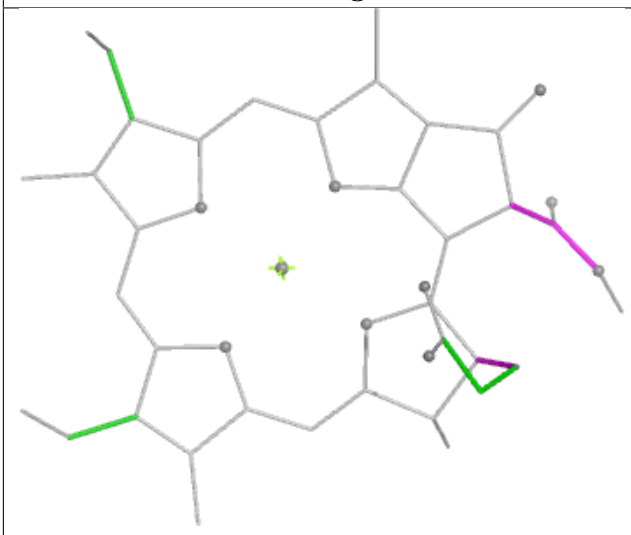
Ligand CLA a 837



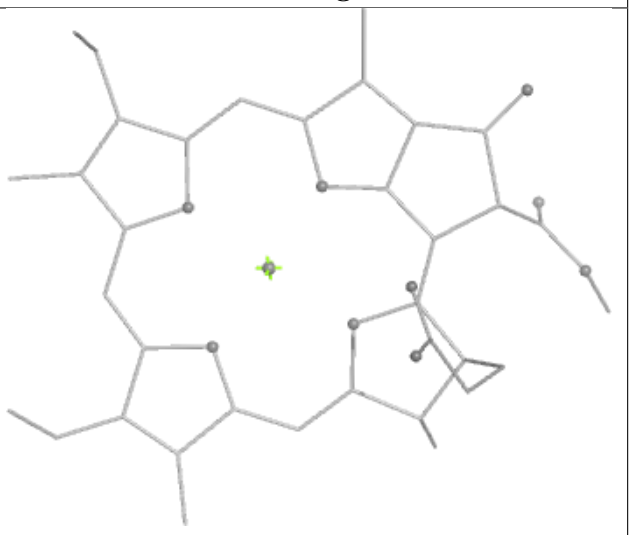
Bond lengths



Bond angles

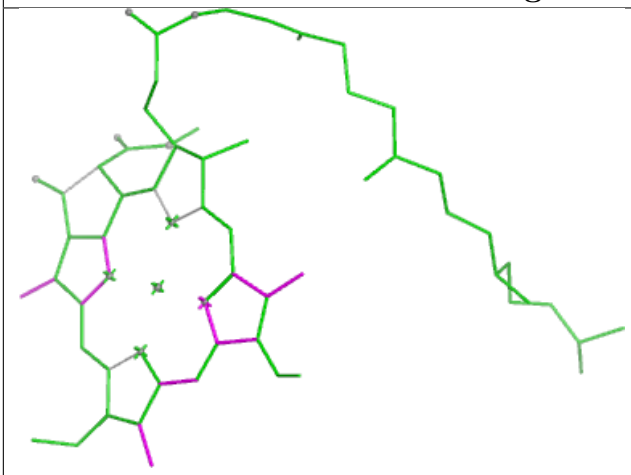


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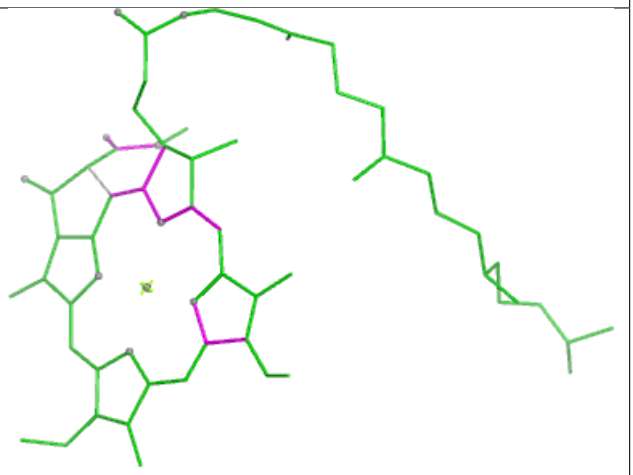


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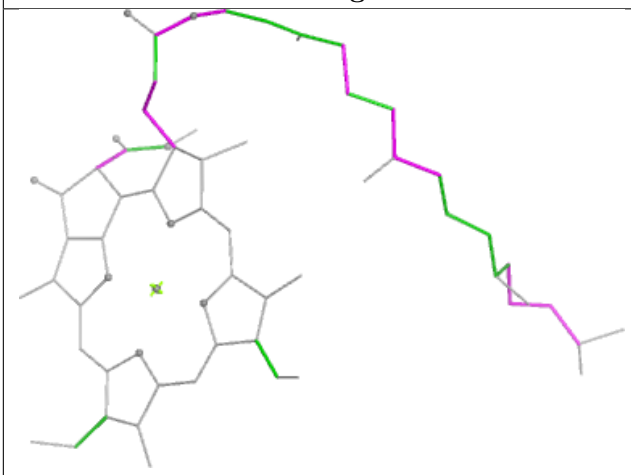
Ligand CLA B 824



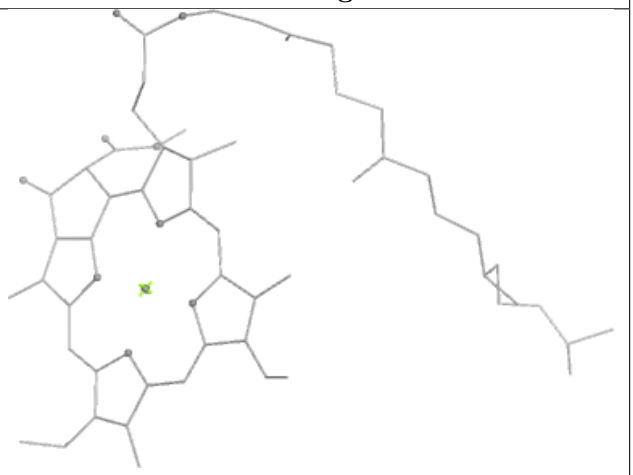
Bond lengths



Bond angles

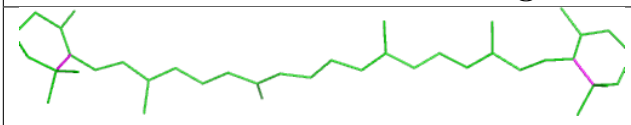


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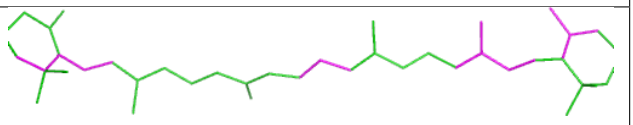


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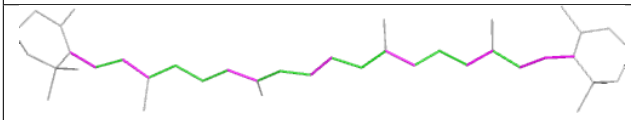
Ligand BCR 1 1648



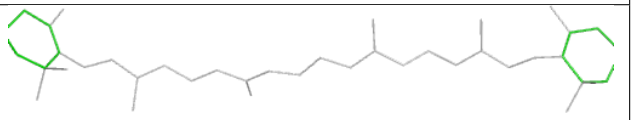
Bond lengths



Bond angles

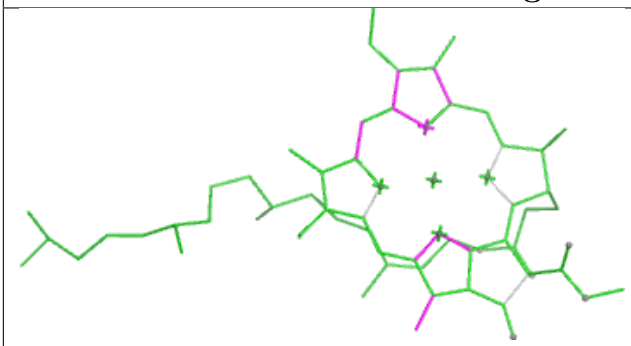


Torsions

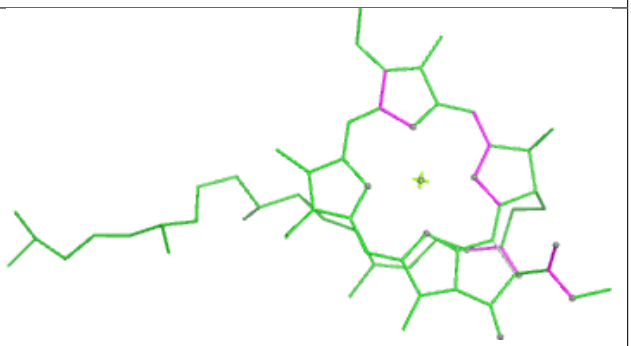


Rings

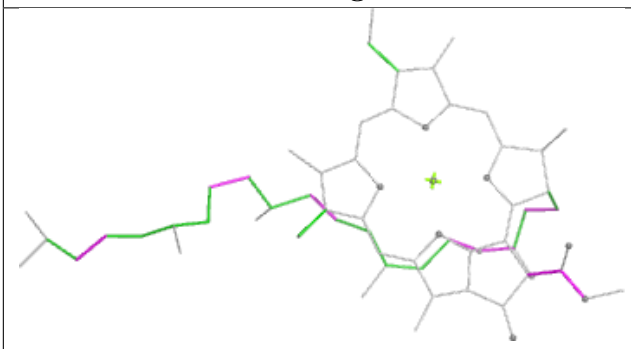
Ligand CLA A 818



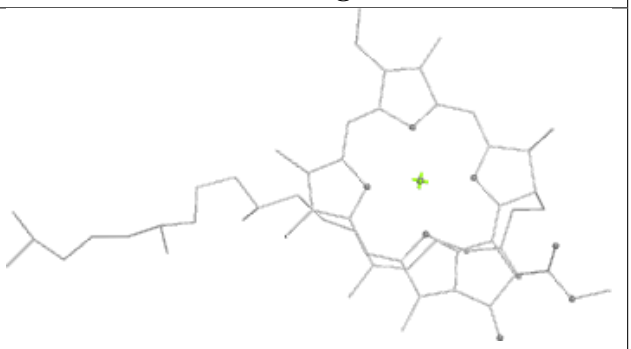
Bond lengths



Bond angles

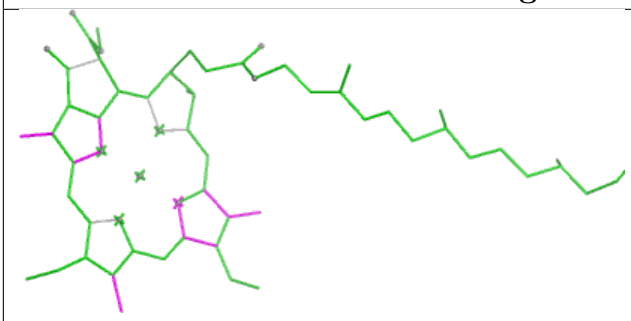


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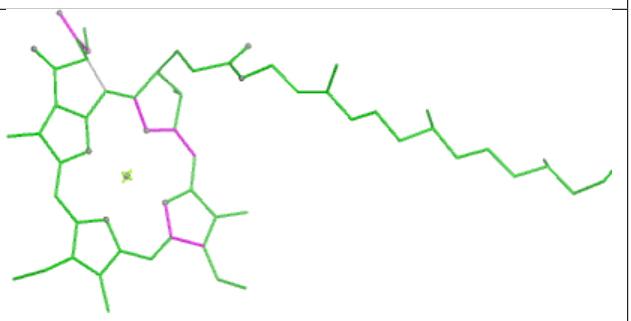


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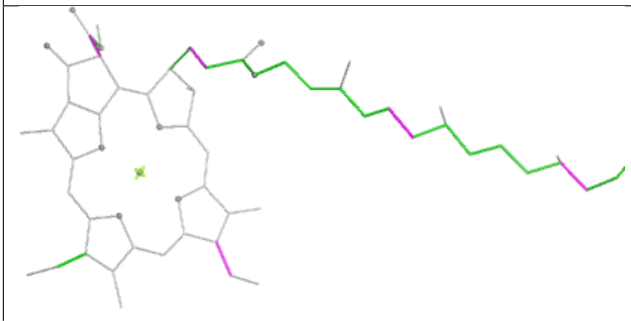
Ligand CLA 1 1636



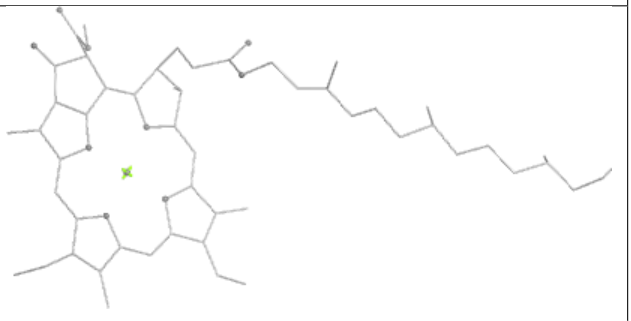
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Bond angles

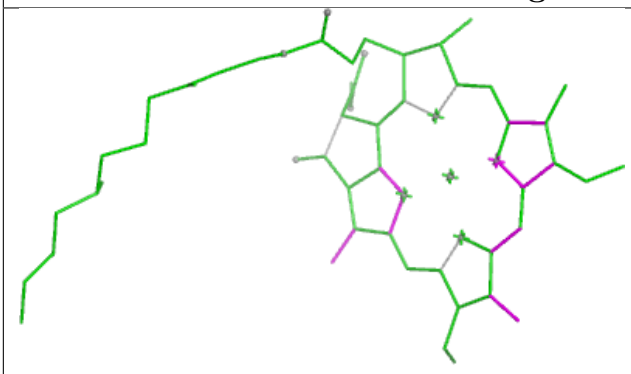


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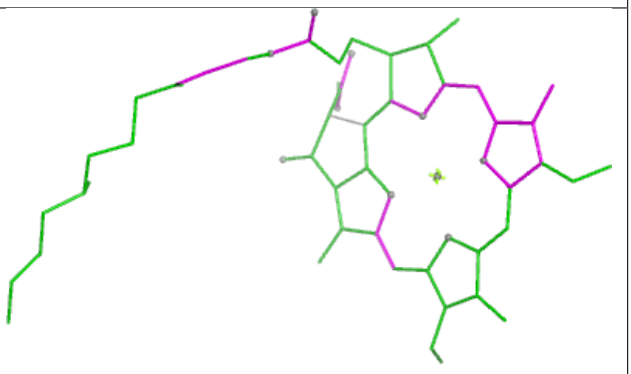


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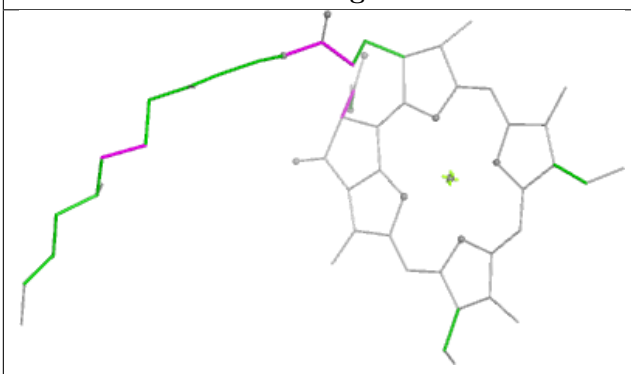
Ligand CLA 9 103



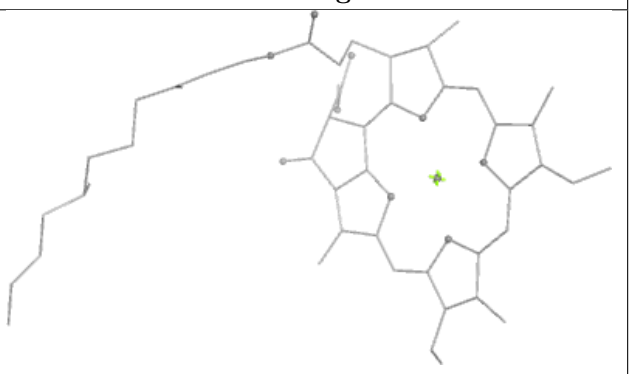
Bond lengths



Bond angles

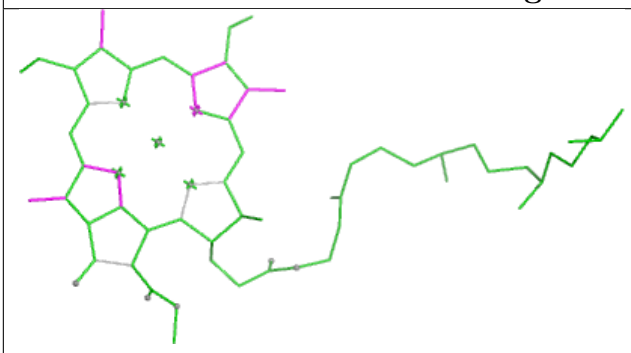


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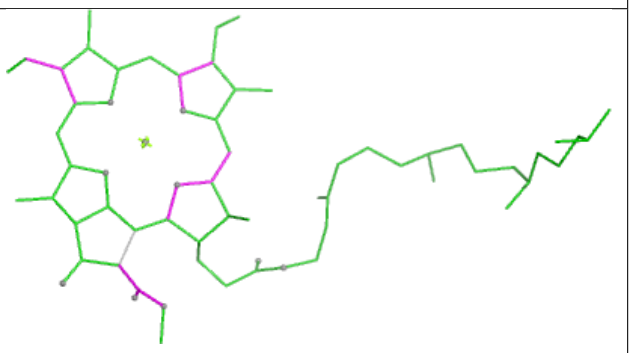


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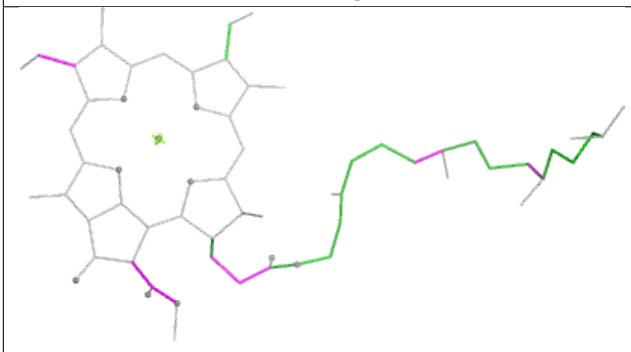
Ligand CLA B 803



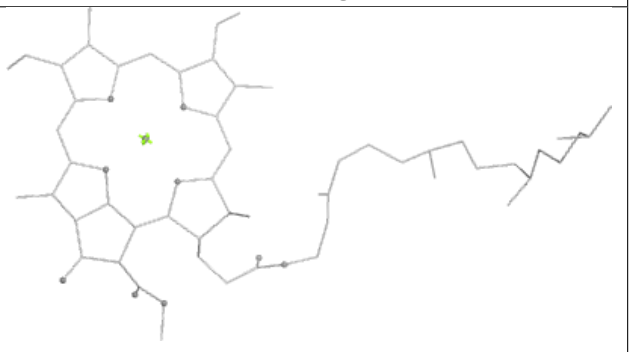
Bond lengths



Bond angles

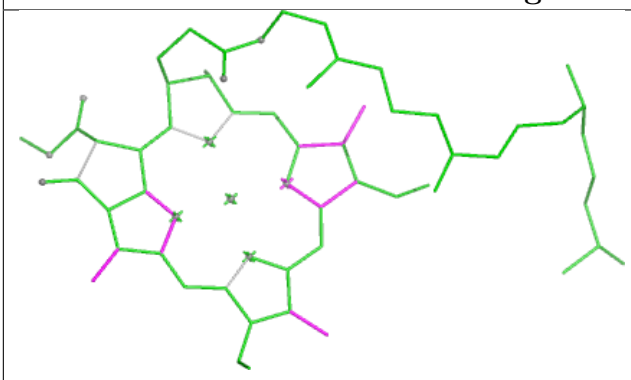


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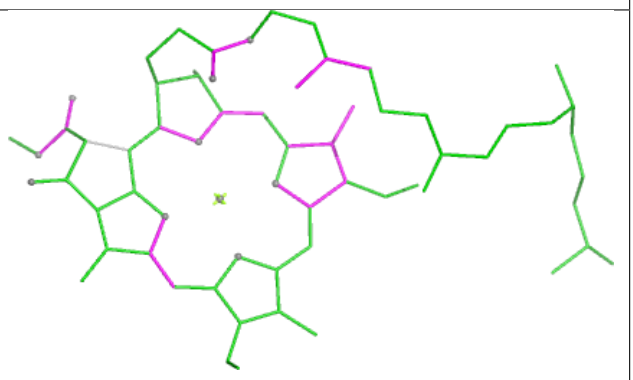


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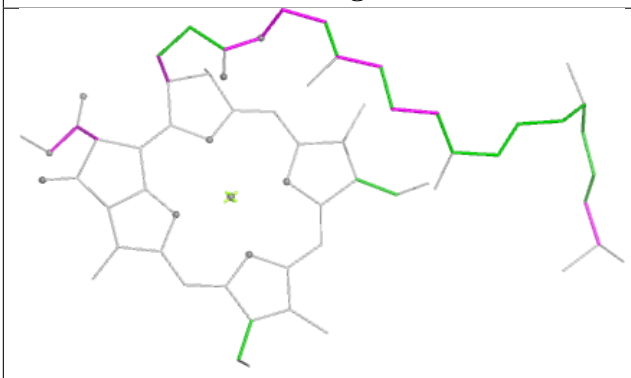
Ligand CLA B 818



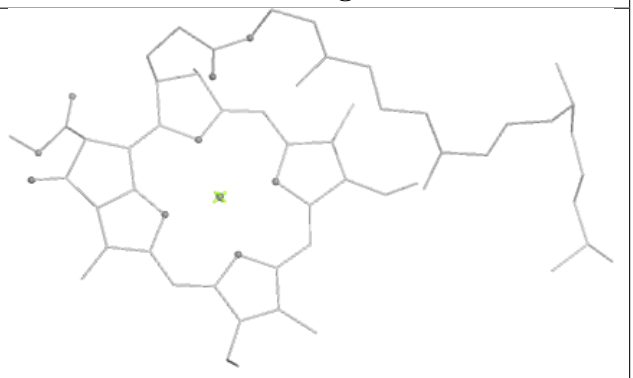
Bond lengths



Bond angles



Torsions

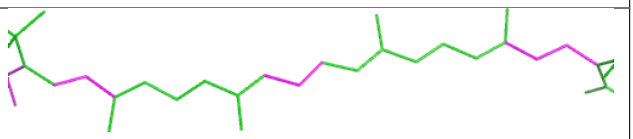


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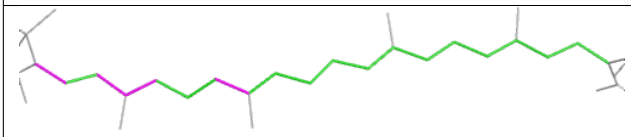
Ligand BCR A 849



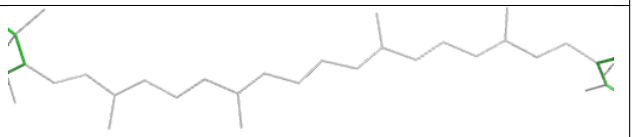
Bond lengths



Bond angles



Torsions

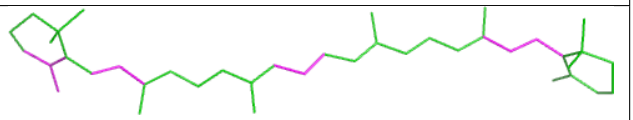


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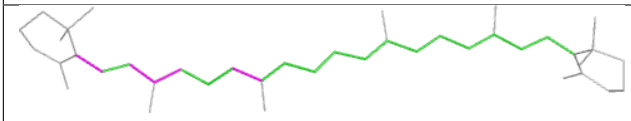
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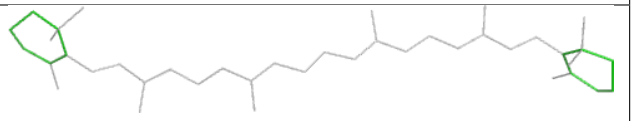
Bond lengths



Bond angles

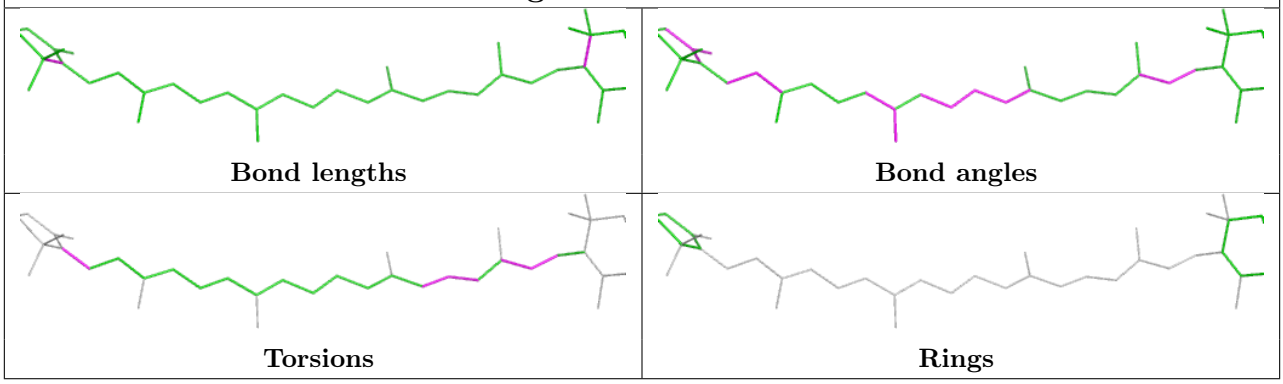


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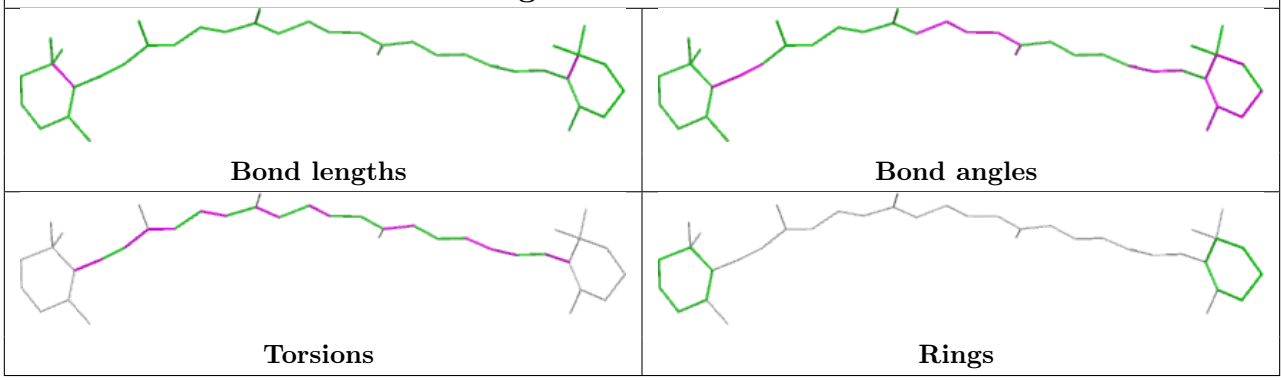


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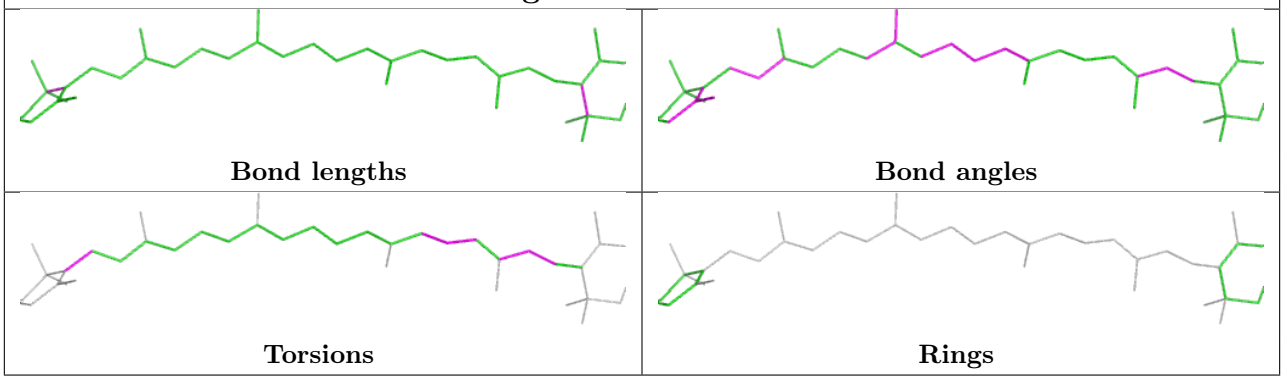
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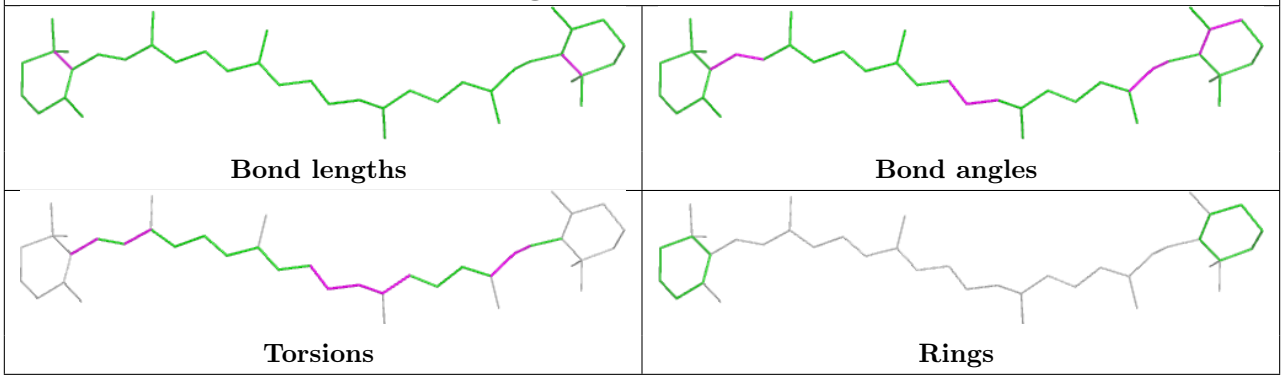
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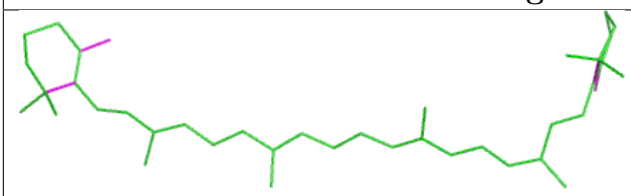
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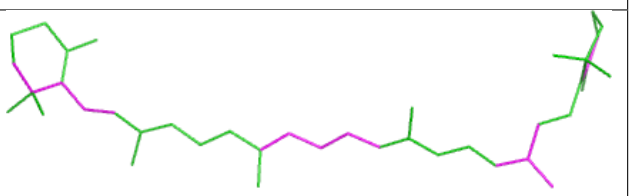
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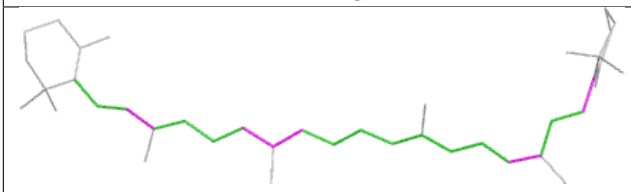
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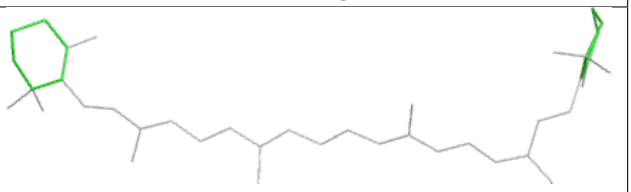
Bond lengths



Bond angles



Torsions

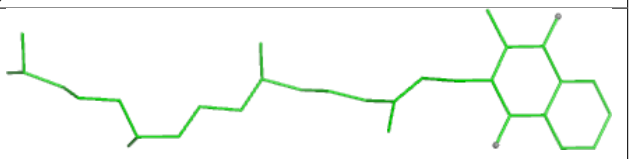


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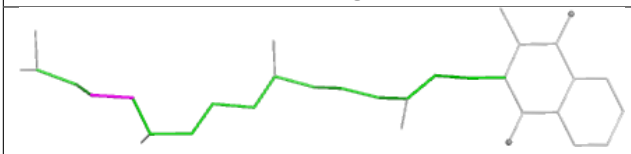
Ligand PQN 1 1646



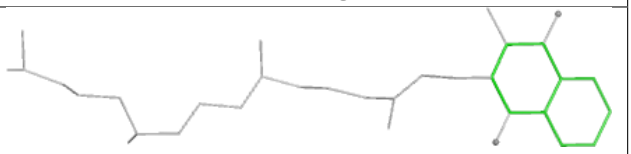
Bond lengths



Bond angles

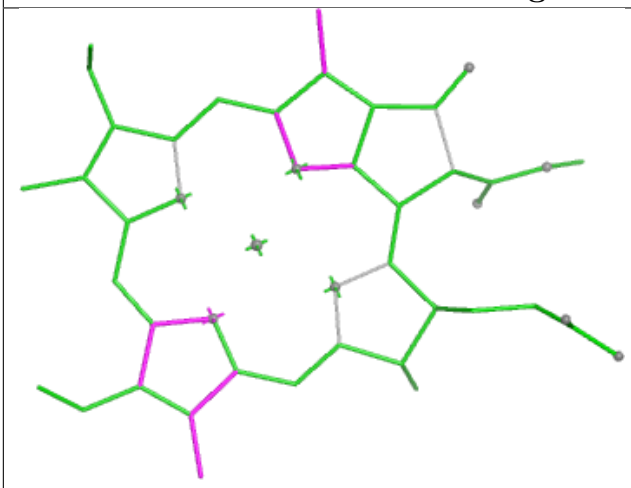


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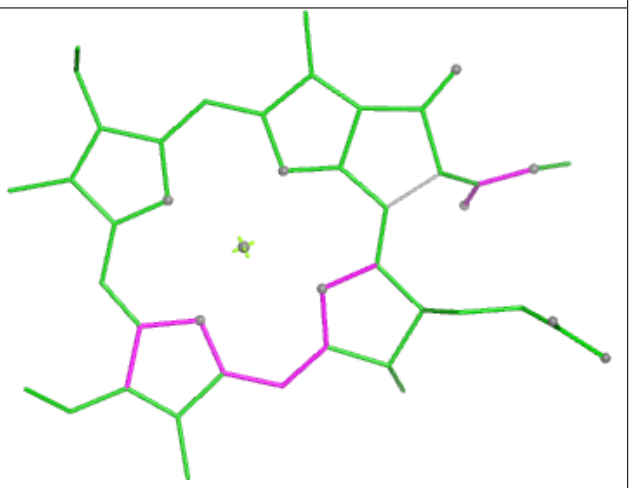


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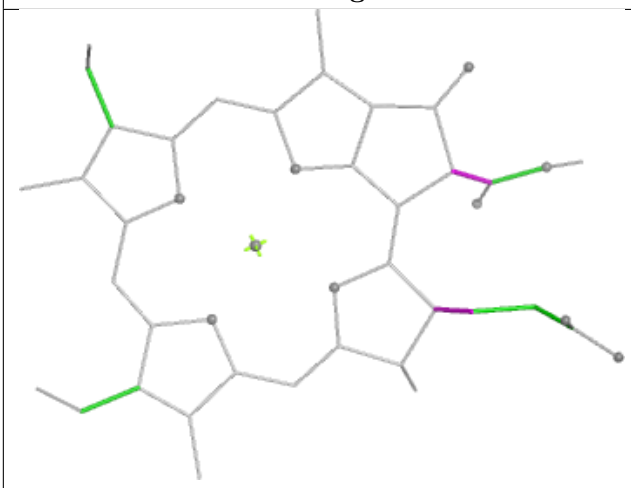
Ligand CLA 2 837



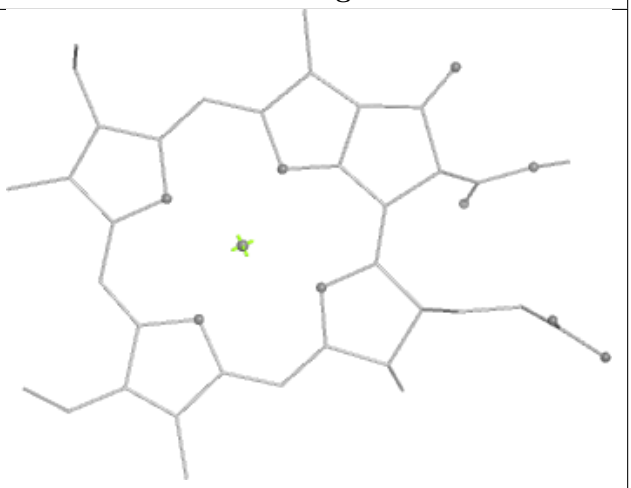
Bond lengths



Bond angles

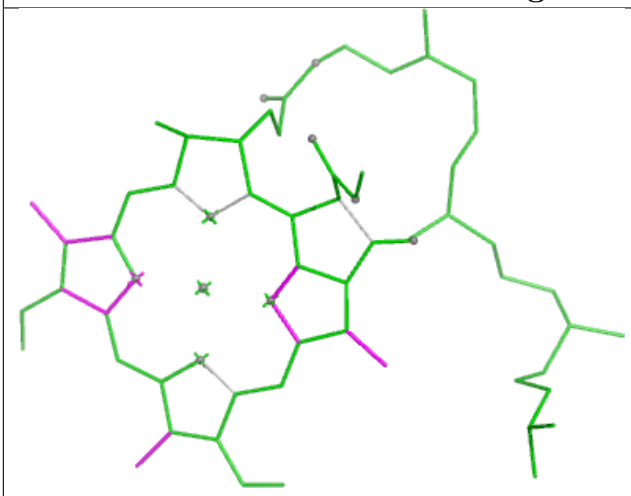


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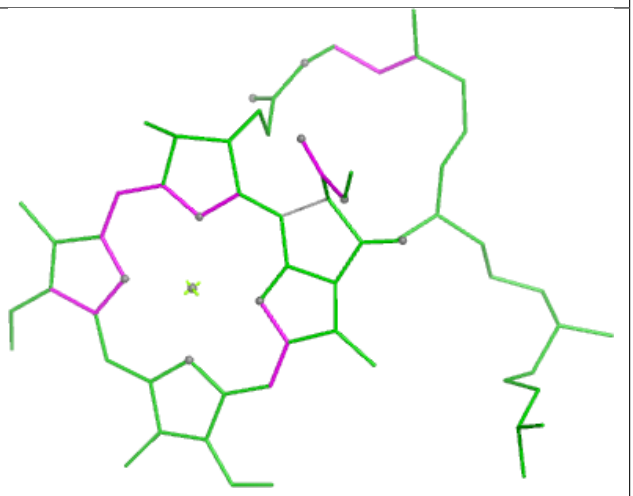


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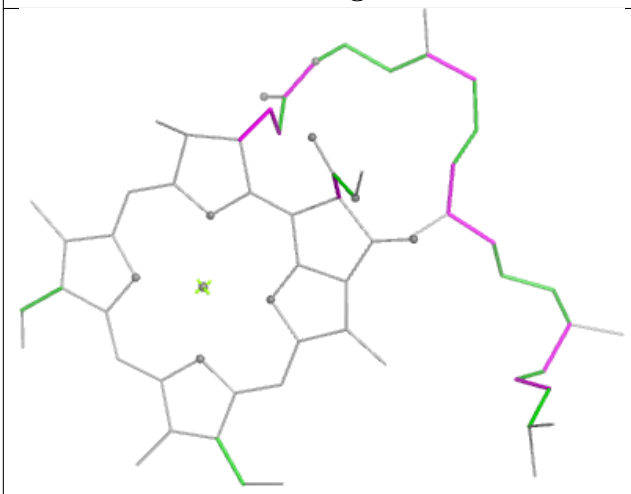
Ligand CLA b 833



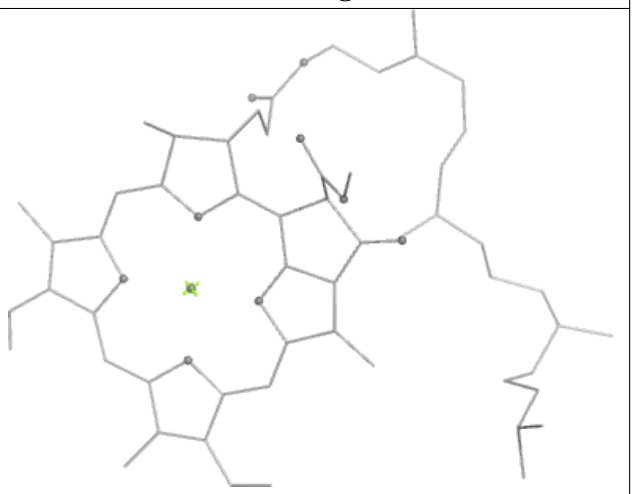
Bond lengths



Bond angles



Torsions

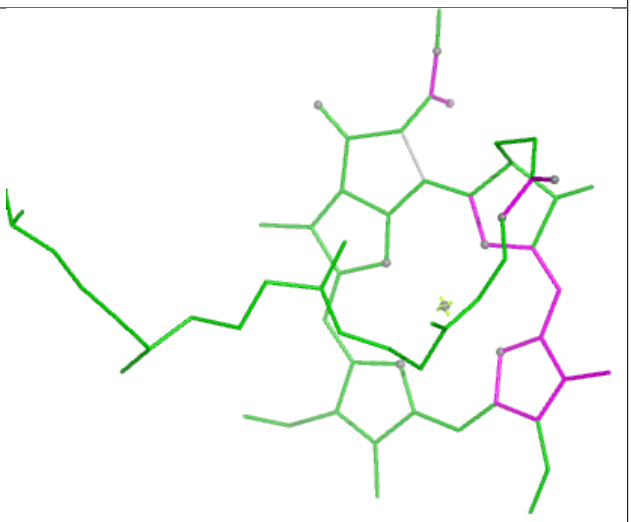


Rings

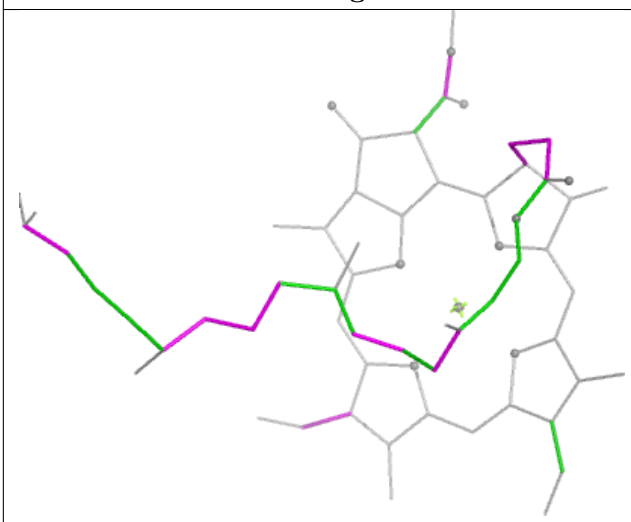
Ligand CLA b 828



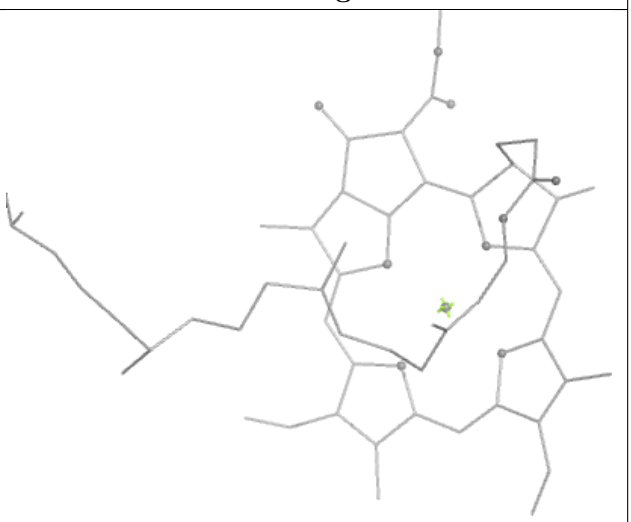
Bond lengths



Bond angles

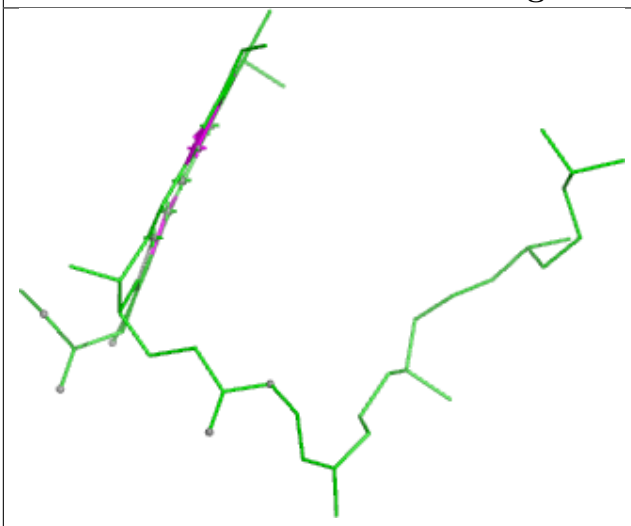


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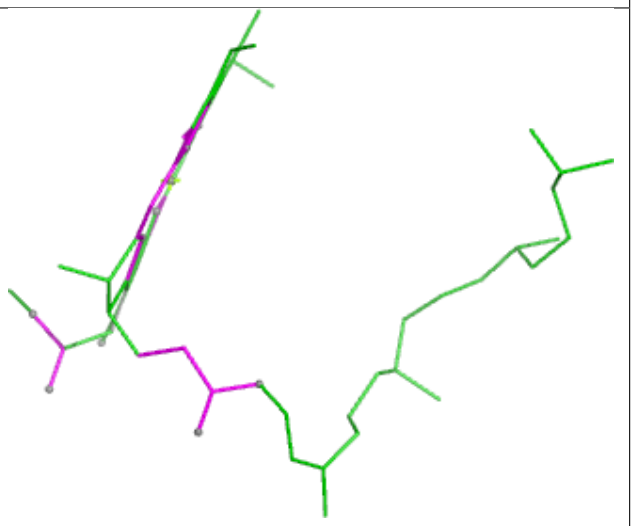


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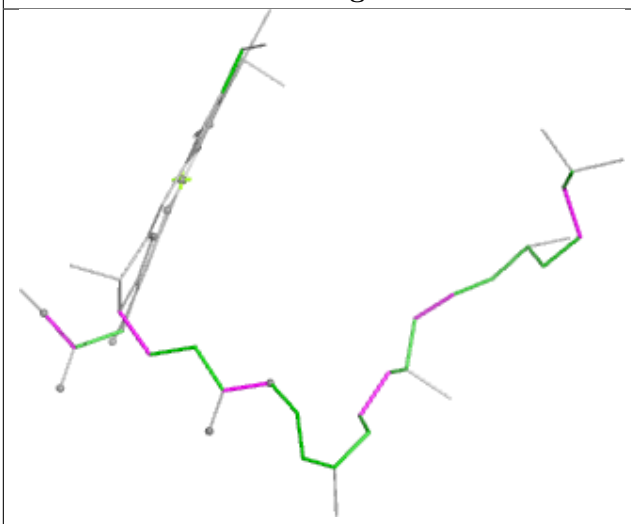
Ligand CLA b 835



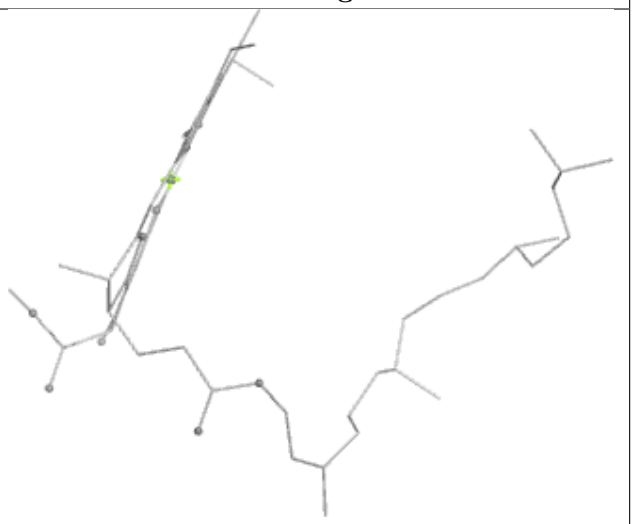
Bond lengths



Bond angles

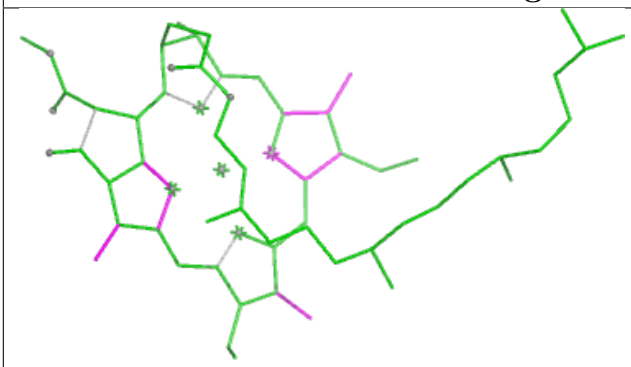


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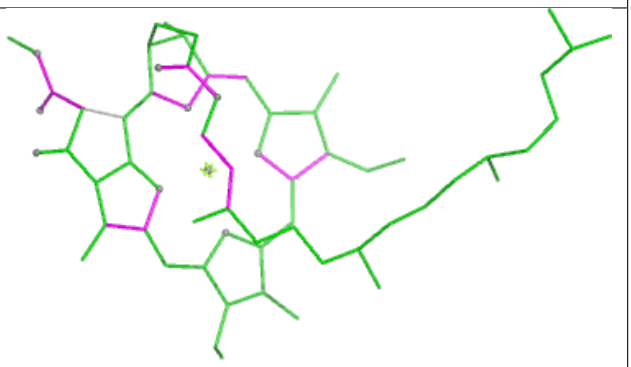


Rings

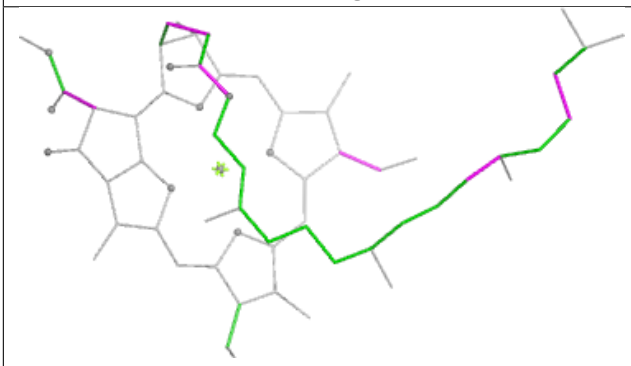
Ligand CLA B 807



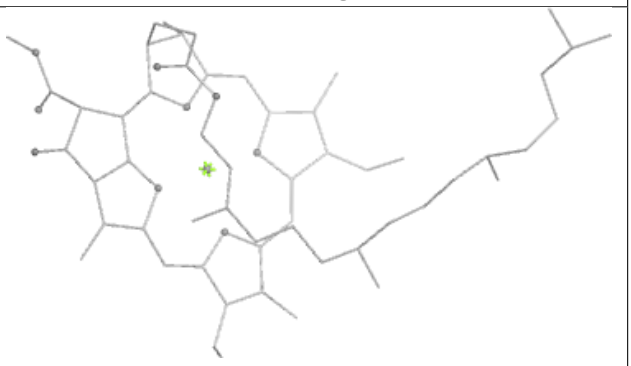
Bond lengths



Bond angles

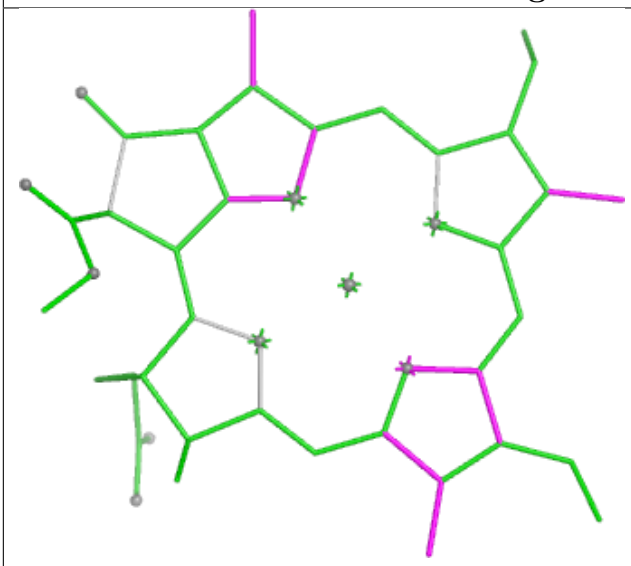


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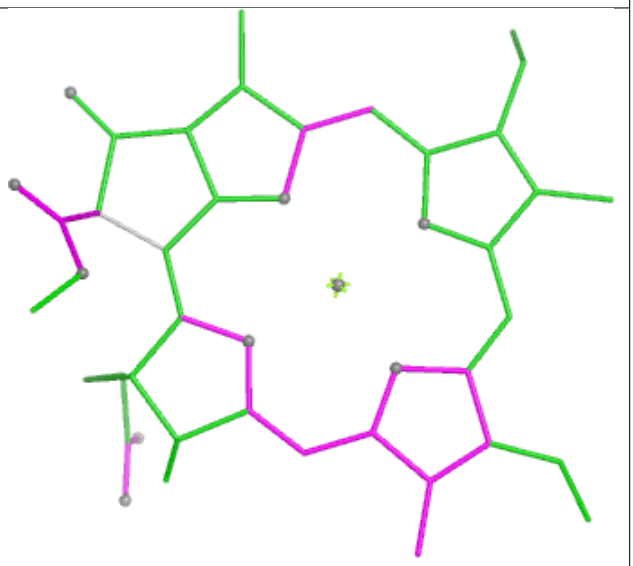


Rings

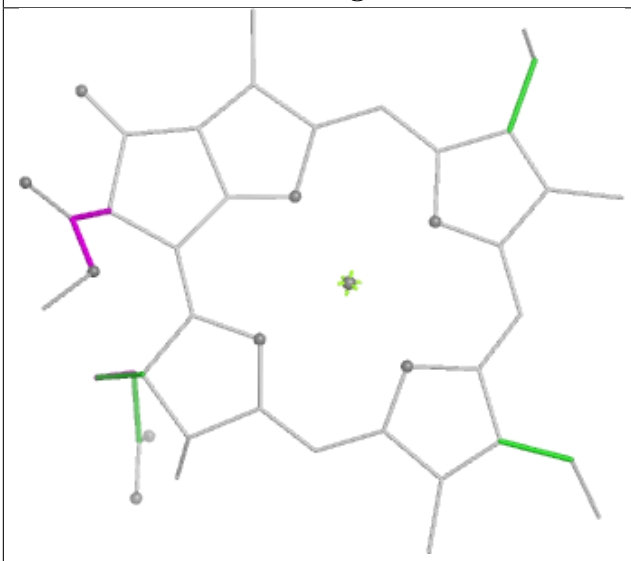
Ligand CLA 2 822



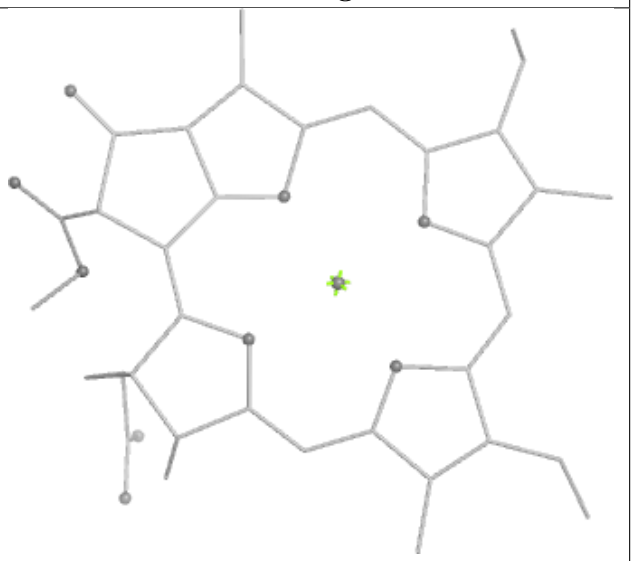
Bond lengths



Bond angles

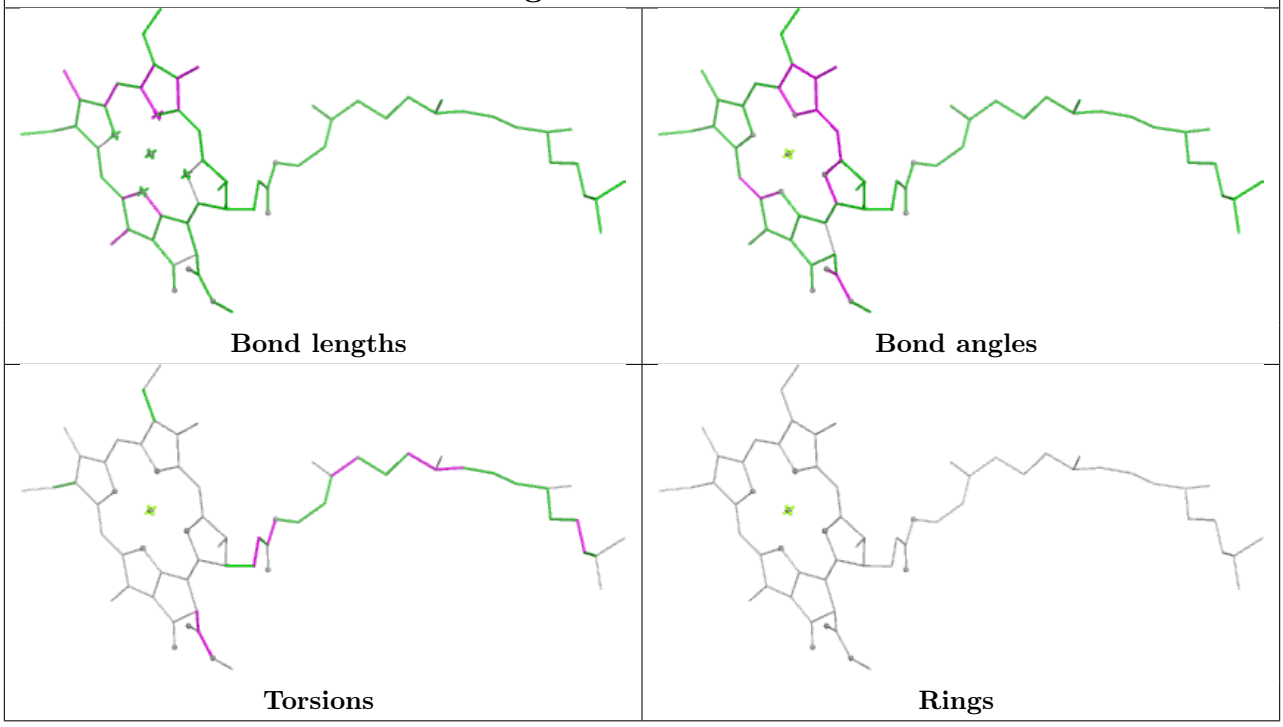


Torsions

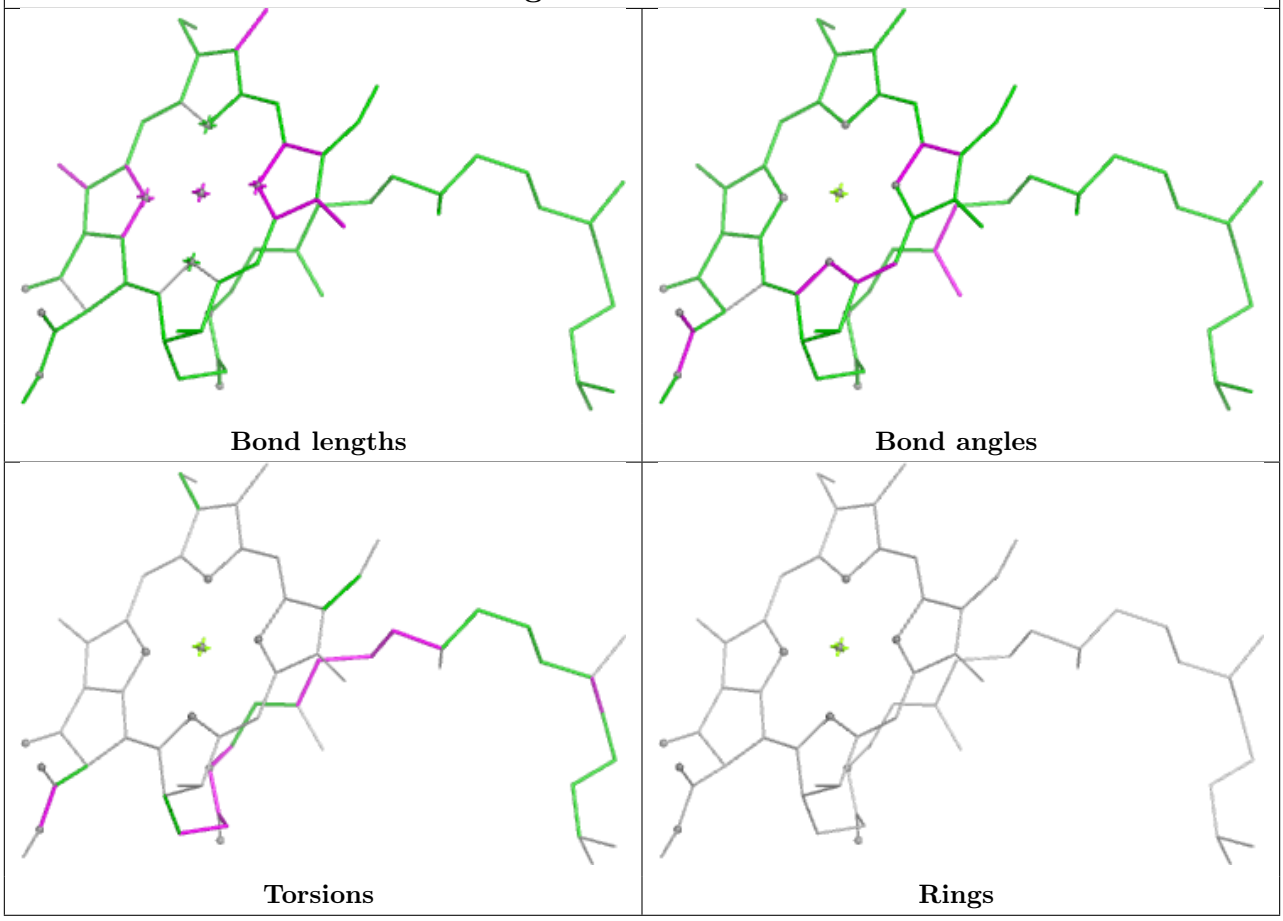


Rings

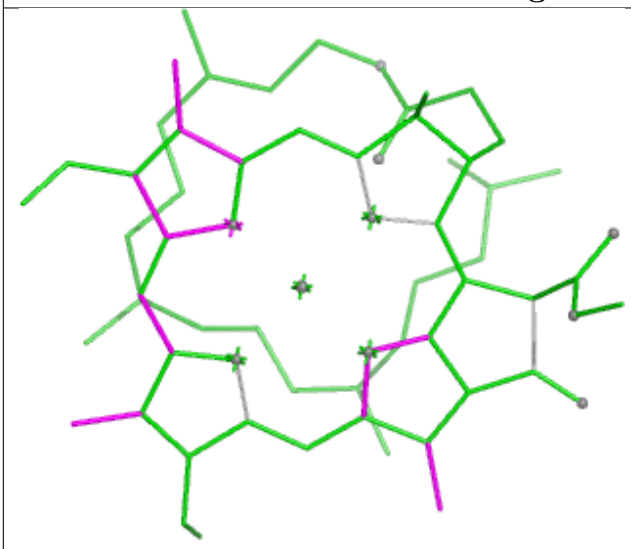
Ligand CLA A 822



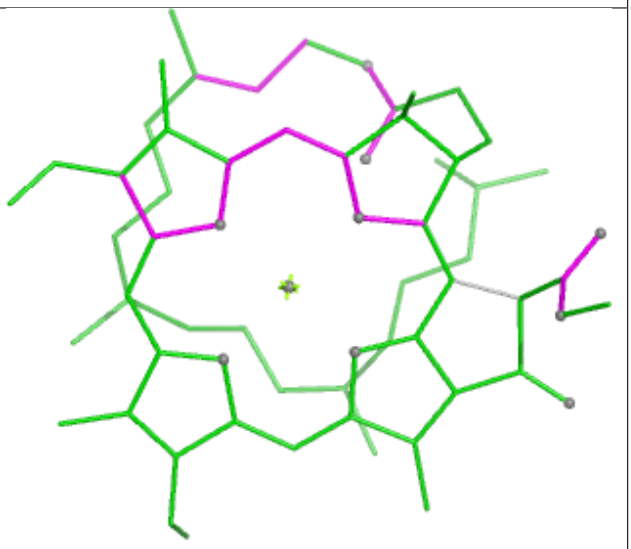
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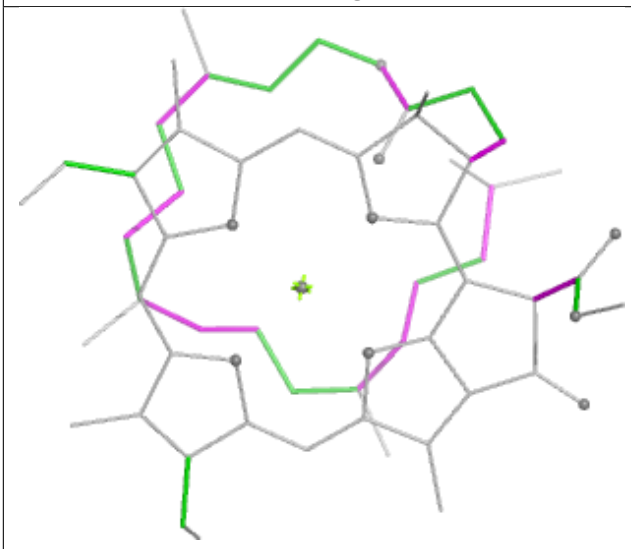
Ligand CLA 0 205



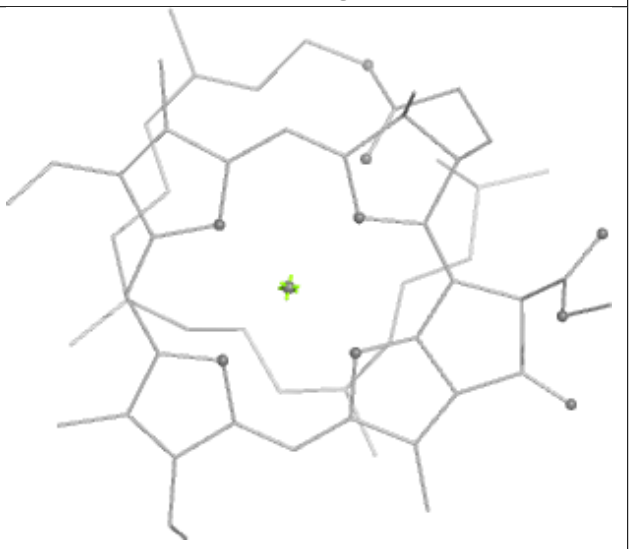
Bond lengths



Bond angles

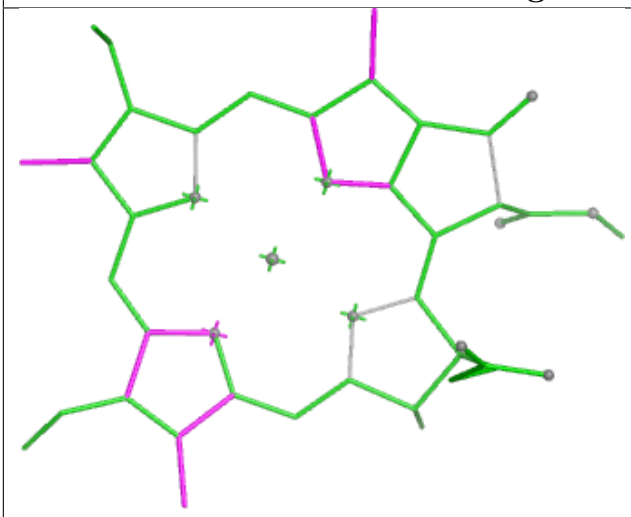


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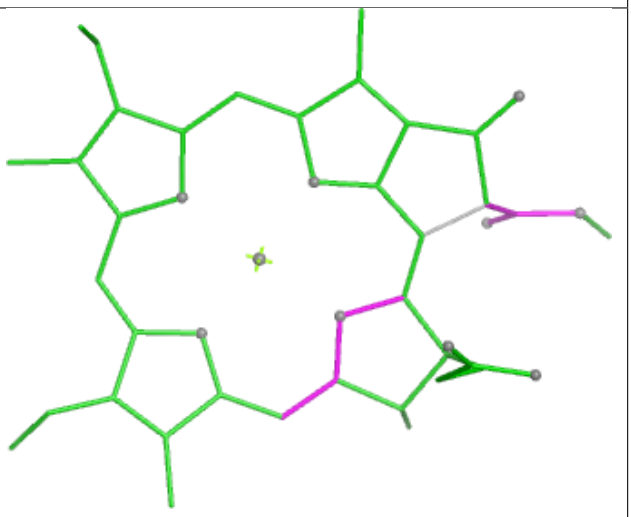


Rings

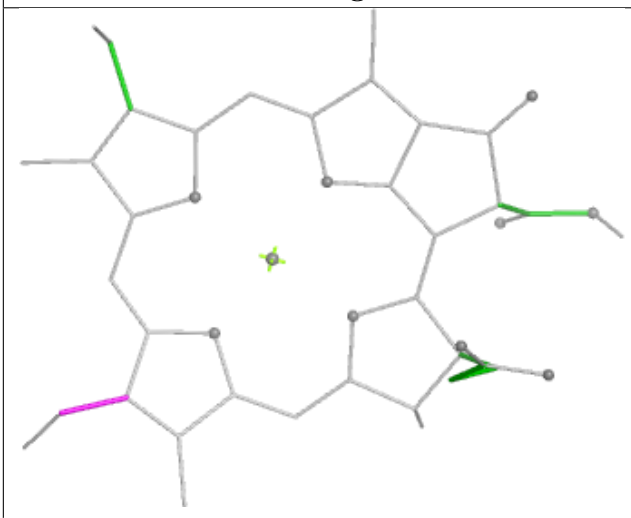
Ligand CLA b 813



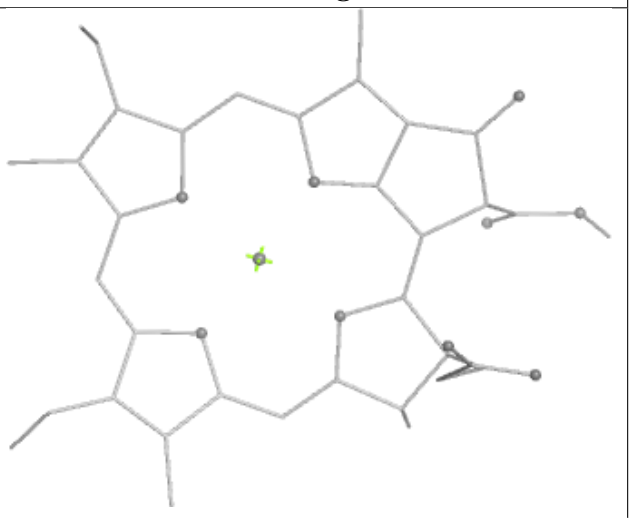
Bond lengths



Bond angles



Torsions



Rings

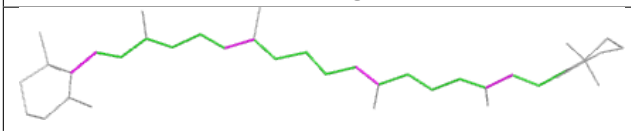
Ligand BCR 0 209



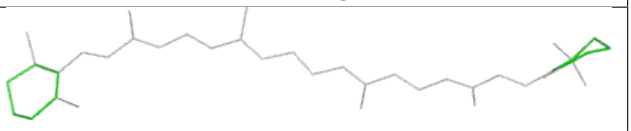
Bond lengths



Bond angles

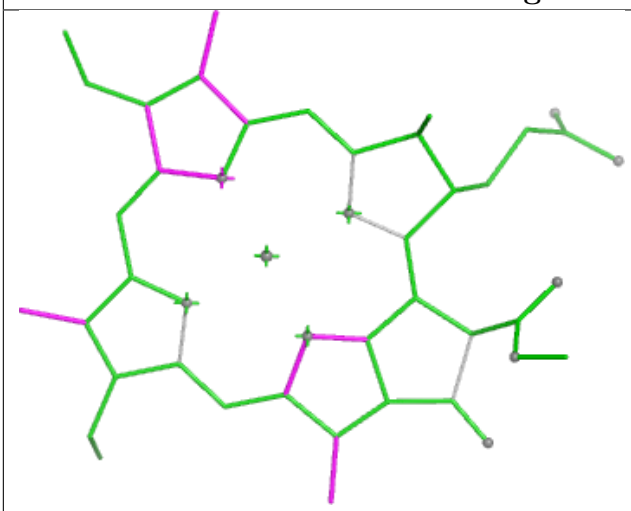


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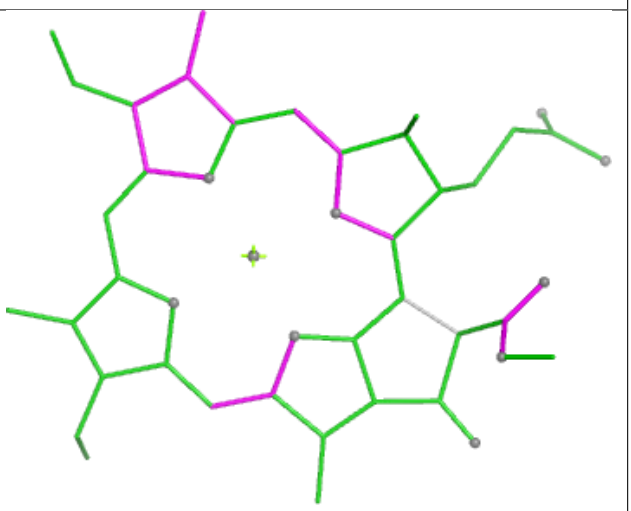


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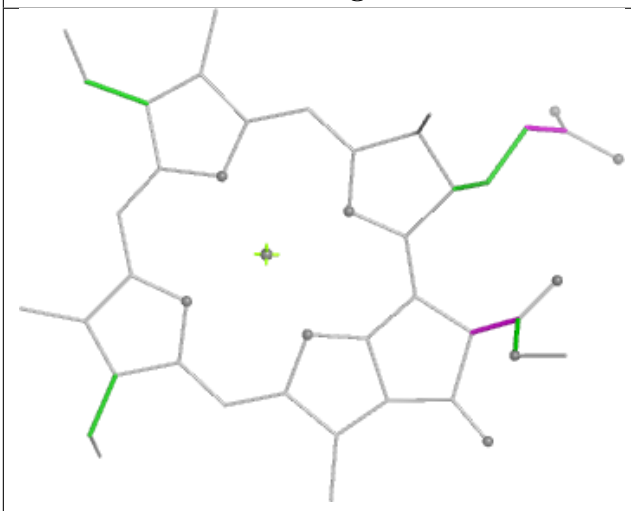
Ligand CLA A 844



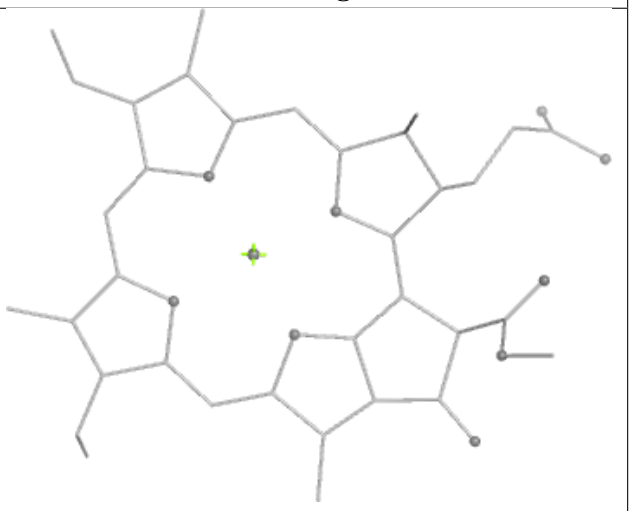
Bond lengths



Bond angles

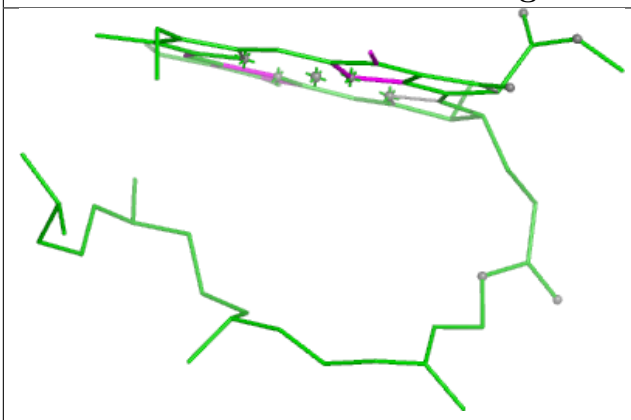


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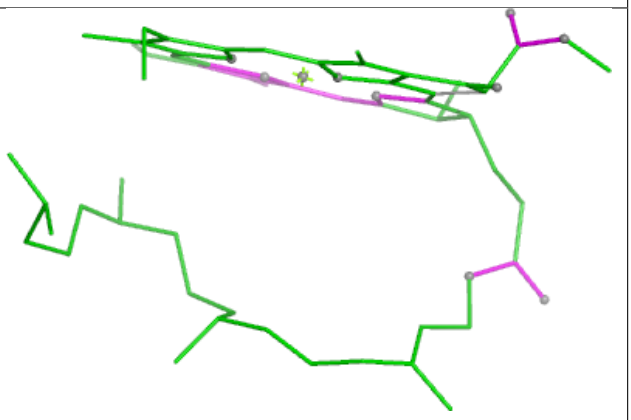


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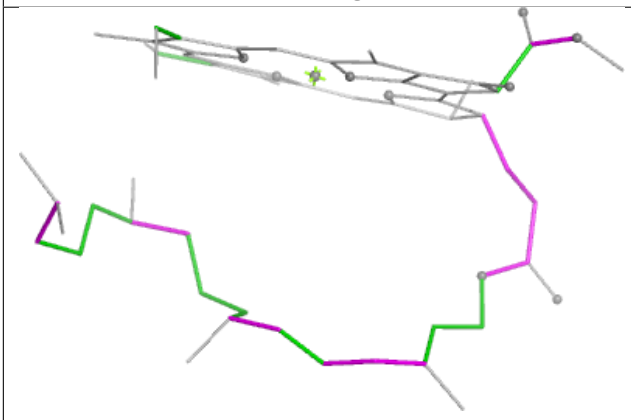
Ligand CLA 1 1622



Bond lengths



Bond angles

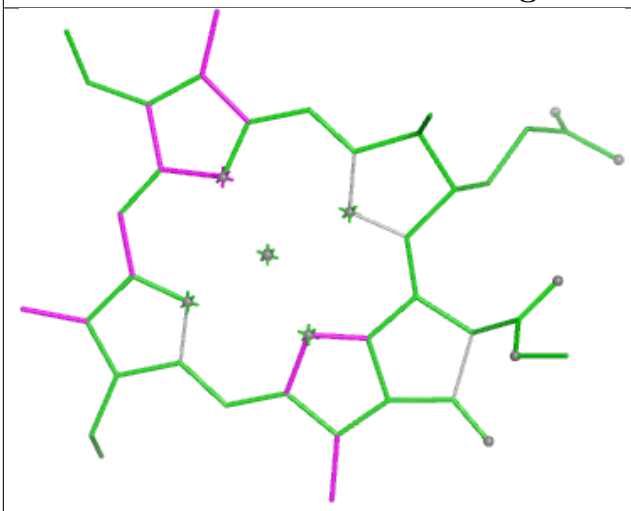


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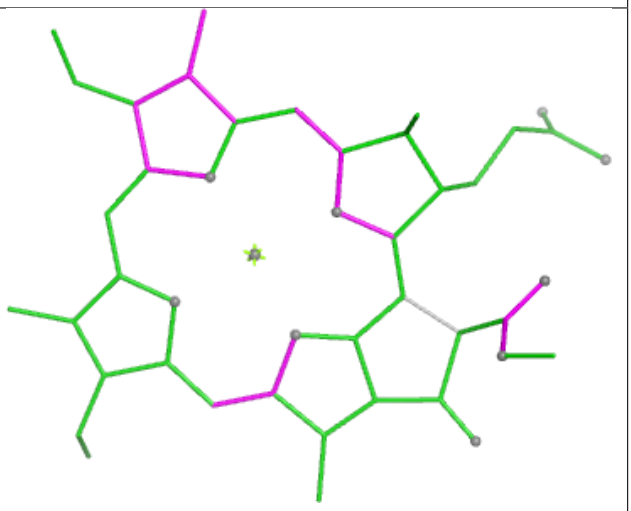


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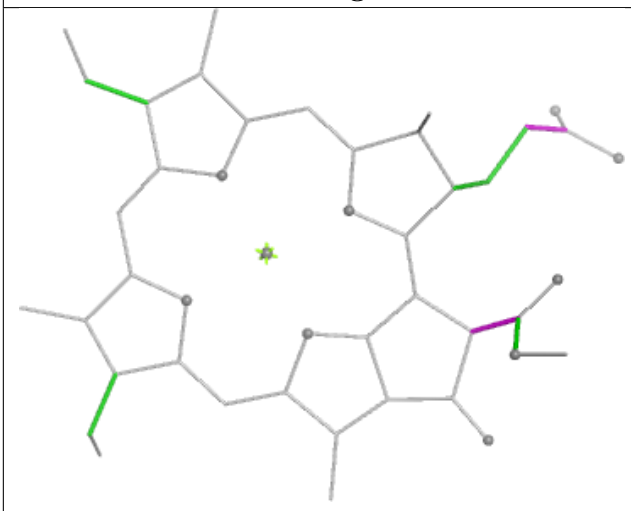
Ligand CLA 1 1645



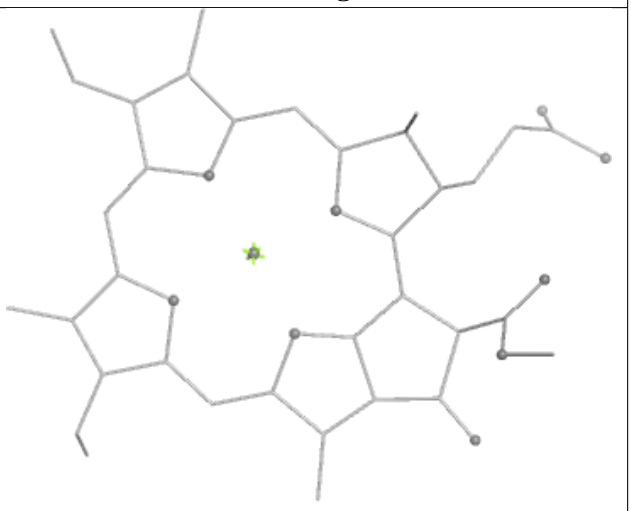
Bond lengths



Bond angles

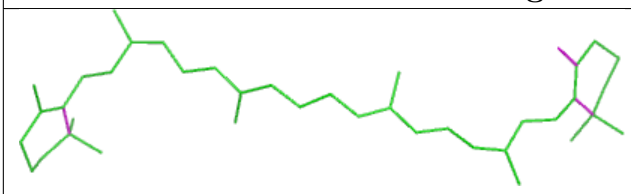


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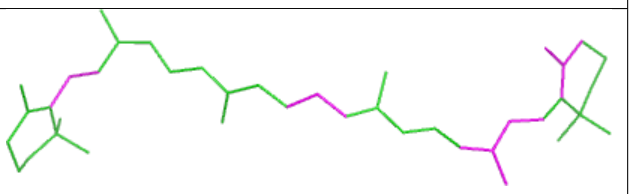


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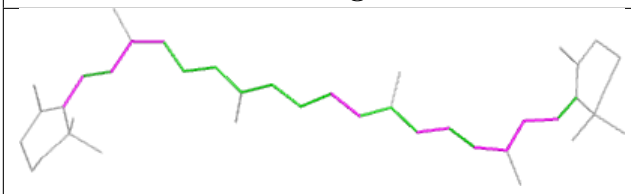
Ligand BCR 2 846



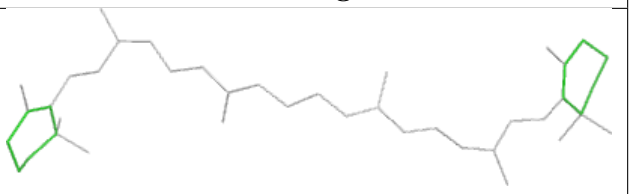
Bond lengths



Bond angles

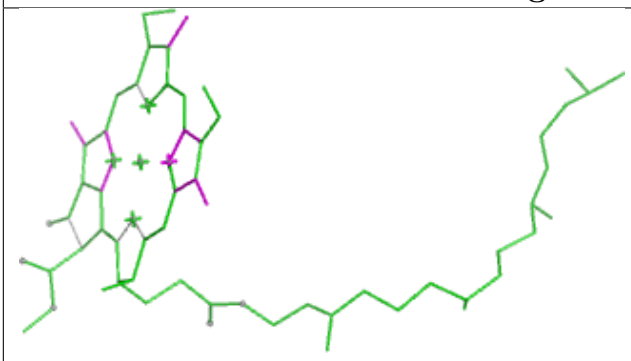


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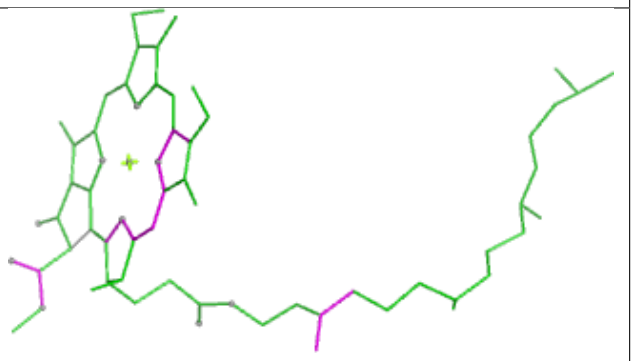


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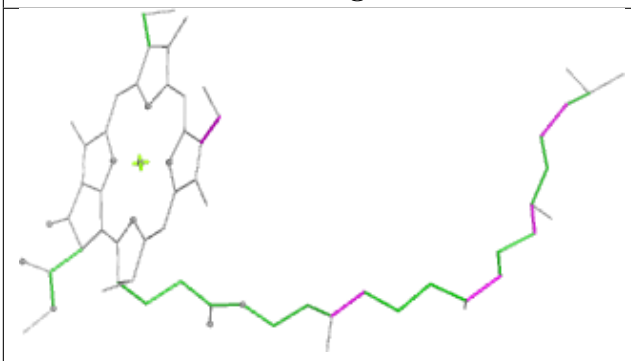
Ligand CLA a 836



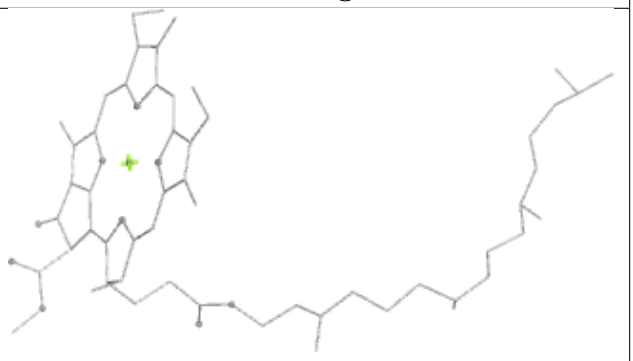
Bond lengths



Bond angles

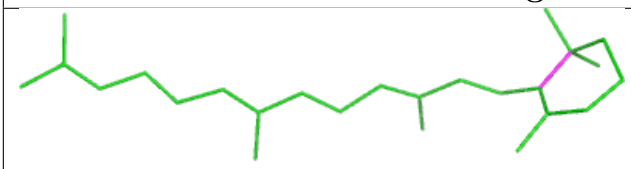


Torsions



Rings

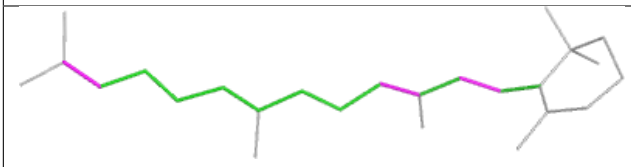
Ligand BCR 9 104



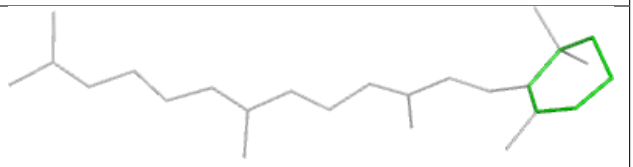
Bond lengths



Bond angles

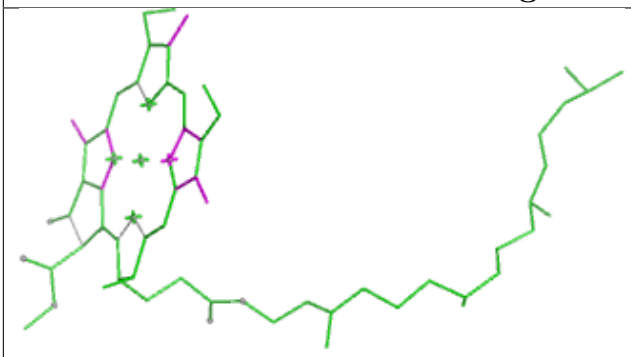


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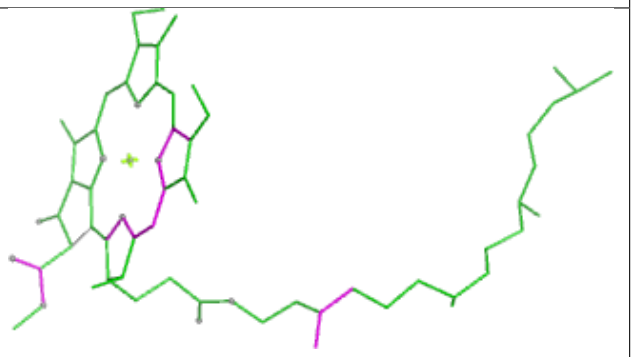


Rings

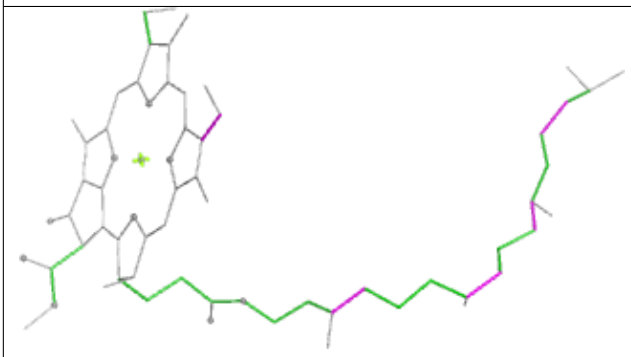
Ligand CLA 1 1637



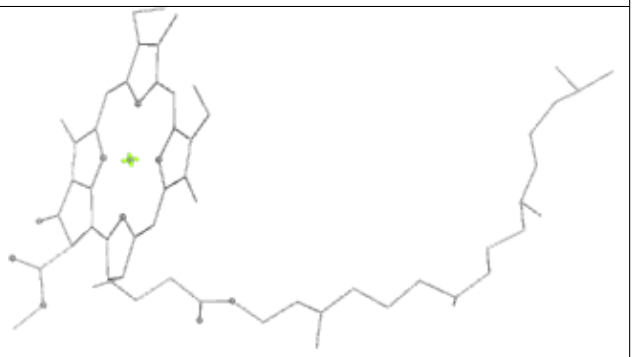
Bond lengths



Bond angles

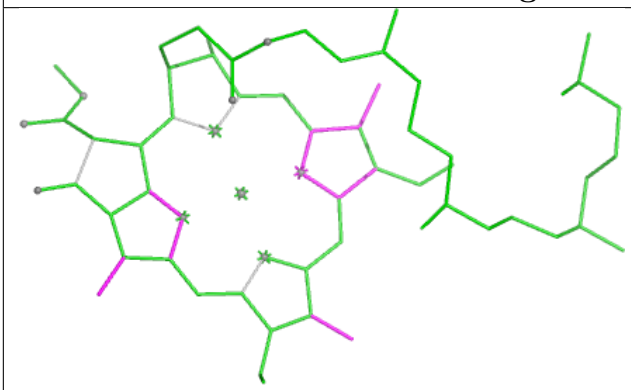


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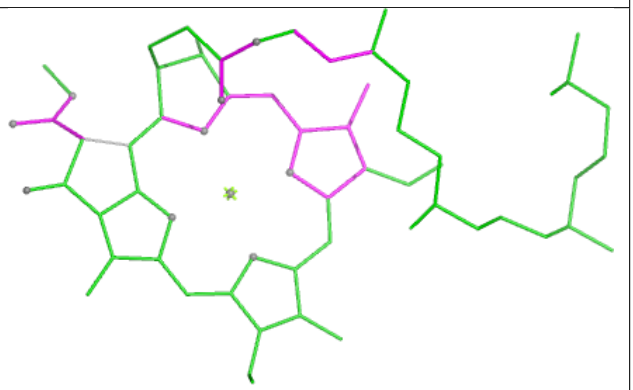


Rings

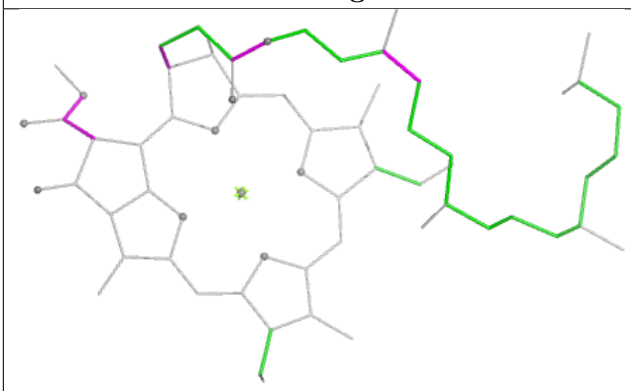
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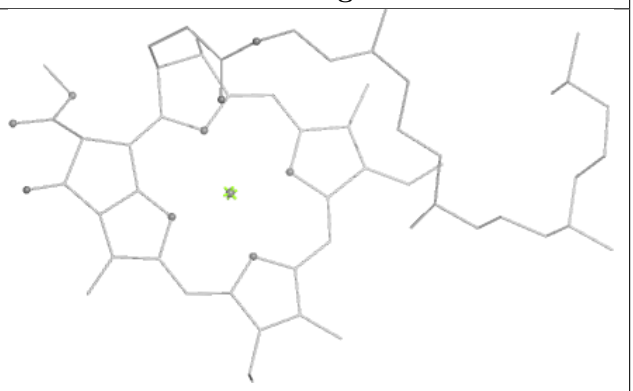
Bond lengths



Bond angles

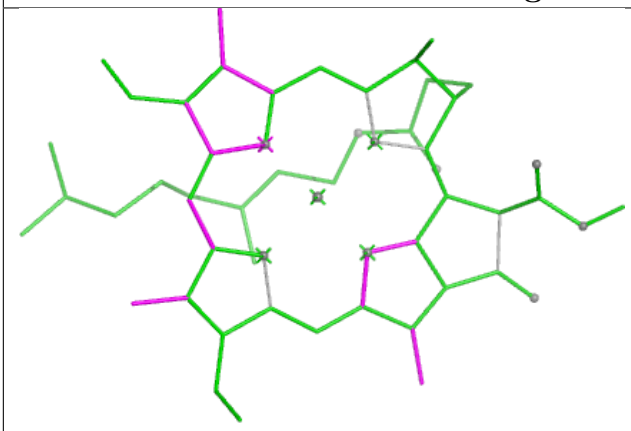


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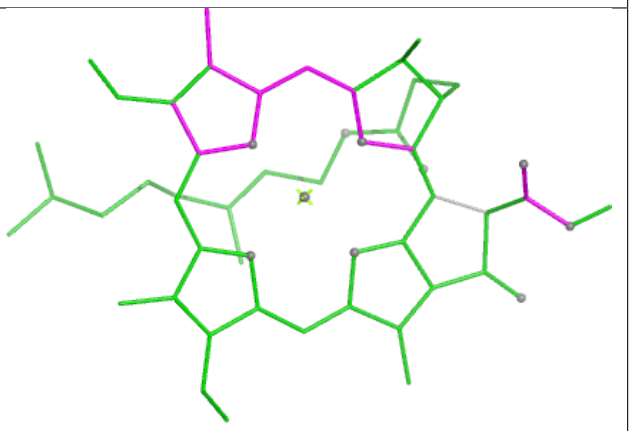


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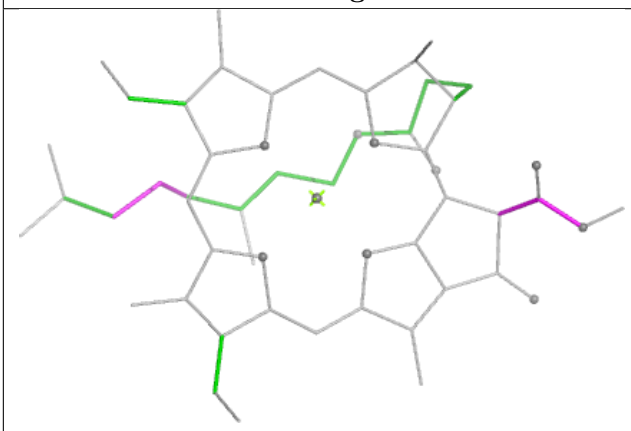
Ligand CLA B 822



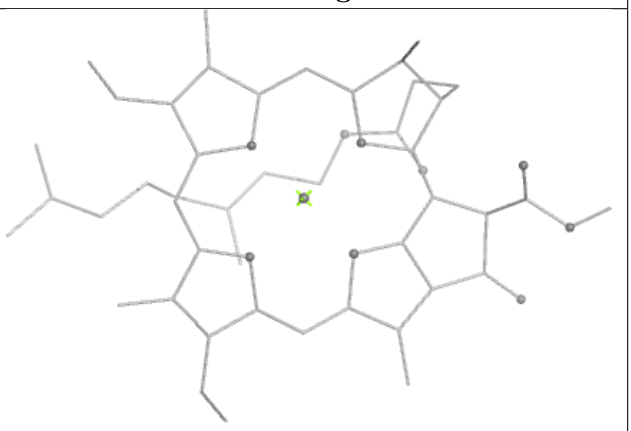
Bond lengths



Bond angles

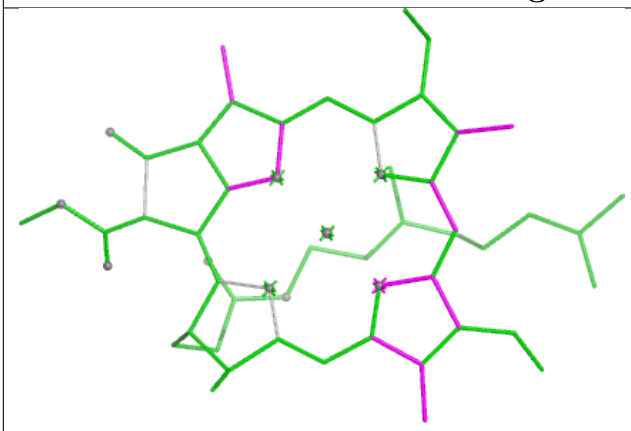


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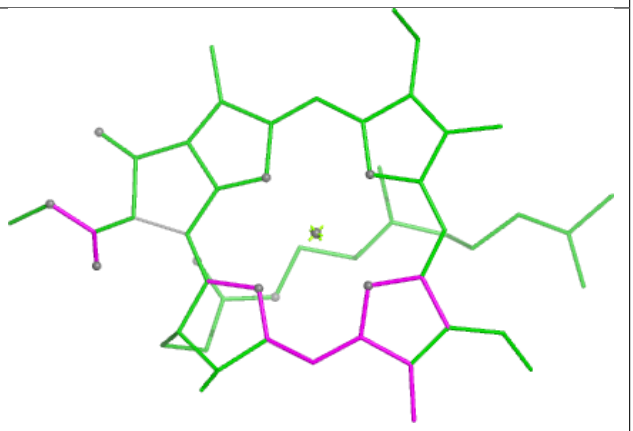


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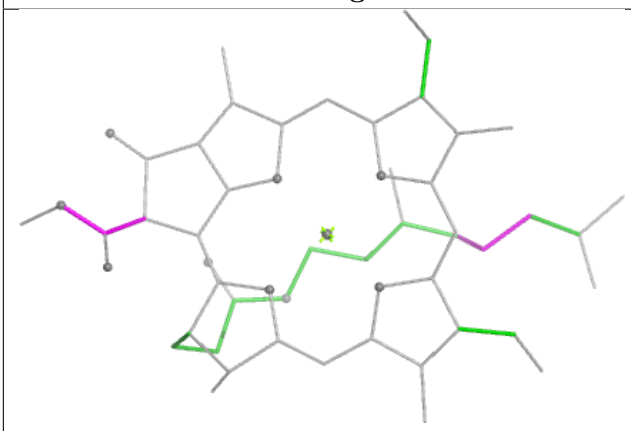
Ligand CLA 2 823



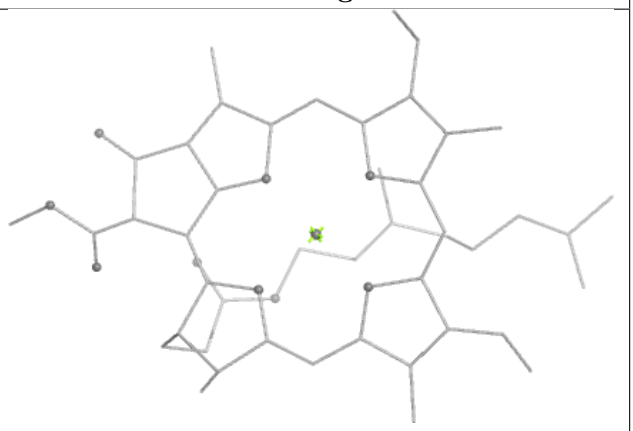
Bond lengths



Bond angles

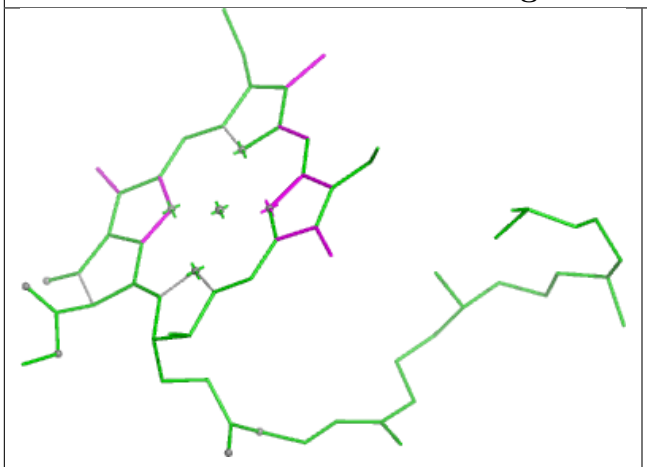


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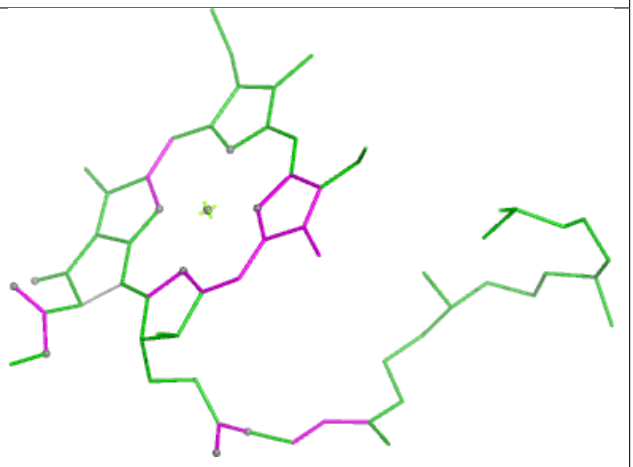


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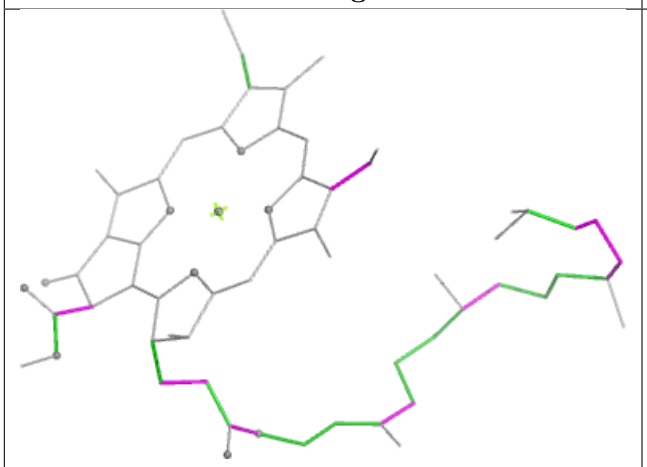
Ligand CLA 1 1626



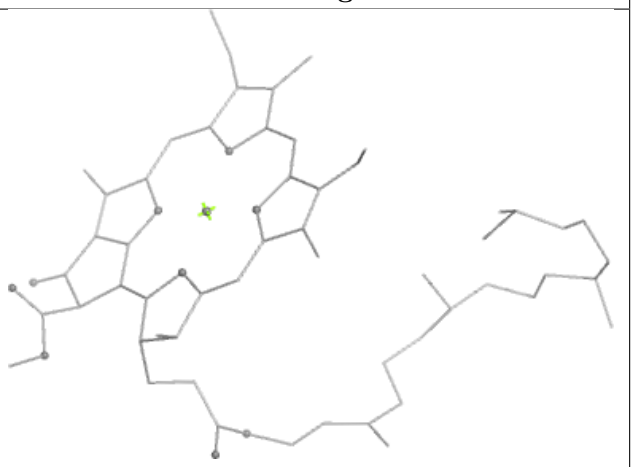
Bond lengths



Bond angles

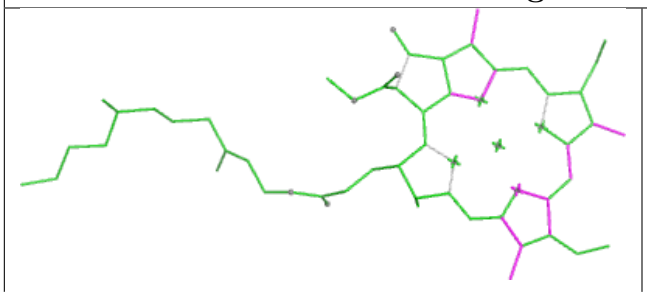


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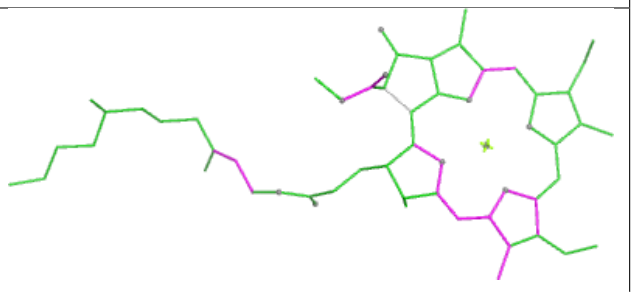


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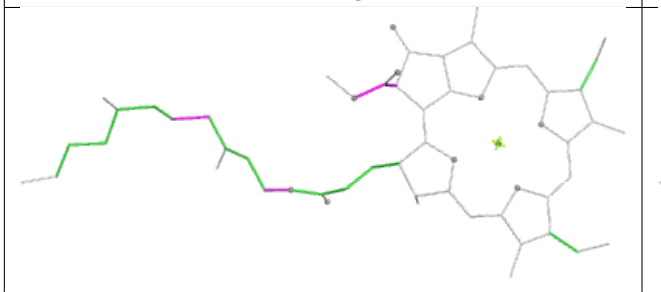
Ligand CLA F 201



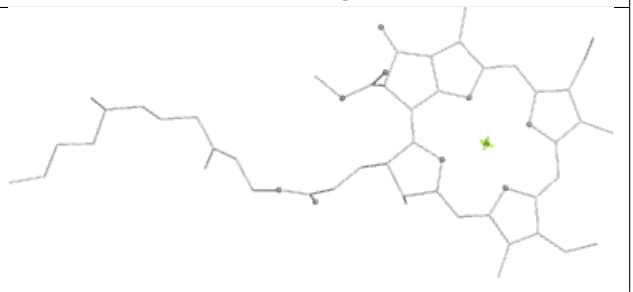
Bond lengths



Bond angles

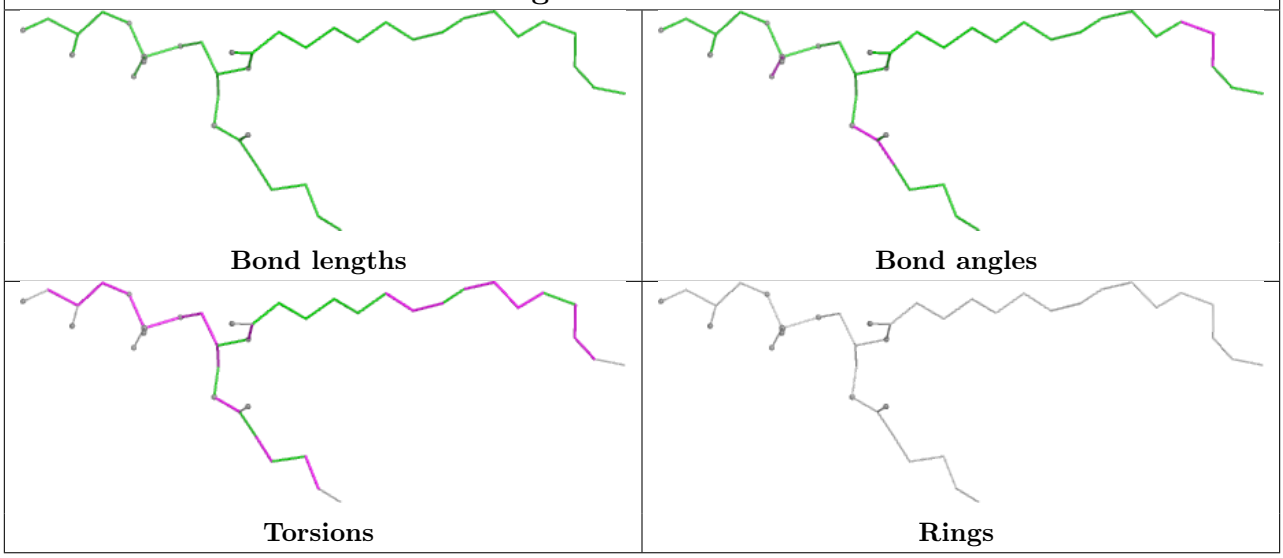


Torsions

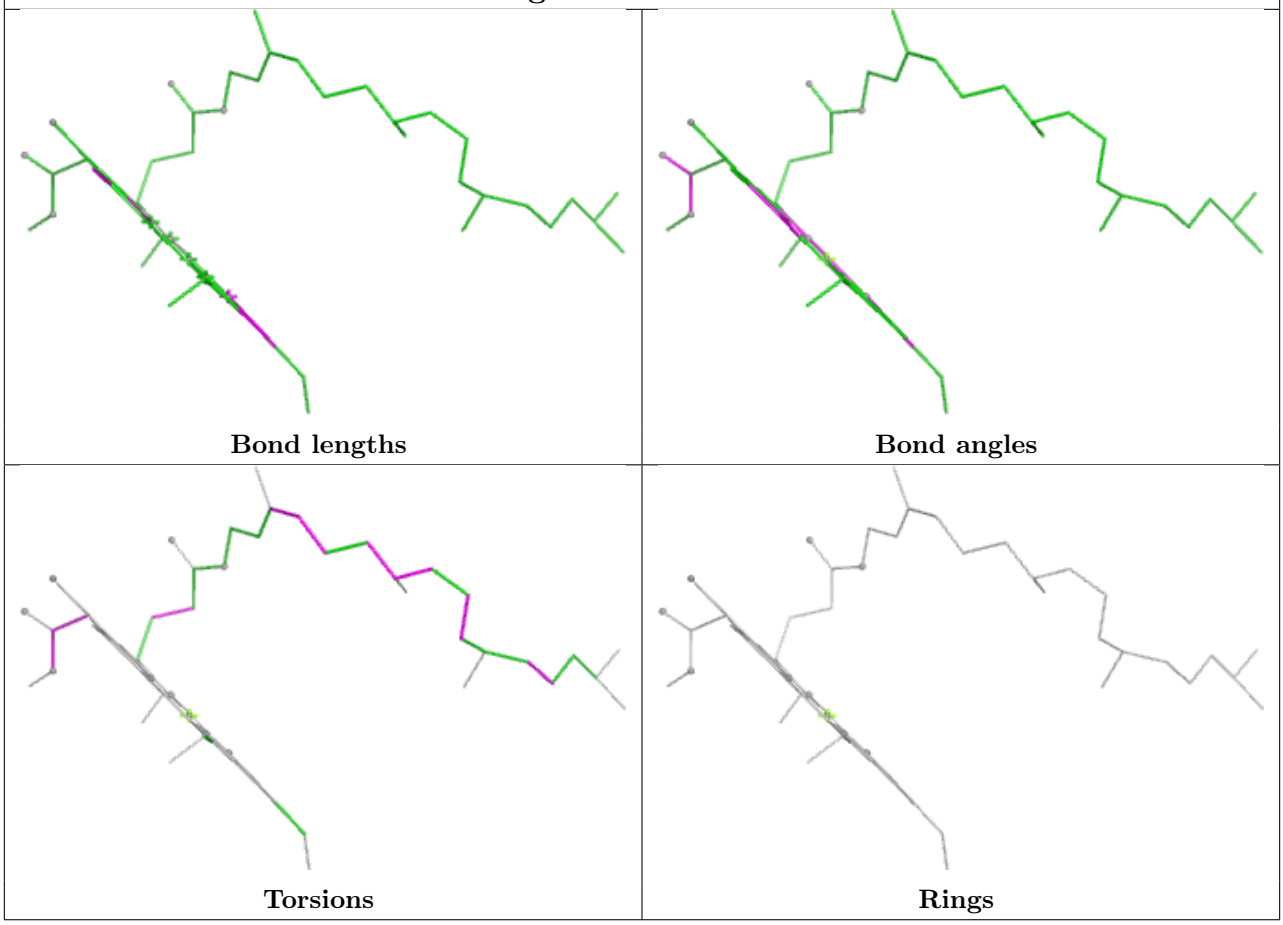


Rings

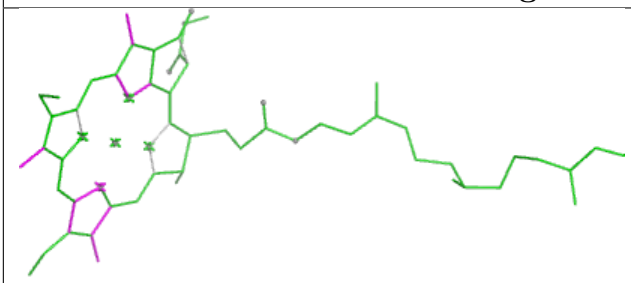
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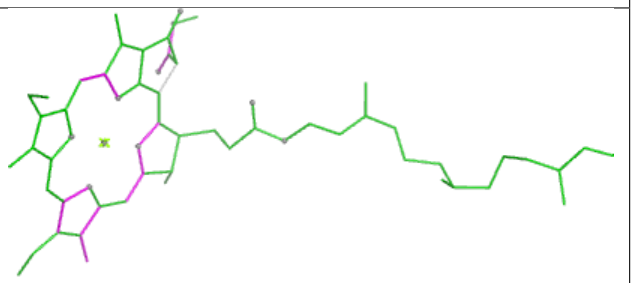
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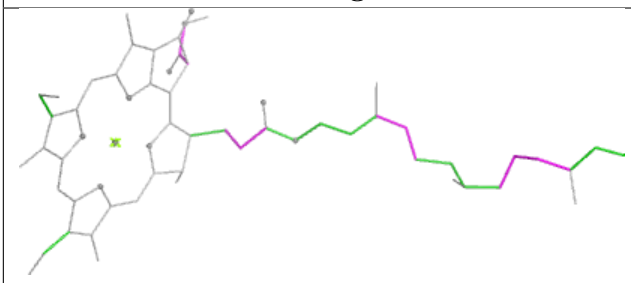
Ligand CLA 1 1611



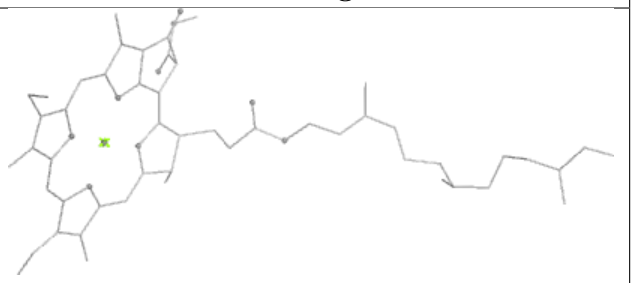
Bond lengths



Bond angles

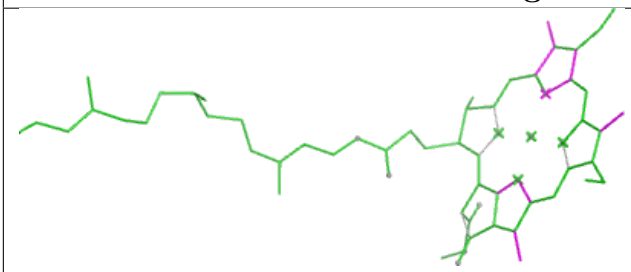


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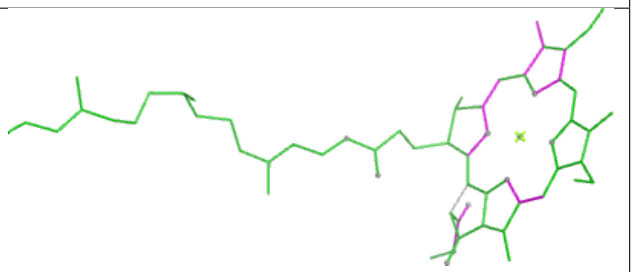


Rings

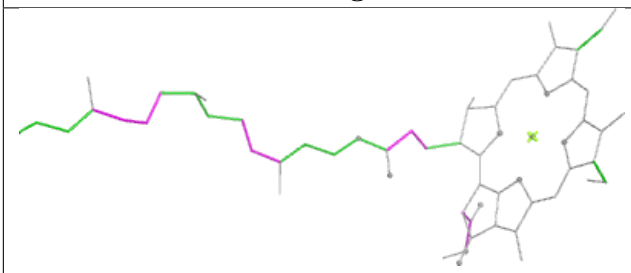
Ligand CLA A 810



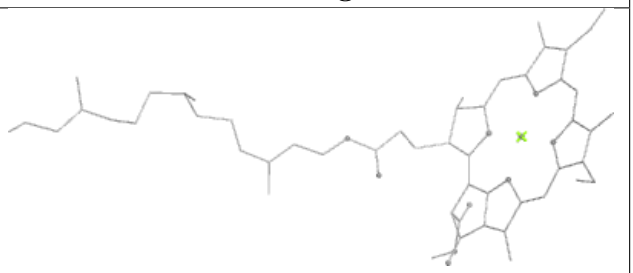
Bond lengths



Bond angles

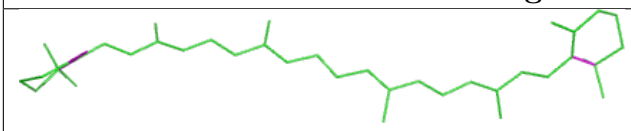


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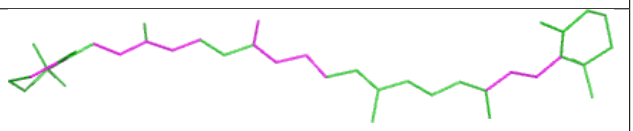


Rings

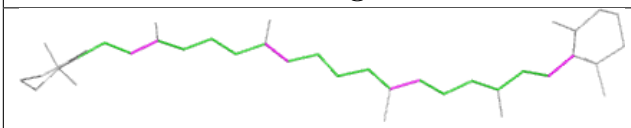
Ligand BCR L 207



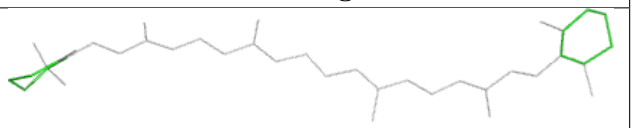
Bond lengths



Bond angles

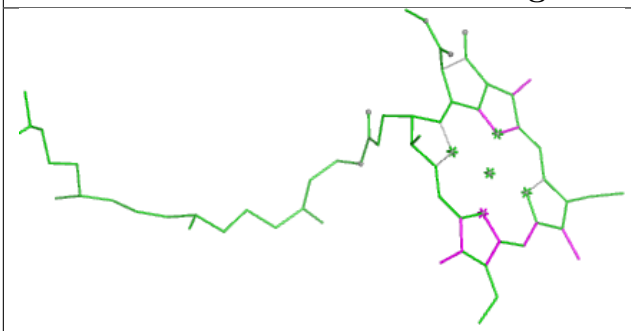


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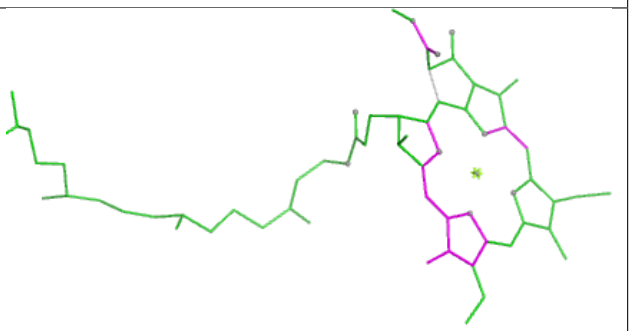


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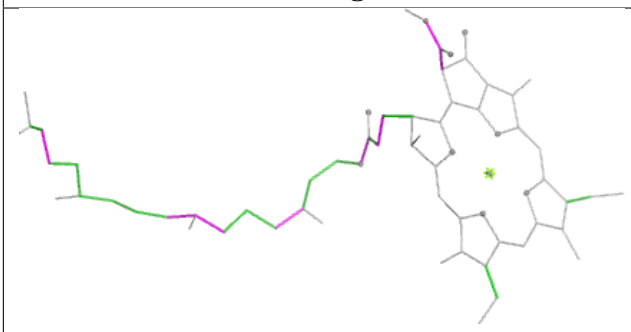
Ligand CLA a 822



Bond lengths



Bond angles



Torsions

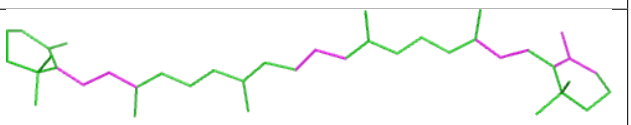


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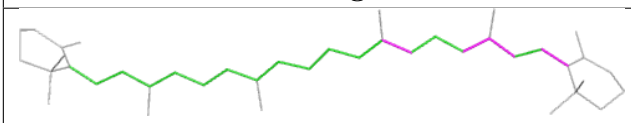
Ligand BCR 1 1650



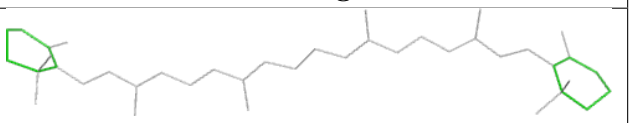
Bond lengths



Bond angles



Torsions

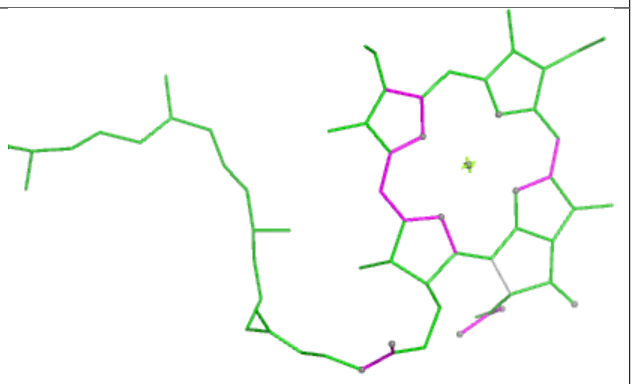


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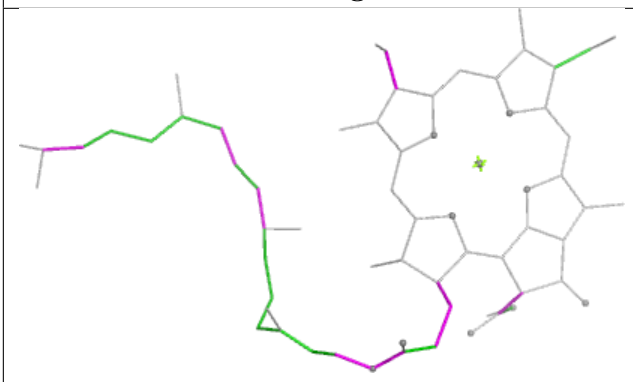
Ligand CLA A 814



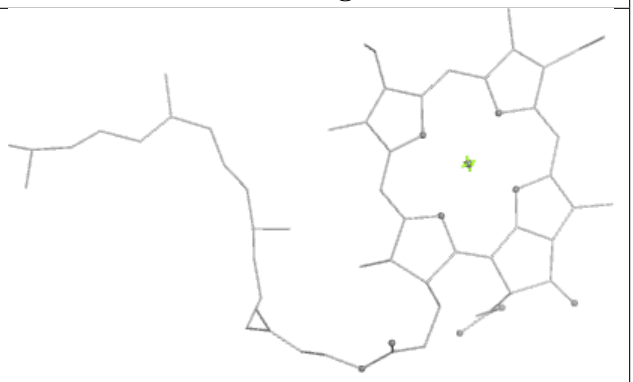
Bond lengths



Bond angles

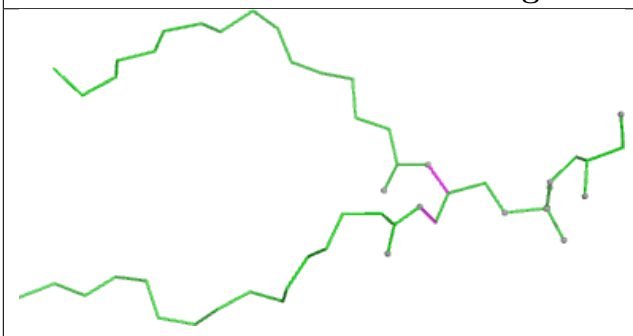


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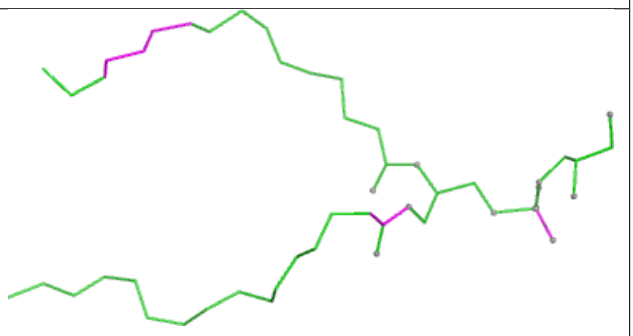


Rings

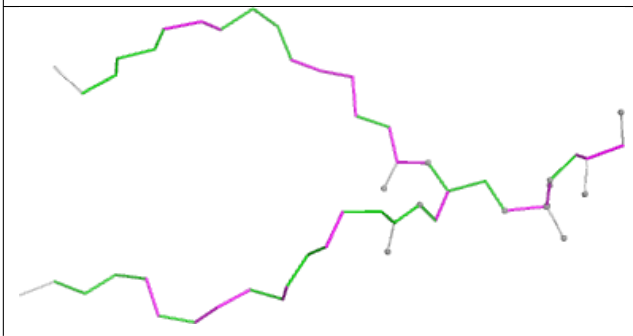
Ligand LHG A 853



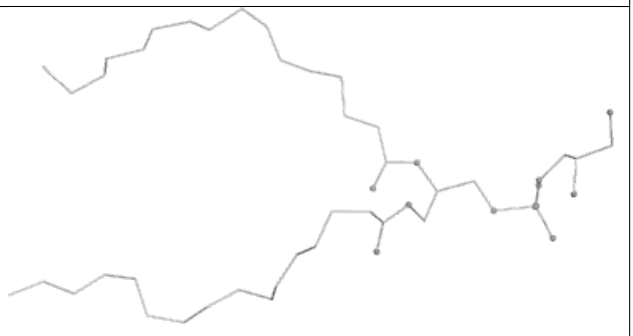
Bond lengths



Bond angles

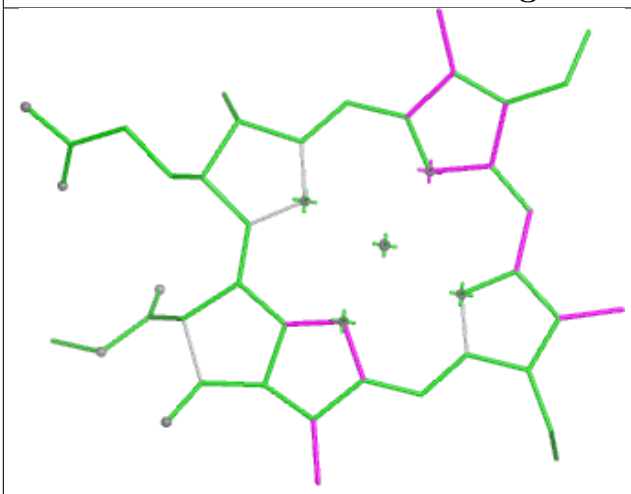


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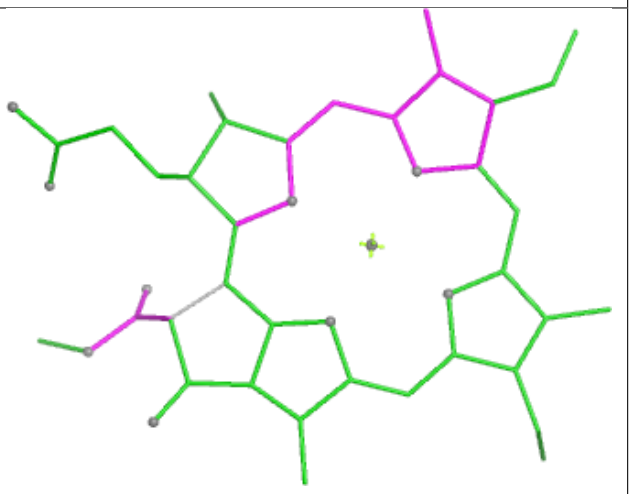


Rings

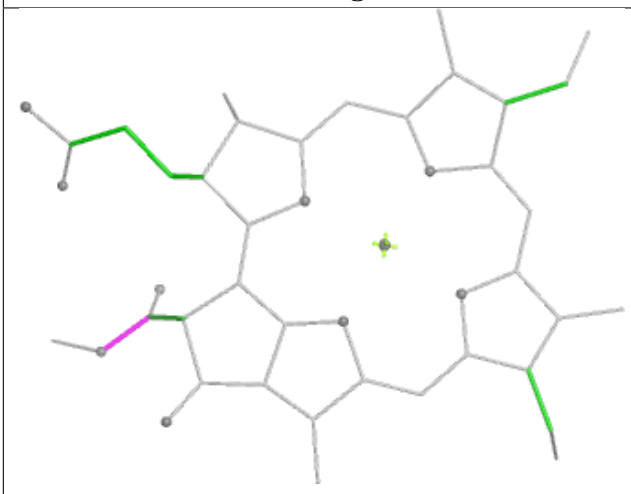
Ligand CLA 8 1301



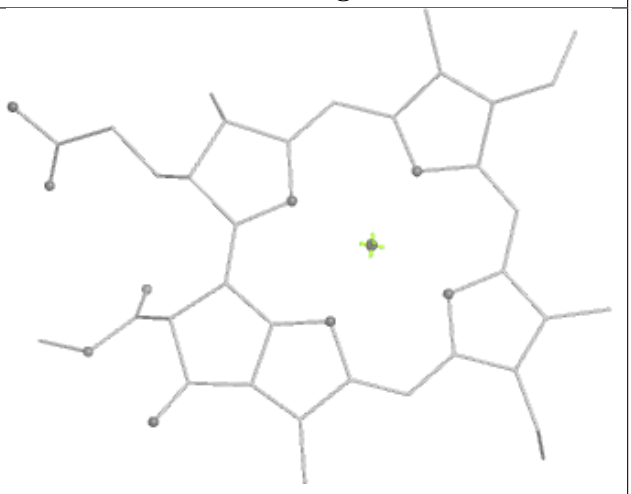
Bond lengths



Bond angles

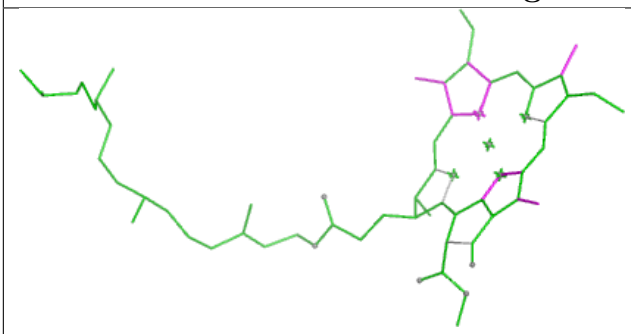


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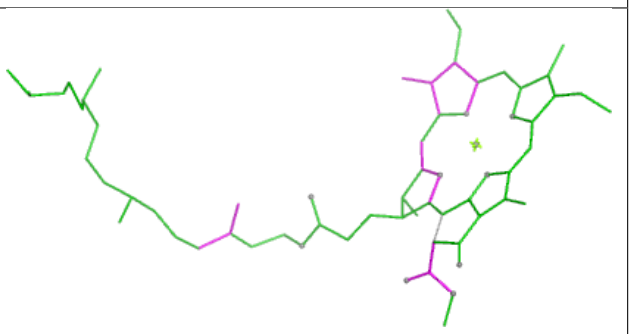


Rings

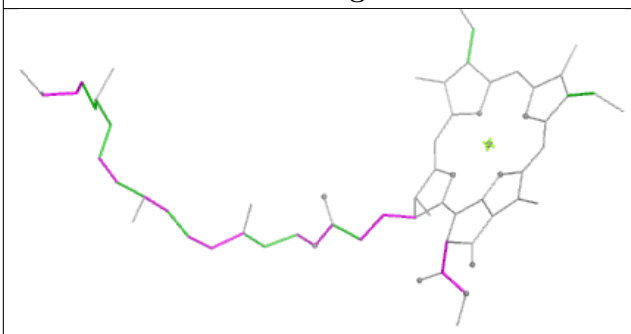
Ligand CLA A 855



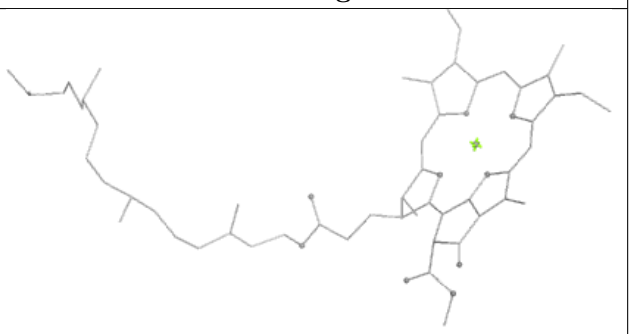
Bond lengths



Bond angles

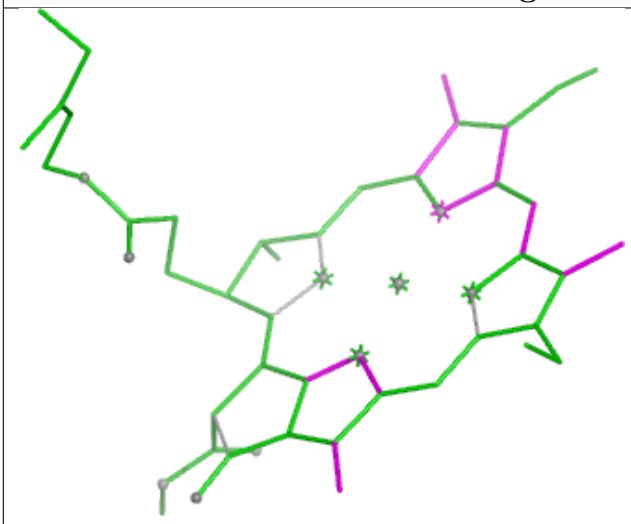


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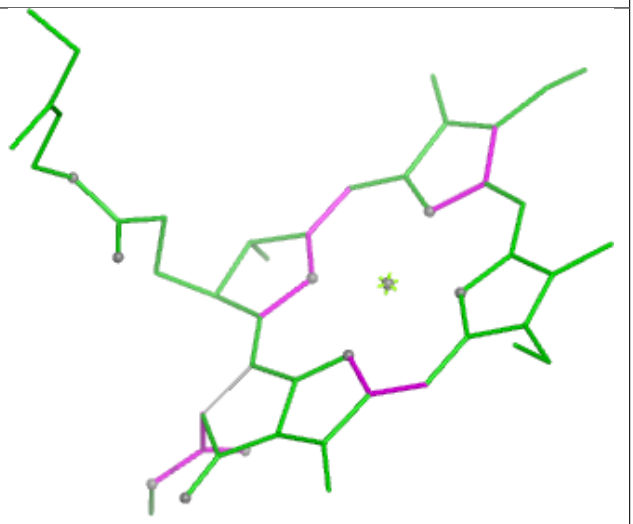


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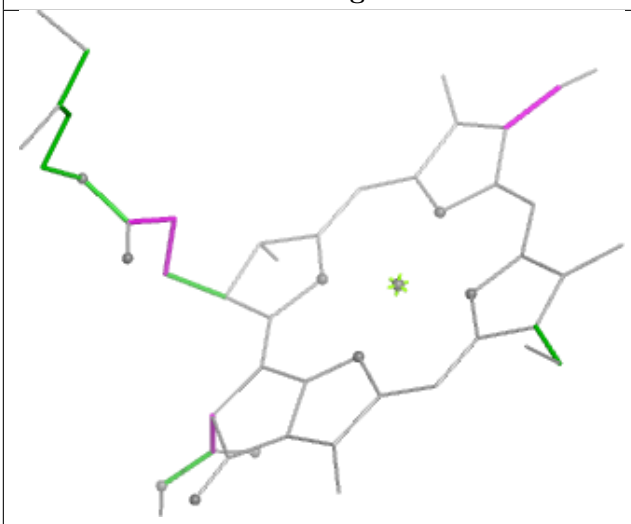
Ligand CLA 1 1609



Bond lengths



Bond angles

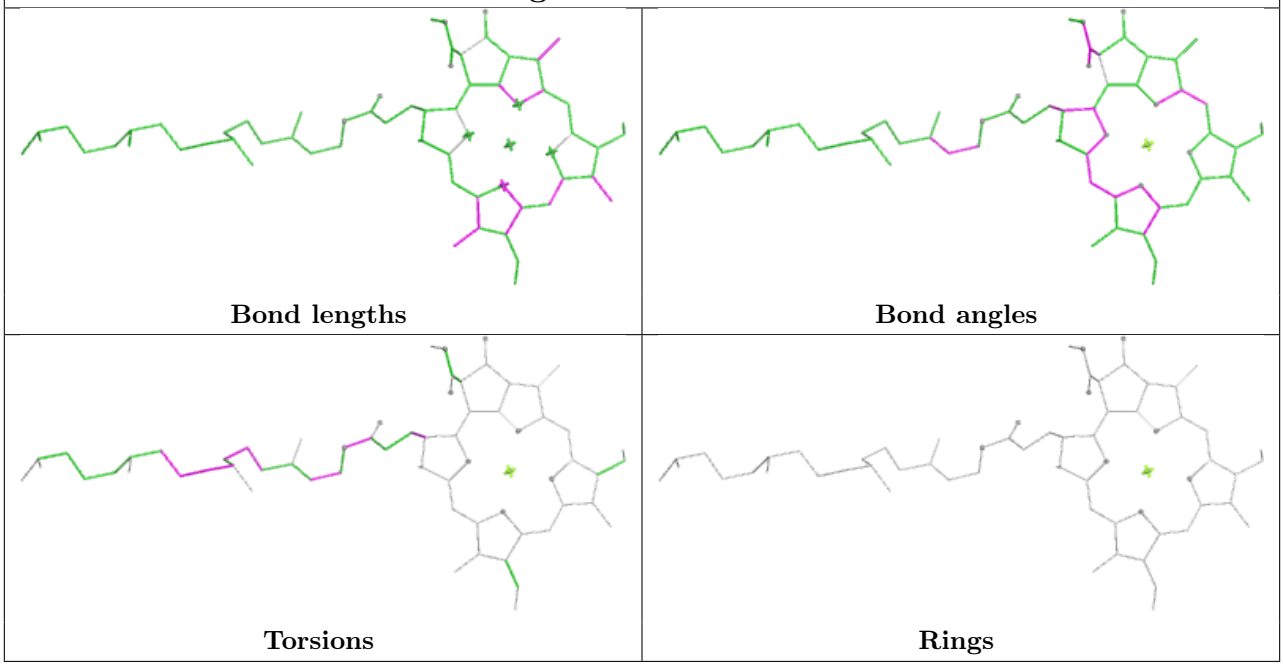


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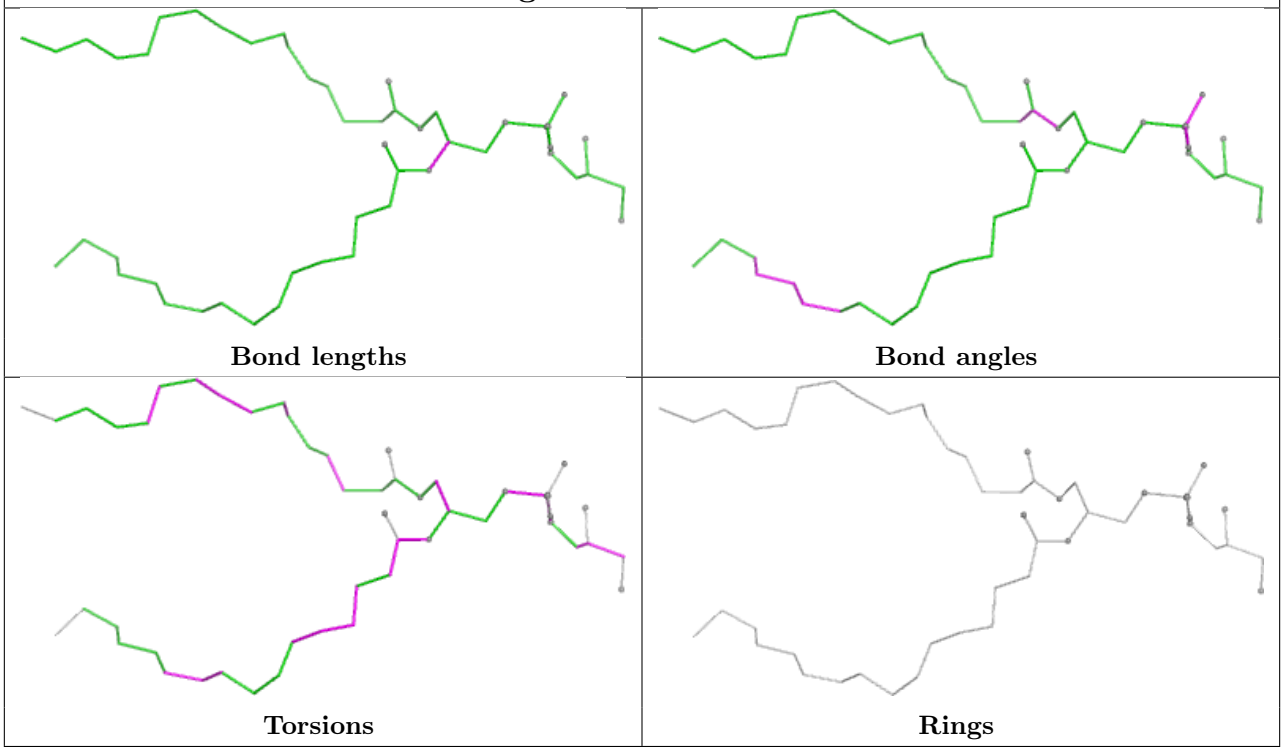


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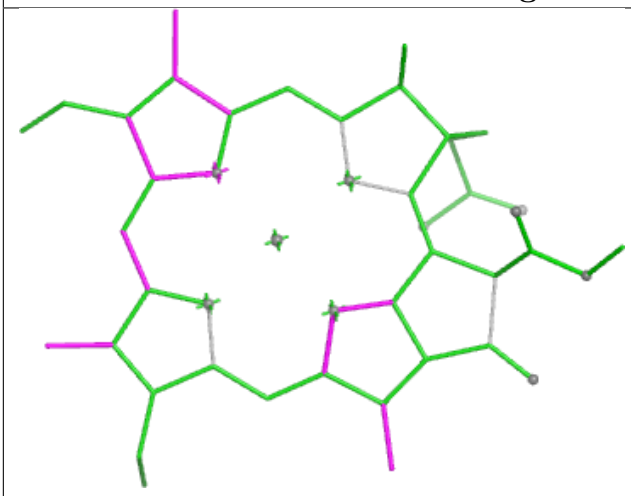
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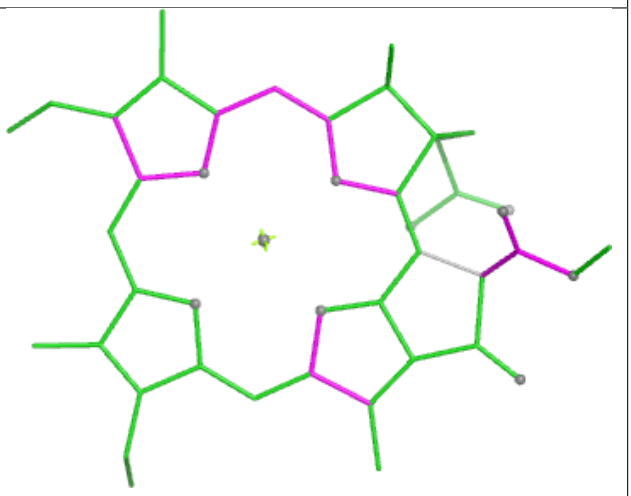
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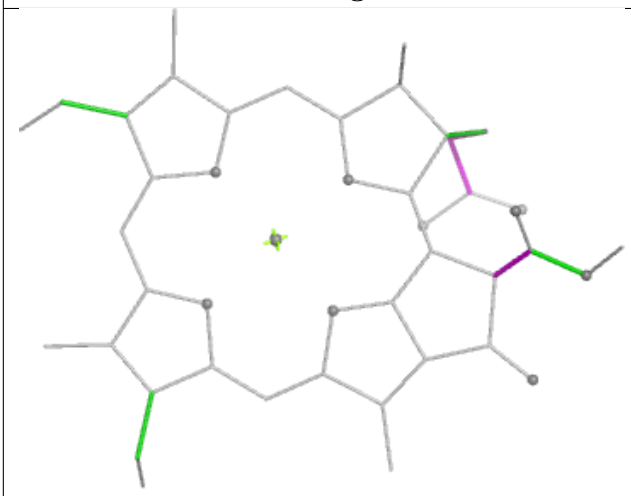
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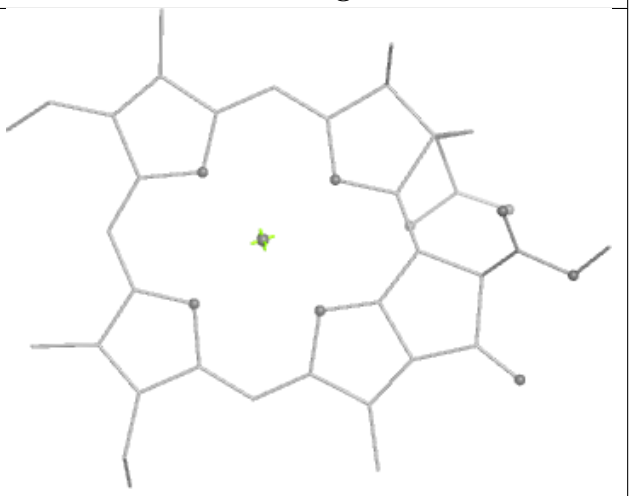
Bond lengths



Bond angles



Torsions

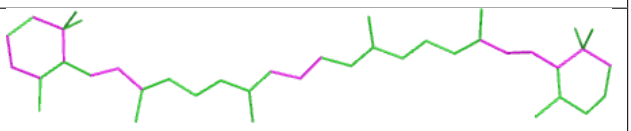


Rings

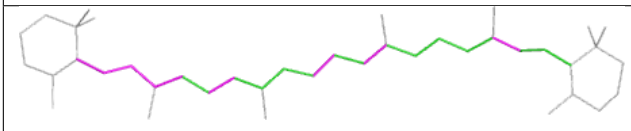
Ligand BCR L 206



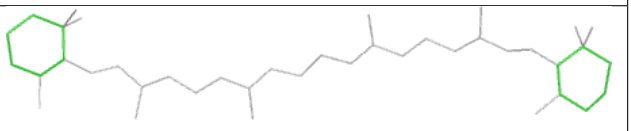
Bond lengths



Bond angles

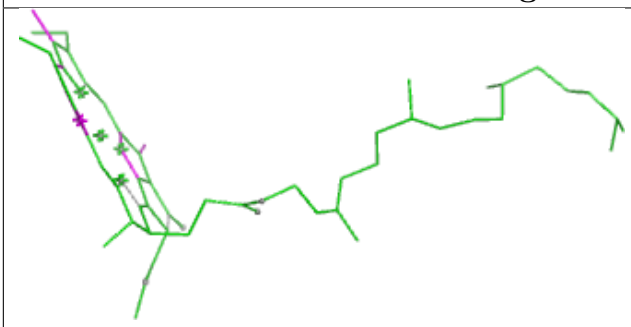


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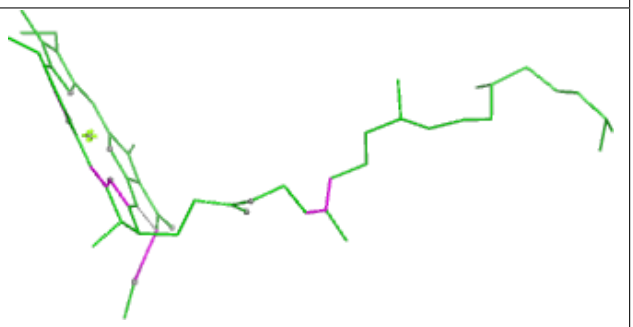


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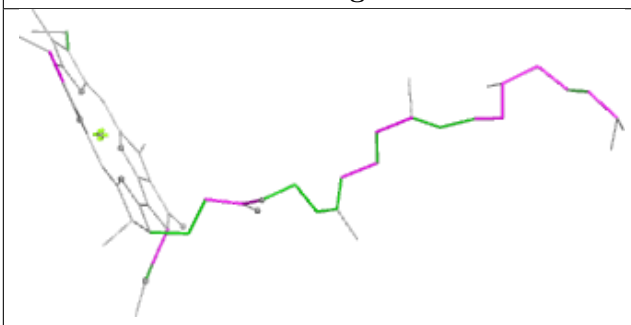
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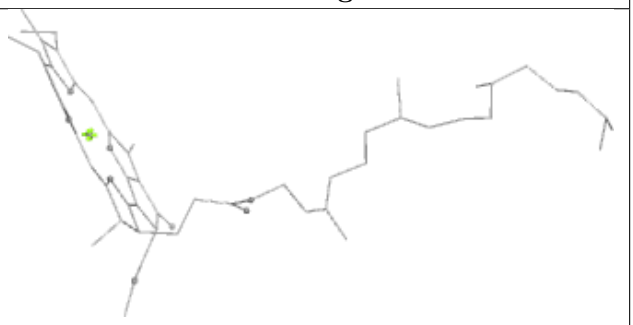
Bond lengths



Bond angles



Torsions

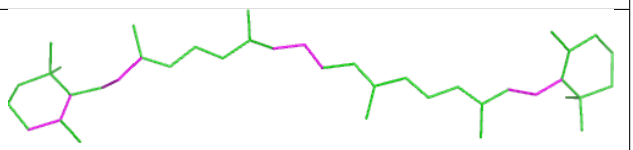


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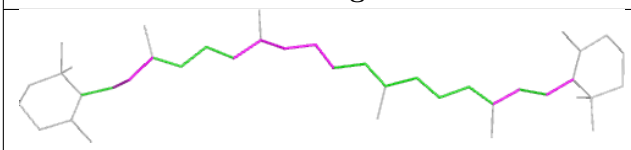
Ligand BCR 2 844



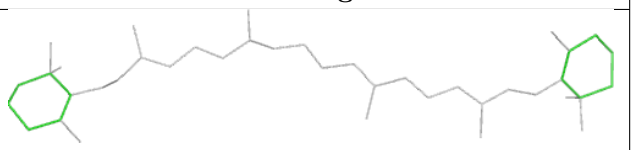
Bond lengths



Bond angles

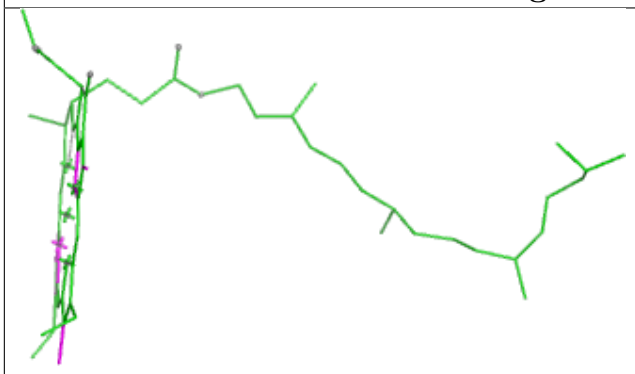


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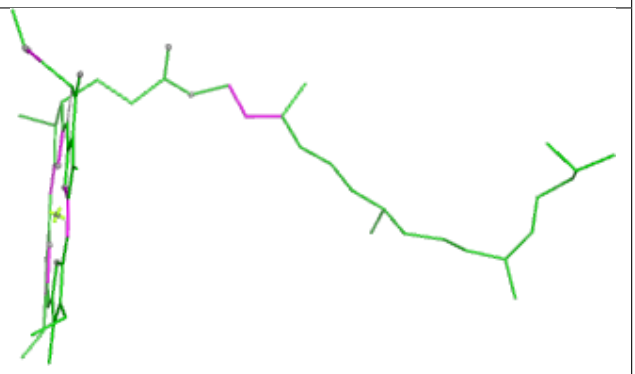


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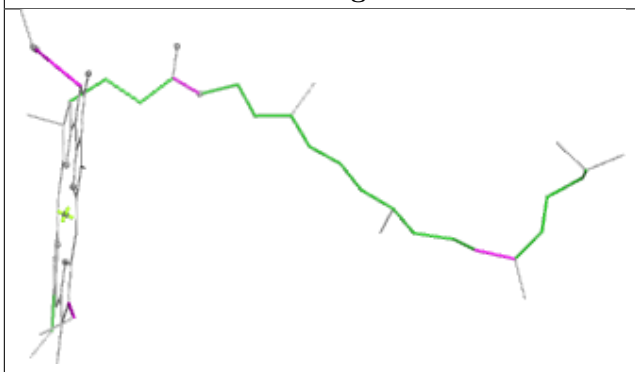
Ligand CLA 2 842



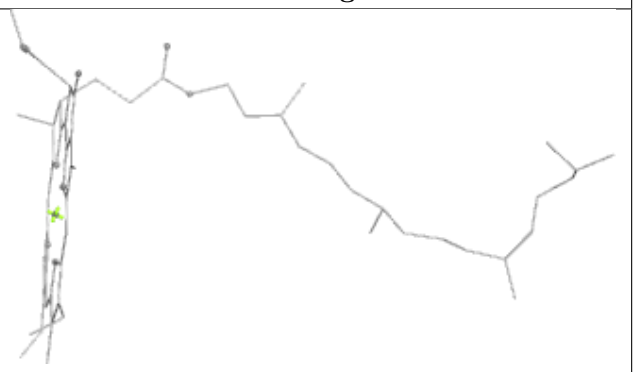
Bond lengths



Bond angles

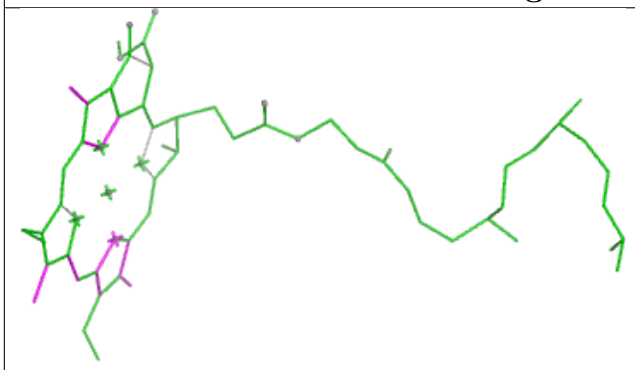


Torsions

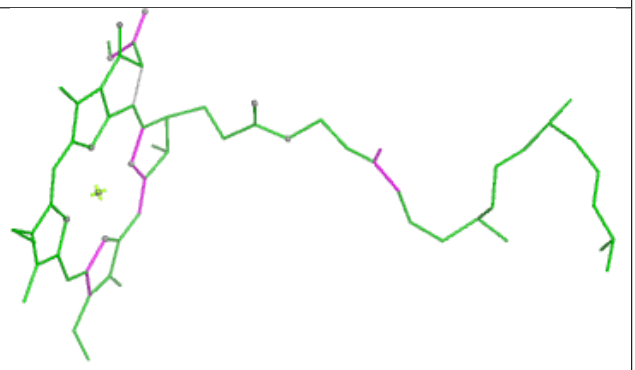


Rings

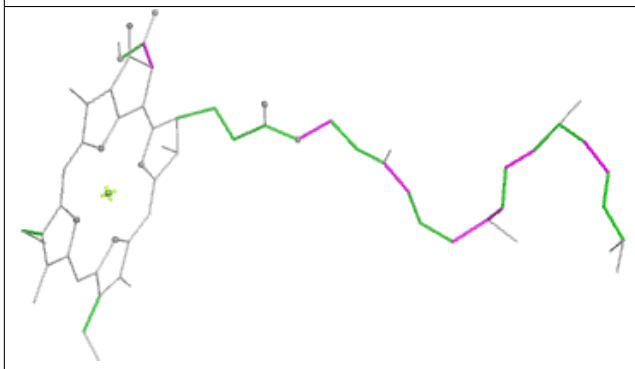
Ligand CLA B 833



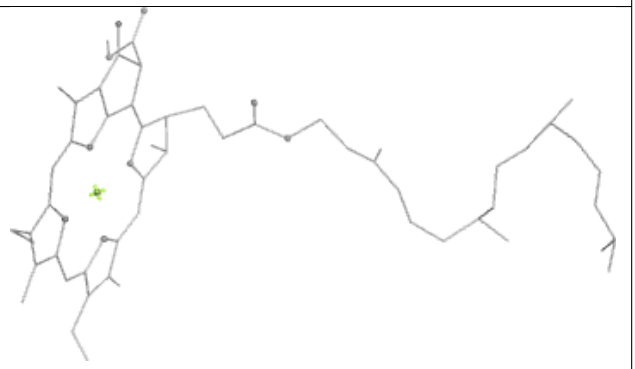
Bond lengths



Bond angles

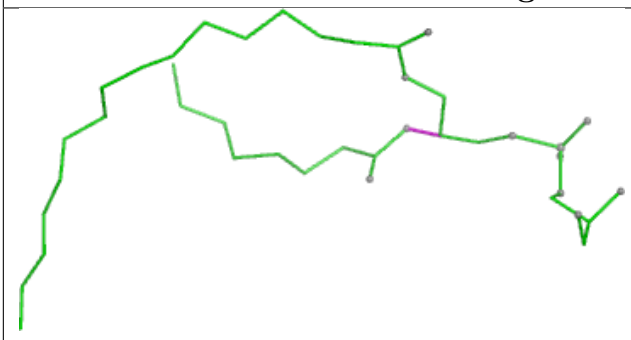


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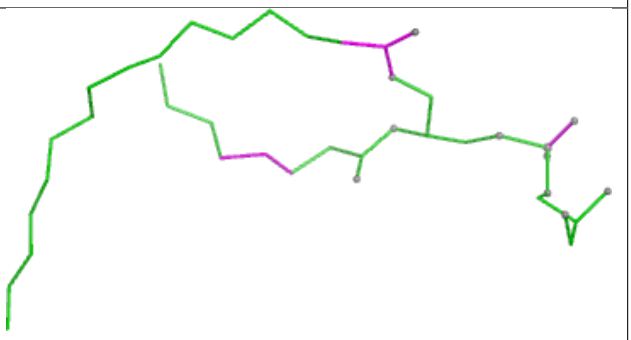


Rings

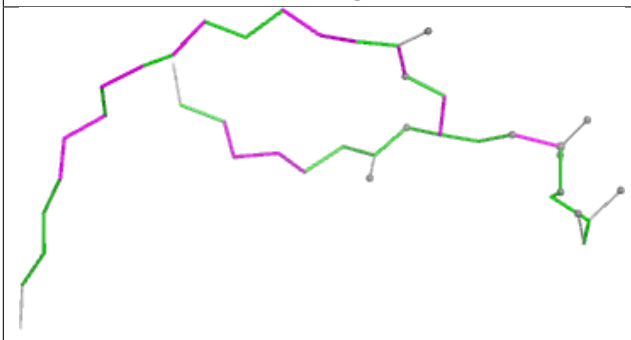
Ligand LHG 1 1655



Bond lengths



Bond angles

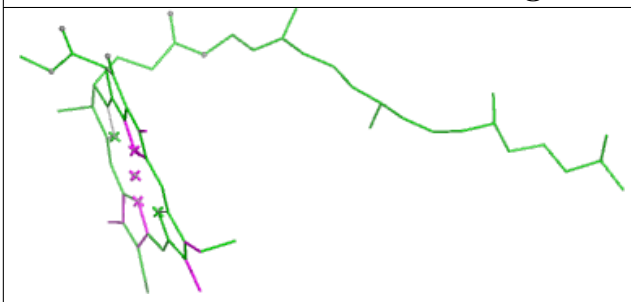


Torsions

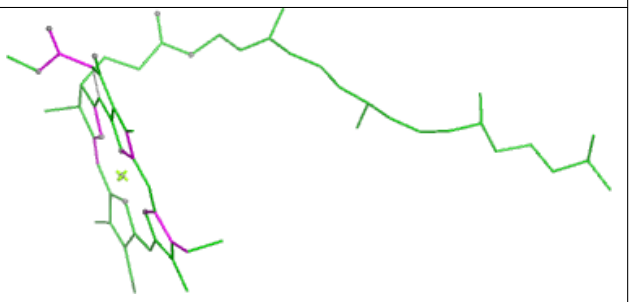


Rings

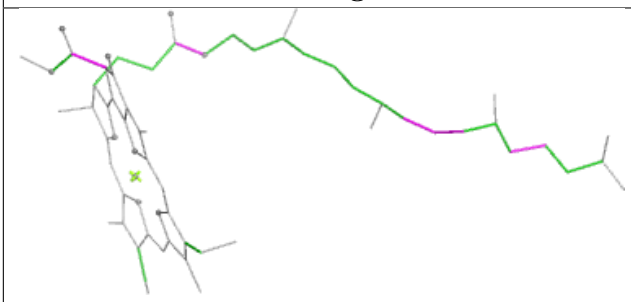
Ligand CLA B 829



Bond lengths



Bond angles

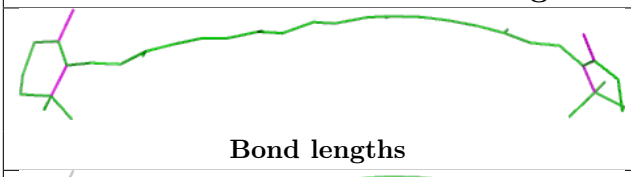


Torsions

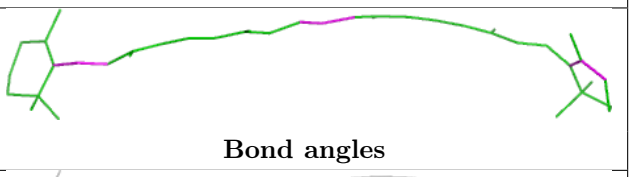


Rings

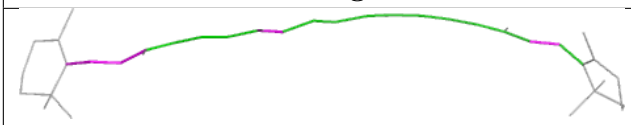
Ligand BCR i 101



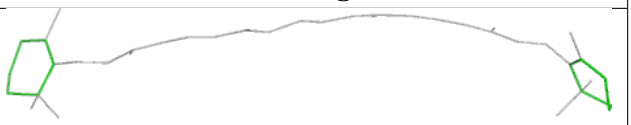
Bond lengths



Bond angles

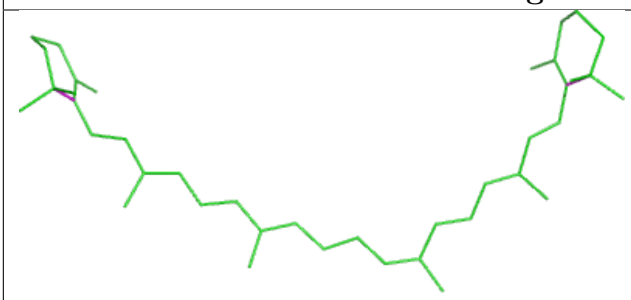


Torsions

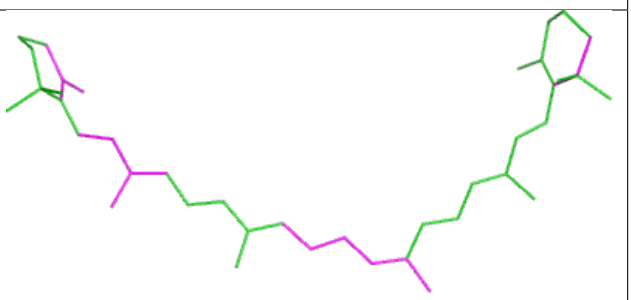


Rings

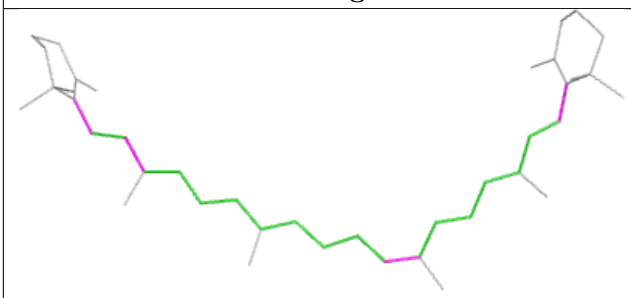
Ligand BCR 6 204



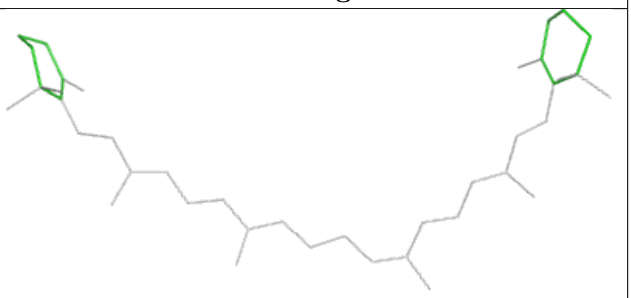
Bond lengths



Bond angles

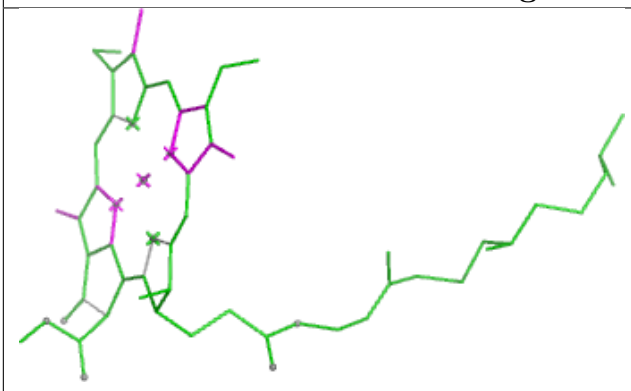


Torsions

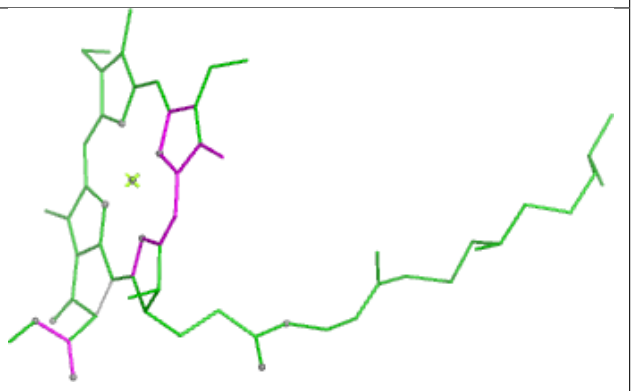


Rings

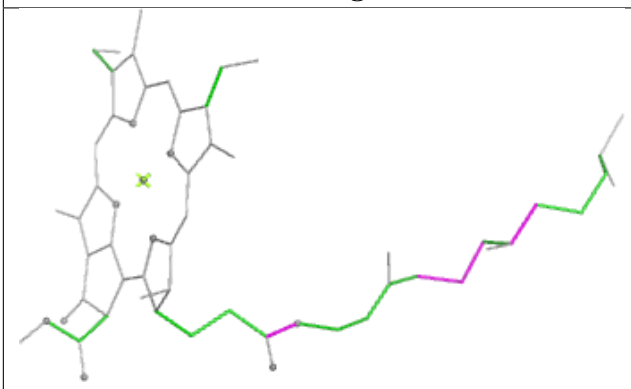
Ligand CLA 1 1633



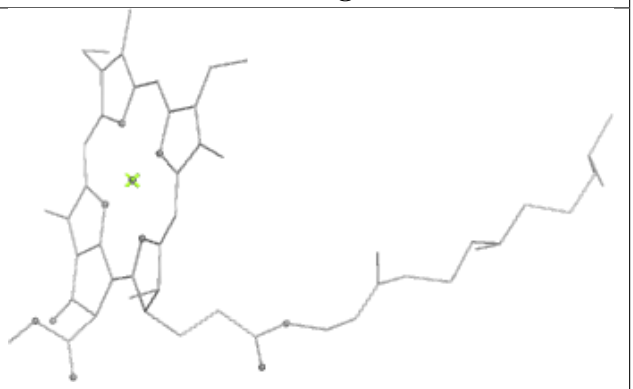
Bond lengths



Bond angles

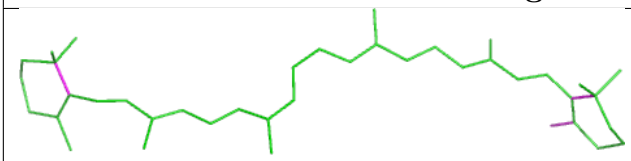


Torsions

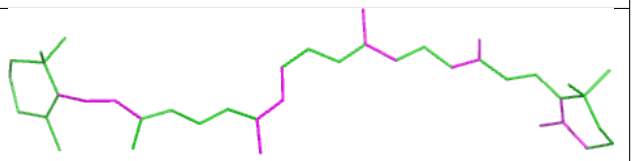


Rings

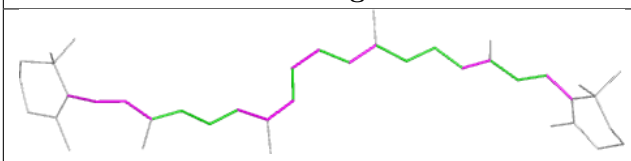
Ligand BCR b 847



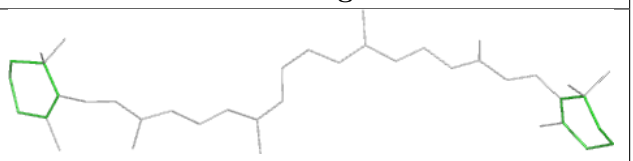
Bond lengths



Bond angles



Torsions

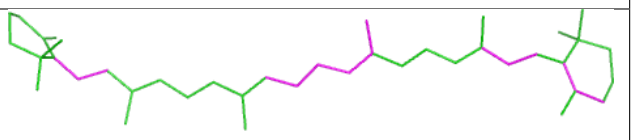


Rings

Ligand BCR b 849



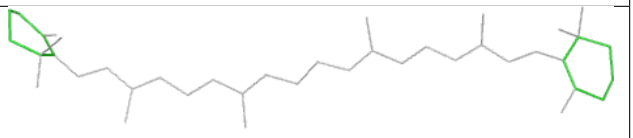
Bond lengths



Bond angles

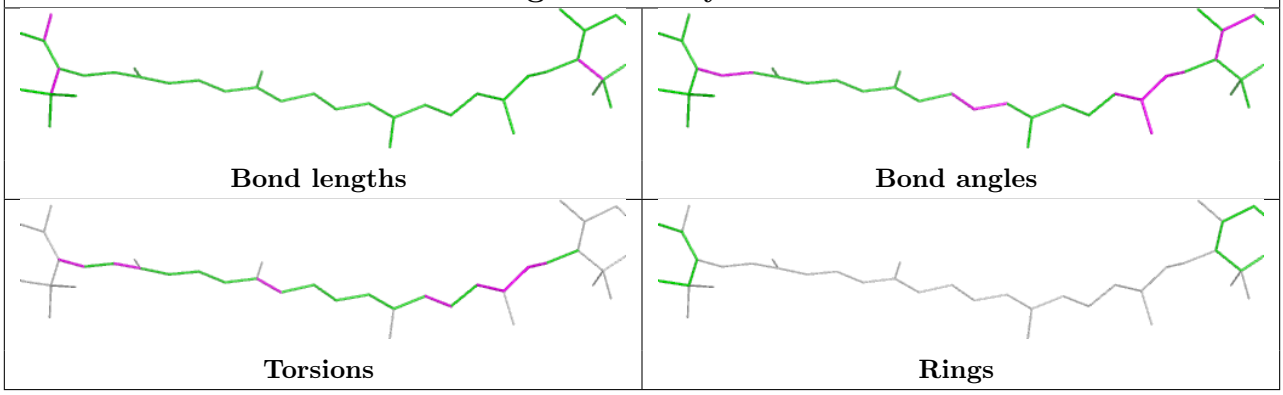


Torsions

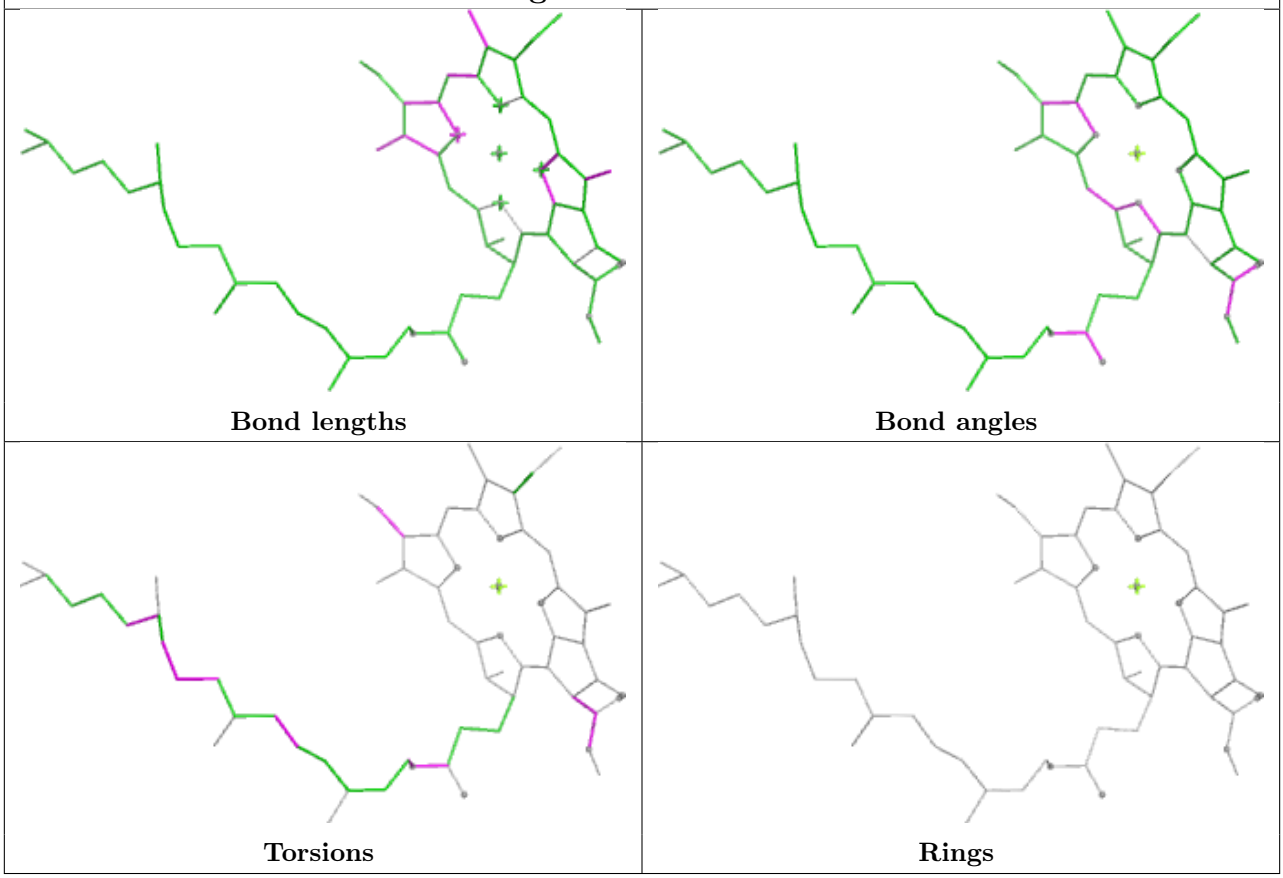


Rings

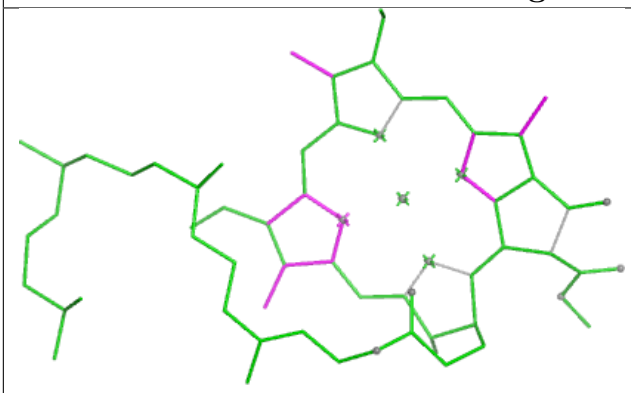
Ligand BCR y 102



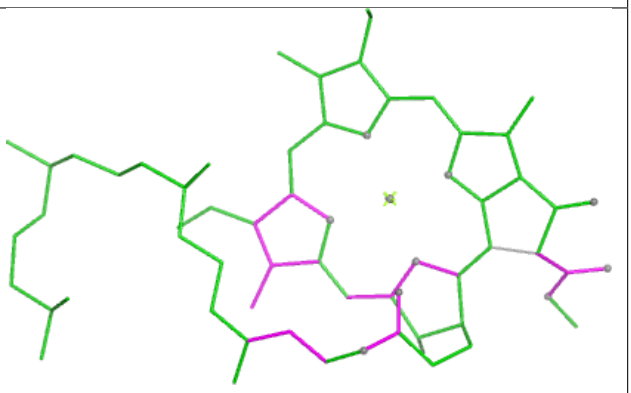
Ligand CLA a 817



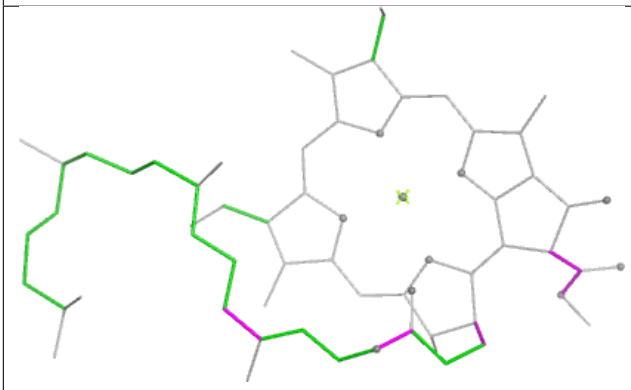
Ligand CLA a 820



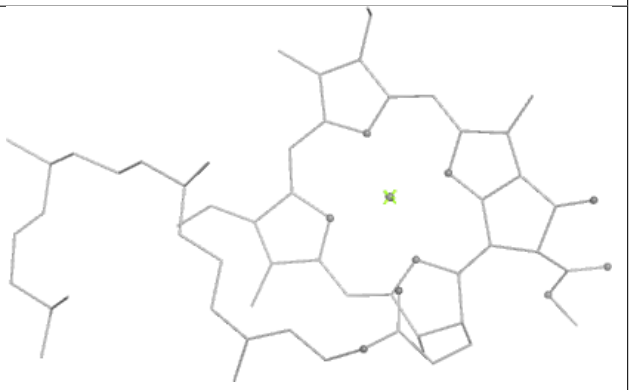
Bond lengths



Bond angles

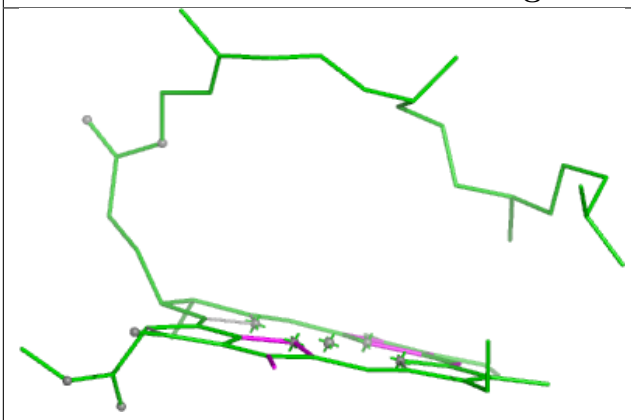


Torsions

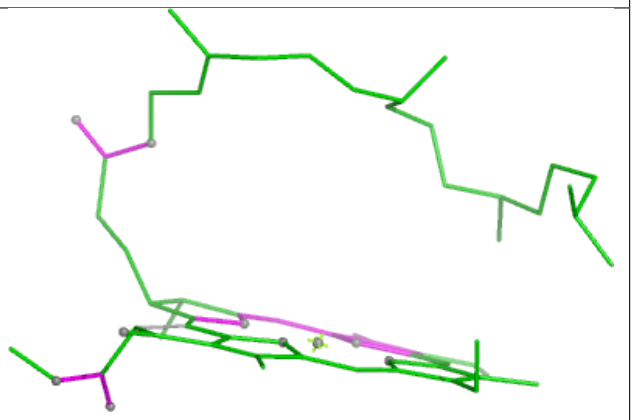


Rings

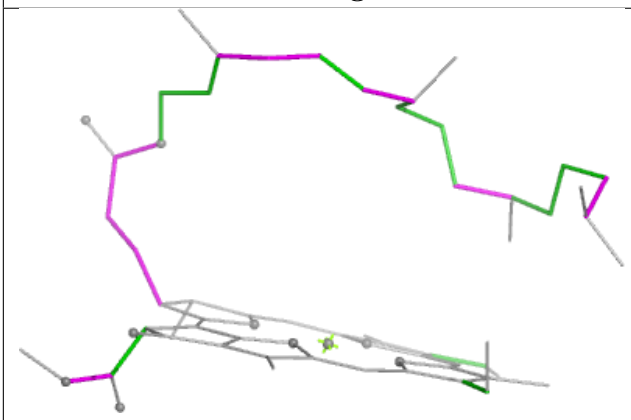
Ligand CLA A 821



Bond lengths



Bond angles

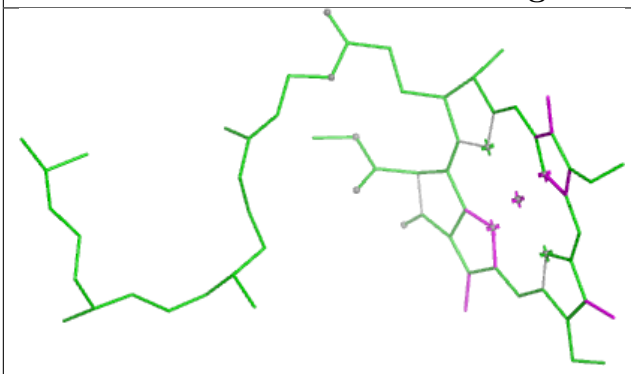


Torsions

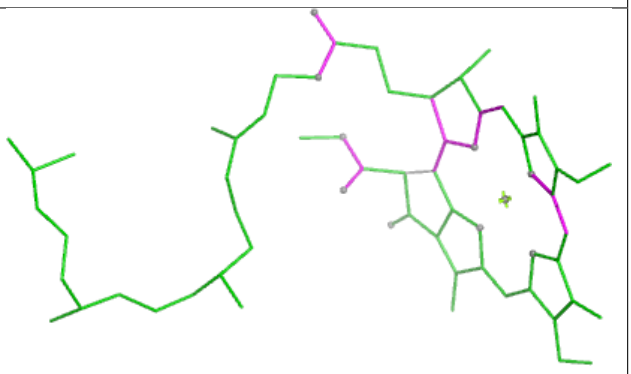


Rings

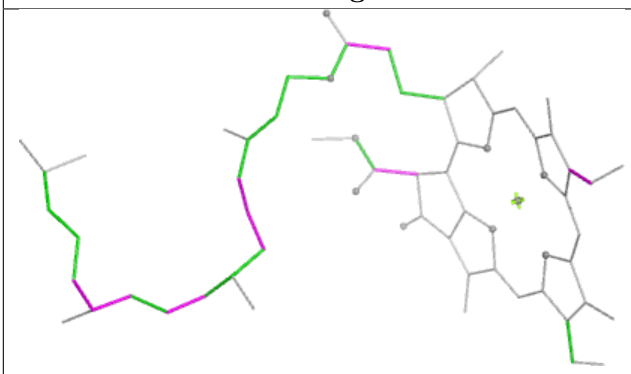
Ligand CL0 A 801



Bond lengths



Bond angles

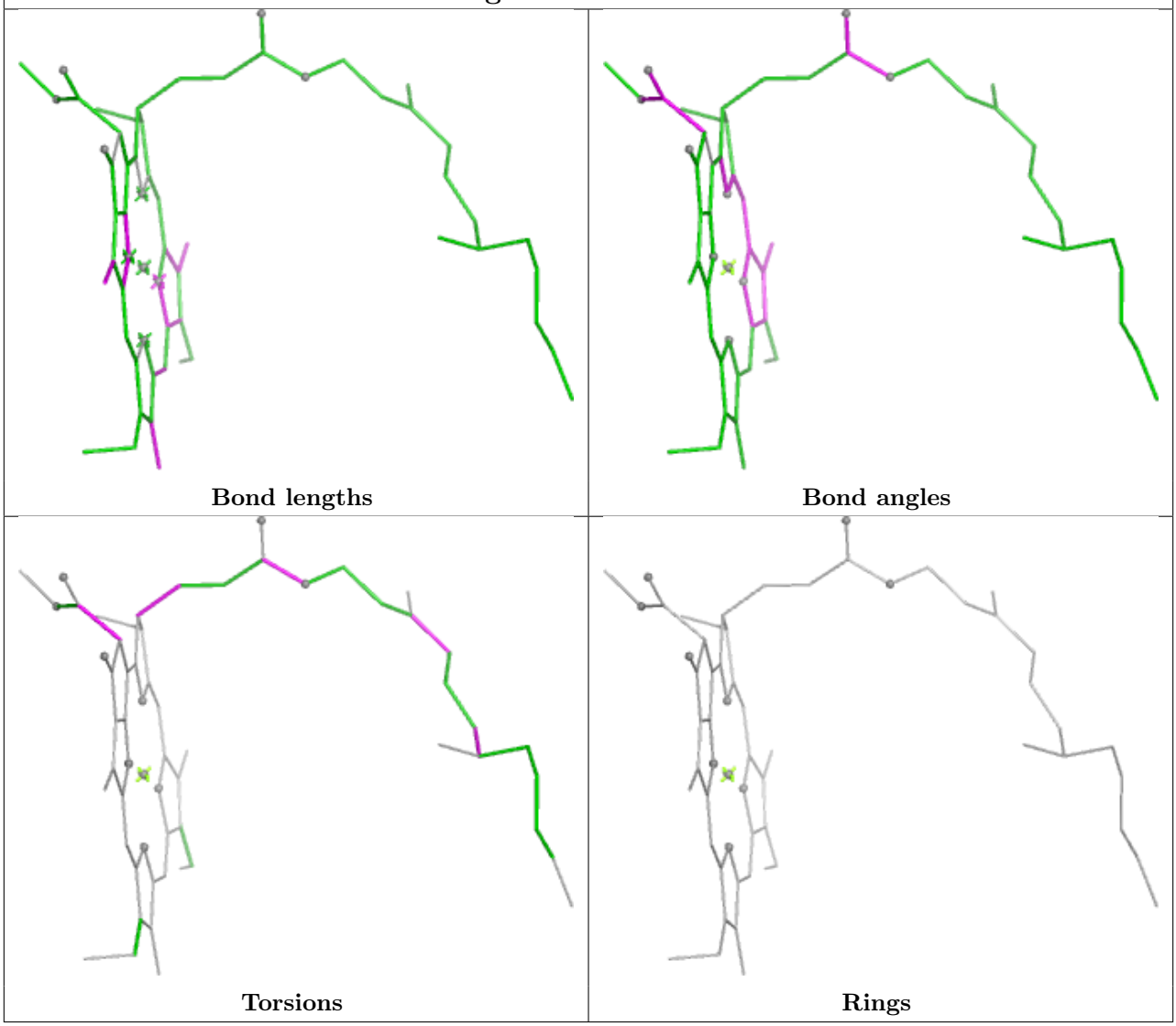


Torsions



Rings

Ligand CLA a 805



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.

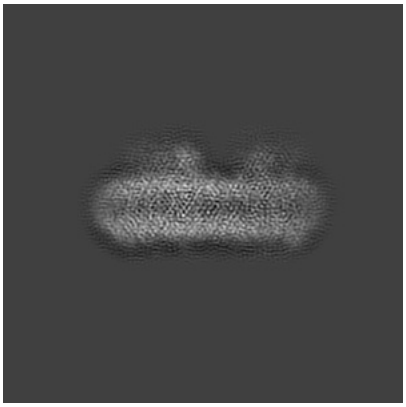
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10559. These allow visual inspection of the internal detail of the map and identification of artifacts.

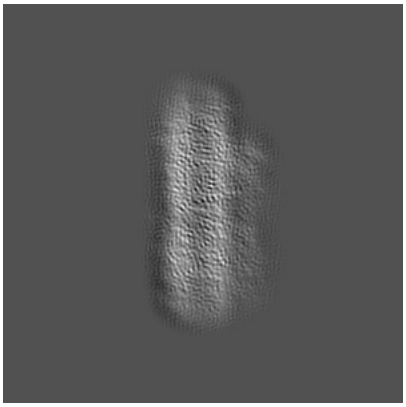
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

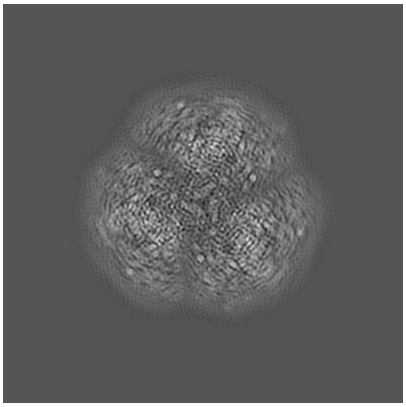
6.1.1 Primary map



X



Y

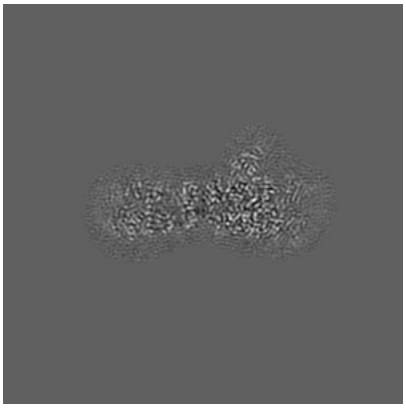


Z

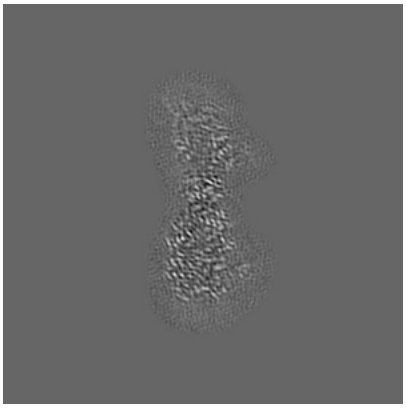
The images above show the map projected in three orthogonal directions.

6.2 Central slices

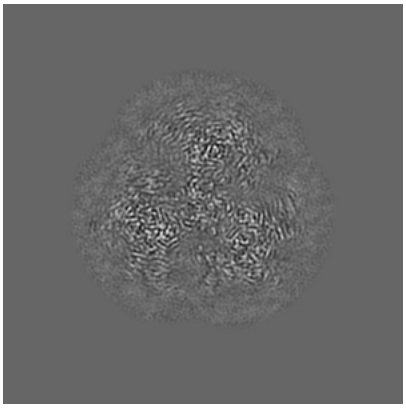
6.2.1 Primary map



X Index: 280



Y Index: 280

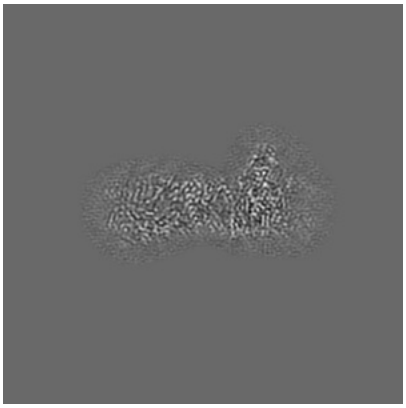


Z Index: 280

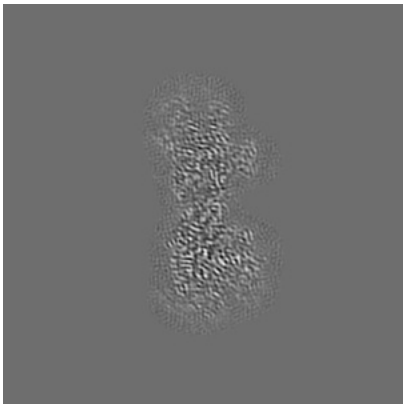
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

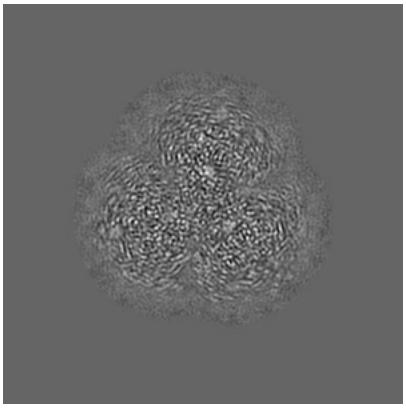
6.3.1 Primary map



X Index: 298



Y Index: 253

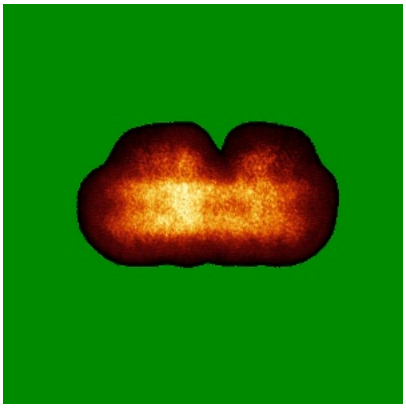


Z Index: 298

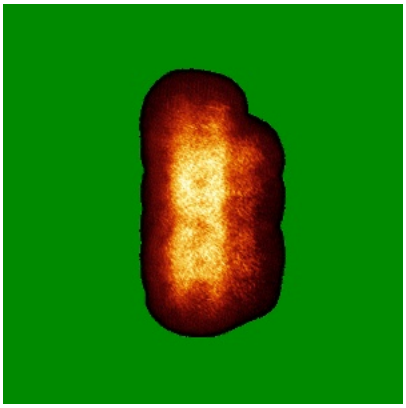
The images above show the largest variance slices of the map in three orthogonal directions.

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

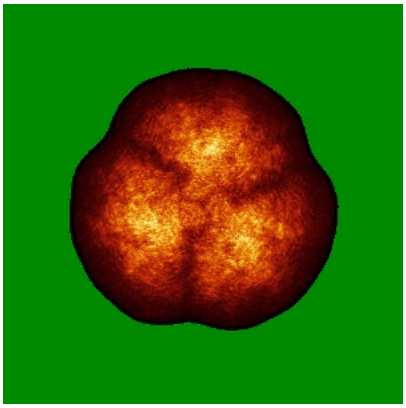
6.4.1 Primary map



X



Y



Z

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 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

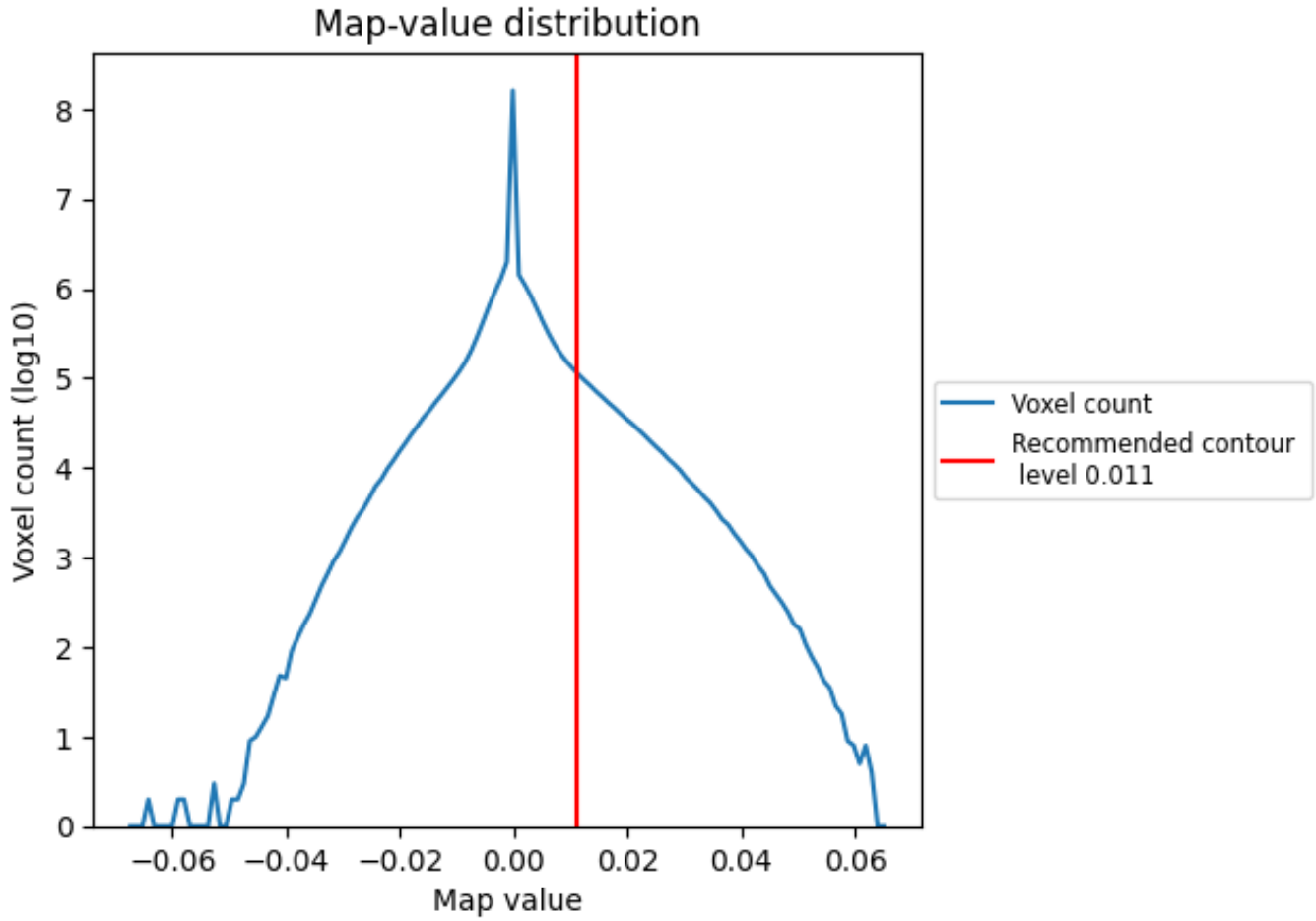
6.6 Mask visualisation (i)

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

7 Map analysis

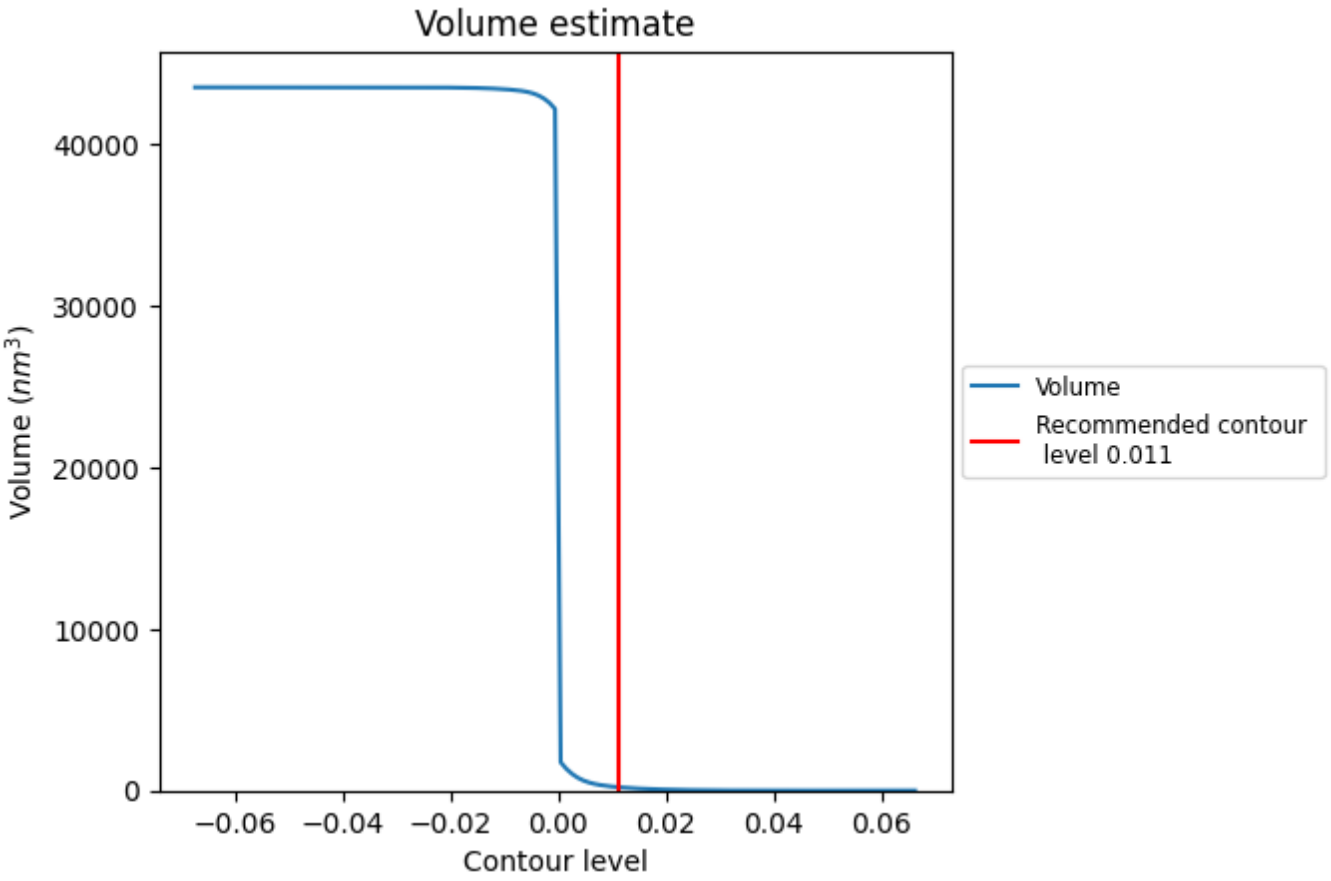
This section contains the results of statistical analysis of the map.

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.

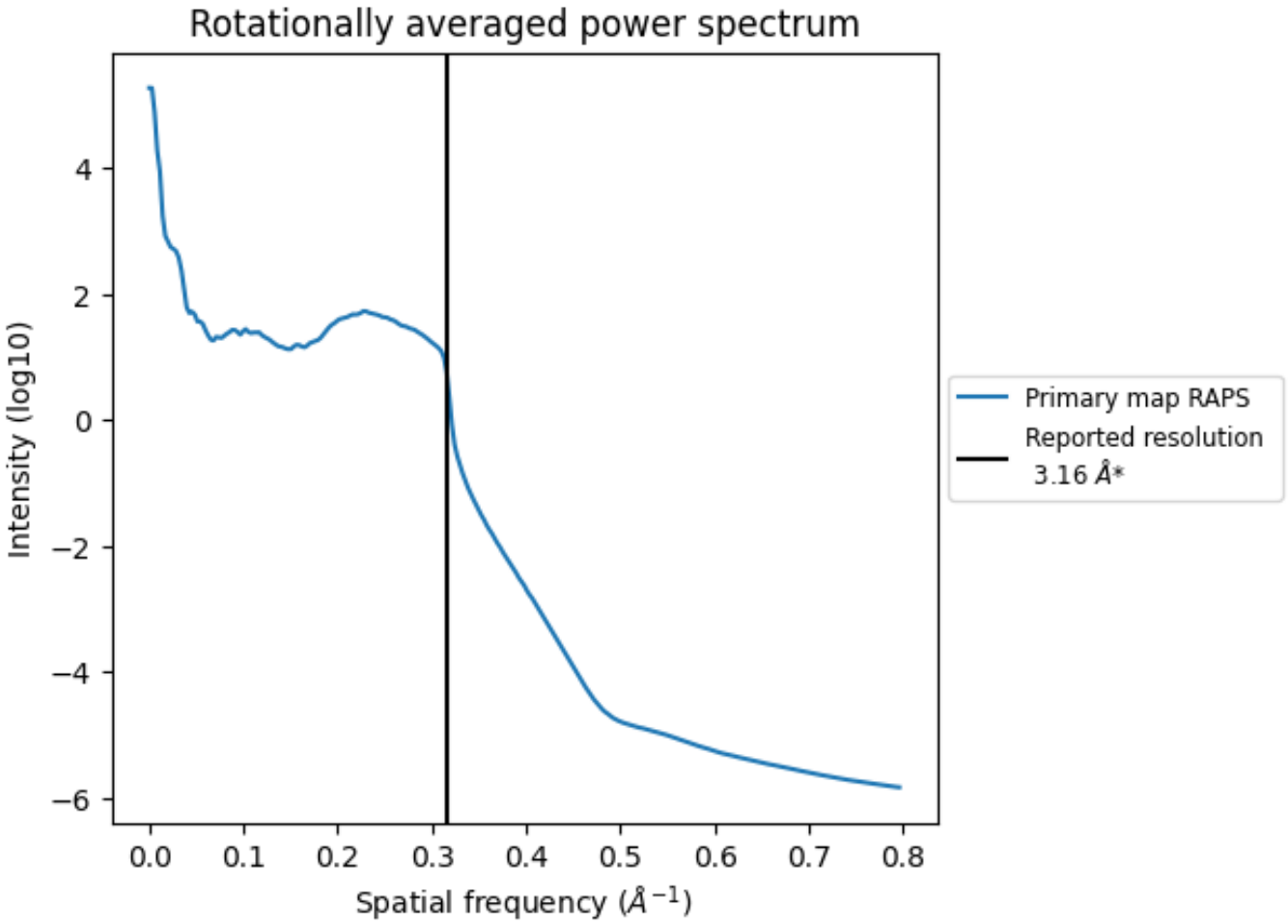
7.2 Volume estimate



The volume at the recommended contour level is 212 nm^3; this corresponds to an approximate mass of 191 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)

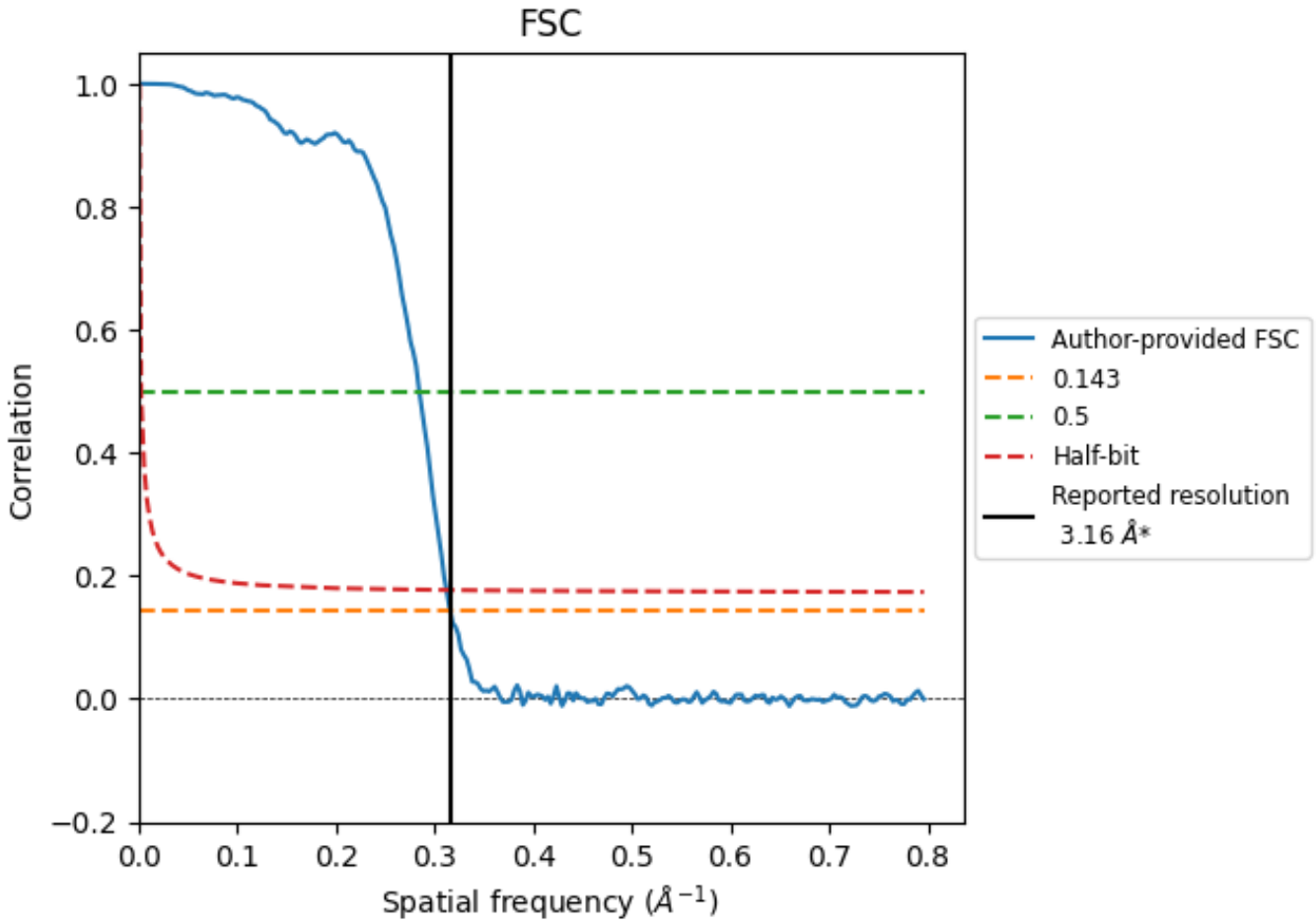


*Reported resolution corresponds to spatial frequency of 0.316 Å^{-1}

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 0.316 $Å^{-1}$

8.2 Resolution estimates (i)

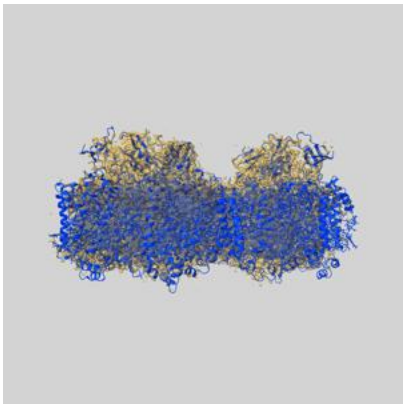
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.17	3.51	3.20
Unmasked-calculated*	-	-	-

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

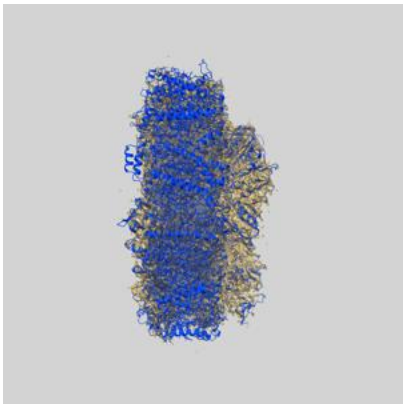
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10559 and PDB model 6TRD. Per-residue inclusion information can be found in section 3 on page 32.

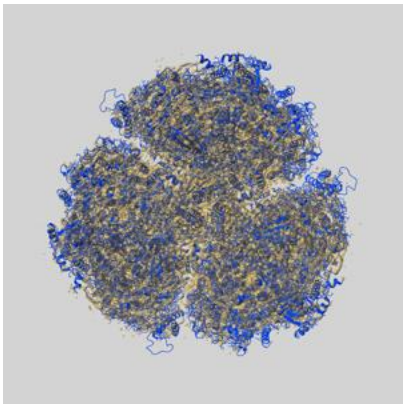
9.1 Map-model overlay



X



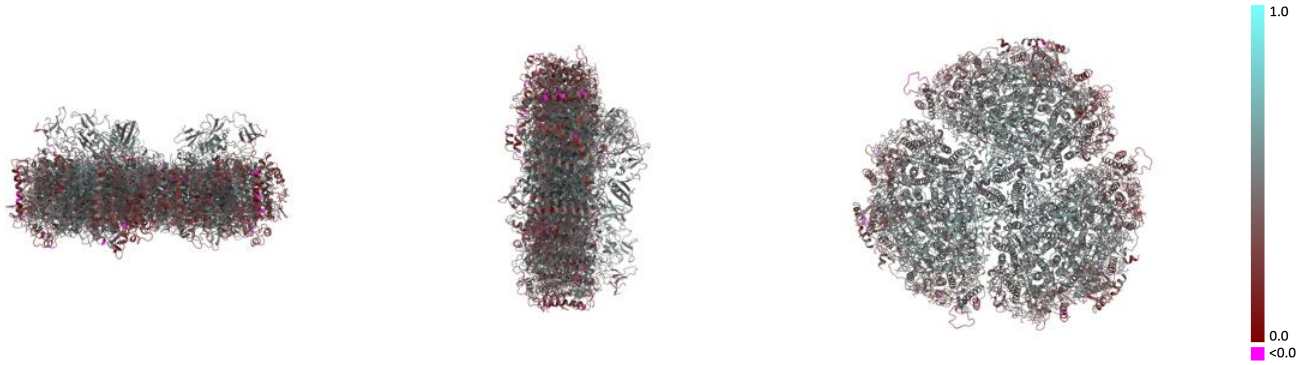
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011 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.

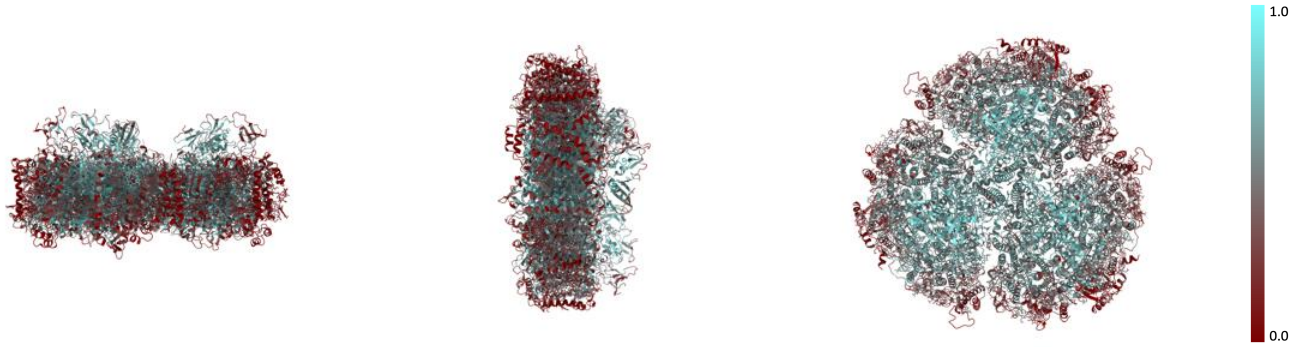
9.2 Q-score mapped to coordinate model



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.

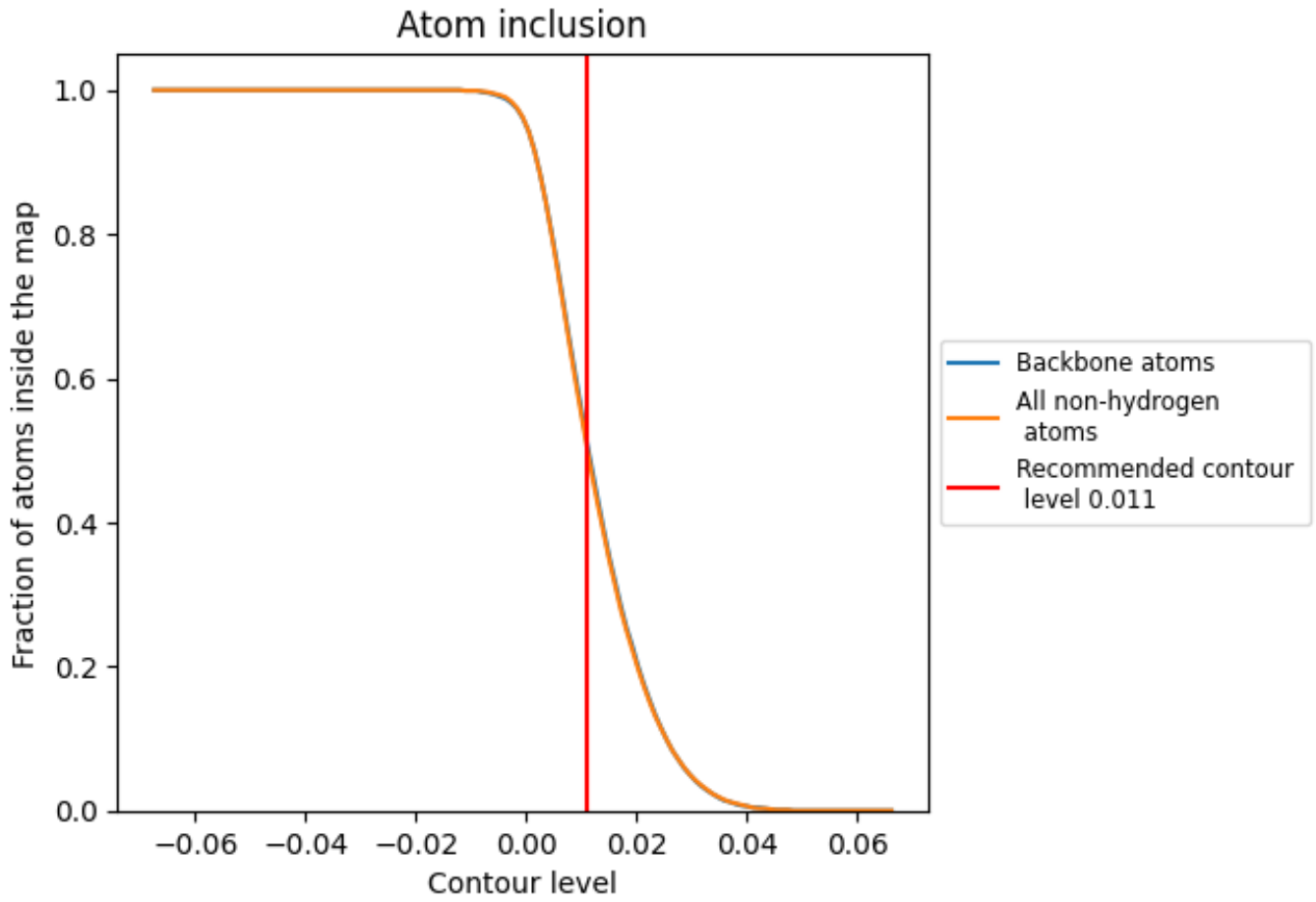
9.3 Atom inclusion mapped to coordinate model



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 (0.011).

9.4 Atom inclusion (i)



At the recommended contour level, 51% of all backbone atoms, 50% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5030	0.4500
0	0.6800	0.5210
1	0.5780	0.4730
2	0.5740	0.4770
3	0.6630	0.4830
4	0.5650	0.4700
5	0.3820	0.4120
6	0.2120	0.3470
7	0.6730	0.5060
8	0.1880	0.3310
9	0.1280	0.3720
A	0.5250	0.4540
B	0.5130	0.4490
C	0.6830	0.4970
D	0.5520	0.4870
E	0.3260	0.4300
F	0.1000	0.2840
I	0.6640	0.5280
J	0.1140	0.3370
K	0.1480	0.3590
L	0.6840	0.5250
M	0.4780	0.4820
X	0.0000	0.1740
a	0.5030	0.4360
b	0.5760	0.4770
c	0.6120	0.4930
d	0.5010	0.4630
e	0.3390	0.4240
f	0.1730	0.3380
i	0.7050	0.5110
j	0.1620	0.3670
k	0.0590	0.2860
l	0.6620	0.5180
m	0.5240	0.4520
x	0.0110	0.2250



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Chain	Atom inclusion	Q-score
y	0.5120	0.4820
z	0.0220	0.2350