Full wwPDB EM Validation Report ⓘ

Apr 23, 2024 – 12:24 am BST

PDB ID	:	7NHO
EMDB ID	:	EMD-12335
Title	:	Structure of PSII-M
Authors	:	Zabret, J.; Bohn, S.; Schuller, S.K.; Arnolds, O.; Chan, A.; Tajkhorshid, E.; Stoll, R.; Engel, B.D.; Rudack, T.; Schuller, J.M.; Nowaczyk, M.M.
Deposited on	:	2021-02-11
Resolution	:	2.66 Å(reported)

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

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

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

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

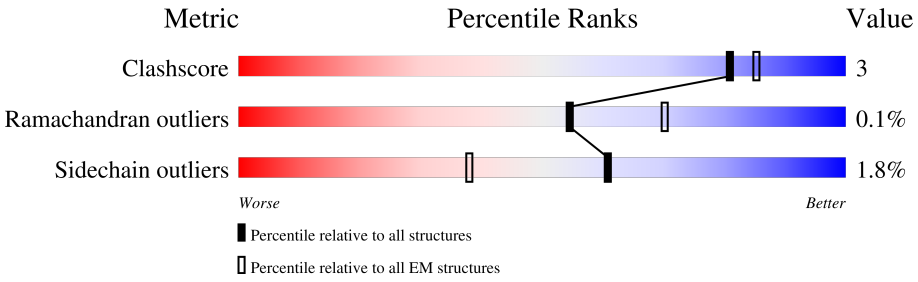
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.66 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	360	87% 5% 7%
2	B	510	91% 5%
3	C	461	6% 91% 5%
4	D	352	89% 7%
5	E	84	15% 86% 6% 8%
6	F	45	13% 82% 16%
7	H	66	5% 94%
8	I	38	87% 8%

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Mol	Chain	Length	Quality of chain
9	K	46	72% 9% 20%
10	L	37	5% 89% 11%
11	M	36	14% 78% 14% 6%
12	T	32	6% 84% 9% 6%
13	X	41	80% 5% 15%
14	y	46	13% 54% 7% 39%
15	Z	62	89% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	PHO	A	404	X	-	-	-
19	PHO	D	405	X	-	-	-
20	CLA	A	405	X	-	-	-
20	CLA	A	406	X	-	-	-
20	CLA	A	407	X	-	-	-
20	CLA	A	408	X	-	-	-
20	CLA	B	602	X	-	-	-
20	CLA	B	603	X	-	-	-
20	CLA	B	604	X	-	-	-
20	CLA	B	605	X	-	-	-
20	CLA	B	606	X	-	-	-
20	CLA	B	607	X	-	-	-
20	CLA	B	608	X	-	-	-
20	CLA	B	609	X	-	-	-
20	CLA	B	610	X	-	-	-
20	CLA	B	611	X	-	-	-
20	CLA	B	612	X	-	-	-
20	CLA	B	613	X	-	-	-
20	CLA	B	614	X	-	-	-
20	CLA	B	615	X	-	-	-
20	CLA	B	616	X	-	-	-
20	CLA	B	617	X	-	-	-
20	CLA	C	502	X	-	-	-
20	CLA	C	503	X	-	-	-
20	CLA	C	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	C	505	X	-	-	-
20	CLA	C	506	X	-	-	-
20	CLA	C	507	X	-	-	-
20	CLA	C	508	X	-	-	-
20	CLA	C	509	X	-	-	-
20	CLA	C	510	X	-	-	-
20	CLA	C	511	X	-	-	-
20	CLA	C	512	X	-	-	-
20	CLA	C	513	X	-	-	-
20	CLA	C	515	X	-	-	-
20	CLA	D	406	X	-	-	-
20	CLA	D	407	X	-	-	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 19800 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	335	2627	1720	432	460	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	485	3812	2505	635	659	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	448	3465	2270	580	602	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	340	2705	1794	440	459	12	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	77	635	417	103	115	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	38	307	207	50	49	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	65	Total	C	N	O	S	0	0
			511	341	82	86	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	35	Total	C	N	O	S	0	0
			286	195	45	45	1		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	34	Total	C	N	O	S	0	0
			267	178	40	48	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	30	Total	C	N	O	S	0	0
			256	180	36	38	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	X	35	Total	C	N	O	0	0
			254	172	38	44		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	y	28	Total	C	N	O	S	0	0
			208	137	36	32	3		

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

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

- Molecule 16 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	Fe	0
			1	1	

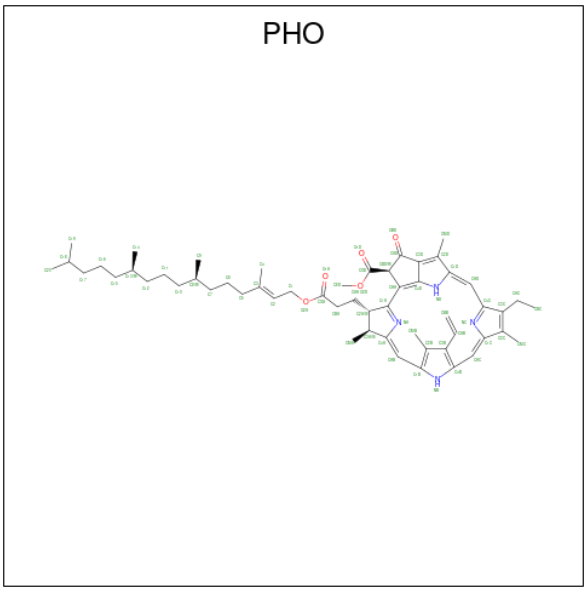
- Molecule 17 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total	Mn	0
			1	1	

- Molecule 18 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

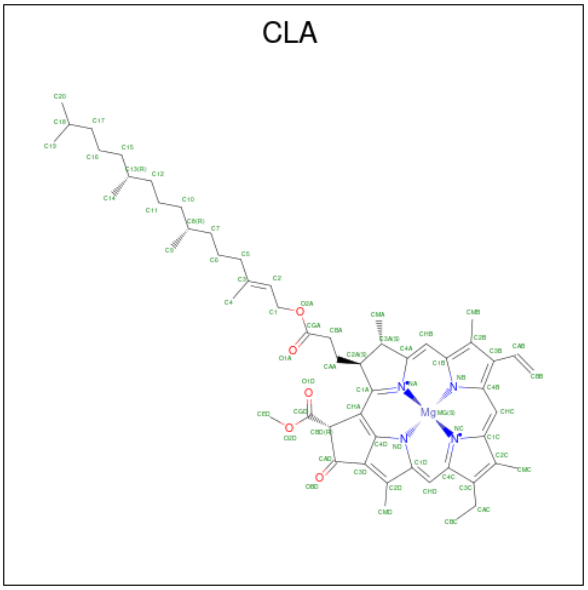
Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Cl	0
			1	1	

- Molecule 19 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 20 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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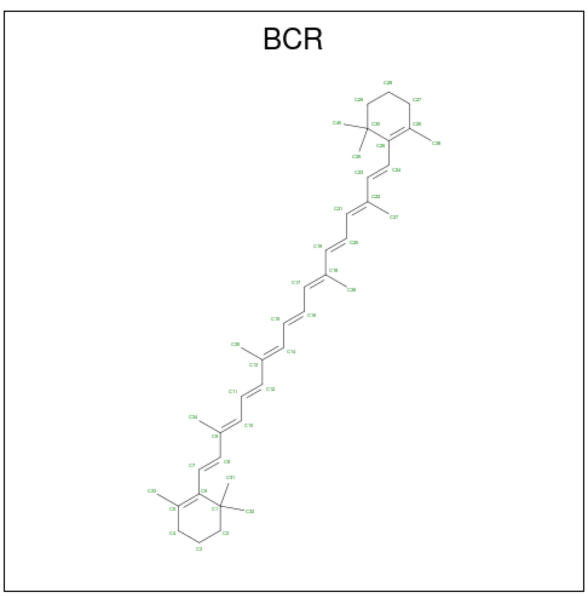
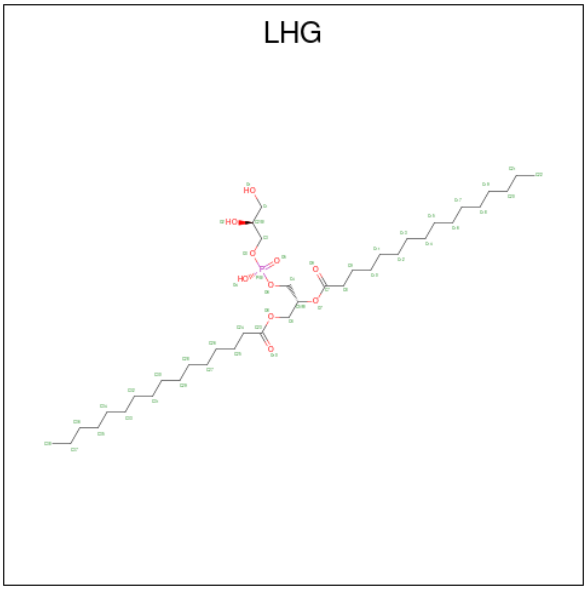
Mol	Chain	Residues	Atoms					AltConf
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	C	1	Total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

- Molecule 21 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	C	1	Total C 40 40	0
21	C	1	Total C 40 40	0
21	F	1	Total C 40 40	0
21	H	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	Z	1	Total C 40 40	0

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

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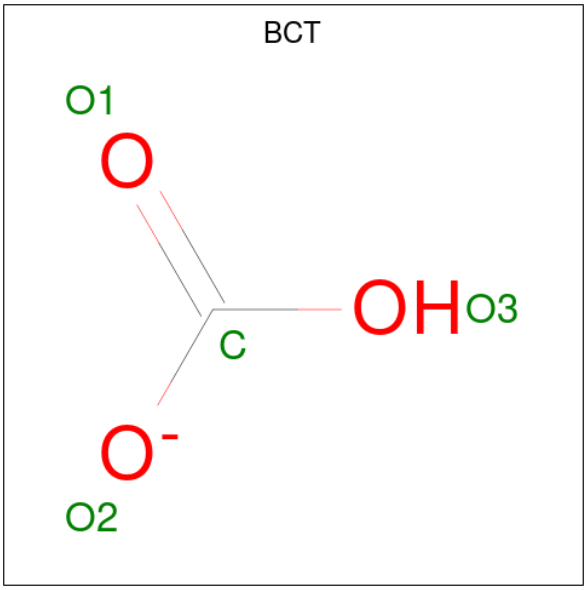
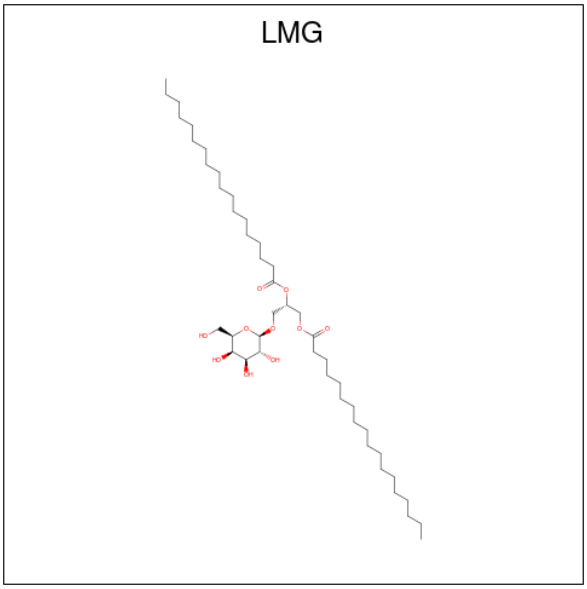
Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



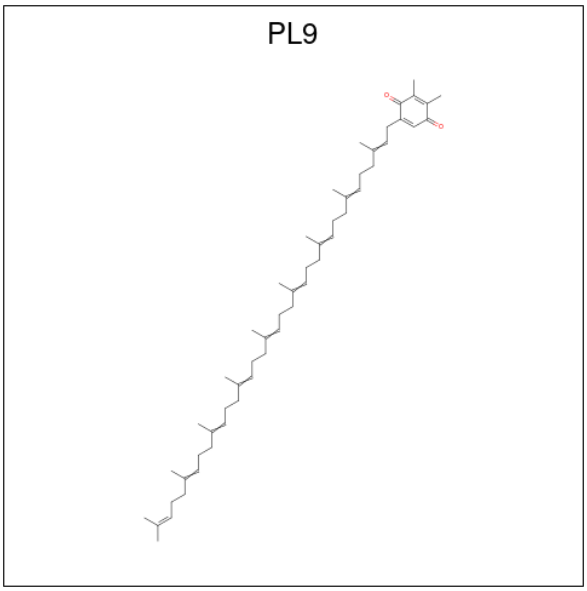
Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	C	O	0
			4	1	3	

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



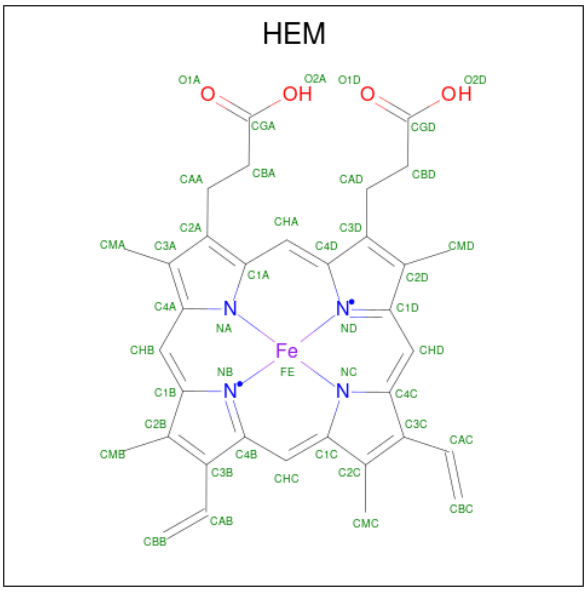
Mol	Chain	Residues	Atoms			AltConf
24	B	1	Total	C	O	0
			55	45	10	
24	C	1	Total	C	O	0
			55	45	10	
24	D	1	Total	C	O	0
			55	45	10	
24	D	1	Total	C	O	0
			55	45	10	
24	D	1	Total	C	O	0
			55	45	10	
24	I	1	Total	C	O	0
			55	45	10	
24	M	1	Total	C	O	0
			55	45	10	

- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



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

- Molecule 26 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



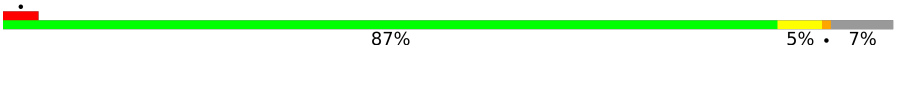
Mol	Chain	Residues	Atoms					AltConf
26	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

3 Residue-property plots (i)

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

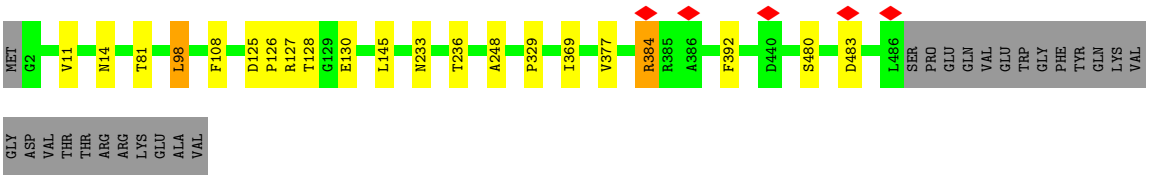
• Molecule 1: Photosystem II protein D1 1

Chain A:



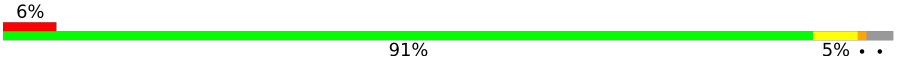
• Molecule 2: Photosystem II CP47 reaction center protein

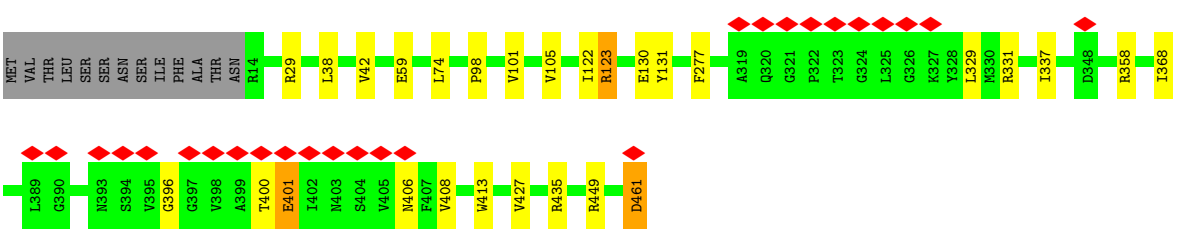
Chain B:



• Molecule 3: Photosystem II CP43 reaction center protein

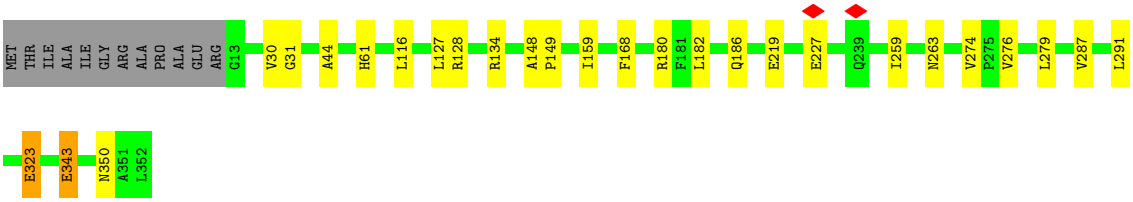
Chain C:



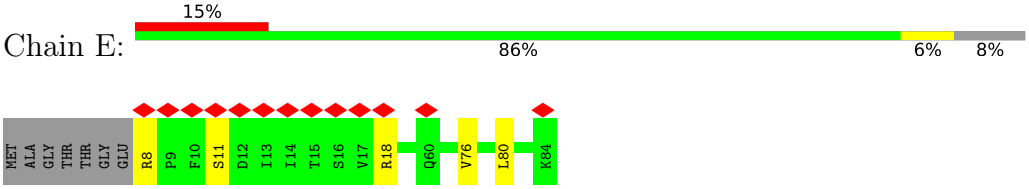


• Molecule 4: Photosystem II D2 protein

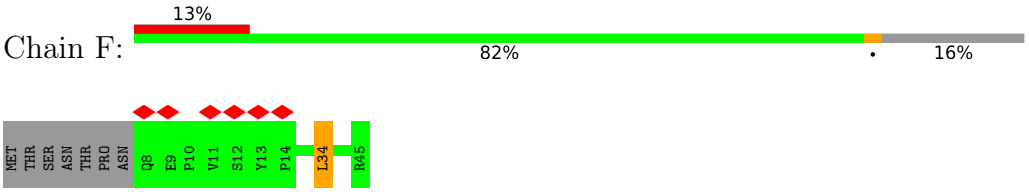
Chain D:



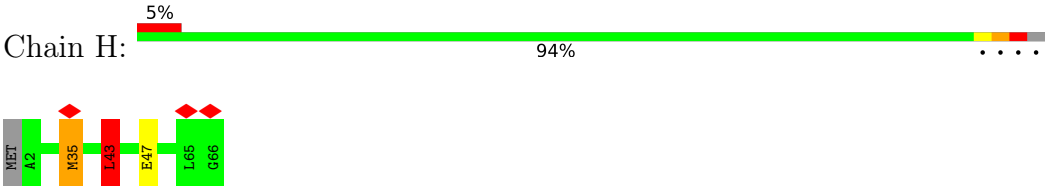
• Molecule 5: Cytochrome b559 subunit alpha



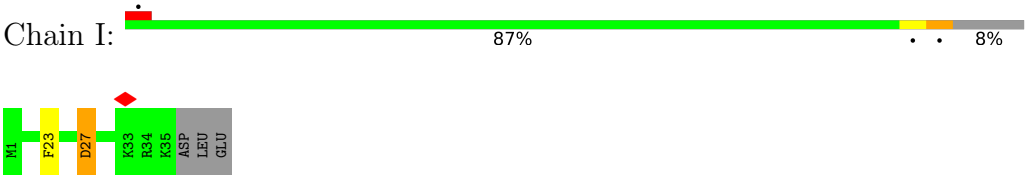
• Molecule 6: Cytochrome b559 subunit beta



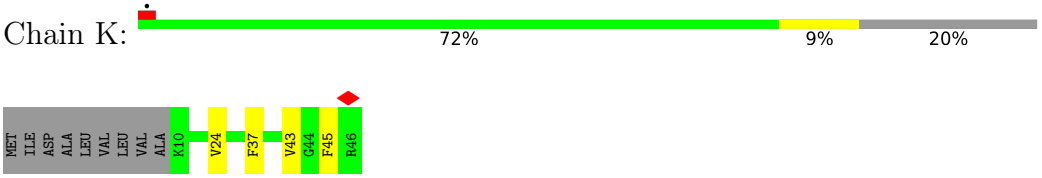
• Molecule 7: Photosystem II reaction center protein H



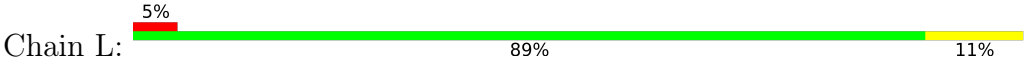
• Molecule 8: Photosystem II reaction center protein I

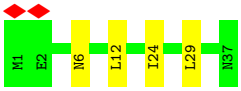


• Molecule 9: Photosystem II reaction center protein K



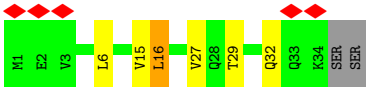
• Molecule 10: Photosystem II reaction center protein L





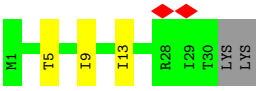
• Molecule 11: Photosystem II reaction center protein M

Chain M:



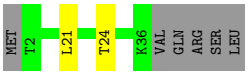
• Molecule 12: Photosystem II reaction center protein T

Chain T:



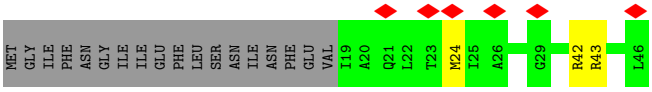
• Molecule 13: Photosystem II reaction center X protein

Chain X:



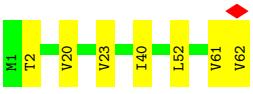
• Molecule 14: Photosystem II reaction center protein Ycf12

Chain y:



• Molecule 15: Photosystem II reaction center protein Z

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	166411	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.062	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	283.4, 283.4, 283.4	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PHO, FE, BCR, CLA, BCT, HEM, LMG, CL, LHG, MN, PL9

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.54	0/2712	0.86	2/3700 (0.1%)
2	B	0.54	0/3947	0.89	5/5379 (0.1%)
3	C	0.55	0/3578	0.92	8/4872 (0.2%)
4	D	0.53	0/2800	0.90	5/3818 (0.1%)
5	E	0.59	0/654	1.00	3/891 (0.3%)
6	F	0.57	0/317	1.05	2/433 (0.5%)
7	H	0.60	0/524	0.99	1/713 (0.1%)
8	I	0.64	0/293	0.95	0/395
9	K	0.58	0/303	0.96	0/416
10	L	0.59	0/311	0.85	0/422
11	M	0.59	0/270	1.05	0/367
12	T	0.56	0/265	0.83	0/359
13	X	0.53	0/257	0.88	0/348
14	y	0.54	0/209	1.01	1/279 (0.4%)
15	Z	0.57	0/490	0.93	0/669
All	All	0.55	0/16930	0.91	27/23061 (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
1	A	0	4
2	B	0	2
3	C	0	1
4	D	0	2
7	H	0	1
8	I	0	1
11	M	0	1
14	y	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	13

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	401	GLU	CA-CB-CG	9.59	134.49	113.40
14	y	43	ARG	NE-CZ-NH2	8.60	124.60	120.30
4	D	323	GLU	OE1-CD-OE2	-6.74	115.21	123.30
3	C	123	ARG	NE-CZ-NH2	6.48	123.54	120.30
2	B	98	LEU	CA-CB-CG	6.41	130.03	115.30
2	B	98	LEU	CB-CG-CD1	-6.40	100.12	111.00
4	D	128	ARG	NE-CZ-NH1	6.37	123.48	120.30
6	F	34	LEU	CB-CG-CD2	5.95	121.12	111.00
7	H	43	LEU	CB-CG-CD1	5.80	120.86	111.00
3	C	449	ARG	NE-CZ-NH1	5.66	123.13	120.30
4	D	134	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	B	384	ARG	CD-NE-CZ	5.61	131.46	123.60
2	B	98	LEU	CB-CA-C	-5.56	99.64	110.20
3	C	29	ARG	NE-CZ-NH1	5.46	123.03	120.30
6	F	34	LEU	CB-CG-CD1	-5.42	101.78	111.00
3	C	331	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	238	LYS	CA-CB-CG	-5.26	101.83	113.40
2	B	392	PHE	CB-CG-CD1	5.19	124.43	120.80
3	C	358	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	A	180	PHE	CB-CG-CD1	5.14	124.40	120.80
4	D	323	GLU	CG-CD-OE2	-5.13	108.04	118.30
5	E	18	ARG	NE-CZ-NH2	-5.12	117.74	120.30
3	C	435	ARG	NE-CZ-NH2	-5.12	117.74	120.30
5	E	8	ARG	NE-CZ-NH2	-5.07	117.77	120.30
4	D	134	ARG	NE-CZ-NH2	-5.06	117.77	120.30
3	C	427	VAL	CA-CB-CG1	5.05	118.48	110.90
5	E	8	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	231	GLU	Sidechain
1	A	238	LYS	Peptide
1	A	244	GLU	Sidechain

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Mol	Chain	Res	Type	Group
1	A	341	LEU	Peptide
2	B	384	ARG	Sidechain
2	B	483	ASP	Sidechain
3	C	461	ASP	Sidechain
4	D	219	GLU	Sidechain
4	D	323	GLU	Sidechain
7	H	35	MET	Peptide
8	I	27	ASP	Sidechain
11	M	32	GLN	Peptide
14	y	42	ARG	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	A	2627	0	2524	9	0
2	B	3812	0	3683	10	0
3	C	3465	0	3389	12	0
4	D	2705	0	2608	15	0
5	E	635	0	625	1	0
6	F	307	0	312	0	0
7	H	511	0	532	1	0
8	I	286	0	308	1	0
9	K	293	0	305	3	0
10	L	304	0	316	3	0
11	M	267	0	289	2	0
12	T	256	0	262	2	0
13	X	254	0	282	1	0
14	y	208	0	237	0	0
15	Z	479	0	516	3	0
16	A	1	0	0	0	0
17	A	1	0	0	0	0
18	A	1	0	0	0	0
19	A	64	0	74	1	0
19	D	64	0	74	3	0
20	A	260	0	284	8	0
20	B	1040	0	1142	14	0
20	C	845	0	928	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	D	130	0	143	5	0
21	A	40	0	56	1	0
21	B	120	0	168	6	0
21	C	80	0	112	3	0
21	F	40	0	56	0	0
21	H	40	0	56	1	0
21	K	40	0	56	1	0
21	Z	40	0	56	0	0
22	A	98	0	148	1	0
23	A	4	0	1	0	0
24	B	55	0	86	1	0
24	C	55	0	86	1	0
24	D	165	0	258	2	0
24	I	55	0	86	0	0
24	M	55	0	86	0	0
25	D	55	0	80	2	0
26	E	43	0	30	1	0
All	All	19800	0	20254	97	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 3.

All (97) 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)
20:A:408:CLA:HMB1	20:A:408:CLA:HBB1	1.66	0.78
20:C:509:CLA:H93	9:K:37:PHE:CZ	2.31	0.65
20:C:515:CLA:HMB1	20:C:515:CLA:HBB1	1.79	0.64
20:C:511:CLA:HMB1	20:C:511:CLA:HBB1	1.80	0.64
20:B:609:CLA:H42	4:D:127:LEU:HD11	1.81	0.62
21:C:514:BCR:H331	21:C:514:BCR:C8	2.28	0.62
3:C:59:GLU:HB3	3:C:74:LEU:HD12	1.81	0.62
4:D:343:GLU:N	4:D:343:GLU:OE1	2.31	0.61
20:B:613:CLA:HMB1	20:B:613:CLA:HBB1	1.83	0.60
20:C:502:CLA:HMB3	21:C:514:BCR:H403	1.83	0.60
2:B:233:ASN:O	2:B:236:THR:HG22	2.01	0.60
1:A:198:HIS:O	1:A:202:VAL:HG12	2.02	0.59
20:A:406:CLA:HBB1	20:A:406:CLA:HMB1	1.86	0.58
3:C:122:ILE:HD11	20:C:511:CLA:H92	1.87	0.57
2:B:329:PRO:HG3	20:B:608:CLA:HED1	1.88	0.56
3:C:131:TYR:CE2	20:C:513:CLA:HED2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:614:CLA:HMD3	21:B:619:BCR:H341	1.88	0.55
4:D:30:VAL:HG13	4:D:31:GLY:H	1.73	0.54
20:C:509:CLA:H93	9:K:37:PHE:HZ	1.73	0.53
1:A:329:GLU:CD	3:C:400:THR:HG21	2.29	0.53
11:M:15:VAL:HG13	11:M:16:LEU:HD23	1.90	0.53
10:L:12:LEU:H	11:M:29:THR:HG21	1.73	0.53
1:A:234:ASN:HB3	4:D:263:ASN:HD21	1.74	0.53
20:B:606:CLA:HBB1	20:B:606:CLA:HHC	1.90	0.52
20:B:610:CLA:HBB1	20:B:610:CLA:HHC	1.91	0.52
20:D:406:CLA:HBC3	20:D:406:CLA:HHD	1.91	0.52
2:B:248:ALA:HB2	20:B:604:CLA:H93	1.90	0.52
7:H:43:LEU:HD12	7:H:47:GLU:HG3	1.92	0.52
3:C:38:LEU:O	3:C:42:VAL:HG12	2.10	0.51
21:K:101:BCR:H331	21:K:101:BCR:C8	2.39	0.51
19:A:404:PHO:HMB3	20:A:406:CLA:C2	2.41	0.50
20:A:405:CLA:H41	20:A:406:CLA:CHC	2.41	0.50
20:A:405:CLA:H43	20:A:406:CLA:HMC2	1.94	0.50
20:B:605:CLA:HMB3	20:B:608:CLA:HAB	1.93	0.50
1:A:224:ILE:HG22	1:A:225:ARG:N	2.28	0.49
3:C:413:TRP:HB3	20:C:505:CLA:HMB2	1.93	0.49
4:D:116:LEU:HD12	20:D:407:CLA:HED3	1.95	0.49
25:D:404:PL9:H262	25:D:404:PL9:H303	1.96	0.48
24:B:601:LMG:H451	20:B:612:CLA:H151	1.95	0.48
1:A:31:GLY:O	1:A:35:VAL:HG13	2.14	0.48
20:D:406:CLA:HBB1	20:D:406:CLA:HHC	1.96	0.48
4:D:44:ALA:HB3	19:D:405:PHO:H92	1.96	0.47
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.97	0.47
20:A:405:CLA:HMC3	4:D:182:LEU:HD13	1.96	0.47
12:T:5:THR:O	12:T:9:ILE:HG13	2.15	0.47
4:D:159:ILE:HG21	4:D:287:VAL:HG23	1.96	0.46
26:E:101:HEM:HMB2	26:E:101:HEM:HBB2	1.97	0.46
3:C:396:GLY:H	3:C:406:ASN:HA	1.80	0.46
4:D:259:ILE:HD12	4:D:259:ILE:O	2.15	0.46
2:B:145:LEU:HD22	20:B:605:CLA:H171	1.97	0.46
20:C:515:CLA:C17	20:C:515:CLA:H141	2.46	0.46
15:Z:2:THR:HG22	15:Z:61:VAL:HG13	1.97	0.46
19:D:405:PHO:HMB1	19:D:405:PHO:HBB1	1.98	0.46
20:C:503:CLA:HBB1	20:C:503:CLA:HMB1	1.97	0.46
2:B:125:ASP:OD2	2:B:126:PRO:HD2	2.17	0.45
20:C:503:CLA:H122	20:C:504:CLA:HMB2	1.99	0.45
24:D:403:LMG:H272	12:T:13:ILE:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:98:PRO:HA	3:C:101:VAL:HG12	1.97	0.45
8:I:23:PHE:CD1	8:I:27:ASP:OD2	2.69	0.45
1:A:150:PRO:HB2	20:A:405:CLA:H93	2.00	0.44
2:B:128:THR:CG2	2:B:130:GLU:OE2	2.65	0.44
15:Z:61:VAL:HG12	15:Z:62:VAL:HG13	2.00	0.44
4:D:291:LEU:N	4:D:291:LEU:HD22	2.33	0.44
20:A:405:CLA:HAA2	20:A:405:CLA:HBD	2.00	0.43
21:B:618:BCR:H20C	21:B:618:BCR:H361	1.83	0.43
1:A:106:LEU:HD11	21:A:409:BCR:H402	2.00	0.43
20:B:609:CLA:C14	20:D:407:CLA:HMB2	2.49	0.43
9:K:43:VAL:O	9:K:43:VAL:HG22	2.18	0.43
3:C:329:LEU:HD13	3:C:337:ILE:CG2	2.49	0.43
20:B:613:CLA:H43	20:B:616:CLA:CGA	2.48	0.43
21:B:620:BCR:H24C	21:B:620:BCR:H371	1.78	0.43
5:E:80:LEU:HD23	5:E:80:LEU:N	2.32	0.43
1:A:335:ASN:O	1:A:336:ALA:HB2	2.19	0.43
4:D:279:LEU:HD12	19:D:405:PHO:HBC3	2.00	0.43
2:B:145:LEU:HD11	20:B:616:CLA:HMB2	2.00	0.43
1:A:227:THR:HG21	1:A:233:ALA:HA	2.00	0.42
2:B:369:ILE:CG2	2:B:377:VAL:HG22	2.49	0.42
4:D:61:HIS:CE1	4:D:168:PHE:CZ	3.08	0.42
21:B:620:BCR:H11C	21:B:620:BCR:H341	1.87	0.42
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.02	0.42
4:D:274:VAL:HG22	25:D:404:PL9:H253	2.02	0.42
3:C:105:VAL:HG11	24:C:501:LMG:H241	2.01	0.42
3:C:368:ILE:N	3:C:368:ILE:HD12	2.35	0.42
21:H:101:BCR:H24C	21:H:101:BCR:H371	1.79	0.41
21:B:618:BCR:H24C	21:B:618:BCR:H371	1.80	0.41
2:B:128:THR:HG23	2:B:130:GLU:OE2	2.19	0.41
21:B:619:BCR:H24C	21:B:619:BCR:H371	1.91	0.41
22:A:411:LHG:H272	22:A:411:LHG:C23	2.50	0.41
20:B:603:CLA:H172	20:B:603:CLA:H13	1.91	0.41
13:X:21:LEU:O	13:X:24:THR:HG22	2.20	0.41
24:D:402:LMG:H351	20:D:406:CLA:H191	2.02	0.41
2:B:11:VAL:HG12	10:L:6:ASN:O	2.21	0.41
3:C:123:ARG:HH21	3:C:123:ARG:HG3	1.85	0.41
20:C:503:CLA:HMB1	20:C:503:CLA:CBB	2.51	0.40
20:C:507:CLA:H43	21:C:514:BCR:HC8	2.03	0.40
15:Z:23:VAL:HG12	15:Z:40:ILE:HG22	2.04	0.40
10:L:24:ILE:HD13	10:L:24:ILE:HA	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	333/360 (92%)	309 (93%)	23 (7%)	1 (0%)	41 56
2	B	483/510 (95%)	459 (95%)	24 (5%)	0	100 100
3	C	446/461 (97%)	420 (94%)	26 (6%)	0	100 100
4	D	338/352 (96%)	326 (96%)	12 (4%)	0	100 100
5	E	75/84 (89%)	68 (91%)	7 (9%)	0	100 100
6	F	36/45 (80%)	33 (92%)	3 (8%)	0	100 100
7	H	63/66 (96%)	56 (89%)	6 (10%)	1 (2%)	9 14
8	I	33/38 (87%)	31 (94%)	2 (6%)	0	100 100
9	K	35/46 (76%)	34 (97%)	0	1 (3%)	4 6
10	L	35/37 (95%)	35 (100%)	0	0	100 100
11	M	32/36 (89%)	31 (97%)	1 (3%)	0	100 100
12	T	28/32 (88%)	28 (100%)	0	0	100 100
13	X	33/41 (80%)	33 (100%)	0	0	100 100
14	y	26/46 (56%)	23 (88%)	3 (12%)	0	100 100
15	Z	60/62 (97%)	55 (92%)	5 (8%)	0	100 100
All	All	2056/2216 (93%)	1941 (94%)	112 (5%)	3 (0%)	54 69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	H	35	MET
1	A	340	PRO
9	K	45	PHE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	271/291 (93%)	269 (99%)	2 (1%)	84 91
2	B	385/407 (95%)	379 (98%)	6 (2%)	62 78
3	C	350/362 (97%)	345 (99%)	5 (1%)	67 81
4	D	275/283 (97%)	270 (98%)	5 (2%)	59 75
5	E	69/73 (94%)	67 (97%)	2 (3%)	42 60
6	F	32/39 (82%)	31 (97%)	1 (3%)	40 57
7	H	54/55 (98%)	53 (98%)	1 (2%)	57 74
8	I	32/35 (91%)	32 (100%)	0	100 100
9	K	30/37 (81%)	29 (97%)	1 (3%)	38 54
10	L	35/35 (100%)	34 (97%)	1 (3%)	42 60
11	M	31/33 (94%)	28 (90%)	3 (10%)	8 11
12	T	27/29 (93%)	27 (100%)	0	100 100
13	X	28/34 (82%)	28 (100%)	0	100 100
14	y	21/37 (57%)	20 (95%)	1 (5%)	25 39
15	Z	52/52 (100%)	50 (96%)	2 (4%)	33 49
All	All	1692/1802 (94%)	1662 (98%)	30 (2%)	61 75

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	SER
1	A	202	VAL
2	B	14	ASN
2	B	81	THR
2	B	98	LEU
2	B	108	PHE
2	B	127	ARG
2	B	480	SER
3	C	130	GLU
3	C	277	PHE

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Mol	Chain	Res	Type
3	C	401	GLU
3	C	408	VAL
3	C	461	ASP
4	D	180	ARG
4	D	186	GLN
4	D	227	GLU
4	D	343	GLU
4	D	350	ASN
5	E	11	SER
5	E	76	VAL
6	F	34	LEU
7	H	43	LEU
9	K	24	VAL
10	L	29	LEU
11	M	6	LEU
11	M	16	LEU
11	M	27	VAL
14	y	24	MET
15	Z	20	VAL
15	Z	52	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	310	GLN
4	D	83	ASN
4	D	186	GLN
4	D	263	ASN
4	D	336	HIS
4	D	350	ASN
7	H	15	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 62 ligands modelled in this entry, 3 are monoatomic - leaving 59 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	$\#\|Z\| > 2$
20	CLA	B	603	-	65,73,73	1.53	10 (15%)	76,113,113	2.10	18 (23%)
19	PHO	D	405	-	51,69,69	1.09	6 (11%)	47,99,99	1.21	3 (6%)
25	PL9	D	404	-	55,55,55	1.07	5 (9%)	68,69,69	1.40	10 (14%)
20	CLA	C	509	-	65,73,73	1.74	13 (20%)	76,113,113	1.74	13 (17%)
21	BCR	C	516	-	41,41,41	0.69	0	56,56,56	1.26	4 (7%)
21	BCR	Z	101	-	41,41,41	0.81	1 (2%)	56,56,56	1.14	4 (7%)
20	CLA	B	608	-	65,73,73	1.66	11 (16%)	76,113,113	1.84	18 (23%)
20	CLA	B	615	-	65,73,73	1.66	11 (16%)	76,113,113	1.94	12 (15%)
24	LMG	D	401	-	55,55,55	1.01	3 (5%)	63,63,63	0.85	0
21	BCR	K	101	-	41,41,41	0.77	1 (2%)	56,56,56	1.41	10 (17%)
24	LMG	M	101	-	55,55,55	1.12	3 (5%)	63,63,63	0.91	1 (1%)
20	CLA	B	614	-	65,73,73	1.87	11 (16%)	76,113,113	1.84	16 (21%)
20	CLA	B	609	-	65,73,73	1.79	8 (12%)	76,113,113	1.57	10 (13%)
20	CLA	C	506	-	65,73,73	1.77	11 (16%)	76,113,113	2.46	24 (31%)
22	LHG	A	411	-	48,48,48	0.82	1 (2%)	51,54,54	0.81	1 (1%)
20	CLA	B	602	-	65,73,73	1.69	8 (12%)	76,113,113	2.30	19 (25%)
21	BCR	C	514	-	41,41,41	0.94	0	56,56,56	1.35	9 (16%)
24	LMG	D	403	-	55,55,55	1.17	4 (7%)	63,63,63	0.99	3 (4%)
24	LMG	D	402	-	55,55,55	1.01	2 (3%)	63,63,63	1.04	4 (6%)
20	CLA	C	504	-	65,73,73	1.74	10 (15%)	76,113,113	1.80	16 (21%)
20	CLA	C	511	3	65,73,73	1.74	13 (20%)	76,113,113	2.11	18 (23%)
20	CLA	B	616	-	65,73,73	1.61	10 (15%)	76,113,113	1.78	15 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	BCR	B	618	-	41,41,41	0.79	1 (2%)	56,56,56	1.10	4 (7%)
22	LHG	A	410	-	48,48,48	0.85	2 (4%)	51,54,54	0.73	1 (1%)
24	LMG	C	501	-	55,55,55	0.95	2 (3%)	63,63,63	0.97	3 (4%)
20	CLA	A	405	-	65,73,73	1.71	12 (18%)	76,113,113	1.66	18 (23%)
19	PHO	A	404	-	51,69,69	1.07	4 (7%)	47,99,99	1.23	5 (10%)
20	CLA	B	610	-	65,73,73	1.71	12 (18%)	76,113,113	2.25	21 (27%)
20	CLA	C	507	-	65,73,73	1.72	11 (16%)	76,113,113	1.88	15 (19%)
21	BCR	A	409	-	41,41,41	0.72	0	56,56,56	0.97	2 (3%)
24	LMG	I	101	-	55,55,55	0.91	1 (1%)	63,63,63	0.99	3 (4%)
20	CLA	A	406	-	65,73,73	1.48	10 (15%)	76,113,113	1.68	20 (26%)
23	BCT	A	412	16	2,3,3	1.29	0	2,3,3	3.38	1 (50%)
20	CLA	B	607	-	65,73,73	1.59	8 (12%)	76,113,113	1.62	10 (13%)
20	CLA	A	407	-	65,73,73	1.60	7 (10%)	76,113,113	1.89	22 (28%)
20	CLA	B	617	-	65,73,73	1.68	14 (21%)	76,113,113	2.06	15 (19%)
21	BCR	H	101	-	41,41,41	0.91	1 (2%)	56,56,56	1.21	6 (10%)
20	CLA	D	406	-	65,73,73	1.63	10 (15%)	76,113,113	1.75	19 (25%)
24	LMG	B	601	-	55,55,55	0.98	1 (1%)	63,63,63	1.13	4 (6%)
20	CLA	C	505	-	65,73,73	1.64	13 (20%)	76,113,113	1.89	23 (30%)
20	CLA	C	503	-	65,73,73	1.49	10 (15%)	76,113,113	1.90	14 (18%)
20	CLA	B	612	-	65,73,73	1.64	9 (13%)	76,113,113	2.11	16 (21%)
20	CLA	B	606	-	65,73,73	1.67	10 (15%)	76,113,113	1.86	16 (21%)
21	BCR	B	619	-	41,41,41	0.85	1 (2%)	56,56,56	1.00	5 (8%)
21	BCR	B	620	-	41,41,41	0.91	0	56,56,56	1.30	10 (17%)
26	HEM	E	101	5	41,50,50	1.47	6 (14%)	45,82,82	1.32	4 (8%)
20	CLA	B	613	-	65,73,73	1.59	8 (12%)	76,113,113	1.87	20 (26%)
21	BCR	F	101	-	41,41,41	0.72	0	56,56,56	1.25	6 (10%)
20	CLA	B	604	-	65,73,73	1.62	9 (13%)	76,113,113	1.96	16 (21%)
20	CLA	B	605	-	65,73,73	1.65	11 (16%)	76,113,113	1.65	15 (19%)
20	CLA	A	408	-	65,73,73	1.62	11 (16%)	76,113,113	1.46	11 (14%)
20	CLA	C	510	-	65,73,73	1.72	12 (18%)	76,113,113	1.68	18 (23%)
20	CLA	C	515	-	65,73,73	1.58	8 (12%)	76,113,113	2.05	18 (23%)
20	CLA	C	512	-	65,73,73	1.74	13 (20%)	76,113,113	1.94	15 (19%)
20	CLA	D	407	-	65,73,73	1.74	10 (15%)	76,113,113	1.64	13 (17%)
20	CLA	C	513	-	65,73,73	1.69	15 (23%)	76,113,113	1.82	18 (23%)
20	CLA	C	508	-	65,73,73	1.55	9 (13%)	76,113,113	1.78	14 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	B	611	-	65,73,73	1.64	13 (20%)	76,113,113	1.96	15 (19%)
20	CLA	C	502	-	65,73,73	1.60	11 (16%)	76,113,113	1.73	14 (18%)

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
20	CLA	B	603	-	2/2/15/20	3/37/115/115	-
19	PHO	D	405	-	1/1/17/22	8/37/103/103	0/5/6/6
25	PL9	D	404	-	-	7/53/73/73	0/1/1/1
20	CLA	C	509	-	2/2/15/20	4/37/115/115	-
21	BCR	C	516	-	-	13/29/63/63	0/2/2/2
21	BCR	Z	101	-	-	5/29/63/63	0/2/2/2
20	CLA	B	608	-	2/2/15/20	7/37/115/115	-
20	CLA	B	615	-	2/2/15/20	5/37/115/115	-
24	LMG	D	401	-	-	18/50/70/70	0/1/1/1
21	BCR	K	101	-	-	13/29/63/63	0/2/2/2
24	LMG	M	101	-	-	6/50/70/70	0/1/1/1
20	CLA	B	614	-	2/2/15/20	5/37/115/115	-
20	CLA	B	609	-	1/1/15/20	5/37/115/115	-
20	CLA	C	506	-	2/2/15/20	8/37/115/115	-
22	LHG	A	411	-	-	19/53/53/53	-
20	CLA	B	602	-	1/1/15/20	10/37/115/115	-
21	BCR	C	514	-	-	7/29/63/63	0/2/2/2
24	LMG	D	403	-	-	8/50/70/70	0/1/1/1
24	LMG	D	402	-	-	9/50/70/70	0/1/1/1
20	CLA	C	504	-	1/1/15/20	8/37/115/115	-
20	CLA	C	511	3	2/2/15/20	8/37/115/115	-
20	CLA	B	616	-	1/1/15/20	8/37/115/115	-
21	BCR	B	618	-	-	5/29/63/63	0/2/2/2
22	LHG	A	410	-	-	13/53/53/53	-
24	LMG	C	501	-	-	14/50/70/70	0/1/1/1
20	CLA	A	405	-	2/2/15/20	7/37/115/115	-
19	PHO	A	404	-	1/1/17/22	7/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	610	-	2/2/15/20	8/37/115/115	-
20	CLA	C	507	-	2/2/15/20	7/37/115/115	-
21	BCR	A	409	-	-	6/29/63/63	0/2/2/2
24	LMG	I	101	-	-	3/50/70/70	0/1/1/1
20	CLA	A	406	-	2/2/15/20	11/37/115/115	-
20	CLA	B	607	-	2/2/15/20	7/37/115/115	-
20	CLA	A	407	-	1/1/15/20	2/37/115/115	-
20	CLA	B	617	-	1/1/15/20	3/37/115/115	-
21	BCR	H	101	-	-	8/29/63/63	0/2/2/2
20	CLA	D	406	-	2/2/15/20	11/37/115/115	-
24	LMG	B	601	-	-	9/50/70/70	0/1/1/1
20	CLA	C	505	-	1/1/15/20	5/37/115/115	-
20	CLA	C	503	-	2/2/15/20	12/37/115/115	-
20	CLA	B	612	-	2/2/15/20	11/37/115/115	-
20	CLA	B	606	-	2/2/15/20	2/37/115/115	-
21	BCR	B	619	-	-	7/29/63/63	0/2/2/2
21	BCR	B	620	-	-	6/29/63/63	0/2/2/2
26	HEM	E	101	5	-	4/12/54/54	-
20	CLA	B	613	-	1/1/15/20	8/37/115/115	-
21	BCR	F	101	-	-	5/29/63/63	0/2/2/2
20	CLA	B	604	-	2/2/15/20	9/37/115/115	-
20	CLA	B	605	-	2/2/15/20	4/37/115/115	-
20	CLA	A	408	-	1/1/15/20	12/37/115/115	-
20	CLA	C	510	-	1/1/15/20	7/37/115/115	-
20	CLA	C	515	-	1/1/15/20	5/37/115/115	-
20	CLA	C	512	-	1/1/15/20	10/37/115/115	-
20	CLA	D	407	-	1/1/15/20	5/37/115/115	-
20	CLA	C	513	-	1/1/15/20	7/37/115/115	-
20	CLA	C	508	-	1/1/15/20	4/37/115/115	-
20	CLA	B	611	-	2/2/15/20	11/37/115/115	-
20	CLA	C	502	-	2/2/15/20	3/37/115/115	-

All (417) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	614	CLA	C4B-NB	10.88	1.44	1.35
20	B	609	CLA	C4B-NB	9.63	1.43	1.35
20	B	602	CLA	C4B-NB	9.54	1.43	1.35
20	A	407	CLA	C4B-NB	9.16	1.43	1.35
20	C	512	CLA	C4B-NB	9.15	1.43	1.35
20	C	504	CLA	C4B-NB	8.54	1.42	1.35
20	A	405	CLA	C4B-NB	8.51	1.42	1.35
20	C	506	CLA	C4B-NB	8.47	1.42	1.35
20	C	509	CLA	C4B-NB	8.42	1.42	1.35
20	B	606	CLA	C4B-NB	8.40	1.42	1.35
20	C	507	CLA	C4B-NB	8.40	1.42	1.35
20	B	604	CLA	C4B-NB	8.31	1.42	1.35
20	C	510	CLA	C4B-NB	8.31	1.42	1.35
20	B	605	CLA	C4B-NB	8.20	1.42	1.35
20	B	612	CLA	C4B-NB	8.19	1.42	1.35
20	B	607	CLA	C4B-NB	8.14	1.42	1.35
20	B	613	CLA	C4B-NB	8.14	1.42	1.35
20	C	511	CLA	C4B-NB	8.00	1.42	1.35
20	B	610	CLA	C4B-NB	7.99	1.42	1.35
20	D	406	CLA	C4B-NB	7.76	1.42	1.35
20	B	617	CLA	C4B-NB	7.71	1.42	1.35
20	B	616	CLA	C4B-NB	7.66	1.42	1.35
20	C	513	CLA	C4B-NB	7.64	1.42	1.35
20	C	502	CLA	C4B-NB	7.63	1.42	1.35
20	C	515	CLA	C4B-NB	7.60	1.42	1.35
20	A	408	CLA	C4B-NB	7.58	1.42	1.35
20	B	608	CLA	C4B-NB	7.57	1.42	1.35
20	B	615	CLA	C4B-NB	7.53	1.41	1.35
20	C	508	CLA	C4B-NB	7.52	1.41	1.35
20	B	611	CLA	C4B-NB	7.22	1.41	1.35
20	B	603	CLA	C4B-NB	7.13	1.41	1.35
20	D	407	CLA	C4B-NB	6.61	1.41	1.35
20	C	505	CLA	C4B-NB	6.56	1.41	1.35
20	C	503	CLA	C4B-NB	6.37	1.40	1.35
20	A	406	CLA	C4B-NB	6.06	1.40	1.35
26	E	101	HEM	C3C-C2C	-4.67	1.33	1.40
20	D	407	CLA	C1D-ND	4.48	1.43	1.37
20	D	407	CLA	C4D-ND	-4.44	1.31	1.37
20	B	617	CLA	C1D-ND	4.42	1.43	1.37
20	C	505	CLA	C4D-ND	-4.35	1.31	1.37
20	C	515	CLA	C1D-ND	3.93	1.42	1.37
20	C	502	CLA	C4D-ND	-3.91	1.32	1.37
20	D	406	CLA	C1D-ND	3.88	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	D	407	CLA	MG-NA	3.86	2.15	2.06
20	A	408	CLA	C4D-ND	-3.86	1.32	1.37
20	B	615	CLA	C3D-CAD	3.85	1.58	1.45
20	C	508	CLA	C1D-ND	3.83	1.42	1.37
20	B	610	CLA	MG-NC	3.83	2.15	2.06
20	A	408	CLA	C1D-ND	3.82	1.42	1.37
20	B	609	CLA	C1D-ND	3.82	1.42	1.37
20	C	511	CLA	C1D-ND	3.77	1.42	1.37
20	B	607	CLA	C1D-ND	3.76	1.42	1.37
20	C	504	CLA	C1D-ND	3.67	1.42	1.37
20	B	610	CLA	C3D-CAD	3.67	1.57	1.45
20	B	605	CLA	C1D-ND	3.66	1.42	1.37
20	A	406	CLA	C1D-ND	3.63	1.42	1.37
20	C	506	CLA	CAA-C2A	3.62	1.60	1.54
20	B	616	CLA	C1D-ND	3.61	1.42	1.37
20	C	505	CLA	MG-ND	-3.57	1.98	2.05
20	B	603	CLA	C1D-ND	3.54	1.42	1.37
20	D	407	CLA	MG-NC	3.53	2.14	2.06
20	C	503	CLA	C4D-ND	-3.52	1.32	1.37
20	A	407	CLA	C1D-ND	3.51	1.42	1.37
20	C	509	CLA	C3D-CAD	3.47	1.56	1.45
20	B	614	CLA	C3D-CAD	3.47	1.56	1.45
20	B	608	CLA	CMB-C2B	-3.46	1.44	1.51
20	C	509	CLA	CHC-C1C	3.46	1.43	1.35
20	C	506	CLA	C3D-CAD	3.45	1.56	1.45
20	B	608	CLA	C4D-ND	-3.43	1.33	1.37
20	B	611	CLA	C1D-ND	3.40	1.42	1.37
20	C	513	CLA	C3D-CAD	3.40	1.56	1.45
20	B	606	CLA	C1D-ND	3.39	1.41	1.37
20	B	609	CLA	C3D-CAD	3.38	1.56	1.45
20	B	604	CLA	C4D-ND	-3.38	1.33	1.37
20	C	504	CLA	C1B-NB	3.37	1.38	1.35
20	C	511	CLA	C1D-C2D	3.36	1.52	1.45
20	B	606	CLA	C4D-ND	-3.34	1.33	1.37
20	C	515	CLA	C3D-CAD	3.34	1.56	1.45
20	B	608	CLA	C3B-C2B	-3.34	1.35	1.40
20	C	504	CLA	CHC-C1C	3.33	1.43	1.35
20	C	510	CLA	MG-NA	3.33	2.14	2.06
20	C	510	CLA	C1D-ND	3.32	1.41	1.37
20	B	613	CLA	C1D-ND	3.30	1.41	1.37
20	C	512	CLA	C1D-ND	3.27	1.41	1.37
20	B	610	CLA	CMD-C2D	-3.27	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	D	407	CLA	MG-ND	-3.26	1.99	2.05
20	C	502	CLA	C1D-ND	3.26	1.41	1.37
20	C	511	CLA	C3D-CAD	3.25	1.56	1.45
20	C	507	CLA	C1D-ND	3.24	1.41	1.37
20	C	511	CLA	OBD-CAD	-3.24	1.16	1.22
20	C	507	CLA	C3D-CAD	3.22	1.56	1.45
20	B	614	CLA	CHC-C1C	3.22	1.43	1.35
20	C	510	CLA	MG-NC	3.22	2.13	2.06
20	C	507	CLA	CMB-C2B	-3.21	1.45	1.51
20	C	509	CLA	C1D-ND	3.19	1.41	1.37
20	B	602	CLA	C1D-ND	3.16	1.41	1.37
20	A	405	CLA	MG-NC	3.15	2.13	2.06
20	B	611	CLA	MG-NC	3.14	2.13	2.06
20	D	406	CLA	CHC-C1C	3.13	1.43	1.35
20	B	615	CLA	C3D-C4D	3.12	1.51	1.44
20	A	405	CLA	MG-ND	-3.12	1.99	2.05
24	M	101	LMG	O1-C1	3.12	1.45	1.40
20	B	617	CLA	C3D-C4D	3.12	1.51	1.44
20	A	405	CLA	CMB-C2B	-3.11	1.45	1.51
20	B	609	CLA	CHC-C1C	3.11	1.42	1.35
20	D	406	CLA	CMB-C2B	-3.10	1.45	1.51
20	B	616	CLA	MG-NA	3.10	2.13	2.06
20	B	617	CLA	OBD-CAD	-3.10	1.17	1.22
20	C	504	CLA	MG-NC	3.09	2.13	2.06
20	C	512	CLA	CHC-C1C	3.09	1.42	1.35
20	B	613	CLA	CHC-C1C	3.09	1.42	1.35
20	C	504	CLA	C4D-ND	-3.09	1.33	1.37
20	B	612	CLA	C3D-CAD	3.08	1.55	1.45
20	C	505	CLA	MG-NC	3.08	2.13	2.06
20	C	511	CLA	CMB-C2B	-3.07	1.45	1.51
20	C	506	CLA	C2A-C1A	-3.06	1.45	1.52
20	B	606	CLA	CHC-C1C	3.06	1.42	1.35
20	B	611	CLA	CHC-C1C	3.06	1.42	1.35
20	B	604	CLA	C1D-ND	3.04	1.41	1.37
20	B	615	CLA	C1D-ND	3.03	1.41	1.37
20	C	506	CLA	C1D-C2D	3.03	1.51	1.45
20	B	610	CLA	C3D-C4D	3.02	1.51	1.44
20	C	510	CLA	MG-ND	-3.02	1.99	2.05
20	B	612	CLA	CMB-C2B	-3.01	1.45	1.51
20	C	502	CLA	CMD-C2D	-3.01	1.44	1.50
20	C	503	CLA	CMB-C2B	-3.00	1.45	1.51
20	C	503	CLA	C1D-ND	3.00	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	613	CLA	CMD-C2D	-2.99	1.44	1.50
20	A	405	CLA	MG-NA	2.99	2.13	2.06
20	C	506	CLA	CHC-C1C	2.98	1.42	1.35
20	C	505	CLA	C1D-ND	2.98	1.41	1.37
20	B	616	CLA	CMD-C2D	-2.98	1.44	1.50
26	E	101	HEM	C3C-CAC	2.97	1.53	1.47
20	B	612	CLA	C3B-C2B	-2.95	1.36	1.40
20	C	511	CLA	C3D-C4D	2.95	1.50	1.44
20	C	510	CLA	CHC-C1C	2.95	1.42	1.35
20	A	405	CLA	CHC-C1C	2.94	1.42	1.35
20	D	407	CLA	CMB-C2B	-2.94	1.45	1.51
20	B	611	CLA	C4D-ND	-2.94	1.33	1.37
20	B	614	CLA	C3D-C4D	2.92	1.50	1.44
20	A	408	CLA	CHC-C1C	2.91	1.42	1.35
20	B	609	CLA	CMB-C2B	-2.91	1.45	1.51
20	B	610	CLA	C1D-ND	2.90	1.41	1.37
20	C	508	CLA	CHC-C1C	2.90	1.42	1.35
20	B	615	CLA	CHC-C1C	2.90	1.42	1.35
20	C	502	CLA	CHC-C1C	2.90	1.42	1.35
20	C	509	CLA	C3B-C2B	-2.90	1.36	1.40
20	C	506	CLA	C1D-ND	2.89	1.41	1.37
20	C	513	CLA	C3B-CAB	-2.89	1.42	1.47
24	D	403	LMG	C7-C8	2.88	1.59	1.50
20	B	615	CLA	C1D-C2D	2.88	1.51	1.45
20	C	505	CLA	C3B-CAB	-2.87	1.42	1.47
20	C	505	CLA	CMB-C2B	-2.87	1.45	1.51
20	B	614	CLA	C1D-ND	2.86	1.41	1.37
20	C	513	CLA	CMB-C2B	-2.86	1.45	1.51
24	D	403	LMG	C9-C8	2.86	1.59	1.50
20	C	507	CLA	CHC-C1C	2.86	1.42	1.35
20	C	504	CLA	MG-NA	2.86	2.13	2.06
20	B	602	CLA	C3B-C2B	-2.85	1.36	1.40
20	C	510	CLA	C3B-C2B	-2.85	1.36	1.40
25	D	404	PL9	C7-C8	-2.85	1.46	1.50
20	C	510	CLA	C4D-ND	-2.85	1.33	1.37
20	D	406	CLA	C3B-C2B	-2.84	1.36	1.40
20	C	513	CLA	MG-NC	2.83	2.13	2.06
20	C	512	CLA	CMB-C2B	-2.83	1.45	1.51
20	B	608	CLA	C1D-ND	2.83	1.41	1.37
20	B	609	CLA	C3D-C4D	2.82	1.50	1.44
20	C	515	CLA	CHC-C1C	2.82	1.42	1.35
20	B	610	CLA	CHC-C1C	2.81	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	509	CLA	C3D-C4D	2.81	1.50	1.44
19	D	405	PHO	CAC-C3C	-2.80	1.47	1.52
20	D	407	CLA	C3B-C2B	-2.80	1.36	1.40
20	B	606	CLA	C1B-NB	2.79	1.37	1.35
20	C	511	CLA	CHC-C1C	2.79	1.42	1.35
20	B	608	CLA	C3B-CAB	-2.79	1.42	1.47
20	C	513	CLA	MG-NA	2.79	2.12	2.06
20	C	515	CLA	C1D-C2D	2.78	1.50	1.45
20	C	507	CLA	C3B-C2B	-2.78	1.36	1.40
20	B	602	CLA	CMB-C2B	-2.77	1.45	1.51
24	M	101	LMG	C9-C8	2.77	1.59	1.50
20	B	611	CLA	C3D-C4D	2.77	1.50	1.44
20	C	505	CLA	MG-NA	2.77	2.12	2.06
24	M	101	LMG	C7-C8	2.77	1.59	1.50
20	A	408	CLA	MG-NC	2.77	2.12	2.06
20	B	604	CLA	CHC-C1C	2.77	1.42	1.35
20	B	608	CLA	CMD-C2D	-2.76	1.45	1.50
20	C	510	CLA	CMB-C2B	-2.76	1.45	1.51
20	B	607	CLA	MG-NC	2.75	2.12	2.06
24	D	403	LMG	C6-C5	2.75	1.61	1.51
20	D	407	CLA	C3B-CAB	-2.74	1.42	1.47
20	B	603	CLA	C4D-ND	-2.73	1.33	1.37
20	B	608	CLA	CHC-C1C	2.72	1.41	1.35
20	B	617	CLA	CHC-C1C	2.71	1.41	1.35
20	B	610	CLA	MG-NA	2.71	2.12	2.06
19	D	405	PHO	CBD-CGD	-2.71	1.48	1.52
20	A	407	CLA	CHC-C1C	2.70	1.41	1.35
20	B	607	CLA	C4D-ND	-2.69	1.34	1.37
20	B	605	CLA	CMB-C2B	-2.69	1.46	1.51
21	B	618	BCR	C30-C25	-2.69	1.50	1.53
20	C	513	CLA	CHC-C1C	2.68	1.41	1.35
20	C	502	CLA	C3B-C2B	-2.68	1.36	1.40
20	C	515	CLA	C3D-C4D	2.67	1.50	1.44
20	A	408	CLA	CMB-C2B	-2.67	1.46	1.51
20	B	607	CLA	CHC-C1C	2.66	1.41	1.35
20	B	608	CLA	MG-ND	-2.66	2.00	2.05
20	C	506	CLA	C1B-NB	2.65	1.37	1.35
20	B	614	CLA	C1D-C2D	2.65	1.50	1.45
20	B	614	CLA	MG-NC	2.65	2.12	2.06
20	B	605	CLA	MG-NA	2.65	2.12	2.06
20	B	612	CLA	CHC-C1C	2.65	1.41	1.35
22	A	410	LHG	O8-C6	-2.65	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	505	CLA	CMD-C2D	-2.64	1.45	1.50
20	C	512	CLA	MG-NC	2.64	2.12	2.06
19	A	404	PHO	CBD-CGD	-2.64	1.48	1.52
20	A	406	CLA	CHC-C1C	2.64	1.41	1.35
20	C	506	CLA	CMB-C2B	-2.63	1.46	1.51
20	B	616	CLA	CHC-C1C	2.63	1.41	1.35
20	B	603	CLA	C3D-C4D	2.63	1.50	1.44
20	D	407	CLA	CHC-C1C	2.63	1.41	1.35
20	B	611	CLA	CMD-C2D	-2.63	1.45	1.50
20	C	507	CLA	CMD-C2D	-2.63	1.45	1.50
20	A	405	CLA	C4D-ND	-2.62	1.34	1.37
20	C	512	CLA	CMD-C2D	-2.62	1.45	1.50
20	B	604	CLA	C1B-NB	2.62	1.37	1.35
20	A	407	CLA	C1D-C2D	2.61	1.50	1.45
20	B	605	CLA	MG-NC	2.61	2.12	2.06
20	C	507	CLA	MG-NC	2.61	2.12	2.06
20	A	408	CLA	MG-NA	2.61	2.12	2.06
20	A	406	CLA	CMB-C2B	-2.61	1.46	1.51
20	B	607	CLA	MG-NA	2.60	2.12	2.06
20	B	603	CLA	CHC-C1C	2.59	1.41	1.35
20	B	612	CLA	CMD-C2D	-2.59	1.45	1.50
20	B	602	CLA	C3D-C4D	2.59	1.50	1.44
20	B	613	CLA	C4D-ND	-2.59	1.34	1.37
20	B	616	CLA	MG-NC	2.58	2.12	2.06
20	C	508	CLA	C4D-ND	-2.58	1.34	1.37
20	B	611	CLA	MG-NA	2.58	2.12	2.06
20	B	606	CLA	MG-NC	2.57	2.12	2.06
20	C	513	CLA	OBD-CAD	-2.57	1.18	1.22
20	B	611	CLA	C1B-NB	2.55	1.37	1.35
20	C	513	CLA	C3D-C4D	2.55	1.49	1.44
20	C	503	CLA	MG-ND	-2.55	2.00	2.05
24	C	501	LMG	C9-C8	2.55	1.58	1.50
21	B	619	BCR	C30-C25	-2.54	1.50	1.53
20	C	509	CLA	CMD-C2D	-2.53	1.45	1.50
20	C	511	CLA	C3B-C2B	-2.52	1.36	1.40
24	D	402	LMG	C3-C2	2.52	1.58	1.52
20	C	509	CLA	CMB-C2B	-2.52	1.46	1.51
20	D	406	CLA	C1D-C2D	2.51	1.50	1.45
20	A	405	CLA	C3B-C2B	-2.48	1.36	1.40
20	C	503	CLA	CHC-C1C	2.48	1.41	1.35
20	B	613	CLA	CMB-C2B	-2.48	1.46	1.51
20	C	512	CLA	MG-NA	2.48	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	407	CLA	CMB-C2B	-2.48	1.46	1.51
20	B	612	CLA	C3D-C4D	2.48	1.49	1.44
21	K	101	BCR	C30-C25	-2.47	1.50	1.53
20	B	605	CLA	C4D-ND	-2.47	1.34	1.37
20	C	508	CLA	CMB-C2B	-2.47	1.46	1.51
20	A	405	CLA	C1D-C2D	2.46	1.50	1.45
20	B	616	CLA	C3D-C4D	2.46	1.49	1.44
19	D	405	PHO	CMB-C2B	-2.46	1.45	1.51
20	C	509	CLA	MG-NC	2.46	2.12	2.06
20	C	513	CLA	MG-ND	-2.45	2.00	2.05
20	B	616	CLA	CMB-C2B	-2.44	1.46	1.51
20	B	611	CLA	C3B-C2B	-2.44	1.37	1.40
20	B	603	CLA	C3B-CAB	-2.43	1.43	1.47
20	C	509	CLA	MG-NA	2.43	2.12	2.06
20	B	615	CLA	C3B-C2B	-2.43	1.37	1.40
20	B	604	CLA	C3D-C2D	-2.42	1.32	1.39
22	A	411	LHG	P-O6	2.42	1.69	1.59
20	C	512	CLA	C1B-NB	2.42	1.37	1.35
20	C	509	CLA	C1D-C2D	2.41	1.50	1.45
19	A	404	PHO	CAC-C3C	-2.41	1.48	1.52
20	C	505	CLA	CHC-C1C	2.41	1.41	1.35
20	C	506	CLA	OBD-CAD	-2.41	1.18	1.22
25	D	404	PL9	C6-C1	-2.41	1.44	1.48
20	B	612	CLA	C1D-ND	2.41	1.40	1.37
20	A	408	CLA	MG-ND	-2.40	2.01	2.05
20	A	406	CLA	MG-NC	2.40	2.12	2.06
20	A	406	CLA	C1D-C2D	2.40	1.50	1.45
20	C	512	CLA	C4D-ND	-2.40	1.34	1.37
20	C	502	CLA	CMC-C2C	-2.39	1.45	1.50
20	A	405	CLA	C1D-ND	2.39	1.40	1.37
20	B	611	CLA	C3B-CAB	-2.39	1.43	1.47
20	C	502	CLA	C3D-C2D	-2.38	1.32	1.39
19	D	405	PHO	CMC-C2C	-2.38	1.45	1.51
24	D	401	LMG	O8-C9	-2.38	1.39	1.45
20	B	608	CLA	MG-NA	2.38	2.11	2.06
20	B	614	CLA	MG-NA	2.37	2.11	2.06
20	B	617	CLA	C1B-NB	2.37	1.37	1.35
20	B	609	CLA	C1D-C2D	2.37	1.50	1.45
20	A	405	CLA	C4C-C3C	2.36	1.49	1.45
20	C	509	CLA	OBD-CAD	-2.36	1.18	1.22
20	B	605	CLA	CHC-C1C	2.35	1.41	1.35
20	D	406	CLA	MG-NA	2.35	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	401	LMG	C3-C2	2.35	1.58	1.52
20	B	613	CLA	MG-NC	2.34	2.11	2.06
20	B	605	CLA	C3D-C4D	2.34	1.49	1.44
20	C	505	CLA	C3B-C2B	-2.33	1.37	1.40
20	D	406	CLA	CMD-C2D	-2.33	1.45	1.50
20	C	504	CLA	C3B-C2B	-2.33	1.37	1.40
20	B	615	CLA	OBD-CAD	-2.32	1.18	1.22
20	B	605	CLA	C3B-C2B	-2.31	1.37	1.40
20	B	617	CLA	CMD-C2D	-2.31	1.45	1.50
20	C	510	CLA	C3B-CAB	-2.31	1.43	1.47
20	C	504	CLA	C3D-C2D	-2.31	1.32	1.39
20	B	605	CLA	CMC-C2C	-2.30	1.45	1.50
21	H	101	BCR	C1-C6	-2.30	1.50	1.53
20	C	502	CLA	C3B-CAB	-2.29	1.43	1.47
20	C	511	CLA	CMD-C2D	-2.29	1.46	1.50
20	C	513	CLA	C3B-C2B	-2.29	1.37	1.40
20	C	503	CLA	C3B-C2B	-2.28	1.37	1.40
20	B	614	CLA	C1C-C2C	2.28	1.49	1.44
20	B	606	CLA	C3D-C2D	-2.27	1.32	1.39
20	C	515	CLA	CMB-C2B	-2.27	1.46	1.51
20	A	406	CLA	C4D-ND	-2.27	1.34	1.37
20	B	602	CLA	CHC-C1C	2.27	1.40	1.35
20	B	603	CLA	CMD-C2D	-2.26	1.46	1.50
20	B	610	CLA	C4C-C3C	2.26	1.48	1.45
20	B	614	CLA	C1B-NB	2.26	1.37	1.35
20	B	617	CLA	C3B-C2B	-2.25	1.37	1.40
20	B	604	CLA	C3B-C2B	-2.25	1.37	1.40
20	B	607	CLA	MG-ND	-2.24	2.01	2.05
20	C	515	CLA	CMD-C2D	-2.24	1.46	1.50
20	C	511	CLA	C1B-NB	2.24	1.37	1.35
20	A	406	CLA	MG-ND	-2.23	2.01	2.05
20	C	508	CLA	C3D-C4D	2.23	1.49	1.44
20	B	617	CLA	CMB-C2B	-2.23	1.47	1.51
20	B	617	CLA	C1D-C2D	2.22	1.49	1.45
20	B	608	CLA	MG-NC	2.22	2.11	2.06
20	C	508	CLA	C3B-CAB	-2.22	1.43	1.47
20	C	513	CLA	C1D-C2D	2.21	1.49	1.45
20	C	506	CLA	C3D-C4D	2.21	1.49	1.44
20	C	512	CLA	C3D-C2D	-2.20	1.33	1.39
24	D	402	LMG	C9-C8	2.20	1.57	1.50
20	C	512	CLA	C3D-C4D	2.20	1.49	1.44
20	B	612	CLA	C1D-C2D	2.20	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	601	LMG	C4-C5	2.20	1.57	1.53
26	E	101	HEM	C4A-CHB	-2.20	1.34	1.41
20	A	408	CLA	C1B-NB	2.19	1.37	1.35
20	A	406	CLA	C1B-NB	2.19	1.37	1.35
20	C	503	CLA	CMD-C2D	-2.19	1.46	1.50
20	B	610	CLA	MG-ND	-2.18	2.01	2.05
20	B	606	CLA	C1C-C2C	2.18	1.48	1.44
21	Z	101	BCR	C1-C6	-2.18	1.50	1.53
20	A	407	CLA	C4D-ND	-2.18	1.34	1.37
20	A	408	CLA	C3C-C2C	2.18	1.41	1.36
20	C	502	CLA	MG-ND	-2.18	2.01	2.05
19	A	404	PHO	CMB-C2B	-2.17	1.46	1.51
24	I	101	LMG	C9-C8	2.17	1.57	1.50
20	A	405	CLA	CMD-C2D	-2.17	1.46	1.50
20	A	406	CLA	C3B-CAB	-2.16	1.43	1.47
20	B	605	CLA	MG-ND	-2.16	2.01	2.05
19	A	404	PHO	CMC-C2C	-2.16	1.46	1.51
20	B	611	CLA	MG-ND	-2.15	2.01	2.05
20	B	615	CLA	CMD-C2D	-2.15	1.46	1.50
20	C	507	CLA	C1D-C2D	2.15	1.49	1.45
20	D	406	CLA	C1B-NB	2.15	1.37	1.35
20	B	610	CLA	OBD-CAD	-2.15	1.18	1.22
20	B	613	CLA	C3D-C2D	-2.14	1.33	1.39
20	C	505	CLA	C3D-C2D	-2.14	1.33	1.39
20	B	604	CLA	C3B-CAB	-2.14	1.43	1.47
20	B	616	CLA	C4D-ND	-2.14	1.34	1.37
20	C	505	CLA	CMC-C2C	-2.13	1.46	1.50
20	C	510	CLA	C3D-C4D	2.12	1.48	1.44
20	B	615	CLA	MG-NC	2.12	2.11	2.06
20	B	615	CLA	C1B-NB	2.11	1.37	1.35
20	C	510	CLA	CMD-C2D	-2.11	1.46	1.50
24	D	403	LMG	C3-C2	2.11	1.57	1.52
22	A	410	LHG	P-O6	2.11	1.67	1.59
20	C	513	CLA	CBD-CGD	-2.11	1.45	1.52
25	D	404	PL9	C53-C6	-2.10	1.46	1.50
25	D	404	PL9	C33-C34	2.10	1.38	1.33
20	D	406	CLA	CMC-C2C	-2.10	1.46	1.50
20	B	611	CLA	CMB-C2B	-2.10	1.47	1.51
20	A	407	CLA	C1B-NB	2.10	1.37	1.35
20	B	603	CLA	CMB-C2B	-2.09	1.47	1.51
20	C	509	CLA	C3B-CAB	-2.09	1.43	1.47
20	B	616	CLA	C3B-CAB	-2.09	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	511	CLA	CHD-C4C	2.09	1.44	1.39
20	B	617	CLA	MG-NA	2.09	2.11	2.06
20	C	502	CLA	CMB-C2B	-2.09	1.47	1.51
24	D	401	LMG	C9-C8	2.09	1.57	1.50
26	E	101	HEM	CAA-C2A	2.09	1.55	1.52
20	B	617	CLA	C3B-CAB	-2.09	1.43	1.47
20	C	512	CLA	C3B-C2B	-2.08	1.37	1.40
20	B	604	CLA	CMB-C2B	-2.08	1.47	1.51
20	C	508	CLA	CMC-C2C	-2.08	1.46	1.50
26	E	101	HEM	CAB-C3B	2.08	1.53	1.47
20	A	408	CLA	C1D-C2D	2.08	1.49	1.45
20	C	507	CLA	C1B-NB	2.08	1.37	1.35
20	B	617	CLA	CMC-C2C	-2.08	1.46	1.50
20	B	603	CLA	C1D-C2D	2.08	1.49	1.45
20	C	512	CLA	C3B-CAB	-2.08	1.43	1.47
20	B	617	CLA	MG-NC	2.07	2.11	2.06
20	C	507	CLA	OBD-CAD	-2.07	1.18	1.22
20	B	609	CLA	MG-NC	2.07	2.11	2.06
20	B	607	CLA	C3B-CAB	-2.07	1.43	1.47
20	C	513	CLA	CMD-C2D	-2.07	1.46	1.50
20	B	602	CLA	OBD-CAD	-2.07	1.18	1.22
20	C	513	CLA	C1C-C2C	2.07	1.48	1.44
20	C	508	CLA	CMD-C2D	-2.06	1.46	1.50
20	C	503	CLA	C3B-CAB	-2.06	1.43	1.47
20	B	610	CLA	CMB-C2B	-2.06	1.47	1.51
20	B	614	CLA	CMB-C2B	-2.06	1.47	1.51
24	C	501	LMG	C7-C8	2.06	1.57	1.50
20	C	503	CLA	CMC-C2C	-2.05	1.46	1.50
19	D	405	PHO	C1C-NC	-2.04	1.32	1.38
20	B	606	CLA	MG-NA	2.04	2.11	2.06
20	B	606	CLA	CMB-C2B	-2.03	1.47	1.51
20	B	602	CLA	CMD-C2D	-2.02	1.46	1.50
20	B	603	CLA	C3D-C2D	-2.02	1.33	1.39
26	E	101	HEM	CMB-C2B	2.02	1.55	1.50
25	D	404	PL9	C38-C39	2.01	1.37	1.33
20	C	504	CLA	CMB-C2B	-2.00	1.47	1.51
19	D	405	PHO	C3B-C2B	-2.00	1.37	1.40
20	C	511	CLA	MG-NA	2.00	2.11	2.06

All (678) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	503	CLA	C4A-NA-C1A	10.38	111.37	106.71
20	B	612	CLA	C4A-NA-C1A	9.87	111.14	106.71
20	B	602	CLA	C4D-C3D-CAD	9.79	119.64	108.10
20	B	617	CLA	C4D-C3D-CAD	9.50	119.29	108.10
20	C	506	CLA	C4A-NA-C1A	9.20	110.84	106.71
20	B	604	CLA	C4A-NA-C1A	9.15	110.82	106.71
20	B	617	CLA	C4A-NA-C1A	8.88	110.70	106.71
20	B	602	CLA	C4A-NA-C1A	8.81	110.67	106.71
20	C	511	CLA	C4D-C3D-CAD	8.76	118.42	108.10
20	C	512	CLA	C4D-C3D-CAD	8.37	117.96	108.10
20	B	614	CLA	C4A-NA-C1A	8.33	110.45	106.71
20	B	603	CLA	C4D-C3D-CAD	8.28	117.86	108.10
20	C	515	CLA	C4A-NA-C1A	8.15	110.37	106.71
20	B	610	CLA	C4D-C3D-CAD	8.14	117.69	108.10
20	B	612	CLA	C4D-C3D-CAD	7.66	117.13	108.10
20	B	606	CLA	C4A-NA-C1A	7.65	110.15	106.71
20	C	515	CLA	C4D-C3D-CAD	7.62	117.08	108.10
20	B	603	CLA	C4A-NA-C1A	7.61	110.13	106.71
20	B	611	CLA	C4D-C3D-CAD	7.49	116.93	108.10
20	A	407	CLA	C4A-NA-C1A	7.49	110.07	106.71
20	C	508	CLA	C4A-NA-C1A	7.46	110.06	106.71
20	B	615	CLA	C4D-C3D-CAD	7.40	116.81	108.10
20	C	512	CLA	C4A-NA-C1A	7.40	110.03	106.71
20	C	506	CLA	C4D-C3D-CAD	7.30	116.70	108.10
20	C	511	CLA	C4A-NA-C1A	7.19	109.94	106.71
20	B	602	CLA	C1D-ND-C4D	-7.12	101.28	106.33
20	C	509	CLA	C4D-C3D-CAD	7.08	116.44	108.10
20	B	616	CLA	C4D-C3D-CAD	6.96	116.30	108.10
20	B	613	CLA	C4D-C3D-CAD	6.95	116.29	108.10
20	B	610	CLA	C2D-C1D-ND	-6.84	105.06	110.10
20	B	611	CLA	C4A-NA-C1A	6.84	109.78	106.71
20	B	615	CLA	C4A-NA-C1A	6.80	109.77	106.71
20	B	609	CLA	C4A-NA-C1A	6.70	109.72	106.71
20	C	508	CLA	C4D-C3D-CAD	6.66	115.94	108.10
20	C	506	CLA	CAA-C2A-C1A	-6.53	90.58	111.97
20	C	513	CLA	C4D-C3D-CAD	6.47	115.72	108.10
20	B	610	CLA	C3D-C2D-C1D	6.36	114.52	105.83
20	B	614	CLA	C4D-C3D-CAD	6.35	115.58	108.10
20	B	604	CLA	C4D-C3D-CAD	6.35	115.58	108.10
20	C	504	CLA	C4D-C3D-CAD	6.32	115.54	108.10
20	B	607	CLA	C4A-NA-C1A	6.31	109.54	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	507	CLA	C4D-C3D-CAD	6.21	115.42	108.10
20	B	605	CLA	C4A-NA-C1A	6.15	109.47	106.71
20	C	502	CLA	C4A-NA-C1A	6.15	109.47	106.71
20	B	605	CLA	C4D-C3D-CAD	6.11	115.30	108.10
20	C	507	CLA	C2D-C1D-ND	-6.05	105.64	110.10
20	B	616	CLA	C4A-NA-C1A	6.01	109.41	106.71
20	B	606	CLA	C4D-C3D-CAD	5.99	115.16	108.10
20	C	507	CLA	C4A-NA-C1A	5.98	109.40	106.71
20	B	610	CLA	C4A-NA-C1A	5.96	109.39	106.71
20	B	613	CLA	C4A-NA-C1A	5.82	109.32	106.71
20	C	506	CLA	C3A-C2A-C1A	5.80	110.03	101.34
20	C	504	CLA	C4A-NA-C1A	5.70	109.27	106.71
20	B	608	CLA	C4A-NA-C1A	5.67	109.25	106.71
20	C	509	CLA	C4A-NA-C1A	5.56	109.21	106.71
20	C	505	CLA	C4A-NA-C1A	5.48	109.17	106.71
20	C	505	CLA	C4D-C3D-CAD	5.32	114.37	108.10
20	B	609	CLA	C4D-C3D-CAD	5.31	114.35	108.10
20	A	405	CLA	C2D-C1D-ND	-5.24	106.24	110.10
20	B	611	CLA	OBD-CAD-C3D	5.14	140.89	128.52
20	D	406	CLA	C4A-NA-C1A	5.05	108.98	106.71
20	C	504	CLA	CMD-C2D-C1D	5.01	133.55	124.71
20	C	503	CLA	C4D-C3D-CAD	4.98	113.97	108.10
20	C	502	CLA	C4D-C3D-CAD	4.90	113.87	108.10
25	D	404	PL9	C7-C3-C4	4.89	120.85	116.88
20	C	506	CLA	C3D-C4D-ND	4.87	118.11	110.24
20	D	406	CLA	C4D-C3D-CAD	4.86	113.82	108.10
20	B	608	CLA	C4D-C3D-CAD	4.83	113.79	108.10
20	B	606	CLA	CMD-C2D-C1D	4.77	133.13	124.71
20	B	611	CLA	O2A-C1-C2	-4.76	96.14	108.64
20	C	513	CLA	CMB-C2B-C1B	-4.75	121.17	128.46
20	C	510	CLA	C4D-C3D-CAD	4.72	113.65	108.10
20	D	407	CLA	CMD-C2D-C1D	4.69	132.97	124.71
20	B	615	CLA	C3D-C2D-C1D	4.69	112.23	105.83
20	A	406	CLA	C4A-NA-C1A	4.64	108.79	106.71
20	B	608	CLA	CAA-C2A-C1A	-4.62	96.85	111.97
20	C	513	CLA	C3B-C4B-NB	-4.59	103.27	109.21
20	B	608	CLA	C3A-C2A-C1A	4.58	108.19	101.34
20	C	507	CLA	C3D-C2D-C1D	4.55	112.04	105.83
20	B	607	CLA	C4D-C3D-CAD	4.54	113.45	108.10
20	D	407	CLA	C6-C5-C3	4.53	125.34	113.45
20	C	515	CLA	C3D-C4D-ND	4.51	117.53	110.24
20	D	406	CLA	C2D-C1D-ND	-4.48	106.80	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	412	BCT	O2-C-O1	4.47	131.15	119.55
20	C	506	CLA	CMB-C2B-C1B	-4.45	121.62	128.46
20	C	511	CLA	C2D-C1D-ND	-4.42	106.85	110.10
20	B	612	CLA	C3D-C2D-C1D	4.40	111.84	105.83
20	B	615	CLA	C3D-C4D-ND	4.37	117.31	110.24
20	C	509	CLA	C2D-C1D-ND	-4.37	106.88	110.10
20	B	616	CLA	OBD-CAD-C3D	4.35	139.00	128.52
20	A	406	CLA	O2A-C1-C2	-4.33	97.26	108.64
20	C	513	CLA	C2D-C1D-ND	-4.29	106.94	110.10
20	C	510	CLA	OBD-CAD-C3D	4.29	138.84	128.52
20	B	611	CLA	C6-C7-C8	-4.28	102.08	115.92
20	B	615	CLA	CAA-C2A-C1A	-4.26	98.01	111.97
20	C	511	CLA	C3D-C2D-C1D	4.26	111.64	105.83
24	B	601	LMG	C1-C2-C3	-4.25	101.14	110.00
20	C	509	CLA	C3D-C2D-C1D	4.25	111.63	105.83
20	A	406	CLA	C4D-C3D-CAD	4.23	113.08	108.10
20	B	606	CLA	CAA-C2A-C1A	-4.22	98.15	111.97
20	C	504	CLA	OBD-CAD-C3D	4.21	138.65	128.52
20	B	613	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
20	B	610	CLA	CAC-C3C-C4C	4.13	130.16	124.81
20	B	608	CLA	CMA-C3A-C4A	4.13	122.86	111.77
20	B	612	CLA	C3D-C4D-ND	4.12	116.91	110.24
20	C	511	CLA	C3D-C4D-ND	4.09	116.86	110.24
20	B	615	CLA	C2D-C1D-ND	-4.09	107.09	110.10
20	C	515	CLA	C1D-ND-C4D	-4.04	103.47	106.33
20	B	612	CLA	C2D-C1D-ND	-4.04	107.13	110.10
20	C	505	CLA	CGD-CBD-CAD	4.03	123.80	110.73
20	B	603	CLA	OBD-CAD-C3D	4.00	138.15	128.52
20	B	602	CLA	OBD-CAD-C3D	4.00	138.15	128.52
20	C	506	CLA	C3D-C2D-C1D	3.97	111.25	105.83
20	A	405	CLA	C4D-C3D-CAD	3.97	112.77	108.10
20	B	604	CLA	CMD-C2D-C1D	3.96	131.69	124.71
20	B	613	CLA	OBD-CAD-C3D	3.91	137.92	128.52
21	F	101	BCR	C32-C1-C6	3.90	116.63	110.30
20	C	506	CLA	C2D-C1D-ND	-3.89	107.24	110.10
20	C	508	CLA	OBD-CAD-C3D	3.88	137.86	128.52
20	C	511	CLA	CMD-C2D-C3D	-3.87	118.70	127.61
20	C	515	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
20	C	511	CLA	CHD-C1D-ND	-3.87	120.90	124.45
20	A	407	CLA	CAA-C2A-C1A	-3.86	99.34	111.97
20	A	407	CLA	C4D-C3D-CAD	3.86	112.64	108.10
20	C	513	CLA	C3D-C2D-C1D	3.85	111.08	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	617	CLA	CMD-C2D-C3D	-3.84	118.77	127.61
20	A	408	CLA	CMD-C2D-C1D	3.84	131.47	124.71
20	B	603	CLA	CMD-C2D-C1D	3.82	131.45	124.71
20	D	406	CLA	C1-C2-C3	3.81	132.64	126.04
20	C	507	CLA	C3D-C4D-ND	3.81	116.40	110.24
21	C	514	BCR	C2-C1-C6	3.81	116.34	110.48
20	B	603	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
20	A	405	CLA	CAC-C3C-C4C	3.78	129.71	124.81
20	C	503	CLA	CAA-C2A-C1A	-3.77	99.62	111.97
21	H	101	BCR	C1-C6-C5	-3.77	117.30	122.61
21	B	618	BCR	C8-C7-C6	-3.77	116.62	127.20
20	B	608	CLA	OBD-CAD-C3D	3.76	137.57	128.52
20	B	609	CLA	C3D-C4D-ND	3.76	116.32	110.24
20	A	407	CLA	CHD-C1D-ND	-3.76	121.00	124.45
20	D	407	CLA	CMB-C2B-C1B	-3.75	122.69	128.46
20	C	507	CLA	C6-C7-C8	-3.74	103.82	115.92
20	C	510	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
20	B	614	CLA	C3D-C4D-ND	3.74	116.29	110.24
24	D	403	LMG	C8-O7-C10	3.74	126.99	117.79
20	C	502	CLA	O2A-C1-C2	-3.72	98.87	108.64
20	B	603	CLA	CMB-C2B-C3B	3.71	131.62	124.68
20	C	515	CLA	C3D-C2D-C1D	3.68	110.86	105.83
21	C	516	BCR	C2-C1-C6	3.67	116.14	110.48
20	B	603	CLA	O2D-CGD-O1D	-3.64	116.72	123.84
20	C	507	CLA	CAA-C2A-C1A	-3.64	100.06	111.97
20	D	407	CLA	C3B-C4B-NB	-3.63	104.52	109.21
20	A	405	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
20	C	513	CLA	CMB-C2B-C3B	3.61	131.44	124.68
20	B	616	CLA	C2A-C1A-CHA	3.61	130.18	123.86
20	B	617	CLA	CMD-C2D-C1D	3.61	131.07	124.71
20	A	407	CLA	CMD-C2D-C1D	3.59	131.04	124.71
20	C	512	CLA	C3B-C4B-NB	-3.56	104.60	109.21
20	C	509	CLA	C3D-C4D-ND	3.54	115.97	110.24
20	C	503	CLA	O2D-CGD-O1D	-3.52	116.96	123.84
20	C	502	CLA	C3B-C4B-NB	-3.51	104.67	109.21
20	C	505	CLA	O2A-C1-C2	-3.51	99.41	108.64
20	C	512	CLA	C6-C7-C8	-3.50	104.60	115.92
19	A	404	PHO	C6-C5-C3	3.50	122.63	113.45
20	B	603	CLA	C3A-C2A-C1A	3.49	106.56	101.34
20	D	407	CLA	CHA-C1A-NA	-3.48	118.42	126.40
20	C	512	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
20	C	504	CLA	C4-C3-C5	3.47	121.11	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	405	CLA	C3B-C4B-NB	-3.46	104.74	109.21
20	A	406	CLA	C2D-C1D-ND	-3.45	107.56	110.10
25	D	404	PL9	C20-C19-C21	3.45	121.07	115.27
20	C	502	CLA	CAA-C2A-C1A	-3.44	100.71	111.97
20	C	505	CLA	C3A-C2A-C1A	3.44	106.49	101.34
20	B	607	CLA	CMD-C2D-C1D	3.43	130.75	124.71
20	C	506	CLA	C1B-CHB-C4A	-3.42	123.34	130.12
20	C	509	CLA	O2A-C1-C2	-3.42	99.65	108.64
20	B	610	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
20	C	505	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
20	B	602	CLA	C2A-C1A-CHA	3.39	129.78	123.86
26	E	101	HEM	CBA-CAA-C2A	3.36	118.35	112.62
20	B	610	CLA	C3D-C4D-ND	3.36	115.67	110.24
20	C	512	CLA	OBD-CAD-C3D	3.36	136.60	128.52
20	C	502	CLA	C3A-C2A-C1A	3.36	106.37	101.34
20	B	604	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
20	C	505	CLA	C3B-C4B-NB	-3.34	104.89	109.21
20	B	606	CLA	OBD-CAD-C3D	3.34	136.55	128.52
20	B	611	CLA	C3B-C4B-NB	-3.34	104.90	109.21
20	B	616	CLA	C6-C7-C8	3.32	126.65	115.92
21	K	101	BCR	C2-C1-C6	3.31	115.58	110.48
20	C	515	CLA	CMB-C2B-C3B	3.31	130.88	124.68
20	B	602	CLA	C9-C8-C10	3.31	123.27	111.29
20	C	512	CLA	O2A-C1-C2	-3.30	99.97	108.64
20	B	607	CLA	CAA-C2A-C3A	3.29	121.79	112.78
20	B	607	CLA	C3B-C4B-NB	-3.29	104.96	109.21
21	B	620	BCR	C38-C26-C25	-3.28	120.84	124.53
20	C	508	CLA	C1D-ND-C4D	-3.28	104.00	106.33
20	C	506	CLA	C2A-C1A-CHA	-3.28	118.12	123.86
20	D	407	CLA	C4D-CHA-C1A	3.28	125.24	121.25
21	B	620	BCR	C32-C1-C6	-3.28	104.99	110.30
20	C	515	CLA	C6-C5-C3	3.27	122.04	113.45
20	B	604	CLA	C1D-ND-C4D	-3.26	104.02	106.33
20	B	614	CLA	C3D-C2D-C1D	3.25	110.26	105.83
20	C	512	CLA	O1D-CGD-CBD	3.24	131.12	124.48
20	A	408	CLA	O2A-C1-C2	-3.24	100.11	108.64
24	D	402	LMG	C8-O7-C10	3.24	125.76	117.79
20	B	616	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
24	I	101	LMG	C3-C4-C5	-3.22	104.49	110.24
19	A	404	PHO	C3D-CAD-CBD	-3.22	103.37	107.61
20	B	609	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
21	C	514	BCR	C1-C6-C5	-3.21	118.09	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	410	LHG	O4-P-O5	3.21	128.09	112.24
22	A	411	LHG	O4-P-O5	3.21	128.09	112.24
20	C	506	CLA	C6-C7-C8	-3.20	105.56	115.92
20	B	608	CLA	CBA-CAA-C2A	3.20	123.32	113.86
20	A	407	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
20	C	502	CLA	CMD-C2D-C1D	3.18	130.31	124.71
20	C	505	CLA	CAA-C2A-C1A	-3.18	101.57	111.97
20	C	511	CLA	CHD-C1D-C2D	3.17	132.14	125.48
20	A	407	CLA	CHB-C4A-NA	3.17	128.90	124.51
20	B	614	CLA	C11-C10-C8	3.17	126.18	115.92
20	B	605	CLA	CMD-C2D-C1D	3.17	130.30	124.71
20	B	610	CLA	CHD-C1D-ND	3.16	127.36	124.45
20	B	611	CLA	C2D-C1D-ND	-3.16	107.78	110.10
20	C	512	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
20	B	606	CLA	CMC-C2C-C1C	3.15	129.84	125.04
20	C	513	CLA	C4A-NA-C1A	3.15	108.12	106.71
20	B	605	CLA	C11-C10-C8	3.14	126.07	115.92
20	C	502	CLA	CAC-C3C-C4C	3.14	128.88	124.81
20	C	504	CLA	CAA-C2A-C1A	-3.13	101.72	111.97
20	C	511	CLA	O1D-CGD-CBD	3.12	130.87	124.48
20	A	406	CLA	C9-C8-C7	3.12	122.59	111.29
20	B	603	CLA	C11-C10-C8	3.11	125.99	115.92
20	C	513	CLA	C3D-C4D-ND	3.10	115.25	110.24
20	C	505	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
20	D	407	CLA	C2A-C1A-CHA	3.10	129.28	123.86
20	B	613	CLA	CMB-C2B-C3B	3.10	130.47	124.68
20	B	608	CLA	C6-C5-C3	3.07	121.50	113.45
21	C	516	BCR	C40-C30-C25	3.07	115.28	110.30
20	B	615	CLA	C11-C10-C8	3.06	125.82	115.92
20	C	505	CLA	OBD-CAD-C3D	3.06	135.89	128.52
20	A	407	CLA	C6-C7-C8	-3.05	106.06	115.92
20	D	406	CLA	CAA-C2A-C1A	-3.05	101.99	111.97
20	A	408	CLA	C4A-NA-C1A	3.05	108.08	106.71
20	C	510	CLA	C3B-C4B-NB	-3.04	105.28	109.21
20	C	506	CLA	CBA-CAA-C2A	3.04	122.83	113.86
21	K	101	BCR	C7-C8-C9	-3.01	121.68	126.23
20	C	510	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
20	C	508	CLA	CMD-C2D-C1D	3.00	130.00	124.71
20	C	512	CLA	C3A-C2A-C1A	2.99	105.82	101.34
20	C	506	CLA	C3B-C4B-NB	-2.99	105.34	109.21
20	C	504	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
21	C	514	BCR	C39-C30-C25	2.98	115.14	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	505	CLA	CMD-C2D-C1D	2.98	129.97	124.71
20	B	602	CLA	C6-C5-C3	2.98	121.27	113.45
20	B	609	CLA	C3D-C2D-C1D	2.98	109.89	105.83
20	B	612	CLA	C9-C8-C10	2.97	122.06	111.29
20	B	602	CLA	CMD-C2D-C1D	2.97	129.94	124.71
20	B	617	CLA	O2A-C1-C2	-2.96	100.85	108.64
20	B	611	CLA	C1-O2A-CGA	2.96	124.21	116.44
20	B	614	CLA	C3A-C2A-C1A	2.95	105.76	101.34
25	D	404	PL9	C36-C34-C33	-2.95	115.15	121.12
21	B	620	BCR	C2-C1-C6	2.95	115.02	110.48
20	A	408	CLA	CHA-C1A-NA	-2.94	119.65	126.40
20	B	608	CLA	O2D-CGD-CBD	2.94	116.49	111.27
20	D	406	CLA	C3D-C4D-ND	2.93	114.98	110.24
20	B	614	CLA	C3B-C4B-NB	-2.92	105.43	109.21
20	C	502	CLA	CMA-C3A-C4A	2.92	119.63	111.77
21	B	618	BCR	C39-C30-C25	2.91	115.02	110.30
20	C	506	CLA	CMA-C3A-C4A	2.91	119.58	111.77
20	D	407	CLA	C2C-C1C-NC	2.90	112.69	109.97
20	B	603	CLA	CMD-C2D-C3D	-2.90	120.94	127.61
20	C	504	CLA	CMD-C2D-C3D	-2.90	120.94	127.61
20	A	408	CLA	C6-C5-C3	2.90	121.06	113.45
20	B	617	CLA	C3D-C2D-C1D	2.89	109.78	105.83
20	C	515	CLA	O2D-CGD-CBD	2.89	116.41	111.27
20	A	407	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
20	B	602	CLA	C3D-C4D-ND	2.89	114.91	110.24
20	B	605	CLA	CGD-CBD-CAD	2.89	120.08	110.73
20	B	602	CLA	CAC-C3C-C4C	2.88	128.55	124.81
20	B	610	CLA	C11-C10-C8	2.88	125.24	115.92
24	B	601	LMG	C1-O6-C5	-2.88	108.03	113.69
20	B	617	CLA	O1D-CGD-CBD	2.88	130.37	124.48
20	B	617	CLA	OBD-CAD-C3D	2.87	135.43	128.52
20	C	510	CLA	CAC-C3C-C4C	2.87	128.53	124.81
20	C	506	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
20	B	610	CLA	C4-C3-C5	2.86	120.08	115.27
20	B	617	CLA	CHB-C4A-NA	2.85	128.46	124.51
20	C	515	CLA	C6-C7-C8	-2.85	106.72	115.92
20	D	406	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
20	C	503	CLA	CGD-CBD-CAD	2.84	119.95	110.73
20	B	605	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
20	B	612	CLA	C6-C7-C8	-2.84	106.75	115.92
20	A	407	CLA	C3D-C4D-ND	2.84	114.82	110.24
20	D	406	CLA	C3A-C2A-C1A	2.83	105.58	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	504	CLA	C1D-ND-C4D	-2.83	104.32	106.33
20	B	603	CLA	C1-C2-C3	2.83	130.94	126.04
20	C	510	CLA	C4A-NA-C1A	2.83	107.98	106.71
20	B	612	CLA	CMA-C3A-C4A	-2.83	104.17	111.77
20	D	406	CLA	C3D-C2D-C1D	2.82	109.69	105.83
20	B	602	CLA	C2D-C1D-ND	2.82	112.18	110.10
20	B	604	CLA	C9-C8-C7	2.82	121.50	111.29
21	K	101	BCR	C31-C1-C6	-2.81	105.73	110.30
20	B	608	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
20	B	604	CLA	O2D-CGD-CBD	2.81	116.26	111.27
20	A	407	CLA	CMD-C2D-C3D	-2.81	121.16	127.61
20	C	503	CLA	C3A-C2A-C1A	2.80	105.54	101.34
20	C	511	CLA	CMD-C2D-C1D	2.80	129.64	124.71
20	C	506	CLA	CMB-C2B-C3B	2.80	129.91	124.68
19	A	404	PHO	C6-C7-C8	2.79	124.95	115.92
20	B	602	CLA	CMD-C2D-C3D	-2.79	121.19	127.61
20	A	407	CLA	C11-C10-C8	2.79	124.94	115.92
20	C	506	CLA	C1D-ND-C4D	-2.79	104.36	106.33
20	A	405	CLA	CHD-C4C-C3C	2.79	128.94	124.84
25	D	404	PL9	C37-C38-C39	-2.78	120.96	127.66
20	C	510	CLA	C2D-C1D-ND	-2.78	108.05	110.10
26	E	101	HEM	CAA-CBA-CGA	-2.78	105.96	113.76
25	D	404	PL9	C21-C19-C18	-2.78	115.50	121.12
20	A	407	CLA	CMC-C2C-C1C	2.78	129.27	125.04
20	C	510	CLA	CMD-C2D-C1D	2.77	129.59	124.71
20	B	610	CLA	CHD-C4C-NC	-2.76	119.86	124.20
20	B	610	CLA	C5-C3-C2	-2.76	115.53	121.12
20	B	608	CLA	CMD-C2D-C1D	2.76	129.57	124.71
21	Z	101	BCR	C33-C5-C6	-2.75	121.44	124.53
20	B	613	CLA	CED-O2D-CGD	2.75	122.15	115.94
20	B	613	CLA	CMD-C2D-C1D	2.74	129.55	124.71
19	D	405	PHO	C3D-CAD-CBD	-2.74	104.00	107.61
20	B	606	CLA	C1B-CHB-C4A	-2.73	124.70	130.12
25	D	404	PL9	C7-C3-C2	-2.73	119.71	123.30
20	D	406	CLA	CHD-C1D-ND	-2.73	121.94	124.45
20	C	509	CLA	C3B-C4B-NB	-2.73	105.68	109.21
20	C	503	CLA	O2D-CGD-CBD	2.73	116.11	111.27
21	K	101	BCR	C34-C9-C10	-2.72	119.11	122.92
20	B	611	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
20	B	617	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
20	C	503	CLA	CAC-C3C-C4C	2.72	128.34	124.81
20	C	508	CLA	CMB-C2B-C1B	-2.71	124.30	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	513	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
20	C	506	CLA	O1D-CGD-CBD	2.70	130.01	124.48
20	B	605	CLA	C6-C5-C3	2.70	120.53	113.45
20	C	508	CLA	C3B-C4B-NB	-2.69	105.73	109.21
20	C	510	CLA	O2A-C1-C2	-2.69	101.56	108.64
20	B	616	CLA	O2A-C1-C2	-2.69	101.56	108.64
20	B	608	CLA	C3B-C4B-NB	-2.69	105.73	109.21
20	A	406	CLA	CMB-C2B-C1B	-2.69	124.33	128.46
20	B	603	CLA	C2A-C1A-CHA	2.68	128.55	123.86
20	C	510	CLA	CHA-C1A-NA	-2.68	120.27	126.40
20	C	507	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
20	B	604	CLA	CAC-C3C-C2C	-2.67	122.97	127.53
20	A	408	CLA	C2A-C1A-CHA	2.66	128.51	123.86
20	B	616	CLA	CHA-C1A-NA	-2.66	120.31	126.40
20	B	606	CLA	CED-O2D-CGD	2.66	121.95	115.94
20	B	616	CLA	CMD-C2D-C1D	2.65	129.39	124.71
20	B	616	CLA	CMB-C2B-C3B	2.65	129.64	124.68
20	A	406	CLA	CBA-CAA-C2A	2.65	121.69	113.86
20	B	608	CLA	CAA-C2A-C3A	-2.65	105.52	112.78
20	B	615	CLA	CAC-C3C-C4C	2.65	128.24	124.81
20	B	610	CLA	C3A-C2A-C1A	2.64	105.29	101.34
19	A	404	PHO	C9-C8-C7	2.63	120.83	111.29
20	A	406	CLA	CMC-C2C-C1C	2.63	129.05	125.04
24	B	601	LMG	C3-C4-C5	-2.63	105.54	110.24
20	B	604	CLA	C3C-C4C-NC	-2.63	107.62	110.57
20	B	613	CLA	C6-C7-C8	-2.63	107.43	115.92
20	A	408	CLA	CAA-C2A-C1A	-2.63	103.37	111.97
20	C	504	CLA	CMA-C3A-C4A	2.63	118.83	111.77
20	B	604	CLA	C4-C3-C5	2.63	119.69	115.27
21	C	514	BCR	C3-C4-C5	-2.62	109.40	114.08
20	C	505	CLA	CMB-C2B-C3B	2.62	129.58	124.68
20	D	406	CLA	CHD-C1D-C2D	2.62	130.97	125.48
20	C	508	CLA	C3A-C2A-C1A	2.62	105.26	101.34
20	C	508	CLA	CMB-C2B-C3B	2.61	129.56	124.68
20	B	606	CLA	CMD-C2D-C3D	-2.59	121.65	127.61
20	B	617	CLA	C2D-C1D-ND	-2.59	108.19	110.10
20	B	606	CLA	C1D-ND-C4D	-2.59	104.49	106.33
20	B	610	CLA	C9-C8-C10	2.59	120.67	111.29
20	B	602	CLA	C3A-C2A-C1A	2.59	105.22	101.34
20	C	509	CLA	C9-C8-C7	2.59	120.66	111.29
21	F	101	BCR	C40-C30-C25	-2.59	106.10	110.30
20	D	406	CLA	CAC-C3C-C4C	2.58	128.16	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	512	CLA	C9-C8-C10	2.58	120.63	111.29
20	C	510	CLA	C6-C5-C3	-2.58	106.70	113.45
20	C	505	CLA	CBC-CAC-C3C	2.57	119.51	112.43
20	C	503	CLA	CHB-C4A-NA	2.57	128.06	124.51
20	B	609	CLA	C11-C10-C8	2.57	124.22	115.92
20	B	616	CLA	CMD-C2D-C3D	-2.57	121.71	127.61
19	A	404	PHO	C1B-NB-C4B	2.56	112.36	107.09
20	B	608	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
20	C	507	CLA	C3B-C4B-NB	-2.55	105.91	109.21
24	I	101	LMG	O6-C1-O1	-2.55	103.92	109.97
20	A	405	CLA	C3D-C2D-C1D	2.55	109.31	105.83
20	A	406	CLA	O1D-CGD-CBD	2.55	129.70	124.48
26	E	101	HEM	CHC-C4B-C3B	2.54	128.46	124.57
20	C	509	CLA	O2A-CGA-O1A	-2.54	117.17	123.59
20	A	405	CLA	CAA-C2A-C1A	-2.54	103.65	111.97
20	D	406	CLA	C9-C8-C7	2.54	120.48	111.29
24	D	403	LMG	C3-C4-C5	-2.54	105.71	110.24
20	B	606	CLA	C3A-C2A-C1A	2.54	105.14	101.34
20	A	406	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
20	B	605	CLA	OBD-CAD-C3D	2.52	134.59	128.52
21	Z	101	BCR	C30-C25-C26	-2.52	119.07	122.61
20	B	605	CLA	C4-C3-C5	2.51	119.50	115.27
20	B	612	CLA	C4-C3-C5	2.51	119.50	115.27
20	B	602	CLA	CMC-C2C-C1C	2.51	128.87	125.04
20	B	604	CLA	OBD-CAD-C3D	2.50	134.54	128.52
20	C	505	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
20	C	506	CLA	C4D-CHA-C1A	-2.50	118.21	121.25
20	D	406	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
21	K	101	BCR	C33-C5-C6	-2.49	121.73	124.53
24	M	101	LMG	C1-O6-C5	-2.49	108.80	113.69
20	A	405	CLA	C3D-C4D-ND	2.49	114.26	110.24
20	A	406	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
20	B	607	CLA	O1D-CGD-CBD	2.48	129.55	124.48
20	B	603	CLA	CHD-C1D-ND	-2.48	122.18	124.45
20	B	611	CLA	C3D-C2D-C1D	2.48	109.21	105.83
20	B	604	CLA	C3B-C4B-NB	-2.47	106.01	109.21
20	C	513	CLA	CHA-C1A-NA	-2.47	120.74	126.40
21	B	619	BCR	C20-C21-C22	2.47	130.84	127.31
20	B	613	CLA	CAC-C3C-C4C	2.46	128.01	124.81
20	B	608	CLA	CMB-C2B-C1B	-2.46	124.68	128.46
20	C	505	CLA	C9-C8-C10	2.46	120.21	111.29
20	C	503	CLA	CMD-C2D-C1D	2.46	129.05	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	605	CLA	C3A-C2A-C1A	2.46	105.02	101.34
20	C	510	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
20	C	515	CLA	CHB-C4A-NA	2.46	127.91	124.51
20	B	607	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
20	C	504	CLA	C3B-C4B-NB	-2.45	106.04	109.21
20	C	502	CLA	C6-C7-C8	-2.45	108.00	115.92
20	B	612	CLA	CHD-C4C-C3C	2.45	128.44	124.84
21	B	620	BCR	C34-C9-C10	-2.45	119.49	122.92
20	C	515	CLA	C2D-C1D-ND	-2.45	108.30	110.10
20	C	510	CLA	C9-C8-C7	2.44	120.13	111.29
20	C	512	CLA	CMD-C2D-C1D	2.44	129.02	124.71
20	B	613	CLA	C3A-C2A-C1A	2.44	104.99	101.34
20	A	405	CLA	CMD-C2D-C3D	-2.44	122.01	127.61
21	B	618	BCR	C40-C30-C25	-2.44	106.35	110.30
20	C	508	CLA	C10-C8-C7	2.43	124.93	112.13
25	D	404	PL9	C37-C36-C34	2.43	120.98	112.98
20	C	509	CLA	C1-C2-C3	2.43	130.25	126.04
20	C	507	CLA	O2D-CGD-CBD	2.43	115.58	111.27
24	I	101	LMG	O2-C2-C1	-2.43	104.15	110.05
20	C	513	CLA	CHD-C4C-NC	-2.43	120.38	124.20
20	C	513	CLA	C9-C8-C7	2.42	120.07	111.29
20	B	604	CLA	CAA-C2A-C3A	2.42	119.41	112.78
21	F	101	BCR	C24-C23-C22	-2.42	122.58	126.23
20	B	604	CLA	CBC-CAC-C3C	2.42	119.10	112.43
20	B	606	CLA	C3B-C4B-NB	-2.42	106.08	109.21
21	B	620	BCR	C8-C9-C10	2.42	122.65	118.94
20	B	605	CLA	C3B-C4B-NB	-2.42	106.09	109.21
20	A	406	CLA	C6-C7-C8	2.41	123.72	115.92
20	B	616	CLA	C3A-C2A-C1A	2.41	104.95	101.34
20	B	607	CLA	CAC-C3C-C4C	2.41	127.93	124.81
20	A	406	CLA	CAA-C2A-C3A	2.41	119.37	112.78
20	A	406	CLA	CAC-C3C-C4C	2.41	127.93	124.81
20	C	511	CLA	OBD-CAD-C3D	2.40	134.31	128.52
19	D	405	PHO	C6-C7-C8	2.40	123.68	115.92
21	H	101	BCR	C4-C5-C6	2.40	126.21	122.73
20	B	608	CLA	C9-C8-C10	2.40	119.97	111.29
20	B	613	CLA	O2D-CGD-CBD	2.40	115.53	111.27
20	B	602	CLA	CHA-C1A-NA	-2.39	120.92	126.40
20	B	614	CLA	C4-C3-C5	2.39	119.30	115.27
20	D	407	CLA	CMB-C2B-C3B	2.39	129.15	124.68
21	H	101	BCR	C31-C1-C6	2.38	114.17	110.30
20	B	614	CLA	CMB-C2B-C1B	-2.38	124.80	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	515	CLA	CAC-C3C-C4C	-2.38	121.72	124.81
20	A	407	CLA	C4-C3-C5	2.38	119.27	115.27
20	B	617	CLA	C3D-C4D-ND	2.37	114.07	110.24
20	C	505	CLA	O2D-CGD-CBD	2.37	115.48	111.27
21	C	516	BCR	C39-C30-C25	-2.37	106.46	110.30
24	B	601	LMG	O6-C5-C6	2.37	112.32	106.44
20	A	407	CLA	CHD-C1D-C2D	2.36	130.44	125.48
20	C	504	CLA	C11-C10-C8	2.36	123.55	115.92
20	B	603	CLA	C9-C8-C7	2.36	119.84	111.29
21	B	619	BCR	C11-C10-C9	-2.36	123.95	127.31
20	D	406	CLA	CMD-C2D-C3D	-2.36	122.20	127.61
20	B	611	CLA	O1D-CGD-CBD	2.35	129.30	124.48
21	H	101	BCR	C38-C26-C25	-2.35	121.89	124.53
20	C	508	CLA	O1D-CGD-CBD	2.35	129.29	124.48
20	C	515	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
21	B	620	BCR	C23-C22-C21	2.35	122.54	118.94
20	B	613	CLA	CMD-C2D-C3D	-2.34	122.22	127.61
20	C	511	CLA	C6-C7-C8	2.34	123.50	115.92
20	C	510	CLA	C2A-C1A-CHA	2.34	127.95	123.86
20	B	612	CLA	O2A-C1-C2	-2.34	102.49	108.64
20	B	603	CLA	O1D-CGD-CBD	2.34	129.27	124.48
20	A	406	CLA	CMB-C2B-C3B	2.34	129.05	124.68
20	C	504	CLA	CAC-C3C-C4C	2.34	127.84	124.81
19	D	405	PHO	C1B-NB-C4B	2.33	111.88	107.09
21	B	620	BCR	C35-C13-C12	-2.33	114.41	118.08
20	C	507	CLA	C11-C10-C8	2.33	123.44	115.92
20	C	512	CLA	C9-C8-C7	2.32	119.69	111.29
20	B	614	CLA	C1D-ND-C4D	-2.31	104.69	106.33
25	D	404	PL9	C11-C9-C8	-2.31	116.44	121.12
20	A	407	CLA	C9-C8-C7	2.31	119.66	111.29
21	K	101	BCR	C35-C13-C12	-2.31	114.44	118.08
20	B	609	CLA	C1-C2-C3	-2.31	122.05	126.04
20	C	511	CLA	O2A-C1-C2	-2.31	102.58	108.64
20	B	610	CLA	CHD-C4C-C3C	2.30	128.22	124.84
20	B	610	CLA	CAA-C2A-C1A	-2.30	104.44	111.97
20	B	613	CLA	C9-C8-C7	2.30	119.61	111.29
20	D	406	CLA	C6-C7-C8	2.30	123.34	115.92
20	C	515	CLA	CHD-C1D-ND	-2.30	122.34	124.45
20	B	602	CLA	CHD-C4C-C3C	2.30	128.22	124.84
21	C	516	BCR	C8-C7-C6	-2.30	120.75	127.20
20	B	614	CLA	CAC-C3C-C4C	-2.29	121.83	124.81
20	C	512	CLA	C1B-CHB-C4A	-2.29	125.58	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	D	406	CLA	CAA-CBA-CGA	-2.29	106.55	113.25
20	C	510	CLA	CMB-C2B-C3B	2.29	128.97	124.68
20	B	602	CLA	CMB-C2B-C1B	-2.29	124.94	128.46
24	D	402	LMG	O3-C3-C2	-2.29	105.05	110.35
20	B	610	CLA	CGD-CBD-CAD	-2.29	103.32	110.73
20	C	505	CLA	CAC-C3C-C4C	2.29	127.78	124.81
20	B	615	CLA	C3A-C2A-C1A	2.29	104.77	101.34
20	C	502	CLA	C4-C3-C5	2.28	119.11	115.27
20	B	614	CLA	C2D-C1D-ND	-2.28	108.42	110.10
20	B	609	CLA	C9-C8-C7	2.28	119.55	111.29
21	A	409	BCR	C11-C10-C9	-2.27	124.07	127.31
20	C	507	CLA	CAC-C3C-C4C	2.27	127.76	124.81
21	C	514	BCR	C12-C13-C14	2.27	122.42	118.94
20	A	406	CLA	C3B-C4B-NB	-2.26	106.28	109.21
20	B	609	CLA	C1D-ND-C4D	-2.26	104.73	106.33
20	B	612	CLA	CAC-C3C-C4C	2.26	127.74	124.81
21	F	101	BCR	C39-C30-C25	2.25	113.95	110.30
20	B	614	CLA	C1-O2A-CGA	2.25	122.35	116.44
21	C	514	BCR	C33-C5-C6	-2.25	122.00	124.53
21	Z	101	BCR	C2-C1-C6	2.24	113.94	110.48
20	A	407	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
20	B	612	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
20	B	605	CLA	C2A-C1A-CHA	2.24	127.78	123.86
20	C	508	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
20	A	405	CLA	CHD-C4C-NC	-2.24	120.68	124.20
20	B	610	CLA	C3B-C4B-NB	-2.24	106.32	109.21
20	A	405	CLA	CED-O2D-CGD	2.24	120.99	115.94
20	B	606	CLA	CHB-C4A-NA	2.23	127.60	124.51
20	A	405	CLA	CMD-C2D-C1D	2.23	128.65	124.71
20	C	511	CLA	C11-C12-C13	2.23	123.13	115.92
21	F	101	BCR	C31-C1-C6	-2.23	106.68	110.30
20	C	502	CLA	OBD-CAD-C3D	2.23	133.88	128.52
21	H	101	BCR	C8-C9-C10	2.22	122.35	118.94
20	C	511	CLA	C3A-C2A-C1A	2.22	104.67	101.34
20	A	408	CLA	C3B-C4B-NB	-2.22	106.34	109.21
25	D	404	PL9	C35-C34-C36	2.22	119.00	115.27
20	A	408	CLA	CAC-C3C-C2C	2.22	131.32	127.53
21	B	620	BCR	C1-C6-C5	-2.21	119.50	122.61
20	B	614	CLA	CMC-C2C-C1C	2.21	128.40	125.04
21	C	514	BCR	C2-C3-C4	-2.20	106.45	111.38
20	C	506	CLA	CHD-C4C-C3C	2.20	128.07	124.84
20	B	609	CLA	C2D-C1D-ND	-2.20	108.48	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	513	CLA	C6-C7-C8	-2.20	108.82	115.92
20	B	616	CLA	C3B-C4B-NB	-2.19	106.38	109.21
20	D	407	CLA	CED-O2D-CGD	2.19	120.89	115.94
20	B	607	CLA	CMD-C2D-C3D	-2.19	122.59	127.61
20	A	405	CLA	C1-C2-C3	-2.18	122.26	126.04
21	K	101	BCR	C38-C26-C25	-2.18	122.08	124.53
20	B	602	CLA	CHD-C4C-NC	-2.18	120.77	124.20
24	C	501	LMG	C6-C5-C4	-2.18	107.90	113.00
24	D	402	LMG	C3-C4-C5	-2.18	106.36	110.24
20	B	610	CLA	CMD-C2D-C1D	-2.18	120.88	124.71
21	B	618	BCR	C38-C26-C25	-2.17	122.09	124.53
21	B	620	BCR	C11-C10-C9	-2.17	124.21	127.31
20	C	506	CLA	CGD-CBD-CAD	-2.17	103.70	110.73
20	A	405	CLA	CMA-C3A-C4A	2.17	117.60	111.77
20	A	405	CLA	C6-C5-C3	2.17	119.14	113.45
20	C	507	CLA	CMA-C3A-C4A	2.17	117.60	111.77
20	C	506	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
20	C	507	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
21	H	101	BCR	C24-C23-C22	-2.17	122.96	126.23
21	K	101	BCR	C1-C6-C5	-2.16	119.56	122.61
20	C	505	CLA	C6-C7-C8	2.16	122.91	115.92
20	B	611	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
20	B	613	CLA	CHD-C4C-C3C	2.16	128.01	124.84
20	D	407	CLA	C1C-C2C-C3C	-2.15	104.69	106.96
20	A	406	CLA	C11-C10-C8	2.15	122.88	115.92
20	B	611	CLA	C9-C8-C7	2.15	119.08	111.29
20	B	616	CLA	CMC-C2C-C1C	2.15	128.31	125.04
20	C	505	CLA	C2D-C1D-ND	-2.15	108.52	110.10
20	B	605	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
20	B	610	CLA	CMB-C2B-C3B	2.15	128.70	124.68
20	D	406	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
21	F	101	BCR	C35-C13-C12	-2.15	114.70	118.08
20	C	515	CLA	C1B-CHB-C4A	-2.15	125.87	130.12
20	B	606	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
20	A	407	CLA	CBC-CAC-C3C	2.14	118.34	112.43
24	D	403	LMG	O7-C10-C11	-2.14	106.88	111.50
20	D	407	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
20	A	406	CLA	C3D-C4D-ND	2.14	113.69	110.24
20	B	615	CLA	C1-O2A-CGA	2.14	122.05	116.44
20	B	603	CLA	CAA-C2A-C1A	-2.13	104.99	111.97
20	B	612	CLA	C1C-C2C-C3C	-2.12	104.72	106.96
26	E	101	HEM	C4B-C3B-C2B	2.12	108.80	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	405	CLA	O2D-CGD-CBD	-2.12	107.50	111.27
20	A	407	CLA	C1D-ND-C4D	-2.12	104.83	106.33
24	C	501	LMG	C8-O7-C10	2.12	123.01	117.79
20	C	511	CLA	CAA-C2A-C1A	-2.12	105.03	111.97
20	B	612	CLA	CAA-C2A-C3A	2.12	118.58	112.78
21	B	619	BCR	C36-C18-C19	-2.12	114.74	118.08
20	B	605	CLA	CAA-CBA-CGA	-2.11	107.07	113.25
20	B	617	CLA	C2A-C1A-CHA	2.11	127.56	123.86
20	C	505	CLA	CMA-C3A-C4A	2.11	117.45	111.77
20	C	515	CLA	C3A-C2A-C1A	2.11	104.50	101.34
20	B	613	CLA	CAA-CBA-CGA	-2.11	107.08	113.25
20	C	515	CLA	C3C-C4C-NC	-2.11	108.20	110.57
20	B	604	CLA	C4D-CHA-C1A	-2.11	118.68	121.25
20	B	613	CLA	C10-C8-C7	2.11	123.20	112.13
20	C	503	CLA	C9-C8-C7	2.10	118.91	111.29
20	C	508	CLA	C6-C5-C3	2.10	118.97	113.45
25	D	404	PL9	O1-C4-C3	-2.10	118.41	120.72
20	C	504	CLA	C9-C8-C7	2.10	118.90	111.29
20	C	510	CLA	CGD-CBD-CAD	2.10	117.54	110.73
20	B	602	CLA	C1-C2-C3	2.10	129.68	126.04
20	C	507	CLA	C3A-C2A-C1A	2.10	104.48	101.34
20	C	506	CLA	CHD-C1D-C2D	2.10	129.88	125.48
21	A	409	BCR	C8-C7-C6	-2.10	121.31	127.20
20	C	511	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
20	B	617	CLA	C3A-C2A-C1A	2.09	104.48	101.34
20	B	606	CLA	C11-C10-C8	2.09	122.69	115.92
20	A	407	CLA	C2D-C1D-ND	-2.09	108.56	110.10
21	B	619	BCR	C1-C6-C5	-2.09	119.67	122.61
20	C	510	CLA	C11-C10-C8	2.09	122.68	115.92
20	A	408	CLA	C4D-CHA-C1A	2.09	123.80	121.25
21	C	514	BCR	C31-C1-C6	-2.09	106.91	110.30
20	B	603	CLA	CAA-CBA-CGA	-2.09	107.14	113.25
20	A	406	CLA	CHD-C4C-C3C	2.09	127.91	124.84
20	B	615	CLA	C10-C8-C7	2.09	123.10	112.13
20	A	406	CLA	C2A-C3A-C4A	2.09	105.24	101.87
20	C	505	CLA	C6-C5-C3	2.08	118.92	113.45
20	B	605	CLA	C9-C8-C7	2.08	118.84	111.29
20	B	616	CLA	C9-C8-C10	2.08	118.84	111.29
20	B	608	CLA	C9-C8-C7	2.08	118.83	111.29
20	B	612	CLA	C2C-C1C-NC	2.08	111.92	109.97
20	A	407	CLA	C3A-C2A-C1A	2.07	104.44	101.34
20	D	406	CLA	O2A-C1-C2	2.07	114.08	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	603	CLA	C3B-C4B-NB	-2.07	106.53	109.21
20	B	613	CLA	C5-C3-C2	-2.07	116.93	121.12
20	C	503	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
20	B	611	CLA	C4D-CHA-C1A	2.07	123.76	121.25
20	C	511	CLA	C1D-ND-C4D	-2.07	104.87	106.33
21	C	514	BCR	C30-C25-C26	-2.07	119.70	122.61
24	D	402	LMG	O6-C1-C2	-2.06	105.98	110.35
20	B	611	CLA	C10-C8-C7	2.06	122.99	112.13
21	Z	101	BCR	C8-C7-C6	-2.06	121.42	127.20
20	A	407	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
20	B	608	CLA	C11-C10-C8	2.06	122.57	115.92
21	B	619	BCR	C32-C1-C6	2.06	113.64	110.30
20	C	505	CLA	C2A-C1A-CHA	2.06	127.45	123.86
20	C	505	CLA	CMC-C2C-C1C	2.06	128.17	125.04
20	C	513	CLA	CMA-C3A-C4A	2.05	117.29	111.77
20	B	610	CLA	CMC-C2C-C1C	2.05	128.16	125.04
20	B	613	CLA	CGD-CBD-CAD	2.05	117.38	110.73
20	C	502	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
20	C	508	CLA	C11-C10-C8	2.05	122.55	115.92
20	C	506	CLA	C9-C8-C10	2.05	118.71	111.29
21	K	101	BCR	C40-C30-C25	-2.05	106.98	110.30
20	B	617	CLA	C1D-ND-C4D	-2.04	104.88	106.33
20	C	513	CLA	CMC-C2C-C1C	2.04	128.15	125.04
20	C	509	CLA	CED-O2D-CGD	2.04	120.55	115.94
21	K	101	BCR	C20-C21-C22	-2.04	124.40	127.31
20	B	615	CLA	C9-C8-C10	2.04	118.67	111.29
21	B	620	BCR	C31-C1-C6	2.04	113.60	110.30
20	C	503	CLA	OBD-CAD-C3D	2.04	133.42	128.52
20	B	606	CLA	C9-C8-C7	2.04	118.66	111.29
20	B	607	CLA	C9-C8-C10	2.04	118.66	111.29
20	C	509	CLA	C5-C3-C2	-2.03	117.00	121.12
20	D	407	CLA	CBA-CAA-C2A	2.03	119.86	113.86
20	B	614	CLA	C1C-C2C-C3C	-2.03	104.82	106.96
20	C	503	CLA	CMB-C2B-C1B	-2.02	125.35	128.46
20	C	509	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
20	A	405	CLA	C9-C8-C7	2.02	118.62	111.29
20	C	513	CLA	C3A-C2A-C1A	2.02	104.37	101.34
20	C	513	CLA	CHB-C4A-NA	2.02	127.31	124.51
20	C	504	CLA	O2A-C1-C2	-2.02	103.32	108.64
20	A	408	CLA	CHD-C1D-ND	-2.02	122.60	124.45
20	C	513	CLA	C2C-C1C-NC	2.02	111.86	109.97
20	B	604	CLA	CHB-C4A-NA	2.02	127.30	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	512	CLA	CMB-C2B-C3B	2.02	128.45	124.68
20	B	613	CLA	O2A-C1-C2	-2.01	103.34	108.64
20	B	613	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
24	C	501	LMG	C3-C4-C5	-2.00	106.67	110.24
20	C	504	CLA	C3A-C2A-C1A	2.00	104.34	101.34
20	B	614	CLA	CAC-C3C-C2C	2.00	130.95	127.53
20	C	502	CLA	CMD-C2D-C3D	-2.00	123.01	127.61

All (57) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	404	PHO	C8
19	D	405	PHO	C8
20	A	405	CLA	ND
20	A	405	CLA	C8
20	A	406	CLA	ND
20	A	406	CLA	C8
20	A	407	CLA	C8
20	A	408	CLA	C8
20	B	602	CLA	C8
20	B	603	CLA	ND
20	B	603	CLA	C8
20	B	604	CLA	ND
20	B	604	CLA	C8
20	B	605	CLA	ND
20	B	605	CLA	C8
20	B	606	CLA	ND
20	B	606	CLA	C8
20	B	607	CLA	ND
20	B	607	CLA	C8
20	B	608	CLA	ND
20	B	608	CLA	C8
20	B	609	CLA	C8
20	B	610	CLA	ND
20	B	610	CLA	C8
20	B	611	CLA	ND
20	B	611	CLA	C8
20	B	612	CLA	ND
20	B	612	CLA	C8
20	B	613	CLA	C8
20	B	614	CLA	ND
20	B	614	CLA	C8

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Mol	Chain	Res	Type	Atom
20	B	615	CLA	ND
20	B	615	CLA	C8
20	B	616	CLA	C8
20	B	617	CLA	C8
20	C	502	CLA	ND
20	C	502	CLA	C8
20	C	503	CLA	ND
20	C	503	CLA	C8
20	C	504	CLA	C8
20	C	505	CLA	C8
20	C	506	CLA	C8
20	C	506	CLA	ND
20	C	507	CLA	ND
20	C	507	CLA	C8
20	C	508	CLA	C8
20	C	509	CLA	ND
20	C	509	CLA	C8
20	C	510	CLA	C8
20	C	511	CLA	ND
20	C	511	CLA	C8
20	C	512	CLA	C8
20	C	513	CLA	C8
20	C	515	CLA	C8
20	D	406	CLA	ND
20	D	406	CLA	C8
20	D	407	CLA	C8

All (442) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	404	PHO	O2A-C1-C2-C3
20	A	405	CLA	C11-C10-C8-C7
20	A	406	CLA	C1A-C2A-CAA-CBA
20	A	406	CLA	C3A-C2A-CAA-CBA
20	B	602	CLA	CHA-CBD-CGD-O1D
20	B	602	CLA	CHA-CBD-CGD-O2D
20	B	602	CLA	O2A-C1-C2-C3
20	B	603	CLA	O2A-C1-C2-C3
20	B	604	CLA	C1A-C2A-CAA-CBA
20	B	604	CLA	C3A-C2A-CAA-CBA
20	B	605	CLA	CHA-CBD-CGD-O1D
20	B	605	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	B	607	CLA	C3A-C2A-CAA-CBA
20	B	608	CLA	CHA-CBD-CGD-O1D
20	B	609	CLA	C1A-C2A-CAA-CBA
20	B	612	CLA	C1A-C2A-CAA-CBA
20	B	612	CLA	C3A-C2A-CAA-CBA
20	C	503	CLA	C6-C7-C8-C9
20	C	504	CLA	C4-C3-C5-C6
20	D	406	CLA	O2A-C1-C2-C3
20	D	407	CLA	C1A-C2A-CAA-CBA
20	D	407	CLA	C3A-C2A-CAA-CBA
20	D	407	CLA	O2A-C1-C2-C3
21	A	409	BCR	C7-C8-C9-C34
21	B	618	BCR	C11-C12-C13-C14
21	B	618	BCR	C11-C12-C13-C35
21	B	619	BCR	C17-C18-C19-C20
21	B	619	BCR	C36-C18-C19-C20
21	B	619	BCR	C23-C24-C25-C30
21	B	620	BCR	C1-C6-C7-C8
21	B	620	BCR	C7-C8-C9-C34
21	B	620	BCR	C17-C18-C19-C20
21	C	514	BCR	C9-C10-C11-C12
21	C	514	BCR	C11-C12-C13-C14
21	C	514	BCR	C11-C12-C13-C35
21	C	516	BCR	C11-C12-C13-C14
21	C	516	BCR	C11-C12-C13-C35
21	C	516	BCR	C21-C22-C23-C24
21	C	516	BCR	C37-C22-C23-C24
21	C	516	BCR	C23-C24-C25-C30
21	F	101	BCR	C7-C8-C9-C34
21	F	101	BCR	C21-C22-C23-C24
21	F	101	BCR	C37-C22-C23-C24
21	H	101	BCR	C7-C8-C9-C10
21	H	101	BCR	C7-C8-C9-C34
21	H	101	BCR	C11-C12-C13-C35
21	H	101	BCR	C17-C18-C19-C20
21	H	101	BCR	C36-C18-C19-C20
21	K	101	BCR	C7-C8-C9-C10
21	K	101	BCR	C11-C12-C13-C14
21	K	101	BCR	C11-C12-C13-C35
21	K	101	BCR	C17-C18-C19-C20
21	K	101	BCR	C36-C18-C19-C20
21	K	101	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
21	K	101	BCR	C37-C22-C23-C24
22	A	410	LHG	C4-O6-P-O5
22	A	411	LHG	O1-C1-C2-C3
22	A	411	LHG	C3-O3-P-O4
24	B	601	LMG	O6-C1-O1-C7
25	D	404	PL9	C26-C27-C28-C29
25	D	404	PL9	C33-C34-C36-C37
25	D	404	PL9	C35-C34-C36-C37
20	C	504	CLA	C2-C3-C5-C6
20	C	502	CLA	C2A-CAA-CBA-CGA
20	D	406	CLA	C4C-C3C-CAC-CBC
21	B	619	BCR	C19-C20-C21-C22
20	B	616	CLA	CBD-CGD-O2D-CED
25	D	404	PL9	C39-C41-C42-C43
20	C	512	CLA	CBD-CGD-O2D-CED
22	A	410	LHG	C26-C27-C28-C29
21	A	409	BCR	C19-C20-C21-C22
21	C	516	BCR	C13-C14-C15-C16
24	D	402	LMG	C31-C32-C33-C34
19	D	405	PHO	C11-C10-C8-C9
20	B	602	CLA	C11-C10-C8-C9
20	B	608	CLA	C6-C7-C8-C9
20	D	407	CLA	C6-C7-C8-C9
21	A	409	BCR	C36-C18-C19-C20
21	B	620	BCR	C11-C12-C13-C35
21	B	620	BCR	C36-C18-C19-C20
21	C	514	BCR	C37-C22-C23-C24
21	C	516	BCR	C36-C18-C19-C20
21	K	101	BCR	C7-C8-C9-C34
21	Z	101	BCR	C7-C8-C9-C34
21	Z	101	BCR	C36-C18-C19-C20
21	A	409	BCR	C17-C18-C19-C20
21	Z	101	BCR	C17-C18-C19-C20
20	B	612	CLA	CBA-CGA-O2A-C1
20	B	615	CLA	CBA-CGA-O2A-C1
22	A	411	LHG	C12-C13-C14-C15
20	B	604	CLA	C11-C10-C8-C7
20	B	611	CLA	C11-C10-C8-C7
20	C	507	CLA	C11-C12-C13-C15
20	C	510	CLA	C11-C10-C8-C7
20	D	407	CLA	C11-C10-C8-C7
21	H	101	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	K	101	BCR	C19-C20-C21-C22
20	D	406	CLA	C2C-C3C-CAC-CBC
20	B	615	CLA	O1A-CGA-O2A-C1
24	C	501	LMG	C39-C40-C41-C42
22	A	411	LHG	C3-O3-P-O6
20	B	609	CLA	C10-C11-C12-C13
21	K	101	BCR	C9-C10-C11-C12
21	K	101	BCR	C20-C21-C22-C37
24	D	403	LMG	C39-C40-C41-C42
24	D	403	LMG	C35-C36-C37-C38
22	A	411	LHG	C28-C29-C30-C31
20	C	515	CLA	C4-C3-C5-C6
24	C	501	LMG	C17-C18-C19-C20
20	A	408	CLA	C14-C13-C15-C16
20	B	603	CLA	C6-C7-C8-C9
20	B	614	CLA	C6-C7-C8-C9
21	C	516	BCR	C7-C8-C9-C34
21	A	409	BCR	C21-C22-C23-C24
21	C	514	BCR	C21-C22-C23-C24
21	C	516	BCR	C7-C8-C9-C10
21	C	516	BCR	C17-C18-C19-C20
21	Z	101	BCR	C7-C8-C9-C10
20	B	610	CLA	C16-C17-C18-C19
20	B	610	CLA	C16-C17-C18-C20
20	D	406	CLA	C8-C10-C11-C12
20	B	609	CLA	C3A-C2A-CAA-CBA
24	I	101	LMG	C28-C29-C30-C31
20	A	406	CLA	C4-C3-C5-C6
20	A	408	CLA	C4-C3-C5-C6
20	B	607	CLA	CBA-CGA-O2A-C1
20	A	406	CLA	C2-C3-C5-C6
20	A	408	CLA	C2-C3-C5-C6
20	C	515	CLA	C2-C3-C5-C6
20	B	612	CLA	O1A-CGA-O2A-C1
21	B	619	BCR	C23-C24-C25-C26
21	B	620	BCR	C5-C6-C7-C8
24	D	401	LMG	C29-C28-O8-C9
20	A	406	CLA	C12-C13-C15-C16
20	A	408	CLA	C12-C13-C15-C16
20	C	503	CLA	C11-C10-C8-C7
20	C	504	CLA	C6-C7-C8-C10
20	C	506	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	C	507	CLA	C11-C10-C8-C7
20	C	508	CLA	C11-C10-C8-C7
20	C	509	CLA	C11-C10-C8-C7
20	C	513	CLA	C6-C7-C8-C10
20	D	406	CLA	C11-C12-C13-C15
20	C	506	CLA	C2C-C3C-CAC-CBC
24	C	501	LMG	O9-C10-O7-C8
24	D	403	LMG	C33-C34-C35-C36
20	B	616	CLA	O1D-CGD-O2D-CED
24	C	501	LMG	C11-C10-O7-C8
20	C	502	CLA	C11-C10-C8-C9
20	C	507	CLA	C11-C12-C13-C14
20	C	509	CLA	C14-C13-C15-C16
20	C	515	CLA	C11-C10-C8-C9
20	D	406	CLA	C11-C10-C8-C9
20	D	406	CLA	C11-C12-C13-C14
20	B	608	CLA	C3-C5-C6-C7
24	B	601	LMG	C11-C12-C13-C14
24	D	403	LMG	C29-C30-C31-C32
21	F	101	BCR	C7-C8-C9-C10
20	B	607	CLA	C1A-C2A-CAA-CBA
20	C	511	CLA	C5-C6-C7-C8
20	C	512	CLA	O1D-CGD-O2D-CED
24	M	101	LMG	C33-C34-C35-C36
20	A	405	CLA	C4-C3-C5-C6
20	C	506	CLA	C4-C3-C5-C6
20	B	607	CLA	O1A-CGA-O2A-C1
24	B	601	LMG	C7-C8-C9-O8
24	D	402	LMG	O1-C7-C8-C9
24	D	401	LMG	O10-C28-O8-C9
20	C	504	CLA	CAA-CBA-CGA-O2A
20	A	408	CLA	CBD-CGD-O2D-CED
21	C	514	BCR	C20-C21-C22-C23
21	K	101	BCR	C11-C10-C9-C8
24	D	401	LMG	O7-C8-C9-O8
20	B	602	CLA	C4-C3-C5-C6
19	D	405	PHO	C6-C7-C8-C10
20	B	602	CLA	C2-C3-C5-C6
20	B	604	CLA	C11-C12-C13-C15
20	B	610	CLA	C11-C10-C8-C7
20	C	509	CLA	C12-C13-C15-C16
20	C	513	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
20	A	406	CLA	C14-C13-C15-C16
20	B	609	CLA	C6-C7-C8-C9
20	B	612	CLA	C11-C10-C8-C9
20	B	615	CLA	C11-C10-C8-C9
20	B	616	CLA	C6-C7-C8-C9
20	B	617	CLA	C6-C7-C8-C9
20	C	505	CLA	C11-C10-C8-C9
20	C	508	CLA	C6-C7-C8-C9
21	K	101	BCR	C15-C16-C17-C18
24	C	501	LMG	C15-C16-C17-C18
24	D	403	LMG	C42-C43-C44-C45
24	D	402	LMG	O6-C5-C6-O5
24	D	401	LMG	C19-C20-C21-C22
20	C	513	CLA	C4-C3-C5-C6
20	B	611	CLA	C2-C3-C5-C6
20	A	406	CLA	C5-C6-C7-C8
20	C	512	CLA	CBA-CGA-O2A-C1
19	A	404	PHO	C10-C11-C12-C13
22	A	410	LHG	C4-C5-C6-O8
20	A	405	CLA	O2A-C1-C2-C3
20	B	611	CLA	C4-C3-C5-C6
24	D	401	LMG	C21-C22-C23-C24
22	A	411	LHG	O1-C1-C2-O2
22	A	411	LHG	C26-C27-C28-C29
20	B	604	CLA	CAA-CBA-CGA-O2A
24	D	402	LMG	C42-C43-C44-C45
24	C	501	LMG	O7-C8-C9-O8
24	D	402	LMG	O1-C7-C8-O7
20	B	608	CLA	C2-C1-O2A-CGA
20	B	616	CLA	C2-C1-O2A-CGA
20	C	513	CLA	C2-C3-C5-C6
20	B	602	CLA	C6-C7-C8-C9
22	A	411	LHG	C2-C3-O3-P
21	C	516	BCR	C23-C24-C25-C26
21	H	101	BCR	C11-C12-C13-C14
20	C	506	CLA	C4C-C3C-CAC-CBC
20	B	611	CLA	C11-C12-C13-C15
20	B	615	CLA	C6-C7-C8-C10
20	C	511	CLA	C6-C7-C8-C10
20	C	512	CLA	C8-C10-C11-C12
21	B	619	BCR	C15-C16-C17-C18
19	D	405	PHO	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
21	Z	101	BCR	C20-C21-C22-C37
20	A	408	CLA	CAD-CBD-CGD-O2D
20	B	610	CLA	CAD-CBD-CGD-O2D
20	B	611	CLA	CAD-CBD-CGD-O2D
20	B	613	CLA	CAD-CBD-CGD-O2D
20	C	505	CLA	CAD-CBD-CGD-O2D
20	C	508	CLA	CAD-CBD-CGD-O2D
20	C	509	CLA	CAD-CBD-CGD-O2D
21	C	516	BCR	C22-C23-C24-C25
20	C	512	CLA	O1A-CGA-O2A-C1
24	C	501	LMG	O6-C1-O1-C7
20	B	613	CLA	C3-C5-C6-C7
20	B	608	CLA	CHA-CBD-CGD-O2D
20	C	503	CLA	CHA-CBD-CGD-O1D
20	C	503	CLA	CHA-CBD-CGD-O2D
20	C	510	CLA	CHA-CBD-CGD-O1D
20	C	510	CLA	CHA-CBD-CGD-O2D
20	C	512	CLA	CHA-CBD-CGD-O1D
22	A	410	LHG	O7-C5-C6-O8
24	B	601	LMG	C15-C16-C17-C18
24	M	101	LMG	C22-C23-C24-C25
20	A	408	CLA	C6-C7-C8-C9
20	B	605	CLA	C11-C10-C8-C9
20	C	511	CLA	C16-C17-C18-C20
20	B	612	CLA	C3-C5-C6-C7
20	C	513	CLA	CAA-CBA-CGA-O2A
21	F	101	BCR	C15-C16-C17-C18
22	A	410	LHG	C4-O6-P-O3
22	A	411	LHG	C31-C32-C33-C34
22	A	410	LHG	C2-C3-O3-P
20	C	513	CLA	C16-C17-C18-C19
20	B	605	CLA	CAD-CBD-CGD-O1D
20	C	503	CLA	CAD-CBD-CGD-O1D
20	C	510	CLA	CAD-CBD-CGD-O1D
24	M	101	LMG	C40-C41-C42-C43
24	M	101	LMG	C30-C31-C32-C33
20	B	604	CLA	C6-C7-C8-C10
24	D	401	LMG	C10-C11-C12-C13
24	D	402	LMG	C29-C30-C31-C32
20	C	507	CLA	C10-C11-C12-C13
24	D	402	LMG	C8-C7-O1-C1
24	M	101	LMG	C8-C7-O1-C1

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Mol	Chain	Res	Type	Atoms
20	C	503	CLA	CBA-CGA-O2A-C1
20	A	408	CLA	C13-C15-C16-C17
19	D	405	PHO	C6-C7-C8-C9
20	A	407	CLA	C11-C10-C8-C9
20	B	611	CLA	C11-C12-C13-C14
24	D	401	LMG	C16-C17-C18-C19
20	B	604	CLA	C3-C5-C6-C7
20	C	503	CLA	C3-C5-C6-C7
25	D	404	PL9	C29-C31-C32-C33
24	D	402	LMG	C13-C14-C15-C16
20	C	503	CLA	O1A-CGA-O2A-C1
21	A	409	BCR	C37-C22-C23-C24
20	B	614	CLA	C16-C17-C18-C20
24	C	501	LMG	C23-C24-C25-C26
20	B	616	CLA	C5-C6-C7-C8
20	B	613	CLA	C8-C10-C11-C12
24	C	501	LMG	C7-C8-O7-C10
24	D	402	LMG	C9-C8-O7-C10
24	D	403	LMG	C9-C8-O7-C10
20	B	614	CLA	C2-C1-O2A-CGA
20	C	504	CLA	C2-C1-O2A-CGA
22	A	411	LHG	C9-C10-C11-C12
22	A	410	LHG	C24-C23-O8-C6
20	A	408	CLA	O1D-CGD-O2D-CED
21	B	618	BCR	C1-C6-C7-C8
24	D	401	LMG	C31-C32-C33-C34
24	D	401	LMG	C29-C30-C31-C32
20	B	612	CLA	C13-C15-C16-C17
22	A	410	LHG	C3-O3-P-O6
22	A	411	LHG	C4-O6-P-O3
20	B	602	CLA	C16-C17-C18-C19
20	A	408	CLA	C11-C10-C8-C7
20	B	613	CLA	C11-C10-C8-C7
20	B	616	CLA	C6-C7-C8-C10
20	C	515	CLA	C6-C7-C8-C9
20	A	405	CLA	C2-C3-C5-C6
19	D	405	PHO	CBA-CGA-O2A-C1
24	D	401	LMG	C4-C5-C6-O5
20	C	503	CLA	CBD-CGD-O2D-CED
22	A	410	LHG	O10-C23-O8-C6
20	B	612	CLA	C2-C1-O2A-CGA
24	D	401	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	A	411	LHG	C24-C25-C26-C27
20	B	608	CLA	C13-C15-C16-C17
24	C	501	LMG	C32-C33-C34-C35
19	A	404	PHO	C11-C10-C8-C9
20	A	405	CLA	C6-C7-C8-C9
20	B	607	CLA	C6-C7-C8-C9
20	B	613	CLA	C6-C7-C8-C9
20	C	505	CLA	C11-C12-C13-C14
24	C	501	LMG	C7-C8-C9-O8
24	D	401	LMG	C7-C8-C9-O8
20	C	511	CLA	C4-C3-C5-C6
20	C	512	CLA	C1A-C2A-CAA-CBA
20	B	611	CLA	C6-C7-C8-C10
22	A	410	LHG	C12-C13-C14-C15
19	A	404	PHO	C16-C17-C18-C19
24	I	101	LMG	C14-C15-C16-C17
20	B	616	CLA	C3-C5-C6-C7
20	C	506	CLA	C2A-CAA-CBA-CGA
22	A	411	LHG	O6-C4-C5-O7
20	C	507	CLA	CAA-CBA-CGA-O2A
20	C	507	CLA	C16-C17-C18-C19
20	B	606	CLA	C4-C3-C5-C6
24	B	601	LMG	O7-C8-C9-O8
20	C	511	CLA	C16-C17-C18-C19
20	A	406	CLA	O1A-CGA-O2A-C1
19	D	405	PHO	C2-C1-O2A-CGA
20	B	615	CLA	C2-C1-O2A-CGA
20	B	614	CLA	C11-C10-C8-C9
20	C	504	CLA	C11-C10-C8-C9
20	C	504	CLA	CAA-CBA-CGA-O1A
22	A	411	LHG	C14-C15-C16-C17
20	B	613	CLA	C2A-CAA-CBA-CGA
21	C	516	BCR	C1-C6-C7-C8
21	B	618	BCR	C19-C20-C21-C22
20	B	613	CLA	C4-C3-C5-C6
20	C	508	CLA	C4-C3-C5-C6
25	D	404	PL9	C20-C19-C21-C22
19	A	404	PHO	C3-C5-C6-C7
24	C	501	LMG	C21-C22-C23-C24
20	B	611	CLA	C16-C17-C18-C20
24	D	403	LMG	C4-C5-C6-O5
20	B	611	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
20	A	406	CLA	CBA-CGA-O2A-C1
26	E	101	HEM	CAD-CBD-CGD-O2D
25	D	404	PL9	C15-C14-C16-C17
20	B	610	CLA	C11-C12-C13-C15
20	B	617	CLA	C6-C7-C8-C10
19	D	405	PHO	O1A-CGA-O2A-C1
20	B	604	CLA	CAA-CBA-CGA-O1A
21	B	619	BCR	C35-C13-C14-C15
20	B	613	CLA	C2-C3-C5-C6
20	C	511	CLA	C2-C3-C5-C6
20	C	502	CLA	C14-C13-C15-C16
20	C	511	CLA	C11-C10-C8-C9
26	E	101	HEM	CAA-CBA-CGA-O2A
19	A	404	PHO	CAD-CBD-CGD-O2D
20	A	405	CLA	CAD-CBD-CGD-O2D
20	B	607	CLA	CAD-CBD-CGD-O2D
20	C	504	CLA	CAD-CBD-CGD-O2D
20	C	507	CLA	CAD-CBD-CGD-O2D
20	C	512	CLA	CAD-CBD-CGD-O2D
24	D	401	LMG	C12-C13-C14-C15
20	B	602	CLA	CAA-CBA-CGA-O2A
20	B	612	CLA	CAA-CBA-CGA-O2A
24	D	401	LMG	C18-C19-C20-C21
19	D	405	PHO	C2C-C3C-CAC-CBC
26	E	101	HEM	CAA-CBA-CGA-O1A
20	C	510	CLA	O2A-C1-C2-C3
20	A	406	CLA	CHA-CBD-CGD-O1D
20	A	406	CLA	CHA-CBD-CGD-O2D
20	B	616	CLA	CHA-CBD-CGD-O2D
20	C	512	CLA	CHA-CBD-CGD-O2D
20	A	408	CLA	CAA-CBA-CGA-O2A
24	B	601	LMG	O1-C7-C8-O7
24	D	401	LMG	C38-C39-C40-C41
24	M	101	LMG	C21-C22-C23-C24
20	C	510	CLA	CAA-CBA-CGA-O2A
22	A	411	LHG	O7-C7-C8-C9
20	B	603	CLA	C12-C13-C15-C16
20	C	503	CLA	C11-C12-C13-C15
19	A	404	PHO	C16-C17-C18-C20
20	B	610	CLA	CAA-CBA-CGA-O2A
20	B	611	CLA	CAA-CBA-CGA-O2A
26	E	101	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
20	B	604	CLA	C11-C12-C13-C14
20	B	606	CLA	C6-C7-C8-C9
20	B	607	CLA	C11-C10-C8-C9
20	B	612	CLA	C6-C7-C8-C9
20	C	506	CLA	C6-C7-C8-C9
20	C	506	CLA	C11-C10-C8-C9
20	D	406	CLA	C13-C15-C16-C17
24	C	501	LMG	C36-C37-C38-C39
22	A	411	LHG	C17-C18-C19-C20
20	B	612	CLA	CAA-CBA-CGA-O1A
21	H	101	BCR	C21-C22-C23-C24
24	D	401	LMG	C36-C37-C38-C39
20	D	406	CLA	C1A-C2A-CAA-CBA
24	C	501	LMG	C41-C42-C43-C44
22	A	411	LHG	O9-C7-C8-C9
24	D	401	LMG	C37-C38-C39-C40
20	C	505	CLA	C10-C11-C12-C13
20	A	408	CLA	CAA-CBA-CGA-O1A
20	B	610	CLA	CAA-CBA-CGA-O1A
20	B	602	CLA	CAA-CBA-CGA-O1A
20	C	510	CLA	CAA-CBA-CGA-O1A
22	A	410	LHG	C3-O3-P-O5
22	A	411	LHG	C4-O6-P-O5
21	B	618	BCR	C20-C21-C22-C37
20	B	611	CLA	CAA-CBA-CGA-O1A
21	C	514	BCR	C18-C19-C20-C21
20	B	614	CLA	CAA-CBA-CGA-O2A
24	D	401	LMG	C32-C33-C34-C35
24	B	601	LMG	C17-C18-C19-C20
24	D	403	LMG	C36-C37-C38-C39
20	B	610	CLA	C11-C12-C13-C14
20	A	407	CLA	CAA-CBA-CGA-O2A
20	B	608	CLA	CAA-CBA-CGA-O2A
24	I	101	LMG	C38-C39-C40-C41
20	A	405	CLA	C11-C12-C13-C15
20	B	609	CLA	C11-C10-C8-C7
20	B	617	CLA	C11-C10-C8-C7
20	C	506	CLA	C12-C13-C15-C16
20	C	512	CLA	C11-C10-C8-C7
20	C	515	CLA	C12-C13-C15-C16
20	C	513	CLA	CAA-CBA-CGA-O1A
20	D	406	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	B	601	LMG	O7-C10-C11-C12
22	A	410	LHG	C34-C35-C36-C37
20	D	406	CLA	CAA-CBA-CGA-O1A
20	C	511	CLA	O1D-CGD-O2D-CED
22	A	411	LHG	O2-C2-C3-O3
20	C	503	CLA	CAA-CBA-CGA-O2A
22	A	410	LHG	O8-C23-C24-C25
20	C	505	CLA	C16-C17-C18-C20
24	B	601	LMG	O9-C10-C11-C12
20	C	503	CLA	O1D-CGD-O2D-CED

There are no ring outliers.

41 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	603	CLA	1	0
19	D	405	PHO	3	0
25	D	404	PL9	2	0
20	C	509	CLA	2	0
20	B	608	CLA	2	0
21	K	101	BCR	1	0
20	B	614	CLA	1	0
20	B	609	CLA	2	0
22	A	411	LHG	1	0
21	C	514	BCR	3	0
24	D	403	LMG	1	0
24	D	402	LMG	1	0
20	C	504	CLA	1	0
20	C	511	CLA	2	0
20	B	616	CLA	2	0
21	B	618	BCR	2	0
24	C	501	LMG	1	0
20	A	405	CLA	5	0
19	A	404	PHO	1	0
20	B	610	CLA	1	0
20	C	507	CLA	1	0
21	A	409	BCR	1	0
20	A	406	CLA	4	0
21	H	101	BCR	1	0
20	D	406	CLA	3	0
24	B	601	LMG	1	0
20	C	505	CLA	1	0

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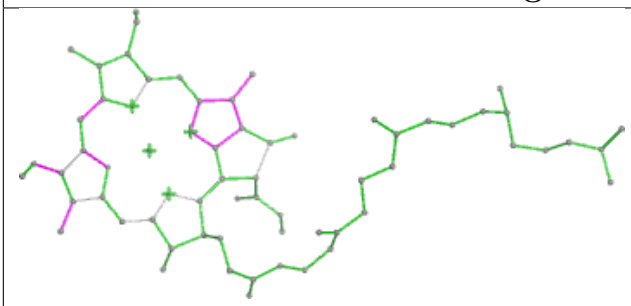
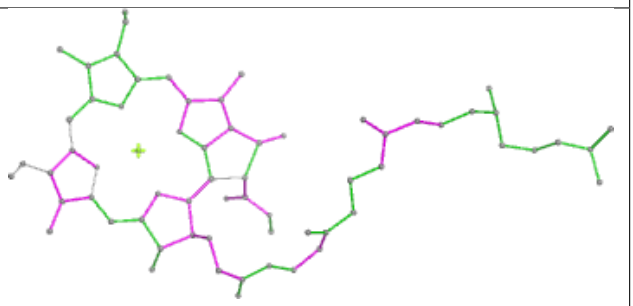
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	C	503	CLA	3	0
20	B	612	CLA	1	0
20	B	606	CLA	1	0
21	B	619	BCR	2	0
21	B	620	BCR	2	0
26	E	101	HEM	1	0
20	B	613	CLA	2	0
20	B	604	CLA	1	0
20	B	605	CLA	2	0
20	A	408	CLA	1	0
20	C	515	CLA	2	0
20	D	407	CLA	2	0
20	C	513	CLA	1	0
20	C	502	CLA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

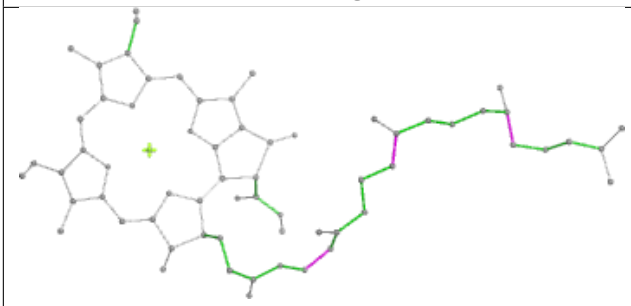
Ligand CLA B 603



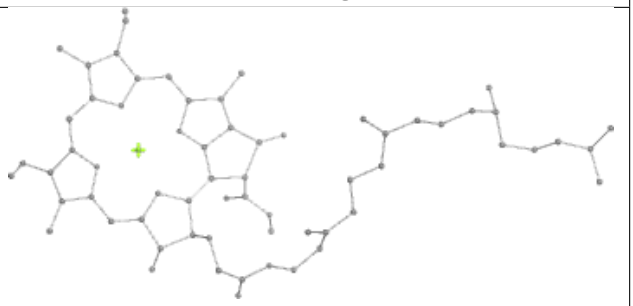
Bond lengths



Bond angles

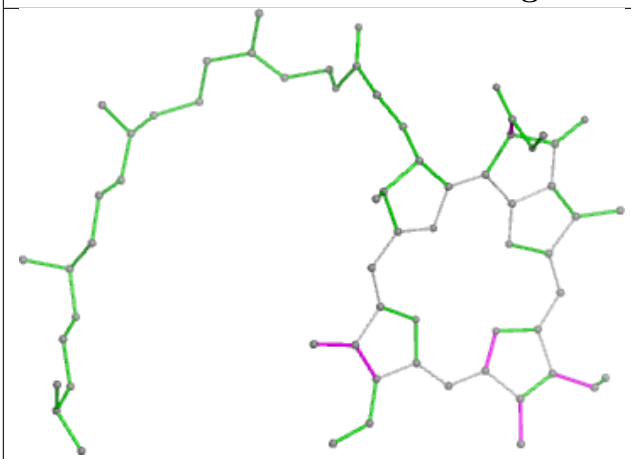


Torsions

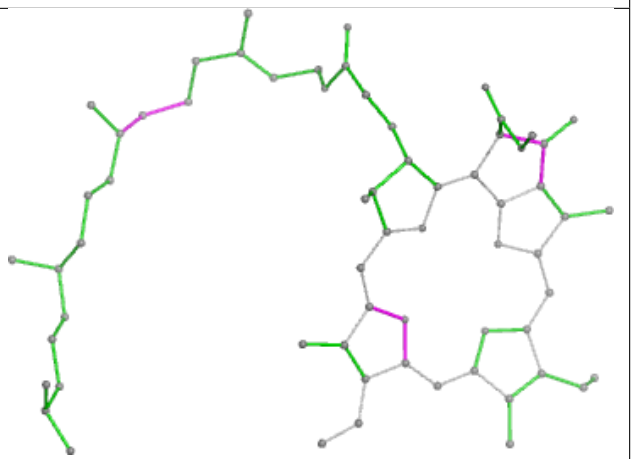


Rings

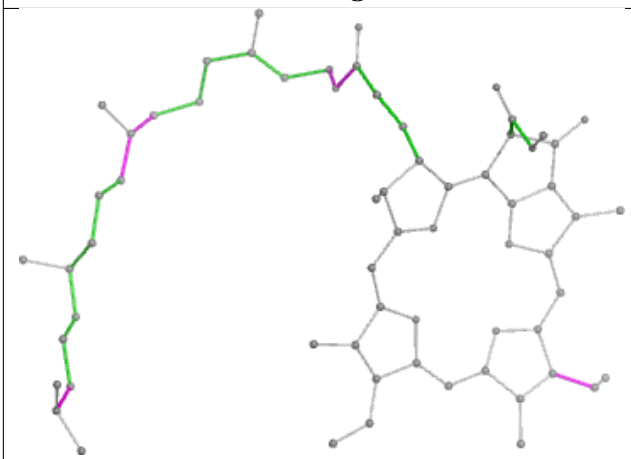
Ligand PHO D 405



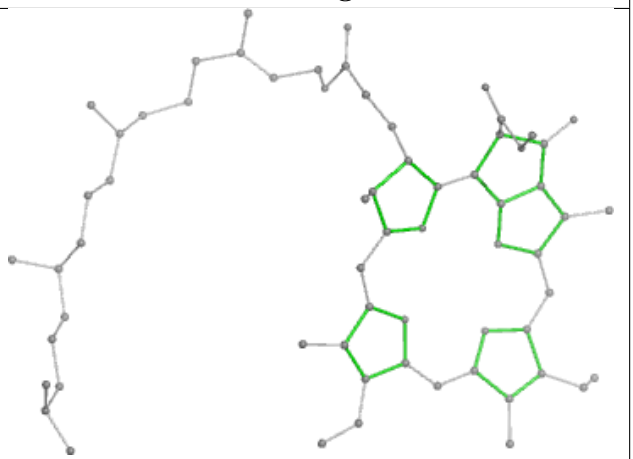
Bond lengths



Bond angles

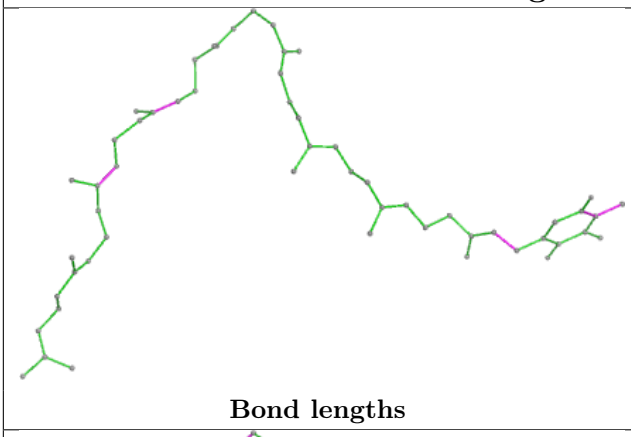


Torsions

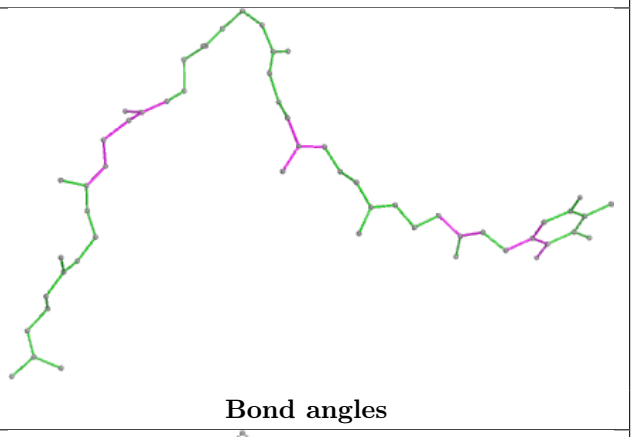


Rings

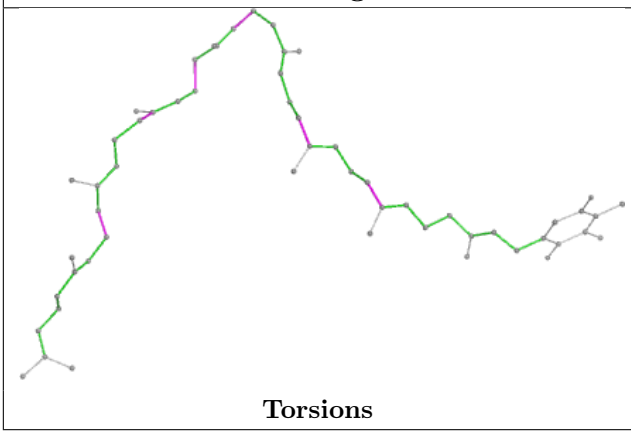
Ligand PL9 D 404



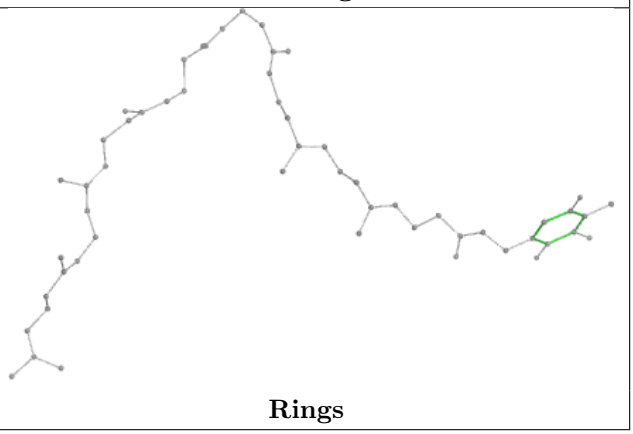
Bond lengths



Bond angles

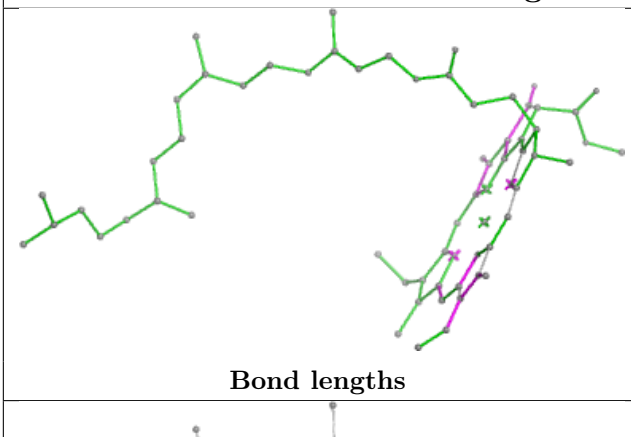


Torsions

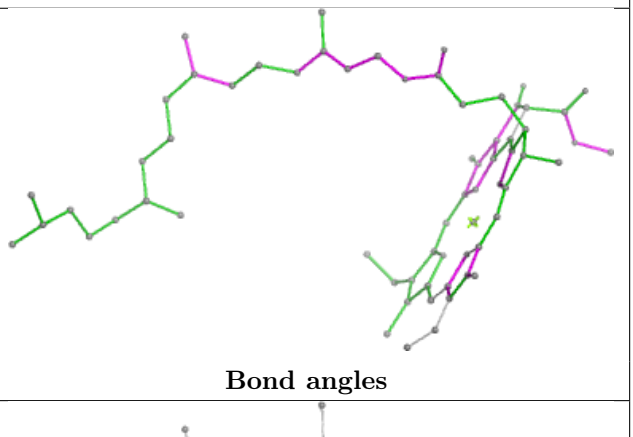


Rings

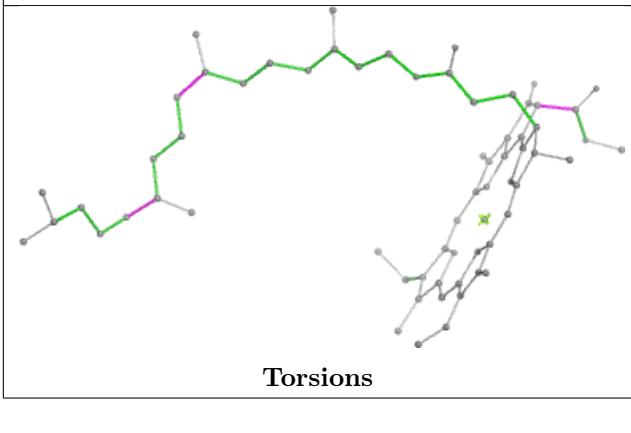
Ligand CLA C 509



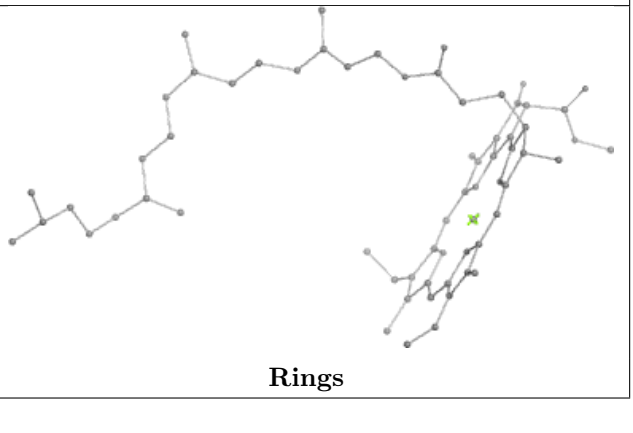
Bond lengths



Bond angles

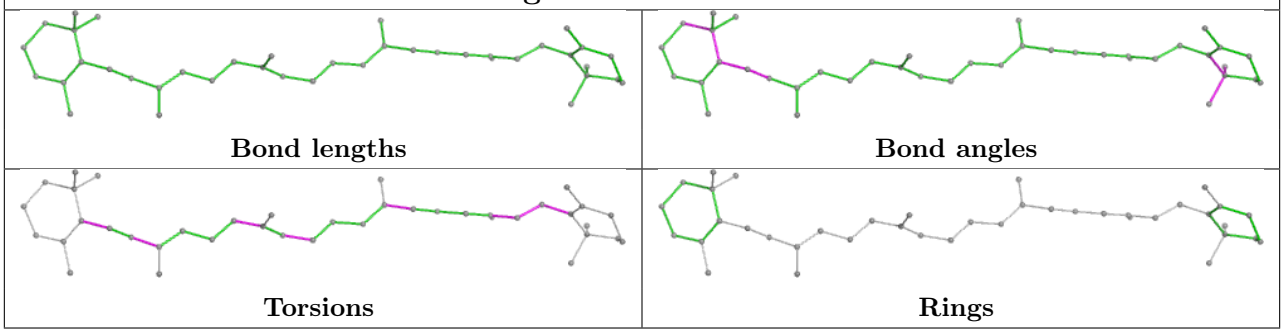


Torsions

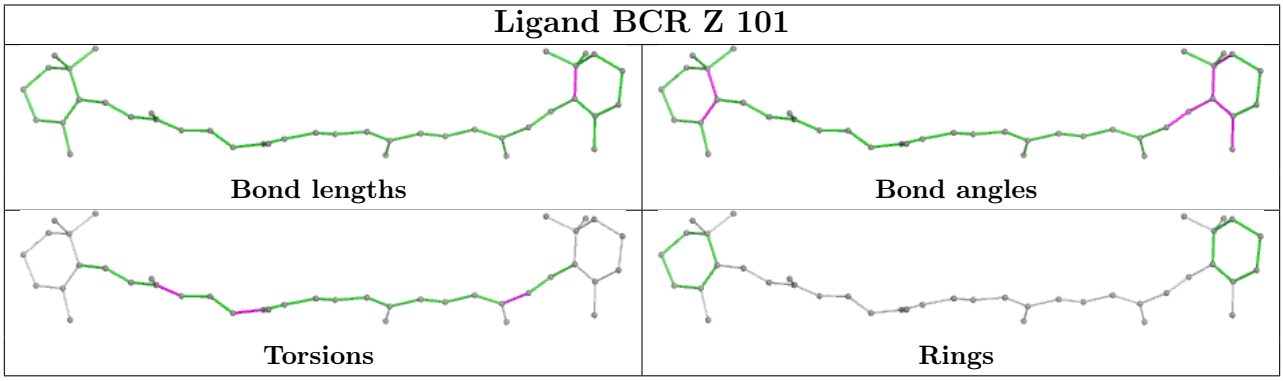


Rings

Ligand BCR C 516



Ligand BCR Z 101



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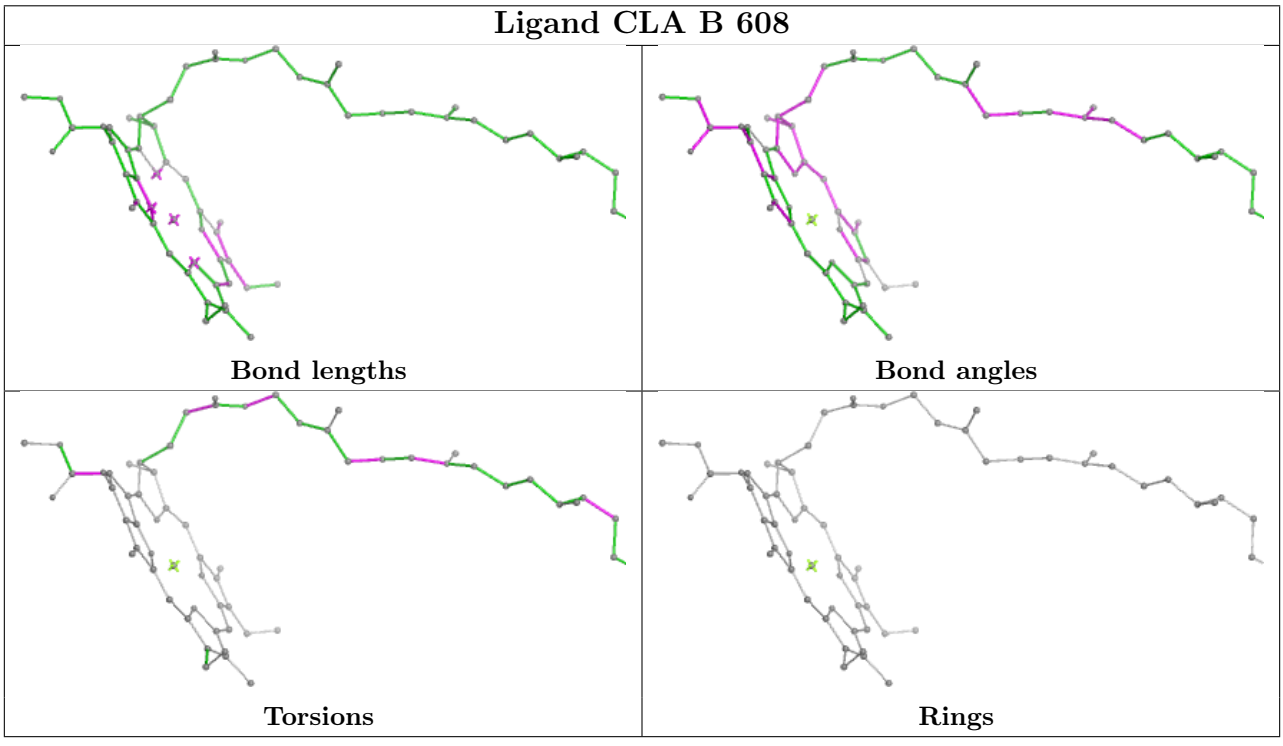

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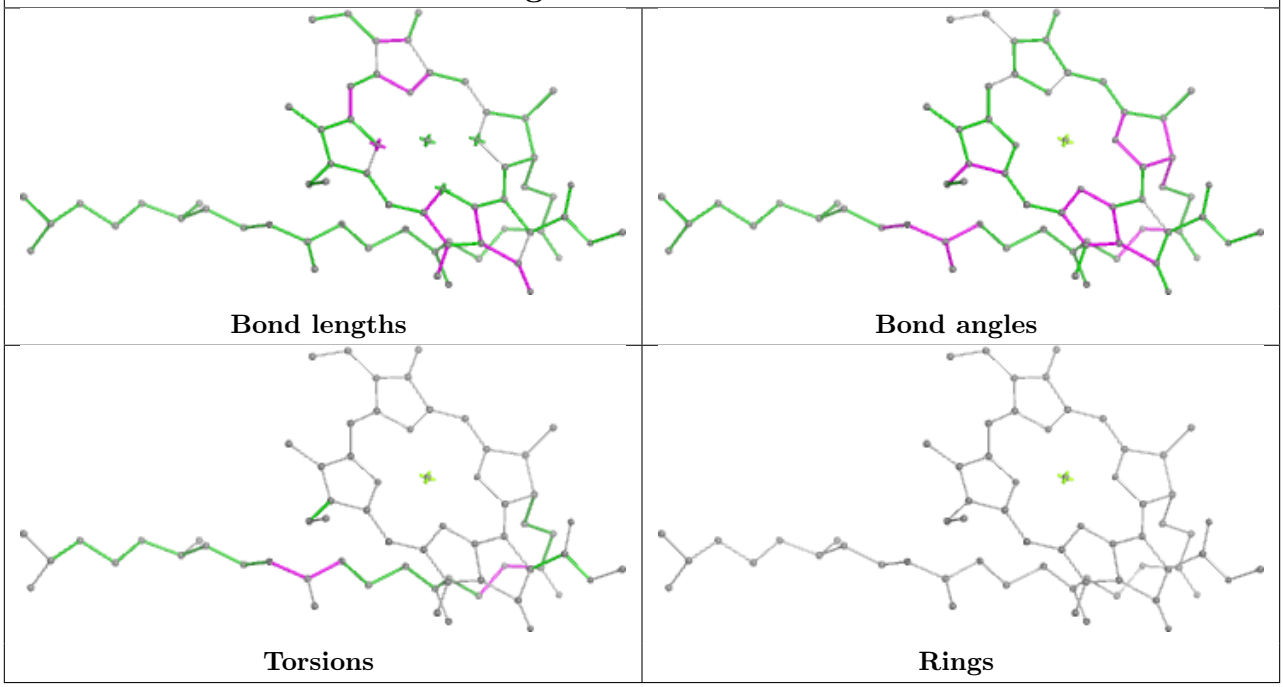

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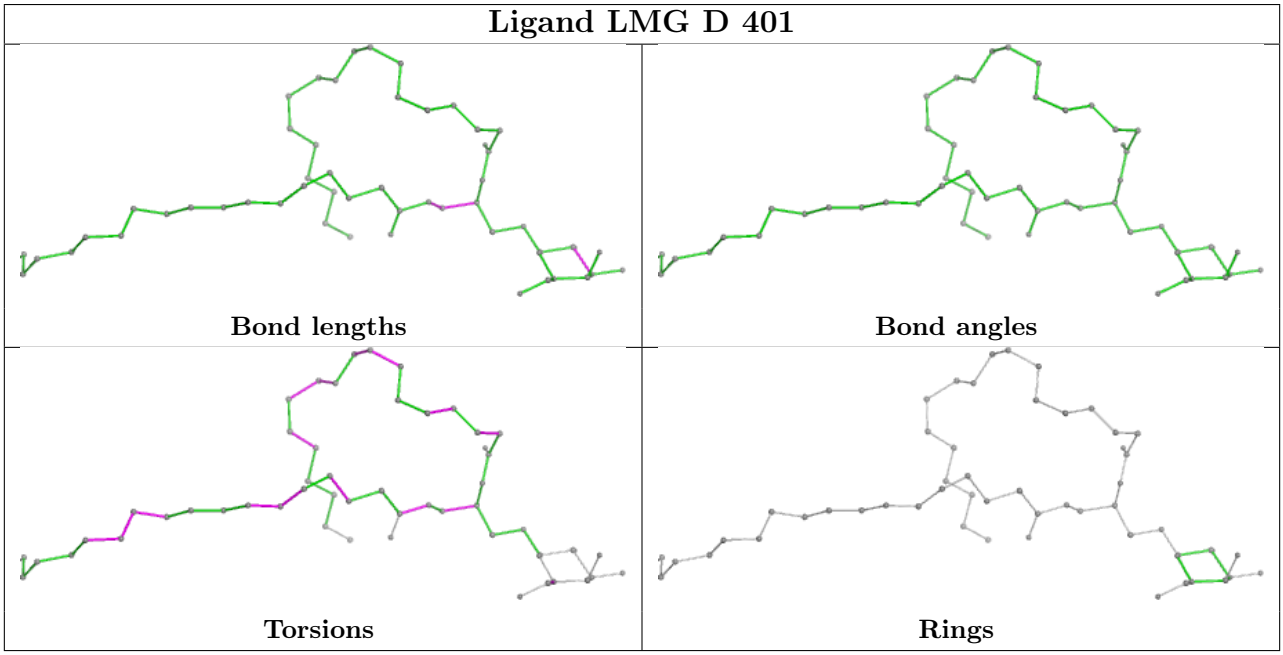

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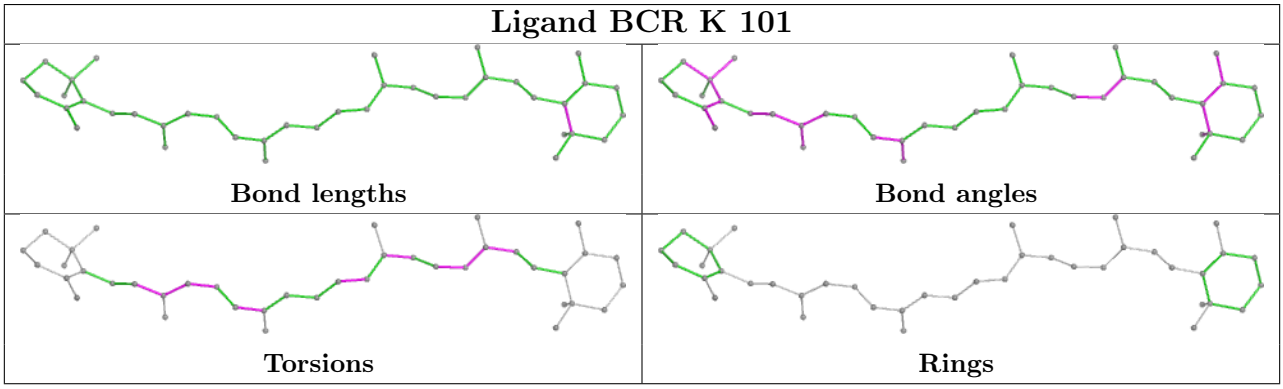


Ligand LMG M 101

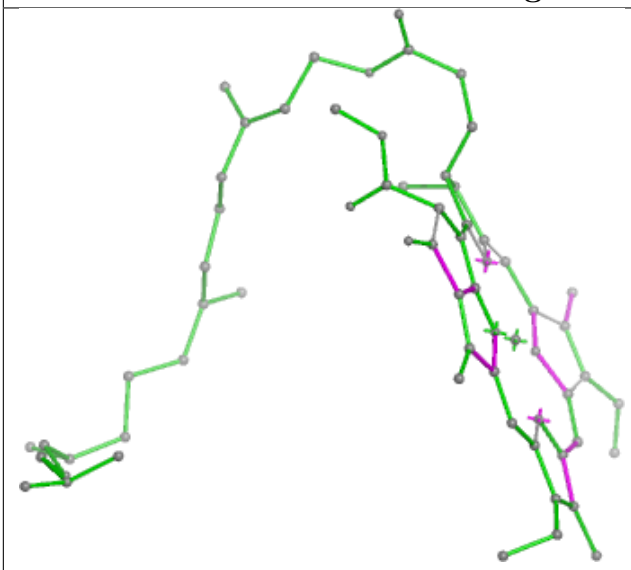
Bond lengths

Bond angles

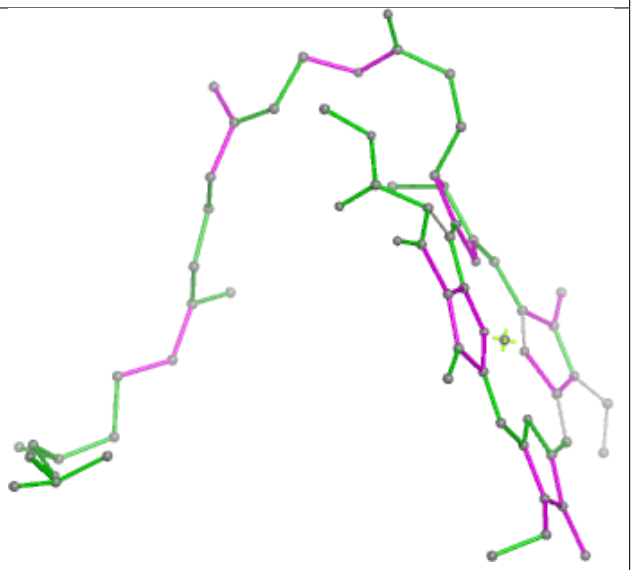
Torsions

Rings

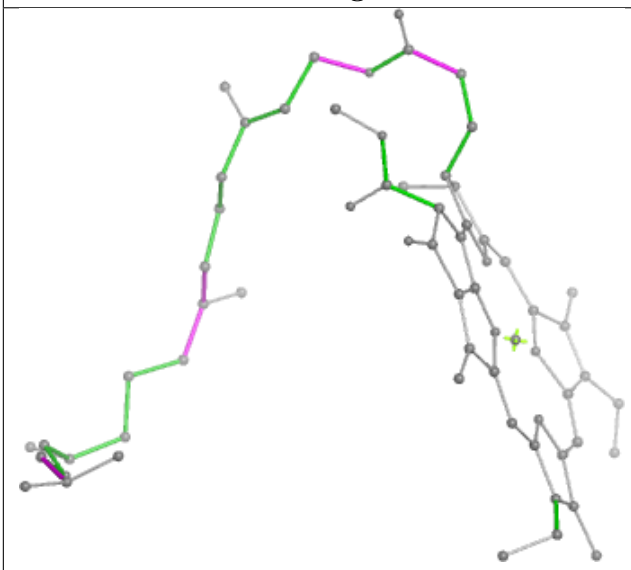
Ligand CLA B 614



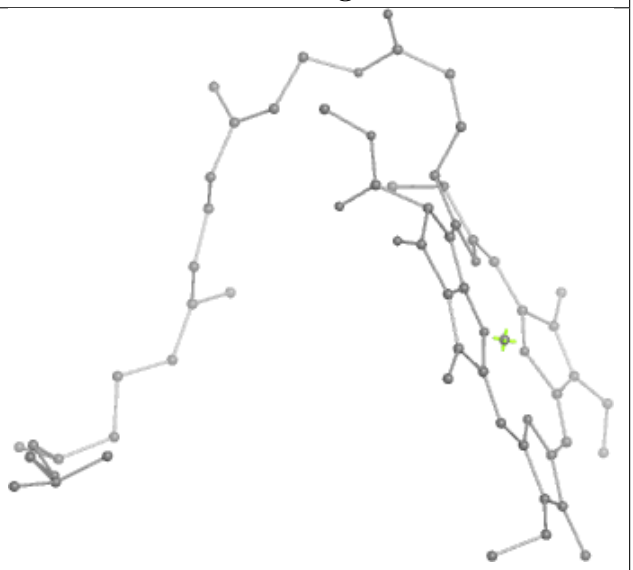
Bond lengths



Bond angles



Torsions



Rings

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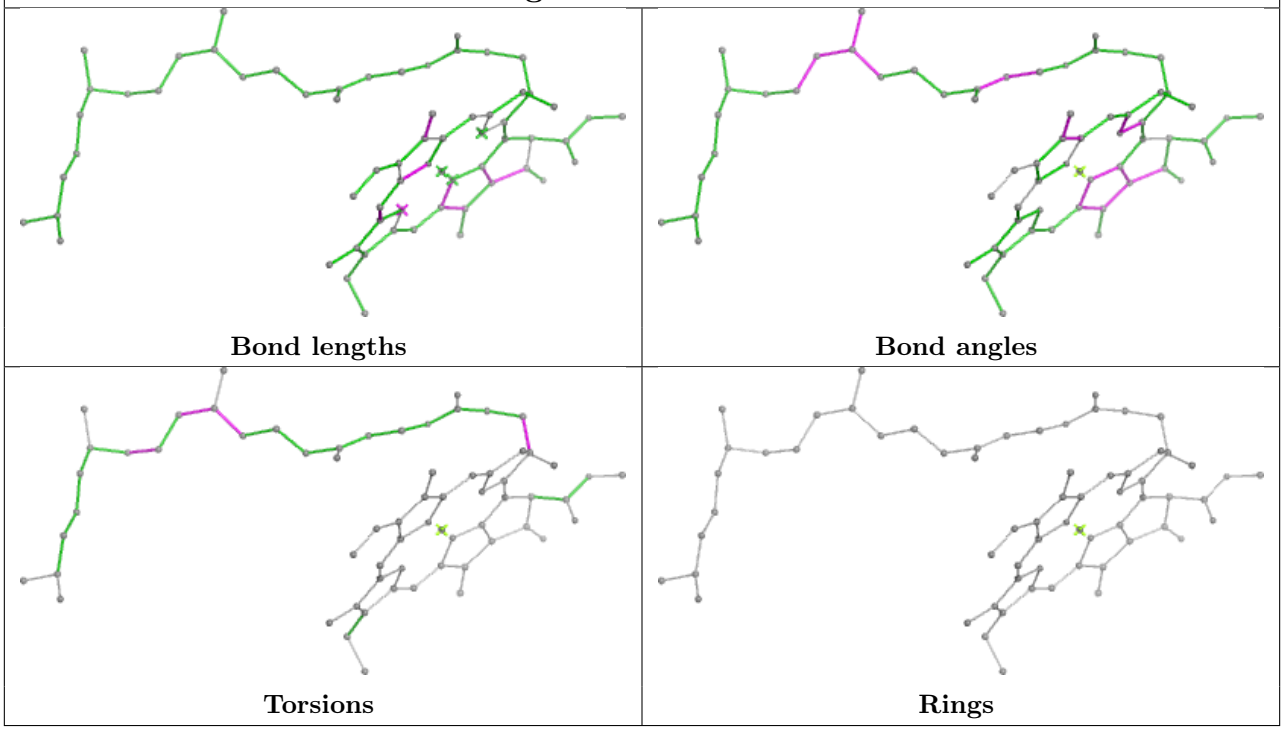
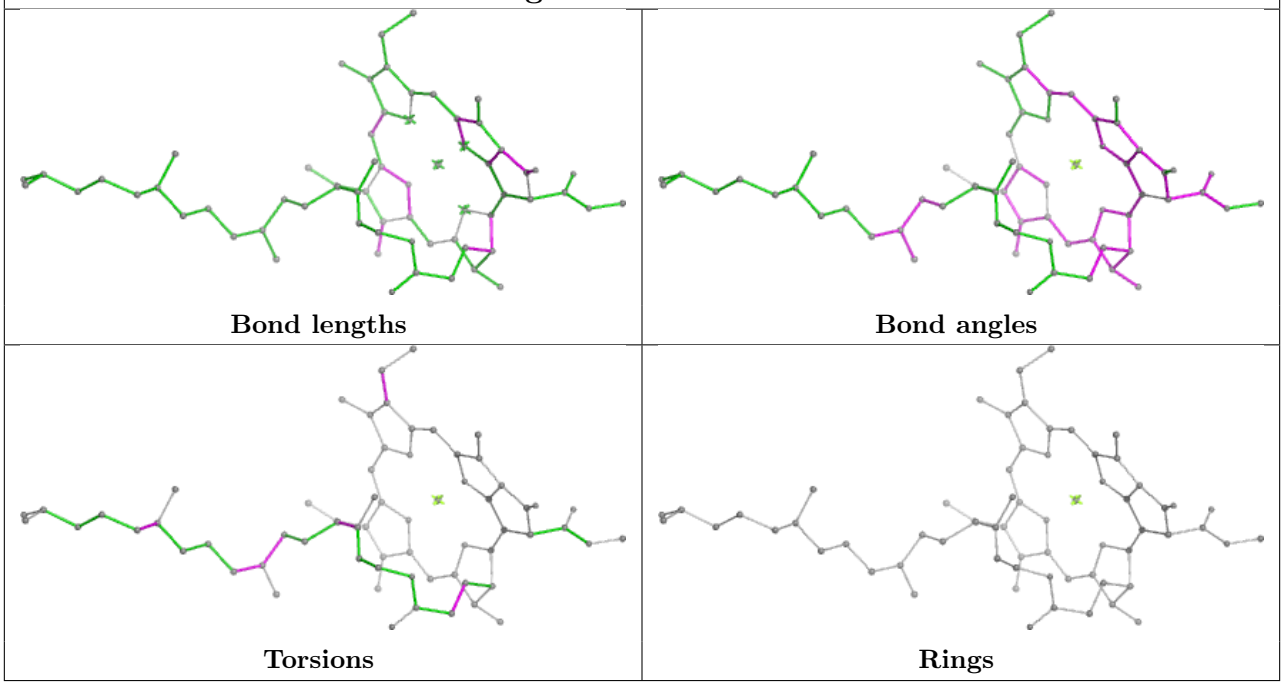
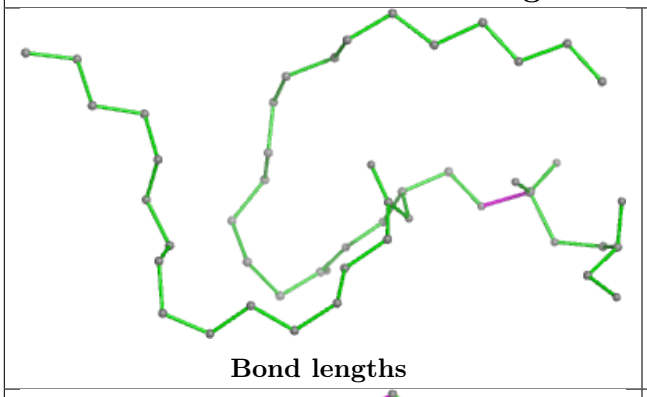


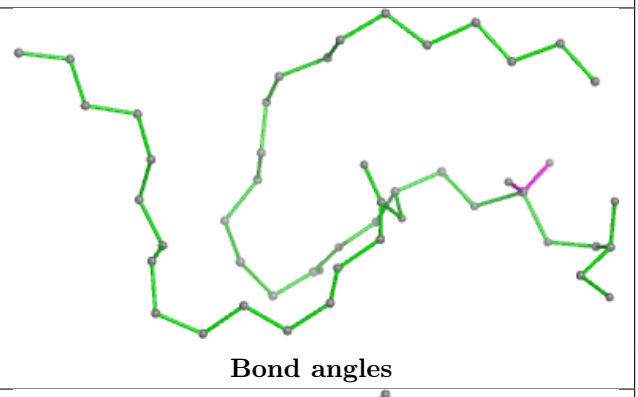
Ligand CLA C 506



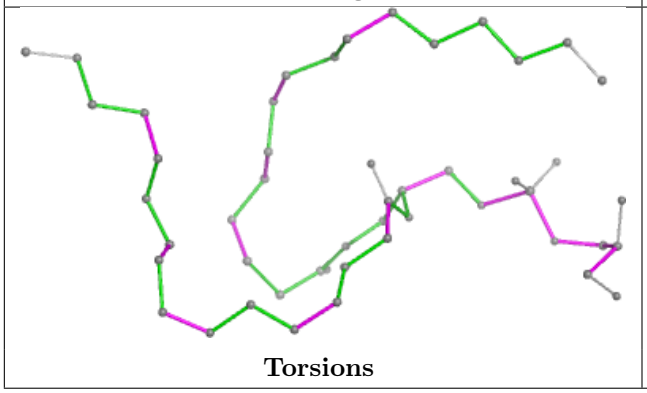
Ligand LHG A 411



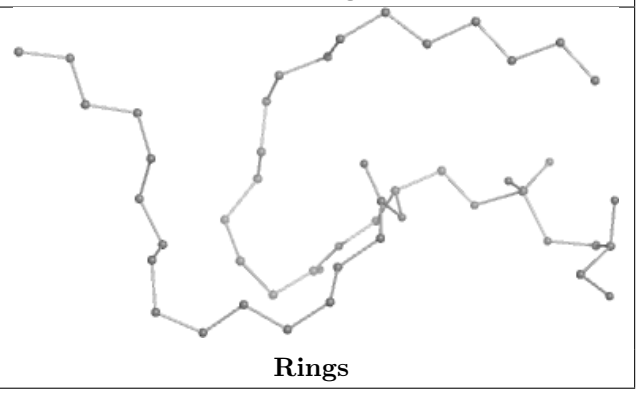
Bond lengths



Bond angles

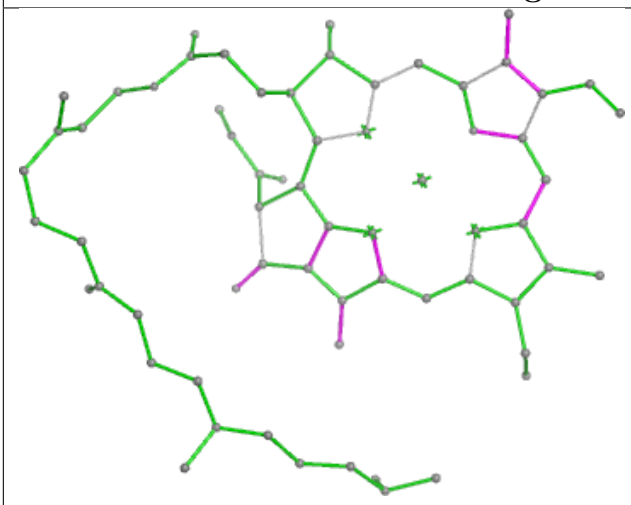


Torsions

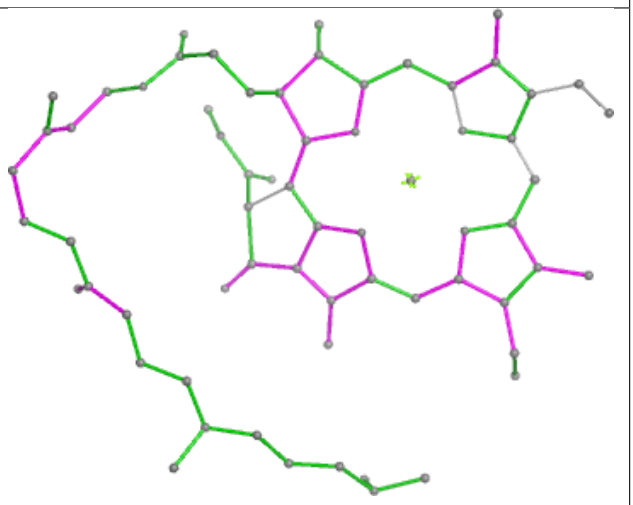


Rings

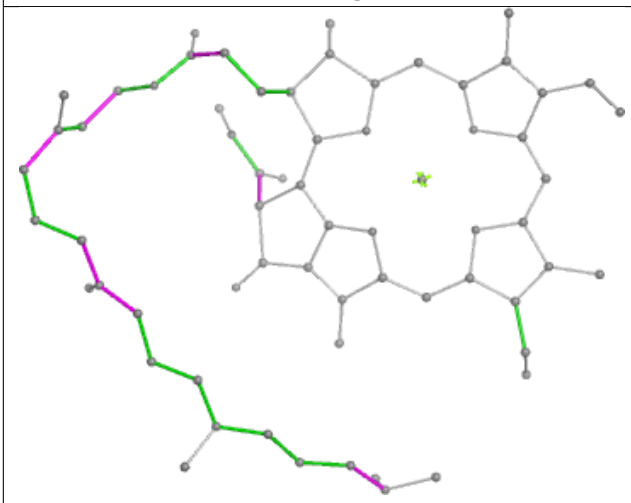
Ligand CLA B 602



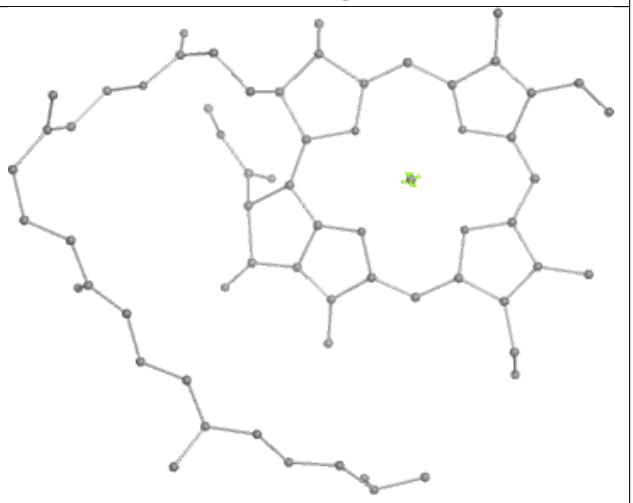
Bond lengths



Bond angles

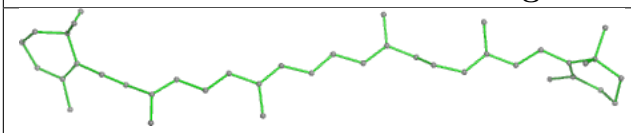


Torsions

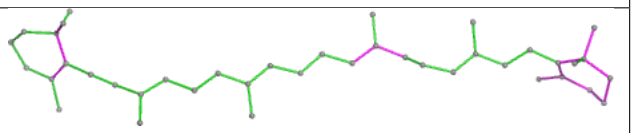


Rings

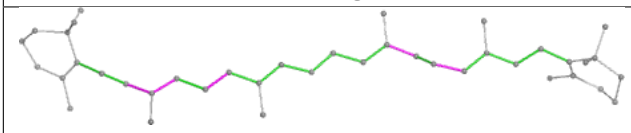
Ligand BCR C 514



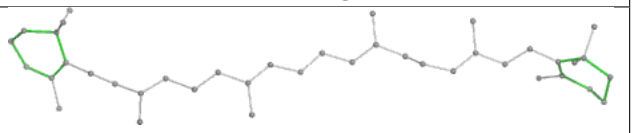
Bond lengths



Bond angles

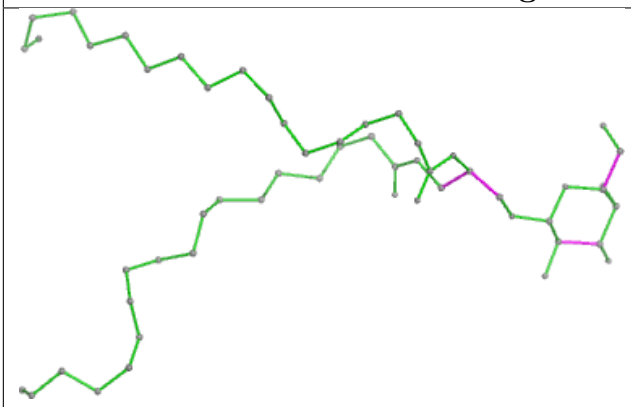


Torsions



Rings

Ligand LMG D 403



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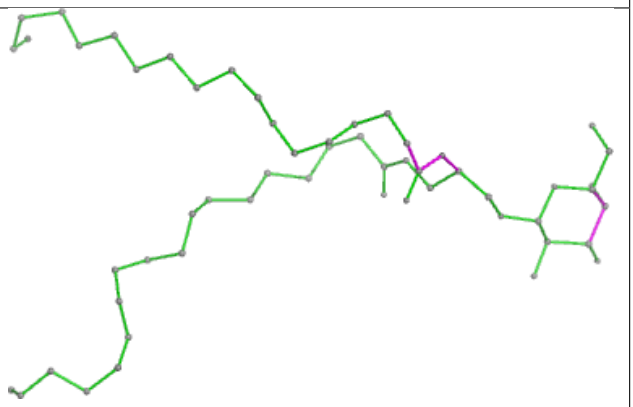
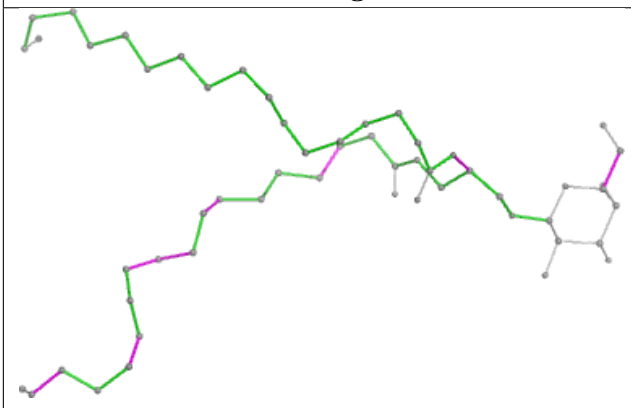
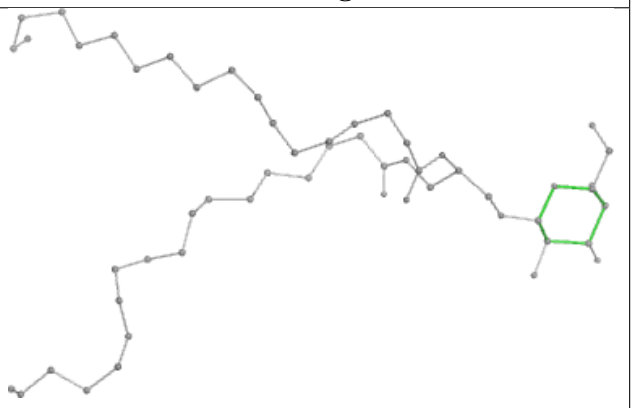


Bond angles

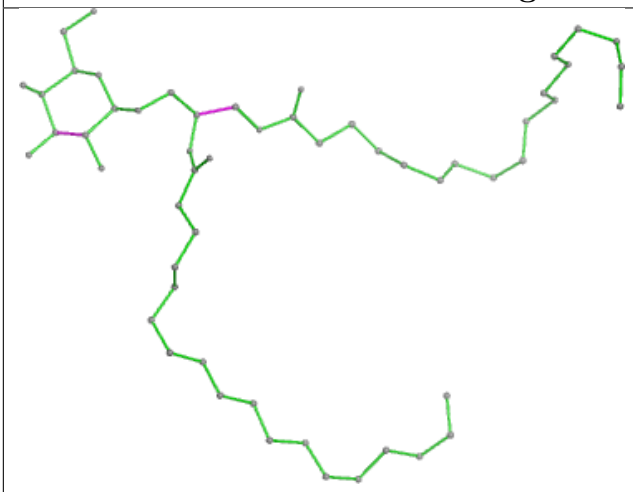


Torsions

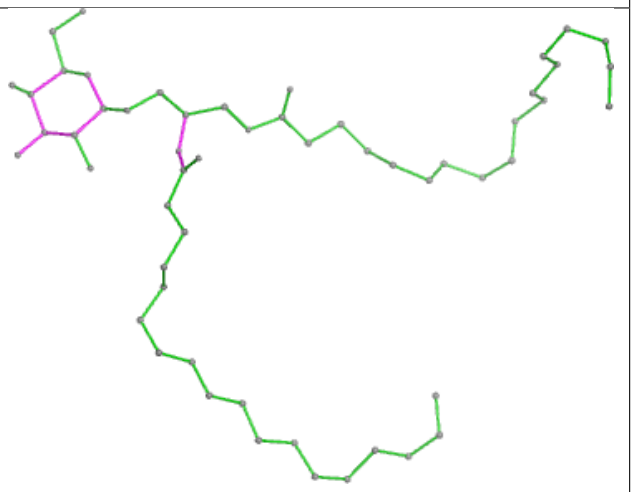


Rings

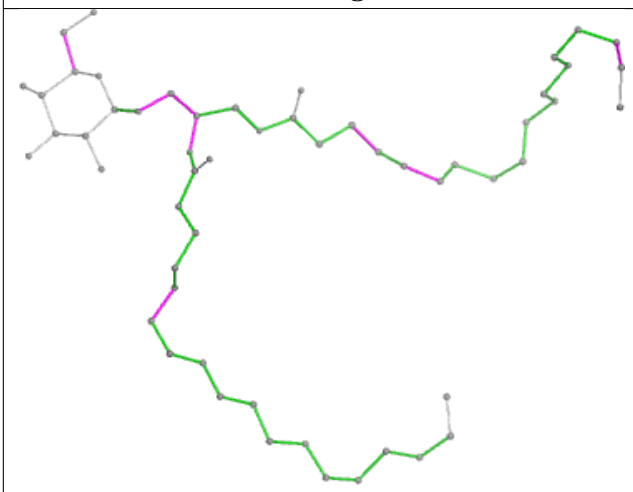
Ligand LMG D 402



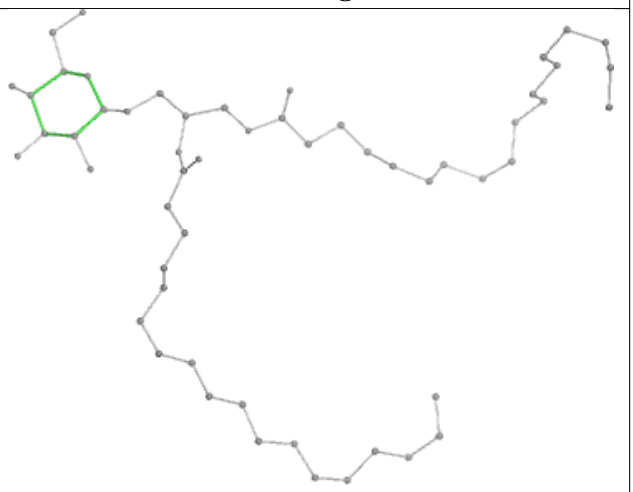
Bond lengths



Bond angles

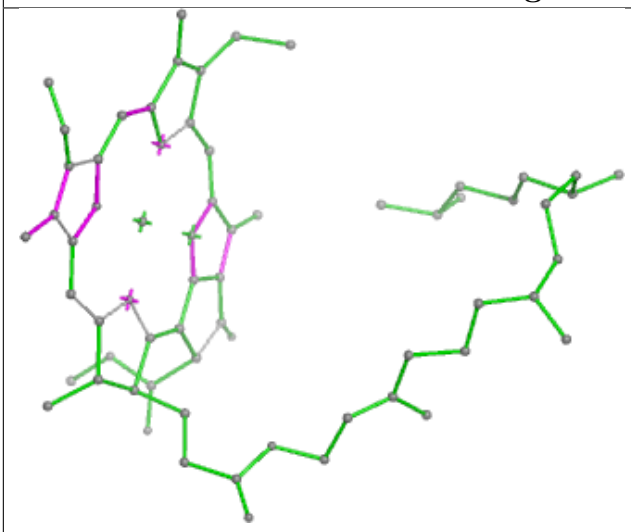


Torsions

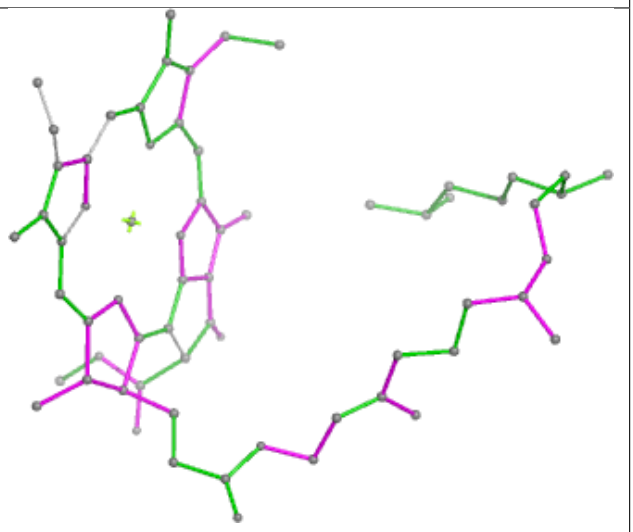


Rings

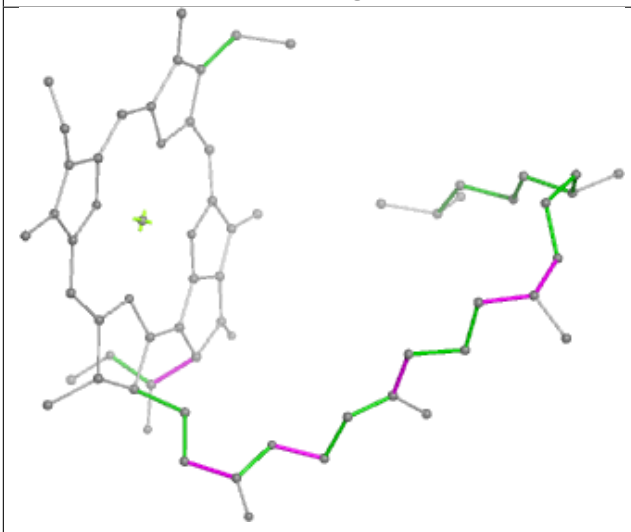
Ligand CLA C 504



Bond lengths



Bond angles



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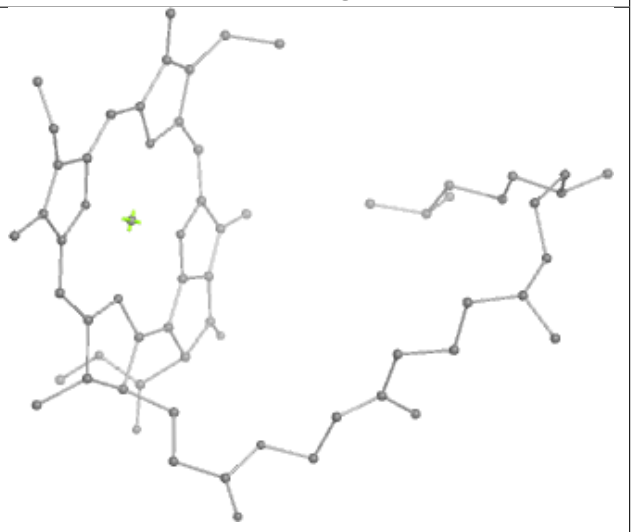
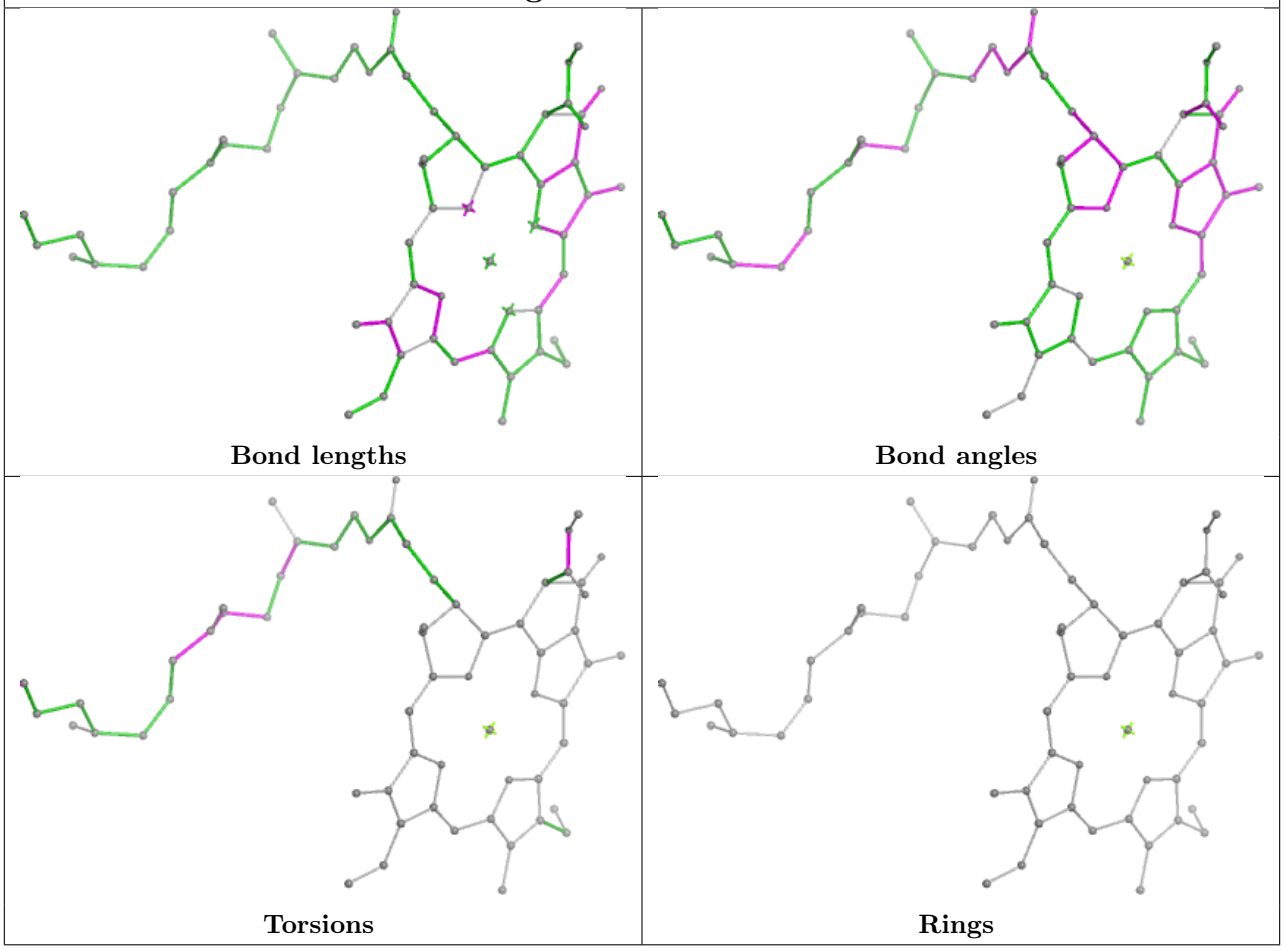
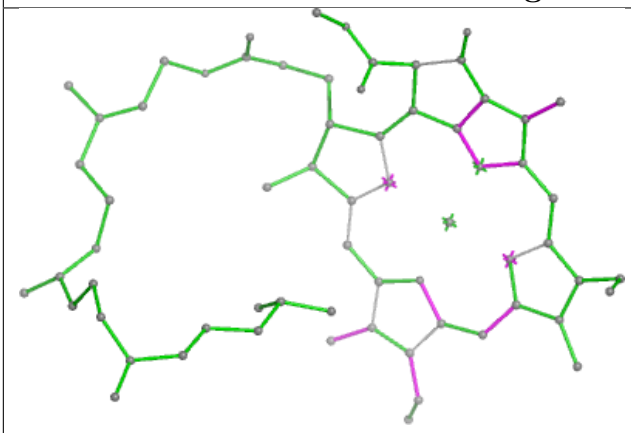


Rings

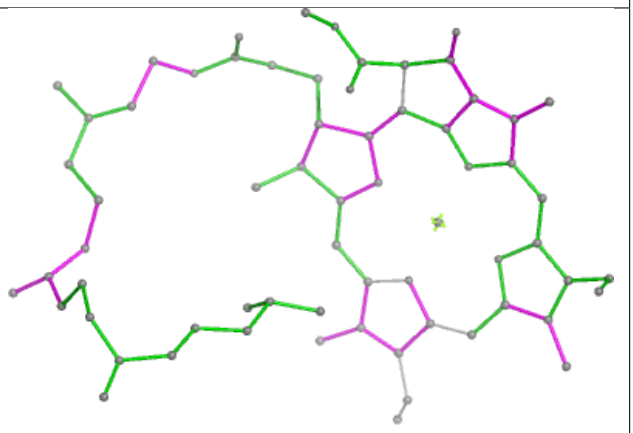
Ligand CLA C 511



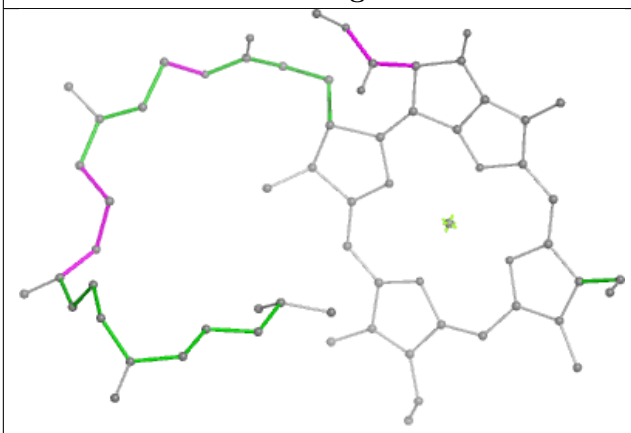
Ligand CLA B 616



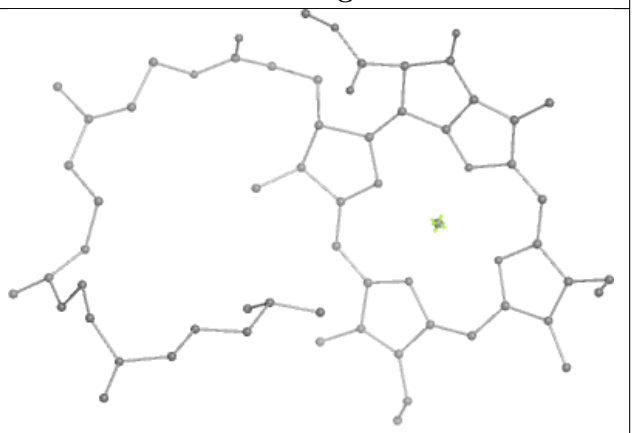
Bond lengths



Bond angles

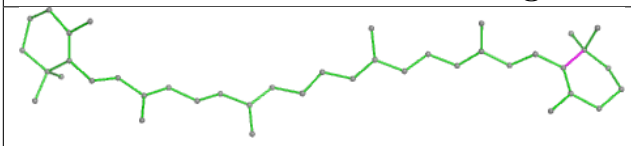


Torsions

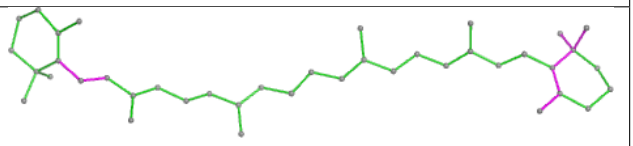


Rings

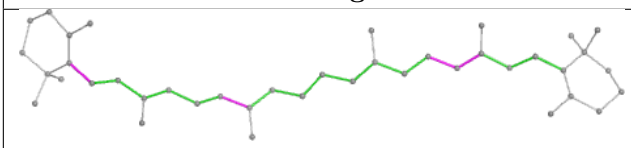
Ligand BCR B 618



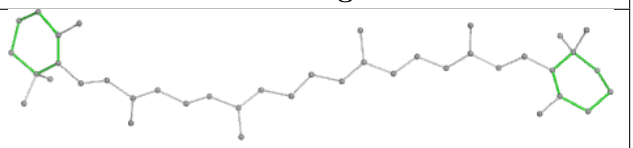
Bond lengths



Bond angles

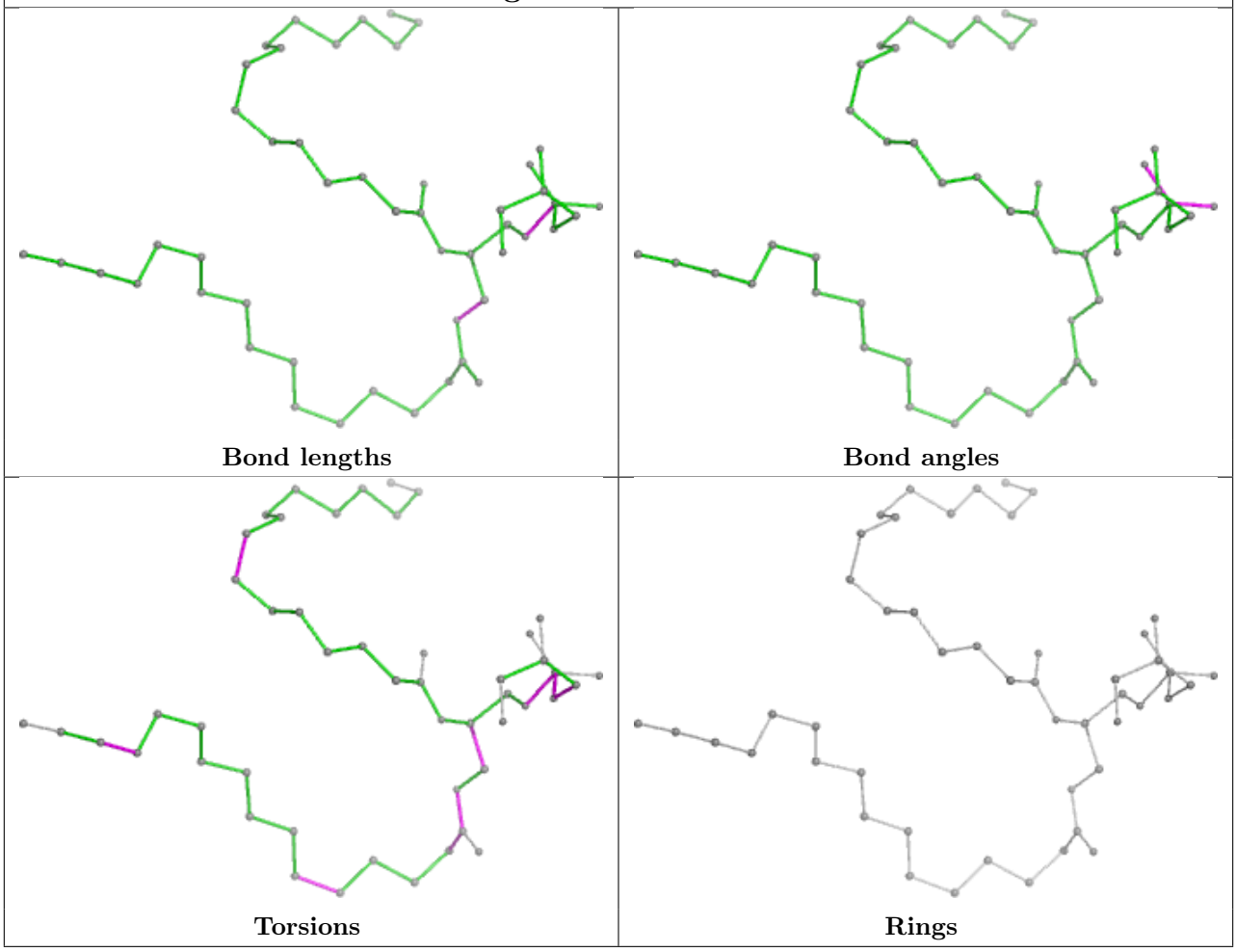


Torsions

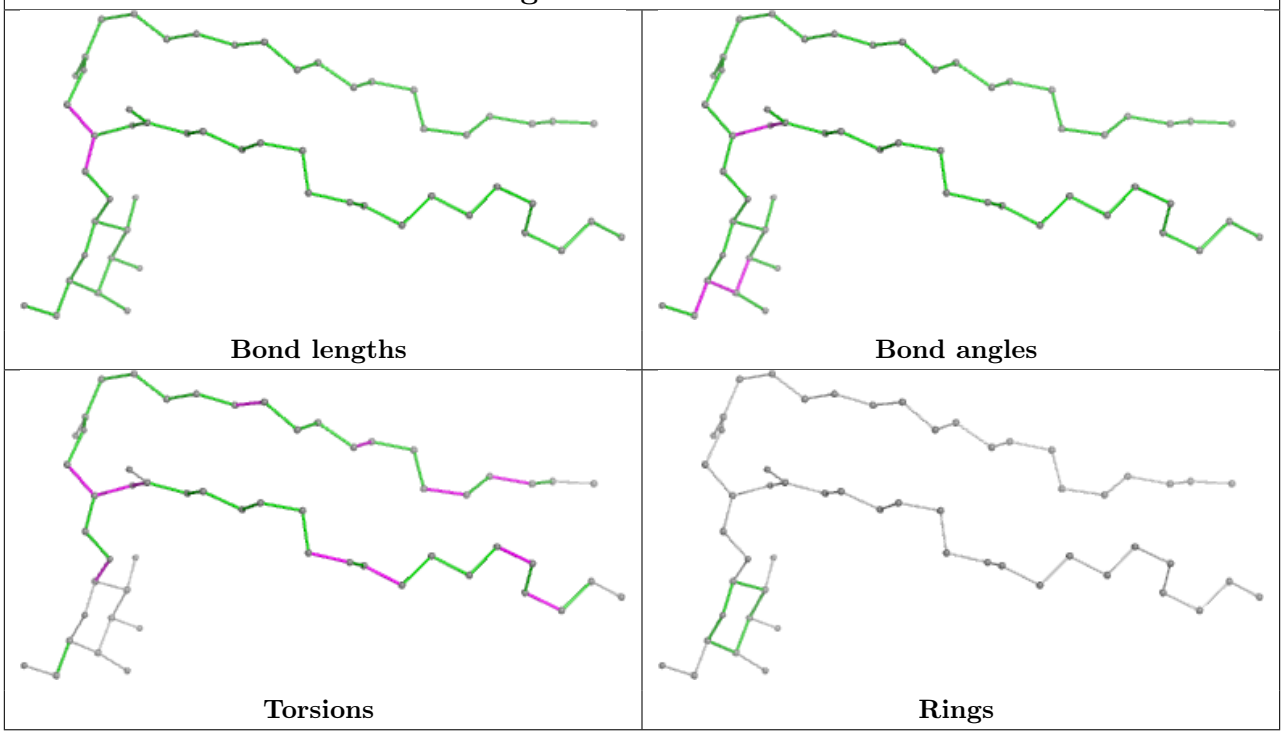


Rings

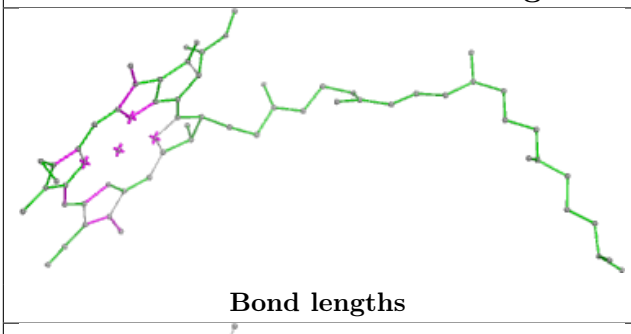
Ligand LHG A 410



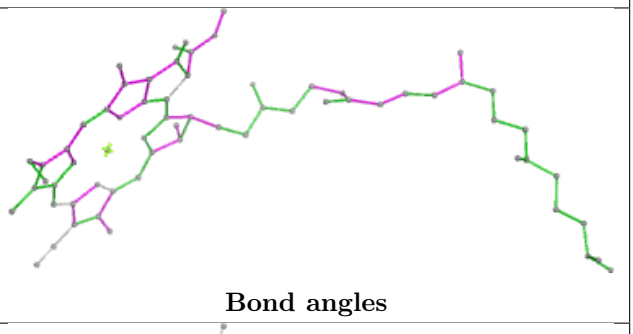
Ligand LMG C 501



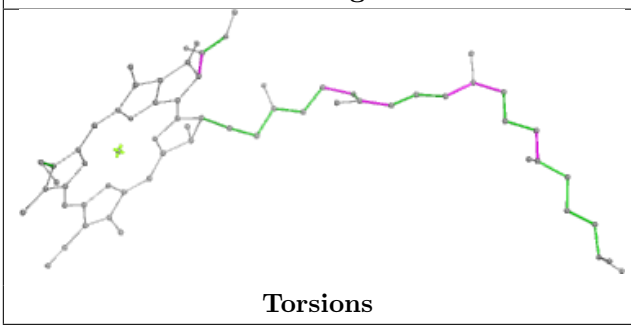
Ligand CLA A 405



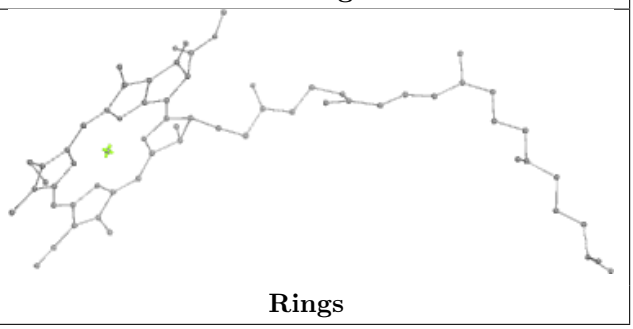
Bond lengths



Bond angles

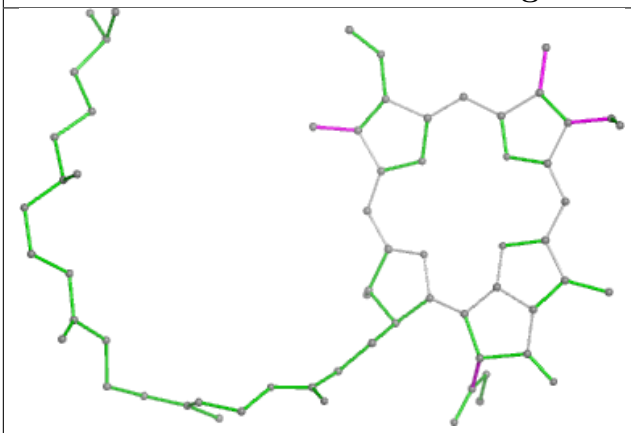


Torsions



Rings

Ligand PHO A 404



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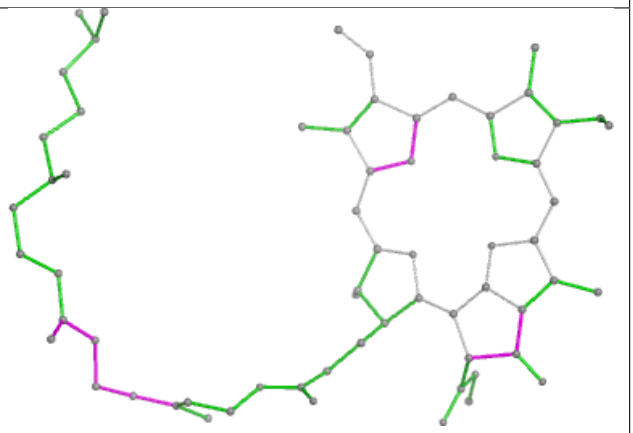
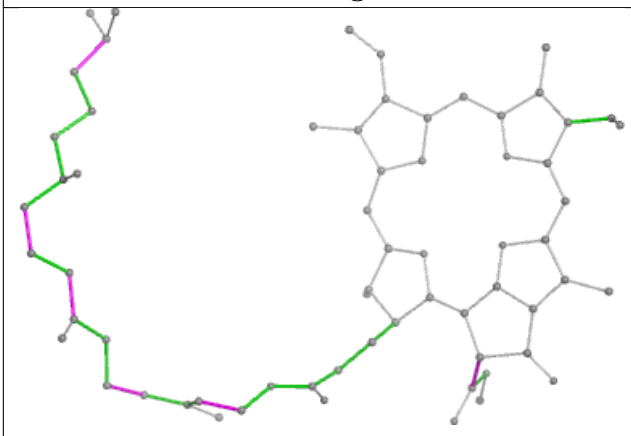
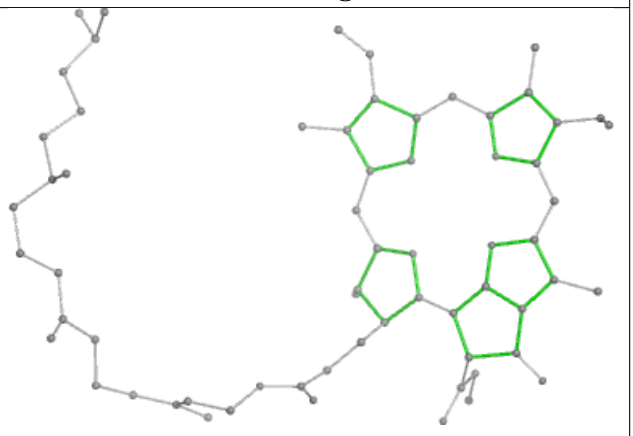


Bond angles

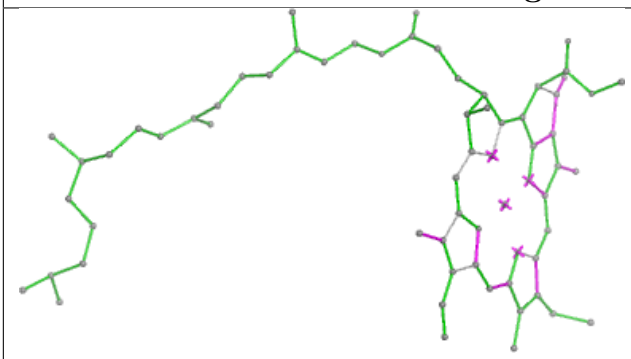


Torsions

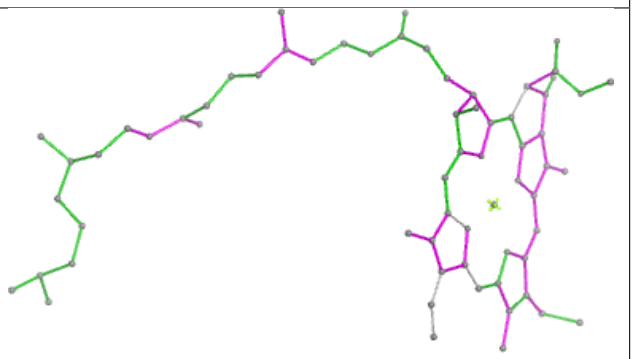


Rings

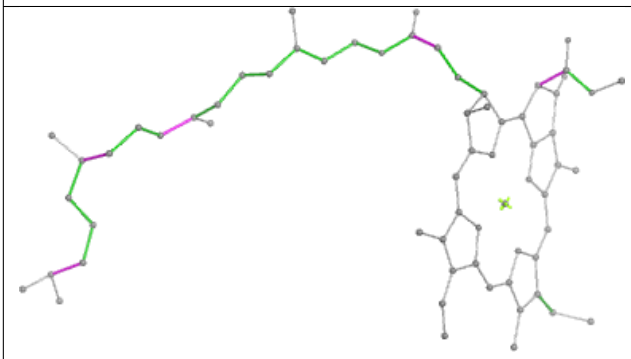
Ligand CLA B 610



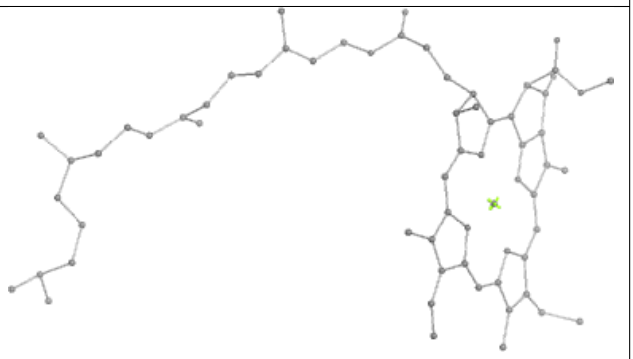
Bond lengths



Bond angles

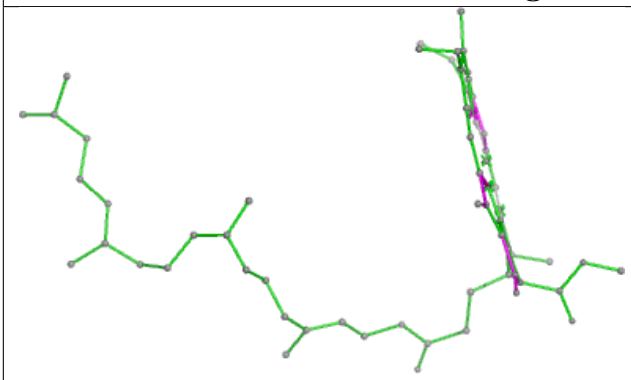


Torsions

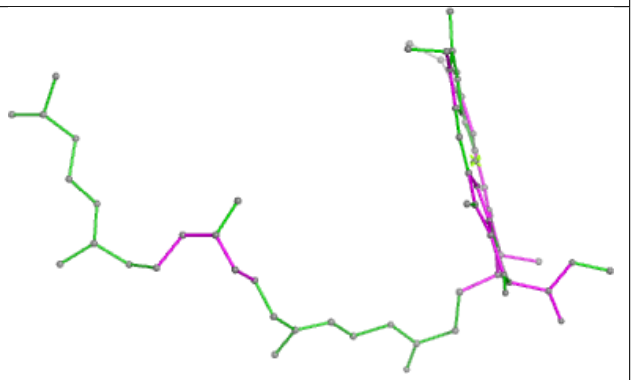


Rings

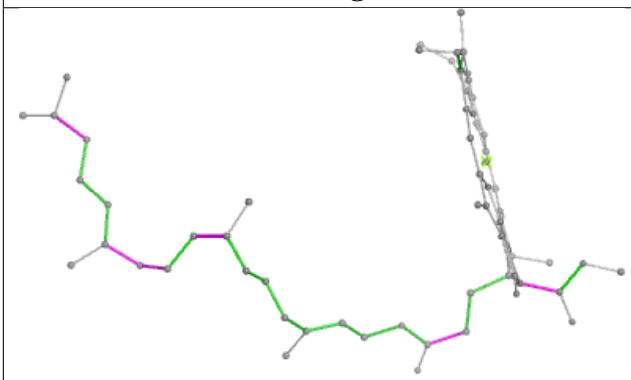
Ligand CLA C 507



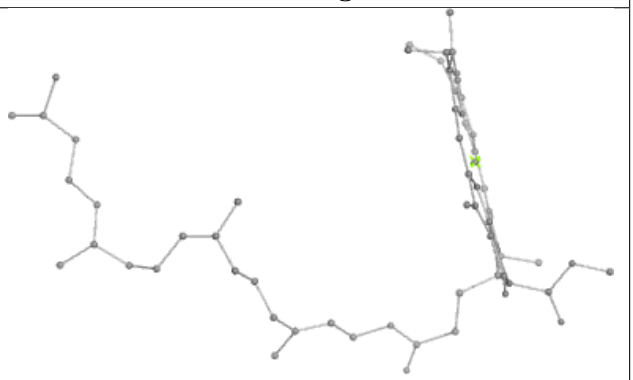
Bond lengths



Bond angles

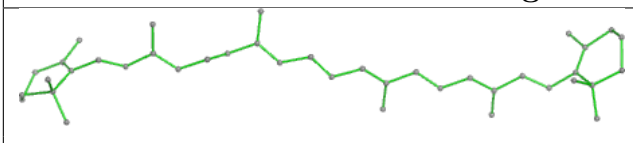


Torsions

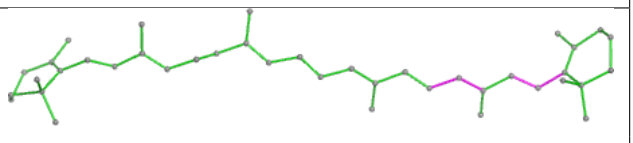


Rings

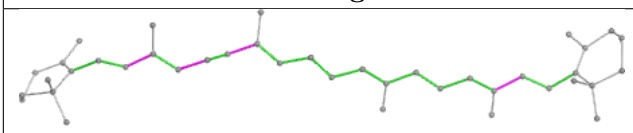
Ligand BCR A 409



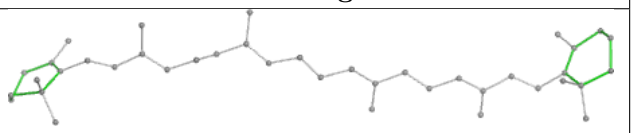
Bond lengths



Bond angles

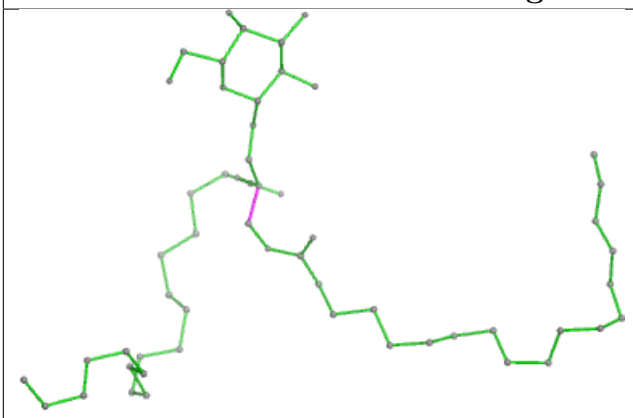


Torsions

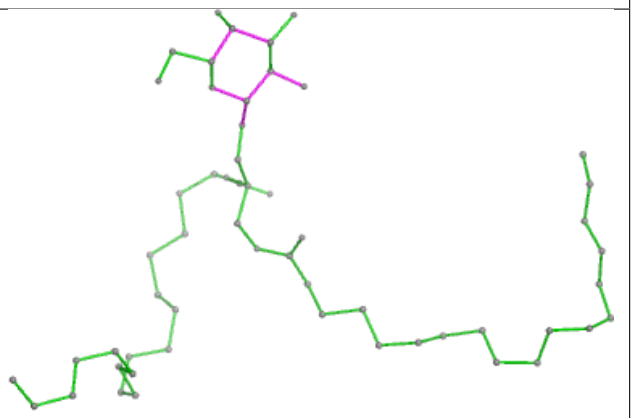


Rings

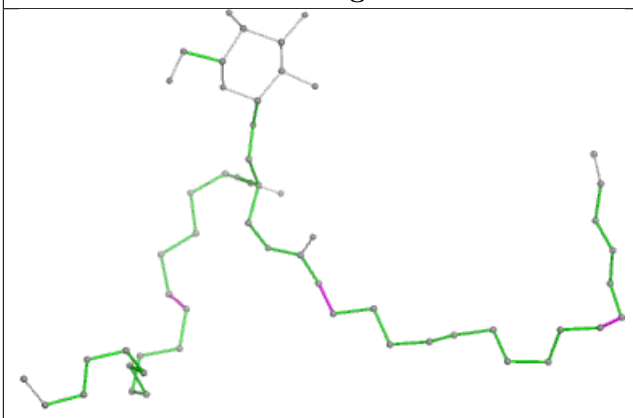
Ligand LMG I 101



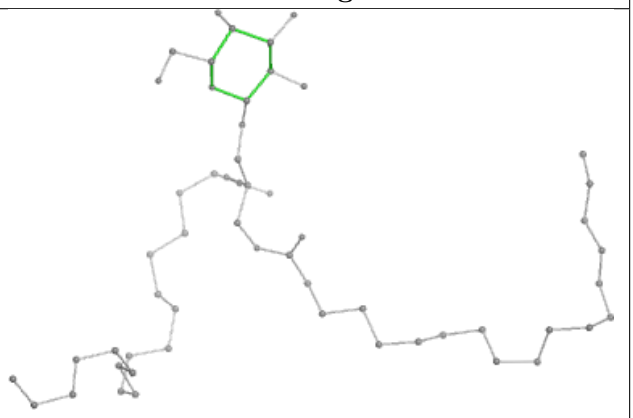
Bond lengths



Bond angles

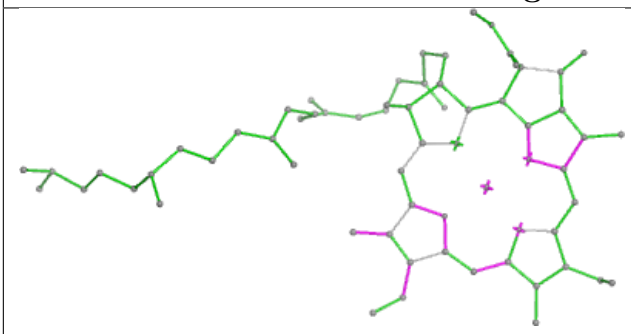


Torsions

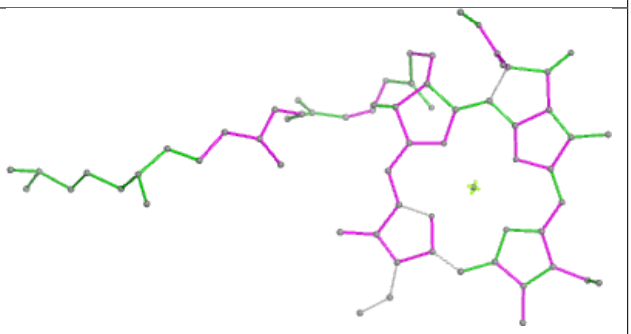


Rings

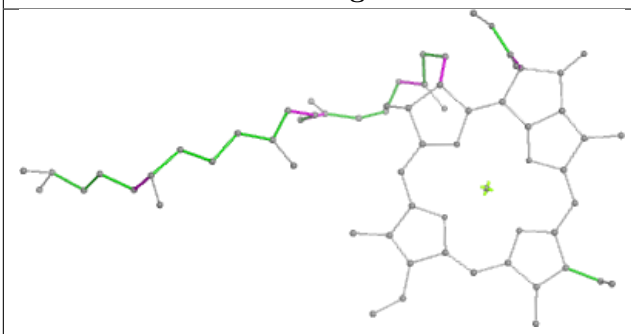
Ligand CLA A 406



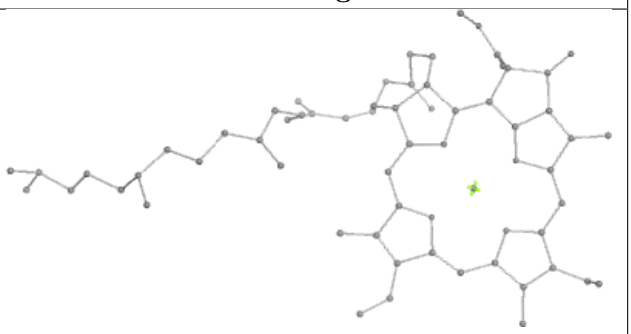
Bond lengths



Bond angles

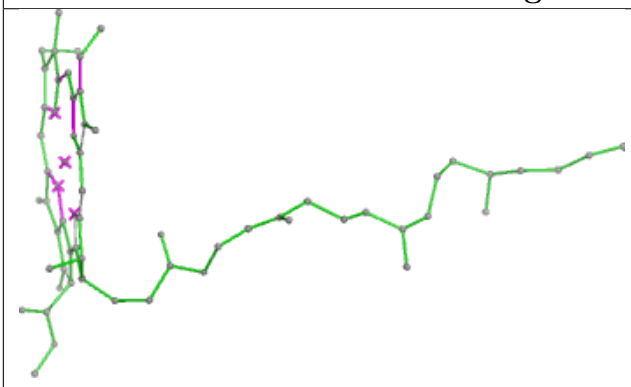


Torsions

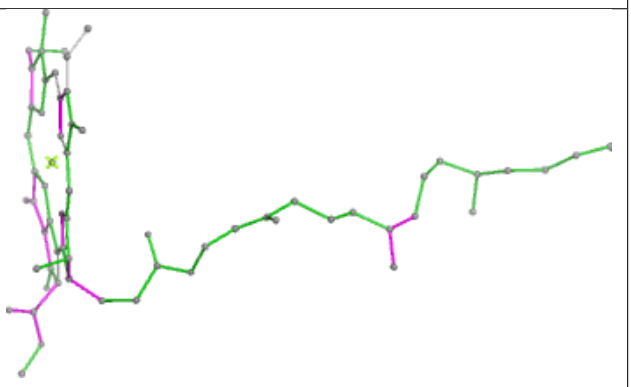


Rings

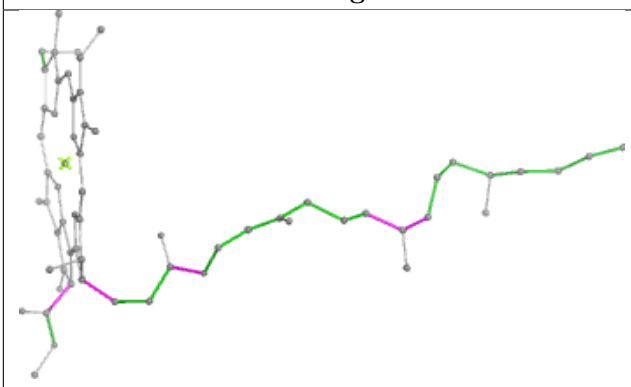
Ligand CLA B 607



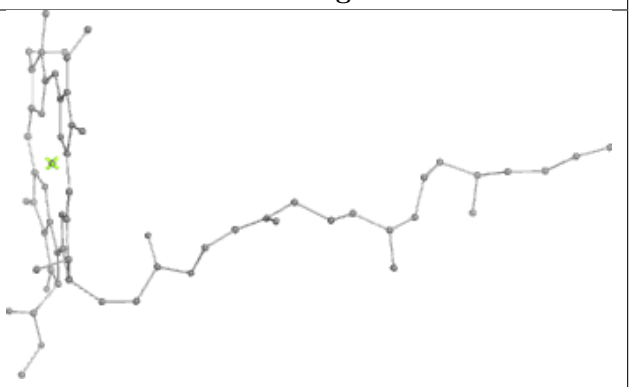
Bond lengths



Bond angles

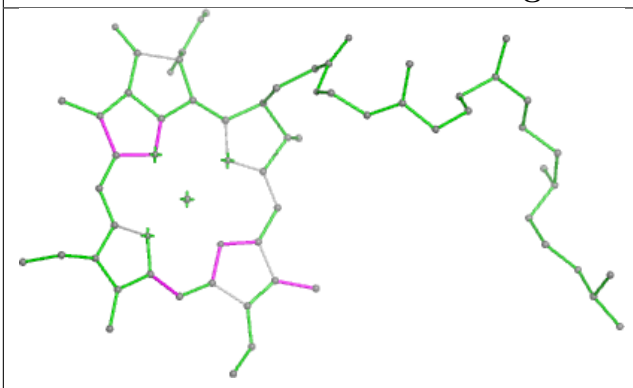


Torsions

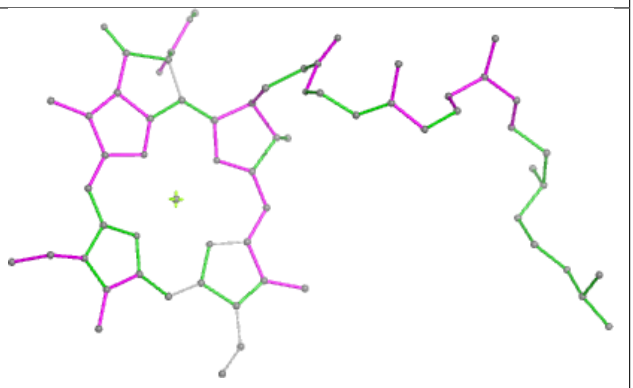


Rings

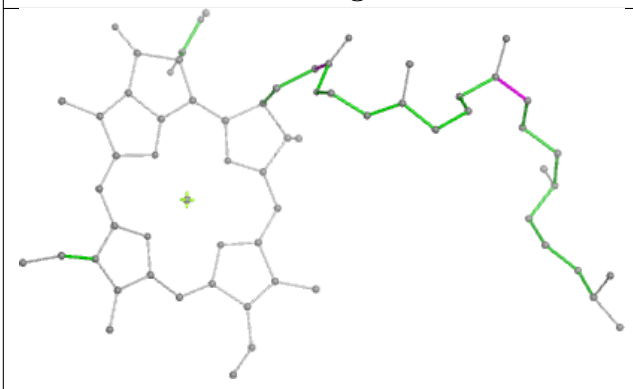
Ligand CLA A 407



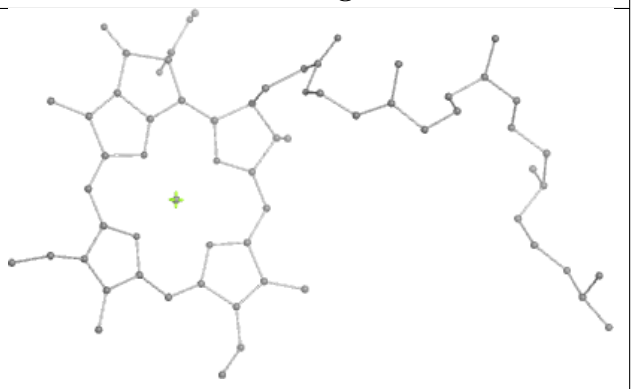
Bond lengths



Bond angles

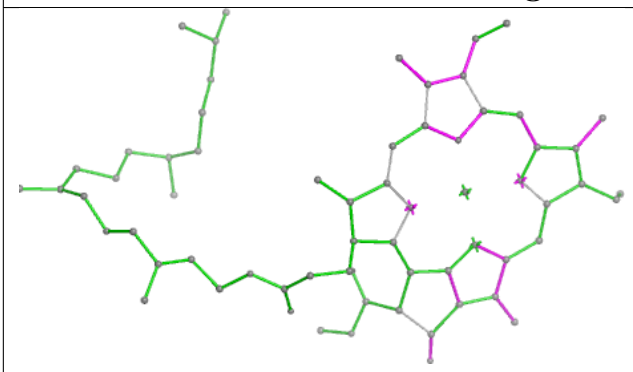


Torsions

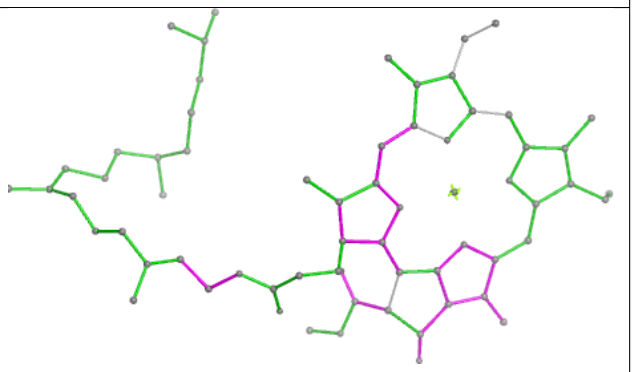


Rings

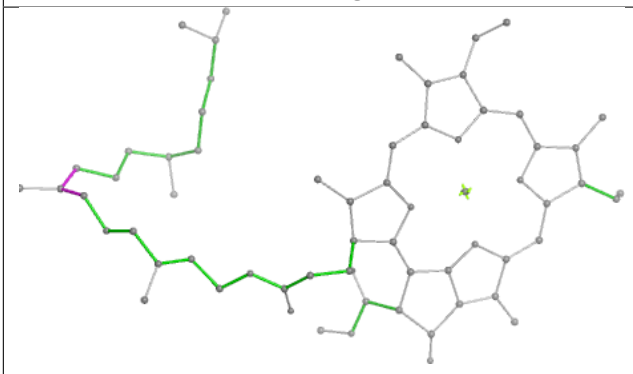
Ligand CLA B 617



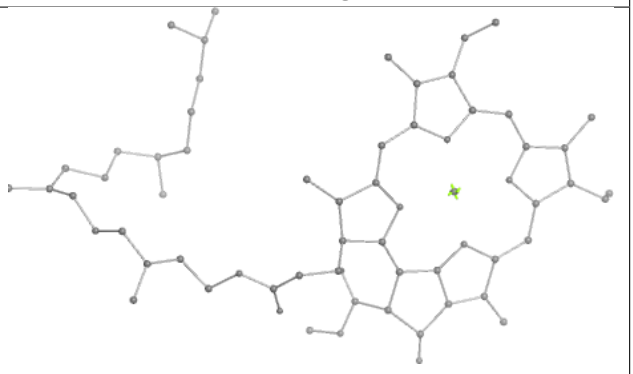
Bond lengths



Bond angles

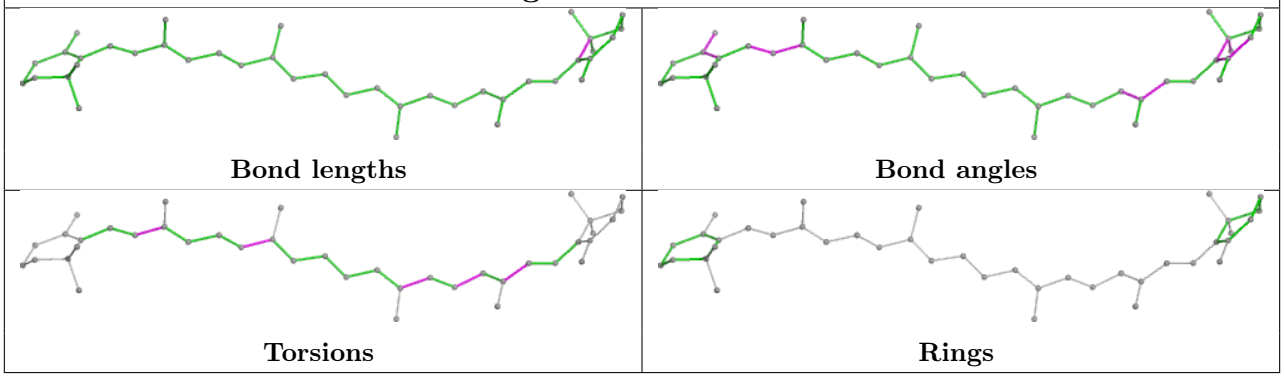


Torsions

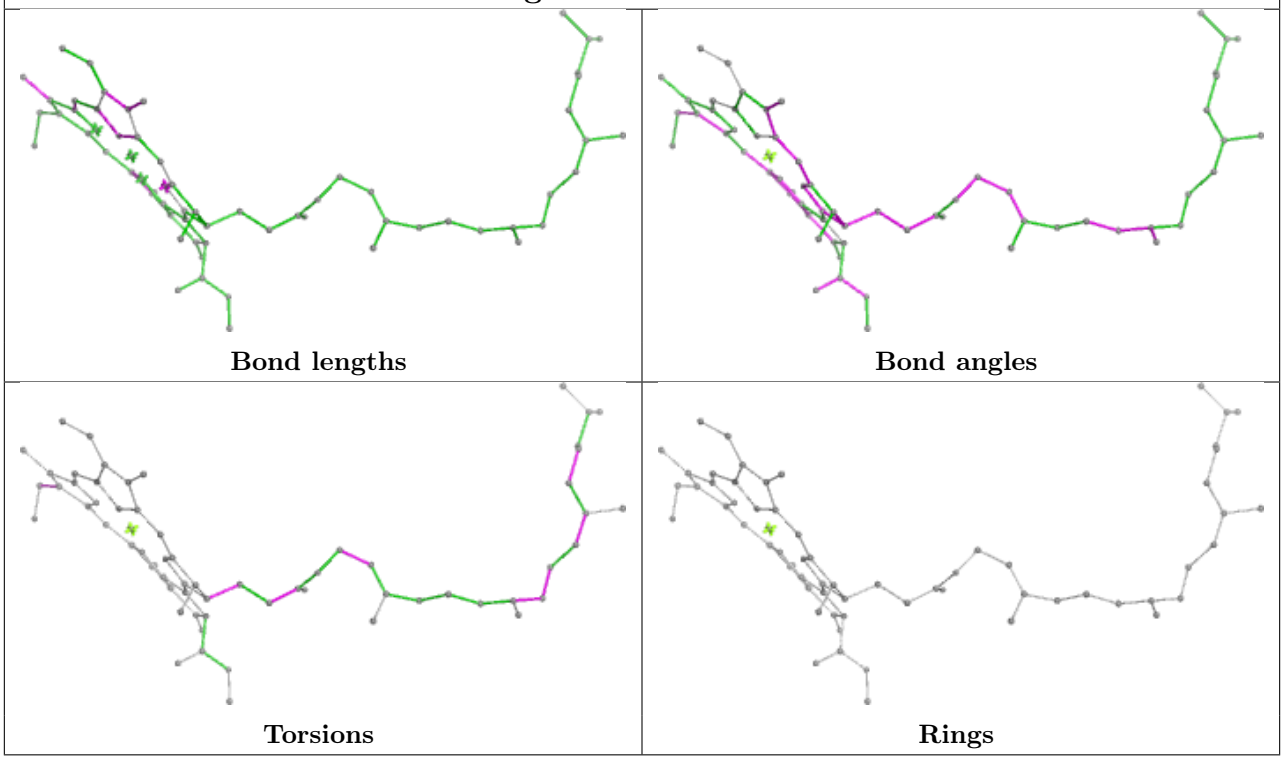


Rings

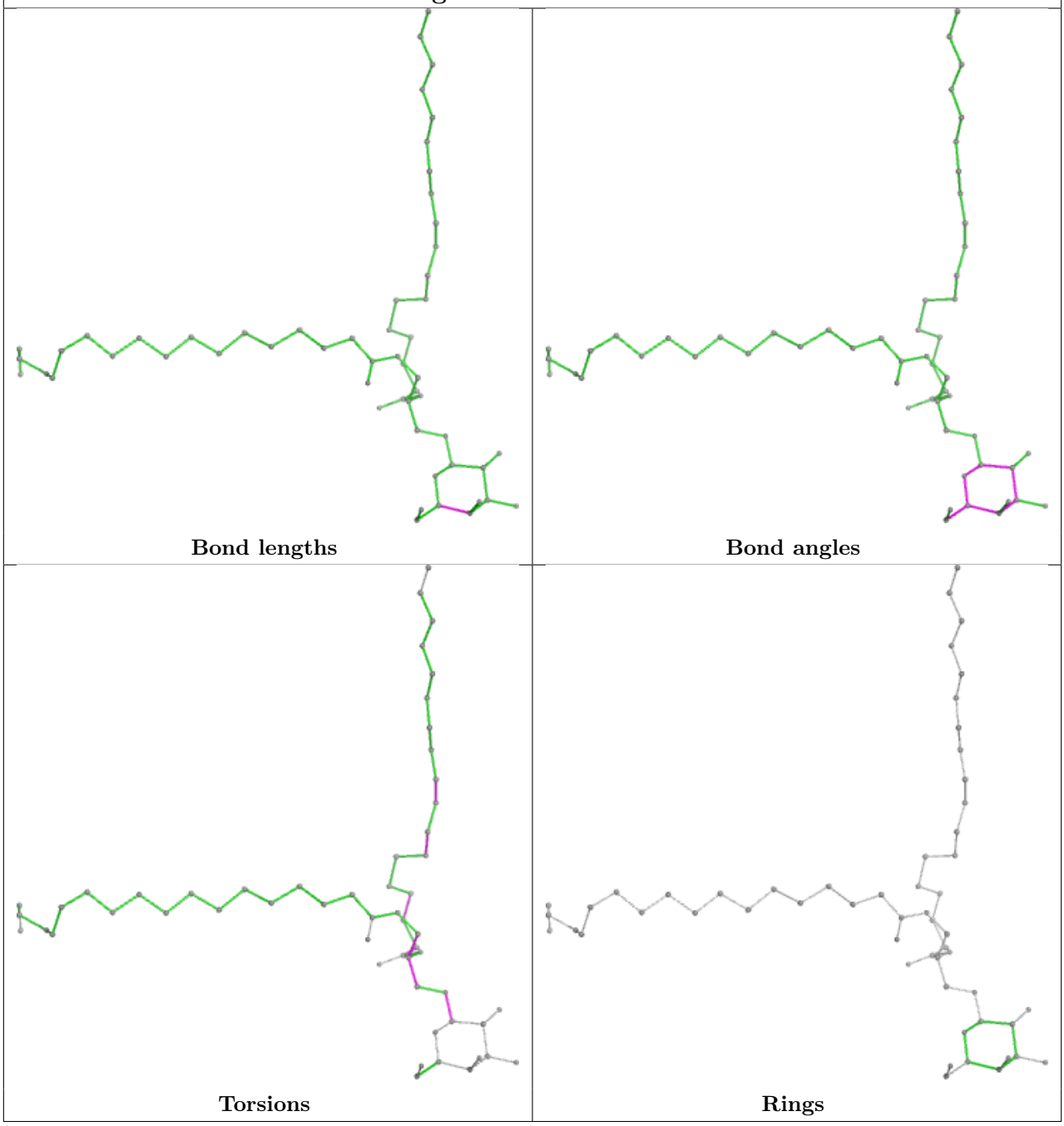
Ligand BCR H 101



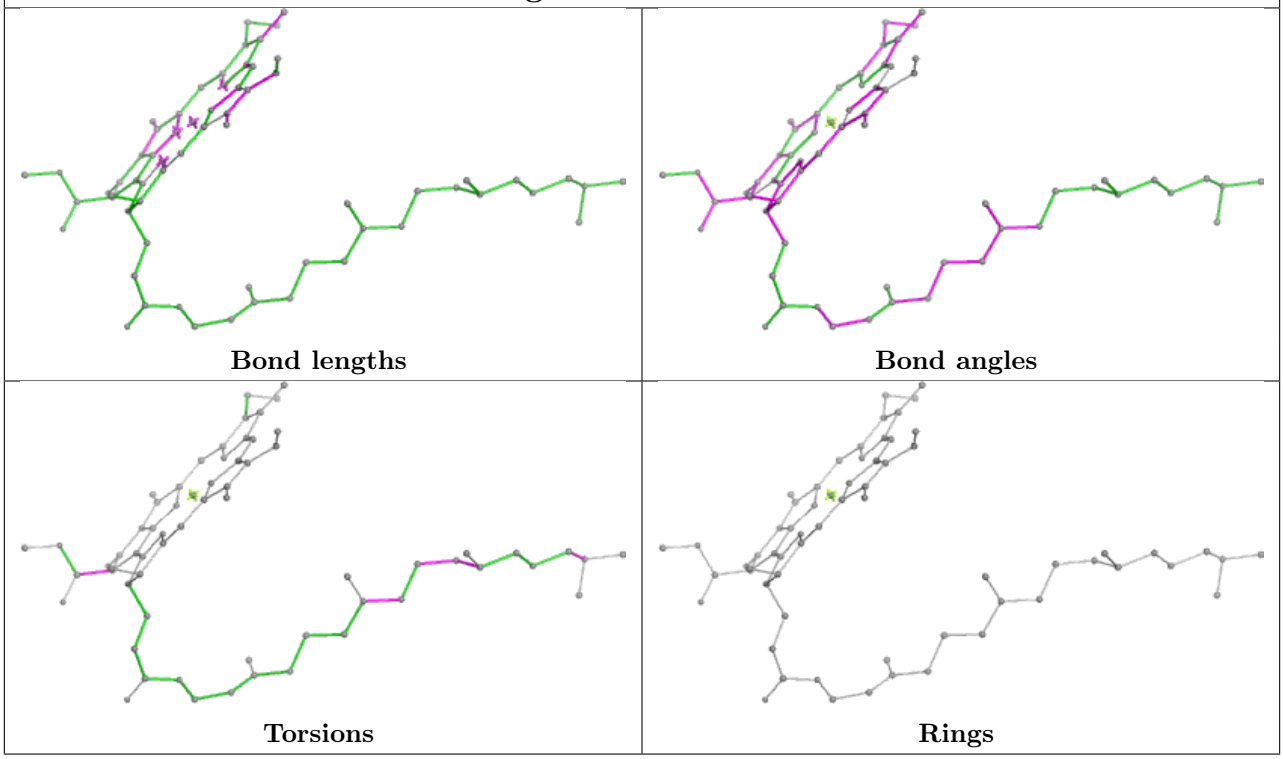
Ligand CLA D 406



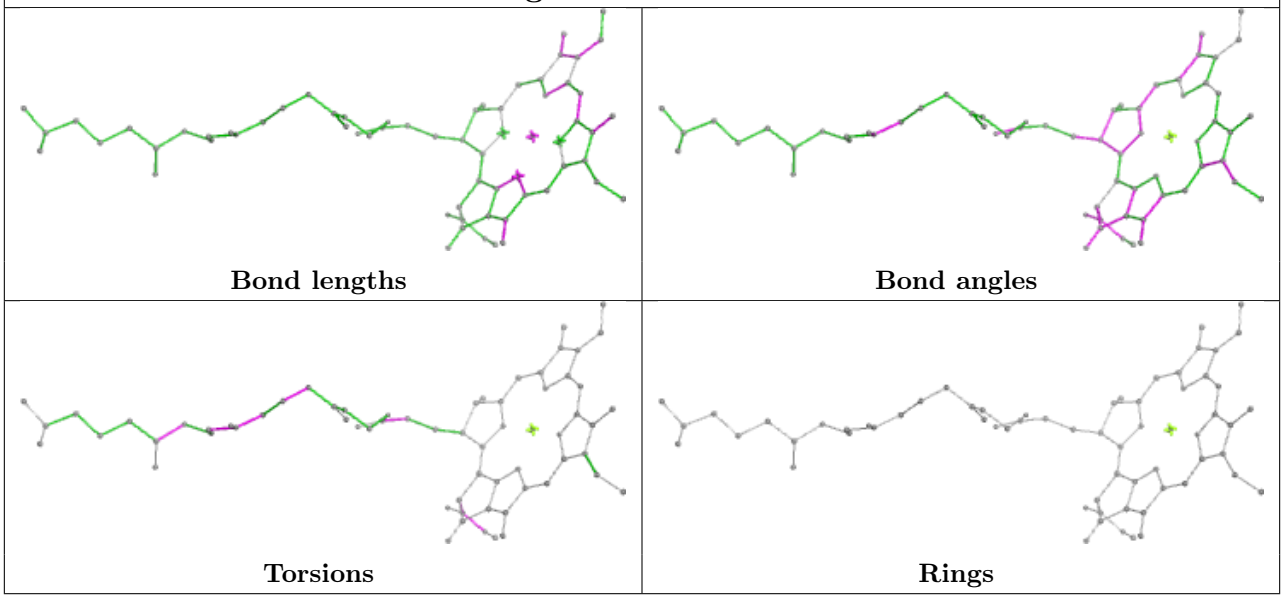
Ligand LMG B 601



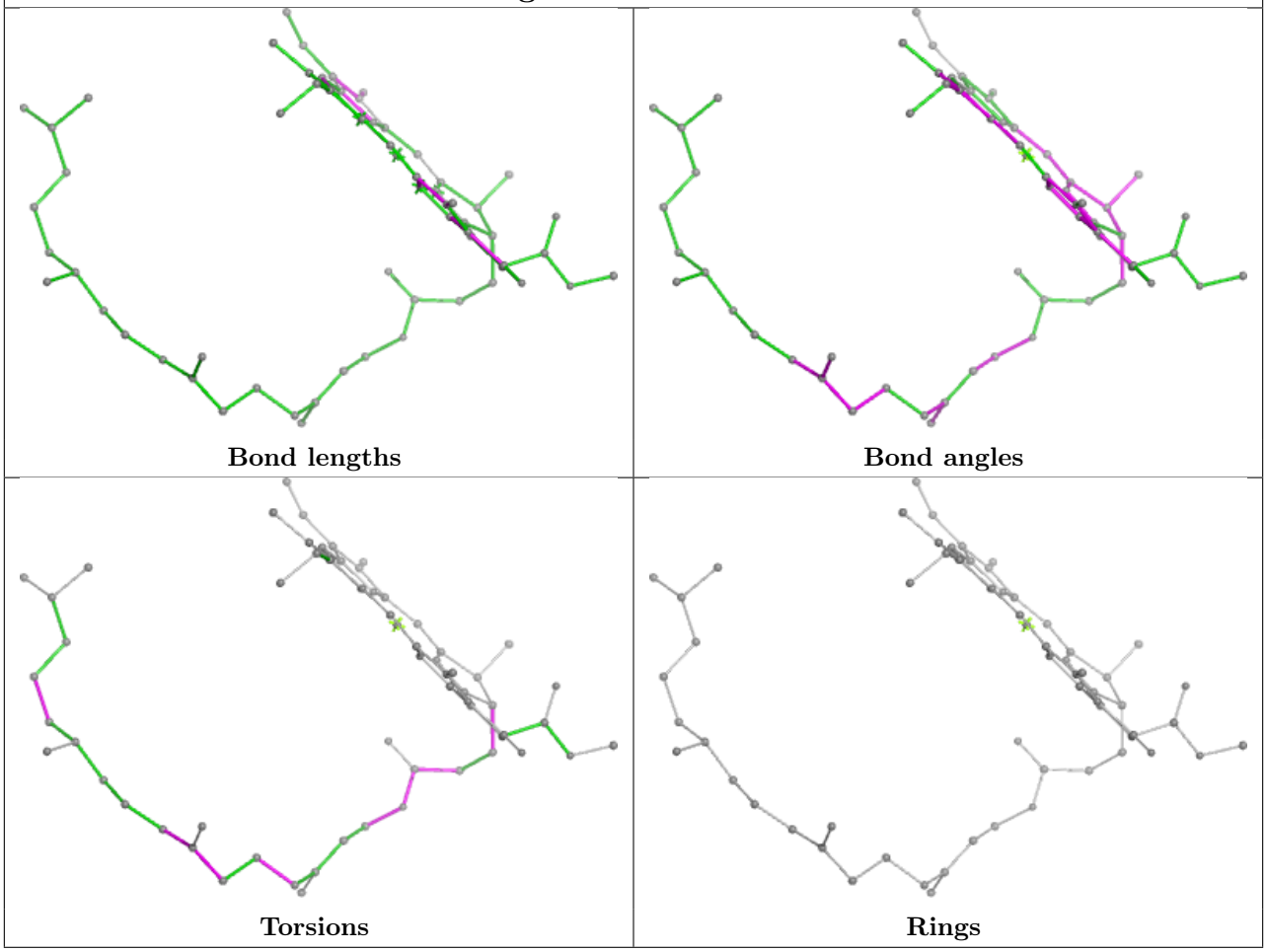
Ligand CLA C 505



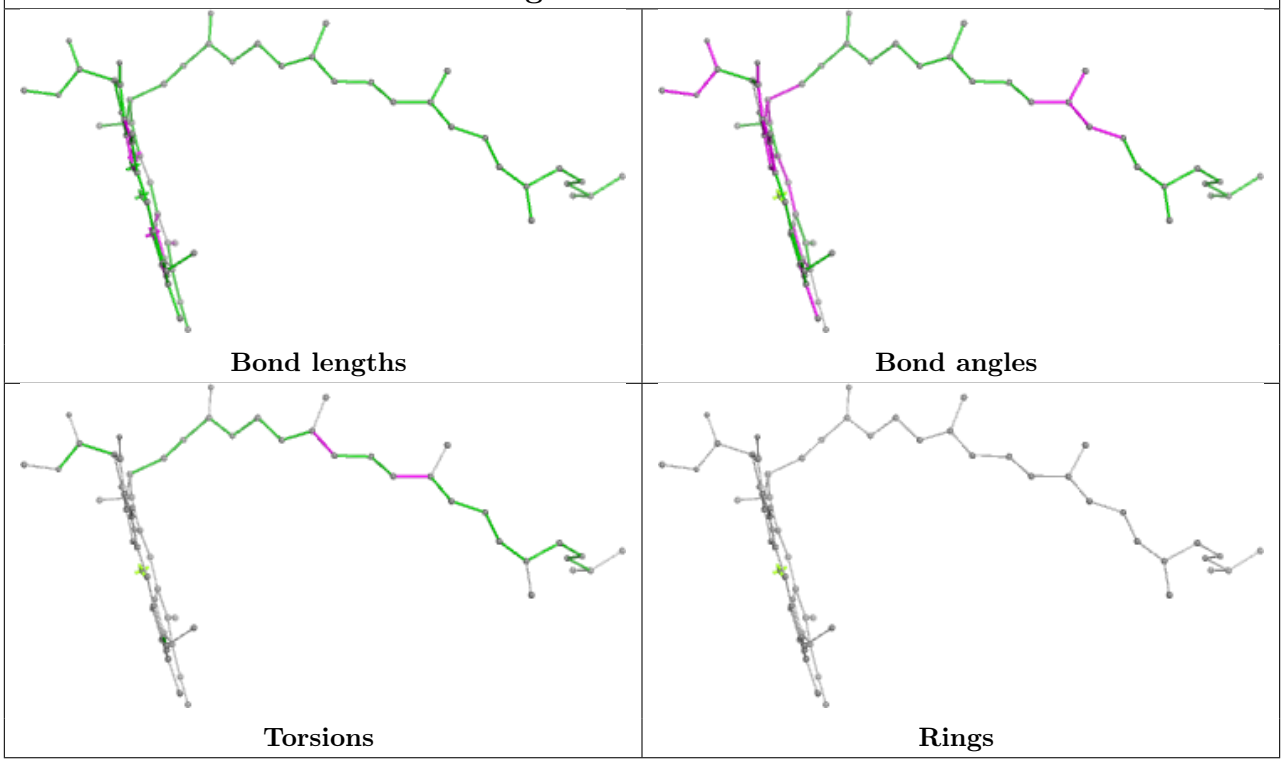
Ligand CLA C 503



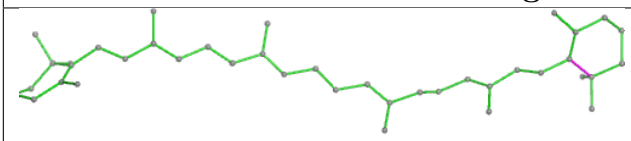
Ligand CLA B 612



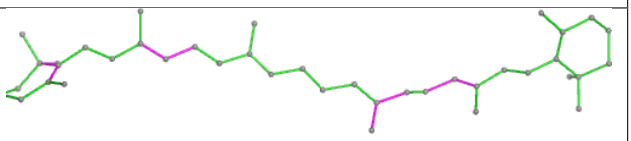
Ligand CLA B 606



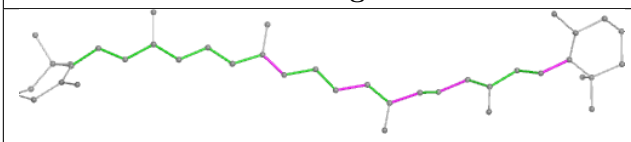
Ligand BCR B 619



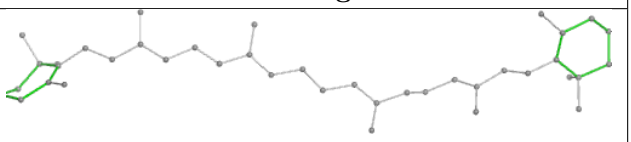
Bond lengths



Bond angles

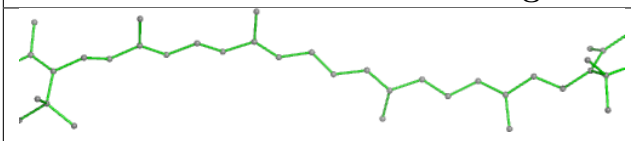


Torsions

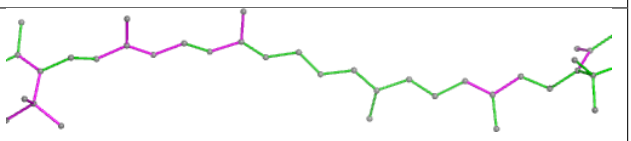


Rings

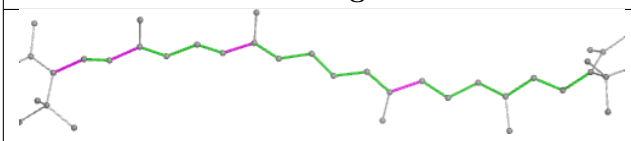
Ligand BCR B 620



Bond lengths



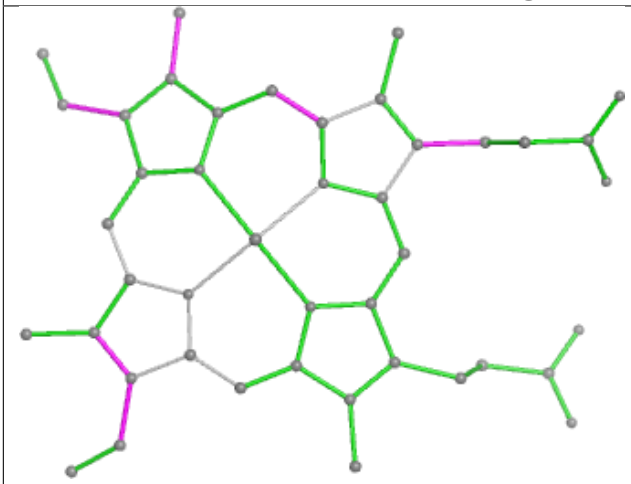
Bond angles



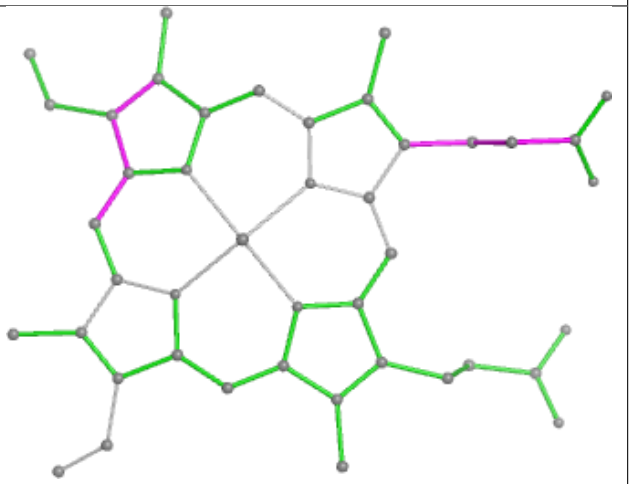
Torsions

Rings

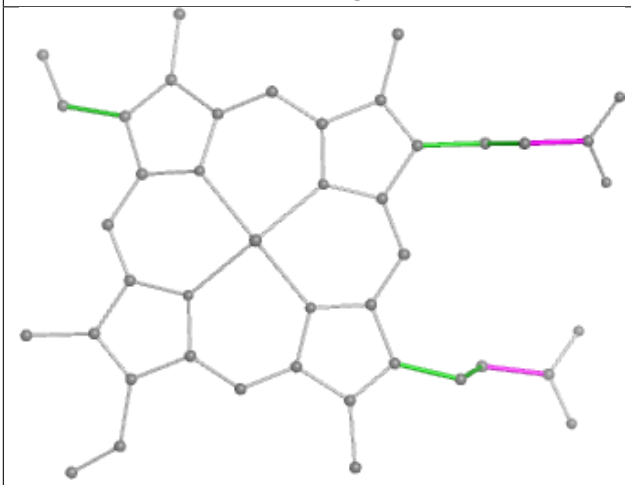
Ligand HEM E 101



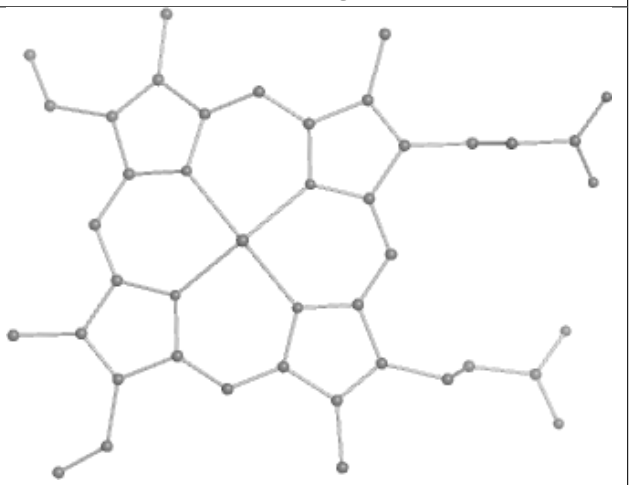
Bond lengths



Bond angles

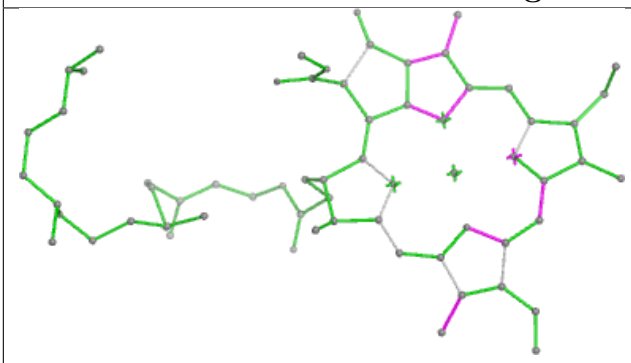


Torsions

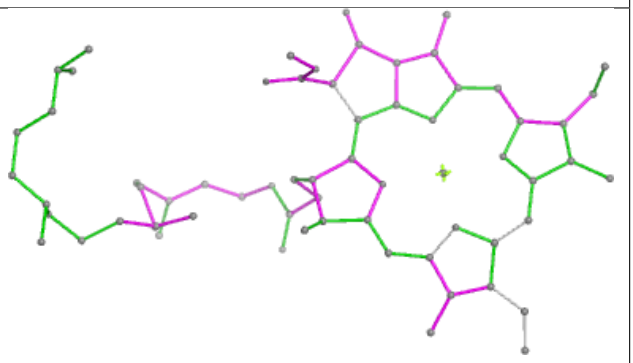


Rings

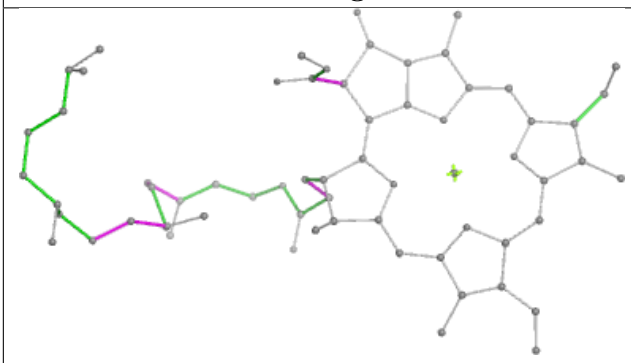
Ligand CLA B 613



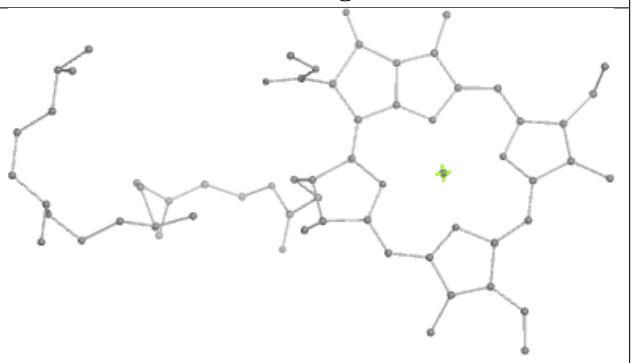
Bond lengths



Bond angles



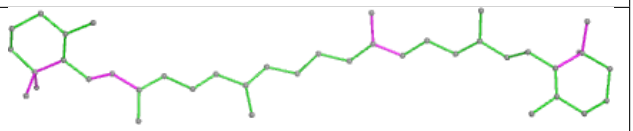
Torsions



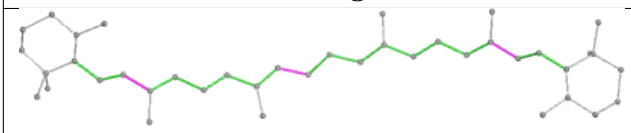
Rings

Ligand BCR F 101

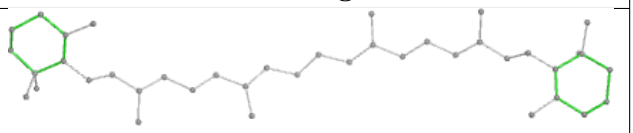
Bond lengths



Bond angles

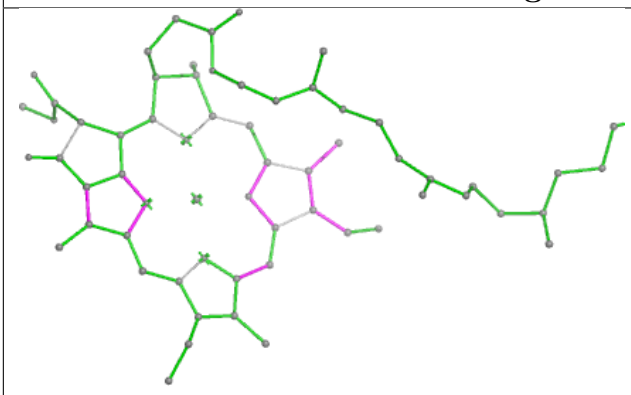


Torsions

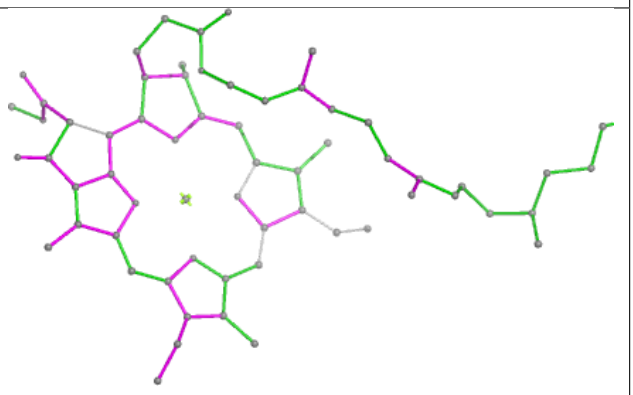


Rings

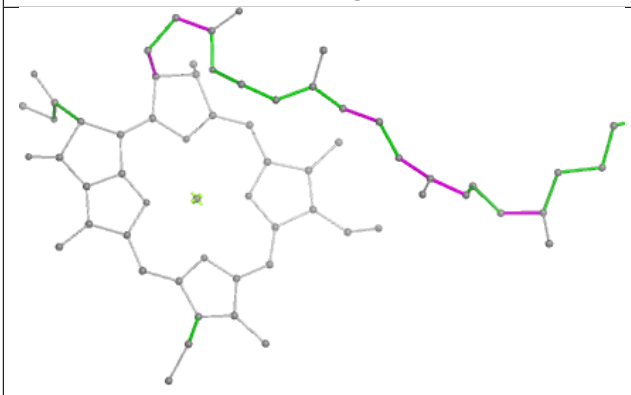
Ligand CLA B 604



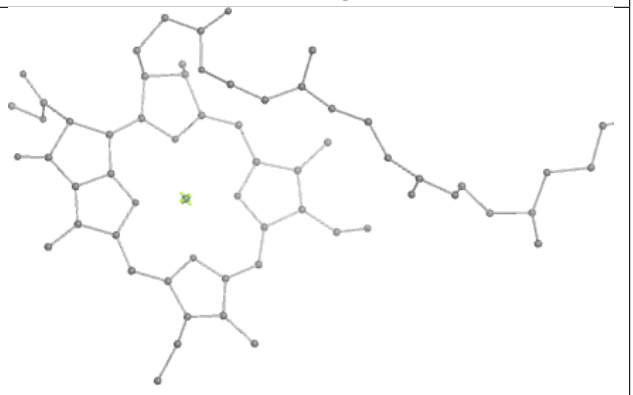
Bond lengths



Bond angles

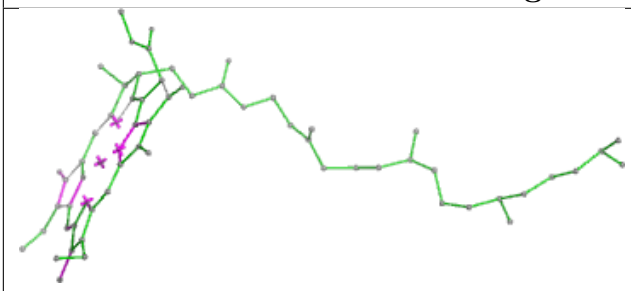


Torsions

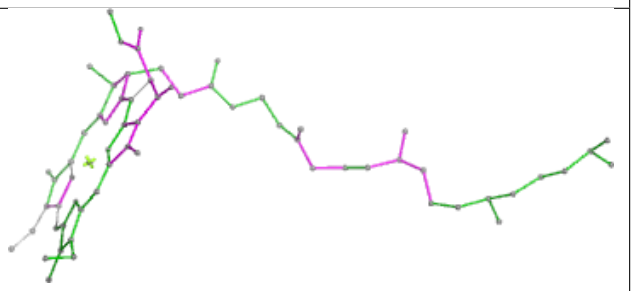


Rings

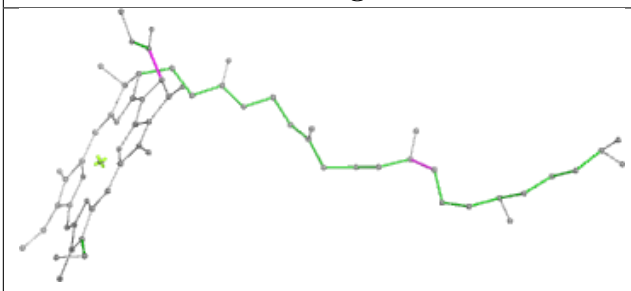
Ligand CLA B 605



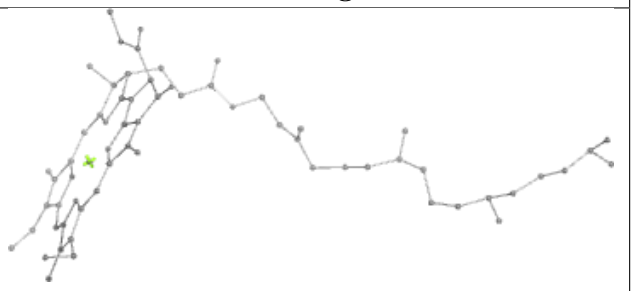
Bond lengths



Bond angles

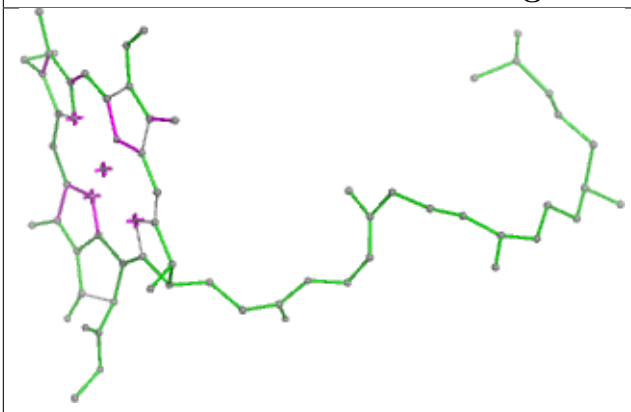


Torsions

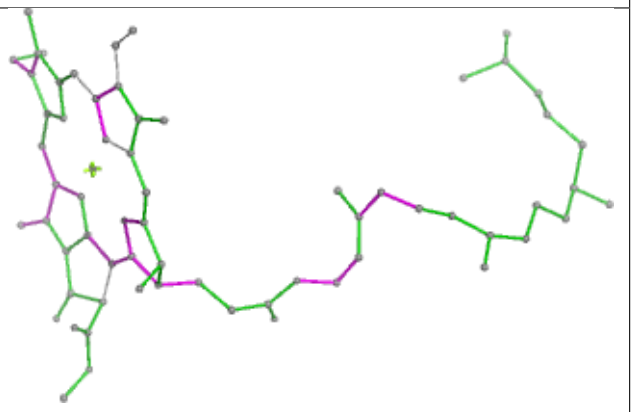


Rings

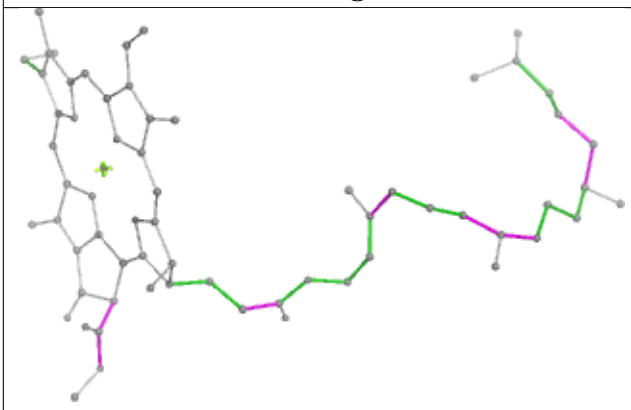
Ligand CLA A 408



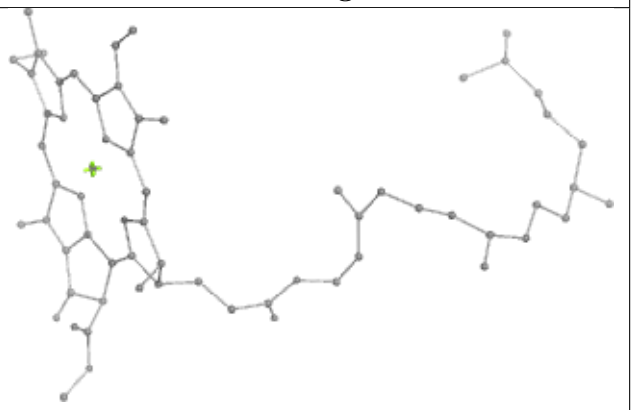
Bond lengths



Bond angles

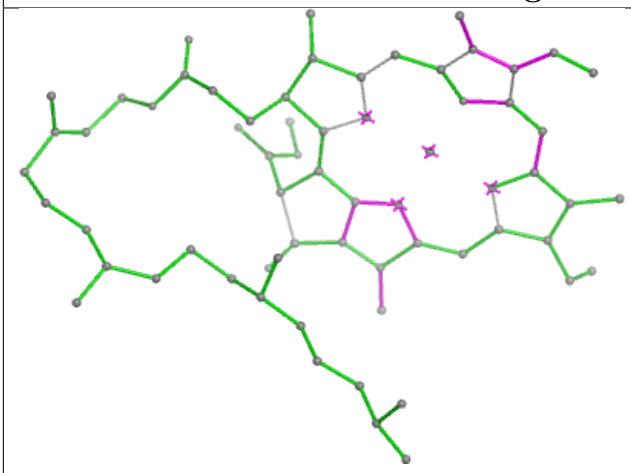


Torsions

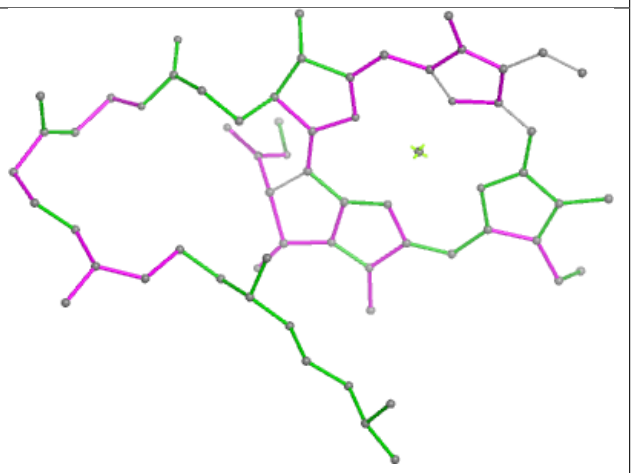


Rings

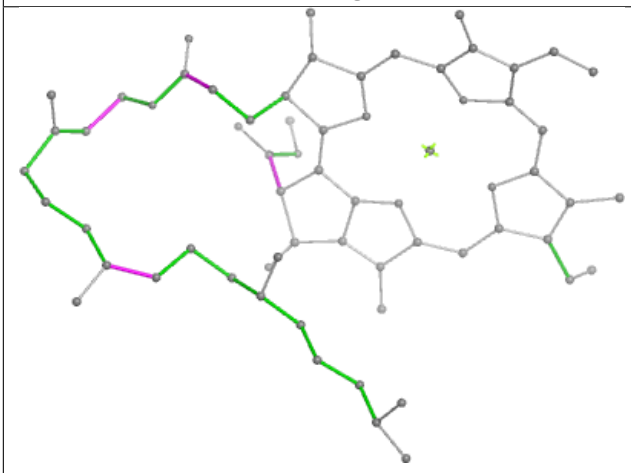
Ligand CLA C 510



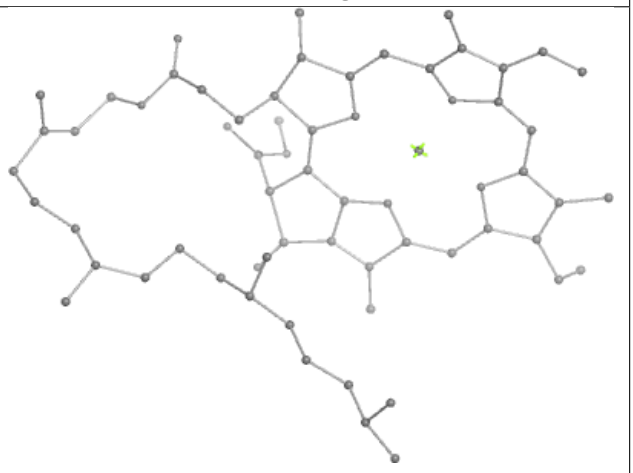
Bond lengths



Bond angles

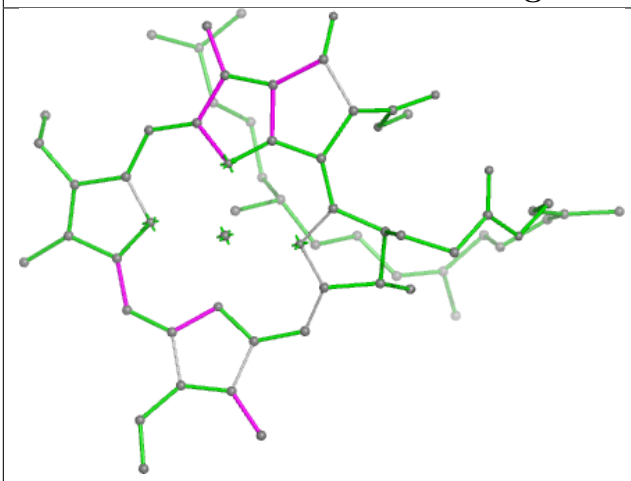


Torsions

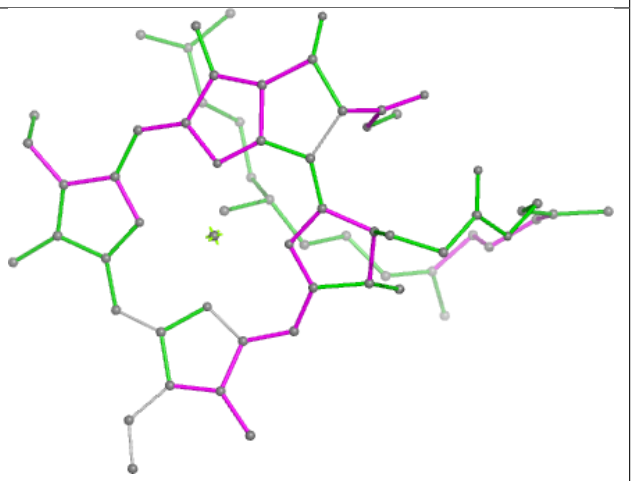


Rings

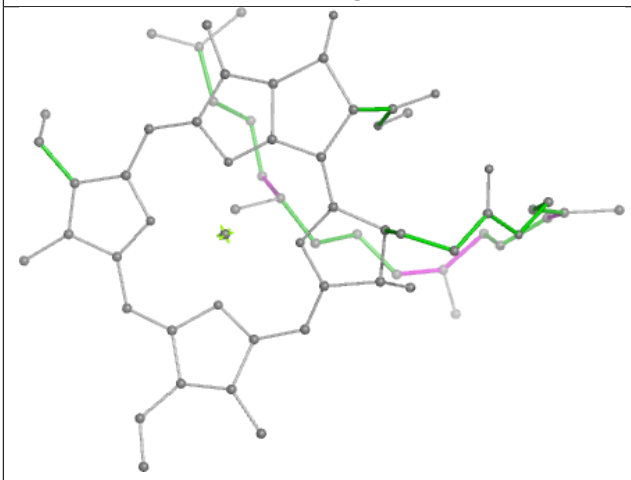
Ligand CLA C 515



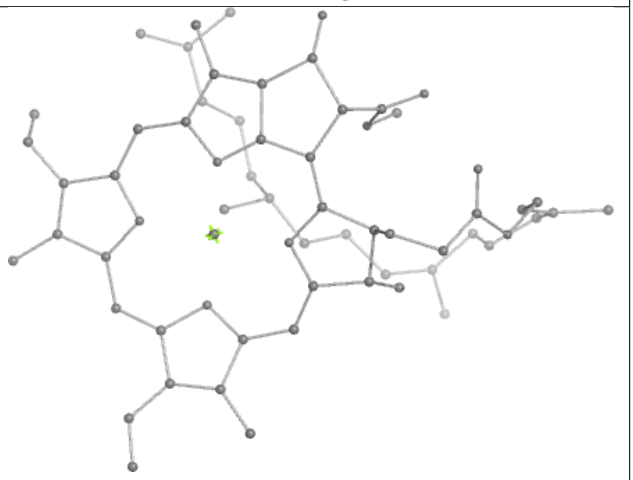
Bond lengths



Bond angles

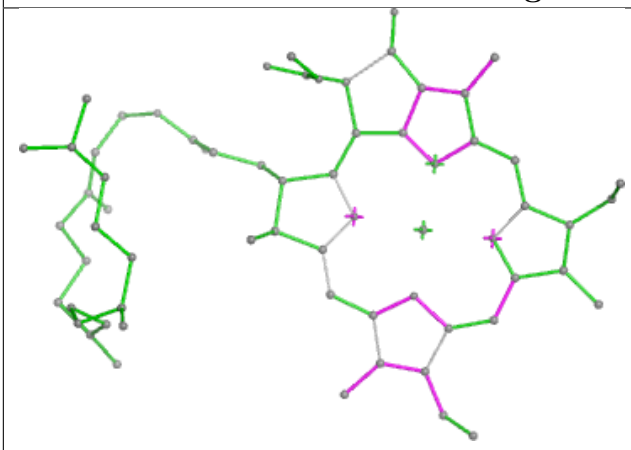


Torsions

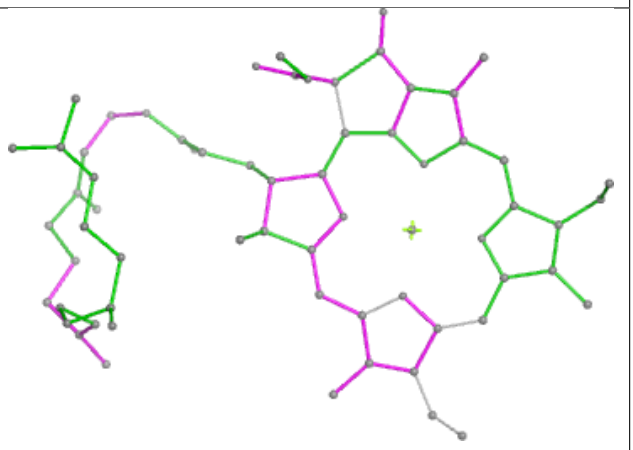


Rings

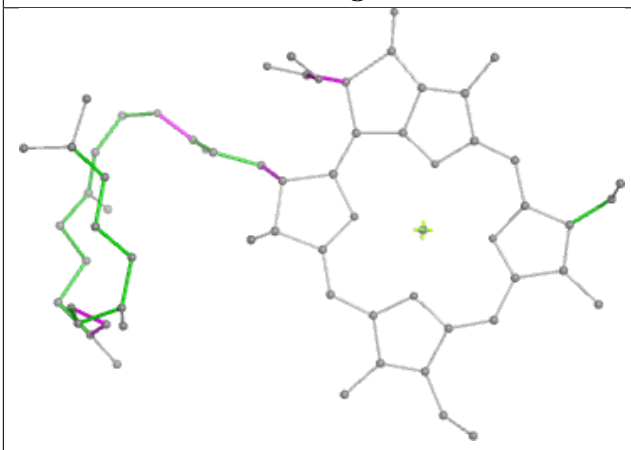
Ligand CLA C 512



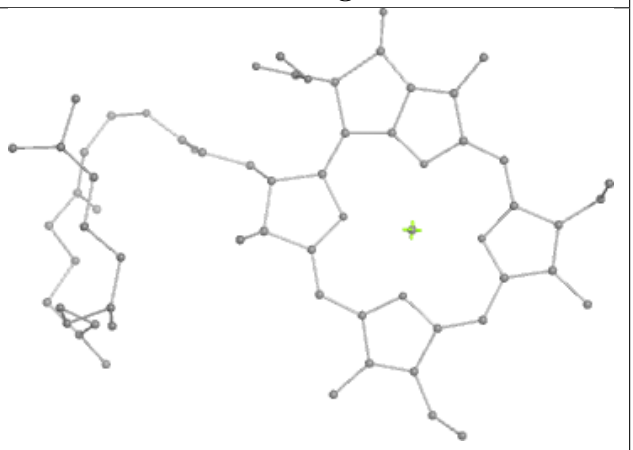
Bond lengths



Bond angles

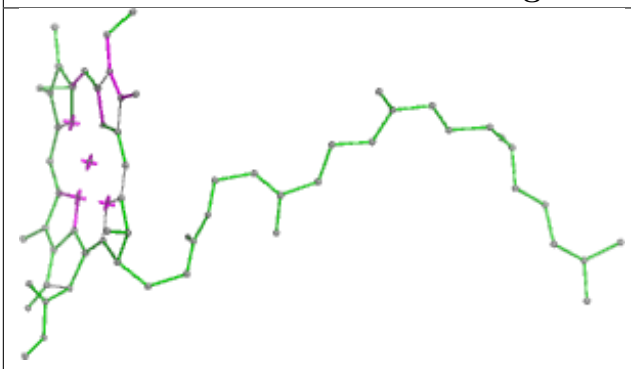


Torsions

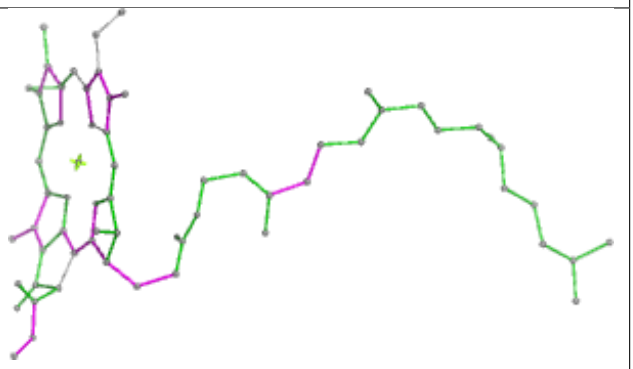


Rings

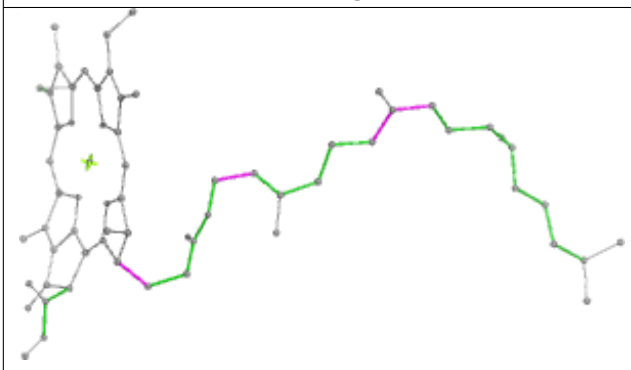
Ligand CLA D 407



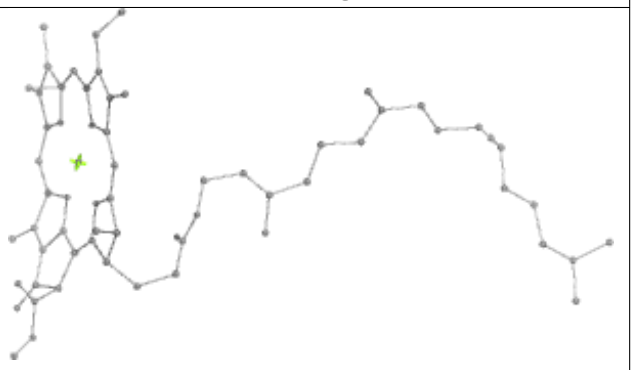
Bond lengths



Bond angles

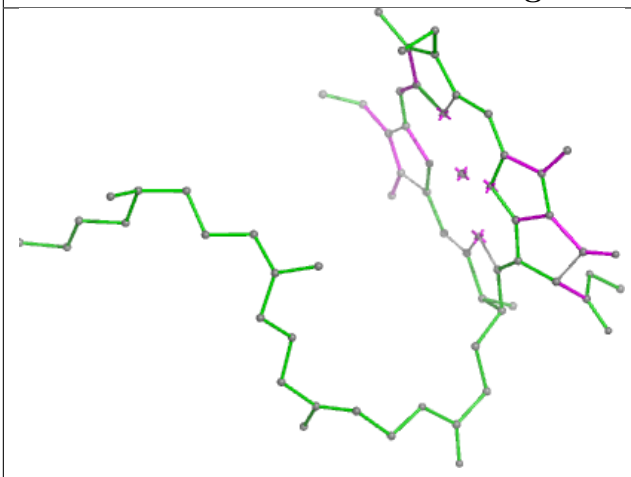


Torsions

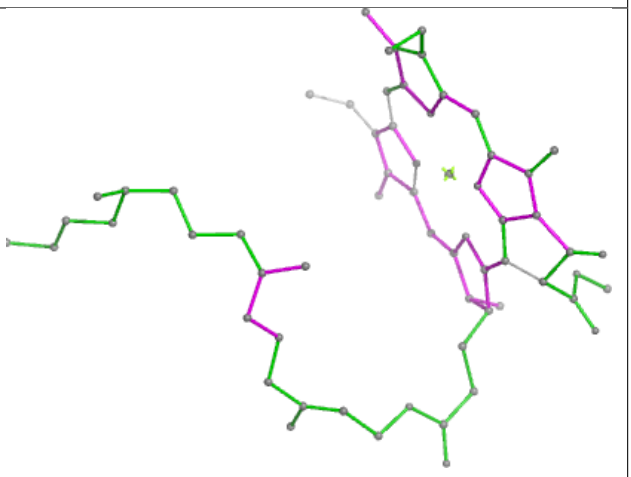


Rings

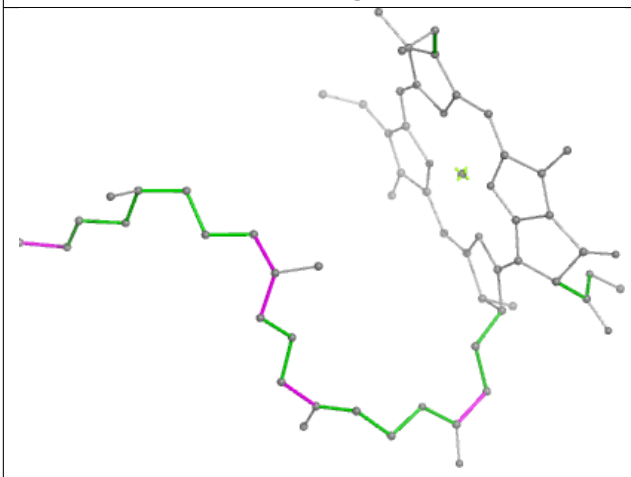
Ligand CLA C 513



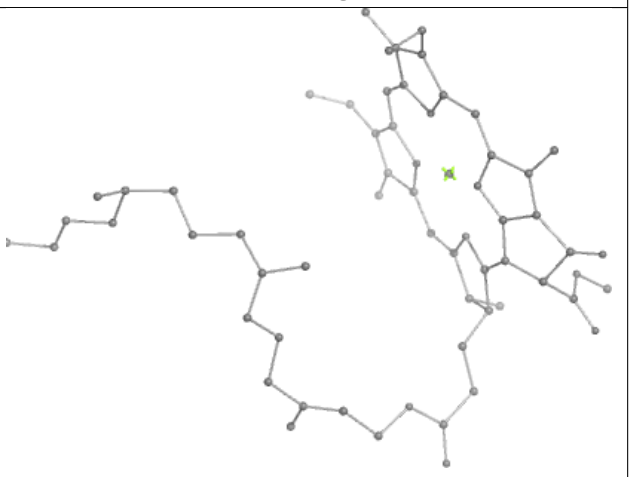
Bond lengths



Bond angles

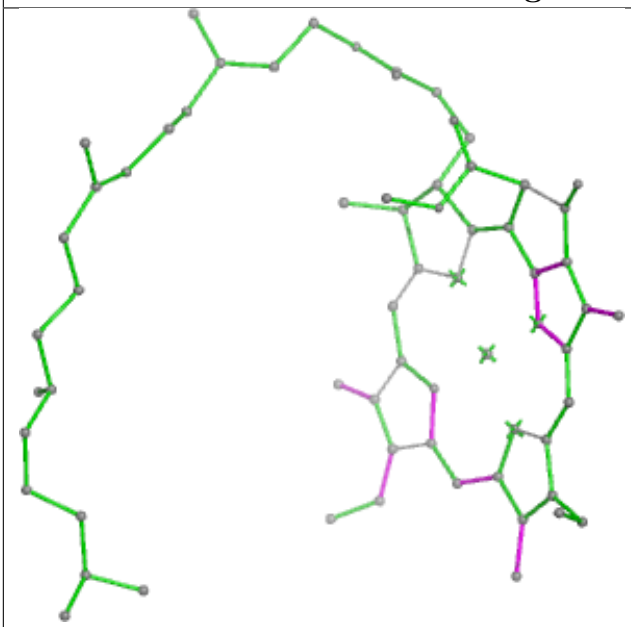


Torsions

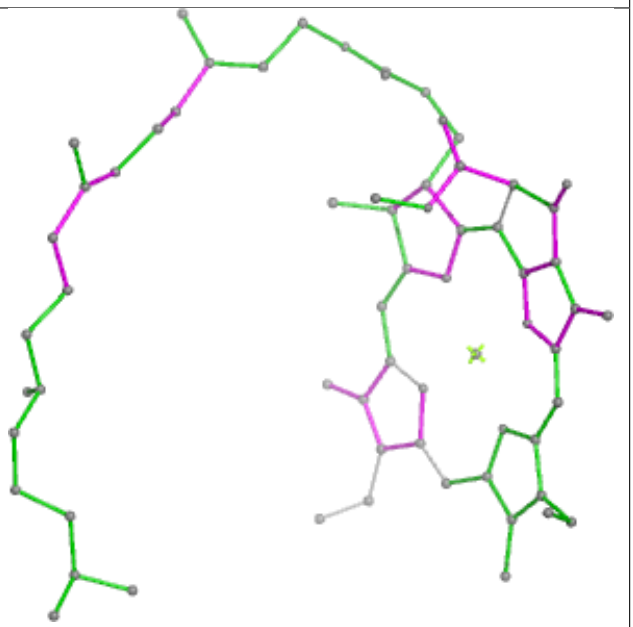


Rings

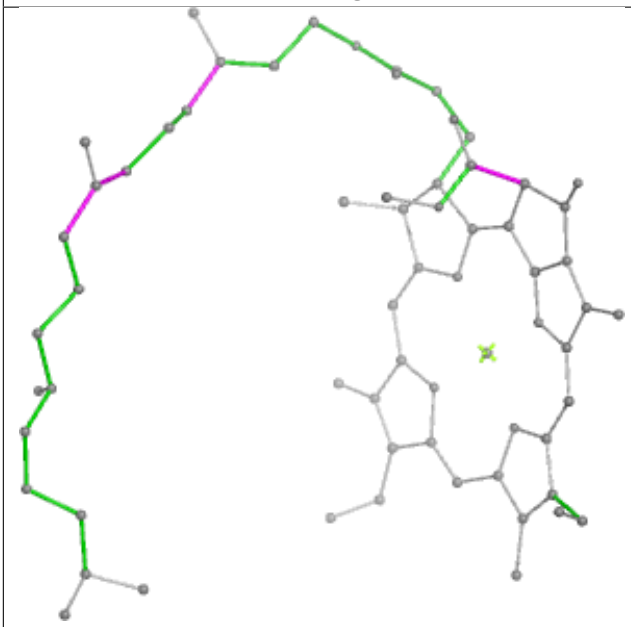
Ligand CLA C 508



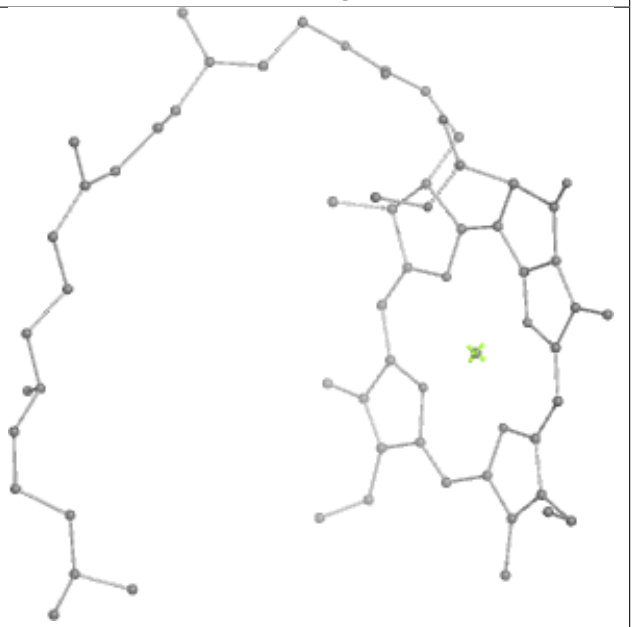
Bond lengths



Bond angles

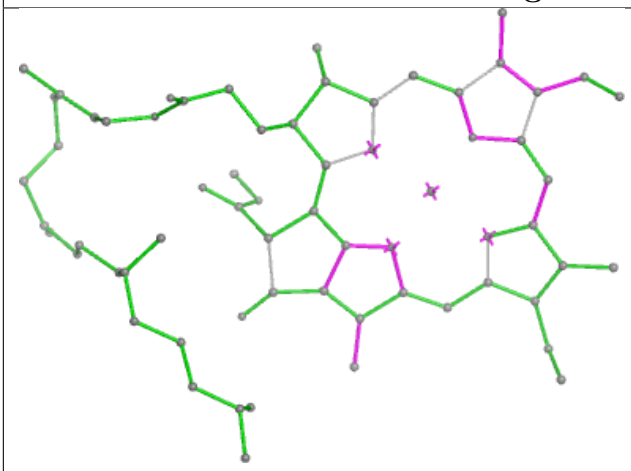


Torsions

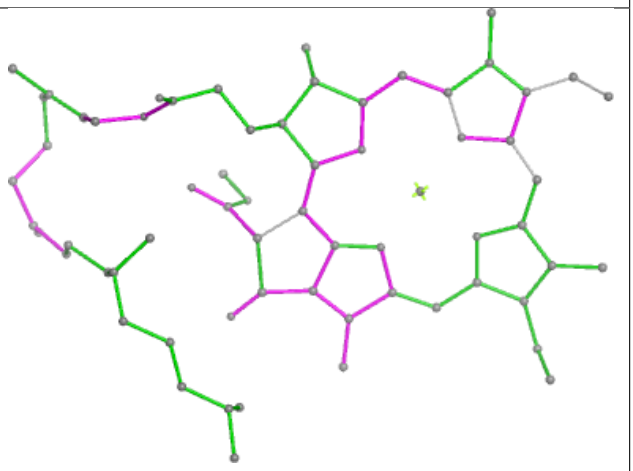


Rings

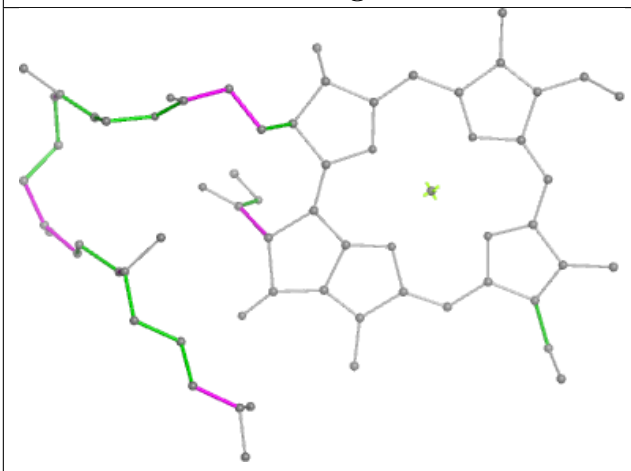
Ligand CLA B 611



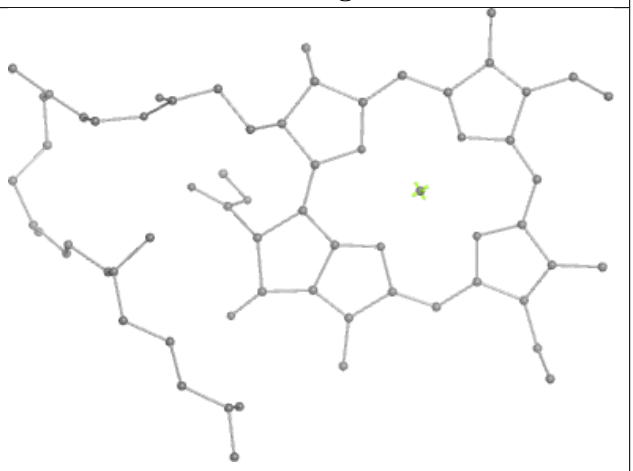
Bond lengths



Bond angles

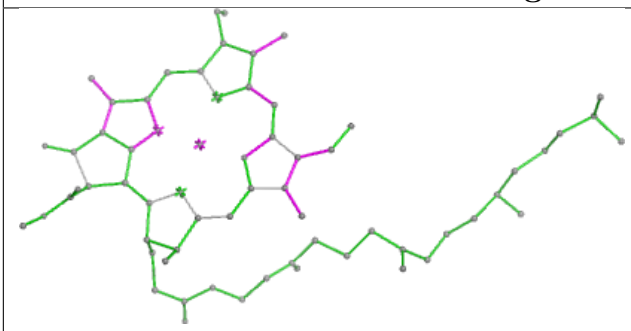


Torsions

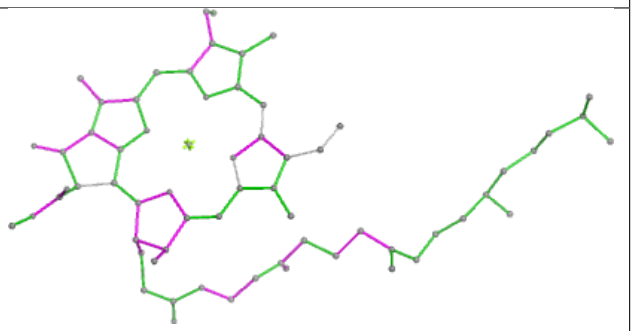


Rings

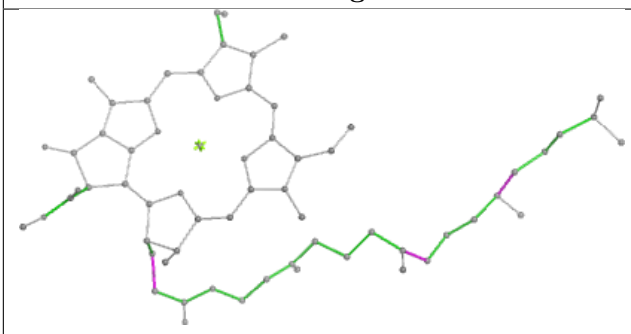
Ligand CLA C 502



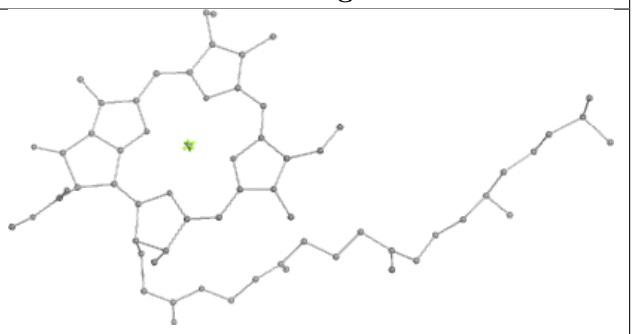
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

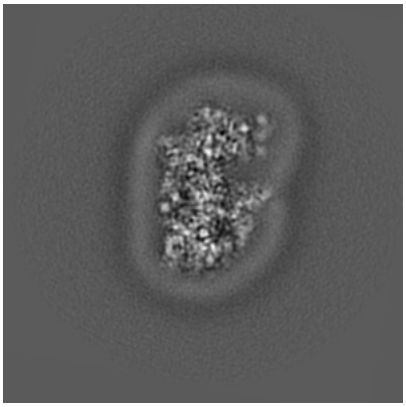
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12335. These allow visual inspection of the internal detail of the map and identification of artifacts.

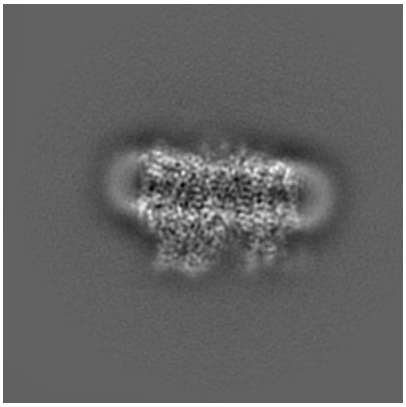
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

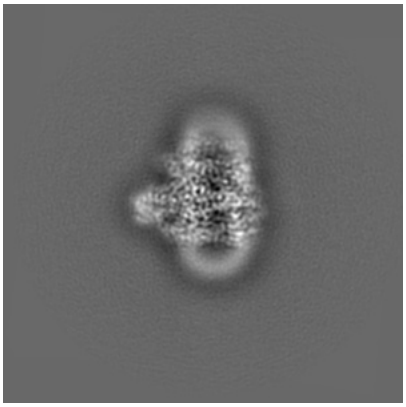
6.1.1 Primary map



X



Y

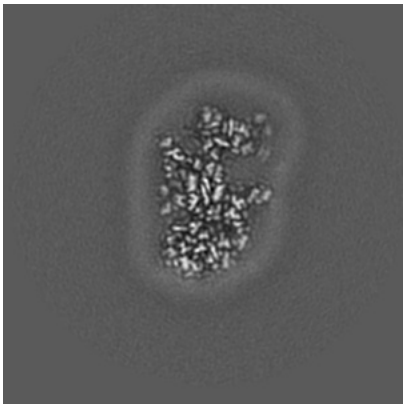


Z

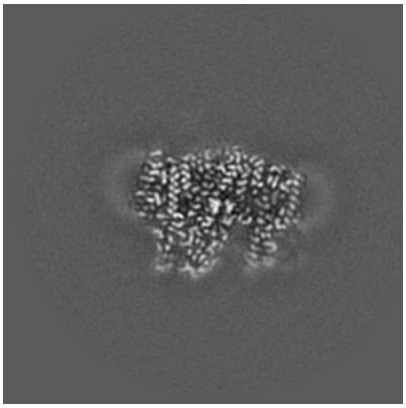
The images above show the map projected in three orthogonal directions.

6.2 Central slices

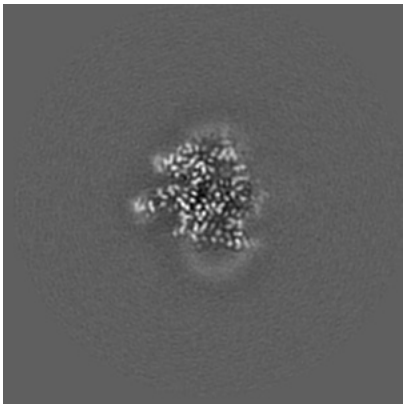
6.2.1 Primary map



X Index: 130



Y Index: 130

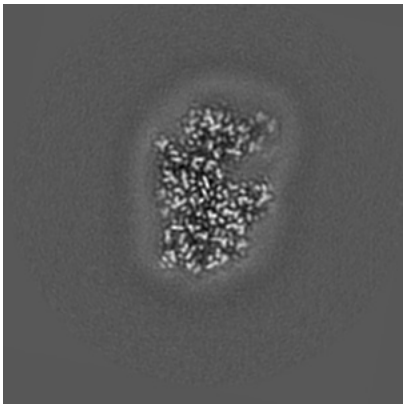


Z Index: 130

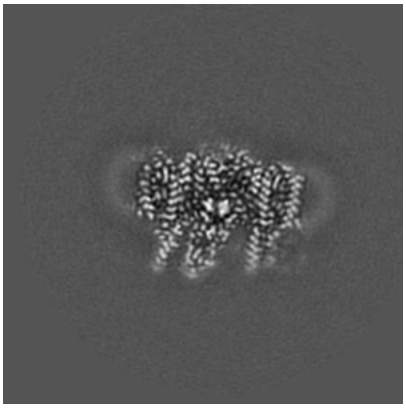
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

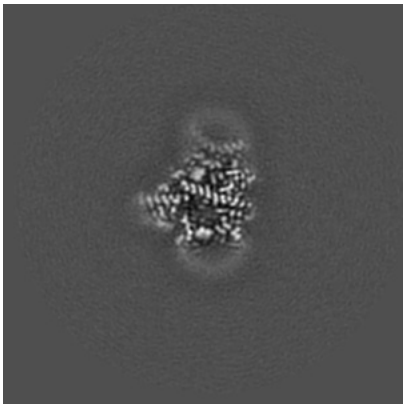
6.3.1 Primary map



X Index: 125



Y Index: 132

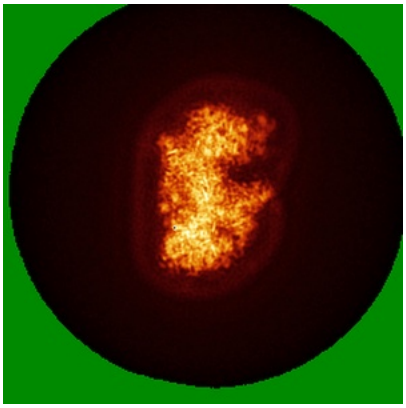


Z Index: 164

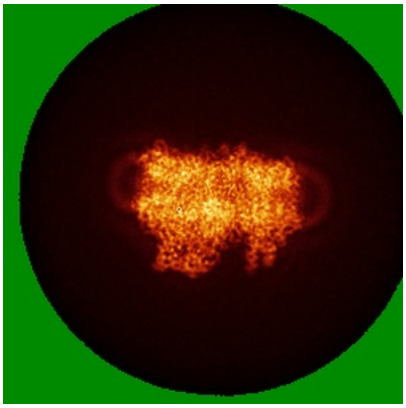
The images above show the largest variance slices of the map in three orthogonal directions.

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

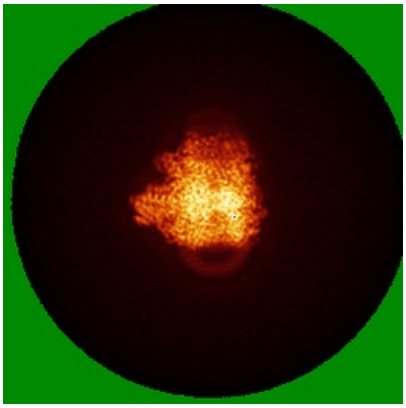
6.4.1 Primary map



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

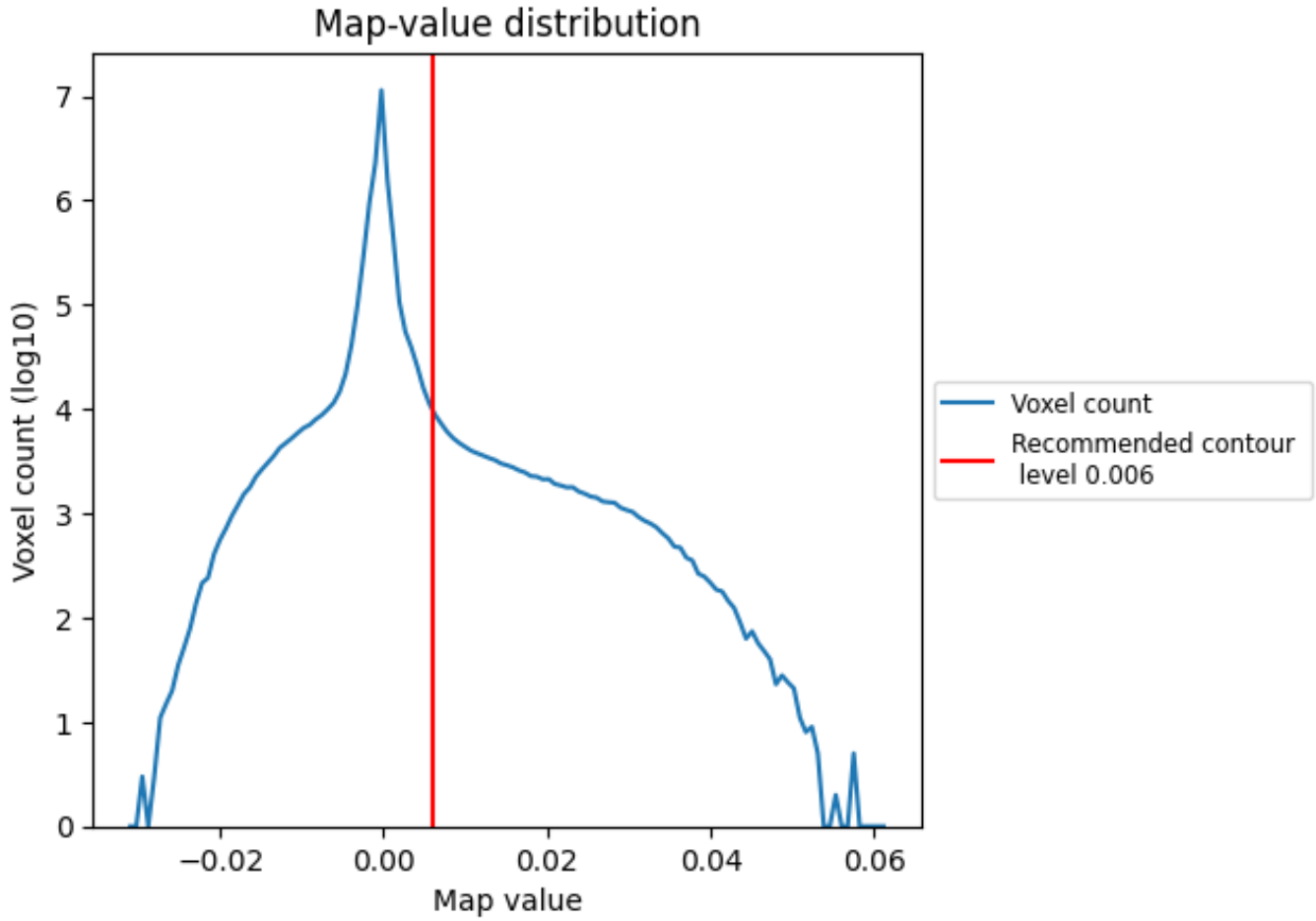
6.6 Mask visualisation (i)

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

7 Map analysis

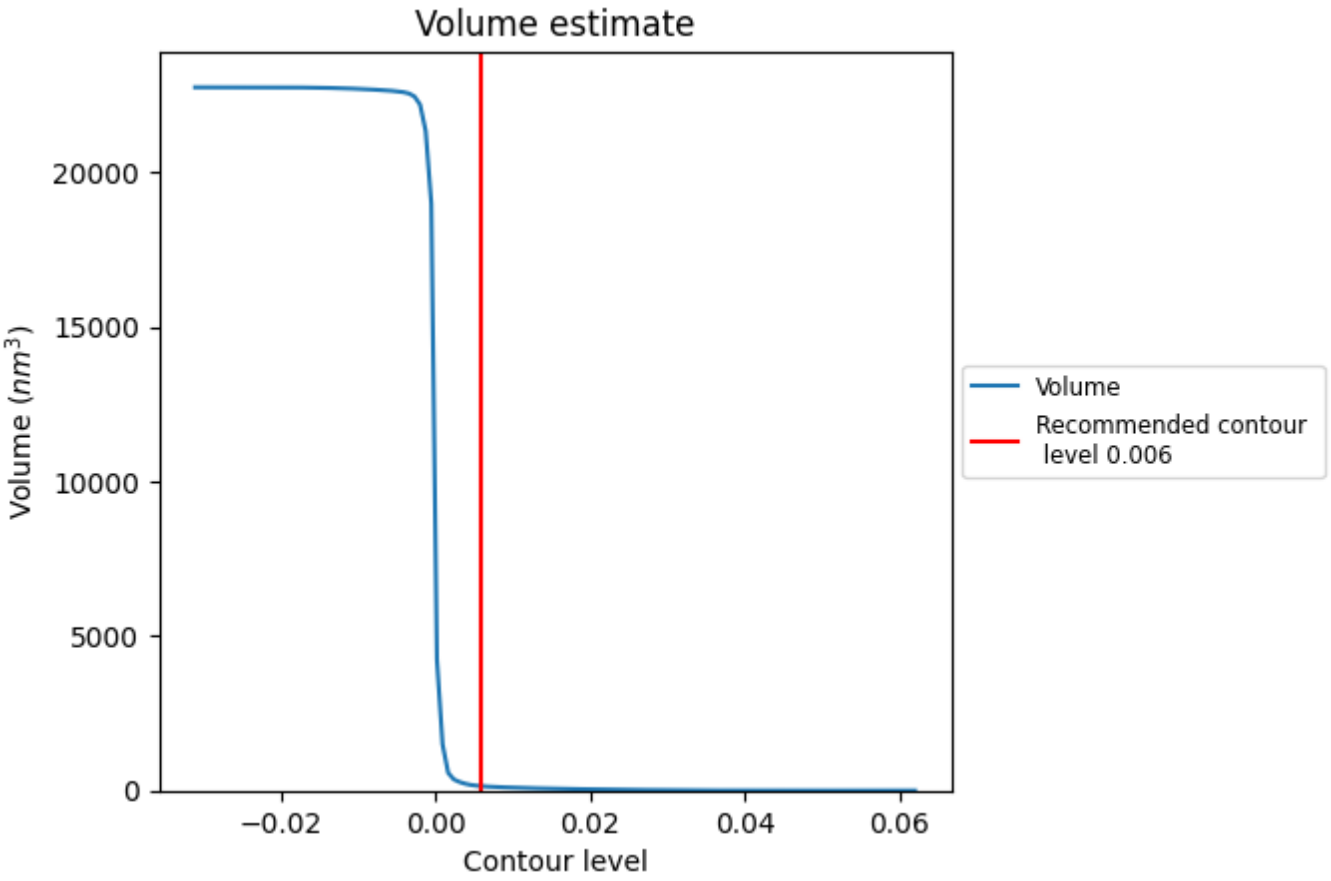
This section contains the results of statistical analysis of the map.

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.

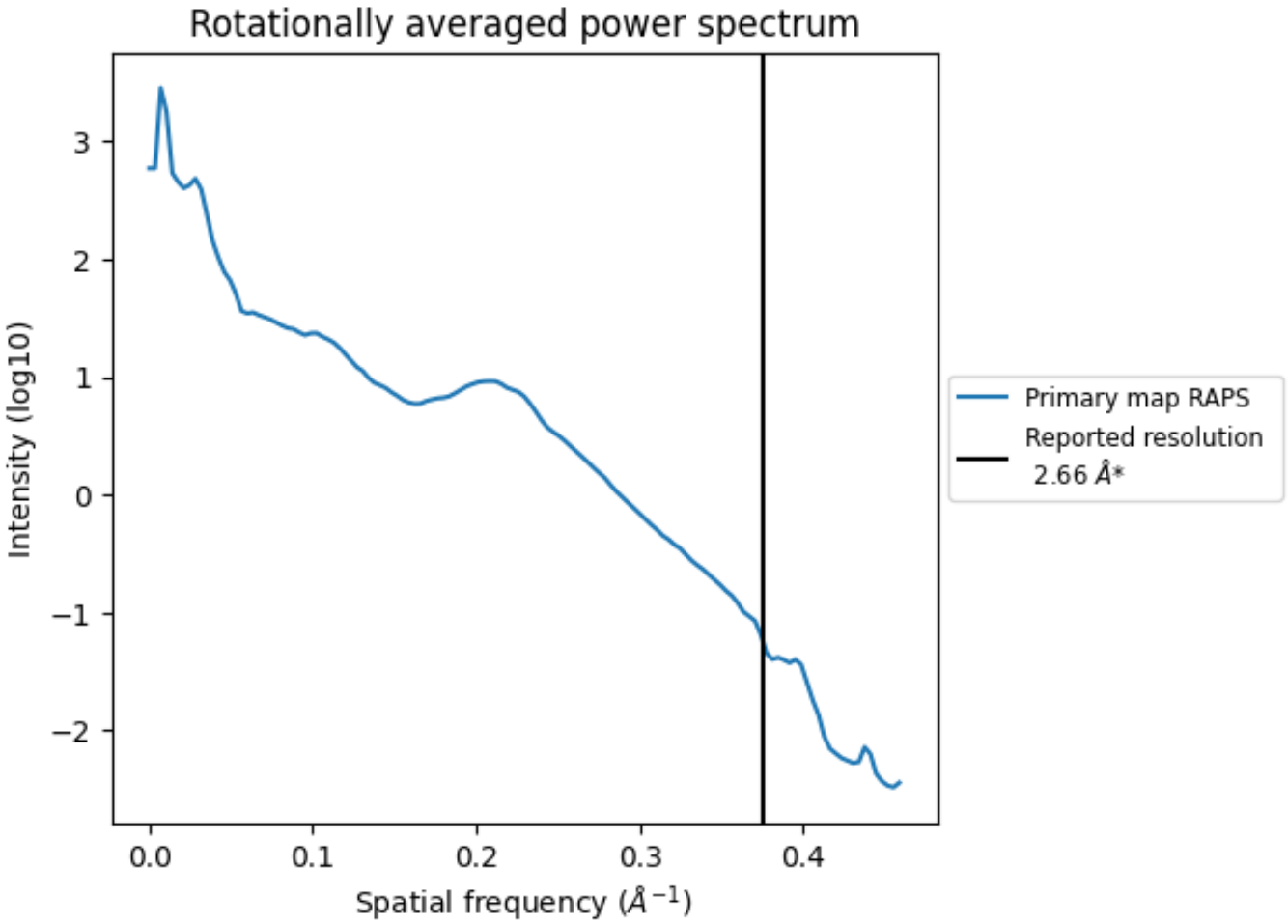
7.2 Volume estimate



The volume at the recommended contour level is 142 nm^3; this corresponds to an approximate mass of 129 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 0.376 $Å^{-1}$

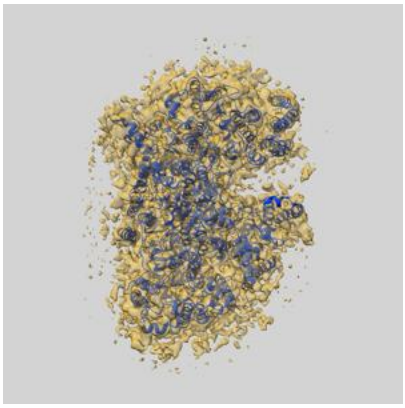
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

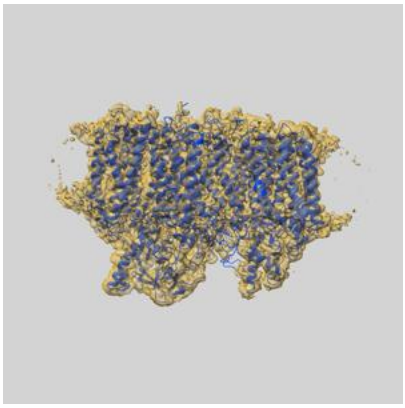
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12335 and PDB model 7NHO. Per-residue inclusion information can be found in section 3 on page 15.

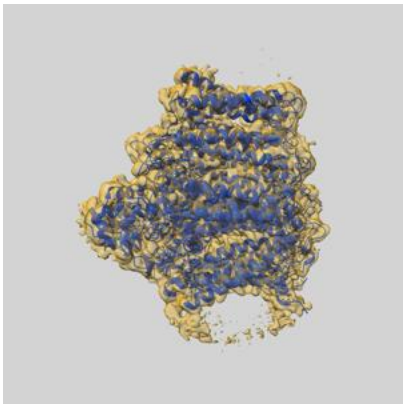
9.1 Map-model overlay



X



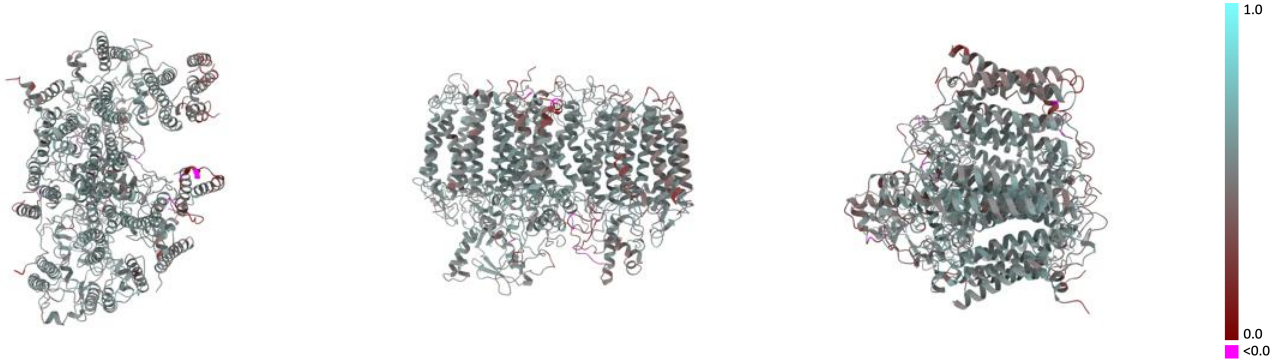
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 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.

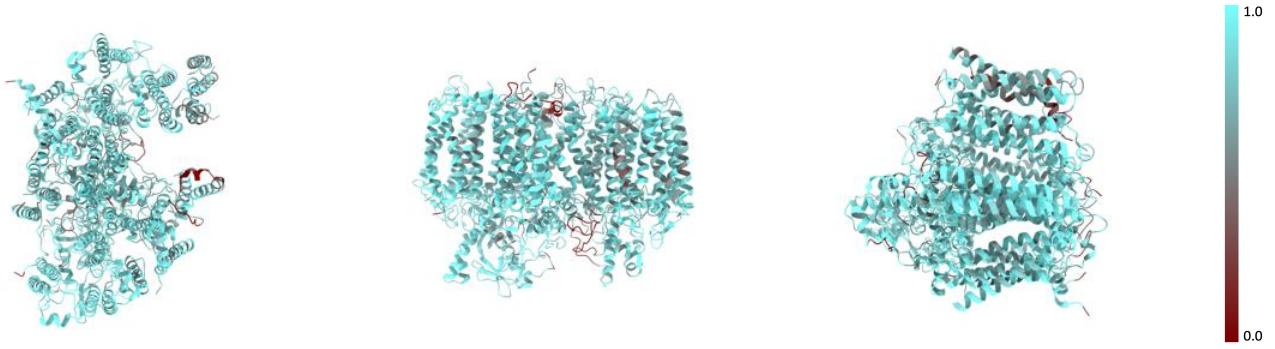
9.2 Q-score mapped to coordinate model



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.

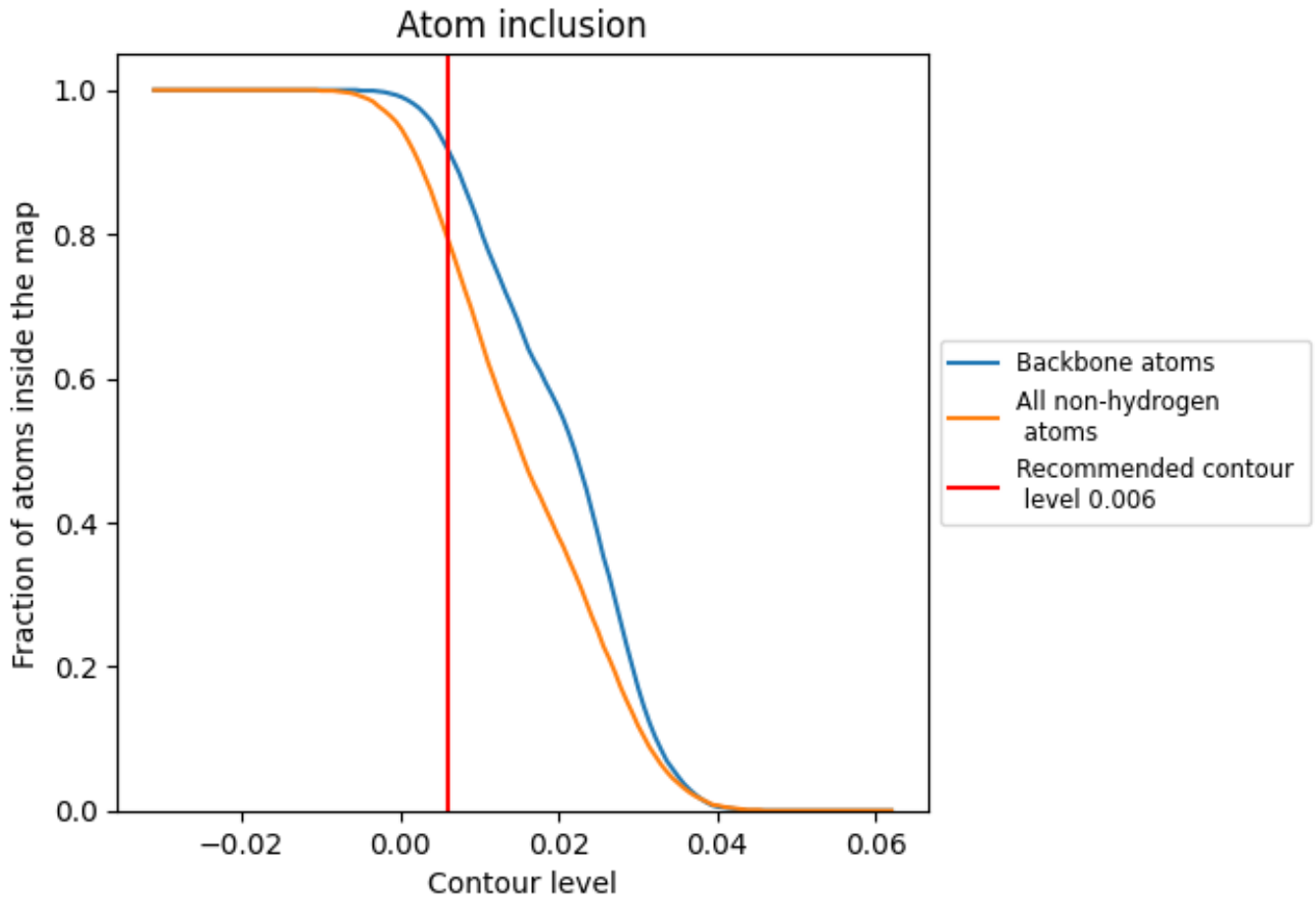
9.3 Atom inclusion mapped to coordinate model



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 (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 79% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7940	0.5010
A	0.7880	0.5100
B	0.8390	0.5250
C	0.7820	0.4940
D	0.8430	0.5380
E	0.7260	0.4090
F	0.6480	0.3980
H	0.8590	0.5020
I	0.7200	0.4590
K	0.7050	0.4700
L	0.8020	0.5040
M	0.5920	0.3780
T	0.7650	0.4940
X	0.7760	0.4730
Z	0.6750	0.4130
y	0.5740	0.3790