Full wwPDB EM Validation Report ⓘ

Dec 4, 2024 – 08:12 PM JST

PDB ID	:	8Y15
EMDB ID	:	EMD-38825
Title	:	Cryo-EM structure of Light-harvesting complex from Spinacia oleracea
Authors	:	Seki, S.; Miyata, T.; Tanaka, H.; Namba, K.; Kurisu, G.; Fujii, R.
Deposited on	:	2024-01-23
Resolution	:	2.17 Å(reported)
Based on initial model	:	1RWT

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:

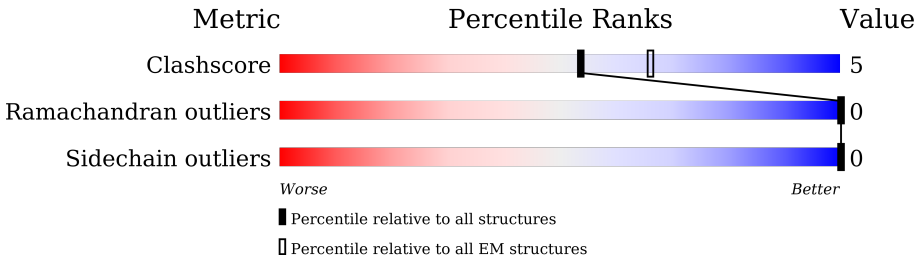
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance

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

The reported resolution of this entry is 2.17 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	216	93% 7%
1	B	216	94% 6%
1	C	216	94% 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CHL	A	601	X	-	-	-
2	CHL	A	605	X	-	-	-
2	CHL	A	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CHL	A	607	X	-	-	-
2	CHL	A	608	X	-	-	-
2	CHL	A	609	X	-	-	-
2	CHL	B	601	X	-	-	-
2	CHL	B	605	X	-	-	-
2	CHL	B	606	X	-	-	-
2	CHL	B	607	X	-	-	-
2	CHL	B	608	X	-	-	-
2	CHL	B	609	X	-	-	-
2	CHL	C	601	X	-	-	-
2	CHL	C	605	X	-	-	-
2	CHL	C	606	X	-	-	-
2	CHL	C	607	X	-	-	-
2	CHL	C	608	X	-	-	-
2	CHL	C	609	X	-	-	-
3	CLA	A	602	X	-	-	-
3	CLA	A	603	X	-	-	-
3	CLA	A	604	X	-	-	-
3	CLA	A	610	X	-	-	-
3	CLA	A	611	X	-	-	-
3	CLA	A	612	X	-	-	-
3	CLA	A	613	X	-	-	-
3	CLA	A	614	X	-	-	-
3	CLA	B	602	X	-	-	-
3	CLA	B	603	X	-	-	-
3	CLA	B	604	X	-	-	-
3	CLA	B	610	X	-	-	-
3	CLA	B	611	X	-	-	-
3	CLA	B	612	X	-	-	-
3	CLA	B	613	X	-	-	-
3	CLA	B	614	X	-	-	-
3	CLA	C	602	X	-	-	-
3	CLA	C	603	X	-	-	-
3	CLA	C	604	X	-	-	-
3	CLA	C	610	X	-	-	-
3	CLA	C	611	X	-	-	-
3	CLA	C	612	X	-	-	-
3	CLA	C	613	X	-	-	-
3	CLA	C	614	X	-	-	-
7	XAT	A	1004	X	-	-	-
7	XAT	B	1004	X	-	-	-
7	XAT	C	1004	X	-	-	-

2 Entry composition (i)

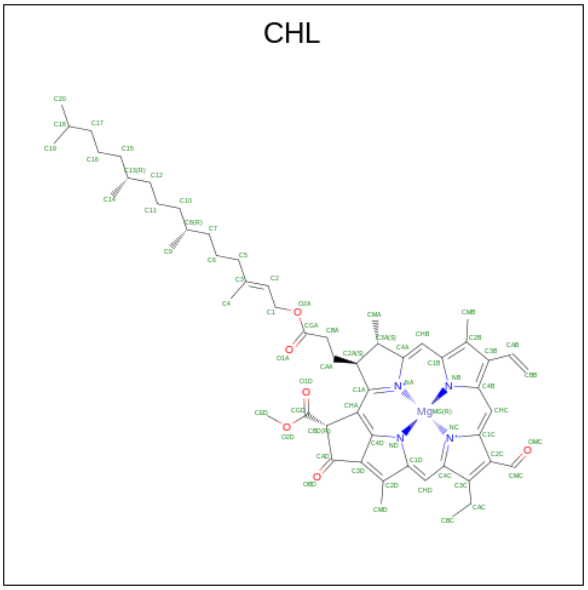
There are 8 unique types of molecules in this entry. The entry contains 8181 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	216	Total	C	N	O	S	0	0
			1650	1072	268	303	7		
1	B	216	Total	C	N	O	S	0	0
			1650	1072	268	303	7		
1	C	216	Total	C	N	O	S	0	0
			1650	1072	268	303	7		

- Molecule 2 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
2	A	1	Total	C	Mg	N	O	0
			51	40	1	4	6	

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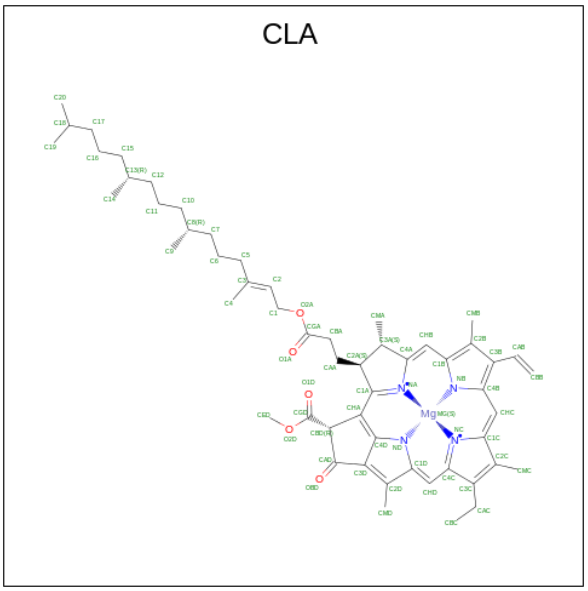
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
2	A	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
2	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
2	B	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
2	B	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
2	B	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
2	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	C	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
2	C	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
2	C	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
2	C	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
2	C	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 3 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
3	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
3	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
3	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
3	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
3	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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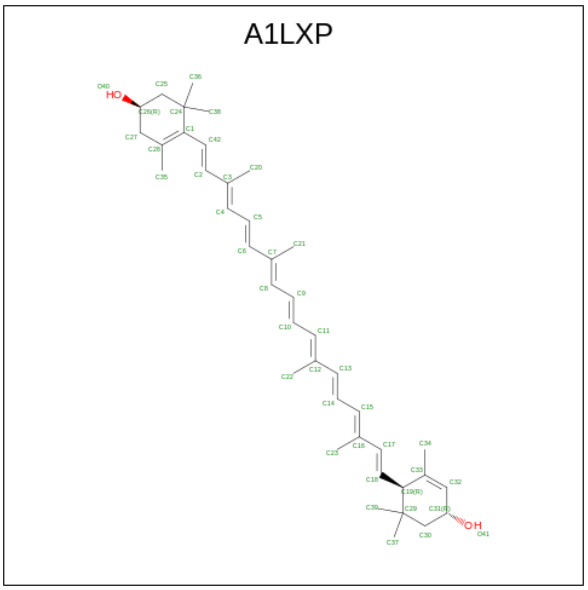
Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
3	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	C	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

- Molecule 4 is Lutein (three-letter code: A1LXP) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



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

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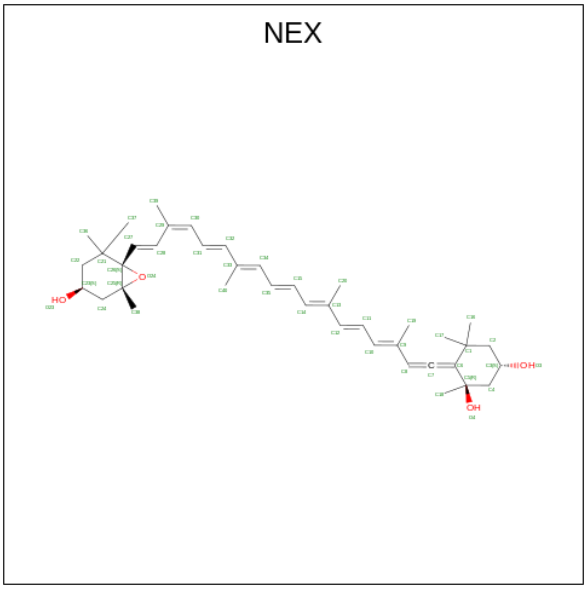
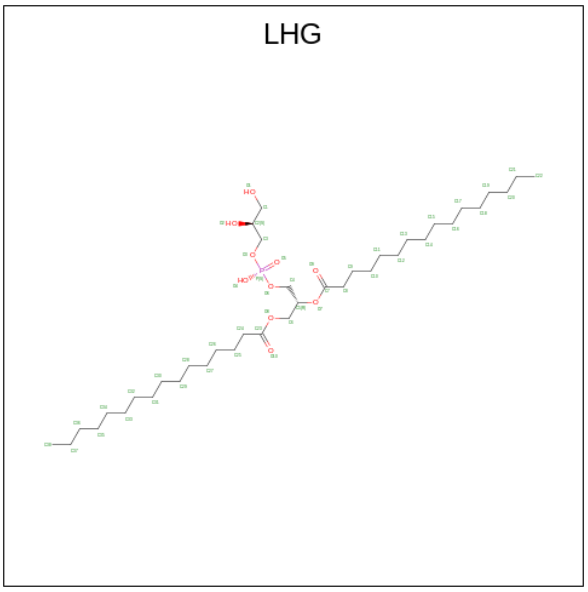
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C O 42 40 2	0
4	B	1	Total C O 42 40 2	0
4	B	1	Total C O 42 40 2	0
4	C	1	Total C O 42 40 2	0
4	C	1	Total C O 42 40 2	0

- Molecule 5 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



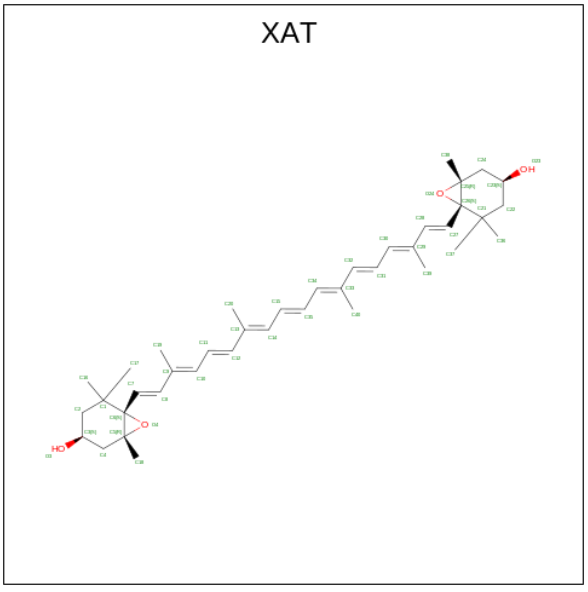
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C O 44 40 4	0
5	B	1	Total C O 44 40 4	0
5	C	1	Total C O 44 40 4	0

- Molecule 6 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C O 44 40 4	0
7	B	1	Total C O 44 40 4	0
7	C	1	Total C O 44 40 4	0

- Molecule 8 is water.

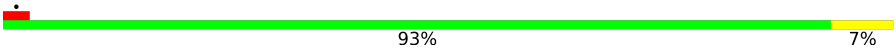
Mol	Chain	Residues	Atoms	AltConf
8	A	45	Total O 45 45	0
8	B	44	Total O 44 44	0
8	C	43	Total O 43 43	0

3 Residue-property plots (i)

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

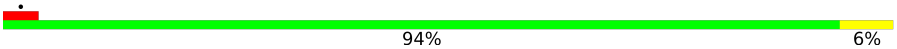
• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

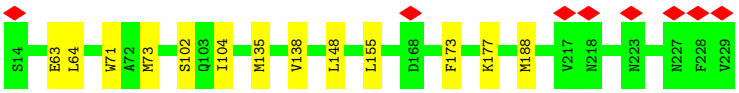
Chain A:



• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

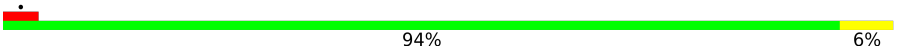
Chain B:





• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	479808	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.880	Depositor
Minimum map value	-1.503	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	219.904, 219.904, 219.904	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.859, 0.859, 0.859	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XAT, LHG, NEX, CHL, CLA, A1LXP

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	0.26	0/1701	0.43	0/2316
1	B	0.25	0/1701	0.42	0/2316
1	C	0.25	0/1701	0.42	0/2316
All	All	0.26	0/5103	0.42	0/6948

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1650	0	1582	10	0
1	B	1650	0	1582	10	0
1	C	1650	0	1582	10	0
2	A	335	0	296	8	0
2	B	335	0	296	10	0
2	C	335	0	296	10	0
3	A	477	0	489	14	0
3	B	477	0	489	12	0
3	C	477	0	489	11	0
4	A	84	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	84	0	0	2	0
4	C	84	0	0	2	0
5	A	44	0	53	0	0
5	B	44	0	53	0	0
5	C	44	0	53	0	0
6	A	49	0	74	2	0
6	B	49	0	74	5	0
6	C	49	0	74	7	0
7	A	44	0	56	3	0
7	B	44	0	56	2	0
7	C	44	0	56	1	0
8	A	45	0	0	0	0
8	B	44	0	0	0	0
8	C	43	0	0	0	0
All	All	8181	0	7650	79	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 5.

All (79) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:HG	2:A:608:CHL:HAB	1.83	0.61
1:B:148:LEU:HG	2:B:608:CHL:HAB	1.83	0.60
7:B:1004:XAT:H12	6:C:1005:LHG:H191	1.83	0.59
7:A:1004:XAT:H363	6:B:1005:LHG:HC41	1.86	0.56
2:A:606:CHL:HBD	2:A:606:CHL:HBA2	1.87	0.56
2:B:606:CHL:HBD	2:B:606:CHL:HBA2	1.87	0.56
1:C:148:LEU:HG	2:C:608:CHL:HAB	1.87	0.56
2:C:606:CHL:HBA2	2:C:606:CHL:HBD	1.87	0.55
7:A:1004:XAT:H361	6:B:1005:LHG:HC92	1.89	0.55
2:B:601:CHL:HED3	6:B:1005:LHG:H142	1.90	0.54
3:C:610:CLA:H8	3:C:612:CLA:H102	1.90	0.54
6:A:1005:LHG:HC41	7:C:1004:XAT:H363	1.89	0.53
3:B:610:CLA:H8	3:B:612:CLA:H102	1.89	0.53
7:B:1004:XAT:H363	6:C:1005:LHG:HC41	1.90	0.53
1:C:64:LEU:HD13	3:C:603:CLA:HBA1	1.90	0.53
3:A:612:CLA:H101	3:A:612:CLA:HMA1	1.91	0.52
3:B:612:CLA:HMA1	3:B:612:CLA:H101	1.92	0.52
3:C:612:CLA:HMA1	3:C:612:CLA:H101	1.91	0.51
2:C:601:CHL:H202	6:C:1005:LHG:H221	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:LEU:HD13	3:B:603:CLA:HBA1	1.93	0.50
3:C:603:CLA:HBB1	2:C:609:CHL:H161	1.94	0.50
1:A:64:LEU:HD13	3:A:603:CLA:HBA1	1.93	0.49
1:C:189:PHE:HZ	6:C:1005:LHG:H151	1.79	0.48
3:A:610:CLA:H8	3:A:612:CLA:H102	1.94	0.48
1:A:63:GLU:HA	1:A:155:LEU:HD11	1.96	0.47
1:B:102:SER:HB3	2:B:607:CHL:HED2	1.97	0.47
3:A:603:CLA:HBB1	2:A:609:CHL:H13	1.95	0.47
1:A:71:TRP:CD1	2:A:609:CHL:HMD3	2.50	0.47
2:C:601:CHL:HBA1	2:C:601:CHL:H3A	1.69	0.46
1:B:71:TRP:CD1	2:B:609:CHL:HMD3	2.51	0.46
1:B:63:GLU:HA	1:B:155:LEU:HD11	1.97	0.46
2:B:601:CHL:HBA1	2:B:601:CHL:H3A	1.68	0.46
6:C:1005:LHG:H301	6:C:1005:LHG:H341	1.97	0.46
3:B:603:CLA:HBB1	2:B:609:CHL:H13	1.98	0.46
3:B:604:CLA:HBD	3:B:604:CLA:HBA1	1.98	0.46
3:A:602:CLA:H41	3:A:602:CLA:H61	1.67	0.45
1:C:135:MET:HA	1:C:138:VAL:HG22	1.97	0.45
1:A:135:MET:HA	1:A:138:VAL:HG22	1.98	0.45
2:B:601:CHL:HMD3	6:B:1005:LHG:HC61	1.97	0.45
1:A:213:LEU:HD21	3:A:614:CLA:HMC3	1.98	0.44
3:A:603:CLA:HAB	4:A:1002:A1LXP:C10	2.47	0.44
3:A:604:CLA:HBA1	3:A:604:CLA:HBD	1.99	0.44
3:B:613:CLA:H51	3:B:613:CLA:C3C	2.47	0.44
1:C:102:SER:HB3	2:C:607:CHL:HED2	1.99	0.44
1:B:135:MET:HA	1:B:138:VAL:HG22	1.99	0.44
7:A:1004:XAT:H10	6:B:1005:LHG:H211	1.99	0.44
1:B:73:MET:SD	3:B:610:CLA:HAB	2.58	0.44
3:A:613:CLA:H51	3:A:613:CLA:C3C	2.47	0.44
3:C:613:CLA:C3C	3:C:613:CLA:H51	2.48	0.43
3:A:603:CLA:C4B	2:A:609:CHL:H111	2.48	0.43
3:C:604:CLA:HBD	3:C:604:CLA:HBA1	2.00	0.43
3:C:610:CLA:H41	3:C:612:CLA:H92	2.00	0.43
1:C:63:GLU:HA	1:C:155:LEU:HD11	1.99	0.43
3:A:603:CLA:HBB1	2:A:609:CHL:H161	2.00	0.43
3:B:603:CLA:HAB	4:B:1002:A1LXP:C10	2.48	0.43
3:B:603:CLA:C4B	2:B:609:CHL:H111	2.49	0.43
3:C:603:CLA:HAB	4:C:1002:A1LXP:C10	2.49	0.43
3:B:610:CLA:H41	3:B:612:CLA:H92	2.01	0.42
1:C:71:TRP:CD1	2:C:609:CHL:HMD3	2.54	0.42
1:A:173:PHE:CZ	1:A:177:LYS:HE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:602:CLA:HMC2	4:B:1002:A1LXP:C14	2.49	0.42
2:C:601:CHL:H162	6:C:1005:LHG:H221	2.01	0.42
3:C:603:CLA:C4B	2:C:609:CHL:H111	2.49	0.42
1:A:102:SER:HB3	2:A:607:CHL:HED2	2.00	0.42
3:A:610:CLA:H41	3:A:612:CLA:H92	2.02	0.42
1:C:73:MET:SD	3:C:610:CLA:HAB	2.60	0.42
1:B:188:MET:HE3	3:B:602:CLA:HMC3	2.01	0.42
2:A:601:CHL:HMA3	6:A:1005:LHG:H121	2.02	0.41
1:C:173:PHE:CZ	1:C:177:LYS:HE3	2.55	0.41
1:B:173:PHE:CZ	1:B:177:LYS:HE3	2.55	0.41
1:A:203:LYS:HD2	1:A:207:GLU:HG2	2.01	0.41
2:C:601:CHL:HMD3	6:C:1005:LHG:HC61	2.01	0.41
2:B:601:CHL:H62	2:B:601:CHL:H41	1.81	0.41
1:C:104:ILE:HD12	1:C:104:ILE:HA	1.90	0.41
1:A:24:TYR:HB3	1:A:44:TYR:HB3	2.03	0.41
3:A:602:CLA:HMC2	4:A:1002:A1LXP:C14	2.51	0.41
3:C:602:CLA:HMC2	4:C:1002:A1LXP:C14	2.50	0.41
1:B:104:ILE:HD12	1:B:104:ILE:HA	1.90	0.40
3:A:613:CLA:H2	3:A:613:CLA:H61	1.82	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	214/216 (99%)	211 (99%)	3 (1%)	0	100	100
1	B	214/216 (99%)	212 (99%)	2 (1%)	0	100	100
1	C	214/216 (99%)	212 (99%)	2 (1%)	0	100	100
All	All	642/648 (99%)	635 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	167/167 (100%)	167 (100%)	0	100	100
1	B	167/167 (100%)	167 (100%)	0	100	100
1	C	167/167 (100%)	167 (100%)	0	100	100
All	All	501/501 (100%)	501 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

57 ligands are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CHL	C	609	1	66,74,74	1.55	5 (7%)	73,114,114	1.70	11 (15%)
3	CLA	B	604	8	55,63,73	2.56	7 (12%)	64,101,113	1.31	9 (14%)
2	CHL	C	605	1	45,53,74	1.91	5 (11%)	46,88,114	2.19	11 (23%)
3	CLA	A	604	8	55,63,73	2.57	8 (14%)	64,101,113	1.32	9 (14%)
2	CHL	C	607	8	46,54,74	1.83	5 (10%)	49,90,114	2.21	10 (20%)
3	CLA	A	610	1	65,73,73	2.35	8 (12%)	76,113,113	1.14	9 (11%)
4	A1LXP	B	1002	-	42,43,43	0.37	0	51,60,60	0.44	0
3	CLA	B	612	1	65,73,73	2.35	8 (12%)	76,113,113	1.18	8 (10%)
3	CLA	A	613	1	65,73,73	2.34	8 (12%)	76,113,113	1.11	8 (10%)
3	CLA	B	613	1	65,73,73	2.33	7 (10%)	76,113,113	1.10	8 (10%)
3	CLA	C	612	1	65,73,73	2.35	7 (10%)	76,113,113	1.18	9 (11%)
6	LHG	B	1005	3	48,48,48	0.24	0	51,54,54	0.27	0
2	CHL	A	609	1	66,74,74	1.54	5 (7%)	73,114,114	1.69	11 (15%)
3	CLA	B	603	1	55,63,73	2.59	8 (14%)	64,101,113	1.31	8 (12%)
6	LHG	C	1005	3	48,48,48	0.24	0	51,54,54	0.26	0
6	LHG	A	1005	3	48,48,48	0.24	0	51,54,54	0.27	0
2	CHL	C	606	8	51,59,74	1.72	5 (9%)	55,96,114	2.09	12 (21%)
5	NEX	B	1003	-	38,46,46	2.32	4 (10%)	50,70,70	0.61	1 (2%)
3	CLA	B	602	1	65,73,73	2.35	8 (12%)	76,113,113	1.08	8 (10%)
3	CLA	A	612	1	65,73,73	2.34	8 (12%)	76,113,113	1.19	9 (11%)
2	CHL	B	608	8	61,69,74	1.61	5 (8%)	67,108,114	1.83	11 (16%)
2	CHL	A	608	8	61,69,74	1.60	5 (8%)	67,108,114	1.82	11 (16%)
5	NEX	A	1003	-	38,46,46	2.43	4 (10%)	50,70,70	0.62	1 (2%)
2	CHL	B	601	1	66,74,74	1.57	5 (7%)	73,114,114	1.78	10 (13%)
2	CHL	C	601	1	66,74,74	1.56	5 (7%)	73,114,114	1.77	11 (15%)
3	CLA	C	610	1	65,73,73	2.35	8 (12%)	76,113,113	1.12	9 (11%)
2	CHL	B	607	8	46,54,74	1.84	5 (10%)	49,90,114	2.22	11 (22%)
3	CLA	C	602	1	65,73,73	2.34	8 (12%)	76,113,113	1.10	9 (11%)
2	CHL	A	605	1	45,53,74	1.91	5 (11%)	46,88,114	2.21	11 (23%)
3	CLA	B	614	1	42,50,73	2.95	8 (19%)	48,85,113	1.44	8 (16%)
2	CHL	A	607	8	46,54,74	1.83	5 (10%)	49,90,114	2.20	10 (20%)
4	A1LXP	A	1001	-	42,43,43	0.37	0	51,60,60	0.41	0
3	CLA	C	614	1	42,50,73	2.95	8 (19%)	48,85,113	1.45	8 (16%)
5	NEX	C	1003	-	38,46,46	2.43	4 (10%)	50,70,70	0.60	1 (2%)
3	CLA	A	602	1	65,73,73	2.34	8 (12%)	76,113,113	1.09	8 (10%)
2	CHL	B	606	8	51,59,74	1.71	5 (9%)	55,96,114	2.09	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CHL	B	605	1	45,53,74	1.92	5 (11%)	46,88,114	2.19	11 (23%)
3	CLA	B	610	1	65,73,73	2.35	8 (12%)	76,113,113	1.12	9 (11%)
3	CLA	B	611	6	65,73,73	2.36	8 (12%)	76,113,113	1.24	8 (10%)
3	CLA	C	613	1	65,73,73	2.33	7 (10%)	76,113,113	1.10	8 (10%)
3	CLA	C	611	6	65,73,73	2.36	8 (12%)	76,113,113	1.25	9 (11%)
2	CHL	A	606	8	51,59,74	1.73	5 (9%)	55,96,114	2.08	13 (23%)
3	CLA	A	611	6	65,73,73	2.36	8 (12%)	76,113,113	1.26	9 (11%)
2	CHL	A	601	1	66,74,74	1.55	5 (7%)	73,114,114	1.81	10 (13%)
7	XAT	B	1004	-	39,47,47	0.09	0	54,74,74	2.51	1 (1%)
7	XAT	C	1004	-	39,47,47	0.09	0	54,74,74	2.53	1 (1%)
7	XAT	A	1004	-	39,47,47	0.09	0	54,74,74	2.53	1 (1%)
4	A1LXP	C	1002	-	42,43,43	0.36	0	51,60,60	0.45	0
4	A1LXP	B	1001	-	42,43,43	0.38	1 (2%)	51,60,60	0.42	0
3	CLA	C	604	8	55,63,73	2.56	7 (12%)	64,101,113	1.33	9 (14%)
3	CLA	C	603	1	55,63,73	2.57	8 (14%)	64,101,113	1.30	9 (14%)
4	A1LXP	C	1001	-	42,43,43	0.38	1 (2%)	51,60,60	0.42	0
2	CHL	C	608	8	61,69,74	1.60	5 (8%)	67,108,114	1.85	11 (16%)
3	CLA	A	603	1	55,63,73	2.57	8 (14%)	64,101,113	1.31	9 (14%)
2	CHL	B	609	1	66,74,74	1.54	5 (7%)	73,114,114	1.70	11 (15%)
3	CLA	A	614	1	42,50,73	2.96	8 (19%)	48,85,113	1.44	8 (16%)
4	A1LXP	A	1002	-	42,43,43	0.37	0	51,60,60	0.45	0

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
2	CHL	C	609	1	4/4/20/26	7/39/137/137	-
3	CLA	B	604	8	2/2/13/20	5/25/103/115	-
2	CHL	C	605	1	3/3/15/26	2/13/112/137	-
3	CLA	A	604	8	2/2/13/20	5/25/103/115	-
2	CHL	C	607	8	3/3/16/26	3/15/113/137	-
3	CLA	A	610	1	2/2/15/20	0/37/115/115	-
4	A1LXP	B	1002	-	-	2/29/67/67	0/2/2/2
3	CLA	B	612	1	2/2/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	A	613	1	2/2/15/20	4/37/115/115	-
3	CLA	B	613	1	2/2/15/20	4/37/115/115	-
3	CLA	C	612	1	2/2/15/20	7/37/115/115	-
6	LHG	B	1005	3	-	11/53/53/53	-
2	CHL	A	609	1	4/4/20/26	6/39/137/137	-
3	CLA	B	603	1	2/2/13/20	3/25/103/115	-
6	LHG	C	1005	3	-	11/53/53/53	-
6	LHG	A	1005	3	-	7/53/53/53	-
2	CHL	C	606	8	3/3/17/26	7/21/119/137	-
5	NEX	B	1003	-	-	2/27/83/83	0/3/3/3
3	CLA	B	602	1	2/2/15/20	9/37/115/115	-
3	CLA	A	612	1	2/2/15/20	7/37/115/115	-
2	CHL	B	608	8	4/4/19/26	5/33/131/137	-
2	CHL	A	608	8	4/4/19/26	6/33/131/137	-
5	NEX	A	1003	-	-	2/27/83/83	0/3/3/3
2	CHL	B	601	1	4/4/20/26	10/39/137/137	-
2	CHL	C	601	1	4/4/20/26	10/39/137/137	-
3	CLA	C	610	1	2/2/15/20	0/37/115/115	-
2	CHL	B	607	8	3/3/16/26	4/15/113/137	-
3	CLA	C	602	1	2/2/15/20	4/37/115/115	-
2	CHL	A	605	1	3/3/15/26	2/13/112/137	-
3	CLA	B	614	1	1/1/10/20	1/10/88/115	-
2	CHL	A	607	8	3/3/16/26	3/15/113/137	-
4	A1LXP	A	1001	-	-	2/29/67/67	0/2/2/2
3	CLA	C	614	1	1/1/10/20	1/10/88/115	-
5	NEX	C	1003	-	-	2/27/83/83	0/3/3/3
3	CLA	A	602	1	2/2/15/20	5/37/115/115	-
2	CHL	B	606	8	3/3/17/26	7/21/119/137	-
2	CHL	B	605	1	3/3/15/26	2/13/112/137	-
3	CLA	B	610	1	2/2/15/20	0/37/115/115	-
3	CLA	B	611	6	2/2/15/20	12/37/115/115	-
3	CLA	C	613	1	2/2/15/20	4/37/115/115	-
3	CLA	C	611	6	2/2/15/20	12/37/115/115	-
2	CHL	A	606	8	3/3/17/26	5/21/119/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	A	611	6	2/2/15/20	12/37/115/115	-
2	CHL	A	601	1	4/4/20/26	11/39/137/137	-
7	XAT	B	1004	-	2/2/12/26	0/31/93/93	0/4/4/4
7	XAT	C	1004	-	2/2/12/26	0/31/93/93	0/4/4/4
7	XAT	A	1004	-	2/2/12/26	0/31/93/93	0/4/4/4
4	A1LXP	C	1002	-	-	2/29/67/67	0/2/2/2
4	A1LXP	B	1001	-	-	2/29/67/67	0/2/2/2
3	CLA	C	604	8	2/2/13/20	5/25/103/115	-
3	CLA	C	603	1	2/2/13/20	3/25/103/115	-
4	A1LXP	C	1001	-	-	2/29/67/67	0/2/2/2
2	CHL	C	608	8	4/4/19/26	8/33/131/137	-
3	CLA	A	603	1	2/2/13/20	3/25/103/115	-
2	CHL	B	609	1	4/4/20/26	6/39/137/137	-
3	CLA	A	614	1	1/1/10/20	1/10/88/115	-
4	A1LXP	A	1002	-	-	2/29/67/67	0/2/2/2

All (291) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	614	CLA	C4B-NB	14.96	1.48	1.35
3	B	603	CLA	C4B-NB	14.95	1.48	1.35
3	A	603	CLA	C4B-NB	14.82	1.48	1.35
3	C	614	CLA	C4B-NB	14.80	1.48	1.35
3	B	614	CLA	C4B-NB	14.78	1.48	1.35
3	C	603	CLA	C4B-NB	14.77	1.48	1.35
3	B	602	CLA	C4B-NB	14.75	1.48	1.35
3	C	612	CLA	C4B-NB	14.70	1.48	1.35
3	A	602	CLA	C4B-NB	14.65	1.48	1.35
3	B	612	CLA	C4B-NB	14.64	1.48	1.35
3	A	604	CLA	C4B-NB	14.61	1.48	1.35
3	C	610	CLA	C4B-NB	14.61	1.48	1.35
3	B	610	CLA	C4B-NB	14.57	1.48	1.35
3	A	610	CLA	C4B-NB	14.56	1.48	1.35
3	B	613	CLA	C4B-NB	14.55	1.48	1.35
3	C	602	CLA	C4B-NB	14.54	1.48	1.35
3	A	612	CLA	C4B-NB	14.54	1.48	1.35
3	A	613	CLA	C4B-NB	14.53	1.48	1.35
3	B	604	CLA	C4B-NB	14.51	1.48	1.35
3	C	604	CLA	C4B-NB	14.50	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	613	CLA	C4B-NB	14.50	1.48	1.35
3	C	611	CLA	C4B-NB	14.43	1.48	1.35
3	B	611	CLA	C4B-NB	14.42	1.48	1.35
3	A	611	CLA	C4B-NB	14.39	1.48	1.35
5	A	1003	NEX	C40-C33	-13.13	1.23	1.50
5	B	1003	NEX	C40-C33	-12.79	1.24	1.50
5	C	1003	NEX	C40-C33	-12.60	1.24	1.50
2	B	605	CHL	C4B-NB	11.35	1.45	1.35
2	C	605	CHL	C4B-NB	11.29	1.45	1.35
2	A	605	CHL	C4B-NB	11.28	1.45	1.35
2	B	601	CHL	C4B-NB	11.17	1.45	1.35
2	C	601	CHL	C4B-NB	11.07	1.45	1.35
2	A	601	CHL	C4B-NB	11.04	1.45	1.35
2	B	608	CHL	C4B-NB	11.01	1.45	1.35
2	C	609	CHL	C4B-NB	11.00	1.45	1.35
2	A	609	CHL	C4B-NB	10.93	1.45	1.35
2	C	608	CHL	C4B-NB	10.93	1.45	1.35
2	B	609	CHL	C4B-NB	10.91	1.44	1.35
2	A	608	CHL	C4B-NB	10.88	1.44	1.35
2	B	607	CHL	C4B-NB	10.85	1.44	1.35
2	A	606	CHL	C4B-NB	10.79	1.44	1.35
2	A	607	CHL	C4B-NB	10.78	1.44	1.35
2	C	606	CHL	C4B-NB	10.77	1.44	1.35
2	C	607	CHL	C4B-NB	10.77	1.44	1.35
2	B	606	CHL	C4B-NB	10.68	1.44	1.35
3	B	614	CLA	C1B-NB	7.70	1.42	1.35
3	A	603	CLA	C1B-NB	7.65	1.42	1.35
3	B	603	CLA	C1B-NB	7.62	1.42	1.35
3	A	611	CLA	C1B-NB	7.60	1.42	1.35
3	C	611	CLA	C1B-NB	7.60	1.42	1.35
3	C	603	CLA	C1B-NB	7.60	1.42	1.35
3	C	614	CLA	C1B-NB	7.59	1.42	1.35
3	B	611	CLA	C1B-NB	7.55	1.41	1.35
3	A	614	CLA	C1B-NB	7.54	1.41	1.35
3	C	610	CLA	C1B-NB	7.54	1.41	1.35
3	A	613	CLA	C1B-NB	7.51	1.41	1.35
3	B	610	CLA	C1B-NB	7.51	1.41	1.35
3	C	613	CLA	C1B-NB	7.48	1.41	1.35
3	C	604	CLA	C1B-NB	7.48	1.41	1.35
3	A	604	CLA	C1B-NB	7.47	1.41	1.35
3	A	610	CLA	C1B-NB	7.47	1.41	1.35
3	C	612	CLA	C1B-NB	7.46	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	CLA	C1B-NB	7.46	1.41	1.35
3	C	602	CLA	C1B-NB	7.46	1.41	1.35
3	B	612	CLA	C1B-NB	7.43	1.41	1.35
3	A	612	CLA	C1B-NB	7.40	1.41	1.35
3	B	604	CLA	C1B-NB	7.37	1.41	1.35
3	B	613	CLA	C1B-NB	7.33	1.41	1.35
3	B	602	CLA	C1B-NB	7.32	1.41	1.35
3	A	604	CLA	MG-ND	-5.02	1.95	2.05
5	C	1003	NEX	C28-C27	5.01	1.43	1.32
3	B	604	CLA	MG-ND	-4.99	1.95	2.05
3	C	604	CLA	MG-ND	-4.98	1.95	2.05
3	B	611	CLA	MG-ND	-4.96	1.96	2.05
3	C	611	CLA	MG-ND	-4.92	1.96	2.05
3	A	611	CLA	MG-ND	-4.91	1.96	2.05
3	C	610	CLA	MG-ND	-4.90	1.96	2.05
3	B	610	CLA	MG-ND	-4.89	1.96	2.05
3	C	602	CLA	MG-ND	-4.87	1.96	2.05
3	A	610	CLA	MG-ND	-4.86	1.96	2.05
3	A	602	CLA	MG-ND	-4.85	1.96	2.05
3	B	602	CLA	MG-ND	-4.85	1.96	2.05
3	C	613	CLA	MG-ND	-4.82	1.96	2.05
3	A	613	CLA	MG-ND	-4.81	1.96	2.05
3	B	613	CLA	MG-ND	-4.79	1.96	2.05
3	A	612	CLA	MG-ND	-4.71	1.96	2.05
3	B	612	CLA	MG-ND	-4.69	1.96	2.05
3	C	612	CLA	MG-ND	-4.68	1.96	2.05
3	B	614	CLA	MG-ND	-4.59	1.96	2.05
3	A	614	CLA	MG-ND	-4.58	1.96	2.05
3	C	614	CLA	MG-ND	-4.57	1.96	2.05
3	B	603	CLA	MG-ND	-4.52	1.96	2.05
3	A	603	CLA	MG-ND	-4.51	1.96	2.05
3	C	603	CLA	MG-ND	-4.51	1.96	2.05
5	A	1003	NEX	C34-C33	-4.40	1.29	1.35
5	C	1003	NEX	C34-C33	-4.35	1.30	1.35
3	A	611	CLA	MG-NA	-4.28	1.96	2.06
3	C	603	CLA	C1D-ND	4.28	1.43	1.37
3	B	611	CLA	MG-NA	-4.27	1.96	2.06
3	C	614	CLA	C1D-ND	4.25	1.43	1.37
3	A	614	CLA	C1D-ND	4.23	1.43	1.37
3	C	611	CLA	MG-NA	-4.22	1.96	2.06
3	B	614	CLA	C1D-ND	4.21	1.43	1.37
3	A	603	CLA	C1D-ND	4.21	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	612	CLA	C1D-ND	4.20	1.42	1.37
3	B	603	CLA	C1D-ND	4.20	1.42	1.37
3	C	604	CLA	MG-NA	-4.17	1.96	2.06
3	A	612	CLA	C1D-ND	4.16	1.42	1.37
3	B	604	CLA	MG-NA	-4.16	1.96	2.06
3	C	612	CLA	C1D-ND	4.14	1.42	1.37
3	A	604	CLA	MG-NA	-4.12	1.96	2.06
3	C	610	CLA	MG-NA	-4.09	1.96	2.06
3	A	610	CLA	MG-NA	-4.08	1.96	2.06
3	B	610	CLA	MG-NA	-4.03	1.96	2.06
3	A	613	CLA	C1D-ND	4.03	1.42	1.37
5	A	1003	NEX	C28-C27	4.03	1.41	1.32
3	A	604	CLA	C1D-ND	3.98	1.42	1.37
3	C	604	CLA	C1D-ND	3.97	1.42	1.37
3	A	611	CLA	C1D-ND	3.97	1.42	1.37
3	B	611	CLA	C1D-ND	3.96	1.42	1.37
3	B	604	CLA	C1D-ND	3.93	1.42	1.37
3	B	613	CLA	C1D-ND	3.93	1.42	1.37
3	C	613	CLA	C1D-ND	3.93	1.42	1.37
3	C	611	CLA	C1D-ND	3.90	1.42	1.37
3	B	610	CLA	C1D-ND	3.89	1.42	1.37
3	C	613	CLA	MG-NA	-3.86	1.97	2.06
3	B	602	CLA	MG-NA	-3.84	1.97	2.06
3	A	610	CLA	C1D-ND	3.83	1.42	1.37
3	A	602	CLA	C1D-ND	3.82	1.42	1.37
3	C	602	CLA	C1D-ND	3.81	1.42	1.37
3	B	613	CLA	MG-NA	-3.81	1.97	2.06
3	A	613	CLA	MG-NA	-3.79	1.97	2.06
3	C	602	CLA	MG-NA	-3.79	1.97	2.06
3	A	602	CLA	MG-NA	-3.77	1.97	2.06
3	B	602	CLA	C1D-ND	3.75	1.42	1.37
3	C	610	CLA	C1D-ND	3.71	1.42	1.37
3	A	614	CLA	MG-NA	-3.68	1.97	2.06
3	B	611	CLA	MG-NC	-3.67	1.97	2.06
3	B	614	CLA	MG-NA	-3.67	1.97	2.06
3	C	614	CLA	MG-NA	-3.63	1.97	2.06
3	A	611	CLA	MG-NC	-3.62	1.97	2.06
3	C	604	CLA	MG-NC	-3.61	1.97	2.06
3	C	611	CLA	MG-NC	-3.61	1.97	2.06
3	A	604	CLA	MG-NC	-3.60	1.97	2.06
5	B	1003	NEX	C28-C27	3.60	1.40	1.32
3	B	604	CLA	MG-NC	-3.59	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	612	CLA	MG-NA	-3.57	1.97	2.06
3	A	612	CLA	MG-NA	-3.56	1.97	2.06
3	A	610	CLA	MG-NC	-3.54	1.97	2.06
3	C	612	CLA	MG-NA	-3.53	1.97	2.06
3	C	610	CLA	MG-NC	-3.51	1.97	2.06
3	B	610	CLA	MG-NC	-3.50	1.98	2.06
3	B	614	CLA	MG-NC	-3.48	1.98	2.06
3	A	614	CLA	MG-NC	-3.47	1.98	2.06
3	C	614	CLA	MG-NC	-3.46	1.98	2.06
3	C	603	CLA	MG-NA	-3.44	1.98	2.06
3	B	603	CLA	MG-NA	-3.42	1.98	2.06
3	A	603	CLA	MG-NA	-3.37	1.98	2.06
3	B	603	CLA	MG-NC	-3.35	1.98	2.06
3	A	603	CLA	MG-NC	-3.34	1.98	2.06
3	B	613	CLA	MG-NC	-3.32	1.98	2.06
3	C	602	CLA	MG-NC	-3.32	1.98	2.06
3	A	613	CLA	MG-NC	-3.31	1.98	2.06
3	A	602	CLA	MG-NC	-3.30	1.98	2.06
5	C	1003	NEX	C39-C29	-3.29	1.44	1.50
3	C	613	CLA	MG-NC	-3.29	1.98	2.06
3	B	602	CLA	MG-NC	-3.27	1.98	2.06
3	C	603	CLA	MG-NC	-3.26	1.98	2.06
3	B	612	CLA	MG-NC	-3.23	1.98	2.06
3	C	612	CLA	MG-NC	-3.23	1.98	2.06
3	A	612	CLA	MG-NC	-3.22	1.98	2.06
5	B	1003	NEX	C34-C33	-3.10	1.31	1.35
5	B	1003	NEX	C39-C29	-2.90	1.44	1.50
5	A	1003	NEX	C39-C29	-2.82	1.45	1.50
3	B	602	CLA	C1C-C2C	2.39	1.49	1.44
3	C	610	CLA	C1D-C2D	-2.34	1.40	1.45
3	A	610	CLA	C1D-C2D	-2.33	1.40	1.45
3	B	610	CLA	C1D-C2D	-2.33	1.40	1.45
3	B	604	CLA	C1D-C2D	-2.33	1.40	1.45
3	C	611	CLA	C1D-C2D	-2.33	1.40	1.45
3	C	612	CLA	C1D-C2D	-2.33	1.40	1.45
3	A	611	CLA	C1D-C2D	-2.33	1.40	1.45
3	B	611	CLA	C1D-C2D	-2.33	1.40	1.45
3	C	602	CLA	C1C-C2C	2.32	1.49	1.44
3	B	612	CLA	C1D-C2D	-2.32	1.40	1.45
3	A	612	CLA	C1D-C2D	-2.32	1.40	1.45
2	B	601	CHL	C3B-C2B	-2.32	1.37	1.40
3	C	604	CLA	C1D-C2D	-2.31	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	CLA	C1D-C2D	-2.31	1.40	1.45
3	A	613	CLA	C1D-C2D	-2.31	1.40	1.45
3	A	602	CLA	C1D-C2D	-2.31	1.40	1.45
3	C	603	CLA	C1D-C2D	-2.31	1.40	1.45
3	C	614	CLA	C1D-C2D	-2.31	1.40	1.45
2	C	607	CHL	C3B-C2B	-2.30	1.37	1.40
3	A	604	CLA	C1D-C2D	-2.30	1.40	1.45
3	B	602	CLA	C1D-C2D	-2.29	1.40	1.45
3	A	614	CLA	C1D-C2D	-2.29	1.40	1.45
3	B	614	CLA	C1D-C2D	-2.28	1.40	1.45
2	B	607	CHL	C3B-C2B	-2.28	1.37	1.40
3	B	603	CLA	C1D-C2D	-2.27	1.40	1.45
2	C	607	CHL	C1D-C2D	-2.27	1.40	1.45
2	A	607	CHL	C1D-C2D	-2.27	1.40	1.45
3	C	613	CLA	C1D-C2D	-2.27	1.40	1.45
2	A	607	CHL	C3B-C2B	-2.27	1.37	1.40
2	C	601	CHL	C3B-C2B	-2.26	1.37	1.40
3	B	613	CLA	C1D-C2D	-2.26	1.40	1.45
3	A	603	CLA	C1D-C2D	-2.26	1.40	1.45
2	B	606	CHL	C1D-C2D	-2.24	1.40	1.45
2	B	607	CHL	C1D-C2D	-2.24	1.40	1.45
2	A	608	CHL	C1D-C2D	-2.23	1.40	1.45
2	B	605	CHL	C3B-C2B	-2.22	1.37	1.40
2	B	608	CHL	C3B-C2B	-2.22	1.37	1.40
2	C	606	CHL	C1D-C2D	-2.22	1.41	1.45
2	C	605	CHL	C3B-C2B	-2.21	1.37	1.40
3	A	602	CLA	C1C-C2C	2.21	1.48	1.44
2	A	605	CHL	C1D-C2D	-2.20	1.41	1.45
2	A	606	CHL	C1D-C2D	-2.20	1.41	1.45
2	A	605	CHL	C3B-C2B	-2.20	1.37	1.40
2	A	601	CHL	C1D-C2D	-2.20	1.41	1.45
2	C	601	CHL	C1D-C2D	-2.20	1.41	1.45
2	A	608	CHL	C3B-C2B	-2.20	1.37	1.40
2	C	608	CHL	C1D-C2D	-2.19	1.41	1.45
2	A	601	CHL	C3B-C2B	-2.19	1.37	1.40
2	B	601	CHL	C1D-C2D	-2.19	1.41	1.45
2	C	605	CHL	C1D-C2D	-2.18	1.41	1.45
2	B	605	CHL	C1D-C2D	-2.17	1.41	1.45
3	C	610	CLA	C1C-C2C	2.17	1.48	1.44
2	B	609	CHL	C1D-C2D	-2.17	1.41	1.45
2	B	608	CHL	C1D-C2D	-2.16	1.41	1.45
2	C	608	CHL	C3B-C2B	-2.15	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	609	CHL	CHC-C1C	2.14	1.40	1.35
2	A	609	CHL	C1D-C2D	-2.14	1.41	1.45
2	C	609	CHL	C1D-C2D	-2.13	1.41	1.45
2	A	609	CHL	CHC-C1C	2.13	1.40	1.35
2	C	601	CHL	CHC-C1C	2.13	1.40	1.35
2	B	601	CHL	CHC-C1C	2.13	1.40	1.35
2	A	608	CHL	CHC-C1C	2.13	1.40	1.35
3	A	614	CLA	C1C-C2C	2.12	1.48	1.44
2	B	608	CHL	CHC-C1C	2.12	1.40	1.35
2	C	609	CHL	CHC-C1C	2.11	1.40	1.35
2	A	609	CHL	C3B-C2B	-2.11	1.37	1.40
3	B	614	CLA	C1C-C2C	2.10	1.48	1.44
2	B	609	CHL	C3B-C2B	-2.10	1.37	1.40
2	C	609	CHL	C3B-C2B	-2.10	1.37	1.40
3	B	610	CLA	C1C-C2C	2.10	1.48	1.44
3	C	614	CLA	C1C-C2C	2.09	1.48	1.44
2	C	608	CHL	CHC-C1C	2.09	1.40	1.35
2	A	606	CHL	C3B-C2B	-2.08	1.37	1.40
2	B	609	CHL	C3D-C4D	-2.08	1.39	1.44
2	A	601	CHL	CHC-C1C	2.08	1.40	1.35
2	A	606	CHL	CHC-C1C	2.07	1.40	1.35
2	A	605	CHL	CHC-C1C	2.07	1.40	1.35
2	B	605	CHL	CHC-C1C	2.07	1.40	1.35
2	C	607	CHL	CHC-C1C	2.06	1.40	1.35
2	C	605	CHL	CHC-C1C	2.06	1.40	1.35
4	B	1001	A1LXP	C30-C31	-2.06	1.49	1.53
2	B	607	CHL	C3D-C4D	-2.06	1.39	1.44
2	C	608	CHL	C3D-C4D	-2.06	1.39	1.44
2	B	608	CHL	C3D-C4D	-2.05	1.39	1.44
2	A	607	CHL	C3D-C4D	-2.05	1.39	1.44
3	C	603	CLA	C1C-C2C	2.05	1.48	1.44
2	C	606	CHL	CHC-C1C	2.05	1.40	1.35
4	C	1001	A1LXP	C30-C31	-2.05	1.49	1.53
2	B	601	CHL	C3D-C4D	-2.05	1.39	1.44
2	C	607	CHL	C3D-C4D	-2.05	1.39	1.44
2	B	606	CHL	CHC-C1C	2.05	1.40	1.35
2	A	605	CHL	C3D-C4D	-2.05	1.39	1.44
2	C	609	CHL	C3D-C4D	-2.05	1.39	1.44
2	A	609	CHL	C3D-C4D	-2.04	1.39	1.44
3	C	611	CLA	C1C-C2C	2.04	1.48	1.44
2	C	605	CHL	C3D-C4D	-2.04	1.39	1.44
2	B	607	CHL	CHC-C1C	2.04	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	CHL	C3D-C4D	-2.04	1.39	1.44
2	A	607	CHL	CHC-C1C	2.04	1.40	1.35
2	B	605	CHL	C3D-C4D	-2.03	1.39	1.44
2	B	606	CHL	C3B-C2B	-2.03	1.37	1.40
2	C	606	CHL	C3D-C4D	-2.02	1.39	1.44
3	B	612	CLA	C1C-C2C	2.02	1.48	1.44
3	A	612	CLA	C1C-C2C	2.02	1.48	1.44
2	A	608	CHL	C3D-C4D	-2.02	1.39	1.44
3	A	603	CLA	C1C-C2C	2.02	1.48	1.44
3	B	611	CLA	C1C-C2C	2.01	1.48	1.44
3	A	604	CLA	C1C-C2C	2.01	1.48	1.44
3	A	610	CLA	C1C-C2C	2.01	1.48	1.44
3	B	603	CLA	C1C-C2C	2.01	1.48	1.44
2	A	606	CHL	C3D-C4D	-2.01	1.39	1.44
3	A	611	CLA	C1C-C2C	2.01	1.48	1.44
3	A	613	CLA	C1C-C2C	2.01	1.48	1.44
2	C	606	CHL	C3B-C2B	-2.00	1.37	1.40
2	A	601	CHL	C3D-C4D	-2.00	1.39	1.44
2	B	606	CHL	C3D-C4D	-2.00	1.39	1.44

All (410) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1004	XAT	O24-C25-C24	-18.28	99.65	113.38
7	C	1004	XAT	O24-C25-C24	-18.28	99.65	113.38
7	B	1004	XAT	O24-C25-C24	-18.17	99.73	113.38
2	A	601	CHL	C4A-NA-C1A	11.46	111.86	106.71
2	B	607	CHL	C4A-NA-C1A	11.41	111.83	106.71
2	A	607	CHL	C4A-NA-C1A	11.39	111.83	106.71
2	C	607	CHL	C4A-NA-C1A	11.32	111.80	106.71
2	B	606	CHL	C4A-NA-C1A	11.31	111.79	106.71
2	C	606	CHL	C4A-NA-C1A	11.28	111.78	106.71
2	A	606	CHL	C4A-NA-C1A	11.21	111.75	106.71
2	B	601	CHL	C4A-NA-C1A	11.09	111.69	106.71
2	C	601	CHL	C4A-NA-C1A	11.00	111.65	106.71
2	C	608	CHL	C4A-NA-C1A	10.93	111.62	106.71
2	A	605	CHL	C4A-NA-C1A	10.82	111.57	106.71
2	B	608	CHL	C4A-NA-C1A	10.76	111.54	106.71
2	C	605	CHL	C4A-NA-C1A	10.69	111.51	106.71
2	B	605	CHL	C4A-NA-C1A	10.62	111.48	106.71
2	A	608	CHL	C4A-NA-C1A	10.61	111.48	106.71
2	B	609	CHL	C4A-NA-C1A	10.27	111.32	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	609	CHL	C4A-NA-C1A	10.19	111.29	106.71
2	A	609	CHL	C4A-NA-C1A	10.12	111.25	106.71
3	C	611	CLA	C4A-NA-C1A	-6.34	103.86	106.71
3	A	611	CLA	C4A-NA-C1A	-6.33	103.86	106.71
3	B	611	CLA	C4A-NA-C1A	-6.24	103.90	106.71
3	C	604	CLA	C4A-NA-C1A	-5.99	104.02	106.71
3	A	604	CLA	C4A-NA-C1A	-5.91	104.05	106.71
3	B	604	CLA	C4A-NA-C1A	-5.80	104.10	106.71
3	A	603	CLA	C4A-NA-C1A	-5.59	104.19	106.71
3	B	603	CLA	C4A-NA-C1A	-5.59	104.19	106.71
3	C	603	CLA	C4A-NA-C1A	-5.37	104.29	106.71
3	A	612	CLA	C4A-NA-C1A	-5.28	104.33	106.71
3	B	612	CLA	C4A-NA-C1A	-5.23	104.35	106.71
3	B	614	CLA	C4A-NA-C1A	-5.21	104.36	106.71
3	C	612	CLA	C4A-NA-C1A	-5.21	104.36	106.71
3	A	614	CLA	C4A-NA-C1A	-5.18	104.38	106.71
3	C	614	CLA	C4A-NA-C1A	-5.16	104.39	106.71
3	A	610	CLA	C4A-NA-C1A	-4.82	104.54	106.71
3	B	610	CLA	C4A-NA-C1A	-4.69	104.60	106.71
3	C	610	CLA	C4A-NA-C1A	-4.68	104.60	106.71
2	A	609	CHL	CHD-C1D-ND	-4.40	120.41	124.45
2	C	609	CHL	CHD-C1D-ND	-4.39	120.42	124.45
3	C	602	CLA	C4A-NA-C1A	-4.39	104.73	106.71
2	B	609	CHL	CHD-C1D-ND	-4.38	120.43	124.45
2	B	608	CHL	CHD-C1D-ND	-4.38	120.43	124.45
3	B	602	CLA	C4A-NA-C1A	-4.37	104.74	106.71
2	A	608	CHL	CHD-C1D-ND	-4.35	120.45	124.45
2	C	608	CHL	CHD-C1D-ND	-4.33	120.48	124.45
3	A	602	CLA	C4A-NA-C1A	-4.26	104.79	106.71
2	B	606	CHL	CHD-C1D-ND	-4.24	120.56	124.45
2	B	605	CHL	CHD-C1D-ND	-4.23	120.57	124.45
2	C	606	CHL	CHD-C1D-ND	-4.22	120.58	124.45
2	A	605	CHL	CHD-C1D-ND	-4.22	120.58	124.45
3	A	613	CLA	C4A-NA-C1A	-4.21	104.81	106.71
2	A	606	CHL	CHD-C1D-ND	-4.20	120.59	124.45
2	B	601	CHL	CHD-C1D-ND	-4.19	120.60	124.45
2	C	601	CHL	CHD-C1D-ND	-4.19	120.61	124.45
2	A	601	CHL	CHD-C1D-ND	-4.19	120.61	124.45
2	C	605	CHL	CHD-C1D-ND	-4.17	120.62	124.45
2	B	607	CHL	CHD-C1D-ND	-4.17	120.62	124.45
2	C	607	CHL	CHD-C1D-ND	-4.16	120.63	124.45
2	A	607	CHL	CHD-C1D-ND	-4.14	120.65	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	613	CLA	C4A-NA-C1A	-4.14	104.85	106.71
3	B	613	CLA	C4A-NA-C1A	-4.13	104.85	106.71
3	A	610	CLA	CHD-C1D-ND	-3.87	120.90	124.45
3	C	614	CLA	CHD-C1D-ND	-3.80	120.96	124.45
3	B	610	CLA	CHD-C1D-ND	-3.74	121.02	124.45
3	C	610	CLA	CHD-C1D-ND	-3.73	121.02	124.45
3	C	602	CLA	CHD-C1D-ND	-3.71	121.04	124.45
3	A	614	CLA	CHD-C1D-ND	-3.70	121.06	124.45
3	A	611	CLA	CHD-C1D-ND	-3.69	121.06	124.45
3	B	614	CLA	CHD-C1D-ND	-3.68	121.07	124.45
3	B	604	CLA	CHD-C1D-ND	-3.67	121.08	124.45
3	A	613	CLA	CHD-C1D-ND	-3.66	121.09	124.45
3	C	604	CLA	CHD-C1D-ND	-3.65	121.10	124.45
3	B	603	CLA	CHD-C1D-ND	-3.65	121.10	124.45
3	C	603	CLA	CHD-C1D-ND	-3.64	121.11	124.45
3	B	602	CLA	CHD-C1D-ND	-3.64	121.11	124.45
3	A	604	CLA	CHD-C1D-ND	-3.64	121.11	124.45
3	A	602	CLA	CHD-C1D-ND	-3.62	121.12	124.45
2	B	606	CHL	CHC-C1C-NC	3.62	129.69	124.20
2	A	605	CHL	CHC-C1C-NC	3.62	129.69	124.20
3	B	613	CLA	CHD-C1D-ND	-3.60	121.14	124.45
2	C	606	CHL	CHC-C1C-NC	3.60	129.67	124.20
2	A	606	CHL	CHC-C1C-NC	3.60	129.67	124.20
2	C	605	CHL	CHC-C1C-NC	3.60	129.66	124.20
2	B	605	CHL	CHC-C1C-NC	3.60	129.66	124.20
3	C	613	CLA	CHD-C1D-ND	-3.59	121.15	124.45
3	B	611	CLA	CHD-C1D-ND	-3.58	121.16	124.45
2	C	607	CHL	CHC-C1C-NC	3.57	129.62	124.20
3	A	603	CLA	CHD-C1D-ND	-3.57	121.17	124.45
3	A	612	CLA	CHD-C1D-ND	-3.57	121.17	124.45
3	B	612	CLA	CHD-C1D-ND	-3.57	121.18	124.45
2	C	608	CHL	CHC-C1C-NC	3.56	129.61	124.20
2	A	609	CHL	CMB-C2B-C1B	-3.55	123.00	128.46
3	C	611	CLA	CHD-C1D-ND	-3.55	121.19	124.45
2	B	607	CHL	CHC-C1C-NC	3.55	129.59	124.20
2	C	609	CHL	CHC-C1C-NC	3.55	129.59	124.20
2	C	606	CHL	CMB-C2B-C1B	-3.55	123.01	128.46
2	B	609	CHL	CMB-C2B-C1B	-3.54	123.03	128.46
2	A	601	CHL	CHC-C1C-NC	3.53	129.56	124.20
2	B	606	CHL	CMB-C2B-C1B	-3.53	123.03	128.46
2	C	609	CHL	CMB-C2B-C1B	-3.53	123.04	128.46
2	B	601	CHL	CHC-C1C-NC	3.53	129.55	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	612	CLA	CHD-C1D-ND	-3.51	121.22	124.45
2	A	608	CHL	CHC-C1C-NC	3.49	129.50	124.20
2	B	608	CHL	CHC-C1C-NC	3.47	129.47	124.20
2	A	606	CHL	CMB-C2B-C1B	-3.47	123.13	128.46
2	A	608	CHL	CMB-C2B-C1B	-3.47	123.13	128.46
2	B	609	CHL	CHC-C1C-NC	3.47	129.46	124.20
2	C	601	CHL	CHC-C1C-NC	3.46	129.46	124.20
2	C	608	CHL	CMB-C2B-C1B	-3.45	123.17	128.46
2	A	609	CHL	CHC-C1C-NC	3.41	129.38	124.20
2	B	608	CHL	CMB-C2B-C1B	-3.40	123.24	128.46
2	A	607	CHL	CHC-C1C-NC	3.39	129.34	124.20
2	A	605	CHL	CMB-C2B-C1B	-3.36	123.30	128.46
2	B	605	CHL	CMB-C2B-C1B	-3.36	123.31	128.46
2	C	605	CHL	CMB-C2B-C1B	-3.35	123.31	128.46
2	A	601	CHL	CMB-C2B-C1B	-3.33	123.35	128.46
2	B	607	CHL	C4D-CHA-C1A	3.30	125.27	121.25
2	C	601	CHL	CMB-C2B-C1B	-3.29	123.41	128.46
2	B	601	CHL	CMB-C2B-C1B	-3.28	123.42	128.46
2	A	607	CHL	CMB-C2B-C1B	-3.28	123.43	128.46
2	C	607	CHL	CMB-C2B-C1B	-3.27	123.44	128.46
2	B	607	CHL	CMB-C2B-C1B	-3.26	123.45	128.46
2	B	607	CHL	CHB-C4A-NA	3.24	128.99	124.51
2	A	607	CHL	C4D-CHA-C1A	3.23	125.17	121.25
2	C	607	CHL	C4D-CHA-C1A	3.22	125.17	121.25
2	A	607	CHL	CHB-C4A-NA	3.22	128.96	124.51
2	C	607	CHL	CHB-C4A-NA	3.20	128.93	124.51
3	C	603	CLA	C1D-ND-C4D	-3.18	104.07	106.33
2	B	605	CHL	C4D-CHA-C1A	3.18	125.12	121.25
2	A	605	CHL	C4D-CHA-C1A	3.17	125.11	121.25
2	B	601	CHL	CHB-C4A-NA	3.16	128.89	124.51
2	C	601	CHL	CHB-C4A-NA	3.15	128.87	124.51
2	C	605	CHL	C4D-CHA-C1A	3.14	125.07	121.25
2	C	608	CHL	C4D-CHA-C1A	3.13	125.06	121.25
2	A	606	CHL	C4D-CHA-C1A	3.13	125.06	121.25
3	B	612	CLA	C1D-ND-C4D	-3.13	104.11	106.33
3	C	614	CLA	C1D-ND-C4D	-3.12	104.12	106.33
2	C	606	CHL	C4D-CHA-C1A	3.11	125.03	121.25
2	B	606	CHL	C4D-CHA-C1A	3.11	125.03	121.25
2	B	601	CHL	C4D-CHA-C1A	3.10	125.02	121.25
2	A	601	CHL	CHB-C4A-NA	3.10	128.79	124.51
3	A	612	CLA	C1D-ND-C4D	-3.09	104.14	106.33
3	A	603	CLA	C1D-ND-C4D	-3.08	104.14	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	603	CLA	C1D-ND-C4D	-3.08	104.14	106.33
3	A	614	CLA	C1D-ND-C4D	-3.08	104.15	106.33
3	C	612	CLA	C1D-ND-C4D	-3.08	104.15	106.33
2	B	608	CHL	C4D-CHA-C1A	3.07	124.99	121.25
2	A	608	CHL	C4D-CHA-C1A	3.07	124.99	121.25
2	B	606	CHL	C2A-C1A-CHA	3.07	129.23	123.86
2	C	608	CHL	CHB-C4A-NA	3.05	128.74	124.51
2	A	601	CHL	C4D-CHA-C1A	3.05	124.96	121.25
2	C	601	CHL	C4D-CHA-C1A	3.05	124.96	121.25
2	B	608	CHL	CHB-C4A-NA	3.04	128.72	124.51
3	B	614	CLA	C1D-ND-C4D	-3.04	104.17	106.33
2	A	606	CHL	C2A-C1A-CHA	3.04	129.17	123.86
2	C	606	CHL	C2A-C1A-CHA	3.04	129.17	123.86
2	A	608	CHL	CHB-C4A-NA	3.02	128.69	124.51
2	C	606	CHL	CHB-C4A-NA	3.00	128.67	124.51
2	A	606	CHL	CHB-C4A-NA	3.00	128.67	124.51
5	A	1003	NEX	O24-C25-C24	2.99	115.63	113.38
2	A	609	CHL	CHB-C4A-NA	2.98	128.64	124.51
2	B	606	CHL	CHB-C4A-NA	2.98	128.63	124.51
3	A	613	CLA	C1D-ND-C4D	-2.98	104.22	106.33
5	B	1003	NEX	O24-C25-C24	2.95	115.59	113.38
2	C	609	CHL	CHB-C4A-NA	2.93	128.56	124.51
2	B	609	CHL	CHB-C4A-NA	2.93	128.56	124.51
2	A	609	CHL	C4D-CHA-C1A	2.92	124.81	121.25
2	A	605	CHL	CHB-C4A-NA	2.91	128.54	124.51
3	B	613	CLA	C1D-ND-C4D	-2.90	104.28	106.33
2	C	609	CHL	C4D-CHA-C1A	2.89	124.77	121.25
5	C	1003	NEX	O24-C25-C24	2.89	115.55	113.38
2	B	609	CHL	C4D-CHA-C1A	2.88	124.76	121.25
2	B	605	CHL	C2A-C1A-CHA	2.88	128.89	123.86
3	C	613	CLA	C1D-ND-C4D	-2.88	104.29	106.33
2	B	607	CHL	C2A-C1A-CHA	2.88	128.89	123.86
2	B	605	CHL	CHB-C4A-NA	2.87	128.49	124.51
2	C	605	CHL	CHB-C4A-NA	2.86	128.47	124.51
2	A	605	CHL	C2A-C1A-CHA	2.86	128.87	123.86
2	C	607	CHL	C2A-C1A-CHA	2.86	128.86	123.86
3	C	602	CLA	C1D-ND-C4D	-2.86	104.31	106.33
2	C	605	CHL	C2A-C1A-CHA	2.85	128.84	123.86
2	A	609	CHL	C2A-C1A-CHA	2.84	128.83	123.86
2	A	607	CHL	C2A-C1A-CHA	2.83	128.81	123.86
3	C	612	CLA	C2C-C1C-NC	2.81	112.60	109.97
3	A	602	CLA	C1D-ND-C4D	-2.81	104.34	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	608	CHL	C2A-C1A-CHA	2.81	128.76	123.86
2	C	609	CHL	C2A-C1A-CHA	2.79	128.74	123.86
3	B	610	CLA	C1D-ND-C4D	-2.79	104.35	106.33
3	B	602	CLA	C1D-ND-C4D	-2.78	104.36	106.33
2	C	608	CHL	C2A-C1A-CHA	2.77	128.70	123.86
3	C	610	CLA	C1D-ND-C4D	-2.77	104.37	106.33
3	A	610	CLA	C1D-ND-C4D	-2.77	104.37	106.33
3	A	612	CLA	C2C-C1C-NC	2.77	112.56	109.97
2	B	609	CHL	C2A-C1A-CHA	2.76	128.69	123.86
2	C	601	CHL	C2A-C1A-CHA	2.76	128.68	123.86
3	B	612	CLA	C2C-C1C-NC	2.75	112.55	109.97
2	A	601	CHL	C2A-C1A-CHA	2.75	128.66	123.86
2	B	608	CHL	C2A-C1A-CHA	2.74	128.64	123.86
2	B	601	CHL	C2A-C1A-CHA	2.73	128.63	123.86
3	B	613	CLA	C2C-C1C-NC	2.72	112.52	109.97
3	C	613	CLA	C2C-C1C-NC	2.70	112.50	109.97
3	C	604	CLA	C1D-ND-C4D	-2.66	104.45	106.33
3	B	604	CLA	C1D-ND-C4D	-2.64	104.46	106.33
3	A	611	CLA	C1D-ND-C4D	-2.64	104.46	106.33
3	A	604	CLA	C1D-ND-C4D	-2.64	104.46	106.33
3	A	613	CLA	C2C-C1C-NC	2.64	112.44	109.97
3	A	612	CLA	CHC-C1C-C2C	-2.62	119.48	126.72
3	C	611	CLA	C1D-ND-C4D	-2.60	104.49	106.33
3	C	603	CLA	C2C-C1C-NC	2.60	112.41	109.97
3	A	603	CLA	C2C-C1C-NC	2.59	112.40	109.97
3	B	603	CLA	C2C-C1C-NC	2.59	112.40	109.97
3	C	612	CLA	CHC-C1C-C2C	-2.59	119.56	126.72
3	B	603	CLA	CHC-C1C-C2C	-2.59	119.57	126.72
3	B	611	CLA	C1D-ND-C4D	-2.58	104.50	106.33
3	B	613	CLA	CHC-C1C-C2C	-2.58	119.58	126.72
3	C	613	CLA	CHC-C1C-C2C	-2.58	119.59	126.72
3	A	603	CLA	C1-C2-C3	-2.58	121.59	126.04
3	A	603	CLA	CHC-C1C-C2C	-2.57	119.60	126.72
3	C	603	CLA	CHC-C1C-C2C	-2.57	119.60	126.72
3	B	612	CLA	CHC-C1C-C2C	-2.57	119.61	126.72
3	A	613	CLA	CHC-C1C-C2C	-2.57	119.61	126.72
3	A	612	CLA	C1-C2-C3	-2.56	121.61	126.04
3	B	603	CLA	C1-C2-C3	-2.56	121.62	126.04
3	C	612	CLA	C1-C2-C3	-2.54	121.65	126.04
3	B	603	CLA	CHC-C1C-NC	2.51	128.01	124.20
3	B	612	CLA	C1-C2-C3	-2.51	121.71	126.04
3	A	602	CLA	C2C-C1C-NC	2.51	112.32	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	611	CLA	CHC-C1C-C2C	-2.50	119.82	126.72
3	A	603	CLA	CHC-C1C-NC	2.49	127.98	124.20
3	C	603	CLA	CHC-C1C-NC	2.48	127.97	124.20
3	A	610	CLA	C2C-C1C-NC	2.48	112.30	109.97
3	A	610	CLA	CHC-C1C-C2C	-2.47	119.88	126.72
3	A	612	CLA	CHC-C1C-NC	2.47	127.95	124.20
3	C	614	CLA	CHC-C1C-C2C	-2.47	119.89	126.72
3	C	604	CLA	CHC-C1C-NC	2.47	127.95	124.20
3	A	614	CLA	CHC-C1C-C2C	-2.47	119.90	126.72
3	C	604	CLA	CHC-C1C-C2C	-2.47	119.90	126.72
3	C	611	CLA	CHC-C1C-C2C	-2.47	119.90	126.72
3	B	604	CLA	CHC-C1C-C2C	-2.46	119.91	126.72
3	B	614	CLA	CHC-C1C-C2C	-2.46	119.91	126.72
3	B	610	CLA	C2C-C1C-NC	2.46	112.28	109.97
3	B	611	CLA	CHC-C1C-C2C	-2.46	119.92	126.72
3	A	611	CLA	C2C-C1C-NC	2.45	112.27	109.97
3	C	603	CLA	C1-C2-C3	-2.45	121.80	126.04
3	A	613	CLA	CHC-C1C-NC	2.45	127.92	124.20
3	A	604	CLA	CHC-C1C-C2C	-2.45	119.95	126.72
3	C	611	CLA	C2C-C1C-NC	2.45	112.26	109.97
3	B	610	CLA	CHC-C1C-C2C	-2.44	119.96	126.72
3	B	611	CLA	CHA-C1A-NA	-2.44	120.81	126.40
3	A	611	CLA	CHA-C1A-NA	-2.44	120.81	126.40
3	C	611	CLA	CHA-C1A-NA	-2.44	120.82	126.40
3	B	604	CLA	CHC-C1C-NC	2.43	127.89	124.20
3	C	613	CLA	CHC-C1C-NC	2.43	127.89	124.20
3	B	614	CLA	C2C-C1C-NC	2.43	112.25	109.97
3	C	610	CLA	CHC-C1C-C2C	-2.43	120.01	126.72
3	A	602	CLA	CHC-C1C-C2C	-2.42	120.02	126.72
3	A	611	CLA	CHC-C1C-NC	2.42	127.88	124.20
3	B	613	CLA	CHC-C1C-NC	2.42	127.88	124.20
3	B	611	CLA	C2C-C1C-NC	2.41	112.23	109.97
3	C	614	CLA	C2C-C1C-NC	2.41	112.23	109.97
3	A	614	CLA	C2C-C1C-NC	2.41	112.23	109.97
3	A	604	CLA	CHC-C1C-NC	2.40	127.84	124.20
3	B	612	CLA	CHC-C1C-NC	2.40	127.84	124.20
3	C	612	CLA	CHC-C1C-NC	2.39	127.84	124.20
3	C	614	CLA	CHC-C1C-NC	2.39	127.83	124.20
3	A	614	CLA	CHC-C1C-NC	2.39	127.83	124.20
3	B	604	CLA	CHA-C1A-NA	-2.39	120.93	126.40
3	C	604	CLA	CHA-C1A-NA	-2.38	120.95	126.40
3	B	611	CLA	CHC-C1C-NC	2.38	127.81	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	610	CLA	CHC-C1C-NC	2.38	127.81	124.20
3	C	610	CLA	CHC-C1C-NC	2.38	127.81	124.20
3	C	611	CLA	CHC-C1C-NC	2.37	127.80	124.20
3	B	614	CLA	CHC-C1C-NC	2.37	127.80	124.20
3	A	604	CLA	CHA-C1A-NA	-2.37	120.97	126.40
3	C	602	CLA	CHC-C1C-C2C	-2.35	120.22	126.72
3	A	604	CLA	C2C-C1C-NC	2.35	112.17	109.97
3	C	610	CLA	C2C-C1C-NC	2.35	112.17	109.97
3	B	602	CLA	CHC-C1C-C2C	-2.34	120.24	126.72
3	B	604	CLA	C2C-C1C-NC	2.34	112.17	109.97
3	B	610	CLA	CHC-C1C-NC	2.33	127.74	124.20
2	C	605	CHL	C3B-C4B-NB	-2.31	106.22	109.21
2	B	605	CHL	C3B-C4B-NB	-2.30	106.23	109.21
2	C	601	CHL	C3B-C4B-NB	-2.30	106.24	109.21
3	C	604	CLA	C2C-C1C-NC	2.30	112.12	109.97
2	A	605	CHL	C3B-C4B-NB	-2.29	106.25	109.21
3	B	602	CLA	C2C-C1C-NC	2.29	112.11	109.97
3	C	602	CLA	C2C-C1C-NC	2.29	112.11	109.97
2	B	601	CHL	C3B-C4B-NB	-2.28	106.27	109.21
3	C	602	CLA	C1-C2-C3	-2.25	122.15	126.04
3	C	602	CLA	CHC-C1C-NC	2.25	127.61	124.20
3	A	602	CLA	CHC-C1C-NC	2.24	127.61	124.20
3	B	602	CLA	CHC-C1C-NC	2.24	127.60	124.20
3	C	610	CLA	C1-C2-C3	-2.23	122.18	126.04
3	B	602	CLA	CHA-C1A-NA	-2.23	121.30	126.40
2	B	607	CHL	C3B-C4B-NB	-2.22	106.34	109.21
3	A	602	CLA	CHA-C1A-NA	-2.21	121.33	126.40
2	A	609	CHL	CMB-C2B-C3B	2.21	128.82	124.68
2	C	606	CHL	CHA-C1A-NA	-2.21	121.34	126.40
2	A	606	CHL	CHA-C1A-NA	-2.21	121.34	126.40
3	A	612	CLA	CHA-C1A-NA	-2.20	121.35	126.40
3	C	614	CLA	CHA-C1A-NA	-2.20	121.35	126.40
2	C	607	CHL	C3B-C4B-NB	-2.20	106.36	109.21
2	B	606	CHL	CHA-C1A-NA	-2.20	121.35	126.40
3	B	612	CLA	CHA-C1A-NA	-2.19	121.38	126.40
2	B	609	CHL	CMB-C2B-C3B	2.19	128.78	124.68
3	C	612	CLA	CHA-C1A-NA	-2.19	121.38	126.40
3	B	613	CLA	CHA-C1A-NA	-2.19	121.38	126.40
2	C	609	CHL	CMB-C2B-C3B	2.19	128.77	124.68
2	B	607	CHL	CHA-C1A-NA	-2.19	121.39	126.40
2	B	609	CHL	C3B-C4B-NB	-2.19	106.38	109.21
3	A	614	CLA	CHA-C1A-NA	-2.19	121.39	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	602	CLA	CHA-C1A-NA	-2.18	121.39	126.40
3	B	614	CLA	CHA-C1A-NA	-2.18	121.40	126.40
2	C	607	CHL	CHA-C1A-NA	-2.18	121.42	126.40
3	C	610	CLA	CHA-C1A-NA	-2.18	121.42	126.40
2	A	607	CHL	CHA-C1A-NA	-2.17	121.42	126.40
2	A	601	CHL	C3B-C4B-NB	-2.17	106.41	109.21
2	C	609	CHL	C3B-C4B-NB	-2.17	106.41	109.21
2	B	606	CHL	CMB-C2B-C3B	2.17	128.73	124.68
2	A	607	CHL	C3B-C4B-NB	-2.16	106.41	109.21
2	A	606	CHL	CMB-C2B-C3B	2.16	128.73	124.68
3	A	613	CLA	CHA-C1A-NA	-2.16	121.45	126.40
3	C	613	CLA	CHA-C1A-NA	-2.16	121.46	126.40
2	B	608	CHL	C3B-C4B-NB	-2.16	106.42	109.21
2	C	606	CHL	CMB-C2B-C3B	2.16	128.71	124.68
2	A	608	CHL	CMB-C2B-C3B	2.15	128.71	124.68
3	A	610	CLA	CHA-C1A-NA	-2.15	121.47	126.40
3	B	610	CLA	CHA-C1A-NA	-2.15	121.48	126.40
2	B	606	CHL	C3B-C4B-NB	-2.14	106.44	109.21
2	A	608	CHL	C3B-C4B-NB	-2.14	106.44	109.21
2	A	606	CHL	C3B-C4B-NB	-2.14	106.45	109.21
2	C	608	CHL	CMB-C2B-C3B	2.13	128.67	124.68
3	A	604	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
3	A	610	CLA	C1-C2-C3	-2.12	122.37	126.04
2	A	609	CHL	C3B-C4B-NB	-2.12	106.47	109.21
3	A	602	CLA	CMB-C2B-C1B	-2.12	125.20	128.46
3	C	604	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
2	C	608	CHL	C3B-C4B-NB	-2.12	106.47	109.21
3	A	603	CLA	CHA-C1A-NA	-2.11	121.56	126.40
3	B	611	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
3	B	603	CLA	CHA-C1A-NA	-2.11	121.58	126.40
3	C	603	CLA	CHA-C1A-NA	-2.10	121.59	126.40
2	C	606	CHL	C3B-C4B-NB	-2.10	106.50	109.21
2	B	608	CHL	CHD-C1D-C2D	2.10	129.88	125.48
3	C	604	CLA	CMB-C2B-C1B	-2.10	125.24	128.46
2	B	608	CHL	CMB-C2B-C3B	2.09	128.59	124.68
2	C	609	CHL	CHD-C1D-C2D	2.09	129.86	125.48
3	A	604	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
2	A	608	CHL	CHD-C1D-C2D	2.09	129.86	125.48
2	B	606	CHL	C1-C2-C3	-2.09	123.38	126.75
2	B	609	CHL	CHD-C1D-C2D	2.09	129.86	125.48
3	A	611	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
2	C	608	CHL	CHD-C1D-C2D	2.08	129.85	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	611	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
2	A	609	CHL	CHD-C1D-C2D	2.08	129.84	125.48
3	B	610	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
3	C	611	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
3	A	610	CLA	CMB-C2B-C1B	-2.07	125.29	128.46
3	B	610	CLA	C1-C2-C3	-2.07	122.47	126.04
2	A	606	CHL	C1-C2-C3	-2.07	123.41	126.75
2	C	607	CHL	CMB-C2B-C3B	2.07	128.54	124.68
2	B	605	CHL	CHA-C1A-NA	-2.06	121.67	126.40
3	B	602	CLA	CMB-C2B-C1B	-2.06	125.29	128.46
3	B	604	CLA	C1B-CHB-C4A	-2.06	126.03	130.12
2	B	601	CHL	CHA-C1A-NA	-2.06	121.68	126.40
3	B	604	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
2	A	607	CHL	CMB-C2B-C3B	2.06	128.52	124.68
3	C	610	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
2	C	601	CHL	CHA-C1A-NA	-2.05	121.69	126.40
3	C	614	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
2	A	609	CHL	CHA-C1A-NA	-2.05	121.70	126.40
3	B	614	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
3	A	611	CLA	CMB-C2B-C1B	-2.05	125.32	128.46
2	A	608	CHL	CHA-C1A-NA	-2.04	121.72	126.40
2	C	606	CHL	C1-C2-C3	-2.04	123.45	126.75
2	A	605	CHL	CHA-C1A-NA	-2.04	121.72	126.40
3	C	613	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
2	C	608	CHL	CHA-C1A-NA	-2.04	121.73	126.40
2	A	606	CHL	CHC-C1C-C2C	-2.04	118.71	126.11
2	B	605	CHL	CHD-C1D-C2D	2.04	129.76	125.48
3	C	602	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
2	B	606	CHL	CHD-C1D-C2D	2.04	129.75	125.48
2	A	606	CHL	CHD-C1D-C2D	2.03	129.75	125.48
2	A	601	CHL	CHA-C1A-NA	-2.03	121.75	126.40
2	C	605	CHL	CHA-C1A-NA	-2.03	121.75	126.40
3	A	614	CLA	CMB-C2B-C1B	-2.03	125.35	128.46
2	A	605	CHL	CMB-C2B-C3B	2.03	128.47	124.68
2	B	608	CHL	CHA-C1A-NA	-2.03	121.76	126.40
2	C	606	CHL	CHD-C1D-C2D	2.03	129.73	125.48
2	A	605	CHL	CHD-C1D-C2D	2.03	129.73	125.48
2	B	607	CHL	CMB-C2B-C3B	2.03	128.47	124.68
2	B	605	CHL	CMB-C2B-C3B	2.02	128.47	124.68
2	C	605	CHL	CHD-C1D-C2D	2.02	129.72	125.48
2	C	609	CHL	CHA-C1A-NA	-2.02	121.77	126.40
3	A	603	CLA	CMB-C2B-C1B	-2.02	125.36	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	603	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
3	A	613	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
2	B	601	CHL	CHD-C1D-C2D	2.01	129.70	125.48
2	C	601	CHL	CMB-C2B-C3B	2.01	128.43	124.68
2	C	605	CHL	CMB-C2B-C3B	2.01	128.43	124.68
2	B	609	CHL	CHA-C1A-NA	-2.01	121.80	126.40
2	B	607	CHL	CHD-C1D-C2D	2.01	129.69	125.48
2	C	601	CHL	CHD-C1D-C2D	2.01	129.69	125.48
3	B	613	CLA	C1-C2-C3	-2.00	122.58	126.04
2	B	606	CHL	CHC-C1C-C2C	-2.00	118.85	126.11
3	A	612	CLA	CMB-C2B-C1B	-2.00	125.39	128.46
3	C	612	CLA	CMB-C2B-C1B	-2.00	125.39	128.46
2	A	601	CHL	CMB-C2B-C3B	2.00	128.42	124.68

All (114) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	CHL	NC
2	A	601	CHL	C8
2	A	601	CHL	NA
2	A	601	CHL	ND
2	A	605	CHL	NC
2	A	605	CHL	NA
2	A	605	CHL	ND
2	A	606	CHL	NC
2	A	606	CHL	NA
2	A	606	CHL	ND
2	A	607	CHL	NC
2	A	607	CHL	NA
2	A	607	CHL	ND
2	A	608	CHL	NC
2	A	608	CHL	C8
2	A	608	CHL	NA
2	A	608	CHL	ND
2	A	609	CHL	NC
2	A	609	CHL	C8
2	A	609	CHL	NA
2	A	609	CHL	ND
2	B	601	CHL	NC
2	B	601	CHL	C8
2	B	601	CHL	NA
2	B	601	CHL	ND

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Mol	Chain	Res	Type	Atom
2	B	605	CHL	NC
2	B	605	CHL	NA
2	B	605	CHL	ND
2	B	606	CHL	NC
2	B	606	CHL	NA
2	B	606	CHL	ND
2	B	607	CHL	NC
2	B	607	CHL	NA
2	B	607	CHL	ND
2	B	608	CHL	NC
2	B	608	CHL	C8
2	B	608	CHL	NA
2	B	608	CHL	ND
2	B	609	CHL	NC
2	B	609	CHL	C8
2	B	609	CHL	NA
2	B	609	CHL	ND
2	C	601	CHL	NC
2	C	601	CHL	C8
2	C	601	CHL	NA
2	C	601	CHL	ND
2	C	605	CHL	NC
2	C	605	CHL	NA
2	C	605	CHL	ND
2	C	606	CHL	NC
2	C	606	CHL	NA
2	C	606	CHL	ND
2	C	607	CHL	NC
2	C	607	CHL	NA
2	C	607	CHL	ND
2	C	608	CHL	NC
2	C	608	CHL	C8
2	C	608	CHL	NA
2	C	608	CHL	ND
2	C	609	CHL	NC
2	C	609	CHL	C8
2	C	609	CHL	NA
2	C	609	CHL	ND
3	A	602	CLA	C8
3	A	602	CLA	ND
3	A	603	CLA	C8
3	A	603	CLA	ND

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Mol	Chain	Res	Type	Atom
3	A	604	CLA	C8
3	A	604	CLA	ND
3	A	610	CLA	C8
3	A	610	CLA	ND
3	A	611	CLA	C8
3	A	611	CLA	ND
3	A	612	CLA	C8
3	A	612	CLA	ND
3	A	613	CLA	C8
3	A	613	CLA	ND
3	A	614	CLA	ND
3	B	602	CLA	C8
3	B	602	CLA	ND
3	B	603	CLA	C8
3	B	603	CLA	ND
3	B	604	CLA	C8
3	B	604	CLA	ND
3	B	610	CLA	C8
3	B	610	CLA	ND
3	B	611	CLA	C8
3	B	611	CLA	ND
3	B	612	CLA	C8
3	B	612	CLA	ND
3	B	613	CLA	C8
3	B	613	CLA	ND
3	B	614	CLA	ND
3	C	602	CLA	C8
3	C	602	CLA	ND
3	C	603	CLA	C8
3	C	603	CLA	ND
3	C	604	CLA	C8
3	C	604	CLA	ND
3	C	610	CLA	C8
3	C	610	CLA	ND
3	C	611	CLA	C8
3	C	611	CLA	ND
3	C	612	CLA	C8
3	C	612	CLA	ND
3	C	613	CLA	C8
3	C	613	CLA	ND
3	C	614	CLA	ND
7	A	1004	XAT	C26

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Mol	Chain	Res	Type	Atom
7	A	1004	XAT	C25
7	B	1004	XAT	C26
7	B	1004	XAT	C25
7	C	1004	XAT	C26
7	C	1004	XAT	C25

All (265) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	CHL	C1A-C2A-CAA-CBA
2	A	601	CHL	C3A-C2A-CAA-CBA
2	A	601	CHL	C1C-C2C-CMC-OMC
2	A	601	CHL	C3C-C2C-CMC-OMC
2	A	605	CHL	C1C-C2C-CMC-OMC
2	A	605	CHL	C3C-C2C-CMC-OMC
2	A	606	CHL	C1A-C2A-CAA-CBA
2	A	609	CHL	C6-C7-C8-C9
2	B	601	CHL	C1A-C2A-CAA-CBA
2	B	601	CHL	C3A-C2A-CAA-CBA
2	B	601	CHL	C1C-C2C-CMC-OMC
2	B	601	CHL	C3C-C2C-CMC-OMC
2	B	605	CHL	C1C-C2C-CMC-OMC
2	B	605	CHL	C3C-C2C-CMC-OMC
2	B	606	CHL	C1A-C2A-CAA-CBA
2	B	606	CHL	C1C-C2C-CMC-OMC
2	B	607	CHL	C3C-C2C-CMC-OMC
2	B	609	CHL	C6-C7-C8-C9
2	C	601	CHL	C1A-C2A-CAA-CBA
2	C	601	CHL	C3A-C2A-CAA-CBA
2	C	601	CHL	C3C-C2C-CMC-OMC
2	C	605	CHL	C1C-C2C-CMC-OMC
2	C	605	CHL	C3C-C2C-CMC-OMC
2	C	606	CHL	C1A-C2A-CAA-CBA
2	C	606	CHL	C1C-C2C-CMC-OMC
2	C	607	CHL	C1C-C2C-CMC-OMC
2	C	607	CHL	C3C-C2C-CMC-OMC
2	C	608	CHL	C1C-C2C-CMC-OMC
2	C	608	CHL	C3C-C2C-CMC-OMC
2	C	609	CHL	C3C-C2C-CMC-OMC
2	C	609	CHL	C6-C7-C8-C9
3	A	604	CLA	C1A-C2A-CAA-CBA
3	A	611	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
3	B	604	CLA	C1A-C2A-CAA-CBA
3	B	611	CLA	C1A-C2A-CAA-CBA
3	C	604	CLA	C1A-C2A-CAA-CBA
3	C	611	CLA	C1A-C2A-CAA-CBA
4	A	1001	A1LXP	C24-C1-C42-C2
4	C	1001	A1LXP	C24-C1-C42-C2
6	A	1005	LHG	C3-O3-P-O6
6	B	1005	LHG	C3-O3-P-O4
6	B	1005	LHG	C4-O6-P-O5
6	C	1005	LHG	C3-O3-P-O4
2	A	608	CHL	C2A-CAA-CBA-CGA
2	B	608	CHL	C2A-CAA-CBA-CGA
2	C	608	CHL	C2A-CAA-CBA-CGA
2	A	601	CHL	C11-C10-C8-C9
2	C	601	CHL	C11-C10-C8-C9
2	B	601	CHL	C5-C6-C7-C8
6	B	1005	LHG	C3-O3-P-O6
6	B	1005	LHG	C4-O6-P-O3
6	C	1005	LHG	C3-O3-P-O6
3	A	602	CLA	C4-C3-C5-C6
2	C	608	CHL	C5-C6-C7-C8
2	A	601	CHL	C11-C12-C13-C14
2	C	601	CHL	C11-C12-C13-C14
3	B	602	CLA	C14-C13-C15-C16
2	A	608	CHL	C5-C6-C7-C8
2	B	608	CHL	C5-C6-C7-C8
3	A	603	CLA	C3A-C2A-CAA-CBA
3	B	603	CLA	C3A-C2A-CAA-CBA
3	C	603	CLA	C3A-C2A-CAA-CBA
6	B	1005	LHG	C23-C24-C25-C26
2	A	609	CHL	C2-C3-C5-C6
3	A	613	CLA	C2-C3-C5-C6
4	B	1001	A1LXP	C24-C1-C42-C2
3	B	613	CLA	C4-C3-C5-C6
3	A	602	CLA	C2-C3-C5-C6
3	B	602	CLA	C12-C13-C15-C16
3	B	613	CLA	C2-C3-C5-C6
3	C	602	CLA	C11-C12-C13-C15
3	C	613	CLA	C2-C3-C5-C6
6	A	1005	LHG	C23-C24-C25-C26
6	C	1005	LHG	C23-C24-C25-C26
3	C	611	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	A	609	CHL	C4-C3-C5-C6
3	A	613	CLA	C4-C3-C5-C6
3	C	613	CLA	C4-C3-C5-C6
3	A	603	CLA	C1A-C2A-CAA-CBA
3	B	603	CLA	C1A-C2A-CAA-CBA
3	C	603	CLA	C1A-C2A-CAA-CBA
3	A	611	CLA	C5-C6-C7-C8
2	B	609	CHL	C4-C3-C5-C6
3	B	611	CLA	C5-C6-C7-C8
2	B	607	CHL	C2A-CAA-CBA-CGA
2	C	601	CHL	C2-C1-O2A-CGA
2	C	601	CHL	C6-C7-C8-C10
3	B	602	CLA	C11-C10-C8-C9
3	C	602	CLA	C11-C12-C13-C14
6	C	1005	LHG	C31-C32-C33-C34
3	B	602	CLA	C4-C3-C5-C6
2	B	609	CHL	C2-C3-C5-C6
2	C	609	CHL	C8-C10-C11-C12
2	B	609	CHL	C8-C10-C11-C12
2	B	606	CHL	C3C-C2C-CMC-OMC
2	C	606	CHL	C3C-C2C-CMC-OMC
2	C	607	CHL	C2A-CAA-CBA-CGA
4	A	1001	A1LXP	C28-C1-C42-C2
4	A	1002	A1LXP	C24-C1-C42-C2
4	B	1002	A1LXP	C24-C1-C42-C2
4	B	1002	A1LXP	C28-C1-C42-C2
4	C	1001	A1LXP	C28-C1-C42-C2
4	C	1002	A1LXP	C24-C1-C42-C2
4	C	1002	A1LXP	C28-C1-C42-C2
2	A	609	CHL	C6-C7-C8-C10
2	B	609	CHL	C6-C7-C8-C10
2	C	609	CHL	C6-C7-C8-C10
3	B	602	CLA	C11-C10-C8-C7
2	A	609	CHL	C8-C10-C11-C12
3	A	612	CLA	CAD-CBD-CGD-O2D
3	B	603	CLA	CAD-CBD-CGD-O2D
3	C	604	CLA	C4-C3-C5-C6
3	A	602	CLA	CHA-CBD-CGD-O1D
3	A	602	CLA	CHA-CBD-CGD-O2D
3	B	602	CLA	CHA-CBD-CGD-O1D
3	B	602	CLA	CHA-CBD-CGD-O2D
3	C	602	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
3	C	602	CLA	CHA-CBD-CGD-O2D
3	A	604	CLA	C4-C3-C5-C6
3	A	612	CLA	C4-C3-C5-C6
3	B	604	CLA	C4-C3-C5-C6
3	A	612	CLA	C11-C10-C8-C9
3	B	602	CLA	C2-C3-C5-C6
6	A	1005	LHG	C3-O3-P-O4
6	B	1005	LHG	C4-O6-P-O4
3	A	614	CLA	CAD-CBD-CGD-O1D
3	B	614	CLA	CAD-CBD-CGD-O1D
3	C	614	CLA	CAD-CBD-CGD-O1D
6	B	1005	LHG	C25-C26-C27-C28
2	A	606	CHL	C3A-C2A-CAA-CBA
2	B	606	CHL	C3A-C2A-CAA-CBA
2	A	607	CHL	C2A-CAA-CBA-CGA
2	B	607	CHL	C1C-C2C-CMC-OMC
2	C	601	CHL	C1C-C2C-CMC-OMC
2	C	609	CHL	C1C-C2C-CMC-OMC
3	C	612	CLA	C4-C3-C5-C6
3	A	604	CLA	C2-C3-C5-C6
3	C	604	CLA	C2-C3-C5-C6
3	B	612	CLA	C4-C3-C5-C6
3	A	612	CLA	C2-C3-C5-C6
3	A	611	CLA	C13-C15-C16-C17
2	C	606	CHL	C2A-CAA-CBA-CGA
4	A	1002	A1LXP	C28-C1-C42-C2
4	B	1001	A1LXP	C28-C1-C42-C2
3	B	604	CLA	C2-C3-C5-C6
6	C	1005	LHG	C4-O6-P-O3
3	C	611	CLA	C12-C13-C15-C16
3	B	612	CLA	C11-C10-C8-C9
3	B	611	CLA	C13-C15-C16-C17
3	B	602	CLA	C3-C5-C6-C7
3	A	602	CLA	C3-C5-C6-C7
3	C	611	CLA	C13-C15-C16-C17
6	C	1005	LHG	C12-C13-C14-C15
2	C	609	CHL	C2-C3-C5-C6
6	B	1005	LHG	C16-C17-C18-C19
2	A	606	CHL	C2A-CAA-CBA-CGA
2	B	606	CHL	C2A-CAA-CBA-CGA
2	C	606	CHL	C3A-C2A-CAA-CBA
2	C	609	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
3	B	611	CLA	C3-C5-C6-C7
3	A	611	CLA	C11-C10-C8-C9
3	A	613	CLA	C6-C7-C8-C9
3	B	611	CLA	C11-C10-C8-C9
3	C	613	CLA	C6-C7-C8-C9
5	A	1003	NEX	C39-C29-C30-C31
5	B	1003	NEX	C39-C29-C30-C31
5	C	1003	NEX	C39-C29-C30-C31
3	B	611	CLA	C4-C3-C5-C6
3	A	611	CLA	C12-C13-C15-C16
3	B	611	CLA	C12-C13-C15-C16
2	B	609	CHL	C3C-C2C-CMC-OMC
6	A	1005	LHG	C4-O6-P-O3
5	A	1003	NEX	C28-C29-C30-C31
5	B	1003	NEX	C28-C29-C30-C31
5	C	1003	NEX	C28-C29-C30-C31
6	C	1005	LHG	C25-C26-C27-C28
2	A	601	CHL	C2-C1-O2A-CGA
2	B	601	CHL	C2-C1-O2A-CGA
3	C	612	CLA	C2-C3-C5-C6
3	B	613	CLA	C6-C7-C8-C9
3	C	611	CLA	C11-C10-C8-C9
3	C	612	CLA	C11-C10-C8-C9
3	A	611	CLA	C3-C5-C6-C7
3	A	611	CLA	C4-C3-C5-C6
3	B	612	CLA	C2-C3-C5-C6
3	C	611	CLA	C3-C5-C6-C7
3	B	604	CLA	CAA-CBA-CGA-O2A
2	B	601	CHL	C4-C3-C5-C6
3	A	612	CLA	C11-C10-C8-C7
3	A	611	CLA	CAA-CBA-CGA-O2A
3	C	611	CLA	CAA-CBA-CGA-O2A
3	C	611	CLA	C14-C13-C15-C16
6	C	1005	LHG	O8-C23-C24-C25
3	A	603	CLA	CAD-CBD-CGD-O2D
3	B	612	CLA	CAD-CBD-CGD-O2D
3	C	612	CLA	CAD-CBD-CGD-O2D
6	B	1005	LHG	C11-C10-C9-C8
3	C	611	CLA	C4-C3-C5-C6
3	A	611	CLA	C2-C3-C5-C6
3	B	611	CLA	C2-C3-C5-C6
3	B	611	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
3	C	604	CLA	CAA-CBA-CGA-O2A
6	B	1005	LHG	O8-C23-C24-C25
2	A	608	CHL	O2A-C1-C2-C3
2	B	608	CHL	O2A-C1-C2-C3
2	C	608	CHL	O2A-C1-C2-C3
3	C	612	CLA	CAA-CBA-CGA-O2A
2	A	601	CHL	CHA-CBD-CGD-O1D
2	A	601	CHL	CHA-CBD-CGD-O2D
2	B	601	CHL	CHA-CBD-CGD-O1D
2	B	601	CHL	CHA-CBD-CGD-O2D
2	C	601	CHL	CHA-CBD-CGD-O1D
2	C	601	CHL	CHA-CBD-CGD-O2D
3	C	603	CLA	CHA-CBD-CGD-O2D
3	B	612	CLA	CAA-CBA-CGA-O2A
6	A	1005	LHG	O8-C23-C24-C25
2	A	607	CHL	CAA-CBA-CGA-O2A
2	C	606	CHL	CAA-CBA-CGA-O2A
3	A	612	CLA	CAA-CBA-CGA-O2A
2	B	606	CHL	CAA-CBA-CGA-O2A
3	A	604	CLA	CAA-CBA-CGA-O2A
2	A	601	CHL	C11-C10-C8-C7
2	C	608	CHL	C6-C7-C8-C10
3	C	611	CLA	C2-C3-C5-C6
2	A	606	CHL	CAA-CBA-CGA-O2A
3	A	611	CLA	CAA-CBA-CGA-O1A
3	B	611	CLA	CAA-CBA-CGA-O1A
3	C	611	CLA	CAA-CBA-CGA-O1A
2	A	606	CHL	CAA-CBA-CGA-O1A
3	A	612	CLA	CAA-CBA-CGA-O1A
6	C	1005	LHG	C4-O6-P-O4
3	B	612	CLA	CAA-CBA-CGA-O1A
3	C	612	CLA	CAA-CBA-CGA-O1A
2	C	606	CHL	CAA-CBA-CGA-O1A
6	A	1005	LHG	O10-C23-C24-C25
6	B	1005	LHG	O10-C23-C24-C25
6	C	1005	LHG	O10-C23-C24-C25
3	C	613	CLA	C2A-CAA-CBA-CGA
2	B	606	CHL	CAA-CBA-CGA-O1A
6	A	1005	LHG	C25-C26-C27-C28
2	A	607	CHL	CAA-CBA-CGA-O1A
2	B	601	CHL	CAD-CBD-CGD-O1D
3	A	604	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
3	B	604	CLA	CAD-CBD-CGD-O1D
3	C	604	CLA	CAD-CBD-CGD-O1D
3	A	611	CLA	C14-C13-C15-C16
3	B	611	CLA	C14-C13-C15-C16
2	C	608	CHL	CAA-CBA-CGA-O2A
6	C	1005	LHG	C15-C16-C17-C18
3	A	613	CLA	C2A-CAA-CBA-CGA
2	B	608	CHL	CAA-CBA-CGA-O2A
2	A	601	CHL	C6-C7-C8-C10
2	A	608	CHL	C6-C7-C8-C10
3	A	611	CLA	C3A-C2A-CAA-CBA
3	B	611	CLA	C3A-C2A-CAA-CBA
3	B	612	CLA	C11-C10-C8-C7
3	C	611	CLA	C3A-C2A-CAA-CBA
3	C	612	CLA	C11-C10-C8-C7
2	C	608	CHL	CAA-CBA-CGA-O1A
2	A	608	CHL	CAA-CBA-CGA-O2A
2	B	607	CHL	CAA-CBA-CGA-O2A
2	A	608	CHL	CAA-CBA-CGA-O1A
2	B	608	CHL	CAA-CBA-CGA-O1A
3	B	613	CLA	C2A-CAA-CBA-CGA
2	A	609	CHL	C15-C16-C17-C18

There are no ring outliers.

43 monomers are involved in 66 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	609	CHL	3	0
3	B	604	CLA	1	0
3	A	604	CLA	1	0
2	C	607	CHL	1	0
3	A	610	CLA	2	0
4	B	1002	A1LXP	2	0
3	B	612	CLA	3	0
3	A	613	CLA	2	0
3	B	613	CLA	1	0
3	C	612	CLA	3	0
6	B	1005	LHG	5	0
2	A	609	CHL	4	0
3	B	603	CLA	4	0
6	C	1005	LHG	7	0
6	A	1005	LHG	2	0

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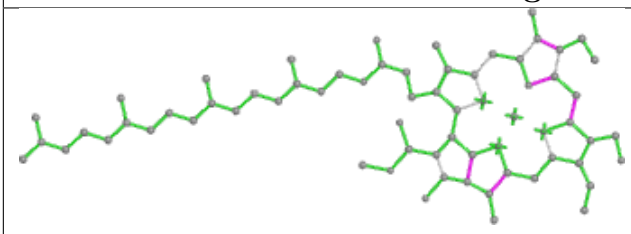
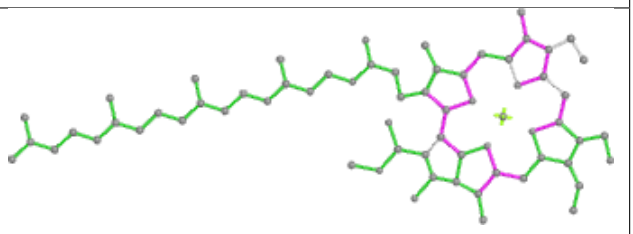
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	606	CHL	1	0
3	B	602	CLA	2	0
3	A	612	CLA	3	0
2	B	608	CHL	1	0
2	A	608	CHL	1	0
2	B	601	CHL	4	0
2	C	601	CHL	4	0
3	C	610	CLA	3	0
2	B	607	CHL	1	0
3	C	602	CLA	1	0
2	A	607	CHL	1	0
3	A	602	CLA	2	0
2	B	606	CHL	1	0
3	B	610	CLA	3	0
3	C	613	CLA	1	0
2	A	606	CHL	1	0
2	A	601	CHL	1	0
7	B	1004	XAT	2	0
7	C	1004	XAT	1	0
7	A	1004	XAT	3	0
4	C	1002	A1LXP	2	0
3	C	604	CLA	1	0
3	C	603	CLA	4	0
2	C	608	CHL	1	0
3	A	603	CLA	5	0
2	B	609	CHL	3	0
3	A	614	CLA	1	0
4	A	1002	A1LXP	2	0

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

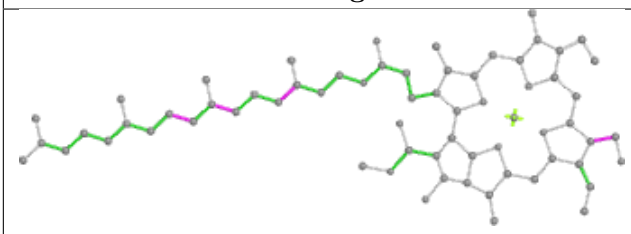
Ligand CHL C 609



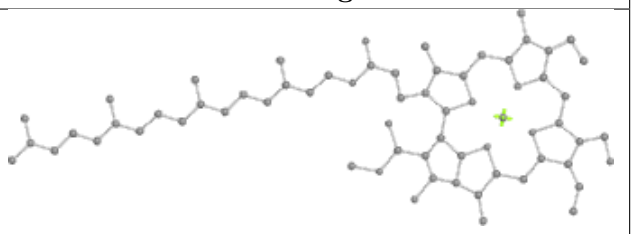
Bond lengths



Bond angles

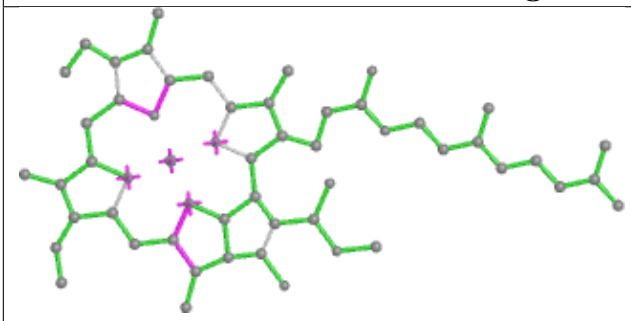


Torsions

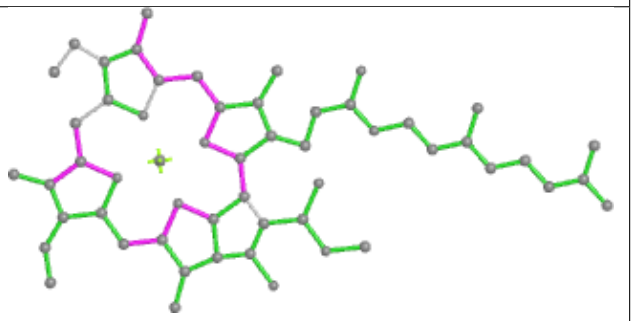


Rings

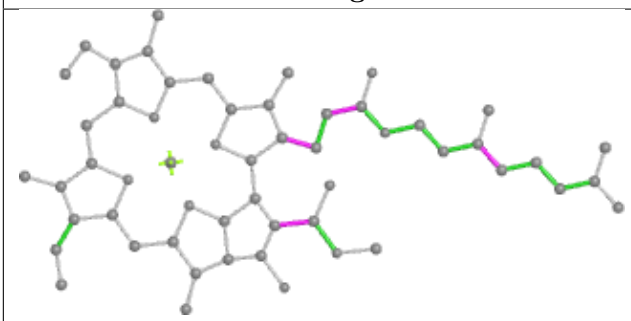
Ligand CLA B 604



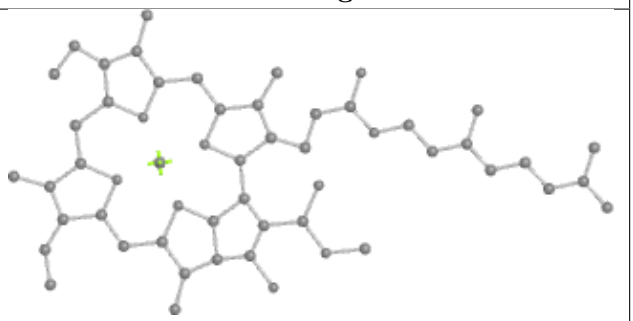
Bond lengths



Bond angles

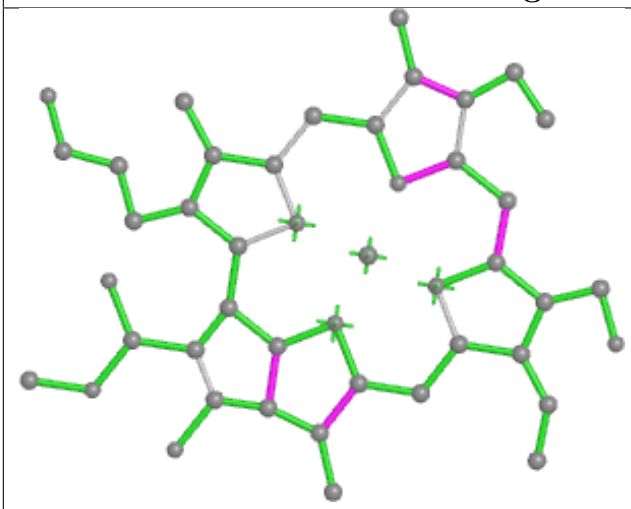


Torsions

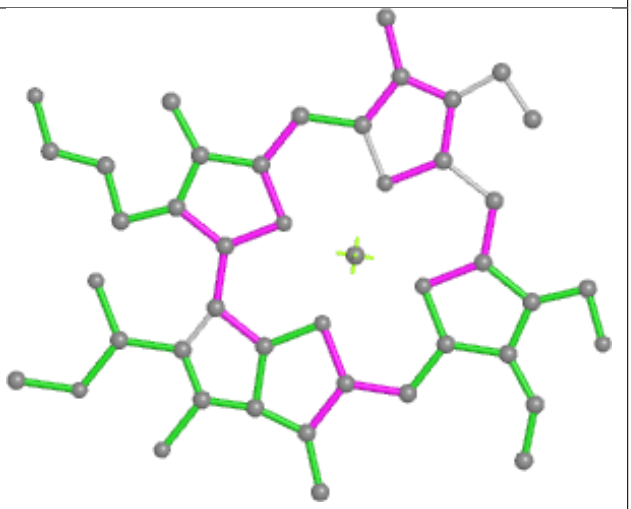


Rings

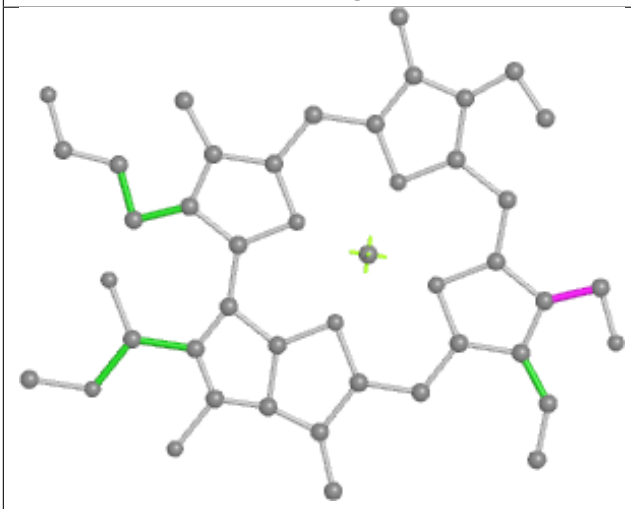
Ligand CHL C 605



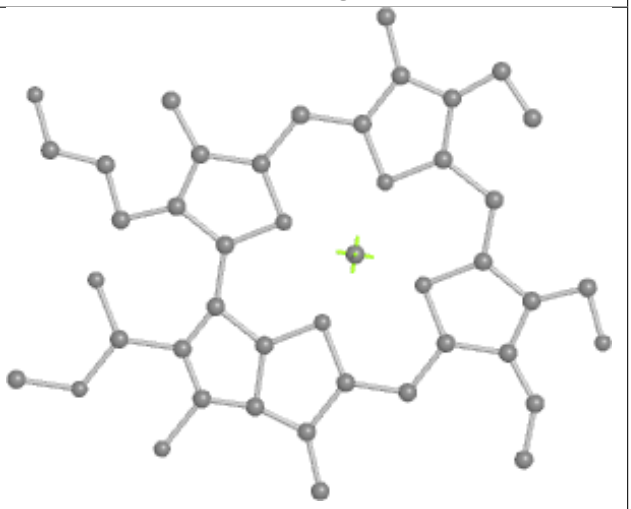
Bond lengths



Bond angles

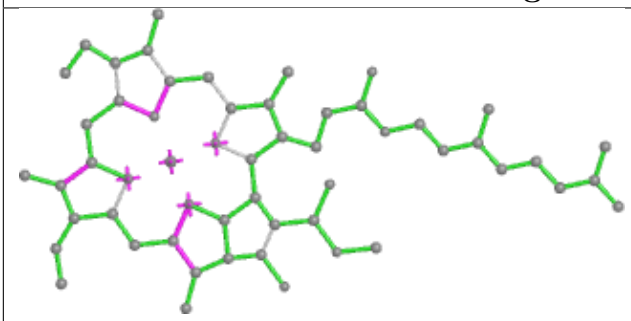


Torsions

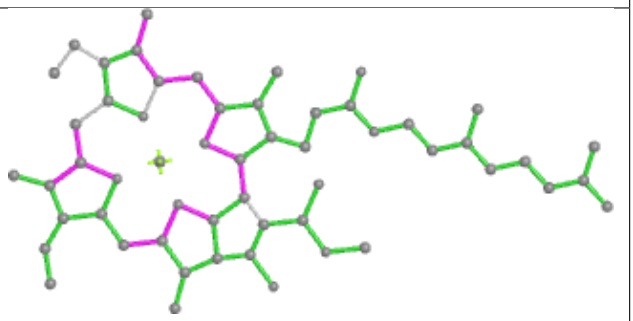


Rings

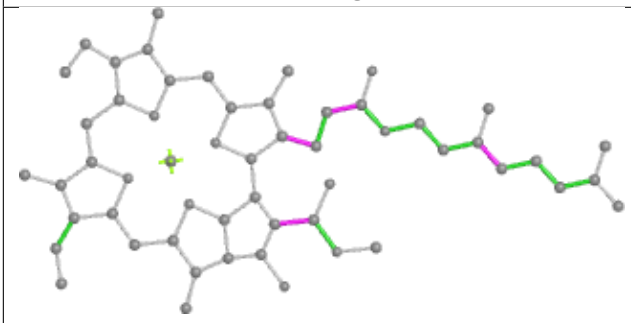
Ligand CLA A 604



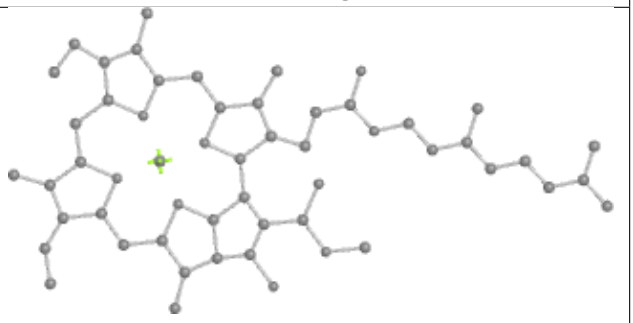
Bond lengths



Bond angles

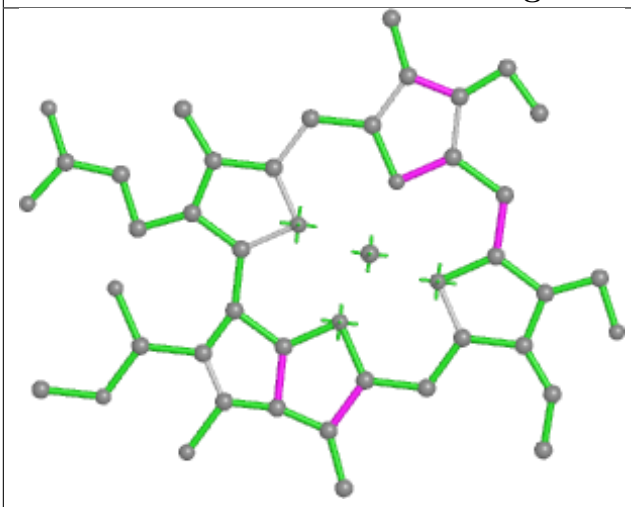


Torsions

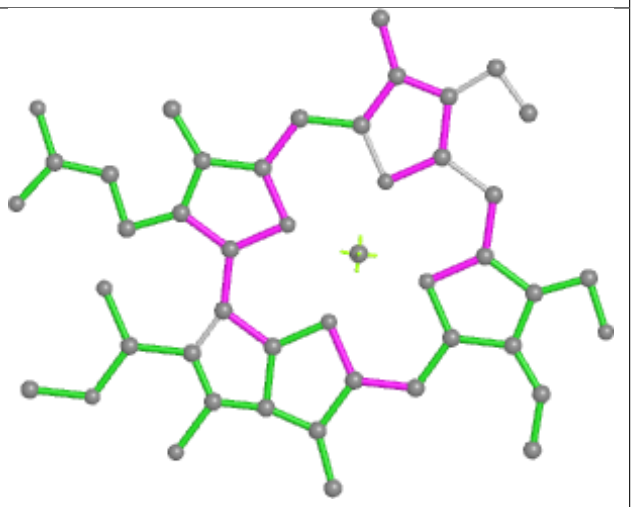


Rings

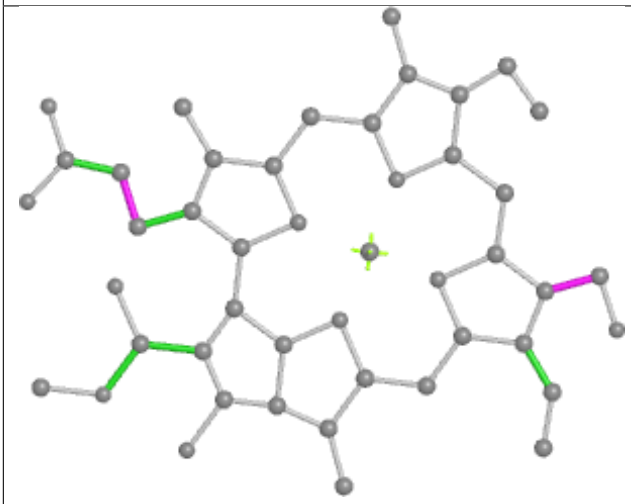
Ligand CHL C 607



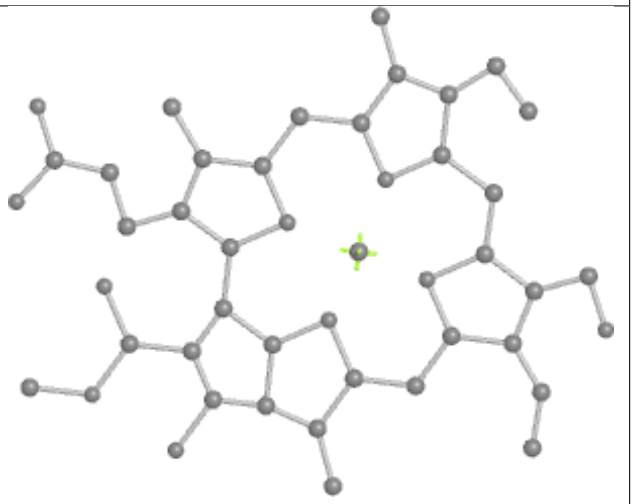
Bond lengths



Bond angles

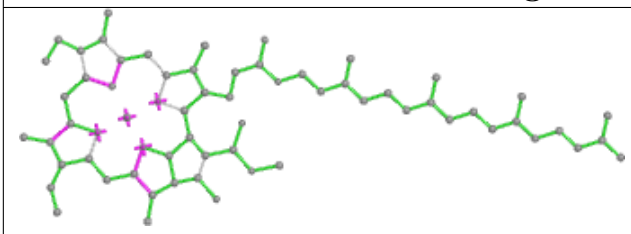


Torsions

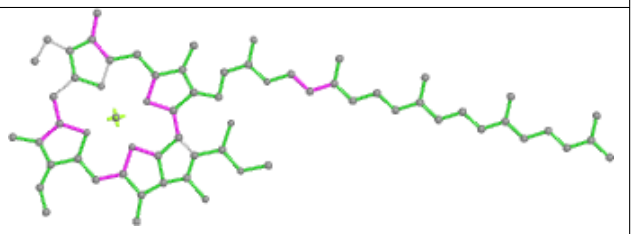


Rings

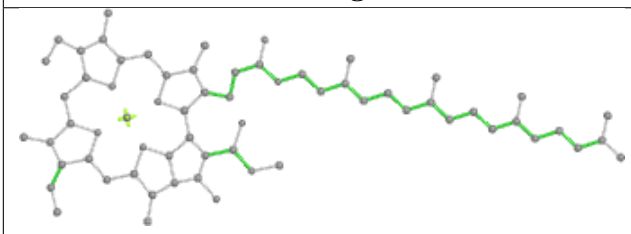
Ligand CLA A 610



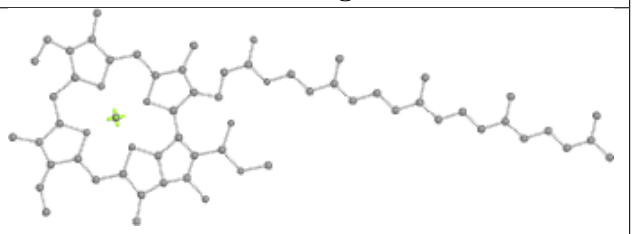
Bond lengths



Bond angles

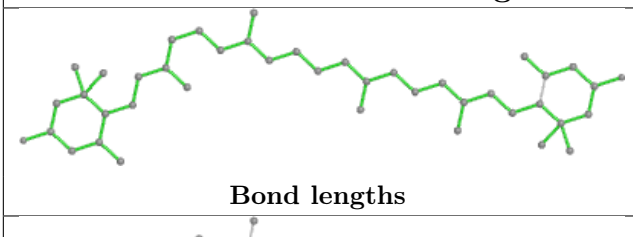


Torsions

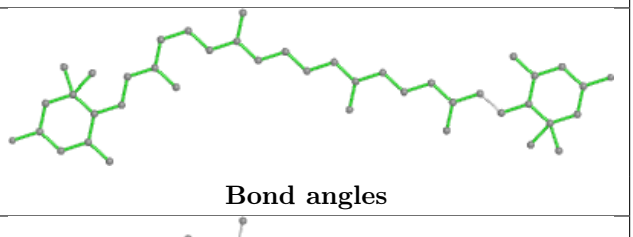


Rings

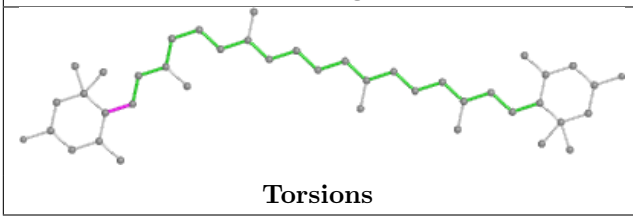
Ligand A1LXP B 1002



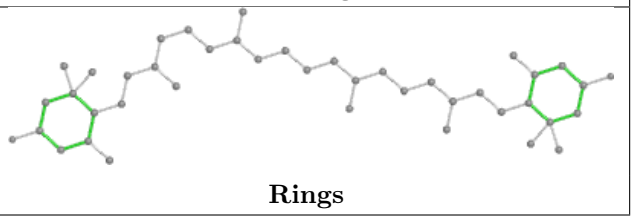
Bond lengths



Bond angles

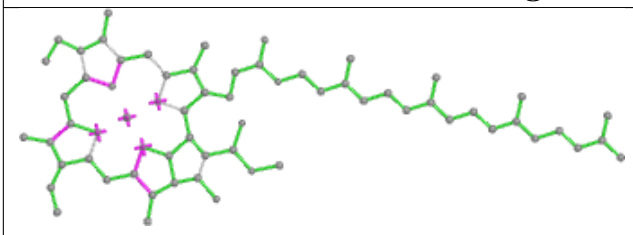


Torsions

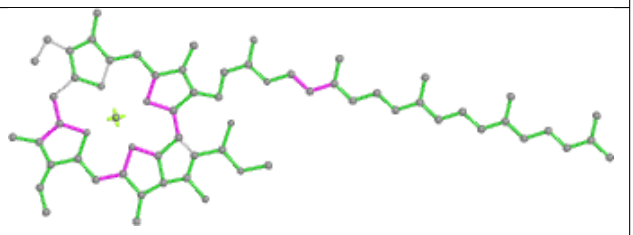


Rings

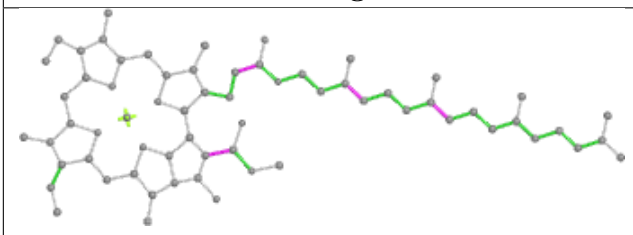
Ligand CLA B 612



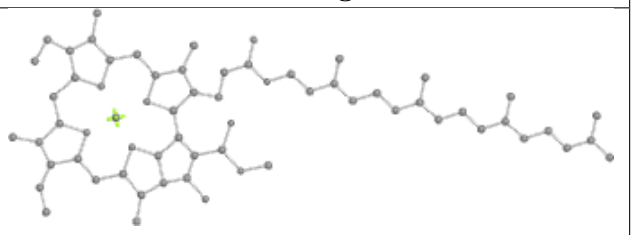
Bond lengths



Bond angles

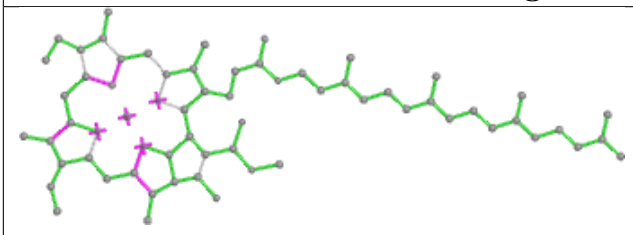


Torsions

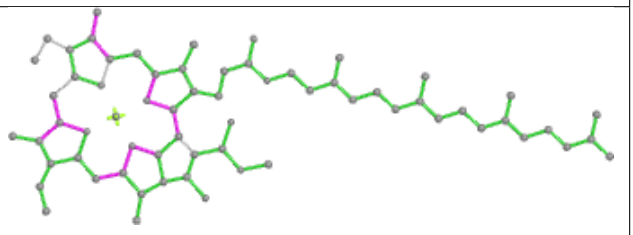


Rings

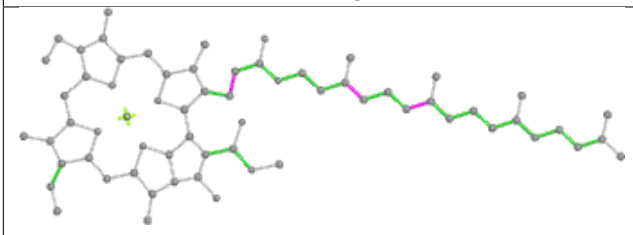
Ligand CLA A 613



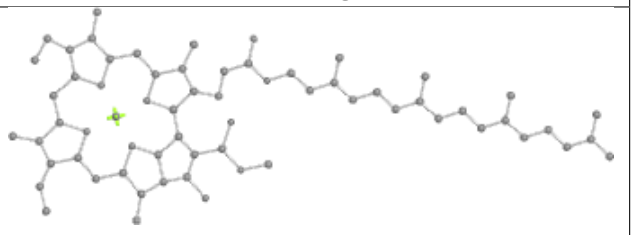
Bond lengths



Bond angles

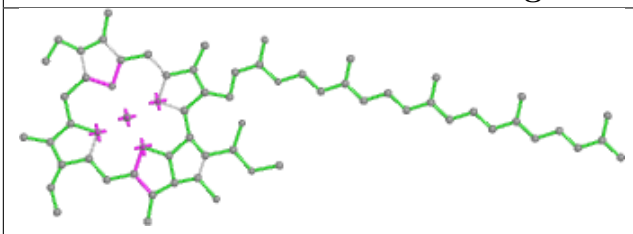


Torsions

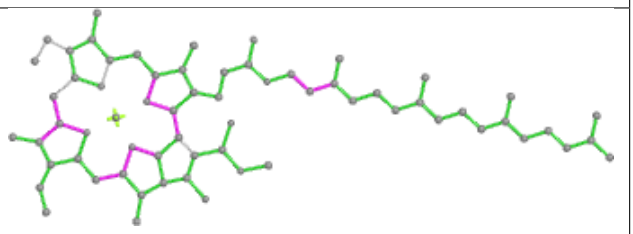


Rings

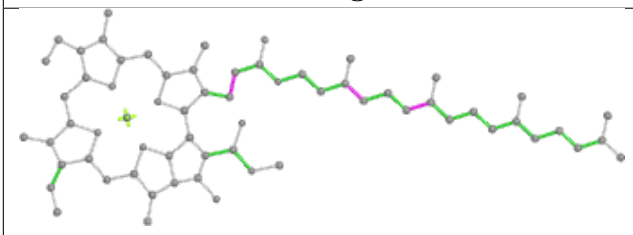
Ligand CLA B 613



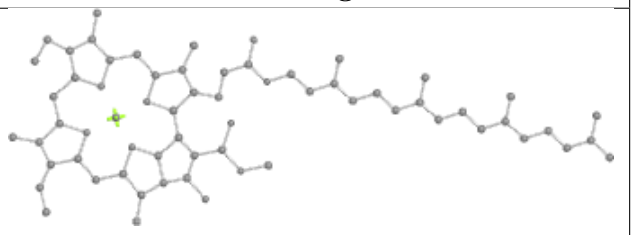
Bond lengths



Bond angles

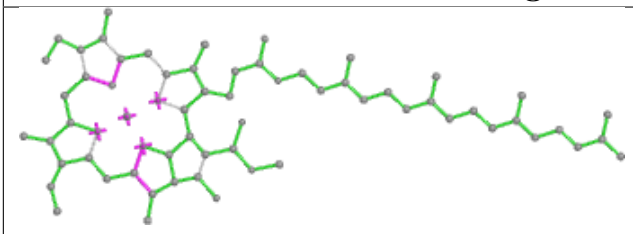


Torsions

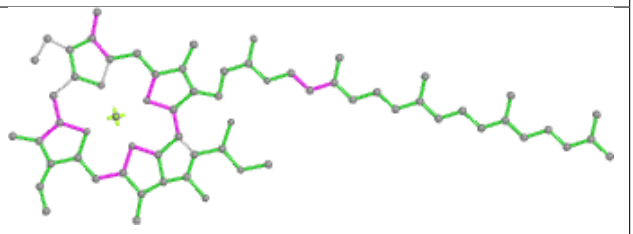


Rings

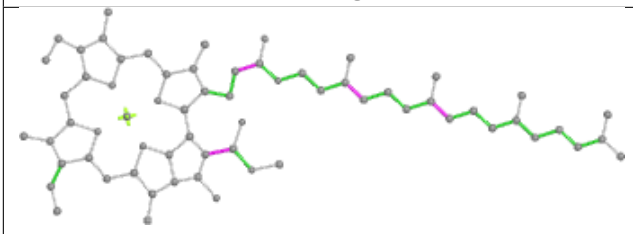
Ligand CLA C 612



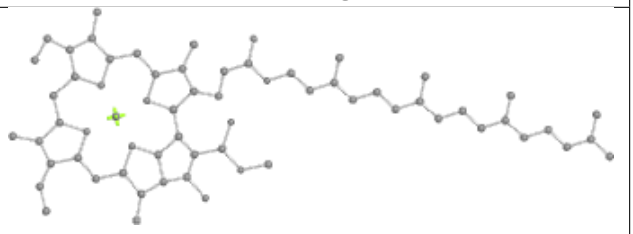
Bond lengths



Bond angles

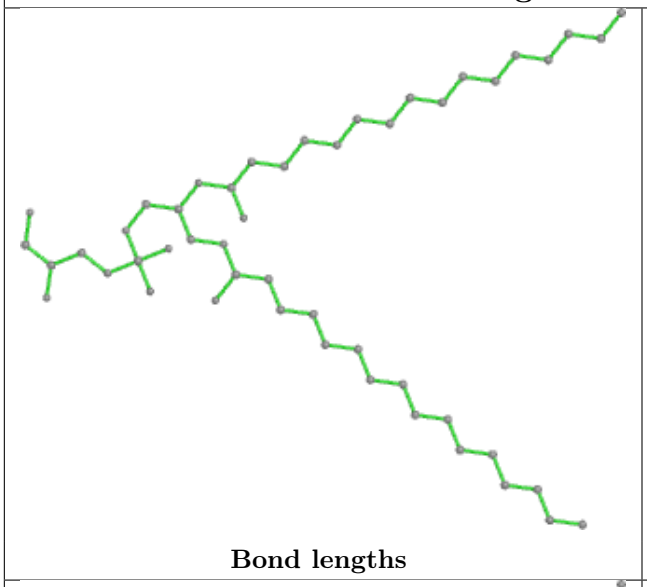


Torsions

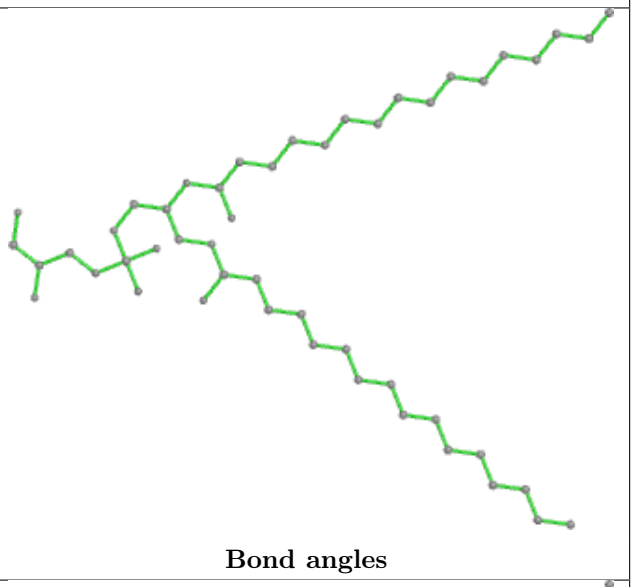


Rings

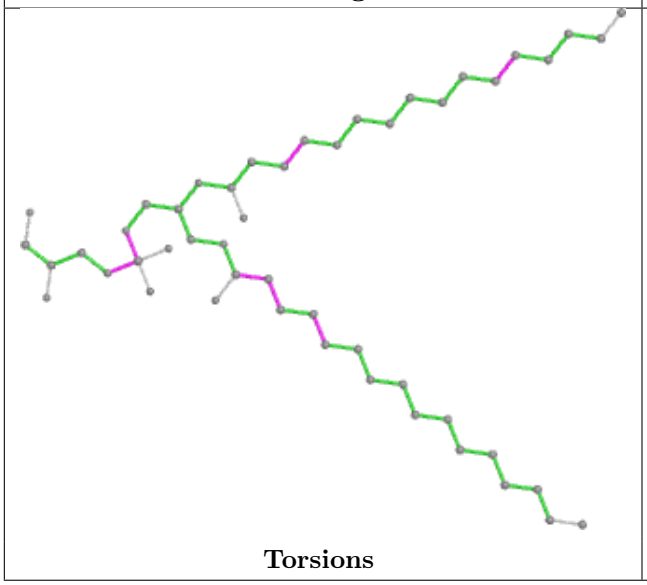
Ligand LHG B 1005



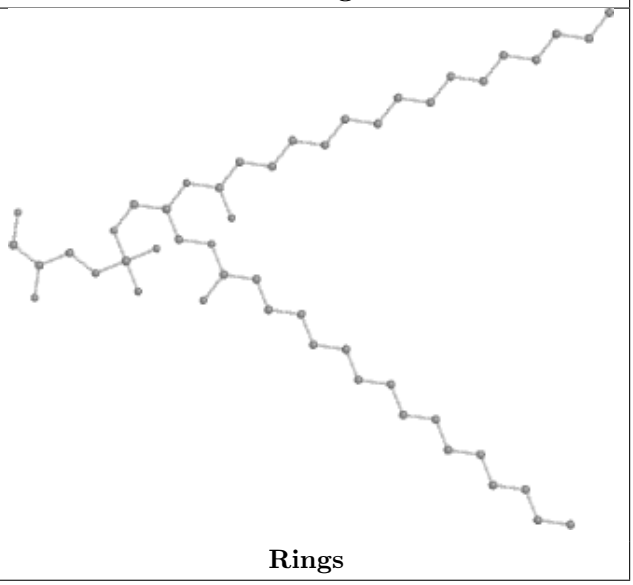
Bond lengths



Bond angles

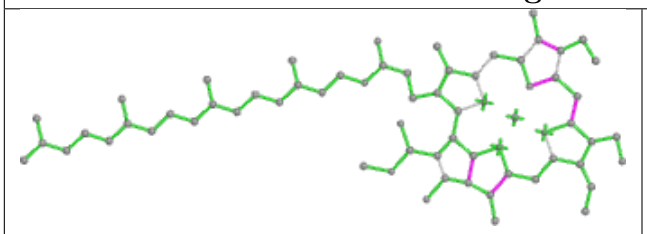


Torsions

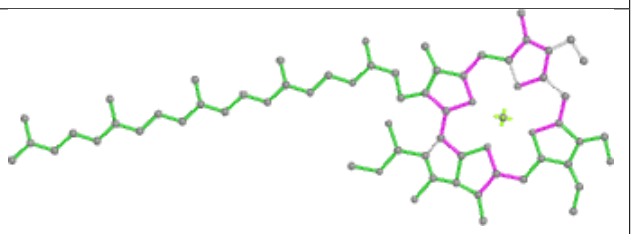


Rings

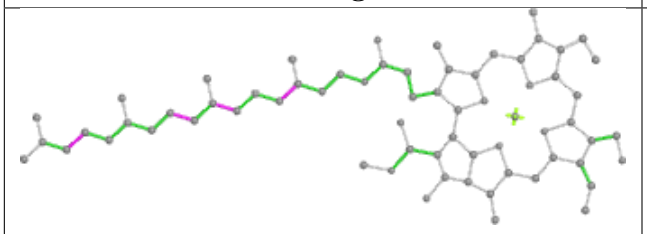
Ligand CHL A 609



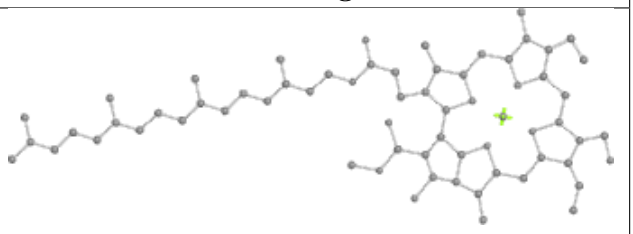
Bond lengths



Bond angles

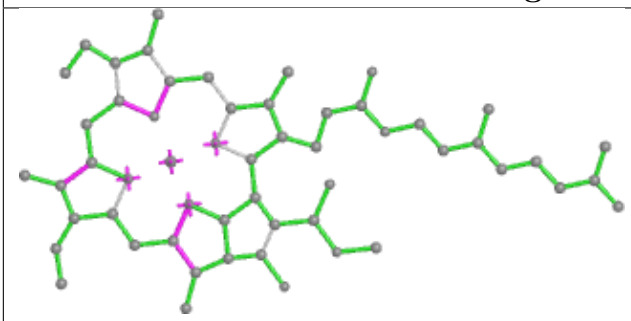


Torsions

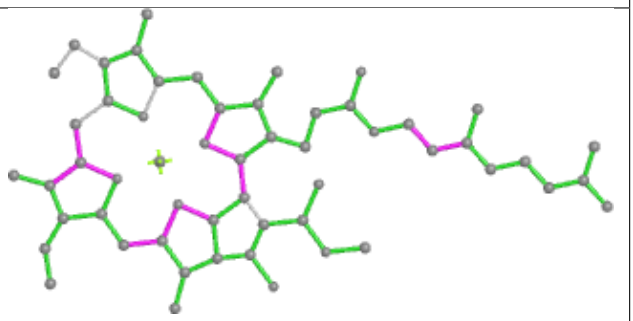


Rings

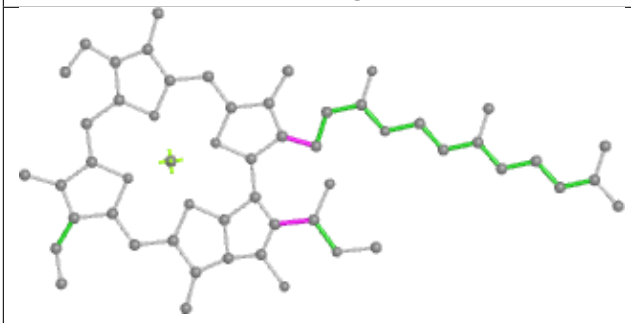
Ligand CLA B 603



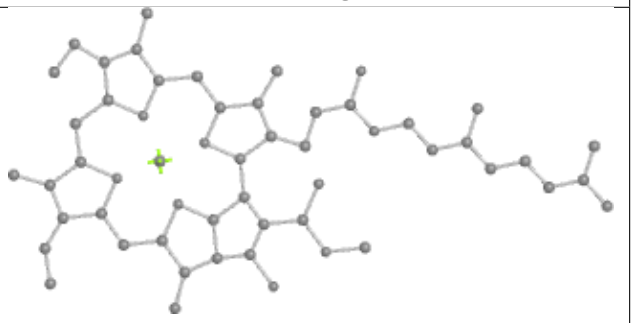
Bond lengths



Bond angles

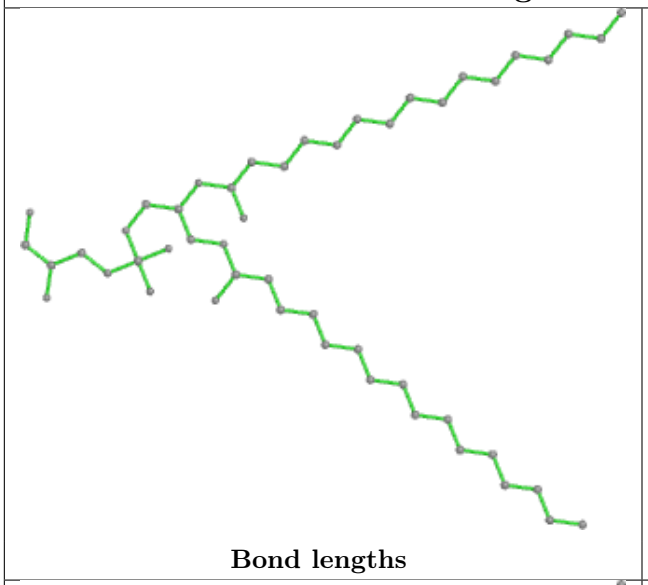


Torsions

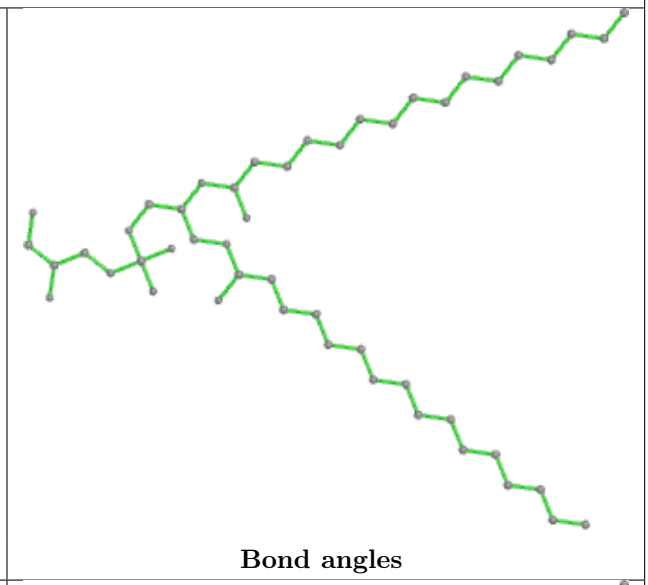


Rings

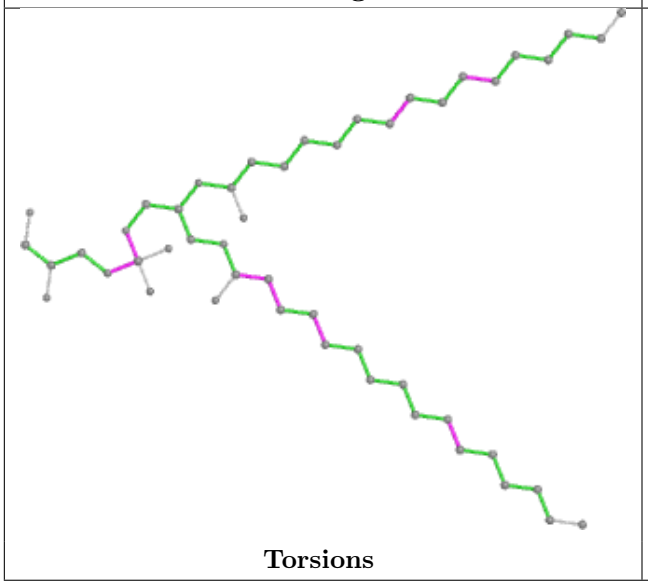
Ligand LHG C 1005



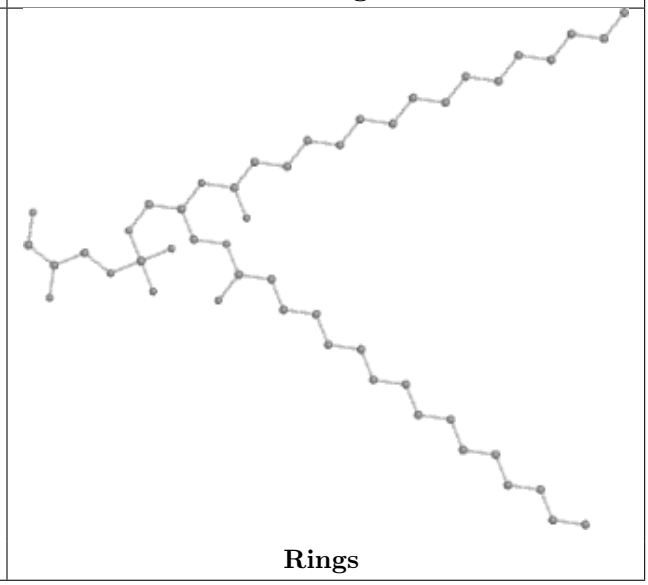
Bond lengths



Bond angles

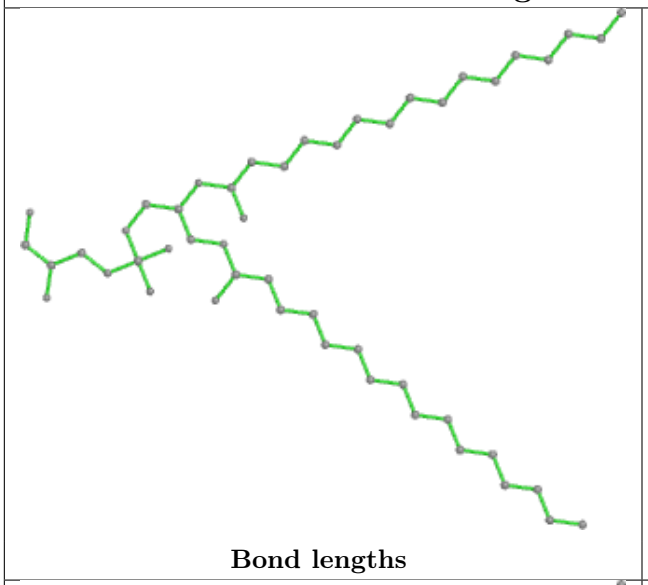


Torsions

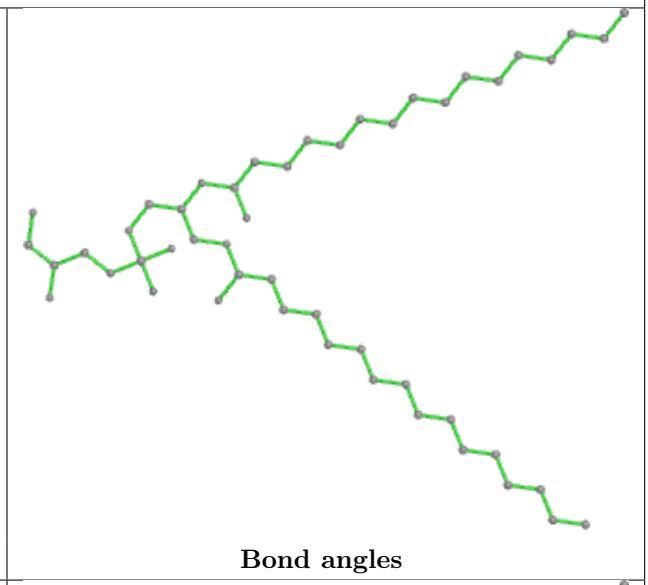


Rings

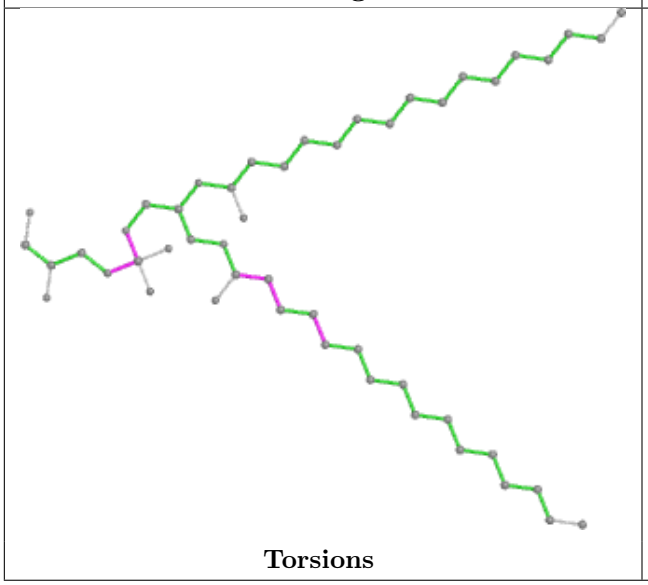
Ligand LHG A 1005



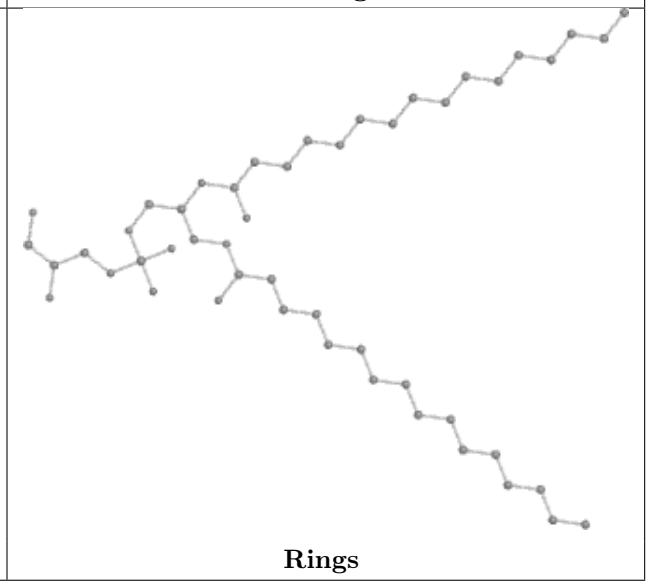
Bond lengths



Bond angles

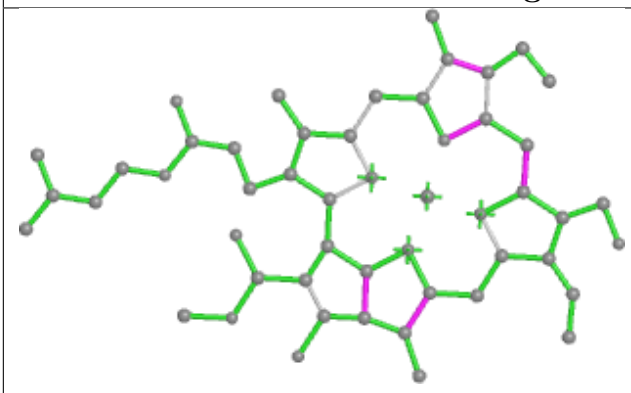


Torsions

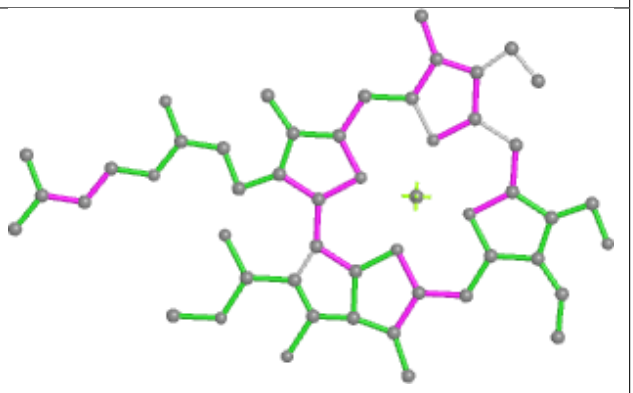


Rings

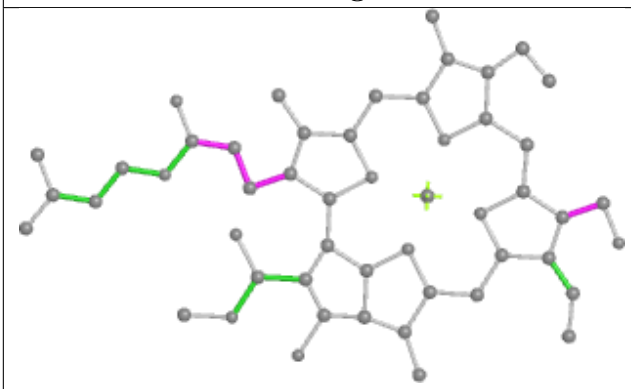
Ligand CHL C 606



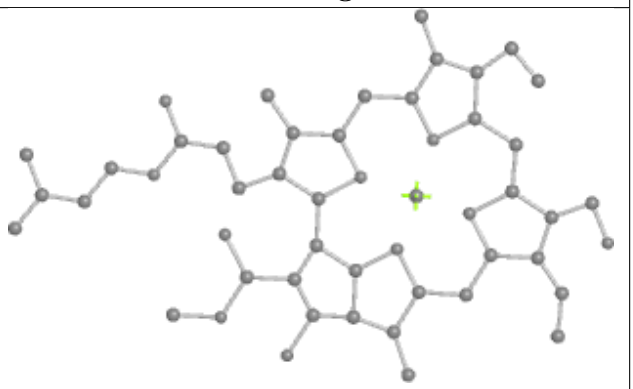
Bond lengths



Bond angles

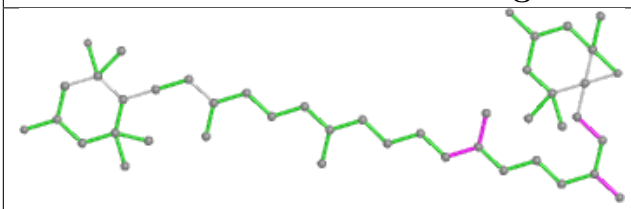


Torsions

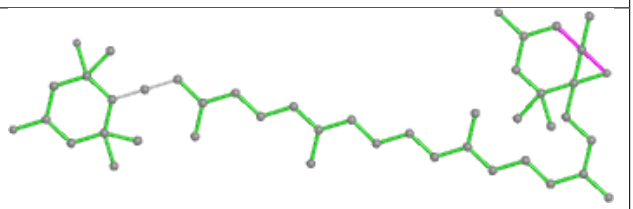


Rings

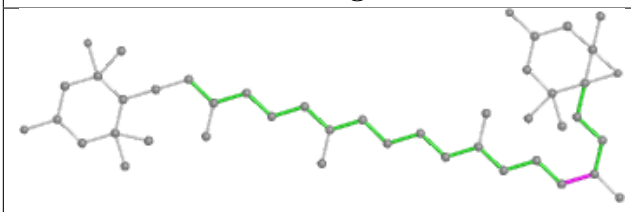
Ligand NEX B 1003



Bond lengths



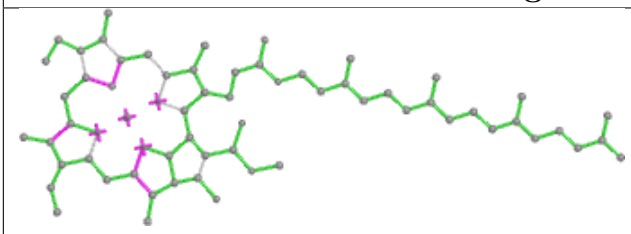
Bond angles



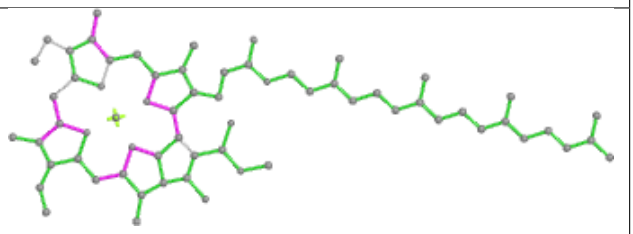
Torsions

Rings

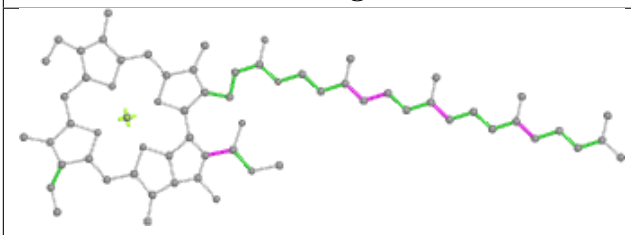
Ligand CLA B 602



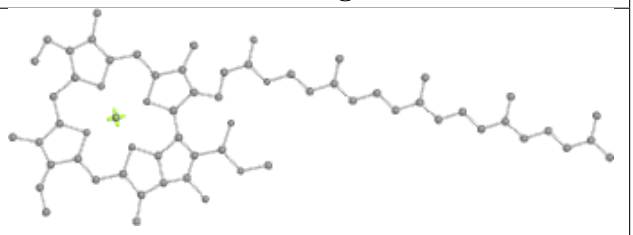
Bond lengths



Bond angles

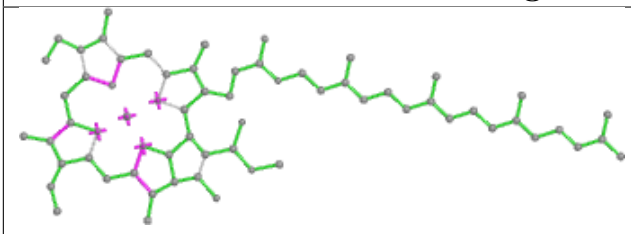


Torsions

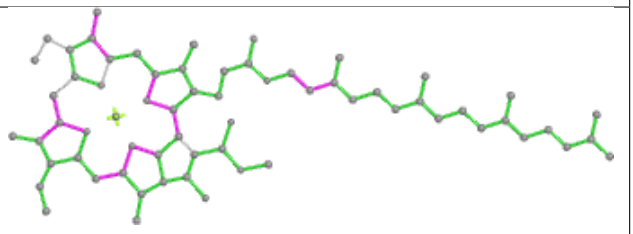


Rings

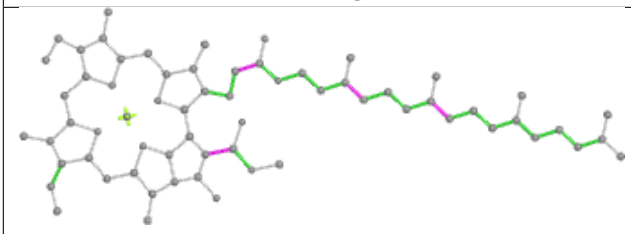
Ligand CLA A 612



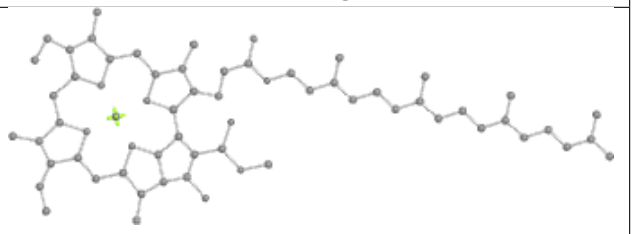
Bond lengths



Bond angles

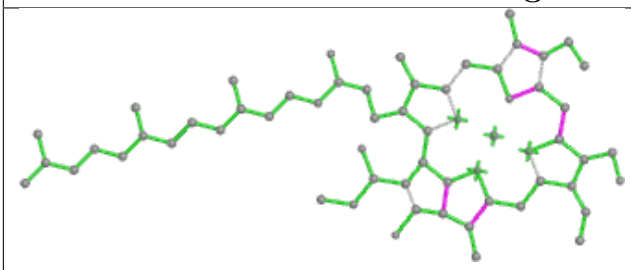


Torsions

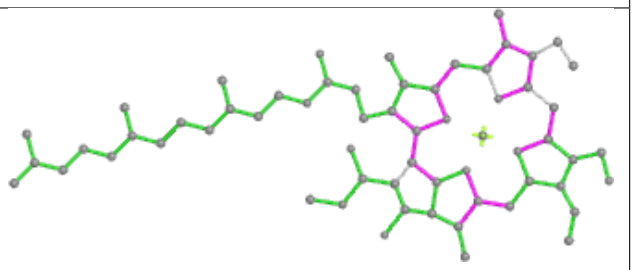


Rings

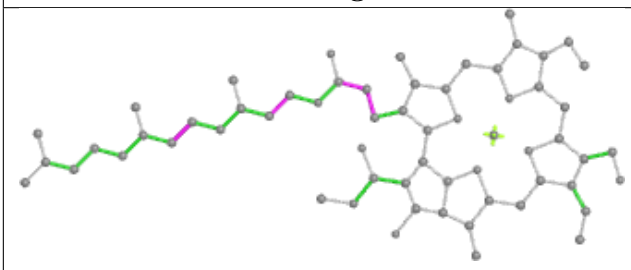
Ligand CHL B 608



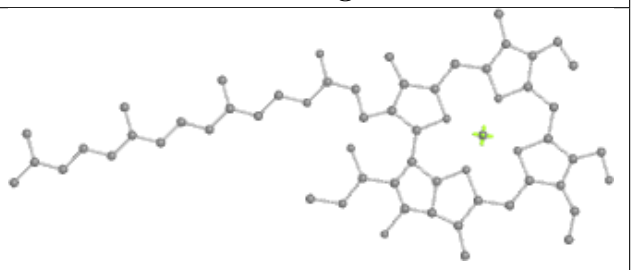
Bond lengths



Bond angles

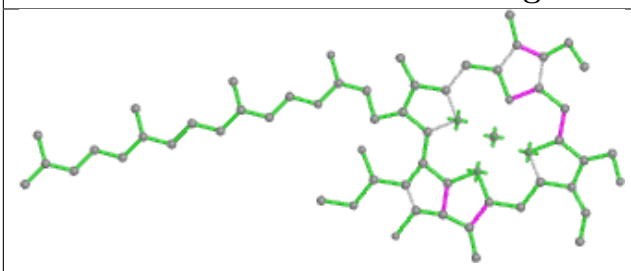


Torsions



Rings

Ligand CHL A 608



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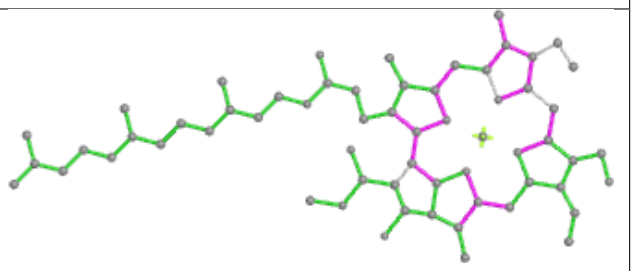
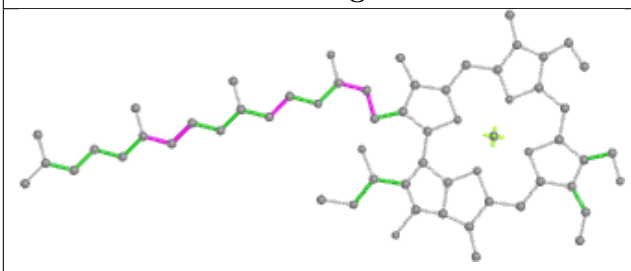
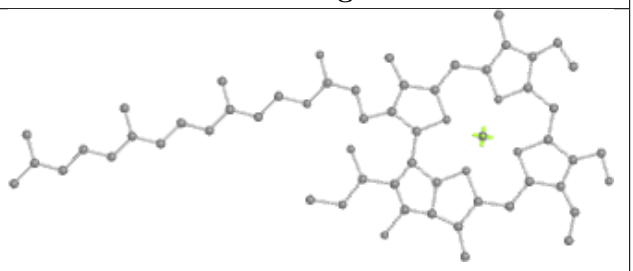


Bond angles

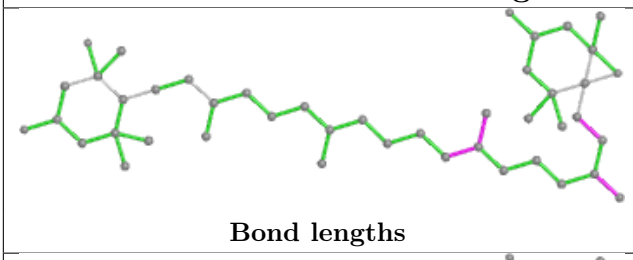


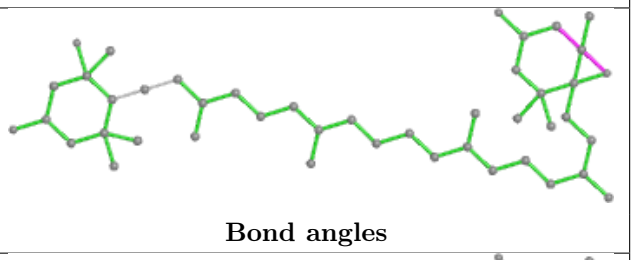
Torsions



Rings

Ligand NEX A 1003


Bond lengths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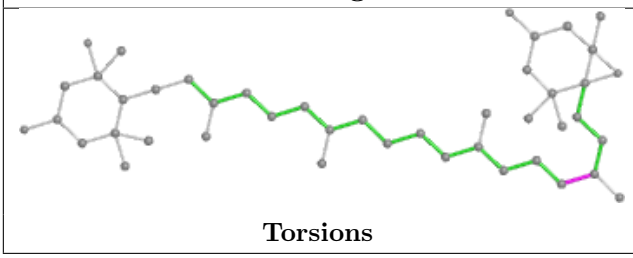
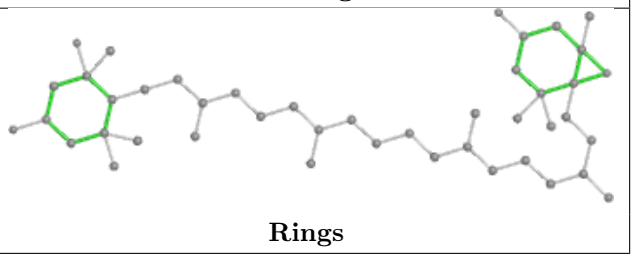
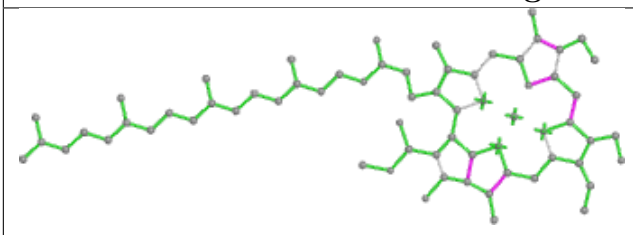
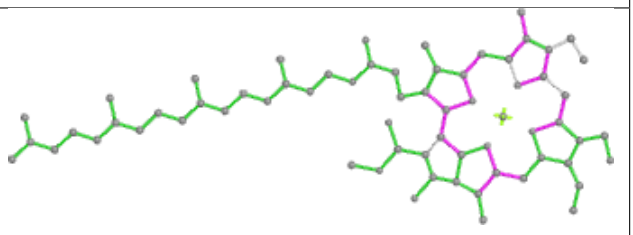
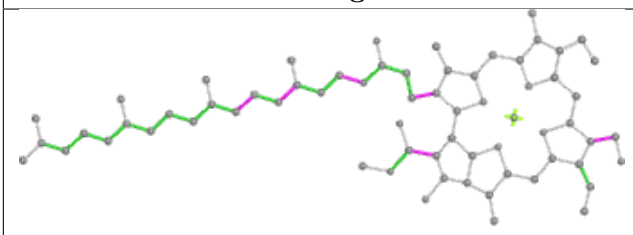

Torsions

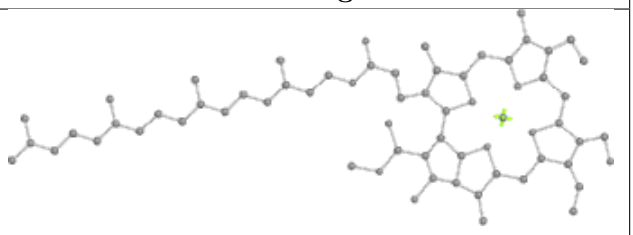

Rings

Ligand CHL B 601

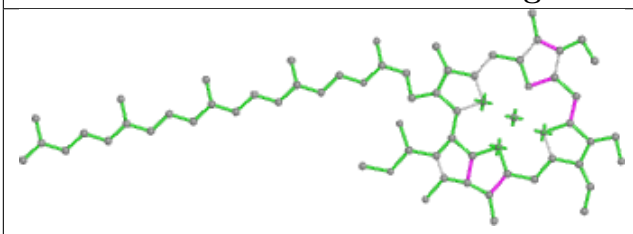

Bond lengths

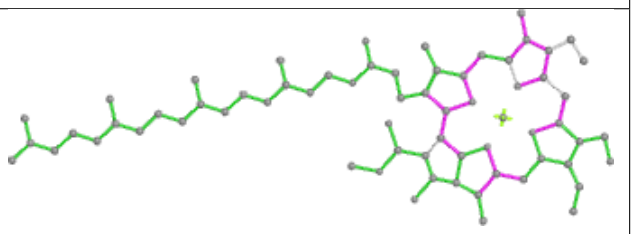

Bond angles

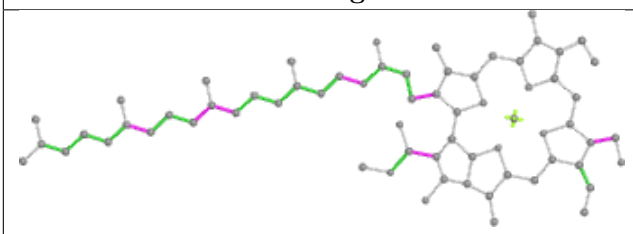

Torsions


Rings

Ligand CHL C 601


Bond lengths


Bond angles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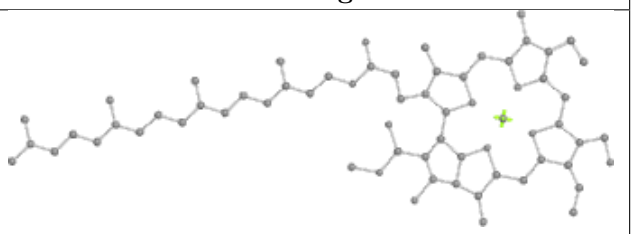
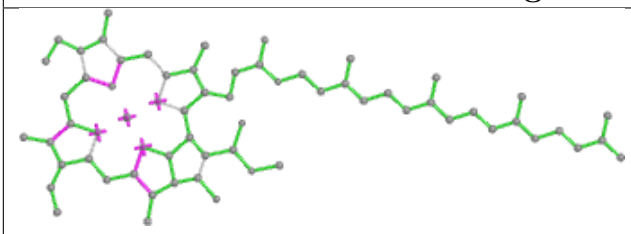
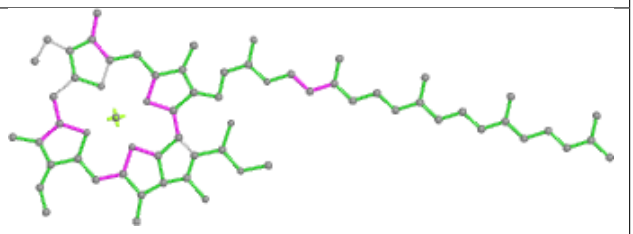

Rings

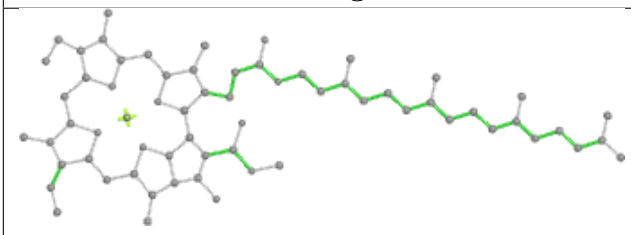
Ligand CLA C 610



Bond lengths



Bond angles



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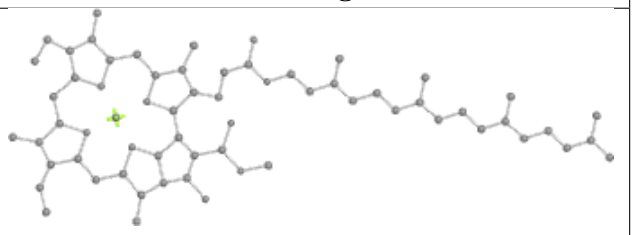
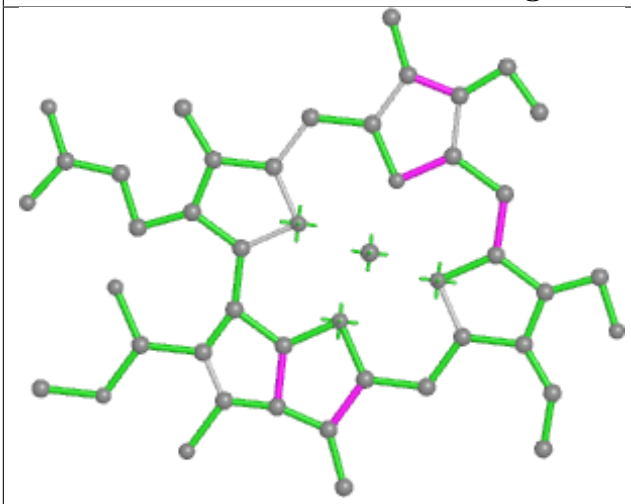
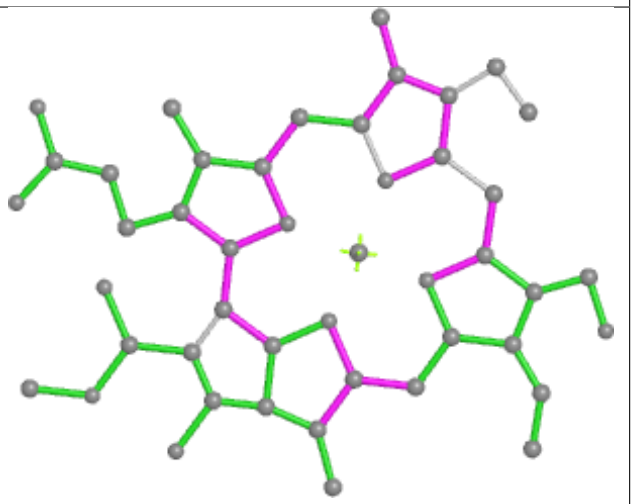


Rings

Ligand CHL B 607



Bond lengths



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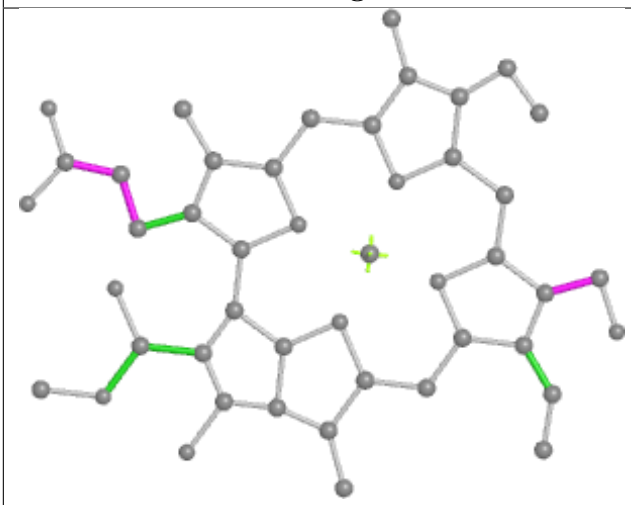

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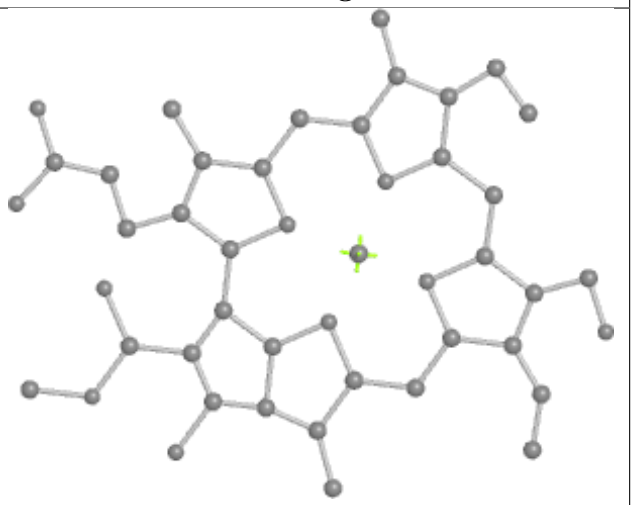
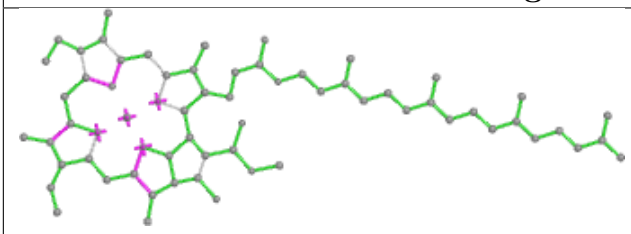
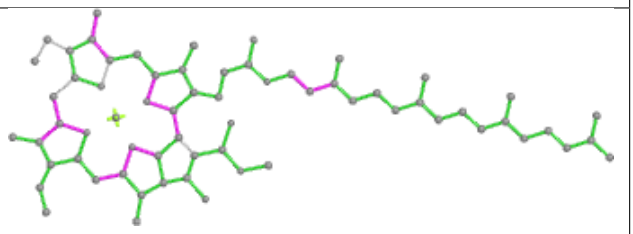


Rings

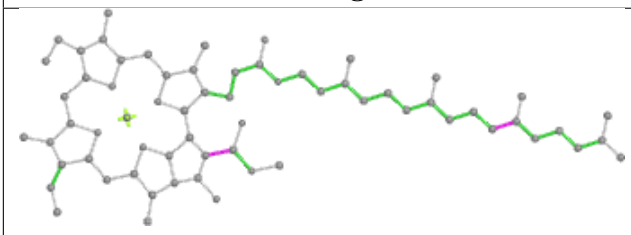
Ligand CLA C 602



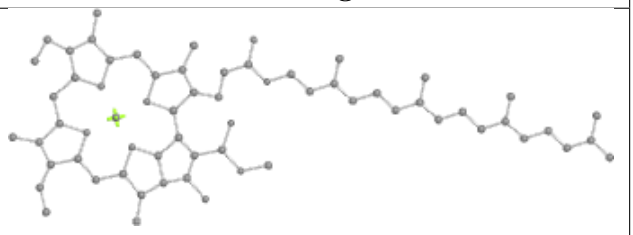
Bond lengths



Bond angles

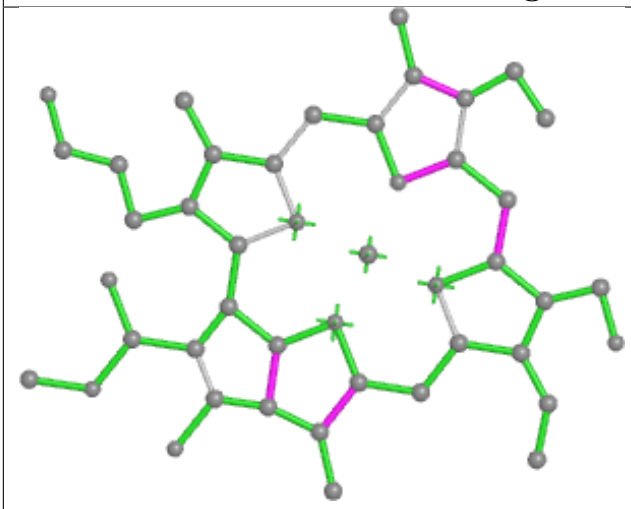


Torsions

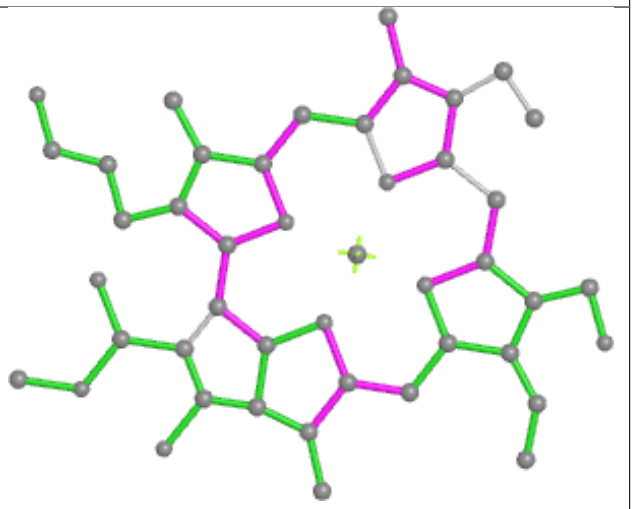


Rings

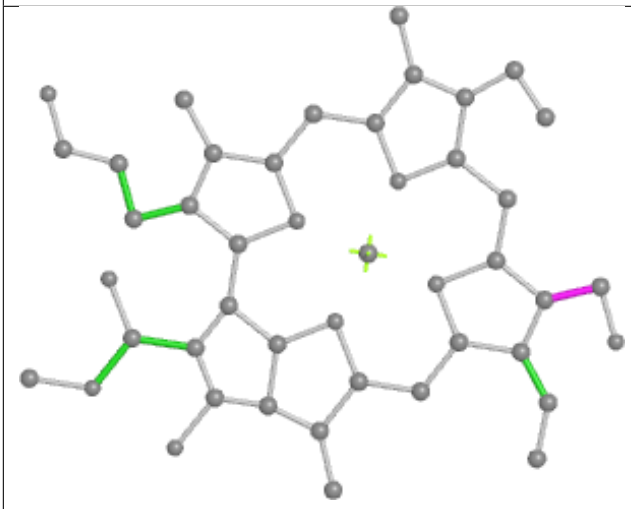
Ligand CHL A 605



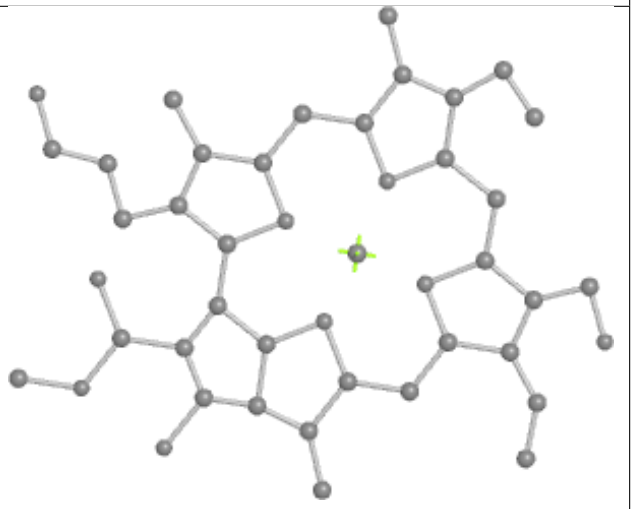
Bond lengths



Bond angles

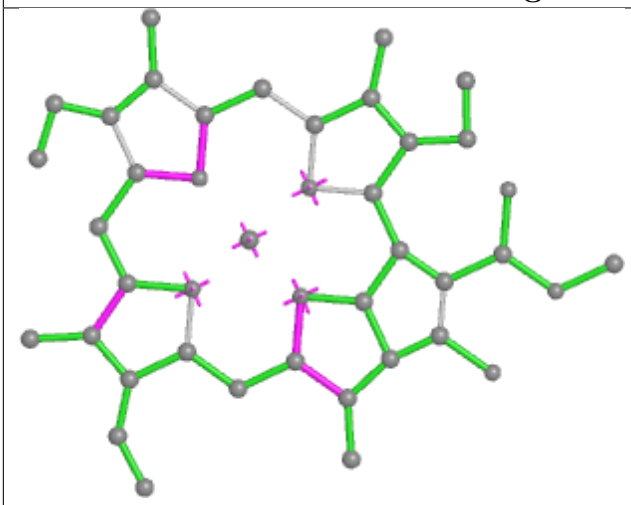


Torsions

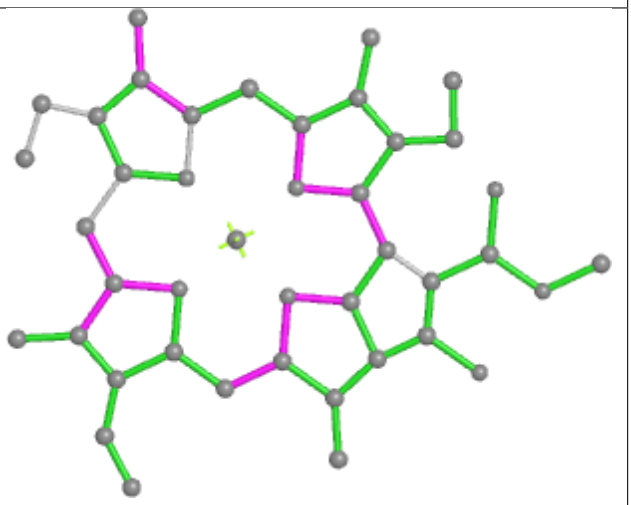


Rings

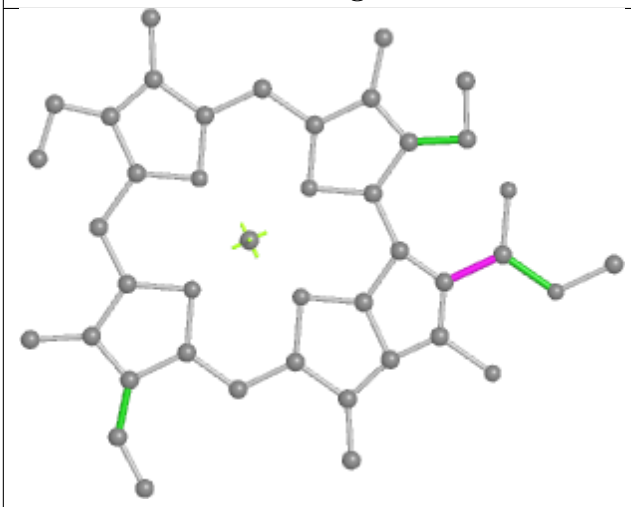
Ligand CLA B 614



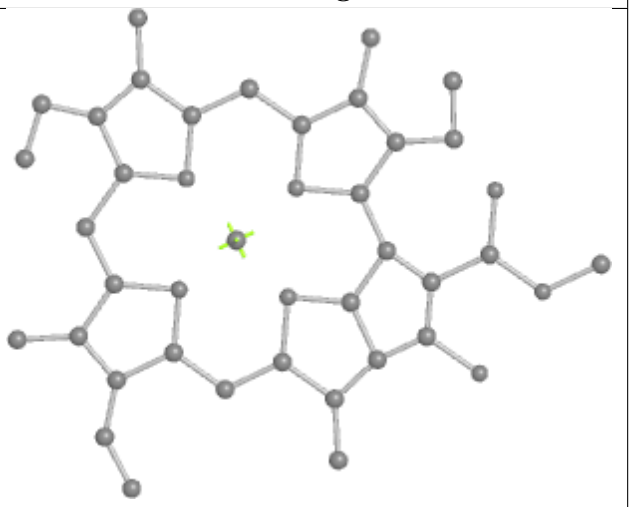
Bond lengths



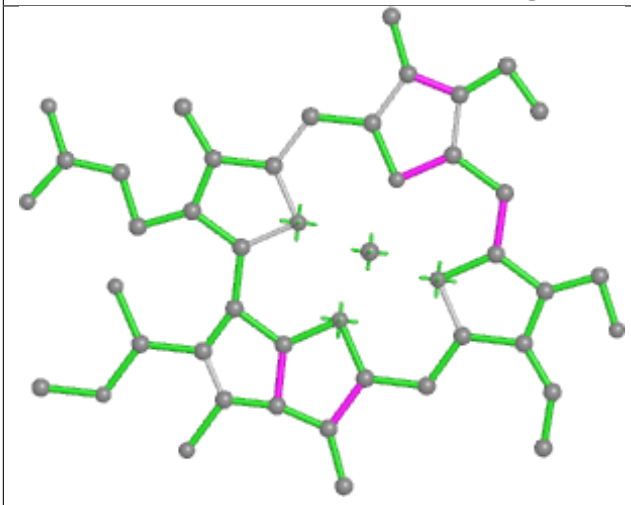
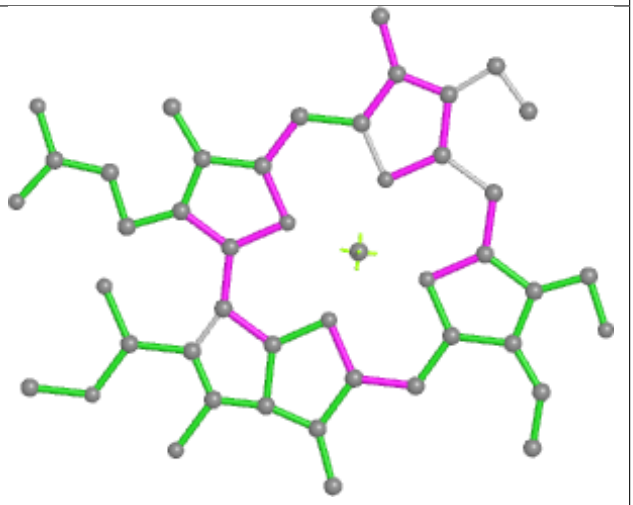
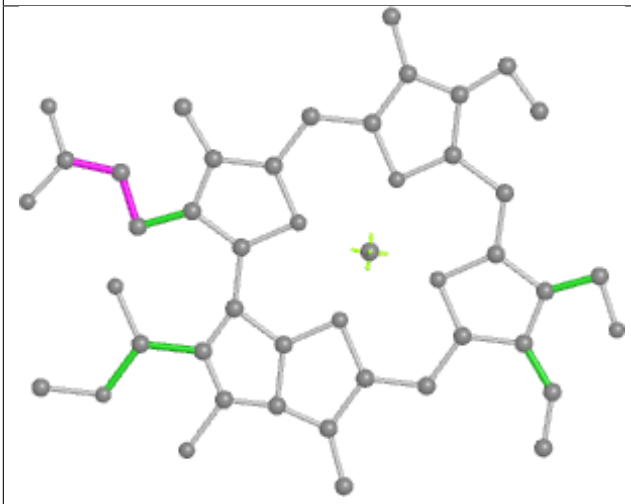
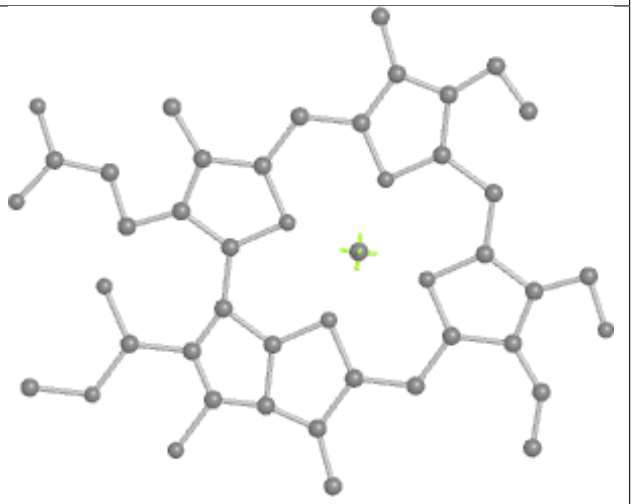
Bond angles

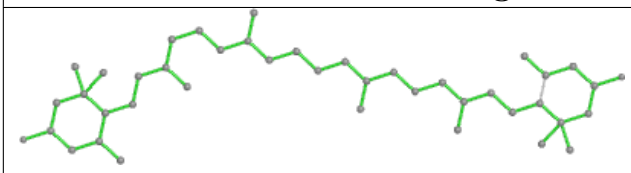
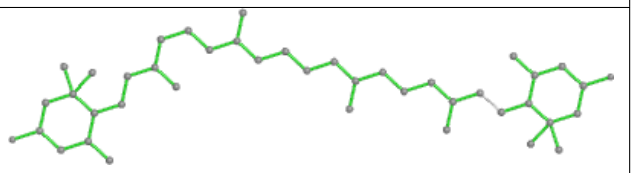
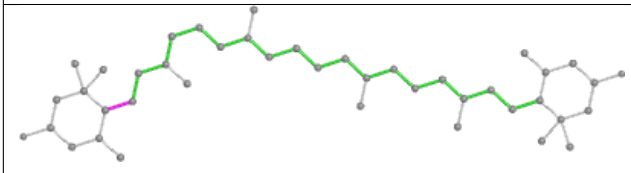
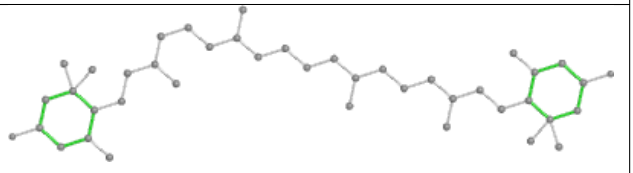


Torsions

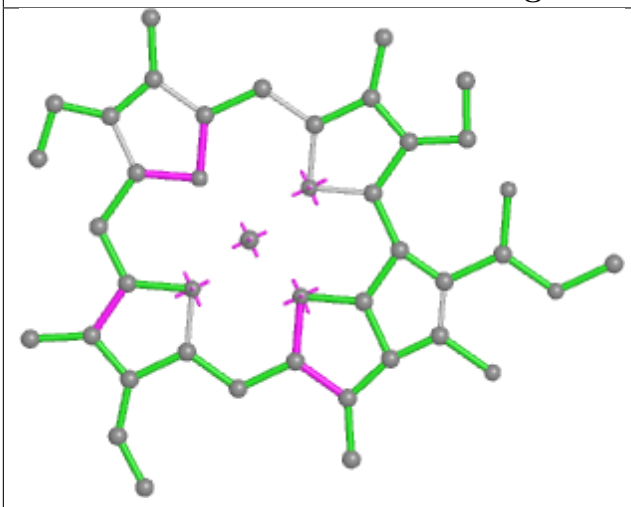


Rings

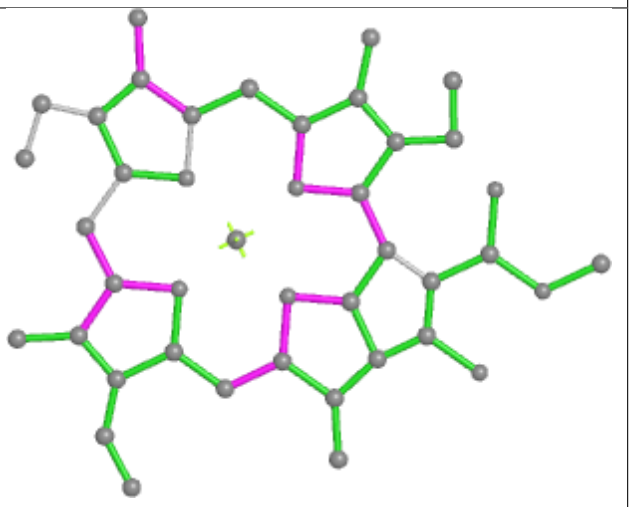
Ligand CHL A 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A1LXP A 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

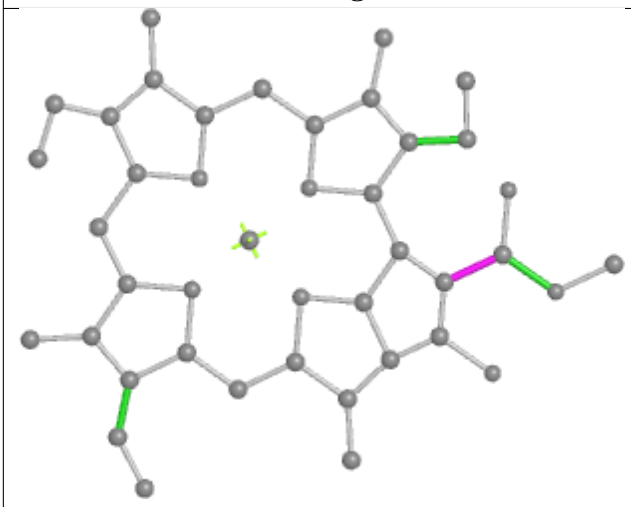
Ligand CLA C 614



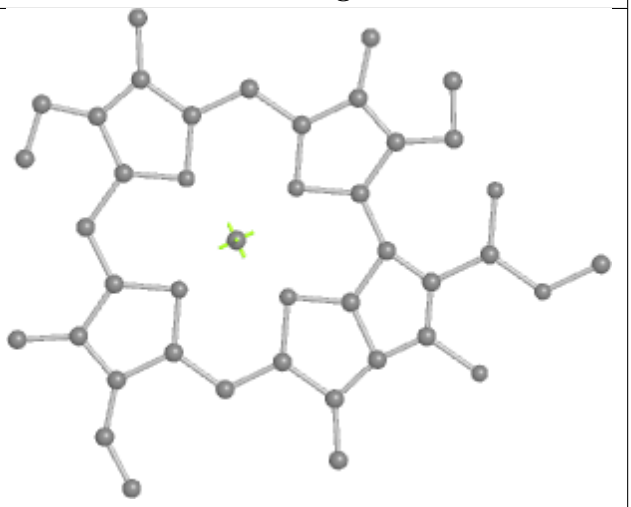
Bond lengths



Bond angles

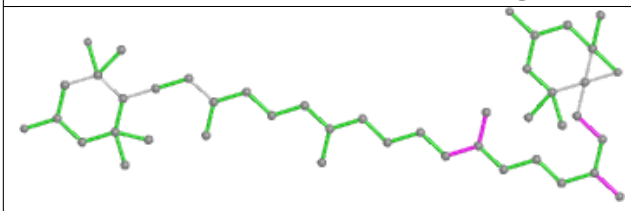


Torsions

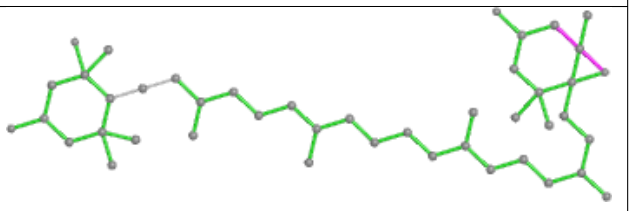


Rings

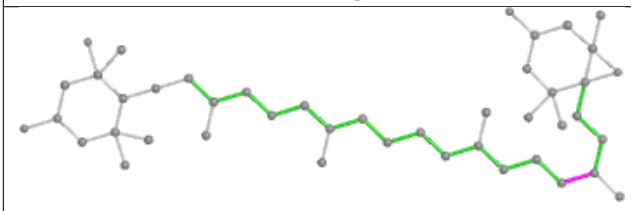
Ligand NEX C 1003



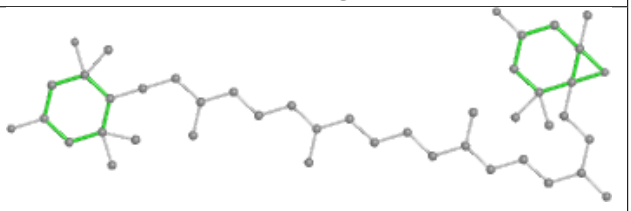
Bond lengths



Bond angles

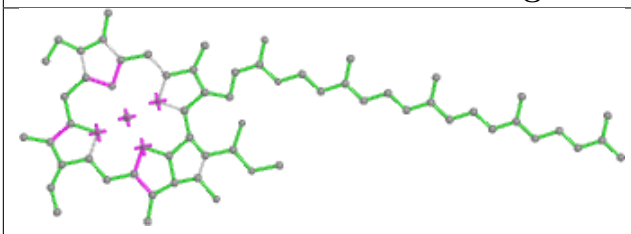


Torsions

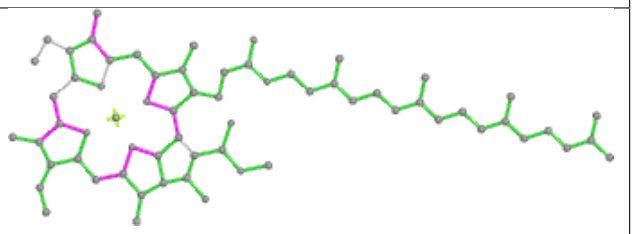


Rings

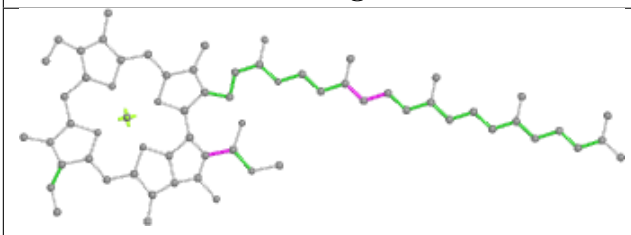
Ligand CLA A 602



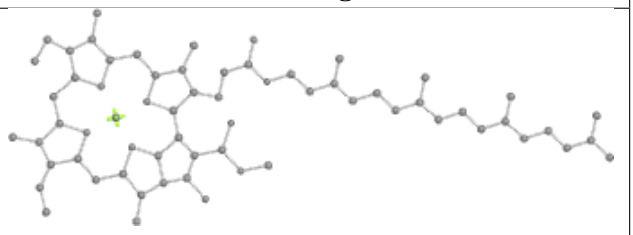
Bond lengths



Bond angles

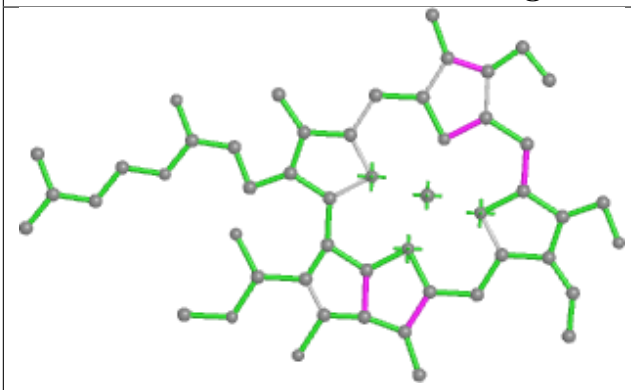


Torsions

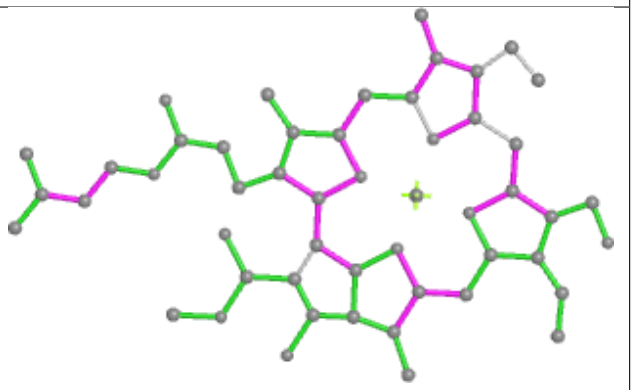


Rings

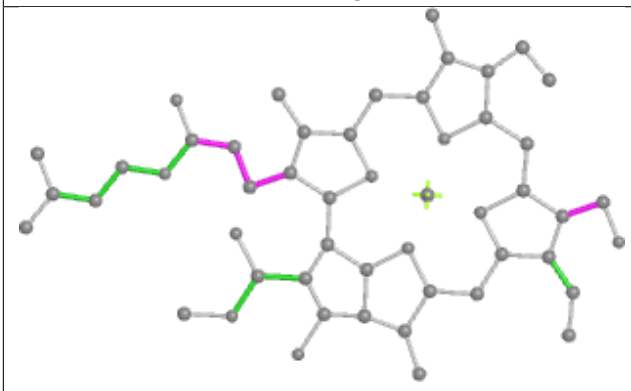
Ligand CHL B 606



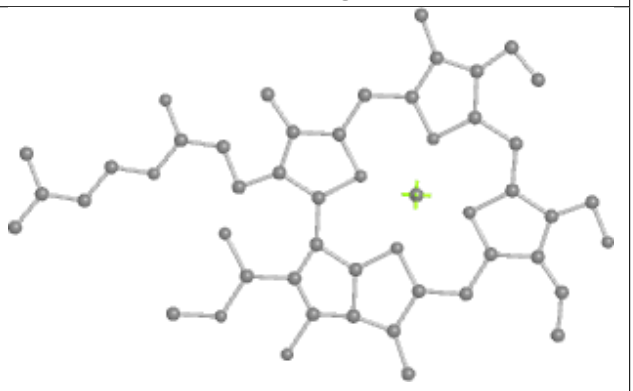
Bond lengths



Bond angles

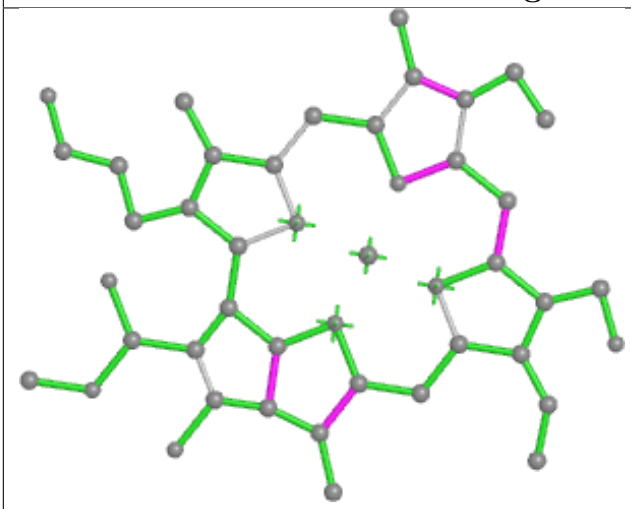


Torsions

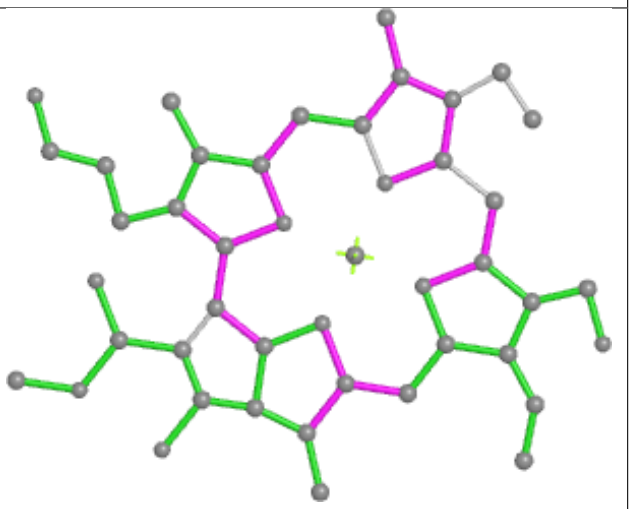


Rings

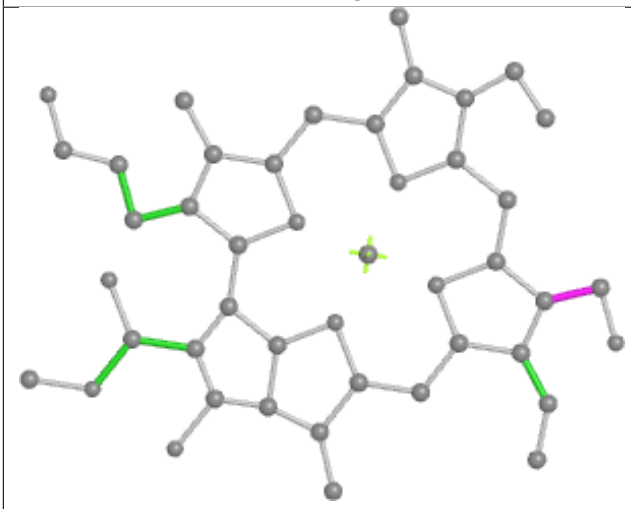
Ligand CHL B 605



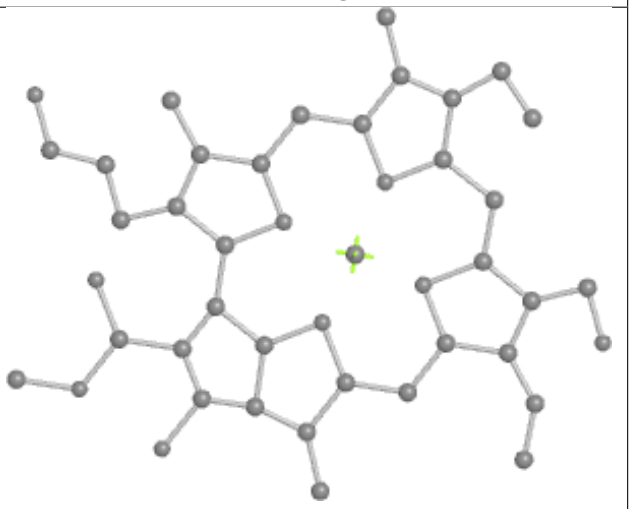
Bond lengths



Bond angles

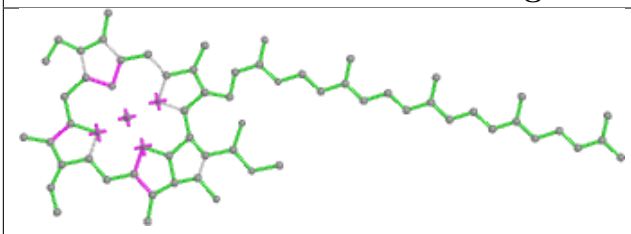


Torsions

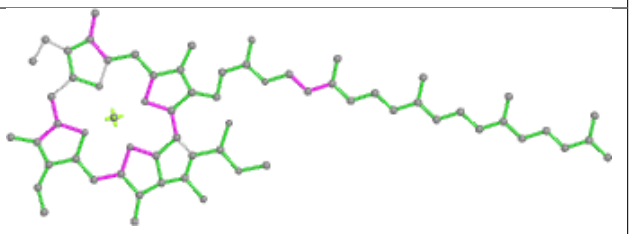


Rings

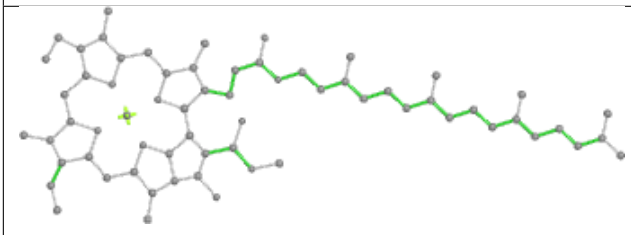
Ligand CLA B 610



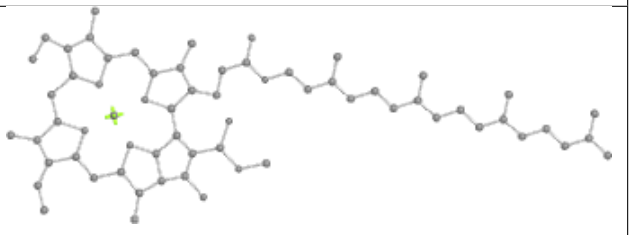
Bond lengths



Bond angles

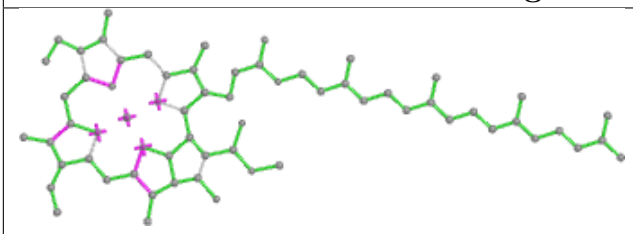


Torsions

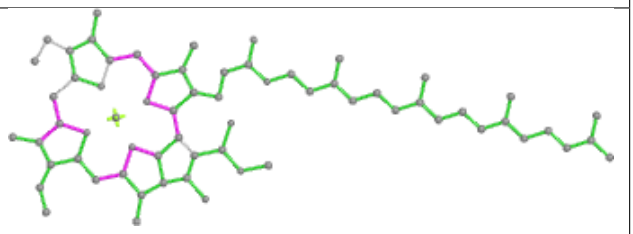


Rings

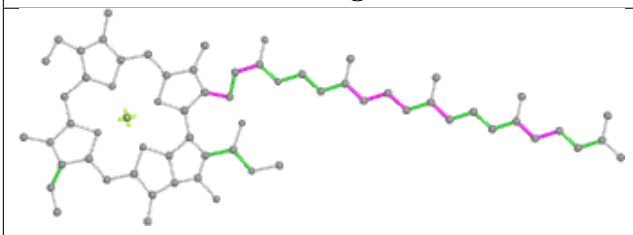
Ligand CLA B 611



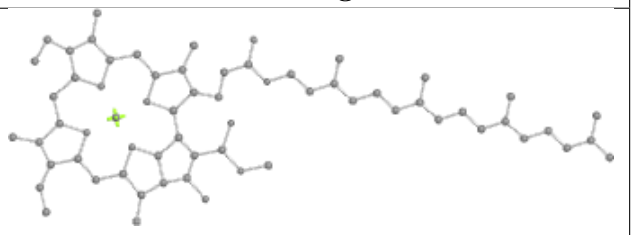
Bond lengths



Bond angles

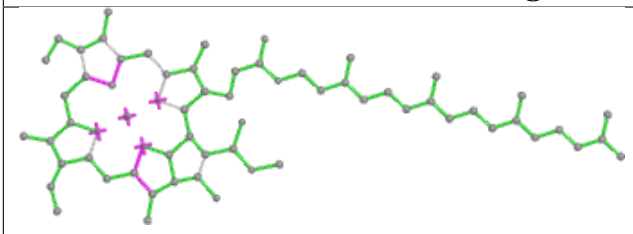


Torsions

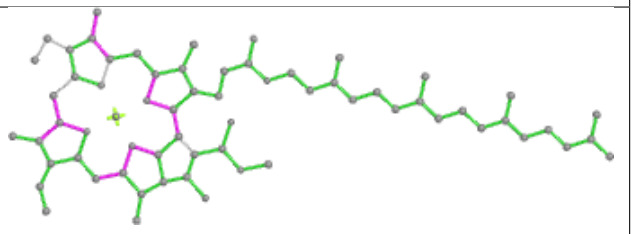


Rings

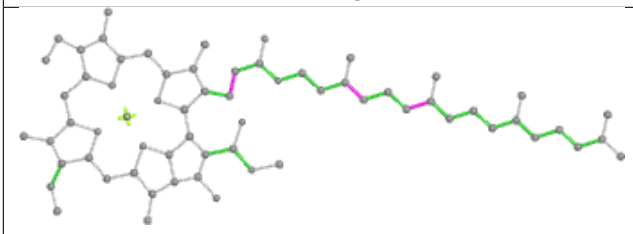
Ligand CLA C 613



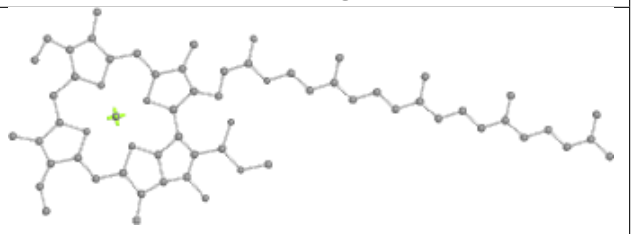
Bond lengths



Bond angles

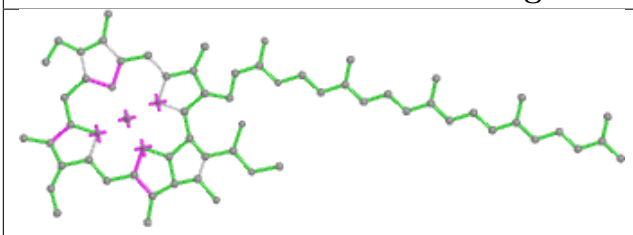


Torsions

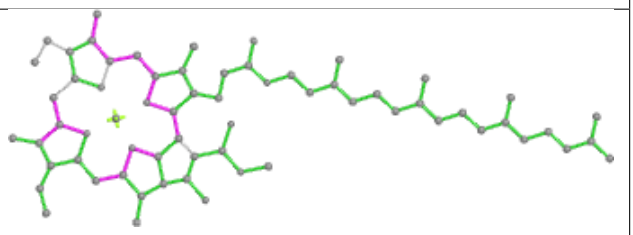


Rings

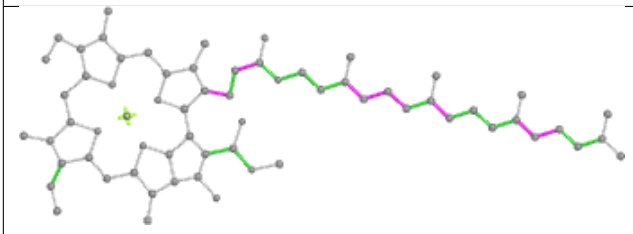
Ligand CLA C 611



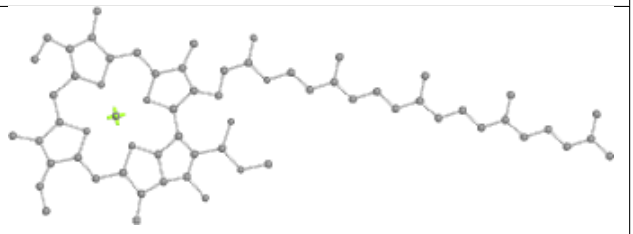
Bond lengths



Bond angles

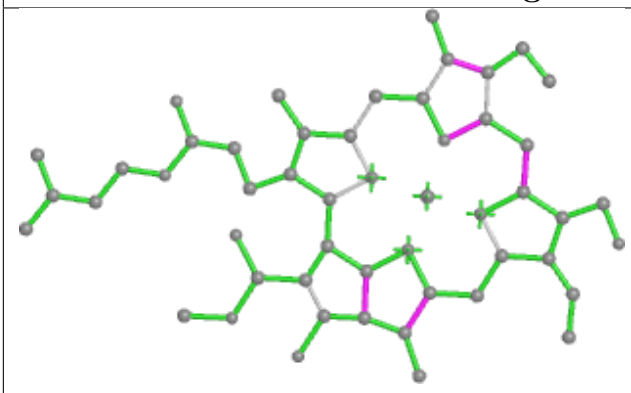


Torsions

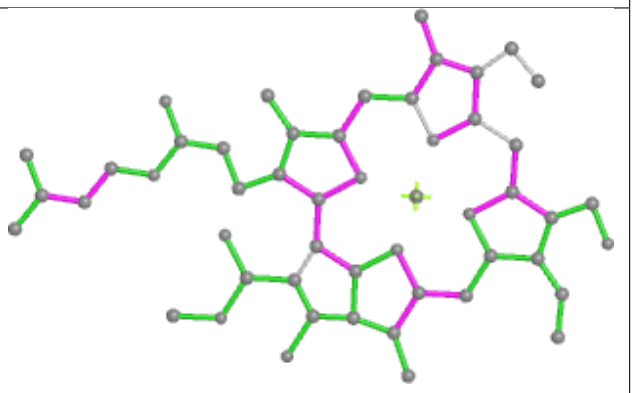


Rings

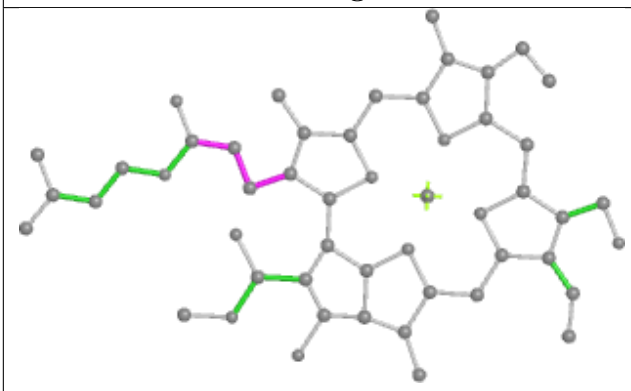
Ligand CHL A 606



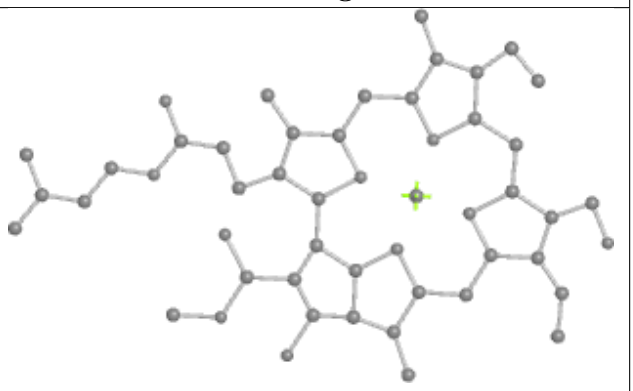
Bond lengths



Bond angles

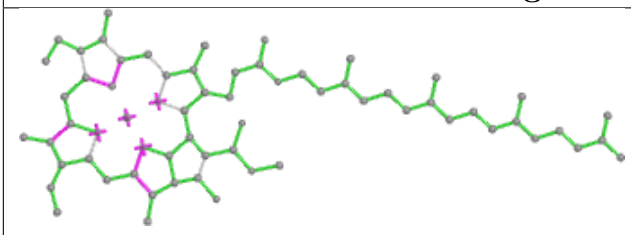


Torsions

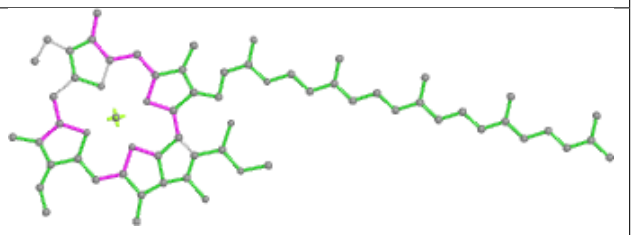


Rings

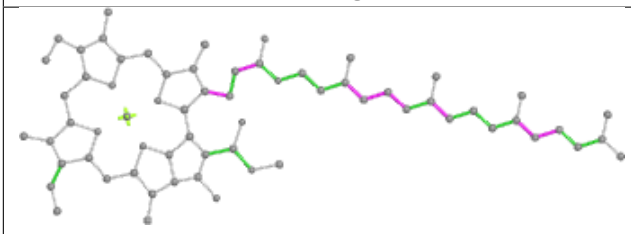
Ligand CLA A 611



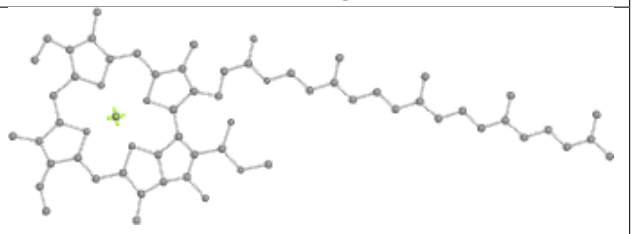
Bond lengths



Bond angles

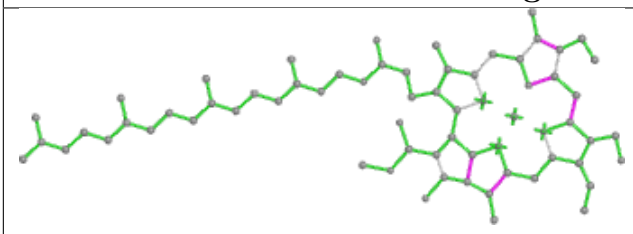


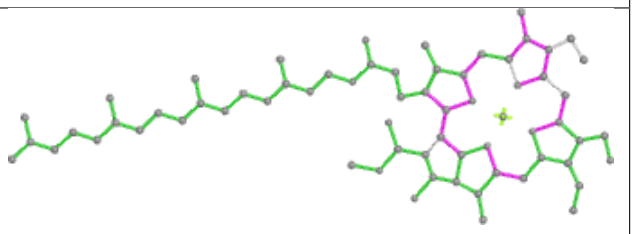
Torsions

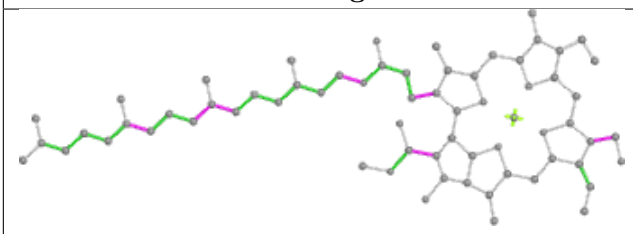


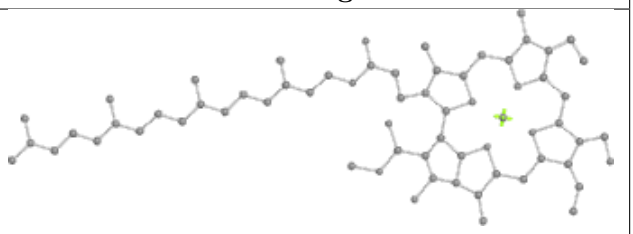
Rings

Ligand CHL A 601

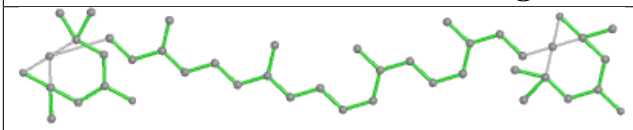

Bond lengths

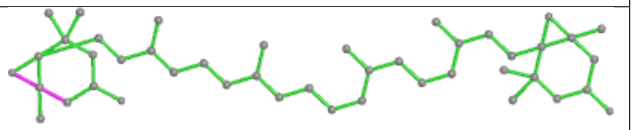

Bond angles

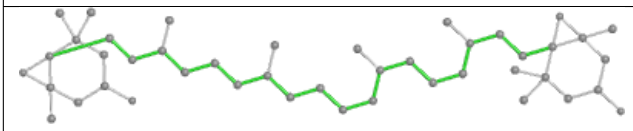

Torsions

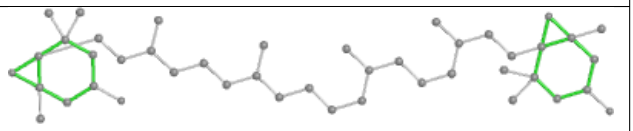

Rings

Ligand XAT B 1004

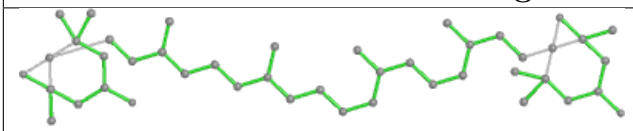

Bond lengths


Bond angles


Torsions


Rings

Ligand XAT C 1004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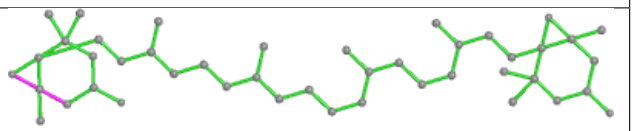
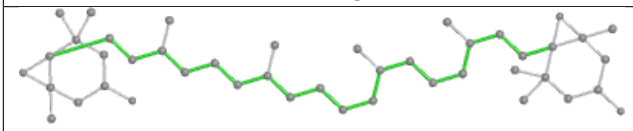

Bond angles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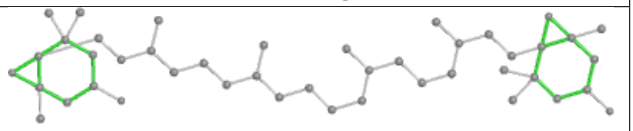
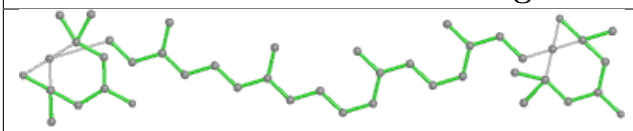

Rings

Ligand XAT A 1004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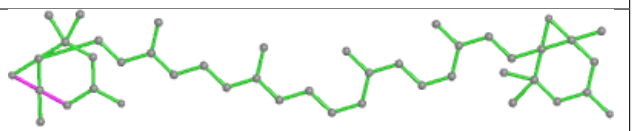
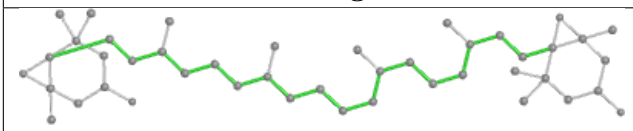
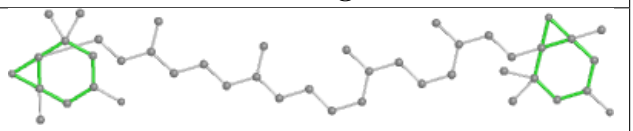
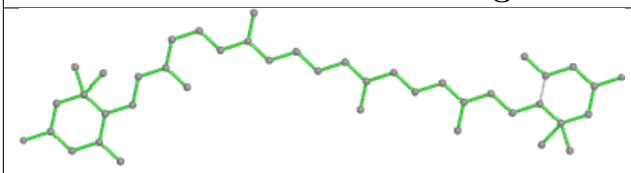

Bond angles

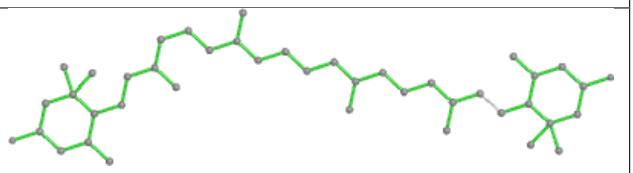

Torsions


Rings

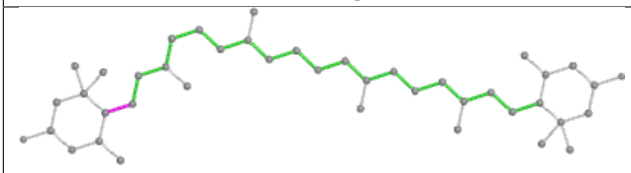
Ligand A1LXP C 1002



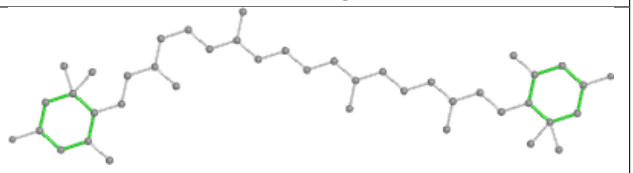
Bond lengths



Bond angles

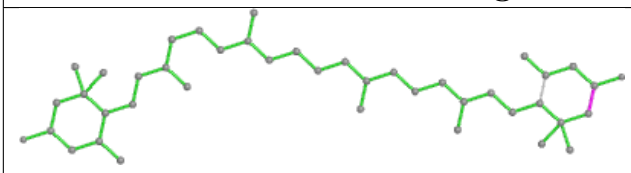


Torsions

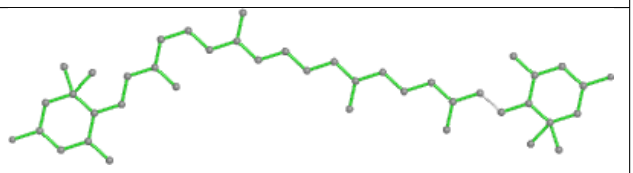


Rings

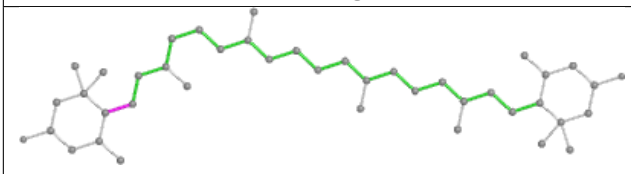
Ligand A1LXP B 1001



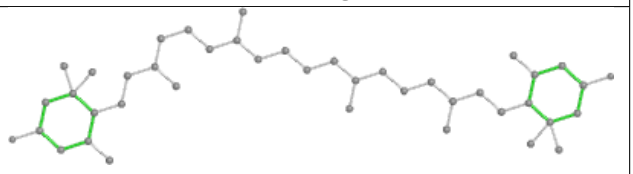
Bond lengths



Bond angles

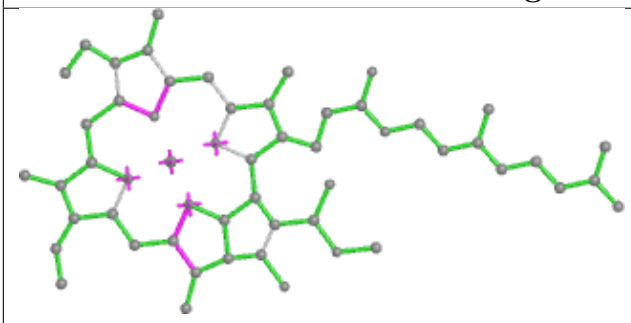


Torsions

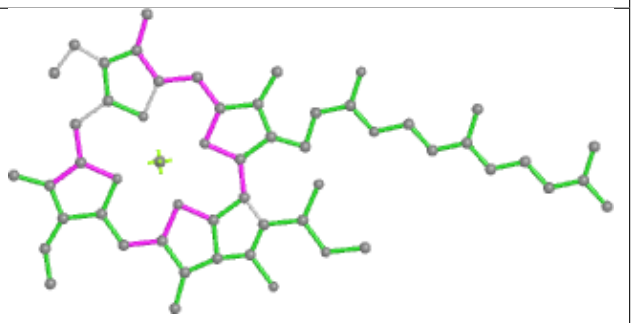


Rings

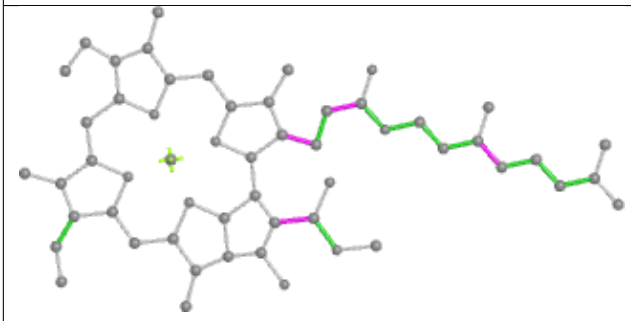
Ligand CLA C 604



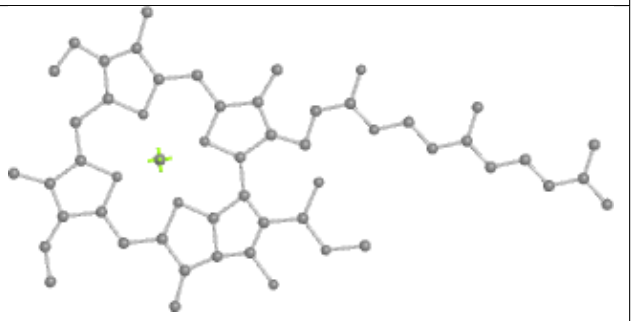
Bond lengths



Bond angles

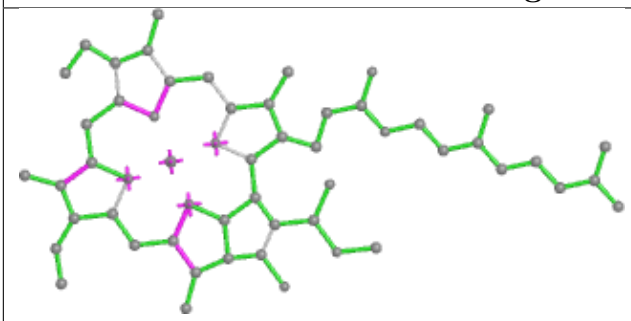


Torsions

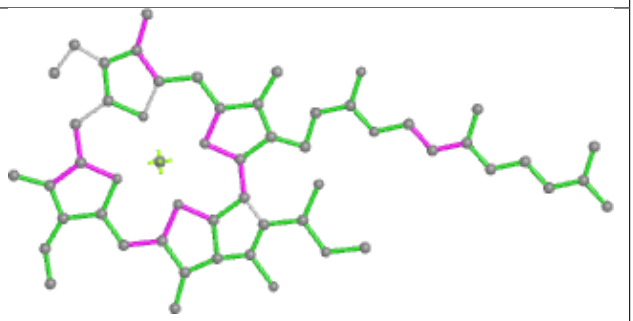


Rings

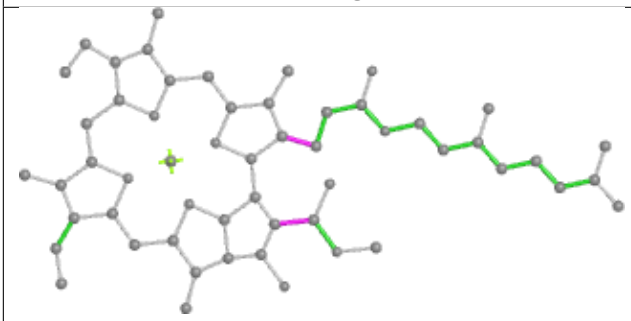
Ligand CLA C 603



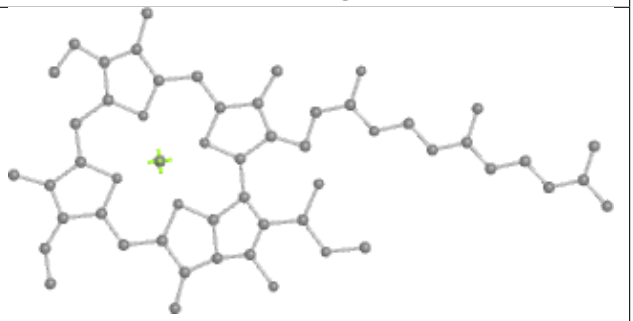
Bond lengths



Bond angles

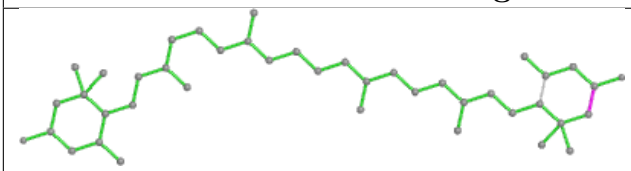


Torsions

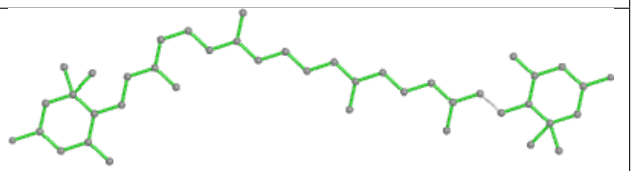


Rings

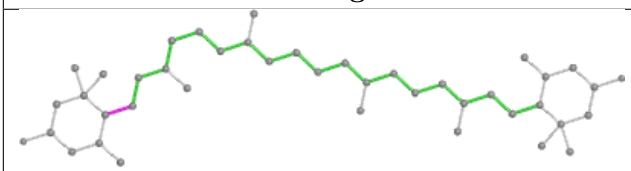
Ligand A1LXP C 1001



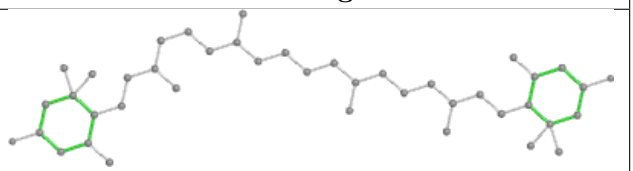
Bond lengths



Bond angles

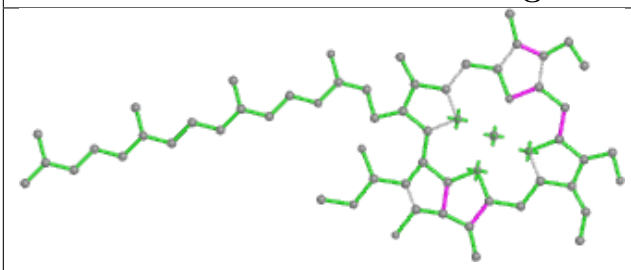


Torsions

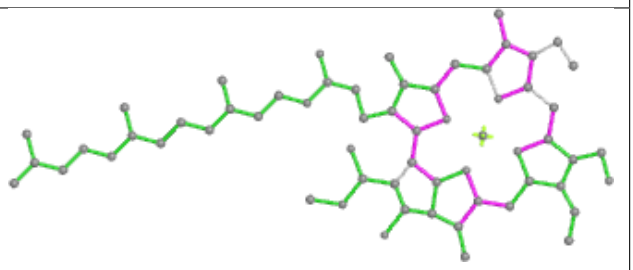


Rings

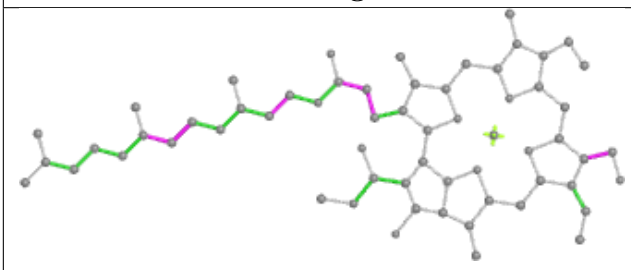
Ligand CHL C 608



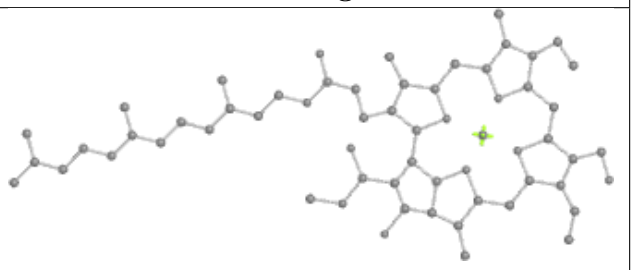
Bond lengths



Bond angles

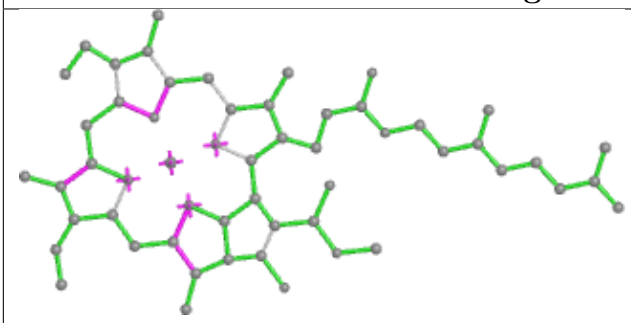


Torsions

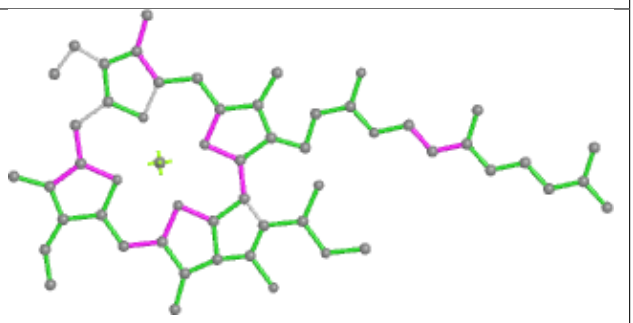


Rings

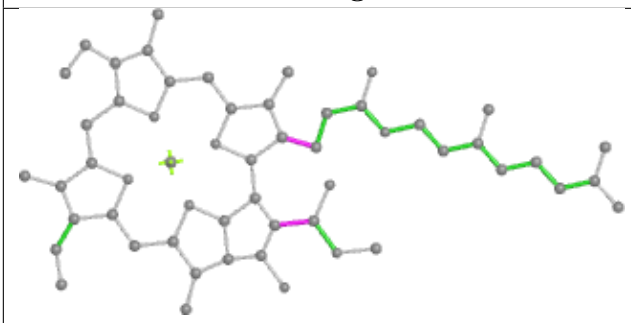
Ligand CLA A 603



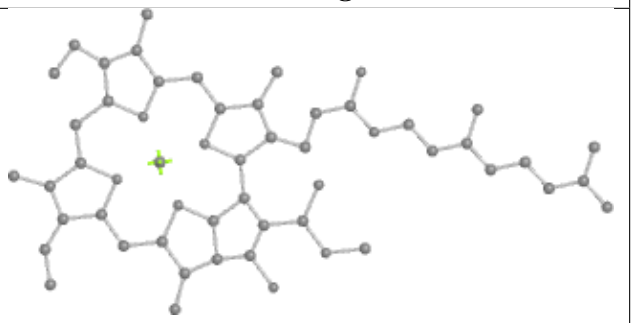
Bond lengths



Bond angles

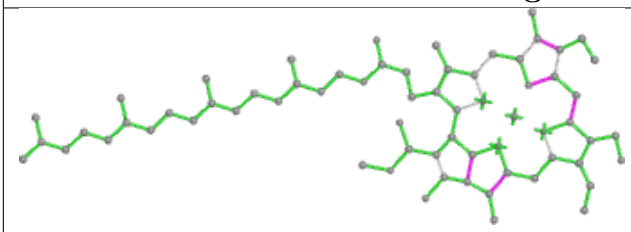


Torsions

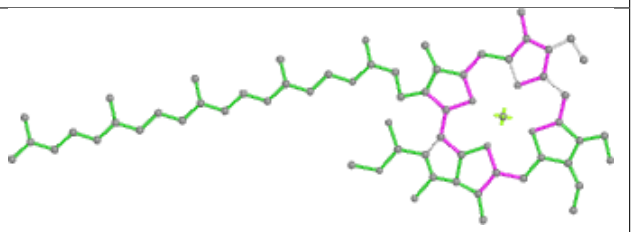


Rings

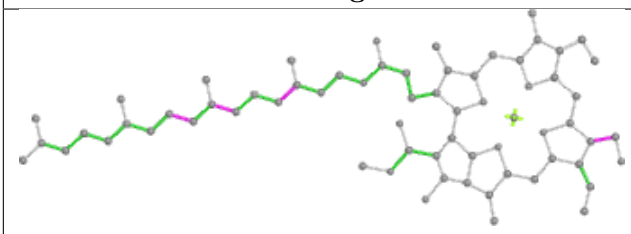
Ligand CHL B 609



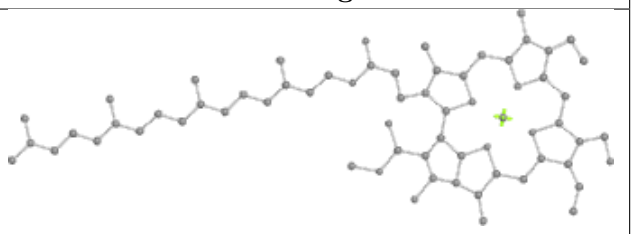
Bond lengths



Bond angles

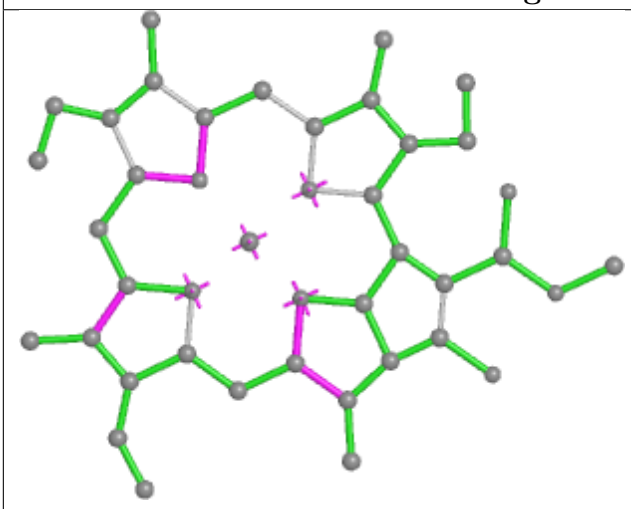


Torsions

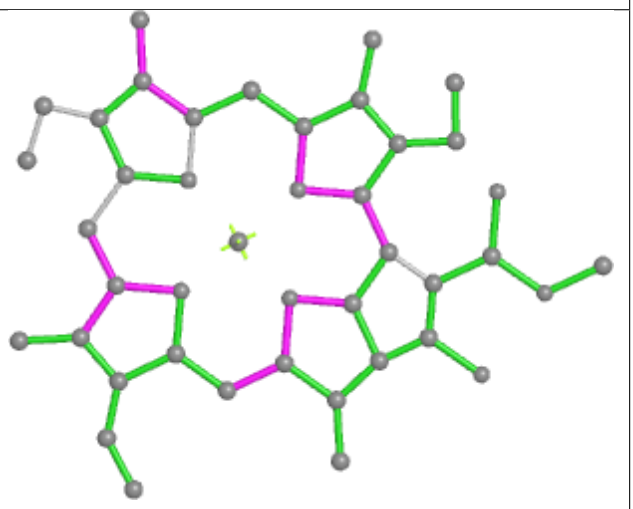


Rings

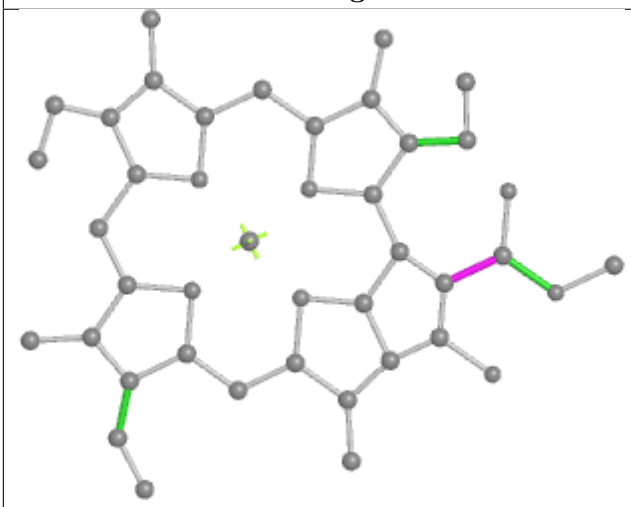
Ligand CLA A 614



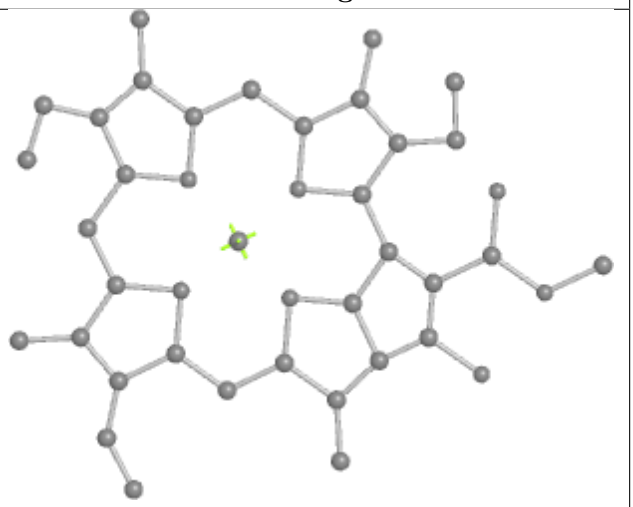
Bond lengths



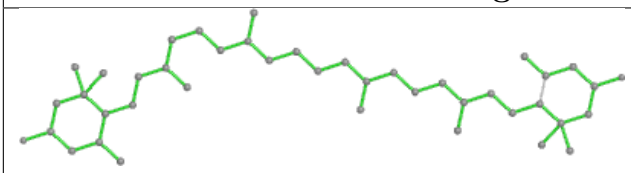
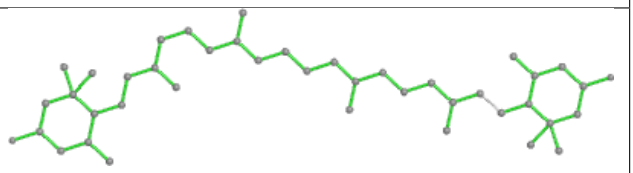
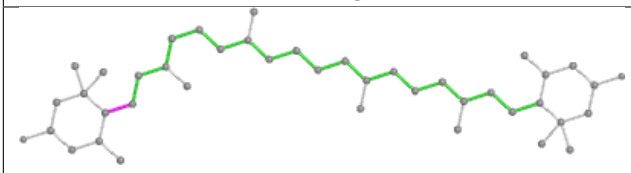
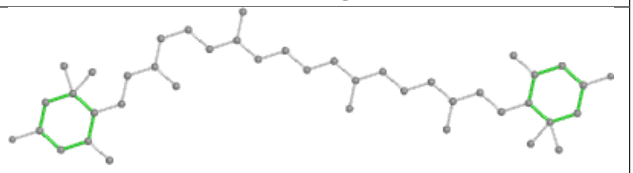
Bond angles



Torsions



Rings

Ligand A1LXP A 1002	
 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.

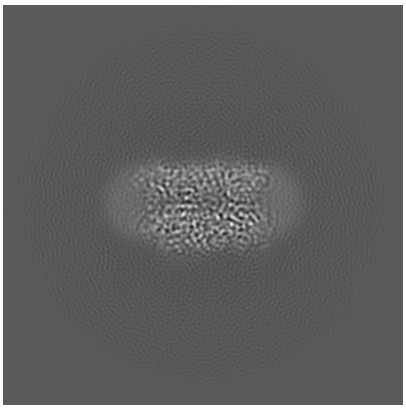
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38825. These allow visual inspection of the internal detail of the map and identification of artifacts.

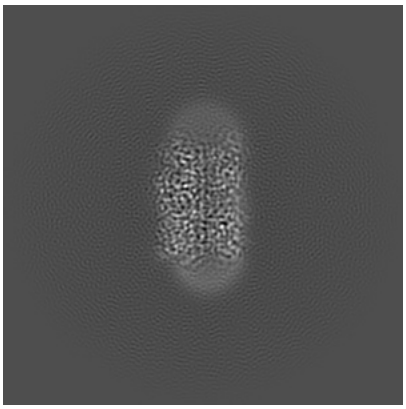
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

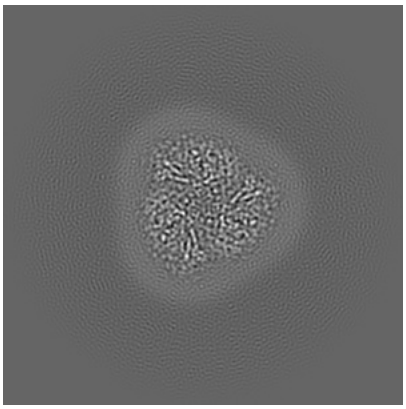
6.1.1 Primary map



X

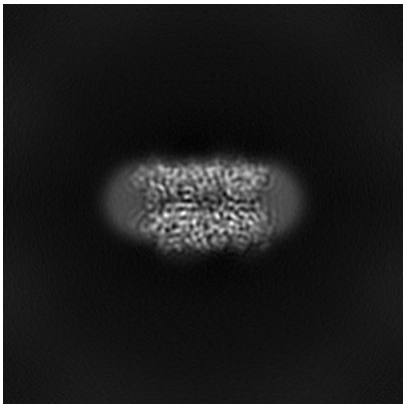


Y

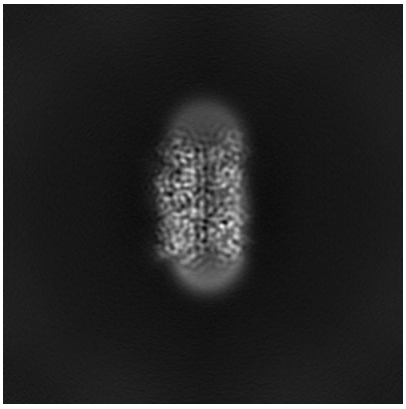


Z

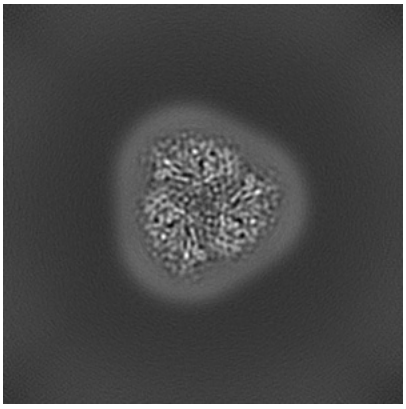
6.1.2 Raw map



X



Y

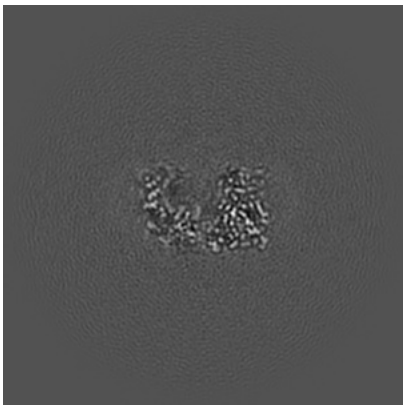


Z

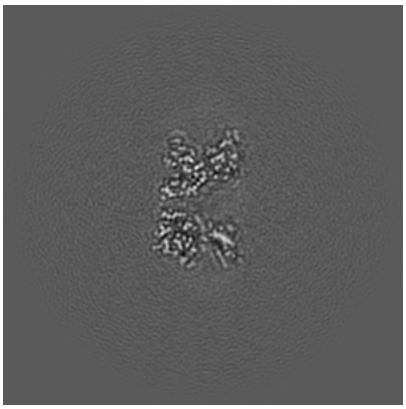
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

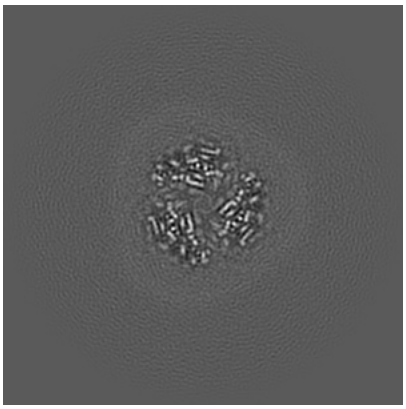
6.2.1 Primary map



X Index: 128

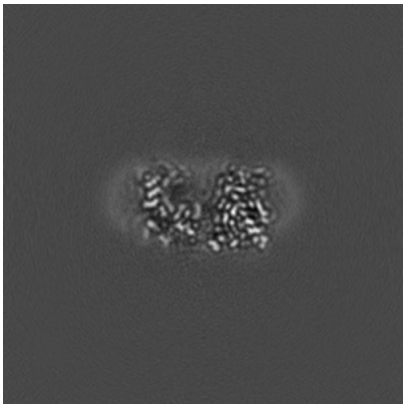


Y Index: 128

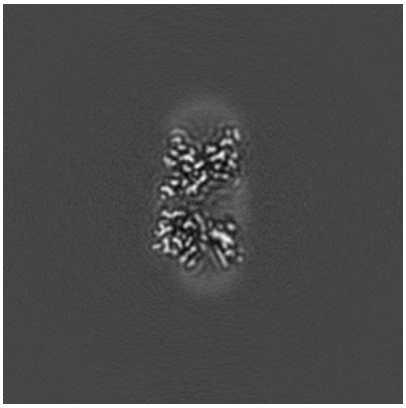


Z Index: 128

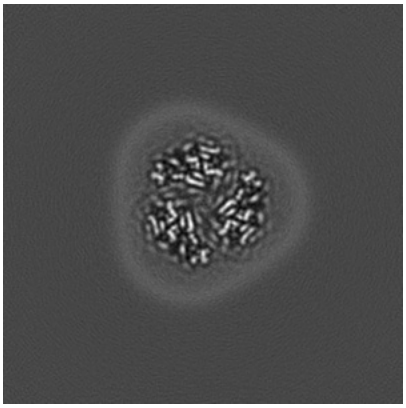
6.2.2 Raw map



X Index: 128



Y Index: 128

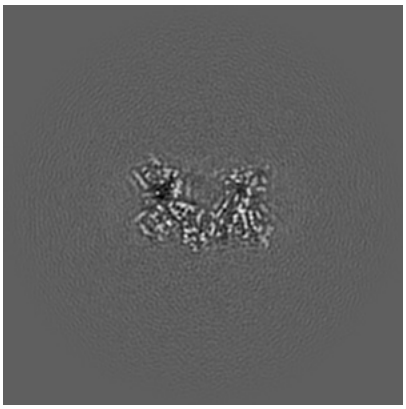


Z Index: 128

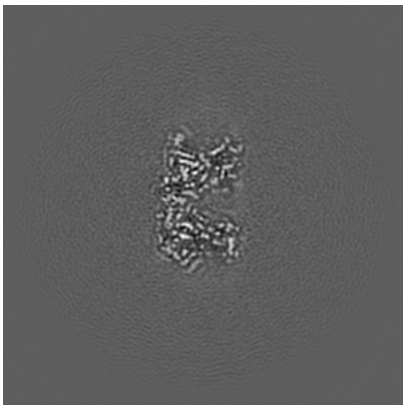
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

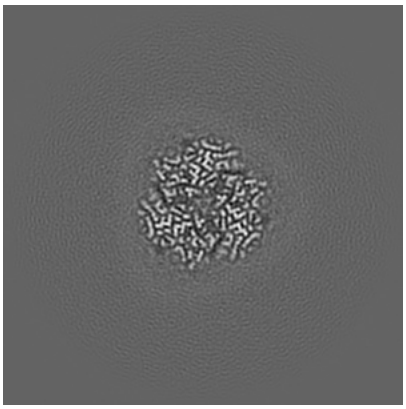
6.3.1 Primary map



X Index: 120

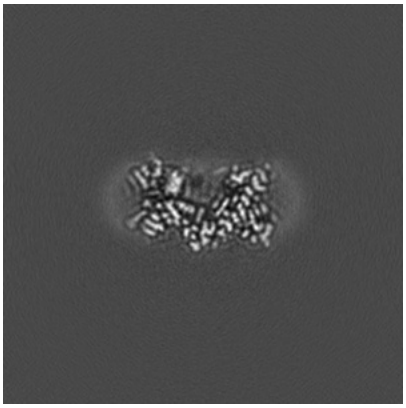


Y Index: 122

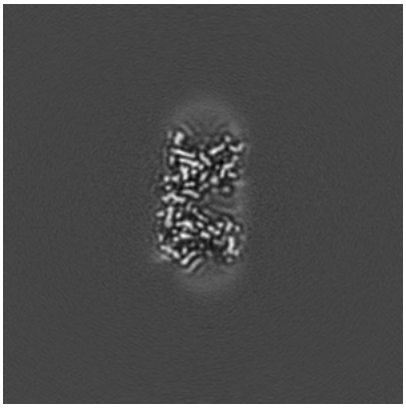


Z Index: 121

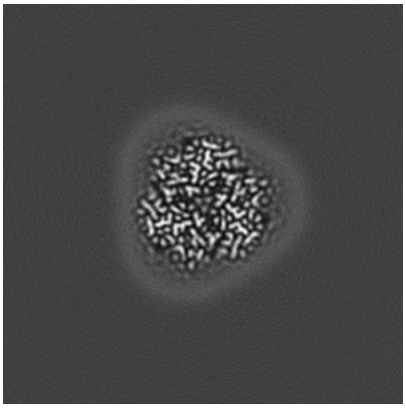
6.3.2 Raw map



X Index: 121



Y Index: 122

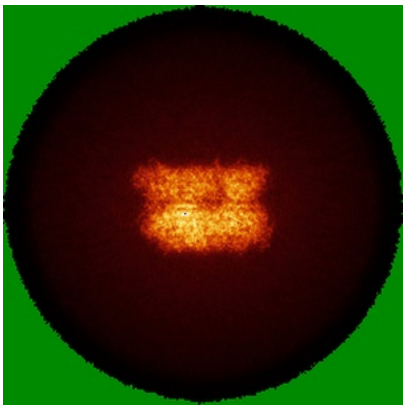


Z Index: 121

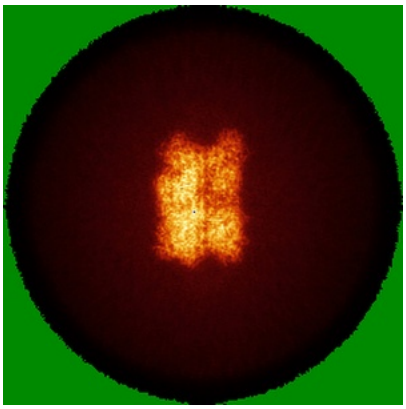
The images above show the largest variance slices of the map in three orthogonal directions.

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

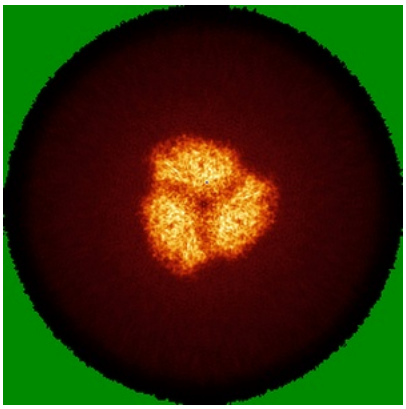
6.4.1 Primary map



X

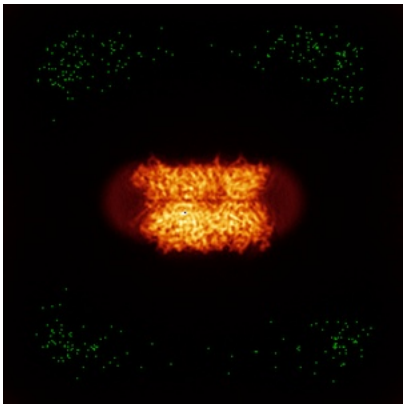


Y

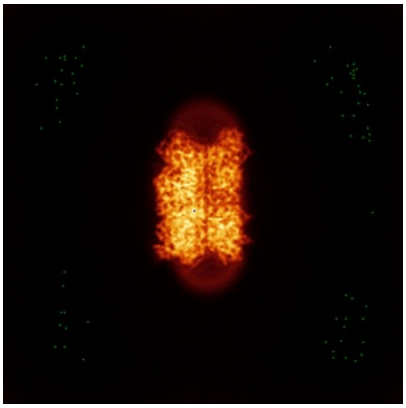


Z

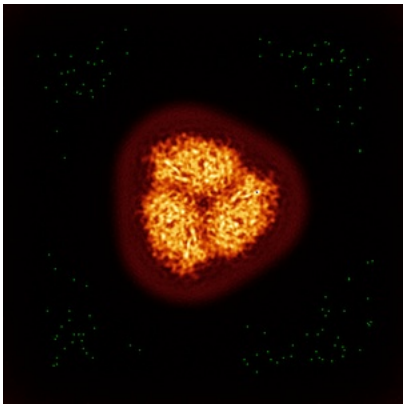
6.4.2 Raw map



X



Y

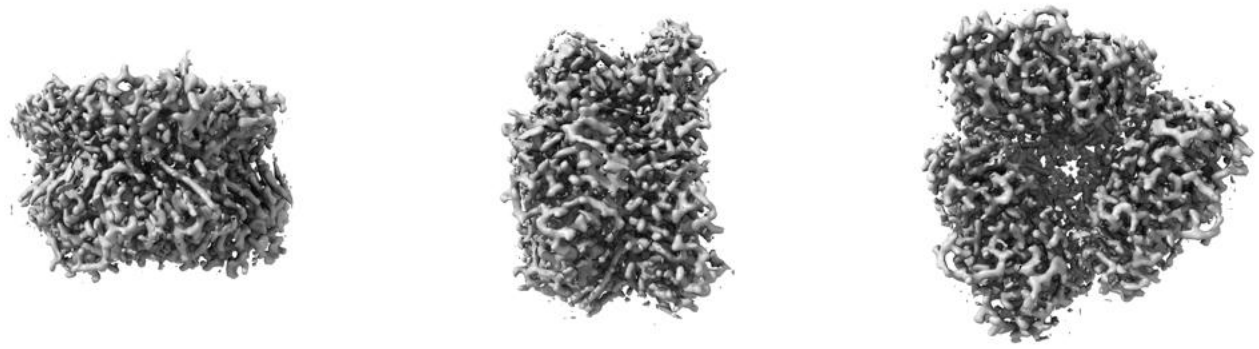


Z

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

6.5 Orthogonal surface views (i)

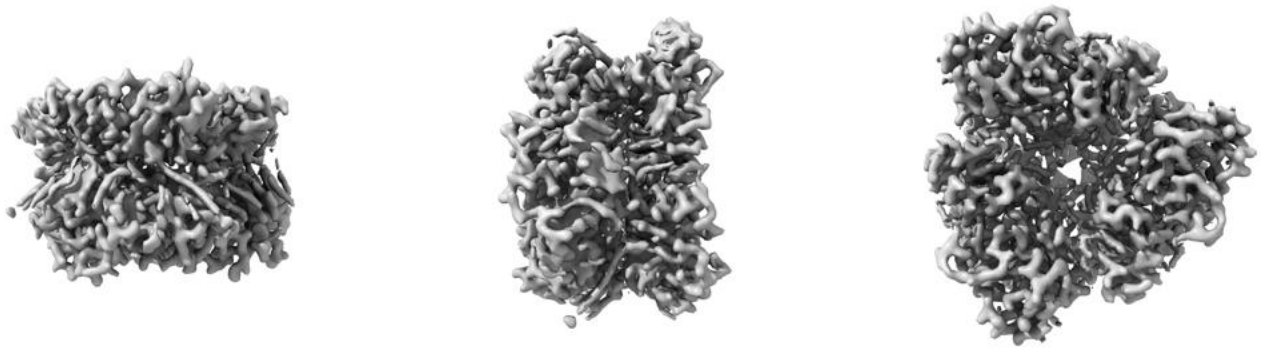
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

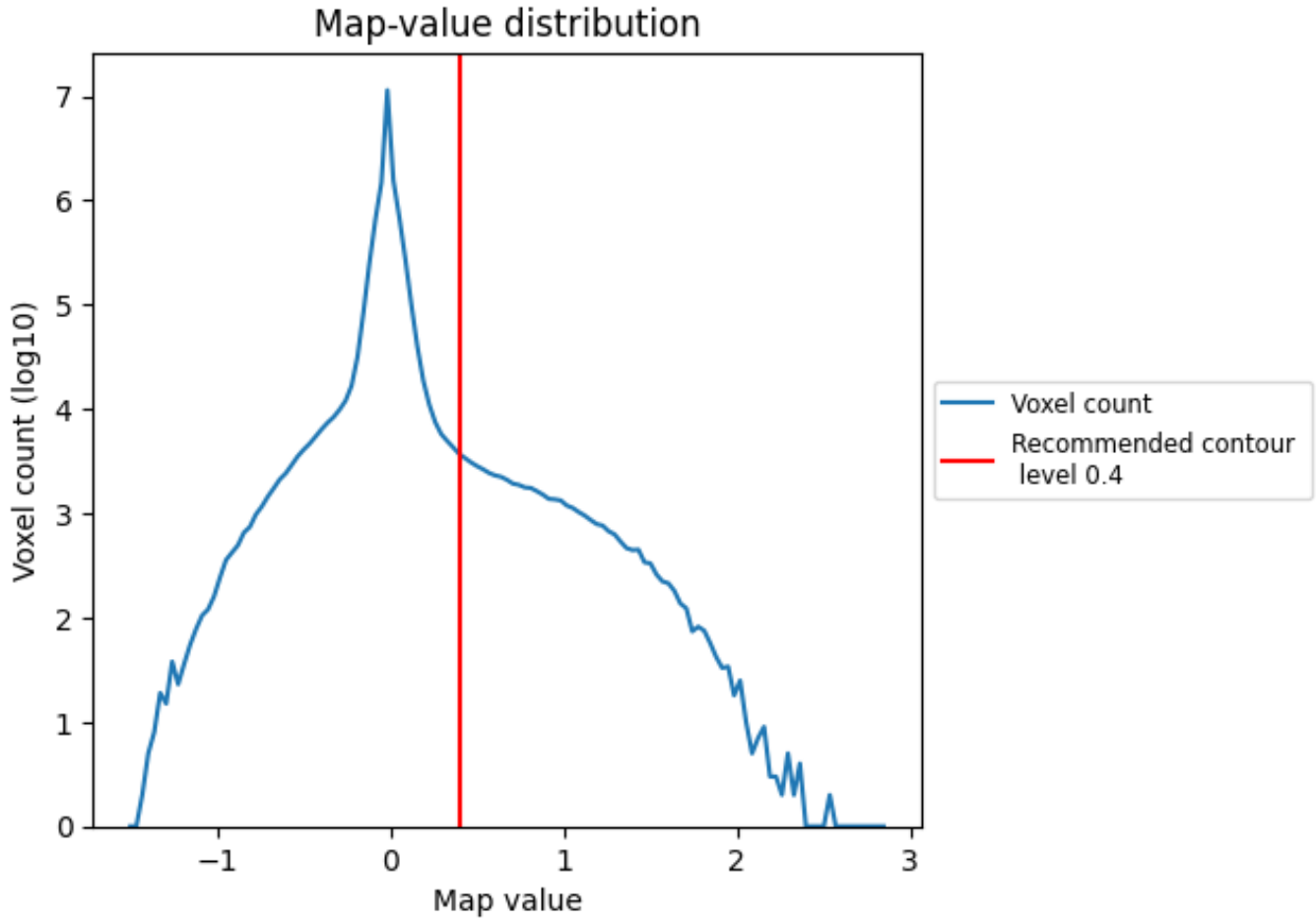
6.6 Mask visualisation (i)

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

7 Map analysis

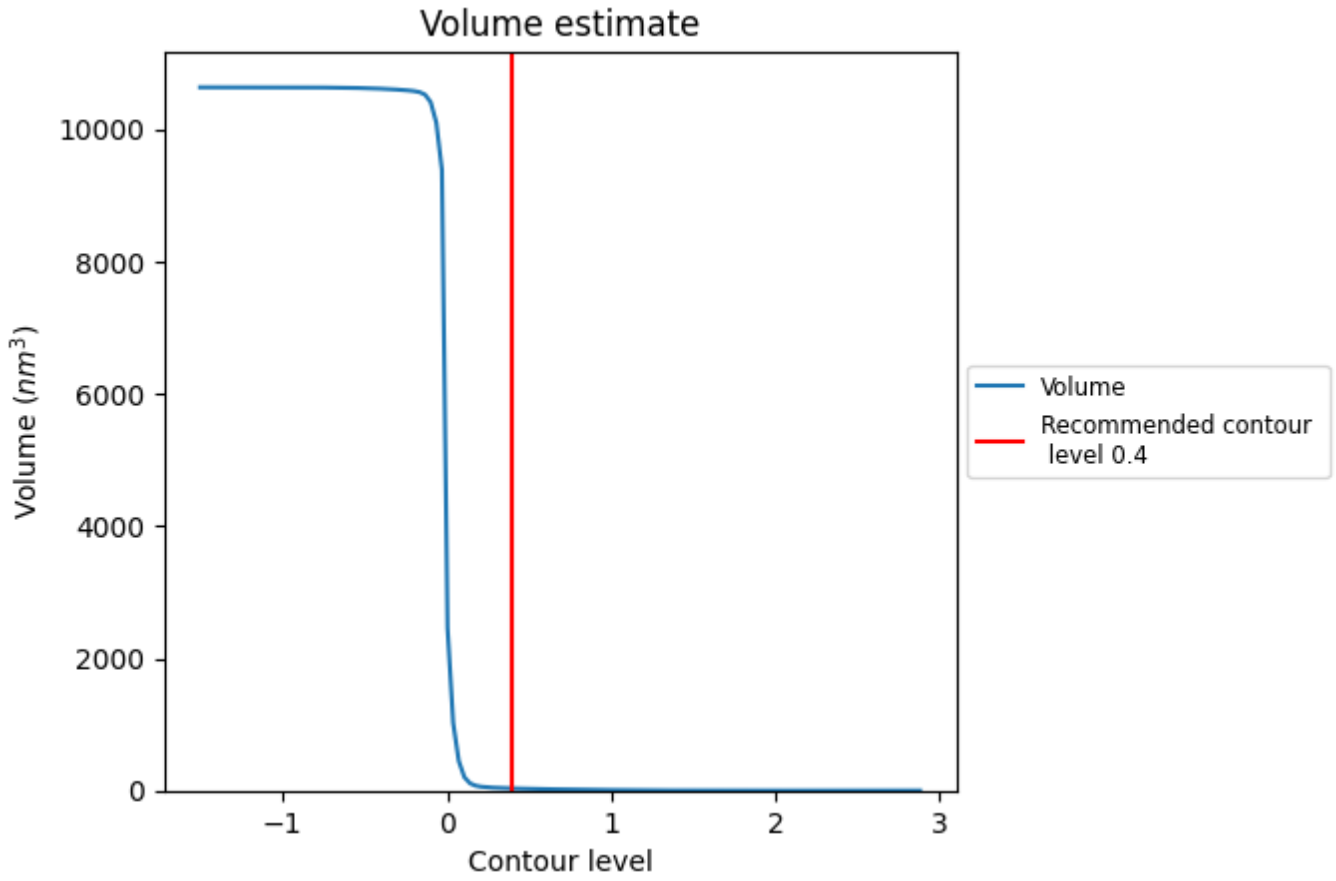
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

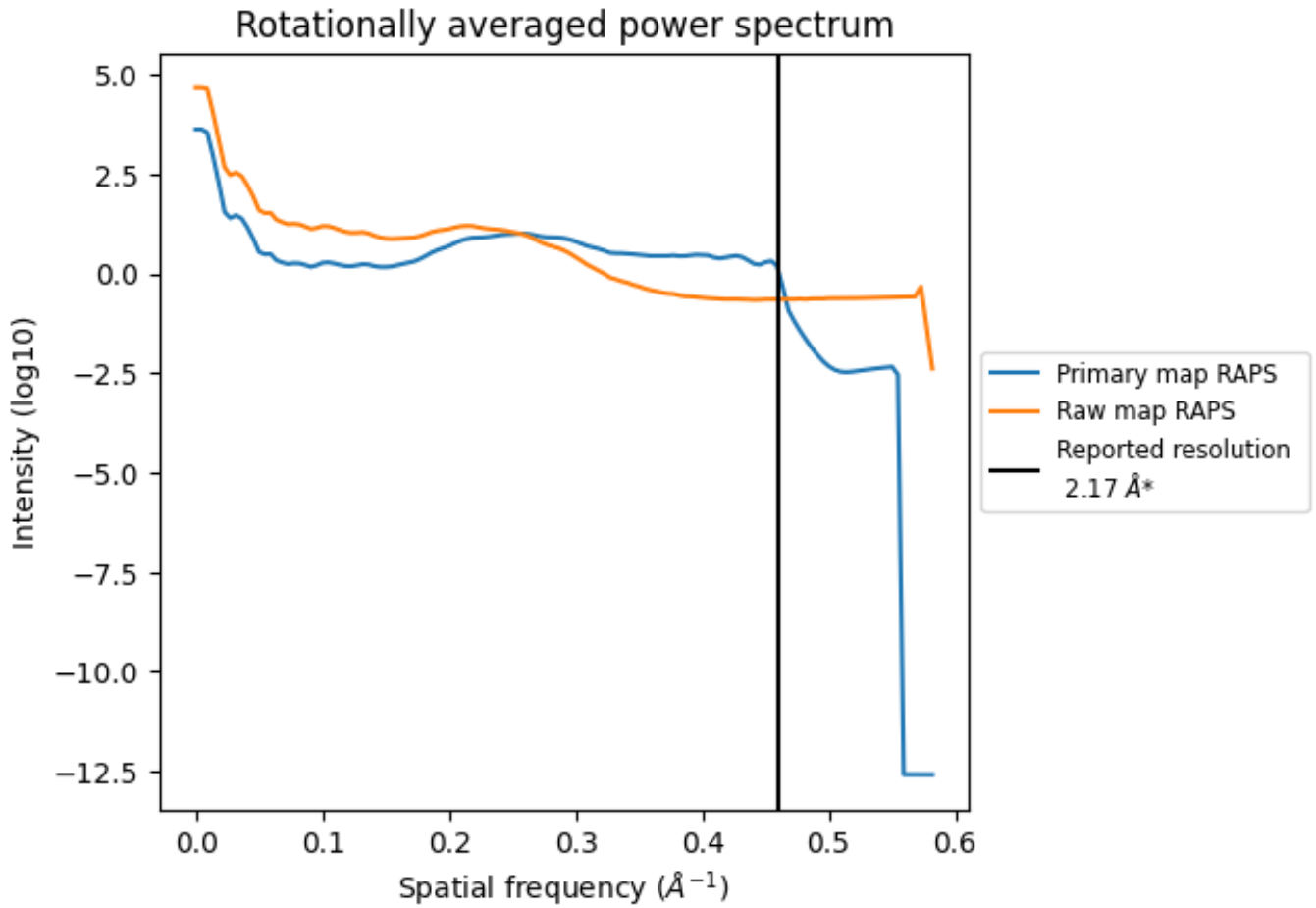
7.2 Volume estimate



The volume at the recommended contour level is 32 nm^3; this corresponds to an approximate mass of 29 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)

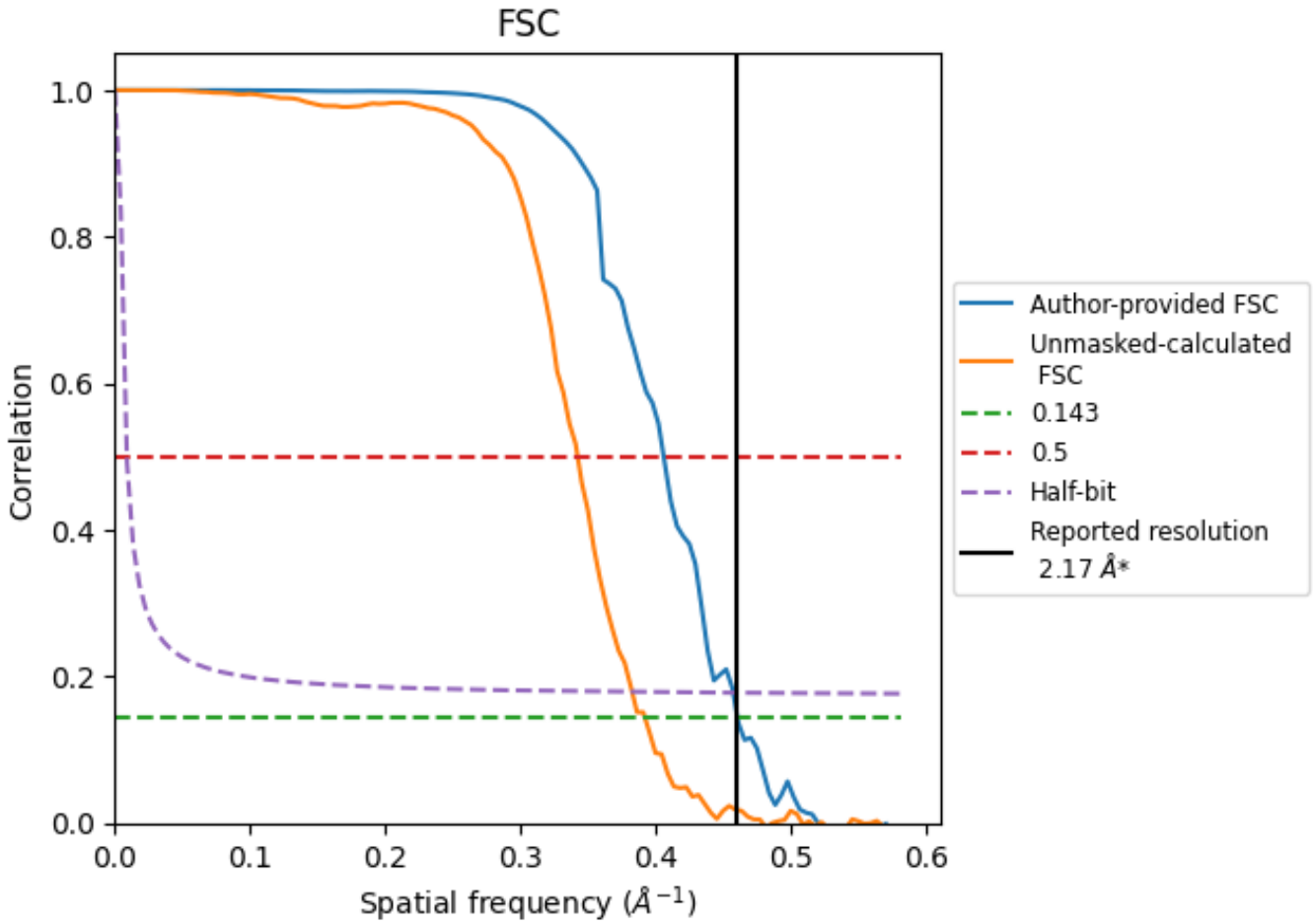


*Reported resolution corresponds to spatial frequency of 0.461 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.461 Å^{-1}

8.2 Resolution estimates (i)

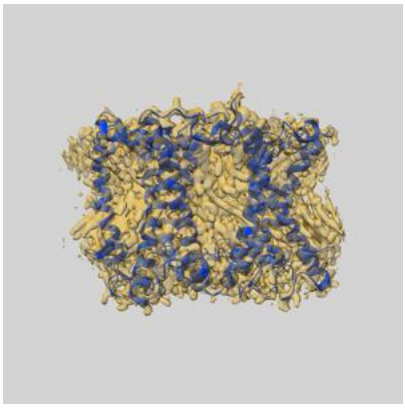
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.17	-	-
Author-provided FSC curve	2.17	2.46	2.19
Unmasked-calculated*	2.55	2.92	2.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.55 differs from the reported value 2.17 by more than 10 %

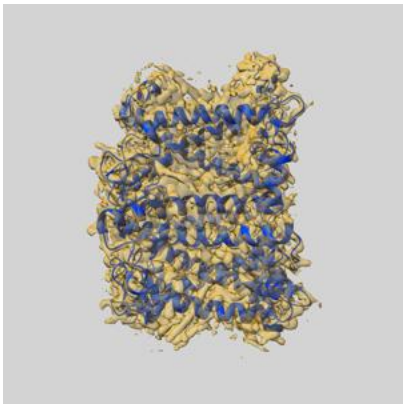
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38825 and PDB model 8Y15. Per-residue inclusion information can be found in section 3 on page 11.

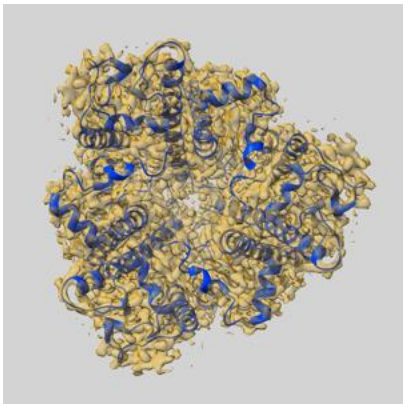
9.1 Map-model overlay



X



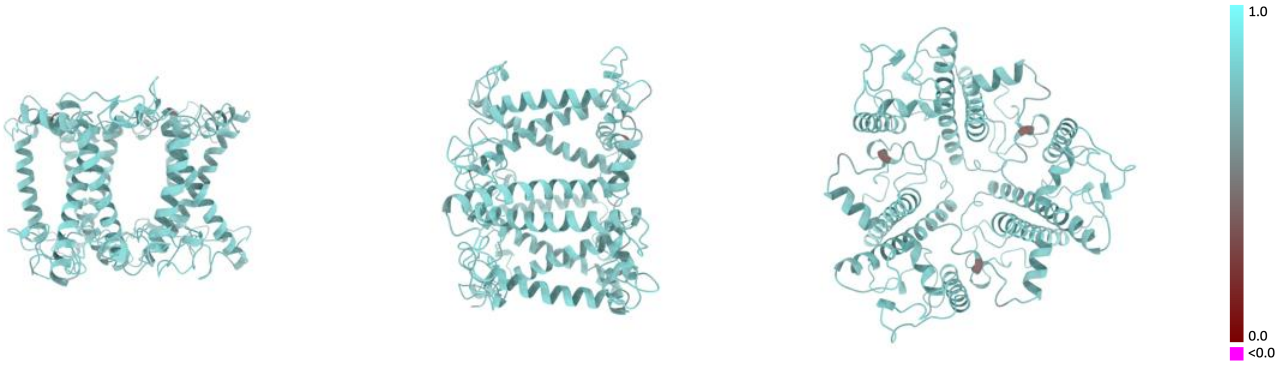
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

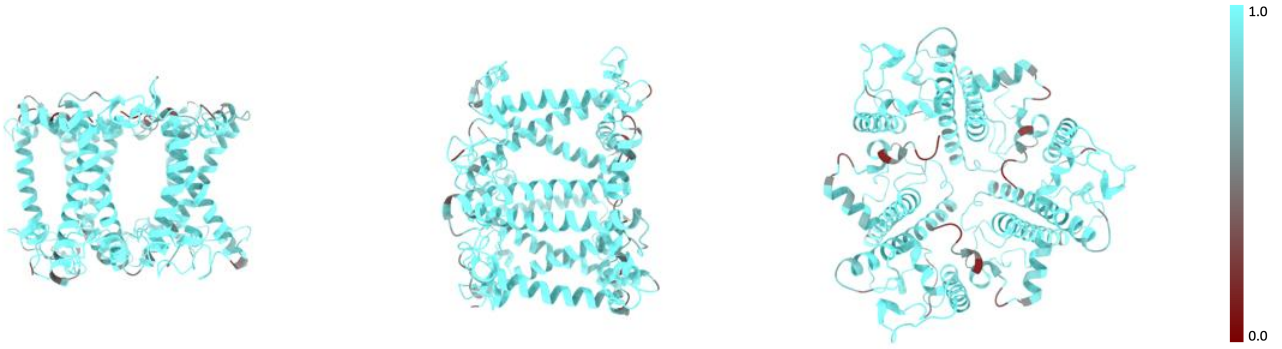
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

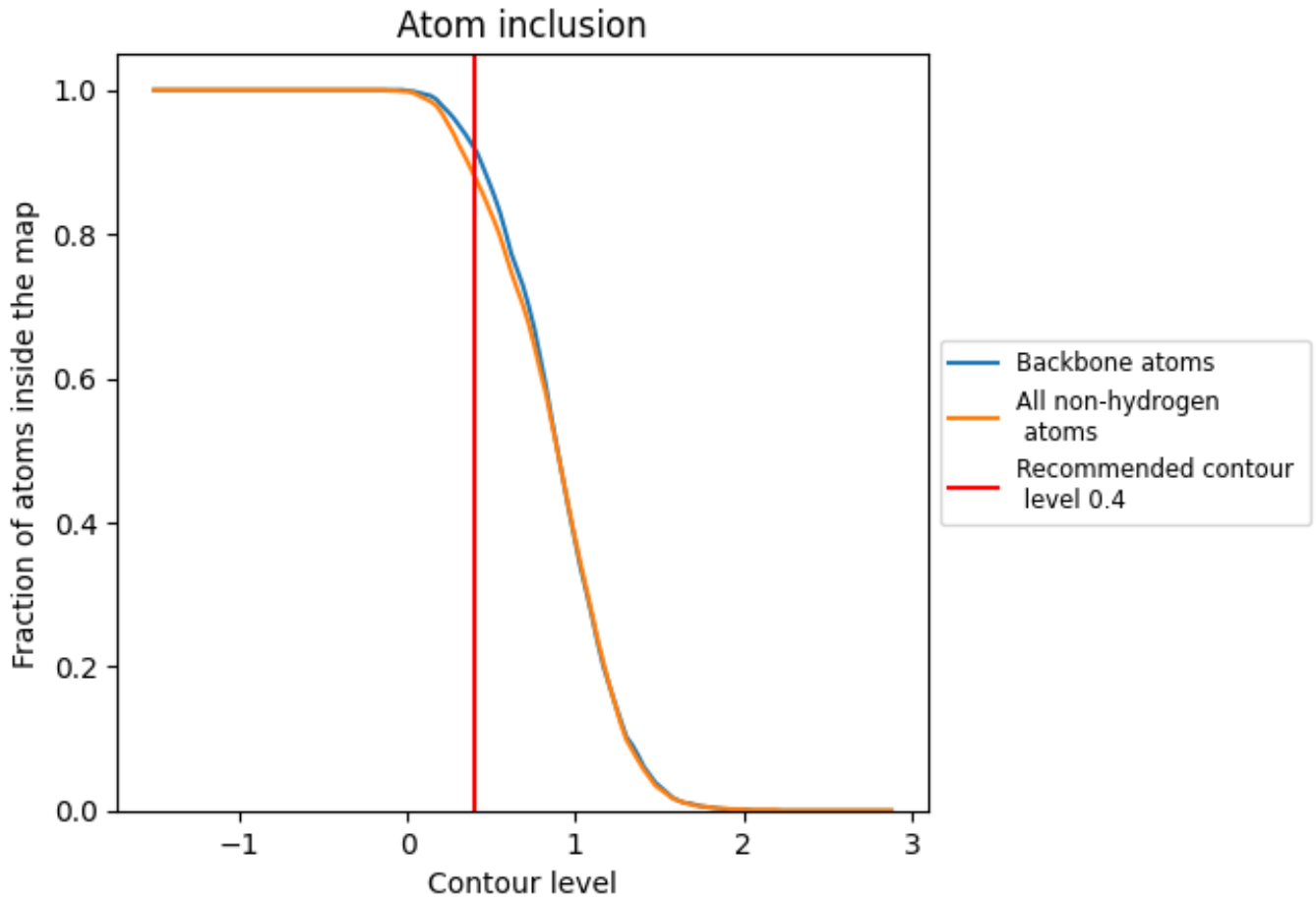
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 88% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8810	0.7090
A	0.8800	0.7090
B	0.8780	0.7090
C	0.8780	0.7090