wwPDB EM Validation Summary Report (i)

Aug 26, 2026 – 01:58 pm BST

PDB ID	:	7R0W / pdb_00007r0w
EMDB ID	:	EMD-14224
Title	:	2.8 Angstrom cryo-EM structure of the dimeric cytochrome b6f-PetP complex from Synechocystis sp. PCC 6803 with natively bound lipids and plastoquinone molecules
Authors	:	Farmer, D.F.; Proctor, M.S.; Malone, L.A.; Swainsbury, D.P.K.; Hawkings, F.R.; Hitchcock, A.; Johnson, M.P.
Deposited on	:	2022-02-02
Resolution	:	2.80 Å(reported)
Based on initial model	:	7PPW

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:

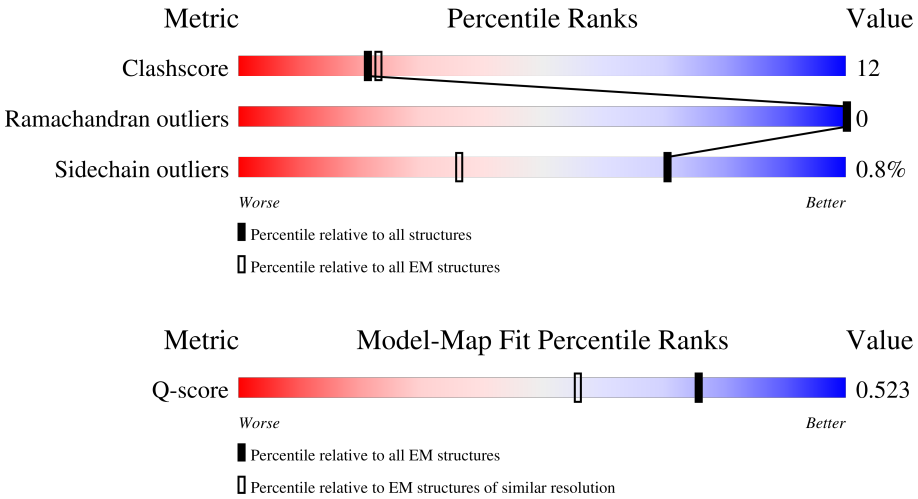
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

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 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	V	65	6%, 52%, 46%
1	X	65	49%, 49%
2	A	222	82%, 18%

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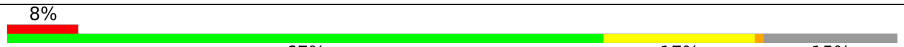
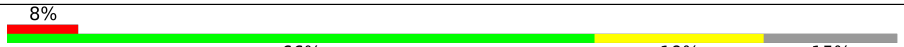
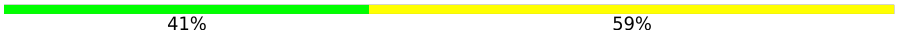
Mol	Chain	Length	Quality of chain
2	I	222	
3	B	160	
3	J	160	
4	C	328	
4	K	328	
5	E	32	
5	M	32	
6	F	36	
6	N	36	
7	G	38	
7	O	38	
8	H	29	
8	P	29	
9	D	192	
9	L	192	

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
14	CLA	B	302	X	-	-	-
14	CLA	J	202	X	-	-	-
15	HEC	C	302	X	-	-	-
15	HEC	K	301	X	-	-	-
16	LMG	N	101	X	-	-	-
17	6PL	H	101	X	-	-	-
17	6PL	P	101	X	-	-	-
19	FES	D	201	-	-	X	-
19	FES	L	202	-	-	X	-

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 16830 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 Uncharacterized protein Cp097, conserved in cyanobacteria.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	64	Total	C	N	O	S	0	0
			500	320	85	94	1		
1	V	64	Total	C	N	O	S	0	0
			500	320	85	94	1		

- Molecule 2 is a protein called Cytochrome b6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	222	Total	C	N	O	S	0	0
			1769	1175	283	299	12		
2	A	222	Total	C	N	O	S	0	0
			1769	1175	283	299	12		

- Molecule 3 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	159	Total	C	N	O	S	0	0
			1223	820	190	206	7		
3	B	159	Total	C	N	O	S	0	0
			1223	820	190	206	7		

- Molecule 4 is a protein called Cytochrome f.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	279	Total	C	N	O	S	0	0
			2115	1356	352	402	5		
4	C	279	Total	C	N	O	S	0	0
			2115	1356	352	402	5		

- Molecule 5 is a protein called Cytochrome B6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	32	Total	C	N	O	S	0	0
			238	165	36	36	1		
5	E	32	Total	C	N	O	S	0	0
			238	165	36	36	1		

- Molecule 6 is a protein called Cytochrome b6-f complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	34	Total	C	N	O	S	0	0
			248	165	38	42	3		
6	F	34	Total	C	N	O	S	0	0
			248	165	38	42	3		

- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	32	Total	C	N	O	S	0	0
			242	166	37	38	1		
7	G	32	Total	C	N	O	S	0	0
			242	166	37	38	1		

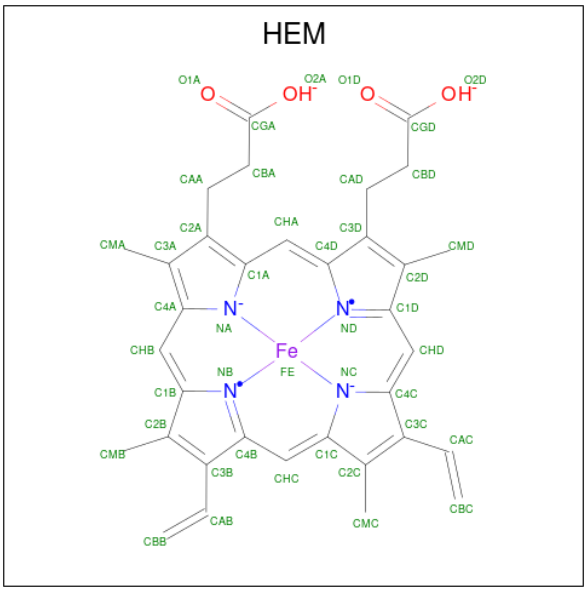
- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	29	Total	C	N	O	S	0	0
			234	159	36	37	2		
8	H	29	Total	C	N	O	S	0	0
			234	159	36	37	2		

- Molecule 9 is a protein called Rieske domain, PetC.

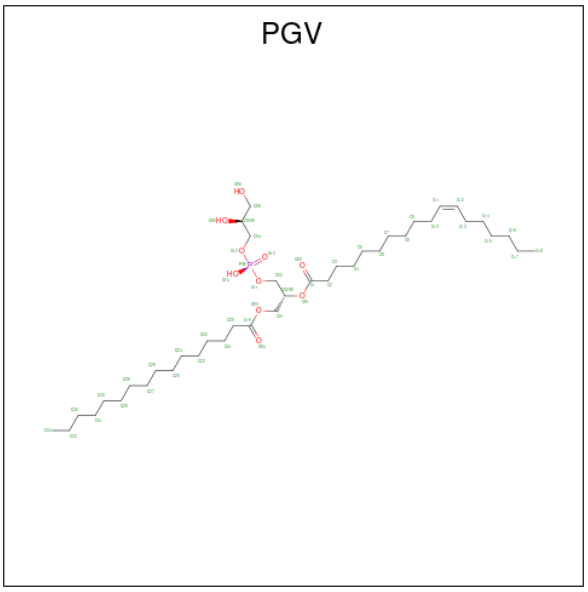
Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	169	Total	C	N	O	S	0	0
			1256	795	215	240	6		
9	L	169	Total	C	N	O	S	0	0
			1256	795	215	240	6		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



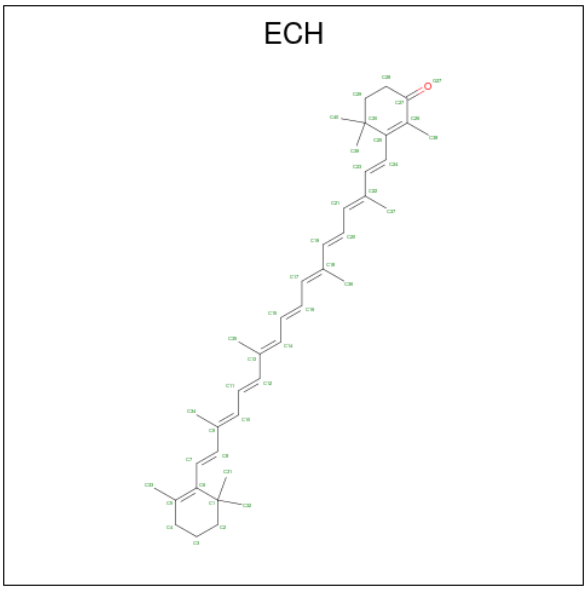
Mol	Chain	Residues	Atoms					AltConf
10	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 11 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



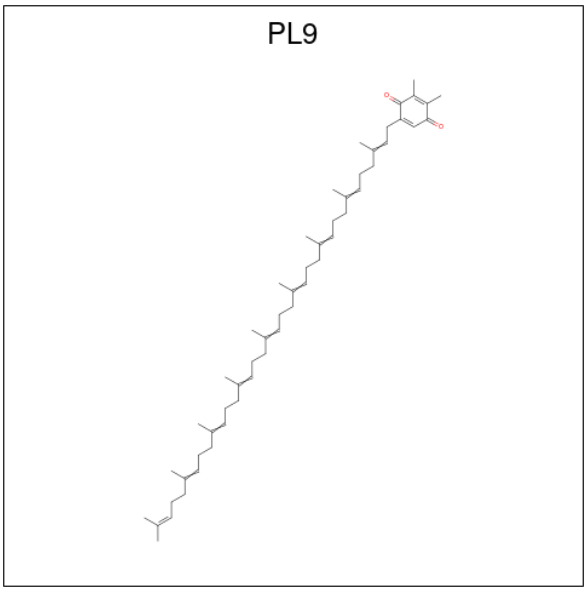
Mol	Chain	Residues	Atoms				AltConf
11	I	1	Total	C	O	P	0
			39	28	10	1	
11	J	1	Total	C	O	P	0
			41	30	10	1	
11	B	1	Total	C	O	P	0
			51	40	10	1	
11	C	1	Total	C	O	P	0
			47	36	10	1	

- Molecule 12 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: $C_{40}H_{54}O$).



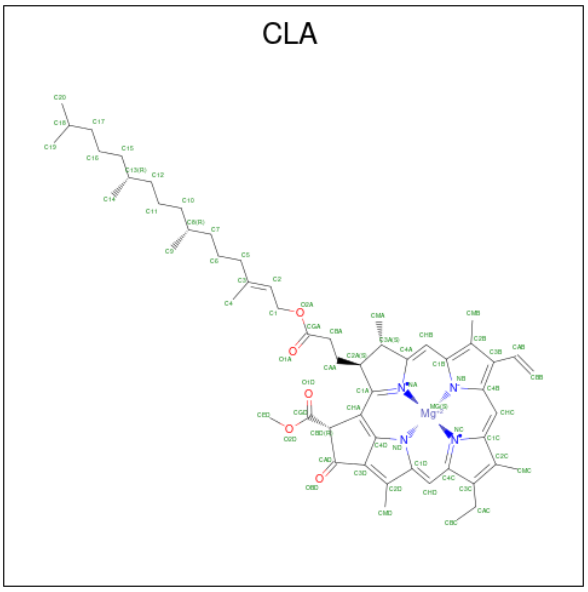
Mol	Chain	Residues	Atoms			AltConf
12	I	1	Total 41	C 40	O 1	0
12	A	1	Total 41	C 40	O 1	0

- Molecule 13 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



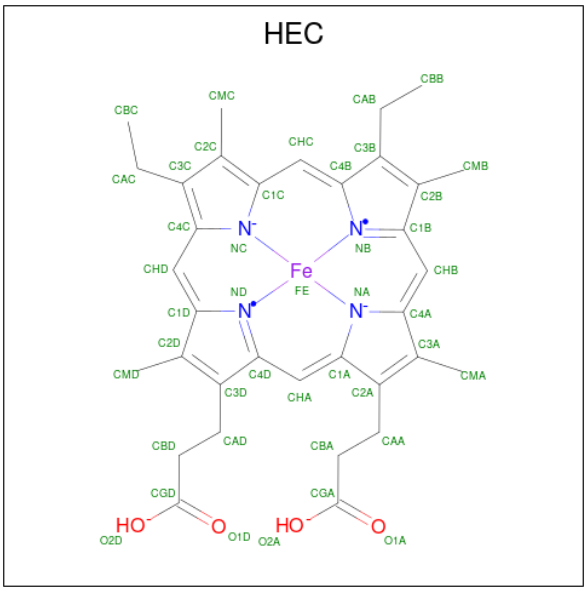
Mol	Chain	Residues	Atoms			AltConf
13	J	1	Total 55	C 53	O 2	0
13	A	1	Total 55	C 53	O 2	0

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 15 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
15	K	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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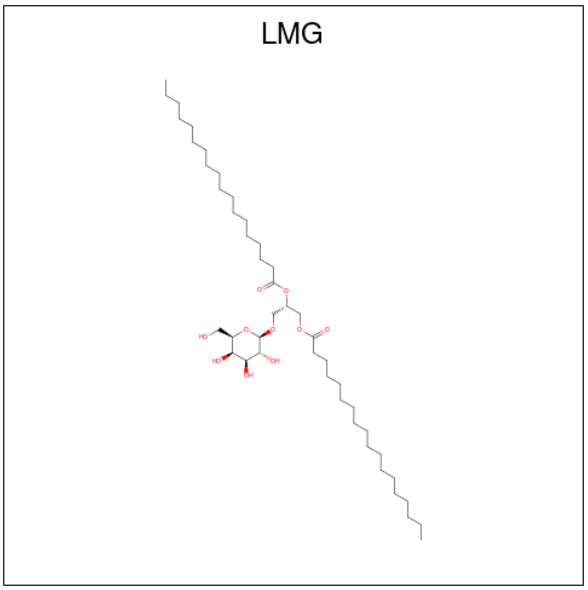
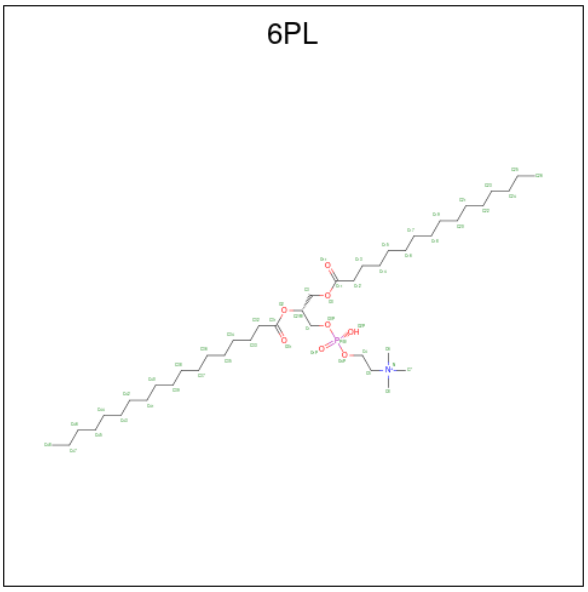
Mol	Chain	Residues	Atoms					AltConf
15	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



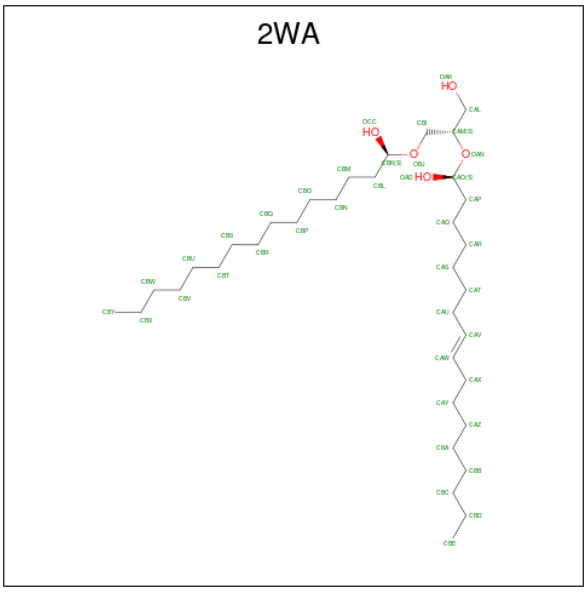
Mol	Chain	Residues	Atoms			AltConf
16	N	1	Total	C	O	0
			55	45	10	

- Molecule 17 is (4S,7R)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: 6PL) (formula: $C_{42}H_{85}NO_8P$).



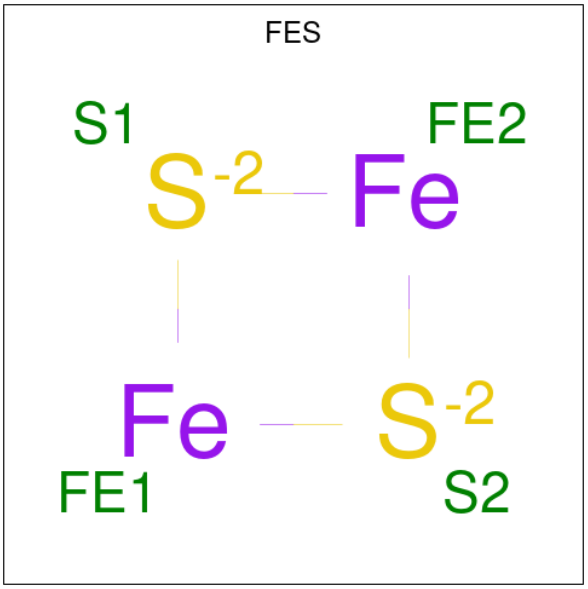
Mol	Chain	Residues	Atoms					AltConf
17	P	1	Total	C	N	O	P	0
			51	41	1	8	1	
17	H	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 18 is (1S,8E)-1-{[(2S)-1-hydroxy-3-{[(1S)-1-hydroxypentadecyl]oxy}propan-2-yl]oxy}heptadec-8-en-1-ol (CCD ID: 2WA) (formula: $C_{35}H_{70}O_5$).



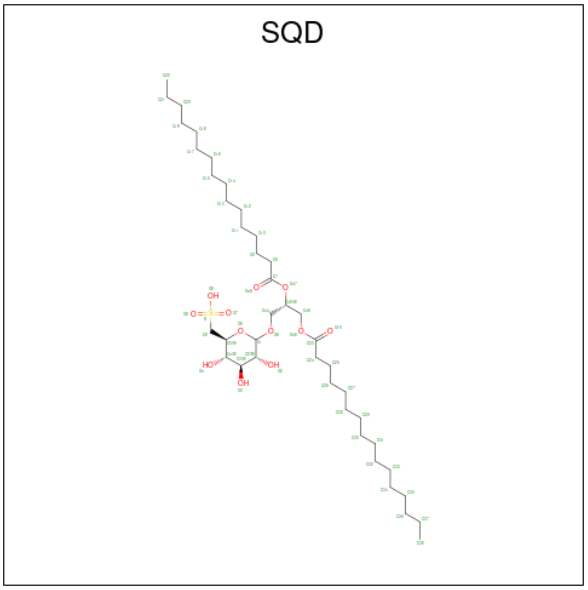
Mol	Chain	Residues	Atoms			AltConf
18	B	1	Total	C	O	0
			40	35	5	

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



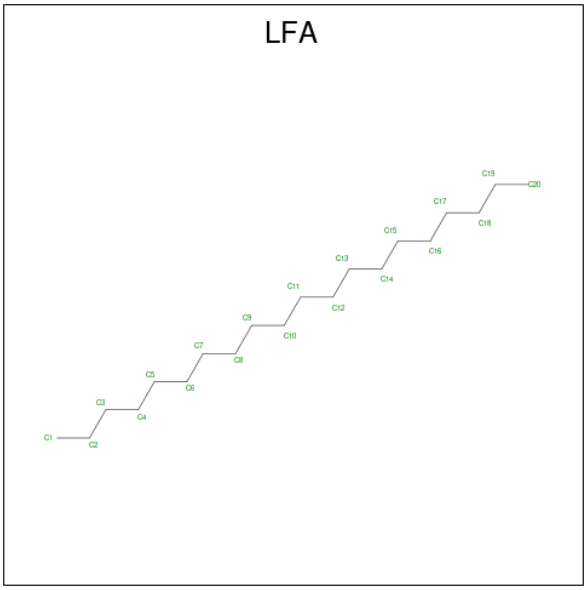
Mol	Chain	Residues	Atoms			AltConf
19	D	1	Total	Fe	S	0
			4	2	2	
19	L	1	Total	Fe	S	0
			4	2	2	

- Molecule 20 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
20	D	1	Total	C	O	S	0
			54	41	12	1	
20	L	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 21 is EICOSANE (CCD ID: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms		AltConf
21	E	1	Total	C	0
			20	20	

- Molecule 22 is water.

Mol	Chain	Residues	Atoms		AltConf
22	I	1	Total	O	0
			1	1	
22	B	1	Total	O	0
			1	1	

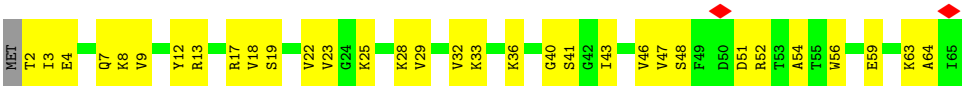
3 Residue-property plots (i)

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

• Molecule 1: Uncharacterized protein Cp097, conserved in cyanobacteria

Chain X:

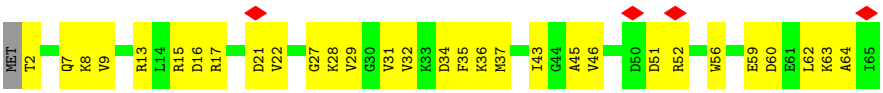




• Molecule 1: Uncharacterized protein Cp097, conserved in cyanobacteria

Chain V:





• Molecule 2: Cytochrome b6

Chain I:

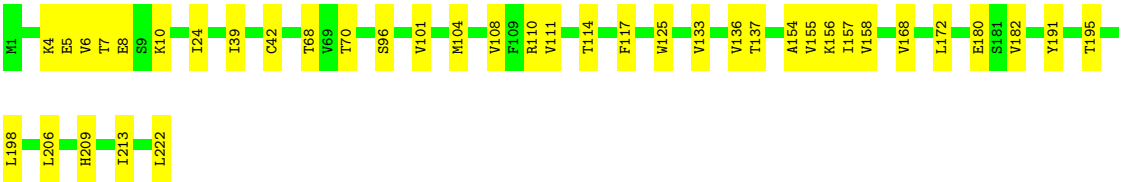




• Molecule 2: Cytochrome b6

Chain A:

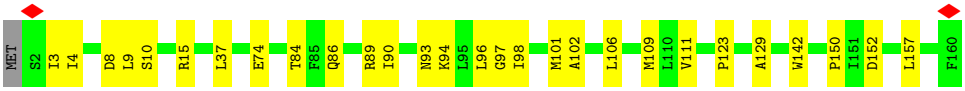




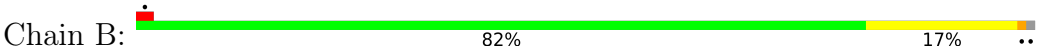
• Molecule 3: Cytochrome b6-f complex subunit 4

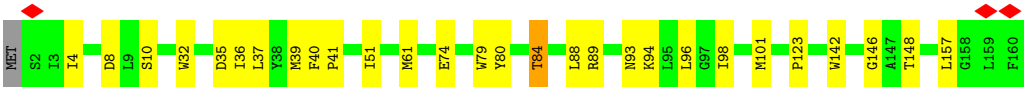
Chain J:





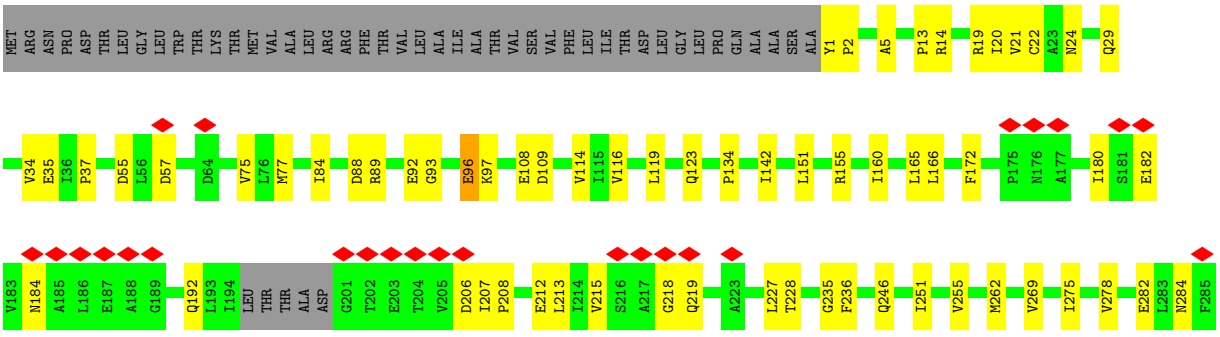
• Molecule 3: Cytochrome b6-f complex subunit 4





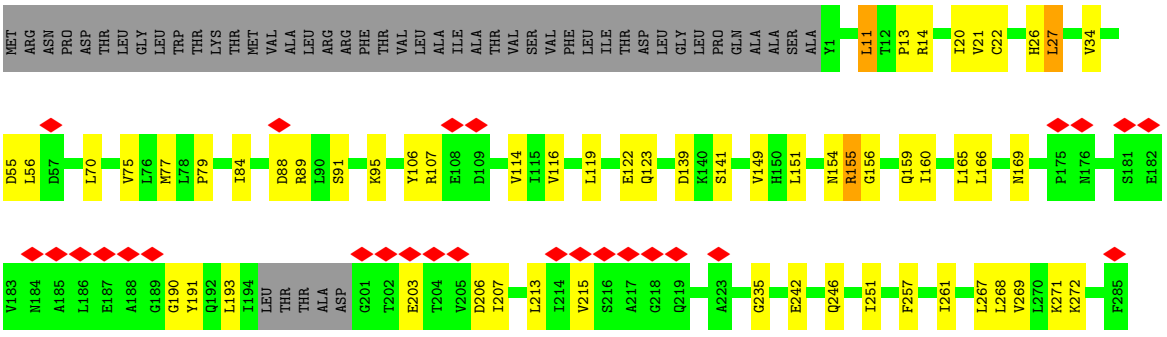
• Molecule 4: Cytochrome f





• Molecule 4: Cytochrome f



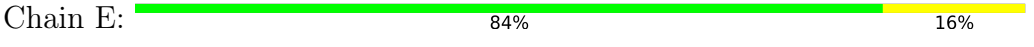


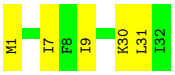
• Molecule 5: Cytochrome B6





• Molecule 5: Cytochrome B6

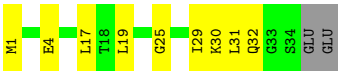




• Molecule 6: Cytochrome b6-f complex subunit 7

Chain N:





• Molecule 6: Cytochrome b6-f complex subunit 7

Chain F:

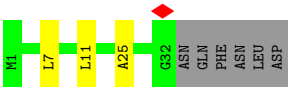




• Molecule 7: Cytochrome b6-f complex subunit 5

Chain O:





• Molecule 7: Cytochrome b6-f complex subunit 5

Chain G:

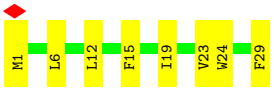




• Molecule 8: Cytochrome b6-f complex subunit 8

Chain P:

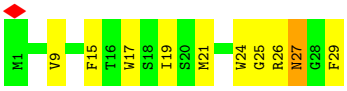




• Molecule 8: Cytochrome b6-f complex subunit 8

Chain H:





• Molecule 9: Rieske domain, PetC

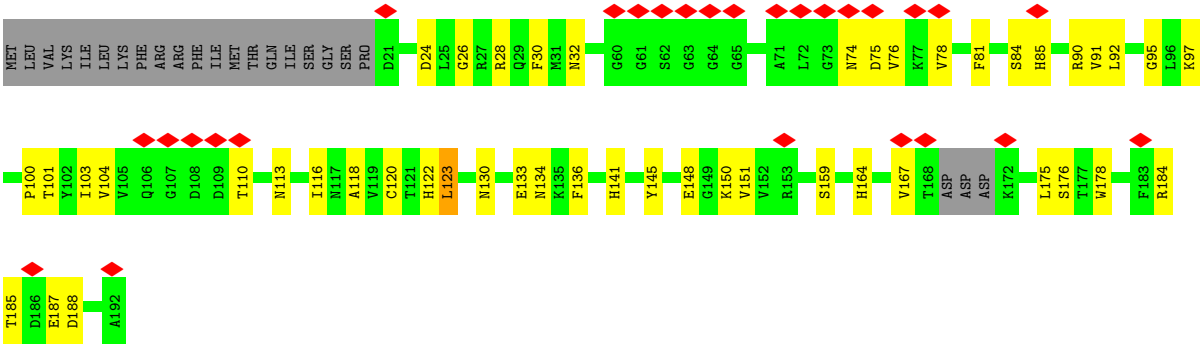
Chain D:





• Molecule 9: Rieske domain, PetC





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	152860	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.986	Depositor
Minimum map value	-0.270	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.132	Depositor
Map size (Å)	211.99998, 211.99998, 211.99998	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SQD, LFA, PGV, FES, CLA, PL9, 2WA, HEC, 6PL, HEM, LMG, ECH

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	V	0.22	0/507	0.54	0/679
1	X	0.27	0/507	0.62	0/679
2	A	0.20	0/1821	0.43	0/2480
2	I	0.22	0/1821	0.43	0/2480
3	B	0.18	0/1261	0.40	0/1721
3	J	0.18	0/1261	0.44	0/1721
4	C	0.14	0/2158	0.38	0/2935
4	K	0.15	0/2158	0.39	0/2935
5	E	0.26	0/242	0.48	0/326
5	M	0.27	0/242	0.56	0/326
6	F	0.27	0/251	0.50	0/337
6	N	0.35	0/251	0.67	0/337
7	G	0.23	0/246	0.44	0/334
7	O	0.21	0/246	0.44	0/334
8	H	0.23	0/241	0.42	0/329
8	P	0.27	0/241	0.46	0/329
9	D	0.18	0/1286	0.45	1/1757 (0.1%)
9	L	0.16	0/1286	0.42	0/1757
All	All	0.19	0/16026	0.44	1/21796 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	97	LYS	CA-CB-CG	5.62	125.34	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	V	500	0	513	30	0
1	X	500	0	513	28	0
2	A	1769	0	1799	35	0
2	I	1769	0	1799	27	0
3	B	1223	0	1268	22	0
3	J	1223	0	1268	24	0
4	C	2115	0	2133	40	0
4	K	2115	0	2133	50	0
5	E	238	0	264	6	0
5	M	238	0	264	13	0
6	F	248	0	268	6	0
6	N	248	0	268	9	0
7	G	242	0	274	9	0
7	O	242	0	274	2	0
8	H	234	0	240	7	0
8	P	234	0	240	9	0
9	D	1256	0	1220	49	0
9	L	1256	0	1219	41	0
10	A	86	0	60	7	0
10	B	43	0	30	2	0
10	I	129	0	90	12	0
11	B	51	0	76	0	0
11	C	47	0	65	0	0
11	I	39	0	47	0	0
11	J	41	0	50	2	0
12	A	41	0	54	5	0
12	I	41	0	54	2	0
13	A	55	0	80	0	0
13	J	55	0	80	4	0
14	B	65	0	71	4	0
14	J	65	0	71	2	0
15	C	43	0	32	5	0
15	K	43	0	31	5	0
16	N	55	0	85	0	0
17	H	52	0	83	1	0
17	P	51	0	78	1	0
18	B	40	0	70	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	D	4	0	0	2	0
19	L	4	0	0	2	0
20	D	54	0	78	4	0
20	L	54	0	78	2	0
21	E	20	0	42	0	0
22	B	1	0	0	0	0
22	I	1	0	0	0	0
All	All	16830	0	17362	402	0

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

The worst 5 of 402 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:42:CYS:SG	10:I:302:HEM:HAB	1.91	1.11
2:I:42:CYS:SG	10:I:302:HEM:CAB	2.40	1.09
2:I:42:CYS:HG	10:I:302:HEM:CAB	1.65	1.09
2:A:42:CYS:SG	10:B:301:HEM:HAB	2.02	1.00
1:V:52:ARG:O	1:V:52:ARG:NH1	2.05	0.90

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	V	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
1	X	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
2	A	220/222 (99%)	211 (96%)	9 (4%)	0	100	100
2	I	220/222 (99%)	213 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
3	J	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
4	C	275/328 (84%)	266 (97%)	9 (3%)	0	100	100
4	K	275/328 (84%)	258 (94%)	17 (6%)	0	100	100
5	E	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
5	M	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
6	F	32/36 (89%)	32 (100%)	0	0	100	100
6	N	32/36 (89%)	32 (100%)	0	0	100	100
7	G	30/38 (79%)	30 (100%)	0	0	100	100
7	O	30/38 (79%)	30 (100%)	0	0	100	100
8	H	27/29 (93%)	27 (100%)	0	0	100	100
8	P	27/29 (93%)	27 (100%)	0	0	100	100
9	D	165/192 (86%)	160 (97%)	5 (3%)	0	100	100
9	L	165/192 (86%)	159 (96%)	6 (4%)	0	100	100
All	All	1996/2204 (91%)	1932 (97%)	64 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	V	54/55 (98%)	53 (98%)	1 (2%)	50	81
1	X	54/55 (98%)	54 (100%)	0	100	100
2	A	192/192 (100%)	192 (100%)	0	100	100
2	I	192/192 (100%)	192 (100%)	0	100	100
3	B	127/128 (99%)	126 (99%)	1 (1%)	73	90
3	J	127/128 (99%)	127 (100%)	0	100	100
4	C	226/266 (85%)	223 (99%)	3 (1%)	61	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	K	226/266 (85%)	225 (100%)	1 (0%)	84 94
5	E	23/23 (100%)	23 (100%)	0	100 100
5	M	23/23 (100%)	22 (96%)	1 (4%)	26 60
6	F	25/27 (93%)	24 (96%)	1 (4%)	28 63
6	N	25/27 (93%)	25 (100%)	0	100 100
7	G	25/31 (81%)	25 (100%)	0	100 100
7	O	25/31 (81%)	25 (100%)	0	100 100
8	H	26/26 (100%)	24 (92%)	2 (8%)	12 36
8	P	26/26 (100%)	26 (100%)	0	100 100
9	D	132/154 (86%)	131 (99%)	1 (1%)	73 90
9	L	132/154 (86%)	129 (98%)	3 (2%)	44 78
All	All	1660/1804 (92%)	1646 (99%)	14 (1%)	70 90

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	30	LYS
8	H	27	ASN
1	V	2	THR
9	L	120	CYS
9	L	123	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
4	C	246	GLN
9	D	74	ASN
9	L	29	GLN
9	D	86	ASN
2	A	22	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

27 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	$\#\|Z\| > 2$
18	2WA	B	303	-	39,39,39	0.53	1 (2%)	39,41,41	0.86	3 (7%)
20	SQD	L	201	-	53,54,54	1.56	7 (13%)	62,65,65	1.81	10 (16%)
13	PL9	J	201	-	55,55,55	0.94	2 (3%)	68,69,69	1.48	11 (16%)
11	PGV	B	304	-	50,50,50	0.49	0	53,56,56	0.63	1 (1%)
12	ECH	A	304	-	42,42,42	0.33	0	55,58,58	0.71	0
14	CLA	B	302	-	69,73,73	1.28	7 (10%)	83,113,113	1.40	13 (15%)
17	6PL	H	101	-	51,51,51	0.49	0	57,59,59	1.23	5 (8%)
12	ECH	I	305	-	42,42,42	0.36	0	55,58,58	0.78	2 (3%)
10	HEM	I	302	22	50,50,50	1.39	6 (12%)	66,82,82	1.20	6 (9%)
17	6PL	P	101	-	50,50,51	0.49	0	56,58,59	1.21	4 (7%)
20	SQD	D	202	-	53,54,54	1.58	8 (15%)	62,65,65	1.27	5 (8%)
19	FES	L	202	9	0,4,4	-	-	-		
16	LMG	N	101	-	55,55,55	0.91	1 (1%)	63,63,63	1.58	10 (15%)
15	HEC	K	301	4	50,50,50	1.78	5 (10%)	68,82,82	1.90	16 (23%)
11	PGV	C	301	-	46,46,50	0.51	0	48,52,56	0.55	0
15	HEC	C	302	4	50,50,50	1.80	6 (12%)	68,82,82	1.75	12 (17%)
19	FES	D	201	9	0,4,4	-	-	-		
10	HEM	B	301	22	50,50,50	1.35	6 (12%)	66,82,82	1.21	5 (7%)
14	CLA	J	202	-	69,73,73	1.27	7 (10%)	83,113,113	1.48	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	HEM	A	302	2	50,50,50	1.32	6 (12%)	66,82,82	1.17	6 (9%)
11	PGV	J	203	-	40,40,50	0.56	0	42,46,56	0.80	2 (4%)
10	HEM	I	303	2	50,50,50	1.38	6 (12%)	66,82,82	1.15	5 (7%)
10	HEM	I	301	2	50,50,50	1.37	6 (12%)	66,82,82	1.16	4 (6%)
13	PL9	A	303	-	55,55,55	0.97	4 (7%)	68,69,69	1.47	7 (10%)
21	LFA	E	101	-	19,19,19	0.32	0	18,18,18	0.59	0
10	HEM	A	301	2	50,50,50	1.36	6 (12%)	66,82,82	1.12	5 (7%)
11	PGV	I	304	-	38,38,50	0.57	0	41,44,56	0.51	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
18	2WA	B	303	-	-	20/41/41/41	-
20	SQD	L	201	-	-	25/49/69/69	0/1/1/1
13	PL9	J	201	-	-	28/53/73/73	0/1/1/1
11	PGV	B	304	-	-	29/55/55/55	-
12	ECH	A	304	-	-	10/29/66/66	0/2/2/2
14	CLA	B	302	-	1/1/15/20	16/39/115/115	-
17	6PL	H	101	-	1/1/5/5	26/55/55/55	-
12	ECH	I	305	-	-	16/29/66/66	0/2/2/2
17	6PL	P	101	-	1/1/5/5	30/54/54/55	-
10	HEM	I	302	22	-	7/14/54/54	-
20	SQD	D	202	-	-	35/49/69/69	0/1/1/1
19	FES	L	202	9	-	-	0/1/1/1
16	LMG	N	101	-	1/1/8/8	19/50/70/70	0/1/1/1
15	HEC	K	301	4	1/1/3/7	7/14/54/54	-
11	PGV	C	301	-	-	30/51/51/55	-
15	HEC	C	302	4	1/1/3/7	7/14/54/54	-
19	FES	D	201	9	-	-	0/1/1/1
10	HEM	B	301	22	-	9/14/54/54	-
14	CLA	J	202	-	1/1/15/20	17/39/115/115	-
10	HEM	A	302	2	-	5/14/54/54	-
11	PGV	J	203	-	-	33/45/45/55	-
10	HEM	I	303	2	-	4/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	HEM	I	301	2	-	4/14/54/54	-
13	PL9	A	303	-	-	18/53/73/73	0/1/1/1
21	LFA	E	101	-	-	8/17/17/17	-
10	HEM	A	301	2	-	3/14/54/54	-
11	PGV	I	304	-	-	21/43/43/55	-

The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	302	HEC	C3D-C2D	7.82	1.53	1.36
15	K	301	HEC	C3D-C2D	7.64	1.53	1.36
15	C	302	HEC	FE-ND	4.80	2.09	1.94
20	L	201	SQD	O48-C23	4.69	1.47	1.33
20	D	202	SQD	O48-C23	4.68	1.47	1.33

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	L	201	SQD	O6-C1-C2	7.55	120.09	108.30
17	P	101	6PL	C1-C2-C3	6.74	127.74	111.79
15	K	301	HEC	CAB-C3B-C4B	6.62	133.40	124.81
16	N	101	LMG	O6-C5-C4	6.16	120.88	109.69
15	K	301	HEC	C1D-ND-C4D	5.89	111.16	105.07

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	J	202	CLA	C8
14	B	302	CLA	C8
15	K	301	HEC	NA
15	C	302	HEC	NA
16	N	101	LMG	C5

5 of 427 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	I	302	HEM	C2B-C3B-CAB-CBB
10	I	302	HEM	C2C-C3C-CAC-CBC
10	I	302	HEM	C4C-C3C-CAC-CBC
10	B	301	HEM	C2B-C3B-CAB-CBB
10	B	301	HEM	C2C-C3C-CAC-CBC

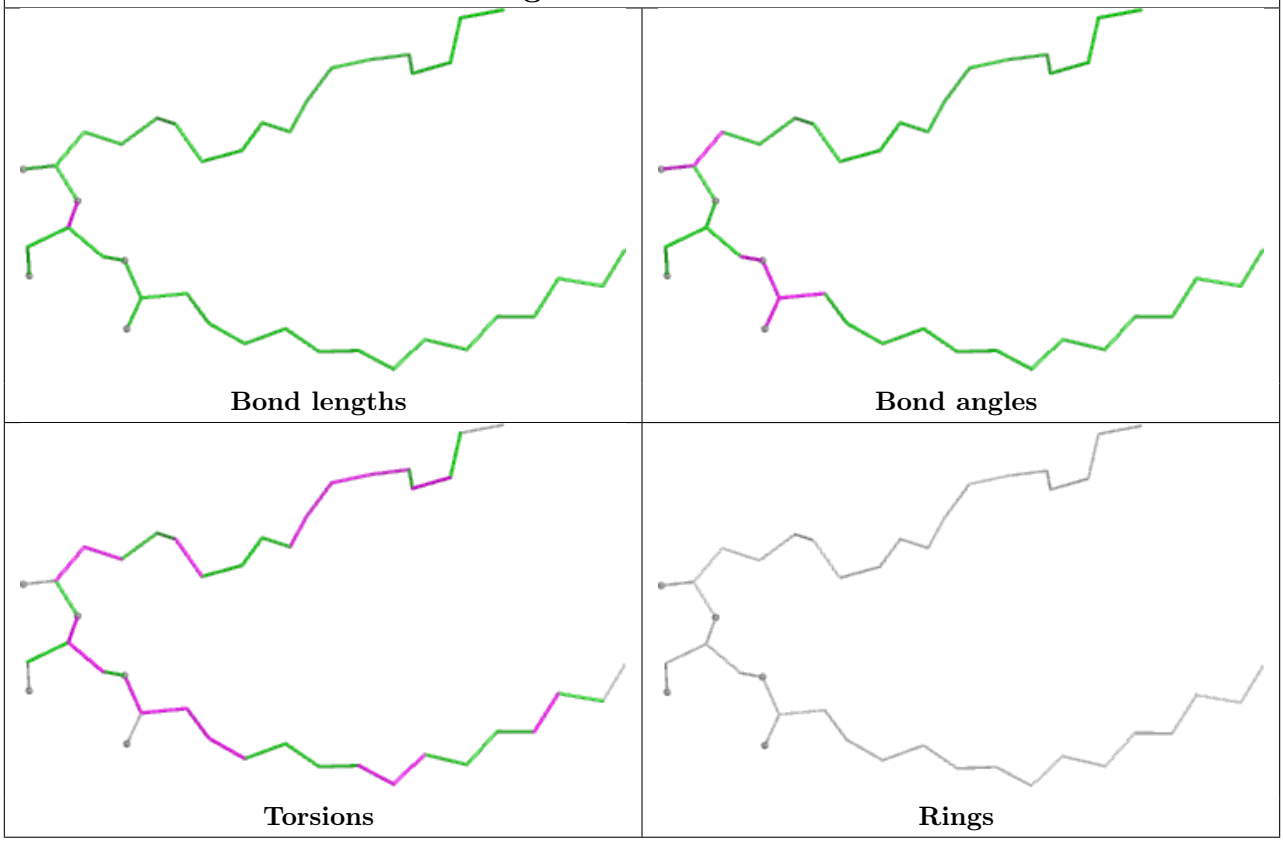
There are no ring outliers.

21 monomers are involved in 64 short contacts:

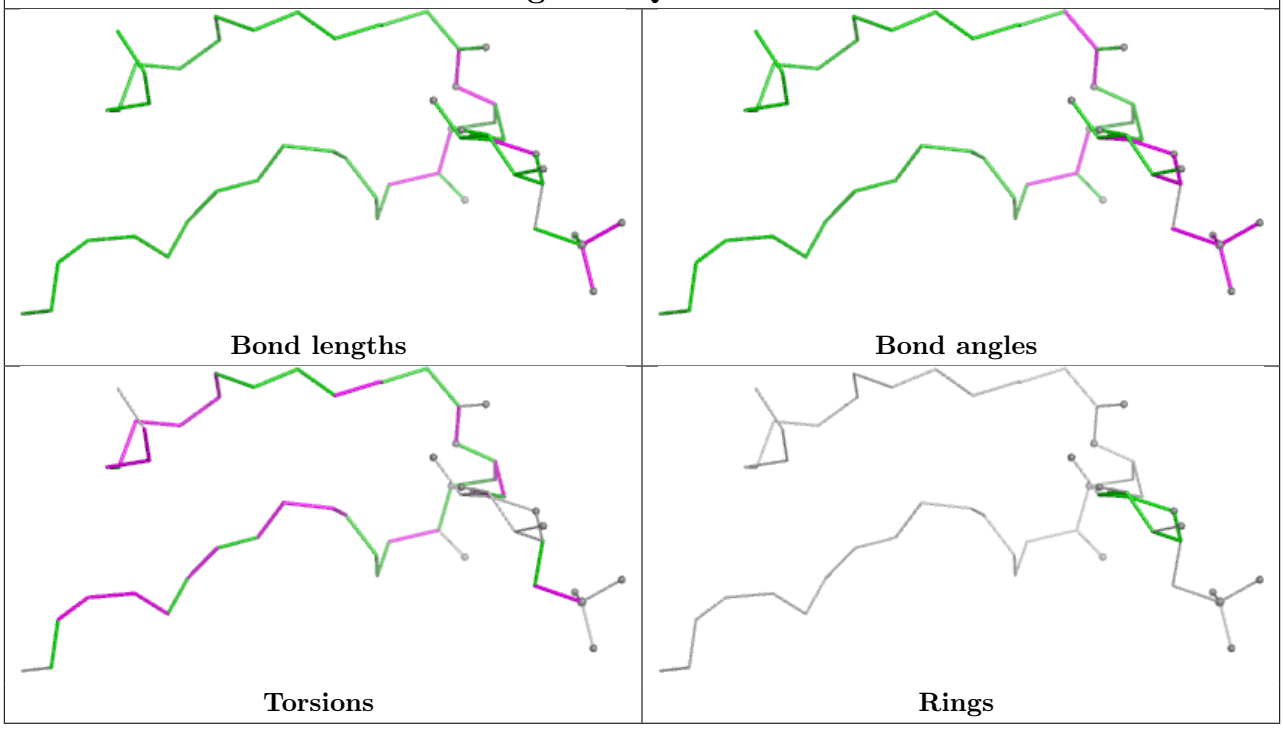
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	303	2WA	2	0
20	L	201	SQD	2	0
13	J	201	PL9	4	0
12	A	304	ECH	5	0
14	B	302	CLA	4	0
17	H	101	6PL	1	0
12	I	305	ECH	2	0
10	I	302	HEM	4	0
17	P	101	6PL	1	0
20	D	202	SQD	4	0
19	L	202	FES	2	0
15	K	301	HEC	5	0
15	C	302	HEC	5	0
19	D	201	FES	2	0
10	B	301	HEM	2	0
14	J	202	CLA	2	0
10	A	302	HEM	1	0
11	J	203	PGV	2	0
10	I	303	HEM	5	0
10	I	301	HEM	3	0
10	A	301	HEM	6	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.

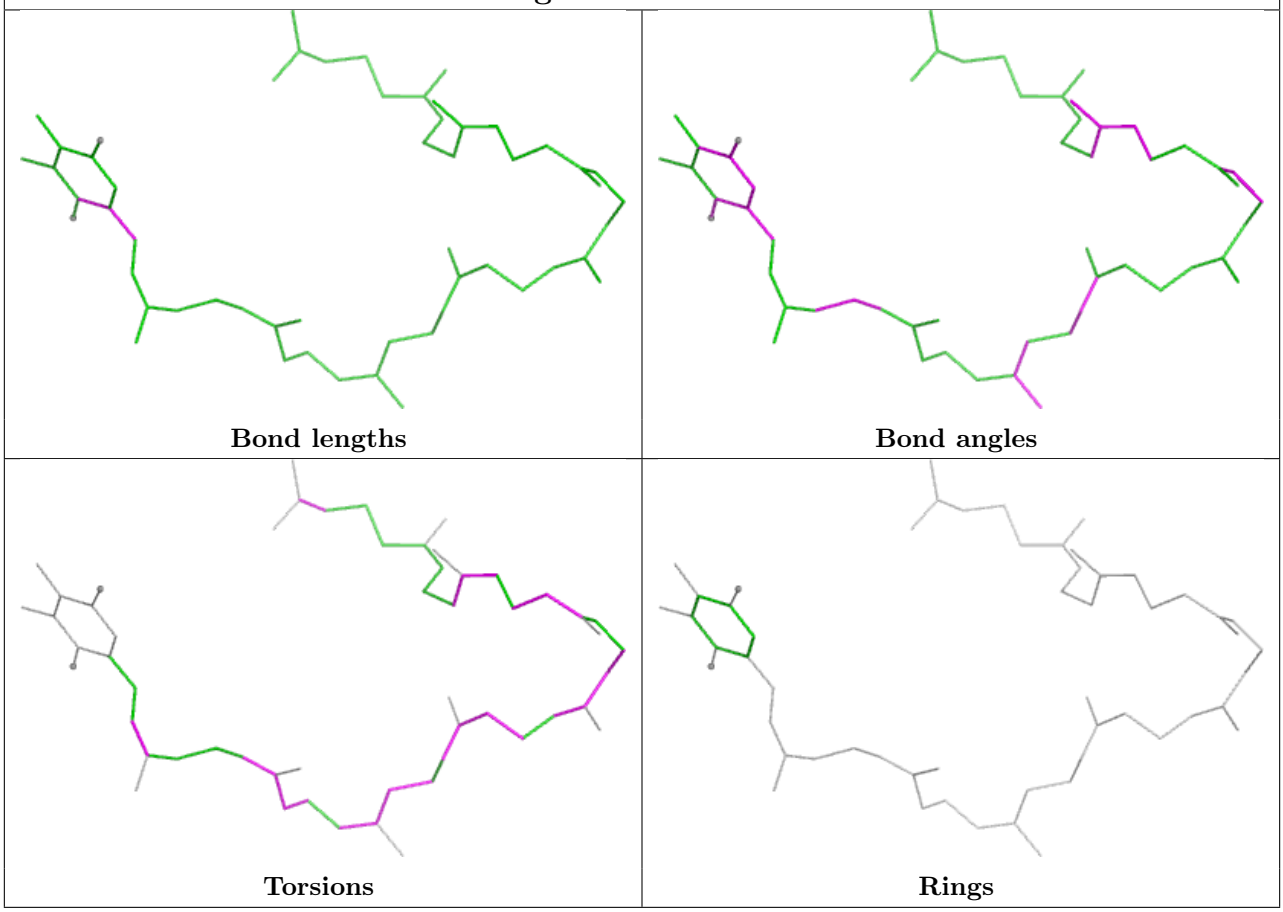
Ligand 2WA B 303



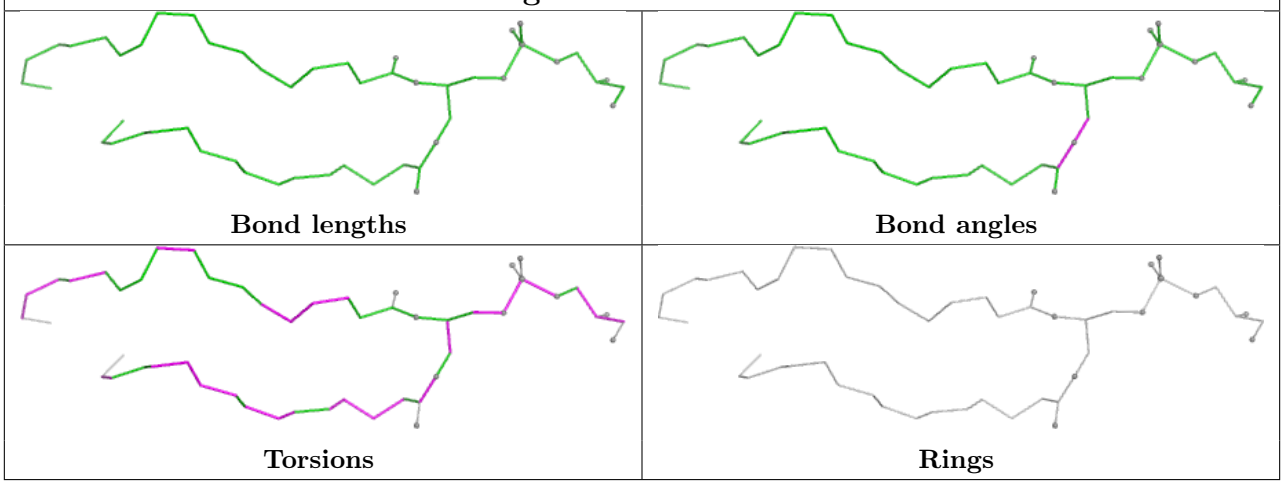
Ligand SQD L 201



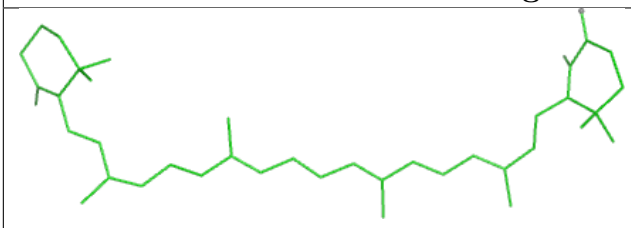
Ligand PL9 J 201



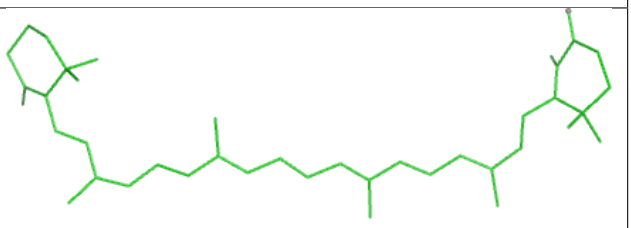
Ligand PGV B 304



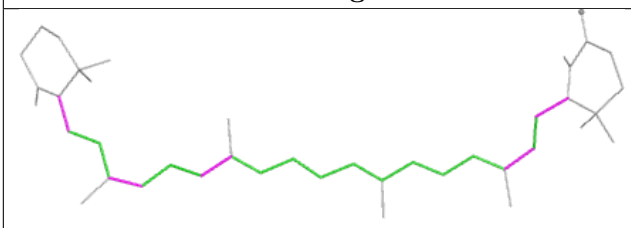
Ligand ECH A 304



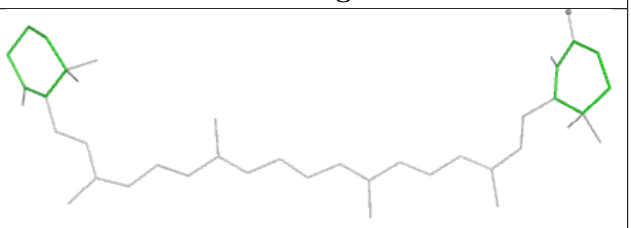
Bond lengths



Bond angles

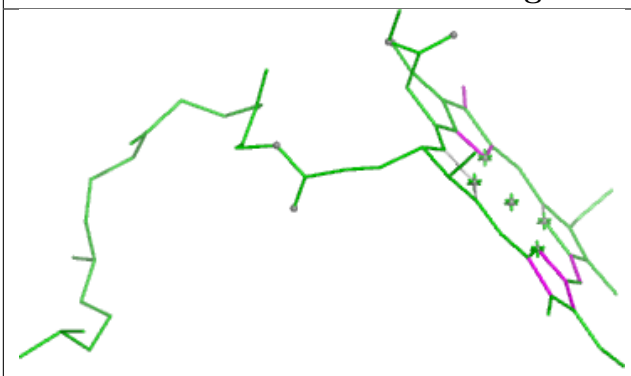


Torsions



Rings

Ligand CLA B 302



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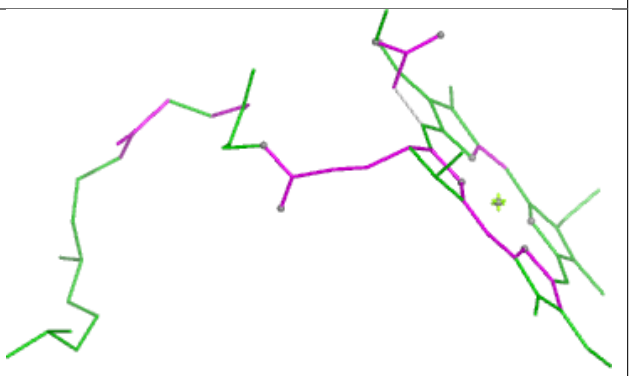
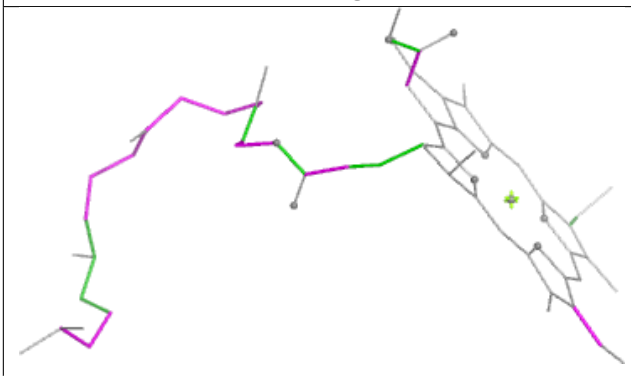


Bond angles



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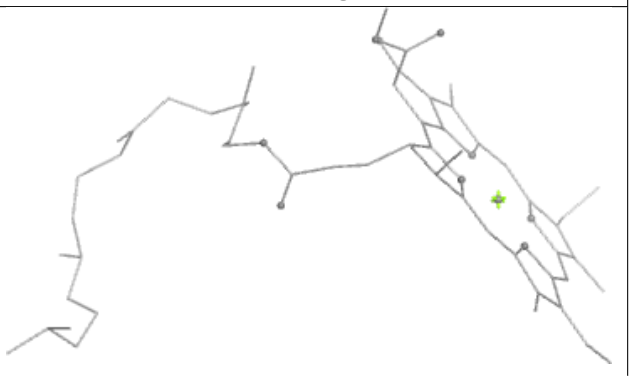
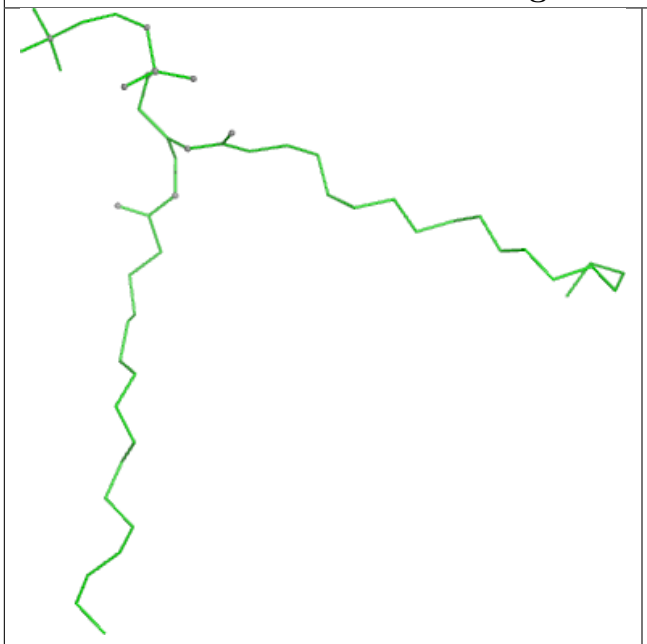


Rings

Ligand 6PL H 101



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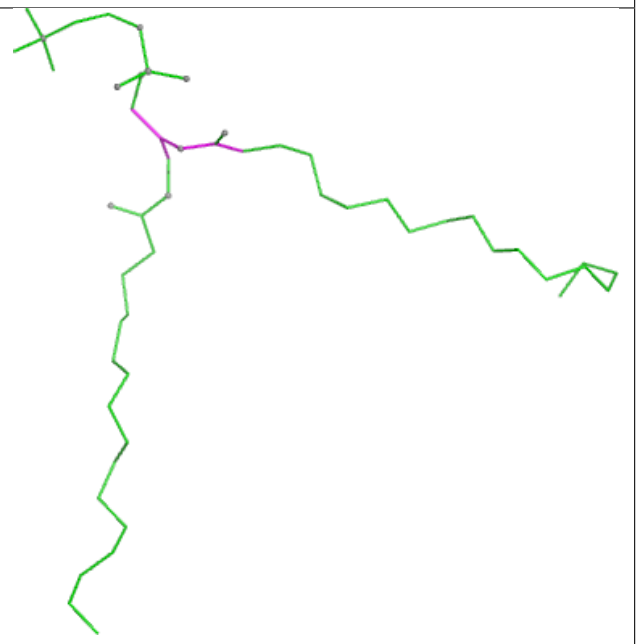
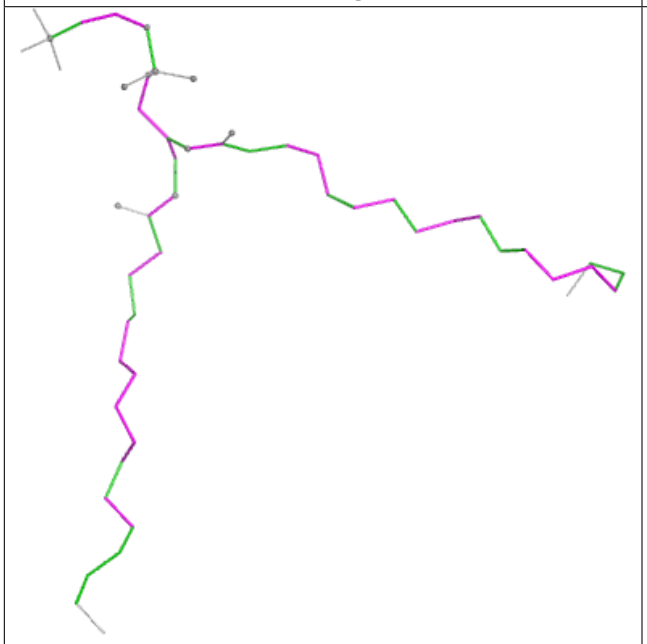


Bond angles

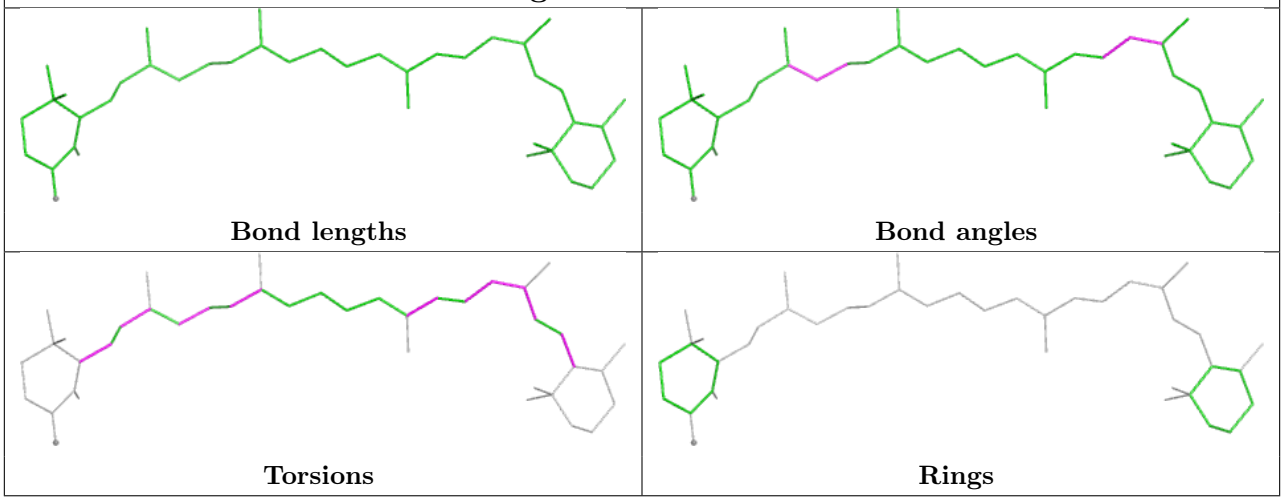


Torsions

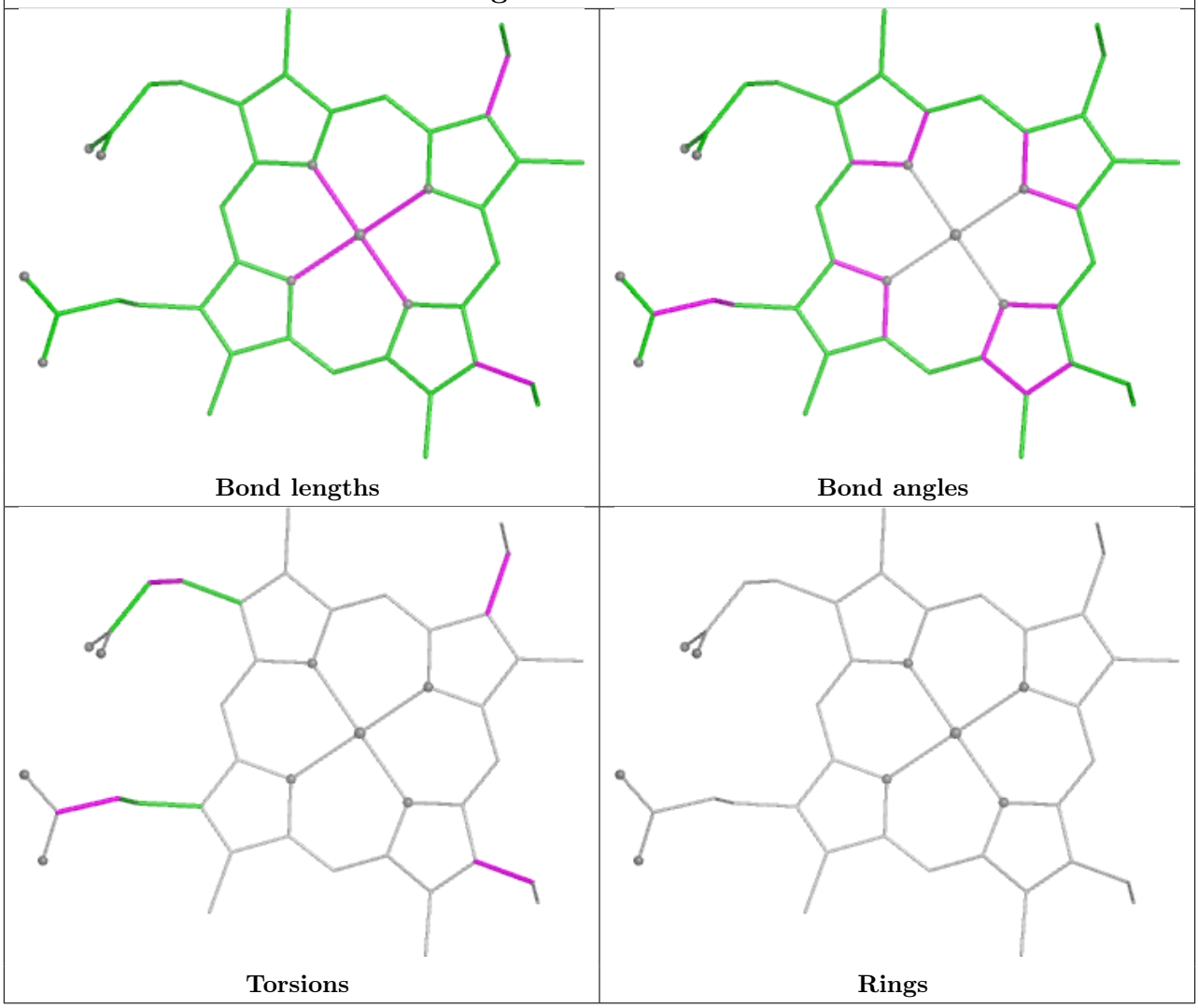


Rings

Ligand ECH I 305



Ligand HEM I 302



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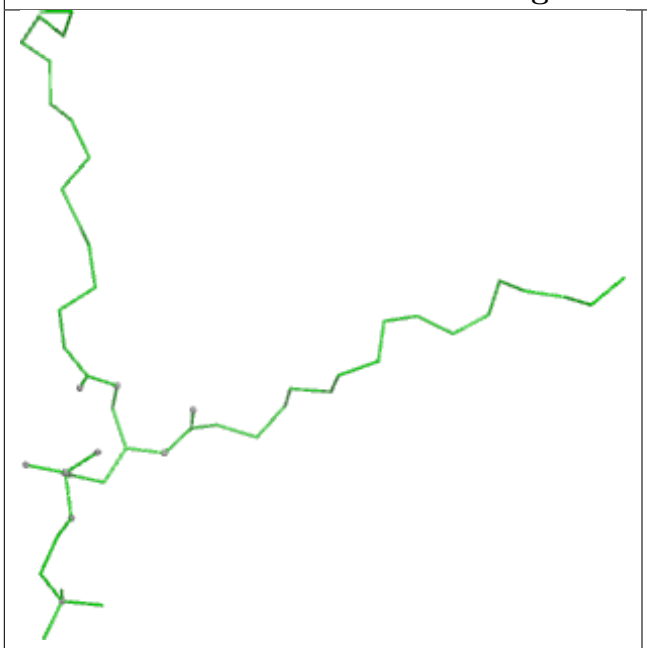

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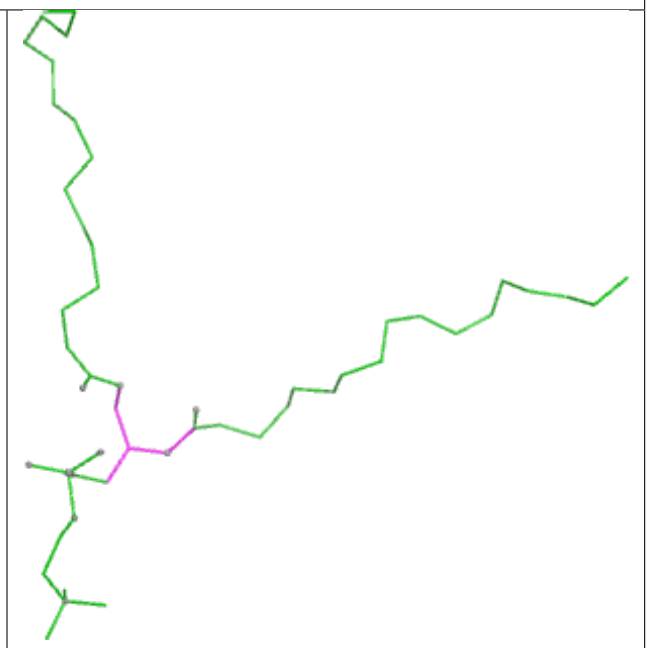
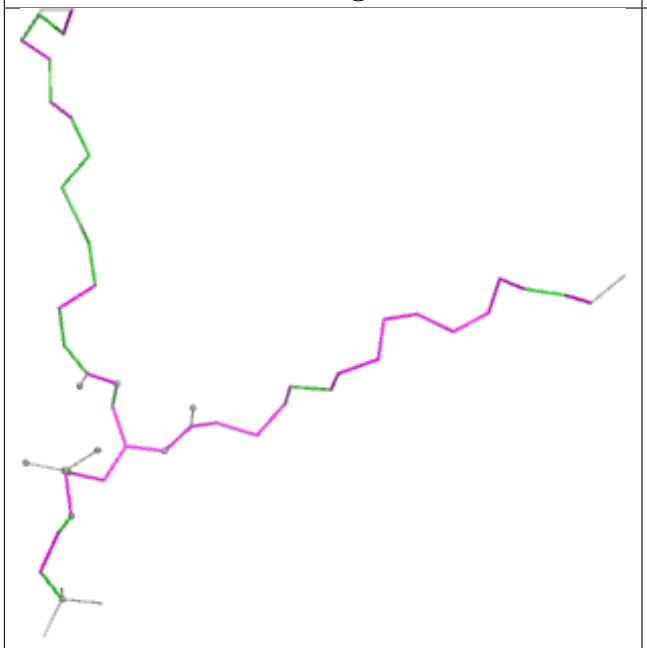


Bond angles



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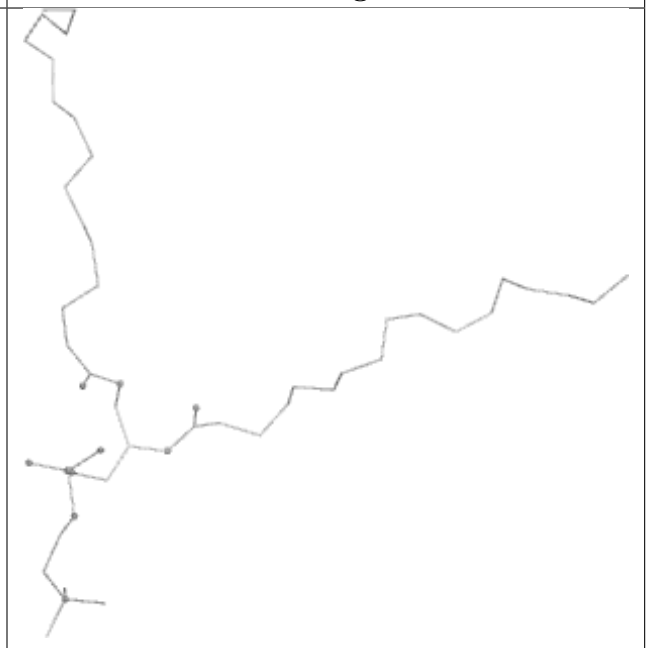
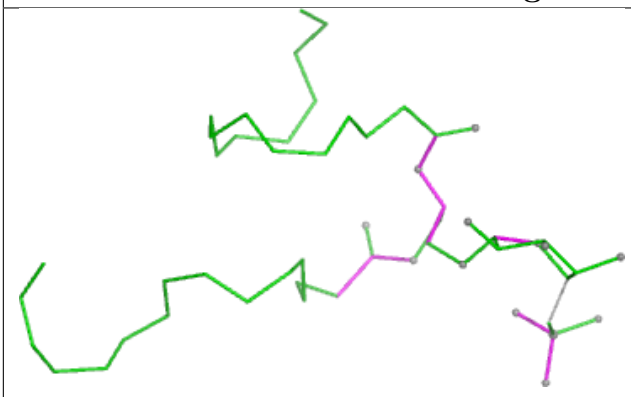


Rings

Ligand SQD D 202



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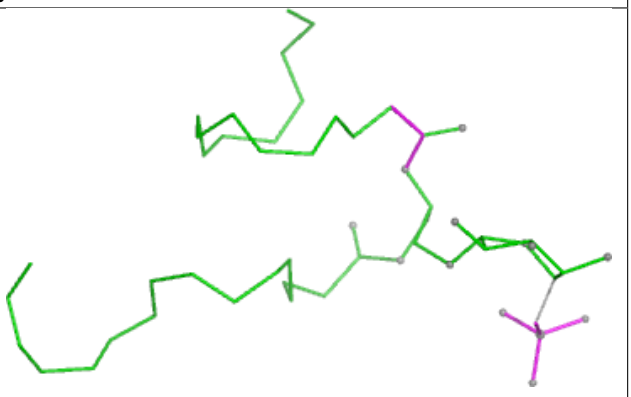
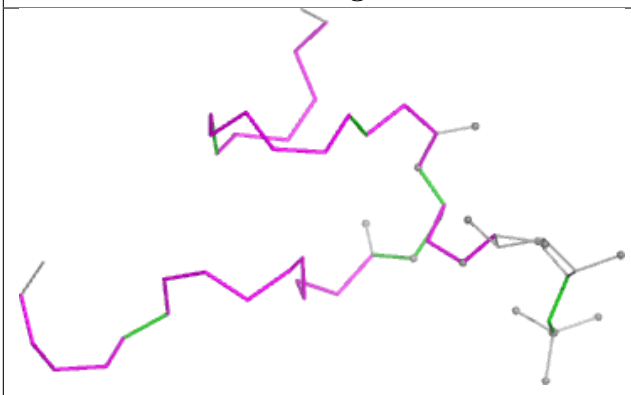


Bond angles



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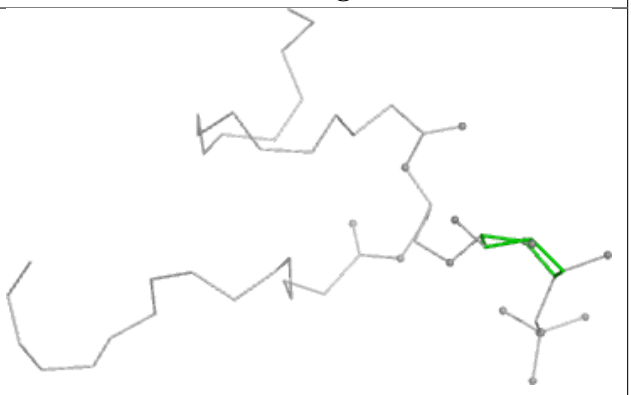
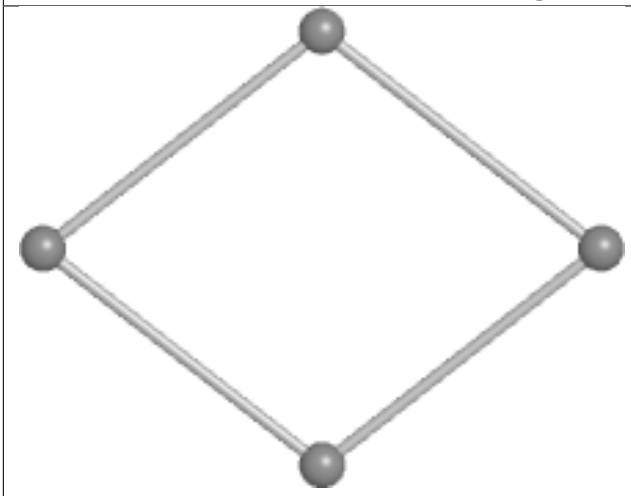


Rings

Ligand FES L 202



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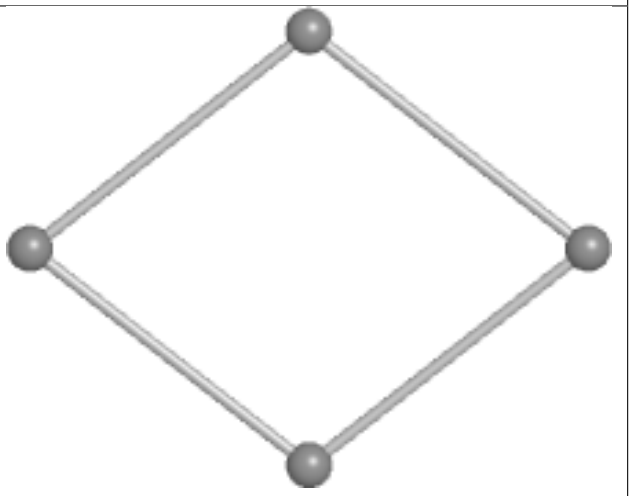
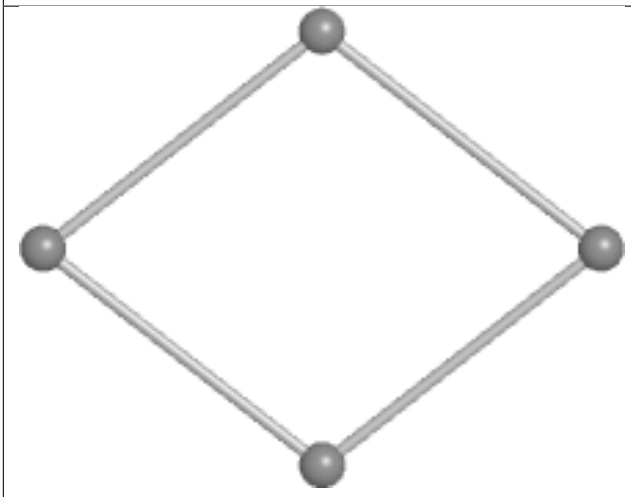


Bond angles



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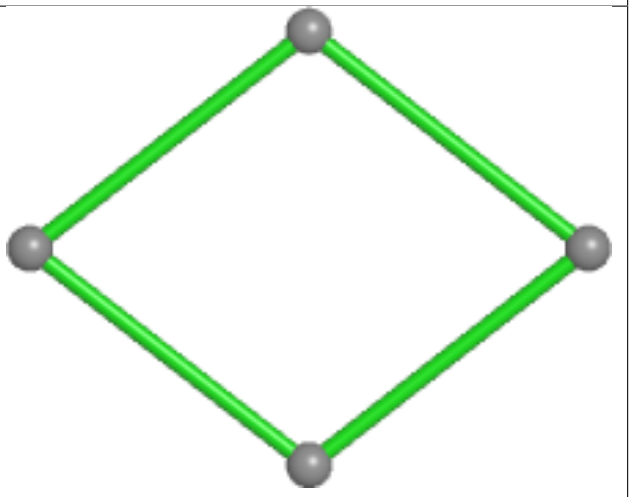
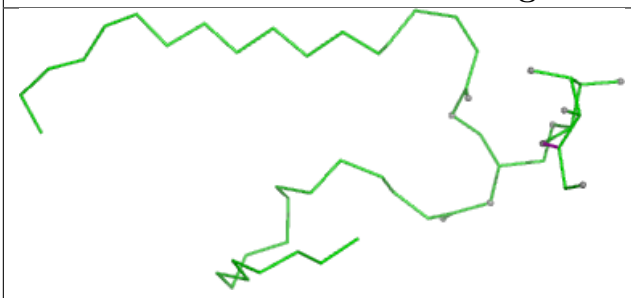


Rings

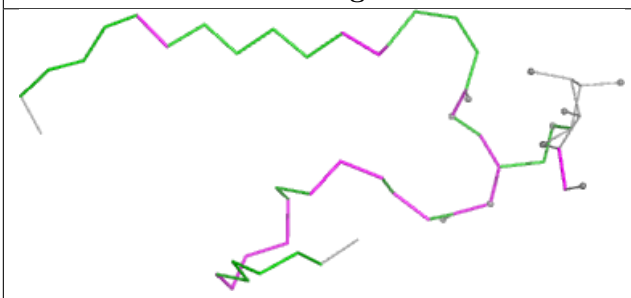
Ligand LMG N 101



Bond lengths



Bond angles



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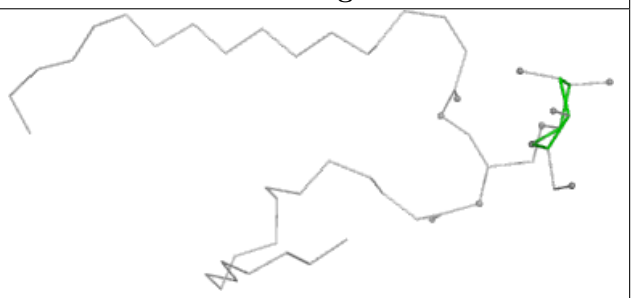
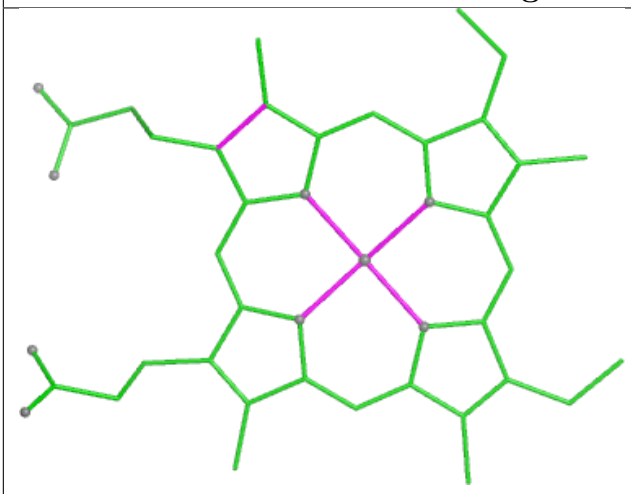


Rings

Ligand HEC K 301



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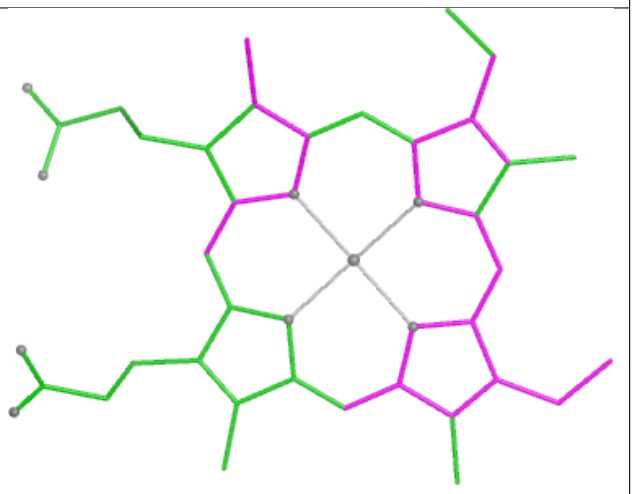

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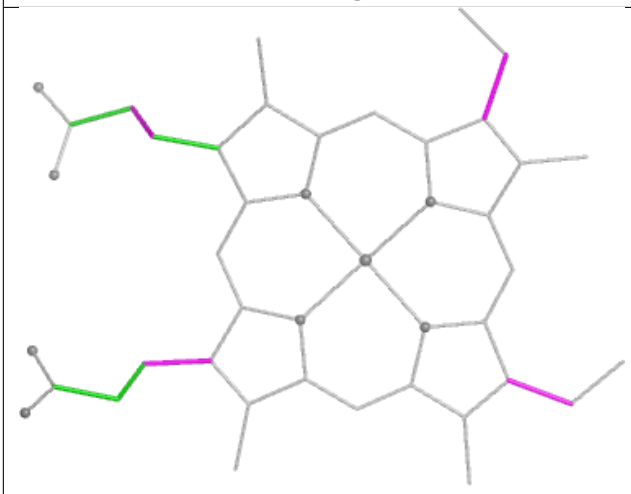

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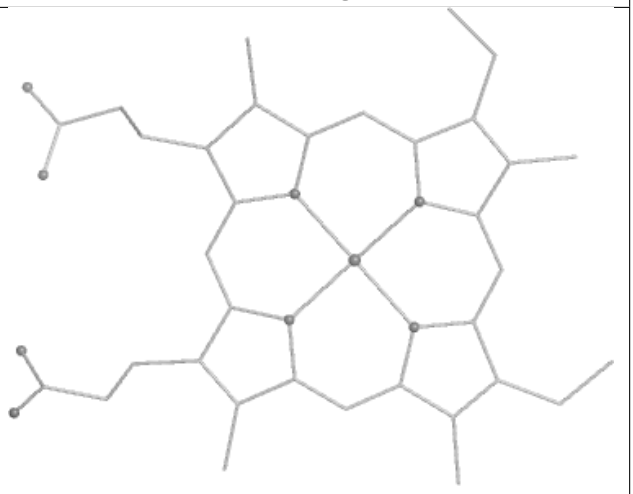
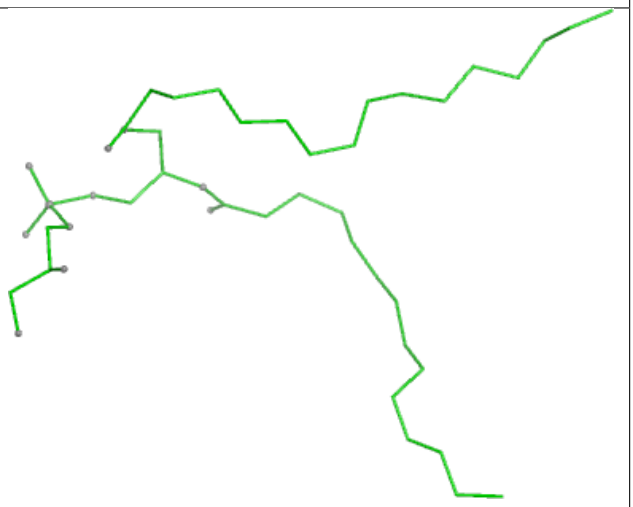


Rings

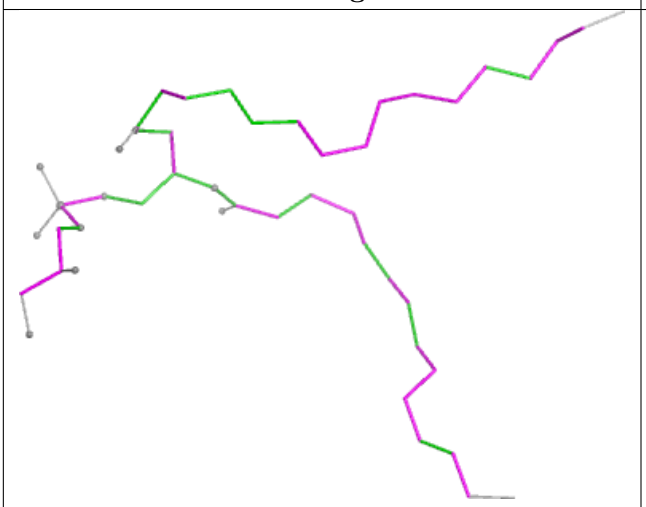
Ligand PGV C 301



Bond lengths



Bond angles

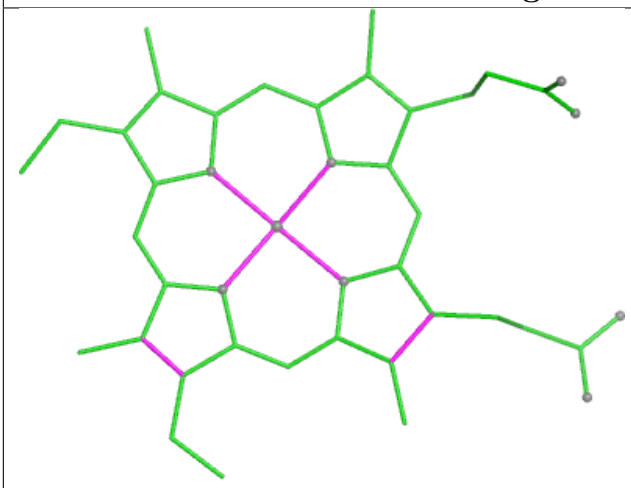


Torsions



Rings

Ligand HEC C 302



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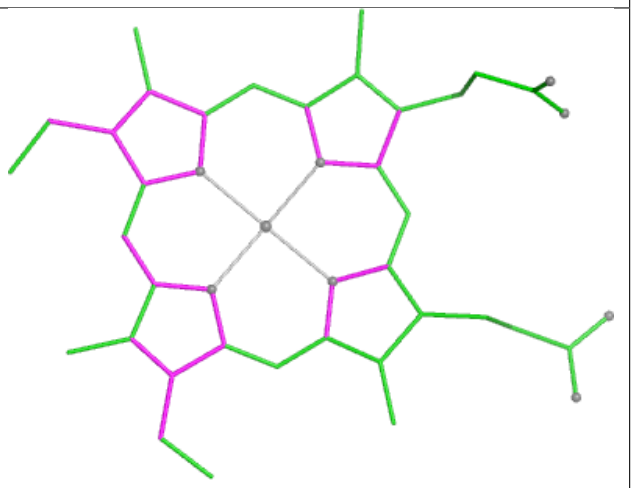
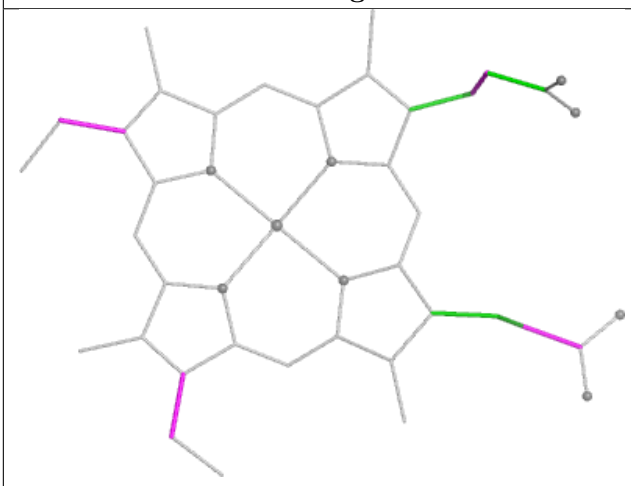


Bond angles



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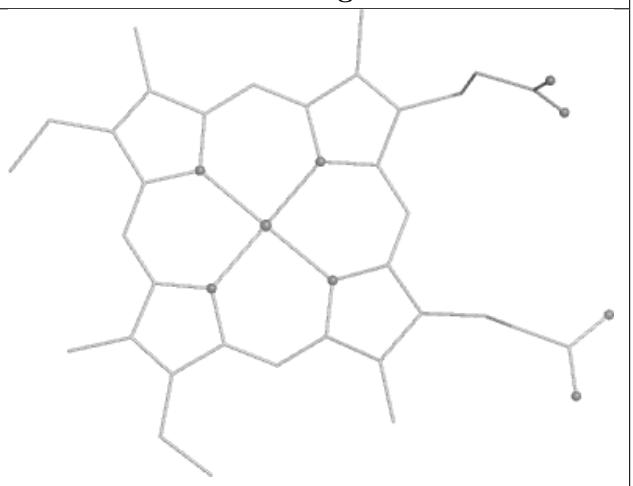
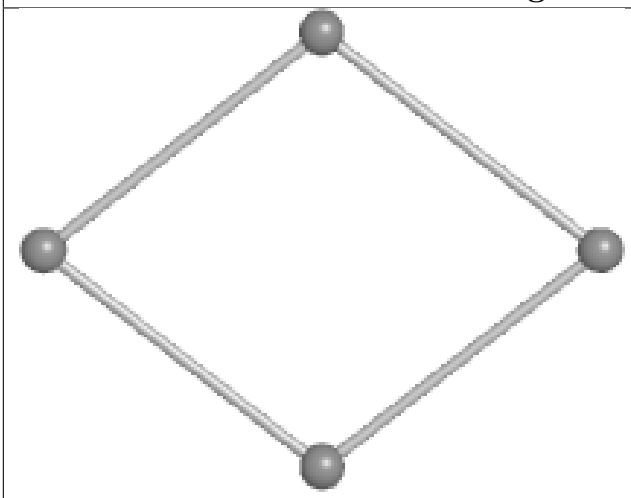


Rings

Ligand FES D 201



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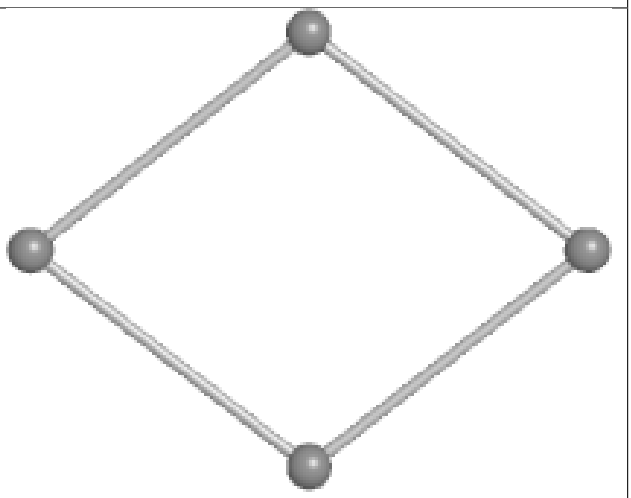
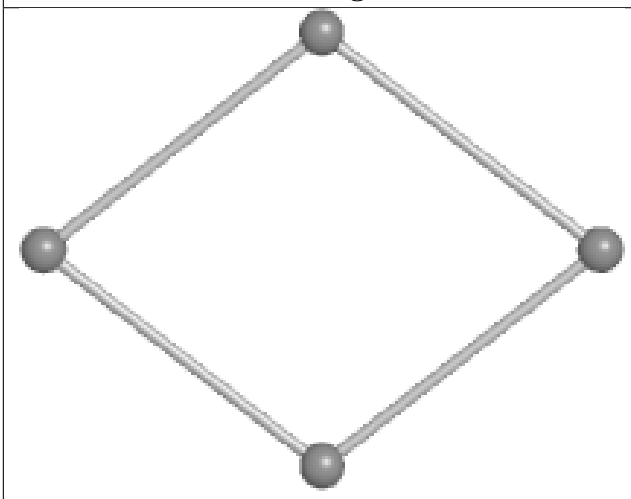


Bond angles



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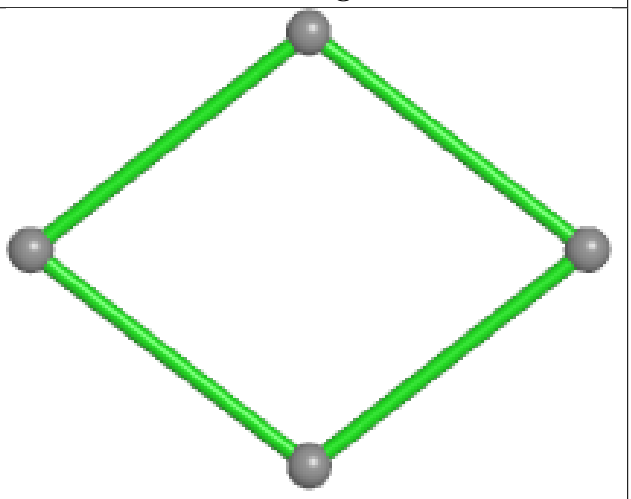
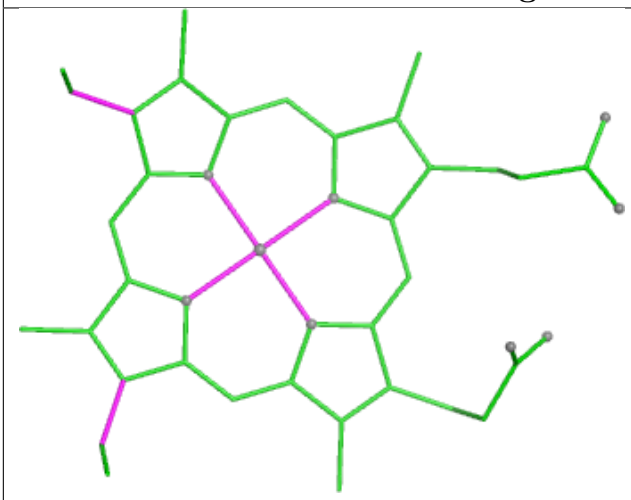


Rings

Ligand HEM B 301



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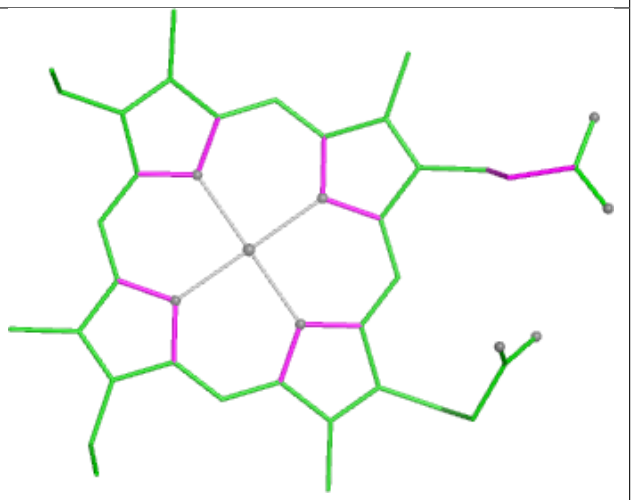

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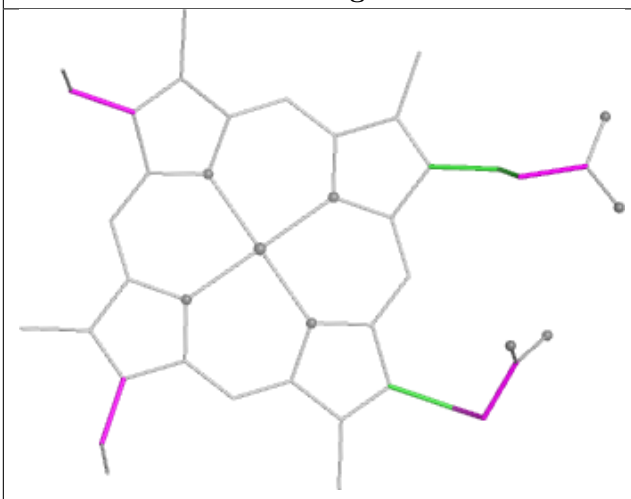

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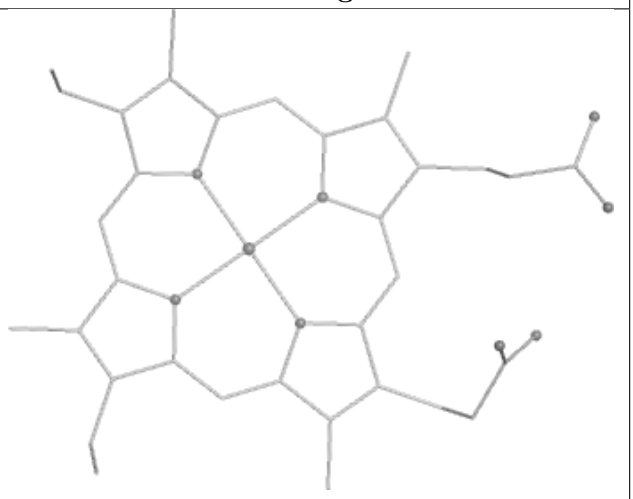
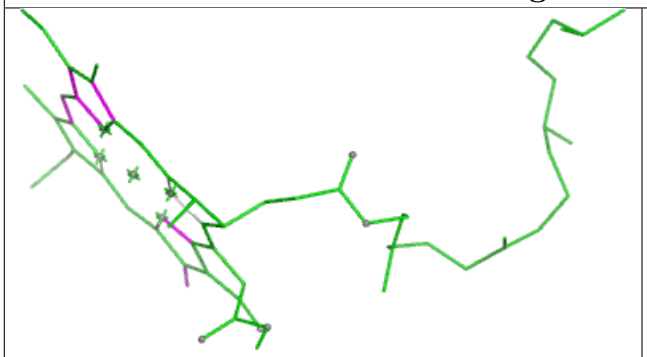


Rings

Ligand CLA J 202



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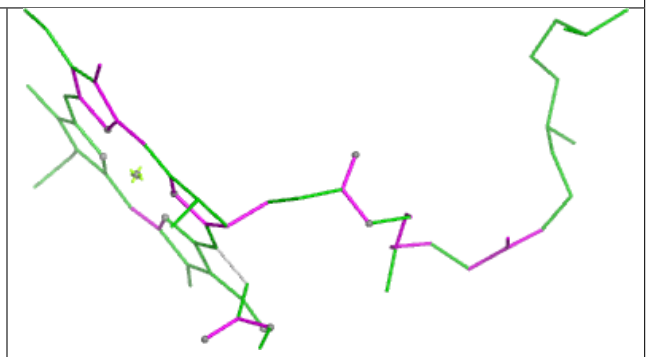
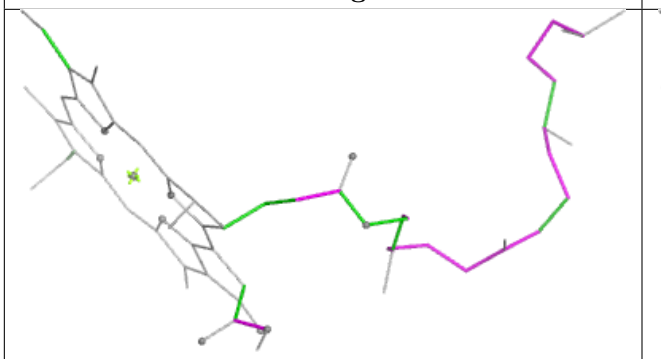


Bond angles



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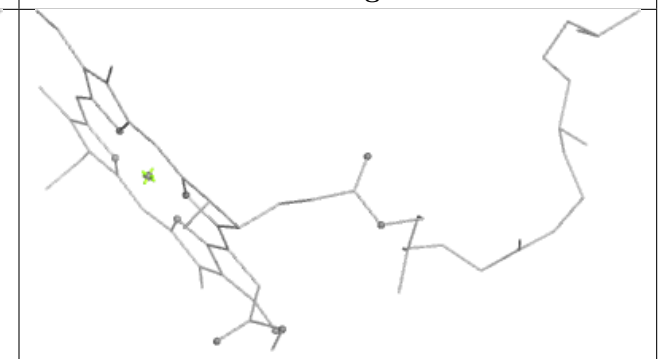
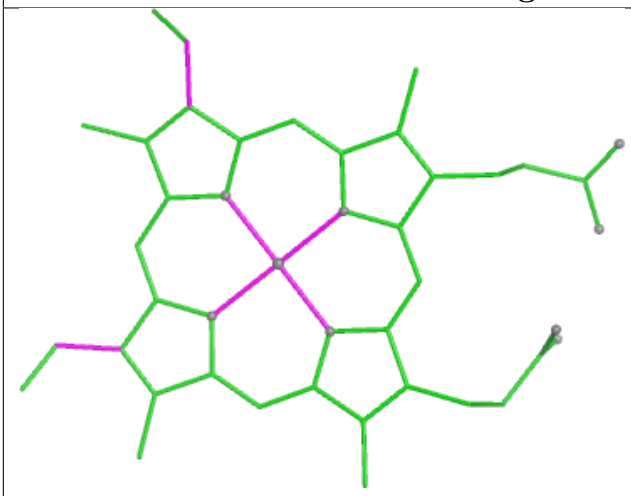


Rings

Ligand HEM A 302



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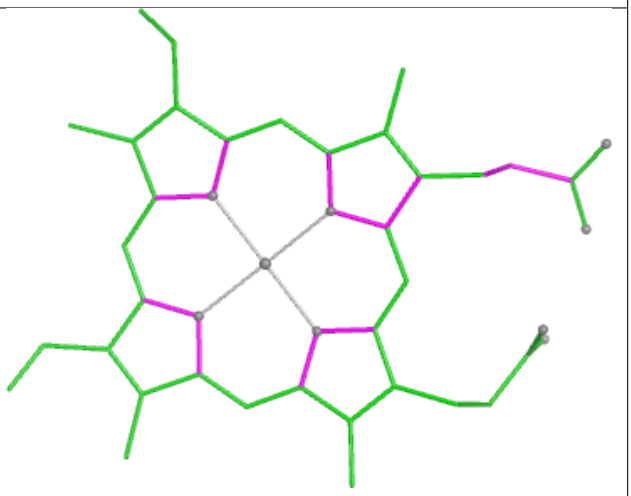
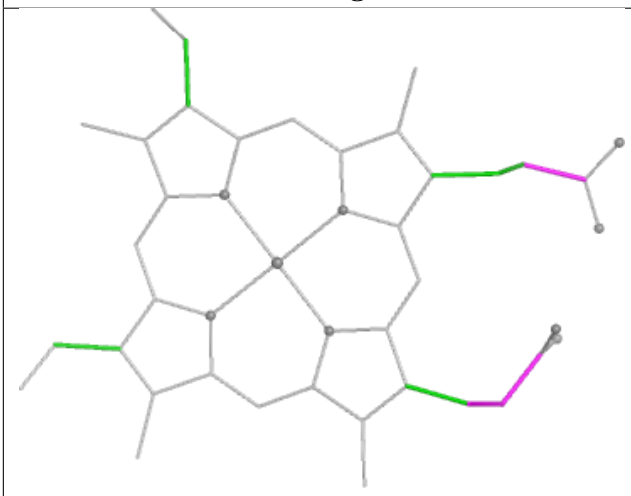


Bond angles



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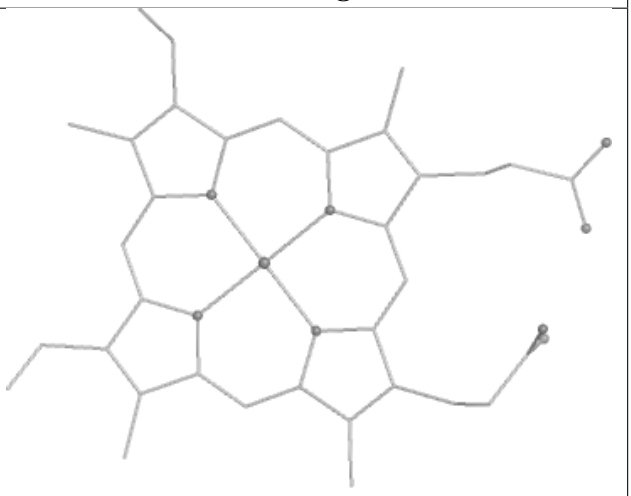
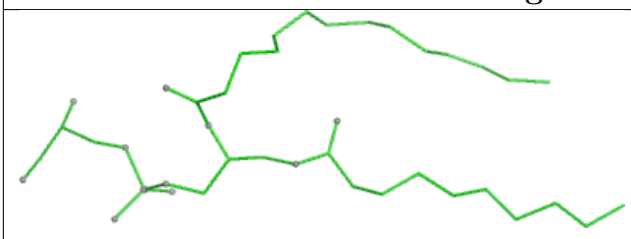


Rings

Ligand PGV J 203



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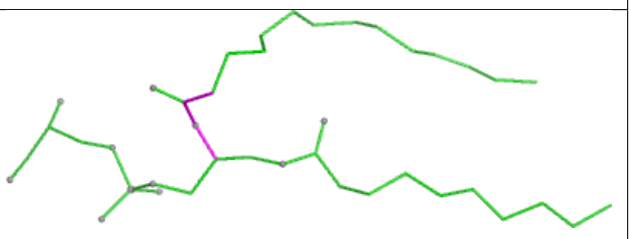
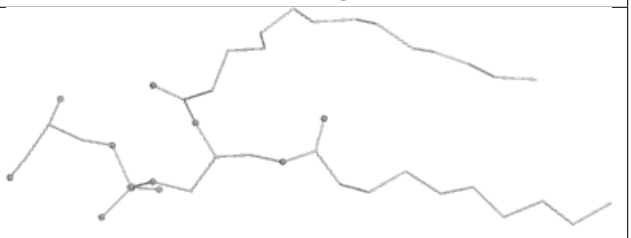


Bond angles

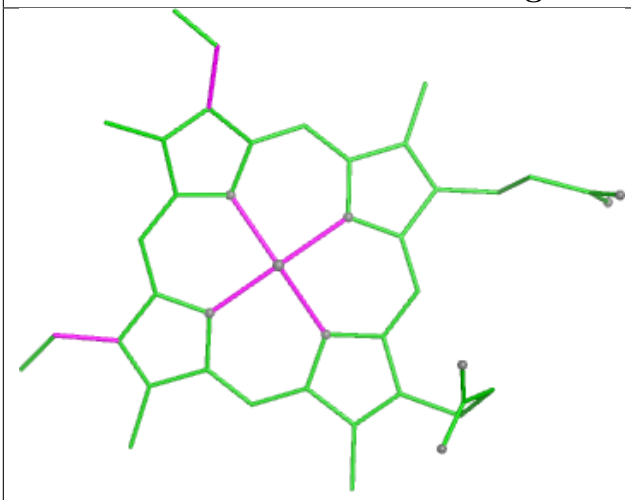


Torsions

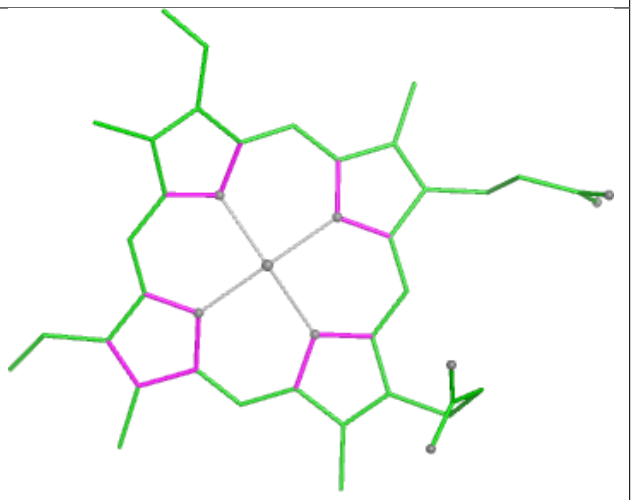


Rings

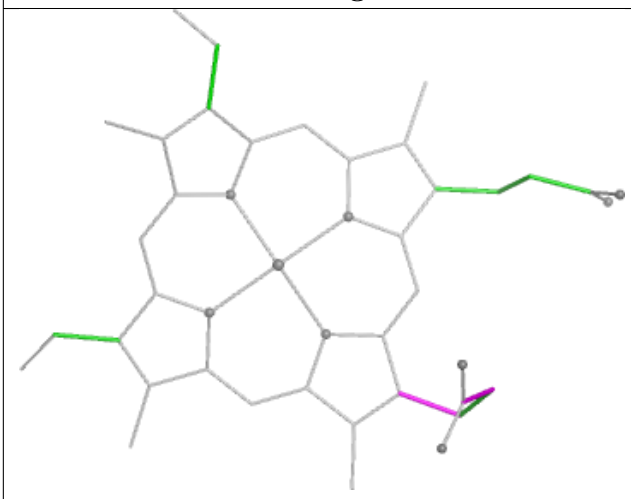
Ligand HEM I 303



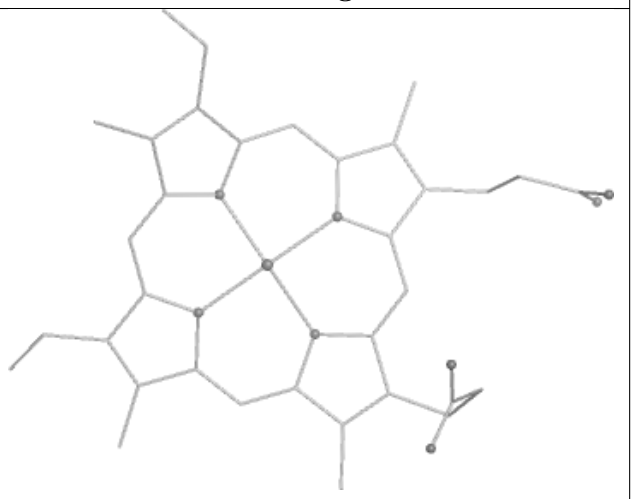
Bond lengths



Bond angles

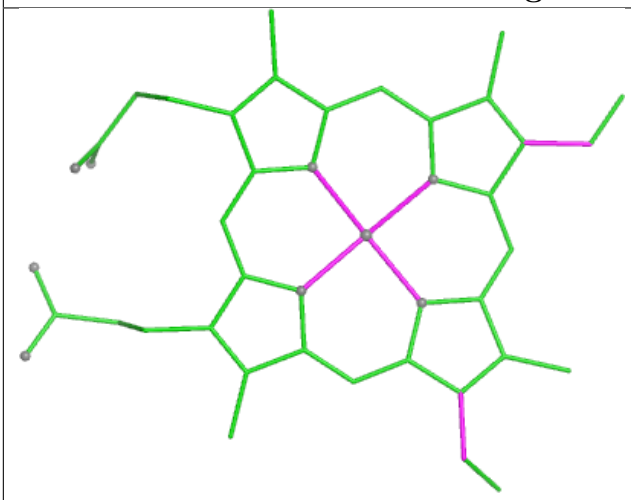


Torsions

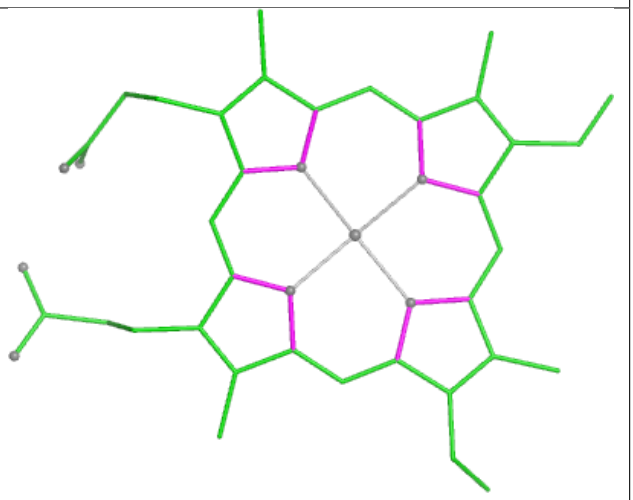


Rings

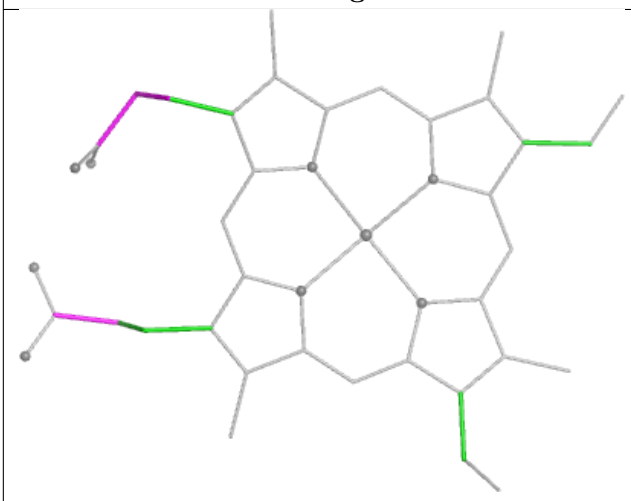
Ligand HEM I 301



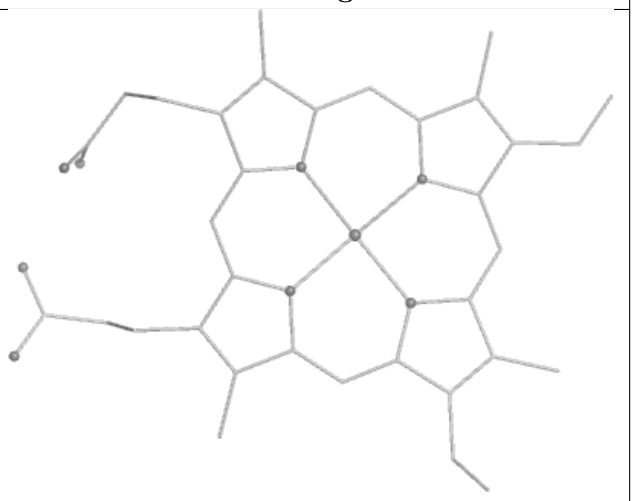
Bond lengths



Bond angles



Torsions

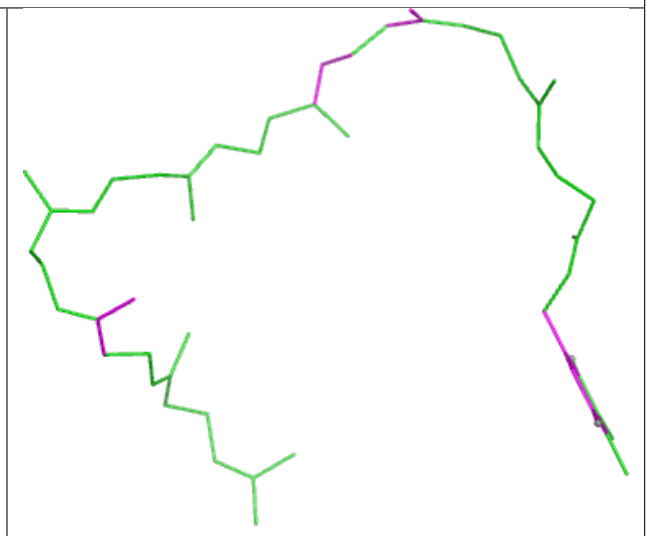


Rings

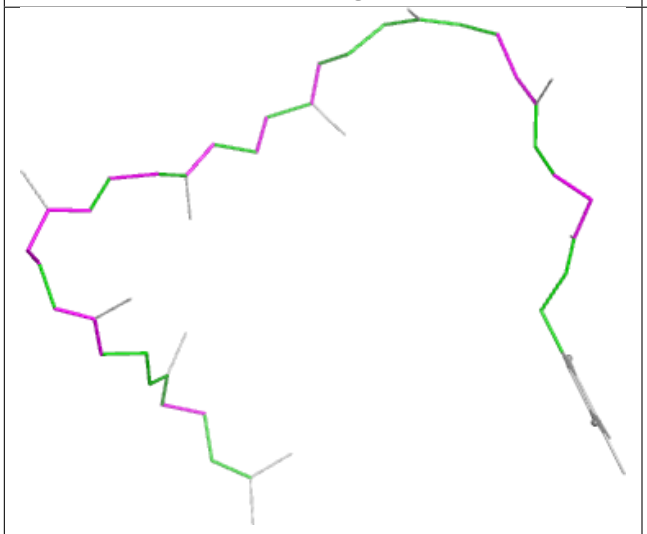
Ligand PL9 A 303



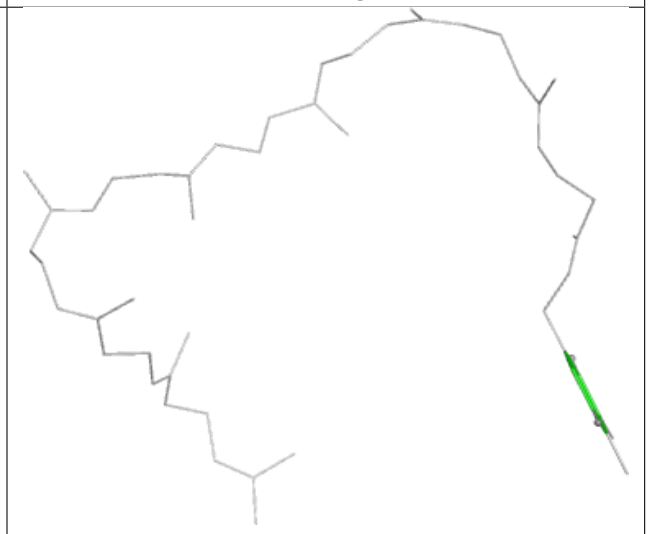
Bond lengths



Bond angles

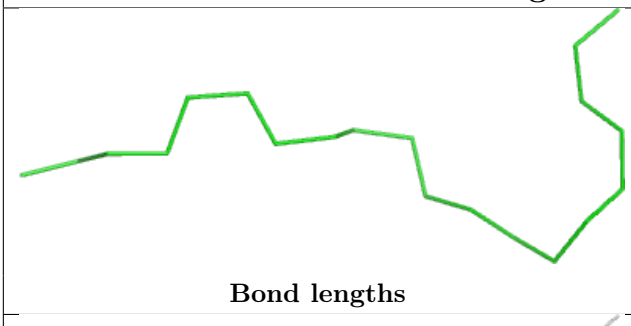


Torsions

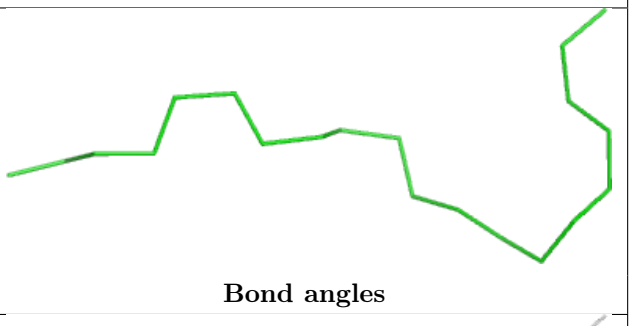


Rings

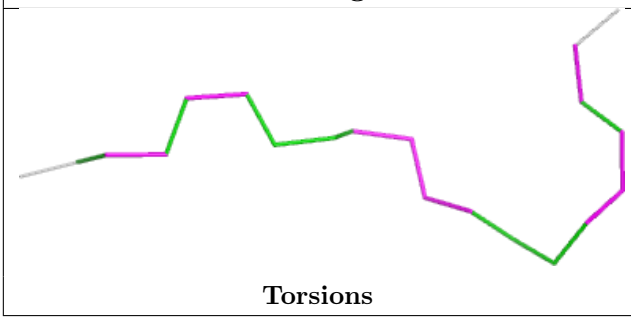
Ligand LFA E 101



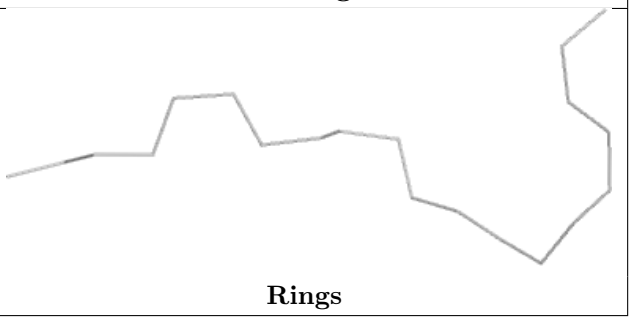
Bond lengths



Bond angles

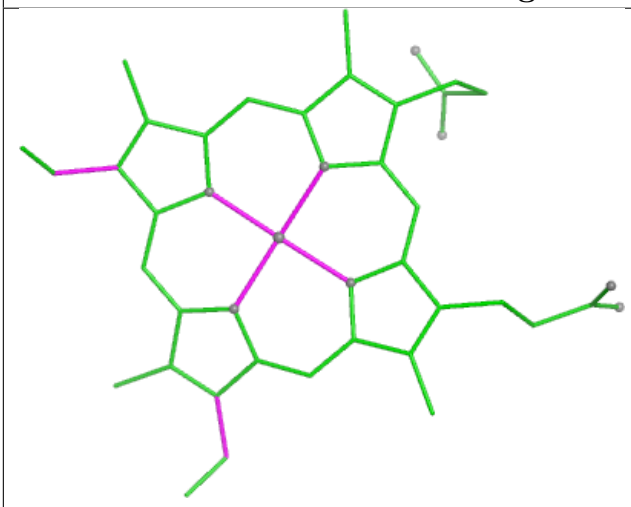


Torsions

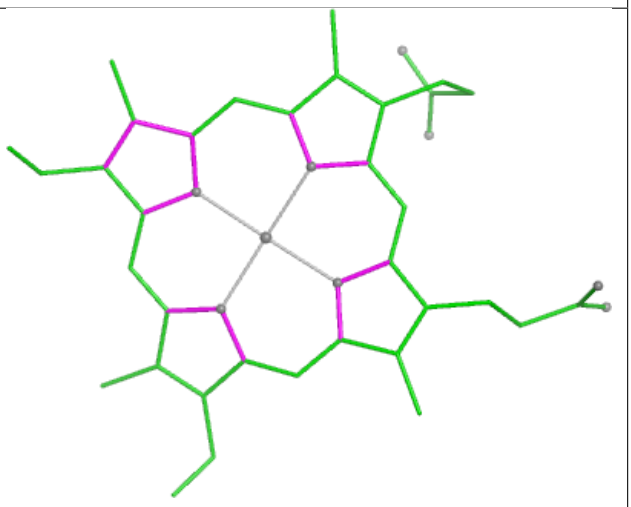


Rings

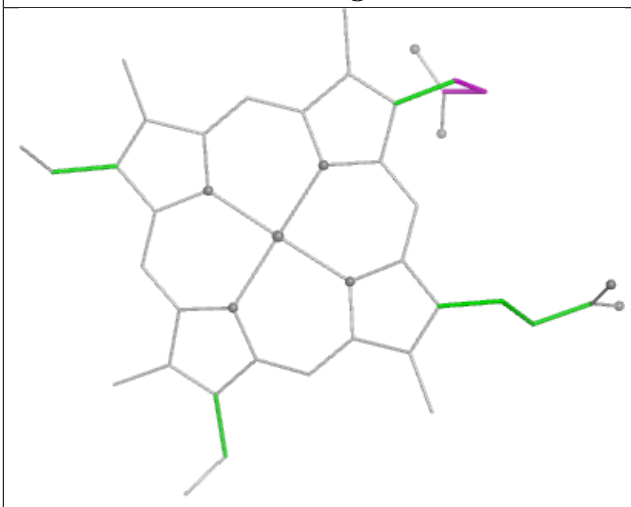
Ligand HEM A 301



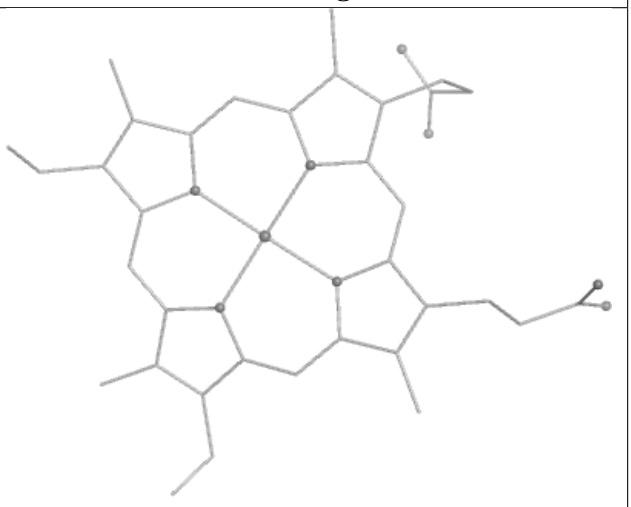
Bond lengths



Bond angles

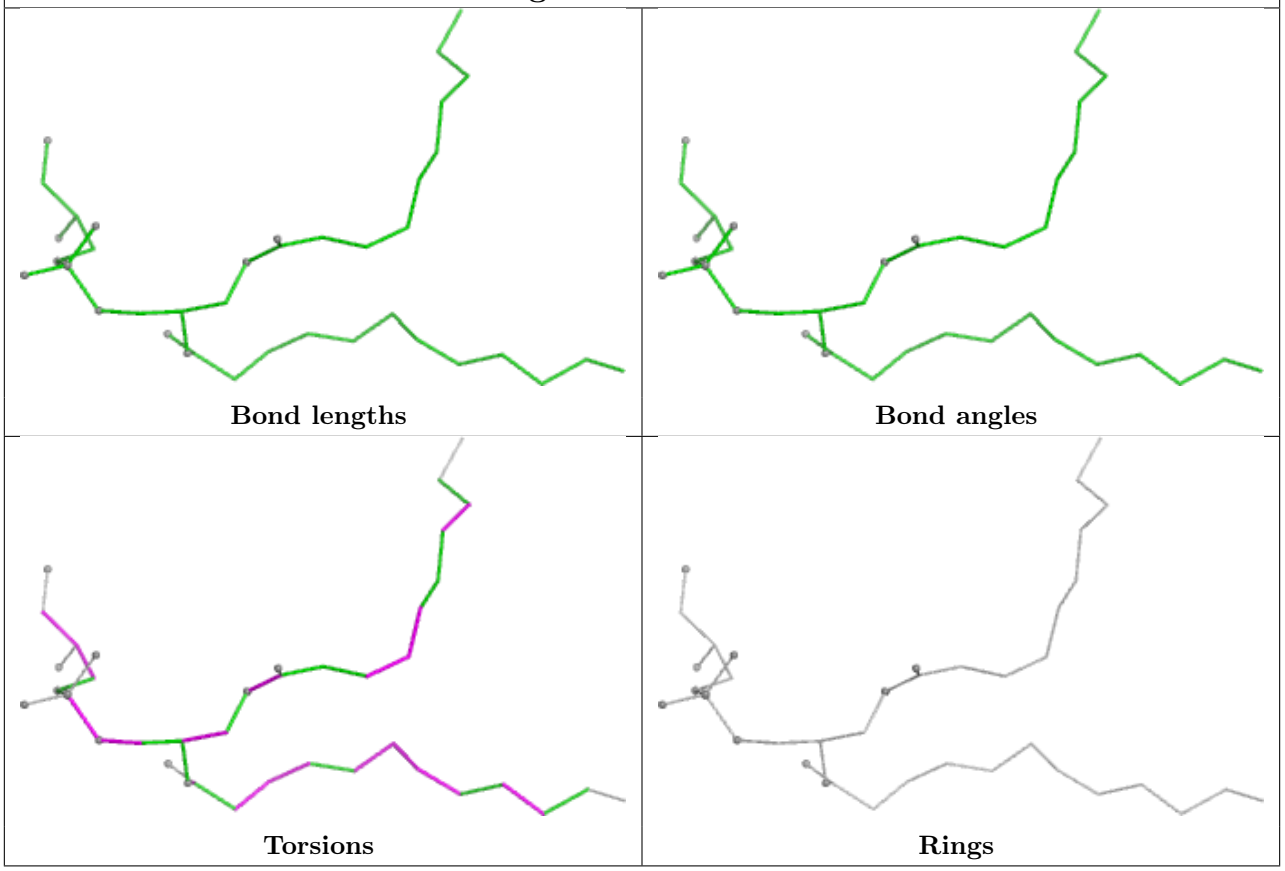


Torsions



Rings

Ligand PGV I 304



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

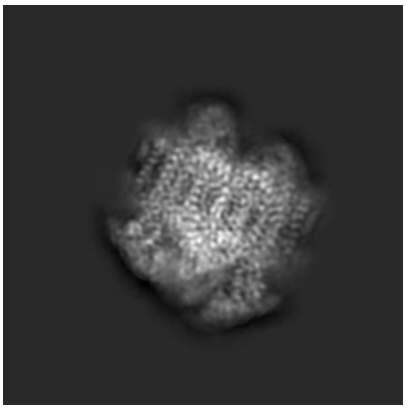
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14224. These allow visual inspection of the internal detail of the map and identification of artifacts.

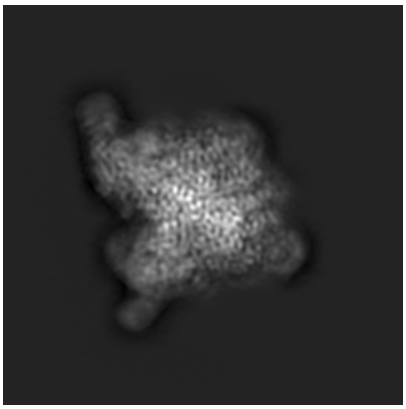
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

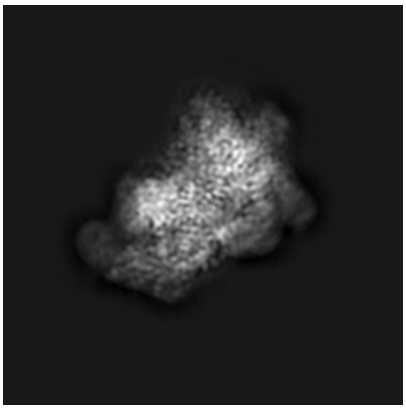
6.1.1 Primary map



X

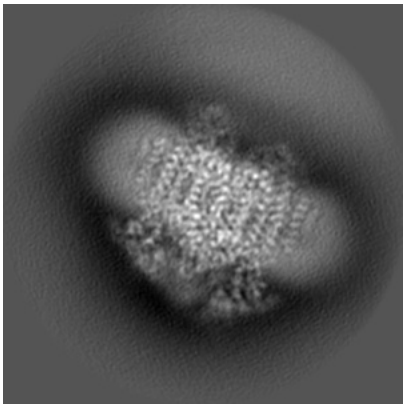


Y

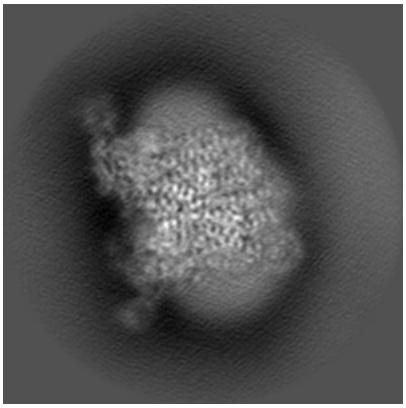


Z

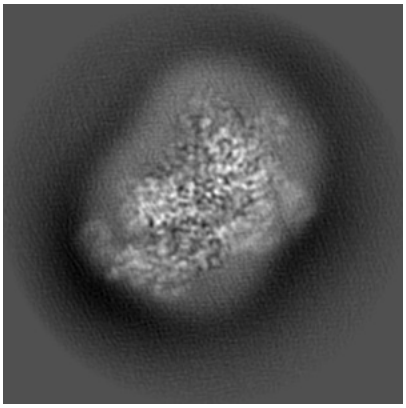
6.1.2 Raw map



X



Y

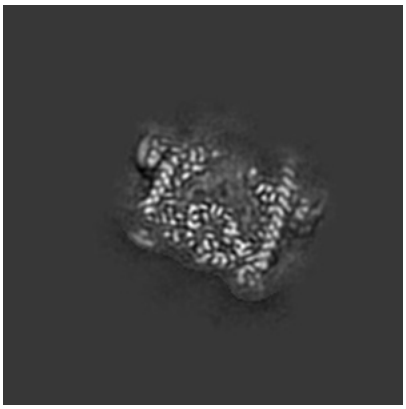


Z

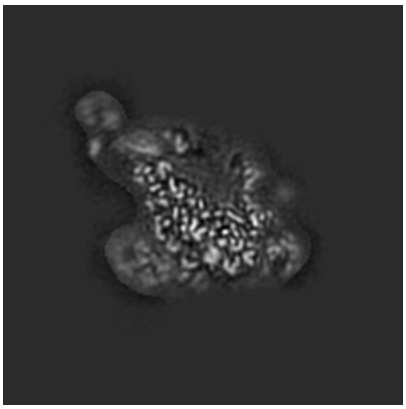
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

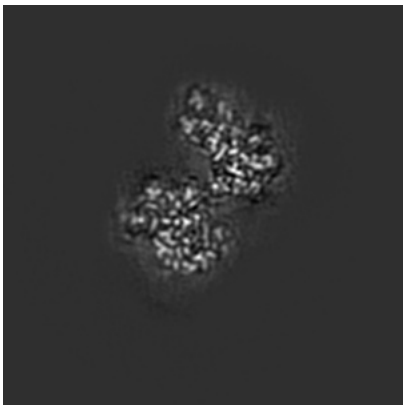
6.2.1 Primary map



X Index: 100

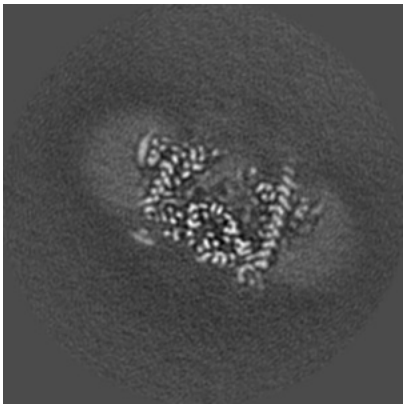


Y Index: 100

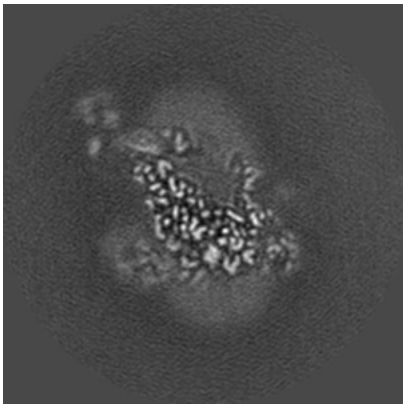


Z Index: 100

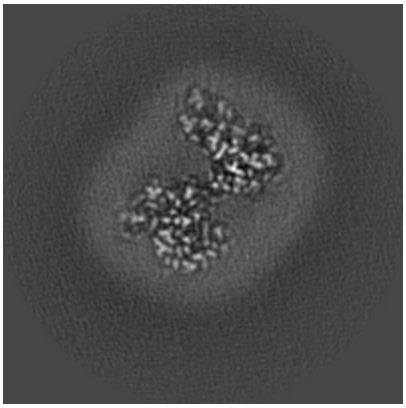
6.2.2 Raw map



X Index: 100



Y Index: 100

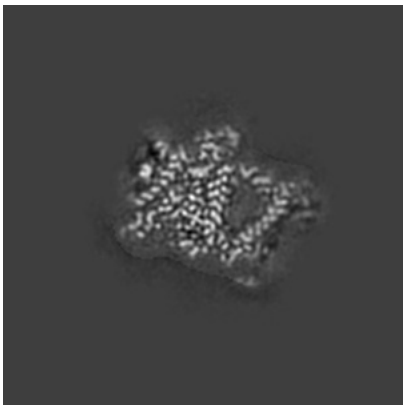


Z Index: 100

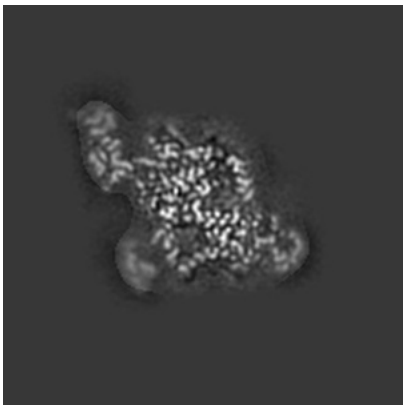
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

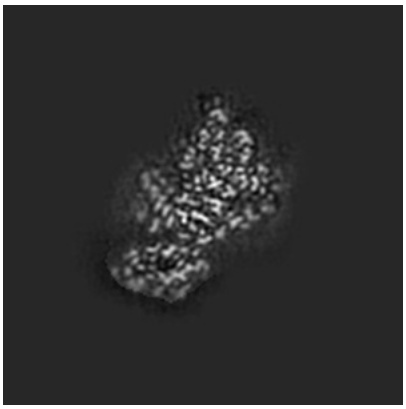
6.3.1 Primary map



X Index: 93

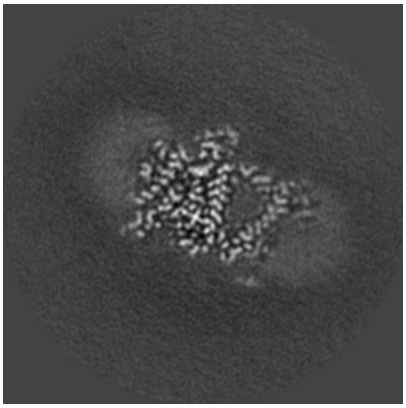


Y Index: 108

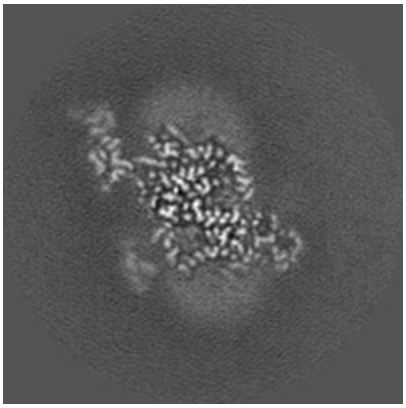


Z Index: 85

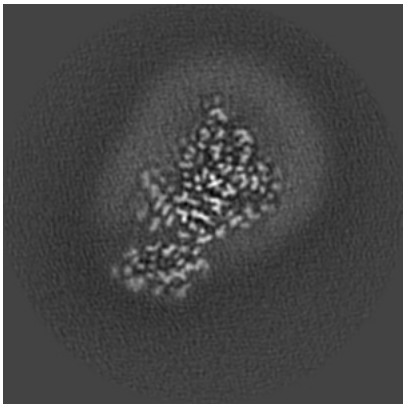
6.3.2 Raw map



X Index: 93



Y Index: 108

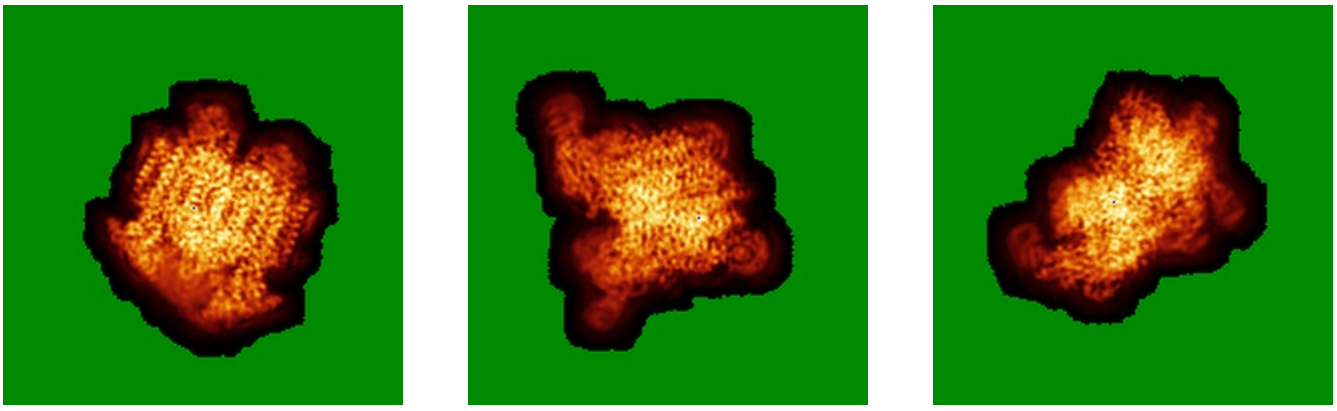


Z Index: 85

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

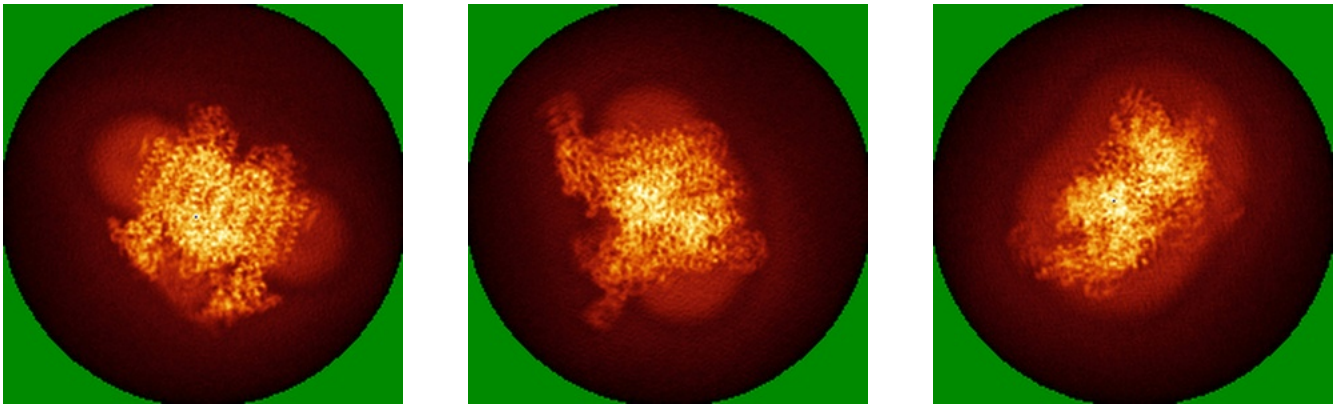
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

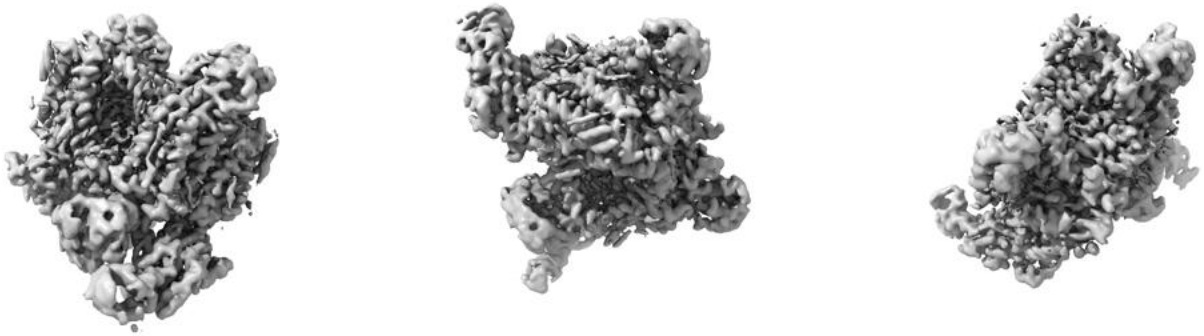


X Y Z

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 0.132. 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.

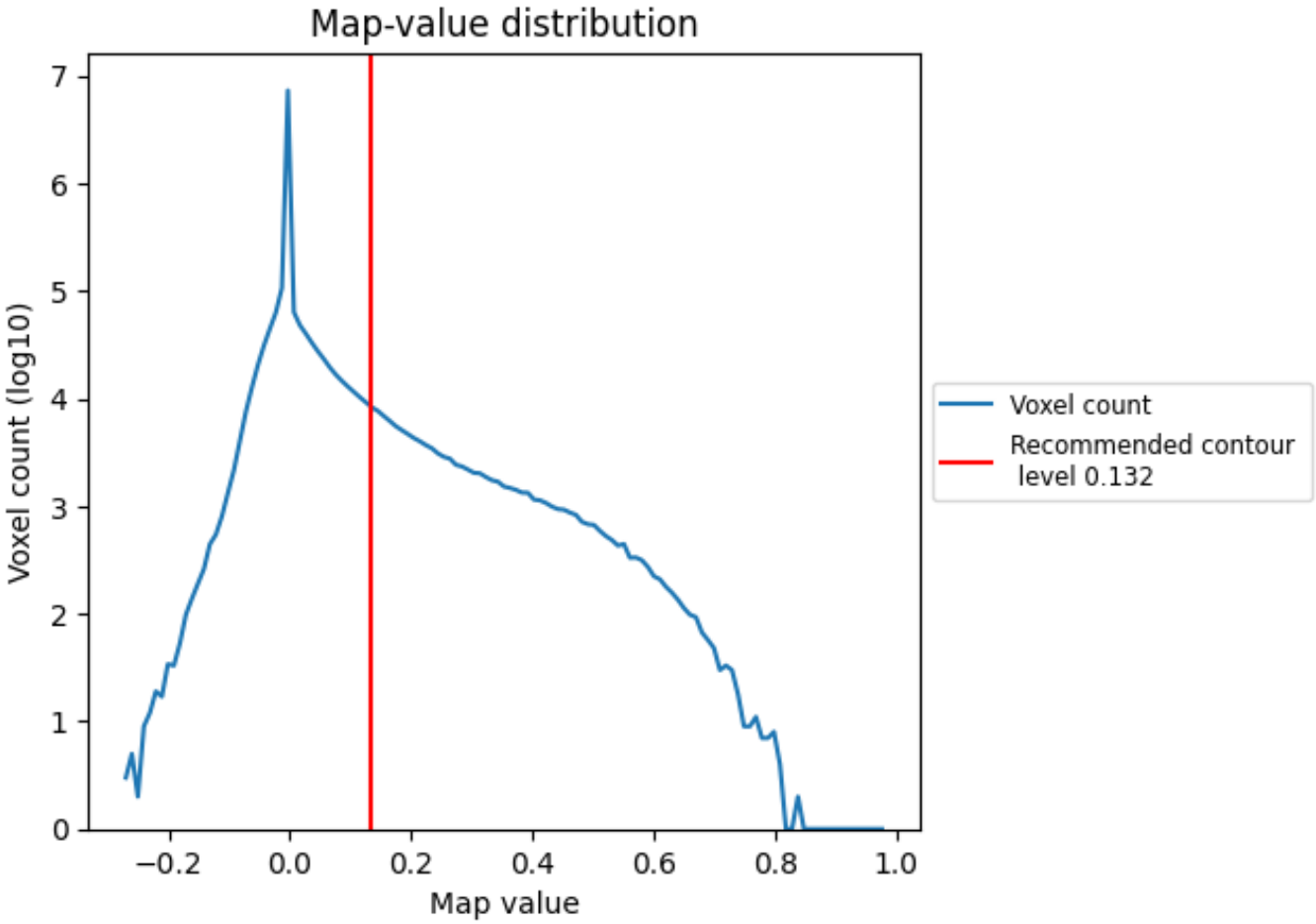
6.6 Mask visualisation (i)

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

7 Map analysis

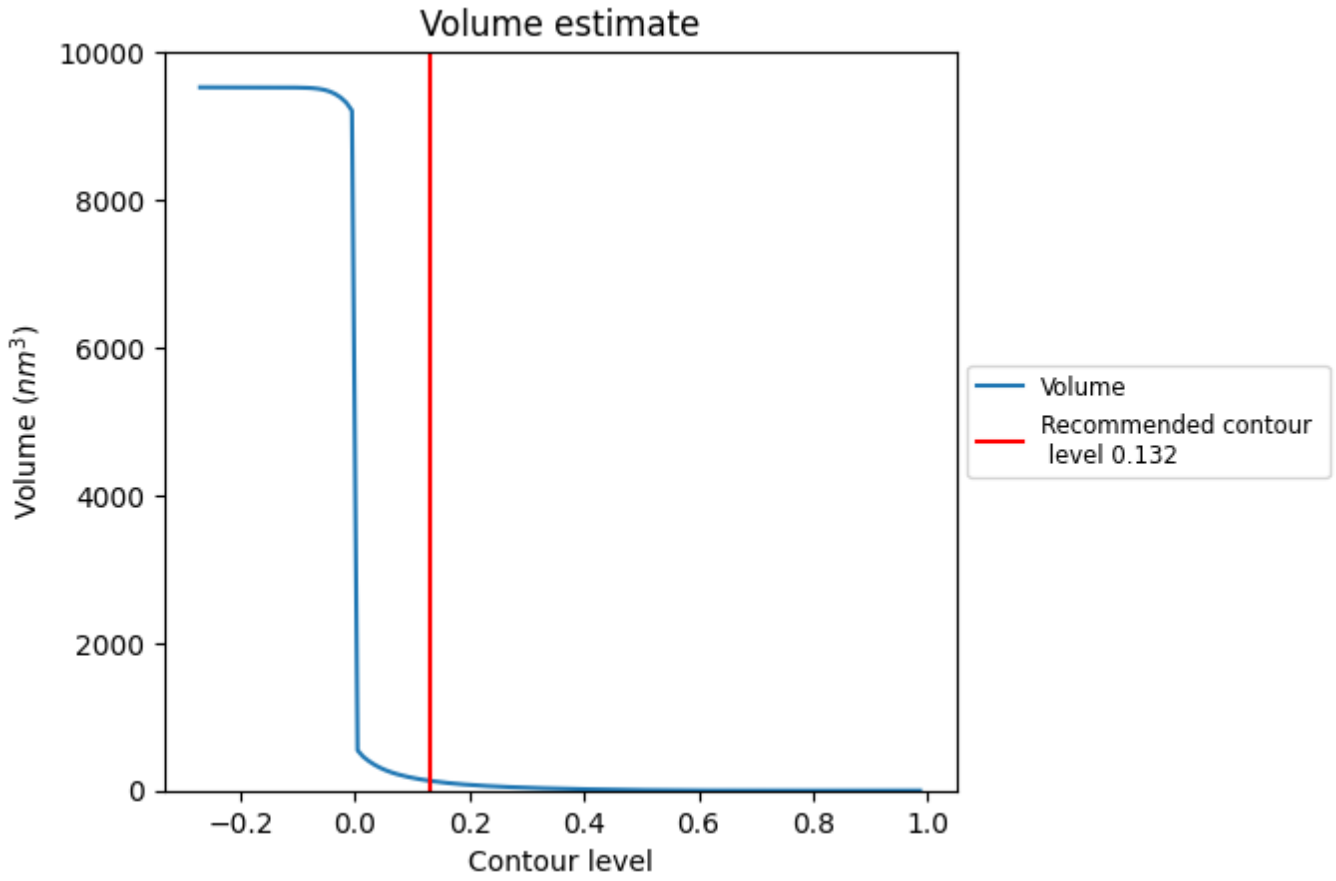
This section contains the results of statistical analysis of the map.

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.

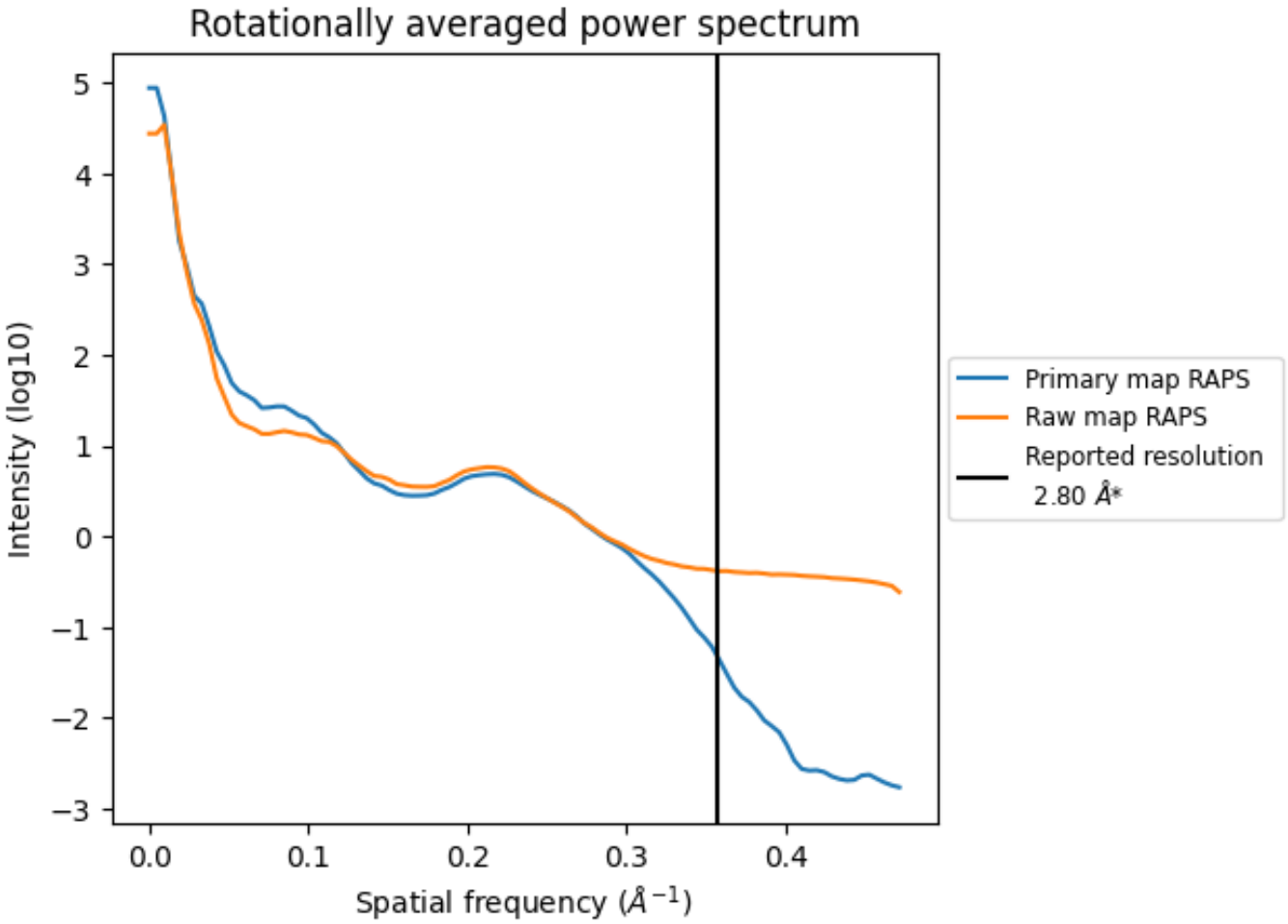
7.2 Volume estimate (i)



The volume at the recommended contour level is 131 nm^3; this corresponds to an approximate mass of 118 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)

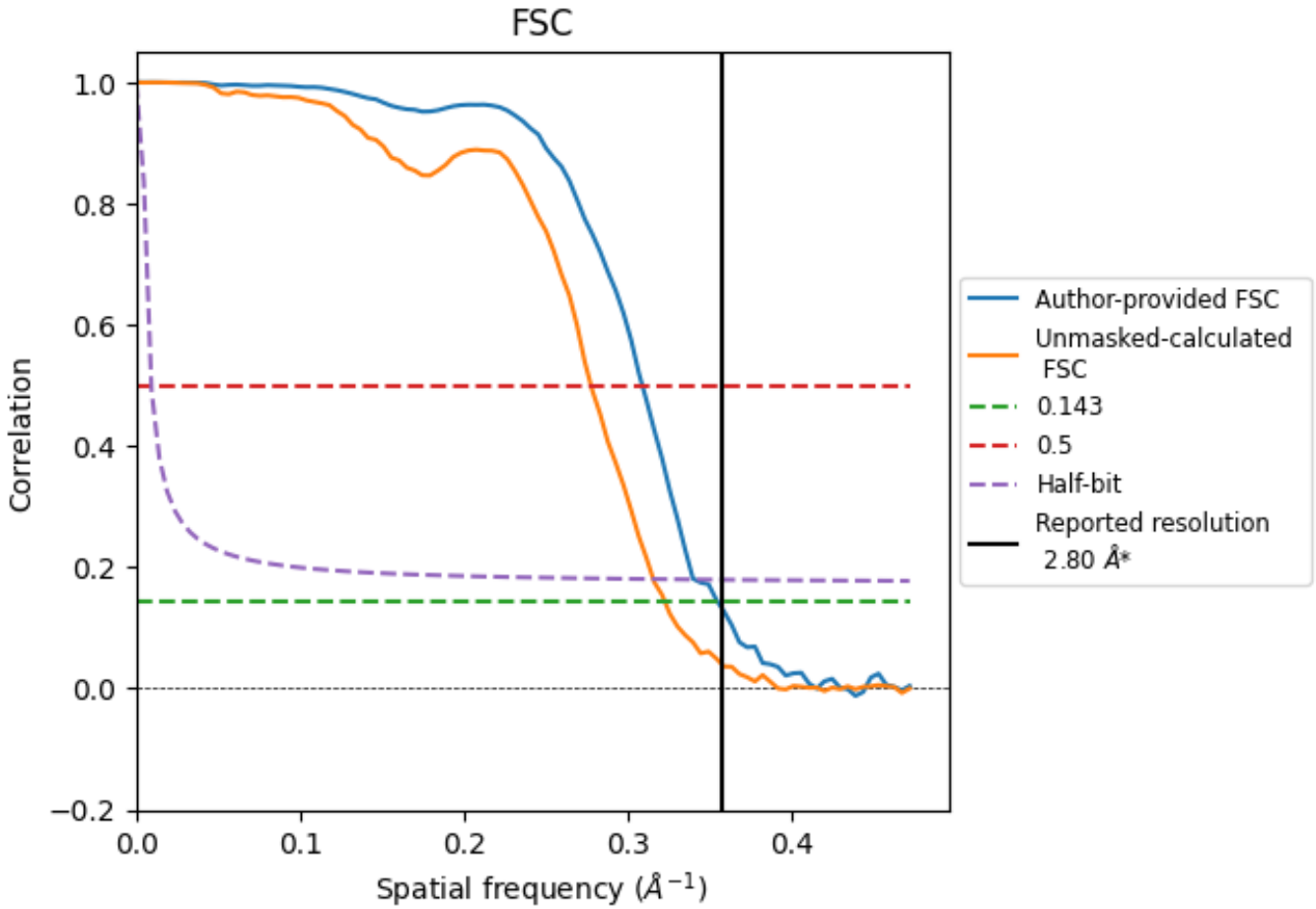


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

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 0.357 Å^{-1}

8.2 Resolution estimates (i)

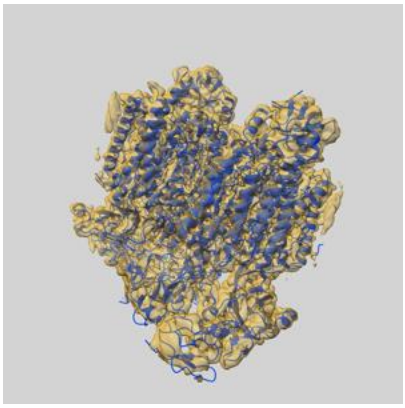
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.82	3.24	2.94
Unmasked-calculated*	3.10	3.60	3.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.10 differs from the reported value 2.8 by more than 10 %

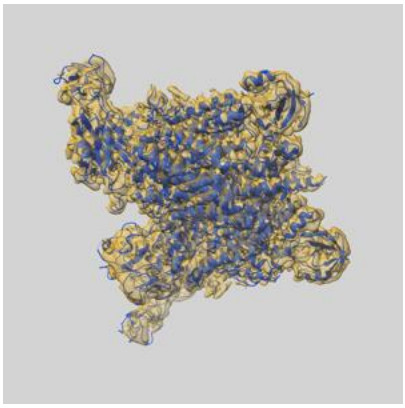
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14224 and PDB model 7R0W. Per-residue inclusion information can be found in section 3 on page 14.

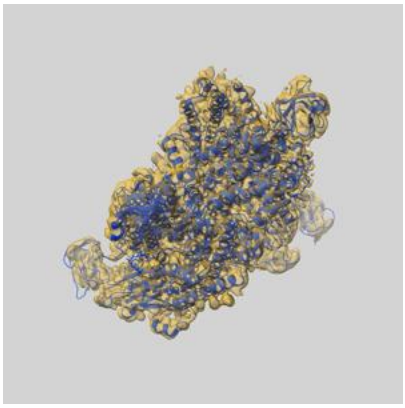
9.1 Map-model overlay



X



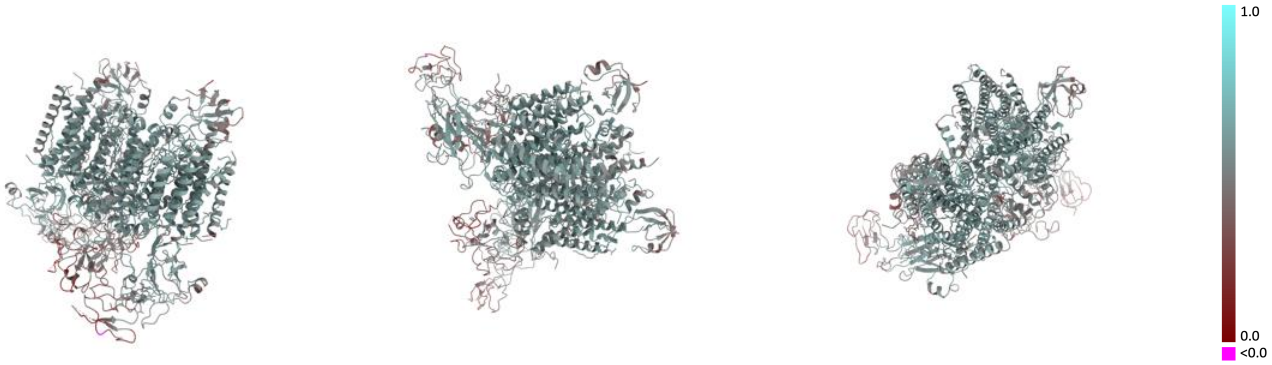
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.132 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

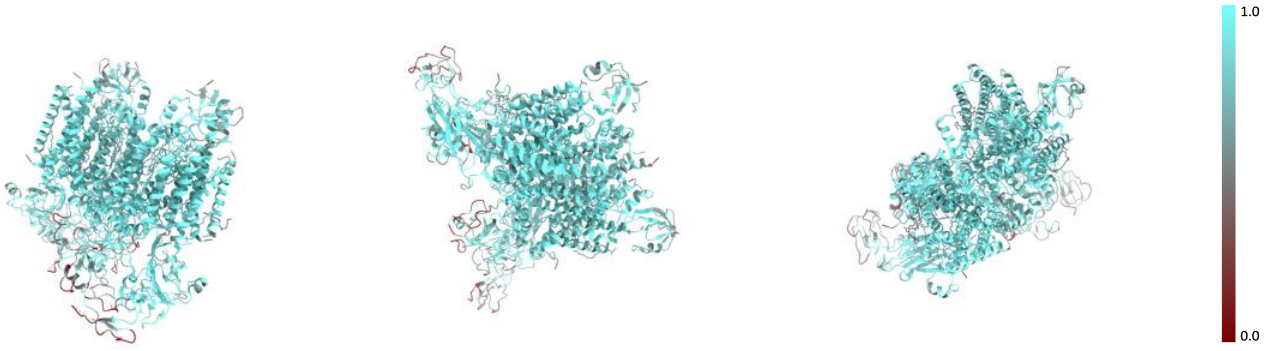
9.2 Q-score mapped to coordinate model



X Y Z

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

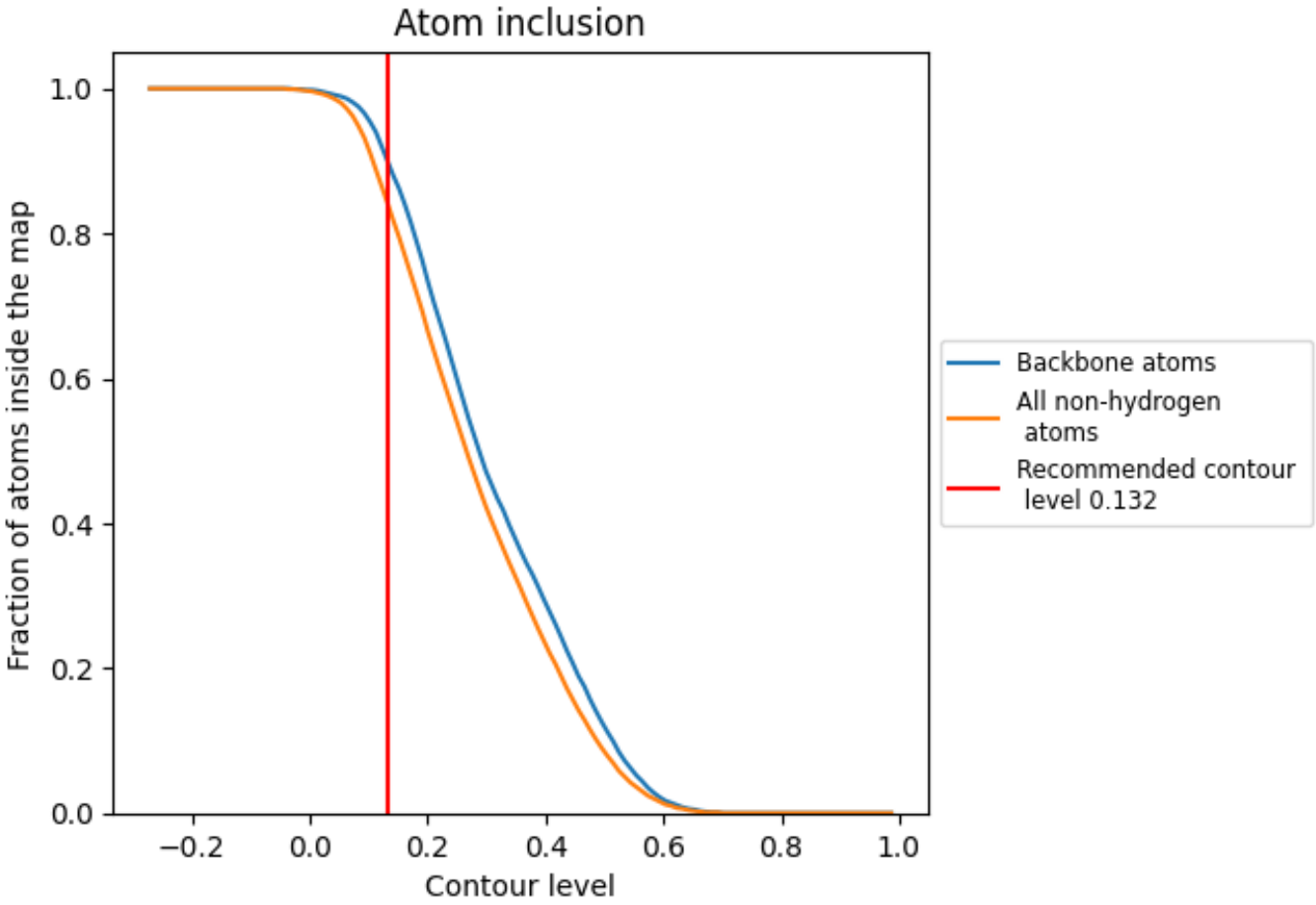
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.132).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 84% 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 (0.132) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8420	0.5230
A	0.9520	0.5910
B	0.8870	0.5630
C	0.8050	0.5040
D	0.6940	0.4050
E	0.8390	0.5420
F	0.9070	0.5350
G	0.9580	0.5720
H	0.9070	0.5670
I	0.9600	0.5890
J	0.8990	0.5670
K	0.8080	0.5060
L	0.7060	0.4120
M	0.8550	0.5130
N	0.8050	0.5080
O	0.9500	0.5880
P	0.9070	0.5640
V	0.7350	0.4680
X	0.7450	0.4690

