wwPDB EM Validation Summary Report

Aug 27, 2026 – 03:35 am BST

PDB ID	:	9F5Z / pdb_00009f5z
EMDB ID	:	EMD-50204
Title	:	Structure of the Chlamydomonas reinhardtii respiratory complex III from respiratory supercomplex
Authors	:	Waltz, F.; Righetto, R.; Kotecha, A.; Engel, B.D.
Deposited on	:	2024-04-30
Resolution	:	2.39 Å(reported)

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 ⓘ symbol.

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

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

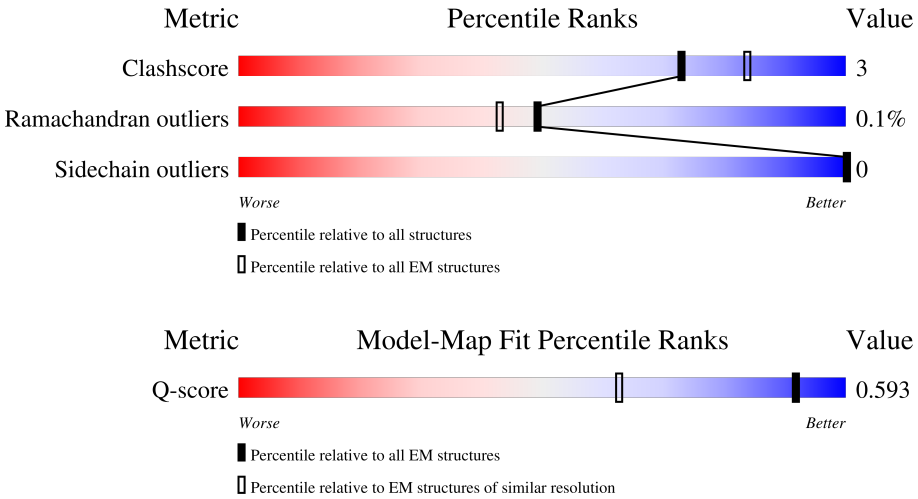
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.39 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.



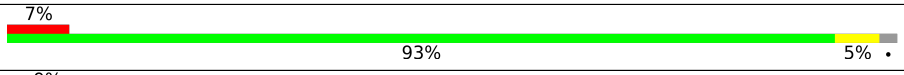
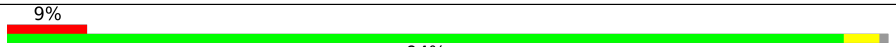
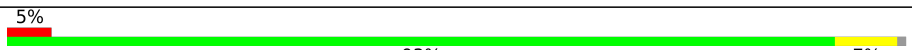
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4884 (1.90 - 2.89)

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	1A	381	93% 6% •
1	1B	381	89% 10% •
2	1C	262	45% 69% 10% 21%
2	1D	262	43% 69% 10% 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	1E	314	
3	1F	314	
4	1G	60	
4	1H	60	
5	1I	69	
5	1J	69	
6	1K	73	
6	1L	73	
7	1M	495	
7	1N	495	
8	1O	59	
8	1P	59	
9	1Q	485	
9	1S	485	
10	1R	123	
10	1T	123	

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 34454 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 Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	376	Total	C	N	O	S	0	0
			2958	1984	466	491	17		
1	1B	376	Total	C	N	O	S	0	0
			2958	1984	466	491	17		

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1C	207	Total	C	N	O	S	0	0
			1602	1017	279	299	7		
2	1D	207	Total	C	N	O	S	0	0
			1602	1017	279	299	7		

- Molecule 3 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1E	243	Total	C	N	O	S	0	0
			1898	1204	326	356	12		
3	1F	243	Total	C	N	O	S	0	0
			1898	1204	326	356	12		

- Molecule 4 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1G	59	Total	C	N	O	S	0	0
			486	316	79	88	3		
4	1H	59	Total	C	N	O	S	0	0
			486	316	79	88	3		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1I	68	Total	C	N	O	S	0	0
			550	347	92	105	6		
5	1J	68	Total	C	N	O	S	0	0
			550	347	92	105	6		

- Molecule 6 is a protein called Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1K	70	Total	C	N	O	S	0	0
			594	386	104	103	1		
6	1L	70	Total	C	N	O	S	0	0
			594	386	104	103	1		

- Molecule 7 is a protein called MPP-Beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1M	464	Total	C	N	O	S	0	0
			3646	2290	641	696	19		
7	1N	464	Total	C	N	O	S	0	0
			3646	2290	641	696	19		

- Molecule 8 is a protein called Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1O	48	Total	C	N	O	S	0	0
			371	249	61	60	1		
8	1P	48	Total	C	N	O	S	0	0
			371	249	61	60	1		

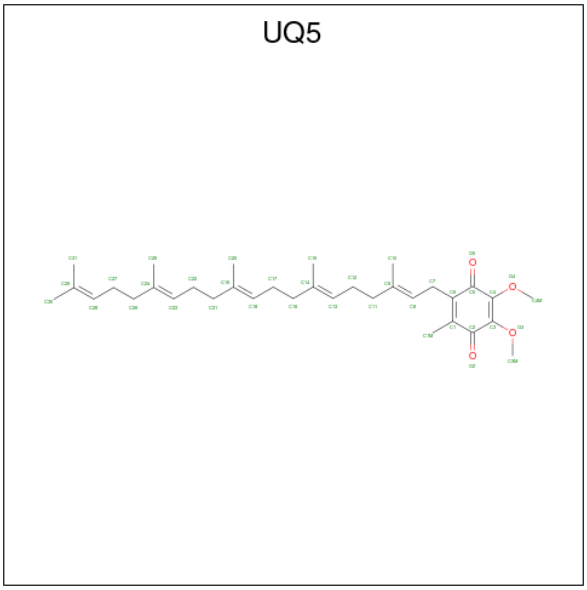
- Molecule 9 is a protein called Alpha-MPP.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1Q	441	Total	C	N	O	S	0	0
			3204	2018	562	619	5		
9	1S	441	Total	C	N	O	S	0	0
			3204	2018	562	619	5		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 7.

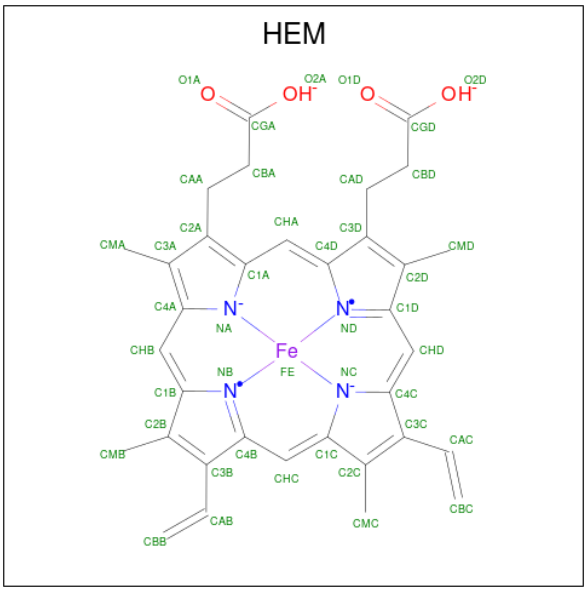
Mol	Chain	Residues	Atoms					AltConf	Trace
10	1R	122	Total	C	N	O	S	0	0
			980	617	178	183	2		
10	1T	122	Total	C	N	O	S	0	0
			980	617	178	183	2		

- Molecule 11 is 2,3-DIMETHOXY-5-METHYL-6-(3,11,15,19-TETRAMETHYL-EICOSA-2,6,10,14,18-PENTAENYL)-[1,4]BENZOQUINONE (CCD ID: UQ5) (formula: $C_{34}H_{50}O_4$).



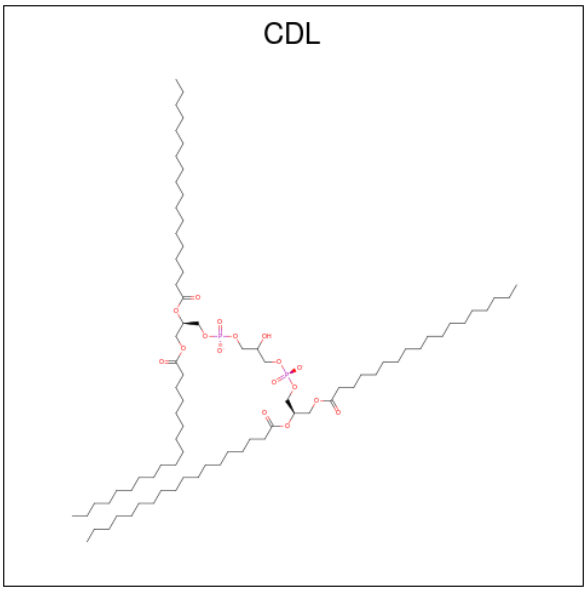
Mol	Chain	Residues	Atoms			AltConf
11	1A	1	Total	C	O	0
			38	34	4	
11	1A	1	Total	C	O	0
			38	34	4	
11	1B	1	Total	C	O	0
			38	34	4	
11	1B	1	Total	C	O	0
			38	34	4	

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



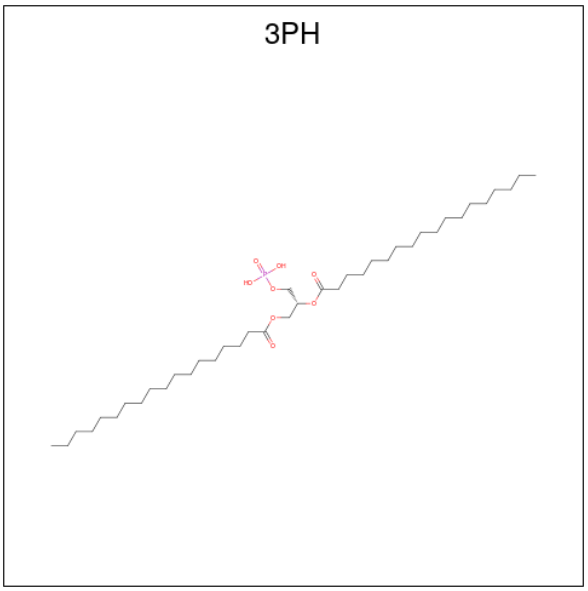
Mol	Chain	Residues	Atoms					AltConf
12	1A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	1A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	1B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	1B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	1E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	1F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 13 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



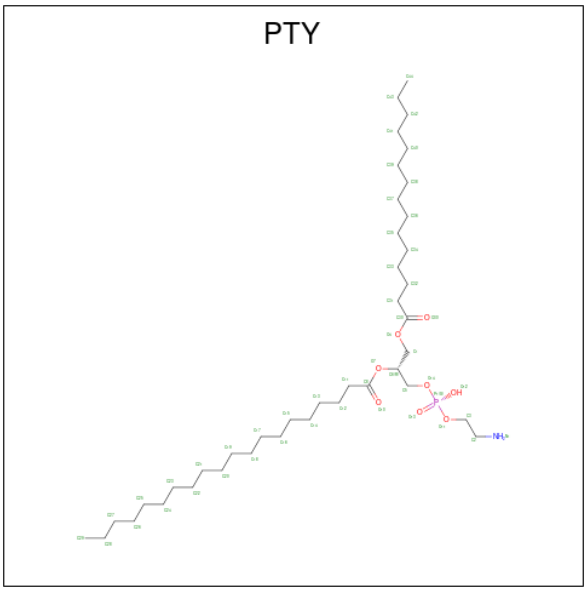
Mol	Chain	Residues	Atoms				AltConf
13	1A	1	Total 59	C 40	O 17	P 2	0
13	1B	1	Total 64	C 45	O 17	P 2	0
13	1B	1	Total 71	C 52	O 17	P 2	0
13	1E	1	Total 53	C 34	O 17	P 2	0
13	1F	1	Total 56	C 37	O 17	P 2	0
13	1K	1	Total 79	C 60	O 17	P 2	0
13	1L	1	Total 59	C 40	O 17	P 2	0
13	1M	1	Total 54	C 35	O 17	P 2	0

- Molecule 14 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



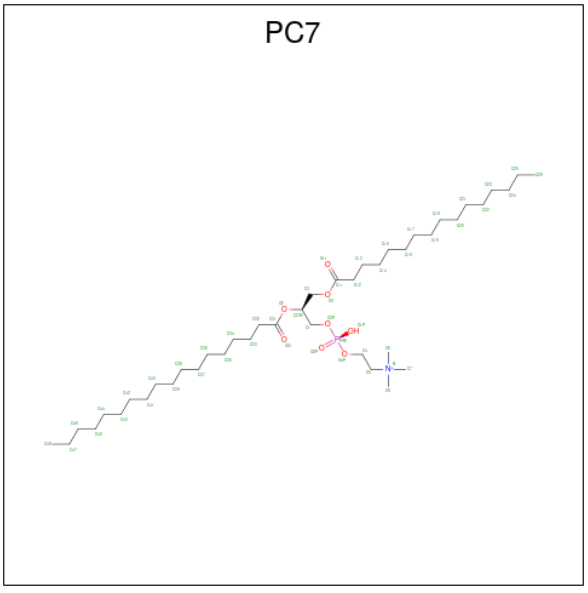
Mol	Chain	Residues	Atoms				AltConf
14	1A	1	Total 31	C 22	O 8	P 1	0
14	1B	1	Total 48	C 39	O 8	P 1	0
14	1B	1	Total 48	C 39	O 8	P 1	0
14	1E	1	Total 40	C 31	O 8	P 1	0
14	1K	1	Total 48	C 39	O 8	P 1	0
14	1K	1	Total 32	C 23	O 8	P 1	0
14	1R	1	Total 37	C 28	O 8	P 1	0

- Molecule 15 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
15	1E	1	Total	C	N	O	P	0
			34	24	1	8	1	
15	1F	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 16 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY) METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: PC7) (formula: $C_{42}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
16	1G	1	Total	C	N	O	P	0
			36	26	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
16	1H	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	1M	1	Total	Zn	0
			1	1	
17	1N	1	Total	Zn	0
			1	1	

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		AltConf
18	1A	48	Total	O	0
			48	48	
18	1B	52	Total	O	0
			52	52	
18	1C	13	Total	O	0
			13	13	
18	1D	12	Total	O	0
			12	12	
18	1E	51	Total	O	0
			51	51	
18	1F	34	Total	O	0
			34	34	
18	1G	7	Total	O	0
			7	7	
18	1H	9	Total	O	0
			9	9	
18	1I	11	Total	O	0
			11	11	
18	1J	3	Total	O	0
			3	3	
18	1K	12	Total	O	0
			12	12	
18	1L	12	Total	O	0
			12	12	
18	1M	76	Total	O	0
			76	76	
18	1N	74	Total	O	0
			74	74	

Continued on next page...

Continued from previous page...

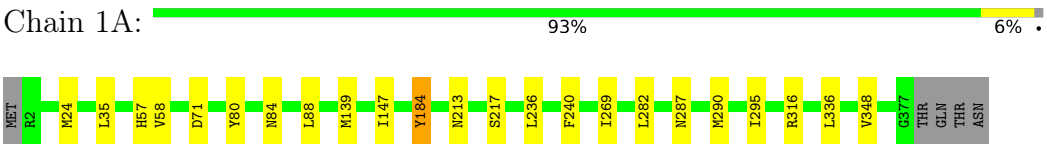
Mol	Chain	Residues	Atoms	AltConf
18	1O	4	Total O 4 4	0
18	1P	6	Total O 6 6	0
18	1Q	27	Total O 27 27	0
18	1R	32	Total O 32 32	0
18	1S	27	Total O 27 27	0
18	1T	28	Total O 28 28	0

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.

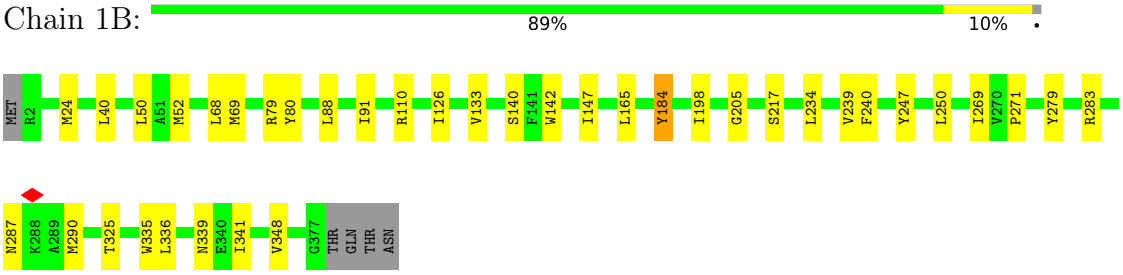
• Molecule 1: Cytochrome b

Chain 1A:



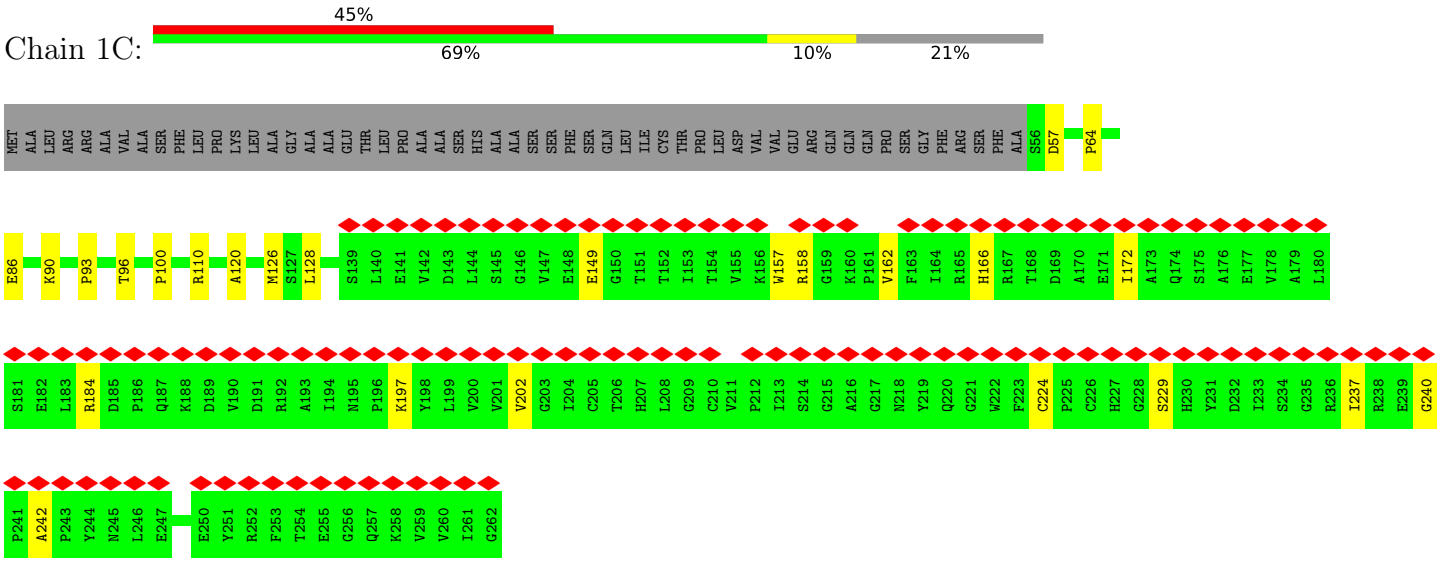
• Molecule 1: Cytochrome b

Chain 1B:

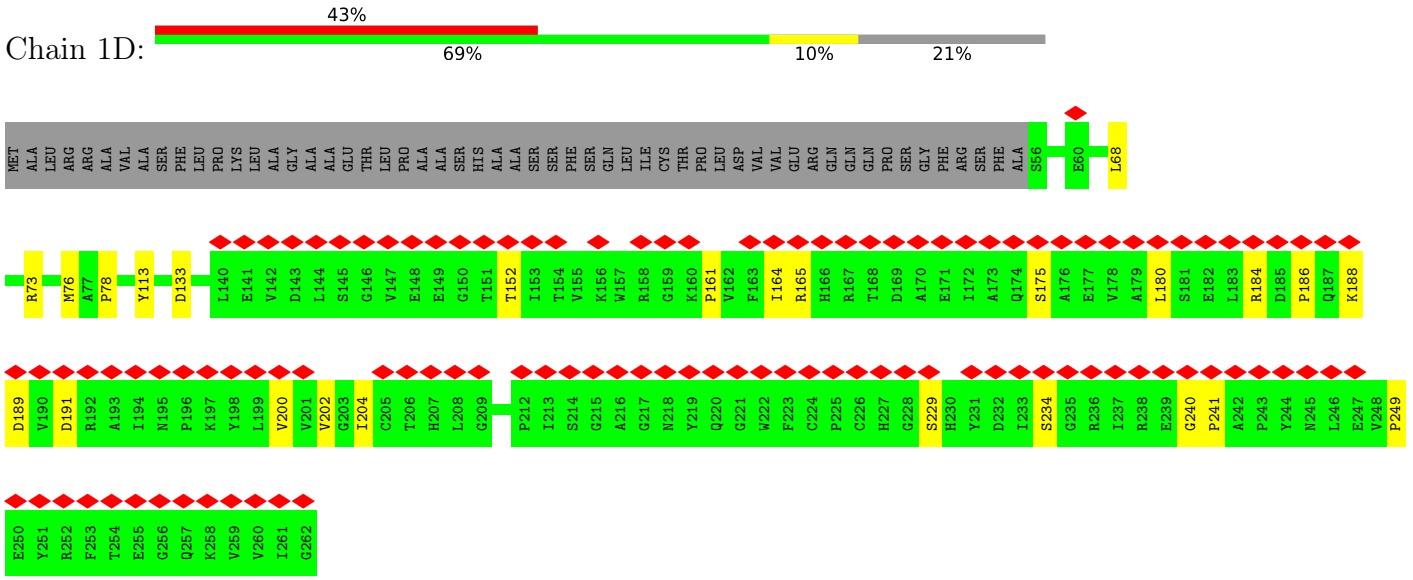


• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

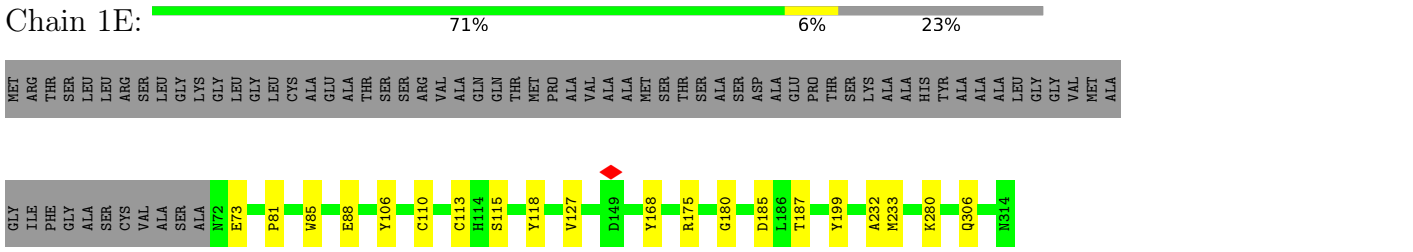
Chain 1C:



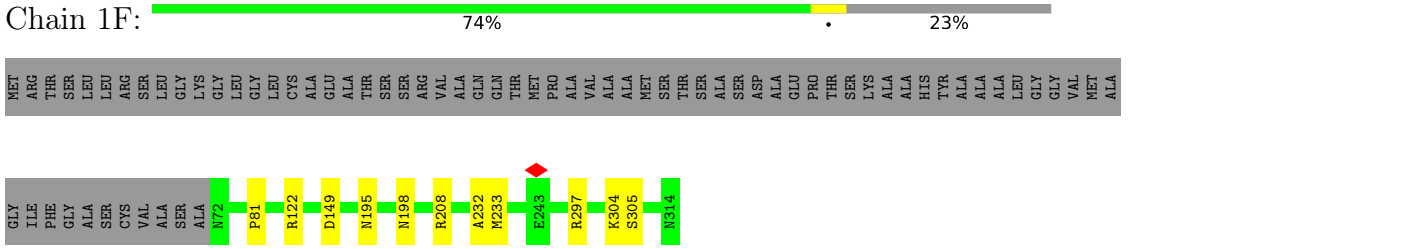
• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial



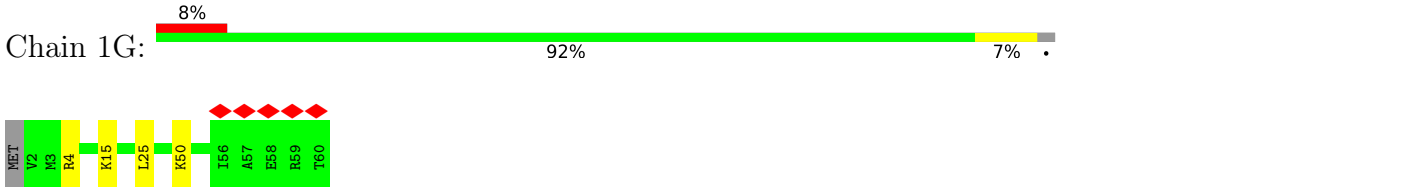
• Molecule 3: Cytochrome c1



• Molecule 3: Cytochrome c1

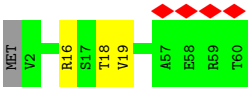


• Molecule 4: Complex III subunit 9



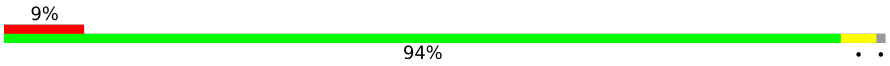
• Molecule 4: Complex III subunit 9

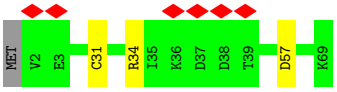




• Molecule 5: Cytochrome b-c1 complex subunit 6

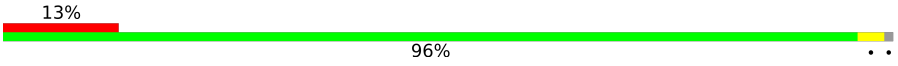
Chain 1I:

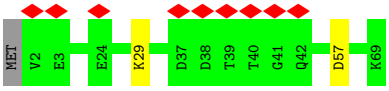




• Molecule 5: Cytochrome b-c1 complex subunit 6

Chain 1J:

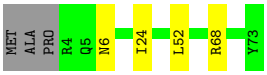




• Molecule 6: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8

Chain 1K:

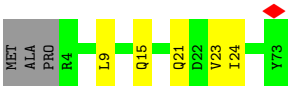




• Molecule 6: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8

Chain 1L:

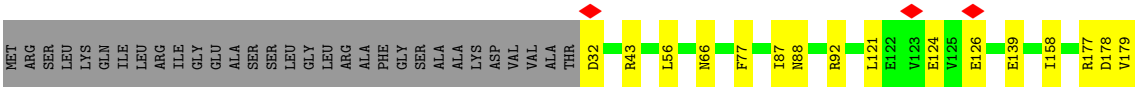


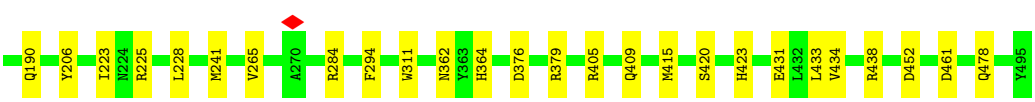


• Molecule 7: MPP-Beta

Chain 1M:



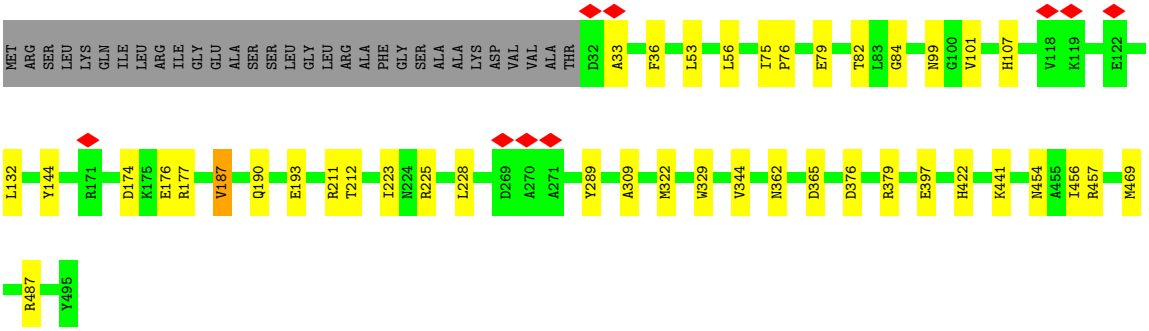




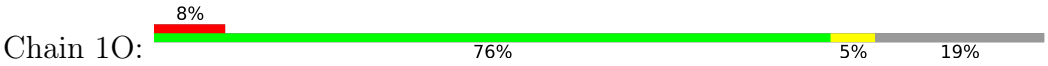
• Molecule 7: MPP-Beta

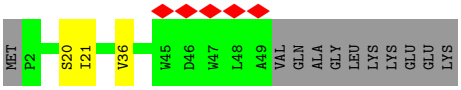
Chain 1N:





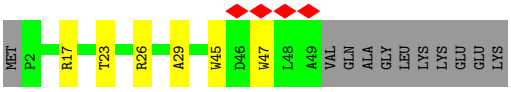
• Molecule 8: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10



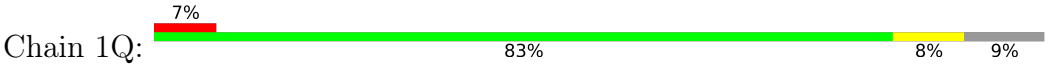


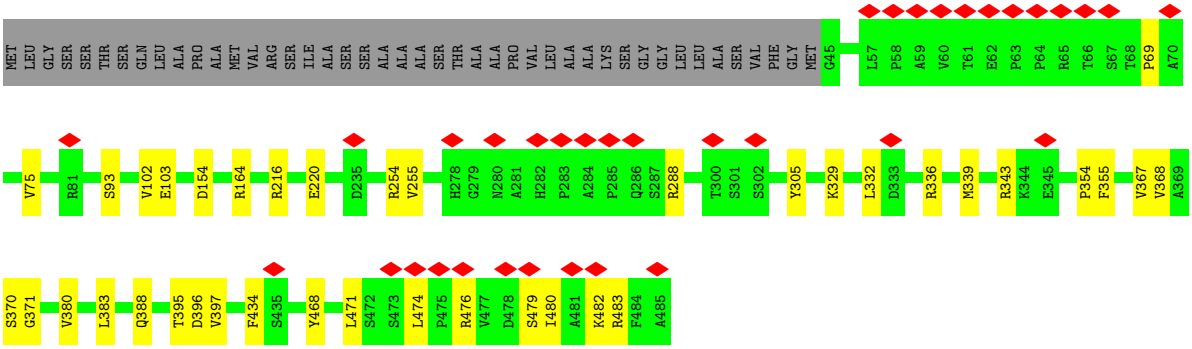
• Molecule 8: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10



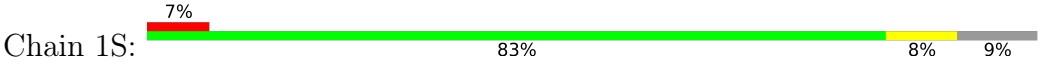


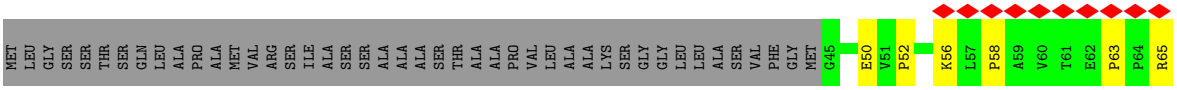
• Molecule 9: Alpha-MPP

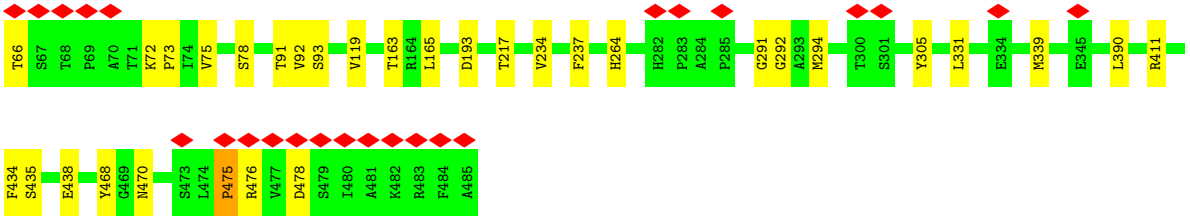




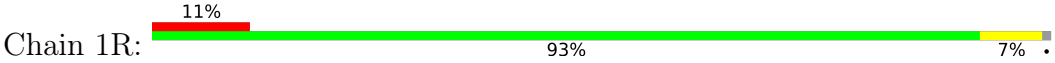
• Molecule 9: Alpha-MPP

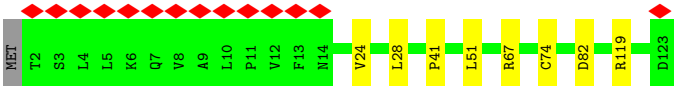




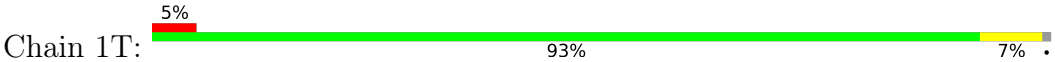


• Molecule 10: Cytochrome b-c1 complex subunit 7





• Molecule 10: Cytochrome b-c1 complex subunit 7





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83443	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.117	Depositor
Minimum map value	-0.534	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.145	Depositor
Map size (Å)	589.6, 589.6, 589.6	wwPDB
Map dimensions	588, 588, 588	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0027211, 1.0027211, 1.0027211	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UQ5, 3PH, PTY, CDL, HEM, ZN, PC7

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	1A	0.25	0/3060	0.48	1/4187 (0.0%)
1	1B	0.26	0/3060	0.48	1/4187 (0.0%)
2	1C	0.18	0/1643	0.36	0/2233
2	1D	0.17	0/1643	0.33	0/2233
3	1E	0.24	0/1953	0.43	1/2654 (0.0%)
3	1F	0.22	0/1953	0.38	0/2654
4	1G	0.23	0/496	0.41	0/667
4	1H	0.22	0/496	0.39	0/667
5	1I	0.23	0/567	0.45	0/766
5	1J	0.21	0/567	0.39	0/766
6	1K	0.25	0/609	0.44	0/817
6	1L	0.22	0/609	0.42	0/817
7	1M	0.23	0/3723	0.42	0/5046
7	1N	0.22	0/3723	0.38	0/5046
8	1O	0.19	0/385	0.44	0/531
8	1P	0.21	0/385	0.52	0/531
9	1Q	0.22	0/3258	0.43	0/4439
9	1S	0.21	0/3258	0.43	1/4439 (0.0%)
10	1R	0.21	0/996	0.35	0/1349
10	1T	0.23	0/996	0.41	0/1349
All	All	0.22	0/33380	0.42	4/45378 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1A	0	1
1	1B	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	184	TYR	N-CA-C	-5.96	104.87	111.36
3	1E	127	VAL	N-CA-C	-5.49	107.51	112.12
9	1S	234	VAL	N-CA-C	-5.43	107.08	111.91
1	1B	184	TYR	N-CA-C	-5.06	105.47	111.69

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1A	184	TYR	Sidechain
1	1B	184	TYR	Sidechain

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	1A	2958	0	2955	15	0
1	1B	2958	0	2953	25	0
2	1C	1602	0	1577	16	0
2	1D	1602	0	1577	15	0
3	1E	1898	0	1800	13	0
3	1F	1898	0	1800	10	0
4	1G	486	0	490	4	0
4	1H	486	0	490	2	0
5	1I	550	0	501	2	0
5	1J	550	0	501	2	0
6	1K	594	0	590	4	0
6	1L	594	0	590	5	0
7	1M	3646	0	3555	29	0
7	1N	3646	0	3555	28	0
8	1O	371	0	372	2	0
8	1P	371	0	372	5	0
9	1Q	3204	0	3271	26	0
9	1S	3204	0	3271	23	0
10	1R	980	0	1004	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	1T	980	0	1005	6	0
11	1A	76	0	100	2	0
11	1B	76	0	100	8	0
12	1A	86	0	60	0	0
12	1B	86	0	60	2	0
12	1E	43	0	30	3	0
12	1F	43	0	30	2	0
13	1A	59	0	62	1	0
13	1B	135	0	159	6	0
13	1E	53	0	50	1	0
13	1F	56	0	56	1	0
13	1K	79	0	105	5	0
13	1L	59	0	62	0	0
13	1M	54	0	52	0	0
14	1A	31	0	35	0	0
14	1B	96	0	150	1	0
14	1E	40	0	56	1	0
14	1K	80	0	112	2	0
14	1R	37	0	50	1	0
15	1E	34	0	41	2	0
15	1F	38	0	49	0	0
16	1G	36	0	46	3	0
16	1H	39	0	52	2	0
17	1M	1	0	0	0	0
17	1N	1	0	0	0	0
18	1A	48	0	0	1	0
18	1B	52	0	0	0	0
18	1C	13	0	0	0	0
18	1D	12	0	0	0	0
18	1E	51	0	0	0	0
18	1F	34	0	0	0	0
18	1G	7	0	0	1	0
18	1H	9	0	0	0	0
18	1I	11	0	0	0	0
18	1J	3	0	0	0	0
18	1K	12	0	0	0	0
18	1L	12	0	0	0	0
18	1M	76	0	0	1	0
18	1N	74	0	0	0	0
18	1O	4	0	0	0	0
18	1P	6	0	0	0	0
18	1Q	27	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	1R	32	0	0	0	0
18	1S	27	0	0	0	0
18	1T	28	0	0	0	0
All	All	34454	0	33746	226	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 226 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)
7:1M:121:LEU:HB3	9:1Q:339:MET:HE1	1.74	0.67
9:1S:50:GLU:HG2	9:1S:52:PRO:HD2	1.79	0.64
9:1Q:216:ARG:HH22	9:1S:470:ASN:HB2	1.64	0.63
2:1D:180:LEU:HB3	2:1D:186:PRO:HB3	1.80	0.63
1:1A:269:ILE:HG22	11:1A:402:UQ5:H3M1	1.81	0.63

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	1A	374/381 (98%)	363 (97%)	11 (3%)	0	100	100
1	1B	374/381 (98%)	366 (98%)	8 (2%)	0	100	100
2	1C	205/262 (78%)	194 (95%)	11 (5%)	0	100	100
2	1D	205/262 (78%)	201 (98%)	4 (2%)	0	100	100
3	1E	241/314 (77%)	236 (98%)	5 (2%)	0	100	100
3	1F	241/314 (77%)	235 (98%)	6 (2%)	0	100	100
4	1G	57/60 (95%)	57 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	1H	57/60 (95%)	57 (100%)	0	0	100	100
5	1I	66/69 (96%)	66 (100%)	0	0	100	100
5	1J	66/69 (96%)	64 (97%)	2 (3%)	0	100	100
6	1K	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
6	1L	68/73 (93%)	65 (96%)	3 (4%)	0	100	100
7	1M	462/495 (93%)	454 (98%)	8 (2%)	0	100	100
7	1N	462/495 (93%)	456 (99%)	5 (1%)	1 (0%)	43	58
8	1O	46/59 (78%)	43 (94%)	3 (6%)	0	100	100
8	1P	46/59 (78%)	44 (96%)	2 (4%)	0	100	100
9	1Q	439/485 (90%)	418 (95%)	20 (5%)	1 (0%)	43	58
9	1S	439/485 (90%)	424 (97%)	13 (3%)	2 (0%)	24	37
10	1R	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
10	1T	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
All	All	4156/4642 (90%)	4047 (97%)	105 (2%)	4 (0%)	49	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	1Q	396	ASP
9	1S	66	THR
7	1N	187	VAL
9	1S	475	PRO

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	1A	312/317 (98%)	312 (100%)	0	100	100
1	1B	312/317 (98%)	312 (100%)	0	100	100
2	1C	171/213 (80%)	171 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1D	171/213 (80%)	171 (100%)	0	100	100
3	1E	191/238 (80%)	191 (100%)	0	100	100
3	1F	191/238 (80%)	191 (100%)	0	100	100
4	1G	52/53 (98%)	52 (100%)	0	100	100
4	1H	52/53 (98%)	52 (100%)	0	100	100
5	1I	58/59 (98%)	58 (100%)	0	100	100
5	1J	58/59 (98%)	58 (100%)	0	100	100
6	1K	62/64 (97%)	62 (100%)	0	100	100
6	1L	62/64 (97%)	62 (100%)	0	100	100
7	1M	390/413 (94%)	390 (100%)	0	100	100
7	1N	390/413 (94%)	390 (100%)	0	100	100
8	1O	38/47 (81%)	38 (100%)	0	100	100
8	1P	38/47 (81%)	38 (100%)	0	100	100
9	1Q	333/362 (92%)	333 (100%)	0	100	100
9	1S	333/362 (92%)	333 (100%)	0	100	100
10	1R	106/107 (99%)	106 (100%)	0	100	100
10	1T	106/107 (99%)	106 (100%)	0	100	100
All	All	3426/3746 (92%)	3426 (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. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
7	1N	198	HIS
9	1S	198	GLN
7	1N	291	HIS
9	1Q	225	HIS
9	1S	211	ASN

5.3.3 RNA

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)

Of 31 ligands modelled in this entry, 2 are monoatomic - leaving 29 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	3PH	1K	102	-	47,47,47	0.64	1 (2%)	51,52,52	0.60	2 (3%)
11	UQ5	1A	401	-	38,38,38	0.53	0	46,49,49	1.08	4 (8%)
13	CDL	1K	101	-	78,78,99	0.42	0	84,90,111	0.28	0
14	3PH	1E	402	-	39,39,47	0.70	1 (2%)	43,44,52	0.64	0
13	CDL	1F	401	-	55,55,99	0.42	0	61,67,111	0.27	0
16	PC7	1H	101	-	38,38,51	0.57	0	44,46,59	0.56	0
14	3PH	1A	406	-	30,30,47	0.78	1 (3%)	34,35,52	0.69	1 (2%)
13	CDL	1A	405	-	58,58,99	0.44	0	64,70,111	0.27	0
14	3PH	1K	103	-	31,31,47	0.78	1 (3%)	35,36,52	0.66	1 (2%)
14	3PH	1R	201	10	36,36,47	0.71	1 (2%)	40,41,52	0.70	1 (2%)
12	HEM	1E	404	3	50,50,50	2.14	10 (20%)	66,82,82	1.47	7 (10%)
12	HEM	1A	403	1	50,50,50	1.49	7 (14%)	66,82,82	1.38	8 (12%)
14	3PH	1B	407	-	47,47,47	0.63	1 (2%)	51,52,52	0.61	0
15	PTY	1E	403	-	33,33,49	0.55	0	36,38,54	0.50	0
12	HEM	1A	404	1	50,50,50	1.31	7 (14%)	66,82,82	1.29	8 (12%)
13	CDL	1M	501	-	53,53,99	0.49	1 (1%)	59,65,111	0.26	0
12	HEM	1F	402	3	50,50,50	2.09	8 (16%)	66,82,82	1.52	10 (15%)
12	HEM	1B	404	1	50,50,50	1.37	7 (14%)	66,82,82	1.24	8 (12%)
11	UQ5	1A	402	-	38,38,38	0.53	0	46,49,49	0.67	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	UQ5	1B	402	-	38,38,38	0.51	0	46,49,49	1.52	6 (13%)
13	CDL	1B	405	-	63,63,99	0.44	1 (1%)	69,75,111	0.25	0
13	CDL	1L	101	-	58,58,99	0.43	0	64,70,111	0.35	0
16	PC7	1G	301	-	35,35,51	0.61	0	41,43,59	0.60	1 (2%)
11	UQ5	1B	401	-	38,38,38	0.46	0	46,49,49	0.73	1 (2%)
14	3PH	1B	406	-	47,47,47	0.63	1 (2%)	51,52,52	0.61	1 (1%)
12	HEM	1B	403	1	50,50,50	1.42	8 (16%)	66,82,82	1.36	10 (15%)
13	CDL	1B	408	1	70,70,99	0.34	0	76,82,111	0.34	0
15	PTY	1F	403	-	37,37,49	0.51	0	40,42,54	0.44	0
13	CDL	1E	401	-	52,52,99	0.44	0	58,64,111	0.25	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
14	3PH	1K	102	-	-	15/49/49/49	-
11	UQ5	1A	401	-	-	10/33/57/57	0/1/1/1
13	CDL	1K	101	-	-	59/89/89/110	-
14	3PH	1E	402	-	-	17/41/41/49	-
13	CDL	1F	401	-	-	32/66/66/110	-
16	PC7	1H	101	-	-	19/42/42/55	-
14	3PH	1A	406	-	-	13/32/32/49	-
13	CDL	1A	405	-	-	34/69/69/110	-
14	3PH	1K	103	-	-	13/33/33/49	-
14	3PH	1R	201	10	-	13/38/38/49	-
12	HEM	1E	404	3	-	4/14/54/54	-
12	HEM	1A	403	1	-	3/14/54/54	-
14	3PH	1B	407	-	-	18/49/49/49	-
15	PTY	1E	403	-	-	15/37/37/53	-
12	HEM	1A	404	1	-	4/14/54/54	-
13	CDL	1M	501	-	-	31/64/64/110	-
12	HEM	1F	402	3	-	4/14/54/54	-
12	HEM	1B	404	1	-	4/14/54/54	-
11	UQ5	1A	402	-	-	9/33/57/57	0/1/1/1
11	UQ5	1B	402	-	-	10/33/57/57	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CDL	1B	405	-	-	49/74/74/110	-
13	CDL	1L	101	-	-	43/69/69/110	-
16	PC7	1G	301	-	-	16/39/39/55	-
11	UQ5	1B	401	-	-	7/33/57/57	0/1/1/1
14	3PH	1B	406	-	-	22/49/49/49	-
12	HEM	1B	403	1	-	4/14/54/54	-
13	CDL	1B	408	1	-	45/81/81/110	-
15	PTY	1F	403	-	-	17/41/41/53	-
13	CDL	1E	401	-	-	41/63/63/110	-

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	1E	404	HEM	C3D-C2D	7.85	1.53	1.36
12	1F	402	HEM	C3D-C2D	7.73	1.53	1.36
12	1F	402	HEM	CBC-CAC	4.94	1.54	1.30
12	1E	404	HEM	CBC-CAC	4.89	1.54	1.30
12	1F	402	HEM	FE-ND	4.88	2.10	1.94

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	1E	404	HEM	C4D-ND-C1D	6.28	111.56	105.07
12	1F	402	HEM	C4D-ND-C1D	5.44	110.69	105.07
11	1B	402	UQ5	C7-C6-C5	5.13	124.65	118.48
11	1B	402	UQ5	C6-C1-C2	4.44	122.69	119.18
12	1A	403	HEM	C3B-C2B-C1B	4.37	109.72	106.49

There are no chirality outliers.

5 of 571 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	1A	401	UQ5	C1-C6-C7-C8
11	1A	401	UQ5	C5-C6-C7-C8
11	1A	401	UQ5	C9-C11-C12-C13
11	1A	401	UQ5	C24-C26-C27-C28
11	1A	402	UQ5	C14-C16-C17-C18

There are no ring outliers.

20 monomers are involved in 42 short contacts:

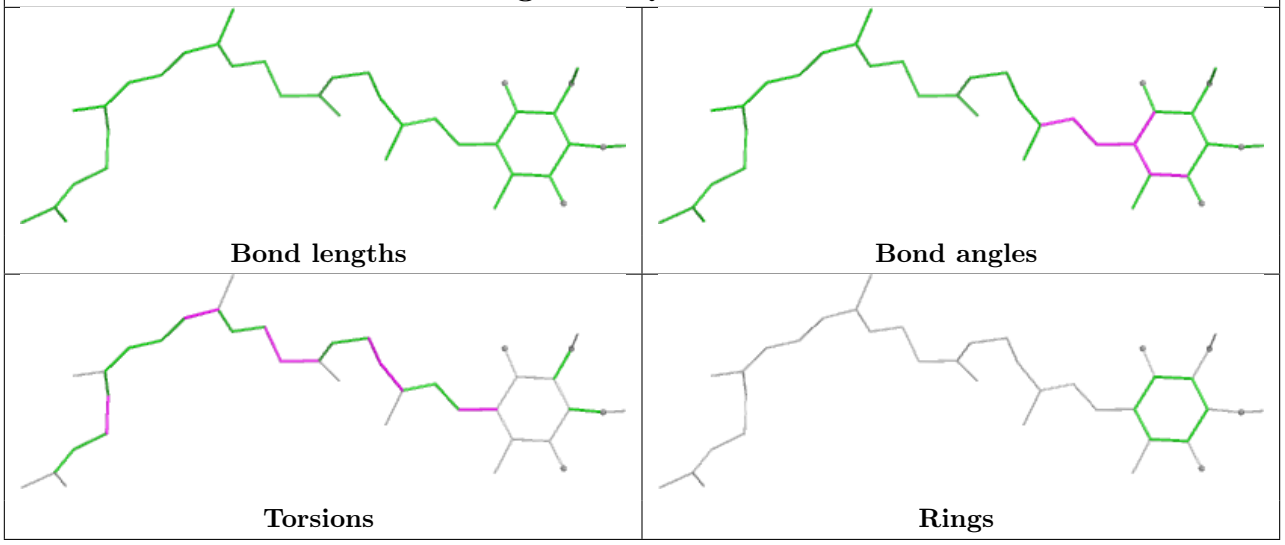
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	1K	102	3PH	1	0
13	1K	101	CDL	5	0
14	1E	402	3PH	1	0
13	1F	401	CDL	1	0
16	1H	101	PC7	2	0
13	1A	405	CDL	1	0
14	1K	103	3PH	1	0
14	1R	201	3PH	1	0
12	1E	404	HEM	3	0
15	1E	403	PTY	2	0
12	1F	402	HEM	2	0
11	1A	402	UQ5	2	0
11	1B	402	UQ5	4	0
13	1B	405	CDL	4	0
16	1G	301	PC7	3	0
11	1B	401	UQ5	4	0
14	1B	406	3PH	1	0
12	1B	403	HEM	2	0
13	1B	408	CDL	2	0
13	1E	401	CDL	1	0

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

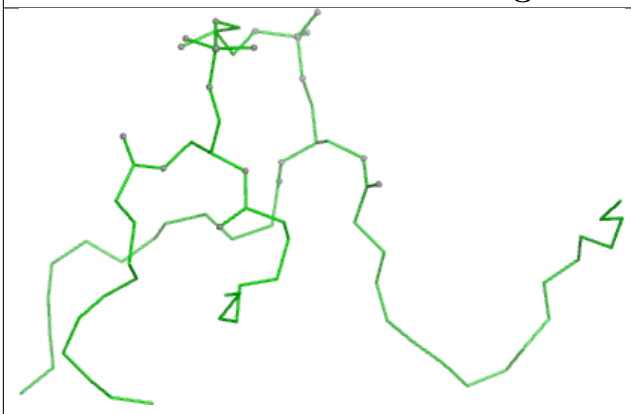
Ligand 3PH 1K 102



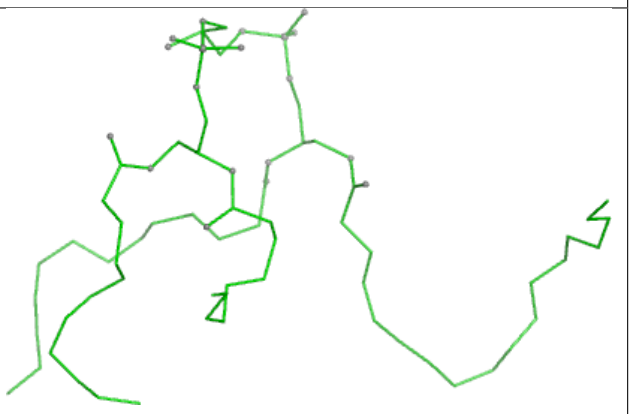
Ligand UQ5 1A 401



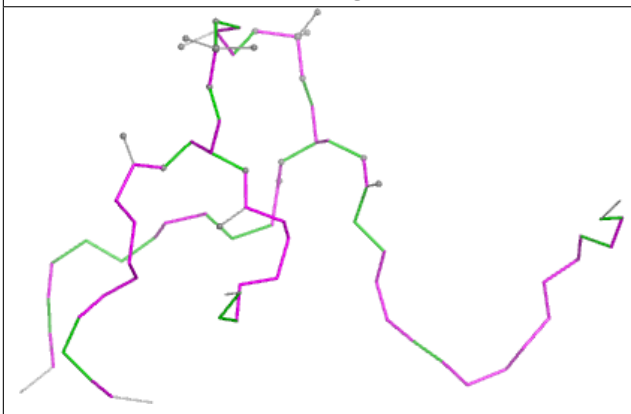
Ligand CDL 1K 101



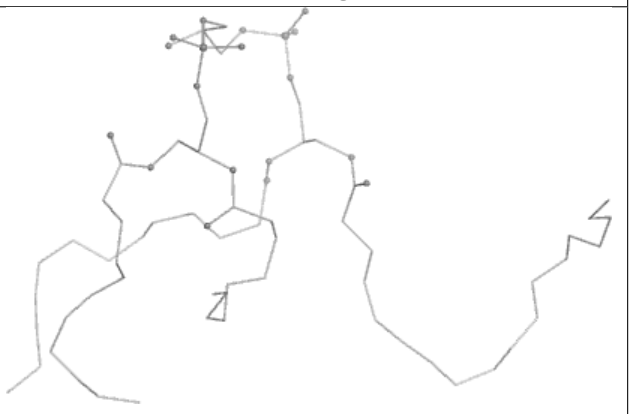
Bond lengths



Bond angles

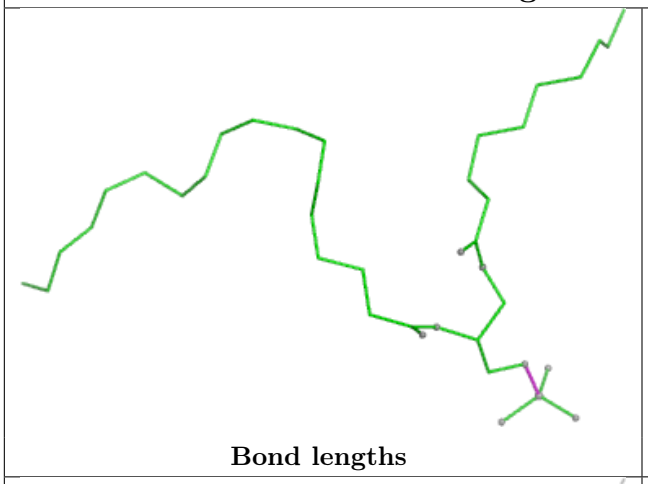


Torsions

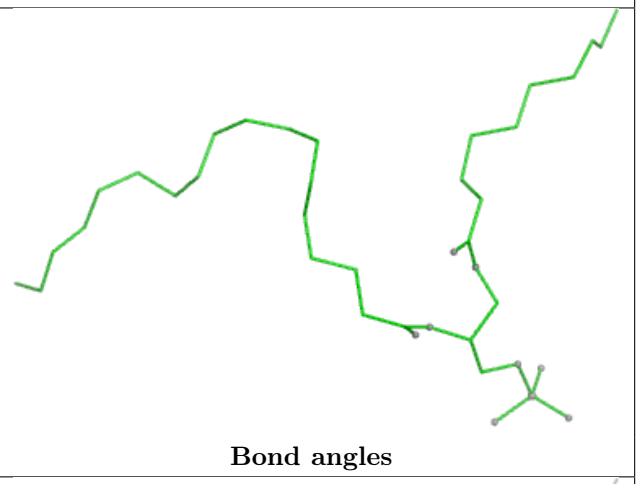


Rings

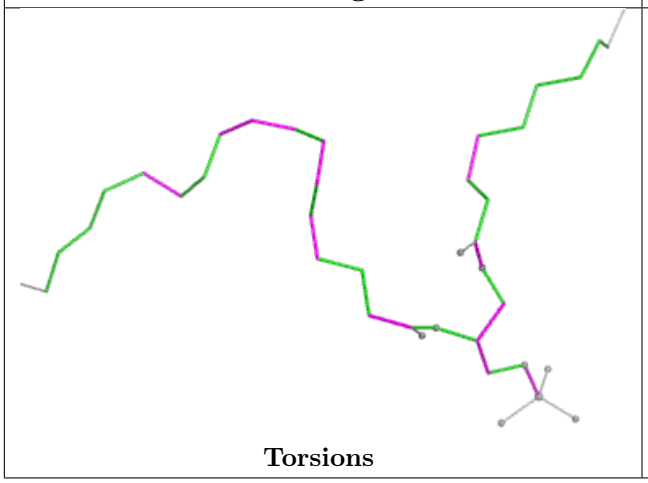
Ligand 3PH 1E 402



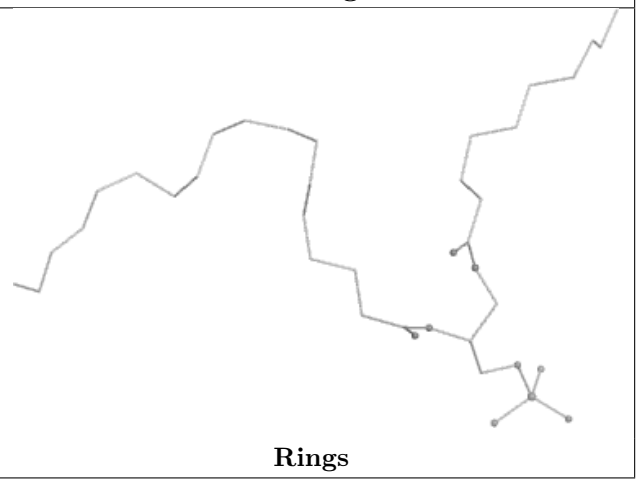
Bond lengths



Bond angles

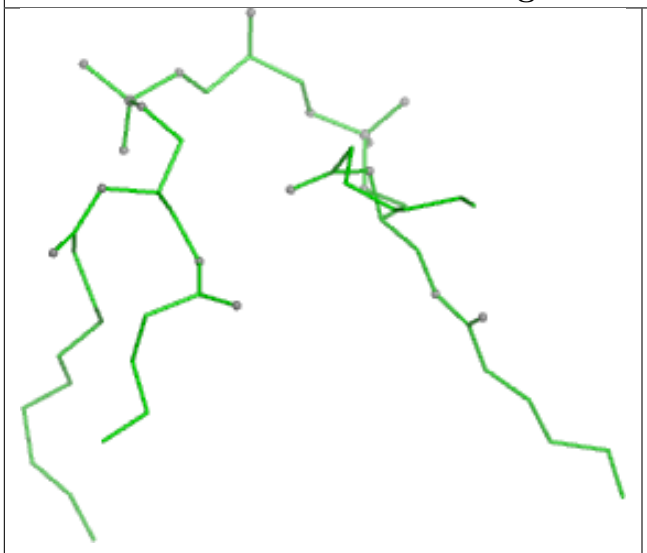


Torsions

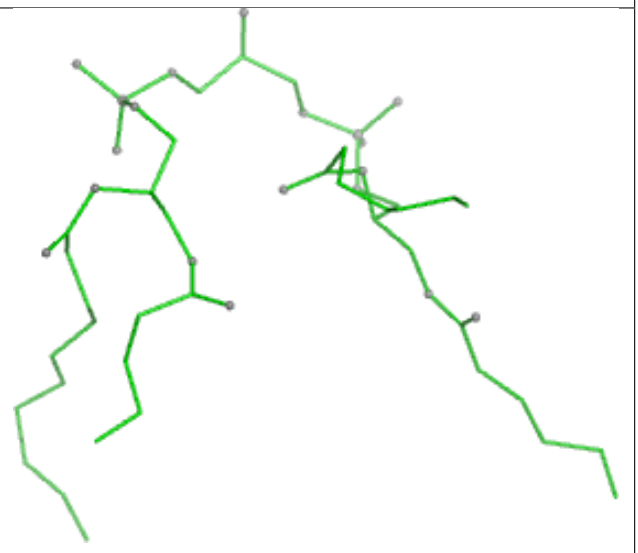


Rings

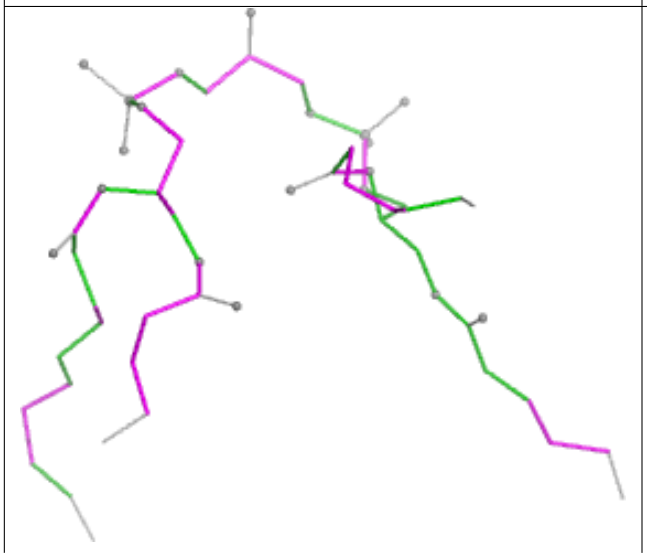
Ligand CDL 1F 401



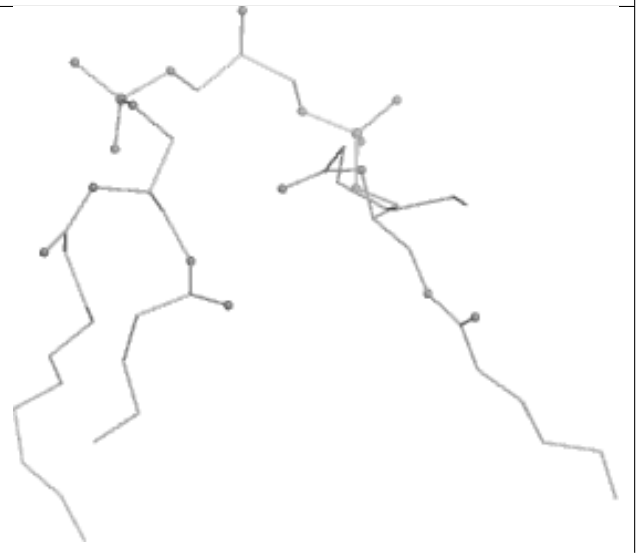
Bond lengths



Bond angles

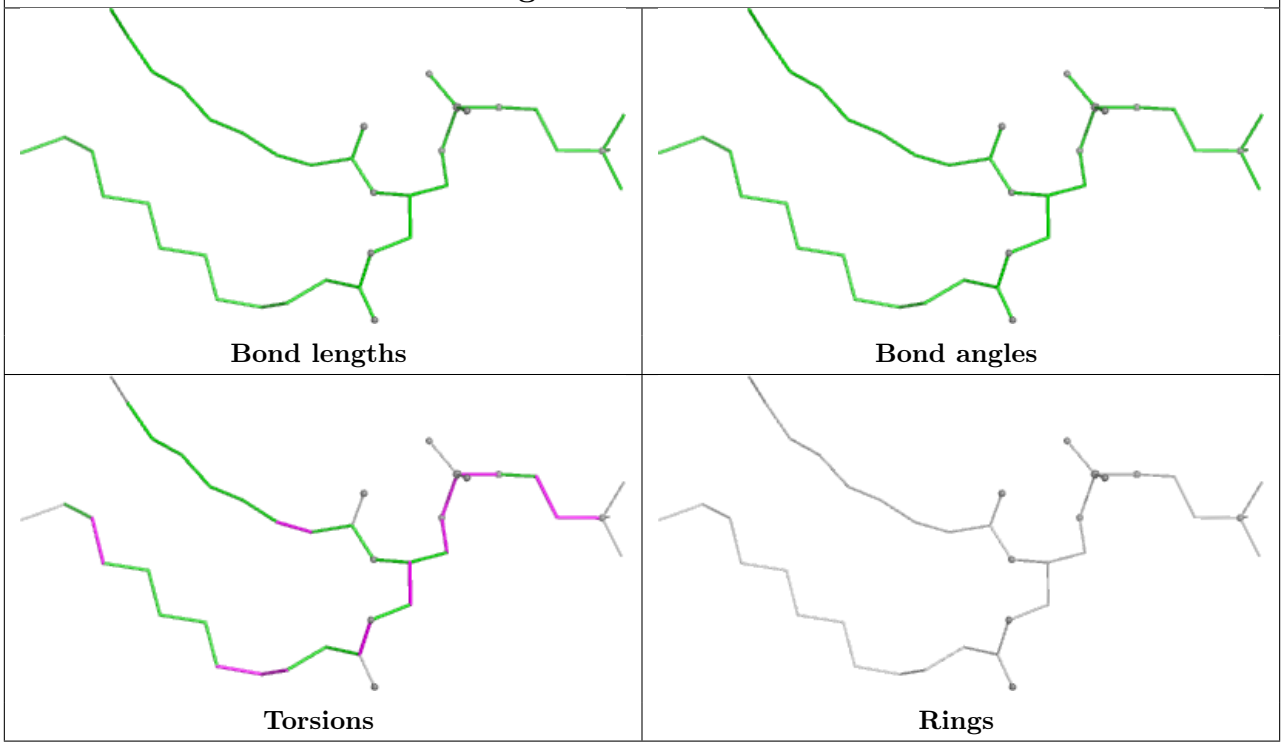


Torsions

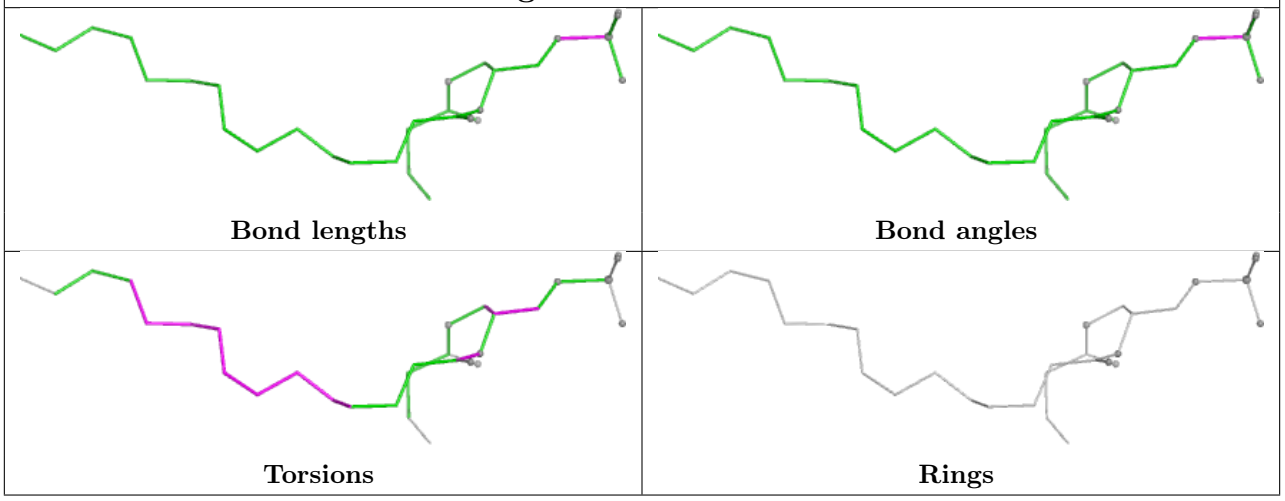


Rings

Ligand PC7 1H 101



Ligand 3PH 1A 406



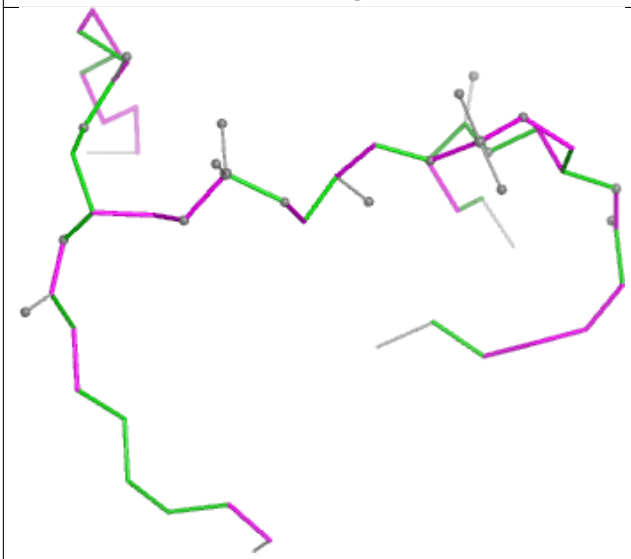
Ligand CDL 1A 405



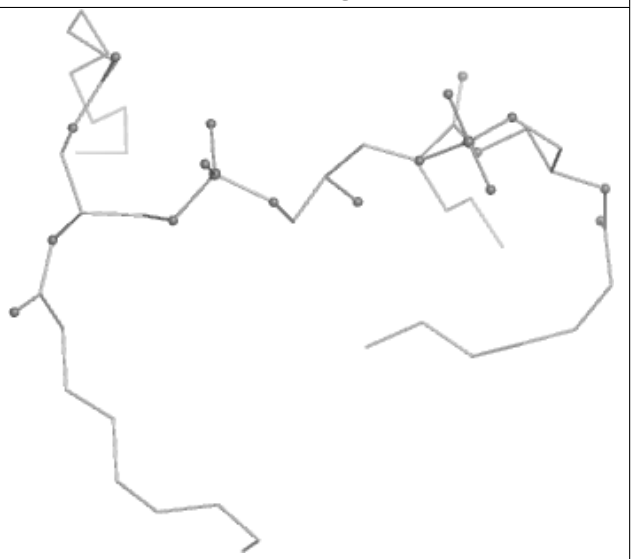
Bond lengths



Bond angles

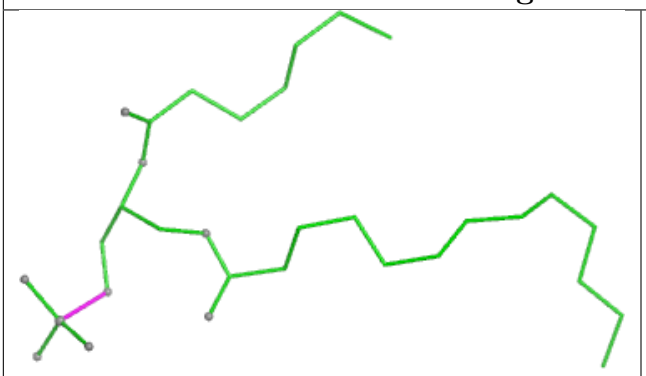


Torsions

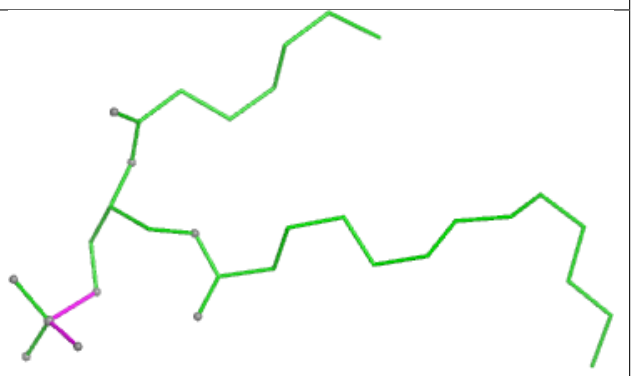


Rings

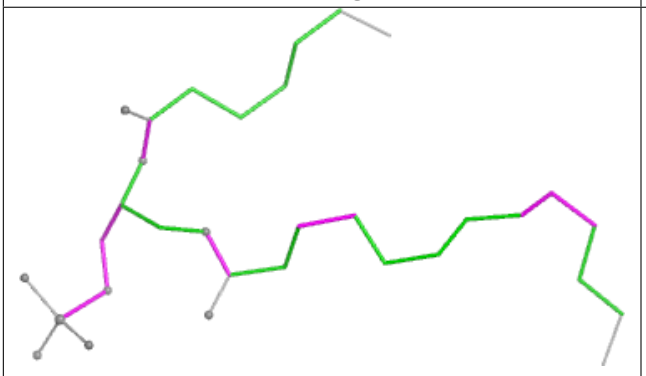
Ligand 3PH 1K 103



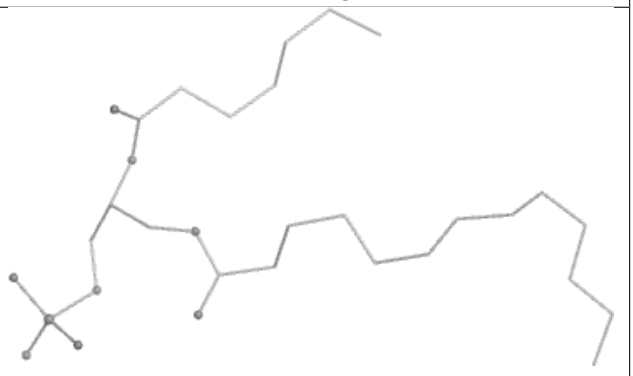
Bond lengths



Bond angles



Torsions



Rings

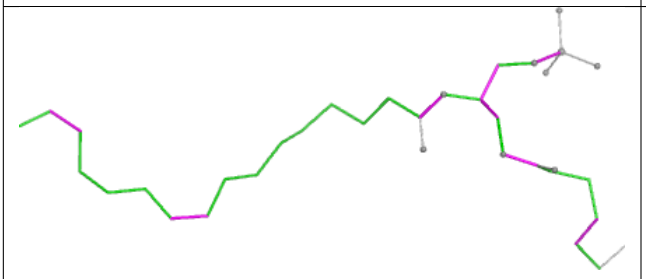
Ligand 3PH 1R 201



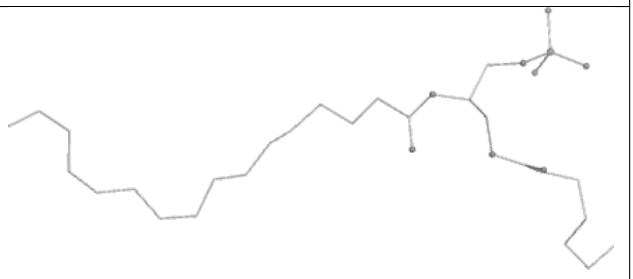
Bond lengths



Bond angles

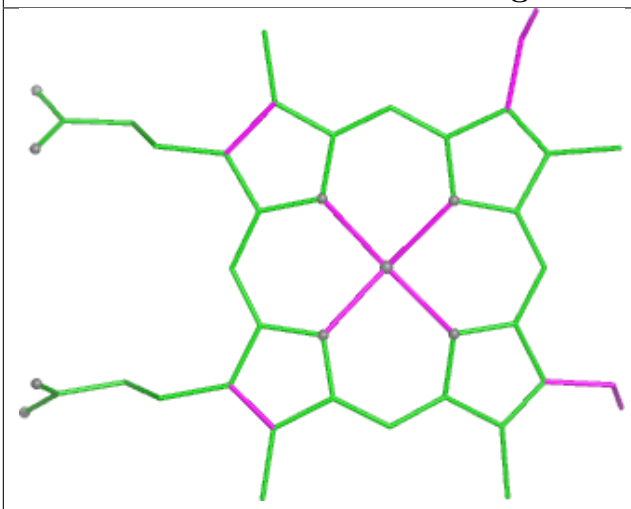


Torsions

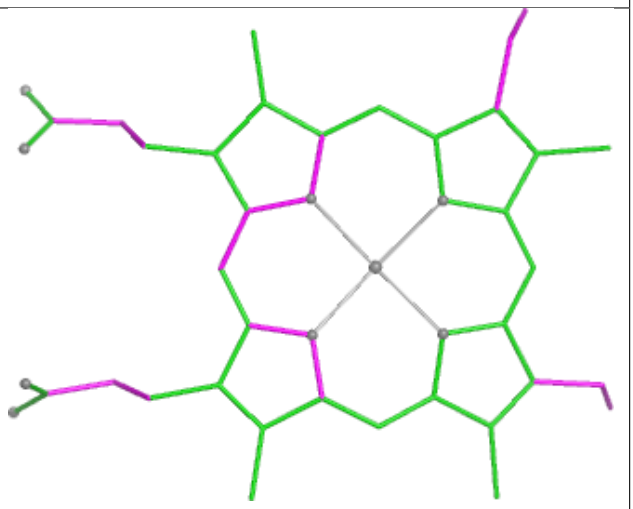


Rings

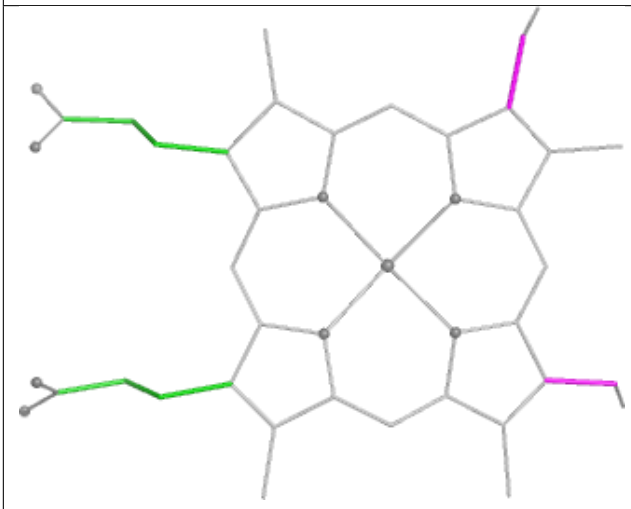
Ligand HEM 1E 404



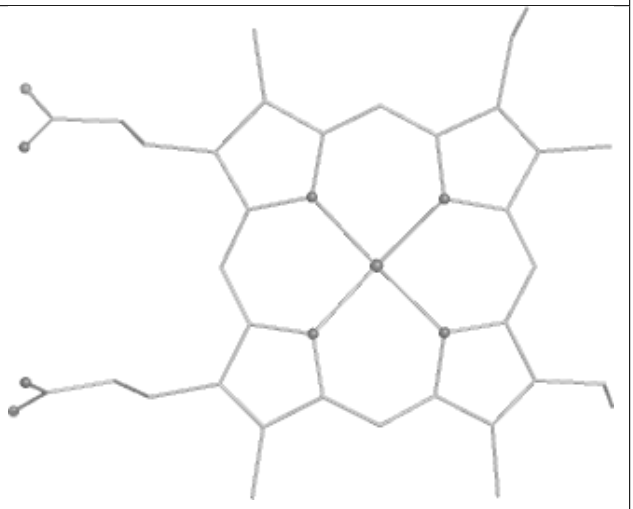
Bond lengths



Bond angles

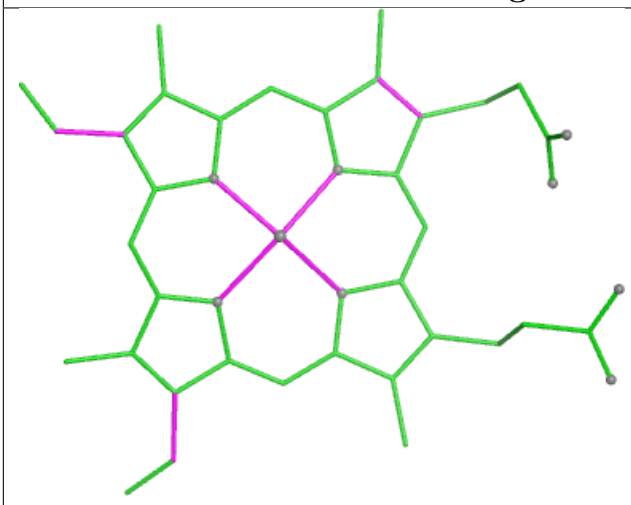


Torsions

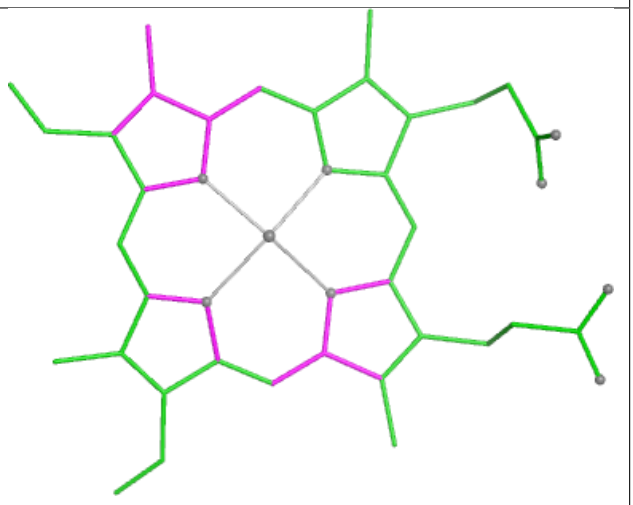


Rings

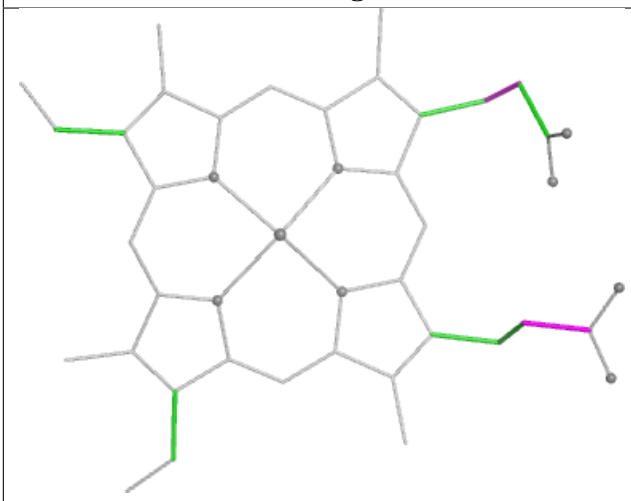
Ligand HEM 1A 403



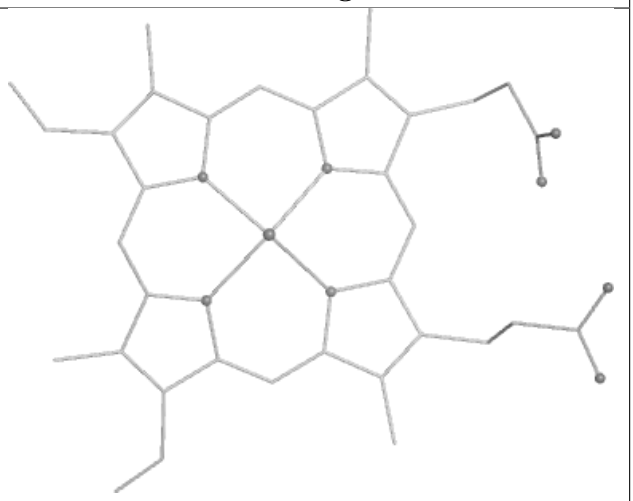
Bond lengths



Bond angles

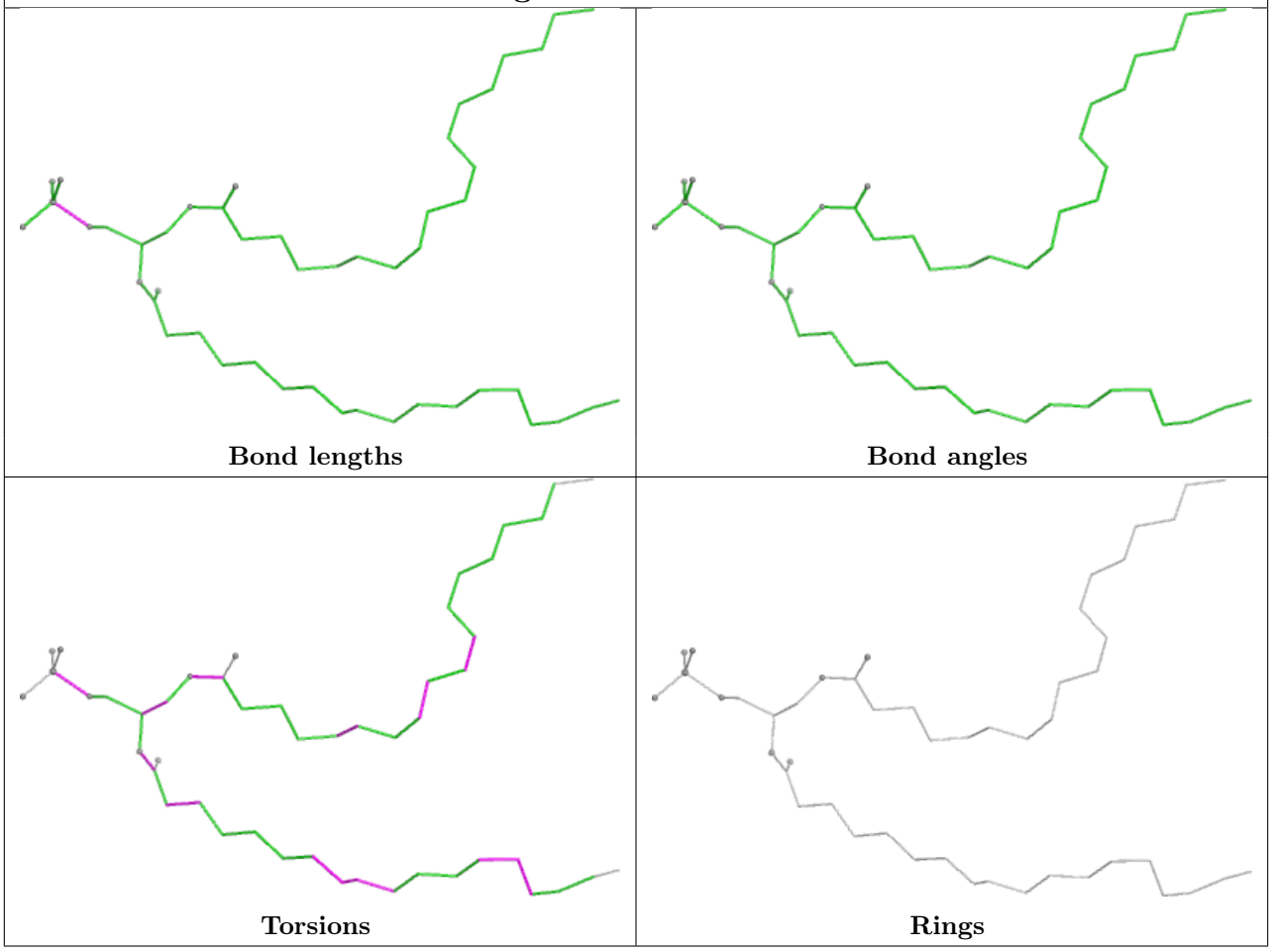


Torsions

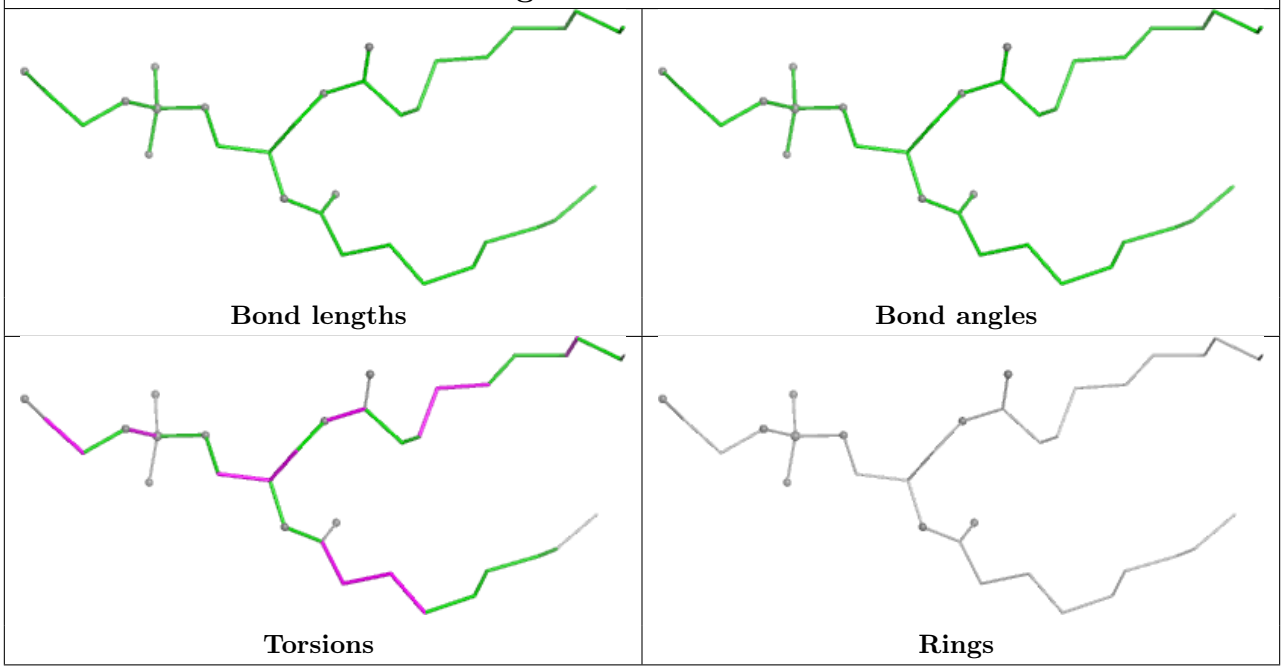


Rings

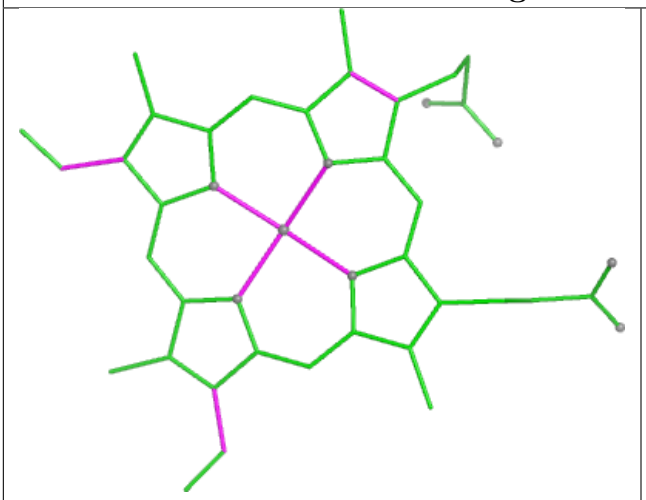
Ligand 3PH 1B 407



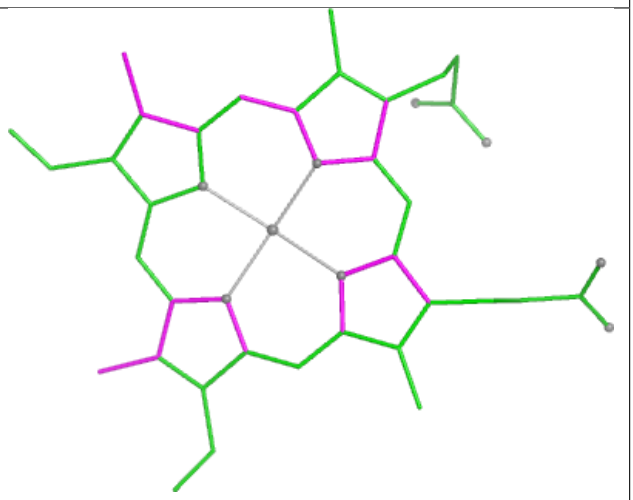
Ligand PTY 1E 403



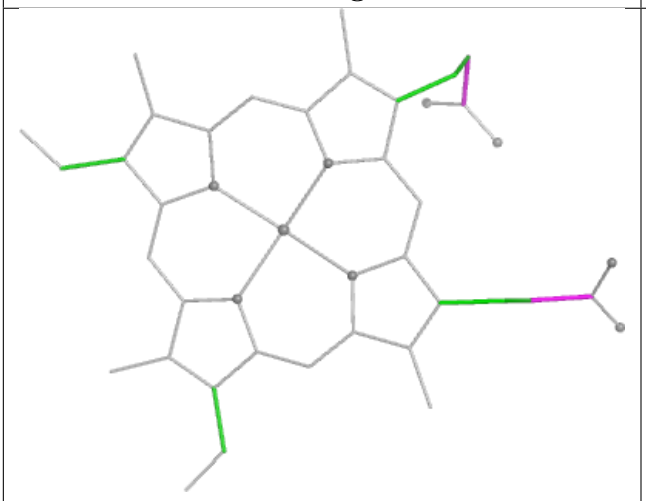
Ligand HEM 1A 404



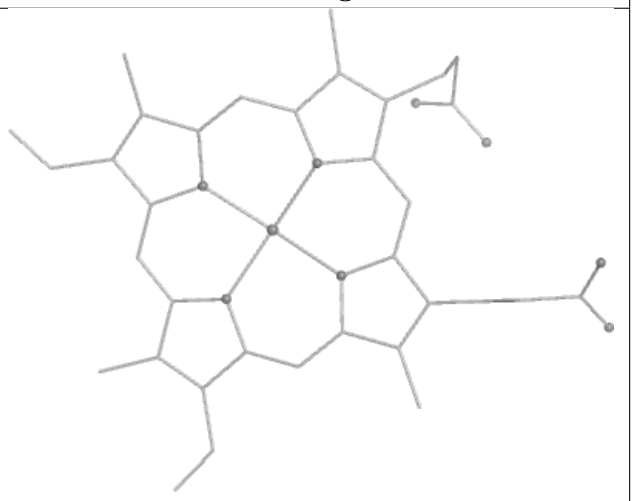
Bond lengths



Bond angles

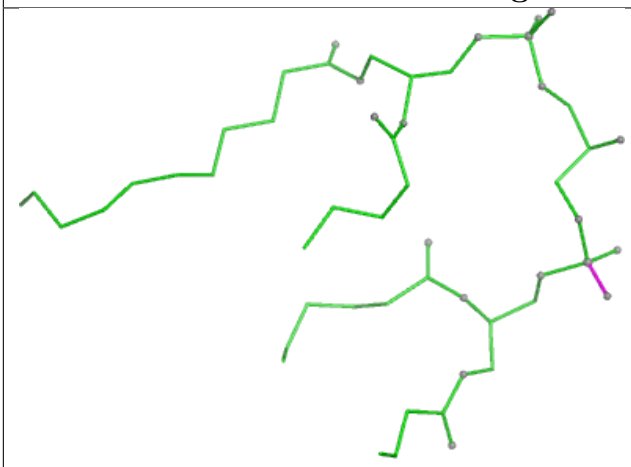


Torsions

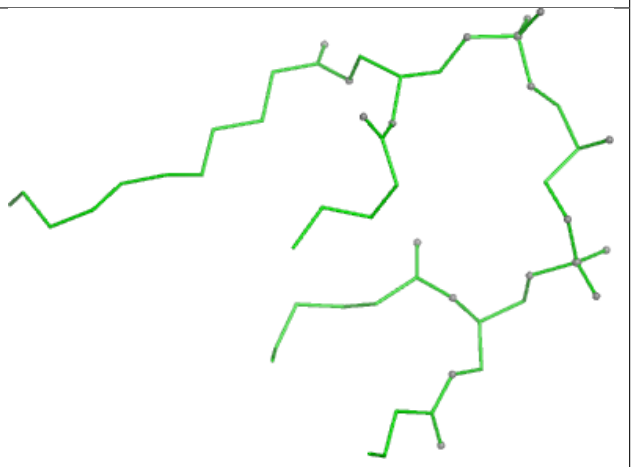


Rings

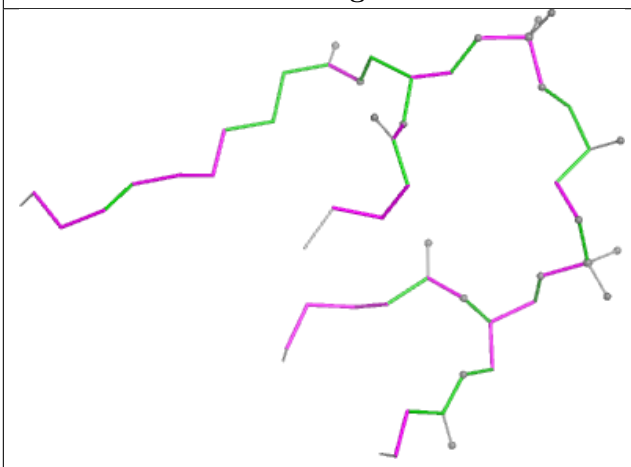
Ligand CDL 1M 501



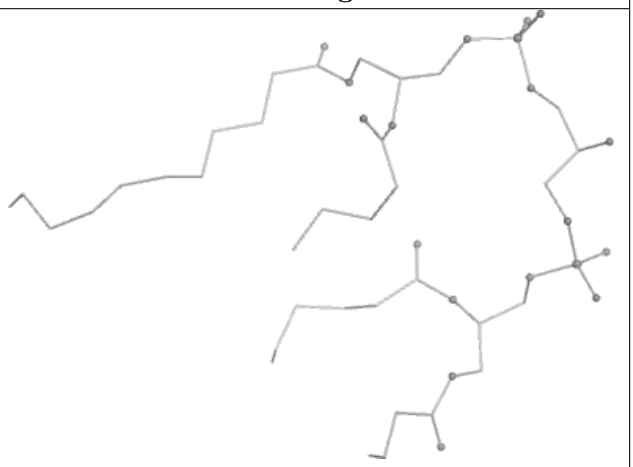
Bond lengths



Bond angles

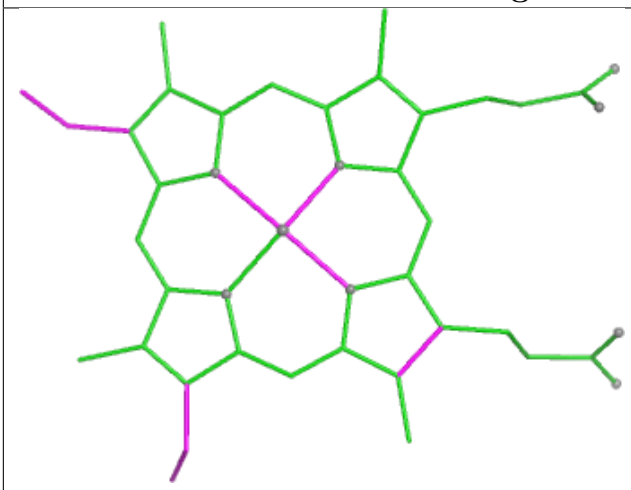


Torsions

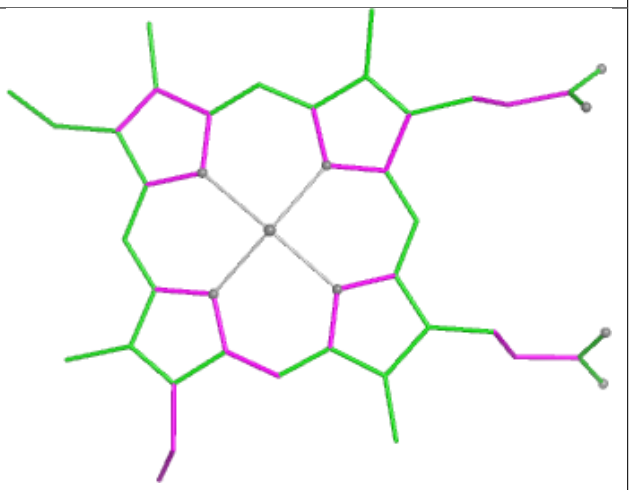


Rings

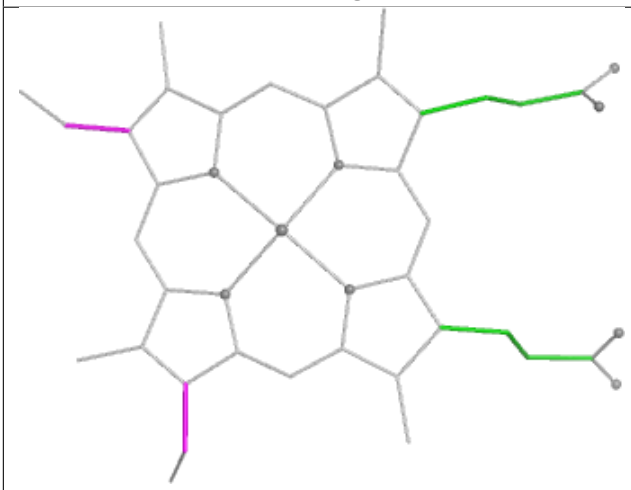
Ligand HEM 1F 402



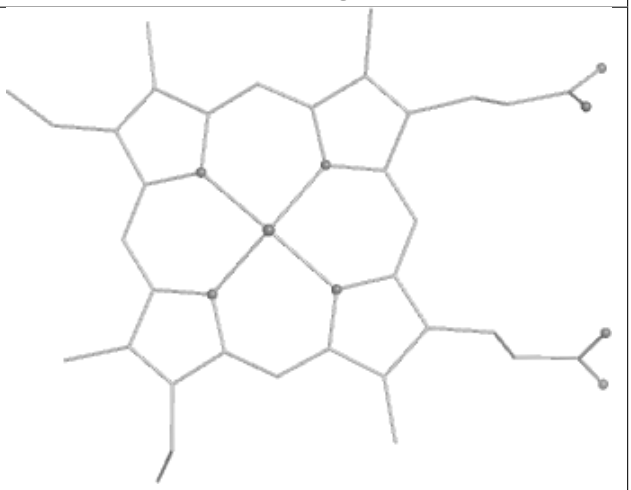
Bond lengths



Bond angles

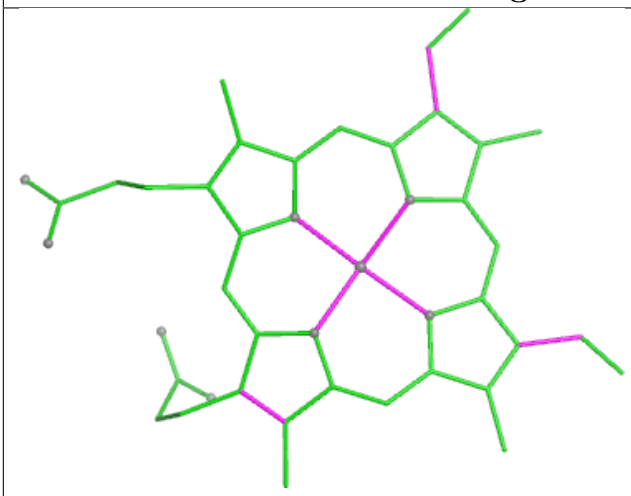


Torsions

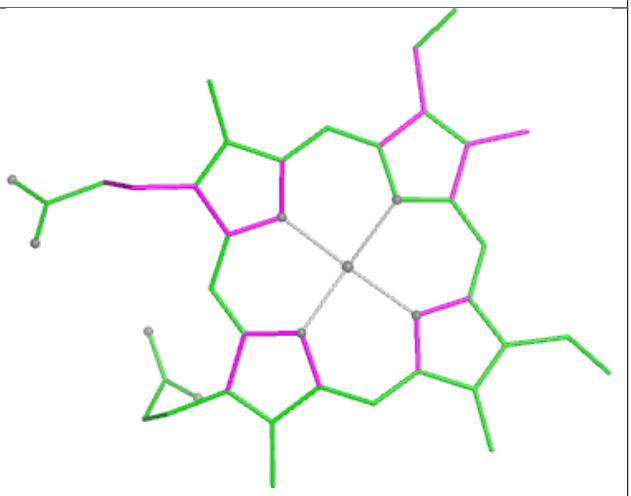


Rings

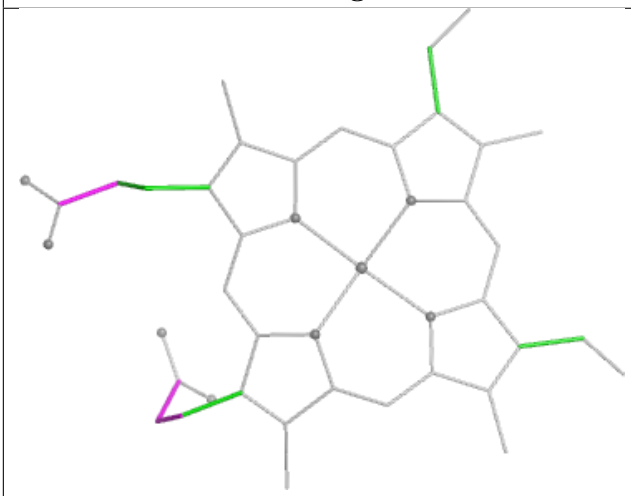
Ligand HEM 1B 404



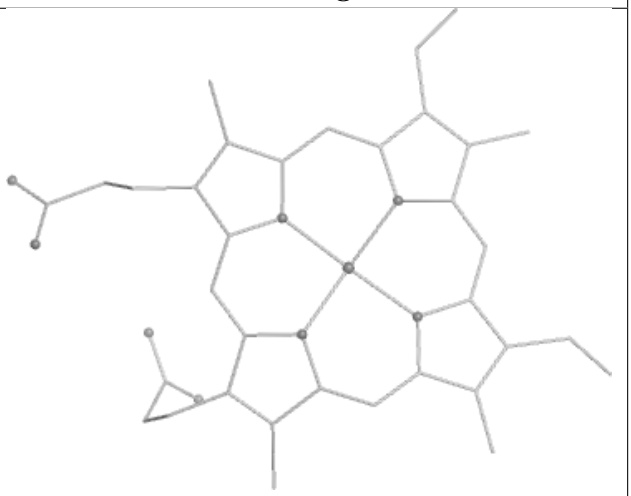
Bond lengths



Bond angles

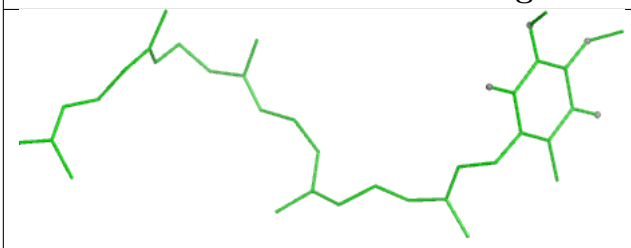


Torsions

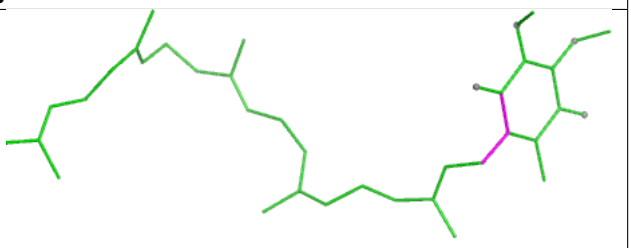


Rings

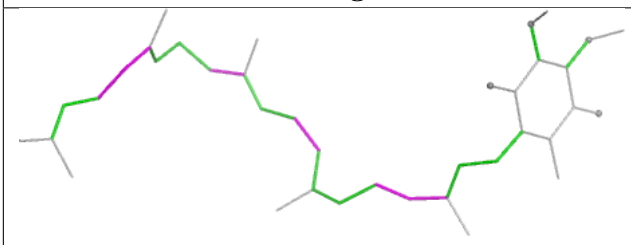
Ligand UQ5 1A 402



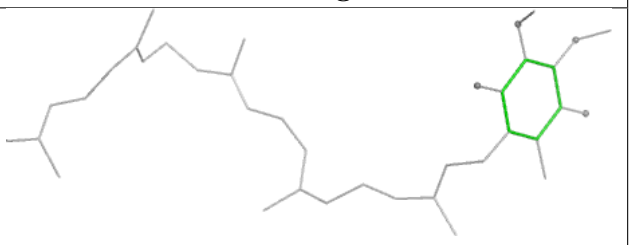
Bond lengths



Bond angles

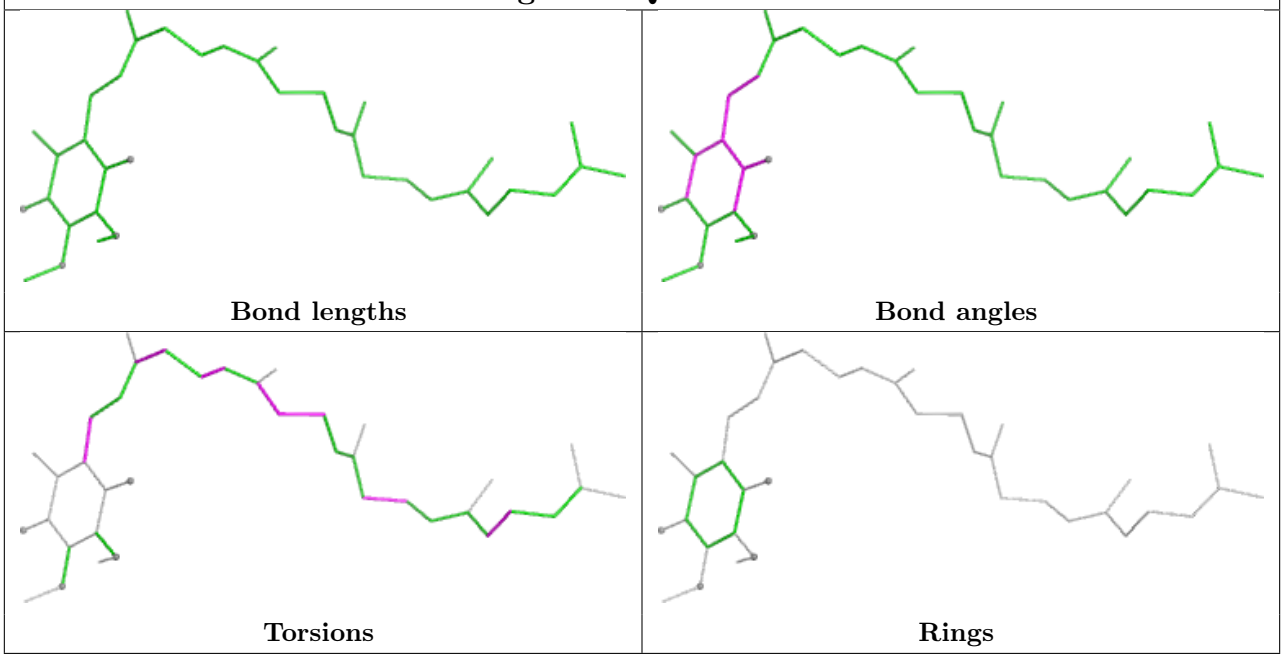


Torsions

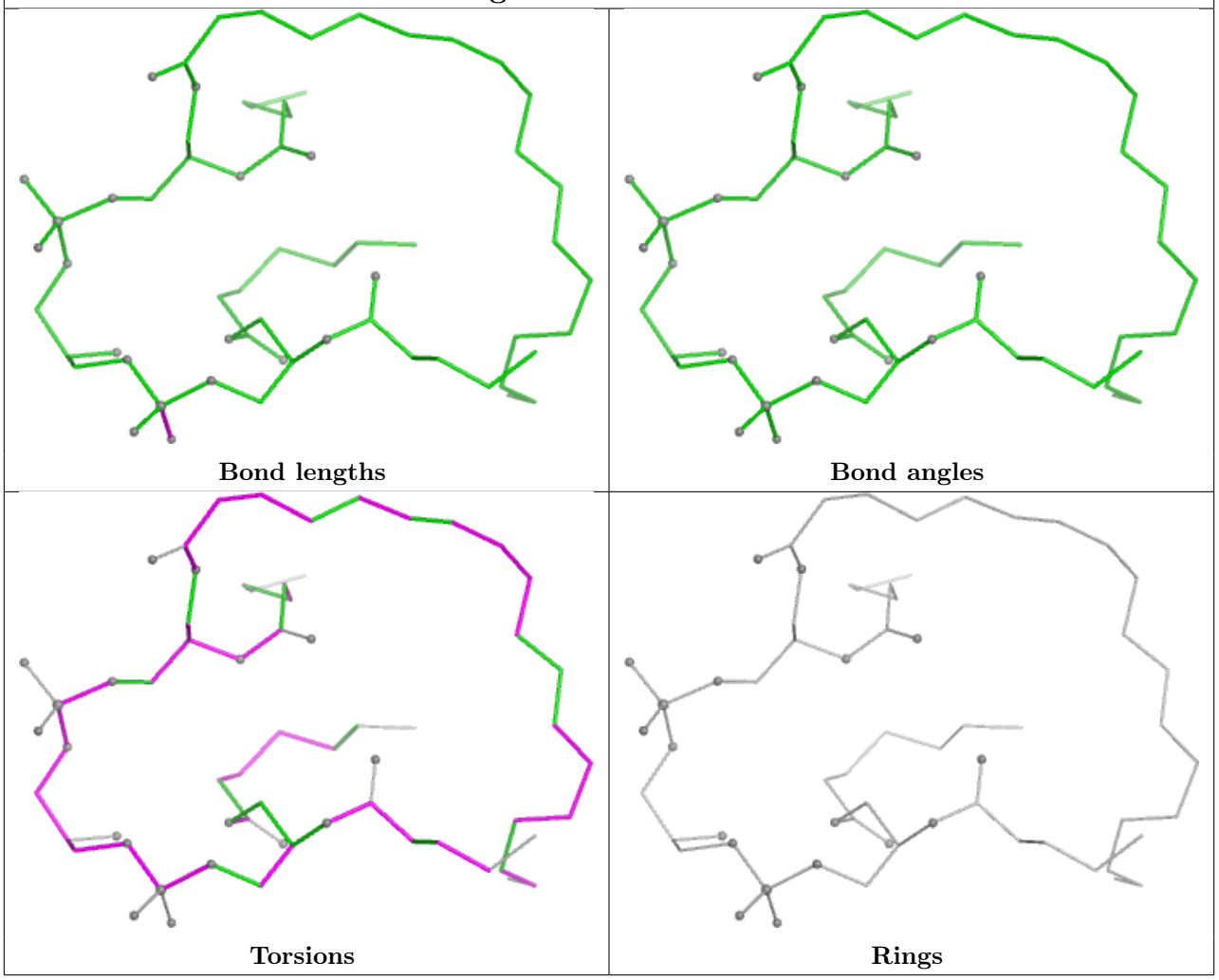


Rings

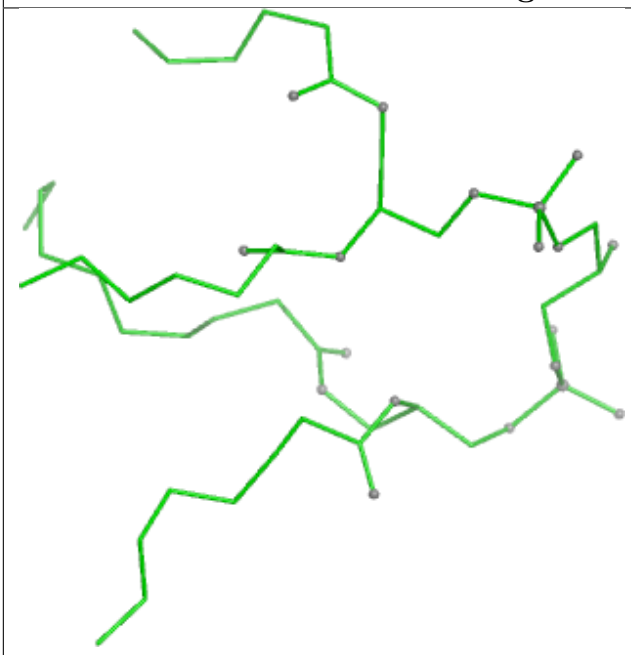
Ligand UQ5 1B 402



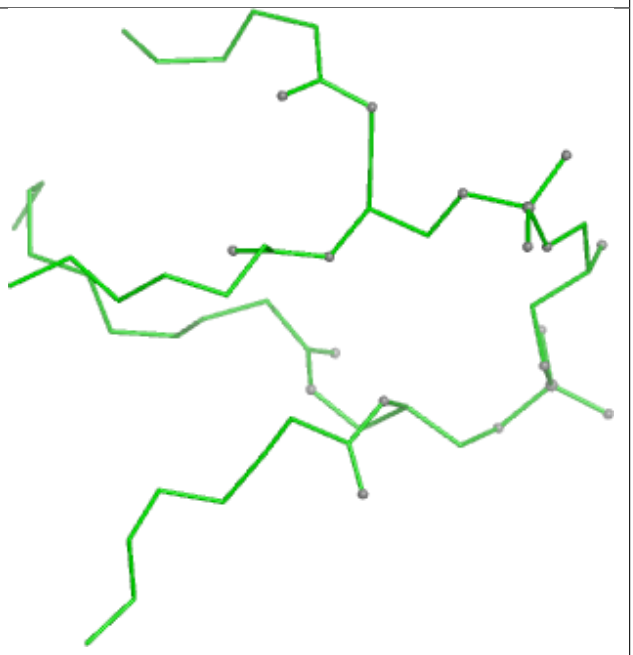
Ligand CDL 1B 405



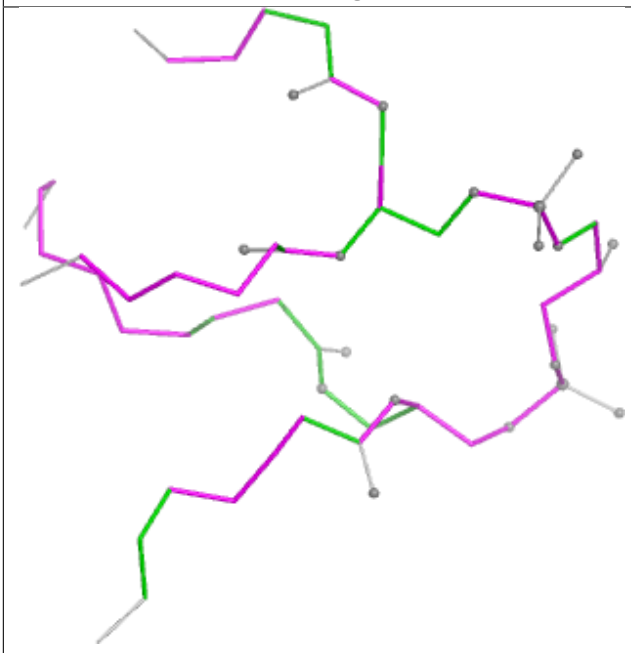
Ligand CDL 1L 101



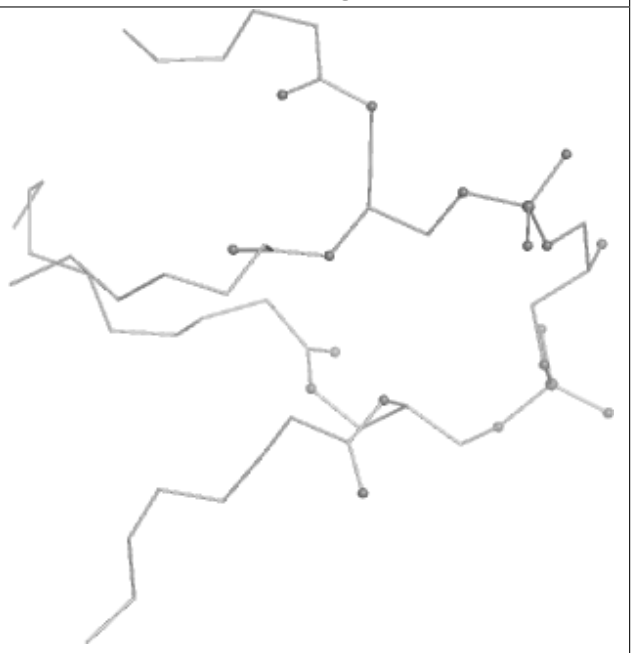
Bond lengths



Bond angles

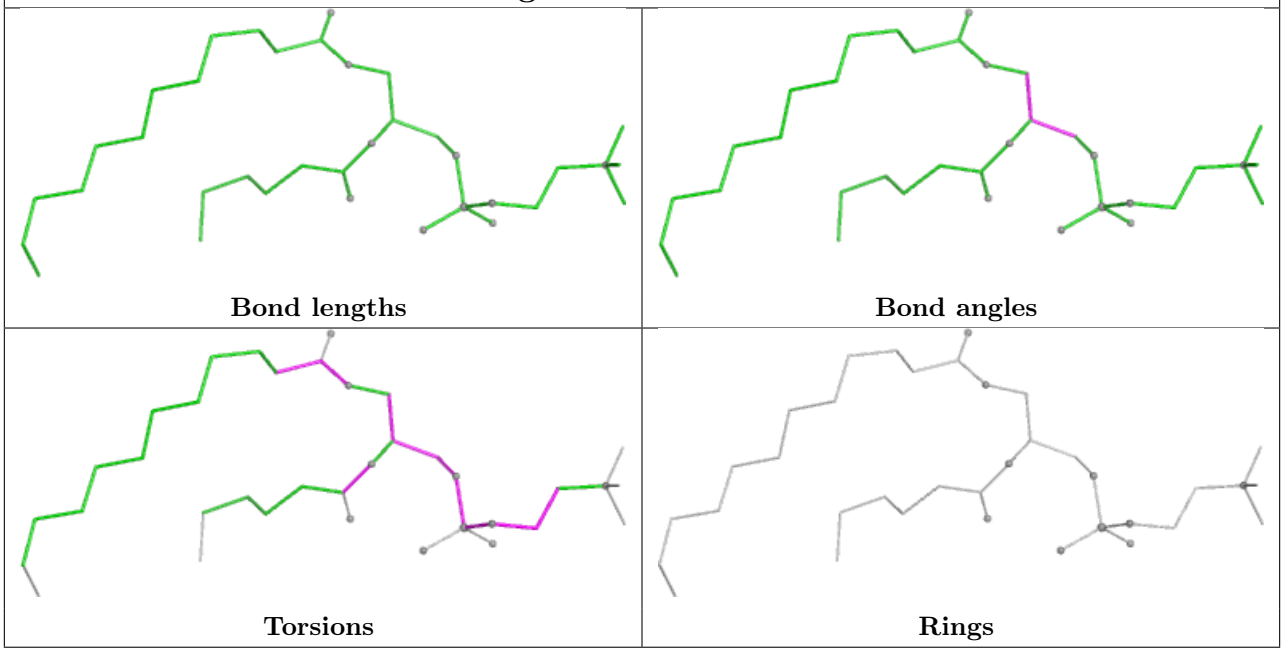


Torsions

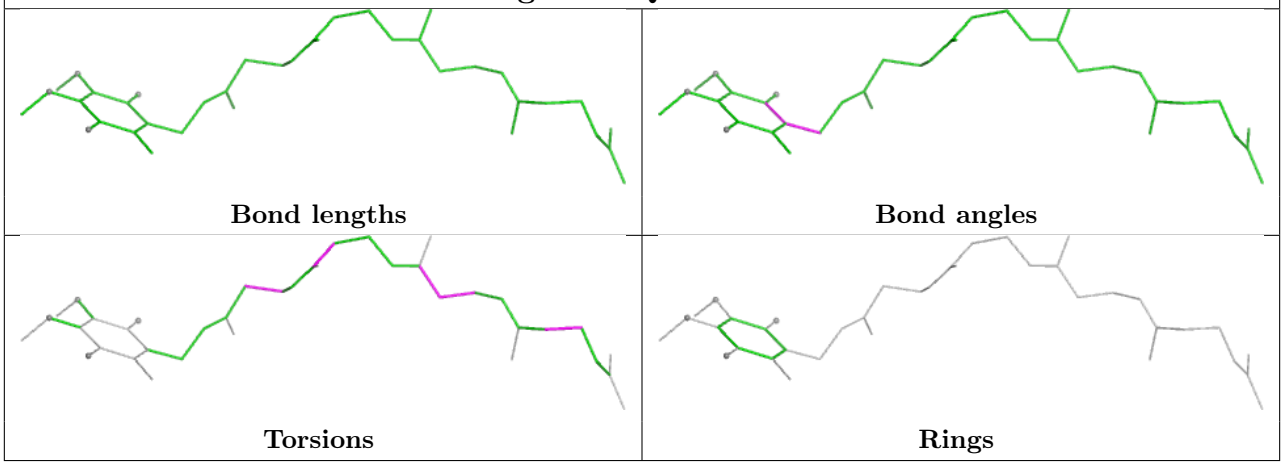


Rings

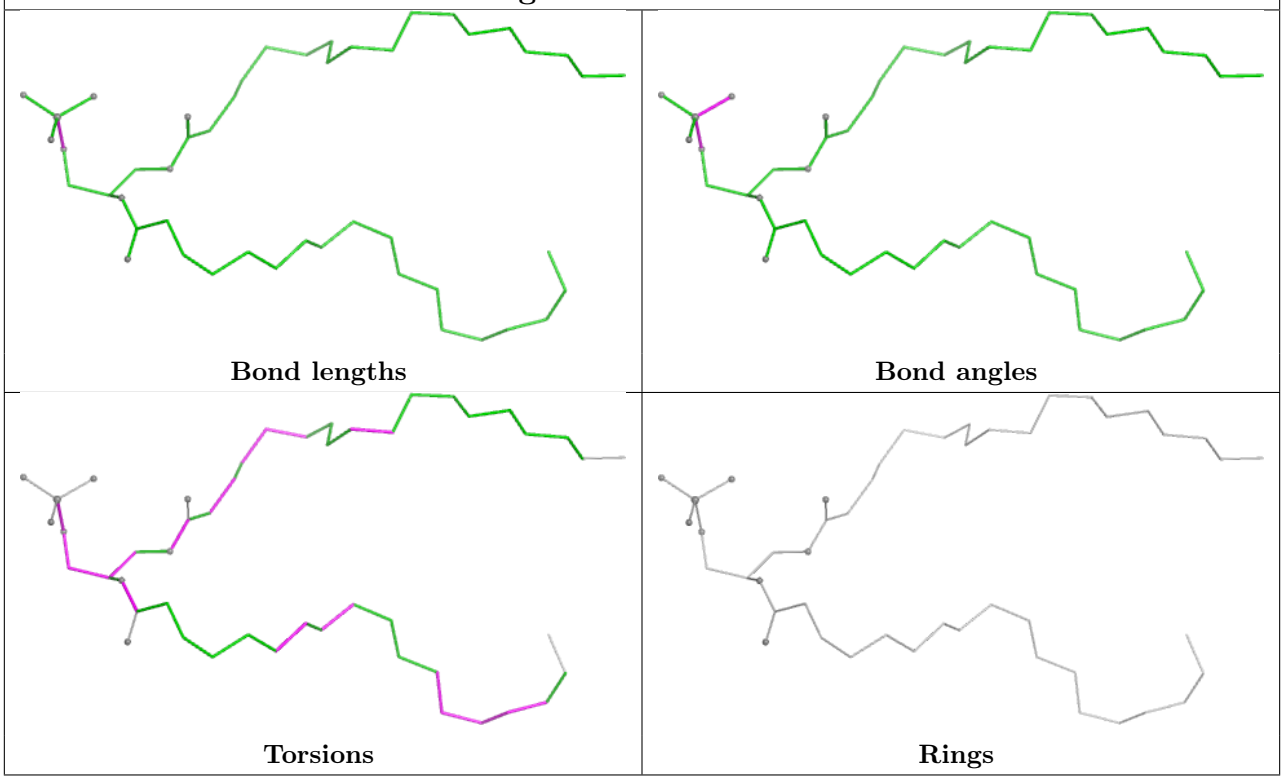
Ligand PC7 1G 301



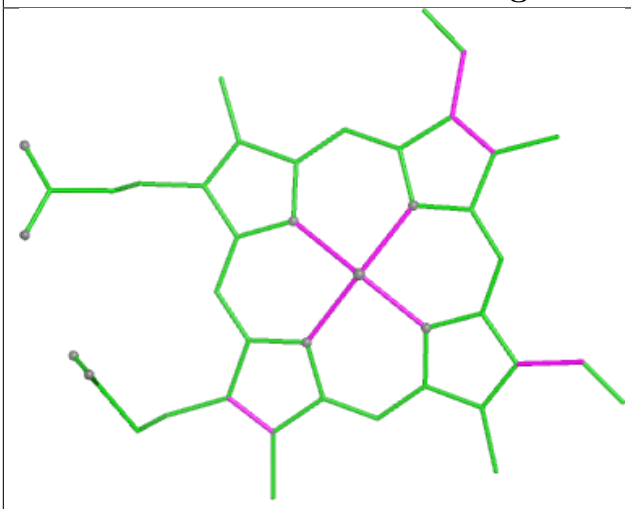
Ligand UQ5 1B 401



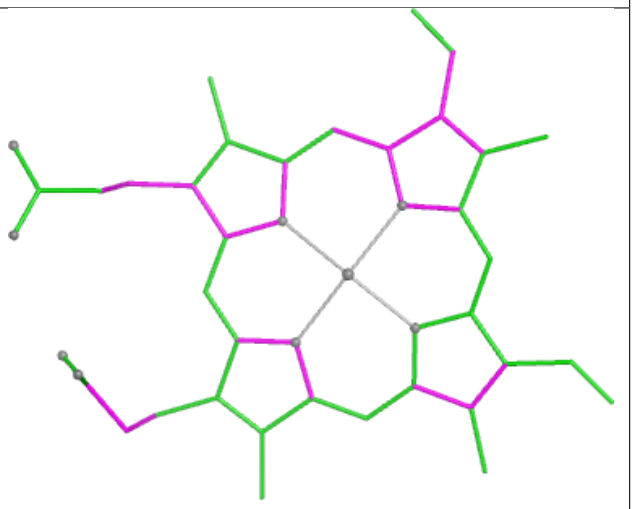
Ligand 3PH 1B 406



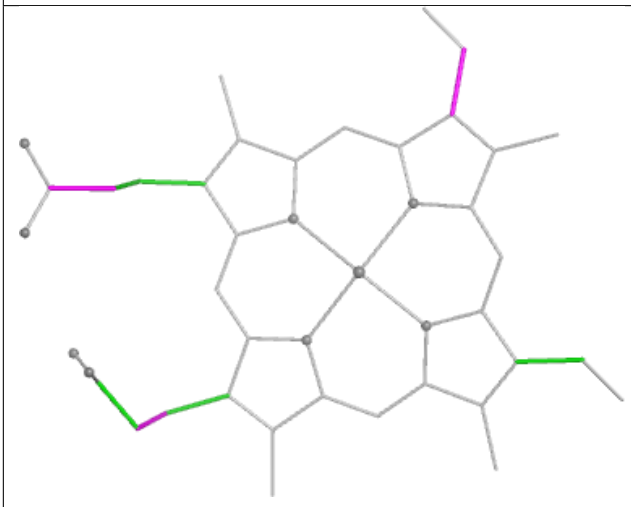
Ligand HEM 1B 403



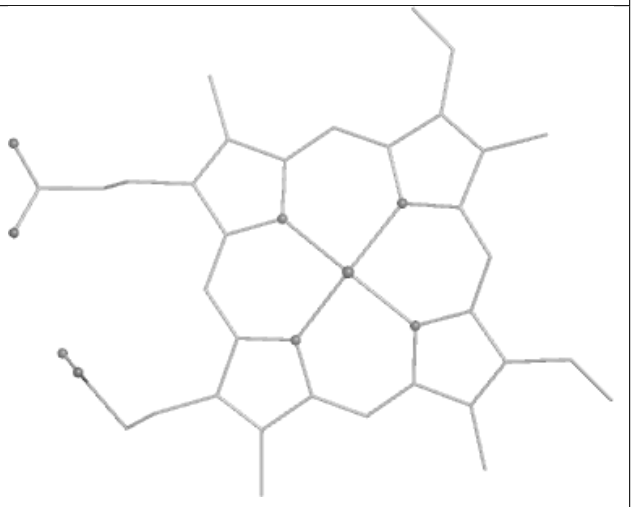
Bond lengths



Bond angles

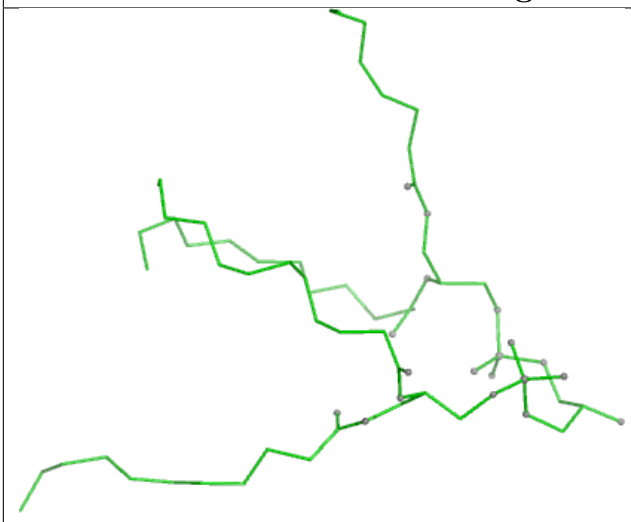


Torsions

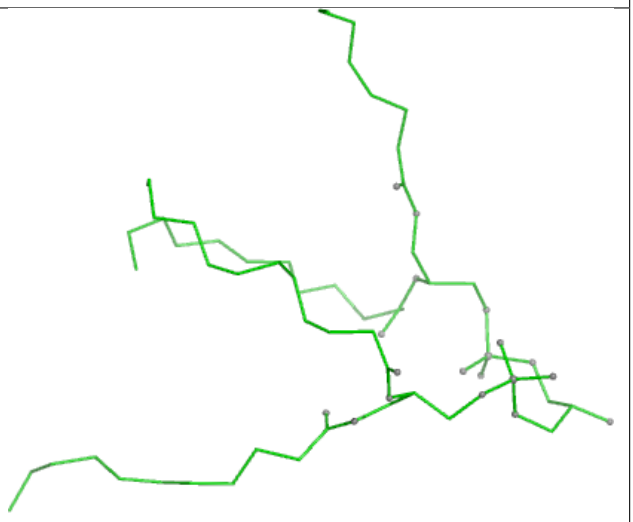


Rings

Ligand CDL 1B 408



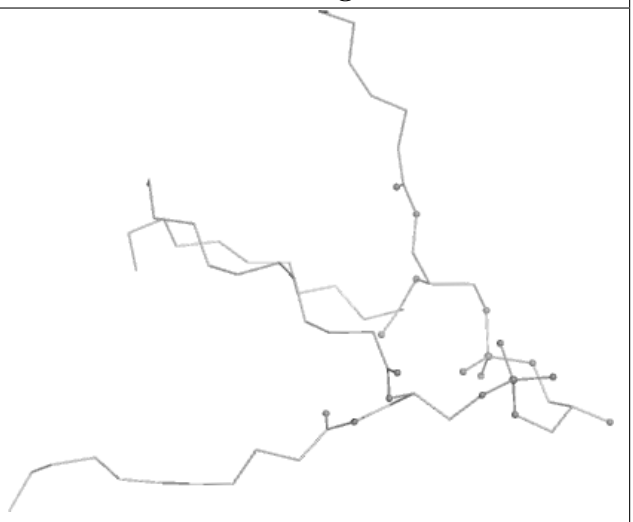
Bond lengths



Bond angles

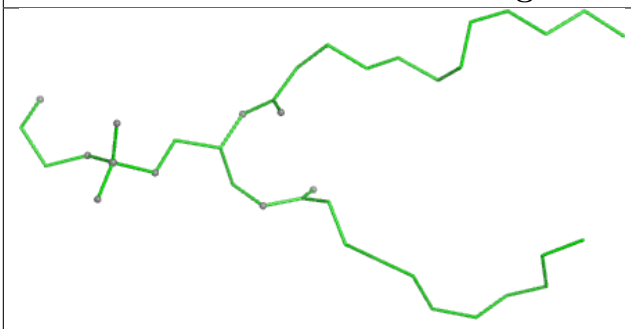


Torsions

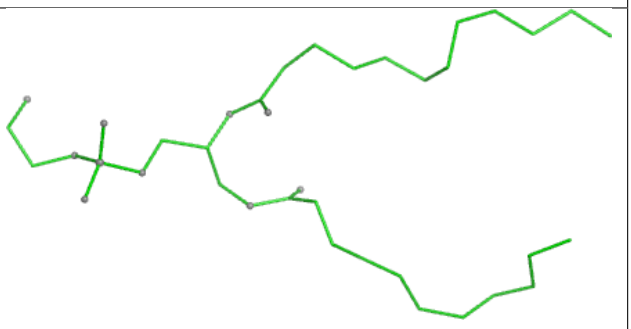


Rings

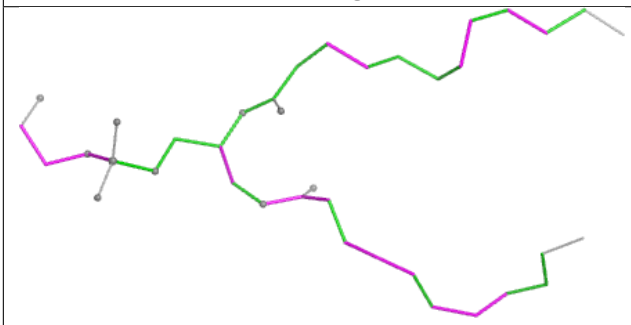
Ligand PTY 1F 403



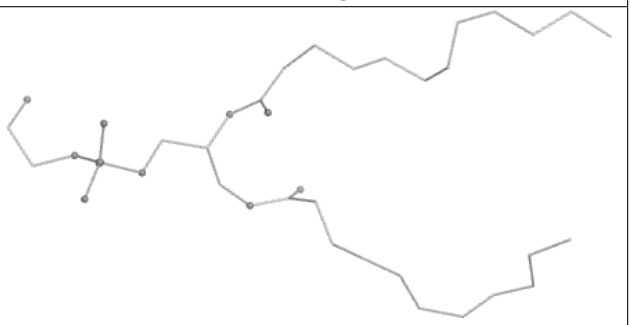
Bond lengths



Bond angles

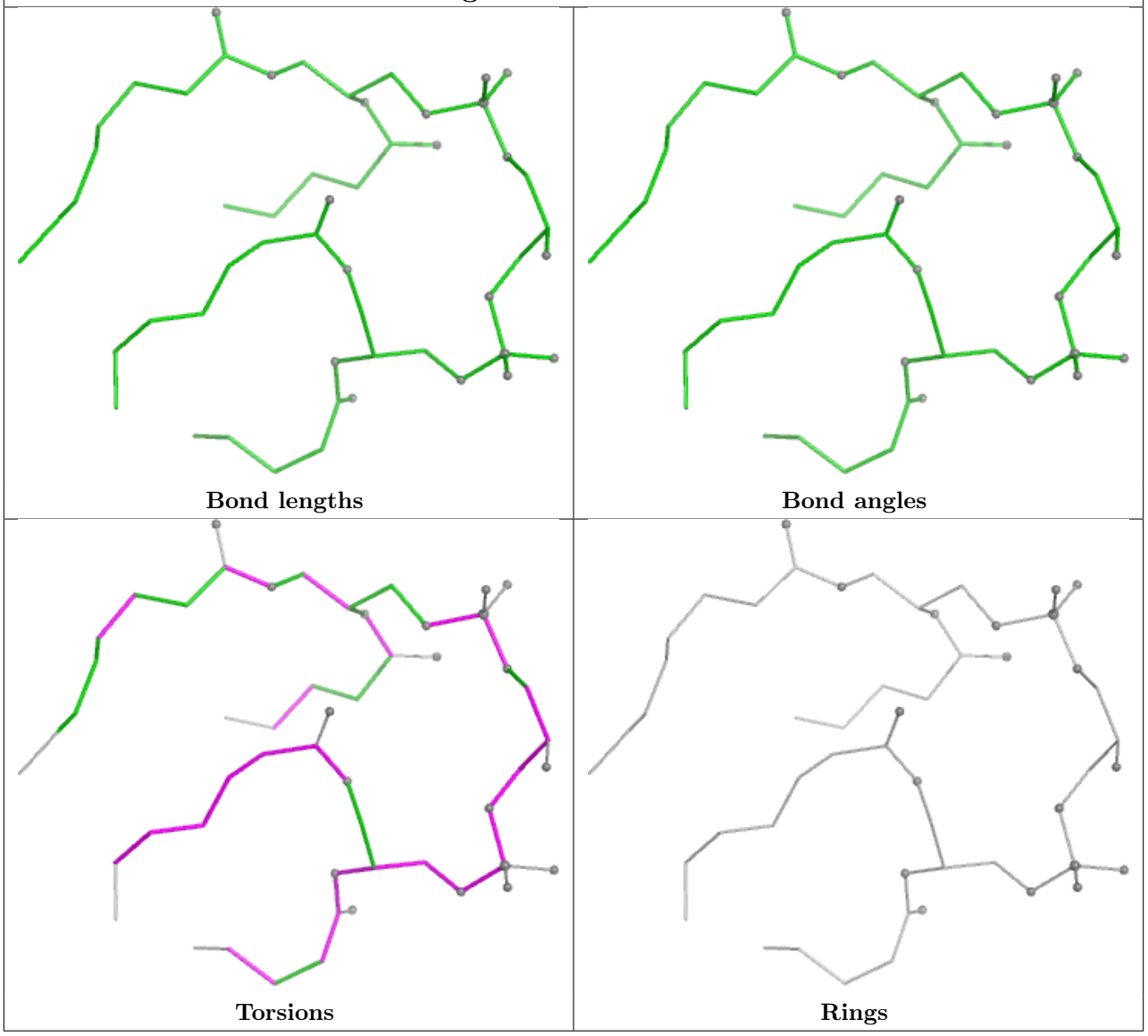


Torsions



Rings

Ligand CDL 1E 401



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-50204. These allow visual inspection of the internal detail of the map and identification of artifacts.

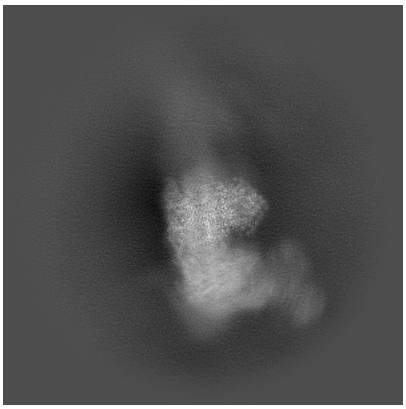
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

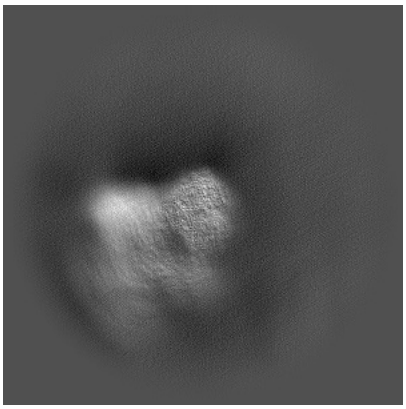
6.1.1 Primary map



X

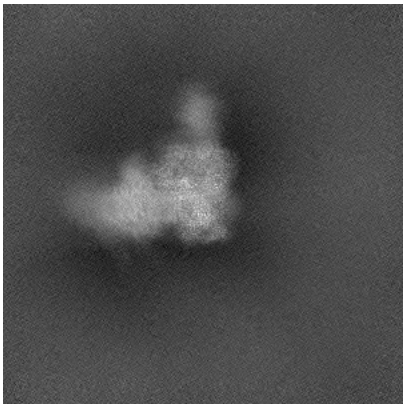


Y

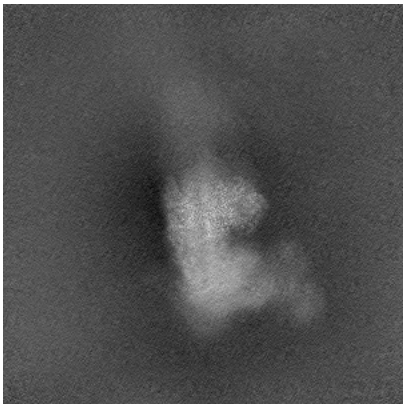


Z

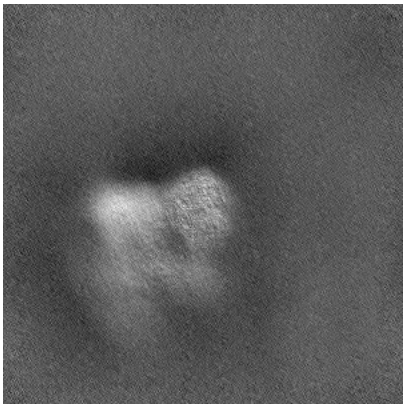
6.1.2 Raw map



X



Y

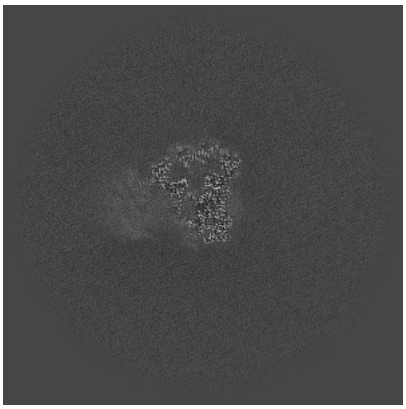


Z

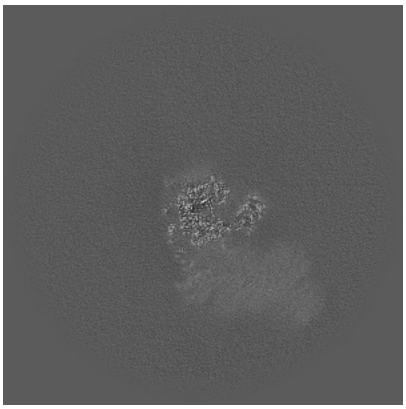
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

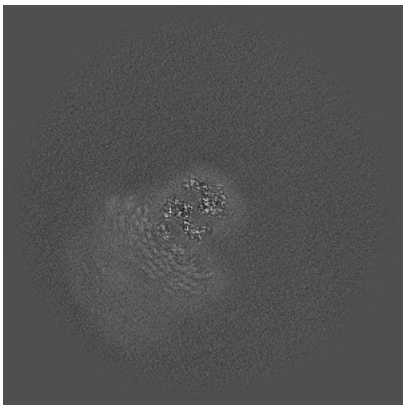
6.2.1 Primary map



X Index: 294

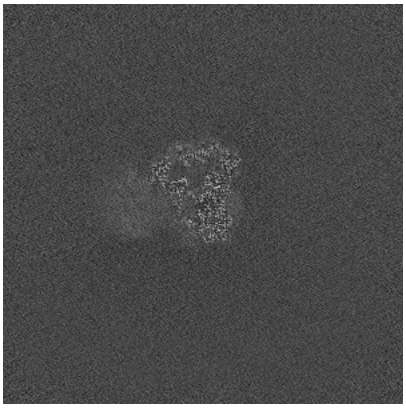


Y Index: 294



Z Index: 294

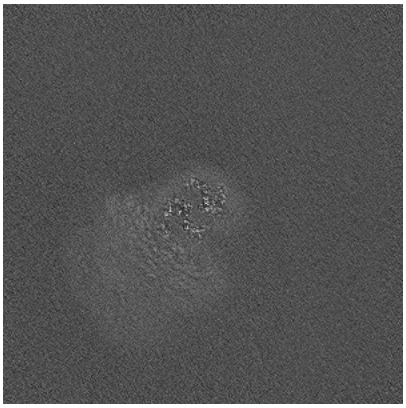
6.2.2 Raw map



X Index: 294



Y Index: 294

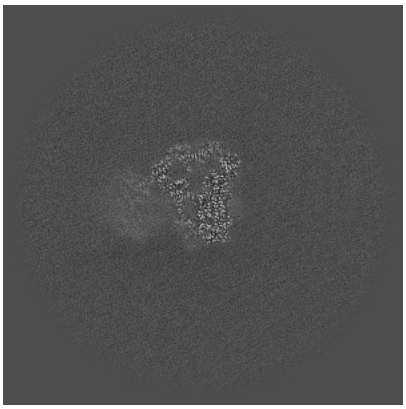


Z Index: 294

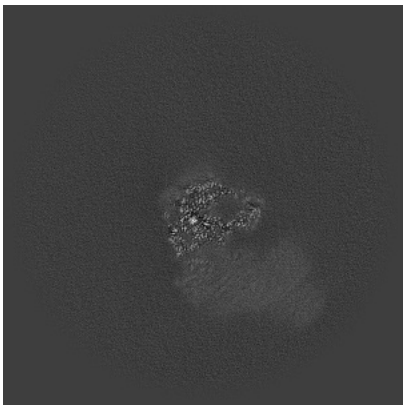
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

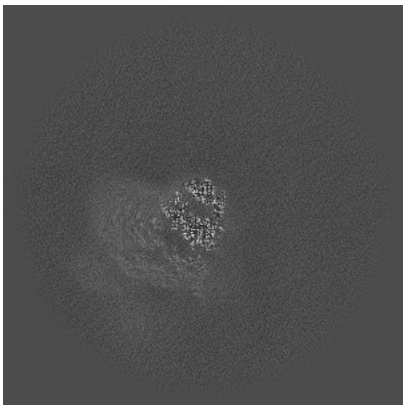
6.3.1 Primary map



X Index: 295

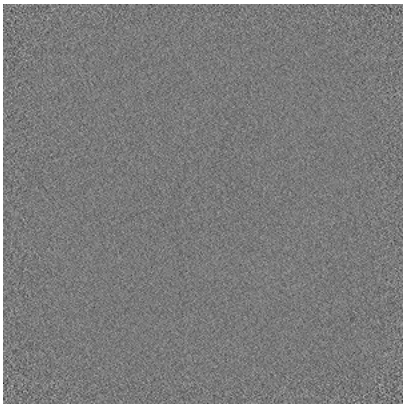


Y Index: 286

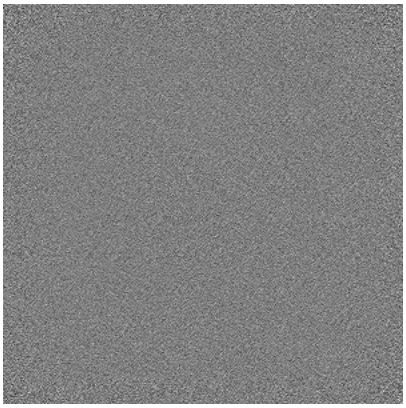


Z Index: 322

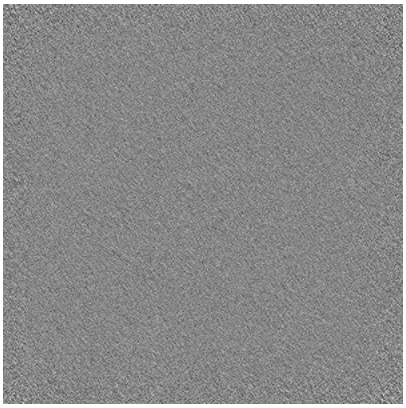
6.3.2 Raw map



X Index: 0



Y Index: 0

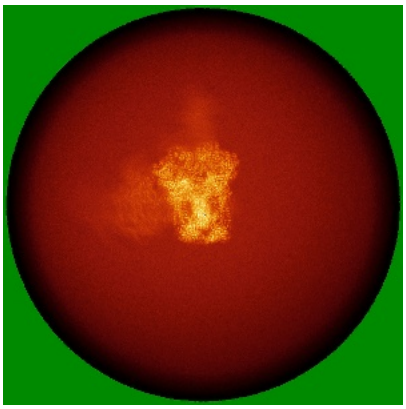


Z Index: 0

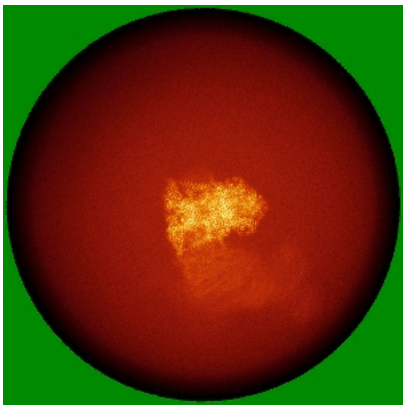
The images above show the largest variance slices of the map in three orthogonal directions.

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

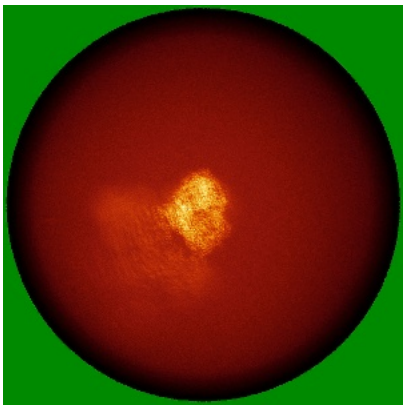
6.4.1 Primary map



X

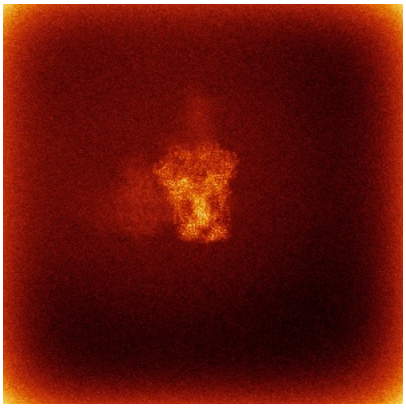


Y

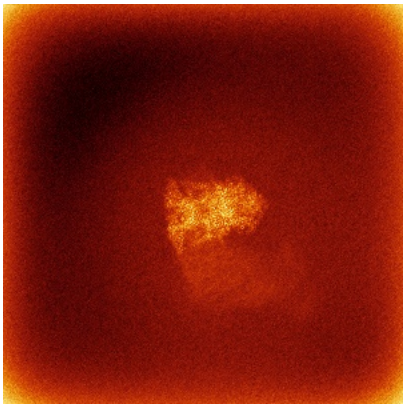


Z

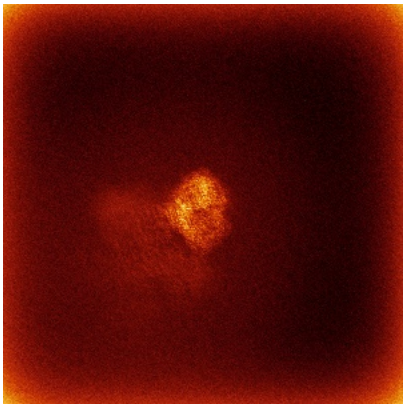
6.4.2 Raw map



X



Y

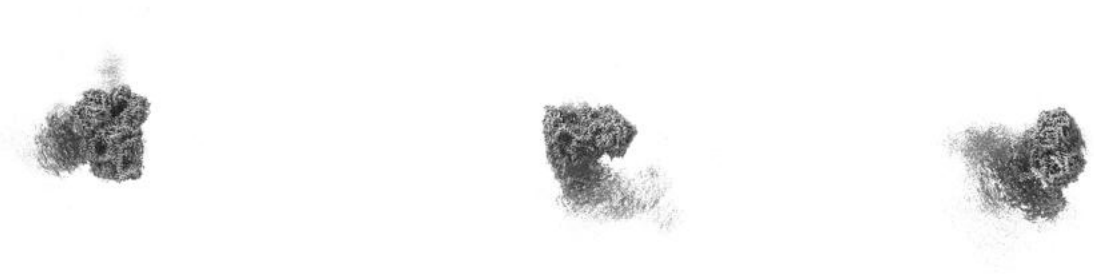


Z

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 0.145. 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.

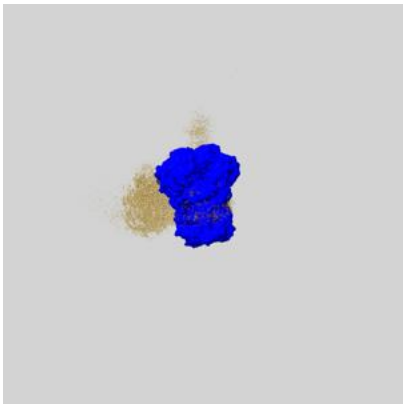
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

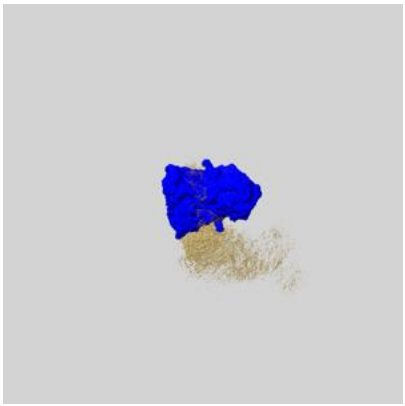
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

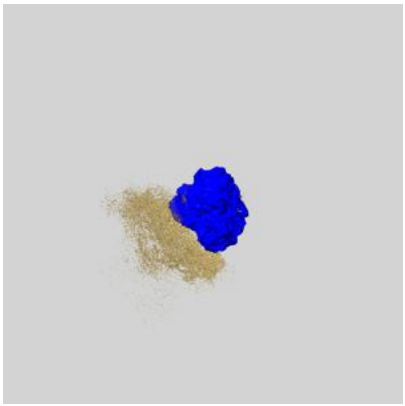
6.6.1 emd_50204_msk_1.map



X



Y

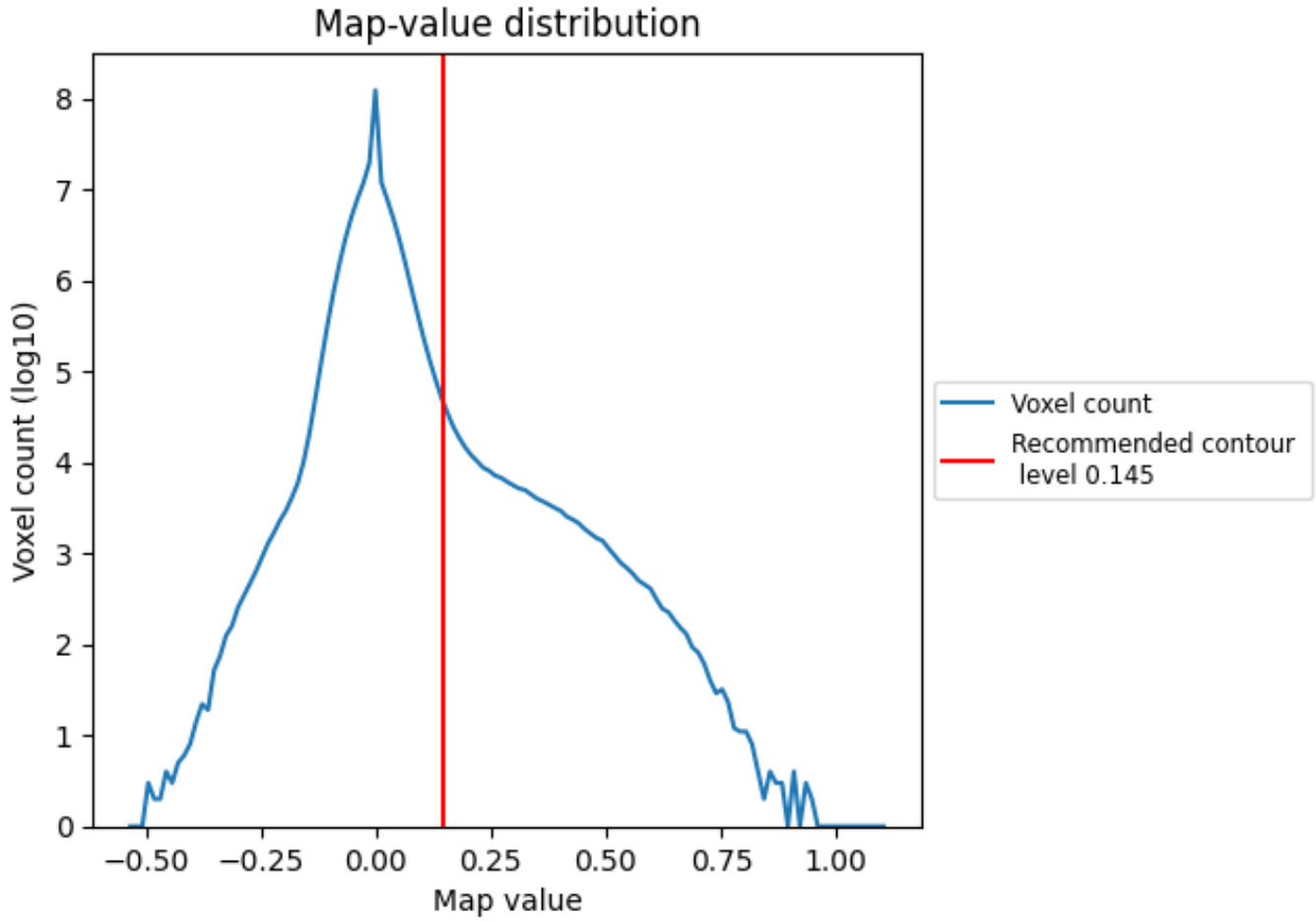


Z

7 Map analysis

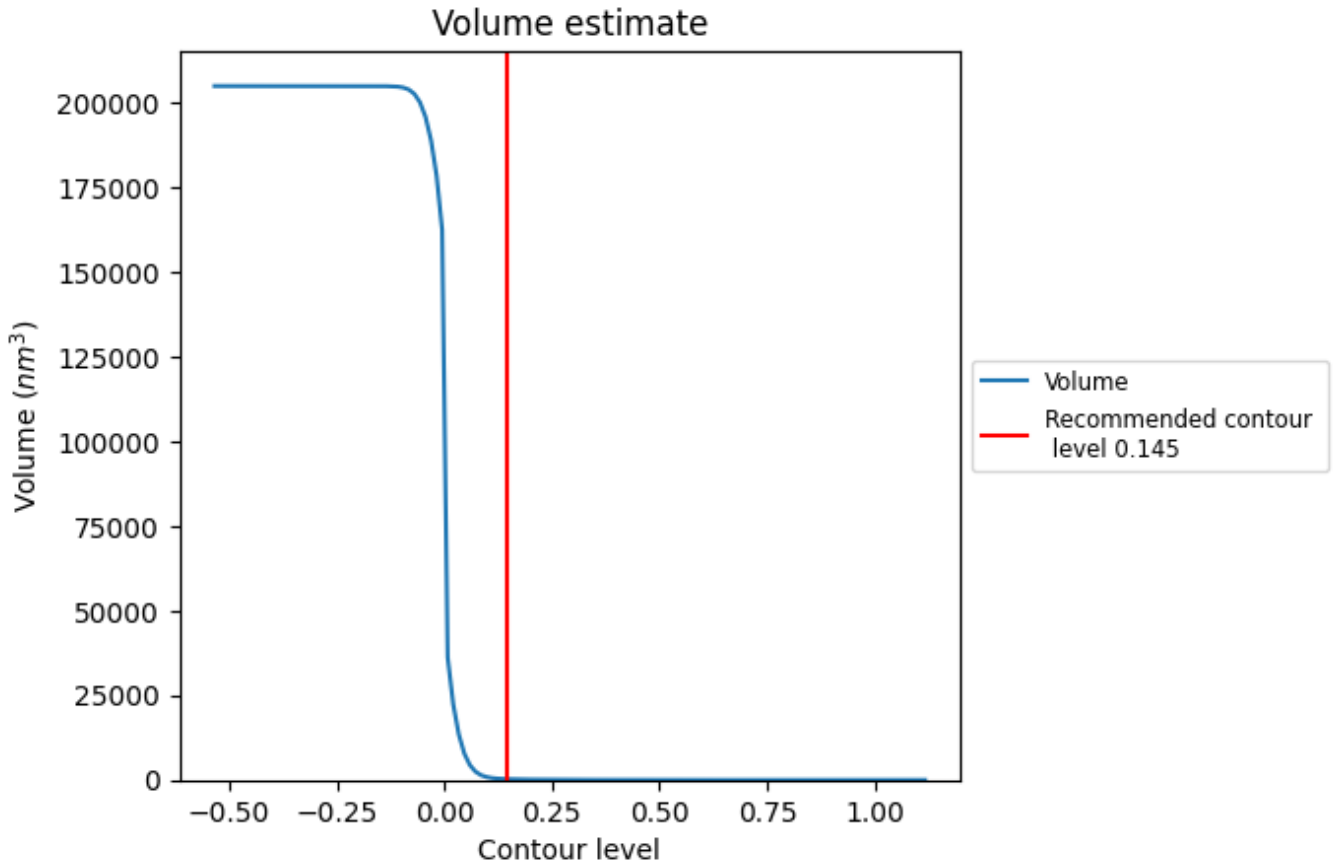
This section contains the results of statistical analysis of the map.

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.

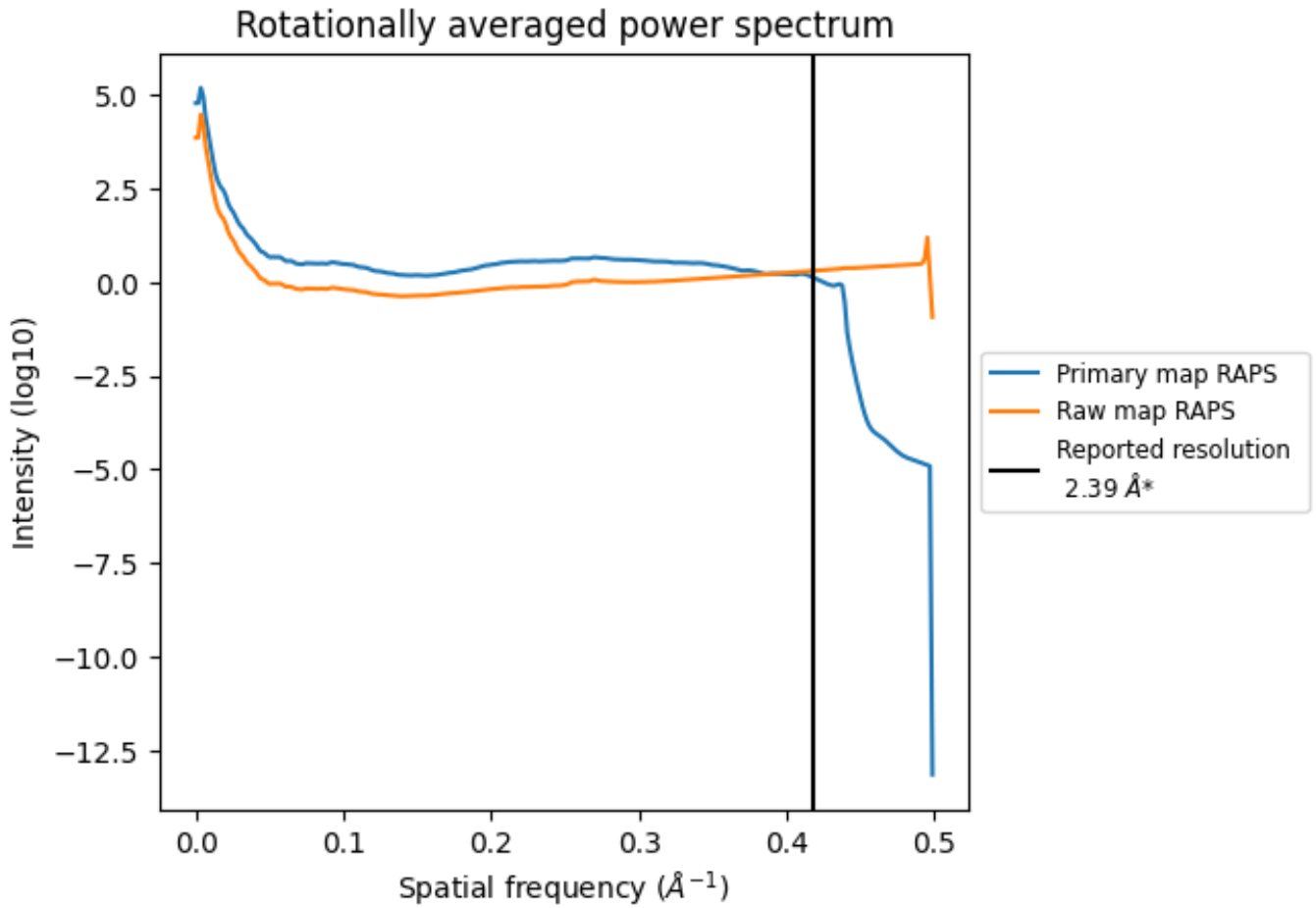
7.2 Volume estimate (i)



The volume at the recommended contour level is 254 nm^3; this corresponds to an approximate mass of 230 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)

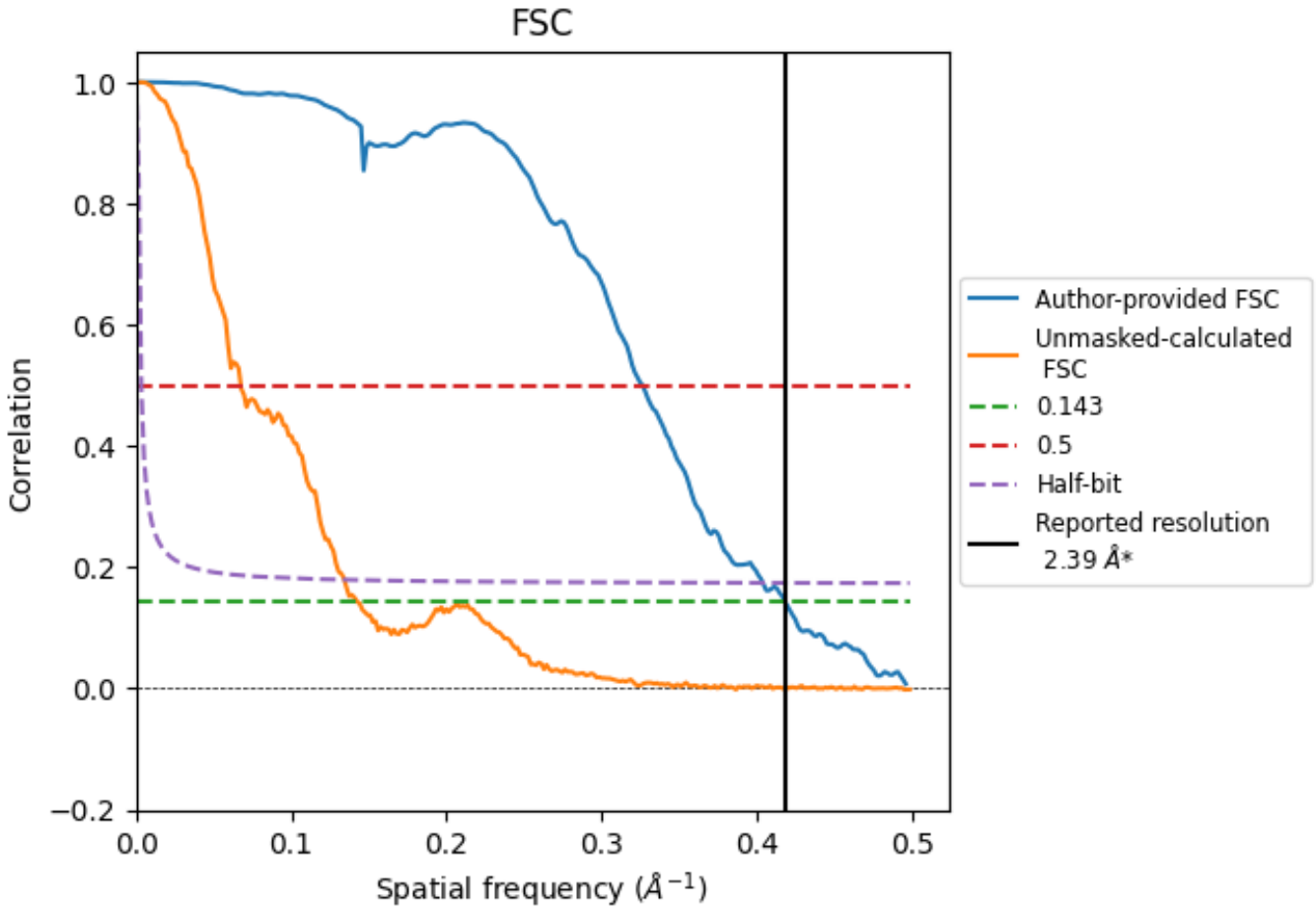


*Reported resolution corresponds to spatial frequency of 0.418 $Å^{-1}$

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 0.418 Å^{-1}

8.2 Resolution estimates (i)

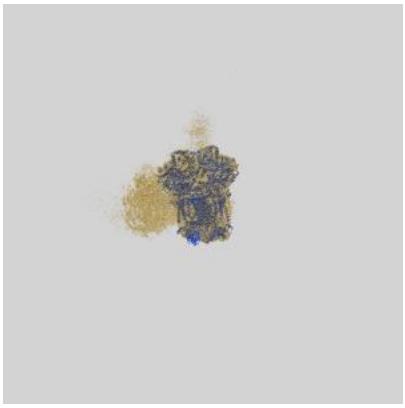
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.39	-	-
Author-provided FSC curve	2.39	3.06	2.48
Unmasked-calculated*	7.02	14.81	7.45

*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 7.02 differs from the reported value 2.39 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50204 and PDB model 9F5Z. Per-residue inclusion information can be found in section 3 on page 13.

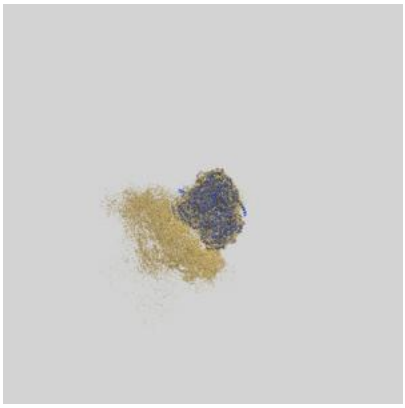
9.1 Map-model overlay



X



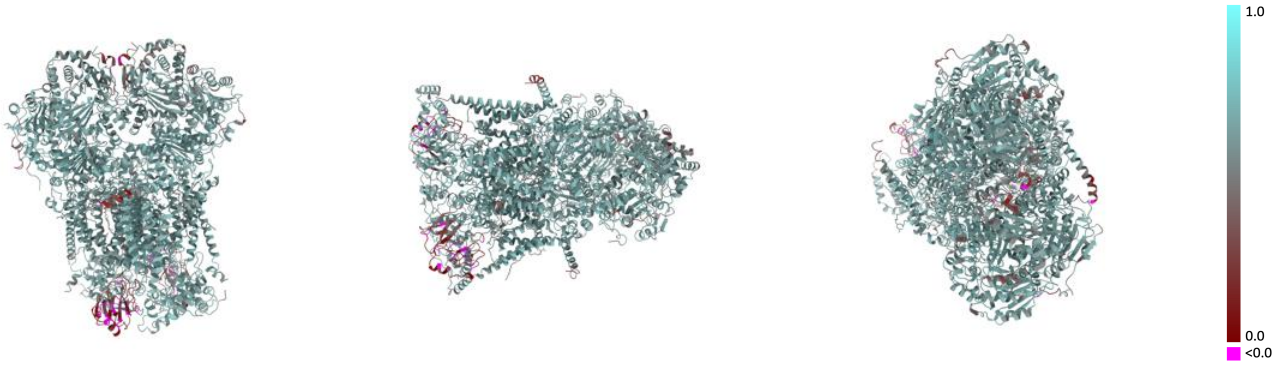
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.145 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.

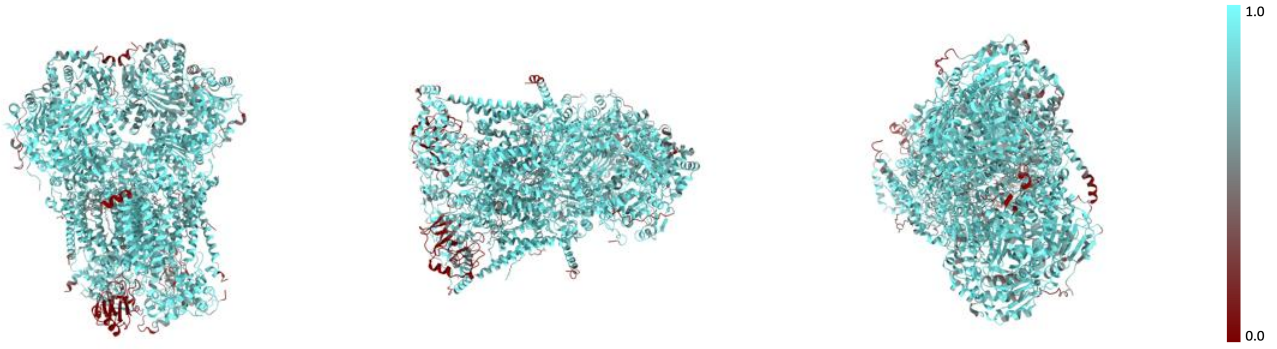
9.2 Q-score mapped to coordinate model (i)



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.

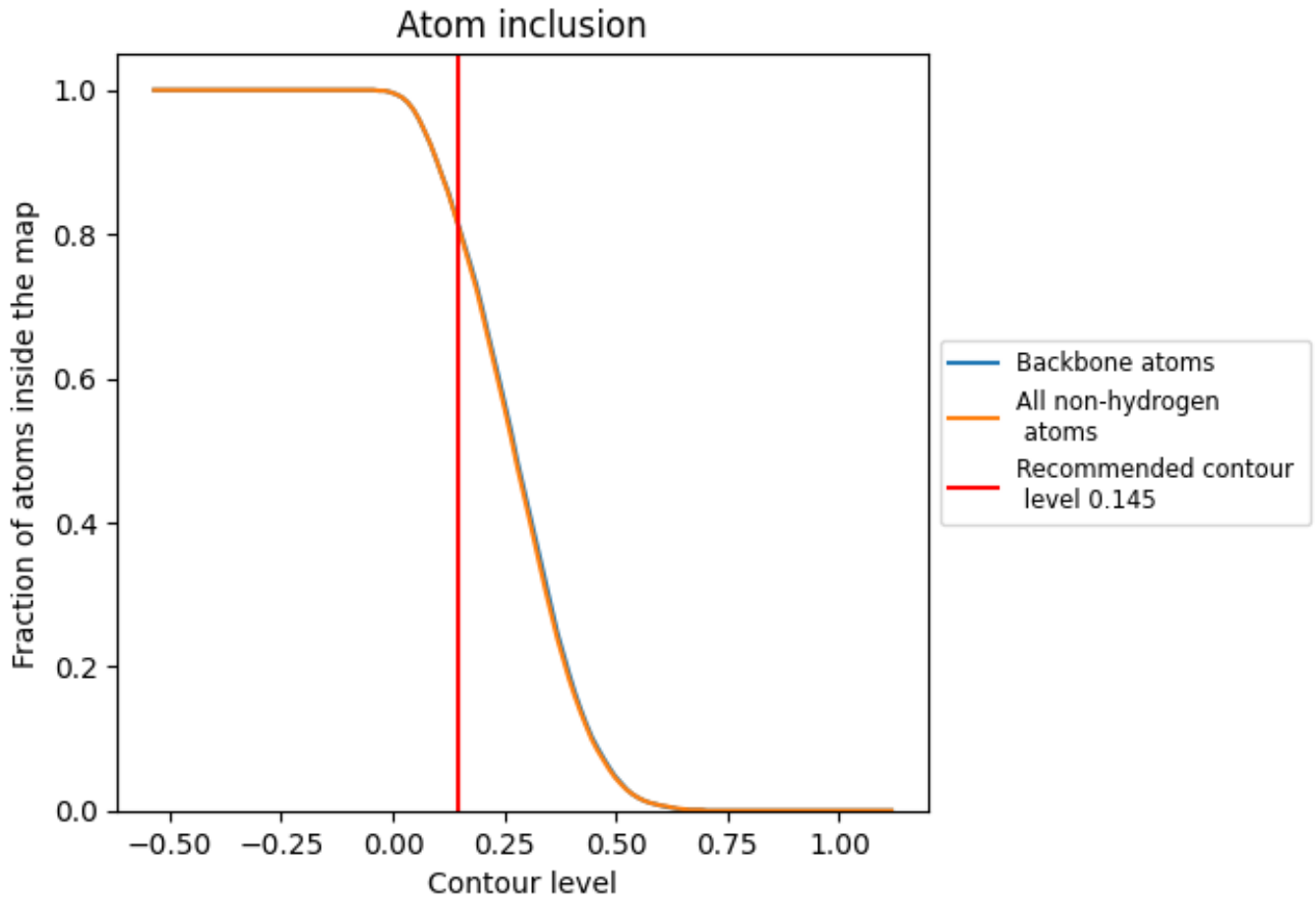
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.145).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 82% 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 (0.145) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8150	0.5930
1A	0.9220	0.6410
1B	0.9120	0.6450
1C	0.4250	0.3640
1D	0.4290	0.3780
1E	0.9040	0.6430
1F	0.8880	0.6290
1G	0.8350	0.6150
1H	0.8340	0.6170
1I	0.8160	0.6070
1J	0.7270	0.5830
1K	0.8440	0.6140
1L	0.8400	0.6020
1M	0.8880	0.6310
1N	0.8760	0.6220
1O	0.7760	0.5900
1P	0.7920	0.5700
1Q	0.7930	0.5750
1R	0.8120	0.5980
1S	0.7770	0.5730
1T	0.8680	0.6350

