wwPDB EM Validation Summary Report (i)

Nov 16, 2022 – 12:17 PM JST

PDB ID	:	6LUM
EMDB ID	:	EMD-0981
Title	:	Structure of Mycobacterium smegmatis succinate dehydrogenase 2
Authors	:	Gao, Y.; Gong, H.; Zhou, X.; Xiao, Y.; Wang, W.; Ji, W.; Wang, Q.; Rao, Z.
Deposited on	:	2020-01-29
Resolution	:	2.84 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 (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:

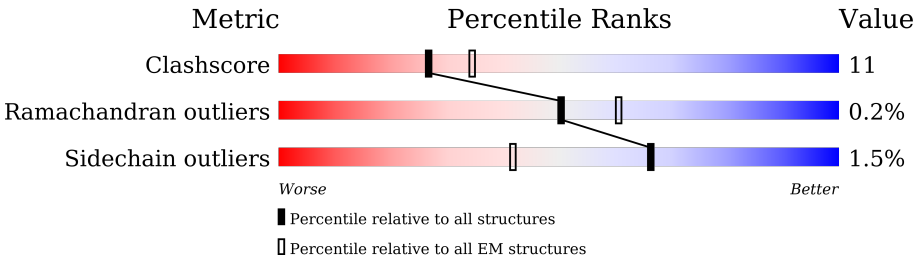
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.84 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	C	138	77% 12% 12%
1	G	138	70% 19% 11%
1	M	138	70% 20% 11%
2	D	166	75% 13% 12%
2	H	166	55% 16% 28%
2	N	166	55% 13% 30%
3	E	32	56% 22% 19%
3	I	32	59% 19% 19%

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Mol	Chain	Length	Quality of chain
3	O	32	59% 19% 19%
4	A	584	70% 22% 8%
4	J	584	71% 21% 9%
4	P	584	6% 65% 28% 8%
5	B	261	72% 19% 9%
5	K	261	71% 24% 5%
5	Q	261	5% 68% 23% 9%

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
15	F3S	Q	303	-	-	X	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 26191 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 Succinate dehydrogenase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	122	Total	C	N	O	S	0	0
			978	649	170	154	5		
1	G	123	Total	C	N	O	S	0	0
			989	658	171	155	5		
1	M	123	Total	C	N	O	S	0	0
			990	660	171	154	5		

- Molecule 2 is a protein called Succinate dehydrogenase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	146	Total	C	N	O	S	0	0
			1193	793	202	191	7		
2	H	120	Total	C	N	O	S	0	0
			991	669	159	157	6		
2	N	116	Total	C	N	O	S	0	0
			961	650	152	153	6		

- Molecule 3 is a protein called Succinate dehydrogenase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	31	Total	C	N	O	S	0	0
			256	179	35	41	1		
3	I	31	Total	C	N	O	S	0	0
			256	179	35	41	1		
3	O	31	Total	C	N	O	S	0	0
			256	179	35	41	1		

- Molecule 4 is a protein called Succinate dehydrogenase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	539	Total	C	N	O	S	0	0
			4129	2575	748	782	24		

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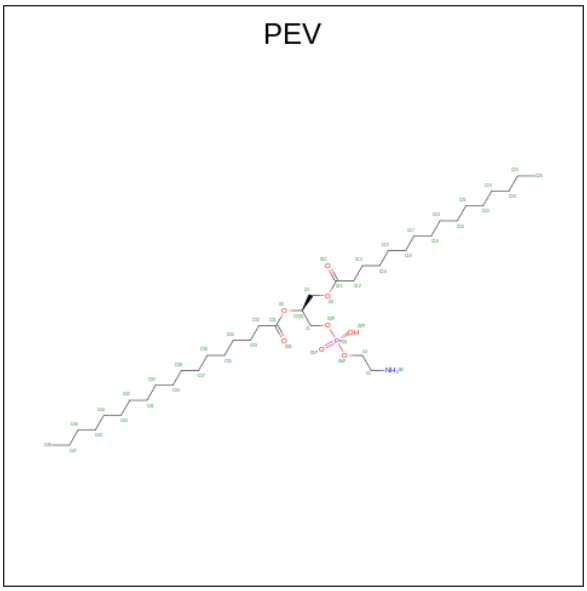
Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	534	Total	C	N	O	S	0	0
			4109	2565	741	779	24		
4	P	539	Total	C	N	O	S	0	0
			4025	2513	722	767	23		

- Molecule 5 is a protein called Succinate dehydrogenase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	238	Total	C	N	O	S	0	0
			1873	1182	335	338	18		
5	K	247	Total	C	N	O	S	0	0
			1938	1225	344	351	18		
5	Q	238	Total	C	N	O	S	0	0
			1849	1170	330	331	18		

- Molecule 6 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PEV) (formula: $C_{39}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	C	1	Total	C	N	O	P	0
			85	65	2	16	2	
6	C	1	Total	C	N	O	P	0
			85	65	2	16	2	
6	G	1	Total	C	N	O	P	0
			44	34	1	8	1	

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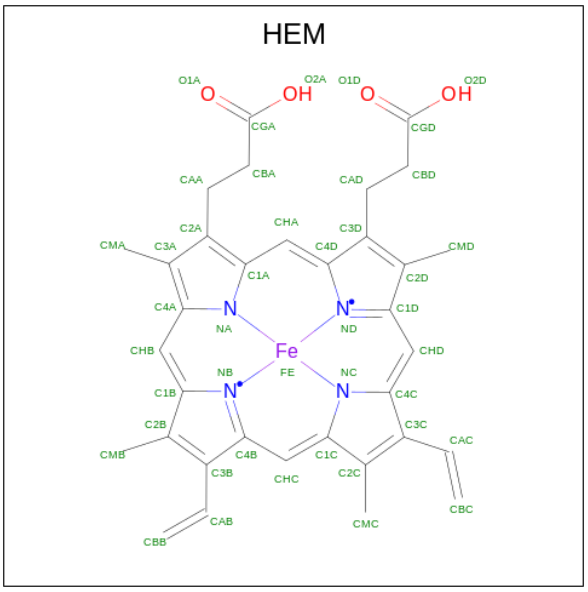
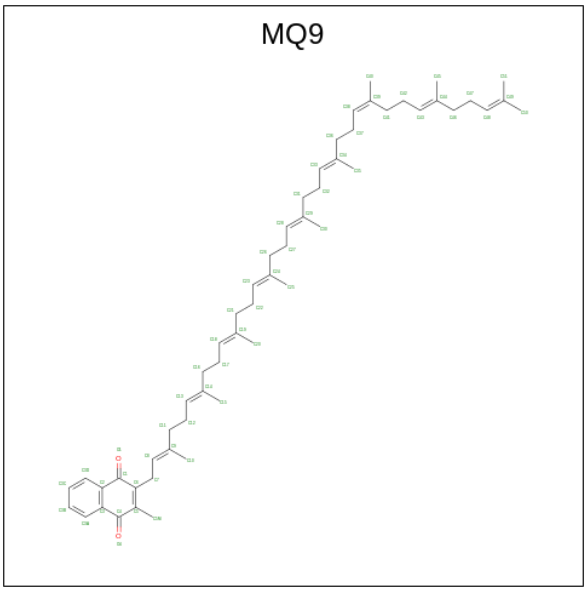
Mol	Chain	Residues	Atoms					AltConf
6	K	1	Total	C	N	O	P	0
			41	31	1	8	1	
6	M	1	Total	C	N	O	P	0
			44	34	1	8	1	
6	Q	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



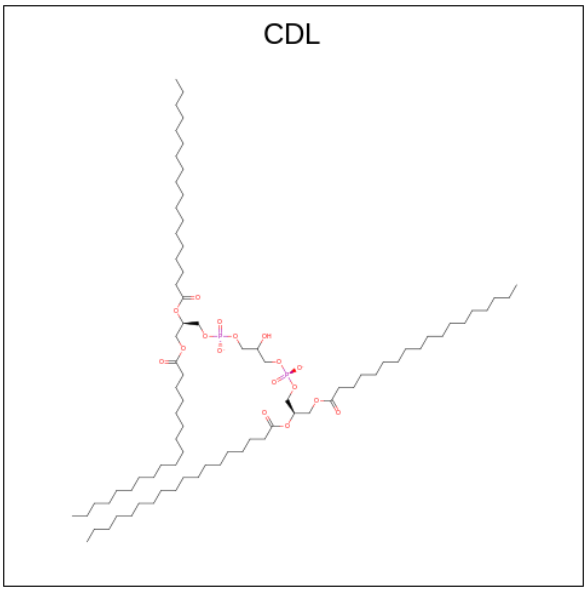
Mol	Chain	Residues	Atoms					AltConf
7	D	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
7	D	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
7	H	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
7	H	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
7	M	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
7	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 8 is MENAQUINONE-9 (three-letter code: MQ9) (formula: $C_{56}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



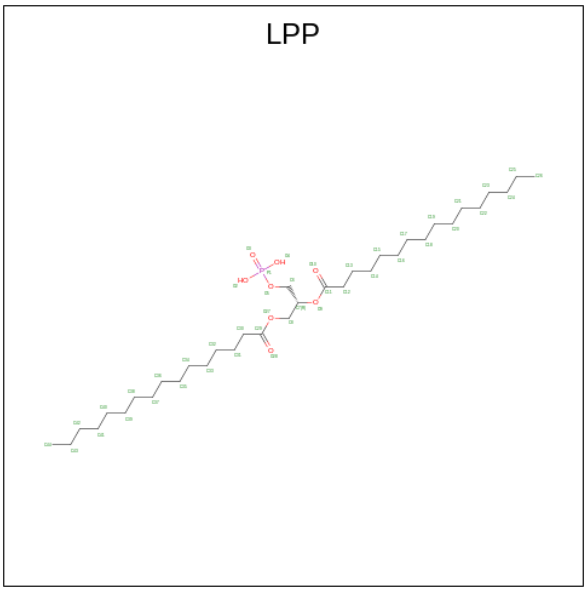
Mol	Chain	Residues	Atoms	AltConf
8	D	1	Total C O 48 44 4	0
8	D	1	Total C O 48 44 4	0
8	H	1	Total C O 23 21 2	0
8	N	1	Total C O 70 64 6	0
8	N	1	Total C O 70 64 6	0
8	N	1	Total C O 70 64 6	0

- Molecule 9 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



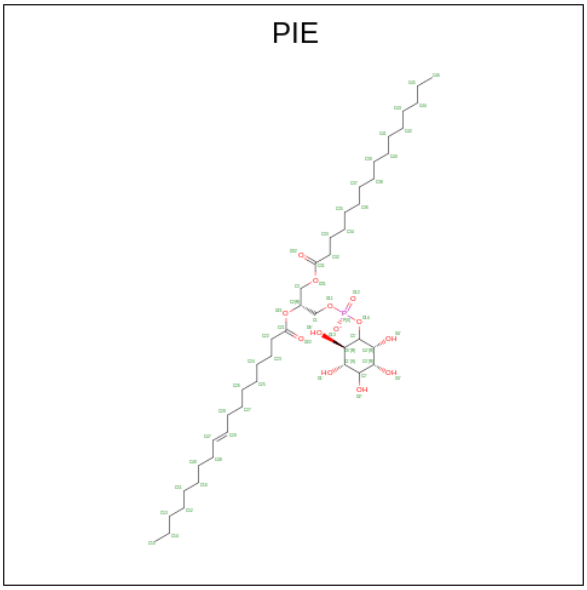
Mol	Chain	Residues	Atoms				AltConf
9	D	1	Total	C	O	P	0
			84	65	17	2	
9	H	1	Total	C	O	P	0
			84	65	17	2	
9	N	1	Total	C	O	P	0
			84	65	17	2	

- Molecule 10 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (three-letter code: LPP) (formula: $C_{35}H_{69}O_8P$).



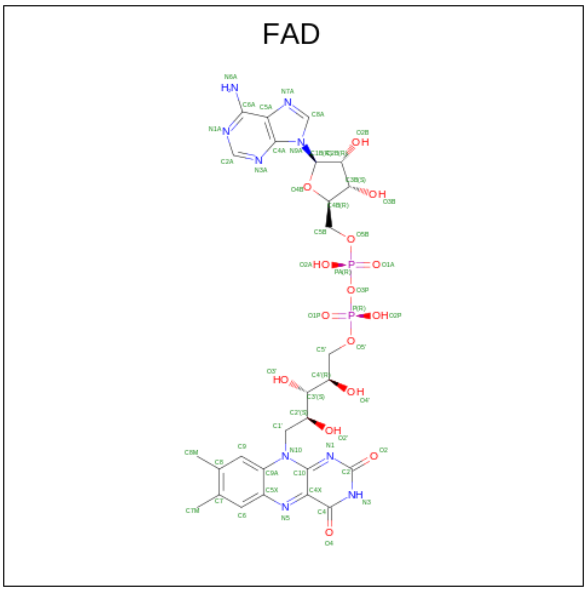
Mol	Chain	Residues	Atoms				AltConf
10	D	1	Total	C	O	P	0
			44	35	8	1	
10	H	1	Total	C	O	P	0
			44	35	8	1	
10	N	1	Total	C	O	P	0
			44	35	8	1	

- Molecule 11 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOINOSITOL (three-letter code: PIE) (formula: $C_{43}H_{80}O_{13}P$) (labeled as "Ligand of Interest" by depositor).



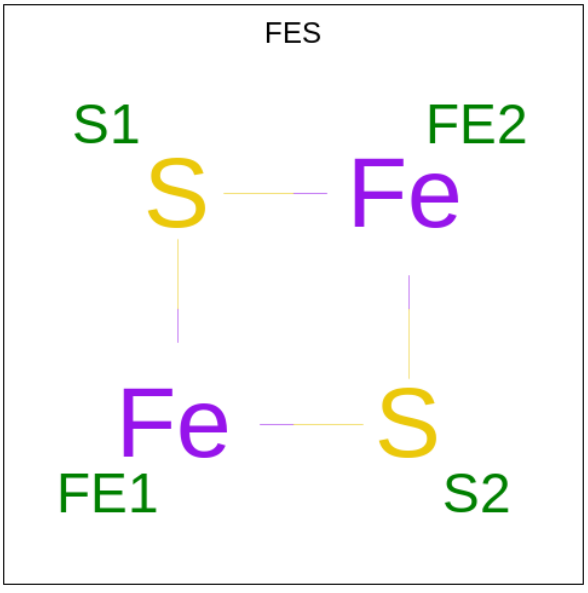
Mol	Chain	Residues	Atoms				AltConf
11	E	1	Total	C	O	P	0
			48	34	13	1	
11	H	1	Total	C	O	P	0
			48	34	13	1	
11	M	1	Total	C	O	P	0
			48	34	13	1	

- Molecule 12 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	N	O	P	0
			53	27	9	15	2	
12	J	1	Total	C	N	O	P	0
			53	27	9	15	2	
12	P	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
13	B	1	Total	Fe	S	0
			4	2	2	

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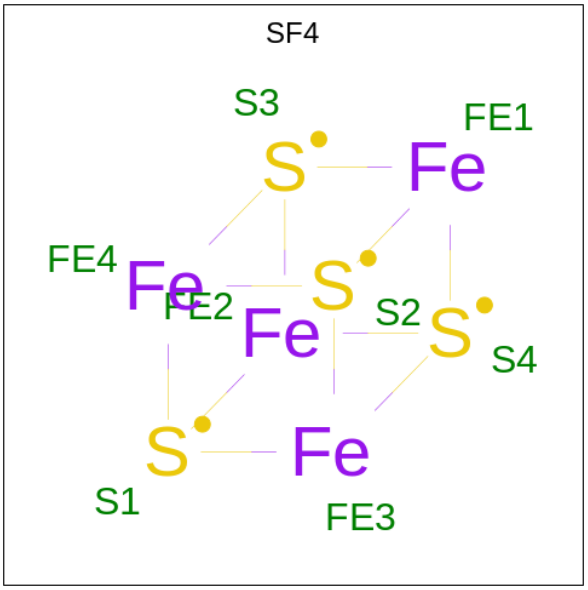
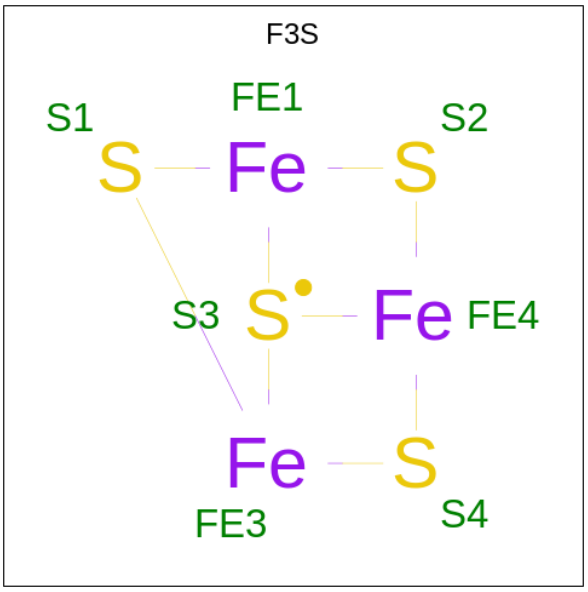
Mol	Chain	Residues	Atoms	AltConf
13	K	1	Total Fe S 4 2 2	0
13	Q	1	Total Fe S 4 2 2	0

- Molecule 14 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
14	B	1	Total Fe S 8 4 4	0
14	K	1	Total Fe S 8 4 4	0
14	Q	1	Total Fe S 8 4 4	0

- Molecule 15 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



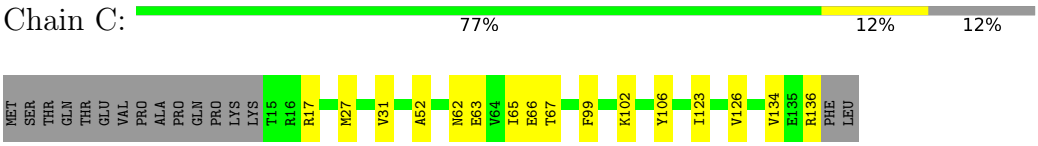
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
15	B	1	7	3	4	0
			Total	Fe	S	
15	K	1	7	3	4	0
			Total	Fe	S	
15	Q	1	7	3	4	0

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.

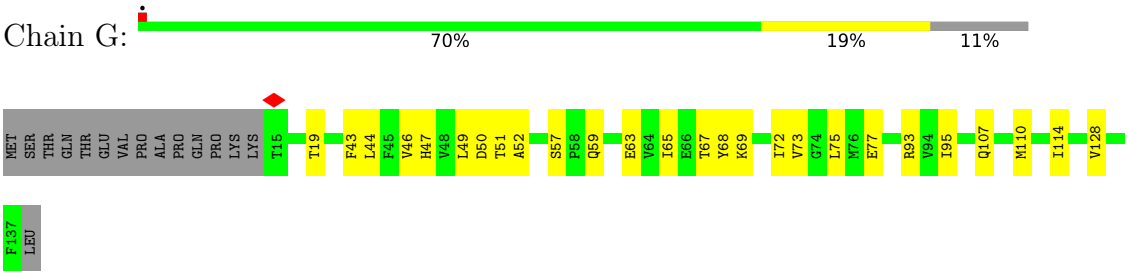
• Molecule 1: Succinate dehydrogenase subunit C

Chain C:



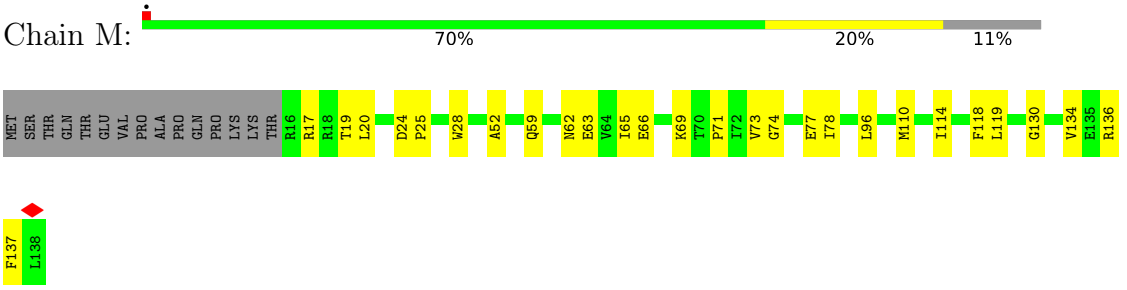
• Molecule 1: Succinate dehydrogenase subunit C

Chain G:



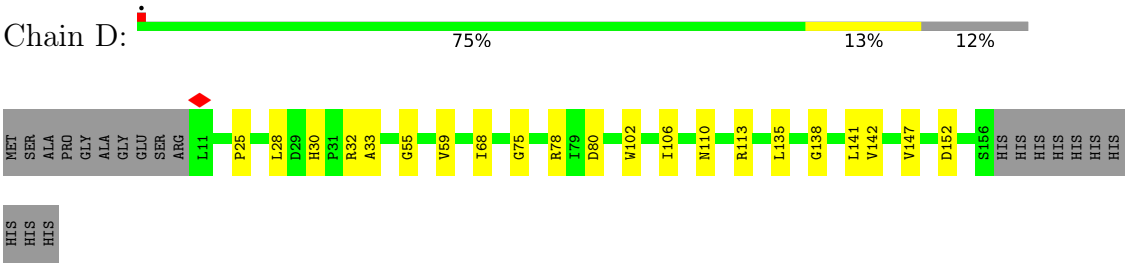
• Molecule 1: Succinate dehydrogenase subunit C

Chain M:



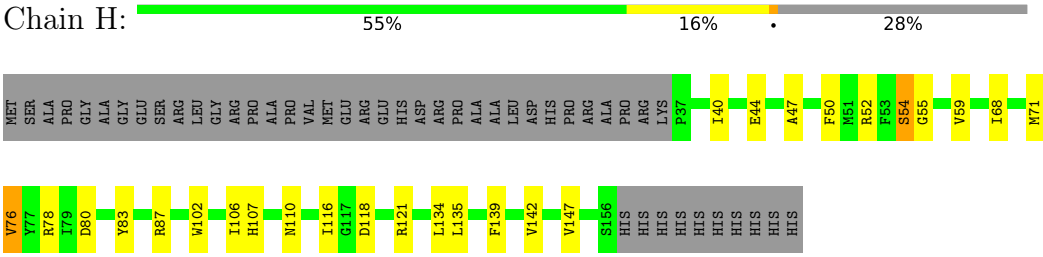
• Molecule 2: Succinate dehydrogenase subunit D

Chain D:



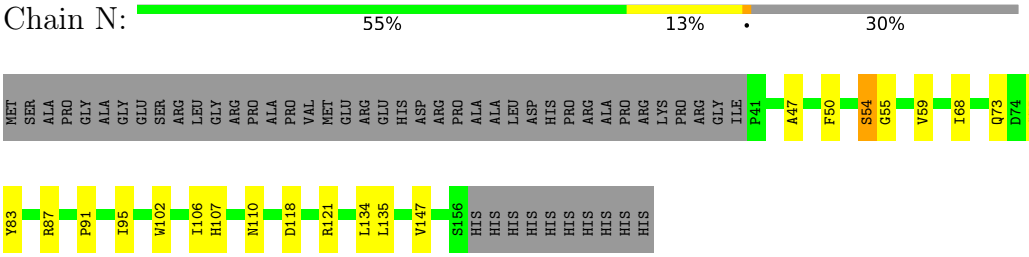
• Molecule 2: Succinate dehydrogenase subunit D

Chain H:



• Molecule 2: Succinate dehydrogenase subunit D

Chain N:



• Molecule 3: Succinate dehydrogenase subunit F

Chain E:

• Molecule 3: Succinate dehydrogenase subunit F

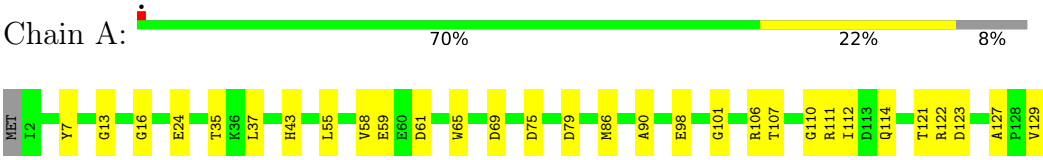
Chain I:

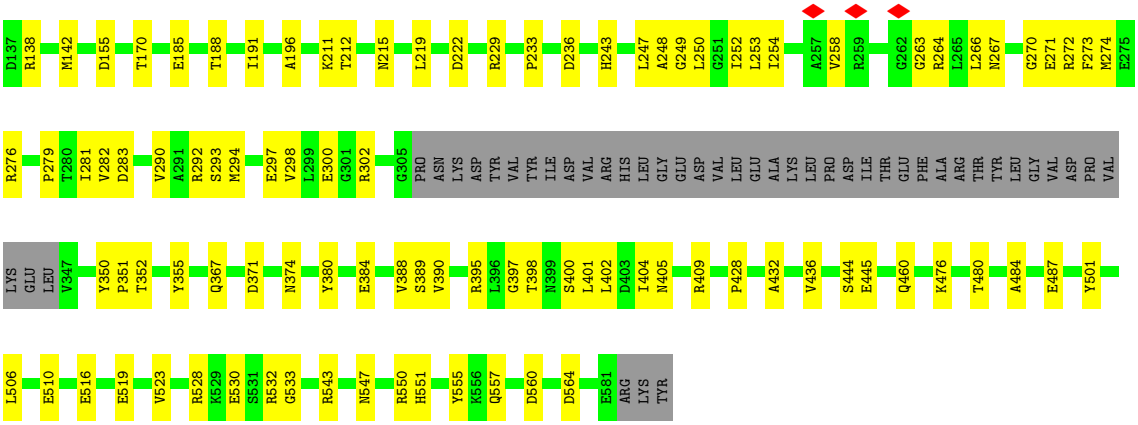
• Molecule 3: Succinate dehydrogenase subunit F

Chain O:

• Molecule 4: Succinate dehydrogenase subunit A

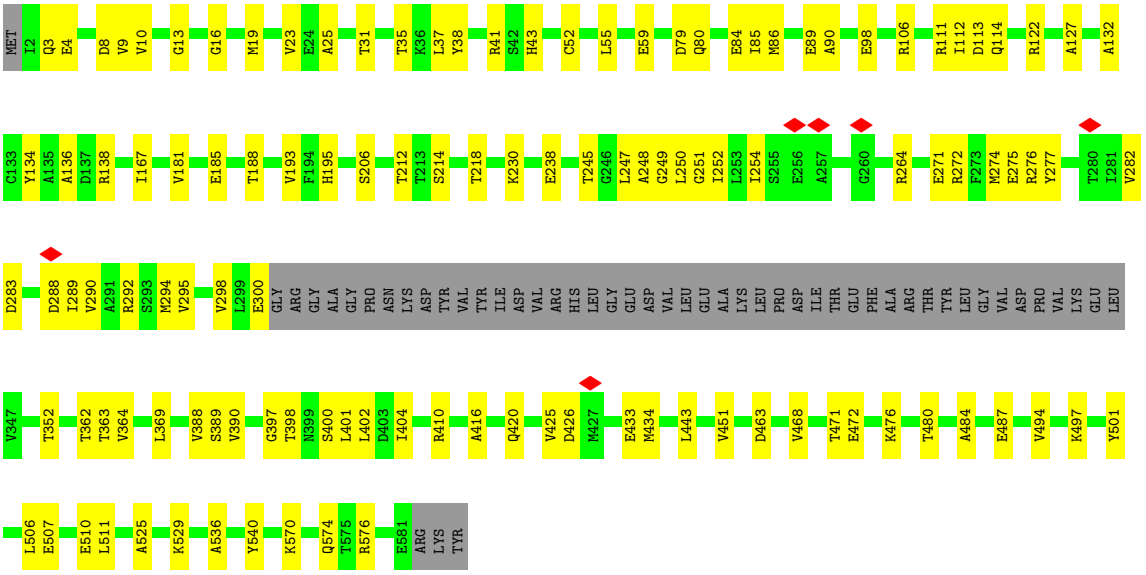
Chain A:





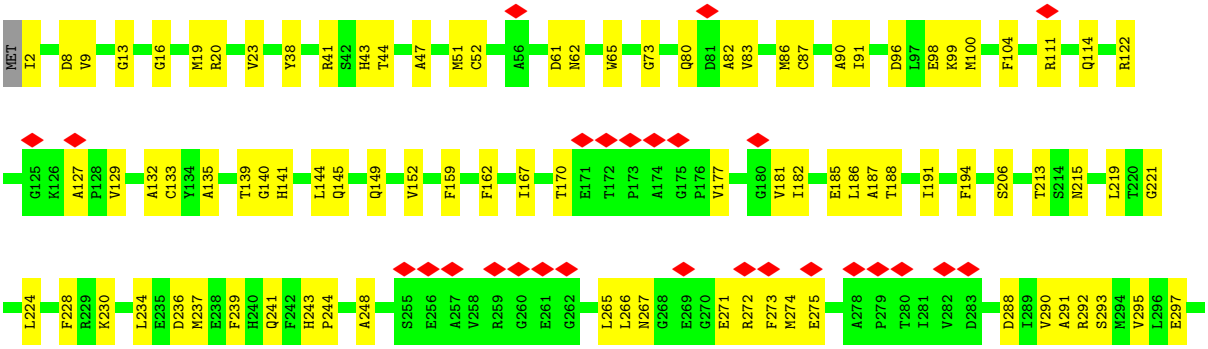
• Molecule 4: Succinate dehydrogenase subunit A

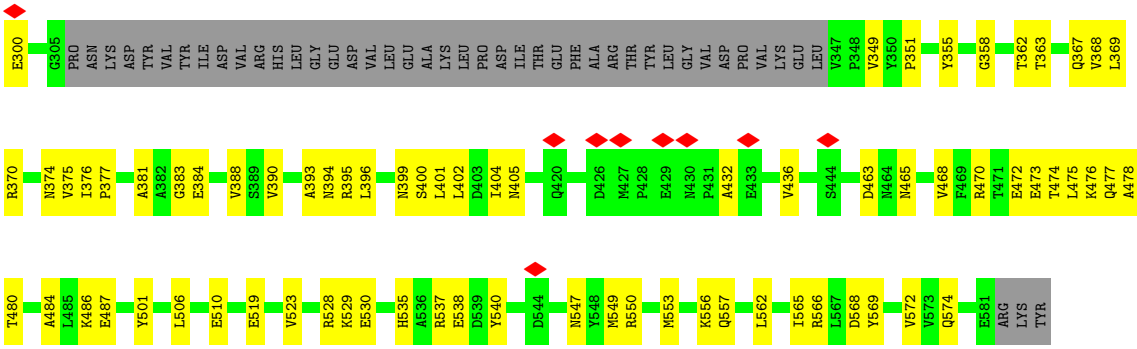
Chain J:



• Molecule 4: Succinate dehydrogenase subunit A

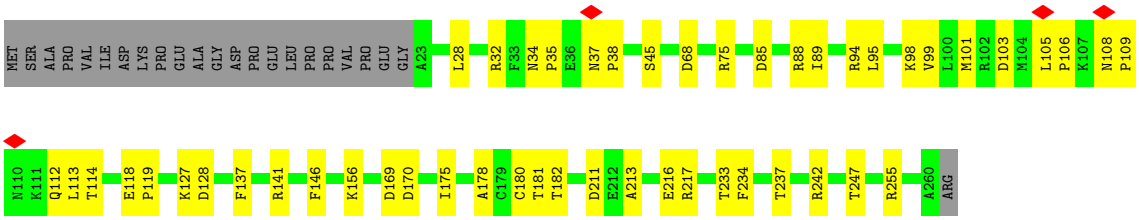
Chain P:





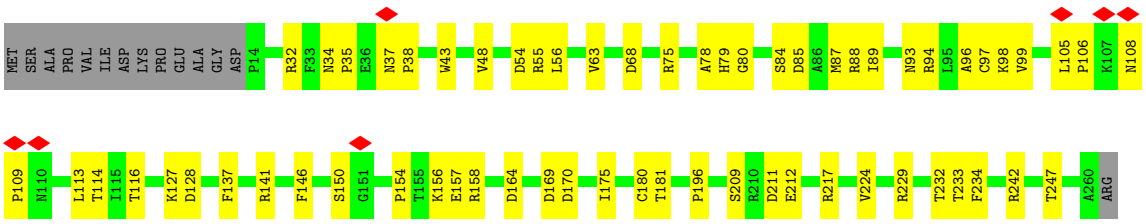
• Molecule 5: Succinate dehydrogenase subunit B

Chain B:



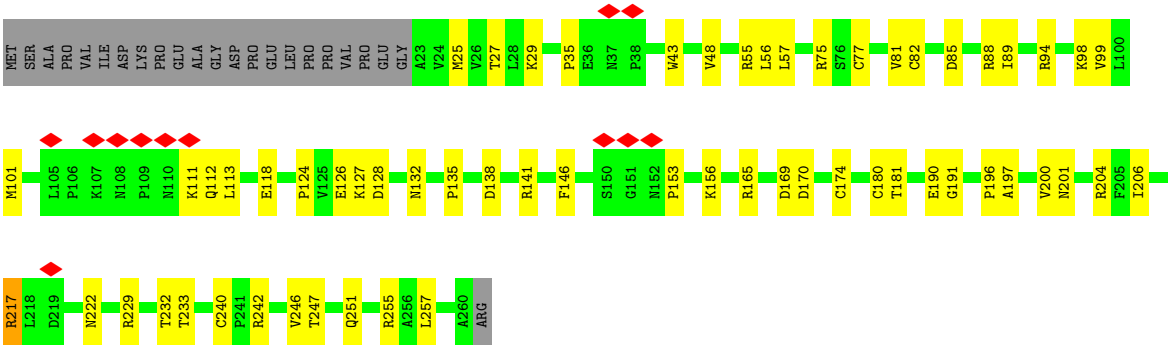
• Molecule 5: Succinate dehydrogenase subunit B

Chain K:



• Molecule 5: Succinate dehydrogenase subunit B

Chain Q:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	461385	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.744	Depositor
Minimum map value	-1.845	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	314.88, 314.88, 314.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, SF4, F3S, HEM, MQ9, FES, PIE, LPP, PEV, FAD

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	C	0.53	0/1003	0.52	0/1363
1	G	0.49	0/1015	0.52	0/1379
1	M	0.44	0/1016	0.51	0/1380
2	D	0.56	0/1234	0.49	0/1680
2	H	0.53	0/1025	0.49	0/1394
2	N	0.54	0/994	0.49	0/1352
3	E	0.53	0/262	0.56	0/359
3	I	0.53	0/262	0.56	0/359
3	O	0.53	0/262	0.56	0/359
4	A	0.46	0/4209	0.53	1/5704 (0.0%)
4	J	0.41	0/4189	0.52	0/5677
4	P	0.33	0/4102	0.52	0/5573
5	B	0.62	0/1916	0.56	0/2605
5	K	0.58	0/1985	0.55	0/2702
5	Q	0.47	0/1891	0.52	0/2573
All	All	0.48	0/25365	0.52	1/34459 (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
5	K	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	101	GLY	C-N-CA	-6.01	106.67	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	K	37	ASN	Peptide
5	K	80	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	978	0	1020	11	0
1	G	989	0	1029	22	0
1	M	990	0	1032	16	0
2	D	1193	0	1184	17	0
2	H	991	0	985	22	0
2	N	961	0	951	16	0
3	E	256	0	271	9	0
3	I	256	0	271	7	0
3	O	256	0	271	8	0
4	A	4129	0	4015	99	0
4	J	4109	0	4003	79	0
4	P	4025	0	3853	130	0
5	B	1873	0	1854	36	0
5	K	1938	0	1918	40	0
5	Q	1849	0	1826	44	0
6	C	85	0	116	0	0
6	G	44	0	61	3	0
6	K	41	0	55	1	0
6	M	44	0	61	1	0
6	Q	41	0	55	0	0
7	D	86	0	60	6	0
7	H	86	0	60	8	0
7	M	43	0	30	3	0
7	N	43	0	30	3	0
8	D	48	0	46	4	0
8	H	23	0	21	0	0
8	N	70	0	65	7	0
9	D	84	0	115	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	H	84	0	115	5	0
9	N	84	0	115	2	0
10	D	44	0	67	2	0
10	H	44	0	67	3	0
10	N	44	0	67	2	0
11	E	48	0	56	4	0
11	H	48	0	56	3	0
11	M	48	0	55	3	0
12	A	53	0	29	18	0
12	J	53	0	29	6	0
12	P	53	0	29	6	0
13	B	4	0	0	0	0
13	K	4	0	0	0	0
13	Q	4	0	0	0	0
14	B	8	0	0	0	0
14	K	8	0	0	0	0
14	Q	8	0	0	1	0
15	B	7	0	0	1	0
15	K	7	0	0	1	0
15	Q	7	0	0	2	0
All	All	26191	0	25943	572	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 11.

The worst 5 of 572 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)
4:J:43:HIS:NE2	12:J:700:FAD:C8M	1.70	1.54
4:A:43:HIS:NE2	12:A:700:FAD:C8M	1.71	1.51
4:P:43:HIS:NE2	12:P:700:FAD:C8M	1.70	1.50
4:J:43:HIS:CE1	12:J:700:FAD:C8M	2.27	1.16
4:A:43:HIS:CE1	12:A:700:FAD:C8M	2.30	1.14

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	C	120/138 (87%)	115 (96%)	5 (4%)	0	100	100
1	G	121/138 (88%)	119 (98%)	2 (2%)	0	100	100
1	M	121/138 (88%)	116 (96%)	5 (4%)	0	100	100
2	D	144/166 (87%)	138 (96%)	6 (4%)	0	100	100
2	H	118/166 (71%)	115 (98%)	3 (2%)	0	100	100
2	N	114/166 (69%)	111 (97%)	3 (3%)	0	100	100
3	E	29/32 (91%)	29 (100%)	0	0	100	100
3	I	29/32 (91%)	29 (100%)	0	0	100	100
3	O	29/32 (91%)	29 (100%)	0	0	100	100
4	A	535/584 (92%)	483 (90%)	51 (10%)	1 (0%)	47	69
4	J	530/584 (91%)	462 (87%)	67 (13%)	1 (0%)	47	69
4	P	535/584 (92%)	492 (92%)	43 (8%)	0	100	100
5	B	236/261 (90%)	197 (84%)	38 (16%)	1 (0%)	34	56
5	K	245/261 (94%)	201 (82%)	43 (18%)	1 (0%)	34	56
5	Q	236/261 (90%)	194 (82%)	41 (17%)	1 (0%)	34	56
All	All	3142/3543 (89%)	2830 (90%)	307 (10%)	5 (0%)	50	69

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	101	MET
4	J	248	ALA
4	A	248	ALA
5	K	96	ALA
5	Q	101	MET

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	C	101/116 (87%)	101 (100%)	0	100 100
1	G	102/116 (88%)	102 (100%)	0	100 100
1	M	102/116 (88%)	102 (100%)	0	100 100
2	D	120/137 (88%)	120 (100%)	0	100 100
2	H	100/137 (73%)	96 (96%)	4 (4%)	31 57
2	N	97/137 (71%)	93 (96%)	4 (4%)	30 56
3	E	27/28 (96%)	19 (70%)	8 (30%)	0 0
3	I	27/28 (96%)	19 (70%)	8 (30%)	0 0
3	O	27/28 (96%)	19 (70%)	8 (30%)	0 0
4	A	421/467 (90%)	421 (100%)	0	100 100
4	J	422/467 (90%)	422 (100%)	0	100 100
4	P	400/467 (86%)	399 (100%)	1 (0%)	92 96
5	B	205/225 (91%)	204 (100%)	1 (0%)	88 94
5	K	213/225 (95%)	211 (99%)	2 (1%)	78 89
5	Q	199/225 (88%)	196 (98%)	3 (2%)	65 82
All	All	2563/2919 (88%)	2524 (98%)	39 (2%)	66 82

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	O	3	LEU
4	P	463	ASP
3	O	7	ILE
3	O	21	VAL
5	Q	204	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	87	HIS
4	P	241	GLN
1	M	132	HIS
4	P	114	GLN
4	P	354	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

39 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	$\#\|Z\| > 2$
12	FAD	J	700	-	53,58,58	1.24	7 (13%)	68,89,89	1.34	12 (17%)
6	PEV	C	201	-	40,40,48	0.95	3 (7%)	43,45,53	0.90	2 (4%)
15	F3S	K	303	5	0,9,9	-	-	-		
11	PIE	H	206	-	48,48,57	1.03	4 (8%)	58,60,69	0.98	3 (5%)
7	HEM	M	201	2	41,50,50	1.42	4 (9%)	45,82,82	1.42	8 (17%)
6	PEV	K	304	-	40,40,48	0.93	4 (10%)	43,45,53	0.98	2 (4%)
11	PIE	E	101	-	48,48,57	1.02	4 (8%)	58,60,69	0.91	2 (3%)
11	PIE	M	202	-	48,48,57	1.04	4 (8%)	58,60,69	1.07	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	HEM	H	202	-	41,50,50	1.52	5 (12%)	45,82,82	1.40	5 (11%)
8	MQ9	H	204	-	24,24,59	4.74	16 (66%)	30,33,75	3.17	12 (40%)
12	FAD	P	700	-	53,58,58	1.29	5 (9%)	68,89,89	1.35	10 (14%)
7	HEM	D	201	2	41,50,50	1.44	5 (12%)	45,82,82	1.51	7 (15%)
13	FES	Q	301	5	0,4,4	-	-	-		
7	HEM	H	203	2	41,50,50	1.50	2 (4%)	45,82,82	1.53	10 (22%)
7	HEM	N	202	1	41,50,50	1.52	5 (12%)	45,82,82	1.39	7 (15%)
13	FES	B	301	5	0,4,4	-	-	-		
10	LPP	N	205	-	43,43,43	0.93	3 (6%)	47,48,48	0.94	2 (4%)
6	PEV	C	202	-	43,43,48	0.94	4 (9%)	46,48,53	0.97	2 (4%)
8	MQ9	N	204	-	24,24,59	4.60	14 (58%)	30,33,75	2.93	12 (40%)
9	CDL	D	204	-	83,83,99	0.94	7 (8%)	89,95,111	1.00	4 (4%)
6	PEV	M	203	-	43,43,48	0.94	4 (9%)	46,48,53	0.98	3 (6%)
10	LPP	H	201	-	43,43,43	0.93	4 (9%)	47,48,48	0.90	2 (4%)
6	PEV	G	201	-	43,43,48	0.94	4 (9%)	46,48,53	0.90	2 (4%)
12	FAD	A	700	-	53,58,58	1.28	5 (9%)	68,89,89	1.35	10 (14%)
14	SF4	K	302	5	0,12,12	-	-	-		
14	SF4	B	302	5	0,12,12	-	-	-		
15	F3S	B	303	5	0,9,9	-	-	-		
6	PEV	Q	304	-	40,40,48	0.94	4 (10%)	43,45,53	0.96	2 (4%)
8	MQ9	N	201	-	24,24,59	4.71	15 (62%)	30,33,75	2.38	9 (30%)
10	LPP	D	206	-	43,43,43	0.93	3 (6%)	47,48,48	0.89	2 (4%)
14	SF4	Q	302	5	0,12,12	-	-	-		
9	CDL	N	206	-	83,83,99	0.93	8 (9%)	89,95,111	0.98	4 (4%)
13	FES	K	301	5	0,4,4	-	-	-		
9	CDL	H	205	-	83,83,99	0.93	8 (9%)	89,95,111	0.98	4 (4%)
8	MQ9	N	203	-	25,25,59	4.71	15 (60%)	31,34,75	3.04	10 (32%)
8	MQ9	D	203	-	25,25,59	4.72	16 (64%)	31,34,75	3.12	11 (35%)
8	MQ9	D	205	-	25,25,59	4.59	14 (56%)	31,34,75	3.18	12 (38%)
7	HEM	D	202	1	41,50,50	1.60	7 (17%)	45,82,82	1.42	5 (11%)
15	F3S	Q	303	5	0,9,9	-	-	-		

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
12	FAD	J	700	-	-	14/30/50/50	0/6/6/6
6	PEV	C	201	-	-	26/44/44/52	-
15	F3S	K	303	5	-	-	0/3/3/3
11	PIE	H	206	-	-	25/43/67/76	0/1/1/1
7	HEM	M	201	2	-	0/12/54/54	-
6	PEV	K	304	-	-	22/44/44/52	-
11	PIE	E	101	-	-	21/43/67/76	0/1/1/1
11	PIE	M	202	-	-	24/43/67/76	0/1/1/1
7	HEM	H	202	-	-	2/12/54/54	-
8	MQ9	H	204	-	-	7/11/31/73	0/2/2/2
12	FAD	P	700	-	-	13/30/50/50	0/6/6/6
7	HEM	D	201	2	-	0/12/54/54	-
13	FES	Q	301	5	-	-	0/1/1/1
7	HEM	H	203	2	-	0/12/54/54	-
7	HEM	N	202	1	-	2/12/54/54	-
13	FES	B	301	5	-	-	0/1/1/1
10	LPP	N	205	-	-	25/45/45/45	-
6	PEV	C	202	-	-	24/47/47/52	-
8	MQ9	N	204	-	-	8/11/31/73	0/2/2/2
9	CDL	D	204	-	-	55/94/94/110	-
6	PEV	M	203	-	-	26/47/47/52	-
10	LPP	H	201	-	-	27/45/45/45	-
6	PEV	G	201	-	-	23/47/47/52	-
12	FAD	A	700	-	-	13/30/50/50	0/6/6/6
14	SF4	K	302	5	-	-	0/6/5/5
14	SF4	B	302	5	-	-	0/6/5/5
15	F3S	B	303	5	-	-	0/3/3/3
6	PEV	Q	304	-	-	25/44/44/52	-
8	MQ9	N	201	-	-	5/11/31/73	0/2/2/2
10	LPP	D	206	-	-	25/45/45/45	-
14	SF4	Q	302	5	-	-	0/6/5/5
9	CDL	N	206	-	-	58/94/94/110	-
13	FES	K	301	5	-	-	0/1/1/1
9	CDL	H	205	-	-	58/94/94/110	-
8	MQ9	N	203	-	-	5/13/33/73	0/2/2/2
8	MQ9	D	203	-	-	7/13/33/73	0/2/2/2
8	MQ9	D	205	-	-	9/13/33/73	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	HEM	D	202	1	-	3/12/54/54	-
15	F3S	Q	303	5	-	-	0/3/3/3

The worst 5 of 203 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	203	MQ9	O4-C4	10.82	1.46	1.23
8	D	203	MQ9	O4-C4	10.78	1.46	1.23
8	H	204	MQ9	O4-C4	10.77	1.46	1.23
8	N	201	MQ9	C8-C9	10.40	1.57	1.33
8	N	204	MQ9	O4-C4	10.31	1.45	1.23

The worst 5 of 180 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	204	MQ9	C7-C8-C9	-10.89	108.66	126.79
8	N	204	MQ9	C7-C8-C9	-8.43	112.75	126.79
8	D	205	MQ9	C7-C8-C9	-8.42	112.78	126.79
8	N	203	MQ9	C7-C8-C9	-8.12	113.27	126.79
8	D	203	MQ9	C7-C8-C9	-8.11	113.29	126.79

There are no chirality outliers.

5 of 552 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	201	PEV	C32-C31-O2-C2
6	C	201	PEV	O4P-C4-C5-N6
6	C	202	PEV	C32-C31-O2-C2
6	C	202	PEV	C4-O4P-P-O3P
6	G	201	PEV	C4-O4P-P-O1P

There are no ring outliers.

30 monomers are involved in 96 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	J	700	FAD	6	0
15	K	303	F3S	1	0
11	H	206	PIE	3	0
7	M	201	HEM	3	0
6	K	304	PEV	1	0
11	E	101	PIE	4	0

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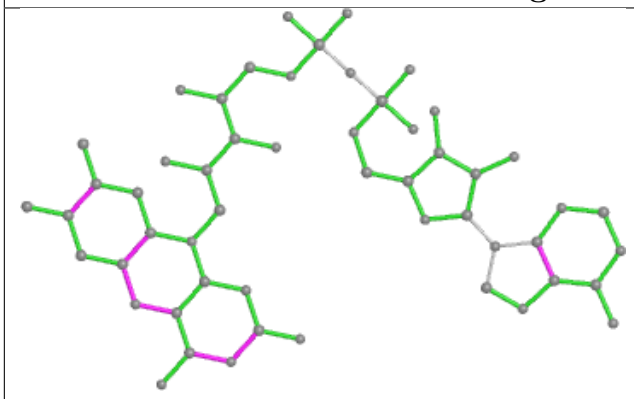
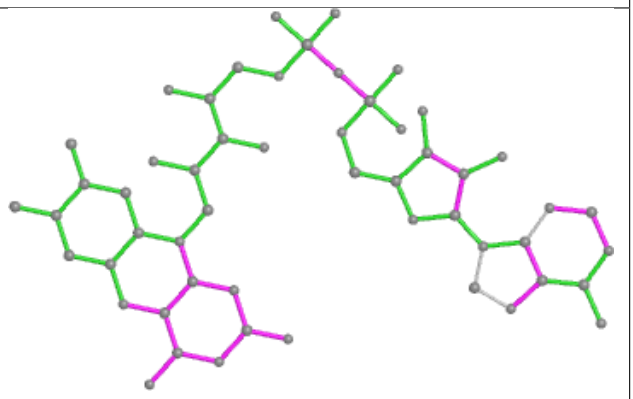
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	M	202	PIE	3	0
7	H	202	HEM	5	0
12	P	700	FAD	6	0
7	D	201	HEM	3	0
7	H	203	HEM	5	0
7	N	202	HEM	3	0
10	N	205	LPP	2	0
8	N	204	MQ9	4	0
9	D	204	CDL	2	0
6	M	203	PEV	1	0
10	H	201	LPP	3	0
6	G	201	PEV	3	0
12	A	700	FAD	18	0
15	B	303	F3S	1	0
8	N	201	MQ9	2	0
10	D	206	LPP	2	0
14	Q	302	SF4	1	0
9	N	206	CDL	2	0
9	H	205	CDL	5	0
8	N	203	MQ9	1	0
8	D	203	MQ9	2	0
8	D	205	MQ9	2	0
7	D	202	HEM	3	0
15	Q	303	F3S	2	0

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

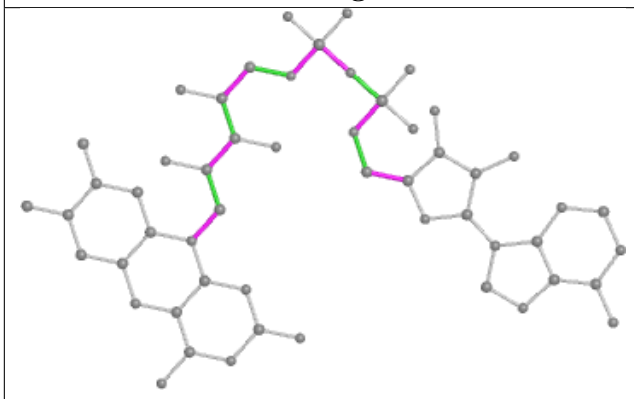
Ligand FAD J 700



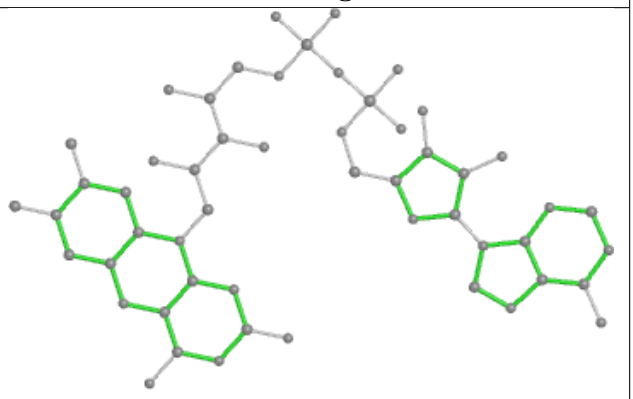
Bond lengths



Bond angles

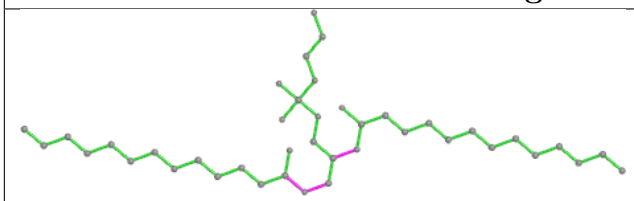


Torsions

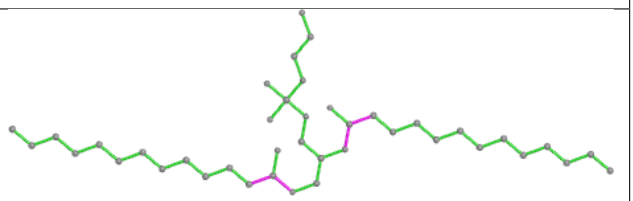


Rings

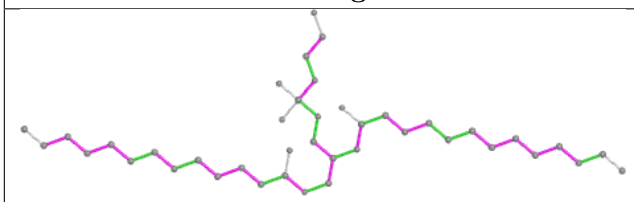
Ligand PEV C 201



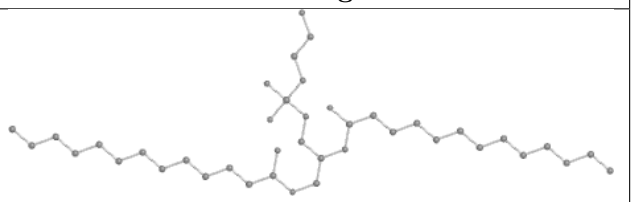
Bond lengths



Bond angles

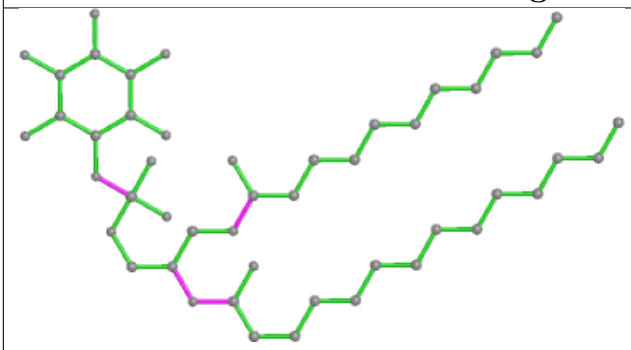


Torsions

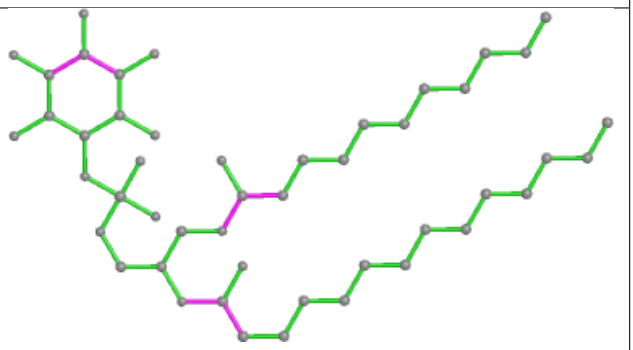


Rings

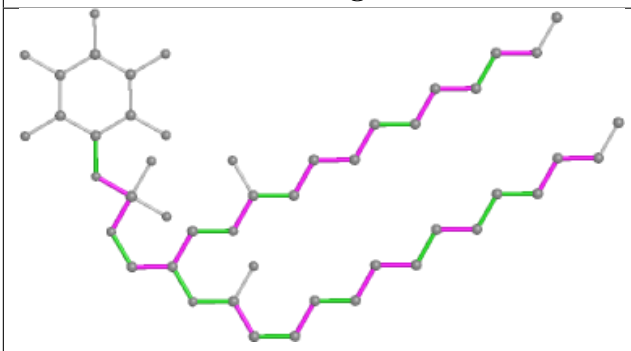
Ligand PIE H 206



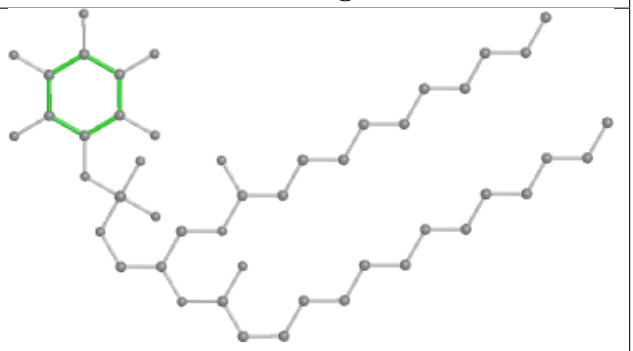
Bond lengths



Bond angles

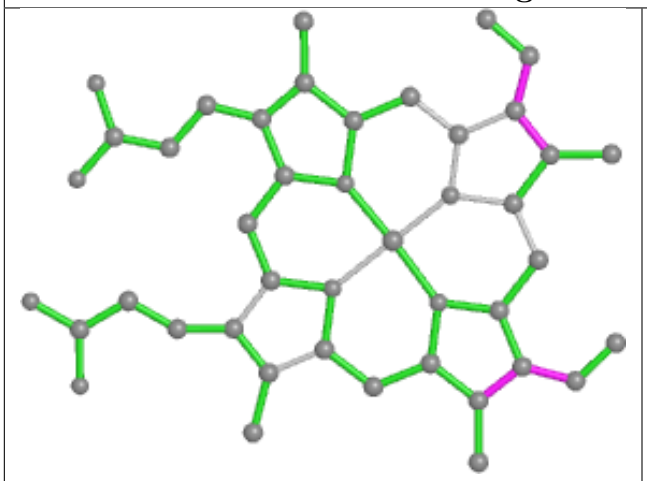


Torsions

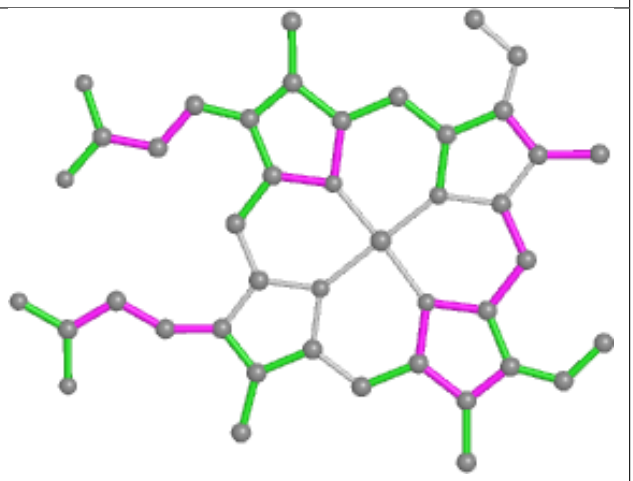


Rings

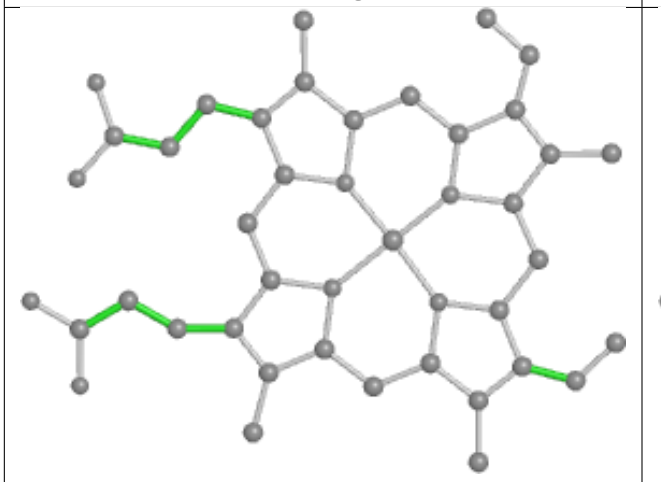
Ligand HEM M 201



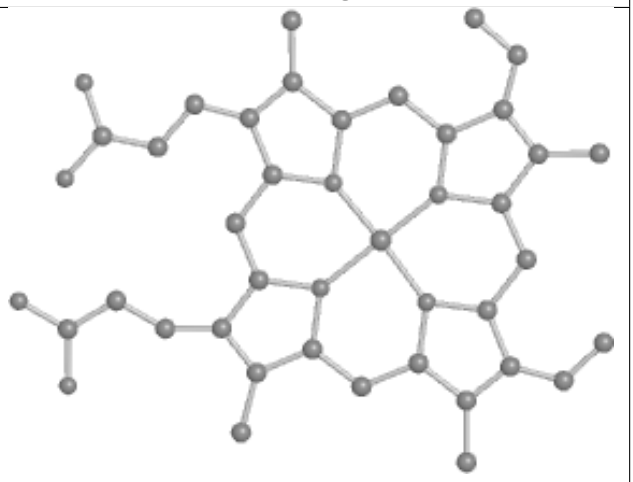
Bond lengths



Bond angles

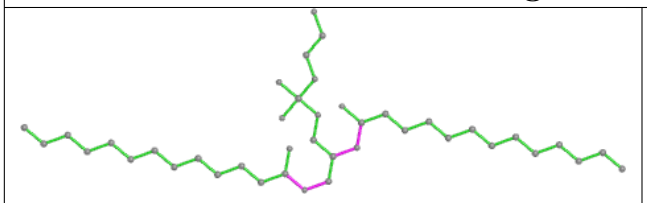


Torsions

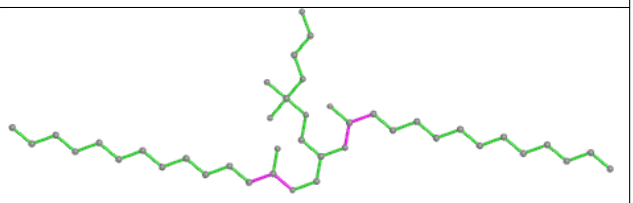


Rings

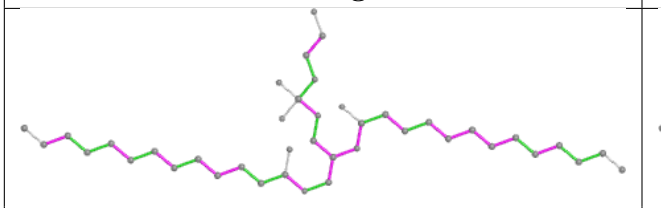
Ligand PEV K 304



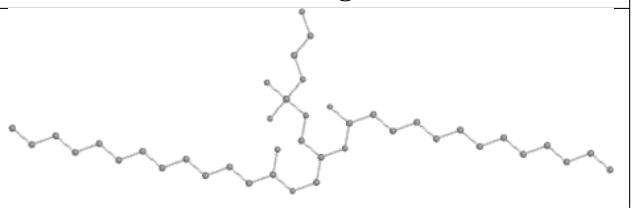
Bond lengths



Bond angles

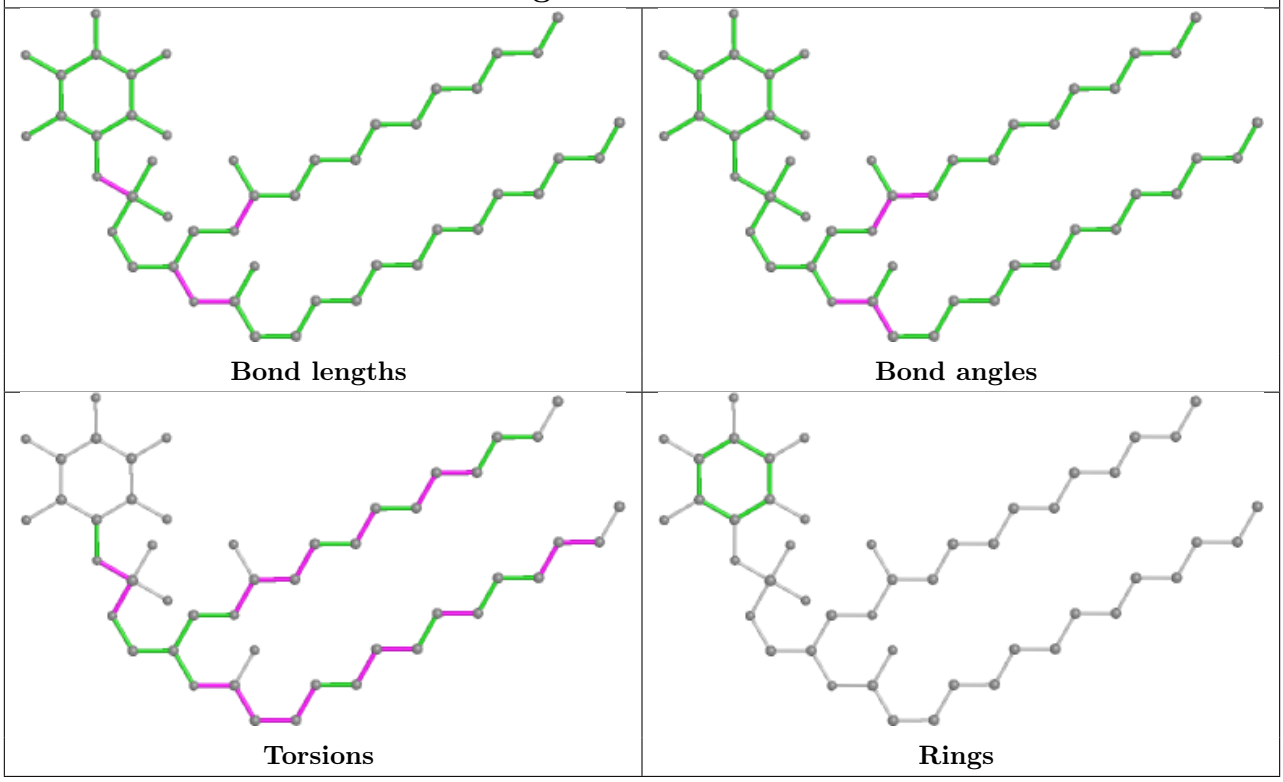


Torsions

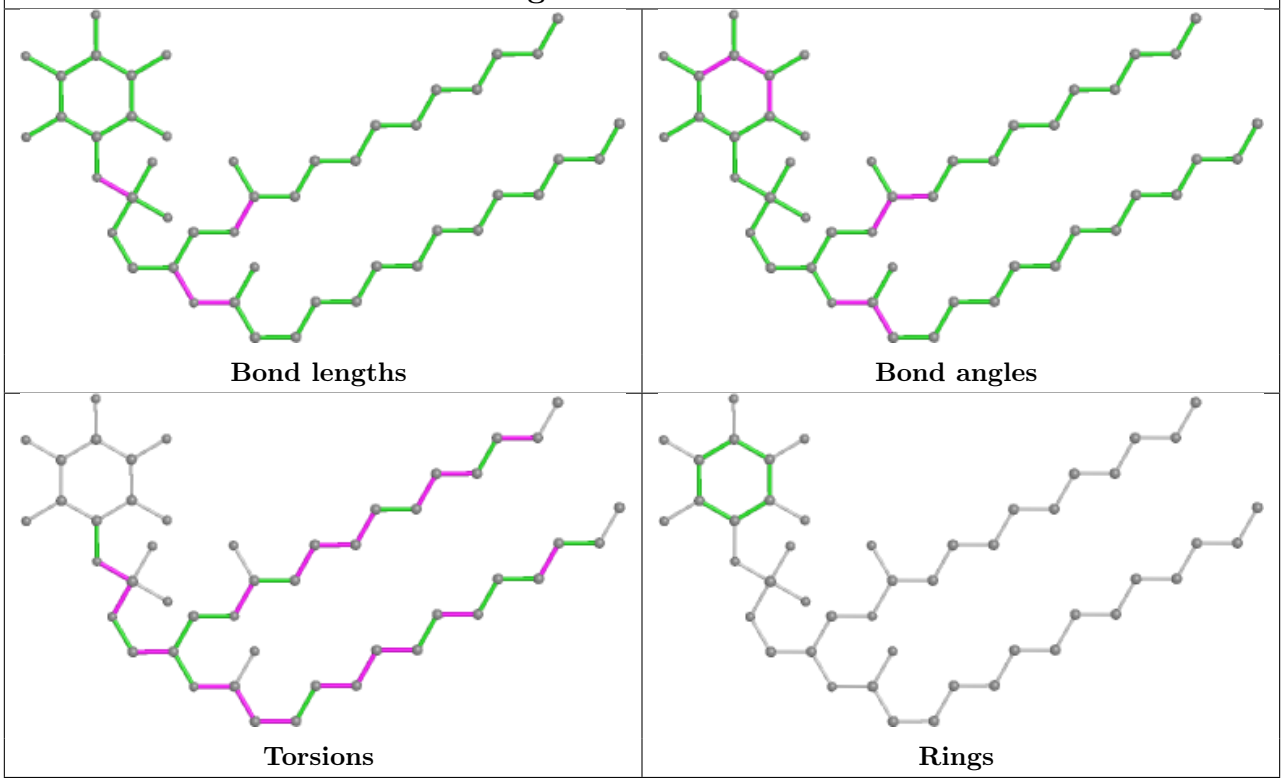


Rings

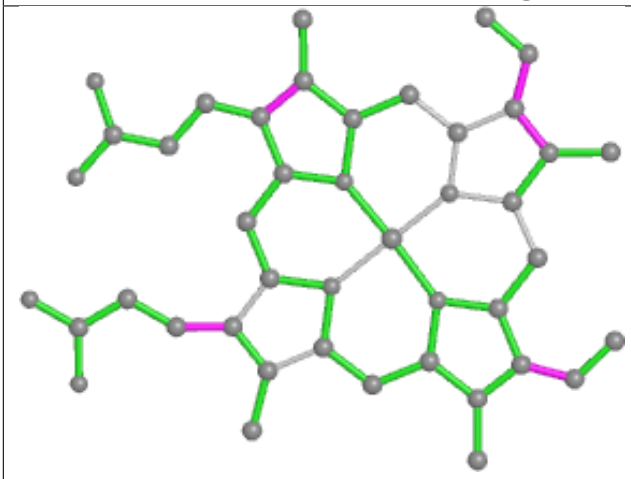
Ligand PIE E 101



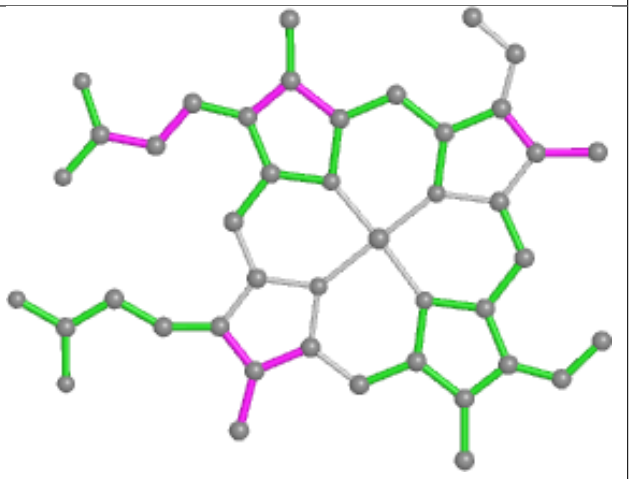
Ligand PIE M 202



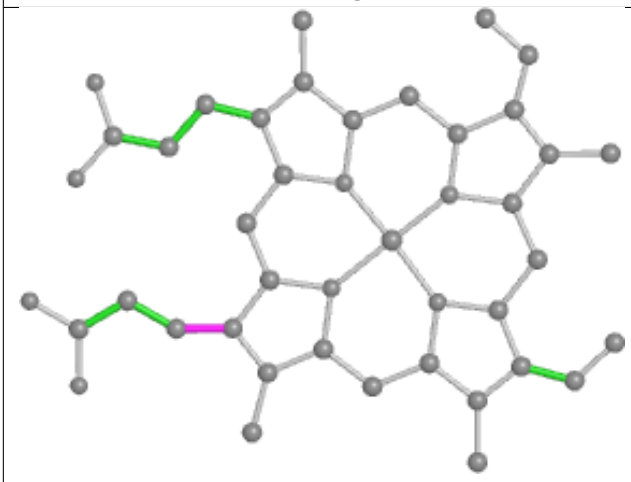
Ligand HEM H 202



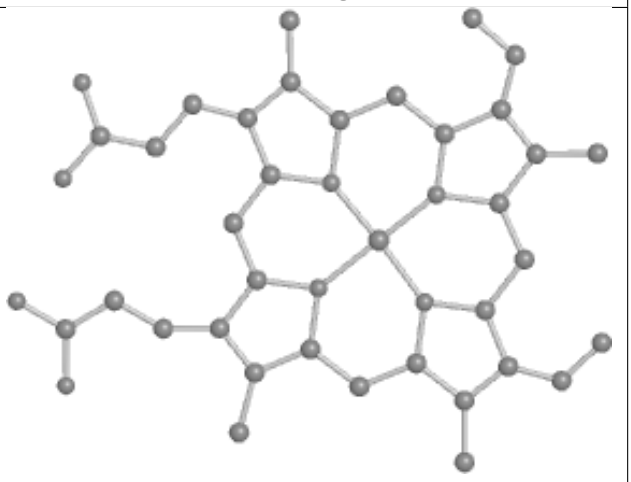
Bond lengths



Bond angles

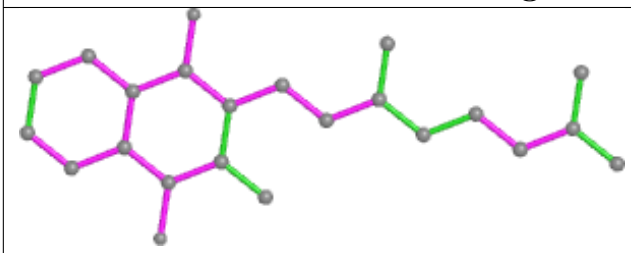


Torsions

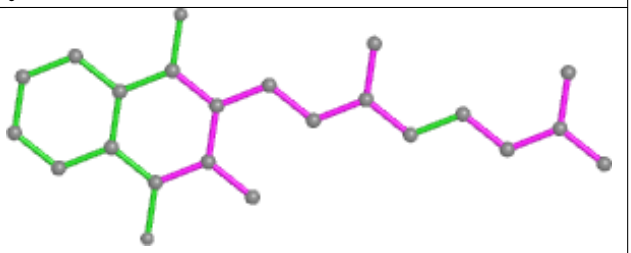


Rings

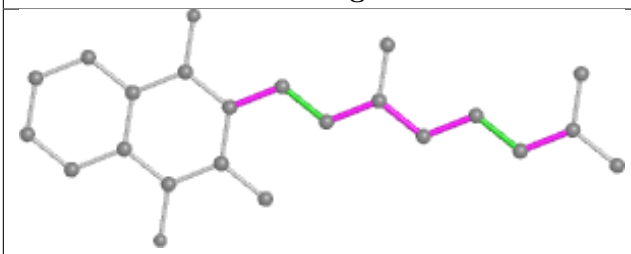
Ligand MQ9 H 204



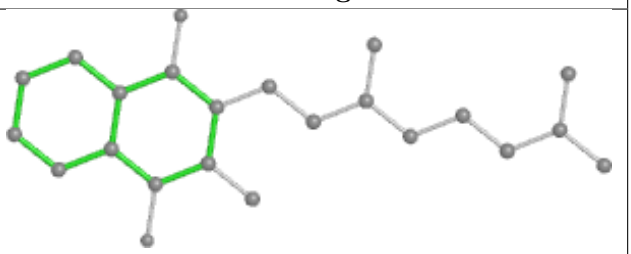
Bond lengths



Bond angles

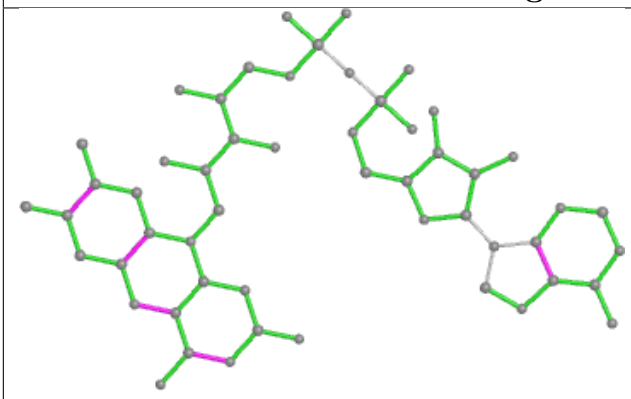


Torsions

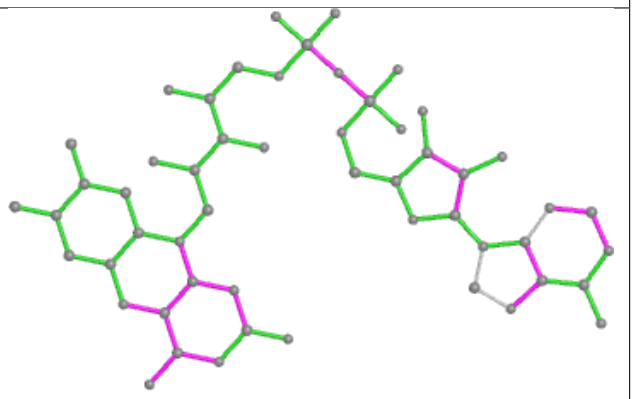


Rings

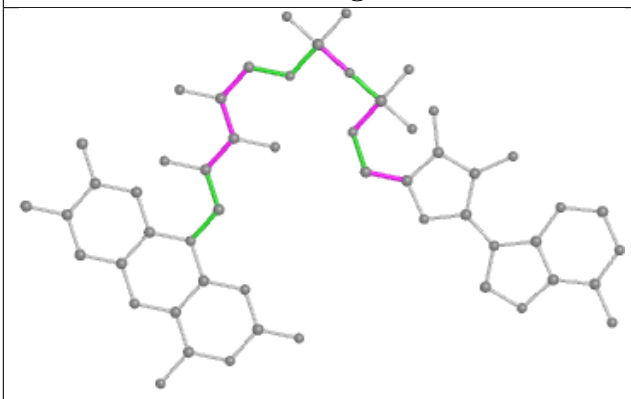
Ligand FAD P 700



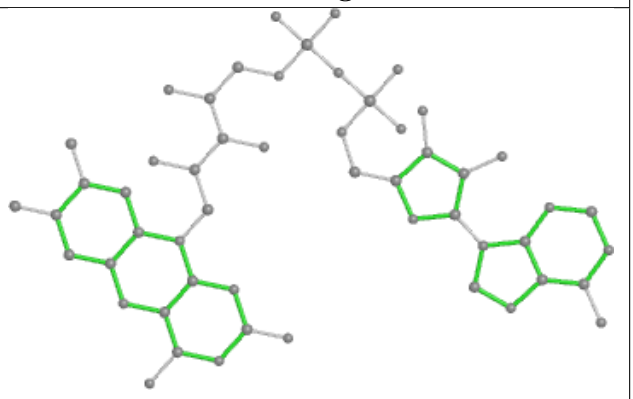
Bond lengths



Bond angles

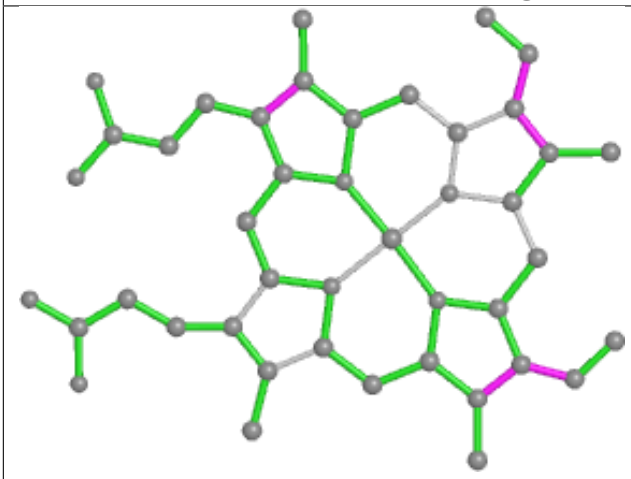


Torsions

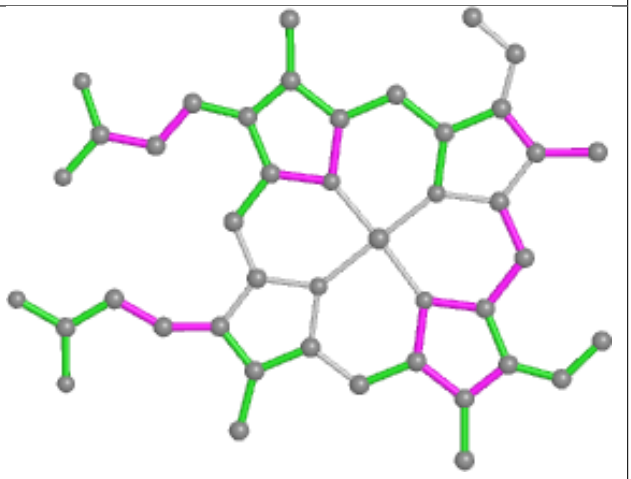


Rings

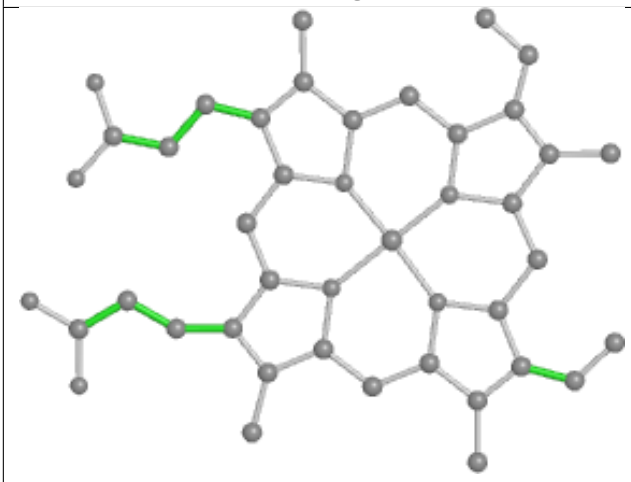
Ligand HEM D 201



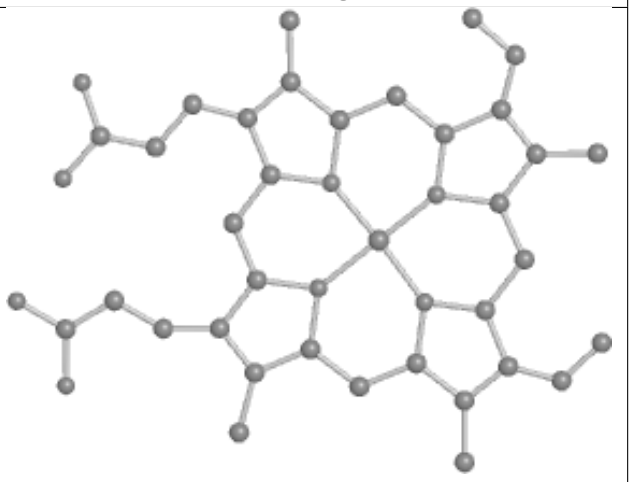
Bond lengths



Bond angles

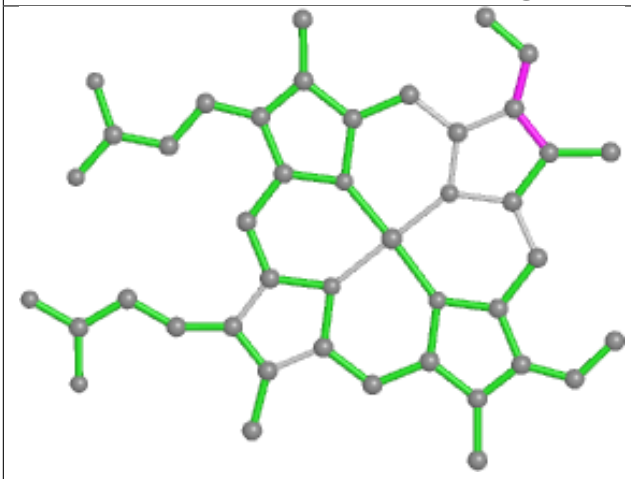


Torsions

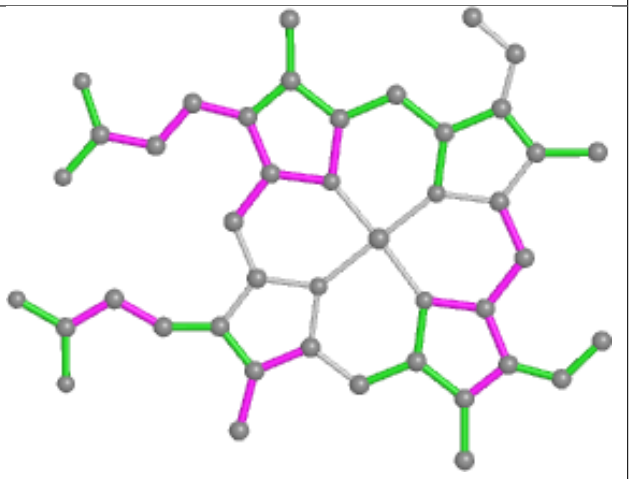


Rings

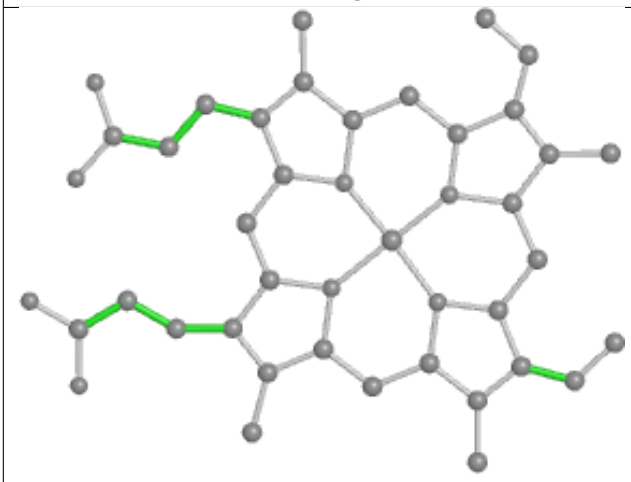
Ligand HEM H 203



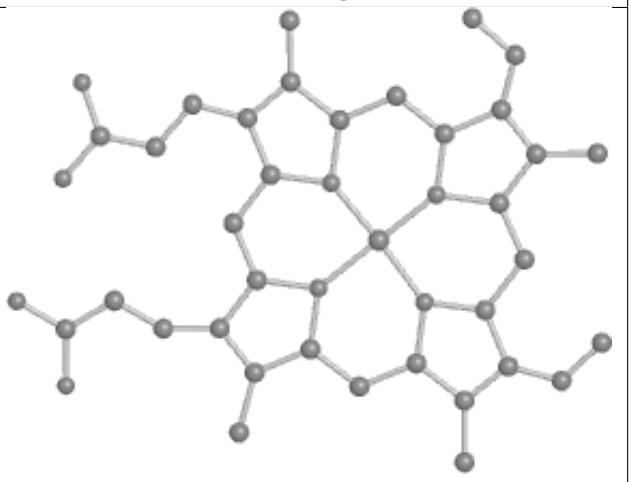
Bond lengths



Bond angles

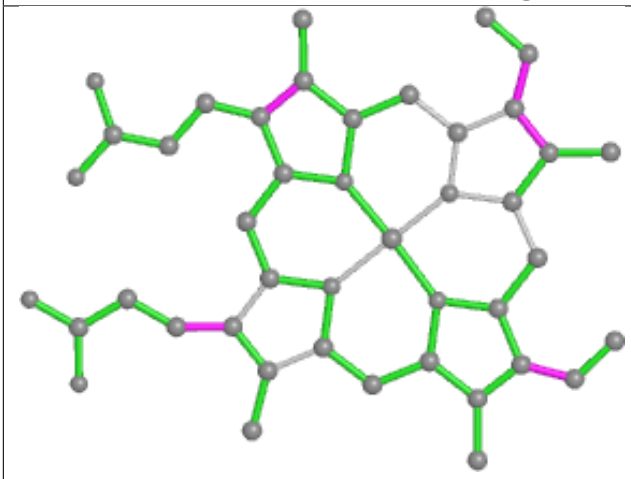


Torsions

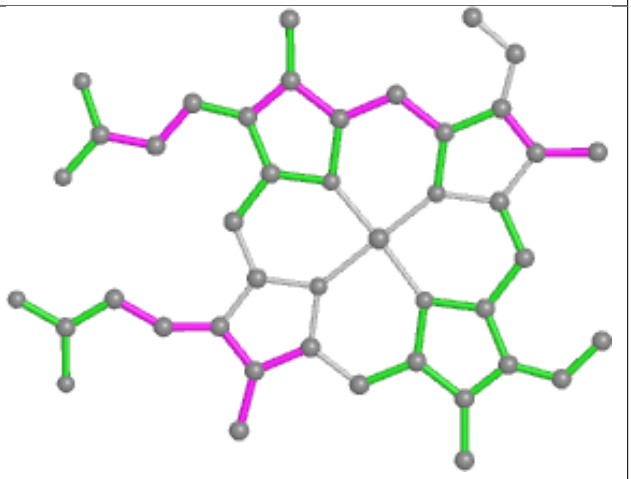


Rings

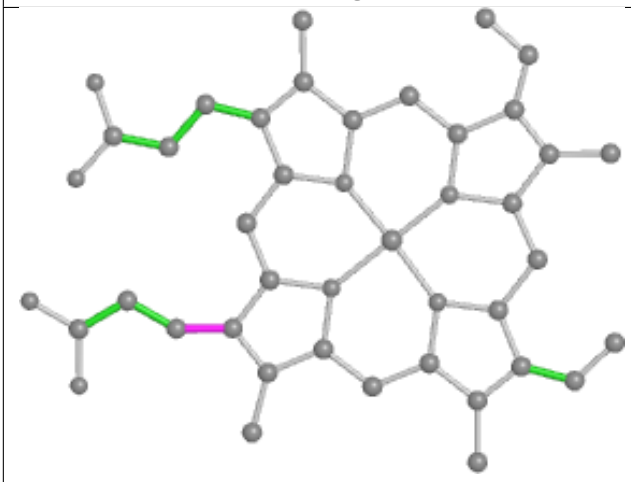
Ligand HEM N 202



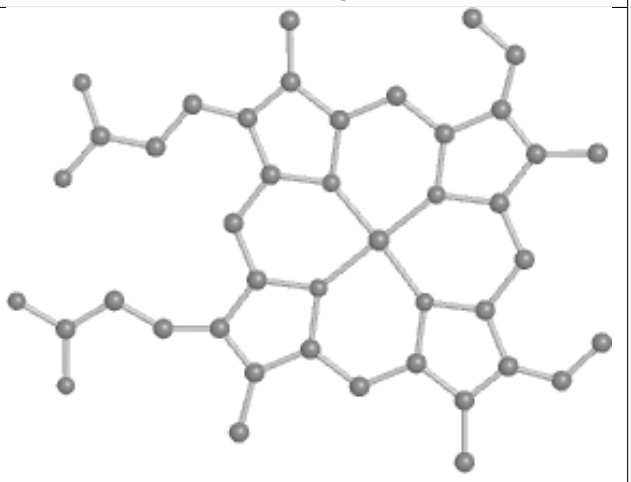
Bond lengths



Bond angles

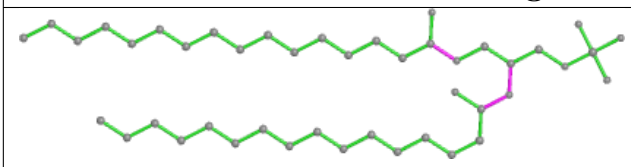


Torsions

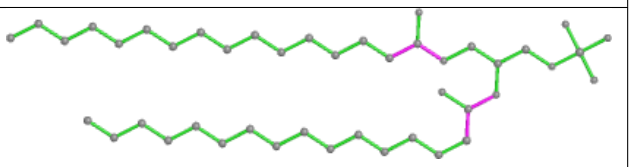


Rings

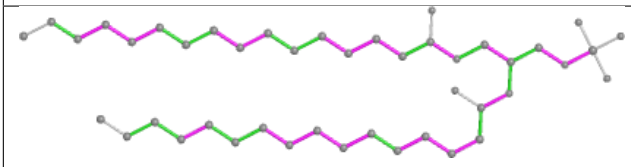
Ligand LPP N 205



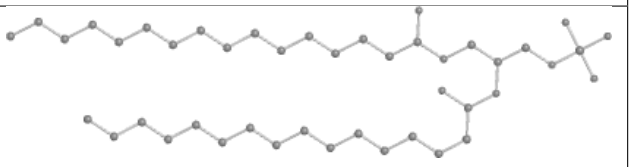
Bond lengths



Bond angles

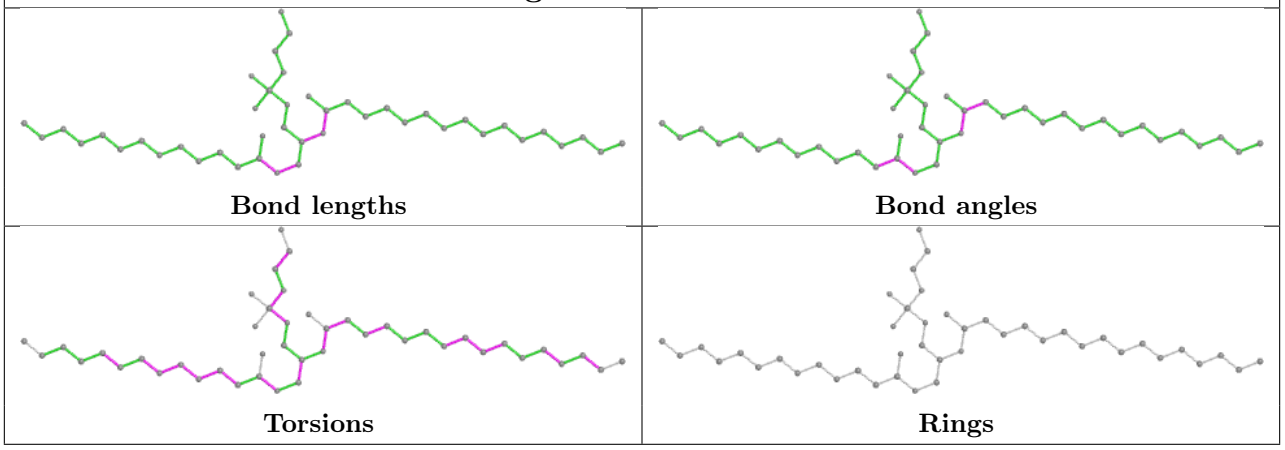


Torsions

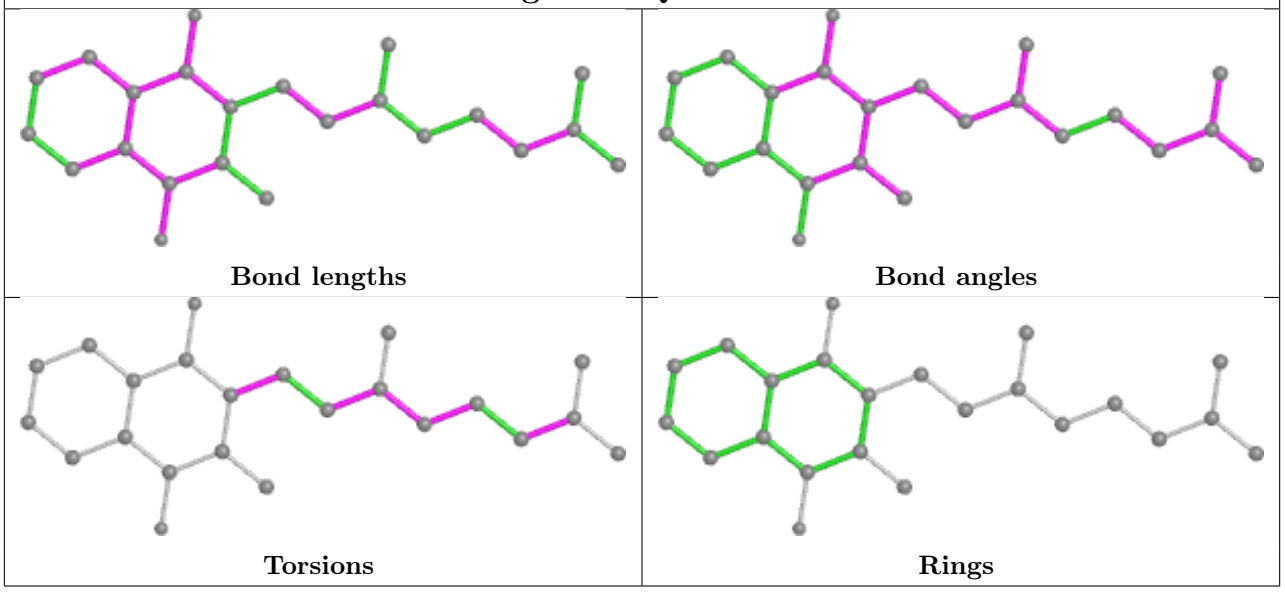


Rings

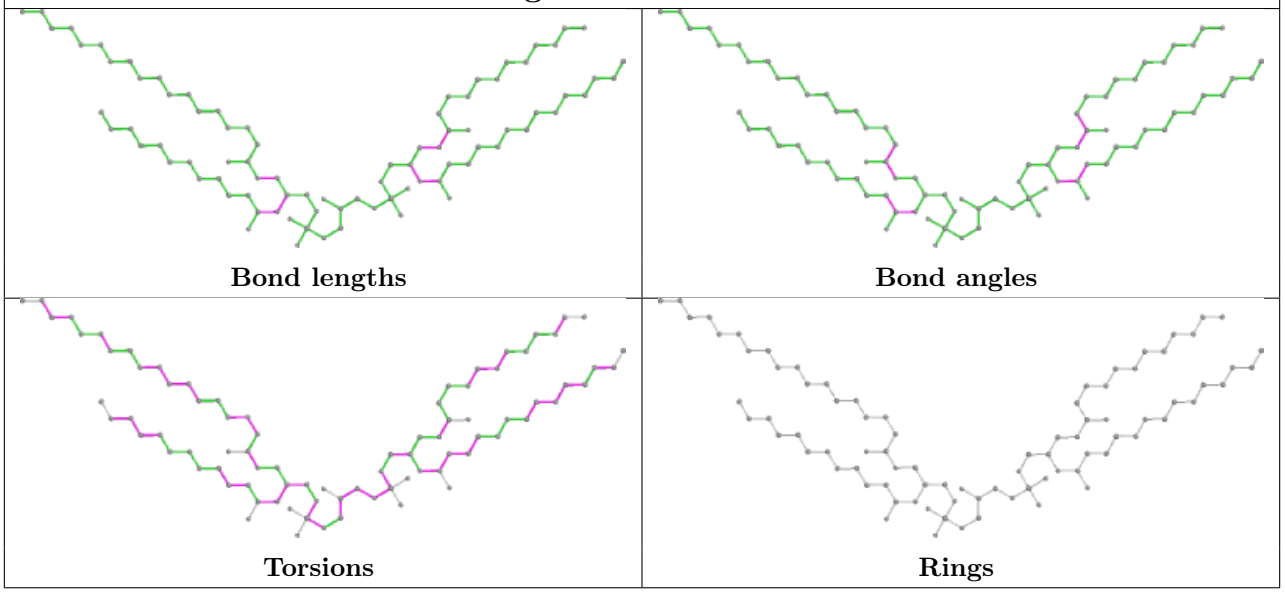
Ligand PEV C 202



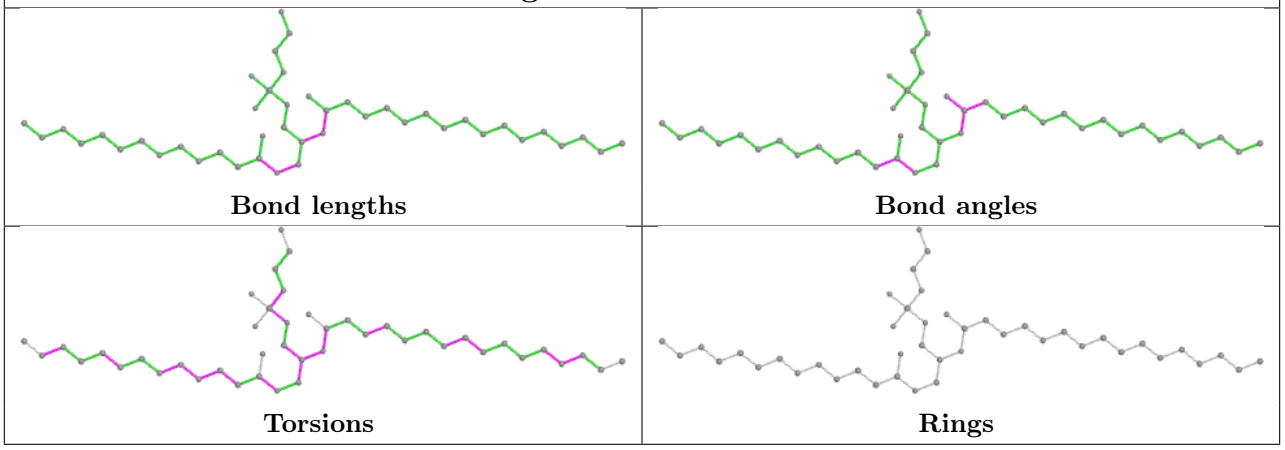
Ligand MQ9 N 204



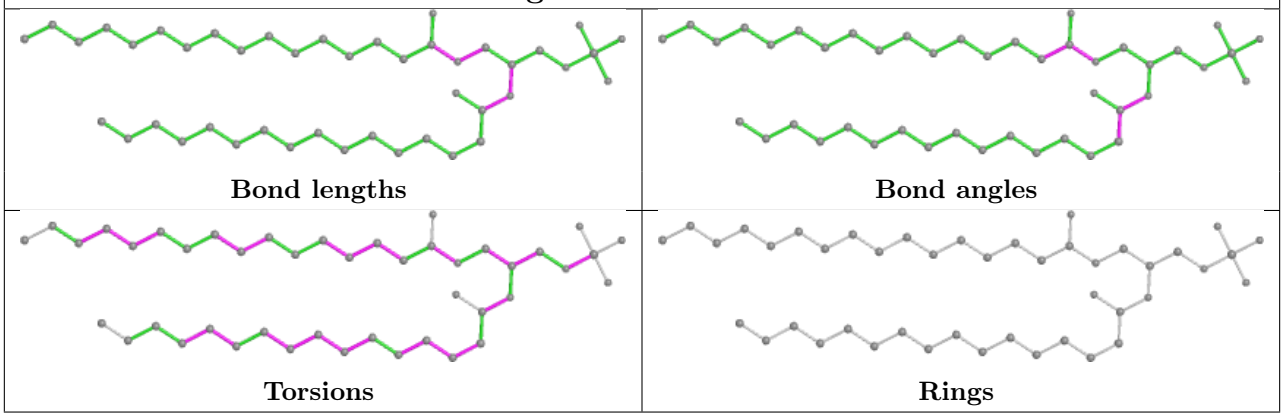
Ligand CDL D 204



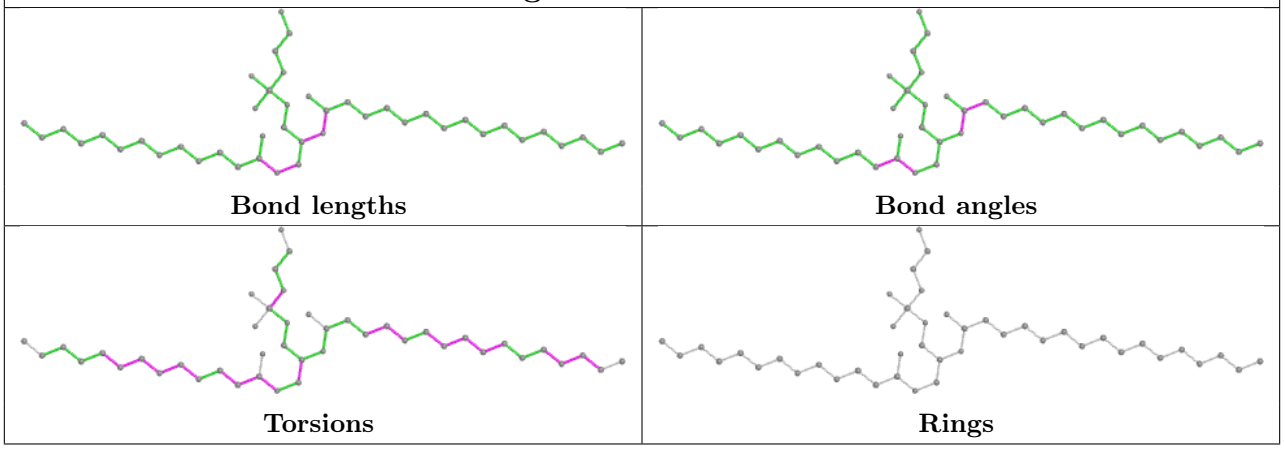
Ligand PEV M 203



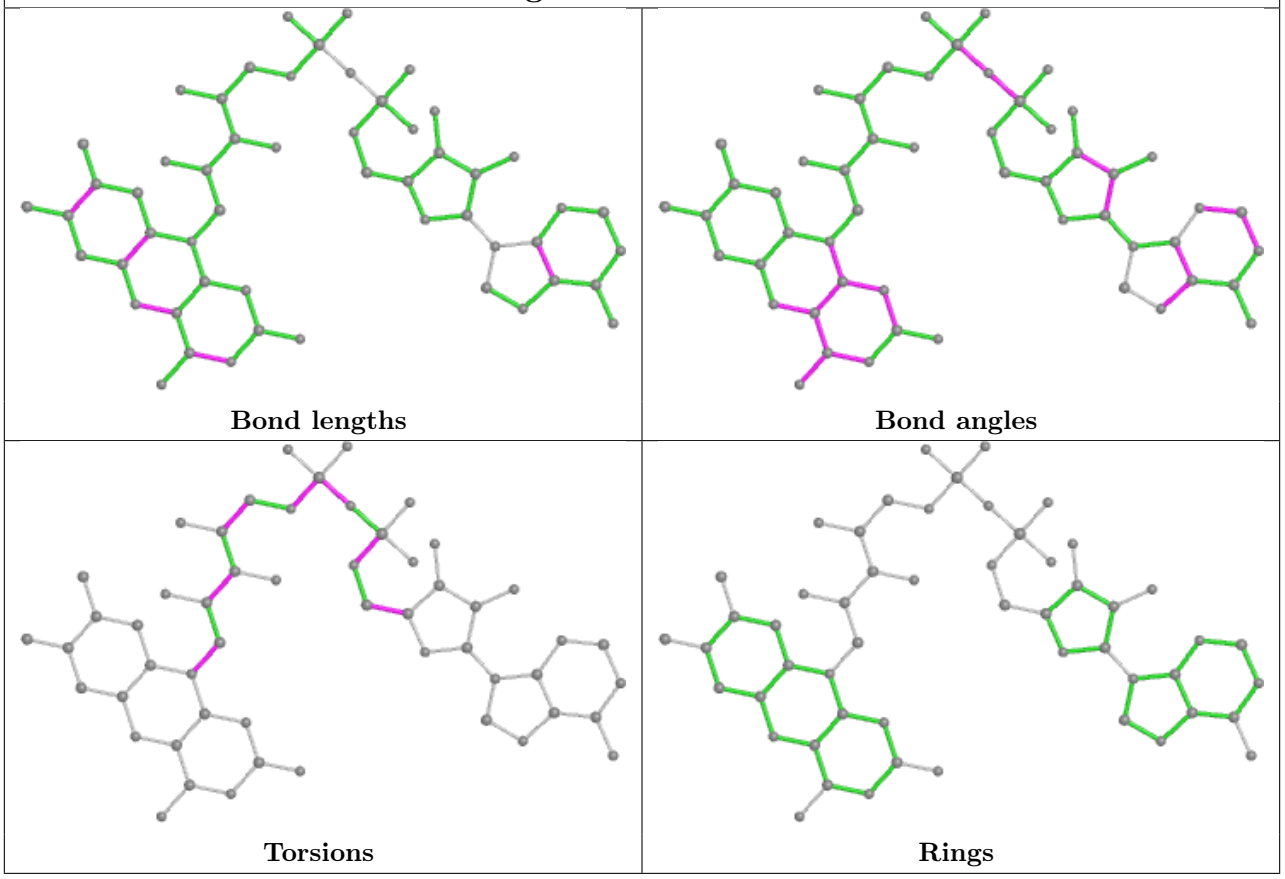
Ligand LPP H 201



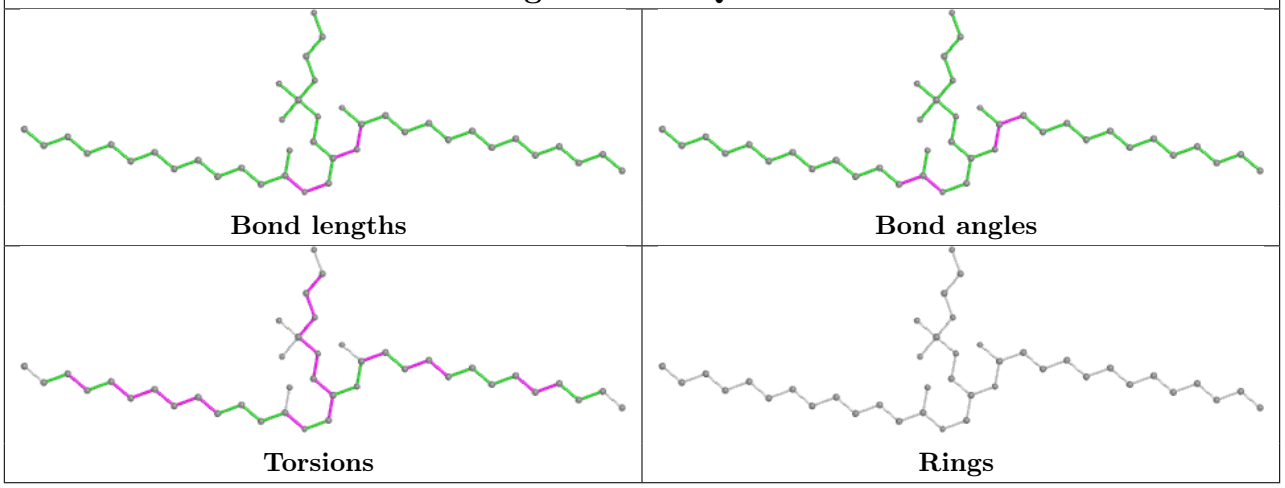
Ligand PEV G 201



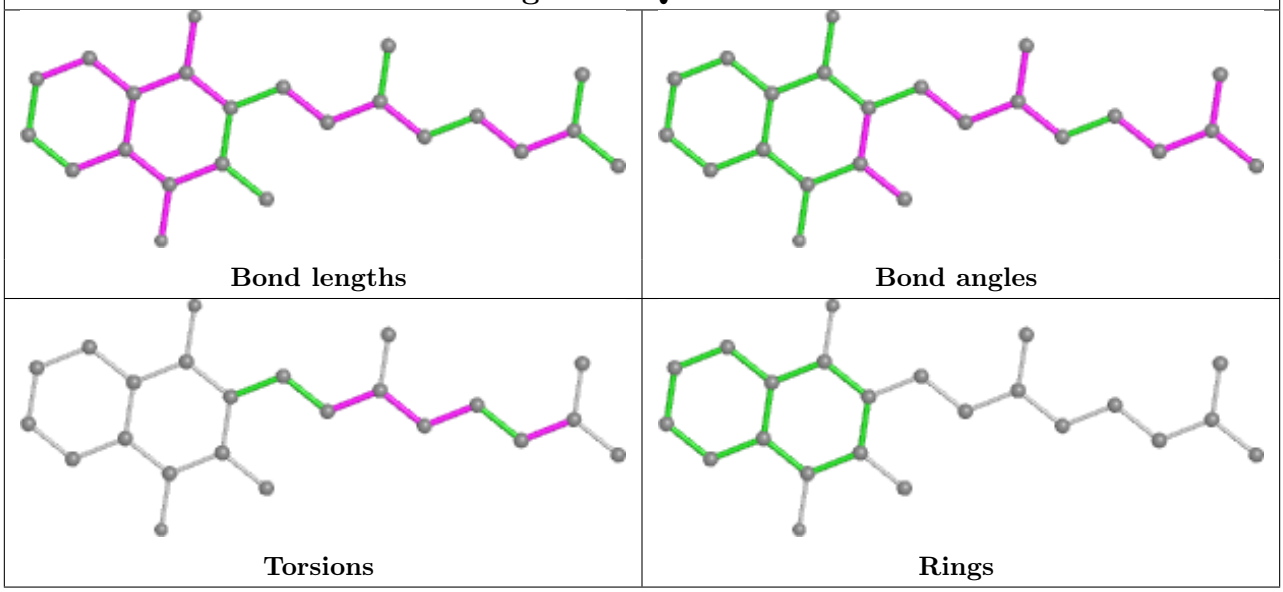
Ligand FAD A 700



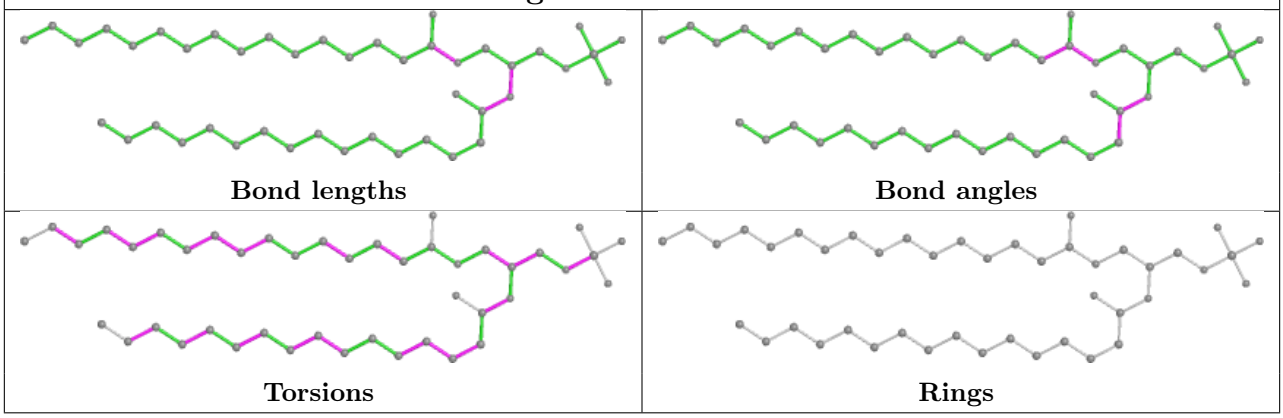
Ligand PEV Q 304



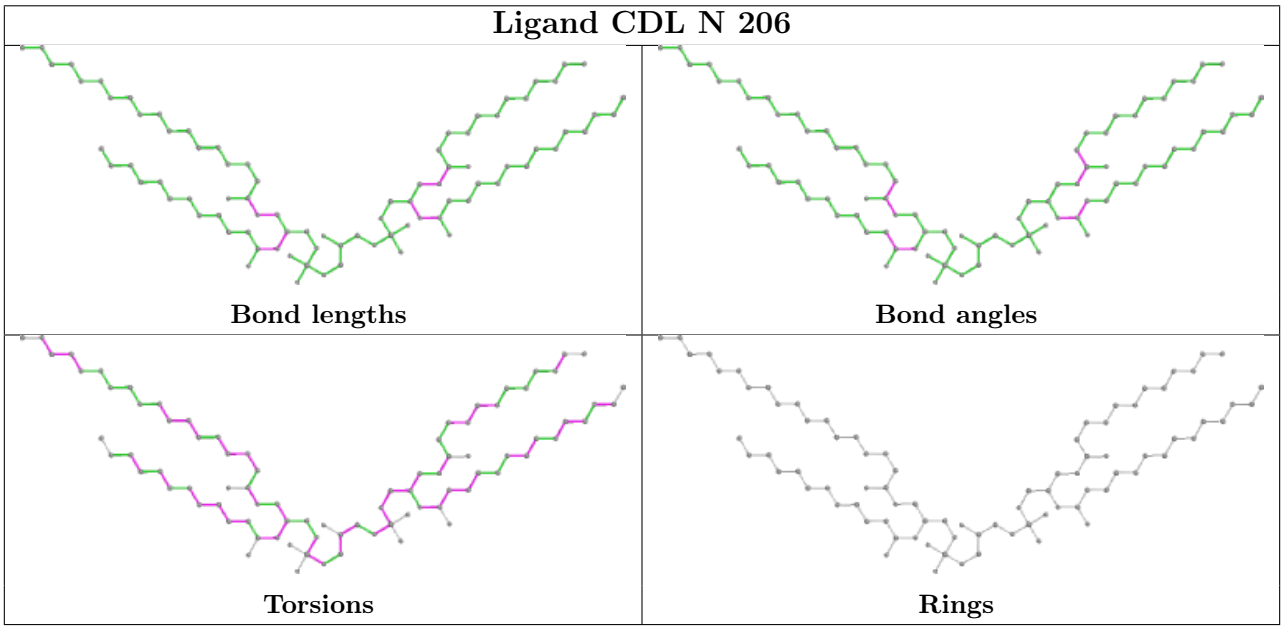
Ligand MQ9 N 201



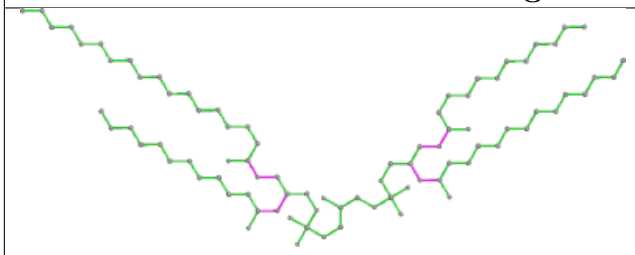
Ligand LPP D 206



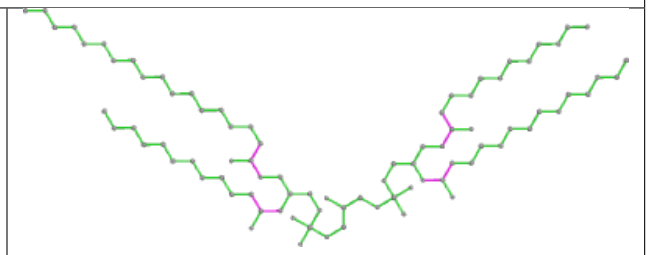
Ligand CDL N 206



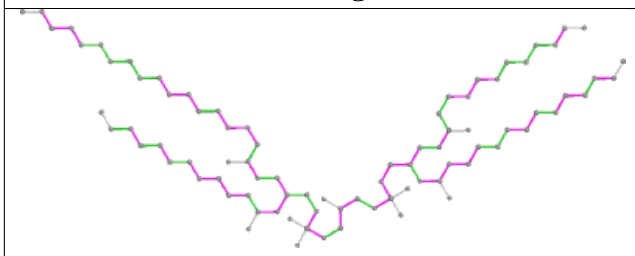
Ligand CDL H 205



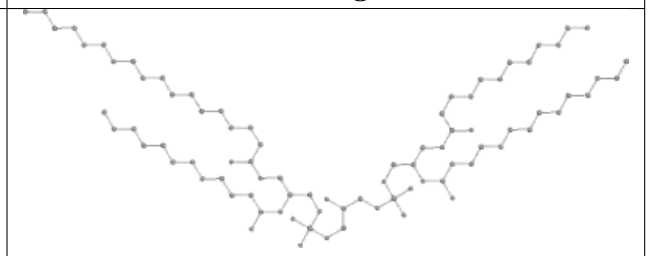
Bond lengths



Bond angles

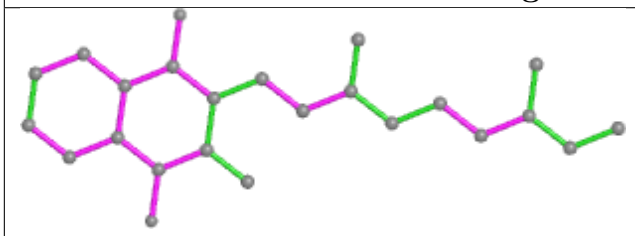


Torsions

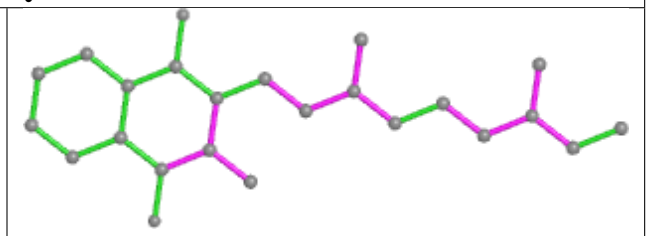


Rings

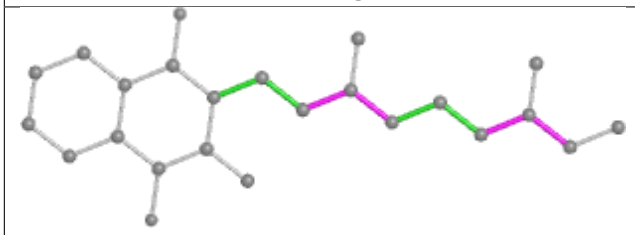
Ligand MQ9 N 203



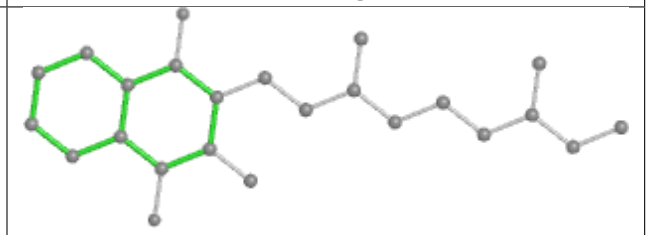
Bond lengths



Bond angles

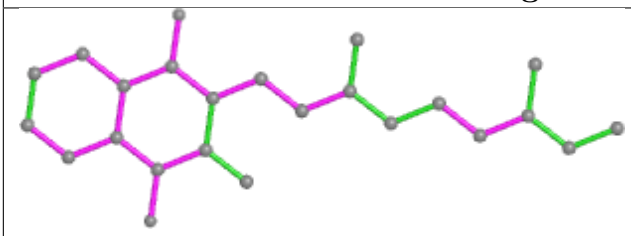


Torsions

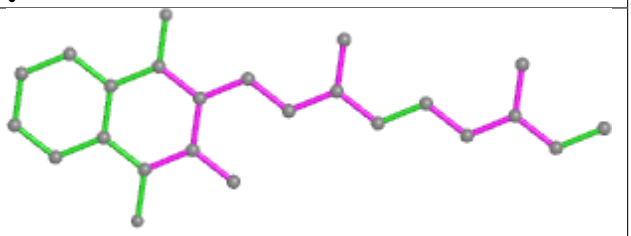


Rings

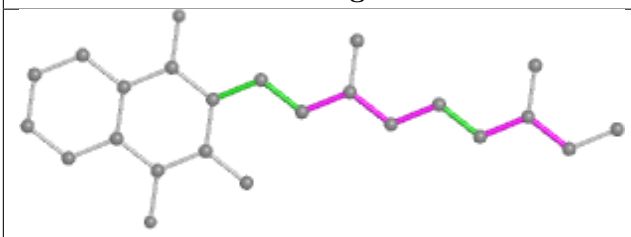
Ligand MQ9 D 203



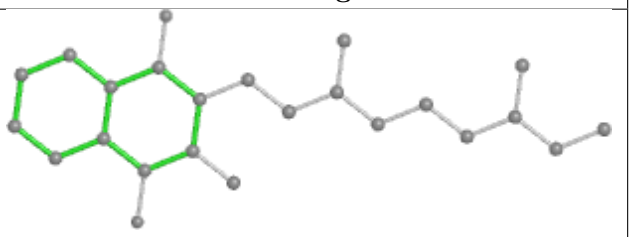
Bond lengths



Bond angles

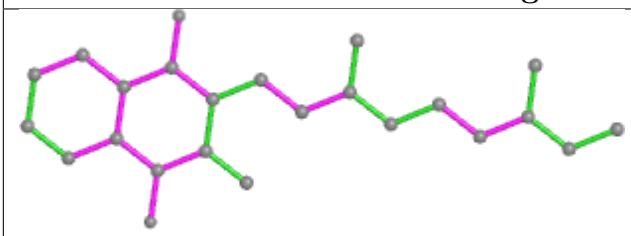


Torsions

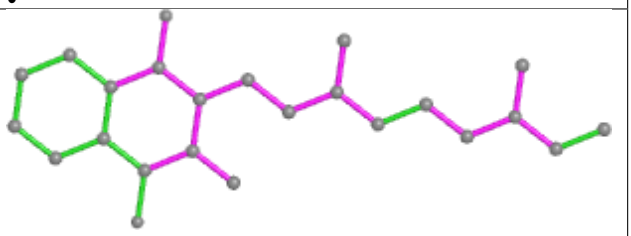


Rings

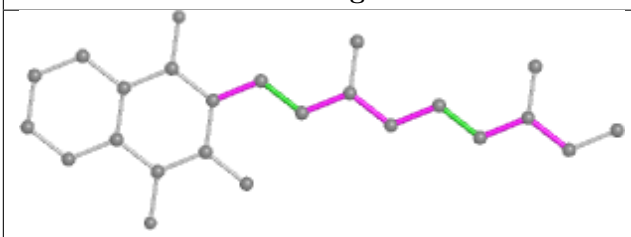
Ligand MQ9 D 205



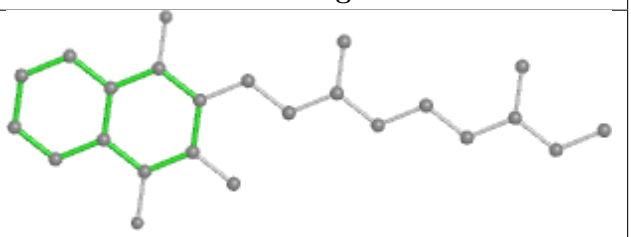
Bond lengths



Bond angles

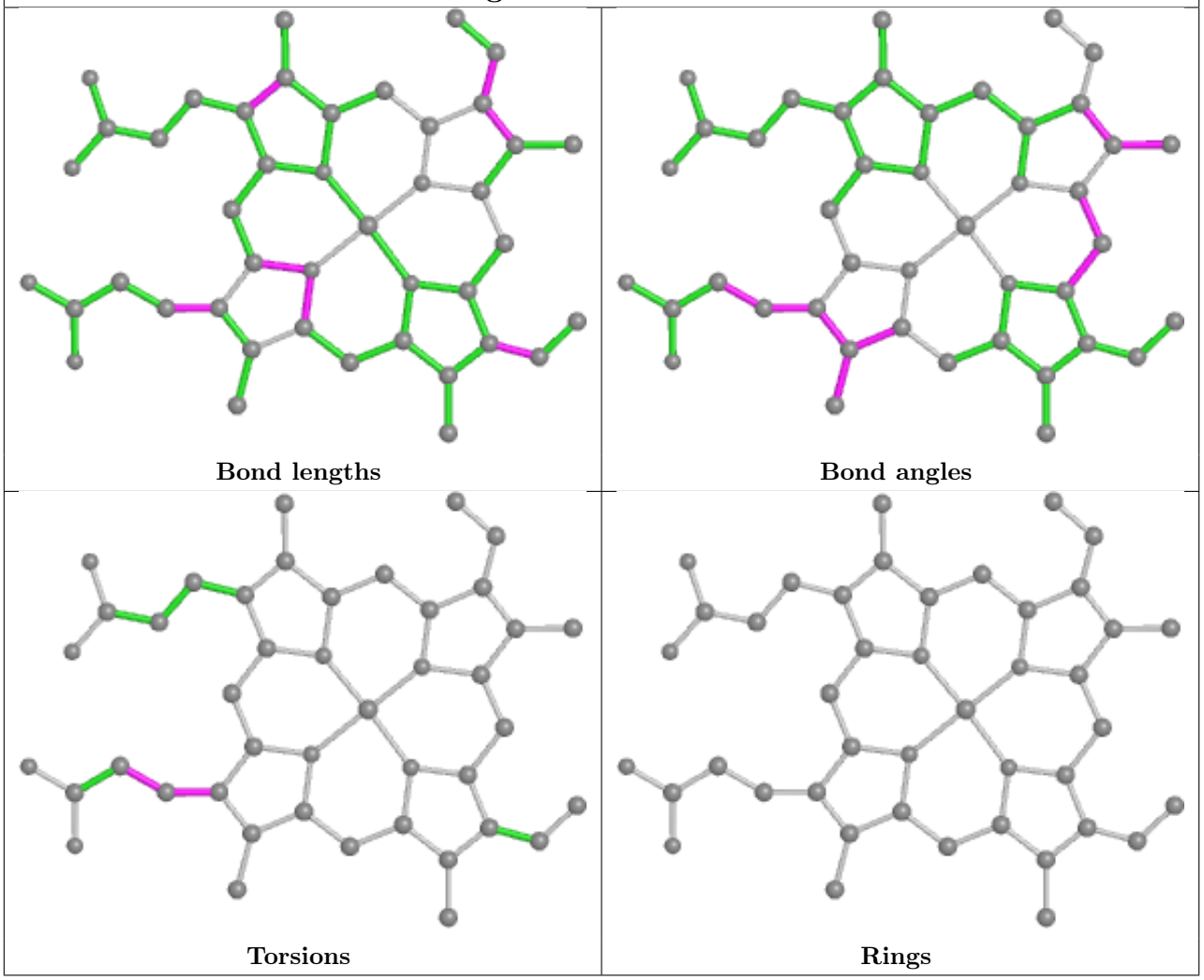


Torsions



Rings

Ligand HEM D 202



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.

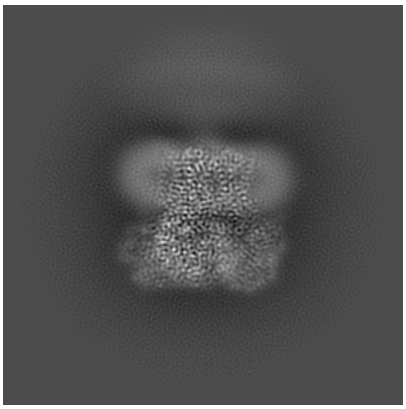
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0981. These allow visual inspection of the internal detail of the map and identification of artifacts.

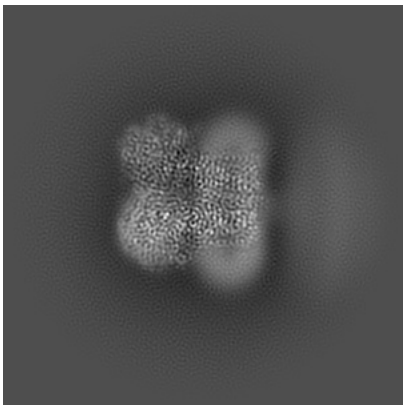
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

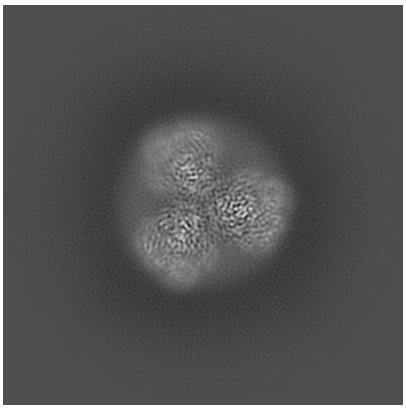
6.1.1 Primary map



X

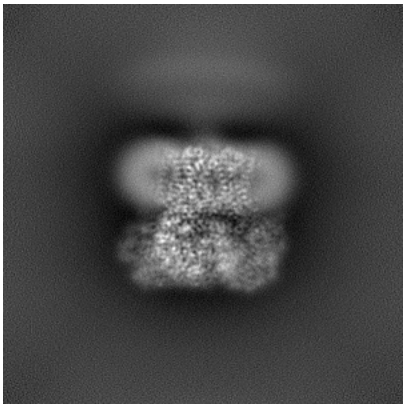


Y

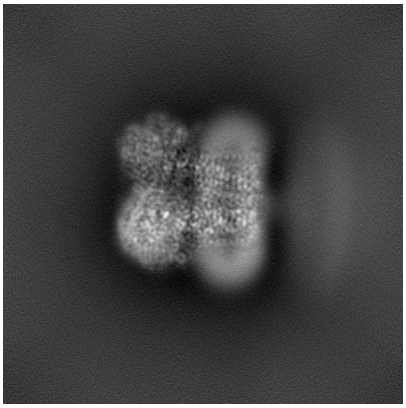


Z

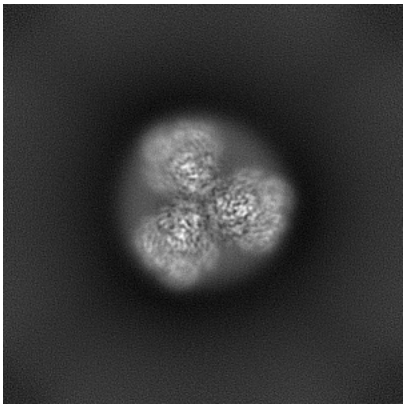
6.1.2 Raw map



X



Y

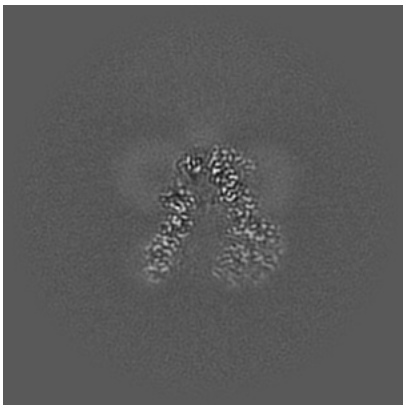


Z

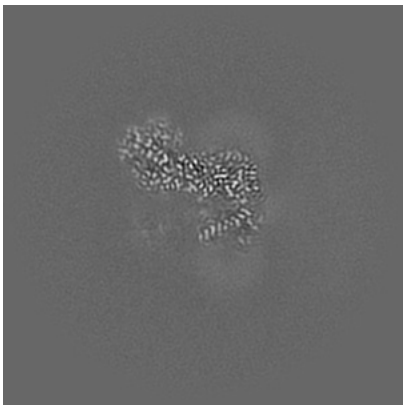
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

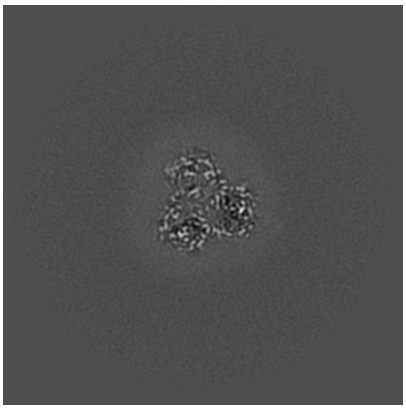
6.2.1 Primary map



X Index: 192

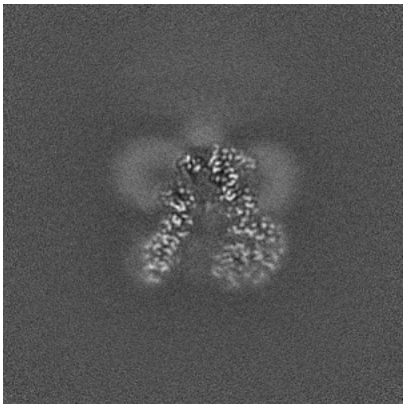


Y Index: 192

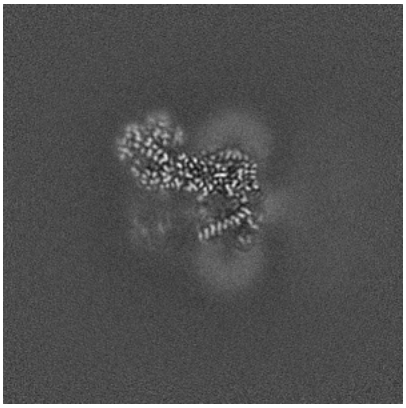


Z Index: 192

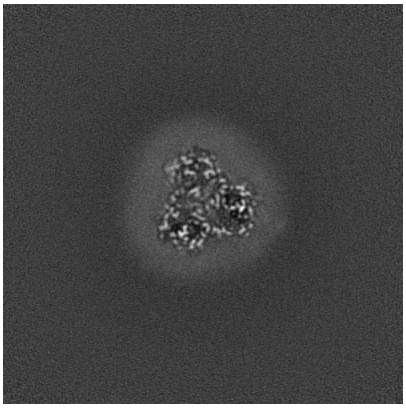
6.2.2 Raw map



X Index: 192



Y Index: 192

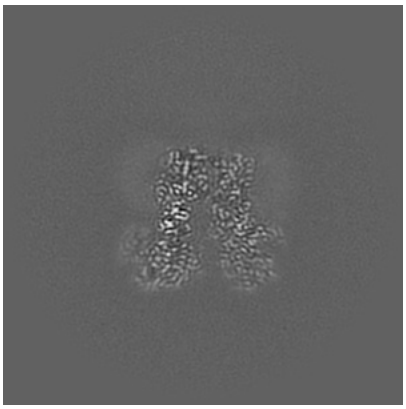


Z Index: 192

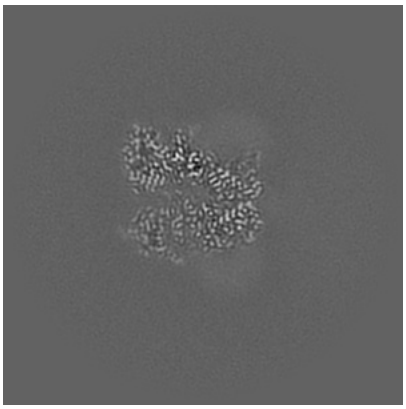
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

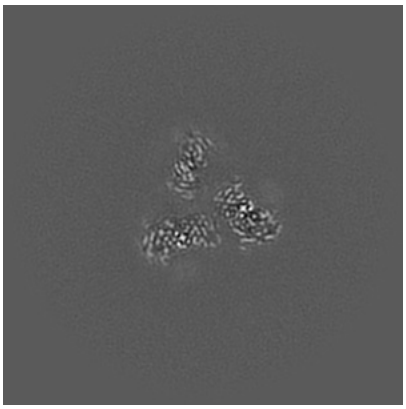
6.3.1 Primary map



X Index: 173

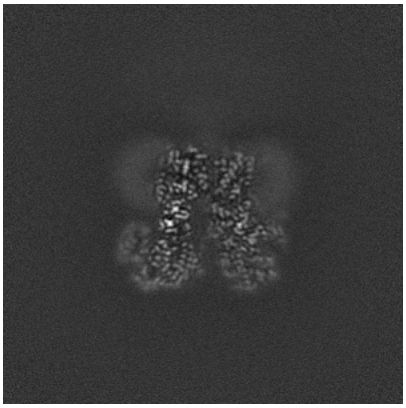


Y Index: 178

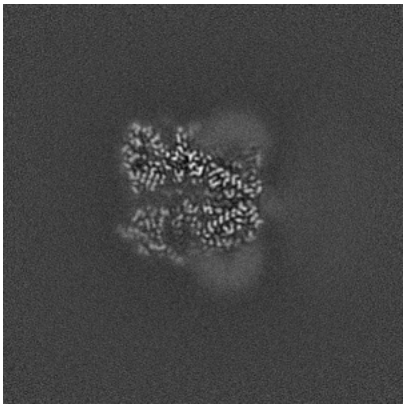


Z Index: 173

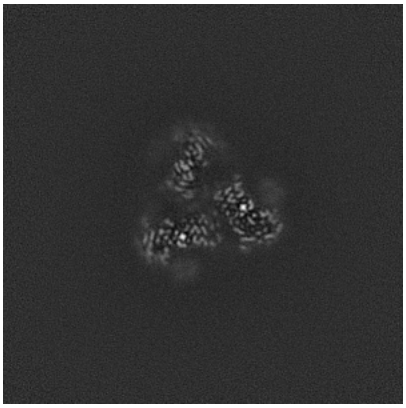
6.3.2 Raw map



X Index: 173



Y Index: 179

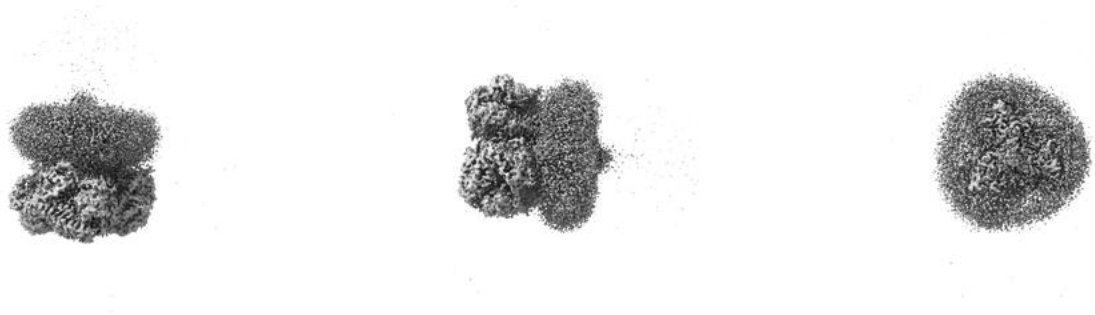


Z Index: 173

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

6.4 Orthogonal surface views (i)

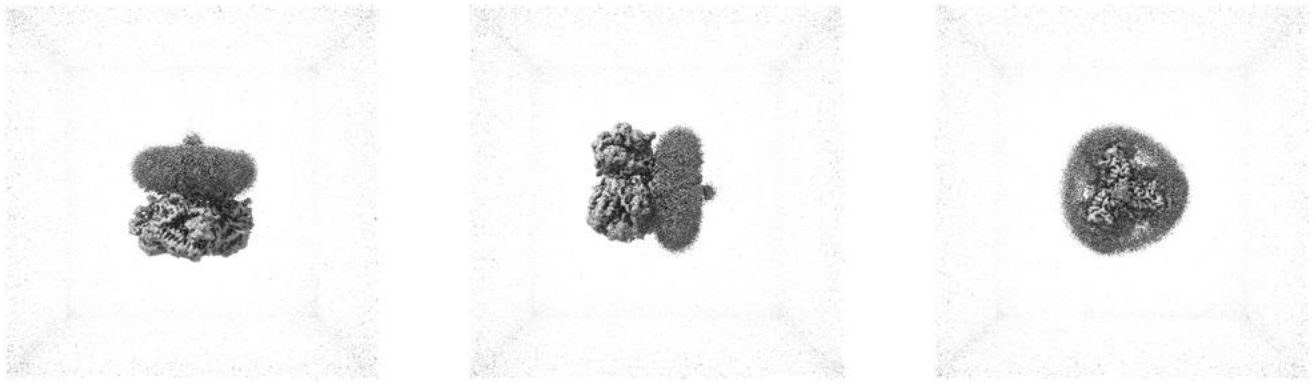
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

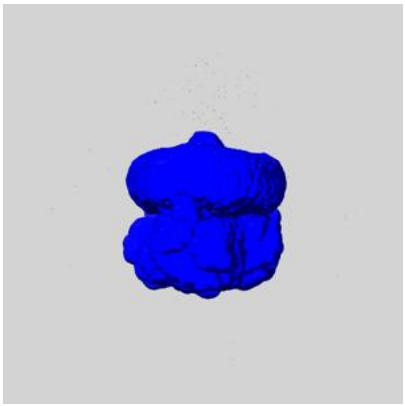
6.5 Mask visualisation (i)

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

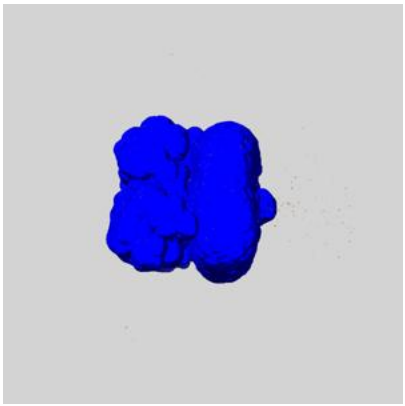
A mask typically either:

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

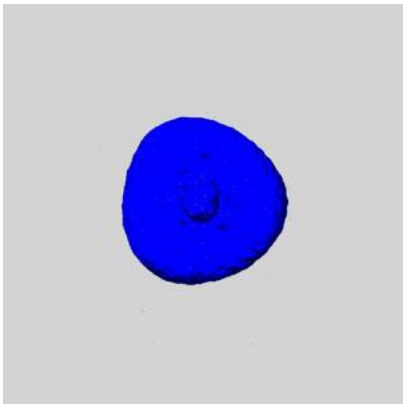
6.5.1 emd_0981_msk_1.map (i)



X



Y

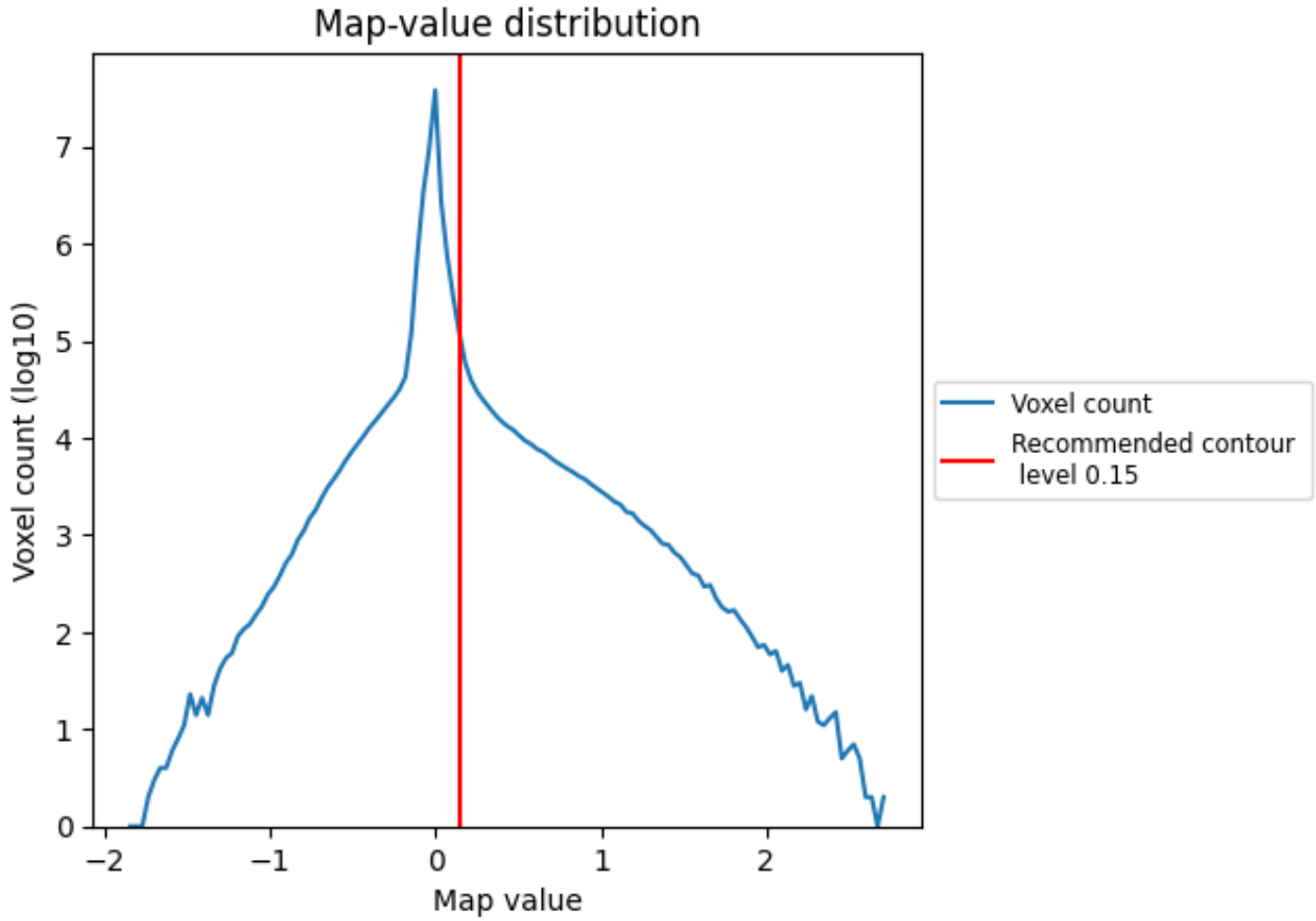


Z

7 Map analysis

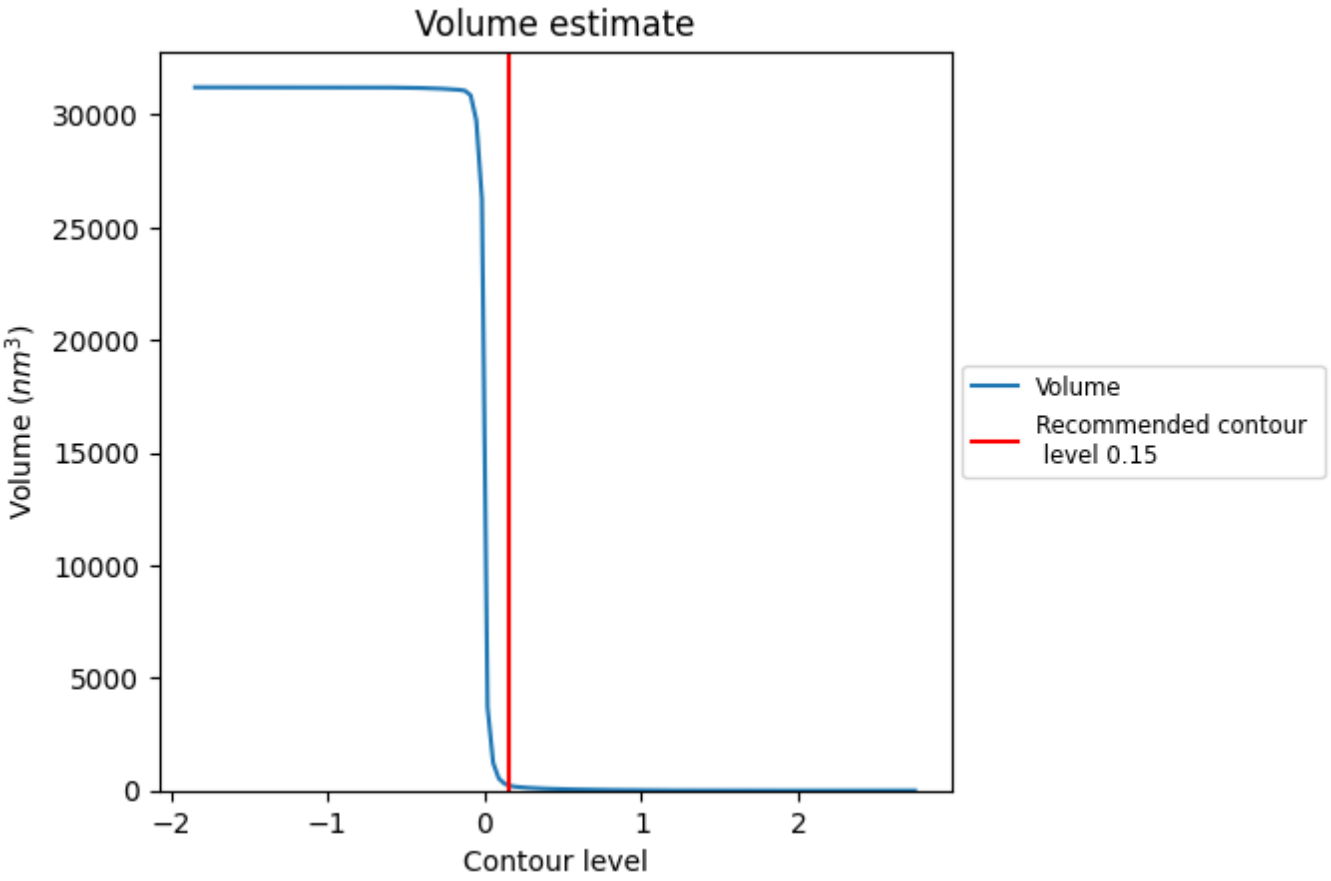
This section contains the results of statistical analysis of the map.

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.

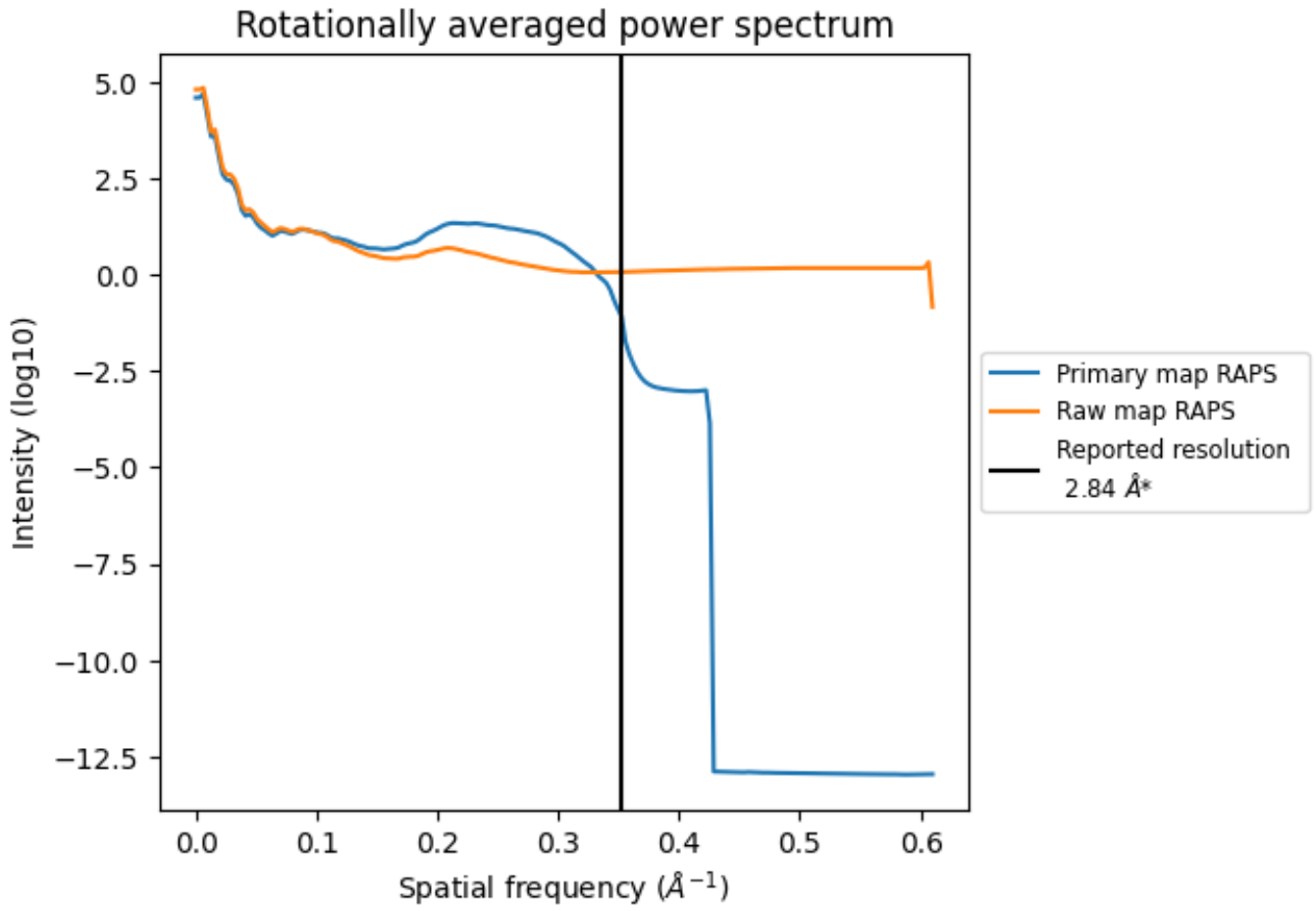
7.2 Volume estimate (i)



The volume at the recommended contour level is 246 nm^3; this corresponds to an approximate mass of 222 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)

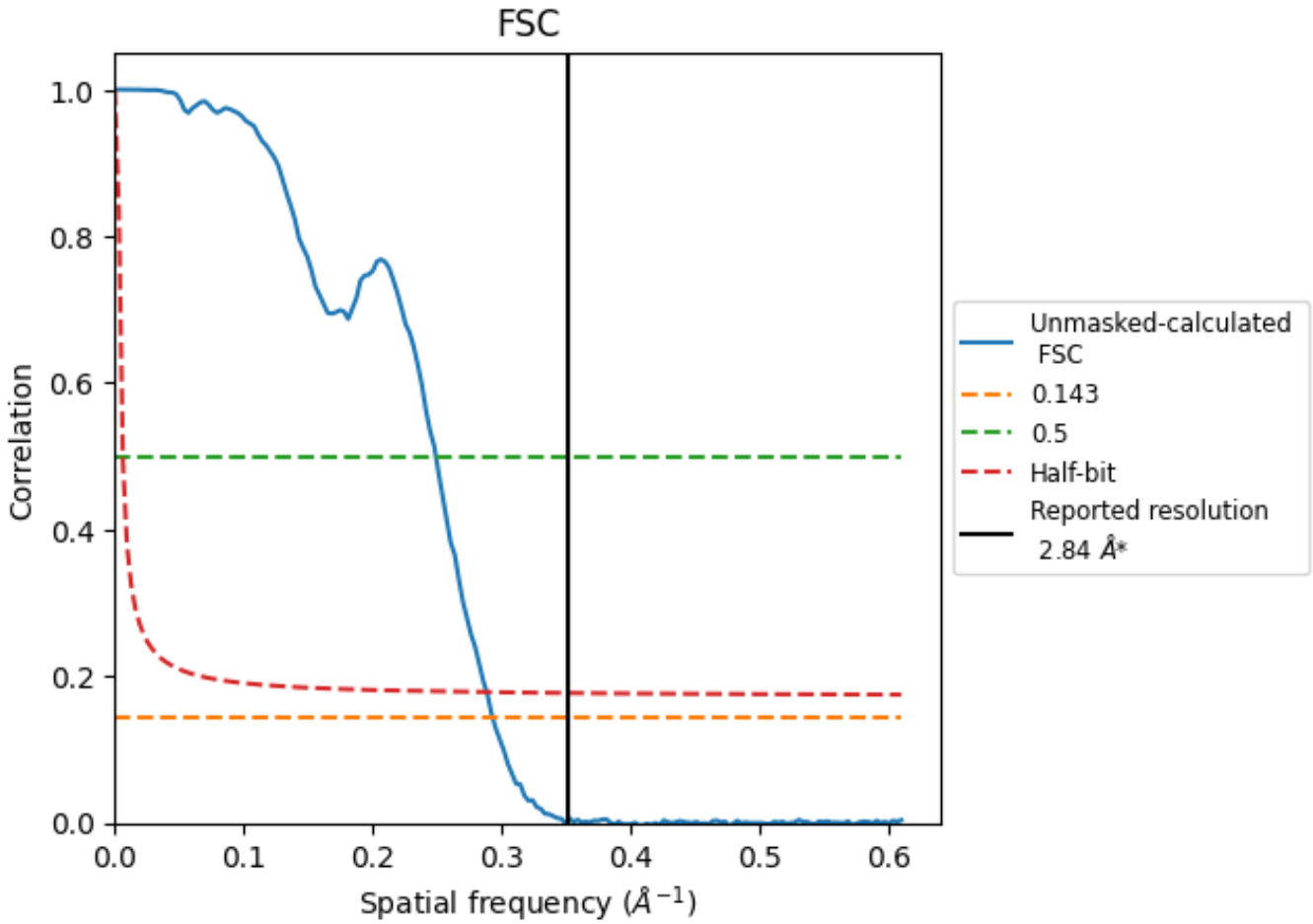


*Reported resolution corresponds to spatial frequency of 0.352 Å^{-1}

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 0.352 Å^{-1}

8.2 Resolution estimates (i)

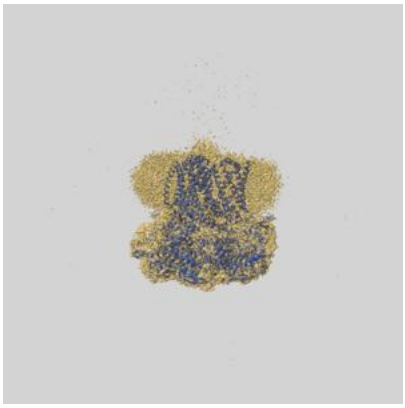
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.41	4.02	3.47

*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 3.41 differs from the reported value 2.84 by more than 10 %

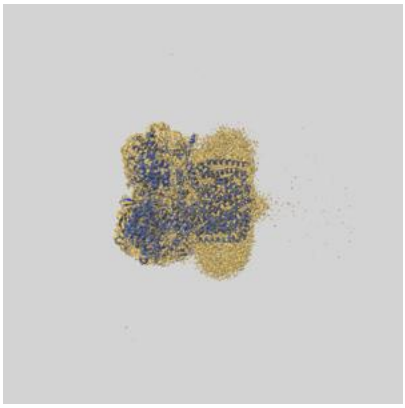
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0981 and PDB model 6LUM. Per-residue inclusion information can be found in section 3 on page 13.

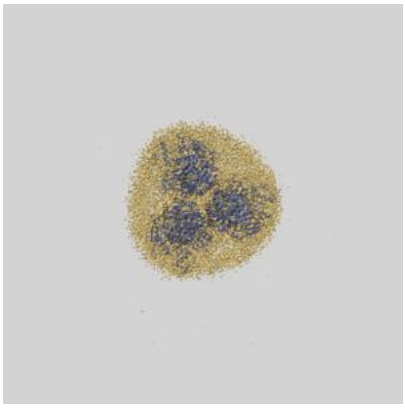
9.1 Map-model overlay



X



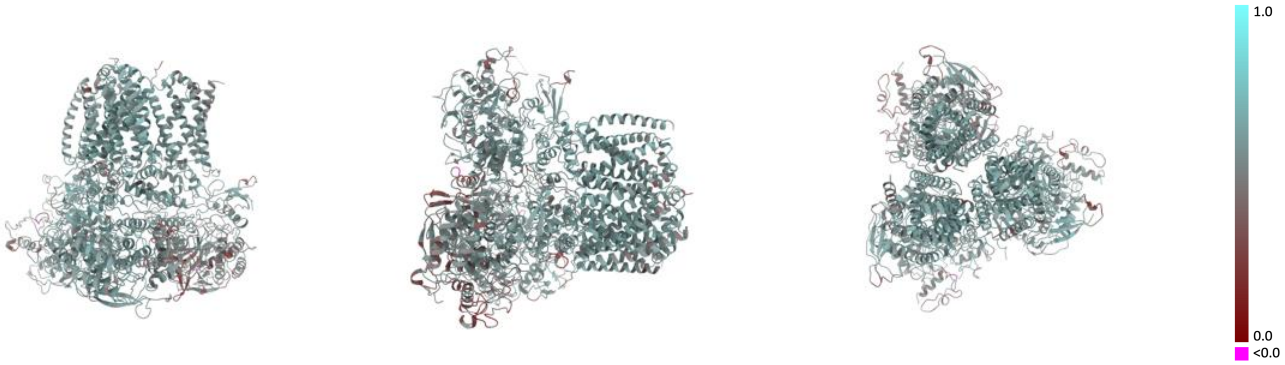
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

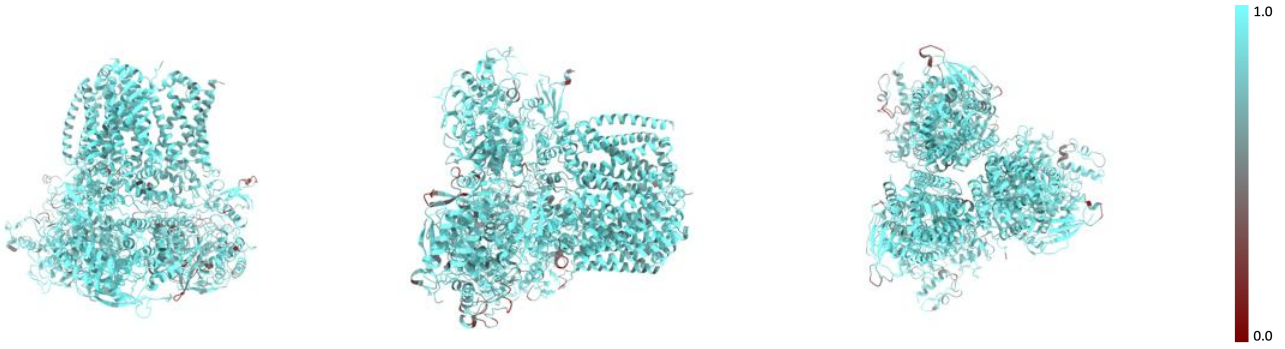
9.2 Q-score mapped to coordinate model



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.

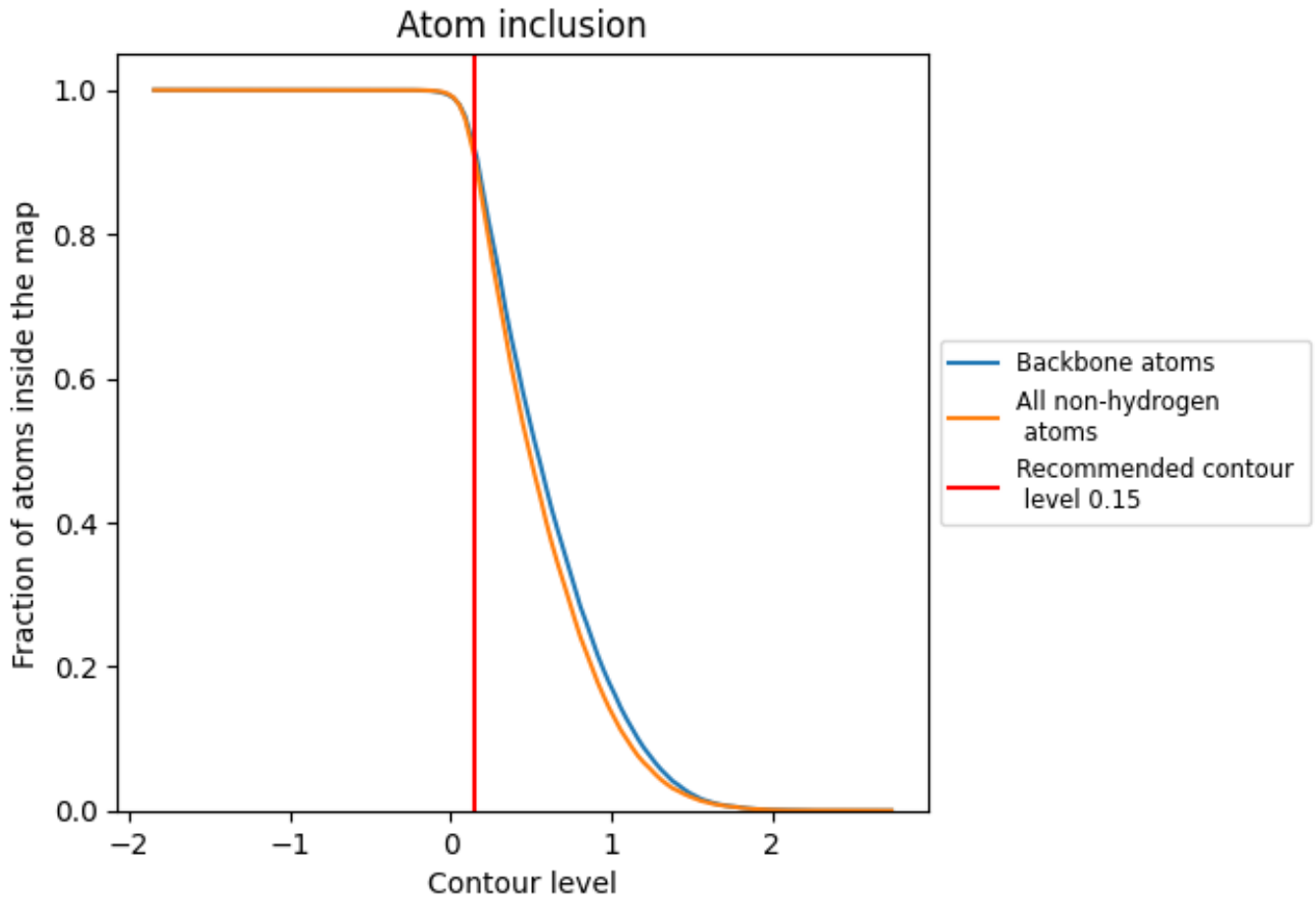
9.3 Atom inclusion mapped to coordinate model



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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 91% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9060	0.5610
A	0.9356	0.5720
B	0.9338	0.5900
C	0.9286	0.5920
D	0.9448	0.6110
E	0.8696	0.5610
G	0.9095	0.5830
H	0.9381	0.5990
I	0.8645	0.5420
J	0.9183	0.5550
K	0.9230	0.5810
M	0.8839	0.5660
N	0.9532	0.5980
O	0.8526	0.5510
P	0.8204	0.4780
Q	0.8886	0.5580