wwPDB EM Validation Summary Report

Oct 5, 2023 – 10:51 AM EDT

PDB ID	:	8SMR
EMDB ID	:	EMD-40601
Title	:	cytochrome bc1-cbb3 supercomplex from Pseudomonas aeruginosa
Authors	:	Di Trani, J.M.; Rubinstein, J.L.
Deposited on	:	2023-04-26
Resolution	:	2.70 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:

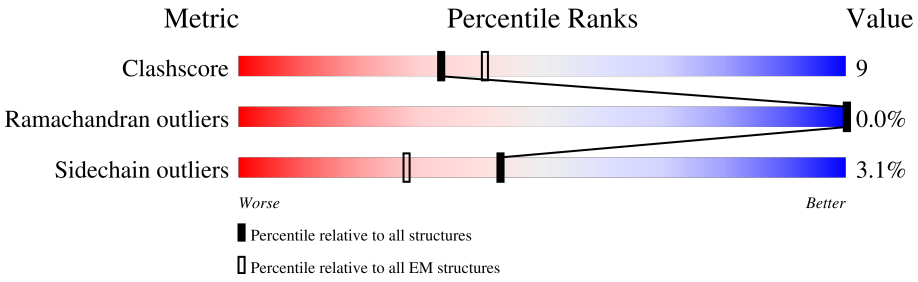
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.70 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	194	12% 79% 18%
1	Z	194	17% 86% 12%
2	D	403	82% 18%
2	I	403	84% 16%
3	J	233	79% 21%
3	M	233	80% 7% 12%
4	K	181	87% 13%
4	N	181	89% 11%

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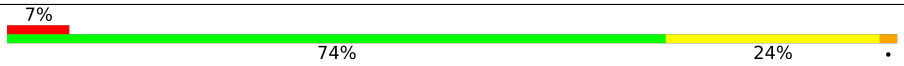
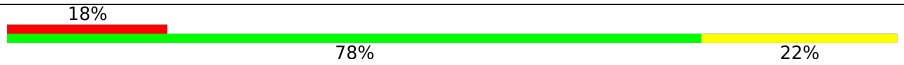
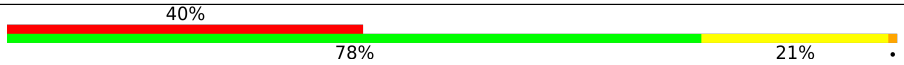
Mol	Chain	Length	Quality of chain
5	L	136	
5	O	136	
6	E	468	
7	F	200	
8	G	312	

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
9	FES	Z	201	-	-	X	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 24154 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 Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	190	Total	C	N	O	S	0	0
			1420	910	245	260	5		
1	Z	194	Total	C	N	O	S	0	0
			1449	926	251	267	5		

- Molecule 2 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	403	Total	C	N	O	S	0	0
			3267	2207	508	533	19		
2	D	403	Total	C	N	O	S	0	0
			3267	2207	508	533	19		

- Molecule 3 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	232	Total	C	N	O	S	0	0
			1842	1188	309	334	11		
3	M	204	Total	C	N	O	S	0	0
			1631	1059	273	290	9		

- Molecule 4 is a protein called Cytochrome c4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	181	Total	C	N	O	S	0	0
			1306	805	235	256	10		
4	N	181	Total	C	N	O	S	0	0
			1306	805	235	256	10		

- Molecule 5 is a protein called Cytochrome C5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	16	Total	C	N	O	S	0	0
			115	73	22	19	1		
5	O	16	Total	C	N	O	S	0	0
			115	73	22	19	1		

- Molecule 6 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	468	Total	C	N	O	S	0	0
			3719	2478	607	609	25		

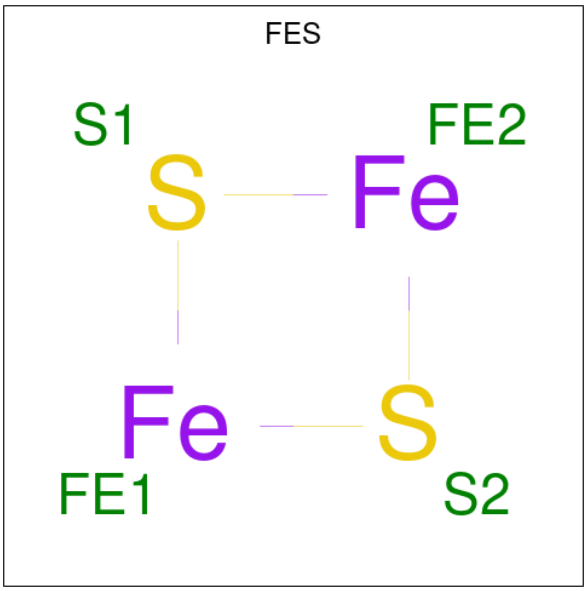
- Molecule 7 is a protein called Cbb3-type Cytochrome C oxidase subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	200	Total	C	N	O	S	0	0
			1499	944	268	280	7		

- Molecule 8 is a protein called Cbb3-type cytochrome c oxidase subunit.

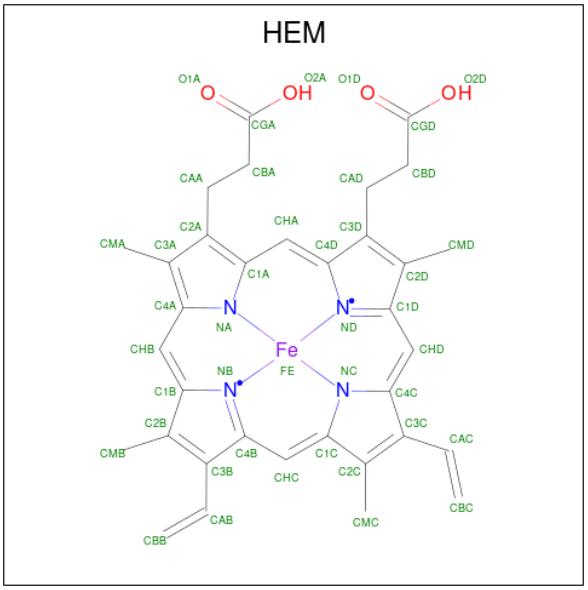
Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	312	Total	C	N	O	S	0	0
			2345	1514	391	425	15		

- Molecule 9 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



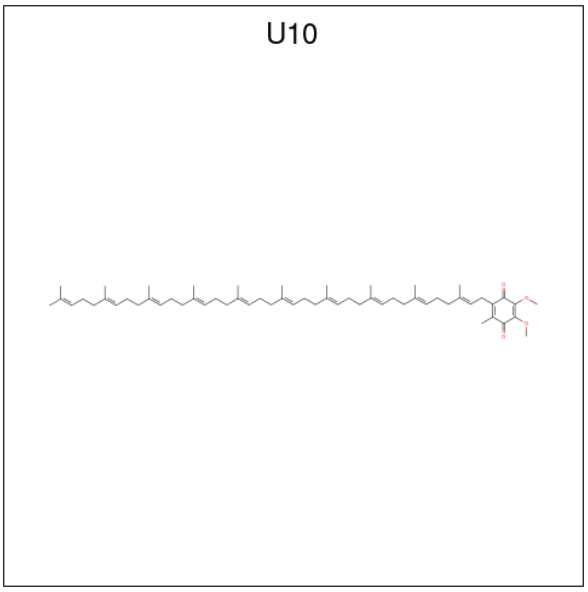
Mol	Chain	Residues	Atoms	AltConf
9	C	1	Total Fe S 4 2 2	0
9	Z	1	Total Fe S 4 2 2	0

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



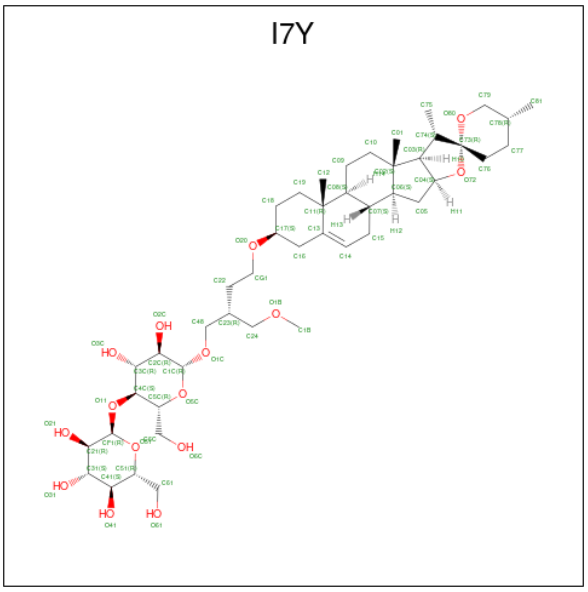
Mol	Chain	Residues	Atoms	AltConf
10	I	1	Total C Fe N O 43 34 1 4 4	0
10	I	1	Total C Fe N O 43 34 1 4 4	0
10	D	1	Total C Fe N O 43 34 1 4 4	0
10	D	1	Total C Fe N O 43 34 1 4 4	0
10	E	1	Total C Fe N O 43 34 1 4 4	0
10	E	1	Total C Fe N O 43 34 1 4 4	0

- Molecule 11 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms	AltConf
11	I	1	Total C O 63 59 4	0
11	D	1	Total C O 63 59 4	0

- Molecule 12 is (2R)-2-(methoxymethyl)-4-{[(25R)-spirost-5-en-3beta-yl]oxy}butyl 4-O-alpha-D-glucopyranosyl-beta-D-glucopyranoside (three-letter code: I7Y) (formula: $C_{45}H_{74}O_{15}$).



Mol	Chain	Residues	Atoms	AltConf
12	I	1	Total C O 31 28 3	0

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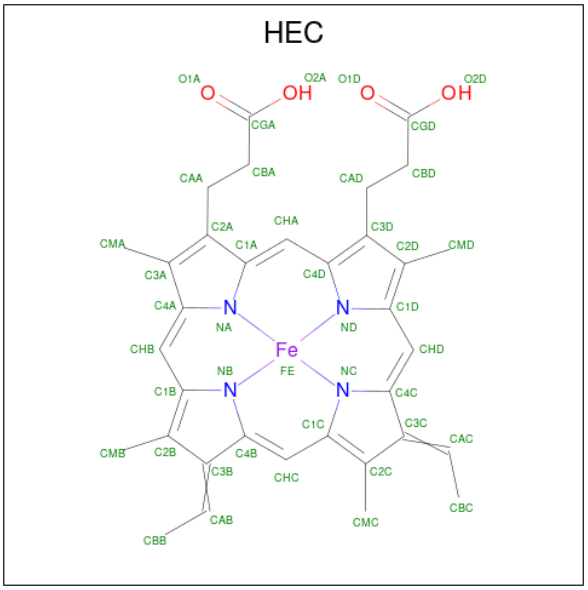
Mol	Chain	Residues	Atoms			AltConf
12	Z	1	Total	C	O	0
			60	45	15	

- Molecule 13 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
13	J	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	K	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	K	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	M	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	G	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	G	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 14 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
14	E	1	Total	Cu	0
			1	1	

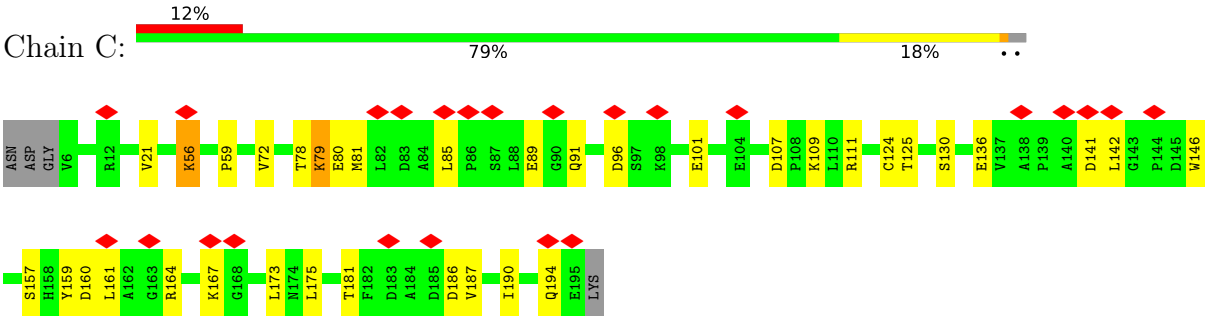
- Molecule 15 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
15	E	2	Total	Ca	0
			2	2	

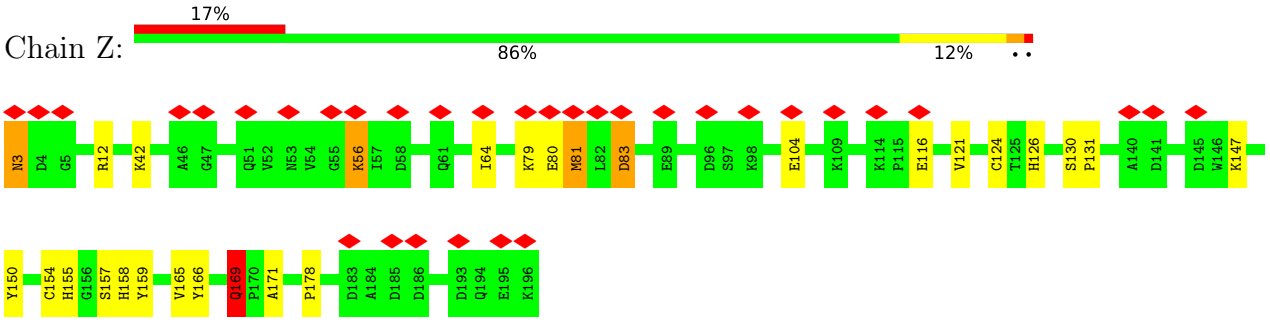
3 Residue-property plots (i)

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.

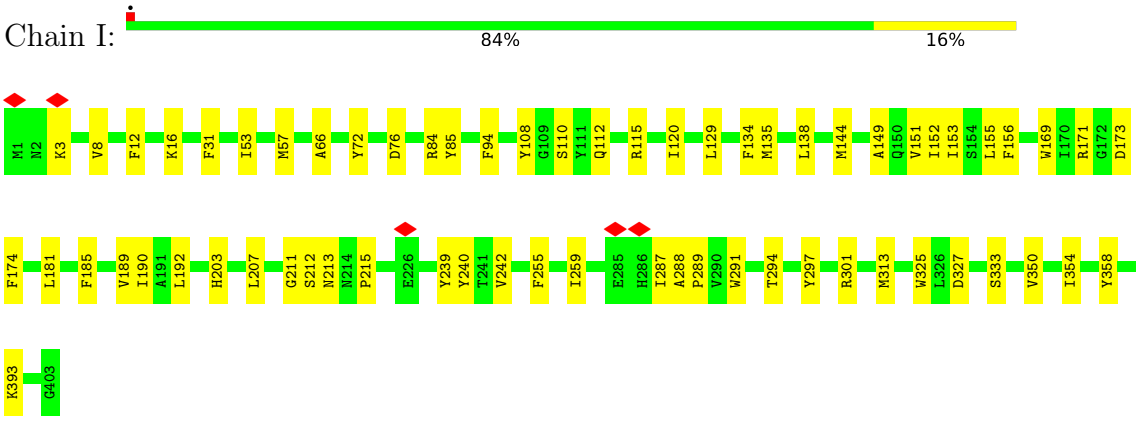
• Molecule 1: Ubiquinol-cytochrome c reductase iron-sulfur subunit



• Molecule 1: Ubiquinol-cytochrome c reductase iron-sulfur subunit

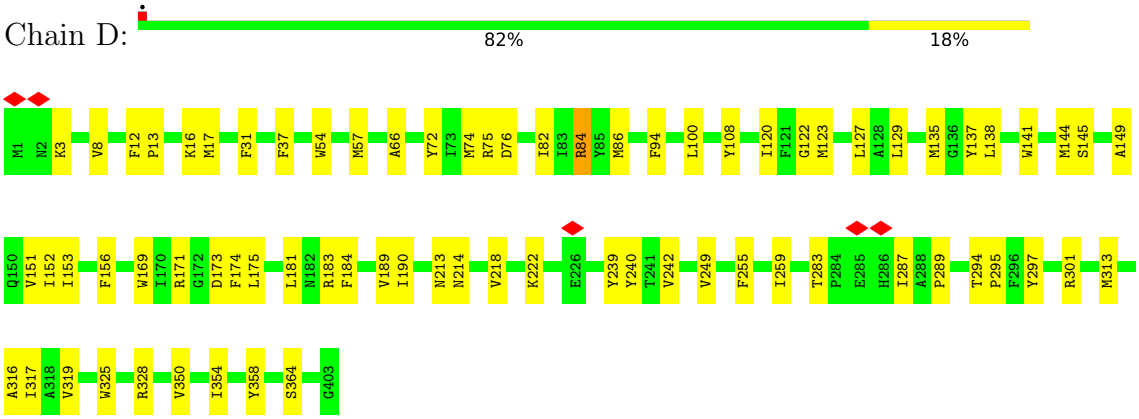


• Molecule 2: Cytochrome b



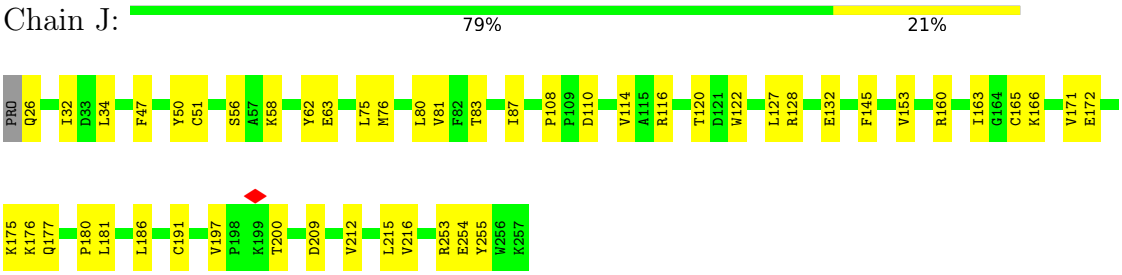
• Molecule 2: Cytochrome b

Chain D:



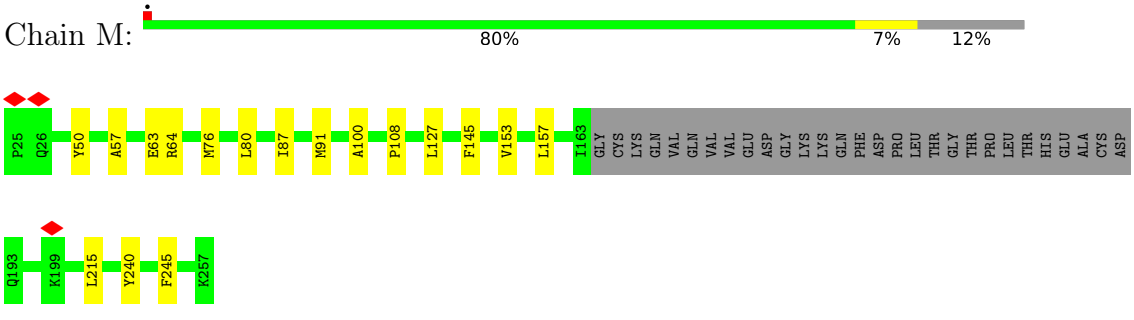
• Molecule 3: Cytochrome c1

Chain J:



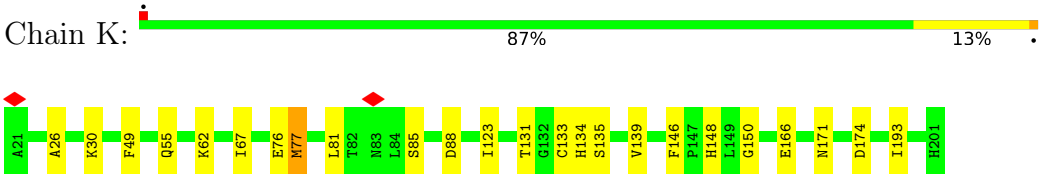
• Molecule 3: Cytochrome c1

Chain M:



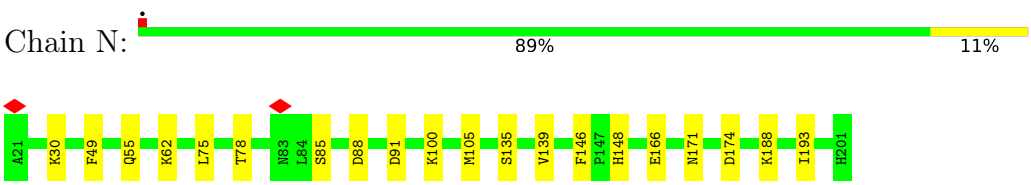
• Molecule 4: Cytochrome c4

Chain K:



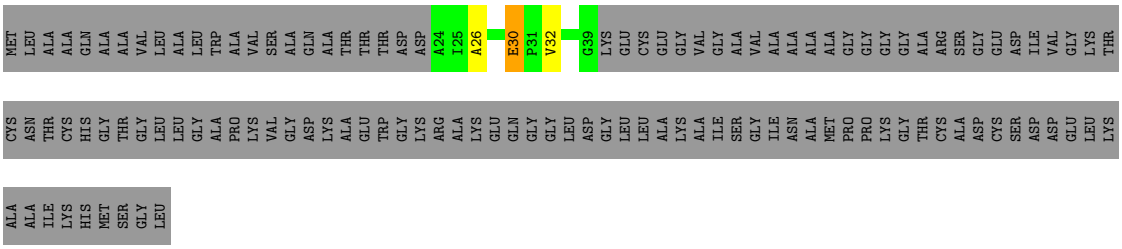
• Molecule 4: Cytochrome c4

Chain N:



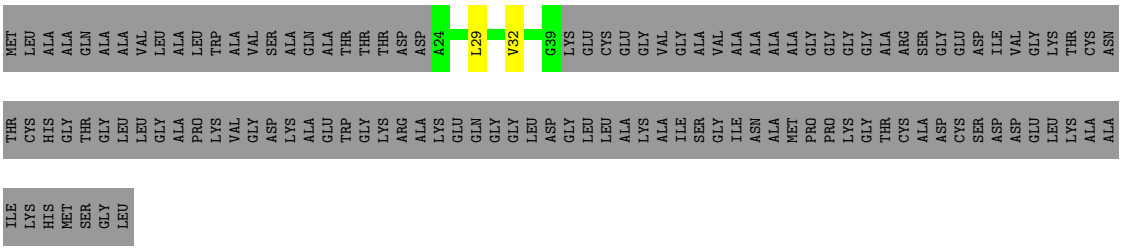
• Molecule 5: Cytochrome C5

Chain L:



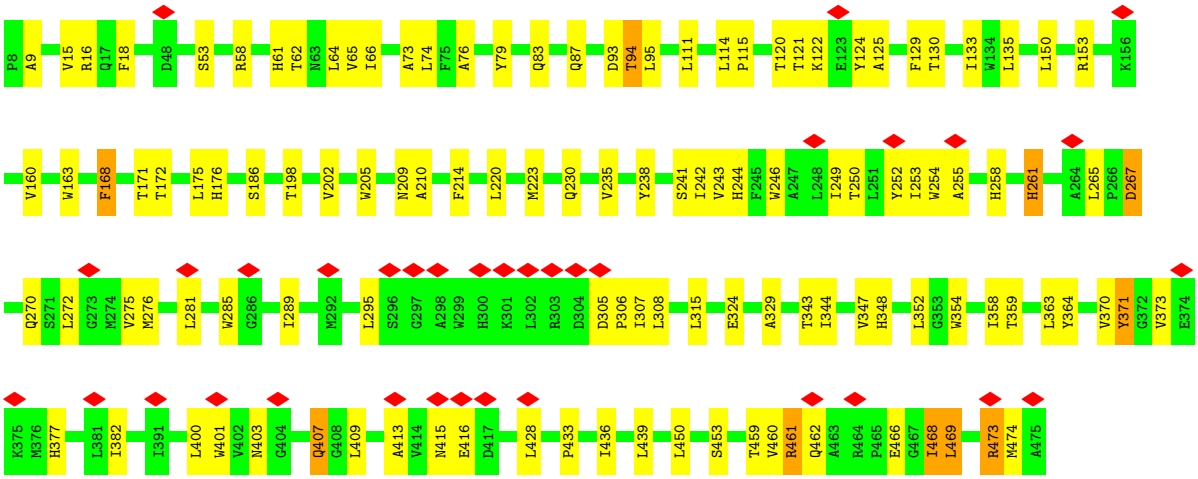
• Molecule 5: Cytochrome C5

Chain O:



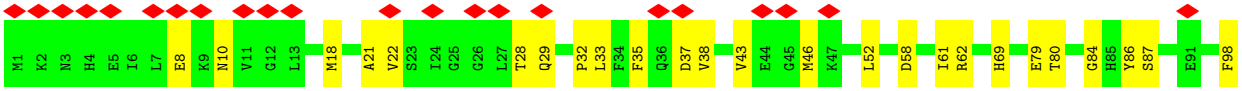
• Molecule 6: cytochrome-c oxidase

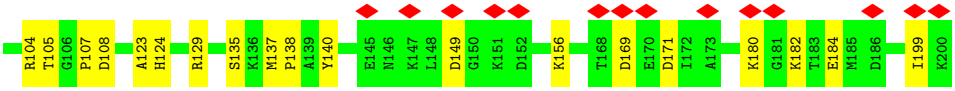
Chain E:



• Molecule 7: Cbb3-type Cytochrome C oxidase subunit II

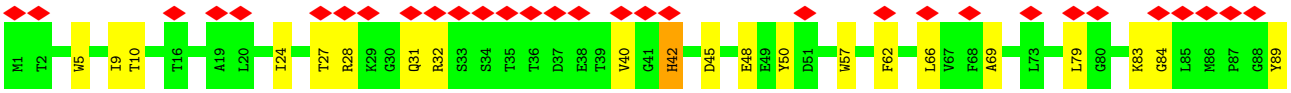
Chain F:

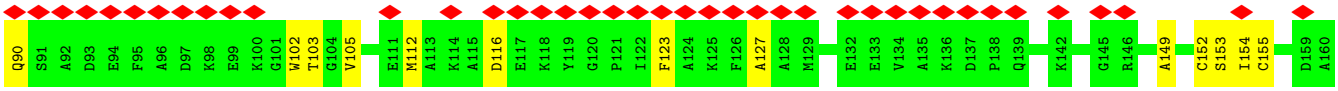


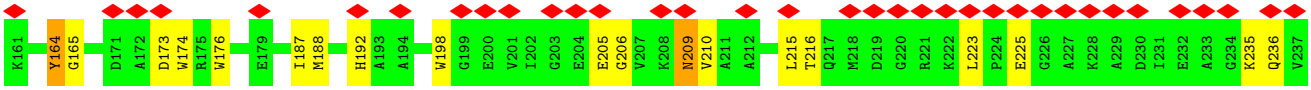


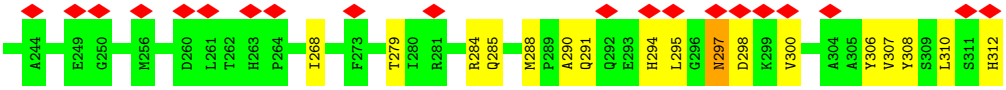
• Molecule 8: Cbb3-type cytochrome c oxidase subunit

Chain G:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48594	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 ($e^-/Å^2$)	51	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	15.242	Depositor
Minimum map value	-7.411	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.182	Depositor
Recommended contour level	1.24	Depositor
Map size (Å)	341.96, 341.96, 341.96	wwPDB
Map dimensions	332, 332, 332	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, CA, HEM, FES, U10, I7Y, CU

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	0.27	0/1461	0.50	0/1997
1	Z	0.30	0/1490	0.56	2/2035 (0.1%)
2	D	0.31	0/3381	0.48	0/4606
2	I	0.27	0/3381	0.46	0/4606
3	J	0.27	0/1889	0.48	0/2564
3	M	0.25	0/1674	0.47	0/2271
4	K	0.24	0/1327	0.45	0/1788
4	N	0.24	0/1327	0.45	0/1788
5	L	0.27	0/115	0.52	0/153
5	O	0.22	0/115	0.47	0/153
6	E	0.28	0/3847	0.49	0/5252
7	F	0.24	0/1533	0.48	0/2083
8	G	0.26	0/2415	0.48	0/3287
All	All	0.27	0/23955	0.48	2/32583 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Z	169	GLN	N-CA-CB	-6.12	99.58	110.60
1	Z	169	GLN	CB-CG-CD	-5.10	98.34	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1420	0	1407	24	0
1	Z	1449	0	1434	21	0
2	D	3267	0	3289	58	0
2	I	3267	0	3289	44	0
3	J	1842	0	1821	39	0
3	M	1631	0	1619	15	0
4	K	1306	0	1279	21	0
4	N	1306	0	1279	11	0
5	L	115	0	129	3	0
5	O	115	0	129	2	0
6	E	3719	0	3712	94	0
7	F	1499	0	1418	31	0
8	G	2345	0	2240	52	0
9	C	4	0	0	1	0
9	Z	4	0	0	2	0
10	D	86	0	60	9	0
10	E	86	0	60	14	0
10	I	86	0	60	12	0
11	D	63	0	90	14	0
11	I	63	0	90	12	0
12	I	31	0	0	3	0
12	Z	60	0	0	3	0
13	F	43	0	30	10	0
13	G	86	0	60	15	0
13	J	43	0	30	11	0
13	K	86	0	60	11	0
13	M	43	0	30	7	0
13	N	86	0	60	7	0
14	E	1	0	0	0	0
15	E	2	0	0	0	0
All	All	24154	0	23675	435	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 9.

The worst 5 of 435 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)
12:I:504:I7Y:C07	12:I:504:I7Y:C15	1.78	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:202:I7Y:C15	12:Z:202:I7Y:C07	1.77	1.58
1:Z:3:ASN:HD22	1:Z:3:ASN:N	1.55	0.97
2:I:129:LEU:HD11	10:I:501:HEM:HBB1	1.56	0.86
12:I:504:I7Y:C15	12:I:504:I7Y:C08	2.55	0.84

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	188/194 (97%)	182 (97%)	6 (3%)	0	100	100
1	Z	192/194 (99%)	185 (96%)	7 (4%)	0	100	100
2	D	401/403 (100%)	393 (98%)	8 (2%)	0	100	100
2	I	401/403 (100%)	396 (99%)	5 (1%)	0	100	100
3	J	230/233 (99%)	227 (99%)	3 (1%)	0	100	100
3	M	200/233 (86%)	197 (98%)	3 (2%)	0	100	100
4	K	179/181 (99%)	175 (98%)	4 (2%)	0	100	100
4	N	179/181 (99%)	175 (98%)	4 (2%)	0	100	100
5	L	14/136 (10%)	14 (100%)	0	0	100	100
5	O	14/136 (10%)	14 (100%)	0	0	100	100
6	E	466/468 (100%)	446 (96%)	19 (4%)	1 (0%)	47	73
7	F	198/200 (99%)	194 (98%)	4 (2%)	0	100	100
8	G	310/312 (99%)	294 (95%)	16 (5%)	0	100	100
All	All	2972/3274 (91%)	2892 (97%)	79 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	E	473	ARG

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	148/151 (98%)	143 (97%)	5 (3%)	37 66
1	Z	151/151 (100%)	143 (95%)	8 (5%)	22 48
2	D	342/342 (100%)	335 (98%)	7 (2%)	55 81
2	I	342/342 (100%)	336 (98%)	6 (2%)	59 83
3	J	195/196 (100%)	190 (97%)	5 (3%)	46 75
3	M	171/196 (87%)	170 (99%)	1 (1%)	86 95
4	K	130/130 (100%)	129 (99%)	1 (1%)	81 93
4	N	130/130 (100%)	126 (97%)	4 (3%)	40 69
5	L	12/90 (13%)	11 (92%)	1 (8%)	11 25
5	O	12/90 (13%)	12 (100%)	0	100 100
6	E	383/383 (100%)	368 (96%)	15 (4%)	32 61
7	F	147/167 (88%)	140 (95%)	7 (5%)	25 53
8	G	226/240 (94%)	211 (93%)	15 (7%)	16 38
All	All	2389/2608 (92%)	2314 (97%)	75 (3%)	43 69

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	F	108	ASP
8	G	235	LYS
7	F	180	LYS
8	G	112	MET
1	Z	147	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	Z	91	GLN
4	N	201	HIS
6	E	208	HIS
6	E	244	HIS
8	G	192	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)

Of 24 ligands modelled in this entry, 3 are monoatomic - leaving 21 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	$\#\|Z\| > 2$
13	HEC	N	501	4	32,50,50	2.27	3 (9%)	24,82,82	1.56	2 (8%)
13	HEC	K	502	4	32,50,50	2.20	3 (9%)	24,82,82	1.56	2 (8%)
11	U10	I	503	-	63,63,63	2.73	17 (26%)	76,79,79	1.76	22 (28%)
13	HEC	F	301	7	32,50,50	2.22	4 (12%)	24,82,82	1.30	1 (4%)
13	HEC	M	500	3	32,50,50	2.22	4 (12%)	24,82,82	1.37	1 (4%)
9	FES	C	201	1	0,4,4	-	-	-		
13	HEC	K	501	4	32,50,50	2.18	3 (9%)	24,82,82	1.61	3 (12%)
10	HEM	D	501	2	41,50,50	1.45	3 (7%)	45,82,82	1.52	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	HEC	J	500	3	32,50,50	2.26	3 (9%)	24,82,82	1.45	5 (20%)
13	HEC	G	401	8	32,50,50	2.13	3 (9%)	24,82,82	1.50	3 (12%)
10	HEM	I	501	2	41,50,50	1.46	3 (7%)	45,82,82	1.50	8 (17%)
13	HEC	N	502	4	32,50,50	2.19	3 (9%)	24,82,82	1.52	4 (16%)
12	I7Y	Z	202	-	67,67,67	4.50	29 (43%)	101,103,103	2.58	24 (23%)
10	HEM	E	504	6,15	41,50,50	1.47	3 (7%)	45,82,82	1.39	6 (13%)
9	FES	Z	201	1	0,4,4	-	-	-		
10	HEM	E	505	6,15	41,50,50	1.50	6 (14%)	45,82,82	1.24	4 (8%)
12	I7Y	I	504	-	36,36,67	5.95	22 (61%)	59,59,103	3.10	17 (28%)
13	HEC	G	402	8	32,50,50	2.20	3 (9%)	24,82,82	1.44	3 (12%)
10	HEM	D	502	2	41,50,50	1.49	5 (12%)	45,82,82	1.40	6 (13%)
10	HEM	I	502	2	41,50,50	1.49	4 (9%)	45,82,82	1.42	6 (13%)
11	U10	D	503	-	63,63,63	2.75	17 (26%)	76,79,79	1.67	20 (26%)

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
13	HEC	N	501	4	-	0/10/54/54	-
13	HEC	K	502	4	-	2/10/54/54	-
11	U10	I	503	-	-	24/63/87/87	0/1/1/1
13	HEC	F	301	7	-	2/10/54/54	-
13	HEC	M	500	3	-	2/10/54/54	-
9	FES	C	201	1	-	-	0/1/1/1
13	HEC	K	501	4	-	2/10/54/54	-
10	HEM	D	501	2	-	1/12/54/54	-
13	HEC	J	500	3	-	0/10/54/54	-
13	HEC	G	401	8	-	4/10/54/54	-
10	HEM	I	501	2	-	7/12/54/54	-
13	HEC	N	502	4	-	2/10/54/54	-
12	I7Y	Z	202	-	-	11/22/150/150	0/8/8/8
10	HEM	E	504	6,15	-	0/12/54/54	-
9	FES	Z	201	1	-	-	0/1/1/1
10	HEM	E	505	6,15	-	4/12/54/54	-
12	I7Y	I	504	-	-	1/2/90/150	0/6/6/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	HEC	G	402	8	-	5/10/54/54	-
10	HEM	D	502	2	-	2/12/54/54	-
10	HEM	I	502	2	-	4/12/54/54	-
11	U10	D	503	-	-	23/63/87/87	0/1/1/1

The worst 5 of 138 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	I	504	I7Y	C15-C07	14.68	1.78	1.53
12	Z	202	I7Y	C15-C07	14.65	1.77	1.53
12	Z	202	I7Y	C07-C08	-14.61	1.25	1.53
12	I	504	I7Y	C07-C08	-14.60	1.25	1.53
12	I	504	I7Y	C10-C02	-13.45	1.30	1.54

The worst 5 of 145 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	I	504	I7Y	C76-C73-C74	15.79	148.17	115.69
12	Z	202	I7Y	C76-C73-C74	15.79	148.16	115.69
12	I	504	I7Y	O80-C73-C74	-7.83	79.89	107.38
12	Z	202	I7Y	O80-C73-C74	-7.83	79.90	107.38
12	Z	202	I7Y	C10-C02-C06	5.10	115.18	107.27

There are no chirality outliers.

5 of 96 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	E	505	HEM	C1A-C2A-CAA-CBA
10	E	505	HEM	C3A-C2A-CAA-CBA
11	I	503	U10	C7-C8-C9-C10
11	I	503	U10	C7-C8-C9-C11
11	I	503	U10	C13-C14-C16-C17

There are no ring outliers.

21 monomers are involved in 131 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	N	501	HEC	4	0
13	K	502	HEC	5	0
11	I	503	U10	12	0

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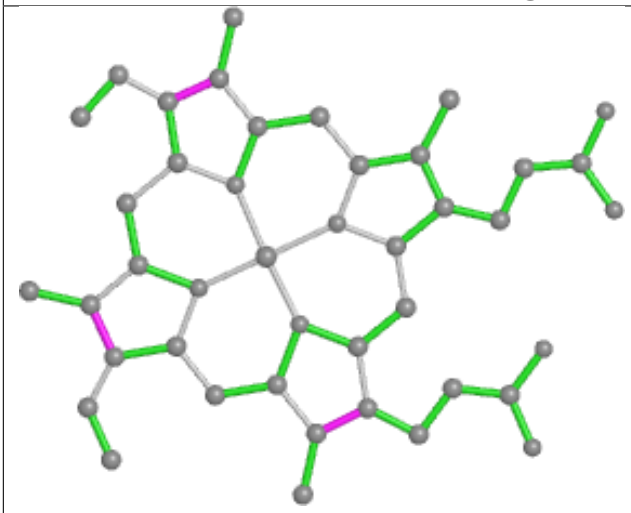
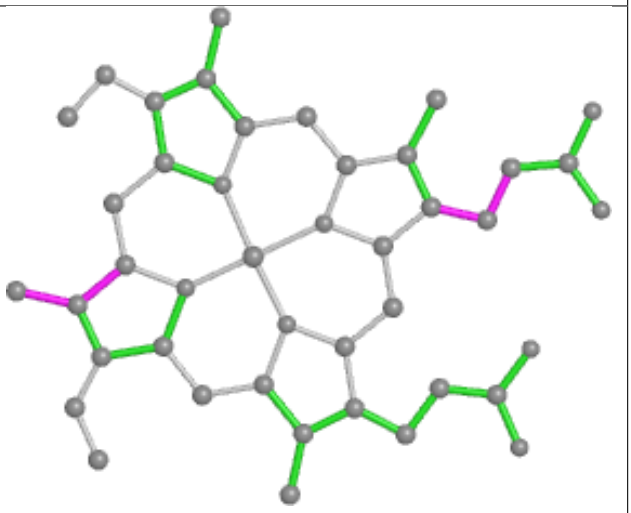
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	F	301	HEC	10	0
13	M	500	HEC	7	0
9	C	201	FES	1	0
13	K	501	HEC	6	0
10	D	501	HEM	4	0
13	J	500	HEC	11	0
13	G	401	HEC	6	0
10	I	501	HEM	7	0
13	N	502	HEC	3	0
12	Z	202	I7Y	3	0
10	E	504	HEM	7	0
9	Z	201	FES	2	0
10	E	505	HEM	7	0
12	I	504	I7Y	3	0
13	G	402	HEC	9	0
10	D	502	HEM	5	0
10	I	502	HEM	5	0
11	D	503	U10	14	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.

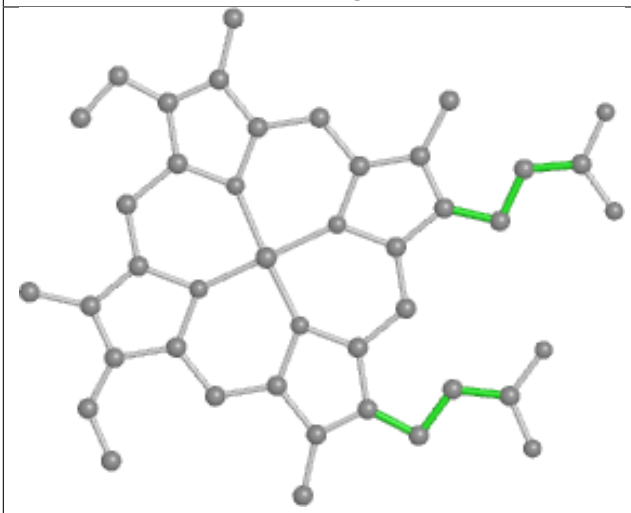
Ligand HEC N 501



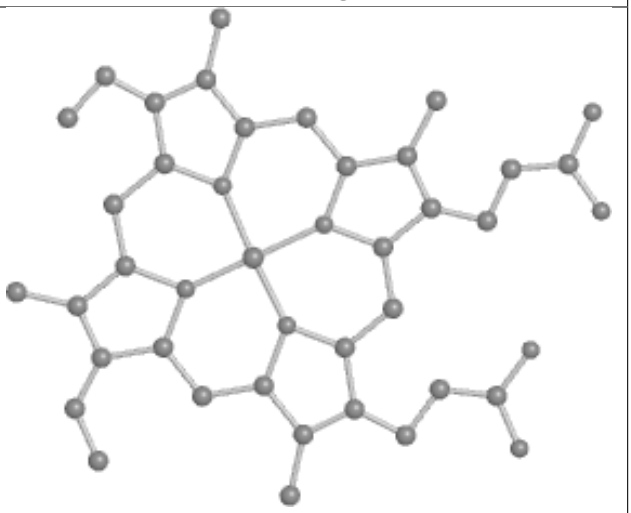
Bond lengths



Bond angles

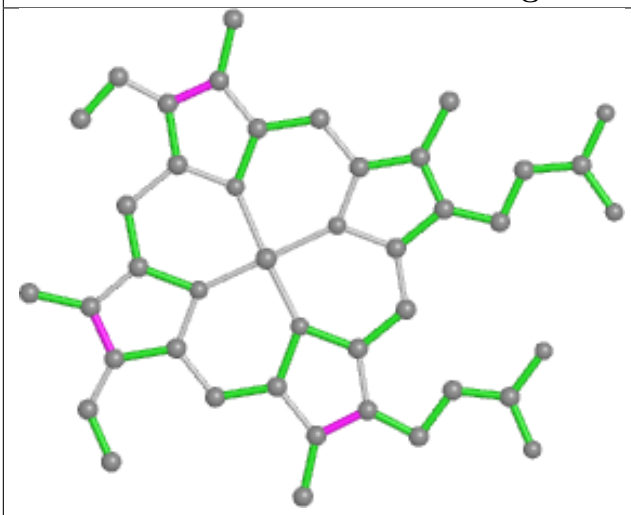


Torsions



Rings

Ligand HEC K 502



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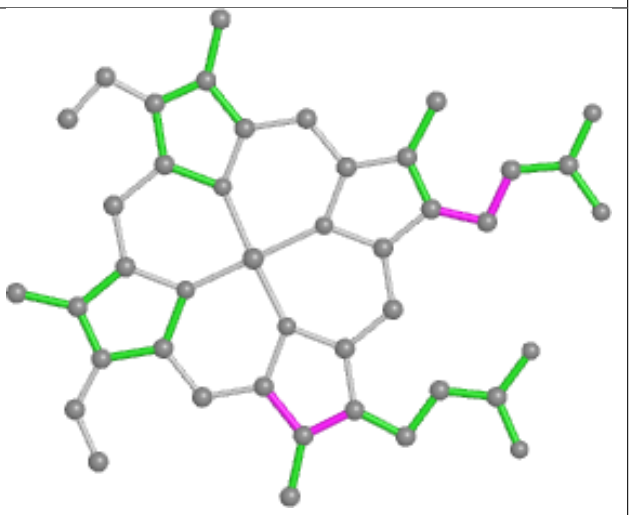

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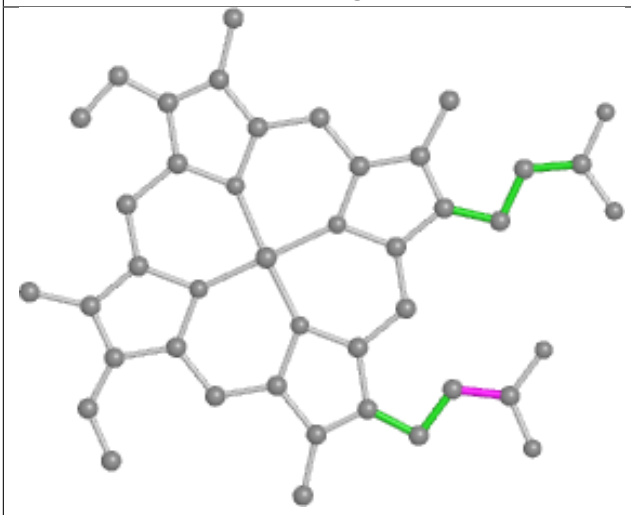

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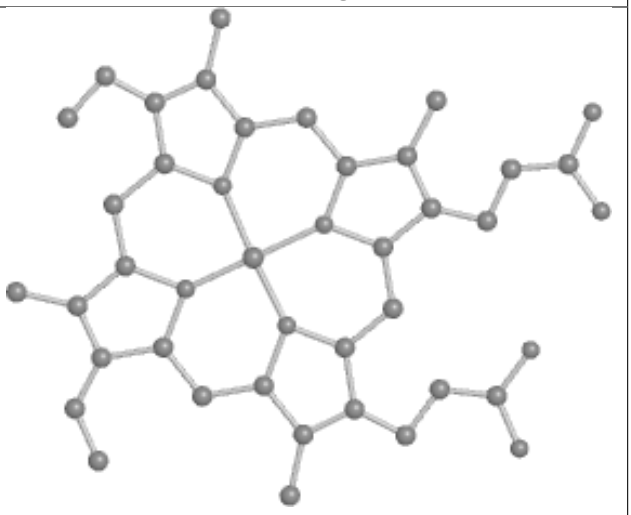
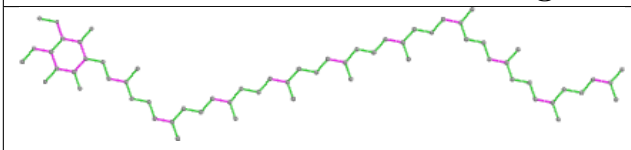


Rings

Ligand U10 I 503



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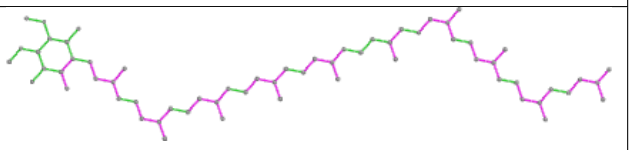

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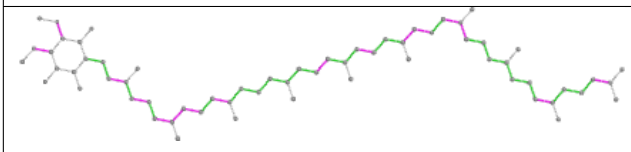
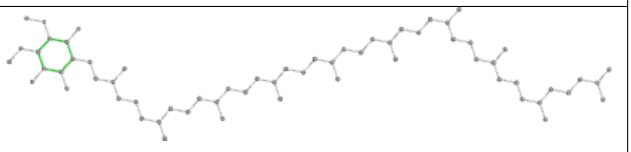
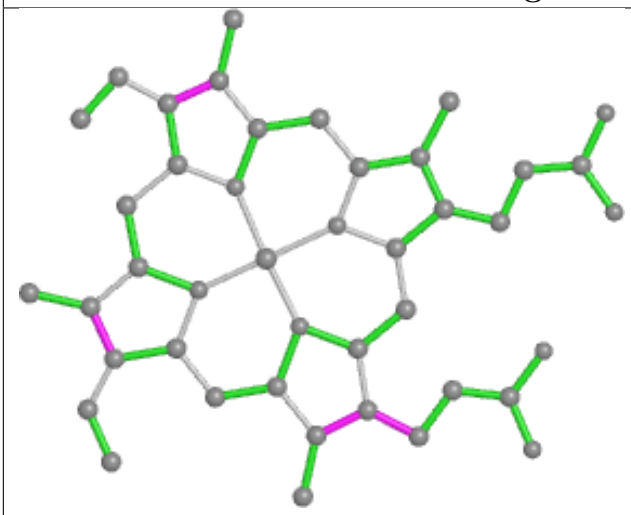


Torsions



Rings

Ligand HEC F 301



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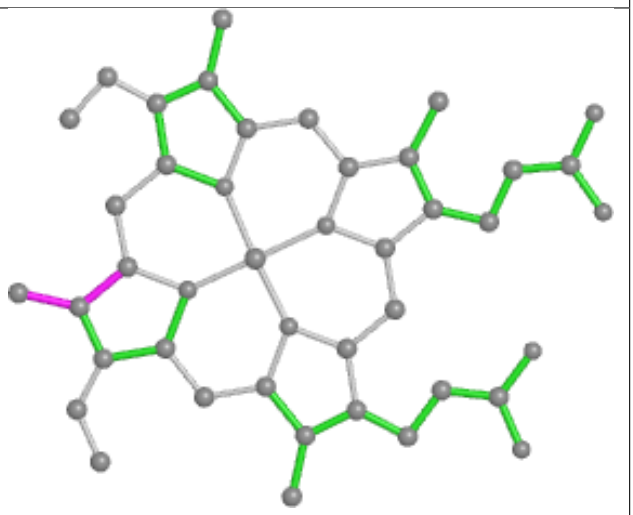
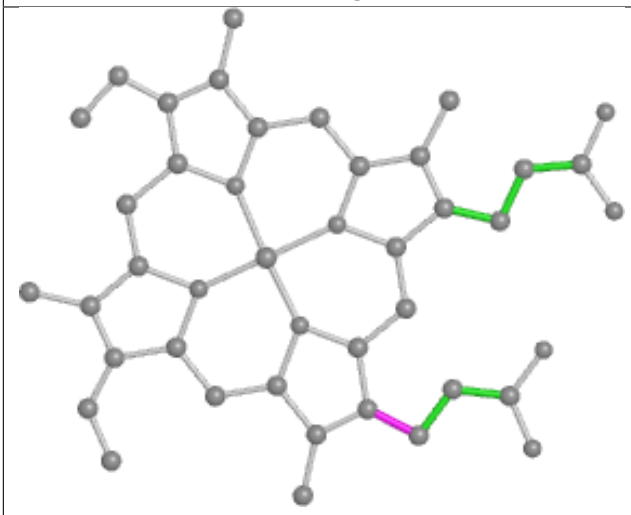


Bond angles



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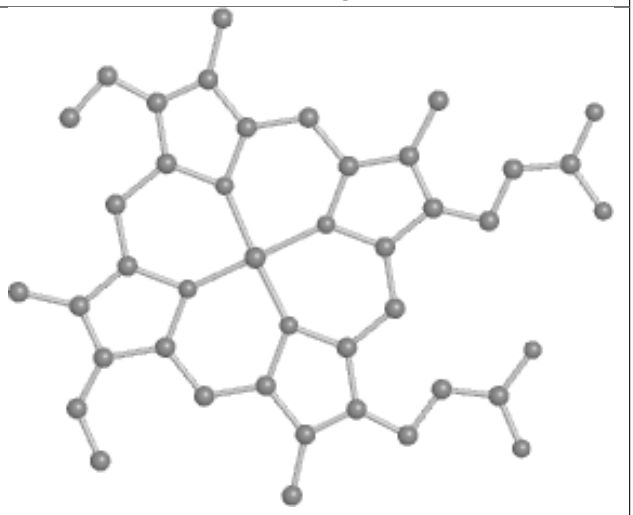
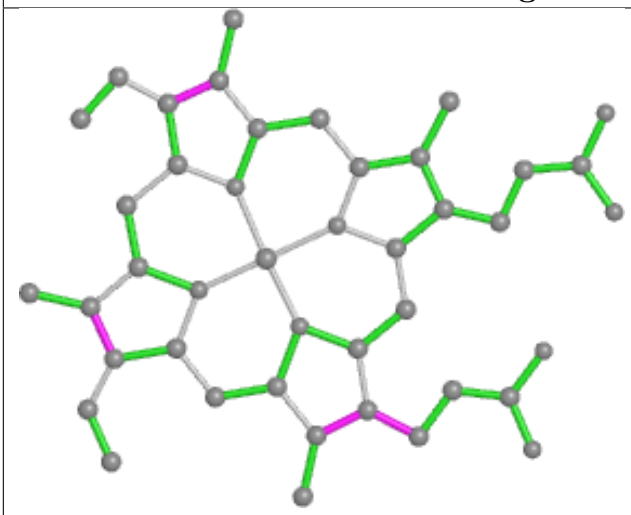
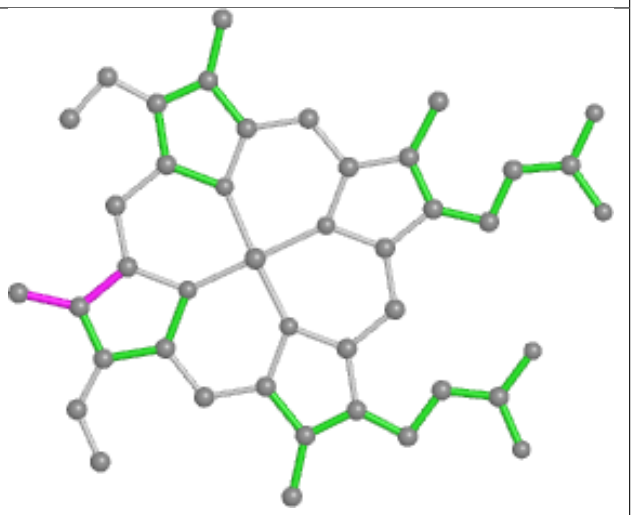


Rings

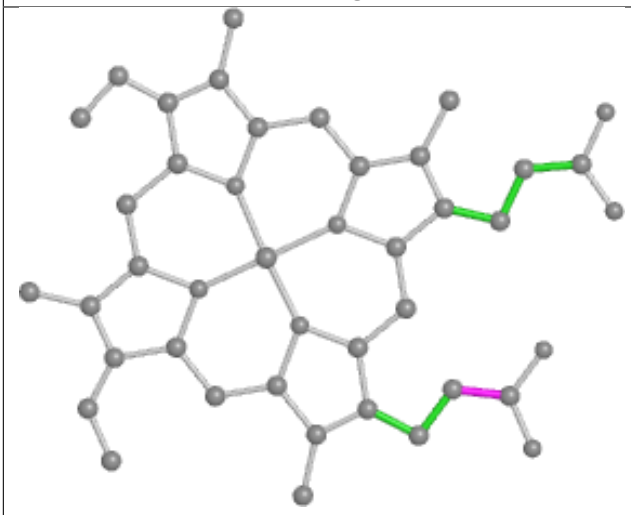
Ligand HEC M 500



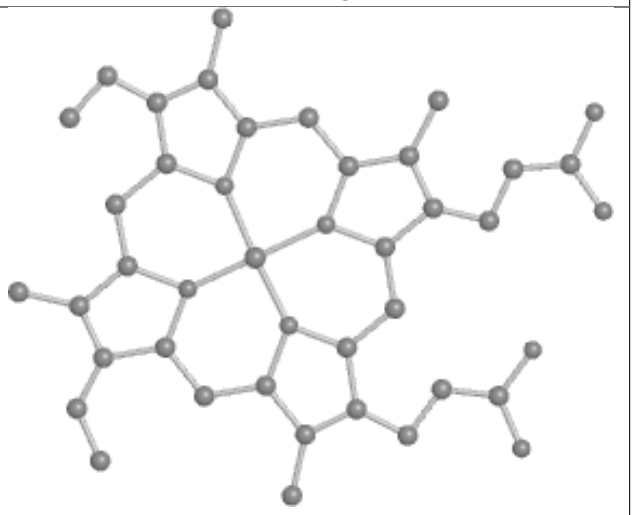
Bond lengths



Bond angles

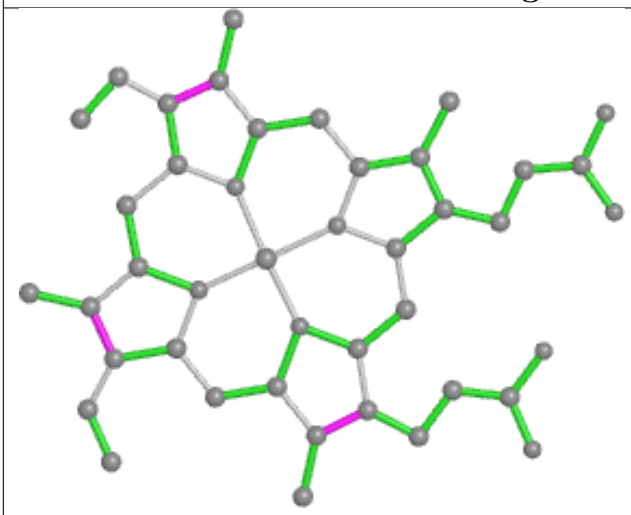


Torsions



Rings

Ligand HEC K 501



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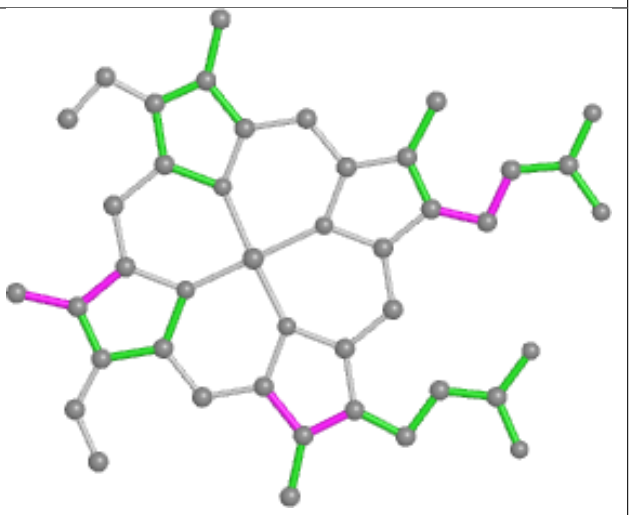
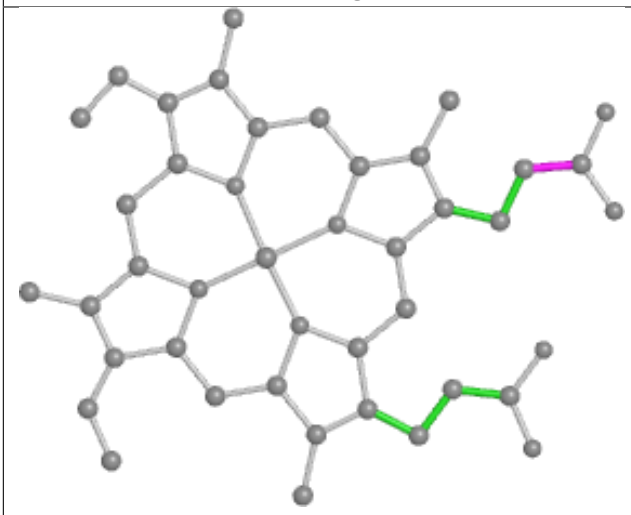
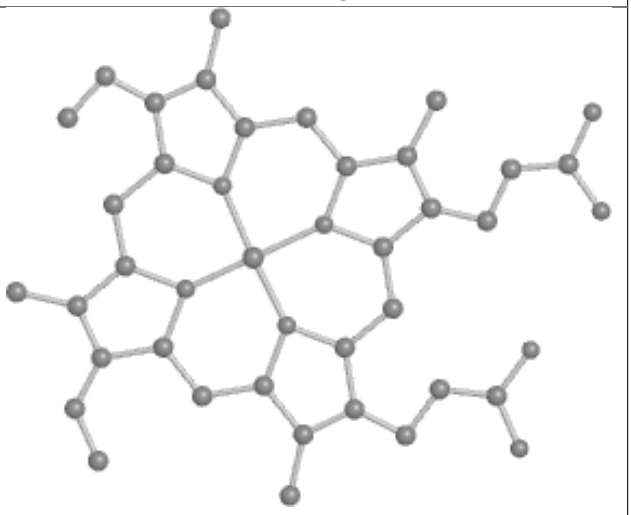


Bond angles

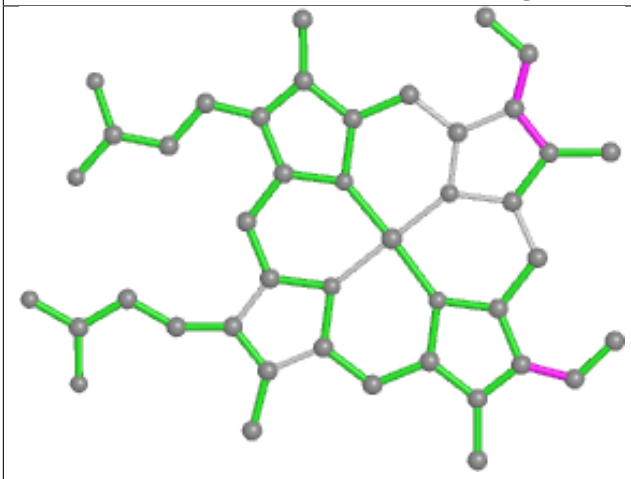


Torsions

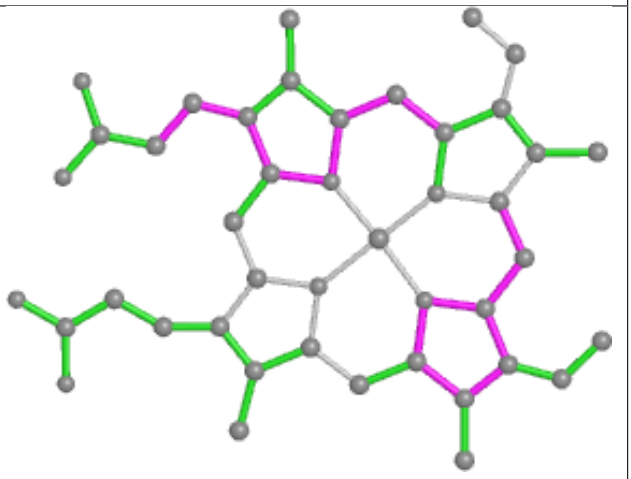


Rings

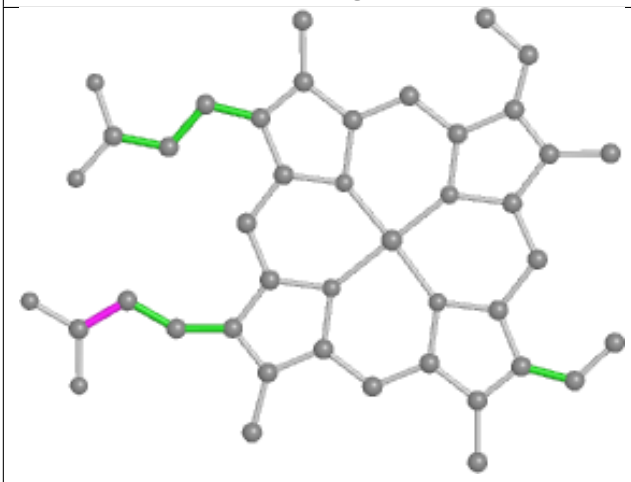
Ligand HEM D 501



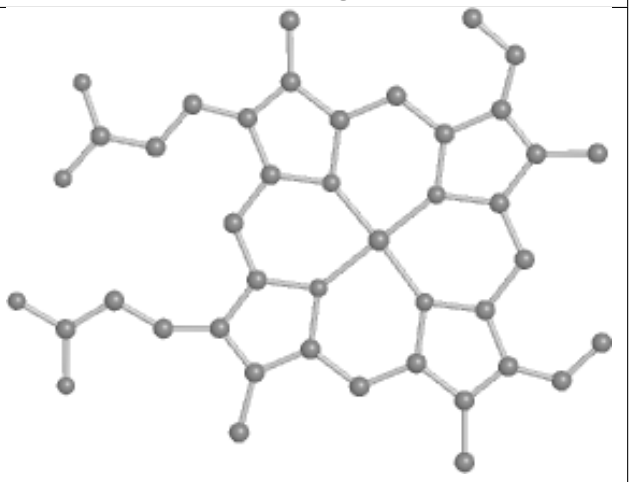
Bond lengths



Bond angles

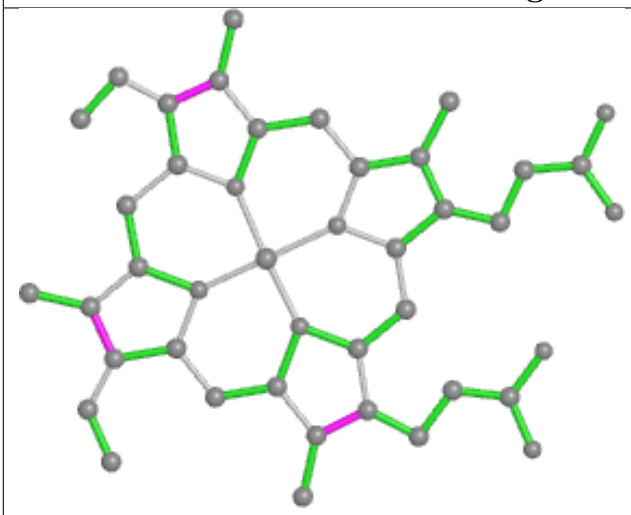


Torsions

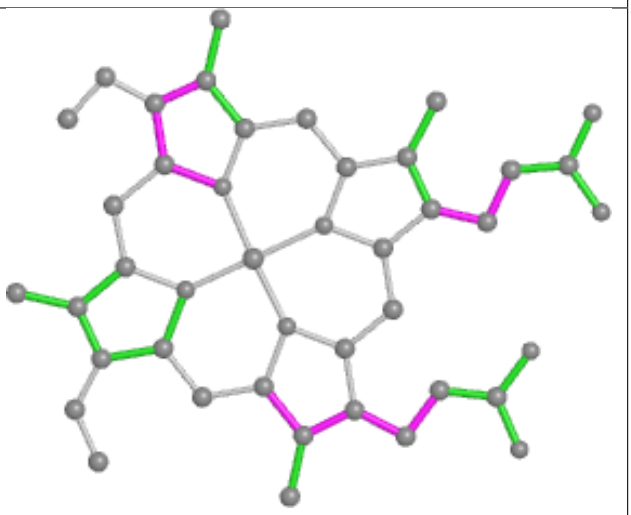


Rings

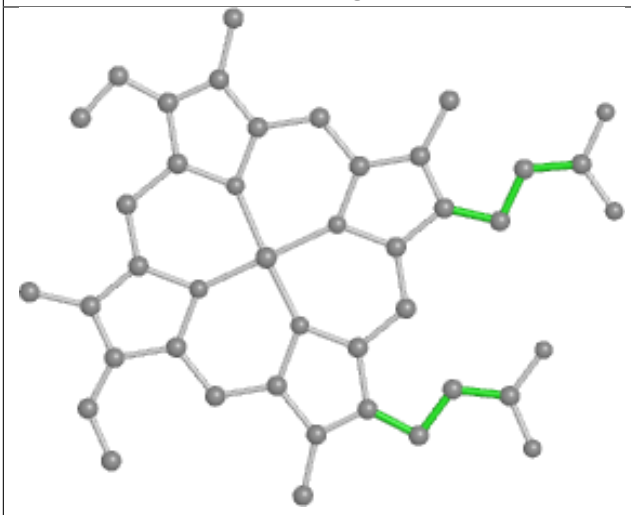
Ligand HEC J 500



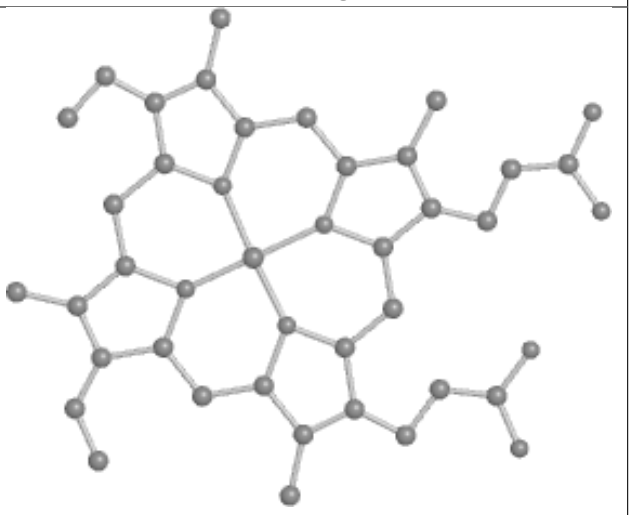
Bond lengths



Bond angles

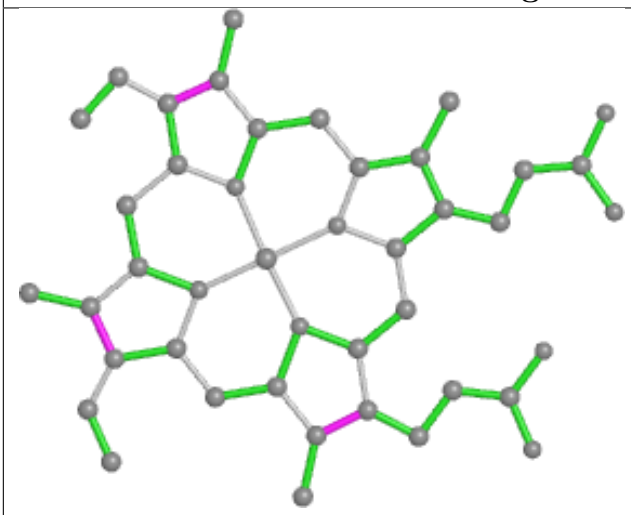


Torsions

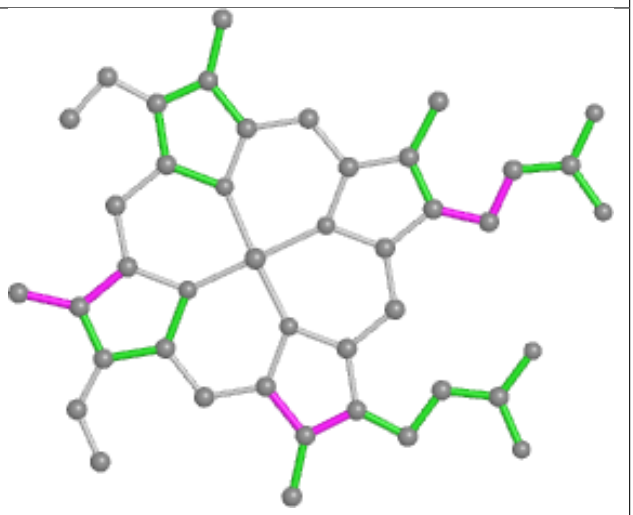


Rings

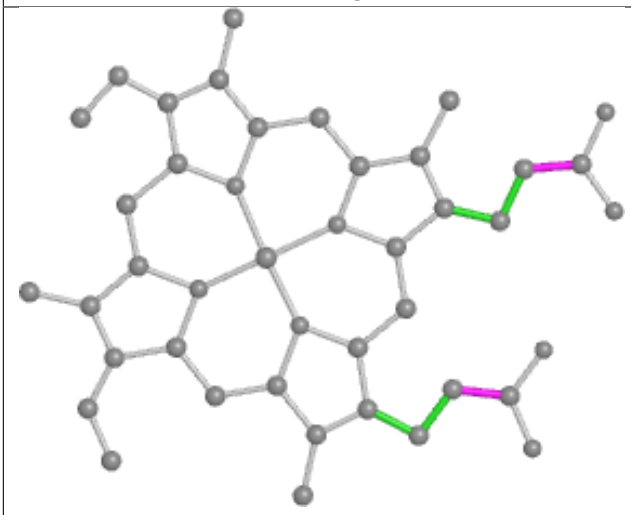
Ligand HEC G 401



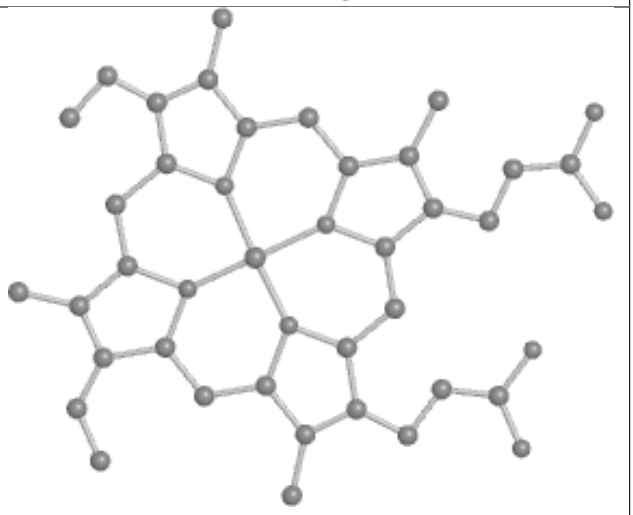
Bond lengths



Bond angles

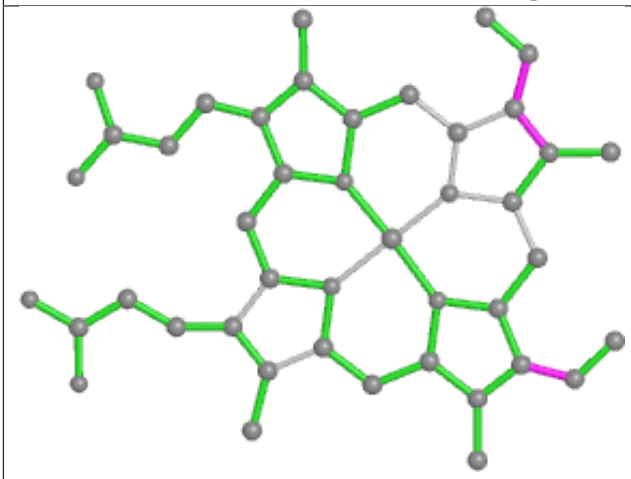


Torsions

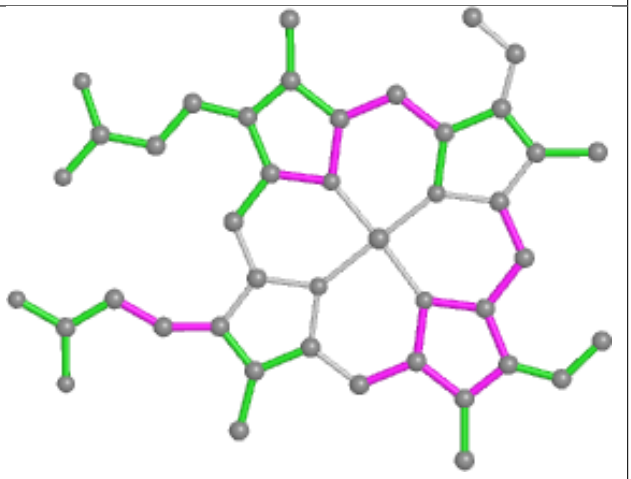


Rings

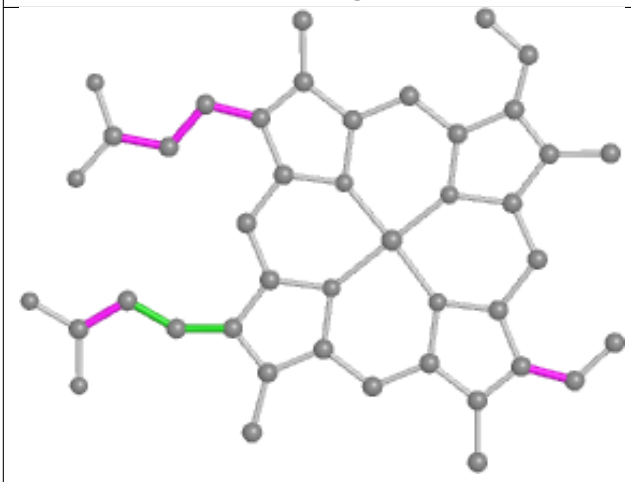
Ligand HEM I 501



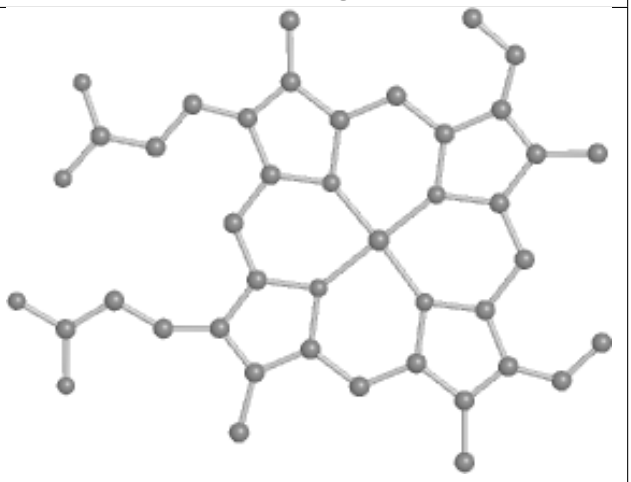
Bond lengths



Bond angles

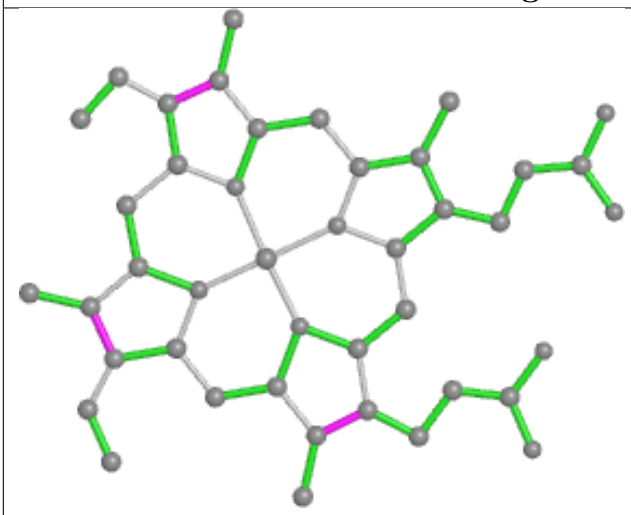


Torsions

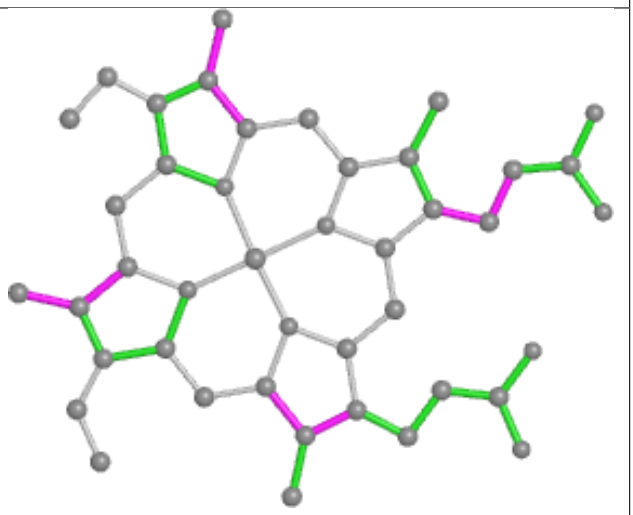


Rings

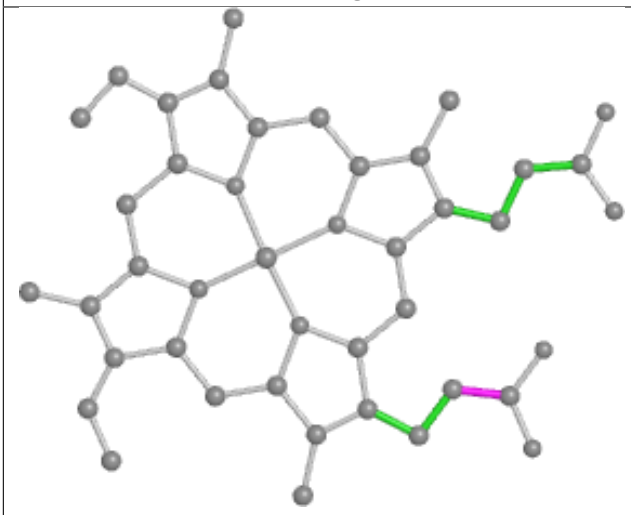
Ligand HEC N 502



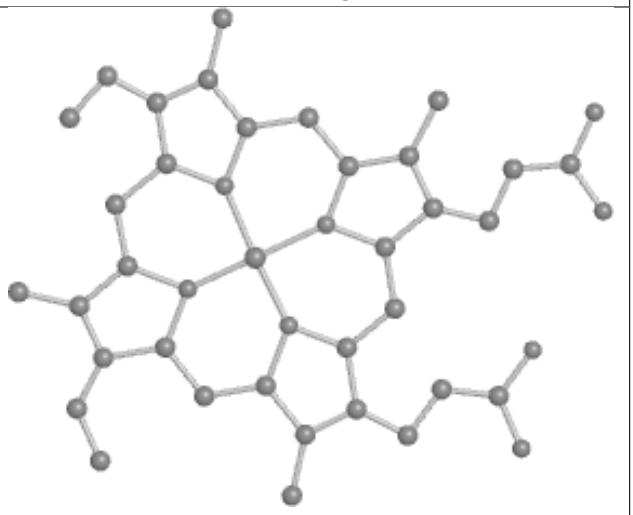
Bond lengths



Bond angles

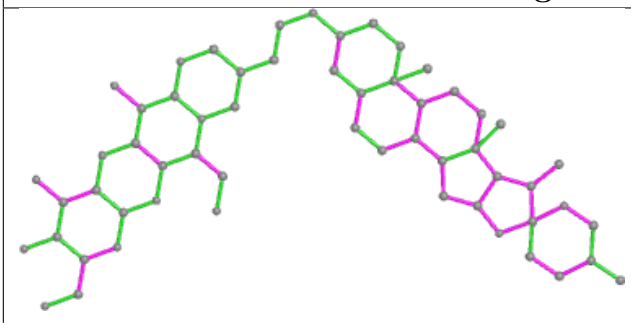


Torsions

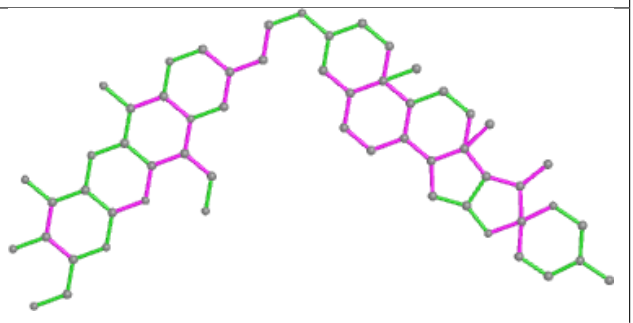


Rings

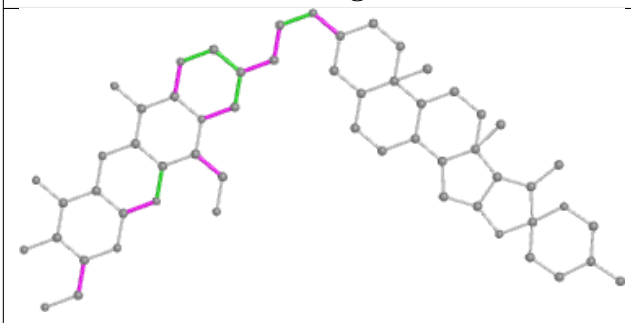
Ligand I7Y Z 202



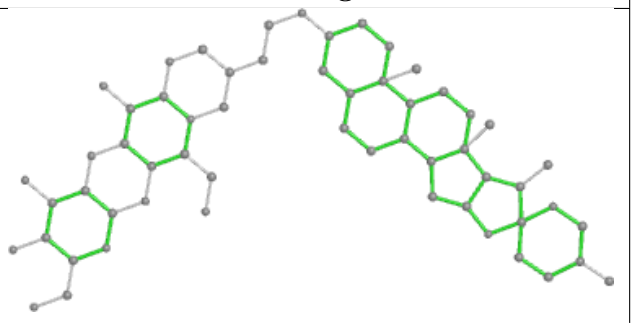
Bond lengths



Bond angles

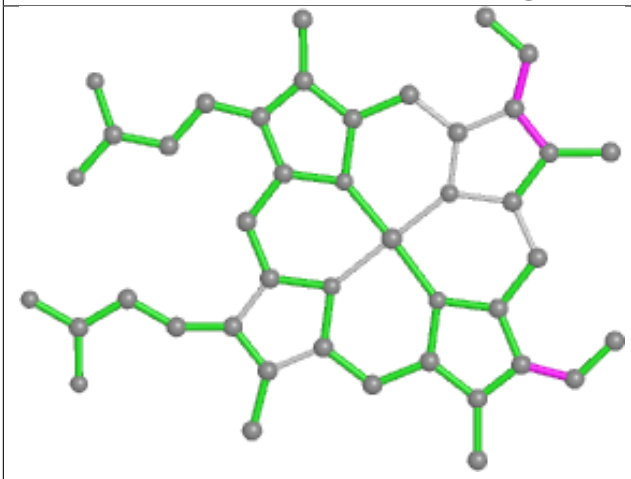


Torsions

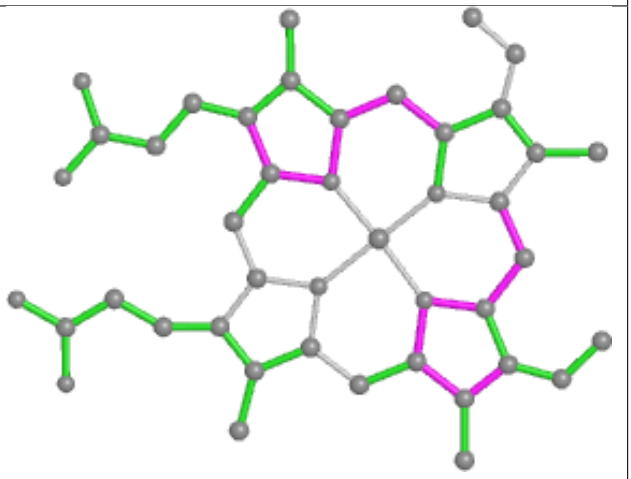


Rings

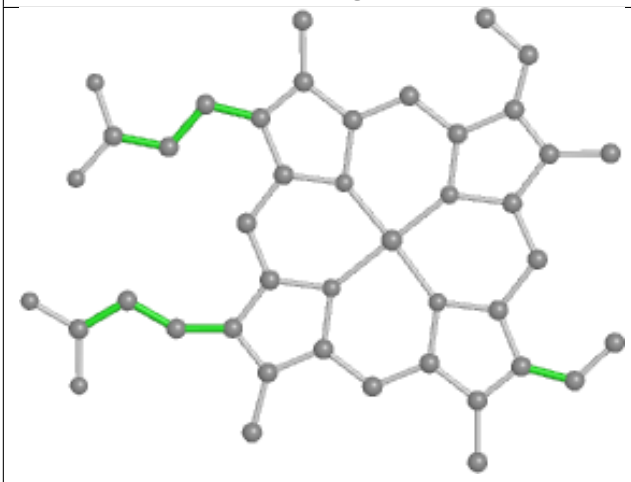
Ligand HEM E 504



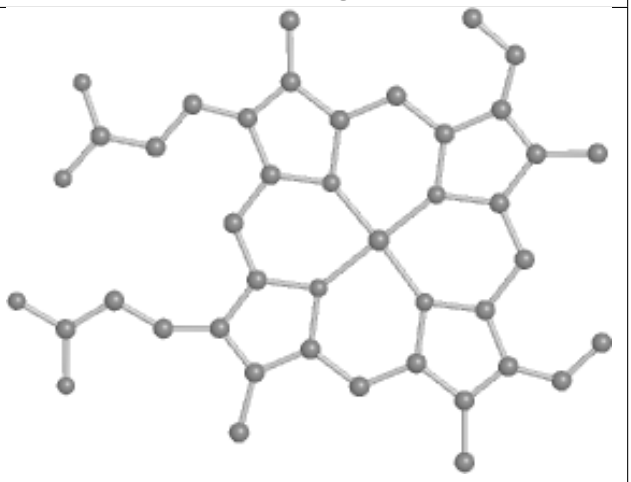
Bond lengths



Bond angles

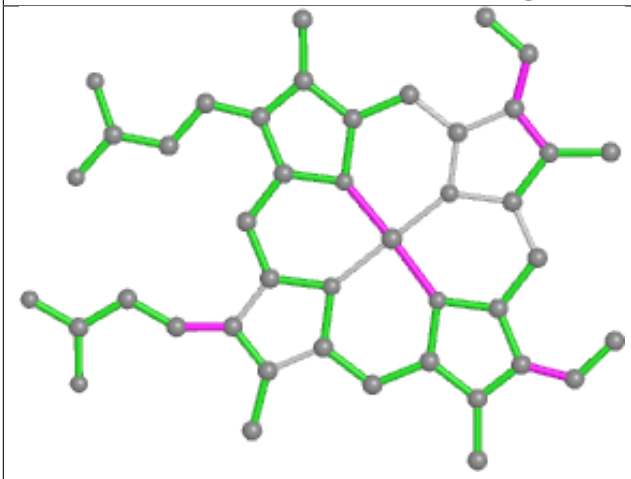


Torsions

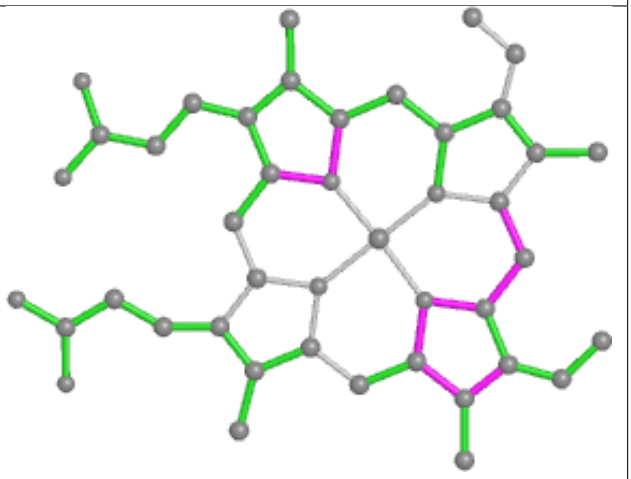


Rings

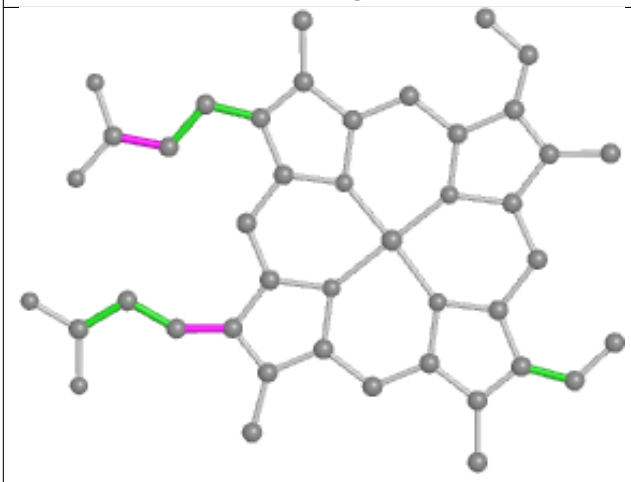
Ligand HEM E 505



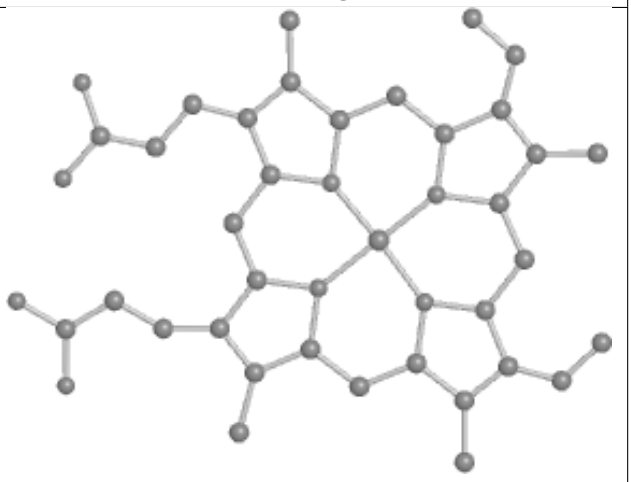
Bond lengths



Bond angles

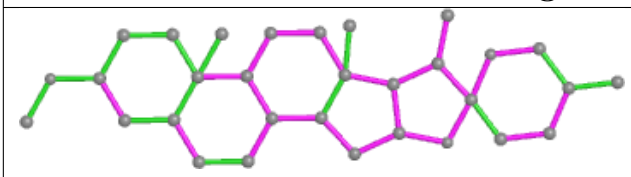


Torsions

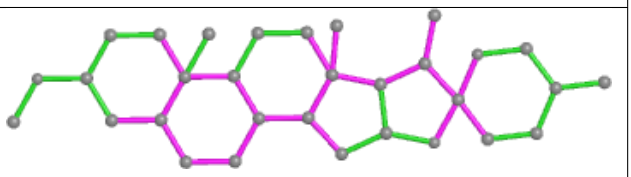


Rings

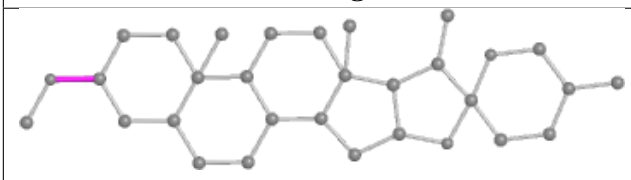
Ligand I7Y I 504



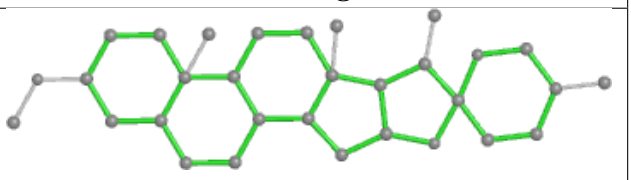
Bond lengths



Bond angles

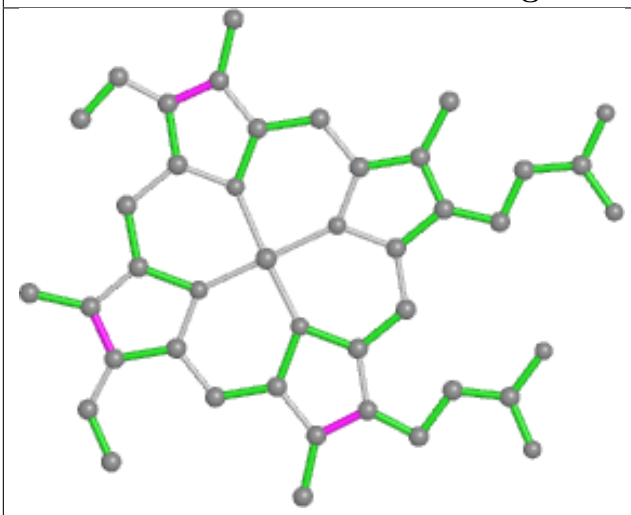


Torsions

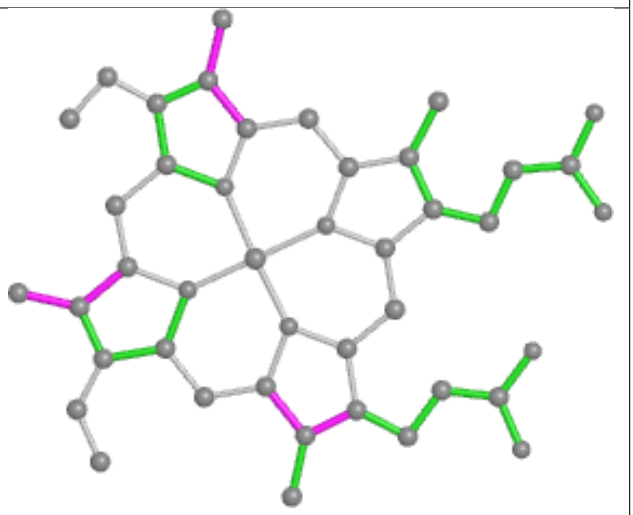


Rings

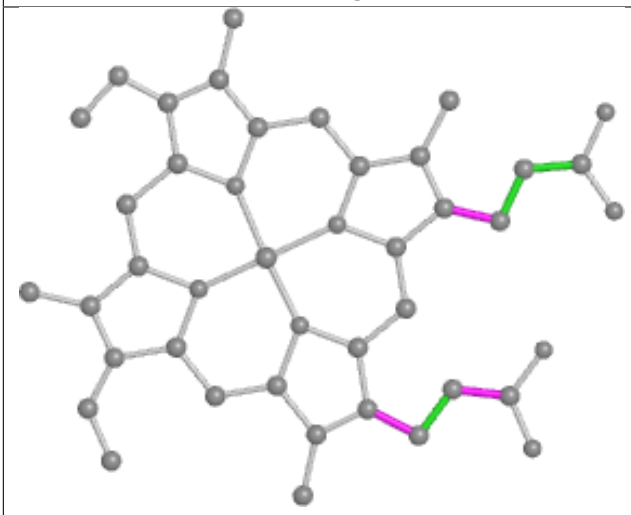
Ligand HEC G 402



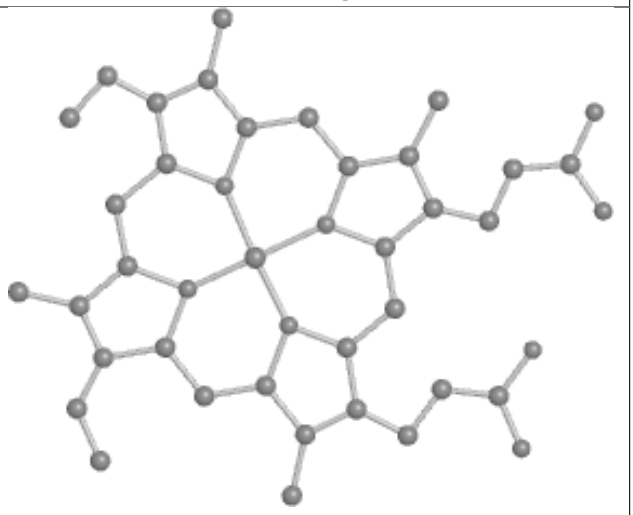
Bond lengths



Bond angles

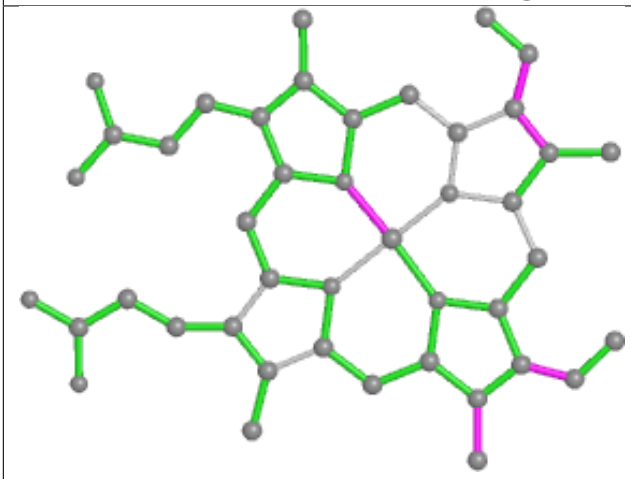


Torsions

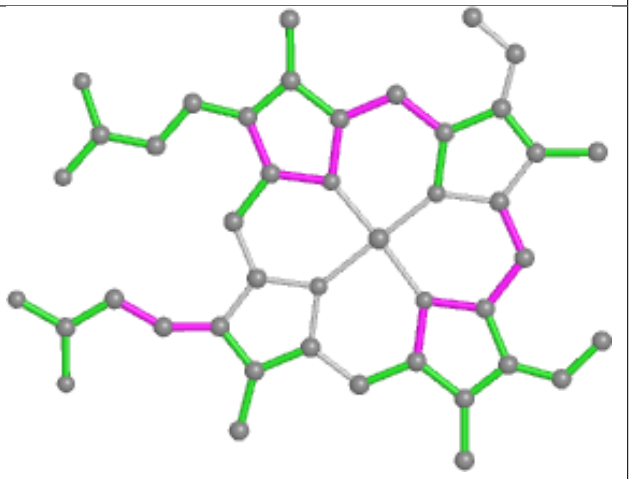


Rings

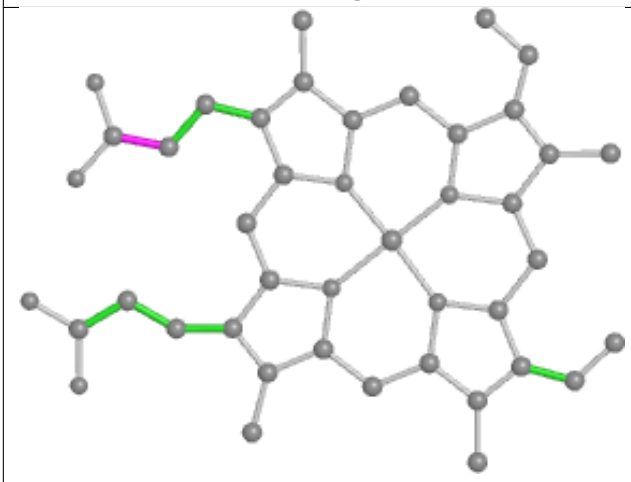
Ligand HEM D 502



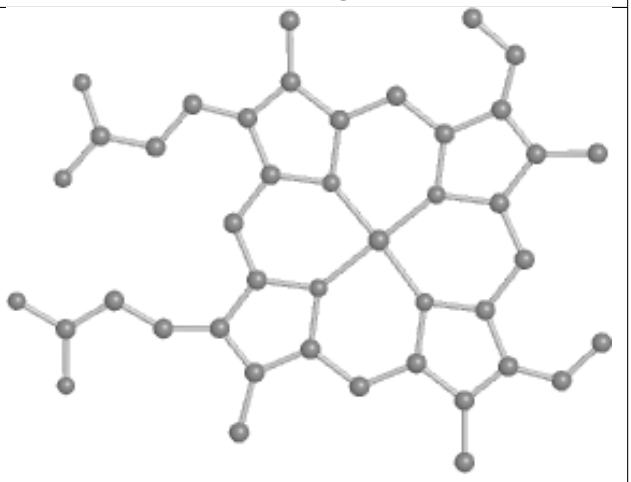
Bond lengths



Bond angles

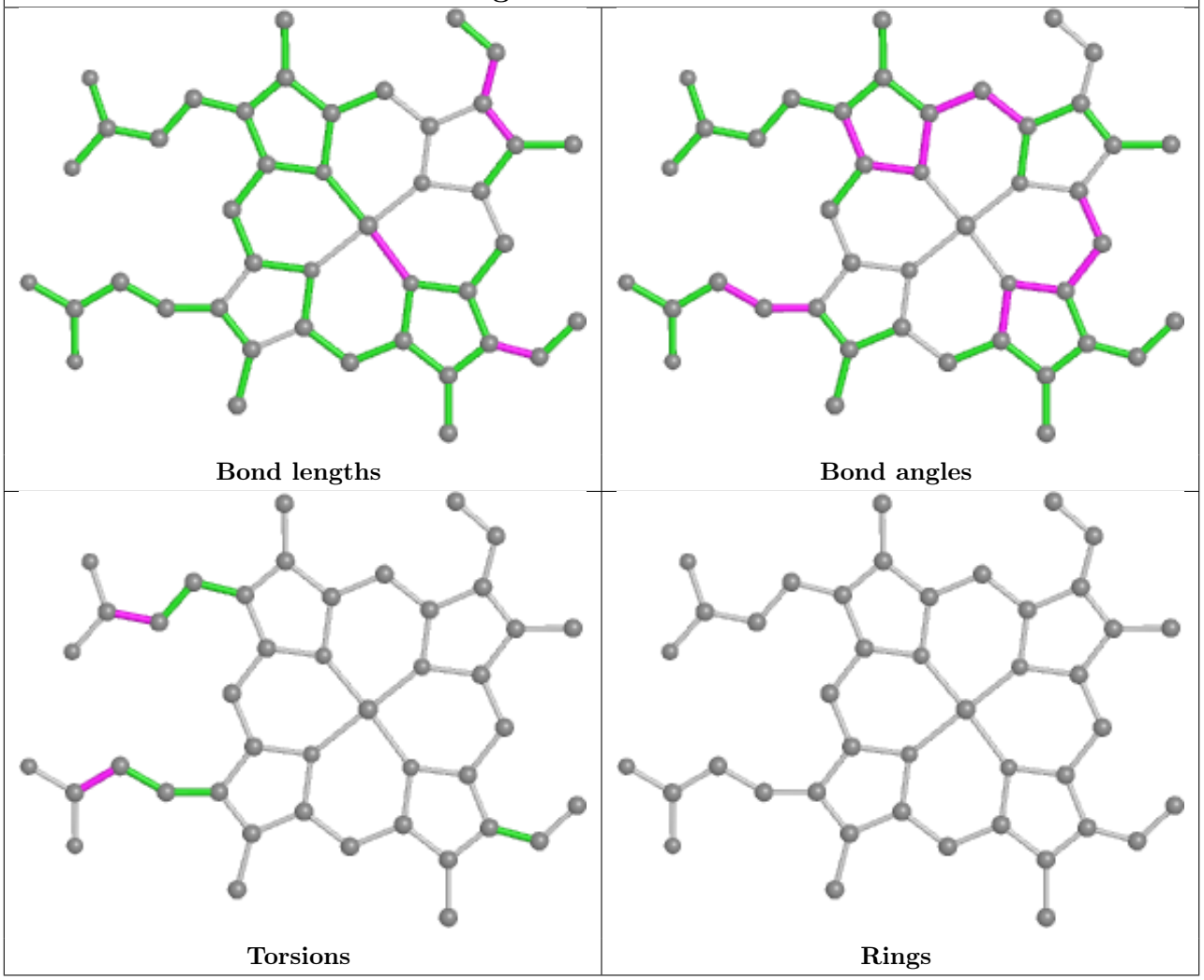


Torsions

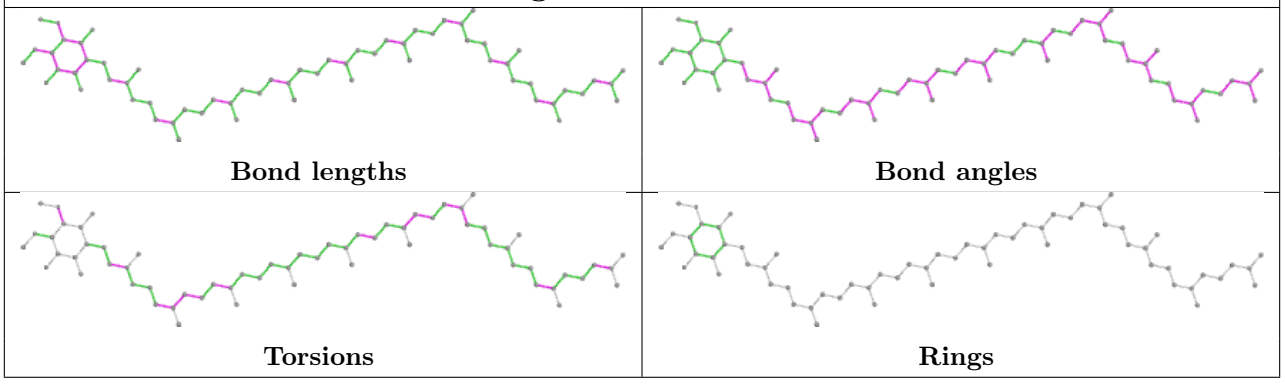


Rings

Ligand HEM I 502



Ligand U10 D 503



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.

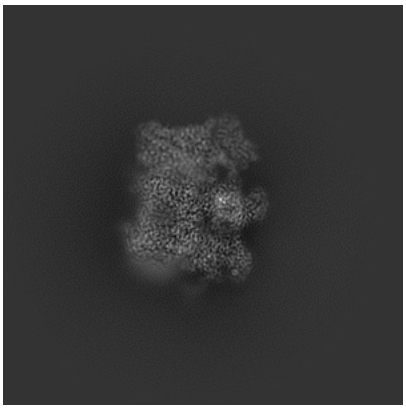
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40601. These allow visual inspection of the internal detail of the map and identification of artifacts.

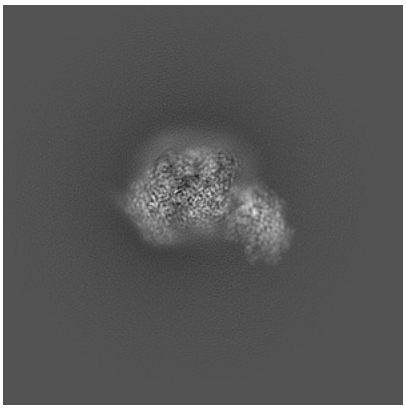
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

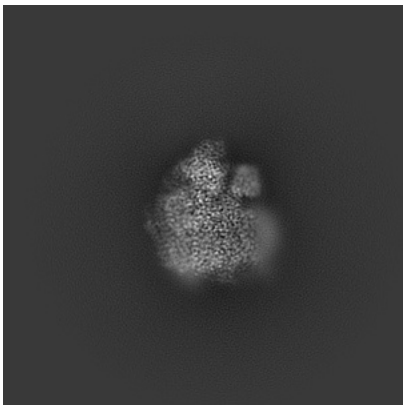
6.1.1 Primary map



X

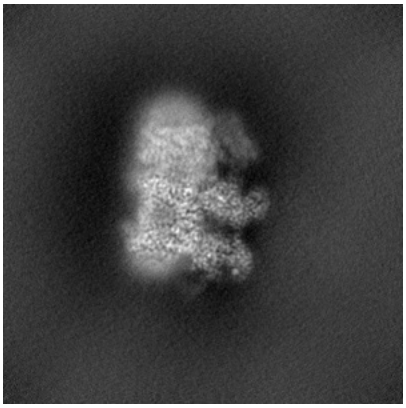


Y

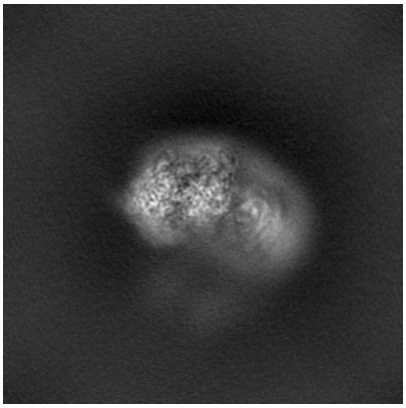


Z

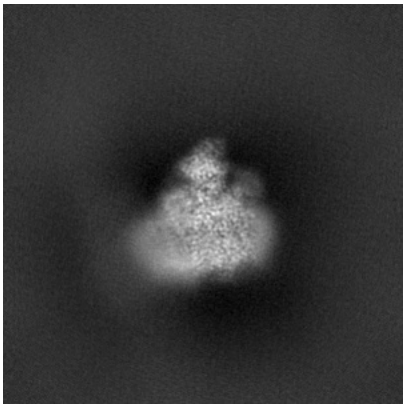
6.1.2 Raw map



X



Y

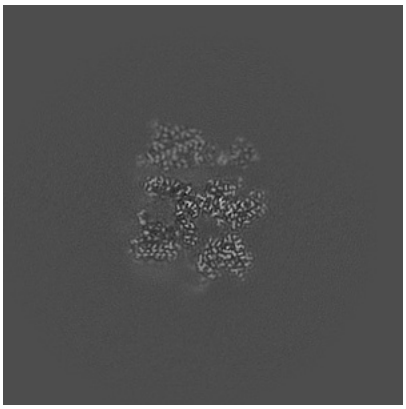


Z

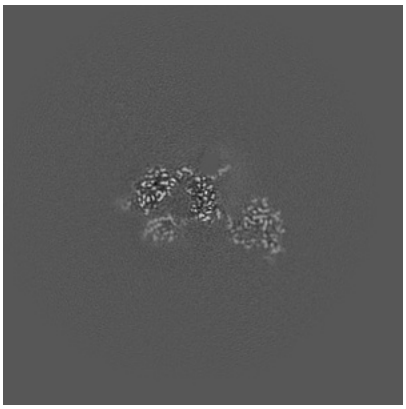
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

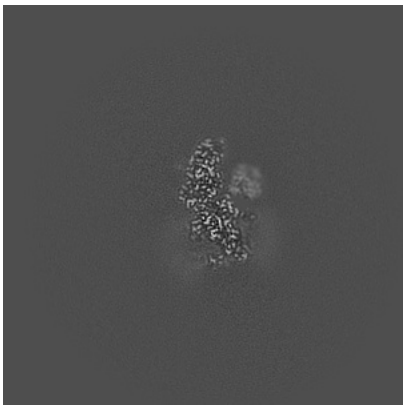
6.2.1 Primary map



X Index: 166

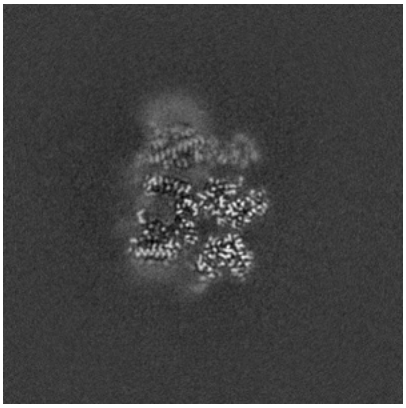


Y Index: 166

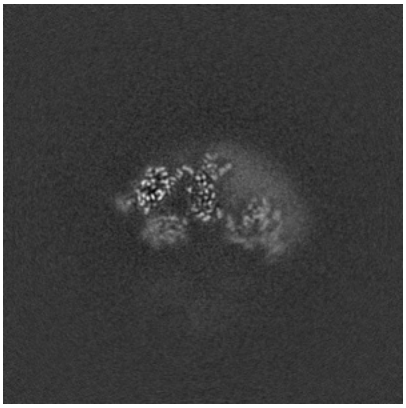


Z Index: 166

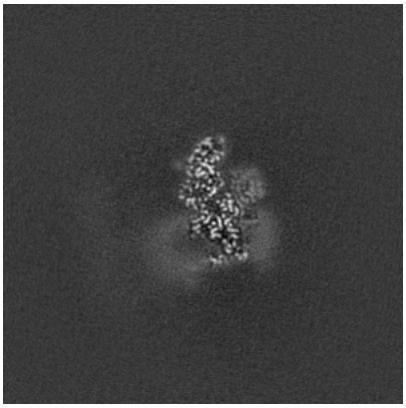
6.2.2 Raw map



X Index: 166



Y Index: 166

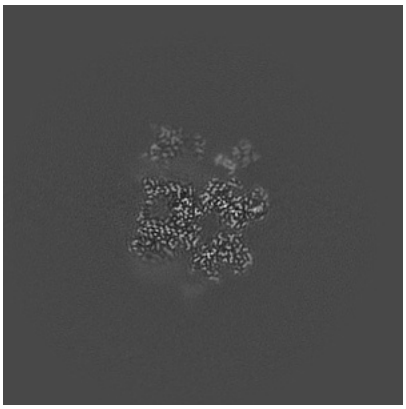


Z Index: 166

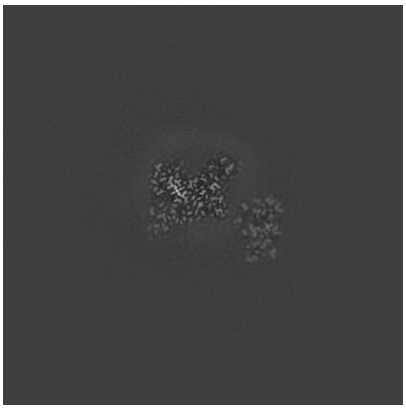
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

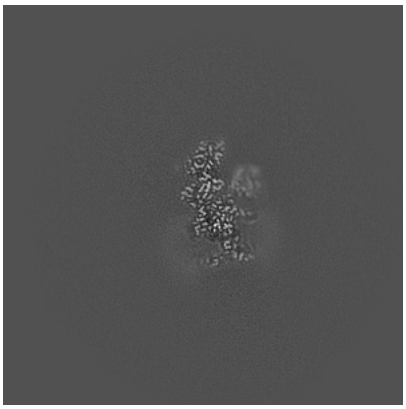
6.3.1 Primary map



X Index: 171

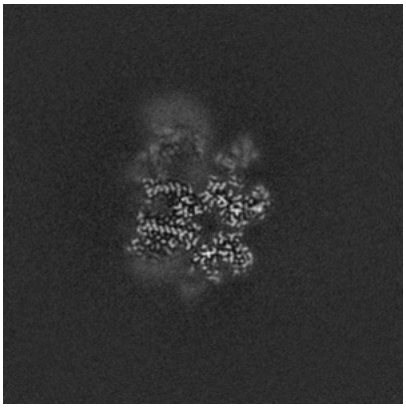


Y Index: 145

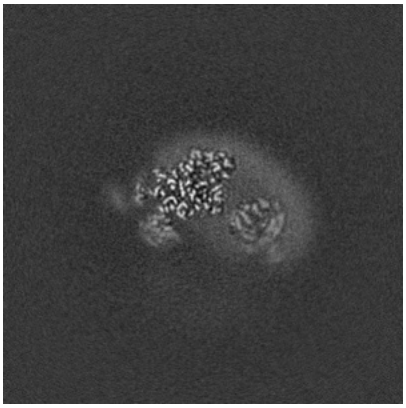


Z Index: 164

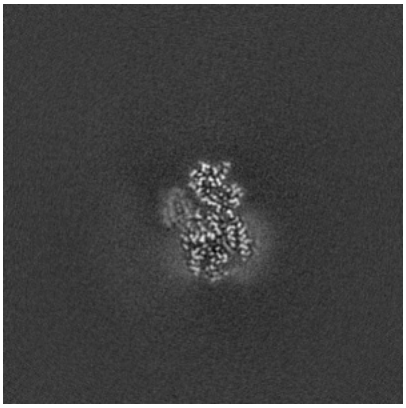
6.3.2 Raw map



X Index: 171



Y Index: 156

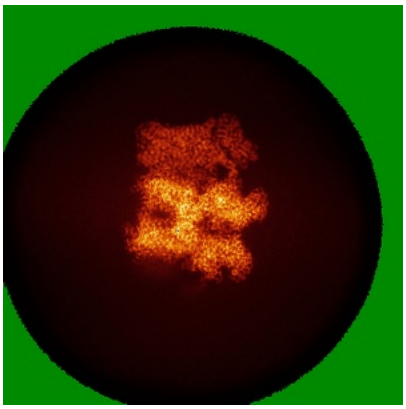


Z Index: 131

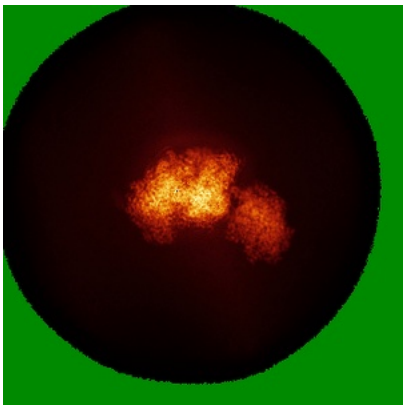
The images above show the largest variance slices of the map in three orthogonal directions.

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

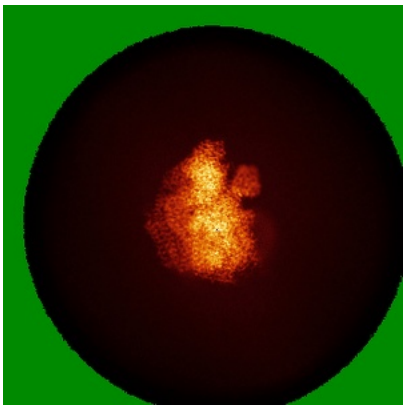
6.4.1 Primary map



X

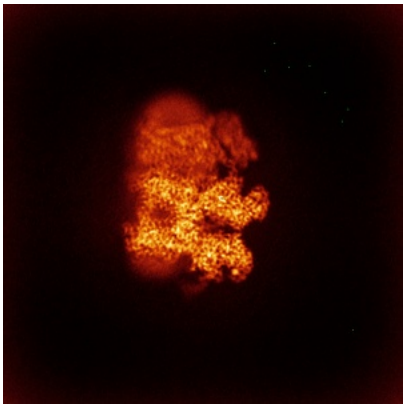


Y

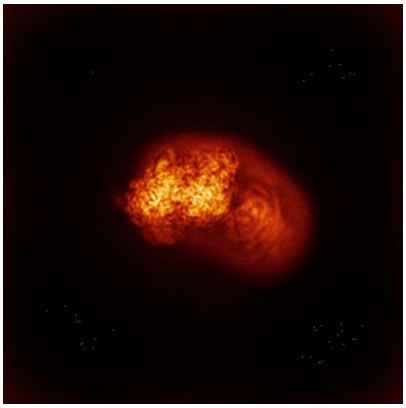


Z

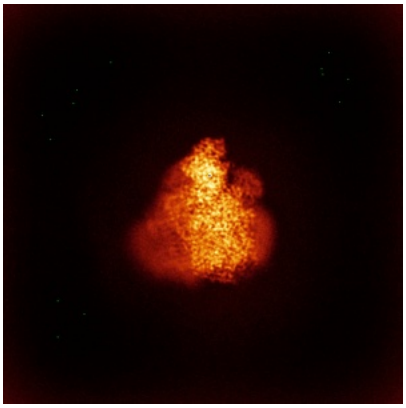
6.4.2 Raw map



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

6.5.2 Raw map

X Y Z

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

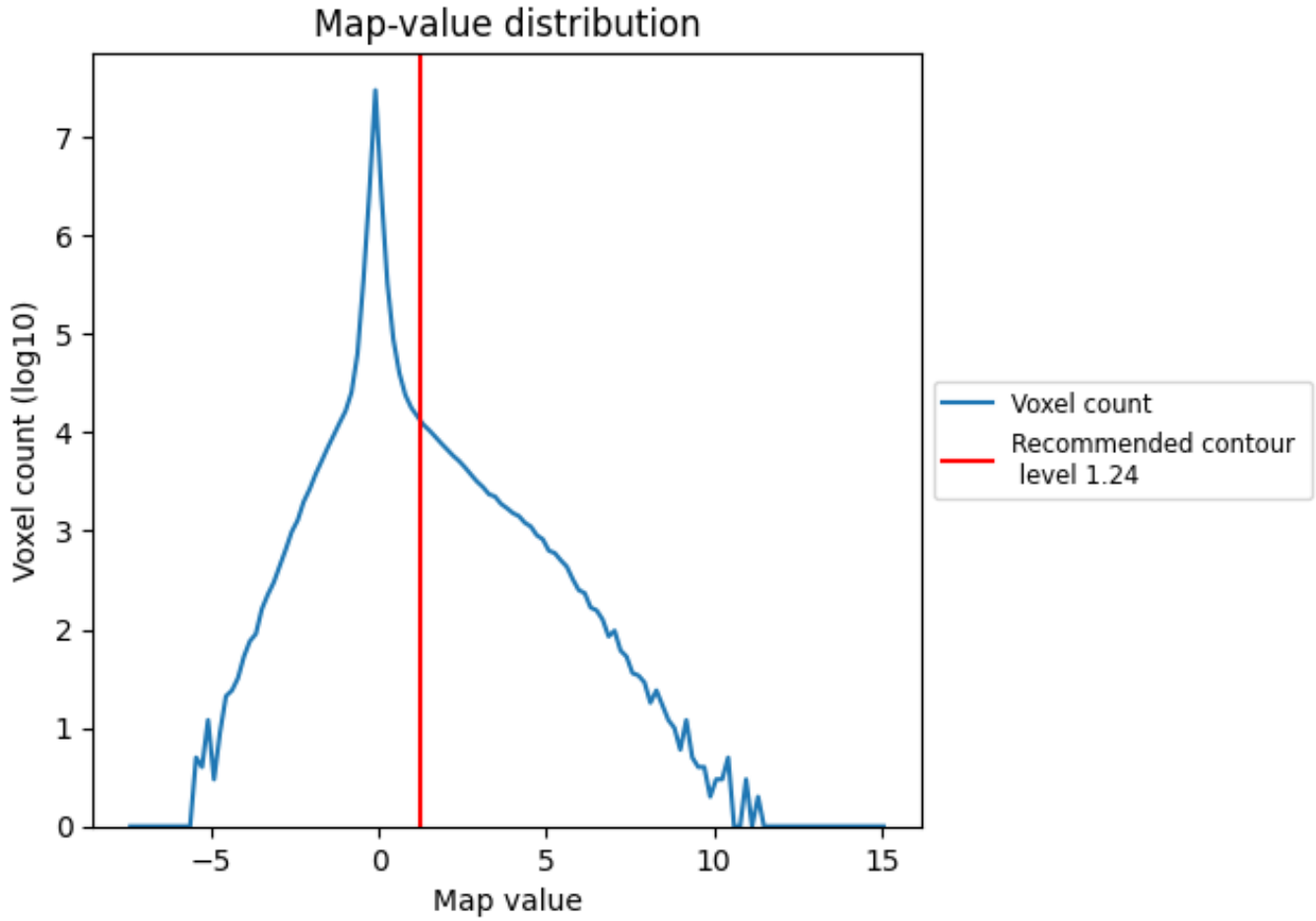
6.6 Mask visualisation (i)

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

7 Map analysis

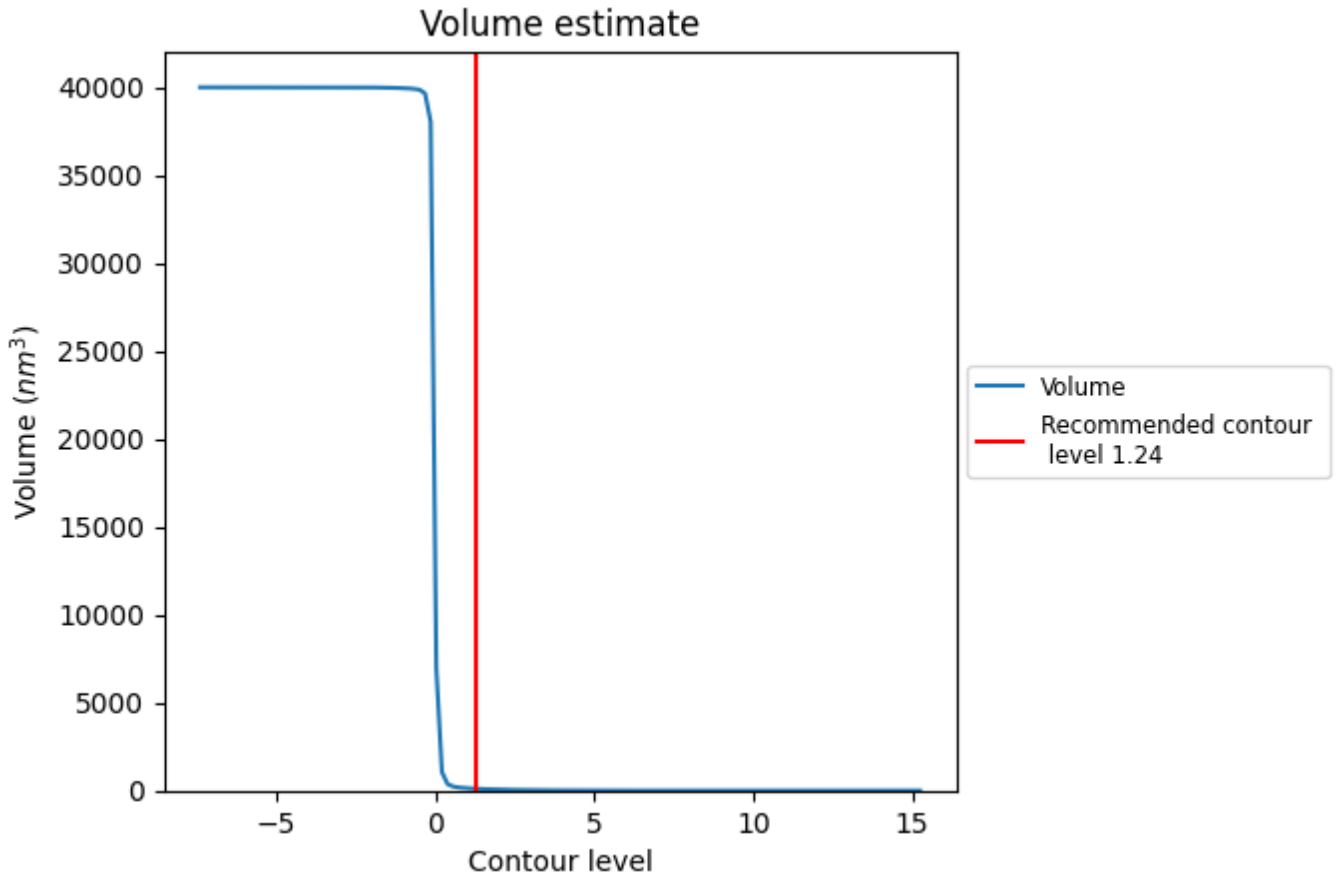
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

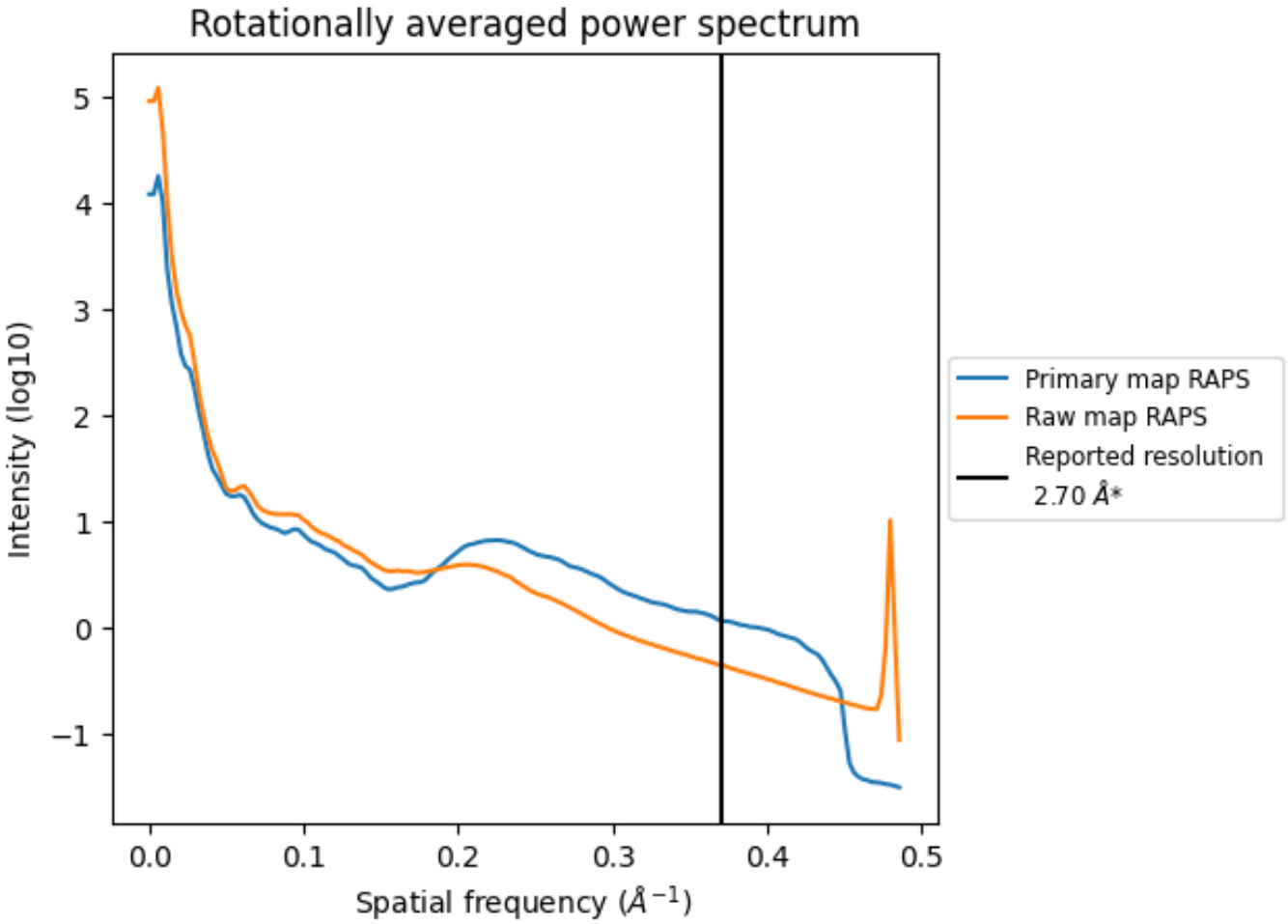
7.2 Volume estimate (i)



The volume at the recommended contour level is 106 nm^3; this corresponds to an approximate mass of 96 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)

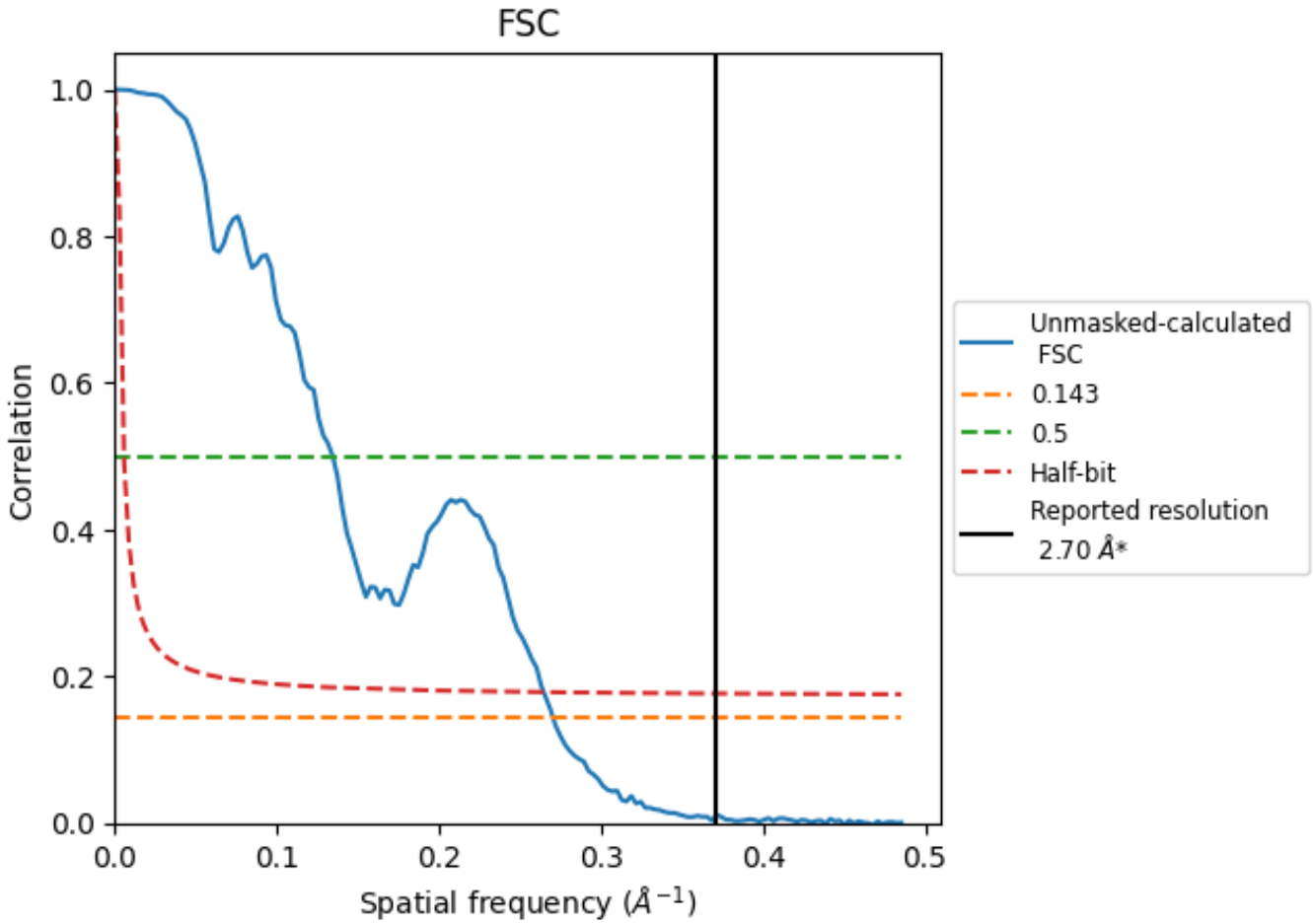


*Reported resolution corresponds to spatial frequency of 0.370 $Å^{-1}$

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 0.370 Å^{-1}

8.2 Resolution estimates (i)

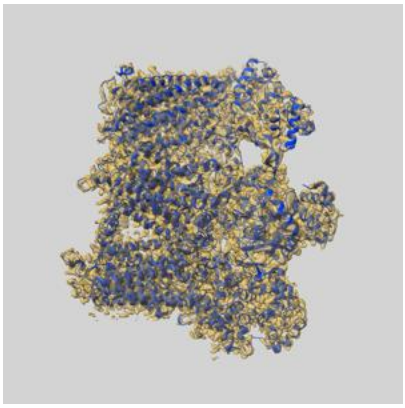
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.70	7.43	3.78

*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 3.70 differs from the reported value 2.7 by more than 10 %

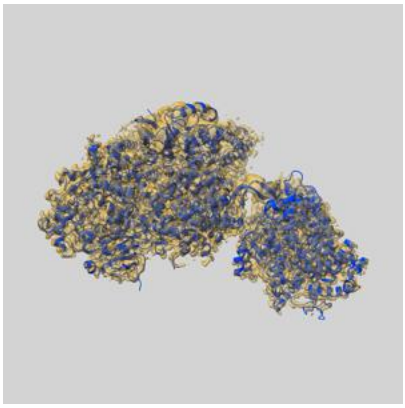
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40601 and PDB model 8SMR. Per-residue inclusion information can be found in section 3 on page 10.

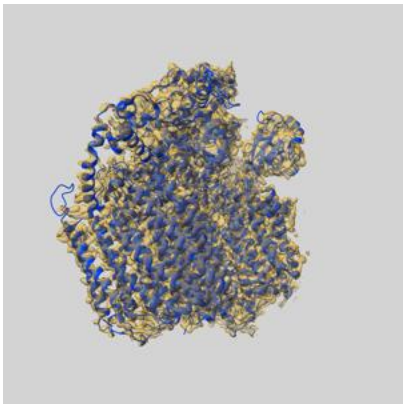
9.1 Map-model overlay



X



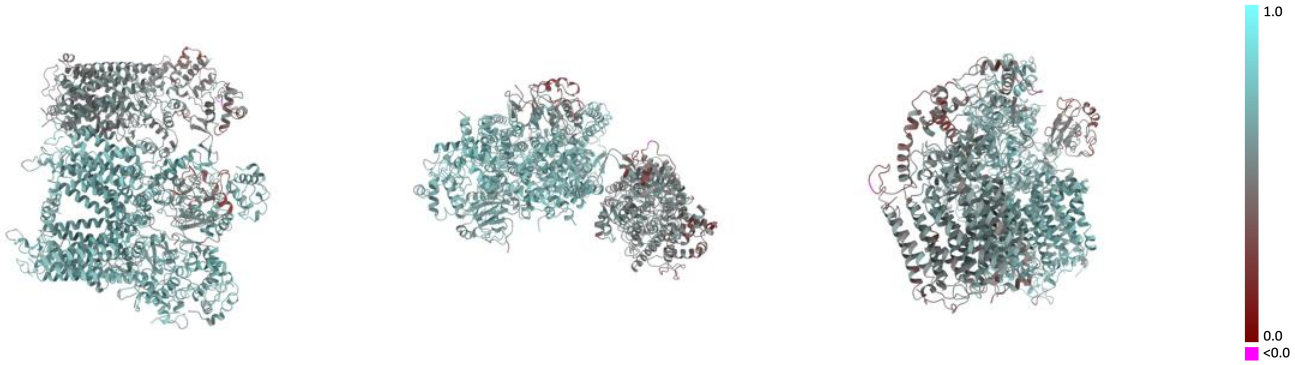
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.24 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.

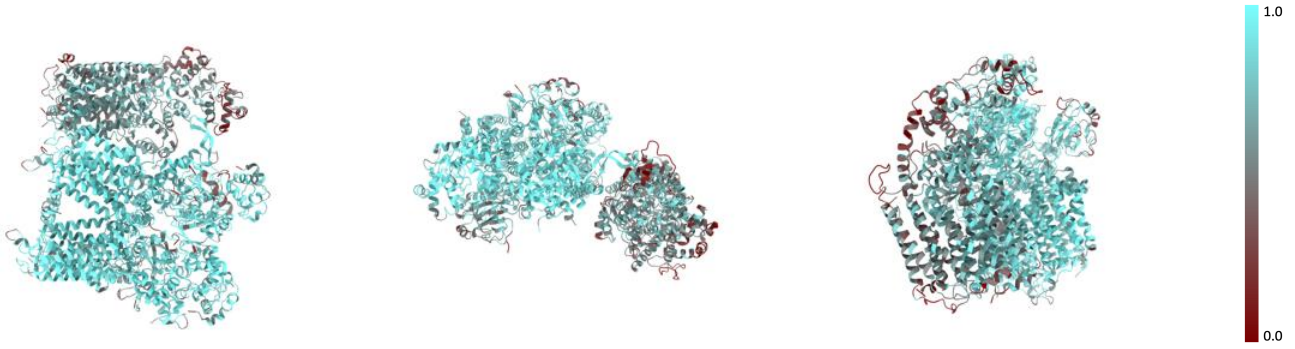
9.2 Q-score mapped to coordinate model (i)



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.

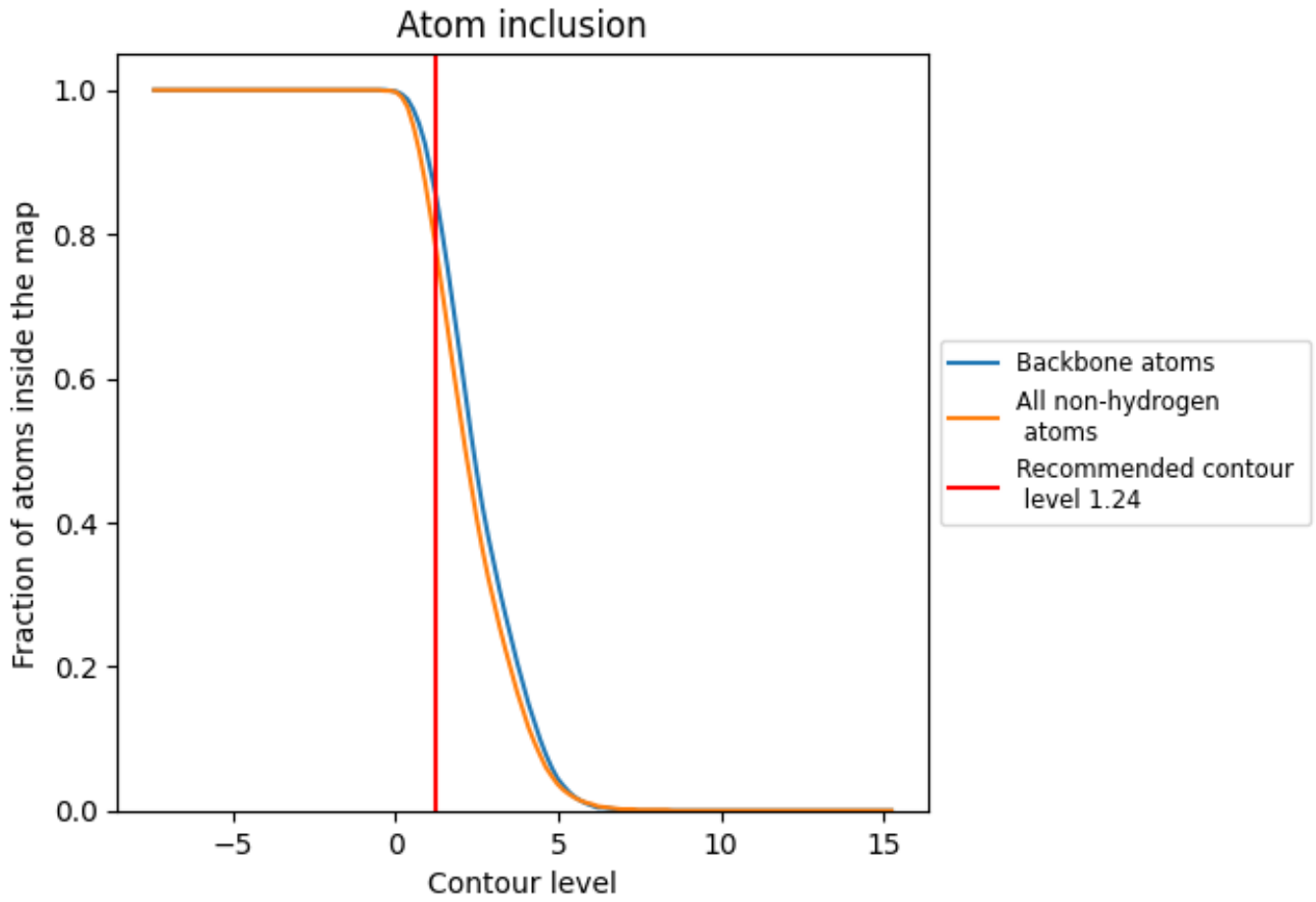
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.24).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 78% 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 (1.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7820	0.6080
C	0.7410	0.4740
D	0.9100	0.6810
E	0.6730	0.5390
F	0.6210	0.5400
G	0.4650	0.4590
I	0.9040	0.6820
J	0.9110	0.6550
K	0.9160	0.6770
L	0.7610	0.6560
M	0.9050	0.6810
N	0.8940	0.6730
O	0.7260	0.6500
Z	0.6820	0.6210