wwPDB EM Validation Summary Report

Nov 20, 2022 – 09:59 am GMT

PDB ID	:	6HWH
EMDB ID	:	EMD-0289
Title	:	Structure of a functional obligate respiratory supercomplex from Mycobacterium smegmatis
Authors	:	Wiseman, B.; Nitharwal, R.G.; Fedotovskaya, O.; Schafer, J.; Guo, H.; Kuang, Q.; Benlekbir, S.; Sjostrand, D.; Adelroth, P.; Rubinstein, J.L.; Brzezinski, P.; Hogbom, M.
Deposited on	:	2018-10-12
Resolution	:	3.30 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:

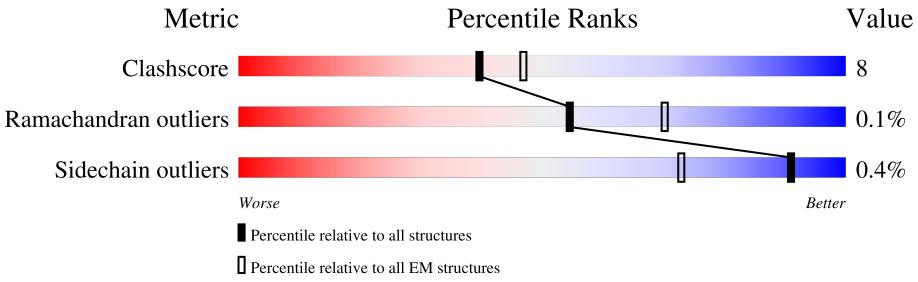
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.30 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	A	408	83% 10% 7%
1	B	408	79% 14% 7%
2	C	74	99%
2	G	74	100%
3	D	65	5% 100%
3	H	65	29% 100%
4	E	20	5% 100%
4	I	20	20% 100%

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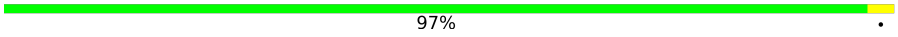
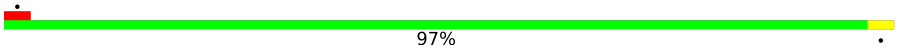
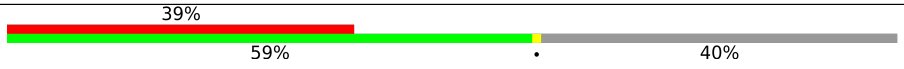
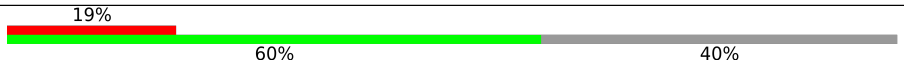
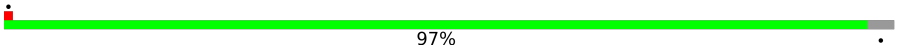
Mol	Chain	Length	Quality of chain
5	F	35	
5	J	35	
6	K	268	
6	M	268	
6	i	268	
6	j	268	
7	L	341	
7	P	341	
8	N	79	
8	R	79	
9	O	157	
9	T	157	
10	Q	583	
10	V	583	
11	S	139	
11	X	139	
12	W	203	
12	Z	203	
13	Y	554	
13	b	554	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	FES	B	501	-	-	X	-
19	HEC	V	804	-	-	X	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 40632 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	A	380	Total	C	N	O	S	0	0
			2960	1914	500	535	11		
1	B	380	Total	C	N	O	S	0	0
			2960	1914	500	535	11		

- Molecule 2 is a protein called Co-purified unknown transmembrane helices built as polyALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	74	Total	C	N	O	0	0
			370	222	74	74		
2	C	74	Total	C	N	O	0	0
			370	222	74	74		

- Molecule 3 is a protein called Co-purified unknown transmembrane helices built as polyALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	65	Total	C	N	O	0	0
			325	195	65	65		
3	D	65	Total	C	N	O	0	0
			325	195	65	65		

- Molecule 4 is a protein called Co-purified unknown peptide built as polyALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	20	Total	C	N	O	0	0
			100	60	20	20		
4	E	20	Total	C	N	O	0	0
			100	60	20	20		

- Molecule 5 is a protein called Co-purified unknown peptide built as polyALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	J	35	Total 175	C 105	N 35	O 35	0	0
5	F	35	Total 175	C 105	N 35	O 35	0	0

- Molecule 6 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	30	Total 211	C 139	N 35	O 33	S 4	0	0
6	K	30	Total 211	C 139	N 35	O 33	S 4	0	0
6	i	162	Total 648	C 324	N 162	O 162		0	0
6	j	162	Total 648	C 324	N 162	O 162		0	0

- Molecule 7 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	281	Total 2236	C 1450	N 368	O 409	S 9	0	0
7	L	281	Total 2236	C 1450	N 368	O 409	S 9	0	0

- Molecule 8 is a protein called MSMEG_4693.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	54	Total 415	C 276	N 67	O 70	S 2	0	0
8	N	54	Total 415	C 276	N 67	O 70	S 2	0	0

- Molecule 9 is a protein called Uncharacterized protein MSMEG_4692/MSMEI_4575.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	142	Total 1019	C 644	N 173	O 200	S 2	0	0
9	O	142	Total 1019	C 644	N 173	O 200	S 2	0	0

- Molecule 10 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	550	Total	C	N	O	S	0	0
			4354	2927	695	709	23		
10	Q	550	Total	C	N	O	S	0	0
			4354	2927	695	709	23		

- Molecule 11 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	X	139	Total	C	N	O	S	0	0
			1077	719	167	188	3		
11	S	139	Total	C	N	O	S	0	0
			1077	719	167	188	3		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	184	Total	C	N	O	S	0	0
			1441	967	229	238	7		
12	W	184	Total	C	N	O	S	0	0
			1441	967	229	238	7		

- Molecule 13 is a protein called Ubiquinol-cytochrome C reductase QcrB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	b	536	Total	C	N	O	S	0	0
			4190	2757	712	703	18		
13	Y	536	Total	C	N	O	S	0	0
			4190	2757	712	703	18		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	547	ASP	-	expression tag	UNP I7FGS8
b	548	TYR	-	expression tag	UNP I7FGS8
b	549	LYS	-	expression tag	UNP I7FGS8
b	550	ASP	-	expression tag	UNP I7FGS8
b	551	ASP	-	expression tag	UNP I7FGS8
b	552	ASP	-	expression tag	UNP I7FGS8
b	553	ASP	-	expression tag	UNP I7FGS8
b	554	LYS	-	expression tag	UNP I7FGS8
Y	547	ASP	-	expression tag	UNP I7FGS8
Y	548	TYR	-	expression tag	UNP I7FGS8
Y	549	LYS	-	expression tag	UNP I7FGS8

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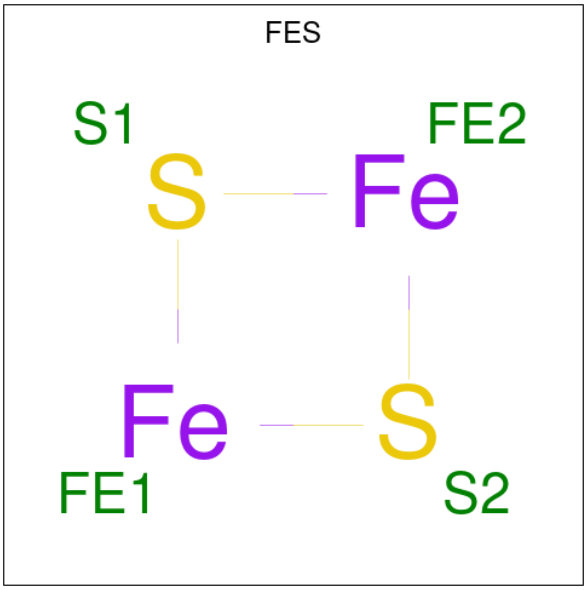
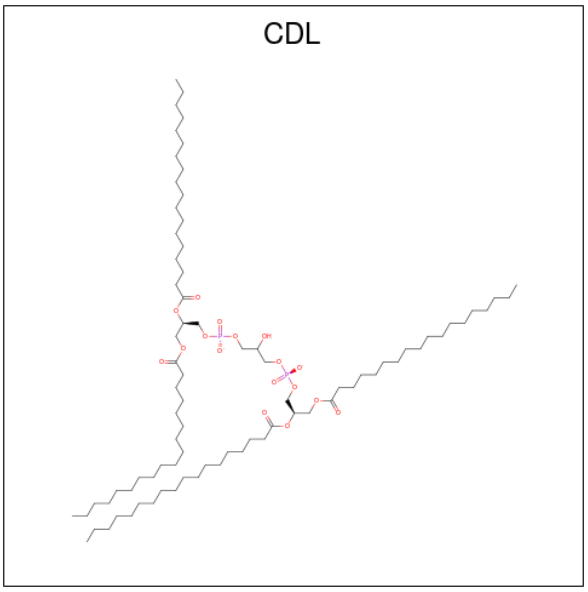
Chain	Residue	Modelled	Actual	Comment	Reference
Y	550	ASP	-	expression tag	UNP I7FGS8
Y	551	ASP	-	expression tag	UNP I7FGS8
Y	552	ASP	-	expression tag	UNP I7FGS8
Y	553	ASP	-	expression tag	UNP I7FGS8
Y	554	LYS	-	expression tag	UNP I7FGS8

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



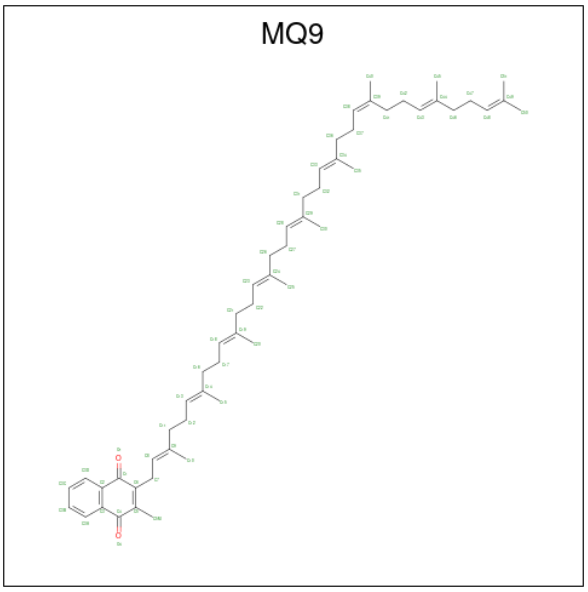
Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	Fe	S	0
			4	2	2	
14	B	1	Total	Fe	S	0
			4	2	2	

- Molecule 15 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
15	M	1	Total	C	O	P	0
			100	81	17	2	
15	V	1	Total	C	O	P	0
			87	68	17	2	
15	b	1	Total	C	O	P	0
			183	145	34	4	
15	b	1	Total	C	O	P	0
			183	145	34	4	
15	K	1	Total	C	O	P	0
			100	81	17	2	
15	Q	1	Total	C	O	P	0
			87	68	17	2	
15	Y	1	Total	C	O	P	0
			183	145	34	4	
15	Y	1	Total	C	O	P	0
			183	145	34	4	

- Molecule 16 is MENAQUINONE-9 (three-letter code: MQ9) (formula: $C_{56}H_{80}O_2$).

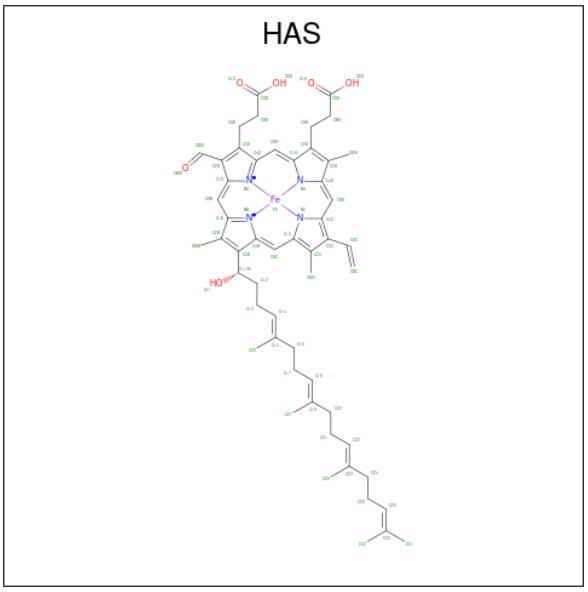


Mol	Chain	Residues	Atoms	AltConf
16	M	1	Total C O 58 56 2	0
16	b	1	Total C O 58 56 2	0
16	Y	1	Total C O 116 112 4	0
16	Y	1	Total C O 116 112 4	0

- Molecule 17 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

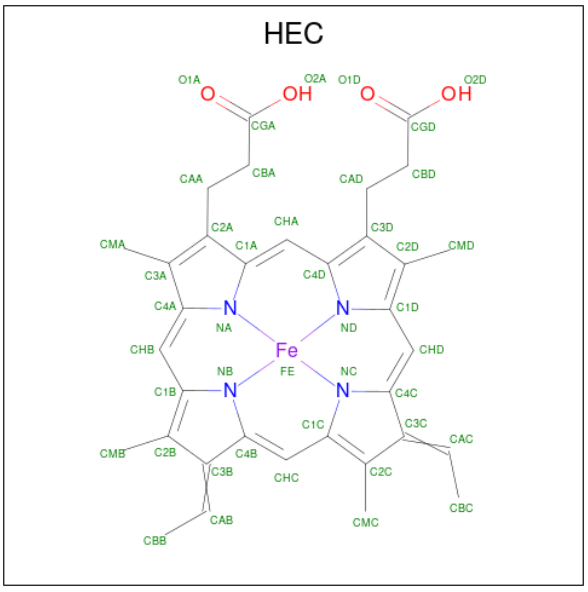
Mol	Chain	Residues	Atoms	AltConf
17	P	2	Total Cu 2 2	0
17	V	1	Total Cu 1 1	0
17	L	2	Total Cu 2 2	0
17	Q	1	Total Cu 1 1	0

- Molecule 18 is HEME-AS (three-letter code: HAS) (formula: $C_{54}H_{64}FeN_4O_6$).



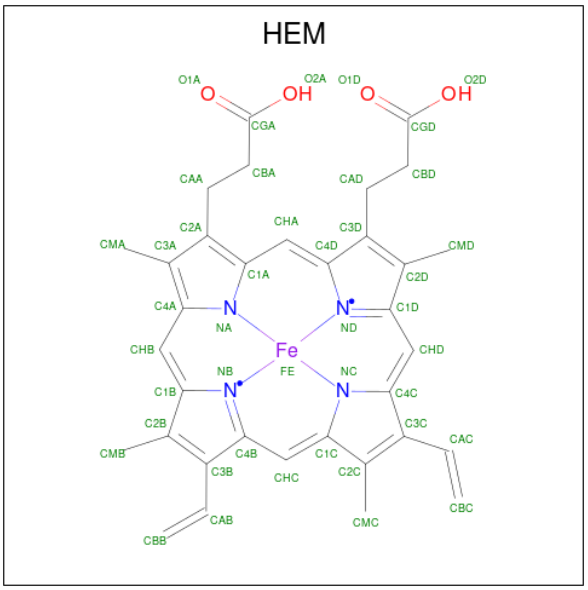
Mol	Chain	Residues	Atoms					AltConf
18	V	1	Total	C	Fe	N	O	0
			130	108	2	8	12	
18	V	1	Total	C	Fe	N	O	0
			130	108	2	8	12	
18	Q	1	Total	C	Fe	N	O	0
			130	108	2	8	12	
18	Q	1	Total	C	Fe	N	O	0
			130	108	2	8	12	

- Molecule 19 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
19	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
19	i	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
19	j	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
19	j	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

- Molecule 20 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



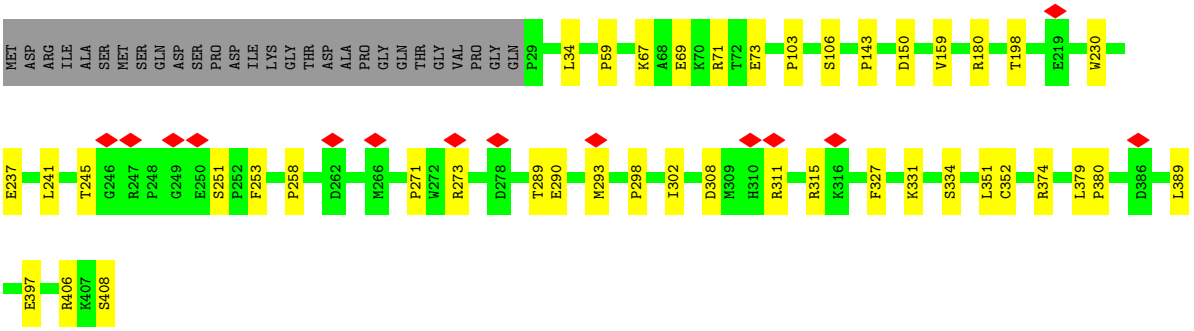
Mol	Chain	Residues	Atoms					AltConf
20	b	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
20	b	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
20	Y	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
20	Y	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

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.

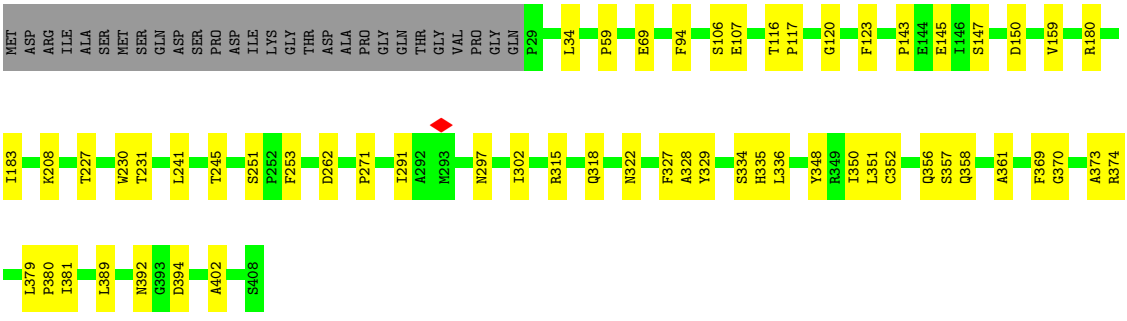
• Molecule 1: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain A:



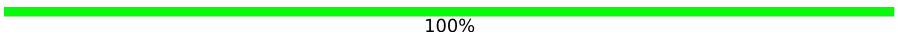
• Molecule 1: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain B:



• Molecule 2: Co-purified unknown transmembrane helices built as polyALA

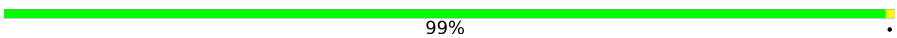
Chain G:



There are no outlier residues recorded for this chain.

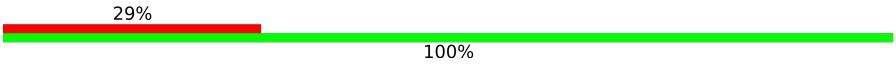
• Molecule 2: Co-purified unknown transmembrane helices built as polyALA

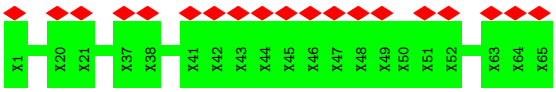
Chain C:



• Molecule 3: Co-purified unknown transmembrane helices built as polyALA

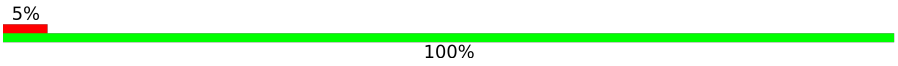
Chain H:





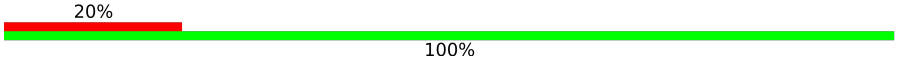
• Molecule 3: Co-purified unknown transmembrane helices built as polyALA

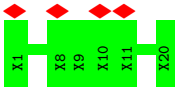
Chain D:



• Molecule 4: Co-purified unknown peptide built as polyALA

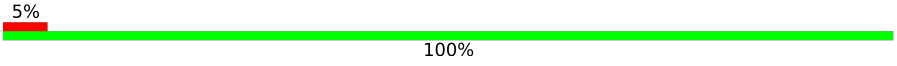
Chain I:





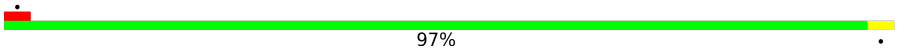
• Molecule 4: Co-purified unknown peptide built as polyALA

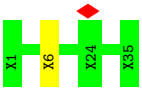
Chain E:



• Molecule 5: Co-purified unknown peptide built as polyALA

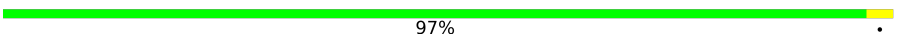
Chain J:





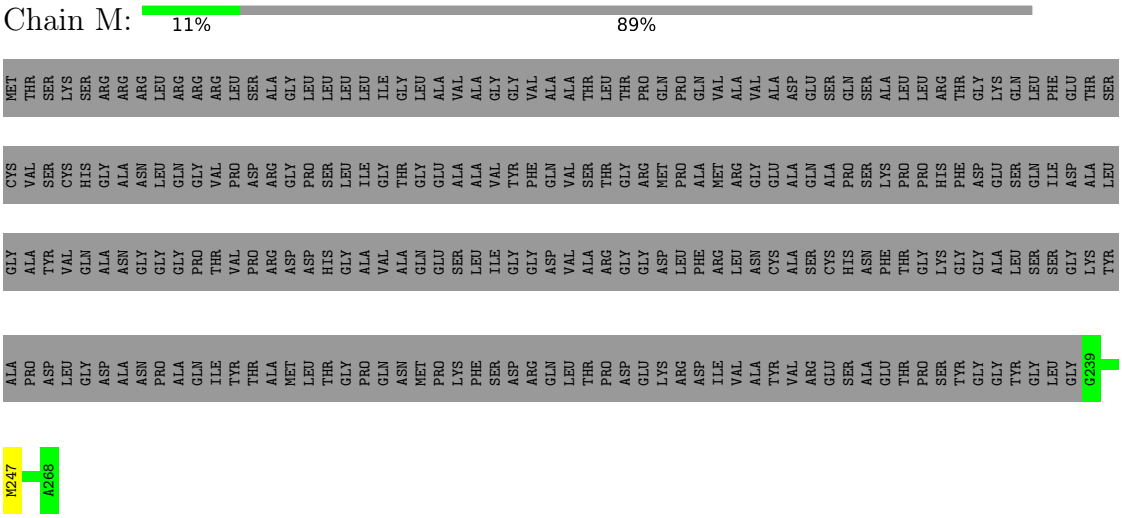
• Molecule 5: Co-purified unknown peptide built as polyALA

Chain F:



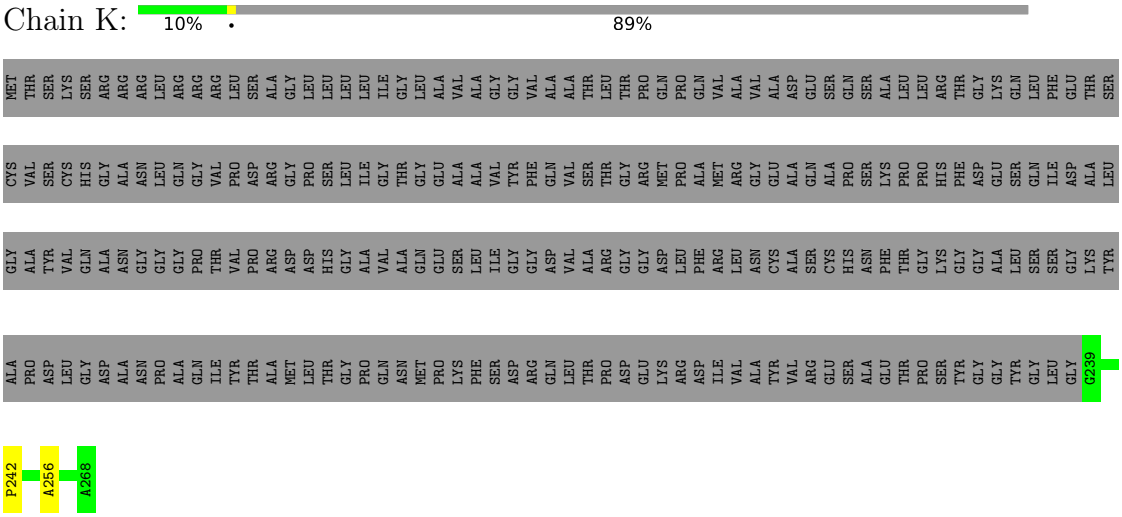
• Molecule 6: Cytochrome bc1 complex cytochrome c subunit

Chain M:



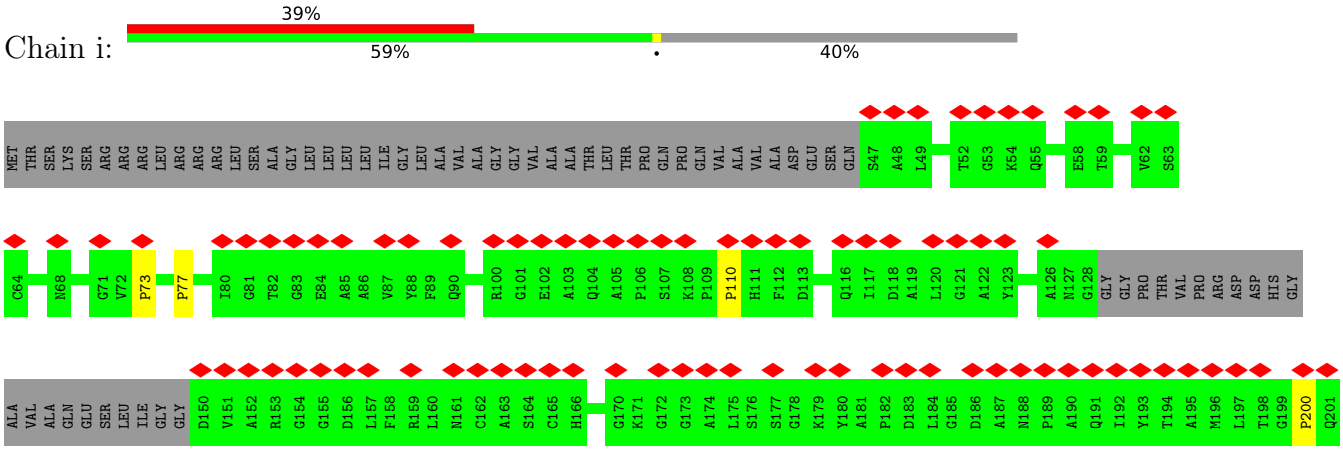
• Molecule 6: Cytochrome bc1 complex cytochrome c subunit

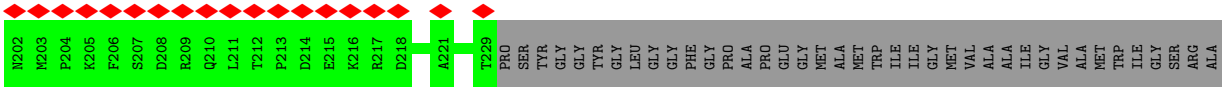
Chain K:



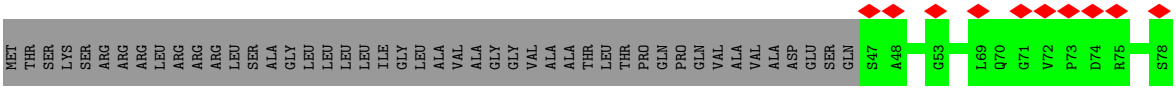
• Molecule 6: Cytochrome bc1 complex cytochrome c subunit

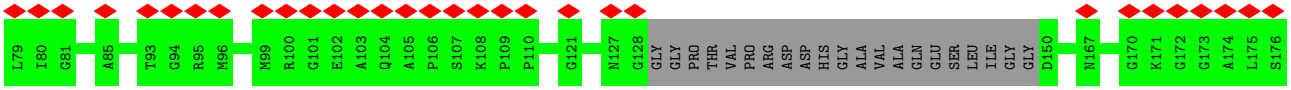
Chain i:

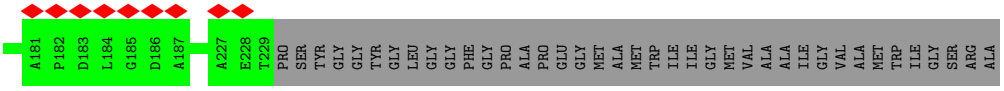




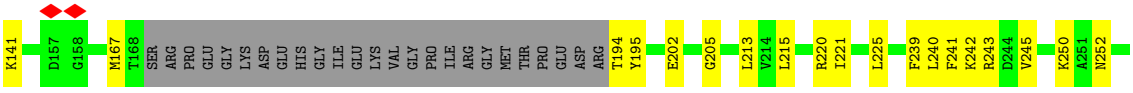
• Molecule 6: Cytochrome bc1 complex cytochrome c subunit

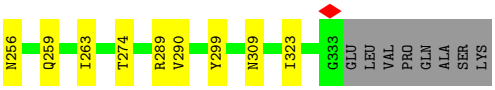




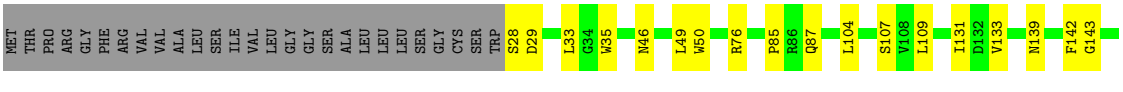


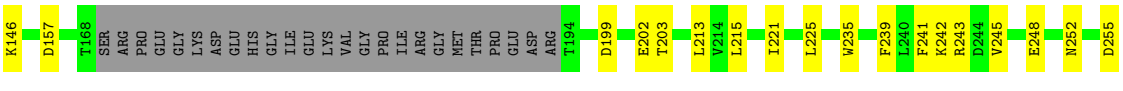
• Molecule 7: Cytochrome c oxidase subunit 2

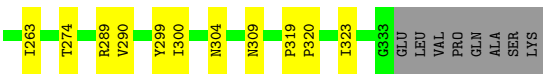




• Molecule 7: Cytochrome c oxidase subunit 2



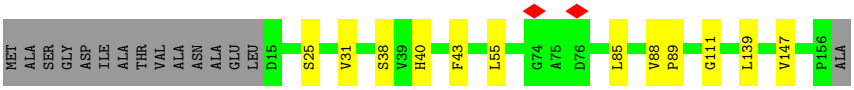




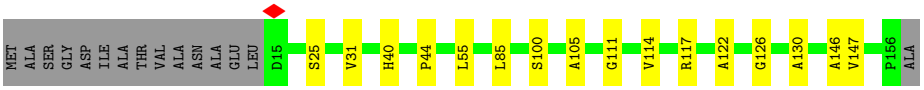
• Molecule 8: MSMEG_4693

• Molecule 8: MSMEG_4693

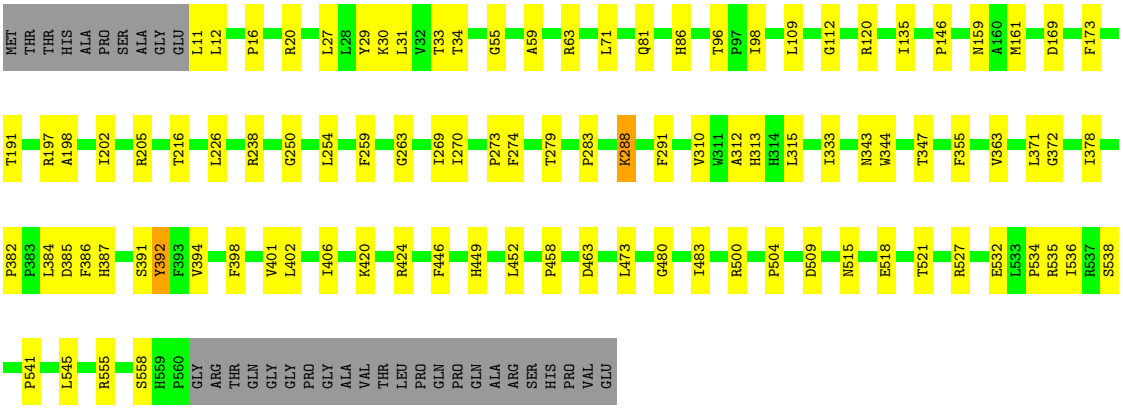
• Molecule 9: Uncharacterized protein MSMEG_4692/MSMEI_4575



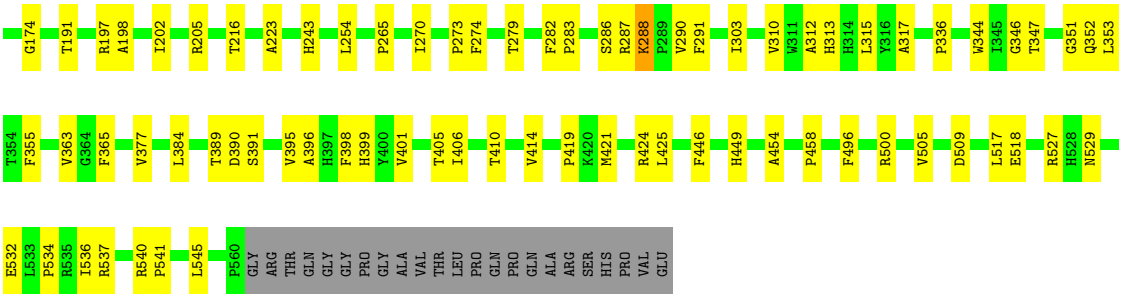
• Molecule 9: Uncharacterized protein MSMEG_4692/MSMEI_4575



• Molecule 10: Cytochrome c oxidase subunit 1



• Molecule 10: Cytochrome c oxidase subunit 1

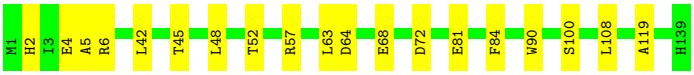


• Molecule 11: Cytochrome c oxidase polypeptide 4

Chain X:

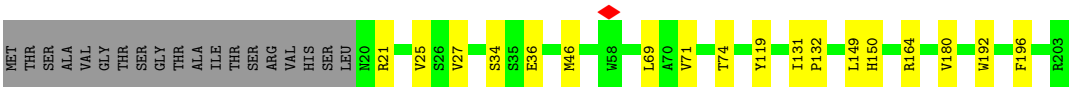
• Molecule 11: Cytochrome c oxidase polypeptide 4

Chain S:



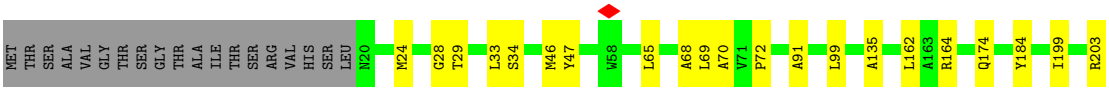
• Molecule 12: Cytochrome c oxidase subunit 3

Chain Z:



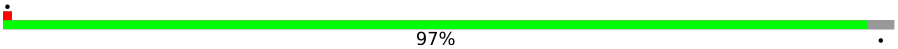
• Molecule 12: Cytochrome c oxidase subunit 3

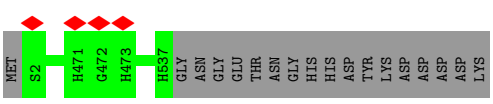
Chain W:



• Molecule 13: Ubiquinol-cytochrome C reductase QcrB

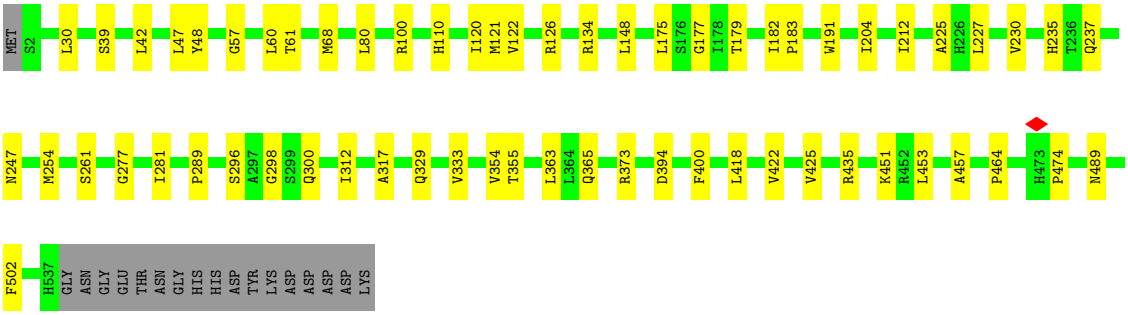
Chain b:





• Molecule 13: Ubiquinol-cytochrome C reductase QcrB

Chain Y:


MET S2 L30 S39 L42 L47 Y48 G57 L60 T61 M68 L80 R100 H110 I120 M121 V122 R126 R134 L148 L175 S176 G177 I178 T179 I182 P183 W191 I204 I212 A225 H226 L227 V230 H235 T236 Q237
N247 M254 S261 G277 I281 P289 S296 A297 G298 S299 Q300 I312 A317 Q329 V333 V354 T355 L363 L364 Q365 R373 D394 F400 L418 V422 V425 R435 K451 R452 L453 A457 P464 H473 P474 N489
F502 H537 GLY ASN GLY GLU THR ASN GLY HIS HIS ASP TYR LYS ASP ASP ASP ASP LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	104198	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 ($e^-/Å^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	5.884	Depositor
Minimum map value	-3.920	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.130	Depositor
Recommended contour level	0.475	Depositor
Map size (Å)	402.8, 402.8, 402.8	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, HEM, MQ9, CU, HAS, FES, CDL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.35	0/3039	0.59	0/4120
1	B	0.40	0/3039	0.61	0/4120
6	K	0.42	0/217	0.56	0/293
6	M	0.41	0/217	0.52	0/293
6	i	0.73	0/646	0.91	0/804
6	j	0.66	0/646	0.97	0/804
7	L	0.44	0/2297	0.63	0/3126
7	P	0.38	0/2297	0.59	0/3126
8	N	0.32	0/430	0.65	0/591
8	R	0.29	0/430	0.63	0/591
9	O	0.38	0/1037	0.57	0/1416
9	T	0.35	0/1037	0.57	0/1416
10	Q	0.51	0/4515	0.68	0/6176
10	V	0.48	0/4515	0.67	0/6176
11	S	0.46	0/1112	0.62	0/1524
11	X	0.42	0/1112	0.59	0/1524
12	W	0.45	0/1488	0.58	0/2032
12	Z	0.40	0/1488	0.56	0/2032
13	Y	0.46	0/4324	0.62	0/5897
13	b	0.41	0/4324	0.61	0/5897
All	All	0.44	0/38210	0.63	0/51958

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	A	2960	0	2963	27	0
1	B	2960	0	2965	45	0
2	C	370	0	80	1	0
2	G	370	0	80	0	0
3	D	325	0	67	0	0
3	H	325	0	67	0	0
4	E	100	0	23	0	0
4	I	100	0	23	0	0
5	F	175	0	38	1	0
5	J	175	0	41	1	0
6	K	211	0	212	2	0
6	M	211	0	212	1	0
6	i	648	0	182	0	0
6	j	648	0	185	0	0
7	L	2236	0	2189	29	0
7	P	2236	0	2189	28	0
8	N	415	0	424	4	0
8	R	415	0	424	3	0
9	O	1019	0	1030	11	0
9	T	1019	0	1030	10	0
10	Q	4354	0	4342	69	0
10	V	4354	0	4341	84	0
11	S	1077	0	1058	20	0
11	X	1077	0	1058	12	0
12	W	1441	0	1439	18	0
12	Z	1441	0	1439	12	0
13	Y	4190	0	4211	45	0
13	b	4190	0	4211	0	0
14	A	4	0	0	0	0
14	B	4	0	0	2	0
15	K	100	0	154	6	0
15	M	100	0	154	4	0
15	Q	87	0	118	3	0
15	V	87	0	118	2	0
15	Y	183	0	266	9	0
15	b	183	0	266	0	0
16	M	58	0	80	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	Y	116	0	160	10	0
16	b	58	0	80	0	0
17	L	2	0	0	0	0
17	P	2	0	0	0	0
17	Q	1	0	0	0	0
17	V	1	0	0	0	0
18	Q	130	0	124	6	0
18	V	130	0	124	7	0
19	V	43	0	32	22	0
19	i	43	0	32	0	0
19	j	86	0	63	0	0
20	Y	86	0	60	6	0
20	b	86	0	60	0	0
All	All	40632	0	38414	391	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 8.

The worst 5 of 391 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)
10:V:161:MET:CG	19:V:804:HEC:HBC2	1.36	1.53
10:V:161:MET:CB	19:V:804:HEC:HBC2	1.58	1.31
10:V:161:MET:CG	19:V:804:HEC:CBC	2.15	1.23
10:V:161:MET:HG2	19:V:804:HEC:CBC	1.73	1.19
10:V:161:MET:O	19:V:804:HEC:HBC1	1.46	1.16

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	378/408 (93%)	335 (89%)	43 (11%)	0	100	100
1	B	378/408 (93%)	335 (89%)	43 (11%)	0	100	100
6	K	28/268 (10%)	27 (96%)	1 (4%)	0	100	100
6	M	28/268 (10%)	26 (93%)	2 (7%)	0	100	100
6	i	158/268 (59%)	143 (90%)	11 (7%)	4 (2%)	5	27
6	j	158/268 (59%)	145 (92%)	13 (8%)	0	100	100
7	L	277/341 (81%)	234 (84%)	43 (16%)	0	100	100
7	P	277/341 (81%)	236 (85%)	41 (15%)	0	100	100
8	N	52/79 (66%)	41 (79%)	11 (21%)	0	100	100
8	R	52/79 (66%)	44 (85%)	8 (15%)	0	100	100
9	O	140/157 (89%)	130 (93%)	10 (7%)	0	100	100
9	T	140/157 (89%)	129 (92%)	11 (8%)	0	100	100
10	Q	548/583 (94%)	504 (92%)	44 (8%)	0	100	100
10	V	548/583 (94%)	504 (92%)	44 (8%)	0	100	100
11	S	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
11	X	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
12	W	182/203 (90%)	166 (91%)	16 (9%)	0	100	100
12	Z	182/203 (90%)	169 (93%)	13 (7%)	0	100	100
13	Y	534/554 (96%)	489 (92%)	45 (8%)	0	100	100
13	b	534/554 (96%)	486 (91%)	48 (9%)	0	100	100
All	All	4868/6000 (81%)	4405 (90%)	459 (9%)	4 (0%)	54	81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	i	73	PRO
6	i	77	PRO
6	i	110	PRO
6	i	200	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	310/333 (93%)	310 (100%)	0	100 100
1	B	310/333 (93%)	310 (100%)	0	100 100
6	K	18/197 (9%)	18 (100%)	0	100 100
6	M	18/197 (9%)	18 (100%)	0	100 100
7	L	239/288 (83%)	237 (99%)	2 (1%)	81 89
7	P	239/288 (83%)	236 (99%)	3 (1%)	69 82
8	N	44/59 (75%)	44 (100%)	0	100 100
8	R	44/59 (75%)	44 (100%)	0	100 100
9	O	105/114 (92%)	105 (100%)	0	100 100
9	T	105/114 (92%)	105 (100%)	0	100 100
10	Q	456/481 (95%)	452 (99%)	4 (1%)	78 87
10	V	456/481 (95%)	451 (99%)	5 (1%)	73 85
11	S	106/106 (100%)	106 (100%)	0	100 100
11	X	106/106 (100%)	106 (100%)	0	100 100
12	W	146/161 (91%)	146 (100%)	0	100 100
12	Z	146/161 (91%)	146 (100%)	0	100 100
13	Y	431/446 (97%)	430 (100%)	1 (0%)	93 97
13	b	431/446 (97%)	431 (100%)	0	100 100
All	All	3710/4370 (85%)	3695 (100%)	15 (0%)	91 95

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	V	527	ARG
10	Q	527	ARG
7	L	76	ARG
13	Y	60	LEU
10	Q	353	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
13	b	365	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 6 are monoatomic - leaving 26 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	FES	A	501	1	0,4,4	-	-	-		
15	CDL	Y	604	-	91,91,99	1.18	7 (7%)	97,103,111	1.04	5 (5%)
16	MQ9	Y	606	-	59,59,59	1.24	7 (11%)	72,75,75	1.47	11 (15%)
14	FES	B	501	1	0,4,4	-	-	-		
15	CDL	b	603	-	91,91,99	1.18	6 (6%)	97,103,111	1.08	4 (4%)
18	HAS	Q	802	10	57,72,72	1.32	8 (14%)	48,109,109	1.52	8 (16%)
18	HAS	Q	801	10	57,72,72	1.34	8 (14%)	48,109,109	1.58	11 (22%)
15	CDL	b	604	-	90,90,99	1.21	8 (8%)	96,102,111	0.97	4 (4%)
15	CDL	K	301	-	99,99,99	1.19	8 (8%)	105,111,111	0.97	4 (3%)
19	HEC	j	302	-	32,50,50	2.24	12 (37%)	24,82,82	1.92	3 (12%)
16	MQ9	M	302	-	59,59,59	1.02	4 (6%)	72,75,75	1.40	11 (15%)
19	HEC	j	301	6	32,50,50	2.26	12 (37%)	24,82,82	1.92	3 (12%)
20	HEM	Y	601	13	41,50,50	1.38	6 (14%)	45,82,82	1.97	12 (26%)
20	HEM	b	601	13	41,50,50	1.44	7 (17%)	45,82,82	2.49	17 (37%)
15	CDL	V	805	-	86,86,99	1.23	9 (10%)	92,98,111	1.01	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	MQ9	b	605	-	59,59,59	0.93	1 (1%)	72,75,75	1.52	15 (20%)
19	HEC	i	301	-	32,50,50	2.25	12 (37%)	24,82,82	1.93	3 (12%)
16	MQ9	Y	605	-	59,59,59	0.88	1 (1%)	72,75,75	1.50	12 (16%)
18	HAS	V	801	10	57,72,72	1.34	7 (12%)	48,109,109	1.66	14 (29%)
15	CDL	M	301	-	99,99,99	1.19	8 (8%)	105,111,111	0.97	4 (3%)
15	CDL	Y	603	-	90,90,99	1.19	8 (8%)	96,102,111	1.03	5 (5%)
20	HEM	Y	602	13	41,50,50	1.47	7 (17%)	45,82,82	2.05	12 (26%)
20	HEM	b	602	13	41,50,50	1.45	7 (17%)	45,82,82	2.48	15 (33%)
18	HAS	V	802	10	57,72,72	1.36	7 (12%)	48,109,109	1.51	9 (18%)
15	CDL	Q	804	-	86,86,99	1.23	8 (9%)	92,98,111	1.06	4 (4%)
19	HEC	V	804	-	32,50,50	2.25	12 (37%)	24,82,82	1.93	3 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FES	A	501	1	-	-	0/1/1/1
15	CDL	Y	604	-	-	61/102/102/110	-
16	MQ9	Y	606	-	-	9/53/73/73	0/2/2/2
14	FES	B	501	1	-	-	0/1/1/1
15	CDL	b	603	-	-	44/102/102/110	-
18	HAS	Q	802	10	-	11/40/122/122	-
18	HAS	Q	801	10	-	8/40/122/122	-
15	CDL	b	604	-	-	55/101/101/110	-
15	CDL	K	301	-	-	56/110/110/110	-
19	HEC	j	302	-	-	3/10/54/54	-
16	MQ9	M	302	-	-	8/53/73/73	0/2/2/2
19	HEC	j	301	6	-	3/10/54/54	-
20	HEM	Y	601	13	-	5/12/54/54	-
20	HEM	b	601	13	-	10/12/54/54	-
15	CDL	V	805	-	-	46/97/97/110	-
16	MQ9	b	605	-	-	15/53/73/73	0/2/2/2
19	HEC	i	301	-	-	3/10/54/54	-
16	MQ9	Y	605	-	-	16/53/73/73	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	HAS	V	801	10	-	11/40/122/122	-
15	CDL	M	301	-	-	55/110/110/110	-
15	CDL	Y	603	-	-	56/101/101/110	-
20	HEM	Y	602	13	-	4/12/54/54	-
20	HEM	b	602	13	-	5/12/54/54	-
18	HAS	V	802	10	-	11/40/122/122	-
15	CDL	Q	804	-	-	47/97/97/110	-
19	HEC	V	804	-	-	3/10/54/54	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	j	301	HEC	C2B-C3B	6.07	1.47	1.40
19	j	301	HEC	C3C-C2C	6.05	1.47	1.40
19	V	804	HEC	C2B-C3B	6.04	1.47	1.40
19	i	301	HEC	C2B-C3B	6.03	1.47	1.40
19	j	302	HEC	C2B-C3B	6.00	1.47	1.40

The worst 5 of 193 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	b	602	HEM	CBA-CAA-C2A	8.62	127.33	112.62
20	b	601	HEM	CBA-CAA-C2A	7.56	125.52	112.62
19	V	804	HEC	C1D-C2D-C3D	-6.10	102.75	107.00
19	i	301	HEC	C1D-C2D-C3D	-6.07	102.77	107.00
19	j	302	HEC	C1D-C2D-C3D	-6.06	102.78	107.00

There are no chirality outliers.

5 of 545 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	M	301	CDL	CA2-OA2-PA1-OA3
15	M	301	CDL	CA2-OA2-PA1-OA4
15	M	301	CDL	CA3-OA5-PA1-OA3
15	V	805	CDL	CA2-OA2-PA1-OA3
15	V	805	CDL	CB2-OB2-PB2-OB3

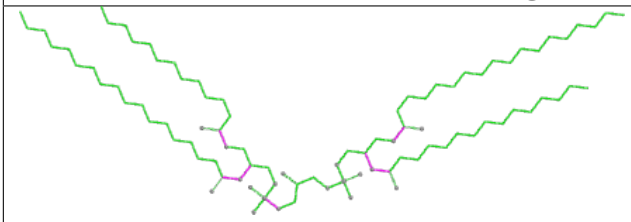
There are no ring outliers.

17 monomers are involved in 79 short contacts:

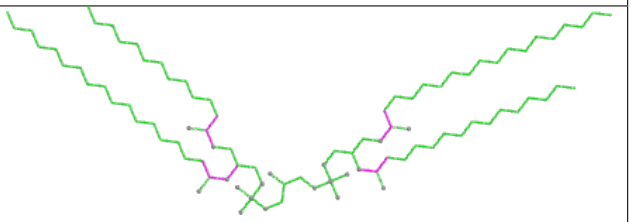
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	Y	604	CDL	8	0
16	Y	606	MQ9	4	0
14	B	501	FES	2	0
18	Q	802	HAS	3	0
18	Q	801	HAS	3	0
15	K	301	CDL	6	0
16	M	302	MQ9	4	0
20	Y	601	HEM	1	0
15	V	805	CDL	2	0
16	Y	605	MQ9	6	0
18	V	801	HAS	5	0
15	M	301	CDL	4	0
15	Y	603	CDL	4	0
20	Y	602	HEM	5	0
18	V	802	HAS	2	0
15	Q	804	CDL	3	0
19	V	804	HEC	22	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.

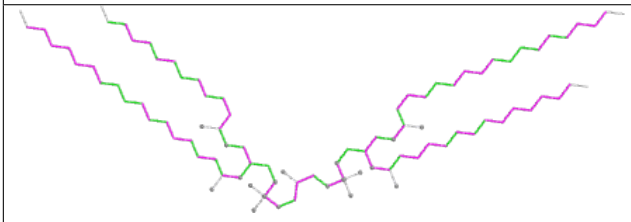
Ligand CDL Y 604



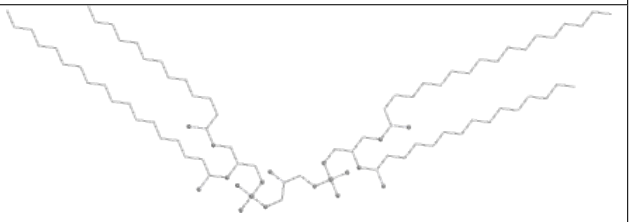
Bond lengths



Bond angles

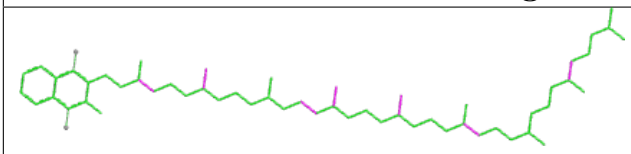


Torsions

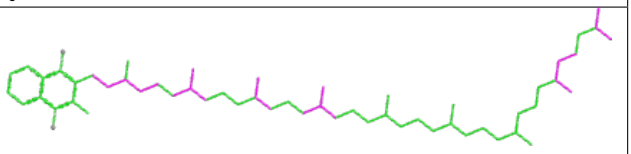


Rings

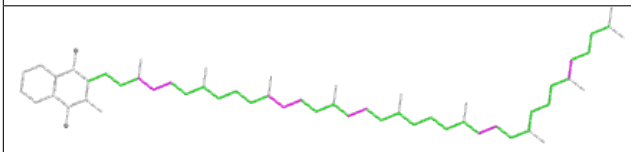
Ligand MQ9 Y 606



Bond lengths



Bond angles



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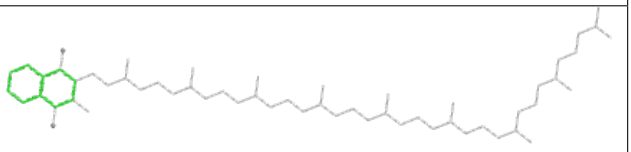
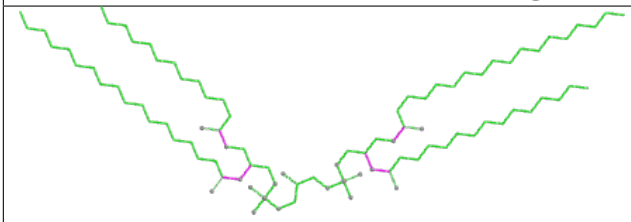


Rings

Ligand CDL b 603



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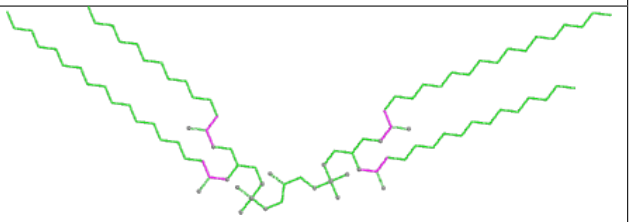
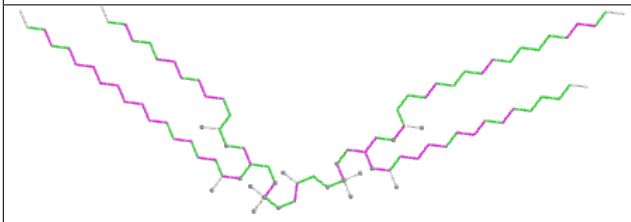


Bond angles



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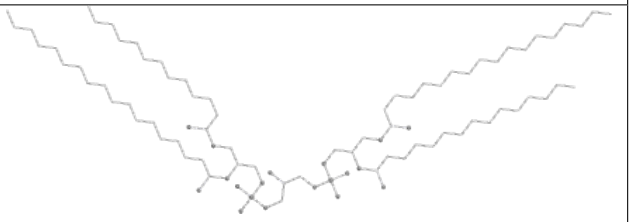
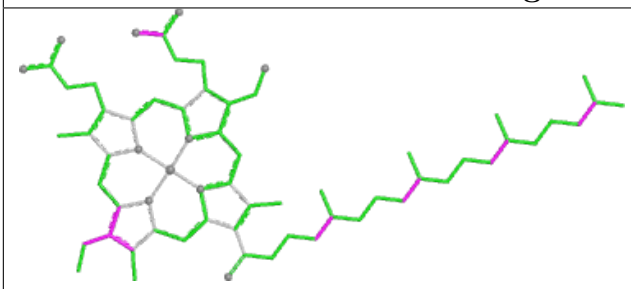
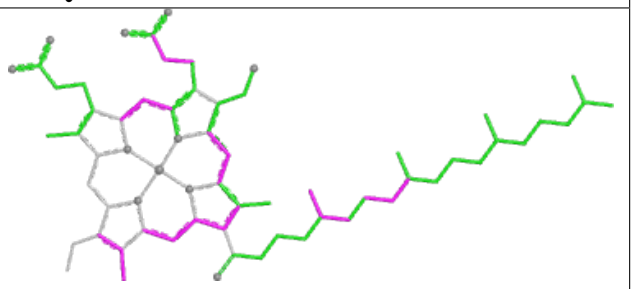
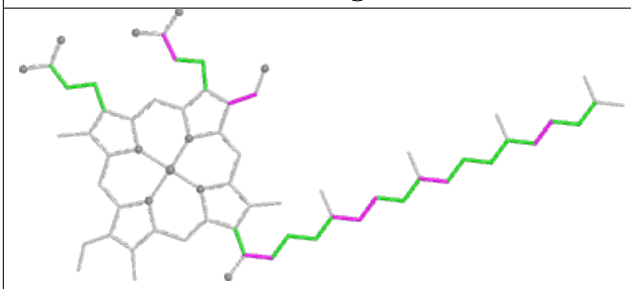
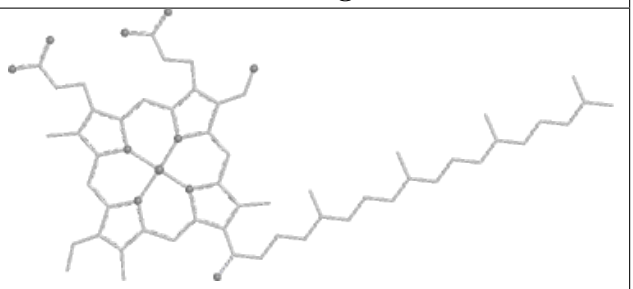


Rings

Ligand HAS Q 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

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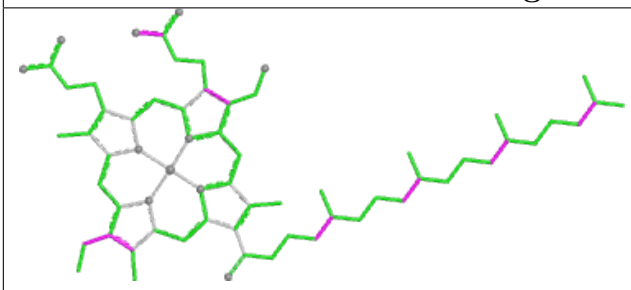
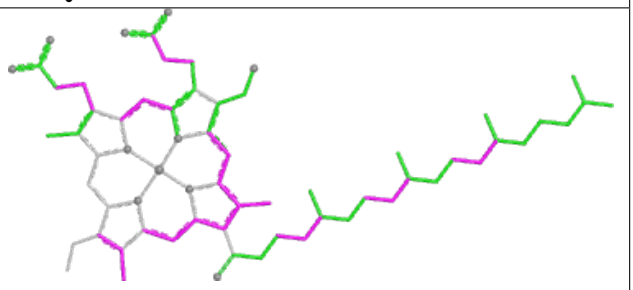
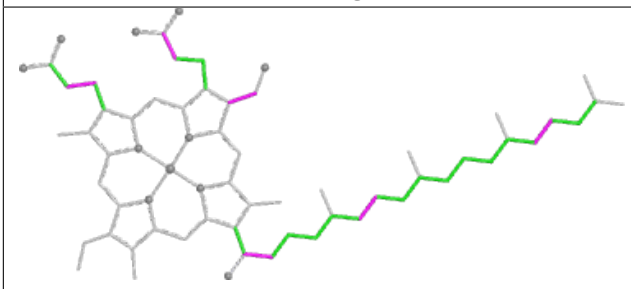
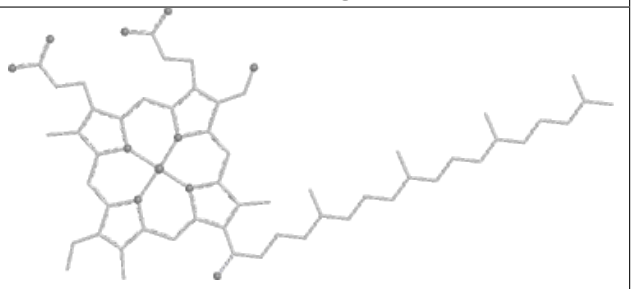
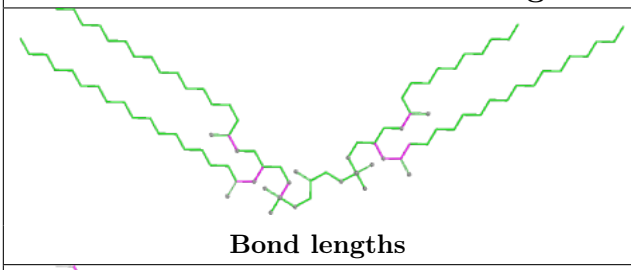
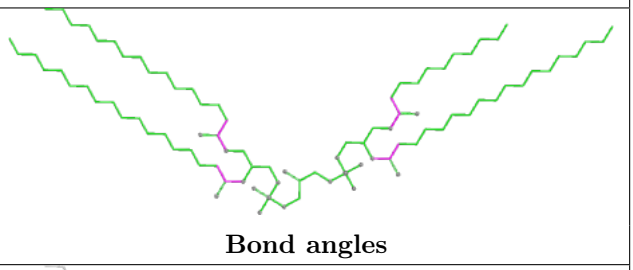
 Bond lengths	 Bond angles
 Torsions	 Rings

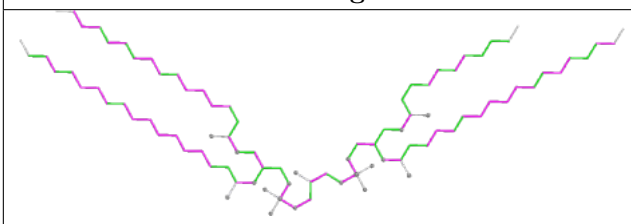
Ligand CDL b 604



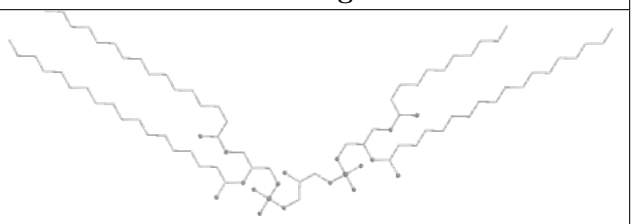
Bond lengths



Bond angles

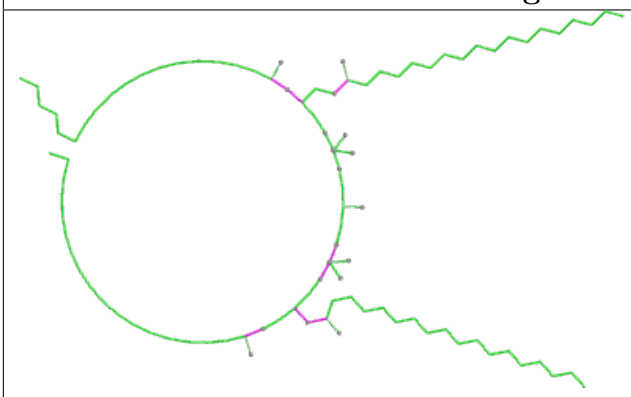


Torsions



Rings

Ligand CDL K 301



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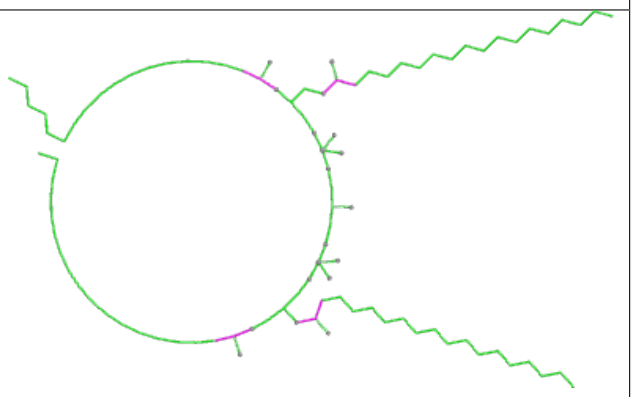

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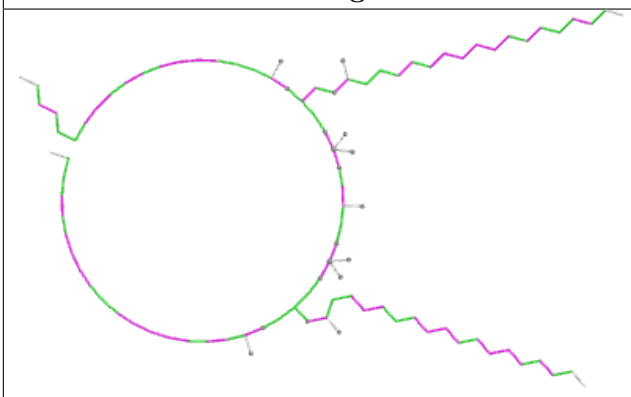

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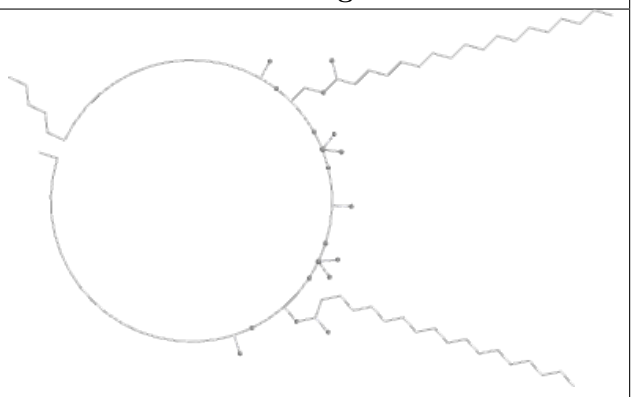
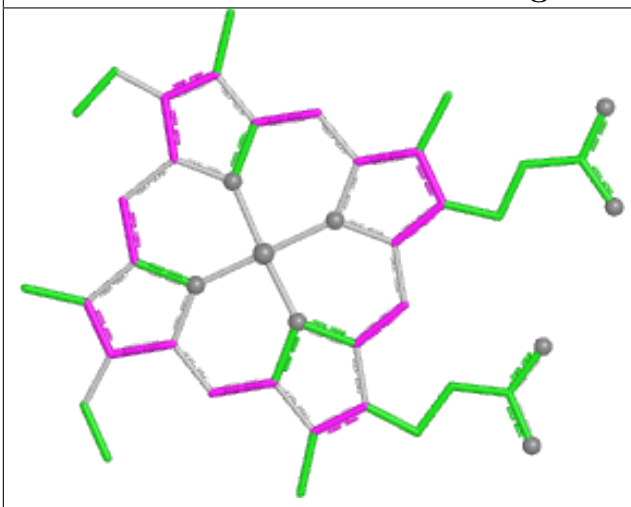


Rings

Ligand HEC j 302



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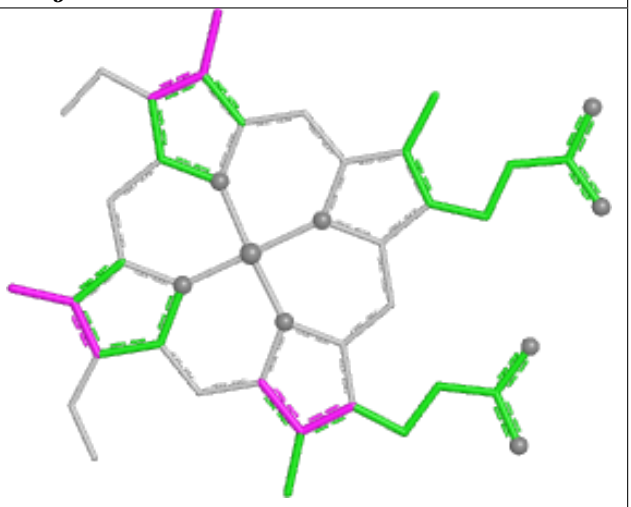

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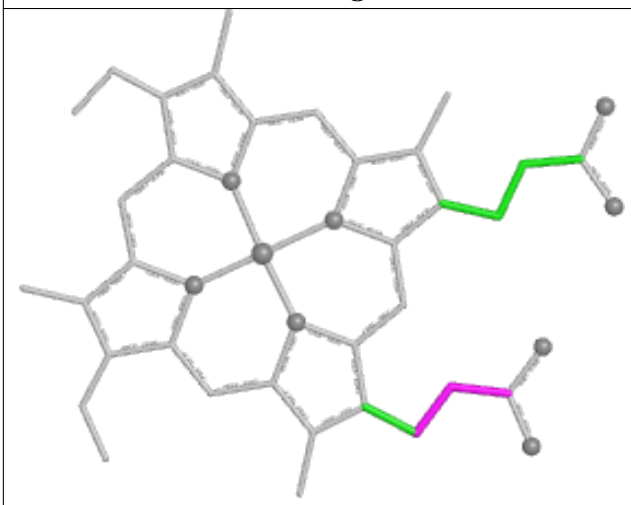

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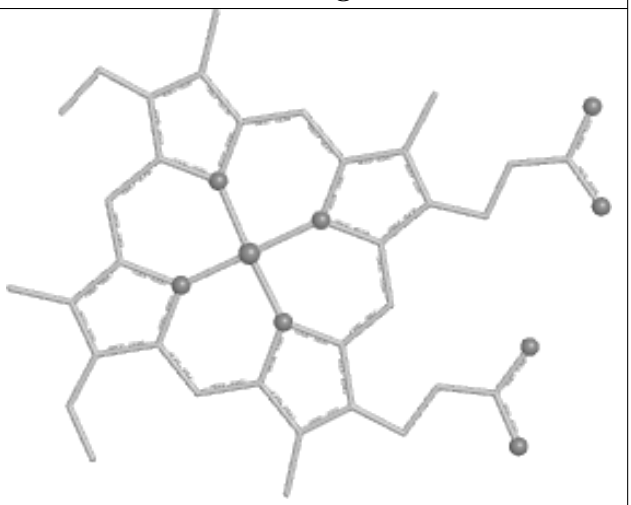
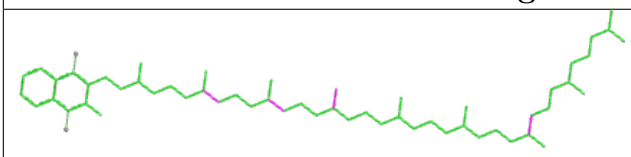


Rings

Ligand MQ9 M 302



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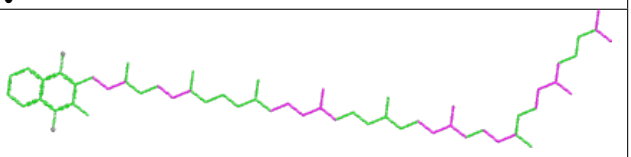

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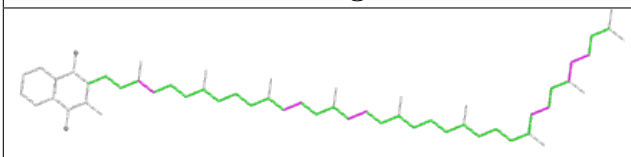

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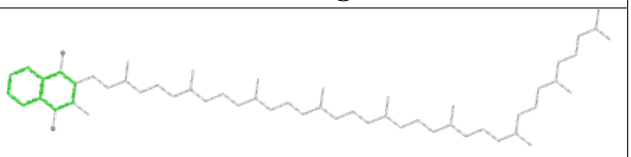
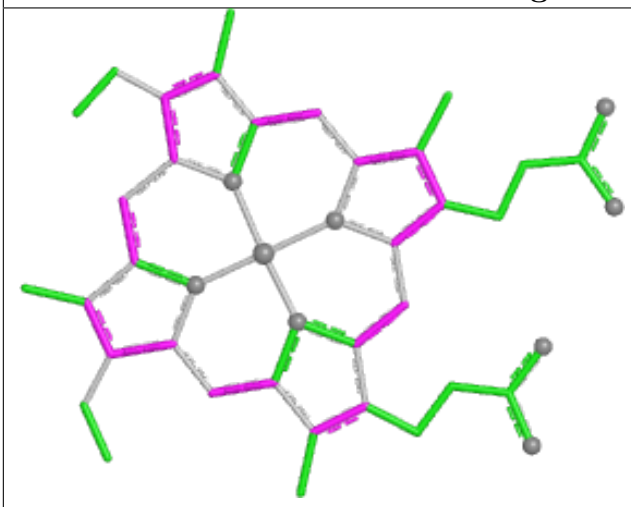


Rings

Ligand HEC j 301



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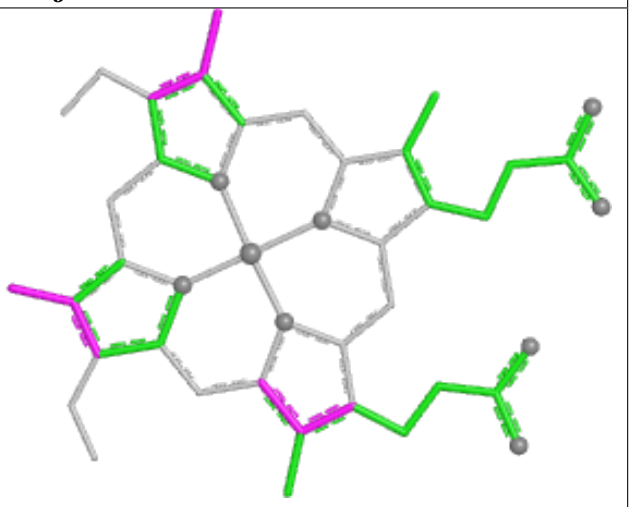
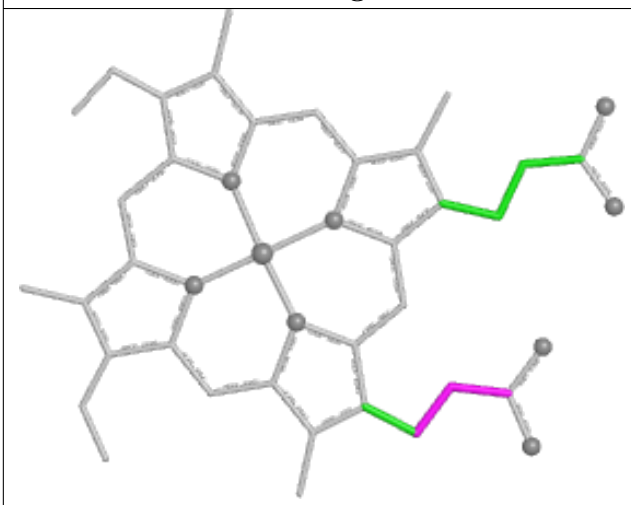
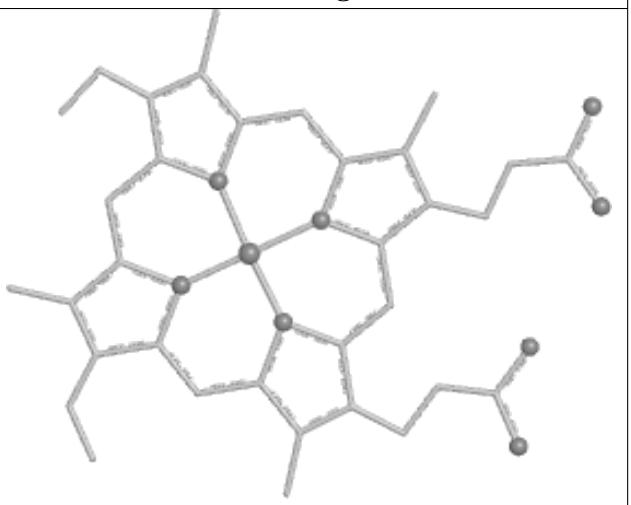


Bond angles

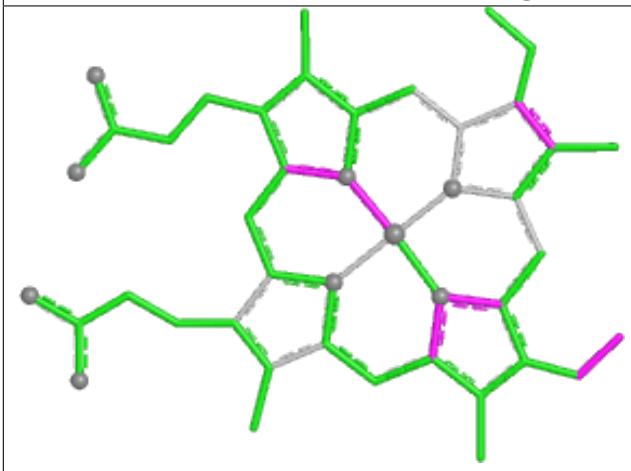


Torsions

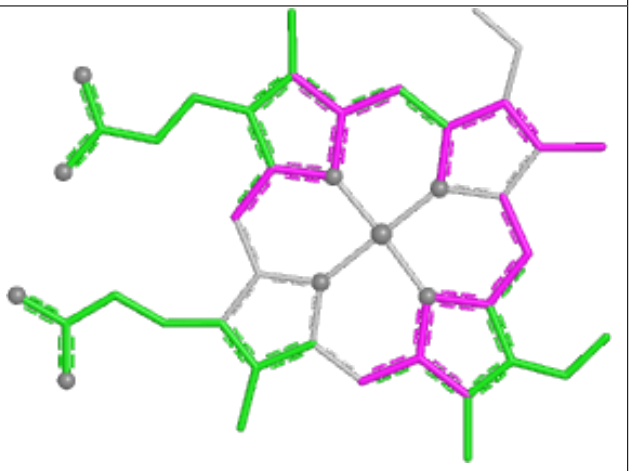


Rings

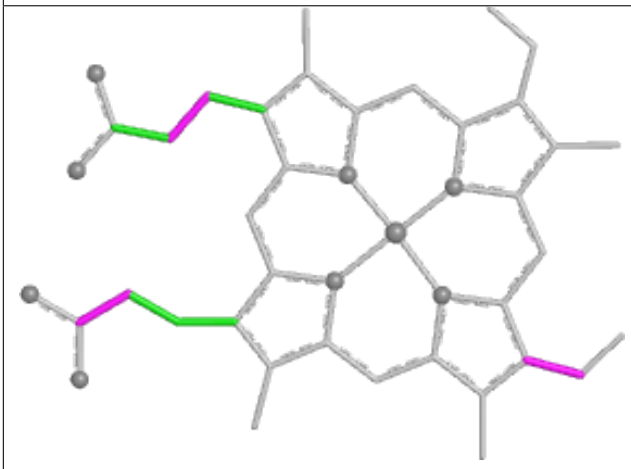
Ligand HEM Y 601



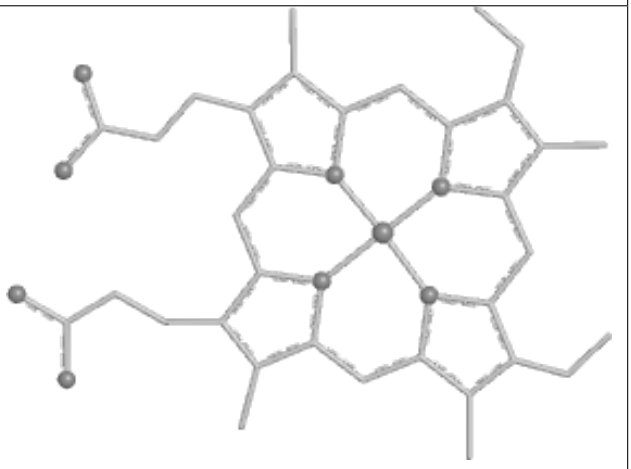
Bond lengths



Bond angles

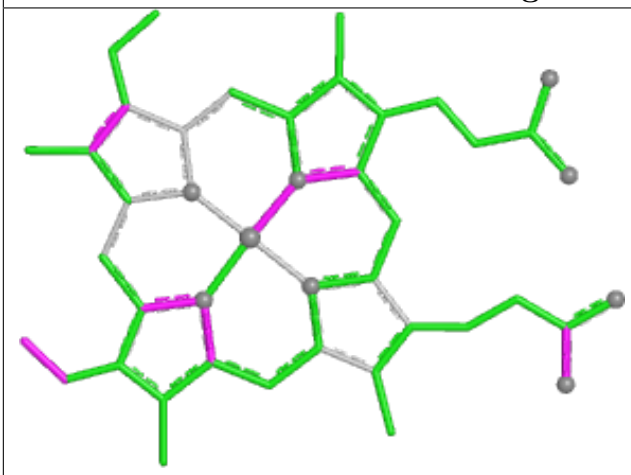


Torsions

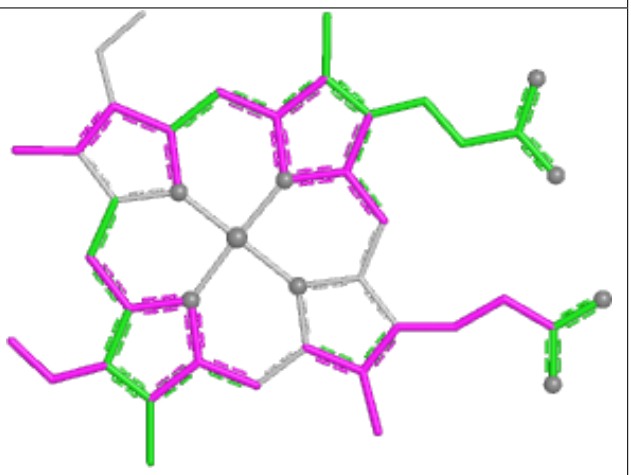


Rings

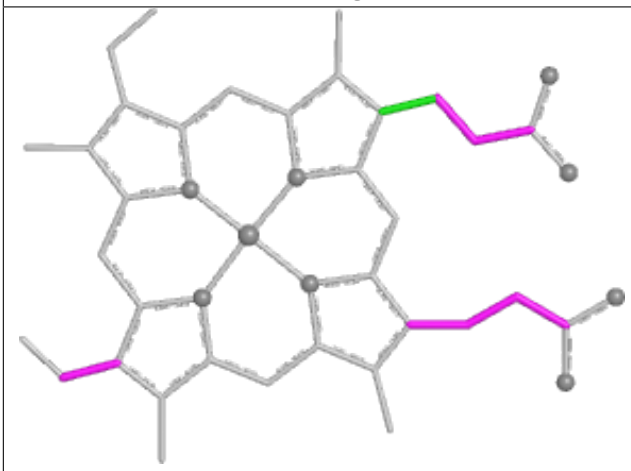
Ligand HEM b 601



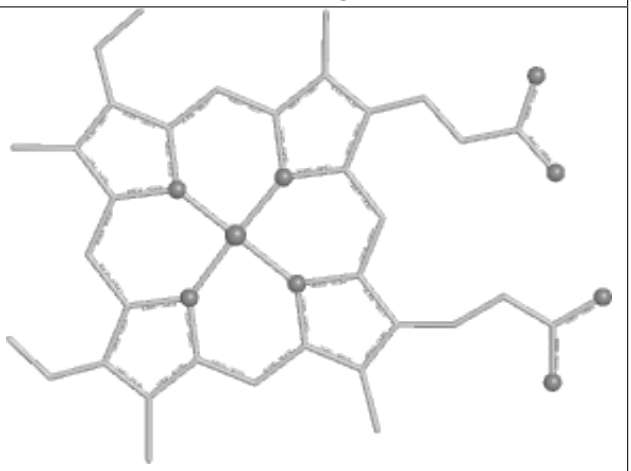
Bond lengths



Bond angles

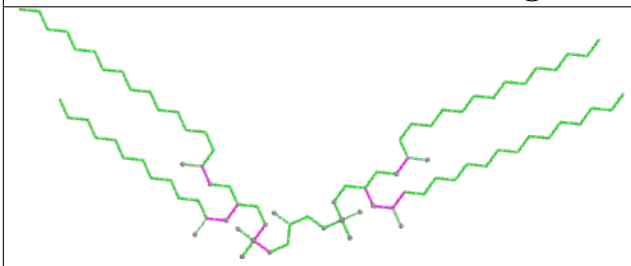


Torsions

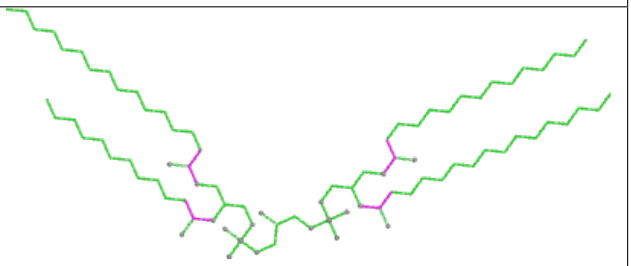


Rings

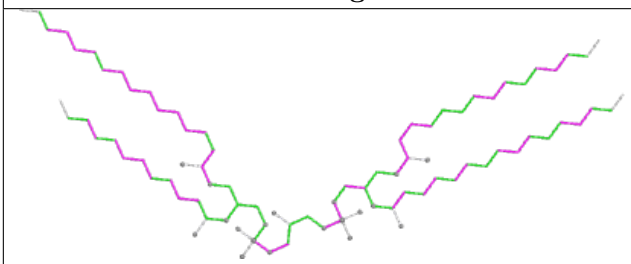
Ligand CDL V 805



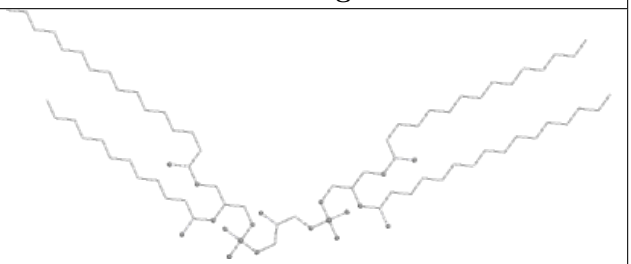
Bond lengths



Bond angles

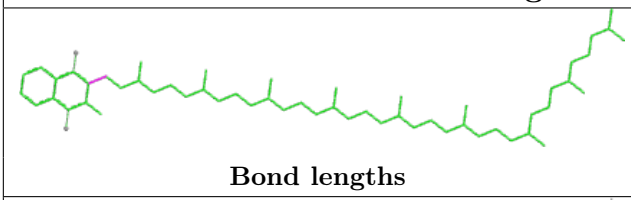


Torsions

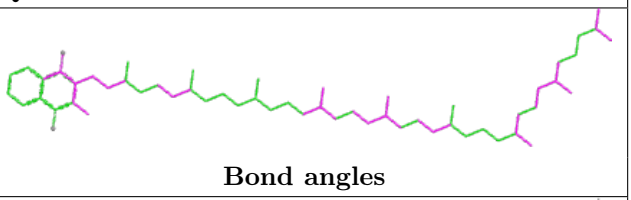


Rings

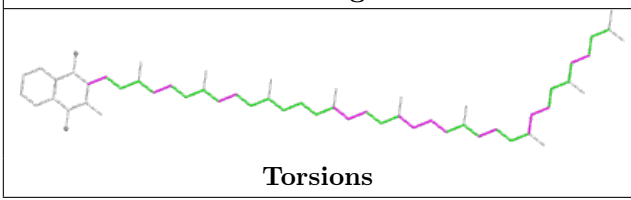
Ligand MQ9 b 605



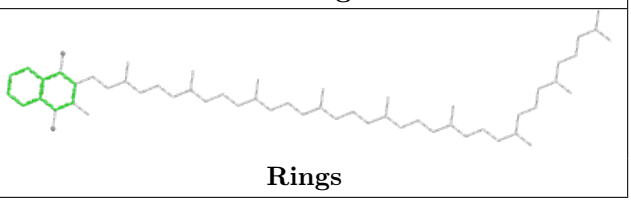
Bond lengths



Bond angles

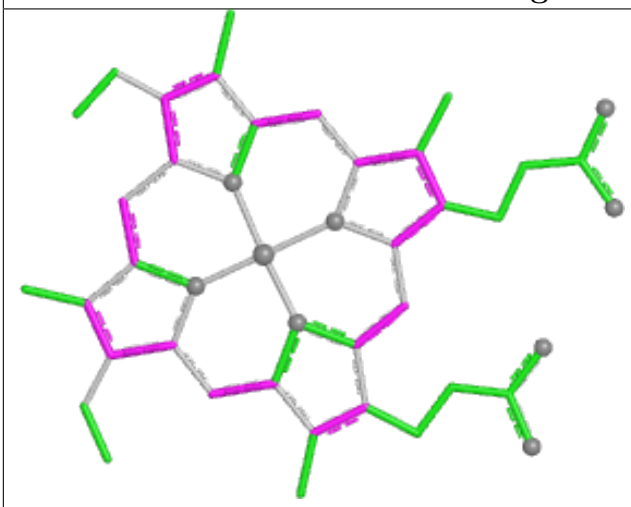


Torsions

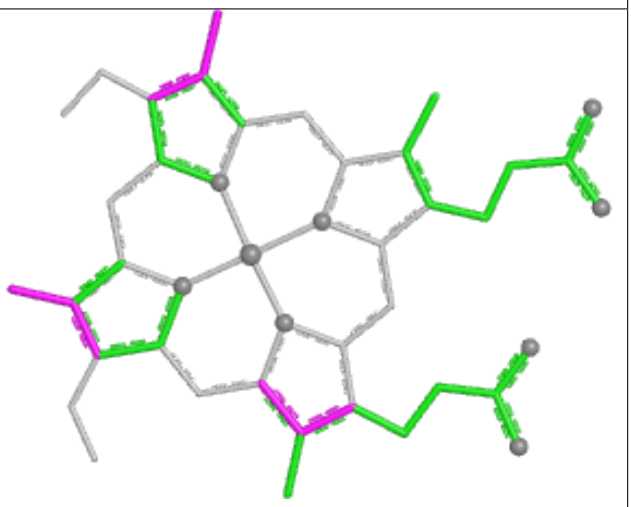


Rings

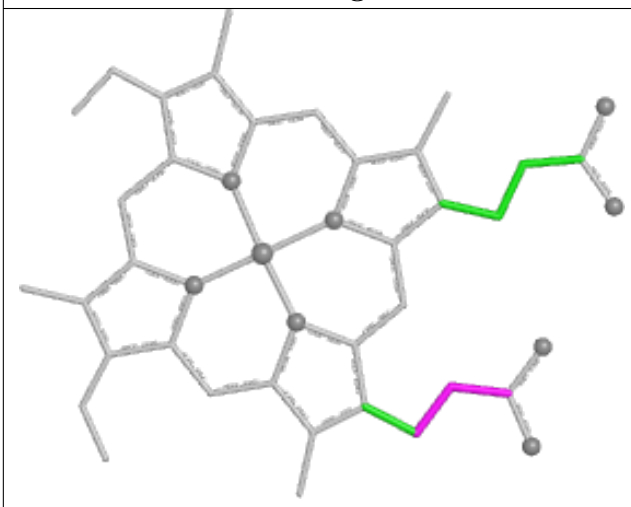
Ligand HEC i 301



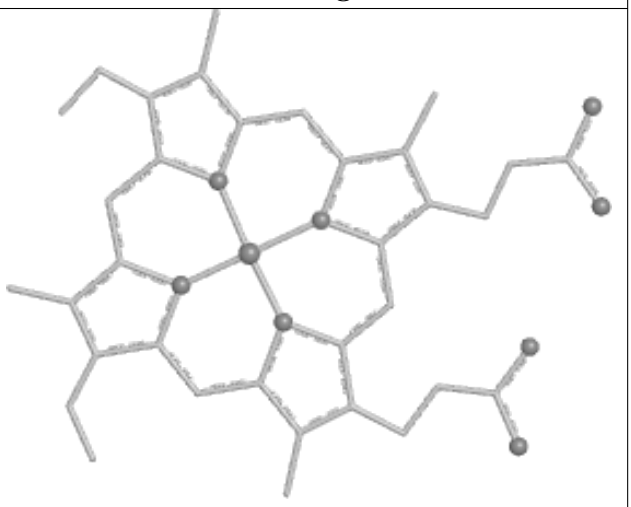
Bond lengths



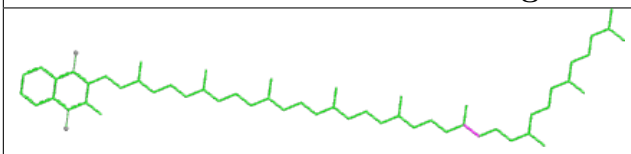
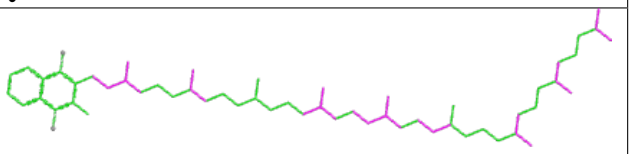
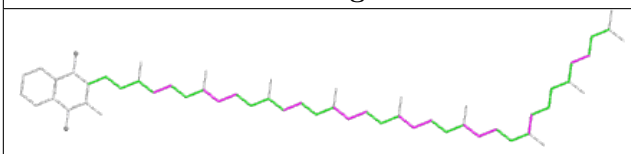
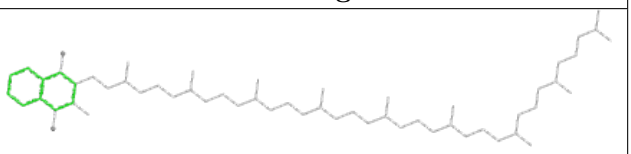
Bond angles

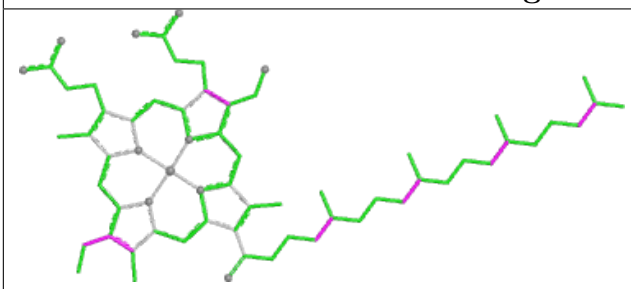
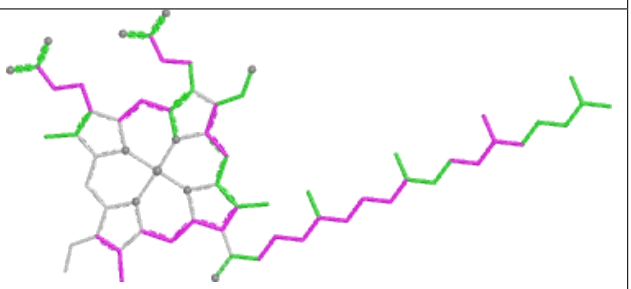
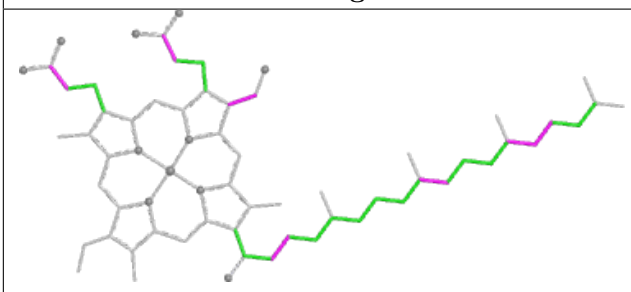
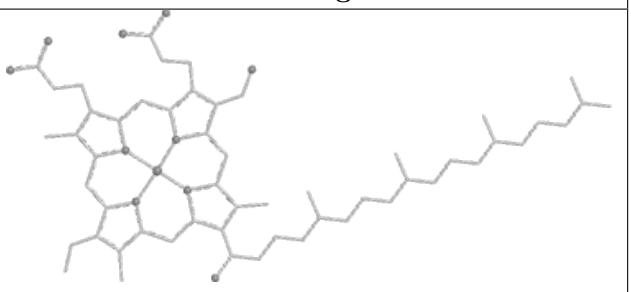


Torsions

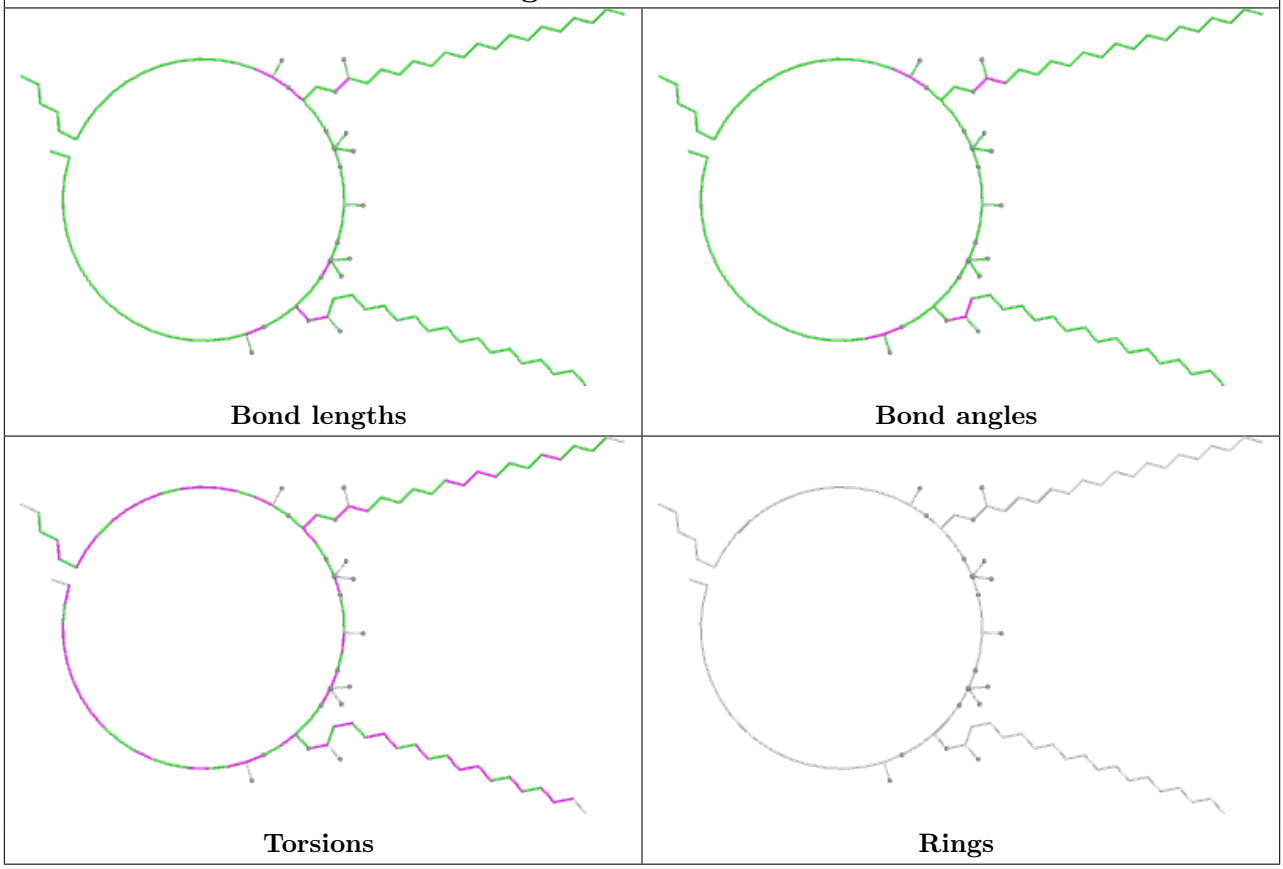


Rings

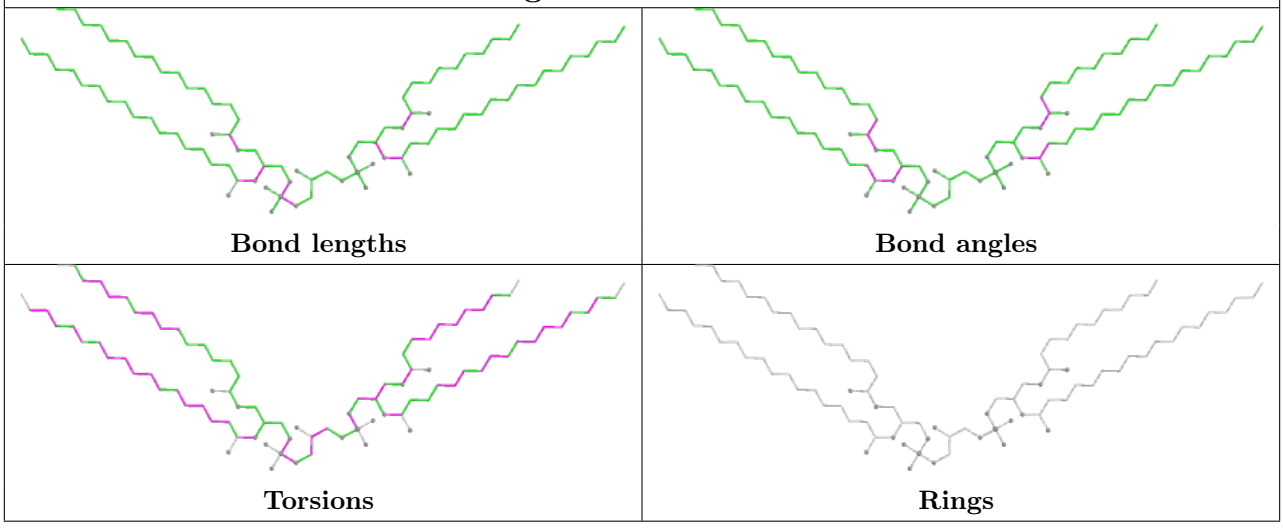
Ligand MQ9 Y 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HAS V 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

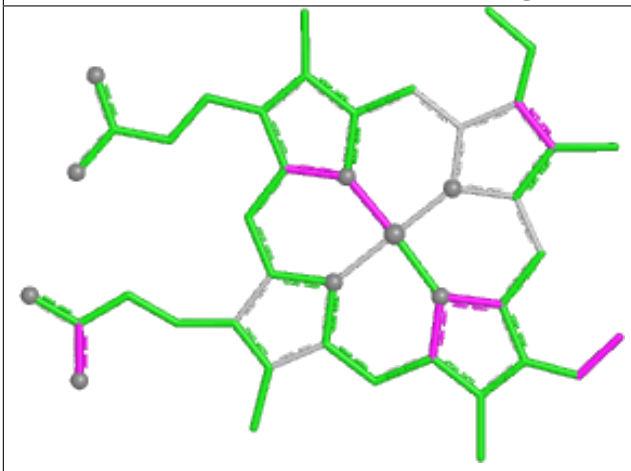
Ligand CDL M 301



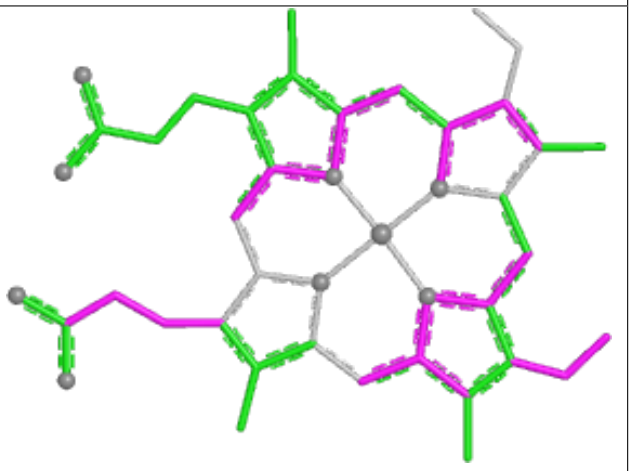
Ligand CDL Y 603



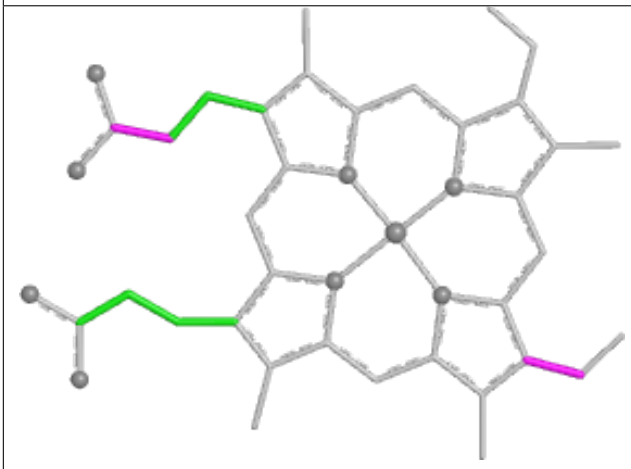
Ligand HEM Y 602



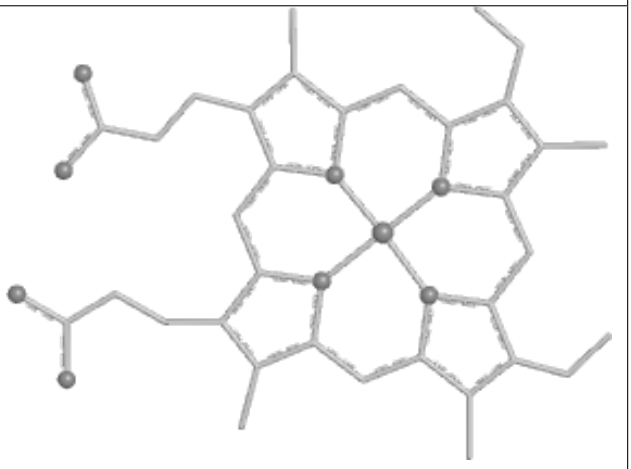
Bond lengths



Bond angles

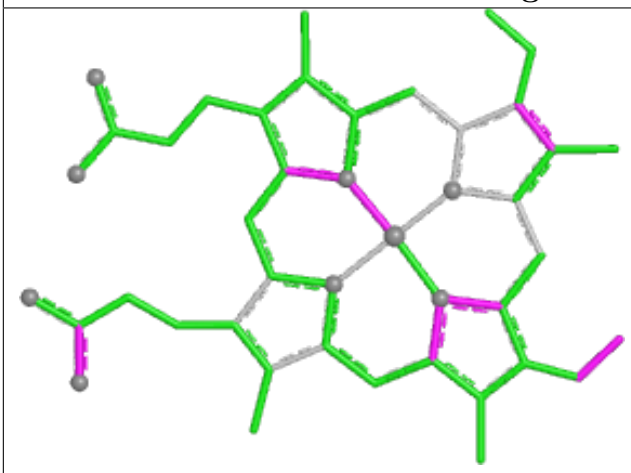


Torsions

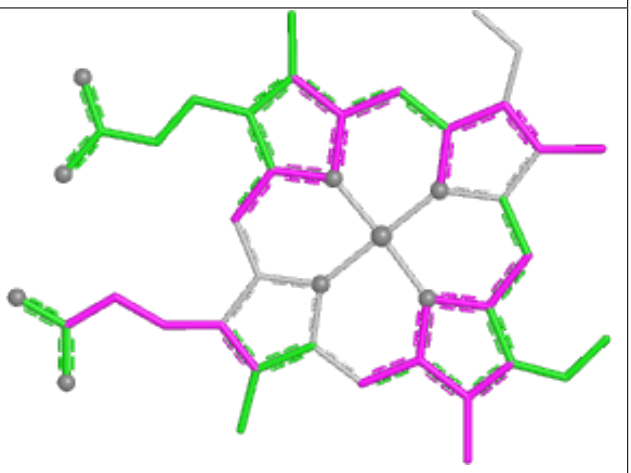


Rings

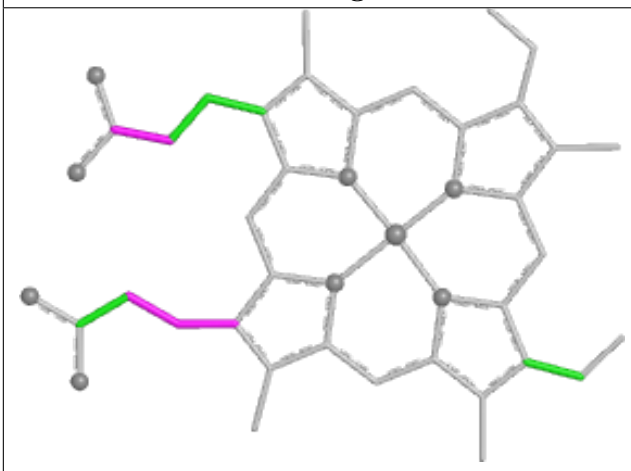
Ligand HEM b 602



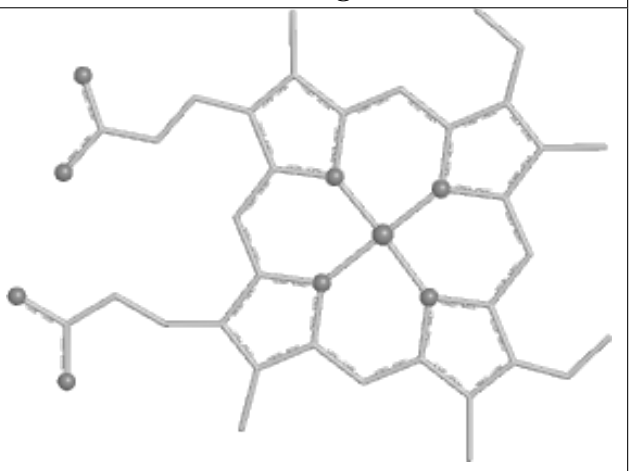
Bond lengths



Bond angles

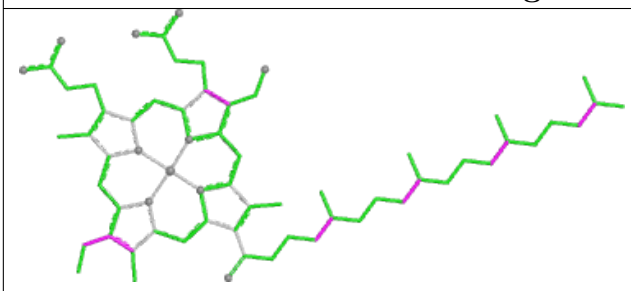


Torsions

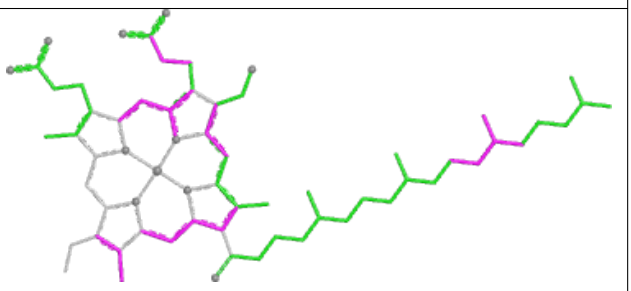


Rings

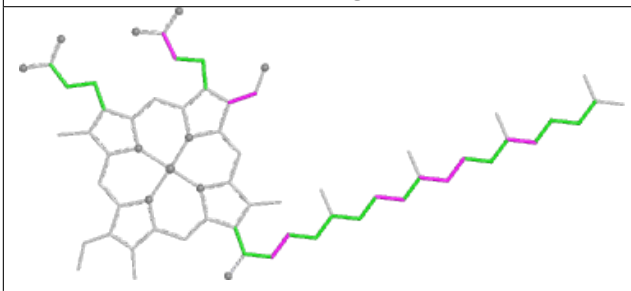
Ligand HAS V 802



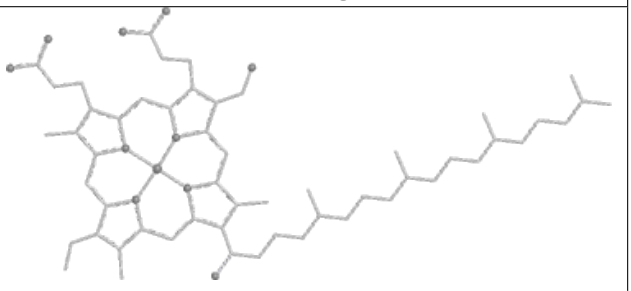
Bond lengths



Bond angles

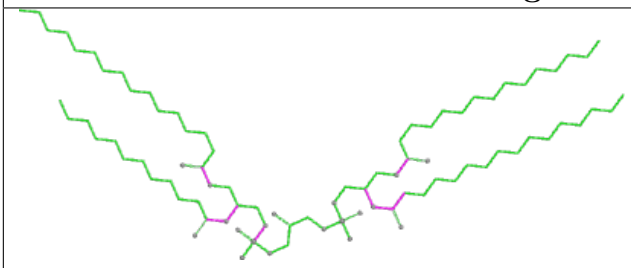


Torsions

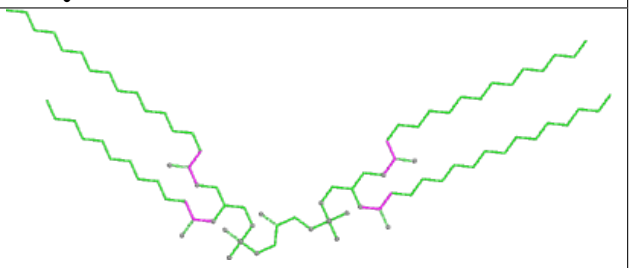


Rings

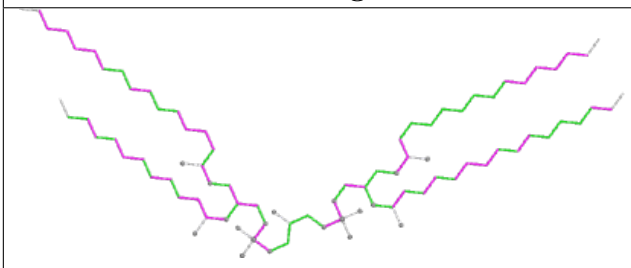
Ligand CDL Q 804



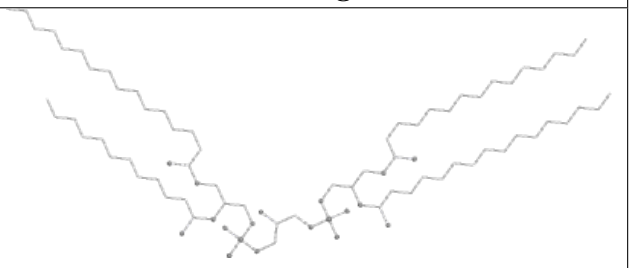
Bond lengths



Bond angles

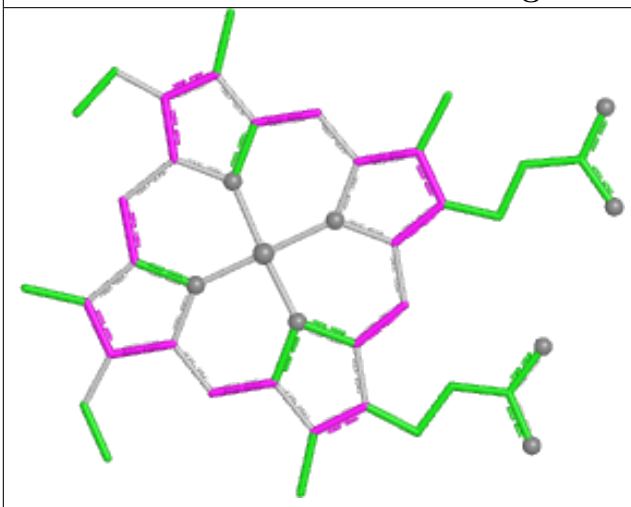


Torsions

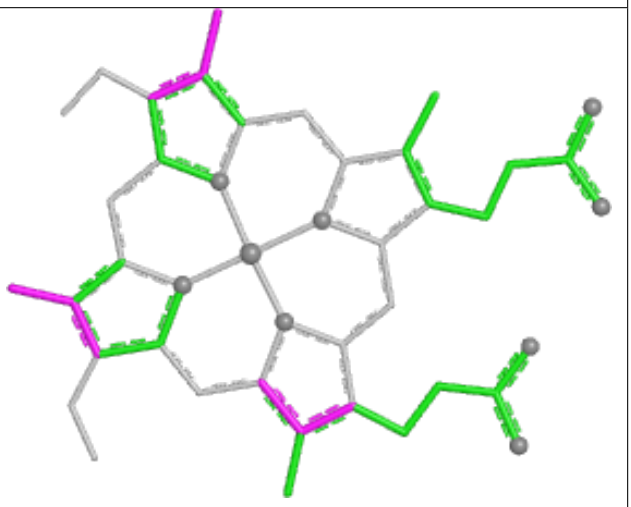


Rings

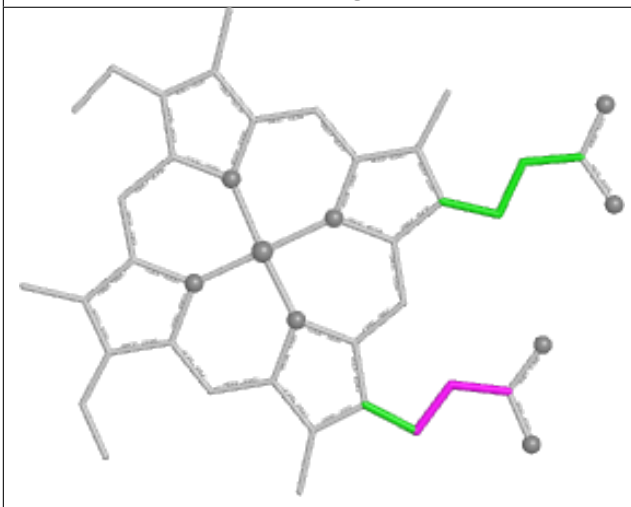
Ligand HEC V 804



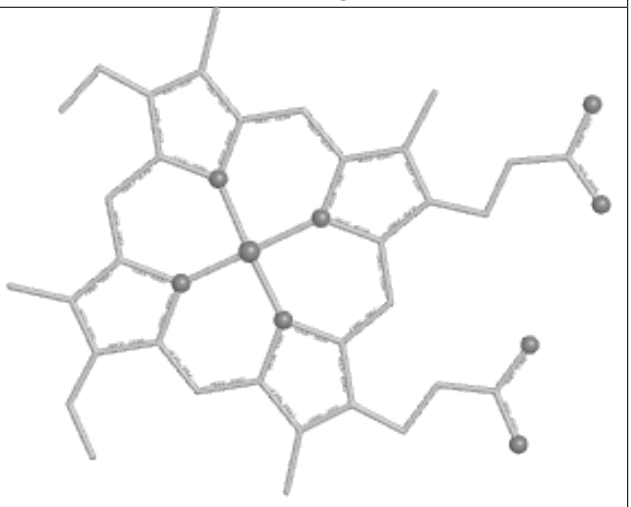
Bond lengths



Bond angles



Torsions



Rings

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.

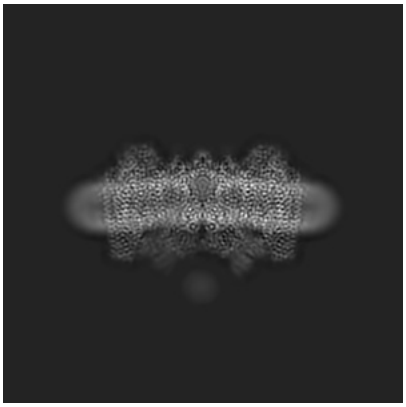
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0289. These allow visual inspection of the internal detail of the map and identification of artifacts.

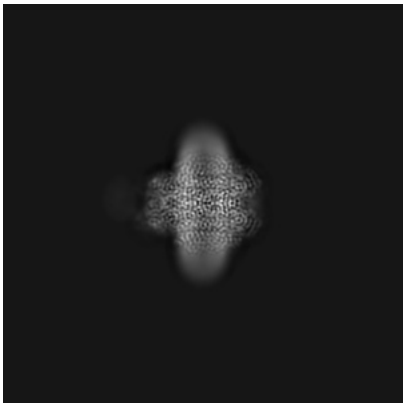
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

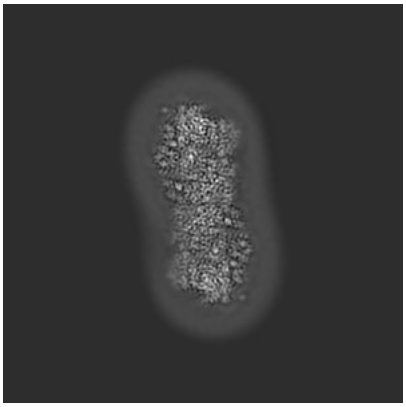
6.1.1 Primary map



X



Y

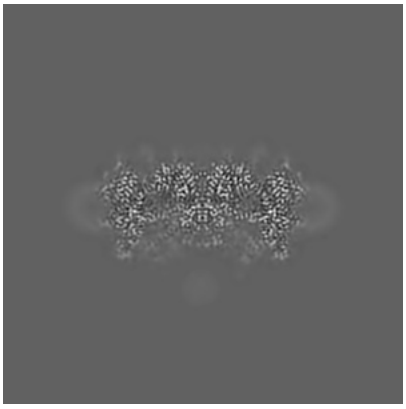


Z

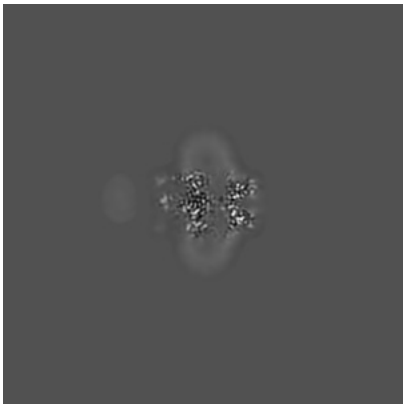
The images above show the map projected in three orthogonal directions.

6.2 Central slices

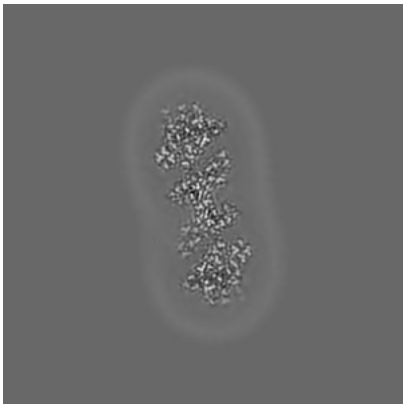
6.2.1 Primary map



X Index: 190



Y Index: 190

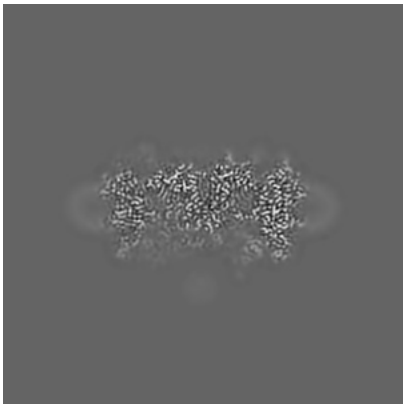


Z Index: 190

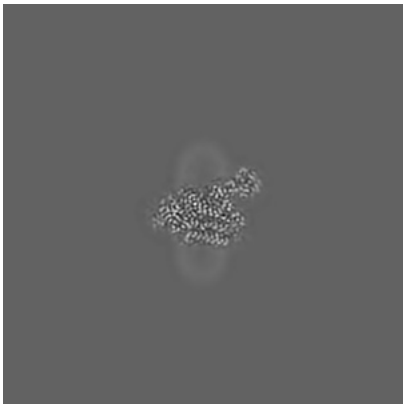
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

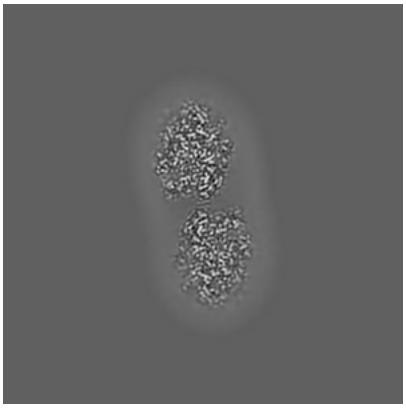
6.3.1 Primary map



X Index: 188



Y Index: 253

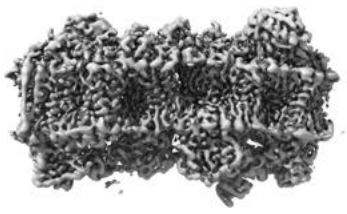


Z Index: 207

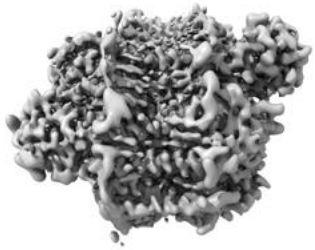
The images above show the largest variance slices of the map in three orthogonal directions.

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

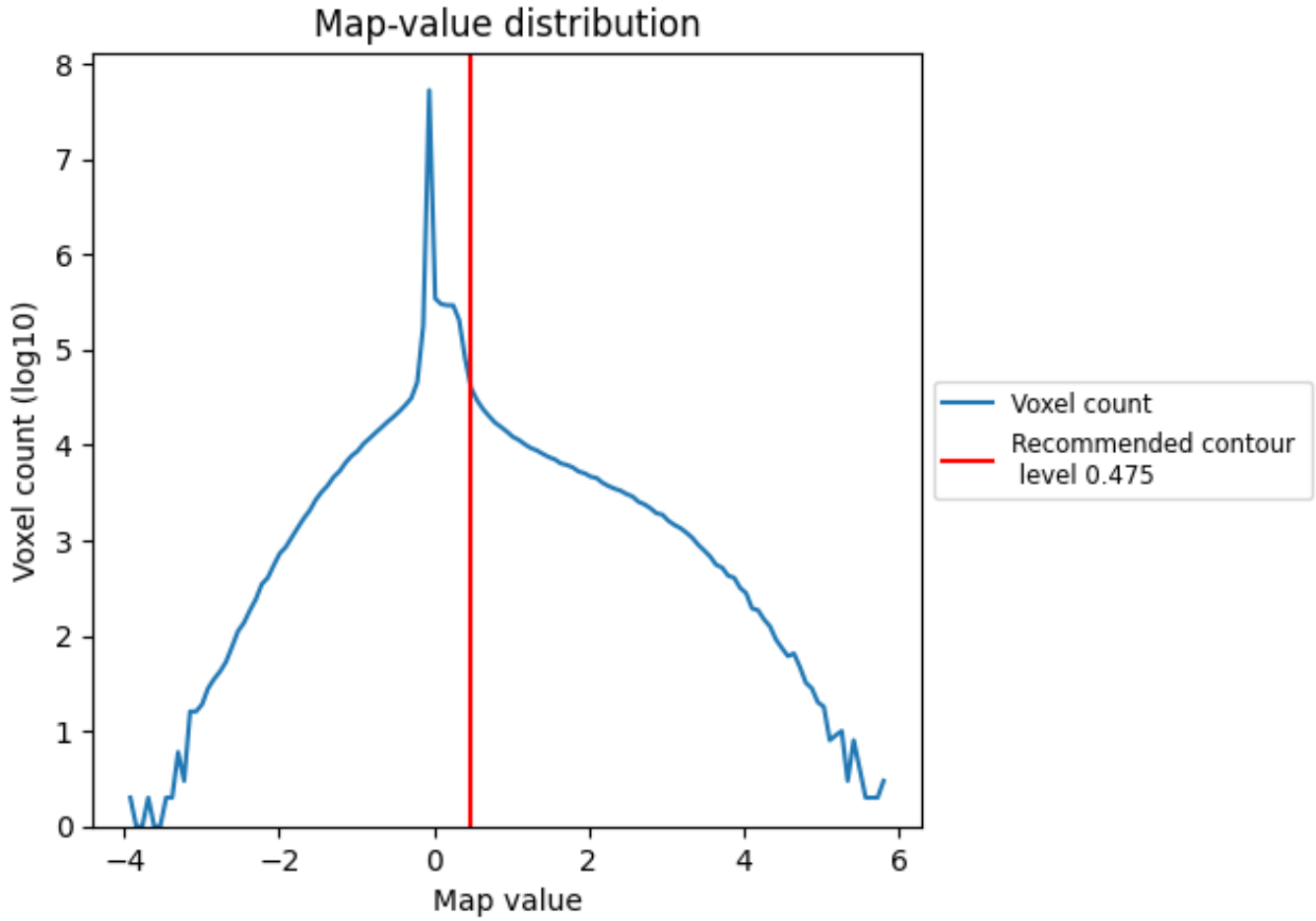
6.5 Mask visualisation (i)

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

7 Map analysis

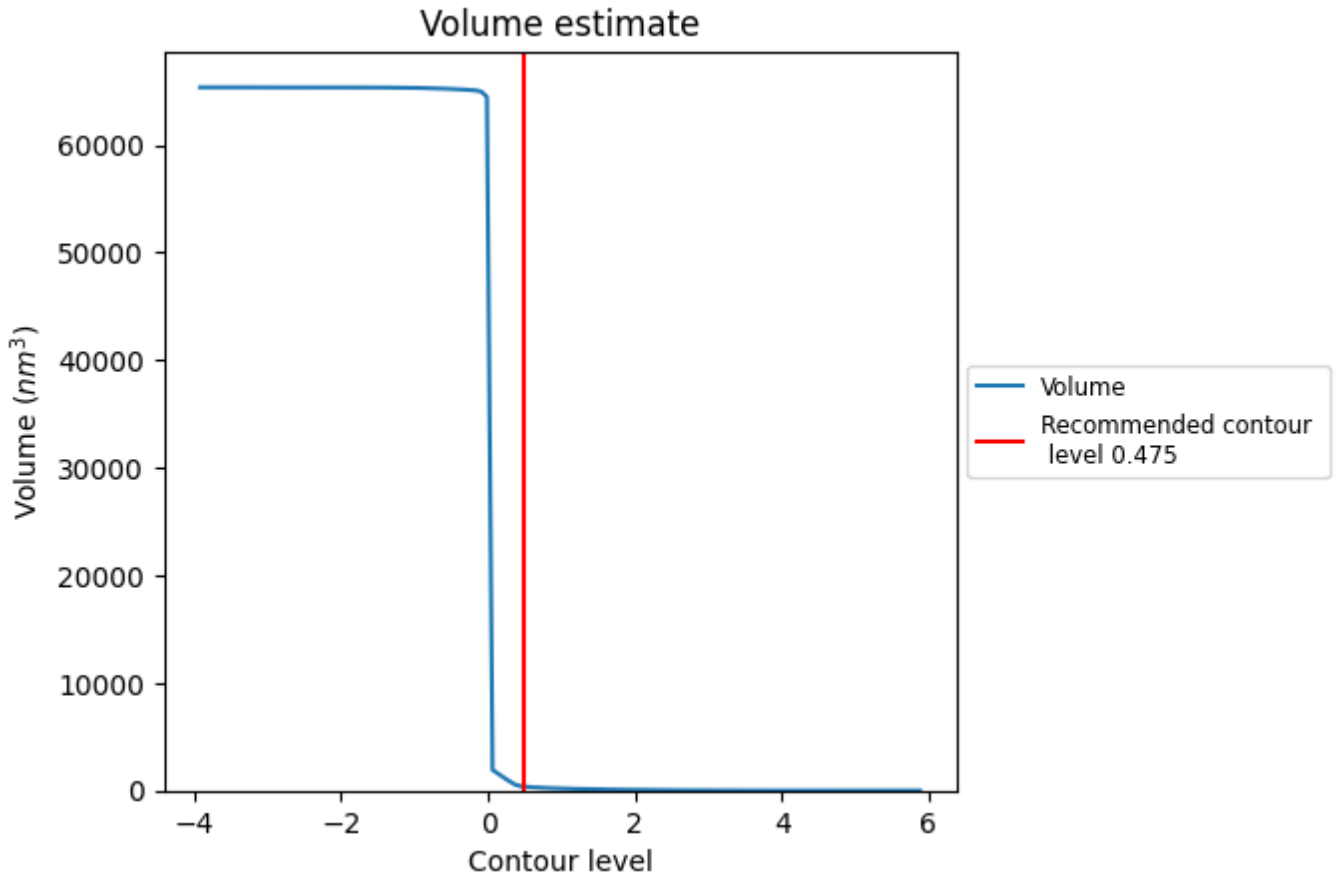
This section contains the results of statistical analysis of the map.

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.

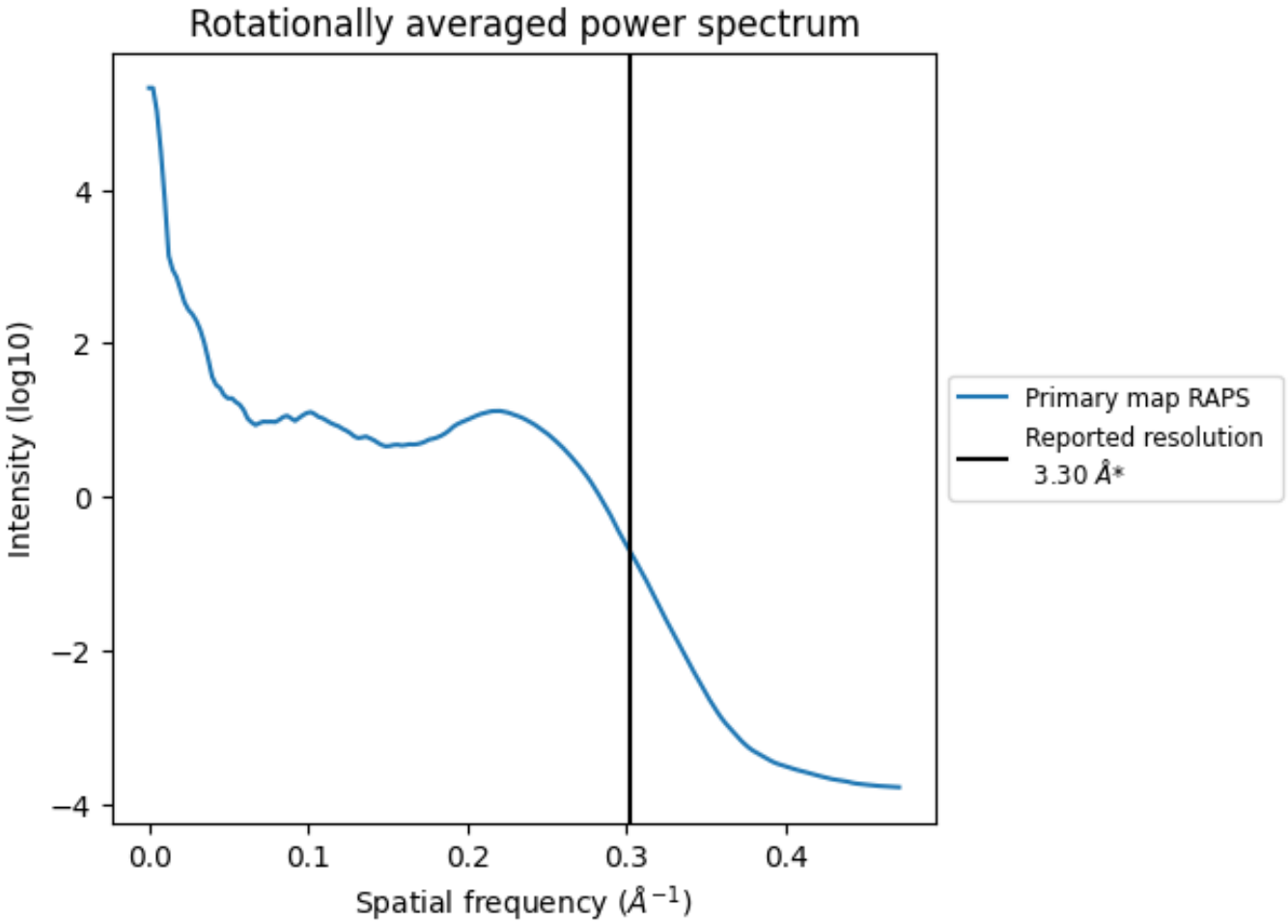
7.2 Volume estimate (i)



The volume at the recommended contour level is 384 nm^3; this corresponds to an approximate mass of 347 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)

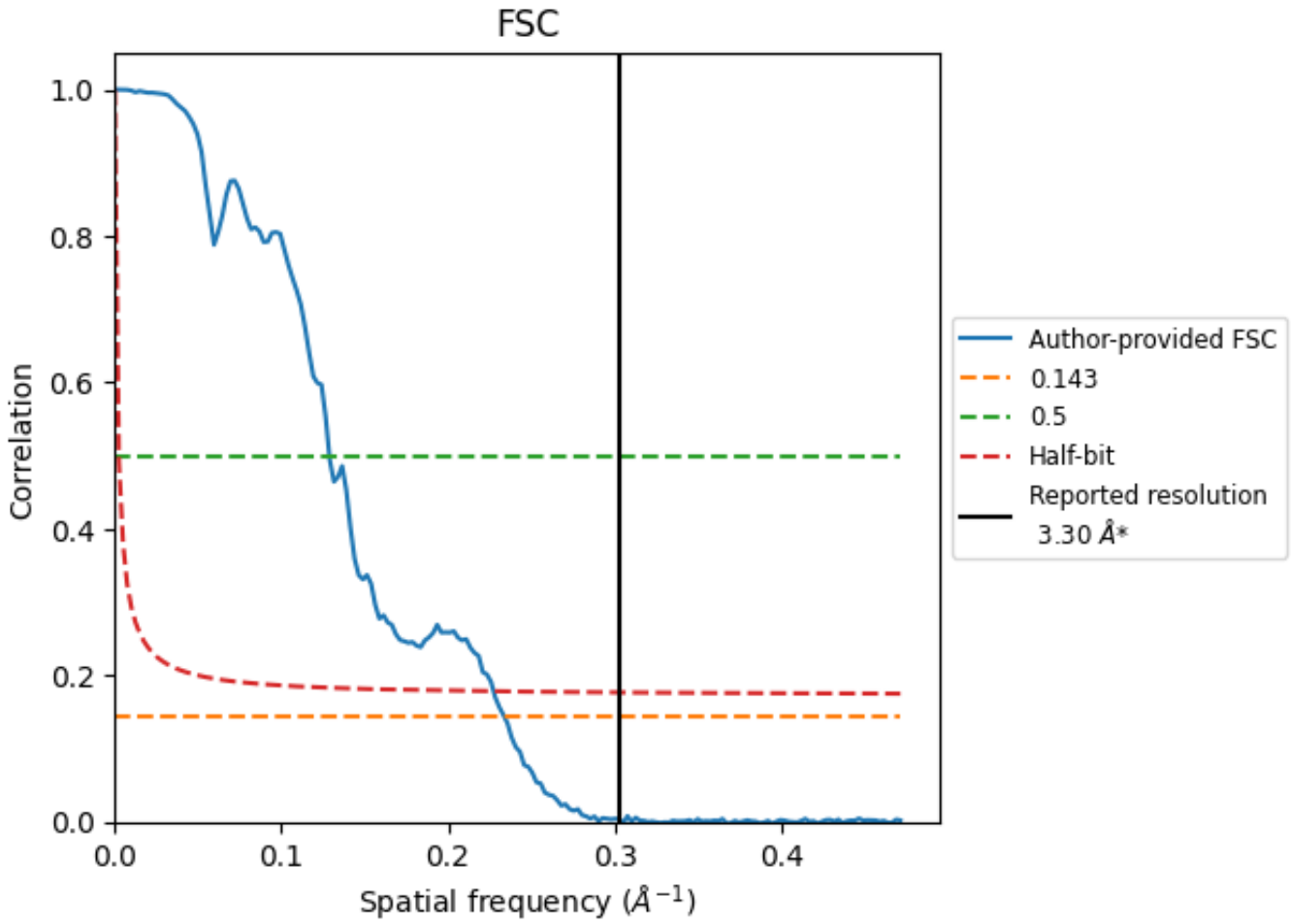


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

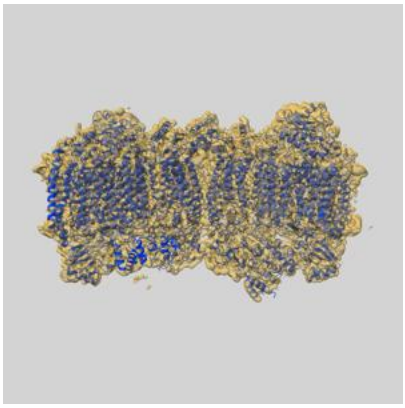
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	4.28	7.76	4.40
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.28 differs from the reported value 3.3 by more than 10 %

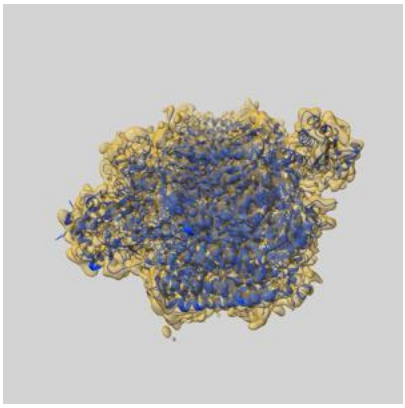
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0289 and PDB model 6HWH. Per-residue inclusion information can be found in section 3 on page 12.

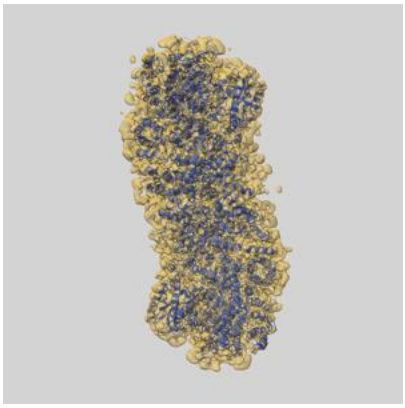
9.1 Map-model overlay



X



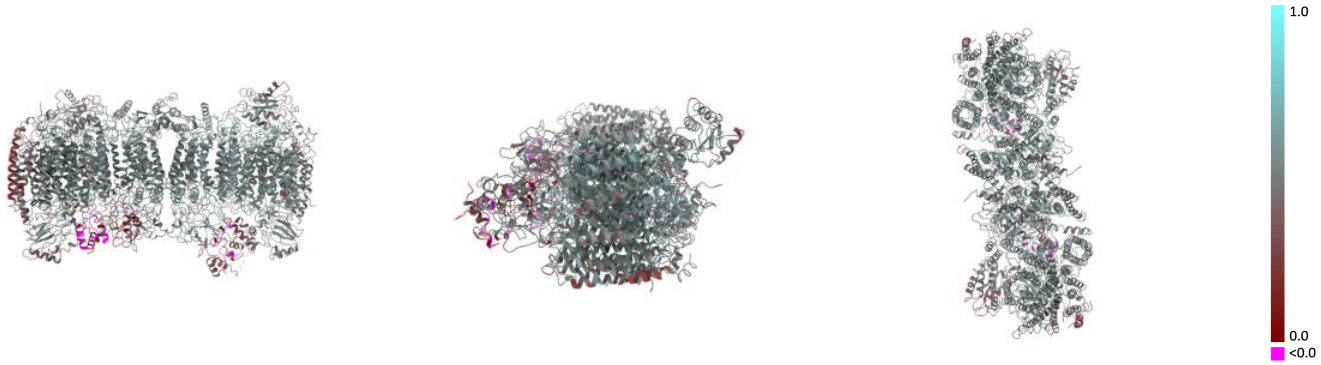
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.475 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.

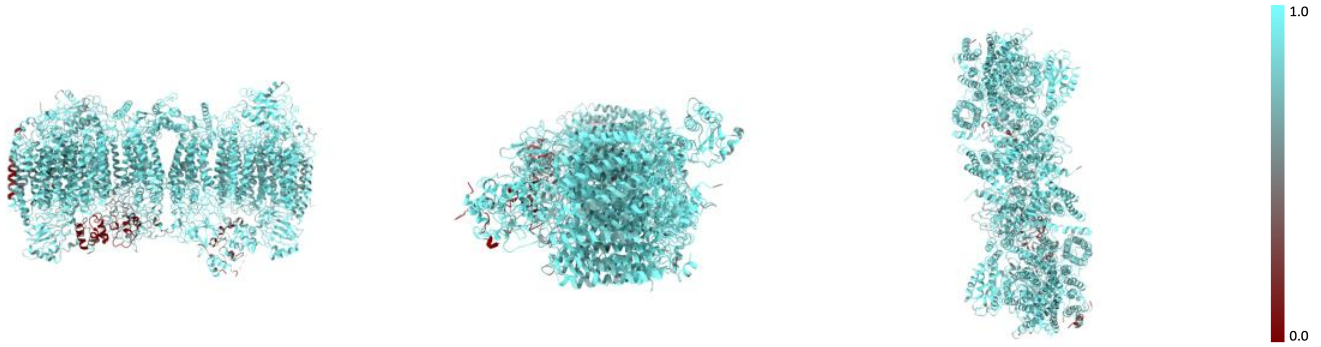
9.2 Q-score mapped to coordinate model



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.

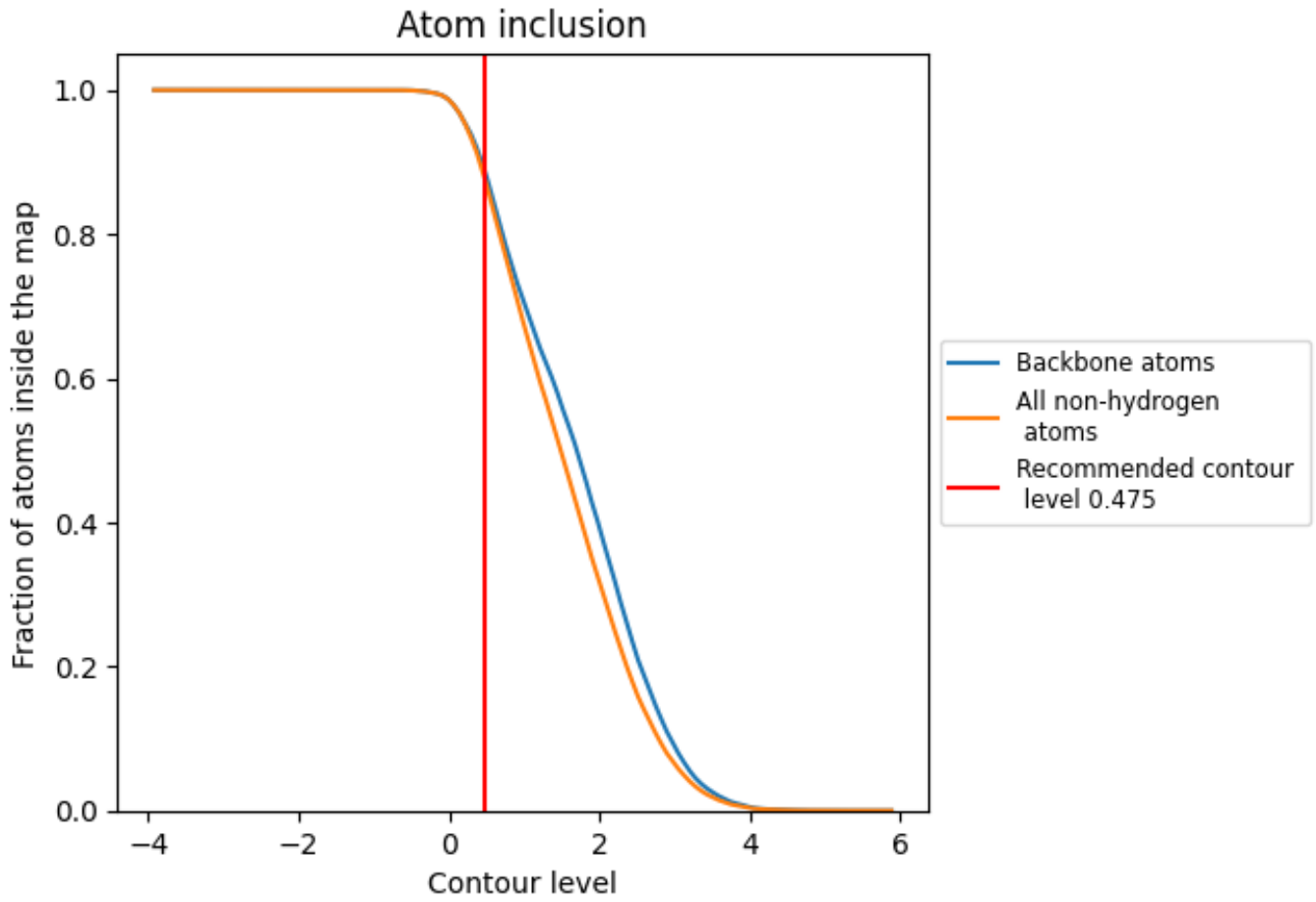
9.3 Atom inclusion mapped to coordinate model



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 (0.475).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.475) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8767	0.5000
A	0.8137	0.4750
B	0.8998	0.5080
C	0.9676	0.5510
D	0.8092	0.4240
E	0.8500	0.4370
F	0.9886	0.5580
G	0.9081	0.5140
H	0.6185	0.3030
I	0.7400	0.4140
J	0.8457	0.5110
K	0.9218	0.5650
L	0.8882	0.4920
M	0.8795	0.5450
N	0.9122	0.4960
O	0.8870	0.4840
P	0.8401	0.4560
Q	0.9283	0.5460
R	0.8537	0.4620
S	0.9186	0.5350
T	0.8600	0.4450
V	0.9068	0.5230
W	0.8988	0.5170
X	0.8988	0.5190
Y	0.9240	0.5450
Z	0.8832	0.5040
b	0.9029	0.5310
i	0.2897	0.1410
j	0.6295	0.1900