wwPDB EM Validation Summary Report

Nov 20, 2022 – 12:26 pm GMT

PDB ID	:	6Q9E
EMDB ID	:	EMD-4481
Title	:	Complex III2 focused refinement from Ovine respiratory supercomplex I+III2
Authors	:	Letts, J.A.; Sazanov, L.A.
Deposited on	:	2018-12-18
Resolution	:	3.90 Å(reported)
Based on initial model	:	1PPJ

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:

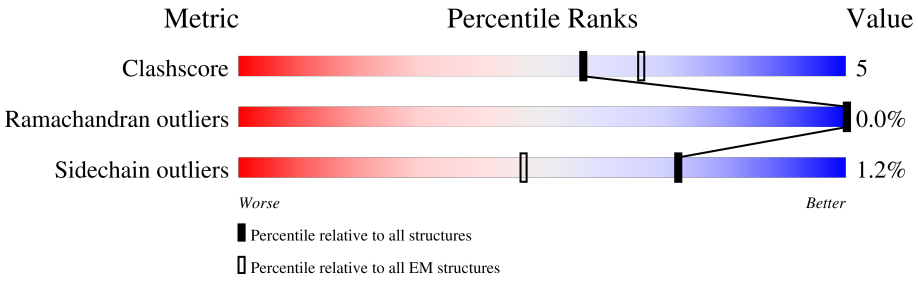
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.90 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.



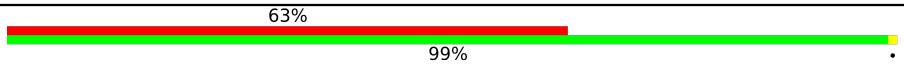
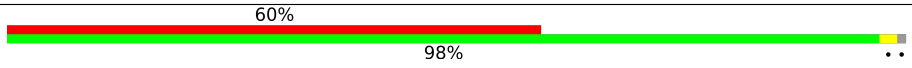
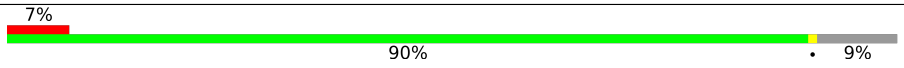
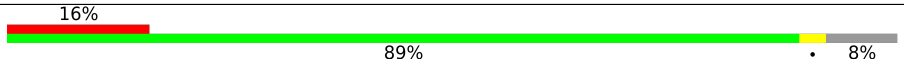
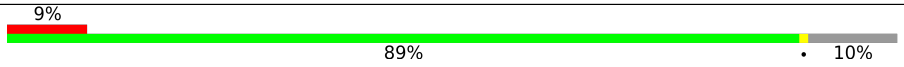
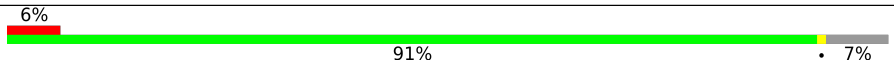
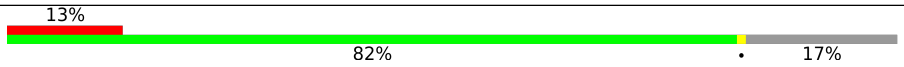
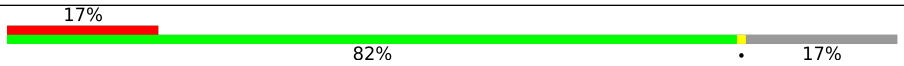
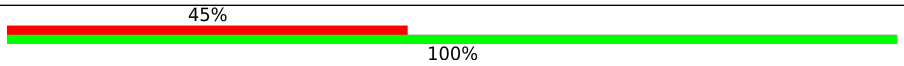
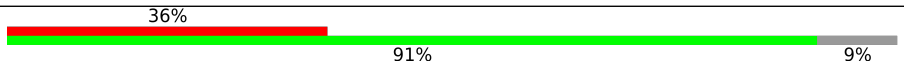
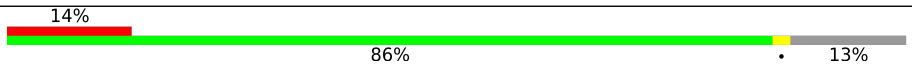
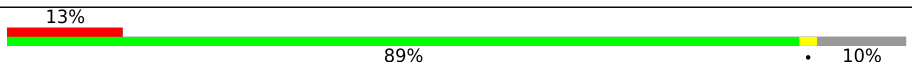
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	a1	446	6% 97%
1	a3	446	6% 98%
2	a2	439	7% 93% 6%
2	a4	439	5% 93% 6%
3	b1	379	8% 99%
3	b2	379	11% 99%
4	c1	240	10% 98%
4	c2	240	10% 98%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	f1	196	
5	f2	196	
6	d1	110	
6	d2	110	
7	q1	81	
7	q2	81	
8	h1	78	
8	h2	78	
9	x1	33	
9	x2	33	
10	i1	63	
10	i2	63	

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 31997 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 core protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a1	439	Total	C	N	O	S	0	0
			3409	2132	603	654	20		
1	a3	444	Total	C	N	O	S	0	0
			3447	2153	608	666	20		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a1	241	ILE	LEU	conflict	UNP W5Q5G6
a1	242	ARG	CYS	conflict	UNP W5Q5G6
a1	244	ARG	PRO	conflict	UNP W5Q5G6
a1	245	GLU	TRP	conflict	UNP W5Q5G6
a1	246	ASP	GLY	conflict	UNP W5Q5G6
a1	249	PRO	ALA	conflict	UNP W5Q5G6
a1	?	-	VAL	deletion	UNP W5Q5G6
a1	?	-	PRO	deletion	UNP W5Q5G6
a1	?	-	GLN	deletion	UNP W5Q5G6
a1	251	ALA	TRP	conflict	UNP W5Q5G6
a1	254	ALA	PRO	conflict	UNP W5Q5G6
a1	255	ILE	PHE	conflict	UNP W5Q5G6
a1	256	ALA	GLN	conflict	UNP W5Q5G6
a1	257	VAL	ILE	conflict	UNP W5Q5G6
a1	258	GLU	ARG	conflict	UNP W5Q5G6
a1	259	GLY	HIS	conflict	UNP W5Q5G6
a3	241	ILE	LEU	conflict	UNP W5Q5G6
a3	242	ARG	CYS	conflict	UNP W5Q5G6
a3	244	ARG	PRO	conflict	UNP W5Q5G6
a3	245	GLU	TRP	conflict	UNP W5Q5G6
a3	246	ASP	GLY	conflict	UNP W5Q5G6
a3	249	PRO	ALA	conflict	UNP W5Q5G6
a3	?	-	VAL	deletion	UNP W5Q5G6
a3	?	-	PRO	deletion	UNP W5Q5G6
a3	?	-	GLN	deletion	UNP W5Q5G6
a3	251	ALA	TRP	conflict	UNP W5Q5G6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
a3	254	ALA	PRO	conflict	UNP W5Q5G6
a3	255	ILE	PHE	conflict	UNP W5Q5G6
a3	256	ALA	GLN	conflict	UNP W5Q5G6
a3	257	VAL	ILE	conflict	UNP W5Q5G6
a3	258	GLU	ARG	conflict	UNP W5Q5G6
a3	259	GLY	HIS	conflict	UNP W5Q5G6

- Molecule 2 is a protein called Ubiquinol-cytochrome c reductase core protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a2	414	Total	C	N	O	S	0	0
			3126	1963	554	601	8		
2	a4	413	Total	C	N	O	S	0	0
			3122	1961	553	600	8		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	b1	378	Total	C	N	O	S	0	0
			3019	2029	471	498	21		
3	b2	378	Total	C	N	O	S	0	0
			3019	2029	471	498	21		

- Molecule 4 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	c1	239	Total	C	N	O	S	0	0
			1909	1219	330	345	15		
4	c2	238	Total	C	N	O	S	0	0
			1903	1216	329	343	15		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f1	196	Total	C	N	O	S	0	0
			1520	958	263	291	8		
5	f2	195	Total	C	N	O	S	0	0
			1514	955	262	289	8		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	d1	100	Total	C	N	O	S	0	0
			886	566	159	159	2		
6	d2	101	Total	C	N	O	S	0	0
			888	566	159	161	2		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d1	1	ALA	-	insertion	UNP W5P642
d1	2	GLY	SER	conflict	UNP W5P642
d1	3	ARG	ASP	conflict	UNP W5P642
d1	4	PRO	LEU	conflict	UNP W5P642
d1	5	ALA	SER	conflict	UNP W5P642
d2	1	ALA	-	insertion	UNP W5P642
d2	2	GLY	SER	conflict	UNP W5P642
d2	3	ARG	ASP	conflict	UNP W5P642
d2	4	PRO	LEU	conflict	UNP W5P642
d2	5	ALA	SER	conflict	UNP W5P642

- Molecule 7 is a protein called Ubiquinol-cytochrome c reductase complex III subunit VII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	q1	73	Total	C	N	O	S	0	0
			618	404	116	97	1		
7	q2	75	Total	C	N	O	S	0	0
			631	413	118	99	1		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h1	65	Total	C	N	O	S	0	0
			532	324	96	107	5		
8	h2	65	Total	C	N	O	S	0	0
			532	324	96	107	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h1	38	GLU	LYS	conflict	UNP W5PZC9
h2	38	GLU	LYS	conflict	UNP W5PZC9

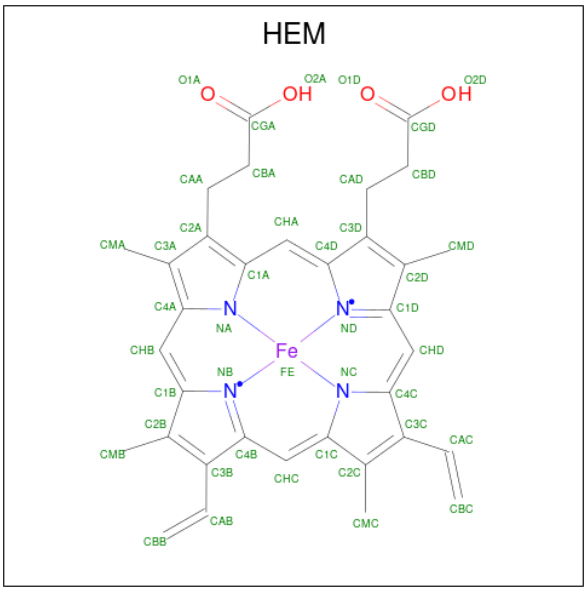
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	x1	33	Total 164	C 98	N 33	O 33	0	0
9	x2	30	Total 150	C 90	N 30	O 30	0	0

- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase, complex III subunit X.

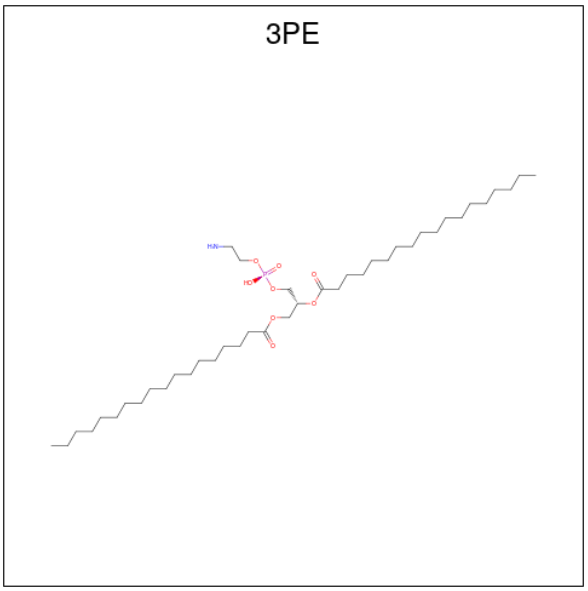
Mol	Chain	Residues	Atoms				AltConf	Trace
10	i1	55	Total 459	C 303	N 80	O 76	0	0
10	i2	57	Total 473	C 312	N 82	O 79	0	0

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



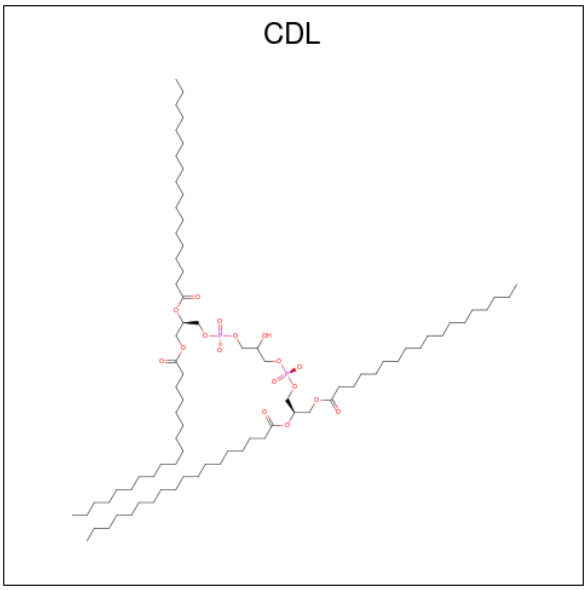
Mol	Chain	Residues	Atoms					AltConf
11	b1	1	Total 86	C 68	Fe 2	N 8	O 8	0
11	b1	1	Total 86	C 68	Fe 2	N 8	O 8	0
11	b2	1	Total 86	C 68	Fe 2	N 8	O 8	0
11	b2	1	Total 86	C 68	Fe 2	N 8	O 8	0

- Molecule 12 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



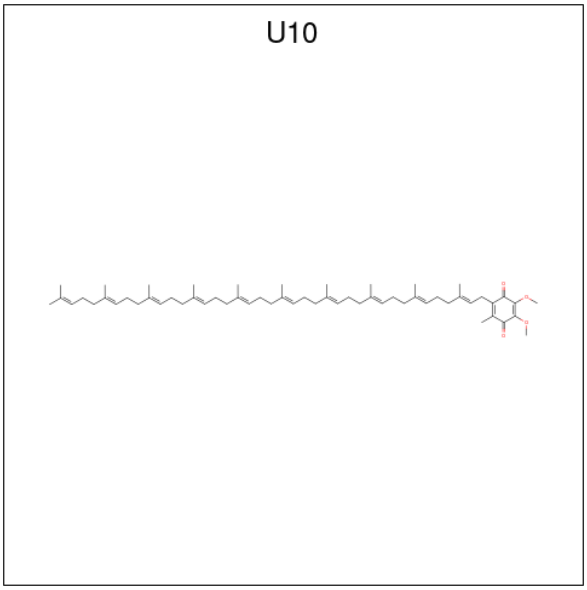
Mol	Chain	Residues	Atoms					AltConf
12	b1	1	Total	C	N	O	P	0
			43	33	1	8	1	
12	c1	1	Total	C	N	O	P	0
			13	5	1	6	1	
12	b2	1	Total	C	N	O	P	0
			37	27	1	8	1	
12	f2	1	Total	C	N	O	P	0
			23	13	1	8	1	

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



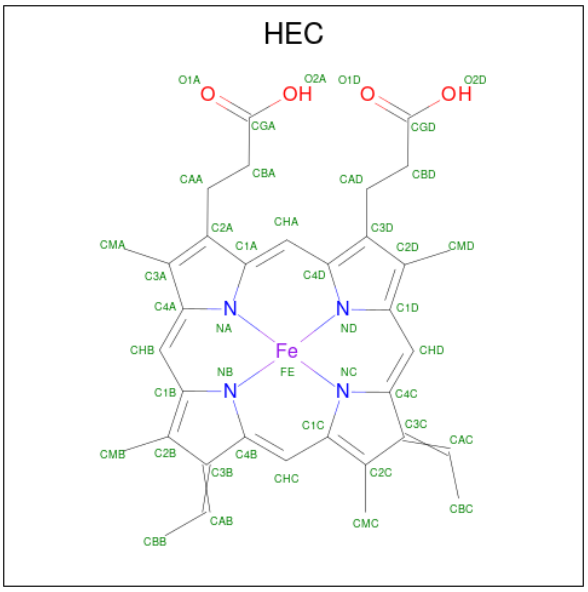
Mol	Chain	Residues	Atoms				AltConf
13	b1	1	Total	C	O	P	0
			80	42	34	4	
13	b1	1	Total	C	O	P	0
			80	42	34	4	
13	c1	1	Total	C	O	P	0
			49	30	17	2	
13	b2	1	Total	C	O	P	0
			41	22	17	2	
13	c2	1	Total	C	O	P	0
			48	29	17	2	

- Molecule 14 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



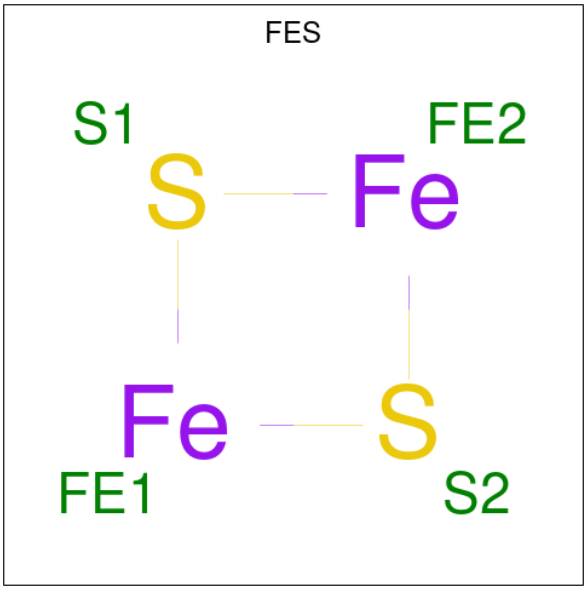
Mol	Chain	Residues	Atoms			AltConf
14	b1	1	Total	C	O	0
			51	43	8	
14	b1	1	Total	C	O	0
			51	43	8	
14	b2	1	Total	C	O	0
			25	21	4	

- Molecule 15 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
15	c1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
15	c2	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



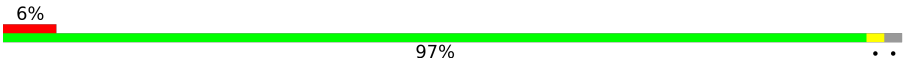
Mol	Chain	Residues	Atoms				AltConf
16	f1	1	Total	Fe	S		0
			4	2	2		
16	f2	1	Total	Fe	S		0
			4	2	2		

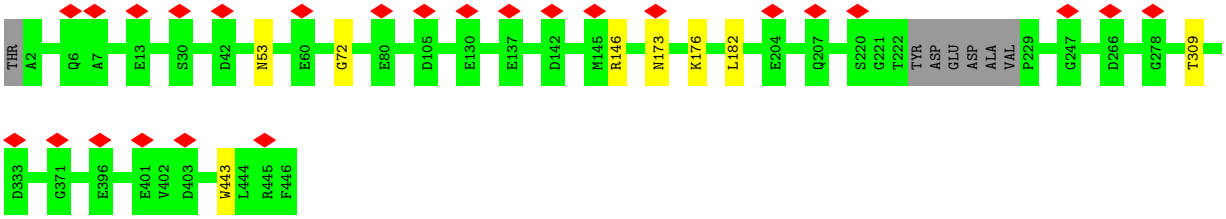
3 Residue-property plots (i)

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 core protein 1

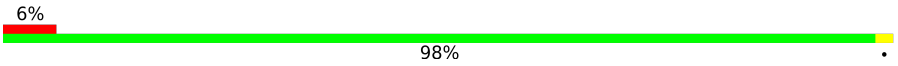
Chain a1:

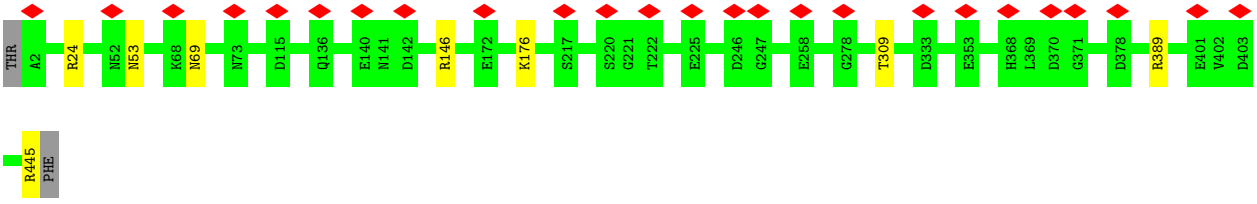




• Molecule 1: Ubiquinol-cytochrome c reductase core protein 1

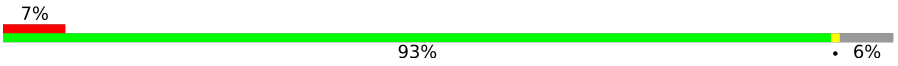
Chain a3:

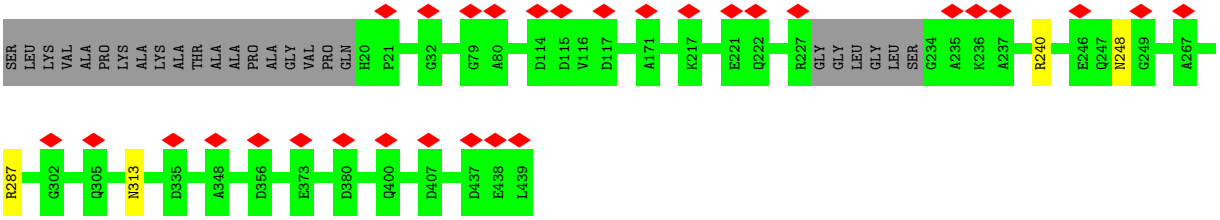




• Molecule 2: Ubiquinol-cytochrome c reductase core protein 2

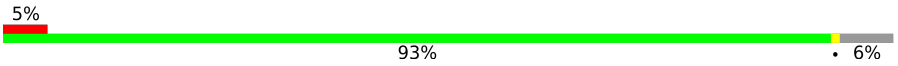
Chain a2:

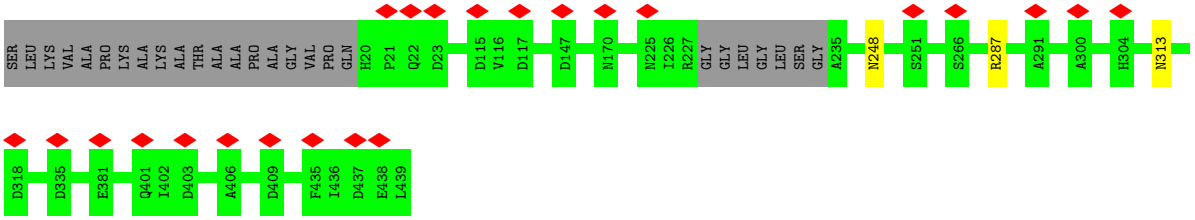




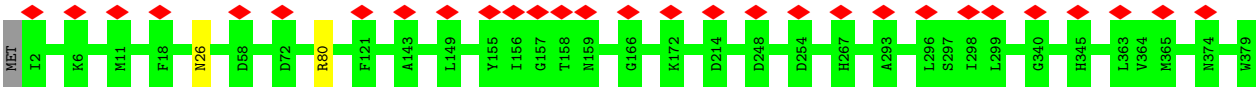
• Molecule 2: Ubiquinol-cytochrome c reductase core protein 2

Chain a4:

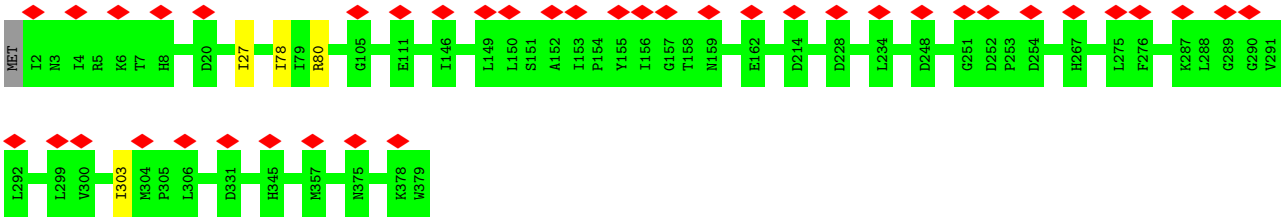




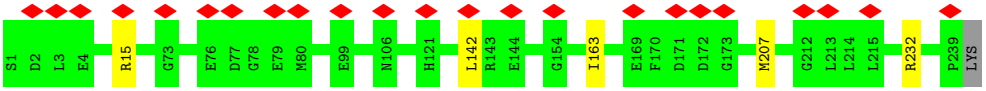
• Molecule 3: Cytochrome b



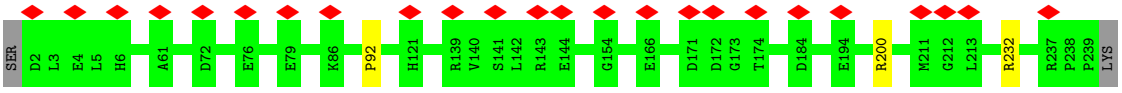
• Molecule 3: Cytochrome b



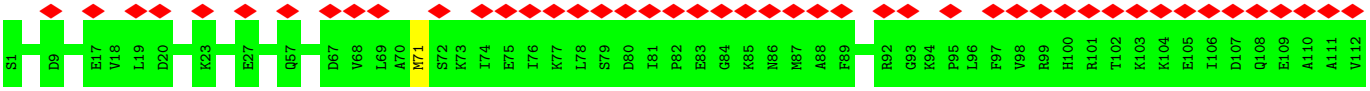
• Molecule 4: Cytochrome c1

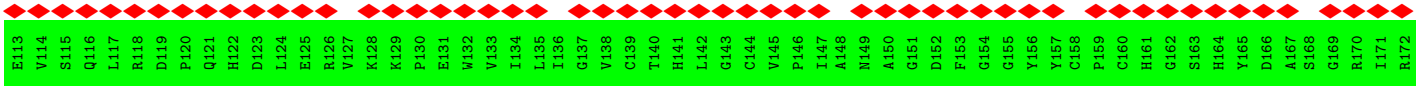


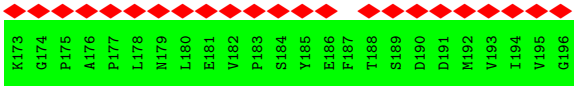
• Molecule 4: Cytochrome c1



• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

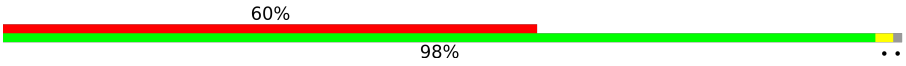


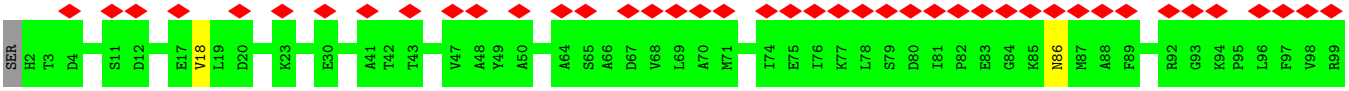


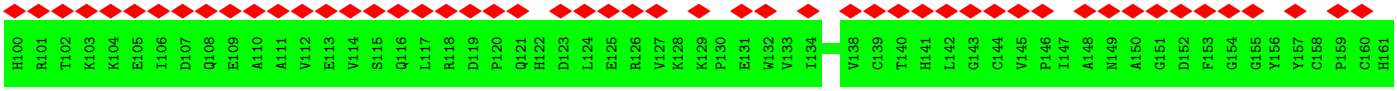


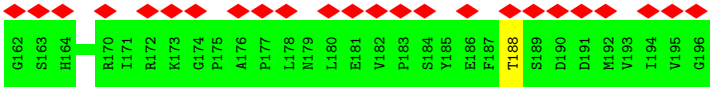
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain f2:



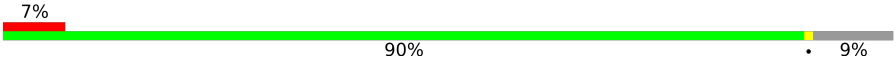


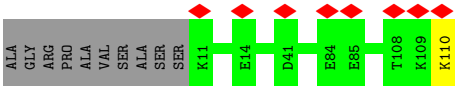




• Molecule 6: Cytochrome b-c1 complex subunit 7

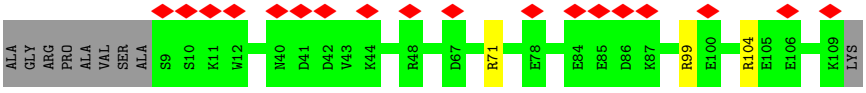
Chain d1:





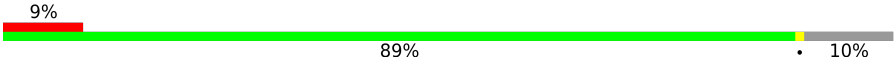
• Molecule 6: Cytochrome b-c1 complex subunit 7

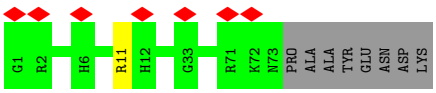
Chain d2:



• Molecule 7: Ubiquinol-cytochrome c reductase complex III subunit VII

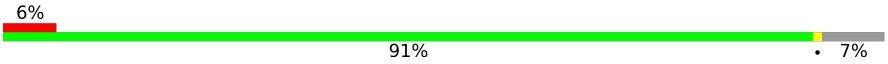
Chain q1:

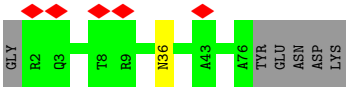




• Molecule 7: Ubiquinol-cytochrome c reductase complex III subunit VII

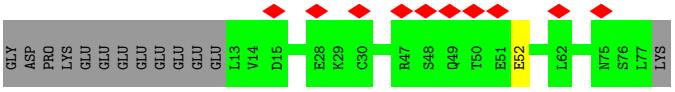
Chain q2:





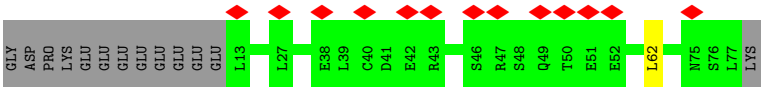
• Molecule 8: Cytochrome b-c1 complex subunit 6

Chain h1:



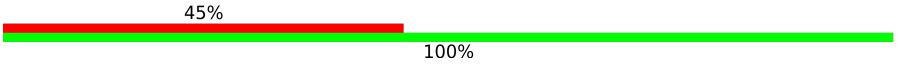
• Molecule 8: Cytochrome b-c1 complex subunit 6

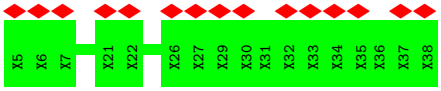
Chain h2:



• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

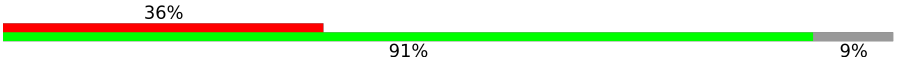
Chain x1:

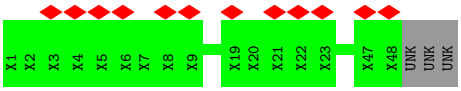




• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

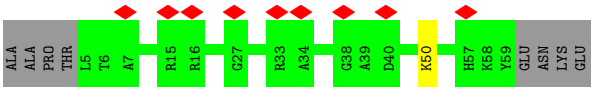
Chain x2:





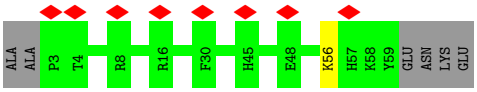
• Molecule 10: Ubiquinol-cytochrome c reductase, complex III subunit X

Chain i1:



• Molecule 10: Ubiquinol-cytochrome c reductase, complex III subunit X

Chain i2:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	102314	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.800	Depositor
Minimum map value	-0.326	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	509.6, 509.6, 509.6	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, HEM, FES, HEC, CDL, U10

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	a1	0.38	0/3479	0.61	0/4719
1	a3	0.37	0/3518	0.59	0/4776
2	a2	0.36	0/3183	0.56	0/4313
2	a4	0.37	0/3179	0.59	0/4308
3	b1	0.41	0/3119	0.61	0/4268
3	b2	0.39	0/3119	0.60	1/4268 (0.0%)
4	c1	0.40	0/1968	0.59	1/2672 (0.0%)
4	c2	0.38	0/1962	0.60	0/2664
5	f1	0.30	0/1554	0.50	0/2101
5	f2	0.31	0/1548	0.55	0/2093
6	d1	0.37	0/906	0.54	0/1213
6	d2	0.34	0/908	0.54	0/1218
7	q1	0.39	0/638	0.57	0/862
7	q2	0.40	0/652	0.58	0/883
8	h1	0.31	0/538	0.62	0/723
8	h2	0.33	0/538	0.71	1/723 (0.1%)
10	i1	0.34	0/471	0.53	0/634
10	i2	0.32	0/486	0.51	0/655
All	All	0.37	0/31766	0.58	3/43093 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a1	0	2
1	a3	0	1
4	c2	0	1
5	f2	0	2
7	q1	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
8	h1	0	1
All	All	0	8

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	h2	62	LEU	CA-CB-CG	5.89	128.85	115.30
4	c1	207	MET	CB-CG-SD	-5.08	97.17	112.40
3	b2	303	ILE	CG1-CB-CG2	-5.06	100.27	111.40

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a1	309	THR	Peptide
1	a1	443	TRP	Peptide
1	a3	309	THR	Peptide
8	h1	52	GLU	Peptide
7	q1	11	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a1	3409	0	3322	0	0
1	a3	3447	0	3350	0	0
2	a2	3126	0	3093	0	0
2	a4	3122	0	3090	0	0
3	b1	3019	0	3082	0	0
3	b2	3019	0	3082	0	0
4	c1	1909	0	1858	0	0
4	c2	1903	0	1850	0	0
5	f1	1520	0	1505	0	0
5	f2	1514	0	1497	0	0
6	d1	886	0	883	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	d2	888	0	880	0	0
7	q1	618	0	628	0	0
7	q2	631	0	639	0	0
8	h1	532	0	509	0	0
8	h2	532	0	509	0	0
9	x1	164	0	40	0	0
9	x2	150	0	44	0	0
10	i1	459	0	462	0	0
10	i2	473	0	477	0	0
11	b1	86	0	60	0	0
11	b2	86	0	60	0	0
12	b1	43	0	63	0	0
12	b2	37	0	48	0	0
12	c1	13	0	12	0	0
12	f2	23	0	20	0	0
13	b1	80	0	48	0	0
13	b2	41	0	26	0	0
13	c1	49	0	42	0	0
13	c2	48	0	40	0	0
14	b1	51	0	54	0	0
14	b2	25	0	27	0	0
15	c1	43	0	30	0	0
15	c2	43	0	30	0	0
16	f1	4	0	0	0	0
16	f2	4	0	0	0	0
All	All	31997	0	31360	0	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 5.

There are no clashes within the asymmetric unit.

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	a1	435/446 (98%)	398 (92%)	36 (8%)	1 (0%)	47 79
1	a3	442/446 (99%)	409 (92%)	33 (8%)	0	100 100
2	a2	410/439 (93%)	382 (93%)	28 (7%)	0	100 100
2	a4	409/439 (93%)	375 (92%)	34 (8%)	0	100 100
3	b1	376/379 (99%)	357 (95%)	19 (5%)	0	100 100
3	b2	376/379 (99%)	356 (95%)	20 (5%)	0	100 100
4	c1	237/240 (99%)	197 (83%)	40 (17%)	0	100 100
4	c2	236/240 (98%)	197 (84%)	39 (16%)	0	100 100
5	f1	194/196 (99%)	177 (91%)	17 (9%)	0	100 100
5	f2	193/196 (98%)	172 (89%)	21 (11%)	0	100 100
6	d1	98/110 (89%)	94 (96%)	4 (4%)	0	100 100
6	d2	99/110 (90%)	95 (96%)	4 (4%)	0	100 100
7	q1	71/81 (88%)	66 (93%)	5 (7%)	0	100 100
7	q2	73/81 (90%)	63 (86%)	10 (14%)	0	100 100
8	h1	63/78 (81%)	56 (89%)	7 (11%)	0	100 100
8	h2	63/78 (81%)	58 (92%)	5 (8%)	0	100 100
10	i1	53/63 (84%)	50 (94%)	3 (6%)	0	100 100
10	i2	55/63 (87%)	51 (93%)	4 (7%)	0	100 100
All	All	3883/4064 (96%)	3553 (92%)	329 (8%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a1	72	GLY

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	a1	366/372 (98%)	361 (99%)	5 (1%)	67 81

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	a3	370/372 (100%)	363 (98%)	7 (2%)	57 75
2	a2	326/341 (96%)	322 (99%)	4 (1%)	71 83
2	a4	326/341 (96%)	323 (99%)	3 (1%)	78 87
3	b1	330/331 (100%)	328 (99%)	2 (1%)	86 91
3	b2	330/331 (100%)	327 (99%)	3 (1%)	78 87
4	c1	205/206 (100%)	201 (98%)	4 (2%)	55 74
4	c2	204/206 (99%)	202 (99%)	2 (1%)	76 86
5	f1	168/168 (100%)	167 (99%)	1 (1%)	86 91
5	f2	167/168 (99%)	166 (99%)	1 (1%)	86 91
6	d1	93/99 (94%)	92 (99%)	1 (1%)	73 84
6	d2	94/99 (95%)	91 (97%)	3 (3%)	39 63
7	q1	66/72 (92%)	66 (100%)	0	100 100
7	q2	67/72 (93%)	66 (98%)	1 (2%)	65 80
8	h1	62/74 (84%)	62 (100%)	0	100 100
8	h2	62/74 (84%)	62 (100%)	0	100 100
10	i1	46/52 (88%)	45 (98%)	1 (2%)	52 71
10	i2	48/52 (92%)	47 (98%)	1 (2%)	53 73
All	All	3330/3430 (97%)	3291 (99%)	39 (1%)	72 83

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

Mol	Chain	Res	Type
3	b2	27	ILE
6	d2	99	ARG
3	b2	78	ILE
4	c2	232	ARG
7	q2	36	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
2	a4	162	ASN
4	c2	23	HIS
2	a4	170	ASN
3	b2	85	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	c2	165	ASN

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)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	3PE	c1	502	-	12,12,50	0.61	0	13,15,55	0.56	0
13	CDL	b1	404	-	41,41,99	0.45	0	47,53,111	0.41	0
13	CDL	b2	404	-	40,40,99	0.47	0	46,52,111	0.64	1 (2%)
11	HEM	b2	402	3	41,50,50	1.41	5 (12%)	45,82,82	1.90	11 (24%)
13	CDL	c2	502	-	47,47,99	0.44	0	53,59,111	0.64	2 (3%)
11	HEM	b1	402	3	41,50,50	1.43	5 (12%)	45,82,82	1.87	13 (28%)
16	FES	f2	202	5	0,4,4	-	-	-		
14	U10	b1	406	-	28,28,63	2.65	12 (42%)	34,37,79	1.52	7 (20%)
13	CDL	b1	405	-	37,37,99	0.44	0	43,49,111	0.42	0
11	HEM	b2	401	3	41,50,50	1.32	4 (9%)	45,82,82	1.72	8 (17%)
16	FES	f1	501	5	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	U10	b2	405	-	25,25,63	2.94	12 (48%)	30,33,79	1.64	7 (23%)
15	HEC	c1	501	4	32,50,50	2.09	4 (12%)	24,82,82	2.61	13 (54%)
12	3PE	b1	403	-	42,42,50	0.33	0	45,47,55	0.33	0
15	HEC	c2	501	4	32,50,50	2.21	4 (12%)	24,82,82	2.50	15 (62%)
12	3PE	b2	403	-	36,36,50	0.35	0	39,41,55	0.33	0
11	HEM	b1	401	3	41,50,50	1.38	4 (9%)	45,82,82	1.87	14 (31%)
14	U10	b1	407	-	23,23,63	2.83	9 (39%)	28,31,79	1.29	5 (17%)
12	3PE	f2	201	-	22,22,50	0.45	0	25,27,55	0.45	0
13	CDL	c1	503	-	48,48,99	0.41	0	54,60,111	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	3PE	c1	502	-	-	8/13/13/54	-
13	CDL	b1	404	-	-	9/52/52/110	-
13	CDL	b2	404	-	-	16/51/51/110	-
11	HEM	b2	402	3	-	5/12/54/54	-
13	CDL	c2	502	-	-	10/58/58/110	-
11	HEM	b1	402	3	-	4/12/54/54	-
16	FES	f2	202	5	-	-	0/1/1/1
14	U10	b1	406	-	-	7/21/45/87	0/1/1/1
13	CDL	b1	405	-	-	11/46/46/110	-
11	HEM	b2	401	3	-	5/12/54/54	-
16	FES	f1	501	5	-	-	0/1/1/1
14	U10	b2	405	-	-	5/18/42/87	0/1/1/1
15	HEC	c1	501	4	-	3/10/54/54	-
12	3PE	b1	403	-	-	14/46/46/54	-
15	HEC	c2	501	4	-	2/10/54/54	-
12	3PE	b2	403	-	-	8/40/40/54	-
11	HEM	b1	401	3	-	3/12/54/54	-
14	U10	b1	407	-	-	1/15/39/87	0/1/1/1
12	3PE	f2	201	-	-	5/26/26/54	-
13	CDL	c1	503	-	-	15/59/59/110	-

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b2	405	U10	C6-C1	10.73	1.54	1.35
14	b1	407	U10	C6-C1	9.91	1.53	1.35
14	b1	406	U10	C6-C1	9.71	1.52	1.35
15	c2	501	HEC	C3C-C2C	-7.82	1.32	1.40
15	c1	501	HEC	C3C-C2C	-7.30	1.33	1.40

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c1	501	HEC	CMB-C2B-C3B	5.84	132.68	125.82
11	b1	402	HEM	CHC-C4B-NB	5.35	130.25	124.43
11	b2	401	HEM	CHC-C4B-NB	5.07	129.94	124.43
11	b1	401	HEM	CHC-C4B-NB	5.07	129.94	124.43
11	b2	402	HEM	CHC-C4B-NB	5.06	129.93	124.43

There are no chirality outliers.

5 of 131 torsion outliers are listed below:

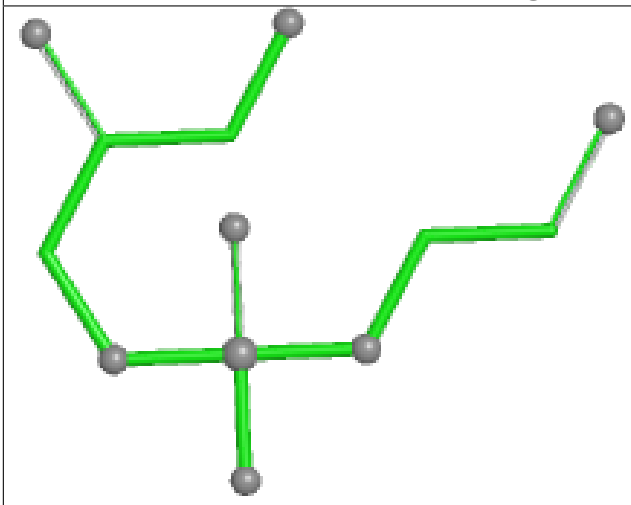
Mol	Chain	Res	Type	Atoms
11	b1	401	HEM	C2B-C3B-CAB-CBB
11	b1	402	HEM	C2B-C3B-CAB-CBB
11	b1	402	HEM	C4B-C3B-CAB-CBB
11	b2	401	HEM	C2A-CAA-CBA-CGA
11	b2	401	HEM	C2B-C3B-CAB-CBB

There are no ring outliers.

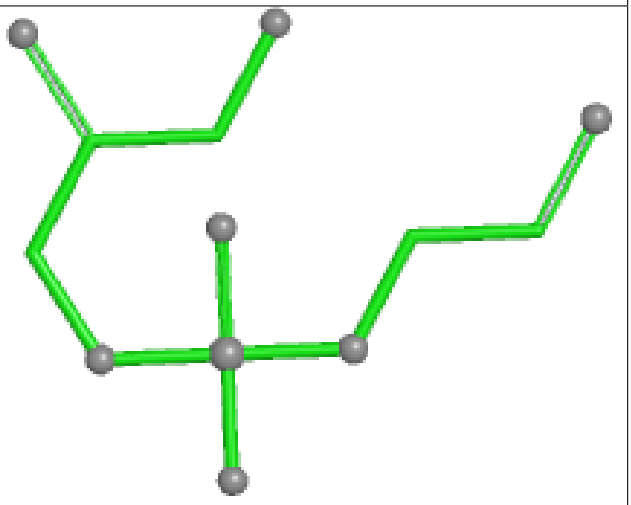
No monomer is involved in short contacts.

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.

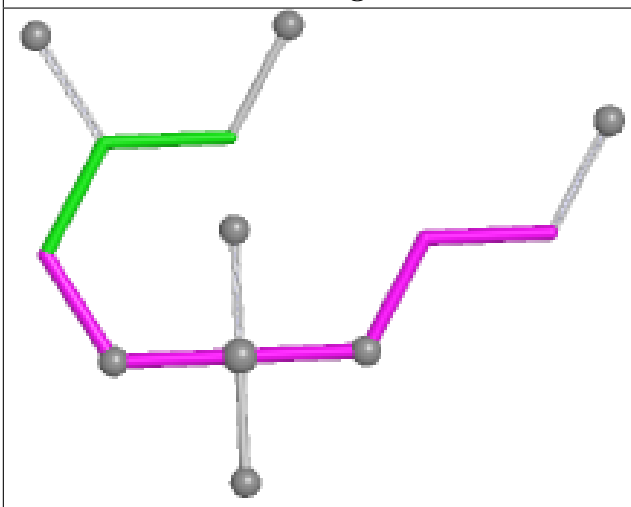
Ligand 3PE c1 502



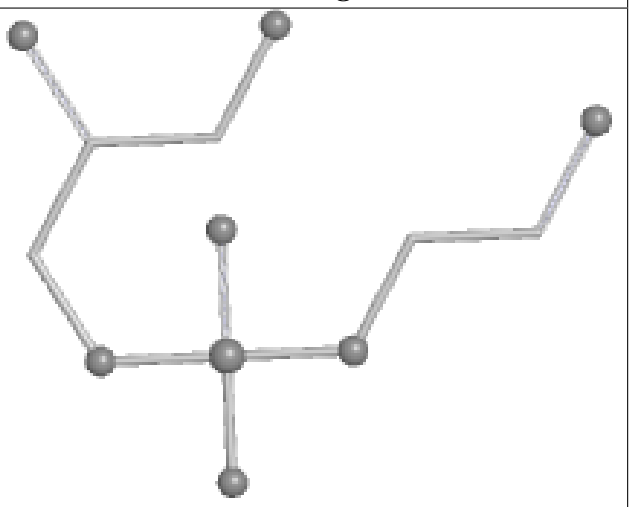
Bond lengths



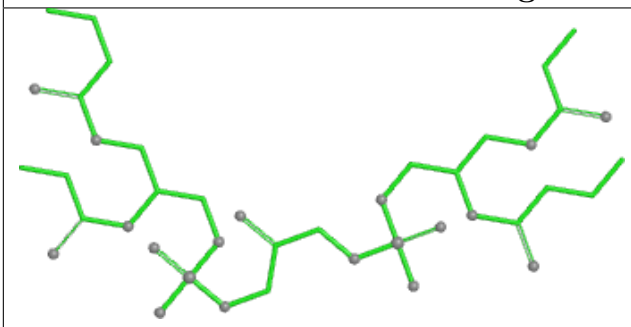
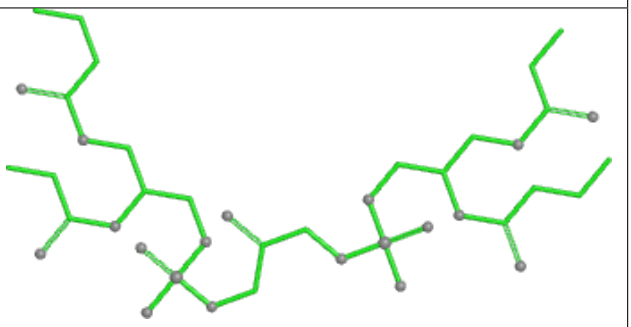
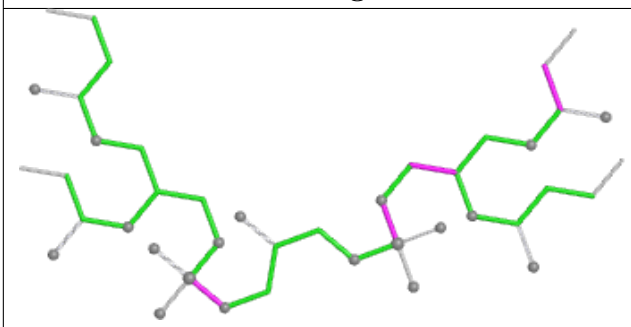
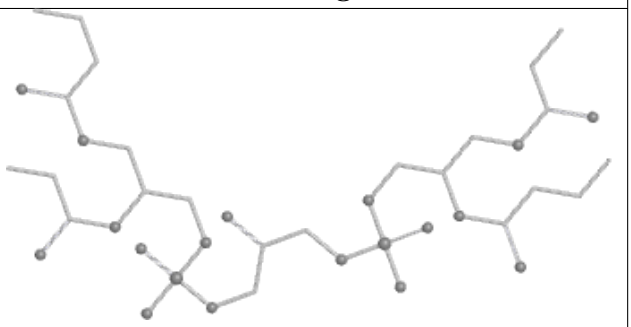
Bond angles

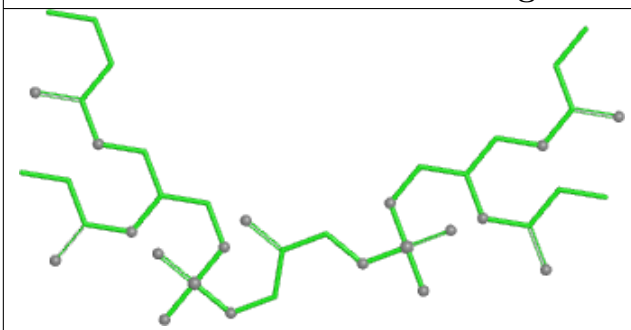
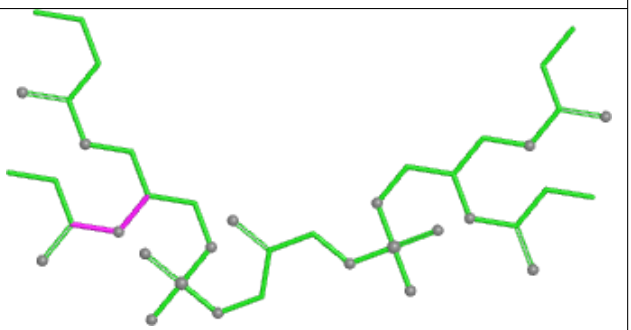
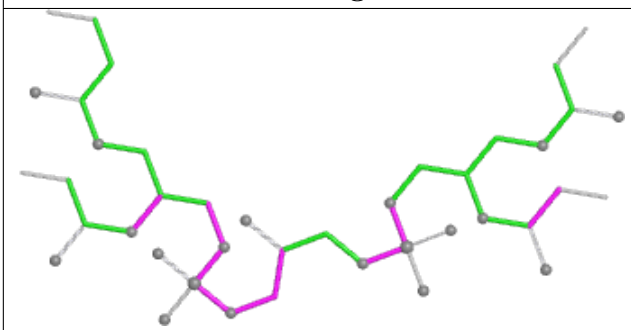
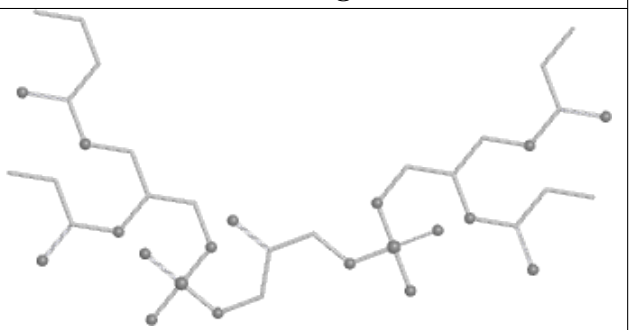


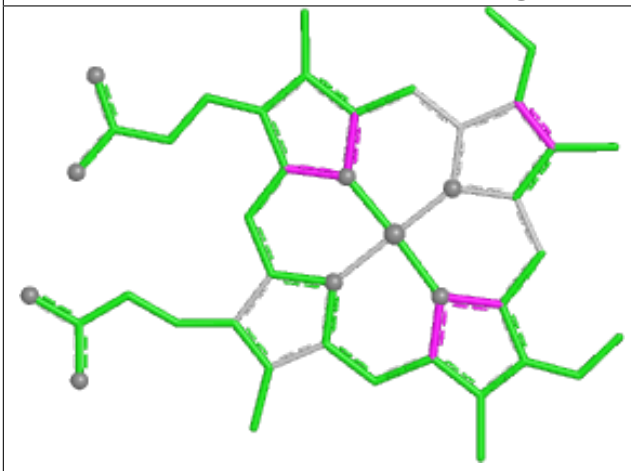
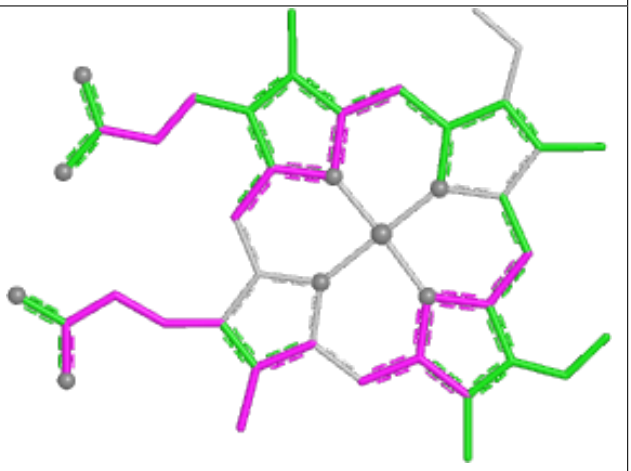
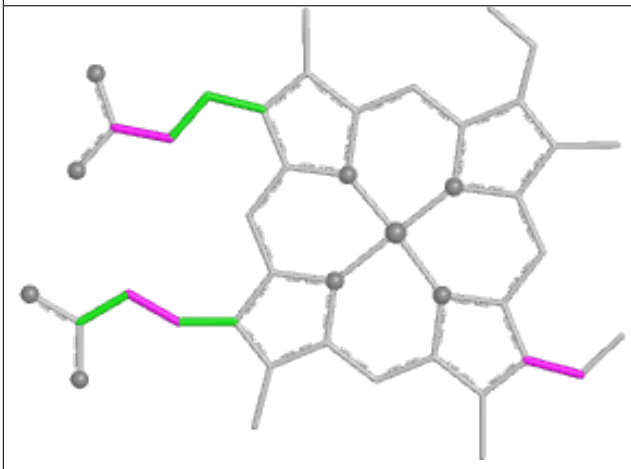
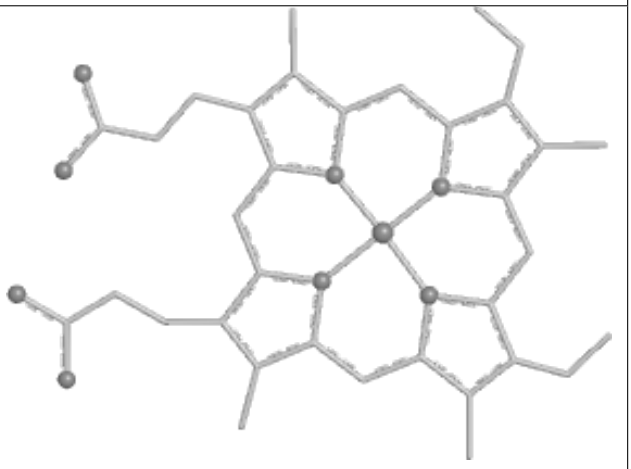
Torsions

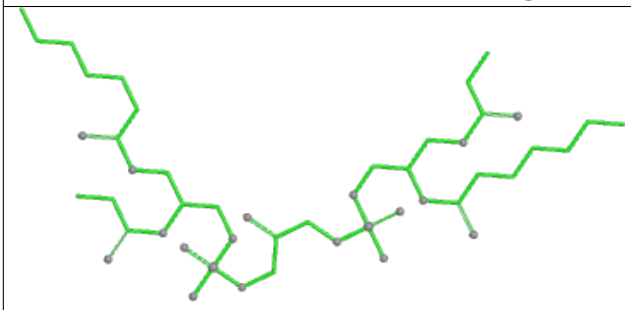
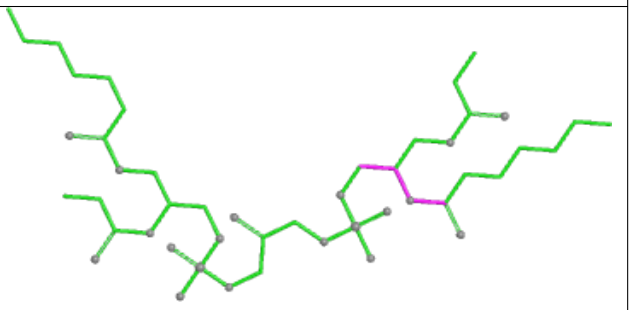
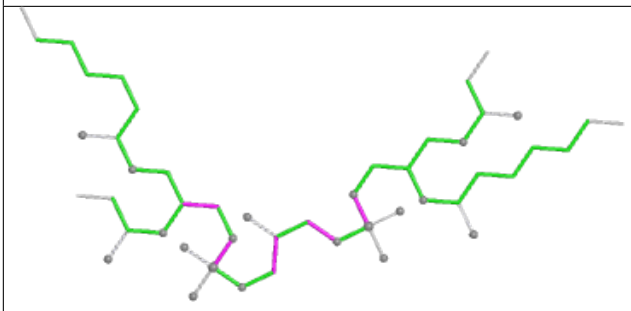
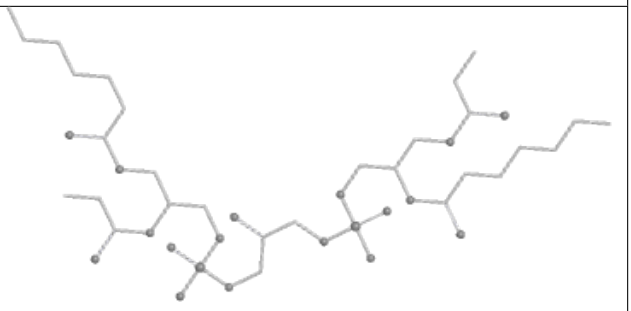


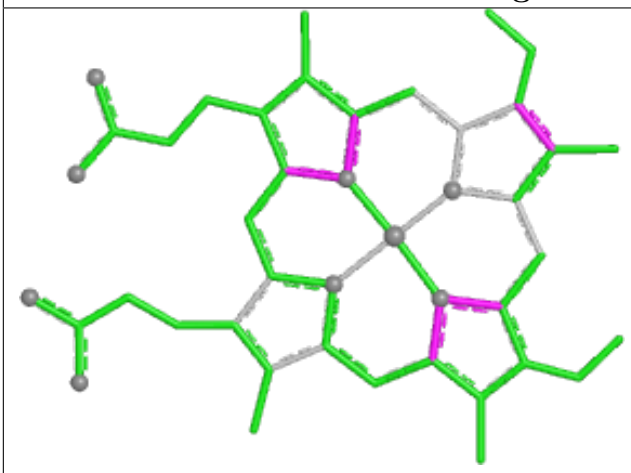
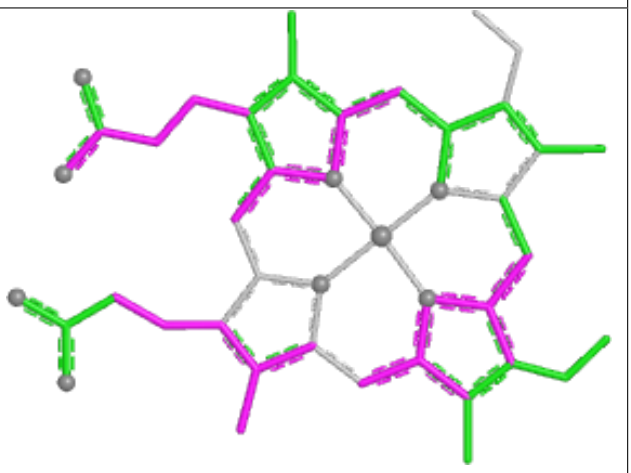
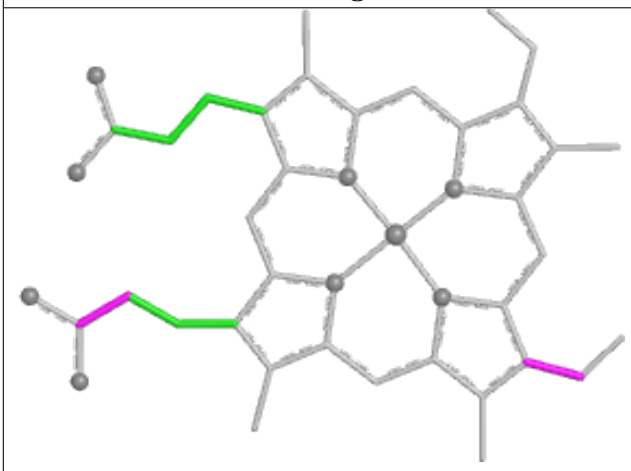
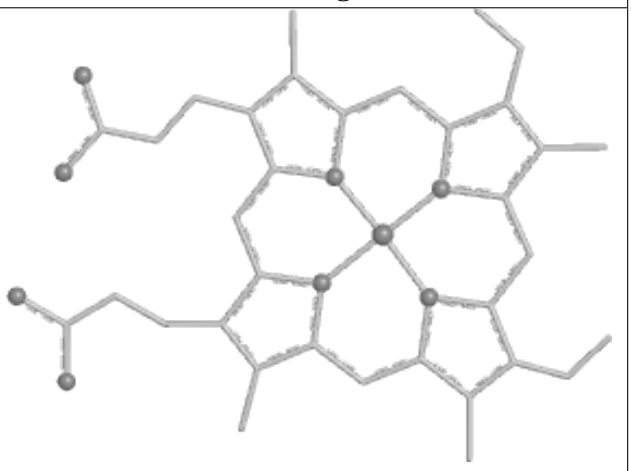
Rings

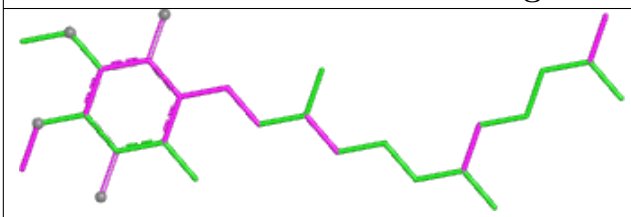
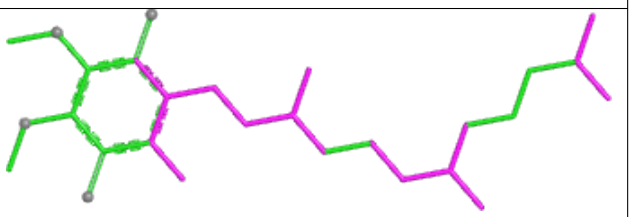
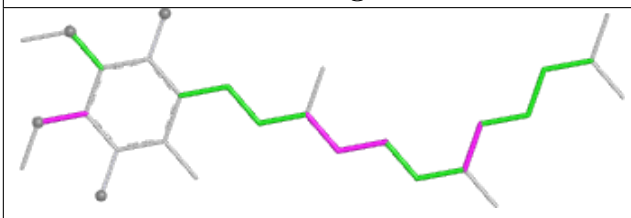
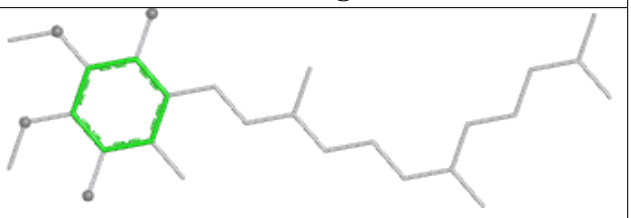
Ligand CDL b1 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

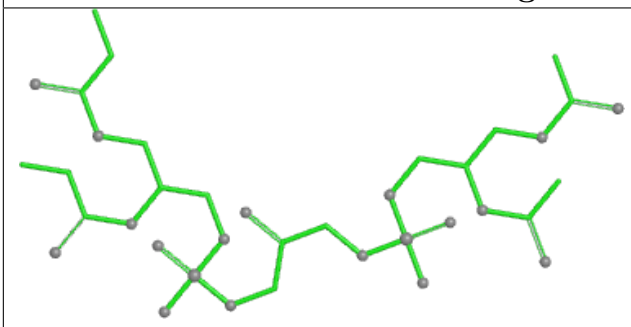
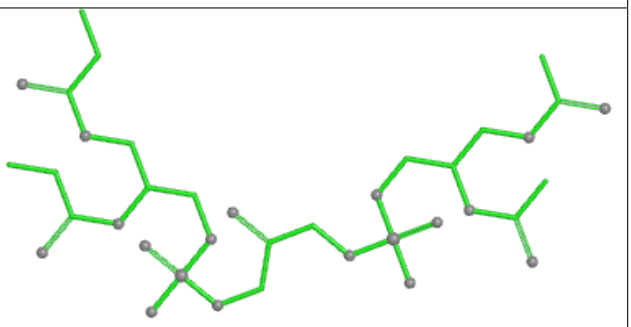
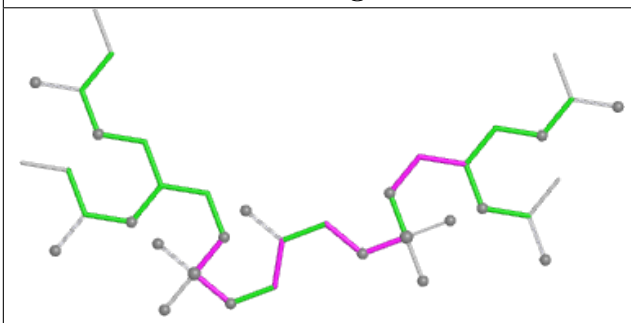
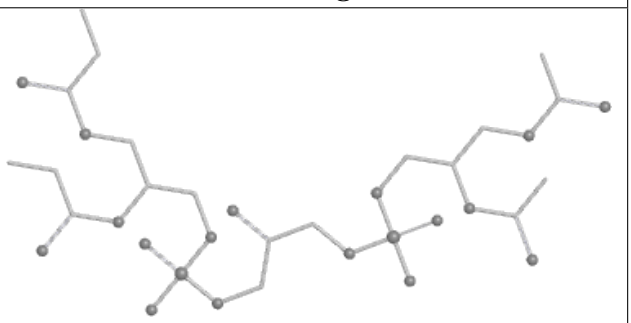
Ligand CDL b2 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

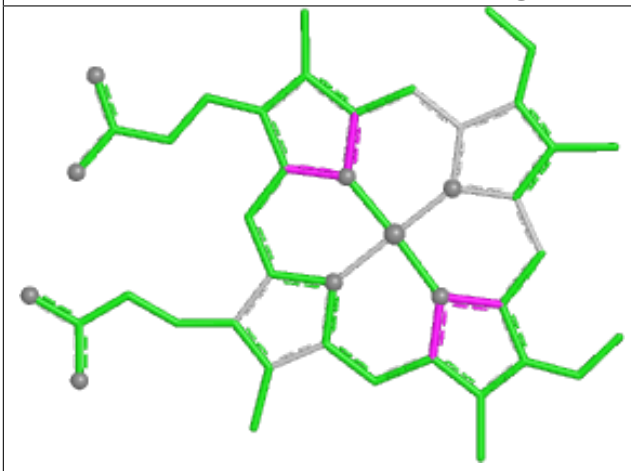
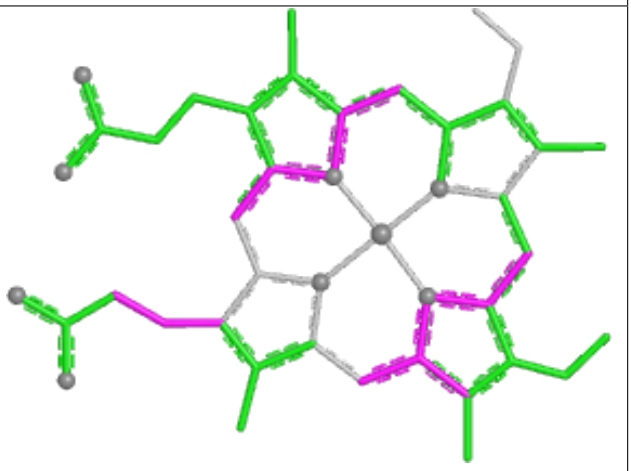
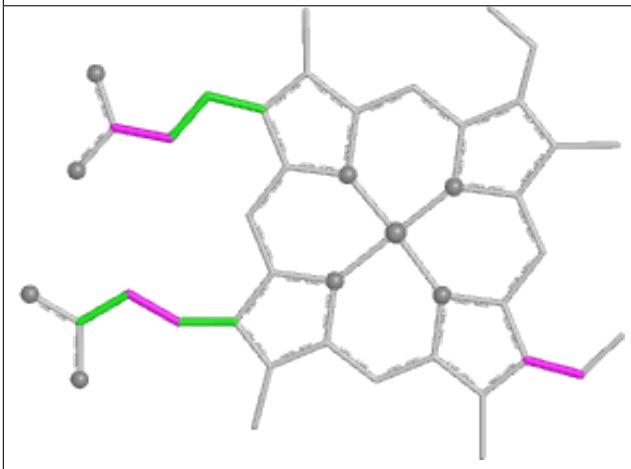
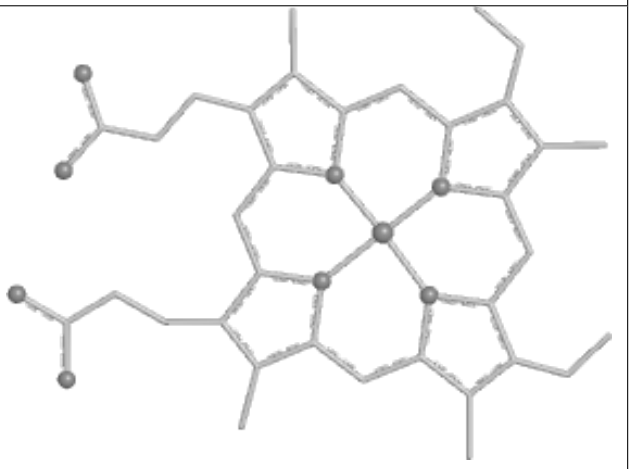
Ligand HEM b2 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

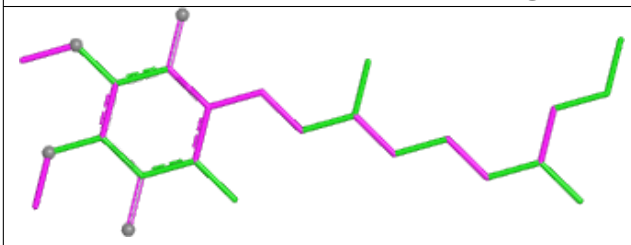
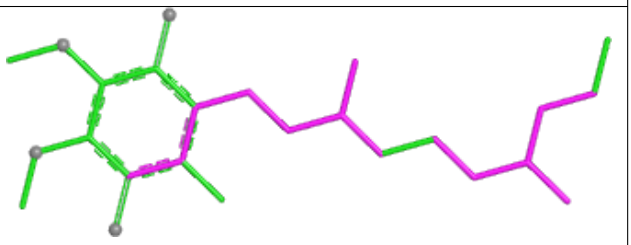
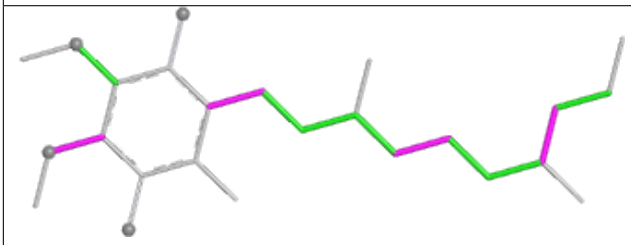
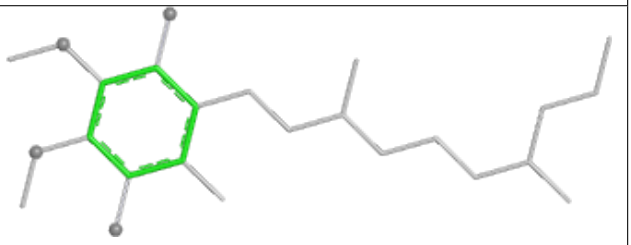
Ligand CDL c2 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand HEM b1 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

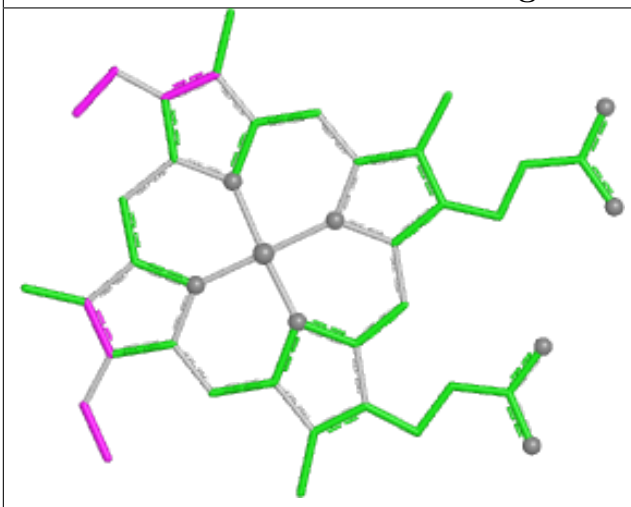
Ligand U10 b1 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL b1 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

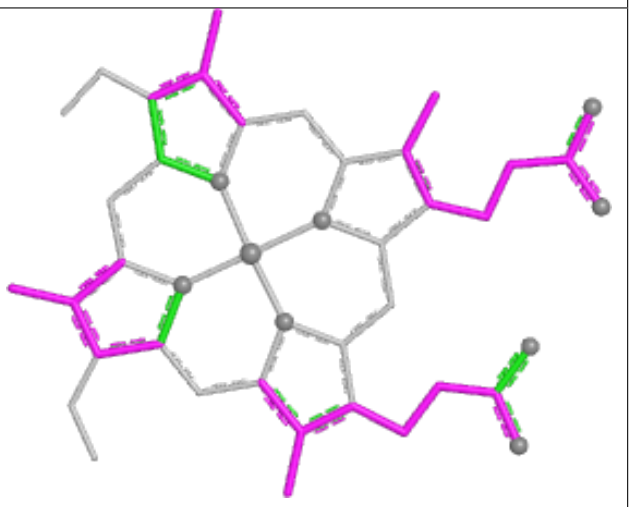
Ligand HEM b2 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand U10 b2 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

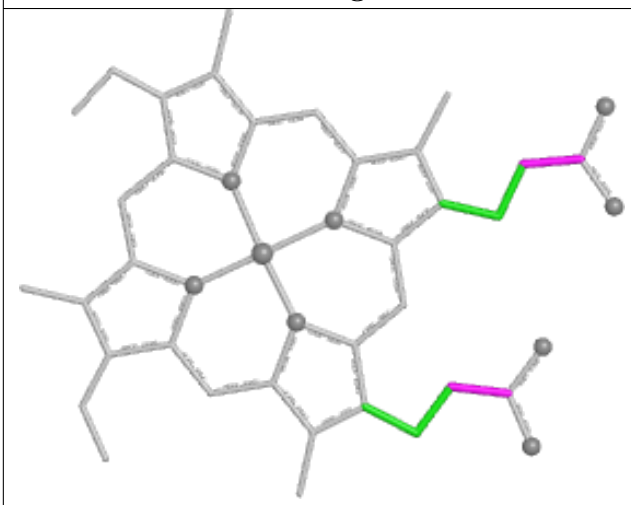
Ligand HEC c1 501



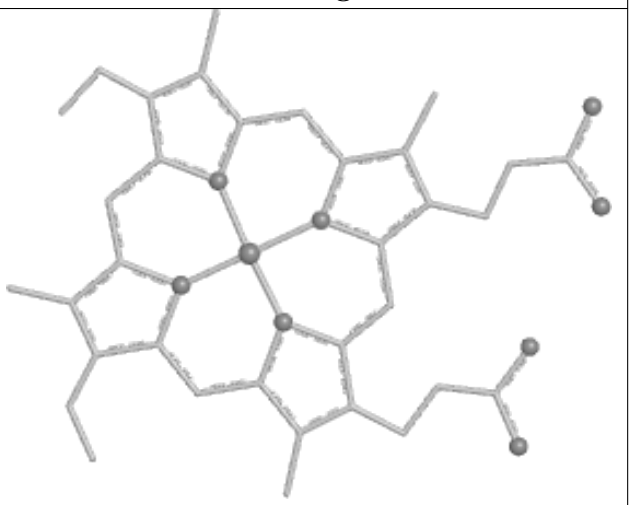
Bond lengths



Bond angles

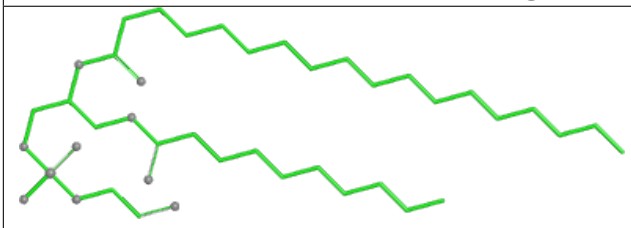


Torsions

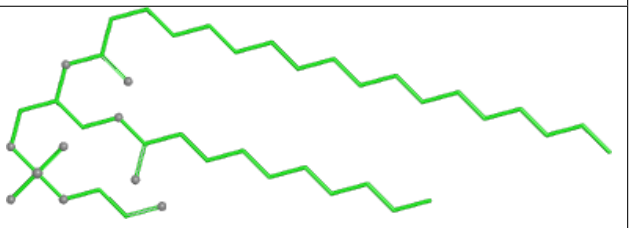


Rings

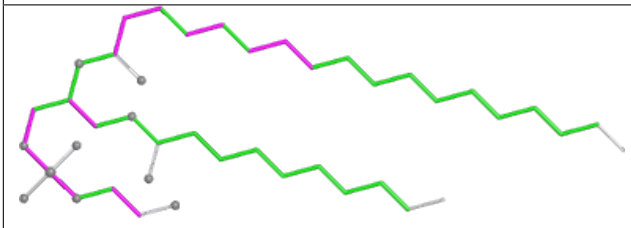
Ligand 3PE b1 403



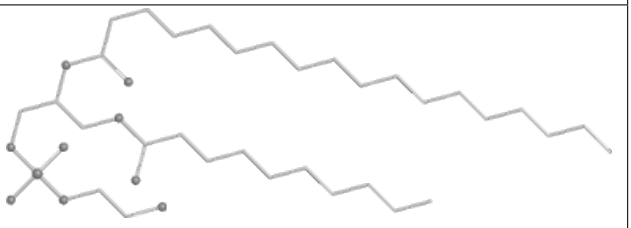
Bond lengths



Bond angles

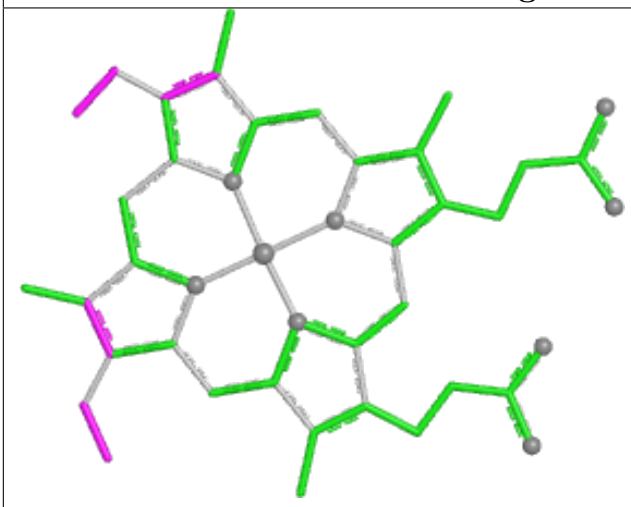


Torsions

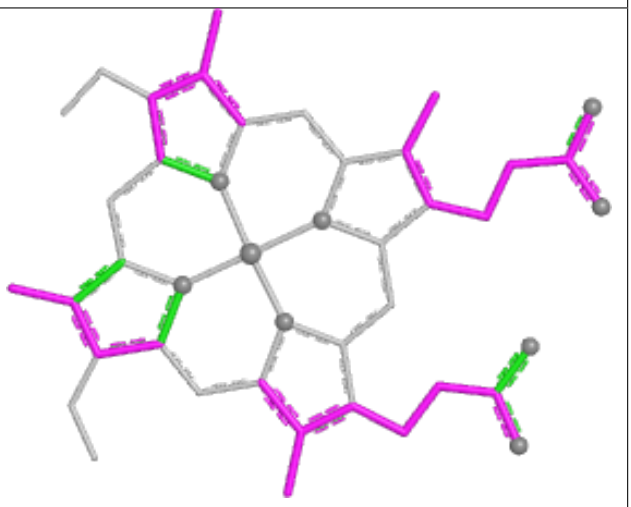


Rings

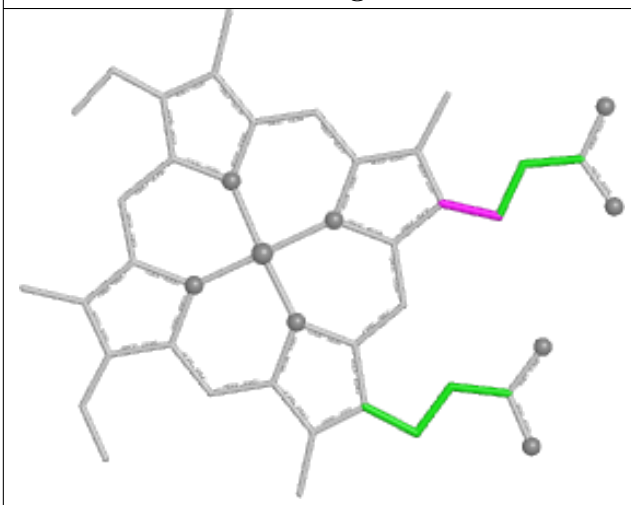
Ligand HEC c2 501



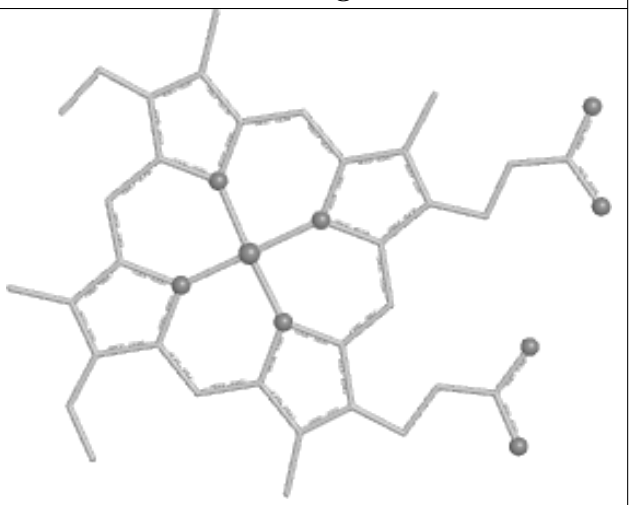
Bond lengths



Bond angles

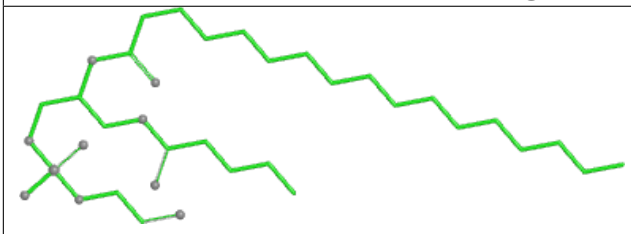


Torsions

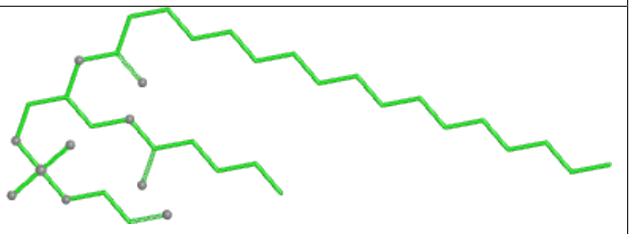


Rings

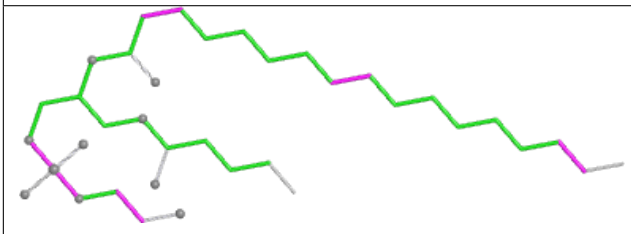
Ligand 3PE b2 403



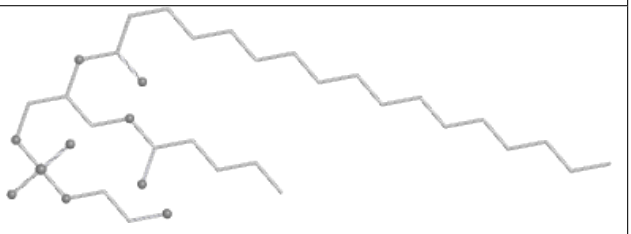
Bond lengths



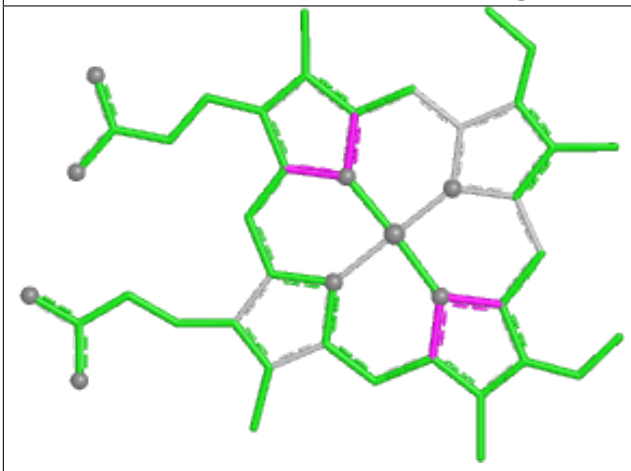
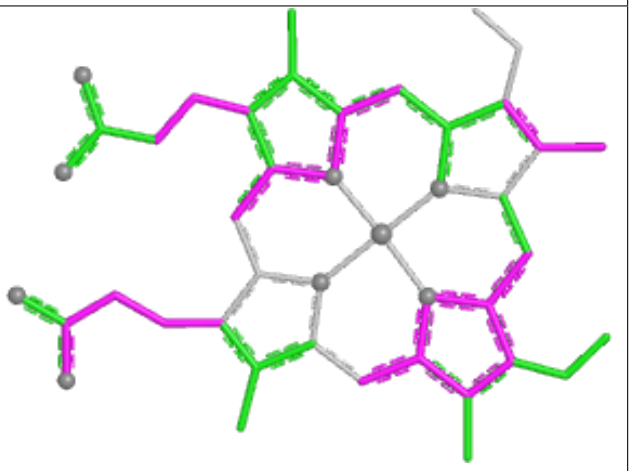
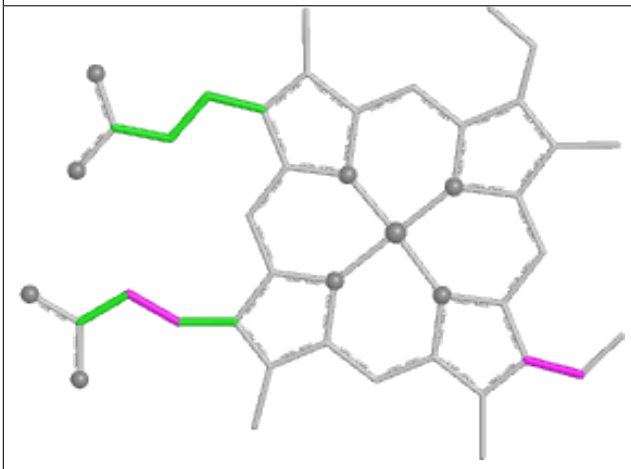
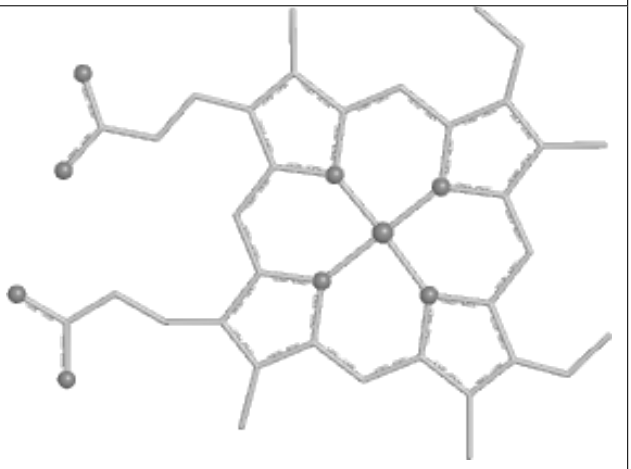
Bond angles

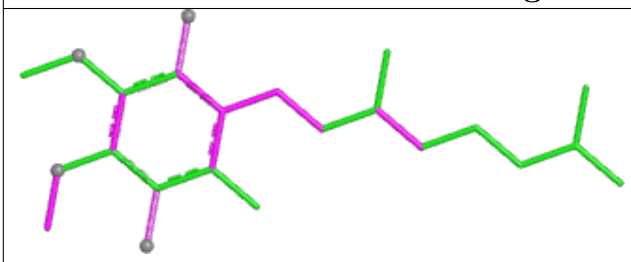
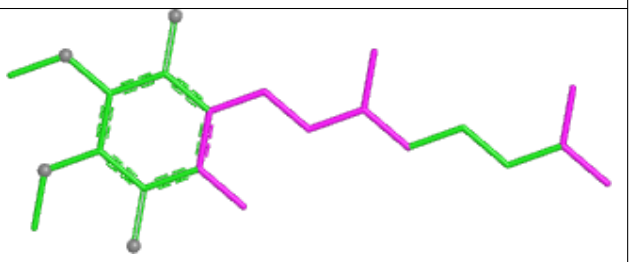
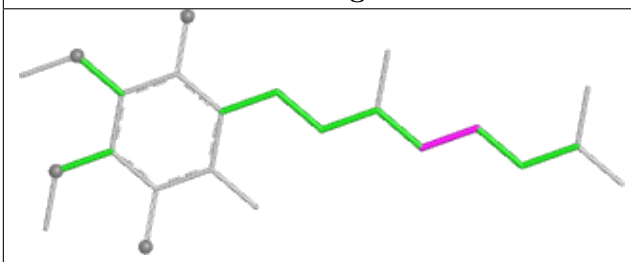
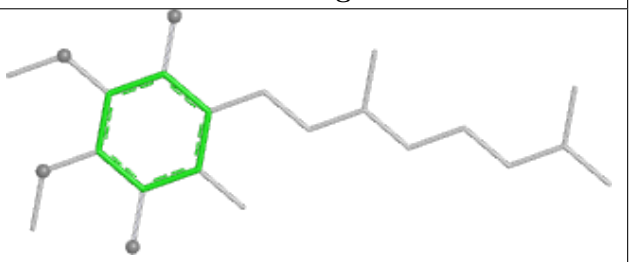


Torsions

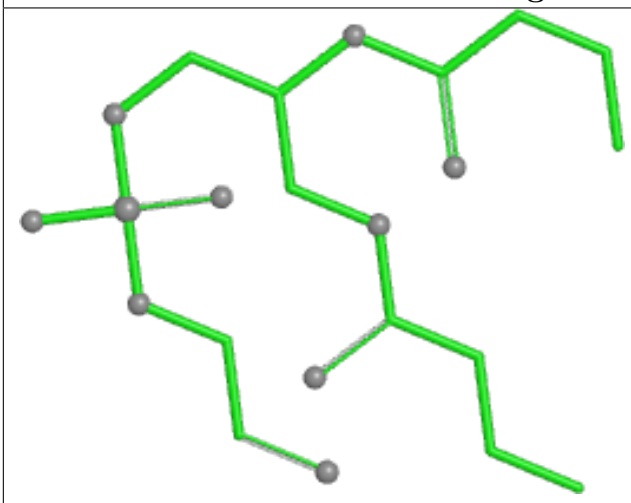


Rings

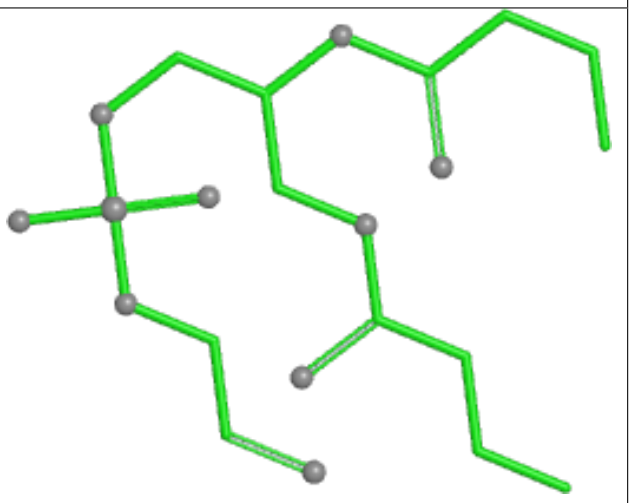
Ligand HEM b1 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand U10 b1 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

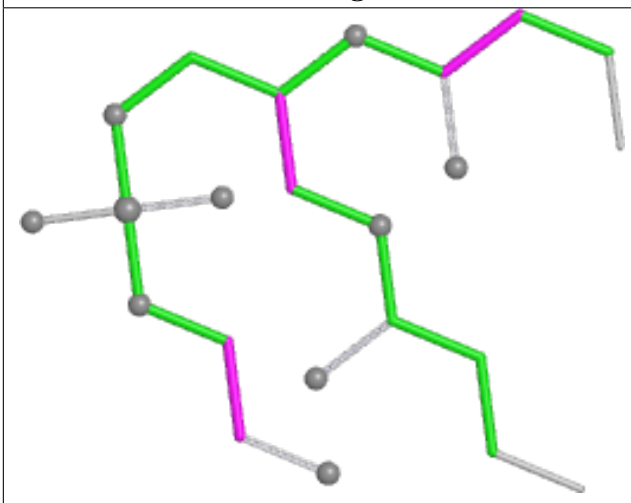
Ligand 3PE f2 201



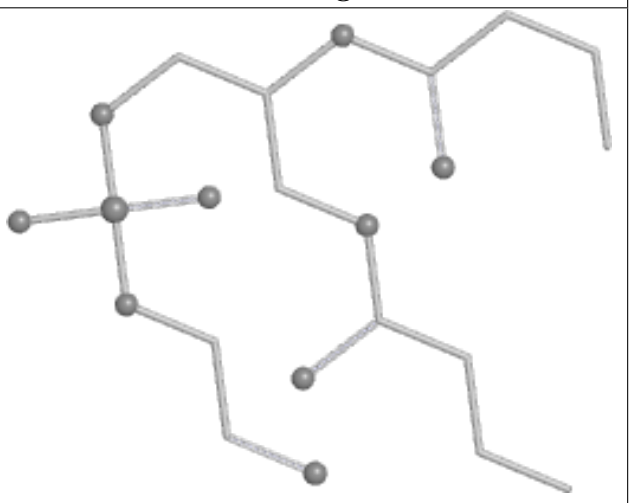
Bond lengths



Bond angles

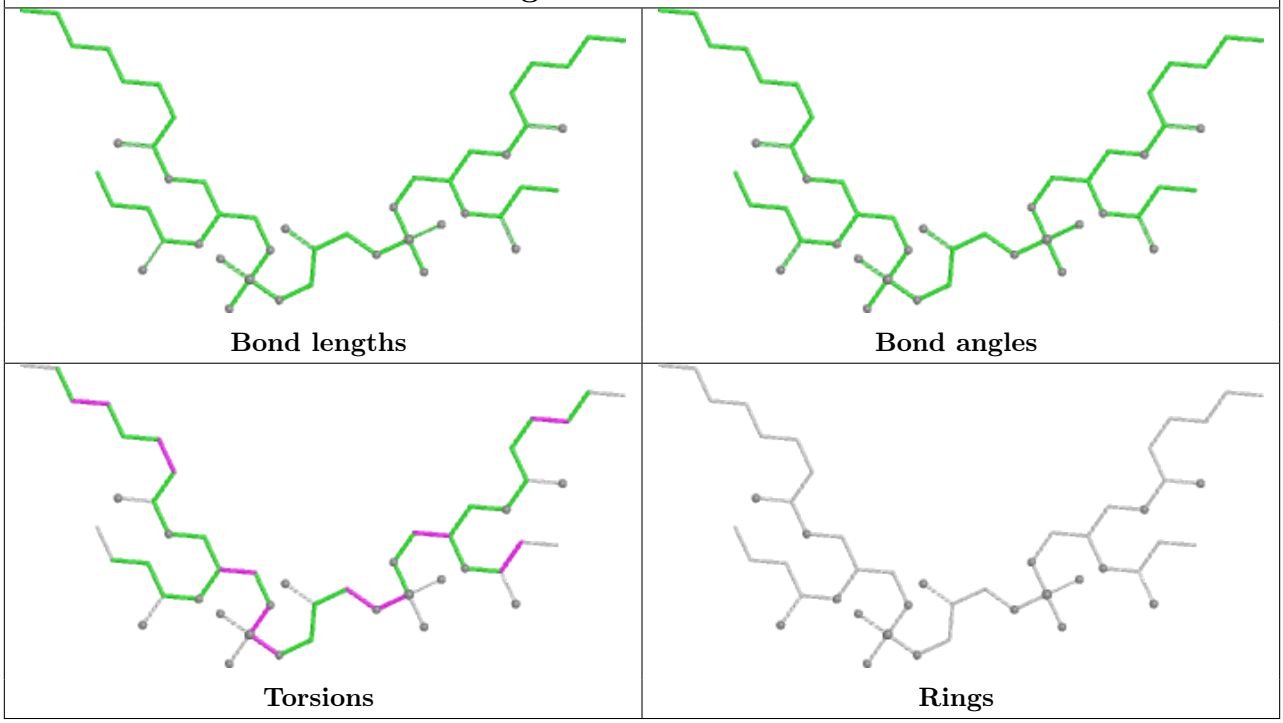


Torsions



Rings

Ligand CDL c1 503



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	x2	1
9	x1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x2	26:UNK	C	45:UNK	N	26.28
1	x1	27:UNK	C	29:UNK	N	5.27

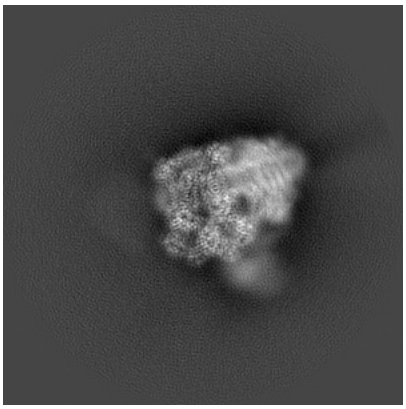
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4481. These allow visual inspection of the internal detail of the map and identification of artifacts.

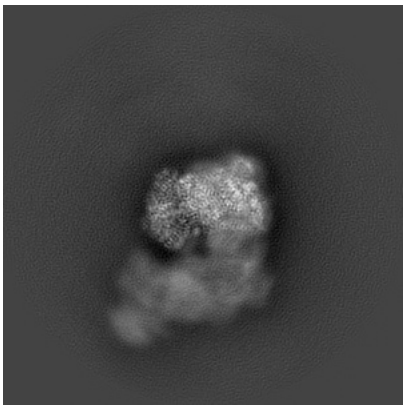
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

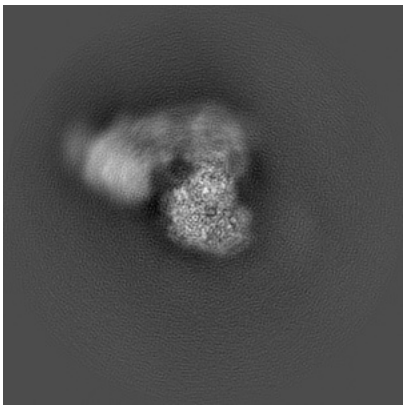
6.1.1 Primary map



X

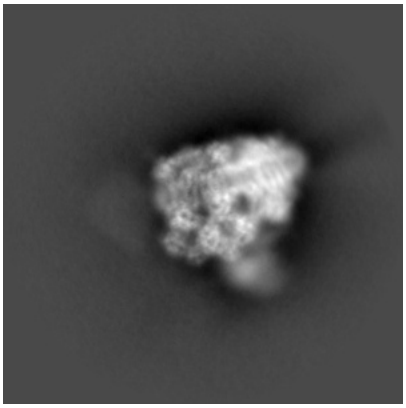


Y

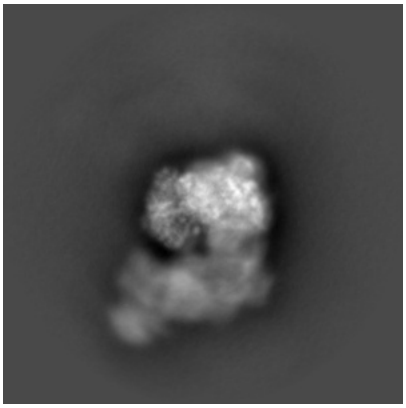


Z

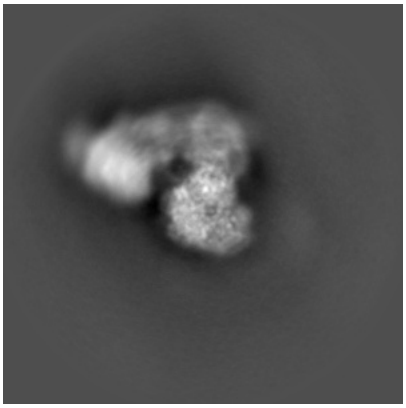
6.1.2 Raw map



X



Y

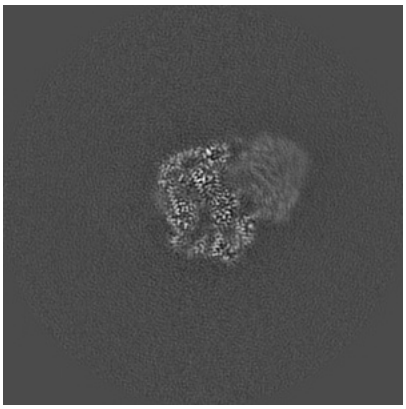


Z

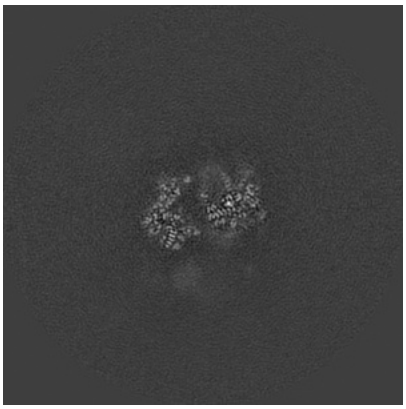
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

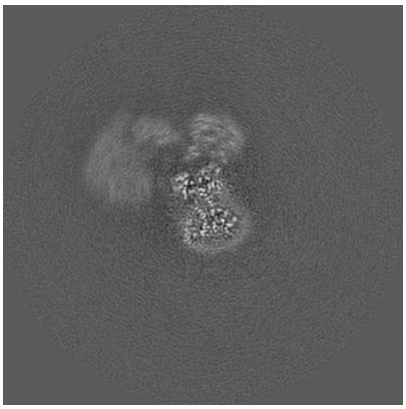
6.2.1 Primary map



X Index: 182

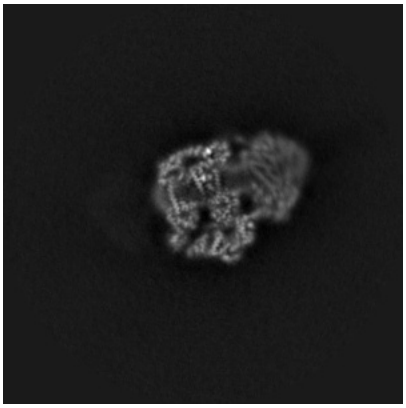


Y Index: 182

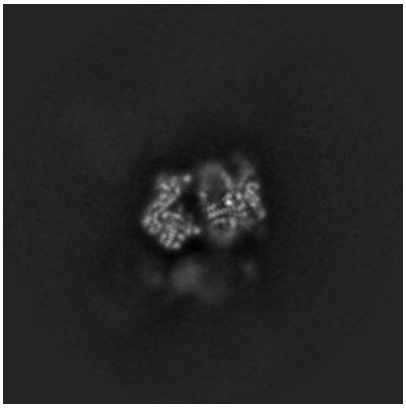


Z Index: 182

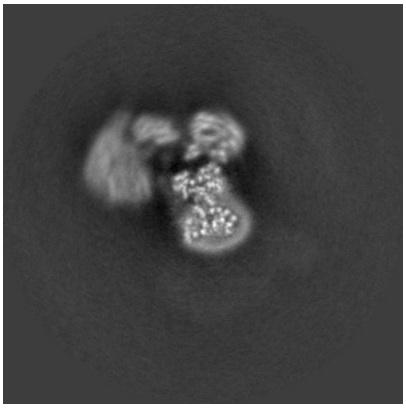
6.2.2 Raw map



X Index: 182



Y Index: 182

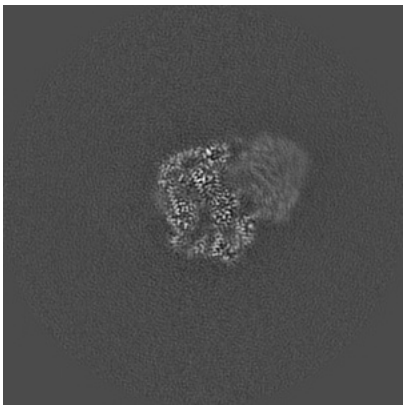


Z Index: 182

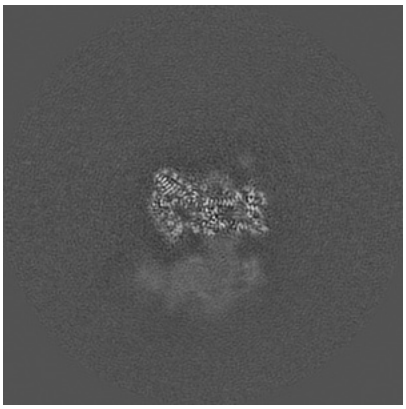
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

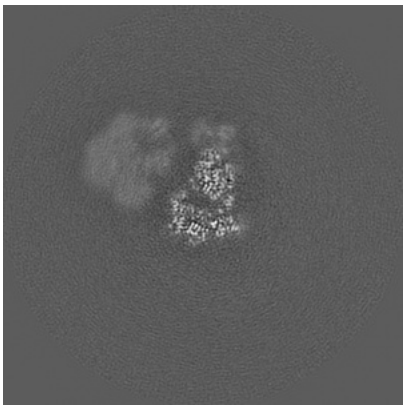
6.3.1 Primary map



X Index: 182

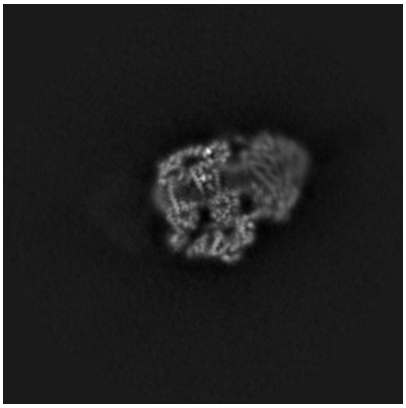


Y Index: 194

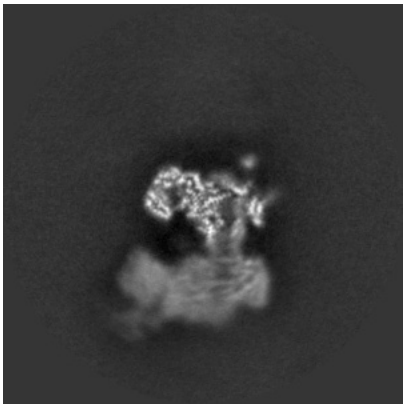


Z Index: 168

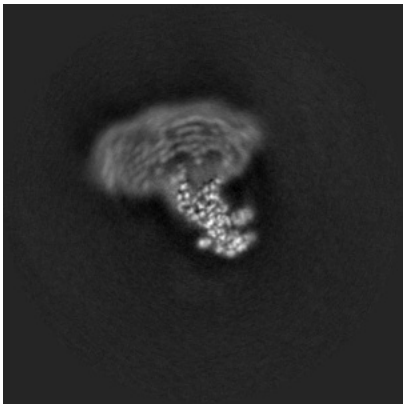
6.3.2 Raw map



X Index: 182



Y Index: 203



Z Index: 210

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

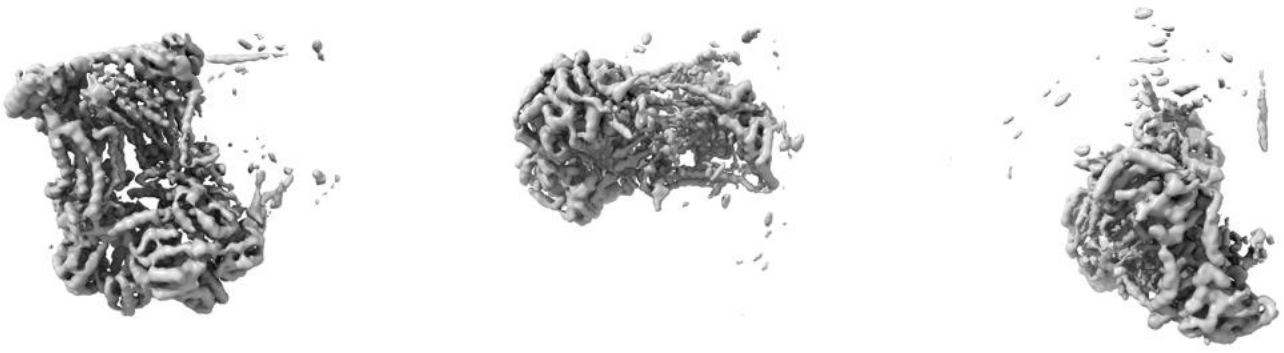
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

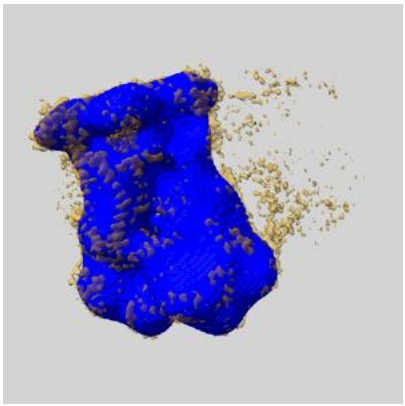
6.5 Mask visualisation (i)

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

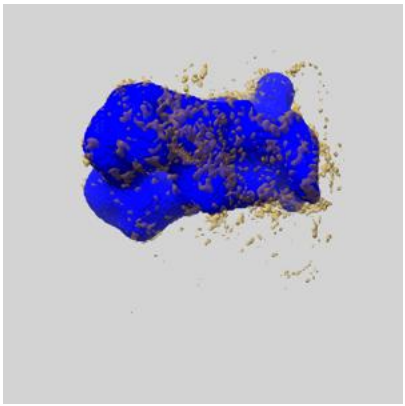
A mask typically either:

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

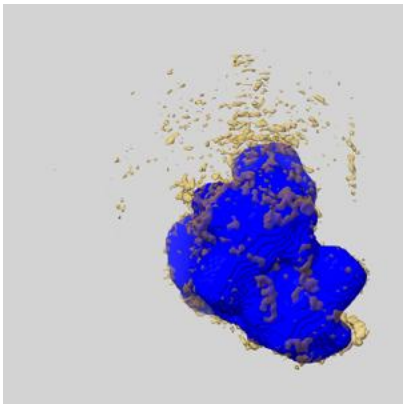
6.5.1 emd_4481_msk_1.map (i)



X



Y

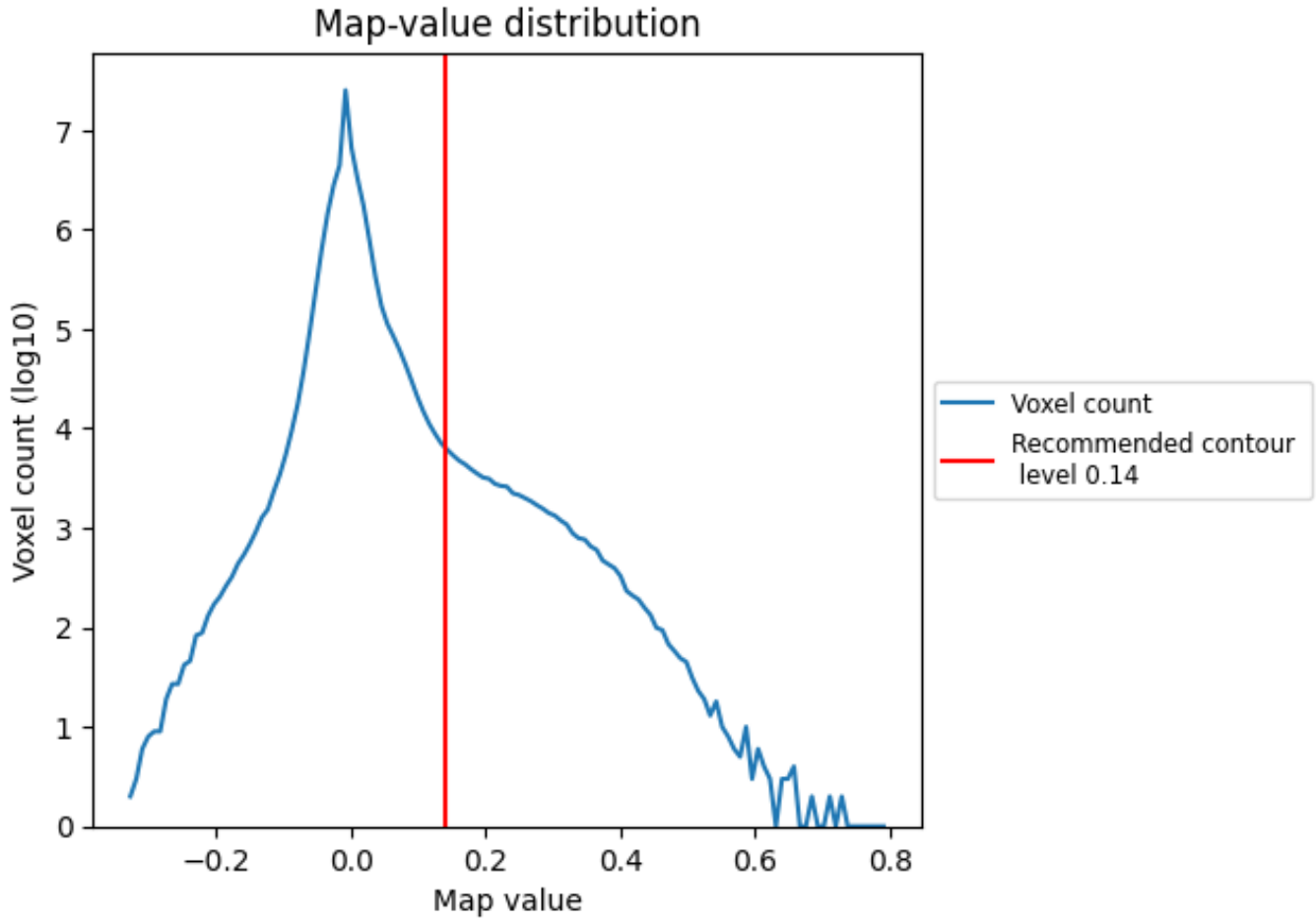


Z

7 Map analysis

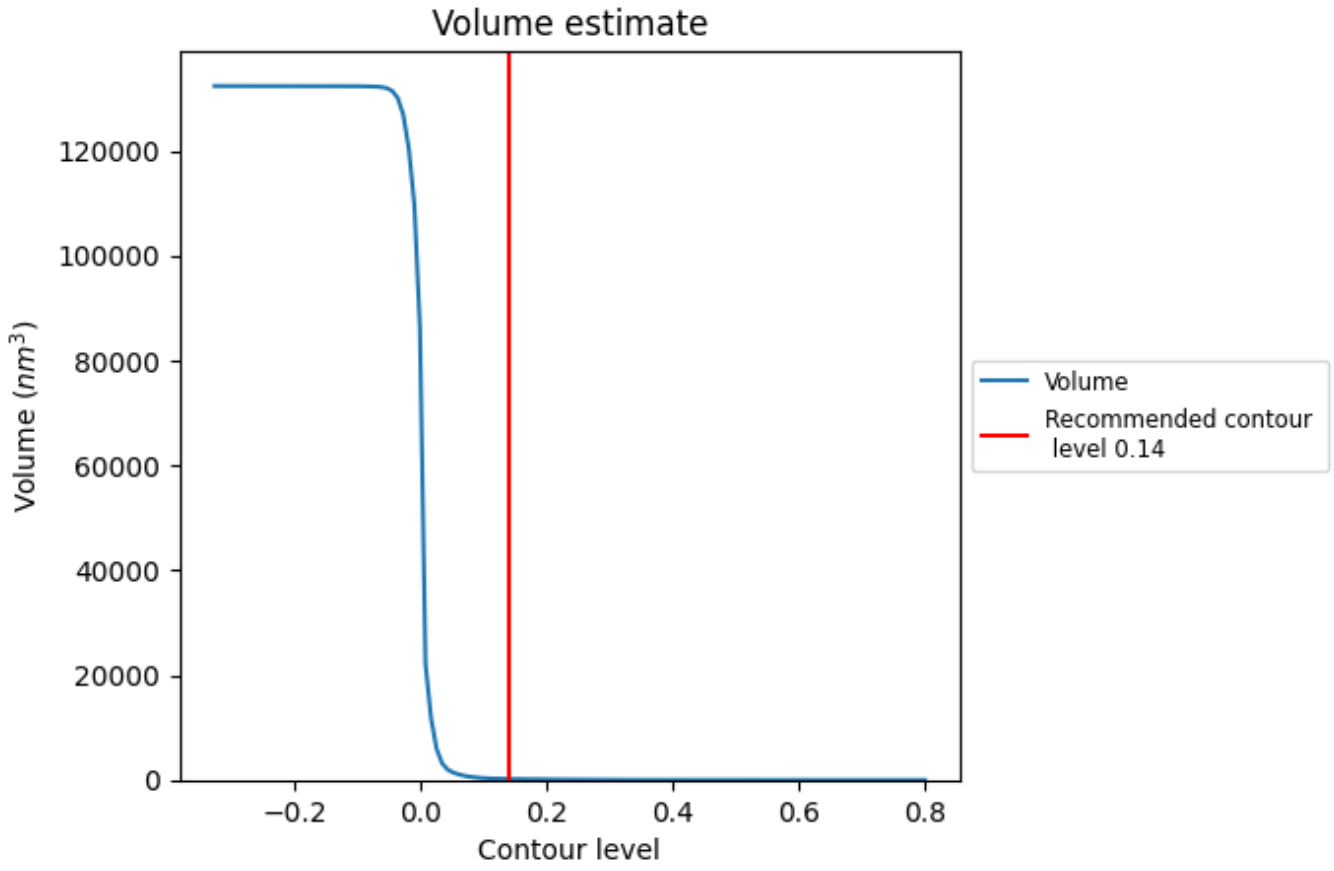
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

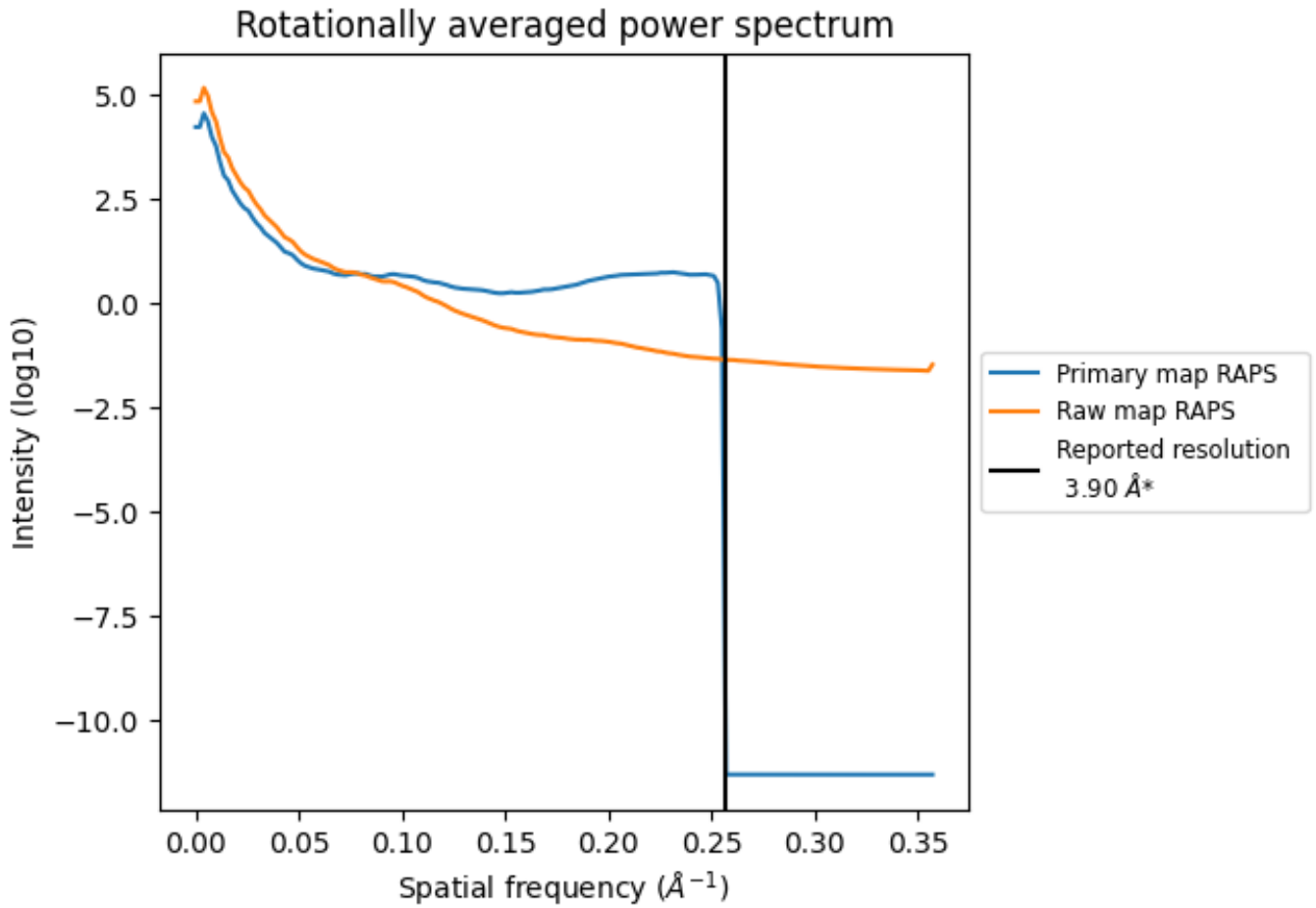
7.2 Volume estimate (i)



The volume at the recommended contour level is 187 nm^3; this corresponds to an approximate mass of 169 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)

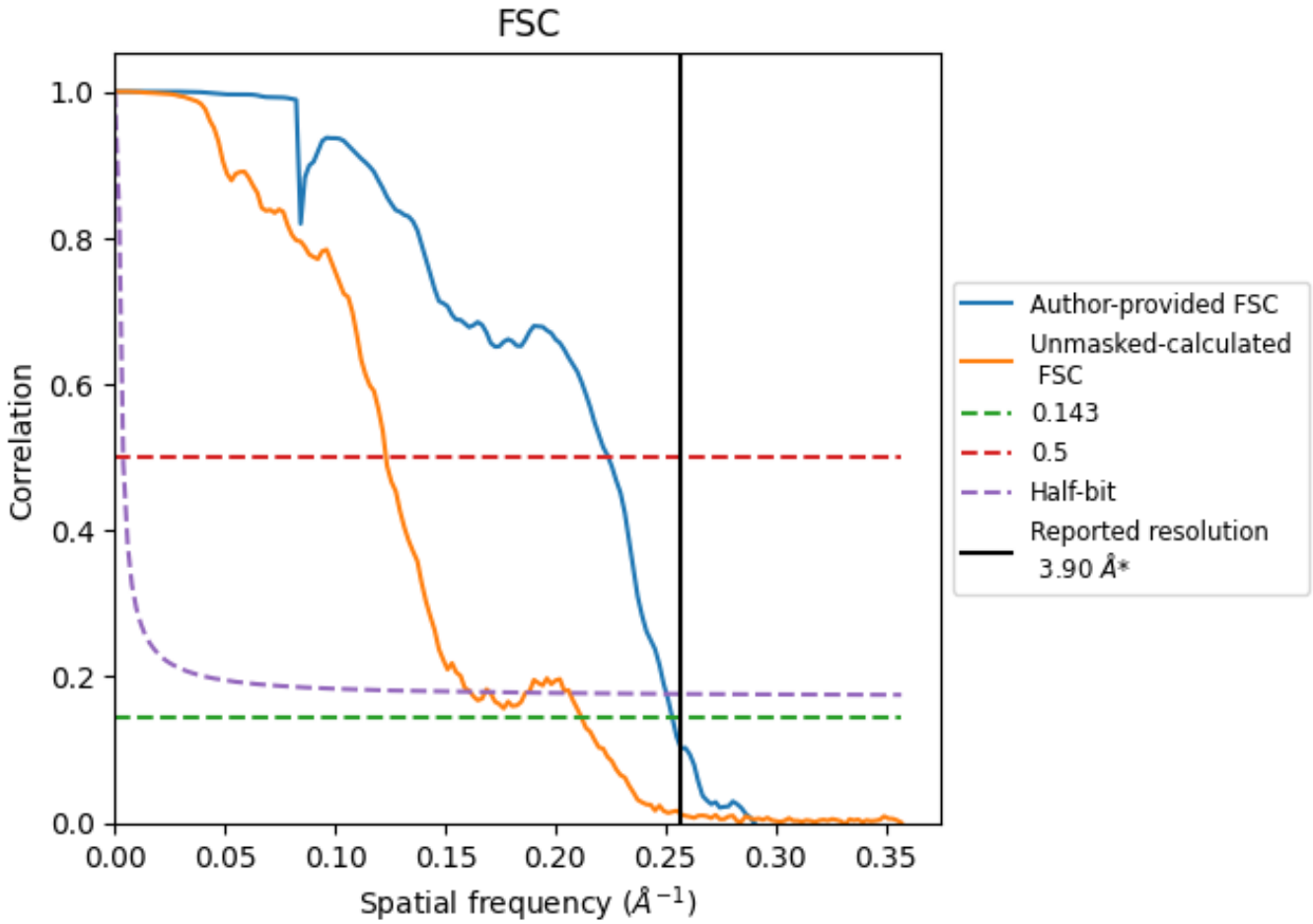


*Reported resolution corresponds to spatial frequency of 0.256 $Å^{-1}$

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 0.256 Å^{-1}

8.2 Resolution estimates (i)

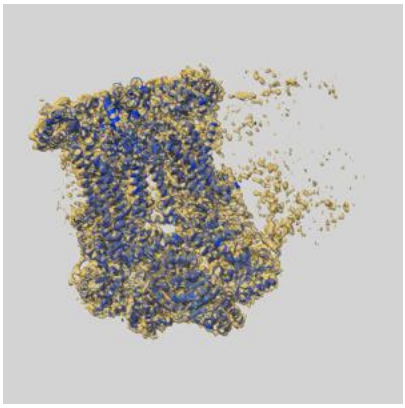
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.95	4.46	3.99
Unmasked-calculated*	4.72	8.12	6.20

*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 4.72 differs from the reported value 3.9 by more than 10 %

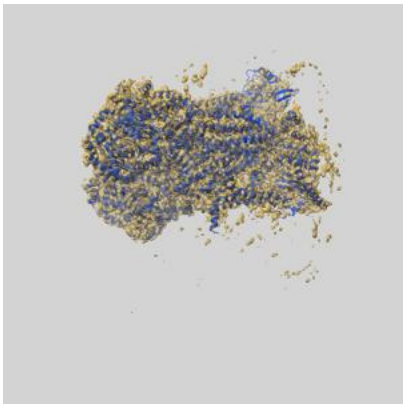
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4481 and PDB model 6Q9E. Per-residue inclusion information can be found in section 3 on page 11.

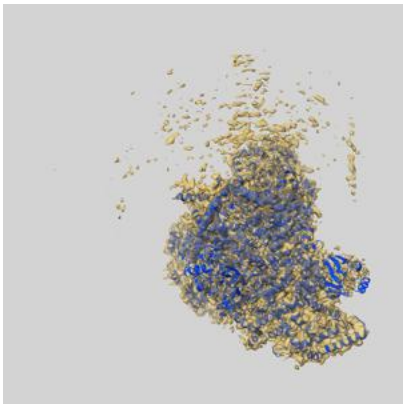
9.1 Map-model overlay



X



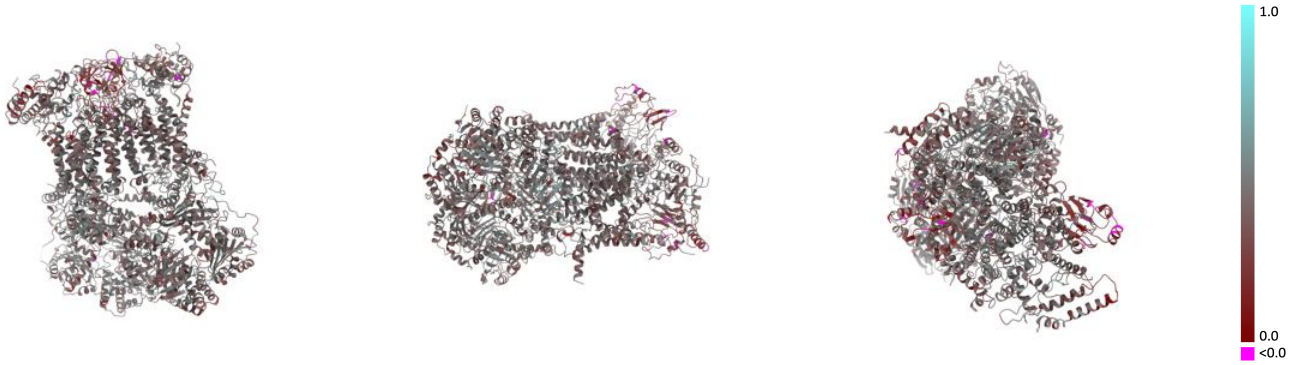
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

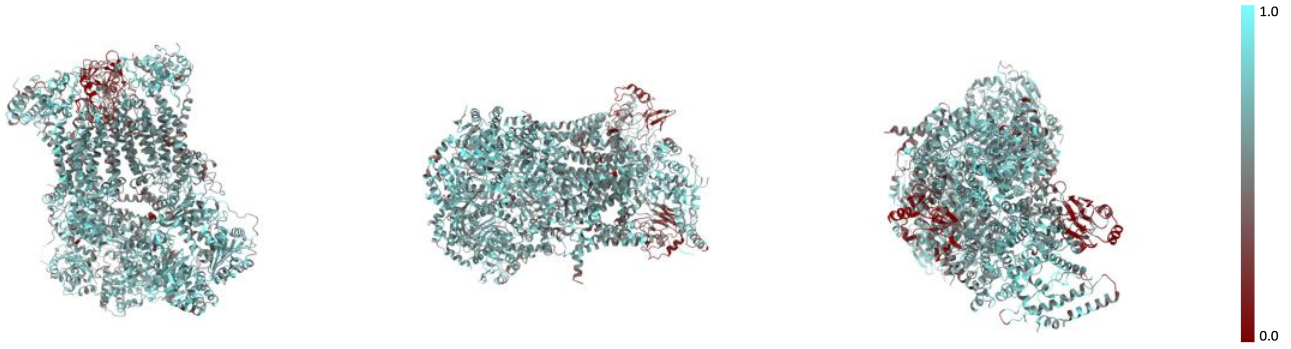
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

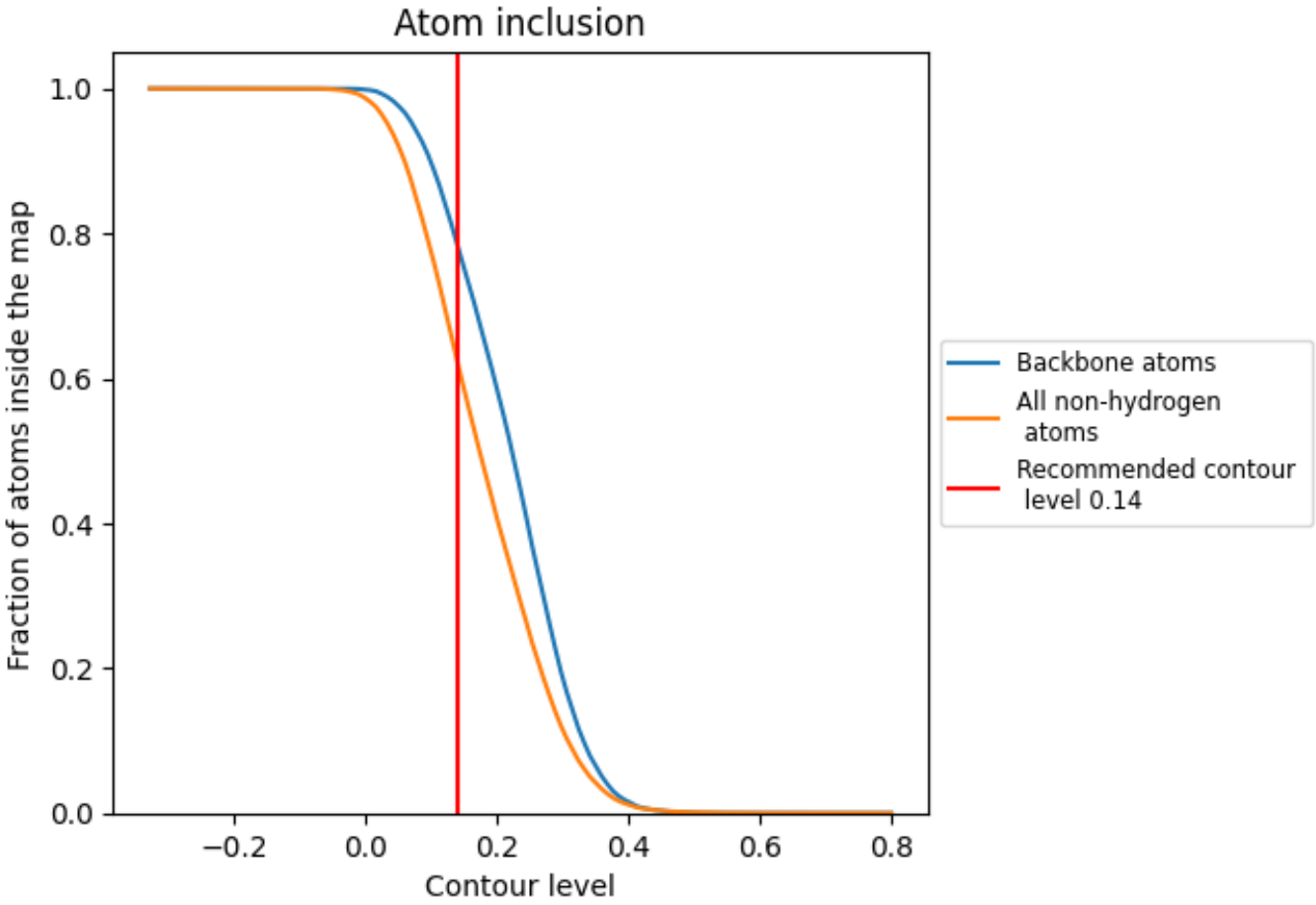
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.14).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 62% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6244	0.4130
a1	0.6927	0.4280
a2	0.6735	0.4250
a3	0.6742	0.4230
a4	0.6848	0.4220
b1	0.6331	0.4370
b2	0.6226	0.4280
c1	0.6944	0.4330
c2	0.6722	0.4280
d1	0.6370	0.4250
d2	0.6051	0.4230
f1	0.2990	0.3090
f2	0.3241	0.3150
h1	0.6154	0.3410
h2	0.6096	0.3390
i1	0.5839	0.3900
i2	0.5488	0.3970
q1	0.6874	0.4320
q2	0.6447	0.4250
x1	0.5549	0.4480
x2	0.5533	0.4630