wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 09:22 am GMT

PDB ID	:	5M3L
EMDB ID	:	EMD-3434
Title	:	Single-particle cryo-EM using alignment by classification (ABC): the structure of Lumbricus terrestris hemoglobin
Authors	:	Afanasyev, P.; Linnemayr-Seer, C.; Ravelli, R.B.G.; Matadeen, R.; De Carlo, S.; Alewijnse, B.; Portugal, R.V.; Pannu, N.S.; Schatz, M.; van Heel, M.
Deposited on	:	2016-10-15
Resolution	:	3.80 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:

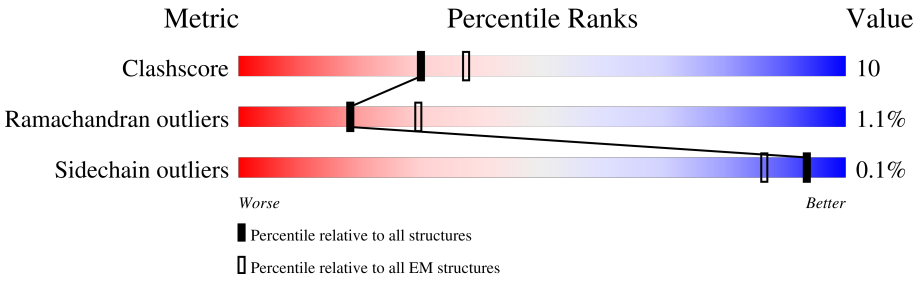
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.80 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	151	25% 79% 17%
1	E	151	38% 74% 21%
1	I	151	30% 81% 14%
2	B	145	21% 86% 14%
2	F	145	19% 86% 14%
2	J	145	35% 85% 14%
3	C	153	23% 89% 8%
3	G	153	33% 88% 10%

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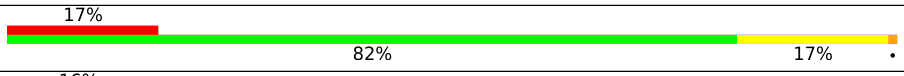
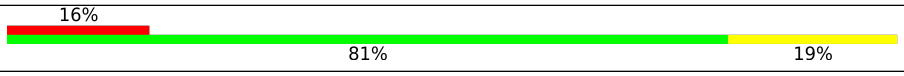
Mol	Chain	Length	Quality of chain
3	K	153	
4	D	140	
4	H	140	
4	L	140	
5	M	217	
6	N	220	
7	O	215	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 19007 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 Extracellular globin-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	147	Total	C	N	O	S	0	0
			1163	750	213	196	4		
1	E	147	Total	C	N	O	S	0	0
			1174	752	219	200	3		
1	I	147	Total	C	N	O	S	0	0
			1168	750	217	198	3		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	LYS	ASP	conflict	UNP P13579
E	78	LYS	ASP	conflict	UNP P13579
I	78	LYS	ASP	conflict	UNP P13579

- Molecule 2 is a protein called Extracellular globin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	145	Total	C	N	O	S	0	0
			1095	698	206	189	2		
2	F	145	Total	C	N	O	S	0	0
			1076	686	206	181	3		
2	J	144	Total	C	N	O	S	0	0
			1089	689	205	192	3		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	66	ASP	GLU	conflict	UNP P02218
F	66	ASP	GLU	conflict	UNP P02218
J	66	ASP	GLU	conflict	UNP P02218

- Molecule 3 is a protein called Extracellular globin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	149	Total	C	N	O	S	0	0
			1152	744	212	193	3		
3	G	149	Total	C	N	O	S	0	0
			1151	739	207	202	3		
3	K	149	Total	C	N	O	S	0	0
			1156	743	212	198	3		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	49	GLU	ASP	conflict	UNP P11069
G	49	GLU	ASP	conflict	UNP P11069
K	49	GLU	ASP	conflict	UNP P11069

- Molecule 4 is a protein called Hemoglobin chain d1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	140	Total	C	N	O	S	0	0
			1088	705	193	186	4		
4	H	140	Total	C	N	O	S	0	0
			1094	705	196	189	4		
4	L	140	Total	C	N	O	S	0	0
			1094	707	196	187	4		

- Molecule 5 is a protein called Hemoglobin linker chain L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	217	Total	C	N	O	S	0	0
			1679	1048	303	318	10		

- Molecule 6 is a protein called Extracellular hemoglobin linker L2 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	220	Total	C	N	O	S	0	0
			1676	1043	314	309	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	55	GLU	THR	conflict	UNP Q2I743

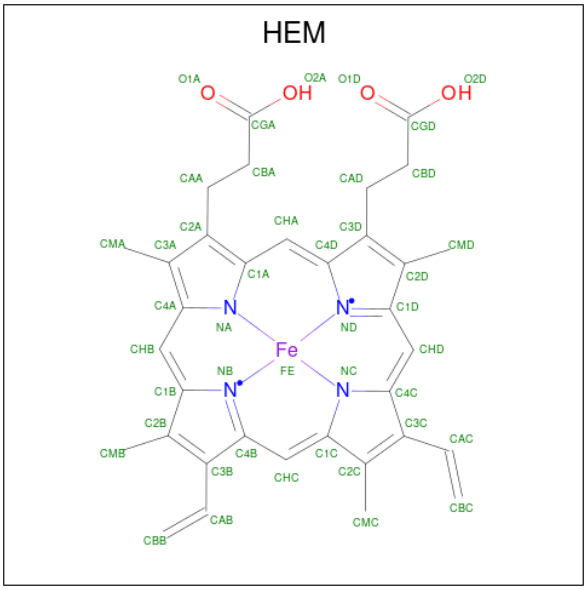
- Molecule 7 is a protein called Extracellular hemoglobin linker L3 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	215	Total	C	N	O	S	0	0
			1636	1015	290	321	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	17	ILE	LEU	conflict	UNP Q2I742
O	113	CYS	VAL	conflict	UNP Q2I742

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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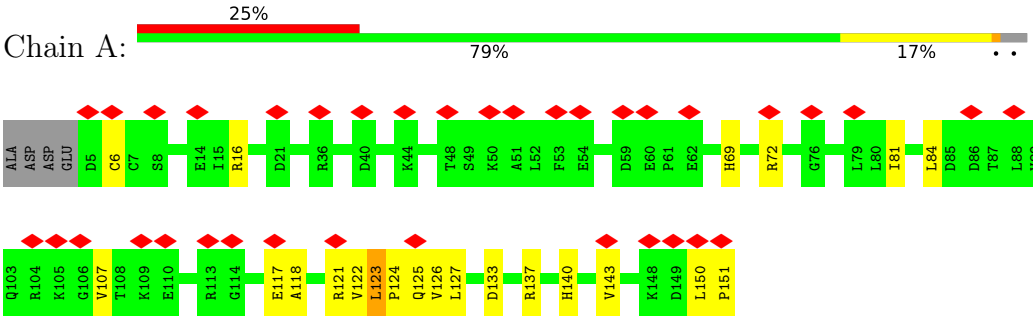
Mol	Chain	Residues	Atoms					AltConf
8	H	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
8	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
8	J	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
8	K	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
8	L	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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.

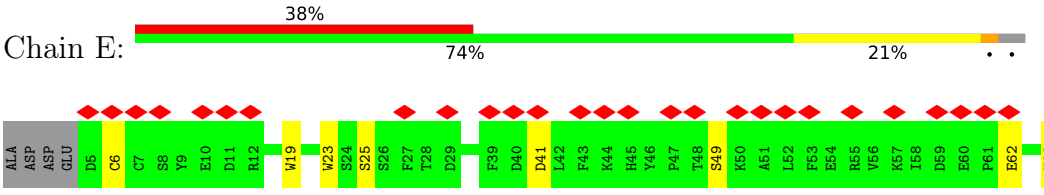
• Molecule 1: Extracellular globin-4

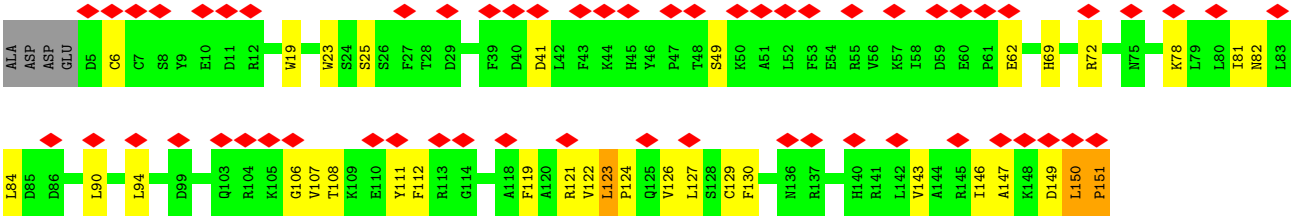
Chain A:



• Molecule 1: Extracellular globin-4

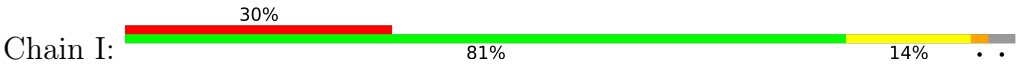
Chain E:

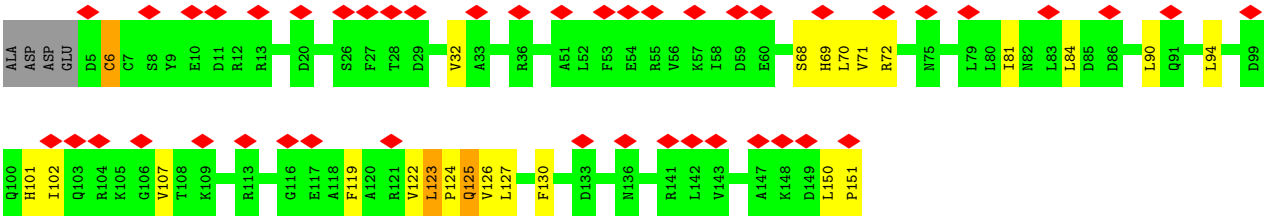




• Molecule 1: Extracellular globin-4

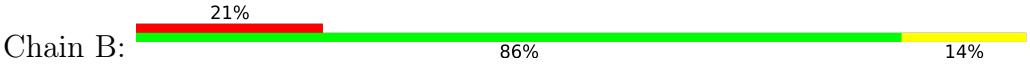
Chain I:

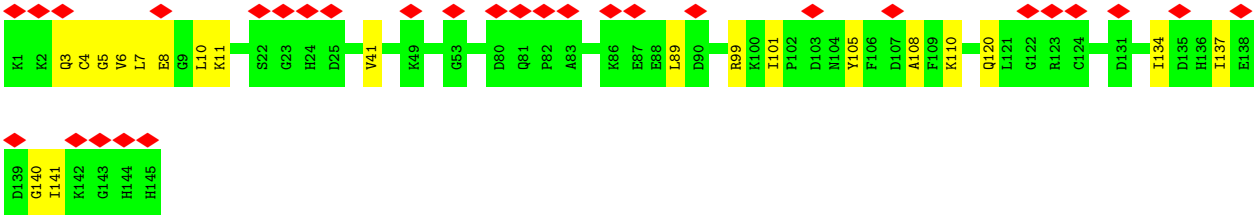




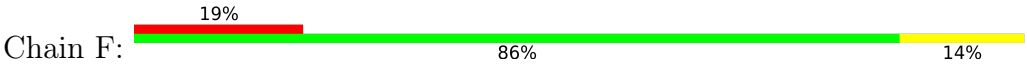
• Molecule 2: Extracellular globin-2

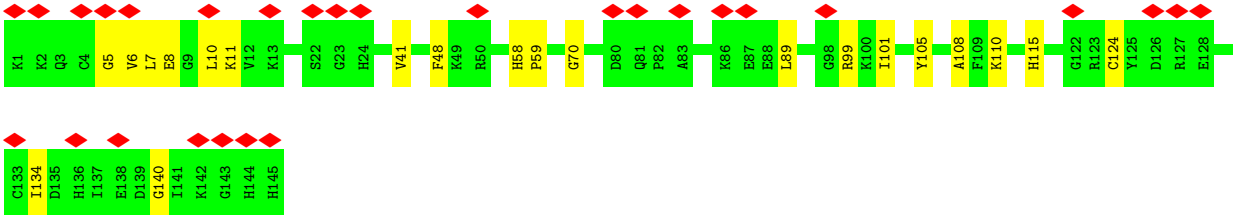
Chain B:



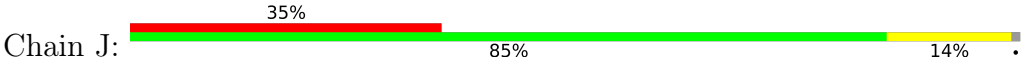


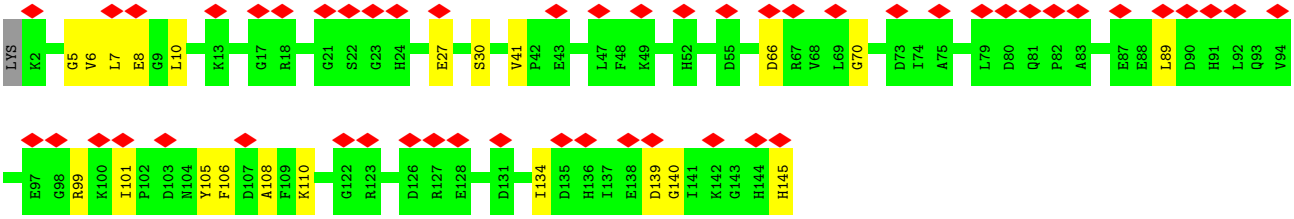
• Molecule 2: Extracellular globin-2



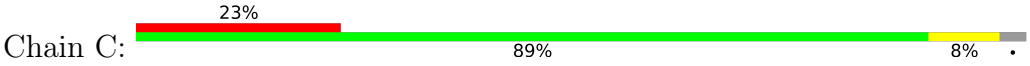


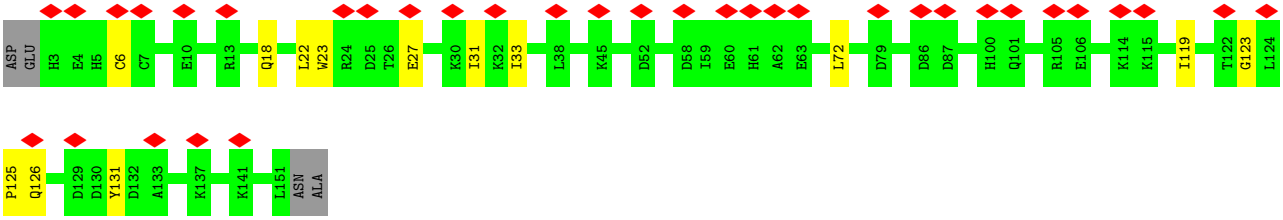
• Molecule 2: Extracellular globin-2



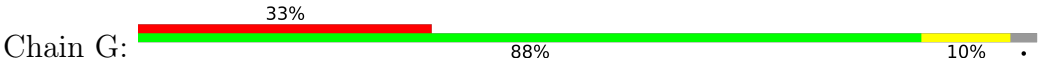


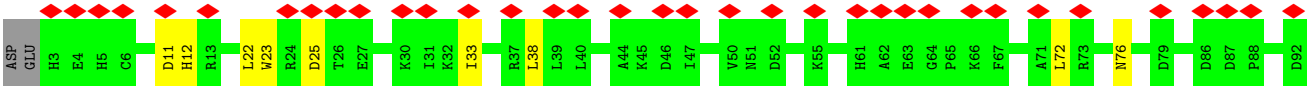
• Molecule 3: Extracellular globin-3

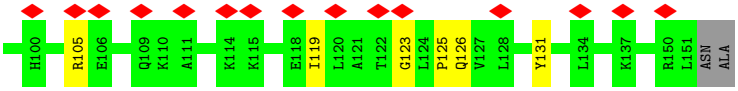




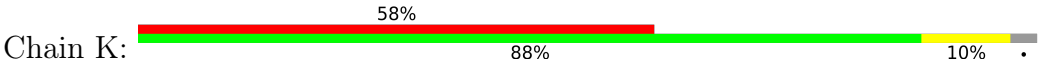
• Molecule 3: Extracellular globin-3

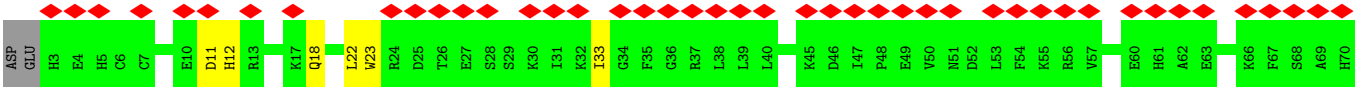


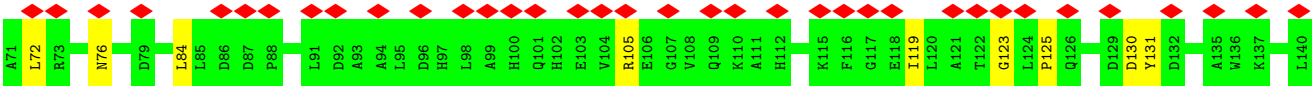


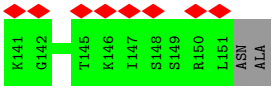


• Molecule 3: Extracellular globin-3

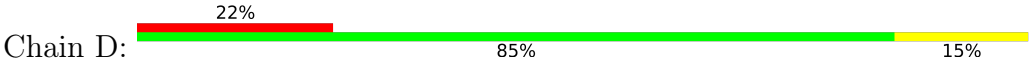


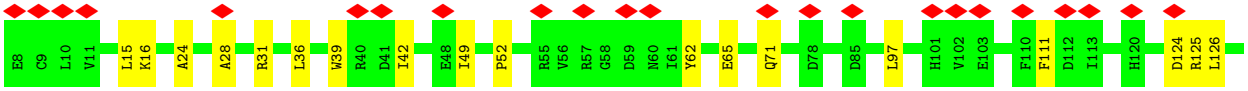


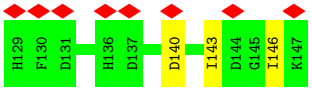




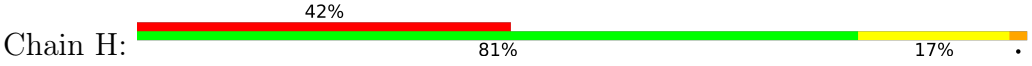
• Molecule 4: Hemoglobin chain d1

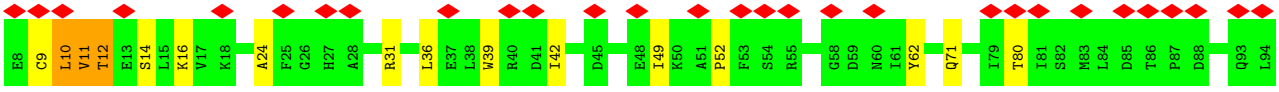


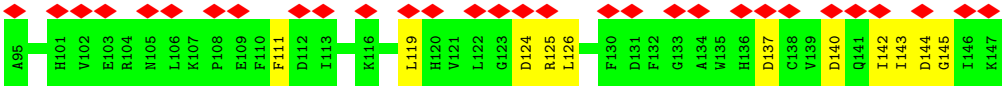




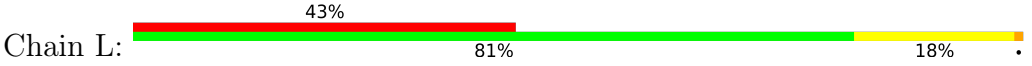
• Molecule 4: Hemoglobin chain d1

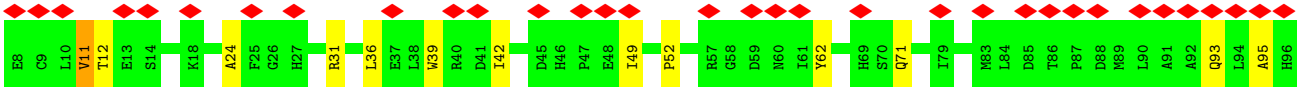


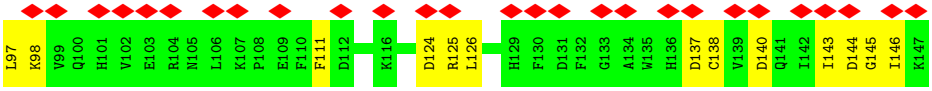




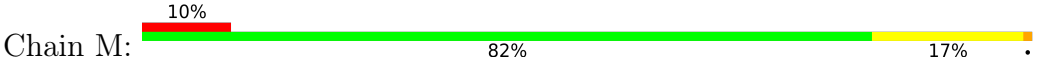
• Molecule 4: Hemoglobin chain d1

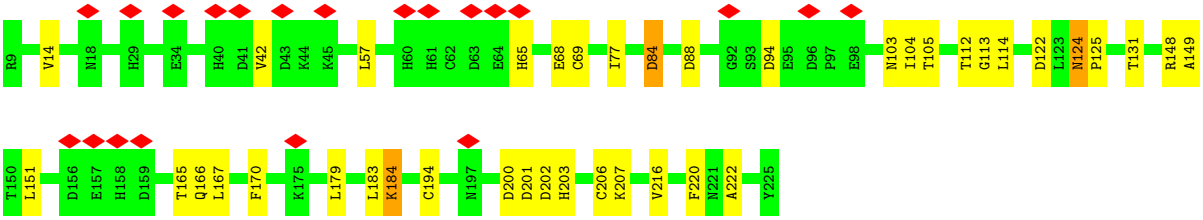




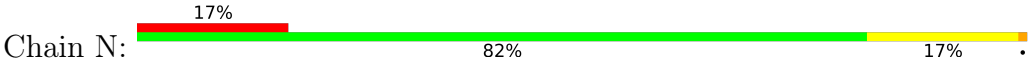


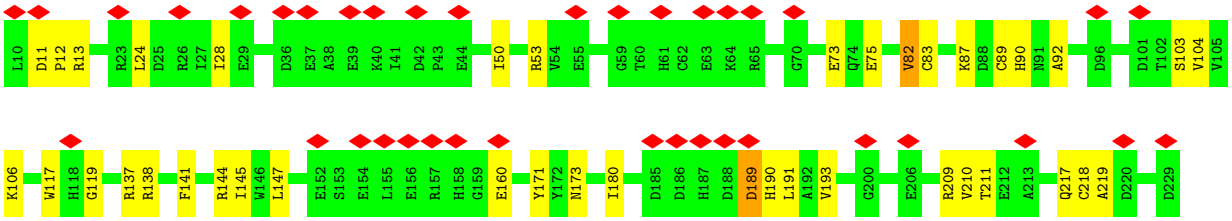
• Molecule 5: Hemoglobin linker chain L1



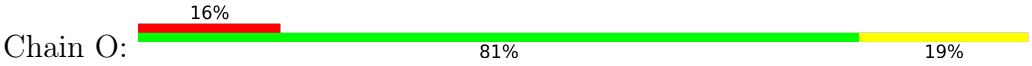


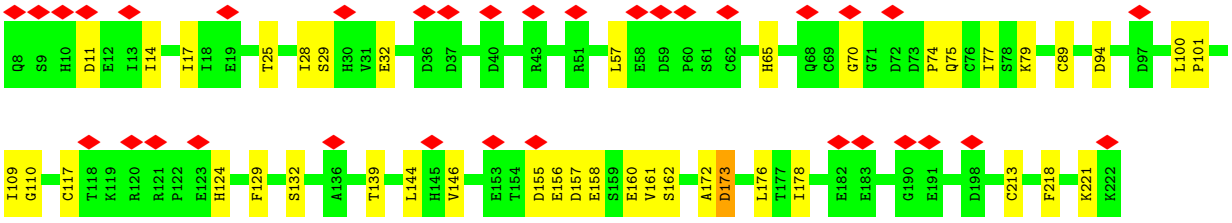
• Molecule 6: Extracellular hemoglobin linker L2 subunit





• Molecule 7: Extracellular hemoglobin linker L3 subunit





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D6	Depositor
Number of particles used	75000	Depositor
Resolution determination method	FSC 1/2 BIT CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; Unsupervised MSA classification of amplitude spectra throughout the full data set ("Full data set CTF correction")	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	10.000	Depositor
Minimum map value	-6.930	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.520	Depositor
Recommended contour level	1.6	Depositor
Map size (Å)	399.6, 399.6, 399.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM

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	0.50	0/1191	0.72	0/1614
1	E	0.55	1/1202 (0.1%)	0.98	3/1626 (0.2%)
1	I	0.47	0/1196	0.68	0/1622
2	B	0.45	0/1122	0.64	0/1520
2	F	0.44	0/1102	0.65	0/1495
2	J	0.42	0/1116	0.63	0/1512
3	C	0.43	0/1177	0.63	0/1592
3	G	0.43	0/1176	0.64	0/1593
3	K	0.41	0/1181	0.61	0/1597
4	D	0.44	0/1118	0.64	0/1518
4	H	0.45	0/1124	0.63	0/1526
4	L	0.44	0/1123	0.63	0/1522
5	M	0.67	0/1716	0.85	3/2328 (0.1%)
6	N	0.56	0/1707	0.77	0/2314
7	O	0.57	0/1671	0.77	1/2261 (0.0%)
All	All	0.50	1/18922 (0.0%)	0.71	7/25640 (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
7	O	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	151	PRO	N-CD	7.66	1.58	1.47

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	150	LEU	C-N-CD	-21.19	73.97	120.60
5	M	84	ASP	CB-CG-OD1	6.40	124.06	118.30
5	M	148	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	E	106	GLY	N-CA-C	5.44	126.69	113.10
1	E	151	PRO	CA-N-CD	-5.35	104.01	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	O	139	THR	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	A	1163	0	1129	27	0
1	E	1174	0	1152	87	0
1	I	1168	0	1130	29	0
2	B	1095	0	1047	12	0
2	F	1076	0	1027	24	0
2	J	1089	0	1032	13	0
3	C	1152	0	1159	9	0
3	G	1151	0	1149	11	0
3	K	1156	0	1163	10	0
4	D	1088	0	1043	17	0
4	H	1094	0	1048	20	0
4	L	1094	0	1060	16	0
5	M	1679	0	1564	27	0
6	N	1676	0	1592	37	0
7	O	1636	0	1494	31	0
8	A	43	0	30	3	0
8	B	43	0	30	4	0
8	C	43	0	30	3	0
8	D	43	0	30	3	0
8	E	43	0	30	2	0
8	F	43	0	30	6	0
8	G	43	0	30	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	43	0	30	2	0
8	I	43	0	30	3	0
8	J	43	0	30	4	0
8	K	43	0	30	5	0
8	L	43	0	30	2	0
All	All	19007	0	18149	370	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 10.

The worst 5 of 370 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)
1:E:107:VAL:CG2	1:E:151:PRO:HB3	1.15	1.63
1:E:150:LEU:HD12	1:E:151:PRO:CD	1.31	1.59
1:E:112:PHE:CE2	1:E:146:ILE:CD1	1.90	1.53
1:E:107:VAL:CG2	1:E:151:PRO:CB	1.93	1.46
1:E:107:VAL:HG21	1:E:151:PRO:CB	1.47	1.43

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	145/151 (96%)	131 (90%)	12 (8%)	2 (1%)	11 46
1	E	145/151 (96%)	131 (90%)	12 (8%)	2 (1%)	11 46
1	I	145/151 (96%)	130 (90%)	12 (8%)	3 (2%)	7 40
2	B	143/145 (99%)	133 (93%)	9 (6%)	1 (1%)	22 60
2	F	143/145 (99%)	132 (92%)	10 (7%)	1 (1%)	22 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	142/145 (98%)	132 (93%)	9 (6%)	1 (1%)	22	60
3	C	147/153 (96%)	137 (93%)	9 (6%)	1 (1%)	22	60
3	G	147/153 (96%)	139 (95%)	8 (5%)	0	100	100
3	K	147/153 (96%)	138 (94%)	9 (6%)	0	100	100
4	D	138/140 (99%)	127 (92%)	11 (8%)	0	100	100
4	H	138/140 (99%)	125 (91%)	10 (7%)	3 (2%)	6	39
4	L	138/140 (99%)	127 (92%)	10 (7%)	1 (1%)	22	60
5	M	215/217 (99%)	190 (88%)	19 (9%)	6 (3%)	5	35
6	N	218/220 (99%)	192 (88%)	22 (10%)	4 (2%)	8	42
7	O	213/215 (99%)	198 (93%)	13 (6%)	2 (1%)	17	54
All	All	2364/2419 (98%)	2162 (92%)	175 (7%)	27 (1%)	18	51

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	125	GLN
4	L	11	VAL
4	H	10	LEU
4	H	12	THR
5	M	184	LYS

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	116/134 (87%)	116 (100%)	0	100	100
1	E	121/134 (90%)	121 (100%)	0	100	100
1	I	117/134 (87%)	117 (100%)	0	100	100
2	B	101/117 (86%)	101 (100%)	0	100	100
2	F	97/117 (83%)	97 (100%)	0	100	100
2	J	103/117 (88%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	114/131 (87%)	114 (100%)	0	100	100
3	G	118/131 (90%)	118 (100%)	0	100	100
3	K	117/131 (89%)	117 (100%)	0	100	100
4	D	109/121 (90%)	109 (100%)	0	100	100
4	H	111/121 (92%)	111 (100%)	0	100	100
4	L	111/121 (92%)	111 (100%)	0	100	100
5	M	176/195 (90%)	176 (100%)	0	100	100
6	N	172/193 (89%)	172 (100%)	0	100	100
7	O	172/193 (89%)	171 (99%)	1 (1%)	86	92
All	All	1855/2090 (89%)	1854 (100%)	1 (0%)	93	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	O	173	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	103	GLN
4	L	93	GLN
4	L	27	HIS
4	L	129	HIS
1	E	69	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	$\#\|Z\| > 2$
8	HEM	C	201	3	41,50,50	1.44	7 (17%)	45,82,82	1.93	16 (35%)
8	HEM	J	201	2	41,50,50	1.33	5 (12%)	45,82,82	1.90	10 (22%)
8	HEM	H	201	4	41,50,50	1.37	7 (17%)	45,82,82	2.01	16 (35%)
8	HEM	L	201	4	41,50,50	1.36	6 (14%)	45,82,82	2.28	16 (35%)
8	HEM	I	201	1	41,50,50	1.38	7 (17%)	45,82,82	1.96	14 (31%)
8	HEM	K	201	3	41,50,50	1.41	6 (14%)	45,82,82	1.90	16 (35%)
8	HEM	B	201	2	41,50,50	1.48	6 (14%)	45,82,82	1.79	11 (24%)
8	HEM	A	201	1	41,50,50	1.35	5 (12%)	45,82,82	2.14	15 (33%)
8	HEM	G	201	3	41,50,50	1.41	6 (14%)	45,82,82	1.89	16 (35%)
8	HEM	D	201	4	41,50,50	1.38	6 (14%)	45,82,82	2.19	18 (40%)
8	HEM	F	201	2	41,50,50	1.49	5 (12%)	45,82,82	2.12	15 (33%)
8	HEM	E	201	1	41,50,50	1.38	7 (17%)	45,82,82	1.93	15 (33%)

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
8	HEM	C	201	3	-	4/12/54/54	-
8	HEM	J	201	2	-	2/12/54/54	-
8	HEM	H	201	4	-	3/12/54/54	-
8	HEM	L	201	4	-	4/12/54/54	-
8	HEM	I	201	1	-	3/12/54/54	-
8	HEM	K	201	3	-	4/12/54/54	-
8	HEM	B	201	2	-	2/12/54/54	-
8	HEM	A	201	1	-	3/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	HEM	G	201	3	-	3/12/54/54	-
8	HEM	D	201	4	-	4/12/54/54	-
8	HEM	F	201	2	-	2/12/54/54	-
8	HEM	E	201	1	-	3/12/54/54	-

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	201	HEM	C1B-NB	-3.85	1.33	1.40
8	F	201	HEM	C1B-NB	-3.81	1.33	1.40
8	C	201	HEM	C1B-NB	-3.73	1.33	1.40
8	A	201	HEM	C1B-NB	-3.65	1.34	1.40
8	G	201	HEM	C4D-ND	-3.63	1.34	1.40

The worst 5 of 178 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	201	HEM	C1B-NB-C4B	5.81	111.07	105.07
8	D	201	HEM	C1B-NB-C4B	5.54	110.80	105.07
8	F	201	HEM	CHC-C4B-NB	5.43	130.33	124.43
8	L	201	HEM	C1B-NB-C4B	5.37	110.62	105.07
8	J	201	HEM	CHC-C4B-NB	5.28	130.16	124.43

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	201	HEM	C1A-C2A-CAA-CBA
8	F	201	HEM	C3A-C2A-CAA-CBA
8	J	201	HEM	C1A-C2A-CAA-CBA
8	J	201	HEM	C3A-C2A-CAA-CBA
8	G	201	HEM	C4D-C3D-CAD-CBD

There are no ring outliers.

12 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	201	HEM	3	0
8	J	201	HEM	4	0
8	H	201	HEM	2	0

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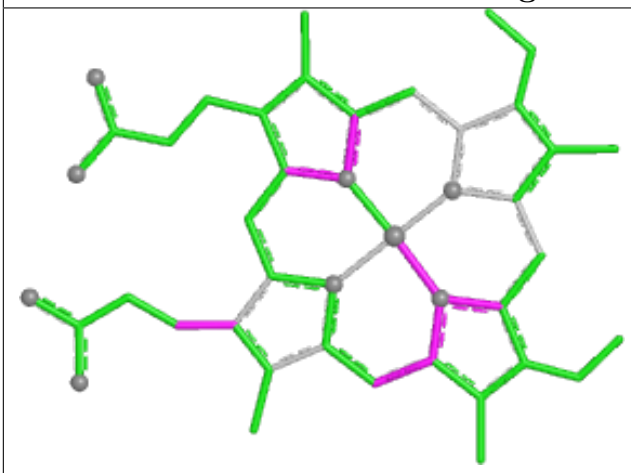
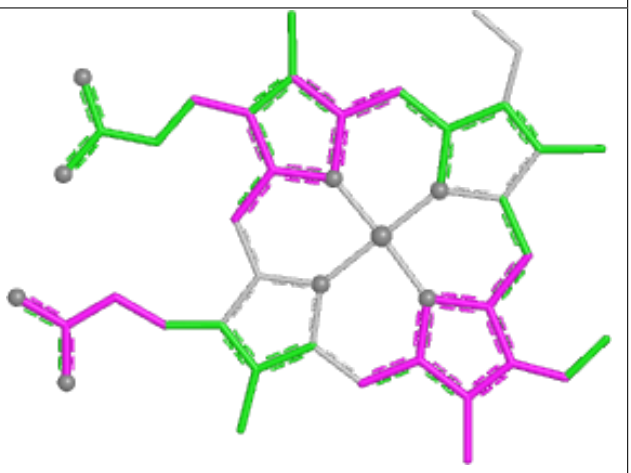
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	201	HEM	2	0
8	I	201	HEM	3	0
8	K	201	HEM	5	0
8	B	201	HEM	4	0
8	A	201	HEM	3	0
8	G	201	HEM	5	0
8	D	201	HEM	3	0
8	F	201	HEM	6	0
8	E	201	HEM	2	0

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

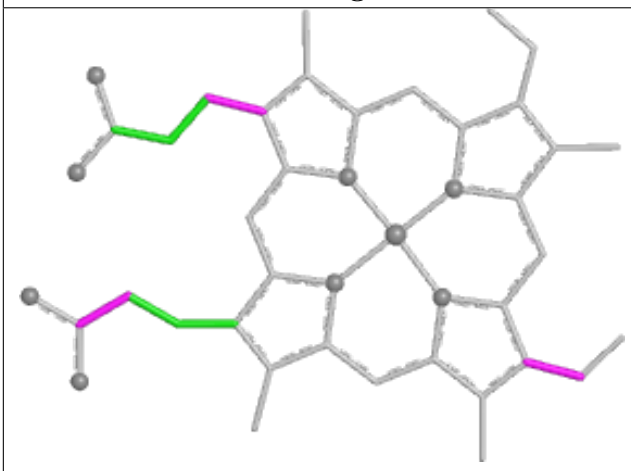
Ligand HEM C 201



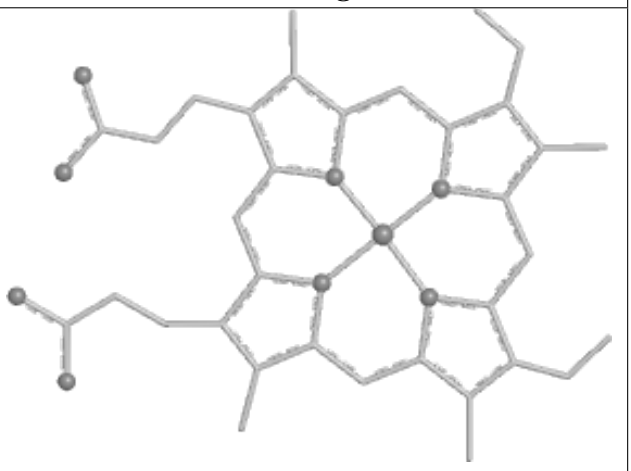
Bond lengths



Bond angles

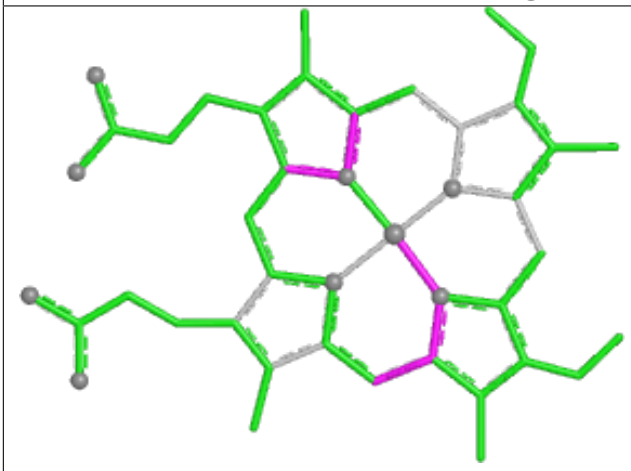


Torsions

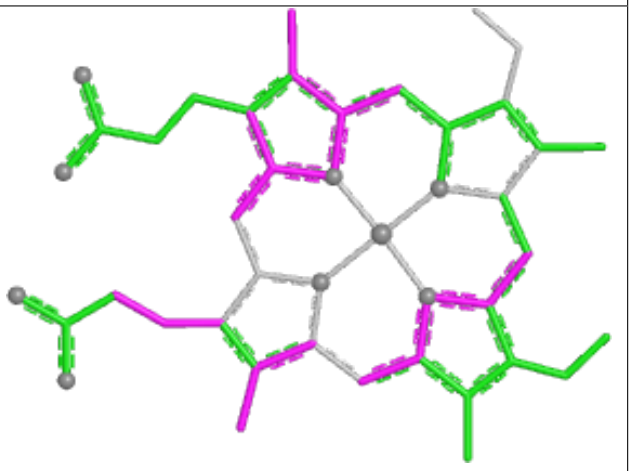


Rings

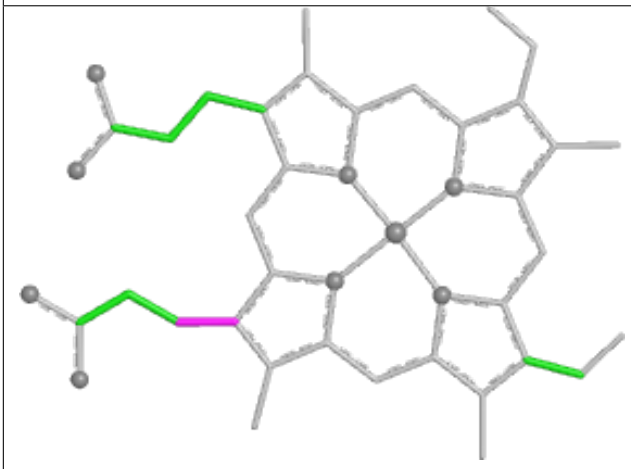
Ligand HEM J 201



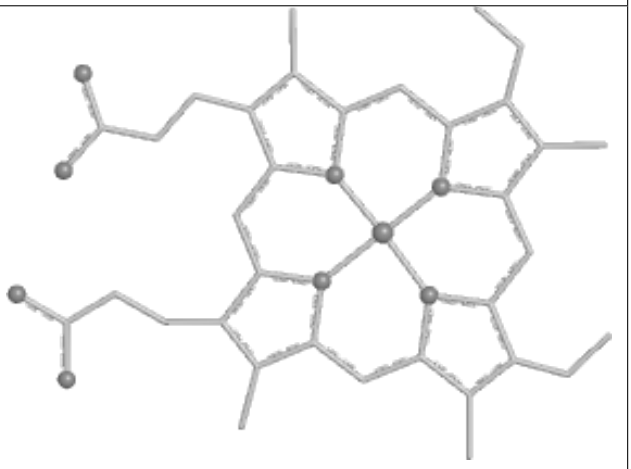
Bond lengths



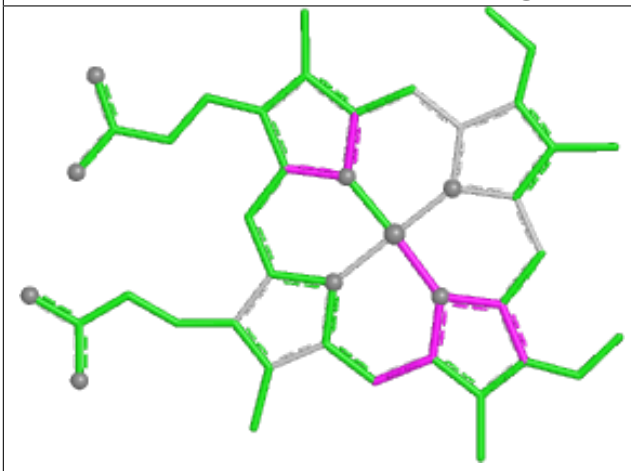
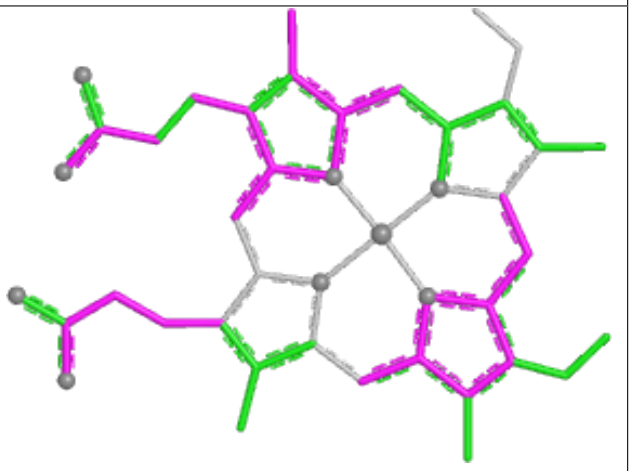
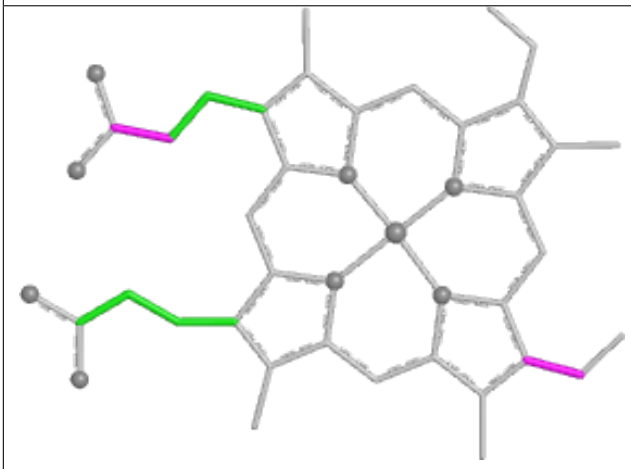
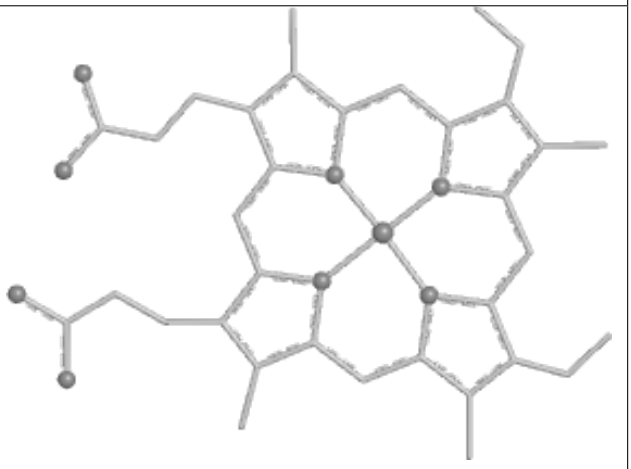
Bond angles



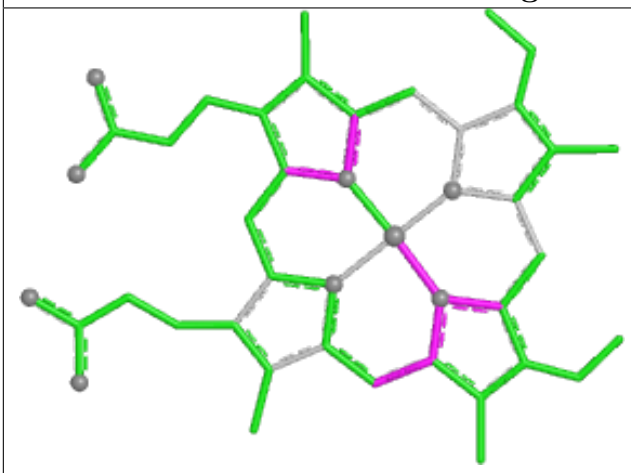
Torsions



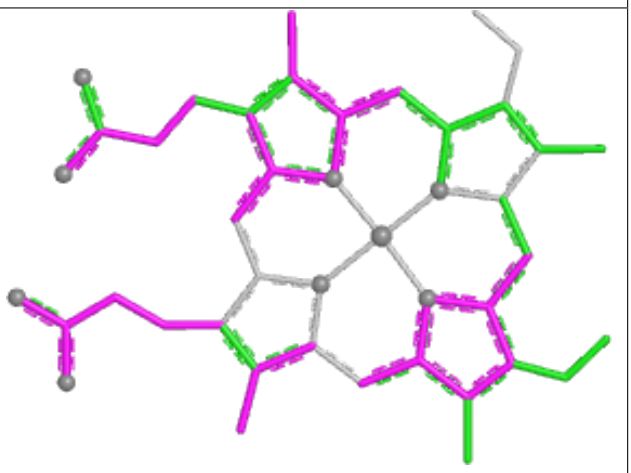
Rings

Ligand HEM H 201	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

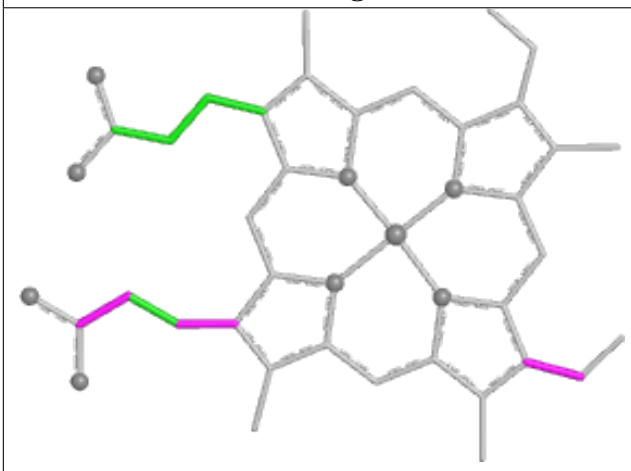
Ligand HEM L 201



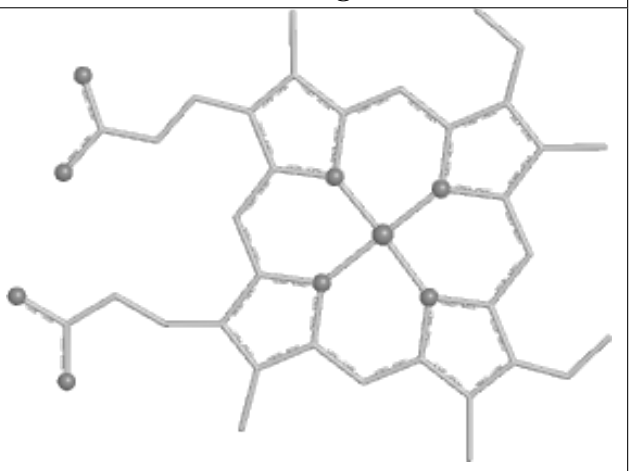
Bond lengths



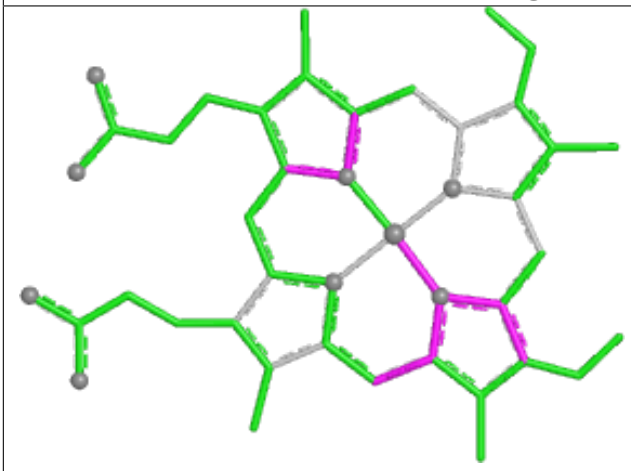
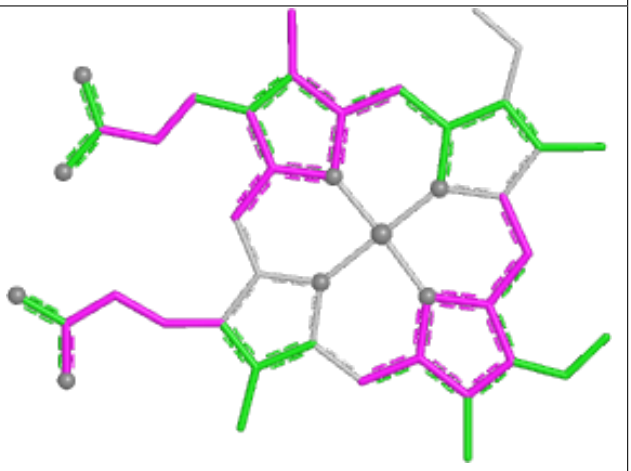
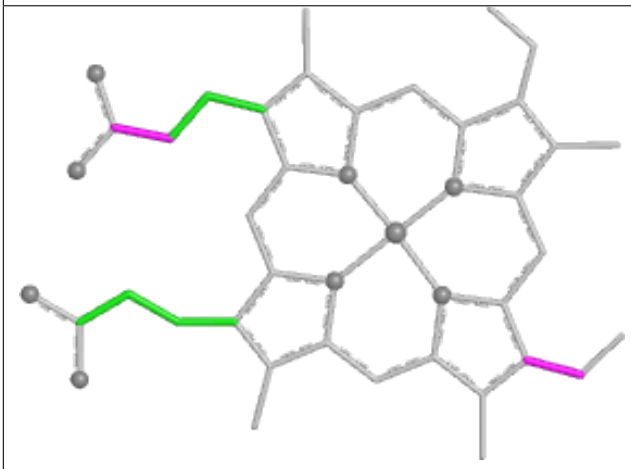
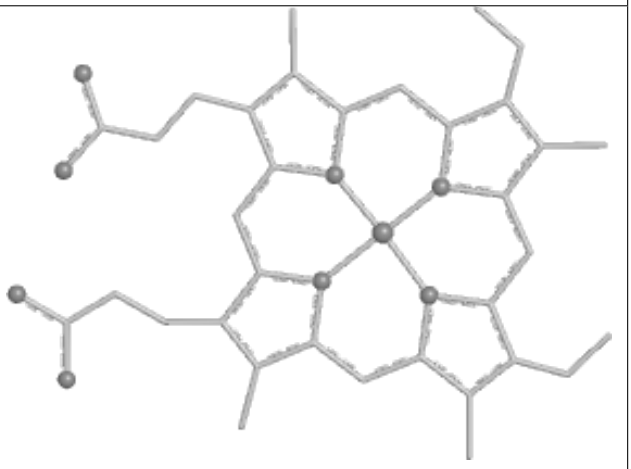
Bond angles

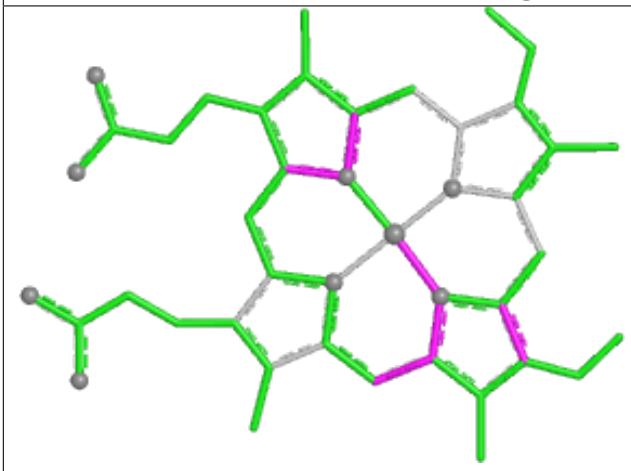
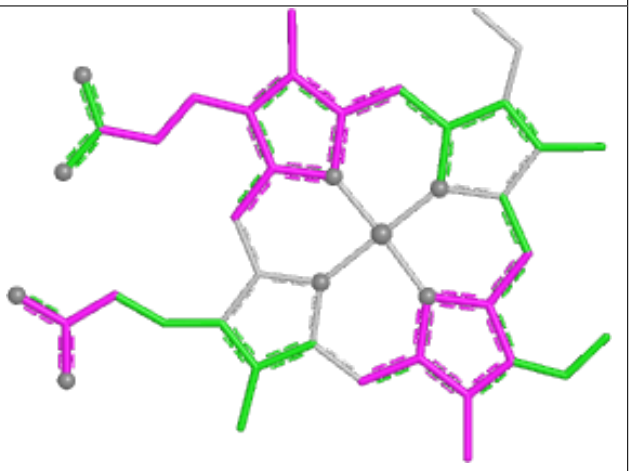
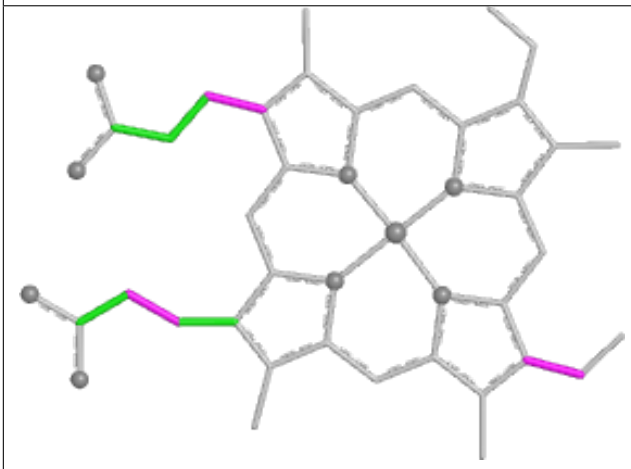
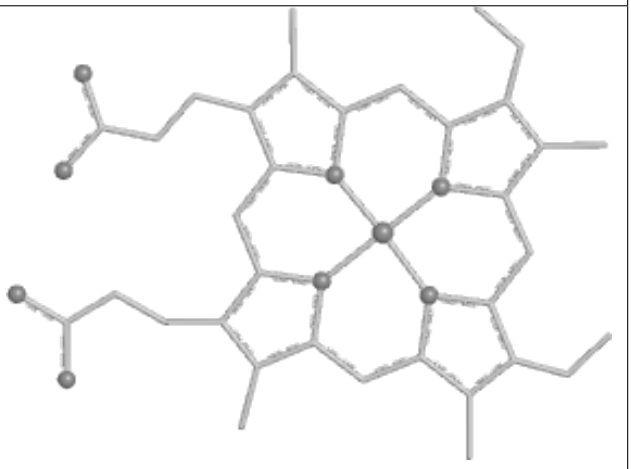


Torsions

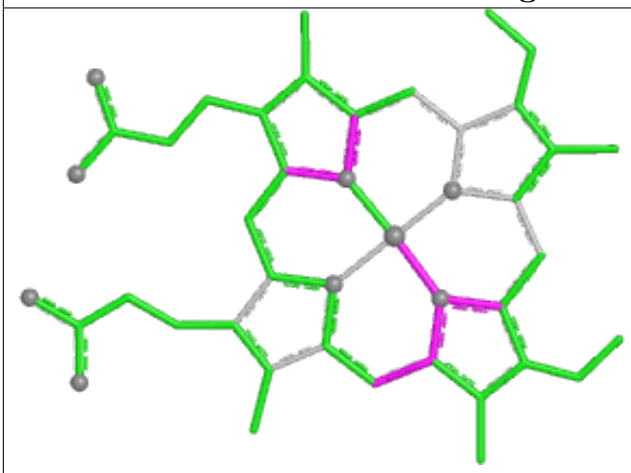


Rings

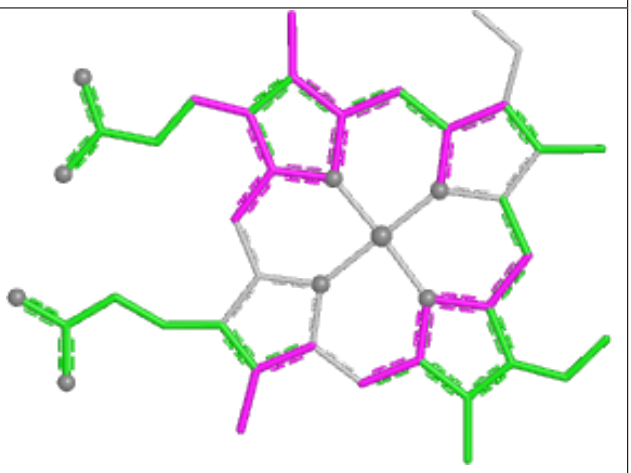
Ligand HEM I 201	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand HEM K 201	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

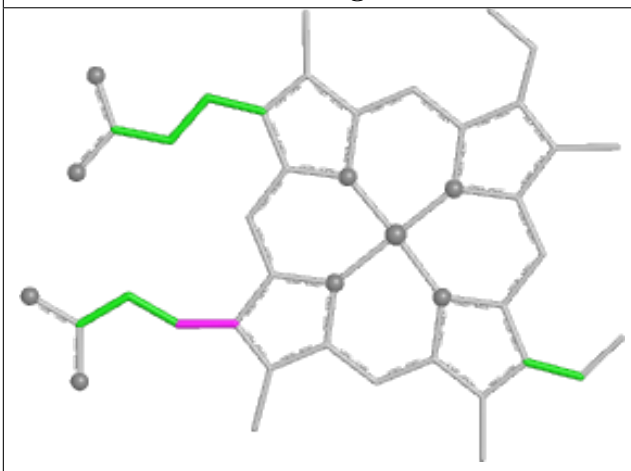
Ligand HEM B 201



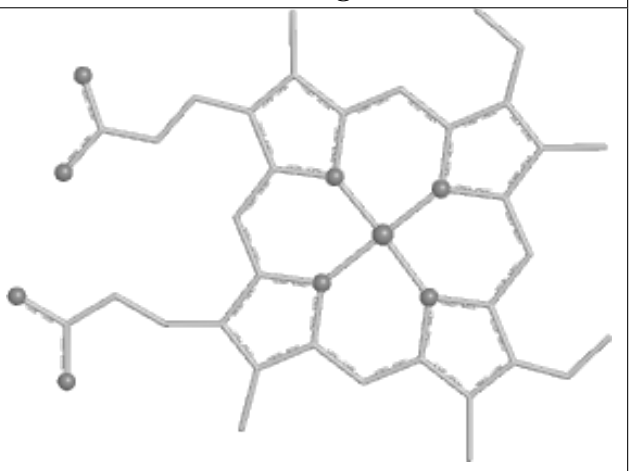
Bond lengths



Bond angles

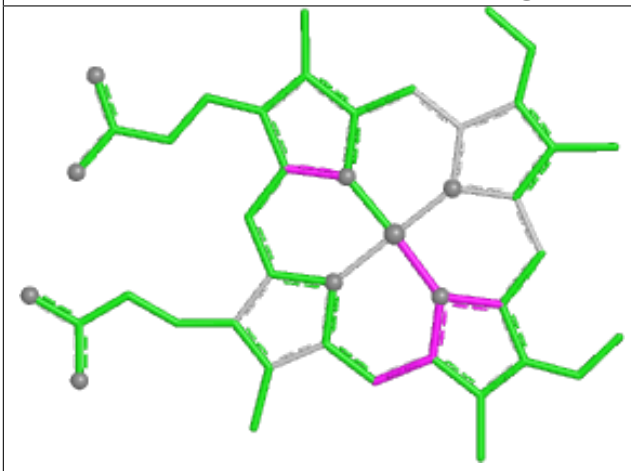


Torsions

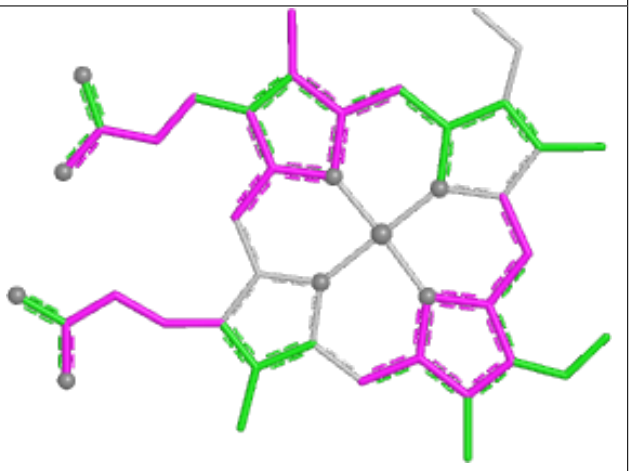


Rings

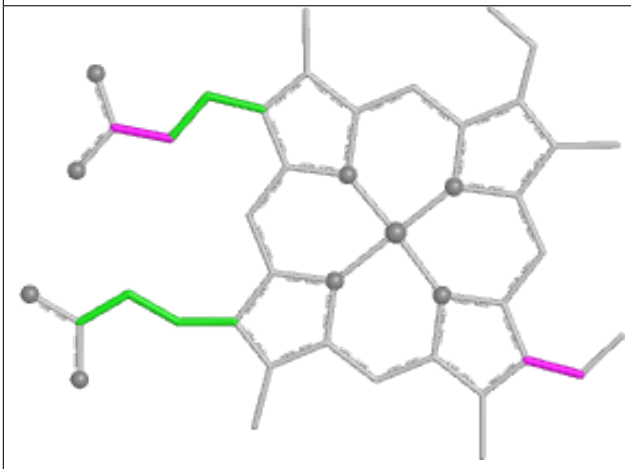
Ligand HEM A 201



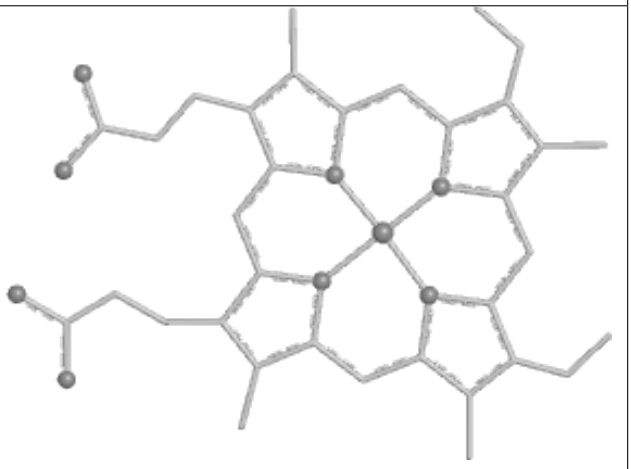
Bond lengths



Bond angles

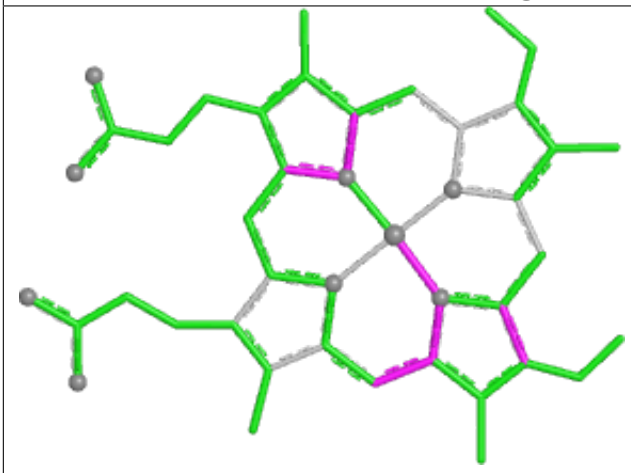


Torsions

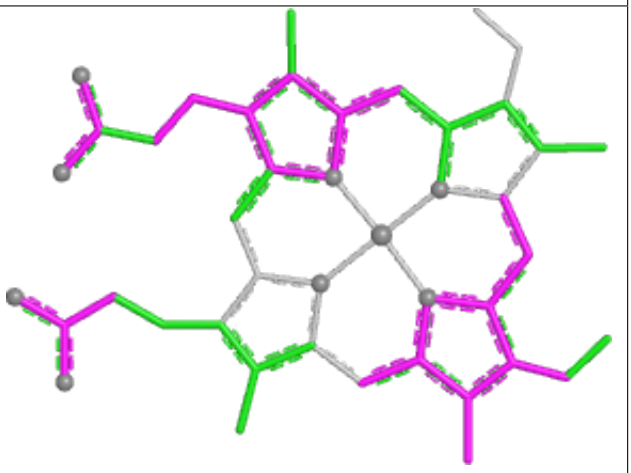


Rings

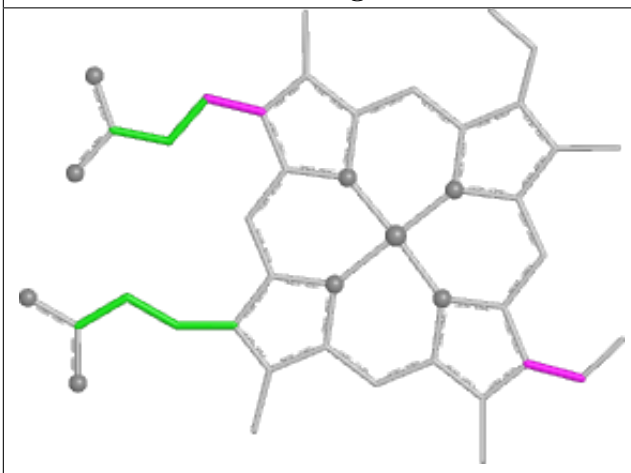
Ligand HEM G 201



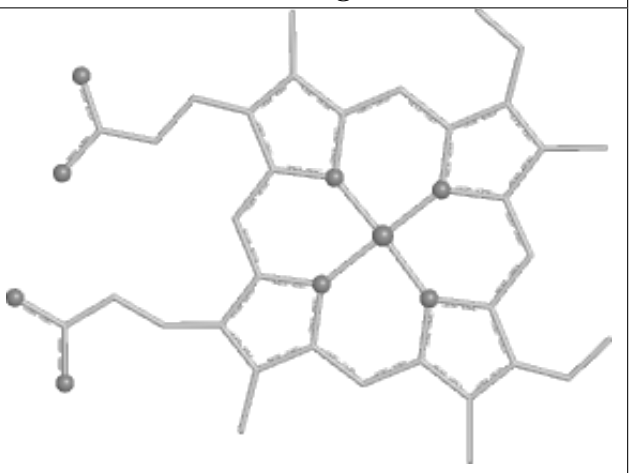
Bond lengths



Bond angles

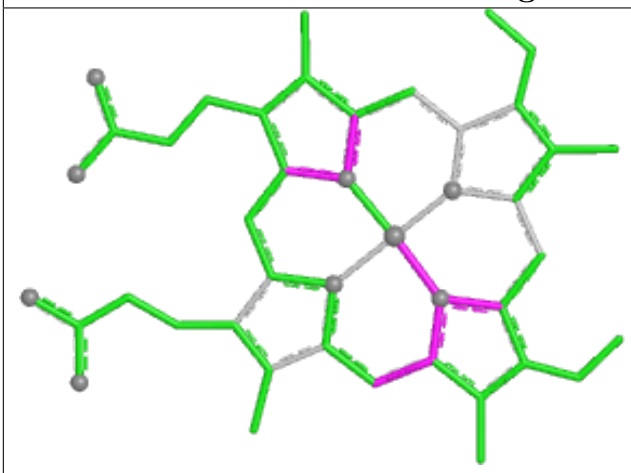


Torsions

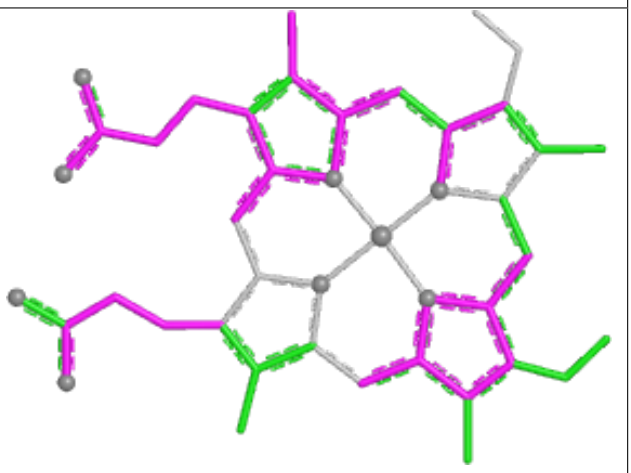


Rings

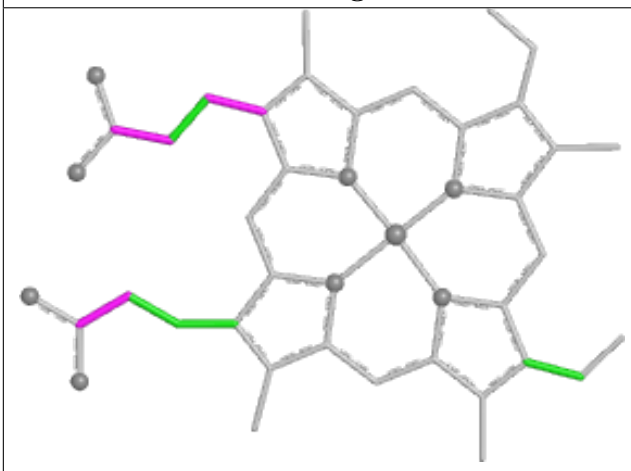
Ligand HEM D 201



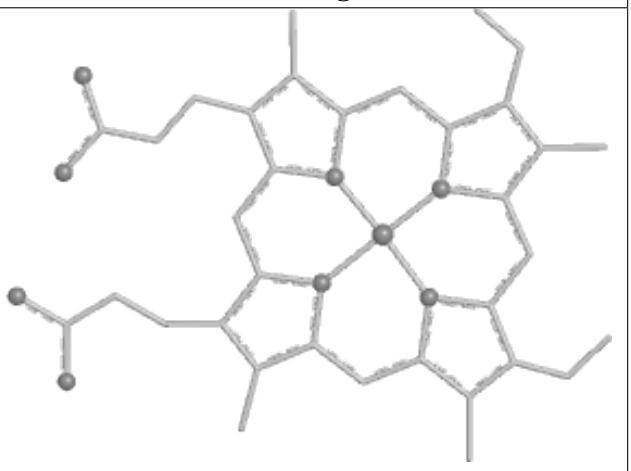
Bond lengths



Bond angles

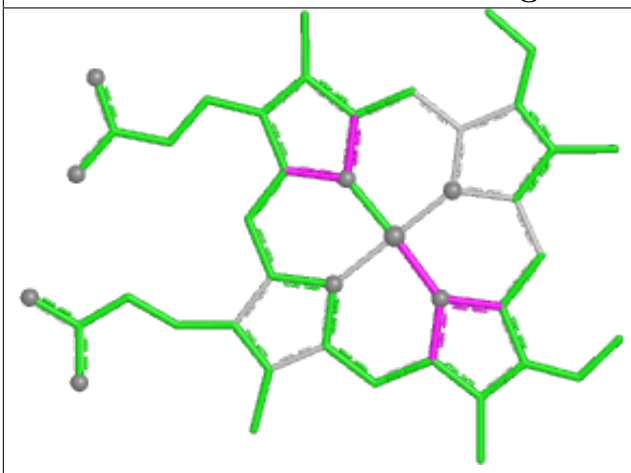


Torsions

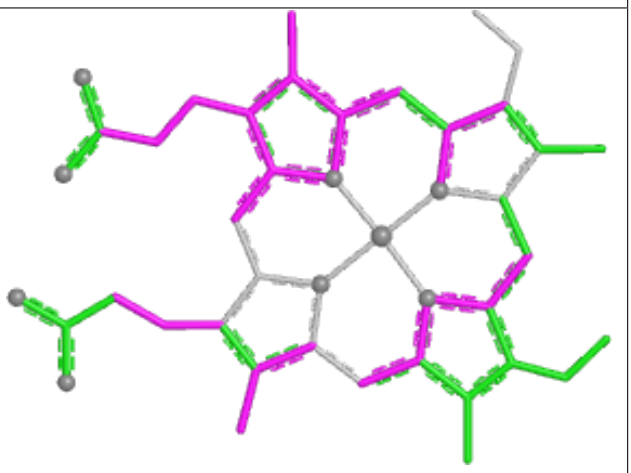


Rings

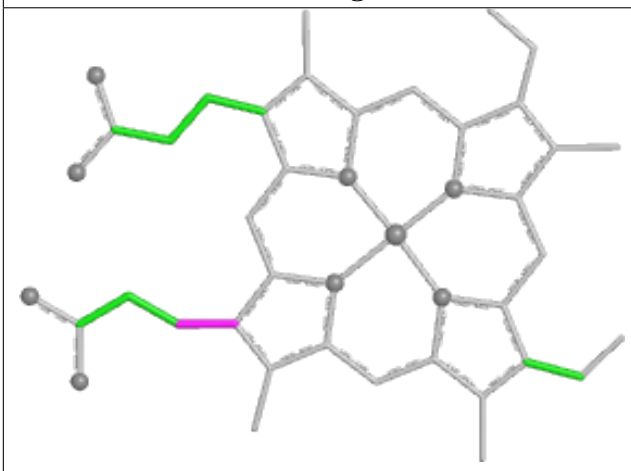
Ligand HEM F 201



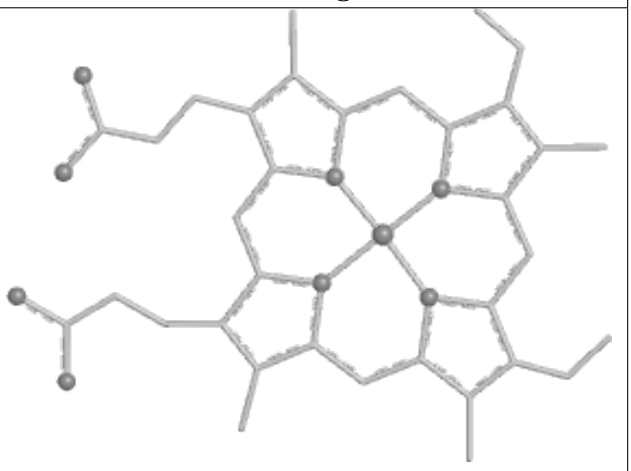
Bond lengths



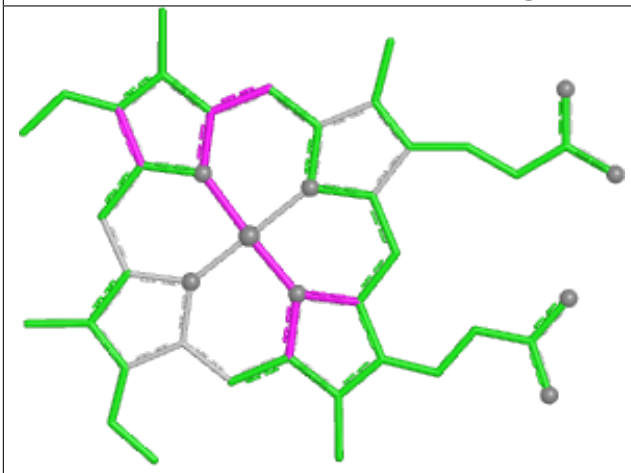
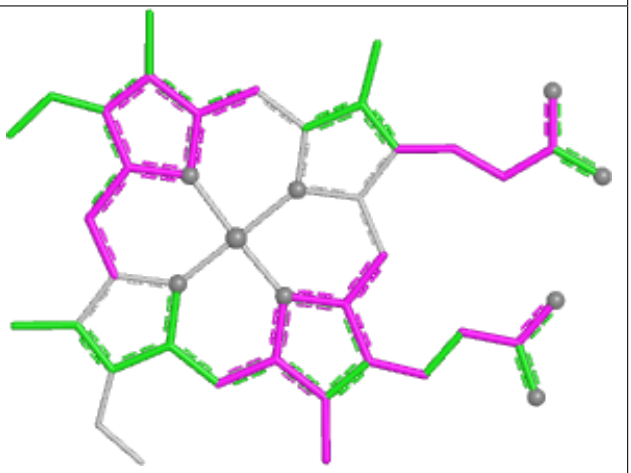
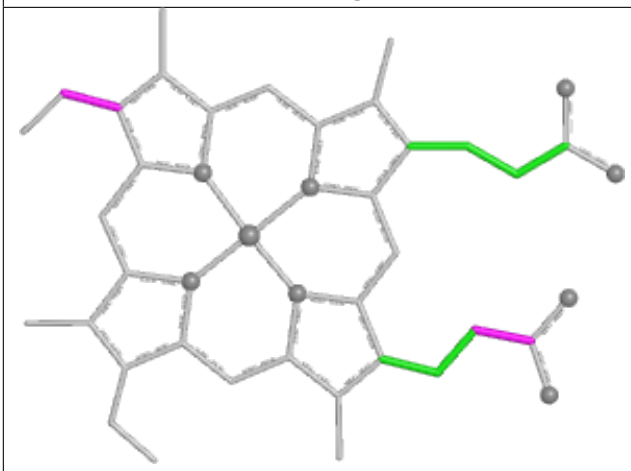
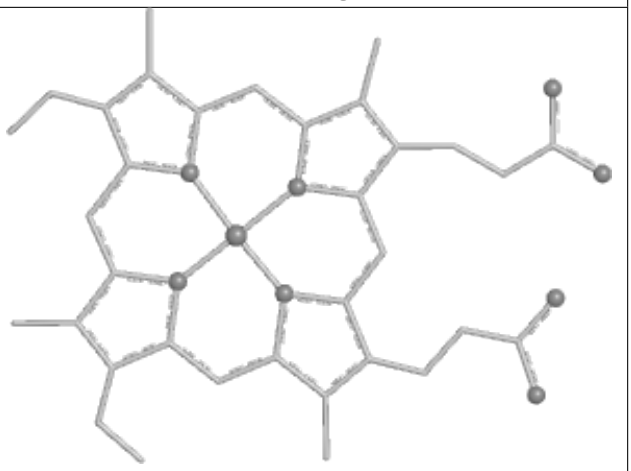
Bond angles



Torsions



Rings

Ligand HEM E 201	
	
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.

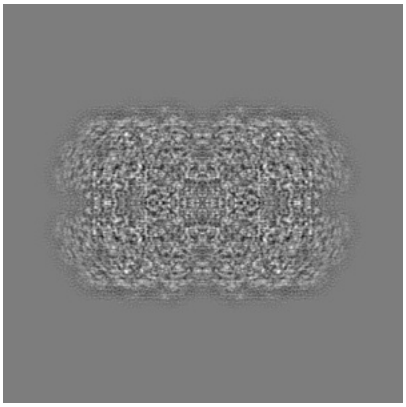
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3434. These allow visual inspection of the internal detail of the map and identification of artifacts.

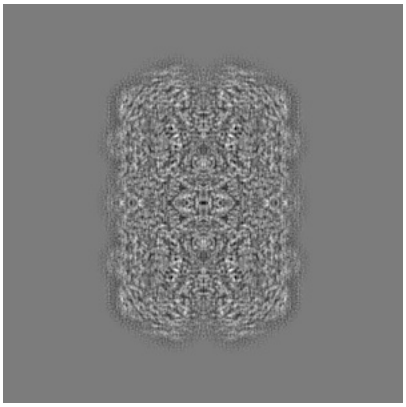
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

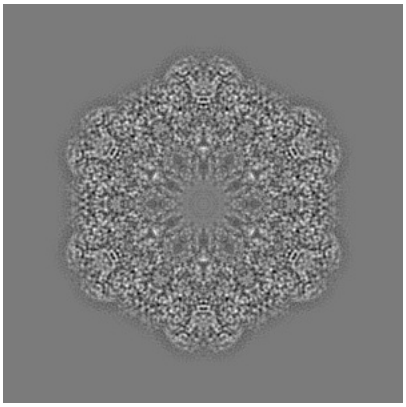
6.1.1 Primary map



X



Y

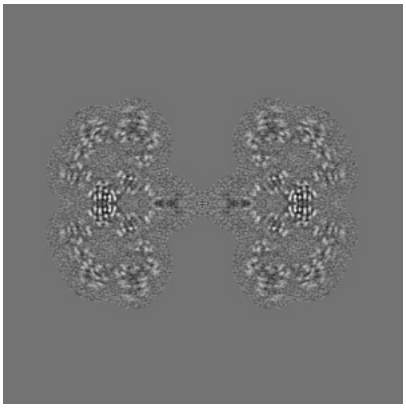


Z

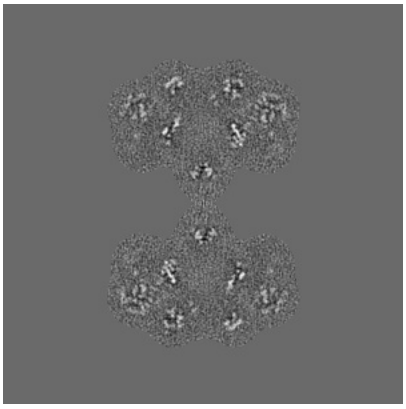
The images above show the map projected in three orthogonal directions.

6.2 Central slices

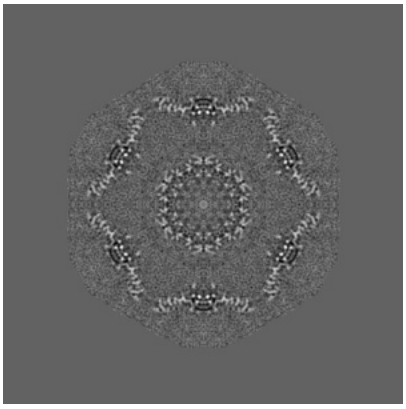
6.2.1 Primary map



X Index: 180



Y Index: 180

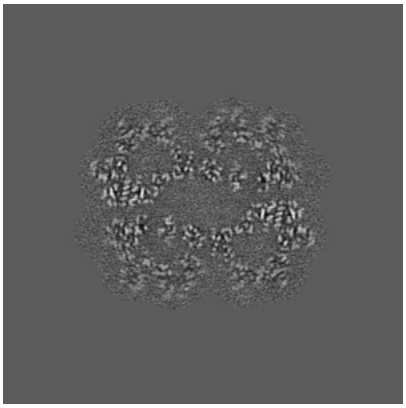


Z Index: 180

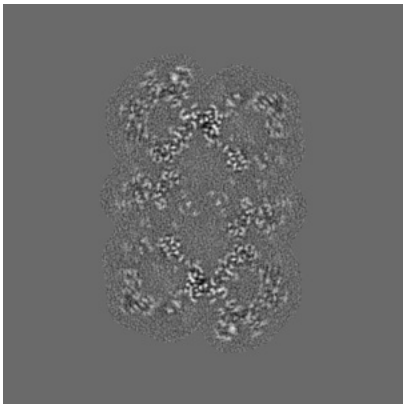
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

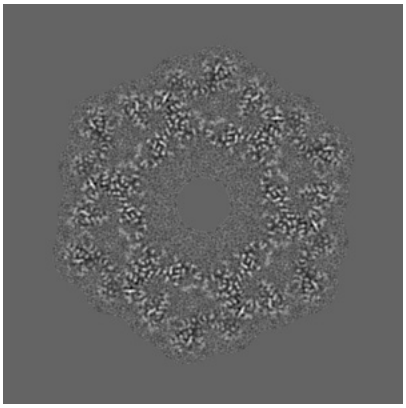
6.3.1 Primary map



X Index: 241



Y Index: 128

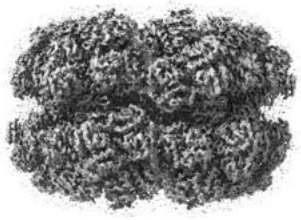


Z Index: 206

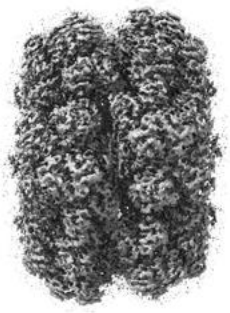
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

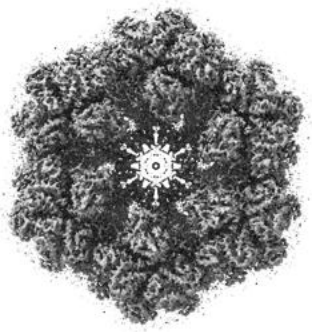
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

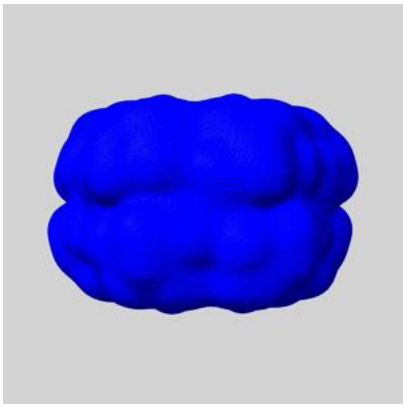
6.5 Mask visualisation (i)

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

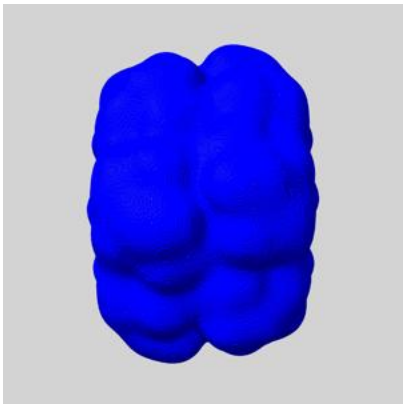
A mask typically either:

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

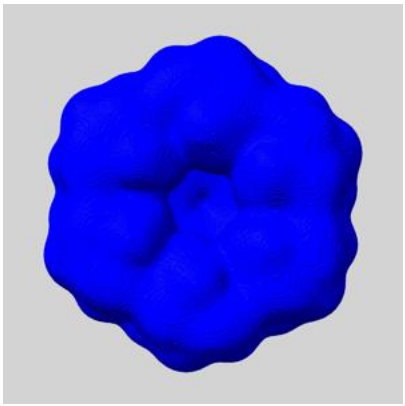
6.5.1 emd_3434_msk.map (i)



X



Y

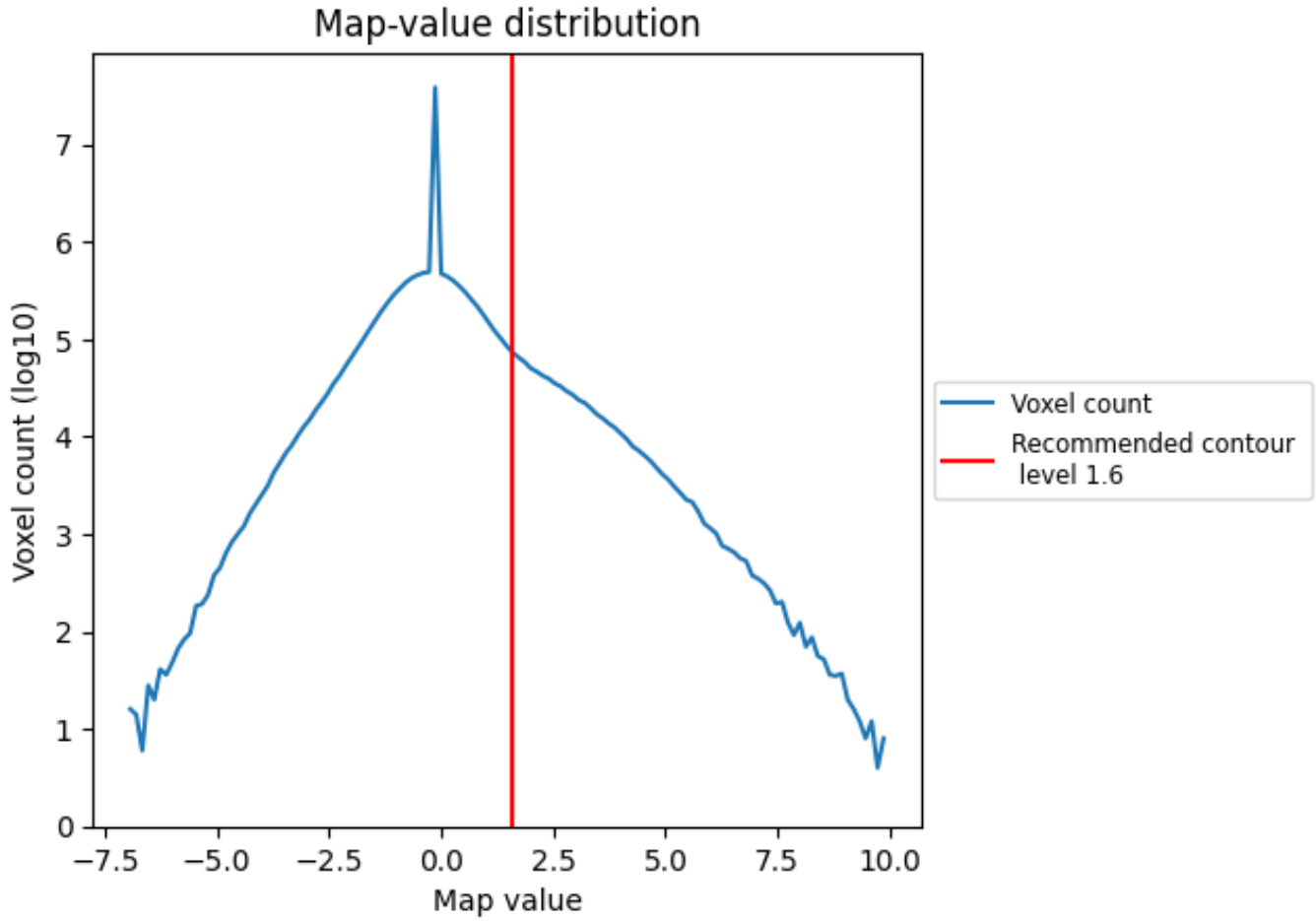


Z

7 Map analysis

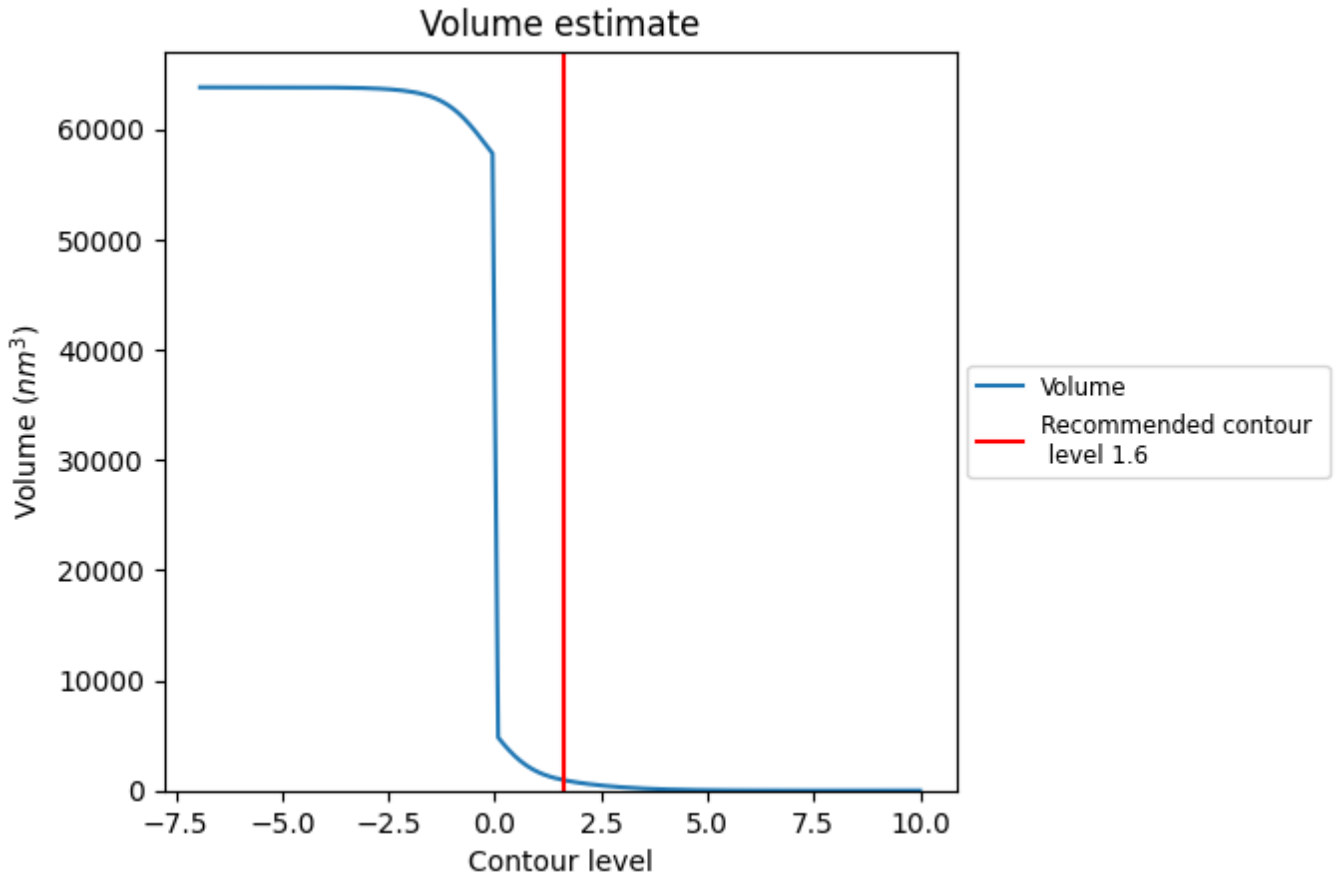
This section contains the results of statistical analysis of the map.

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.

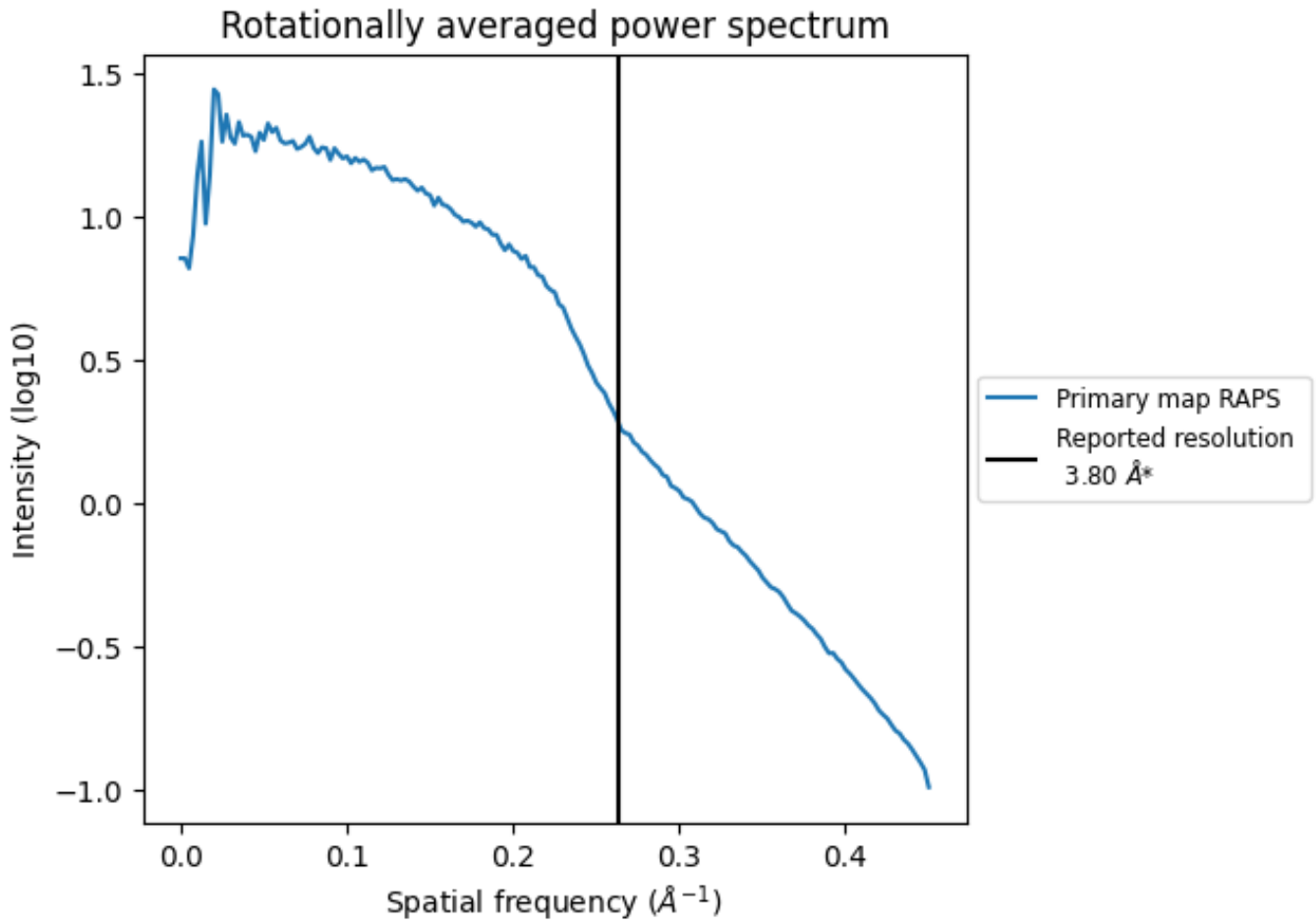
7.2 Volume estimate (i)



The volume at the recommended contour level is 969 nm^3; this corresponds to an approximate mass of 876 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)

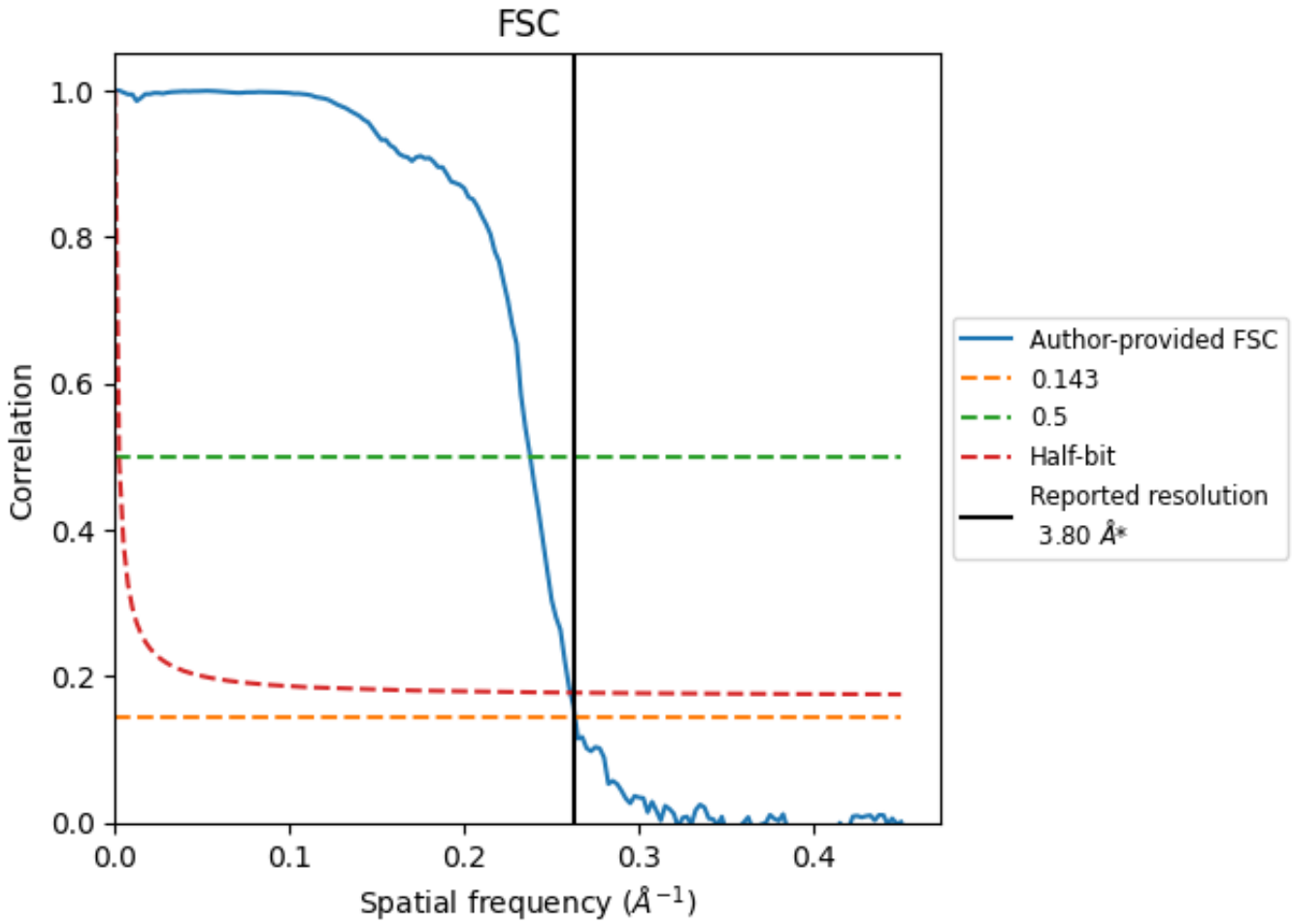


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

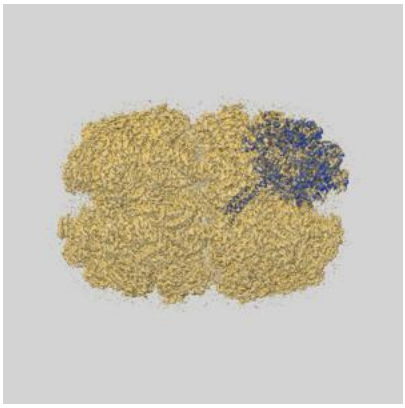
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	3.80
Author-provided FSC curve	3.79	4.20	3.83
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

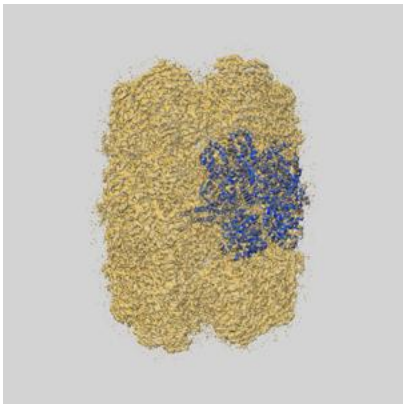
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3434 and PDB model 5M3L. Per-residue inclusion information can be found in section 3 on page 8.

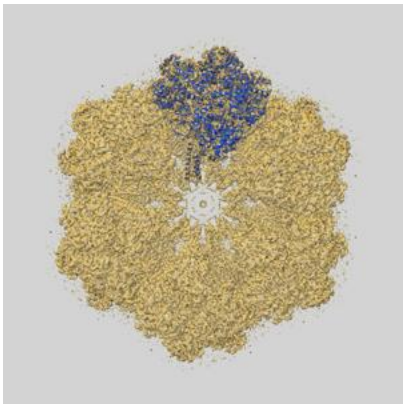
9.1 Map-model overlay



X



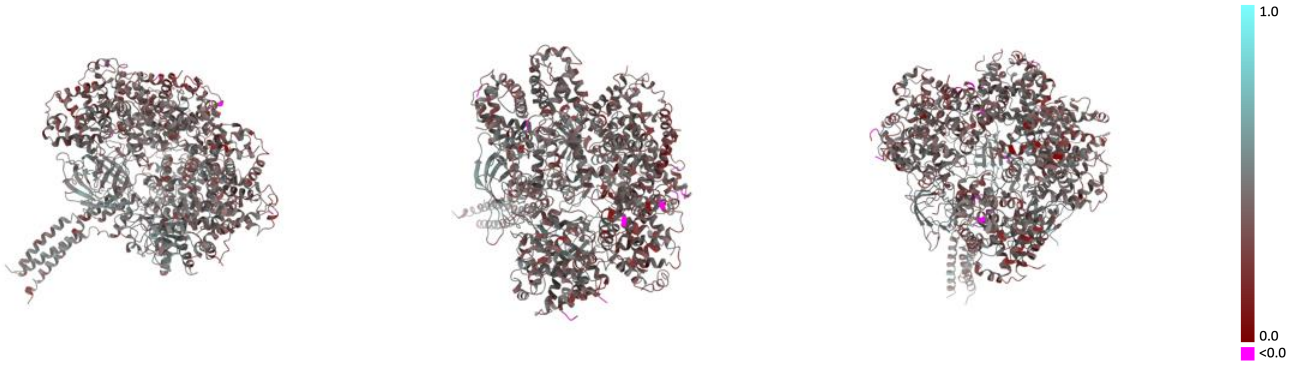
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

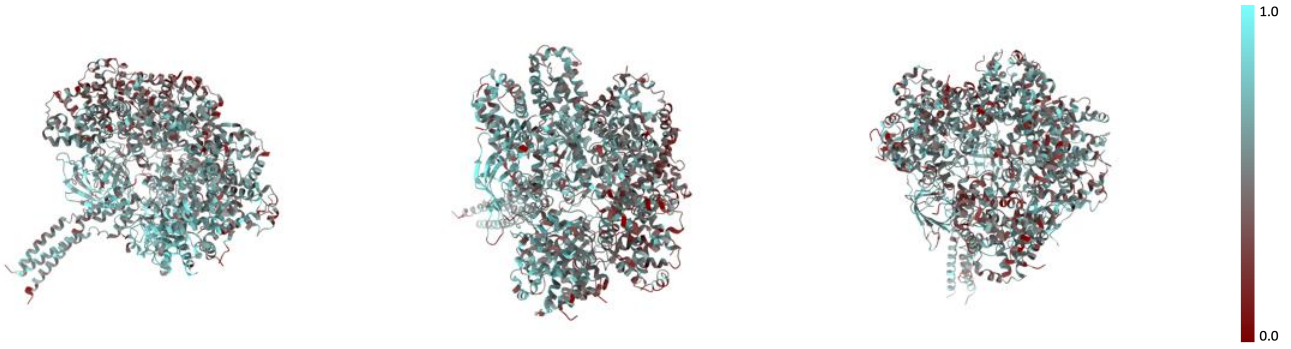
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

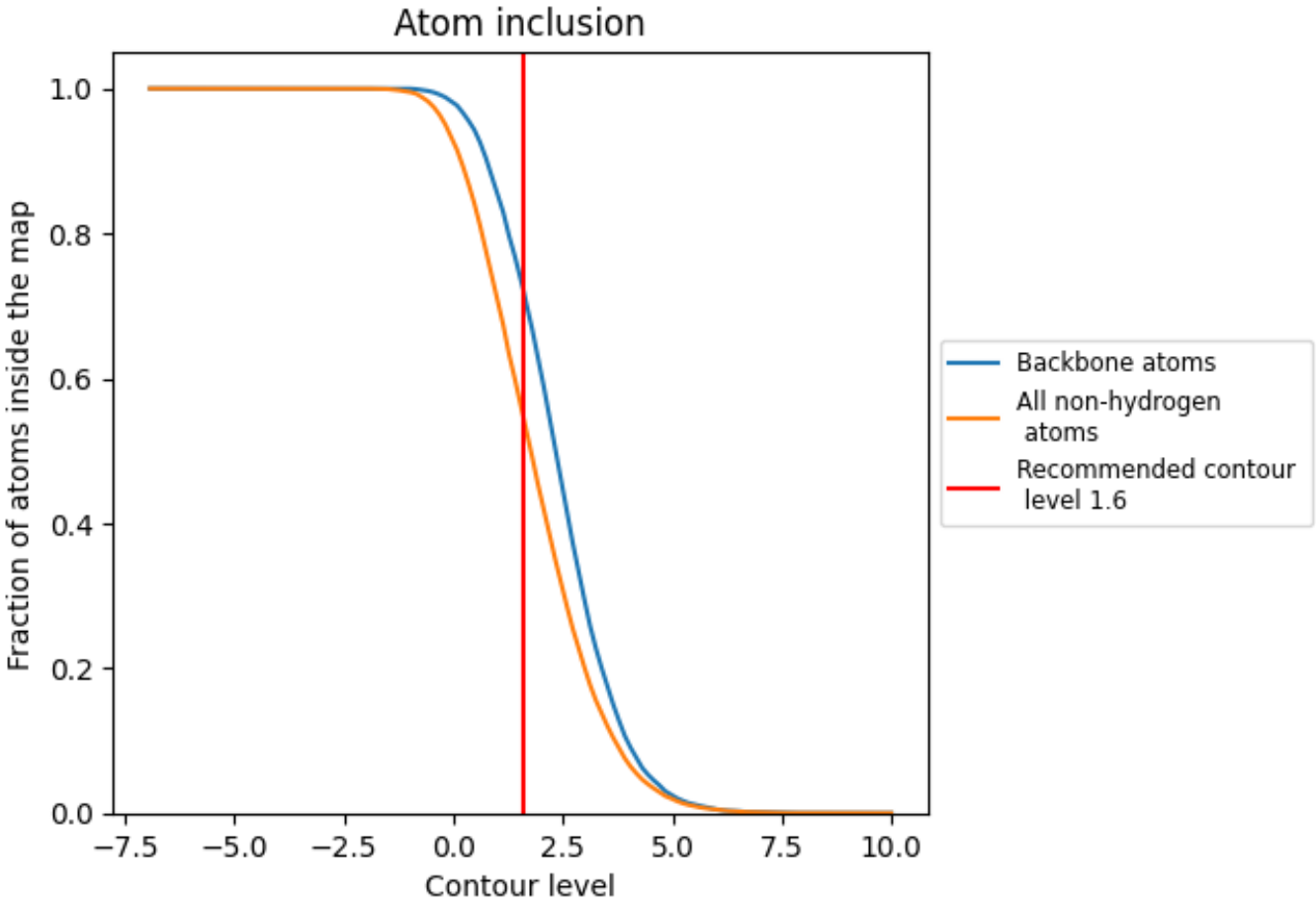
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.6).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5461	0.4090
A	0.5666	0.4010
B	0.6160	0.4240
C	0.5601	0.4040
D	0.5662	0.4070
E	0.4598	0.3790
F	0.6059	0.4200
G	0.5026	0.3850
H	0.4565	0.3410
I	0.5106	0.3980
J	0.4909	0.3820
K	0.3900	0.3660
L	0.4816	0.3600
M	0.6729	0.4770
N	0.6122	0.4570
O	0.6005	0.4600