wwPDB EM Validation Summary Report

Nov 3, 2024 – 03:24 PM EST

PDB ID	:	7TLJ
EMDB ID	:	EMD-25989
Title	:	Rhodobacter sphaeroides Mitochondrial respiratory chain complex
Authors	:	Xia, D.; Zhou, F.; Esser, L.; Huang, R.
Deposited on	:	2022-01-18
Resolution	:	2.91 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

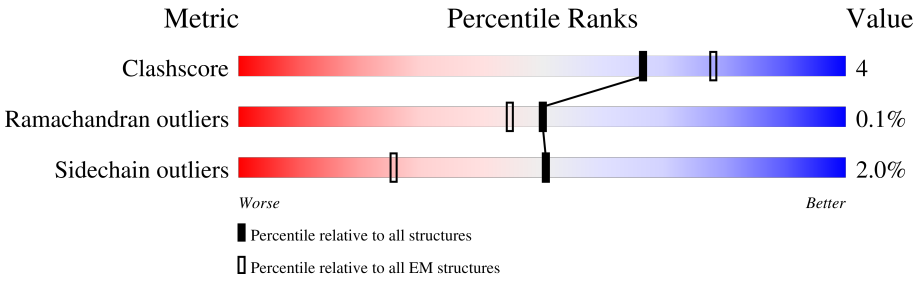
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.91 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	445	88% 8% ·
1	E	445	87% 9% ·
2	B	272	86% 8% 6%
2	F	272	85% 9% 6%
3	C	187	86% 10% ·
3	G	187	86% 9% · ·
4	D	124	17% · 81%
4	H	124	19% · 81%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 28105 atoms, of which 13863 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 Cytochrome b.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	428	Total	C	H	N	O	S	0	0
			6850	2319	3415	545	556	15		
1	E	428	Total	C	H	N	O	S	0	0
			6851	2319	3416	545	556	15		

- Molecule 2 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	256	Total	C	H	N	O	S	0	0
			3794	1240	1841	326	374	13		
2	F	256	Total	C	H	N	O	S	0	0
			3794	1240	1841	326	374	13		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	98	PRO	ALA	conflict	UNP Q02760
B	264	GLY	-	expression tag	UNP Q02760
B	265	THR	-	expression tag	UNP Q02760
B	266	GLY	-	expression tag	UNP Q02760
B	267	HIS	-	expression tag	UNP Q02760
B	268	HIS	-	expression tag	UNP Q02760
B	269	HIS	-	expression tag	UNP Q02760
B	270	HIS	-	expression tag	UNP Q02760
B	271	HIS	-	expression tag	UNP Q02760
B	272	HIS	-	expression tag	UNP Q02760
F	98	PRO	ALA	conflict	UNP Q02760
F	264	GLY	-	expression tag	UNP Q02760
F	265	THR	-	expression tag	UNP Q02760
F	266	GLY	-	expression tag	UNP Q02760
F	267	HIS	-	expression tag	UNP Q02760
F	268	HIS	-	expression tag	UNP Q02760
F	269	HIS	-	expression tag	UNP Q02760

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Chain	Residue	Modelled	Actual	Comment	Reference
F	270	HIS	-	expression tag	UNP Q02760
F	271	HIS	-	expression tag	UNP Q02760
F	272	HIS	-	expression tag	UNP Q02760

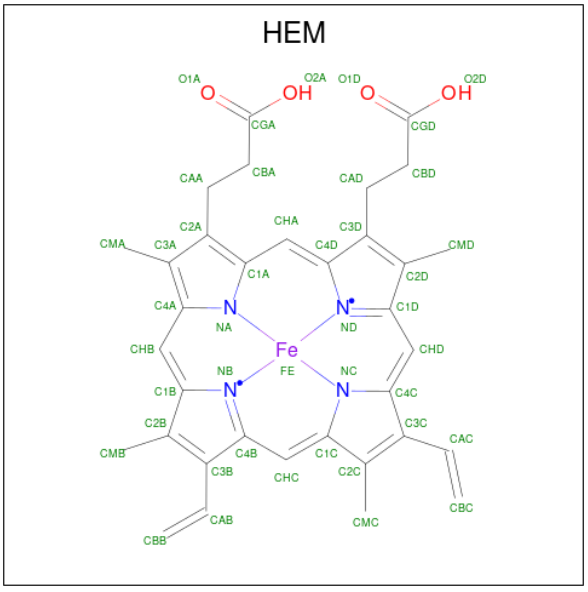
- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	179	Total	C	H	N	O	S	0	0
			2648	845	1307	237	253	6		
3	G	179	Total	C	H	N	O	S	0	0
			2648	845	1307	237	253	6		

- Molecule 4 is a protein called 14 kDa peptide of ubiquinol-cytochrome c2 oxidoreductase complex.

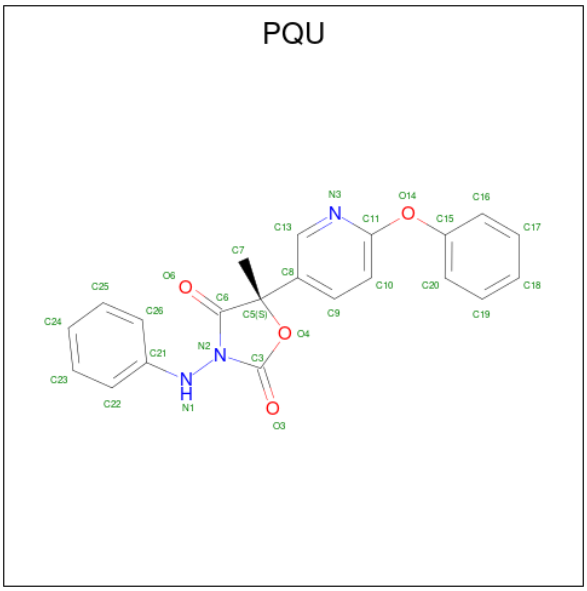
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	24	Total	C	H	N	O	0	0
			378	127	192	32	27		
4	H	24	Total	C	H	N	O	0	0
			378	127	192	32	27		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



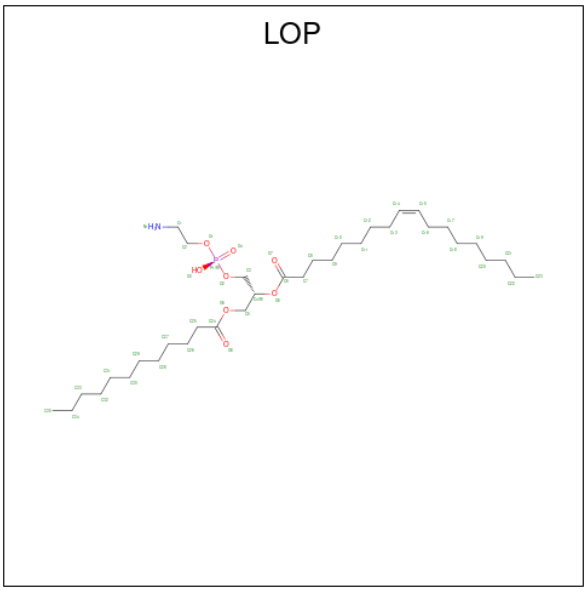
Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
5	A	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
5	E	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
5	E	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 6 is (5S)-3-anilino-5-methyl-5-(6-phenoxypyridin-3-yl)-1,3-oxazolidine-2,4-dione (three-letter code: PQU) (formula: $C_{21}H_{17}N_3O_4$) (labeled as "Ligand of Interest" by depositor).



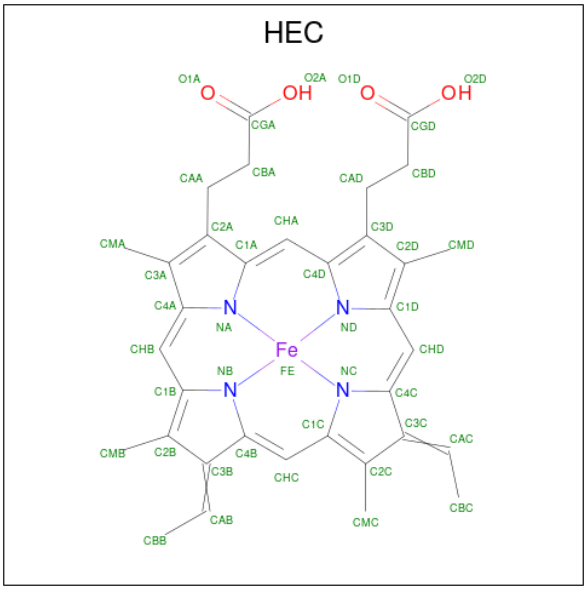
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	H	N	O	0
			45	21	17	3	4	
6	E	1	Total	C	H	N	O	0
			45	21	17	3	4	

- Molecule 7 is (1R)-2-{[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (three-letter code: LOP) (formula: $C_{35}H_{68}NO_8P$).



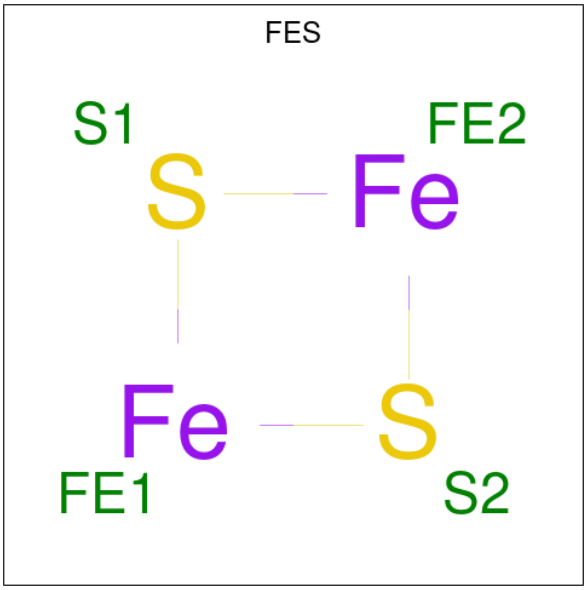
Mol	Chain	Residues	Atoms						AltConf
7	A	1	Total	C	H	N	O	P	0
			112	35	67	1	8	1	
7	E	1	Total	C	H	N	O	P	0
			112	35	67	1	8	1	

- Molecule 8 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms						AltConf
8	B	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	
8	F	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	

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



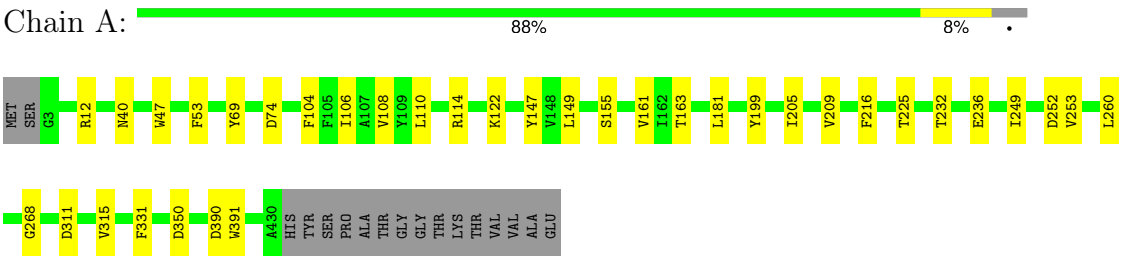
Mol	Chain	Residues	Atoms	AltConf
9	C	1	Total Fe S 4 2 2	0
9	G	1	Total Fe S 4 2 2	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

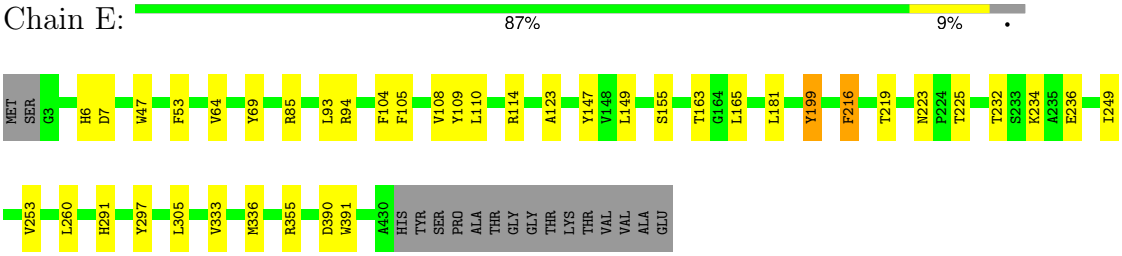
• Molecule 1: Cytochrome b

Chain A:



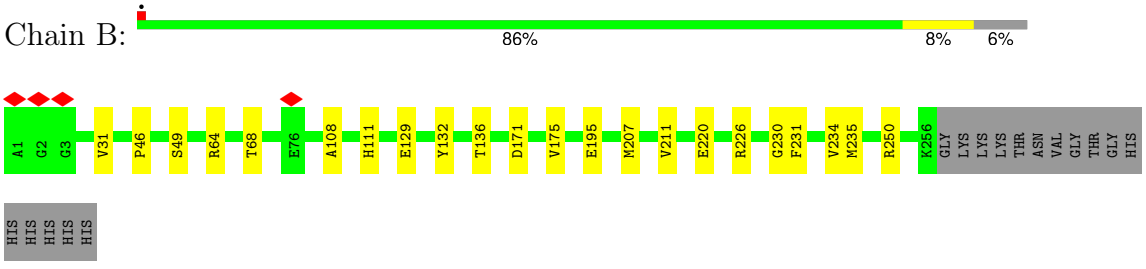
• Molecule 1: Cytochrome b

Chain E:



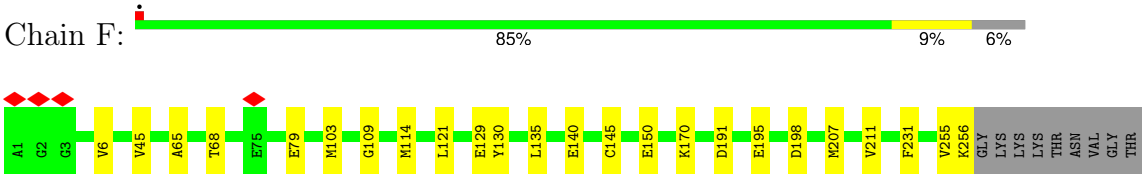
• Molecule 2: Cytochrome c1

Chain B:



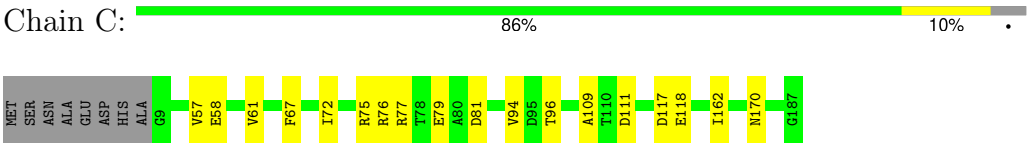
• Molecule 2: Cytochrome c1

Chain F:



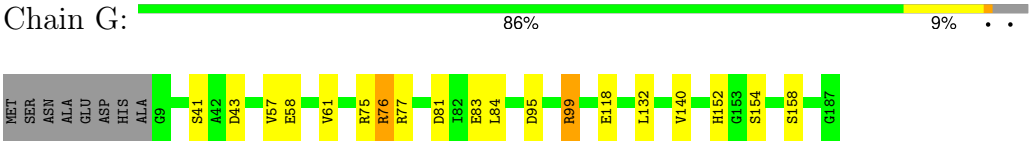
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain C:



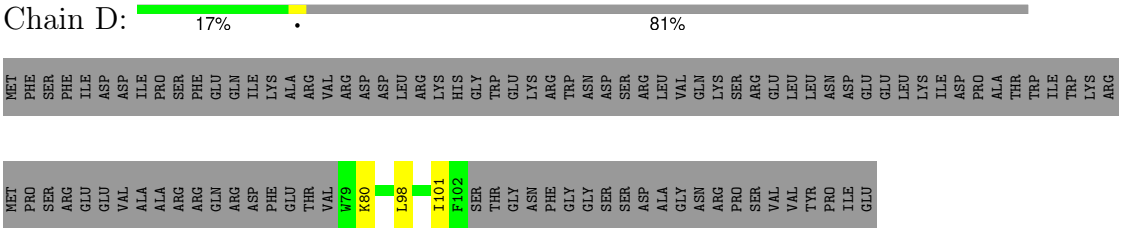
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain G:



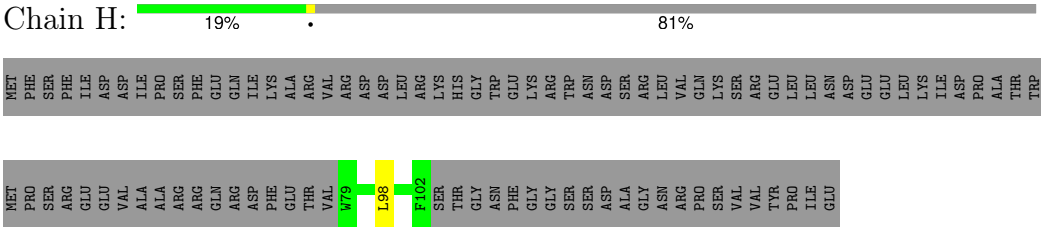
• Molecule 4: 14 kDa peptide of ubiquinol-cytochrome c2 oxidoreductase complex

Chain D:



• Molecule 4: 14 kDa peptide of ubiquinol-cytochrome c2 oxidoreductase complex

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	725256	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 ($e^-/Å^2$)	54.5	Depositor
Minimum defocus (nm)	836	Depositor
Maximum defocus (nm)	3434	Depositor
Magnification	60241	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	11.122	Depositor
Minimum map value	-3.397	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.277	Depositor
Recommended contour level	1.7	Depositor
Map size (Å)	318.72, 318.72, 318.72	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LOP, HEM, HEC, FES, PQU

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	0.31	0/3565	0.46	0/4891
1	E	0.31	0/3565	0.47	0/4891
2	B	0.30	0/2010	0.47	0/2733
2	F	0.32	0/2010	0.54	0/2733
3	C	0.26	0/1371	0.51	0/1868
3	G	0.30	0/1371	0.57	0/1868
4	D	0.26	0/191	0.48	0/256
4	H	0.26	0/191	0.49	0/256
All	All	0.30	0/14274	0.49	0/19496

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3435	3415	3420	17	0
1	E	3435	3416	3420	25	0
2	B	1953	1841	1848	14	0
2	F	1953	1841	1848	15	0
3	C	1341	1307	1307	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1341	1307	1307	10	0
4	D	186	192	192	2	0
4	H	186	192	192	2	0
5	A	86	60	60	5	0
5	E	86	60	60	7	0
6	A	28	17	0	0	0
6	E	28	17	0	0	0
7	A	45	67	67	1	0
7	E	45	67	67	0	0
8	B	43	32	30	3	0
8	F	43	32	30	6	0
9	C	4	0	0	0	0
9	G	4	0	0	1	0
All	All	14242	13863	13848	104	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 4.

The worst 5 of 104 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:223:ASN:OD1	1:E:225:THR:OG1	2.02	0.78
3:G:41:SER:OG	3:G:43:ASP:OD1	2.05	0.75
2:B:207:MET:O	2:B:211:VAL:HG23	1.88	0.74
3:C:75:ARG:NH1	3:C:81:ASP:OD2	2.21	0.74
2:F:130:TYR:OH	8:F:1001:HEC:O2A	2.07	0.73

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	426/445 (96%)	422 (99%)	4 (1%)	0	100	100
1	E	426/445 (96%)	418 (98%)	8 (2%)	0	100	100
2	B	254/272 (93%)	246 (97%)	8 (3%)	0	100	100
2	F	254/272 (93%)	241 (95%)	13 (5%)	0	100	100
3	C	177/187 (95%)	170 (96%)	7 (4%)	0	100	100
3	G	177/187 (95%)	163 (92%)	13 (7%)	1 (1%)	22	51
4	D	22/124 (18%)	21 (96%)	1 (4%)	0	100	100
4	H	22/124 (18%)	22 (100%)	0	0	100	100
All	All	1758/2056 (86%)	1703 (97%)	54 (3%)	1 (0%)	50	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	140	VAL

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	353/366 (96%)	345 (98%)	8 (2%)	45	75
1	E	353/366 (96%)	347 (98%)	6 (2%)	56	82
2	B	203/216 (94%)	200 (98%)	3 (2%)	60	84
2	F	203/216 (94%)	196 (97%)	7 (3%)	32	65
3	C	138/144 (96%)	138 (100%)	0	100	100
3	G	138/144 (96%)	135 (98%)	3 (2%)	47	76
4	D	15/105 (14%)	14 (93%)	1 (7%)	13	37
4	H	15/105 (14%)	15 (100%)	0	100	100
All	All	1418/1662 (85%)	1390 (98%)	28 (2%)	50	78

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	104	PHE
3	G	118	GLU
1	E	291	HIS
2	F	231	PHE
1	E	216	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	ASN
2	B	62	GLN
2	B	69	GLN
2	F	157	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
7	LOP	A	1004	-	44,44,44	1.51	4 (9%)	47,49,49	1.32	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	PQU	E	1003	-	30,31,31	0.86	2 (6%)	36,44,44	1.29	4 (11%)
8	HEC	B	1001	2	32,50,50	2.07	3 (9%)	30,82,82	2.34	7 (23%)
9	FES	C	1001	3	0,4,4	-	-	-		
5	HEM	E	1001	1	42,50,50	1.45	5 (11%)	46,82,82	1.29	3 (6%)
7	LOP	E	1004	-	44,44,44	1.51	3 (6%)	47,49,49	1.48	9 (19%)
5	HEM	E	1002	1	42,50,50	1.45	5 (11%)	46,82,82	1.23	6 (13%)
8	HEC	F	1001	2	32,50,50	2.09	3 (9%)	30,82,82	2.27	6 (20%)
9	FES	G	1001	3	0,4,4	-	-	-		
6	PQU	A	1003	-	30,31,31	0.85	2 (6%)	36,44,44	1.34	6 (16%)
5	HEM	A	1001	1	42,50,50	1.45	5 (11%)	46,82,82	1.31	4 (8%)
5	HEM	A	1002	1	42,50,50	1.46	5 (11%)	46,82,82	1.25	6 (13%)

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
7	LOP	A	1004	-	-	18/48/48/48	-
6	PQU	E	1003	-	-	0/14/33/33	0/4/4/4
8	HEC	B	1001	2	-	0/10/54/54	-
9	FES	C	1001	3	-	-	0/1/1/1
5	HEM	E	1001	1	-	3/12/54/54	-
7	LOP	E	1004	-	-	24/48/48/48	-
5	HEM	E	1002	1	-	3/12/54/54	-
8	HEC	F	1001	2	-	0/10/54/54	-
9	FES	G	1001	3	-	-	0/1/1/1
6	PQU	A	1003	-	-	0/14/33/33	0/4/4/4
5	HEM	A	1001	1	-	3/12/54/54	-
5	HEM	A	1002	1	-	1/12/54/54	-

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	1001	HEC	C2B-C3B	-6.33	1.33	1.40
8	B	1001	HEC	C2B-C3B	-6.26	1.33	1.40
7	A	1004	LOP	P1-O4	6.24	1.72	1.50
7	E	1004	LOP	P1-O4	6.23	1.72	1.50
8	F	1001	HEC	C3C-C2C	-5.84	1.34	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1001	HEC	CBB-CAB-C3B	-7.81	109.20	127.49
8	F	1001	HEC	CBB-CAB-C3B	-7.51	109.90	127.49
8	F	1001	HEC	CBC-CAC-C3C	-5.81	113.89	127.49
8	B	1001	HEC	CBC-CAC-C3C	-5.55	114.50	127.49
7	E	1004	LOP	O5-C6-C7	4.53	121.28	111.48

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1004	LOP	C2-O1-P1-O2
7	A	1004	LOP	C2-O1-P1-O3
7	E	1004	LOP	C2-O1-P1-O2
7	E	1004	LOP	C2-O1-P1-O3
7	E	1004	LOP	C3-O2-P1-O1

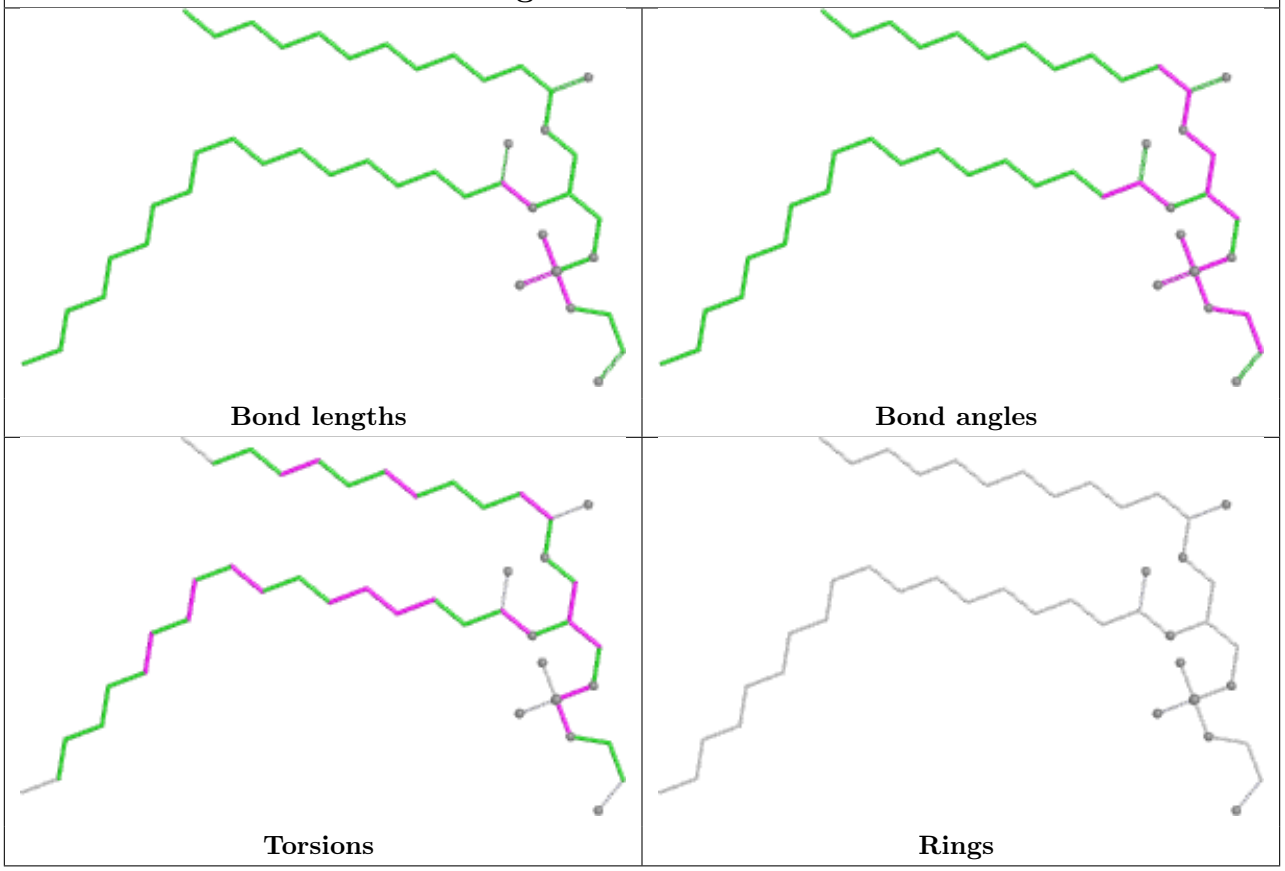
There are no ring outliers.

8 monomers are involved in 23 short contacts:

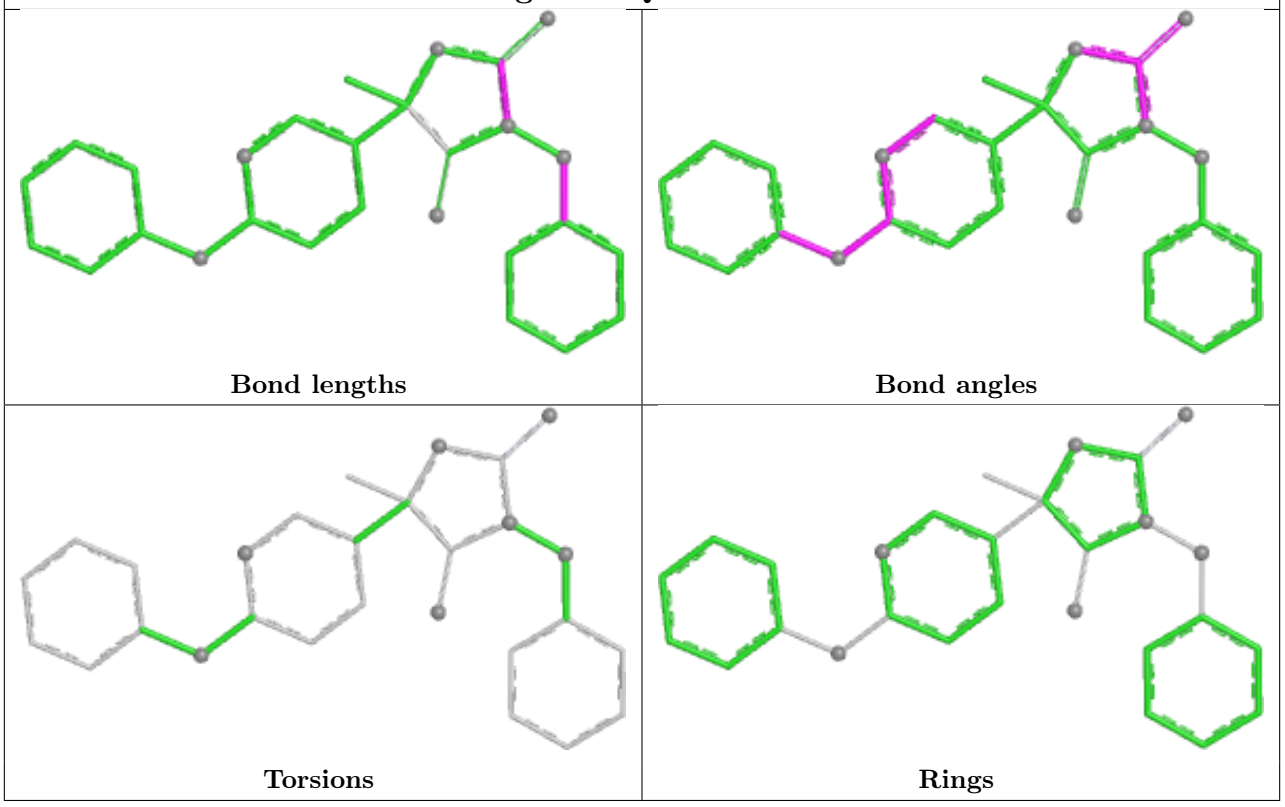
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1004	LOP	1	0
8	B	1001	HEC	3	0
5	E	1001	HEM	4	0
5	E	1002	HEM	3	0
8	F	1001	HEC	6	0
9	G	1001	FES	1	0
5	A	1001	HEM	2	0
5	A	1002	HEM	3	0

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.

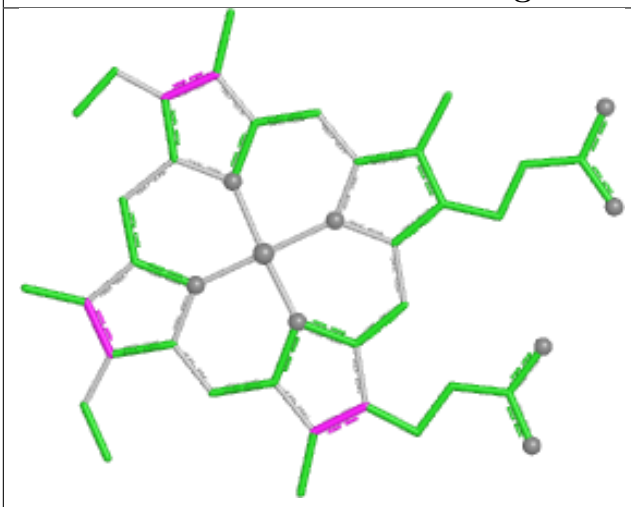
Ligand LOP A 1004



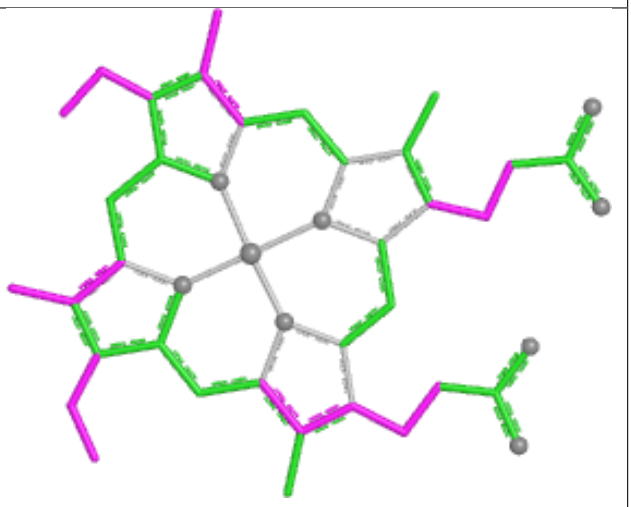
Ligand PQU E 1003



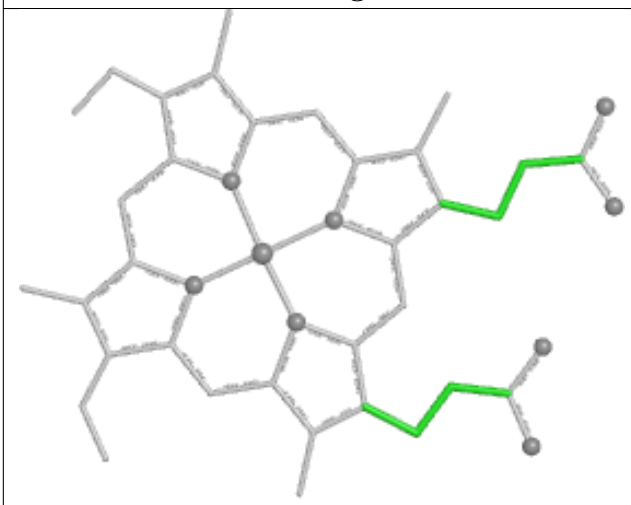
Ligand HEC B 1001



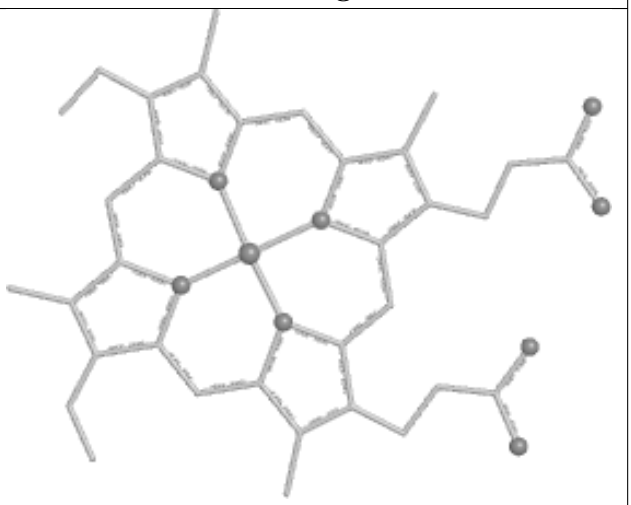
Bond lengths



Bond angles

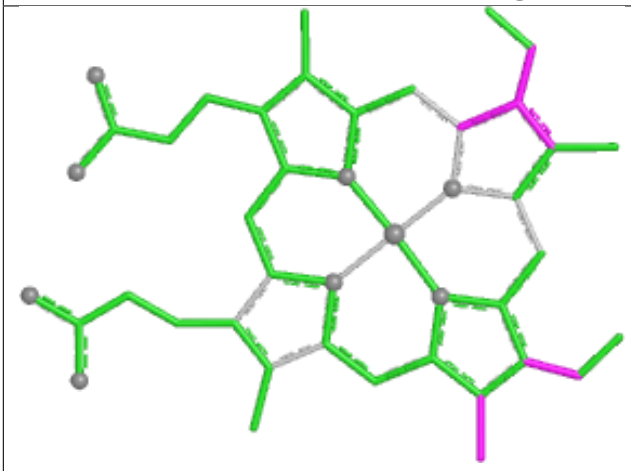


Torsions

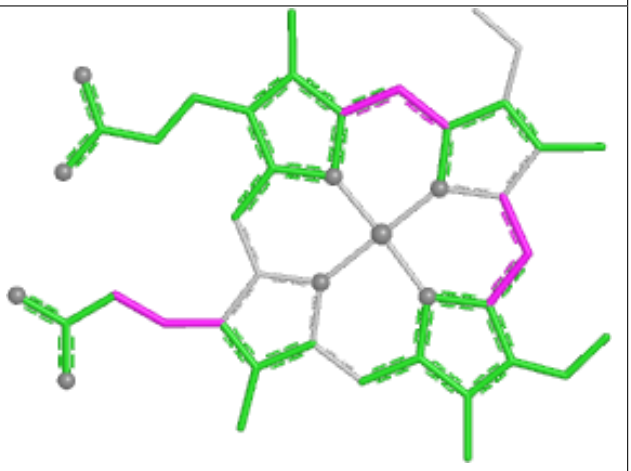


Rings

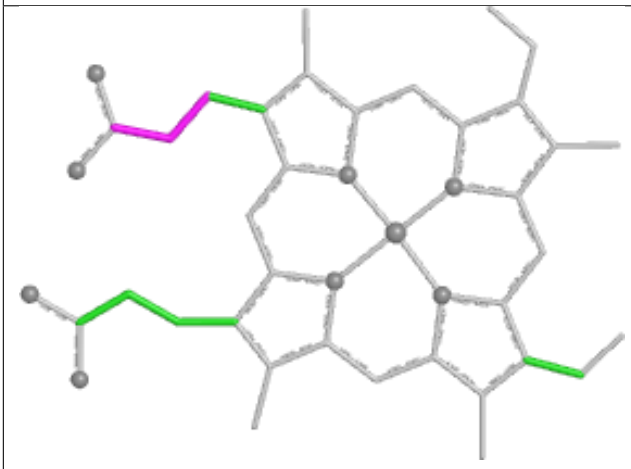
Ligand HEM E 1001



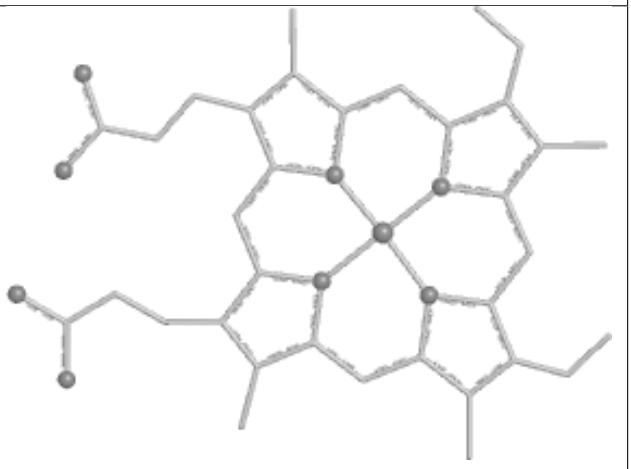
Bond lengths



Bond angles

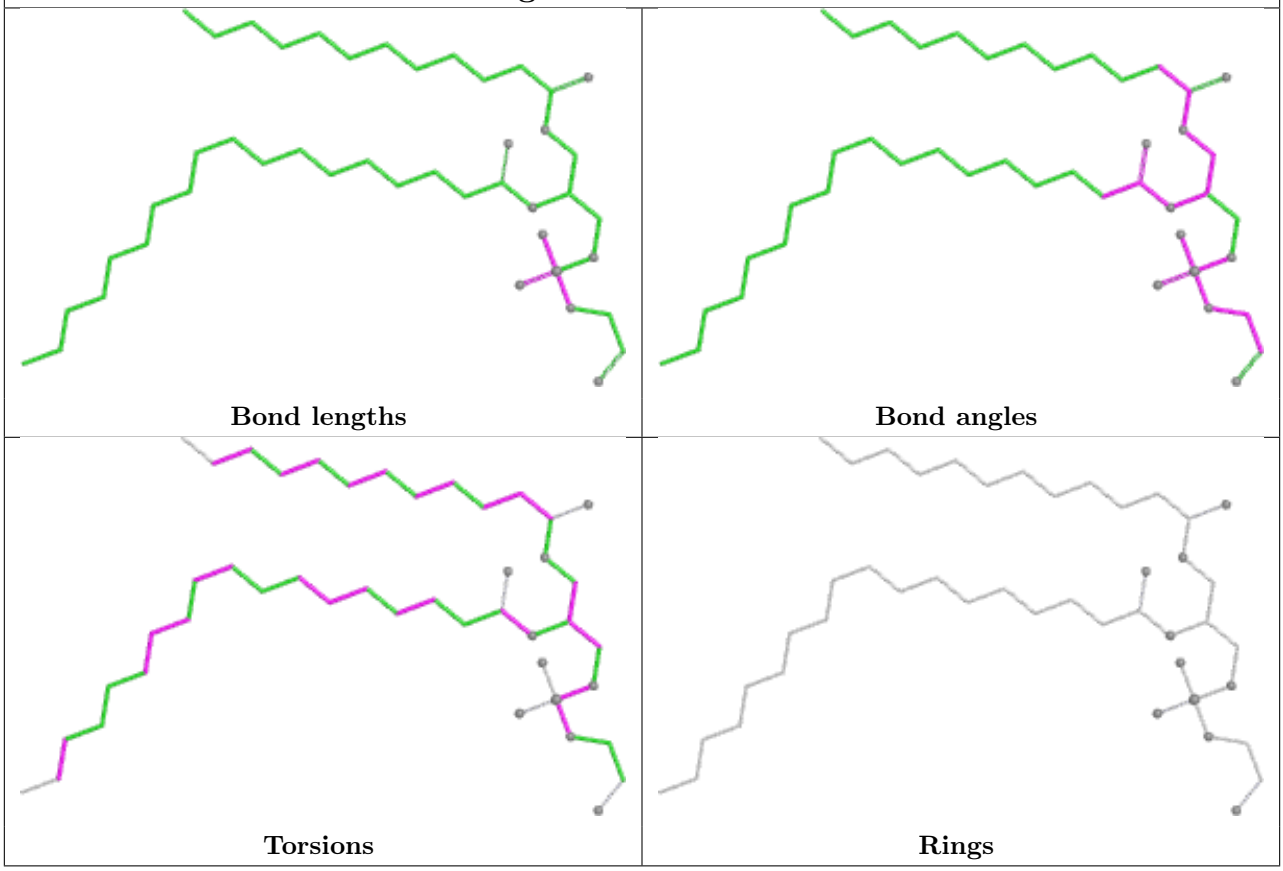


Torsions

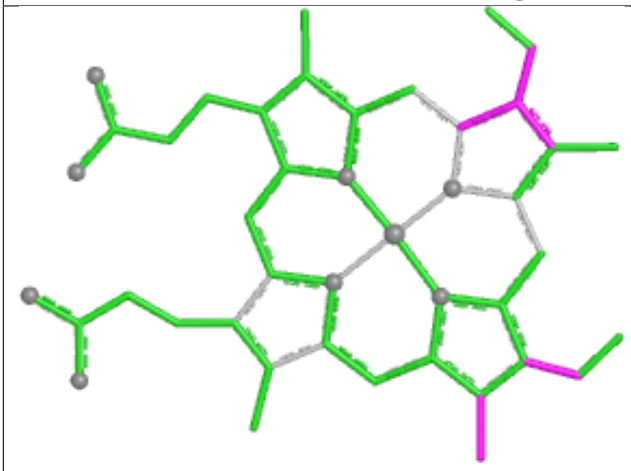


Rings

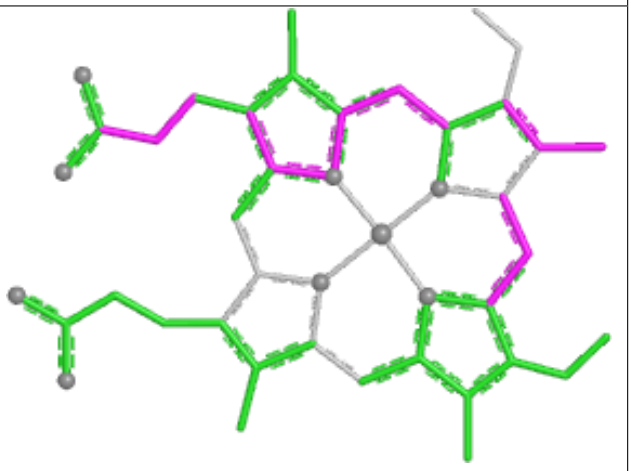
Ligand LOP E 1004



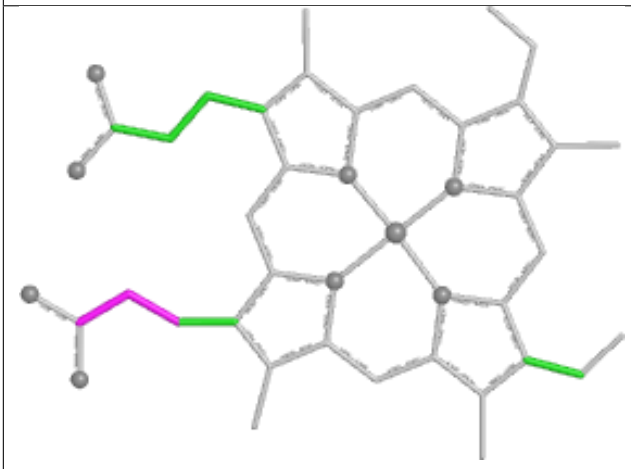
Ligand HEM E 1002



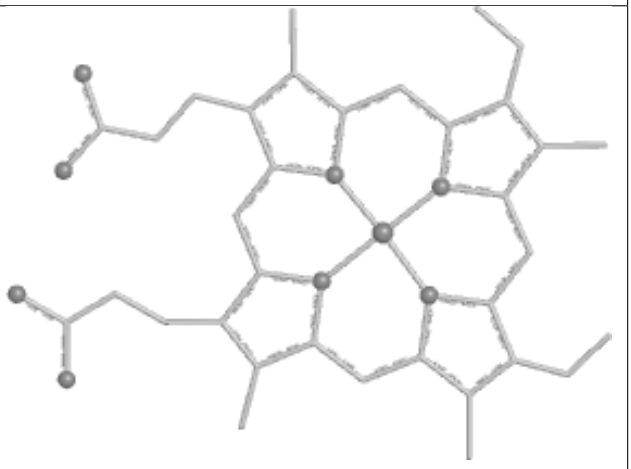
Bond lengths



Bond angles

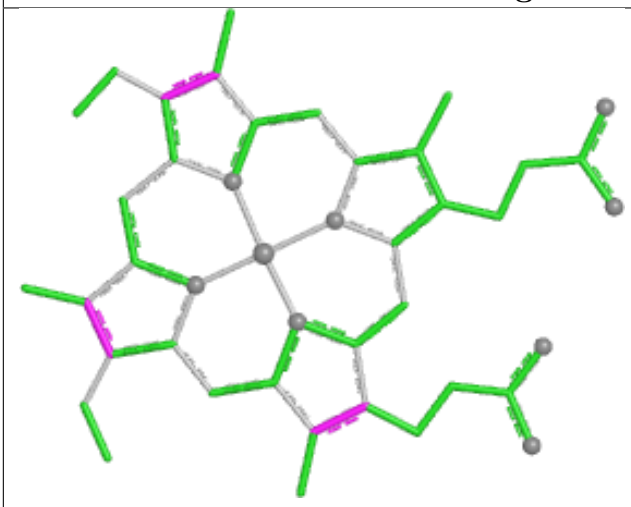


Torsions

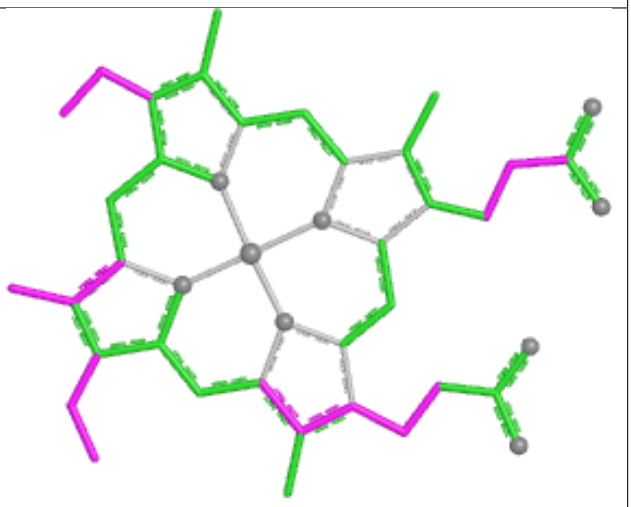


Rings

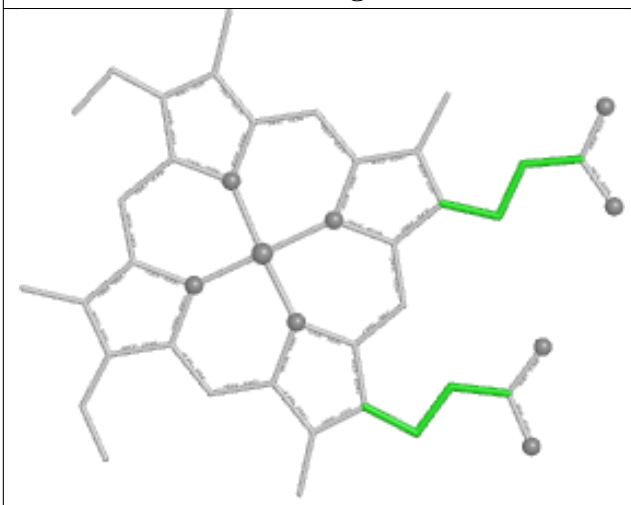
Ligand HEC F 1001



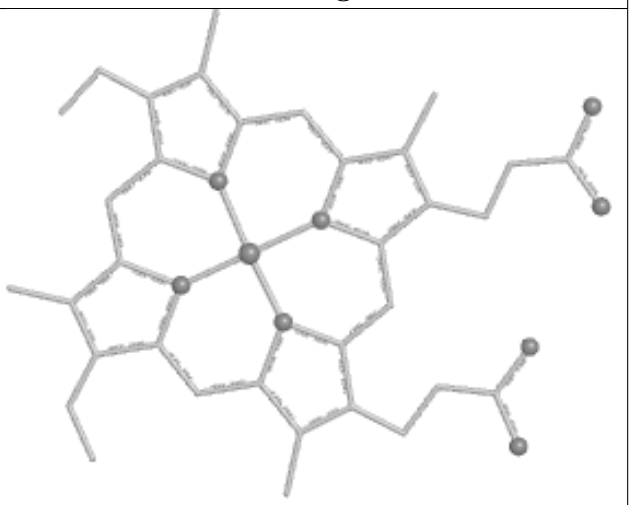
Bond lengths



Bond angles

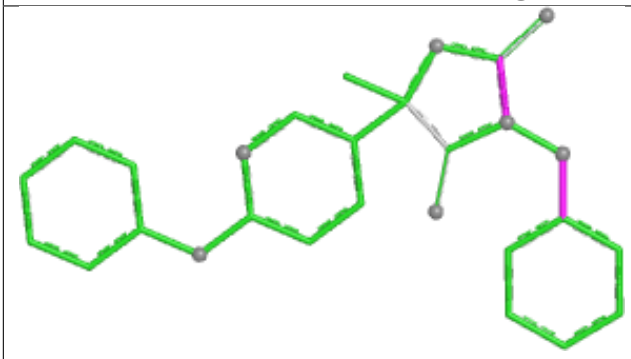


Torsions

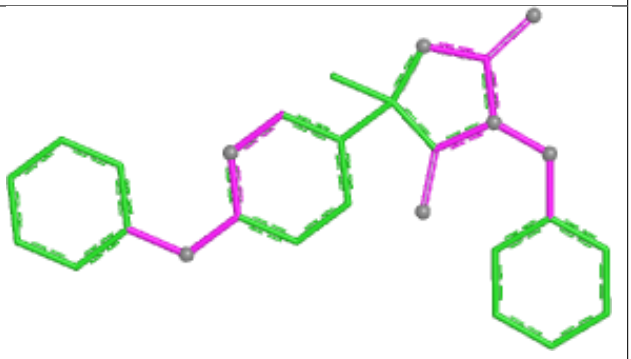


Rings

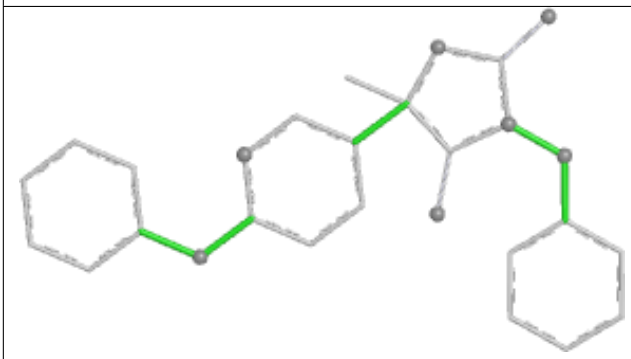
Ligand PQU A 1003



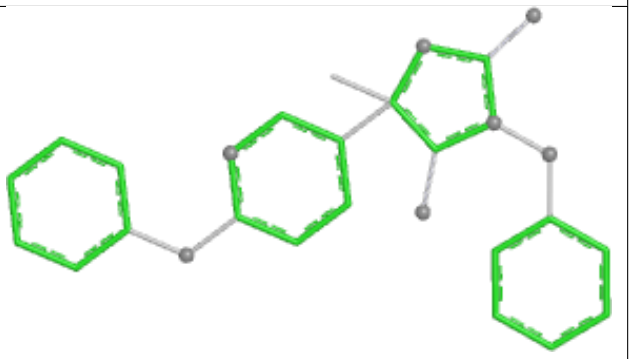
Bond lengths



Bond angles

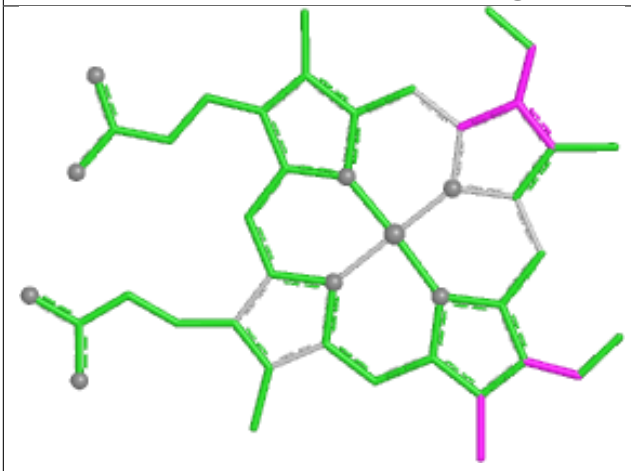


Torsions

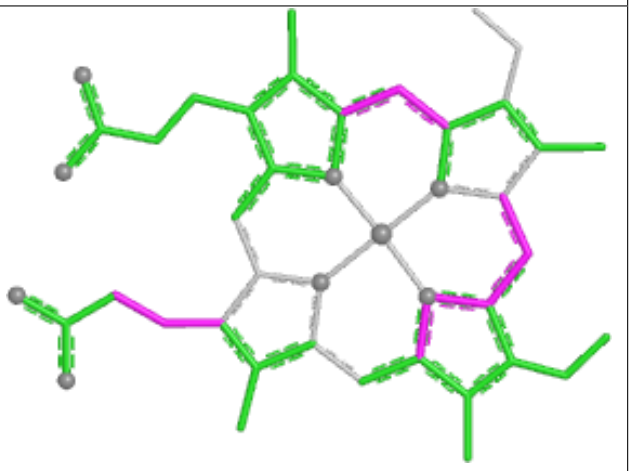


Rings

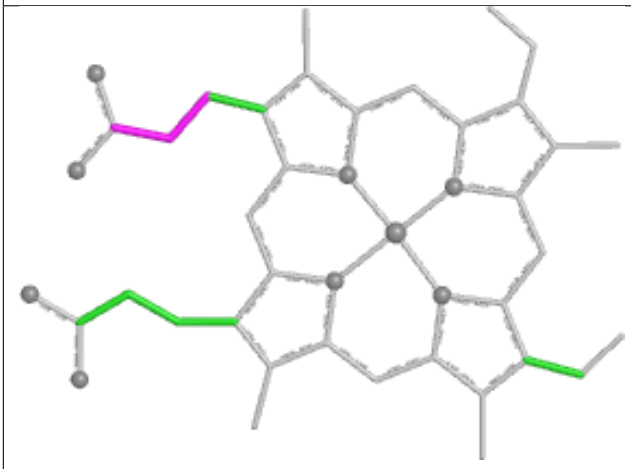
Ligand HEM A 1001



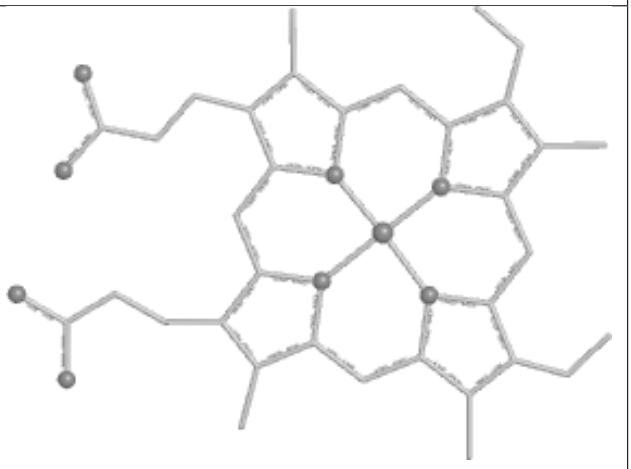
Bond lengths



Bond angles

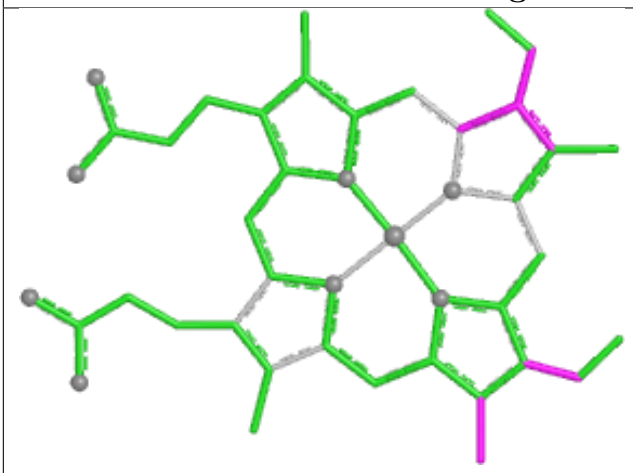


Torsions

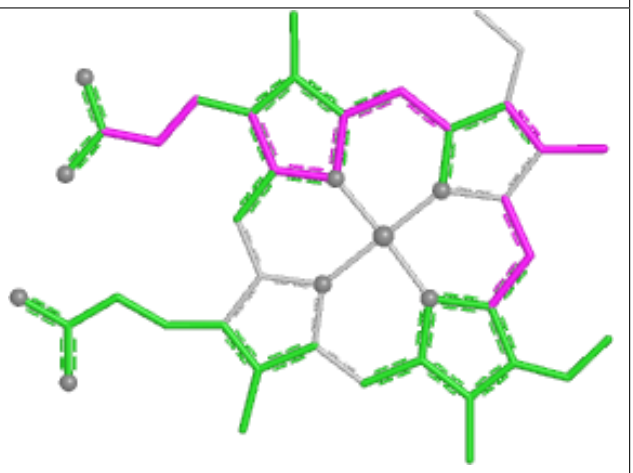


Rings

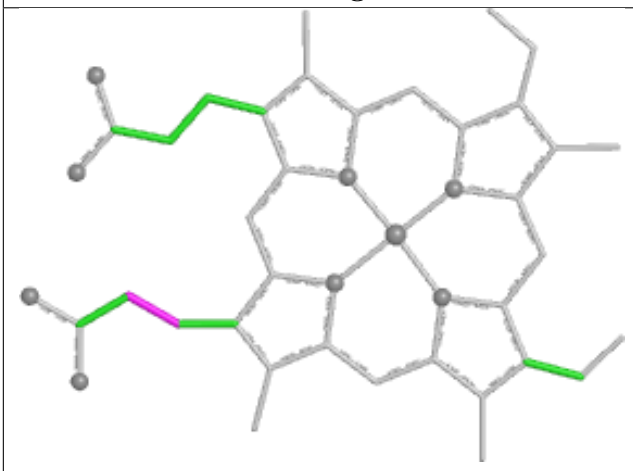
Ligand HEM A 1002



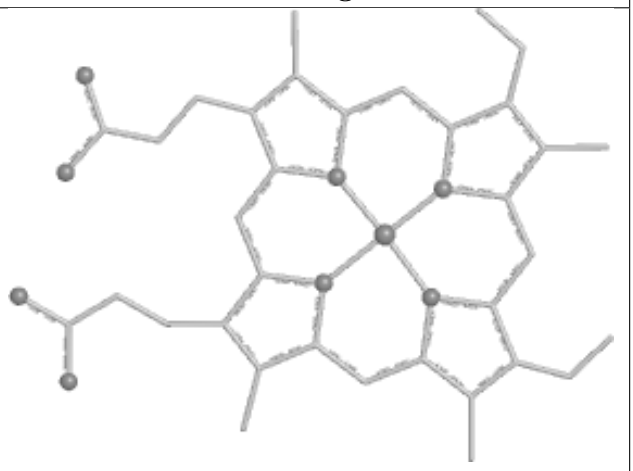
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

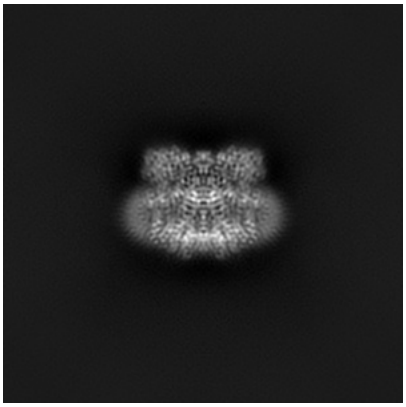
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25989. These allow visual inspection of the internal detail of the map and identification of artifacts.

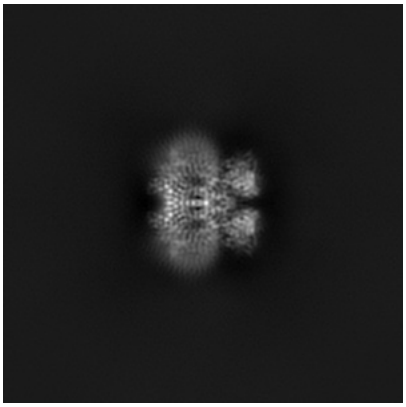
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

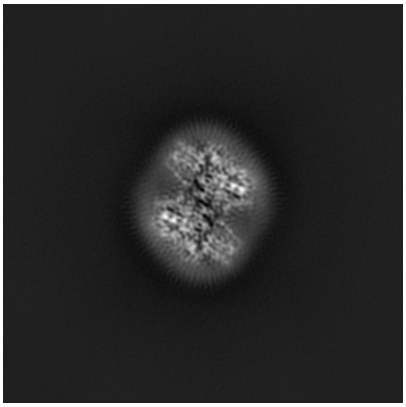
6.1.1 Primary map



X



Y



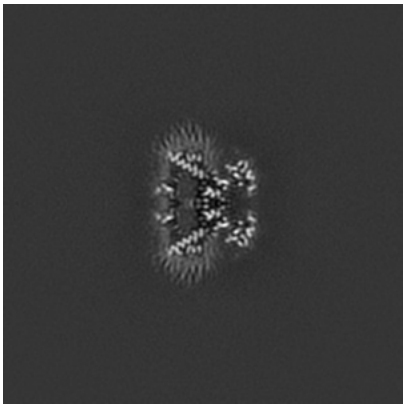
Z

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

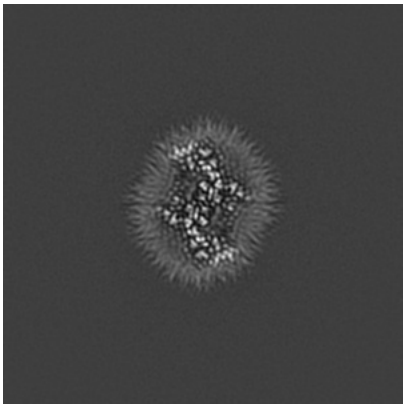
6.2 Central slices

6.2.1 Primary map

X Index: 192



Y Index: 192



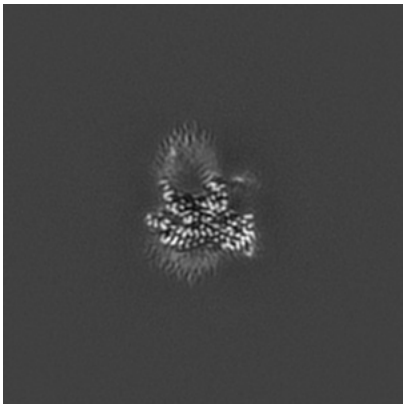
Z Index: 192

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

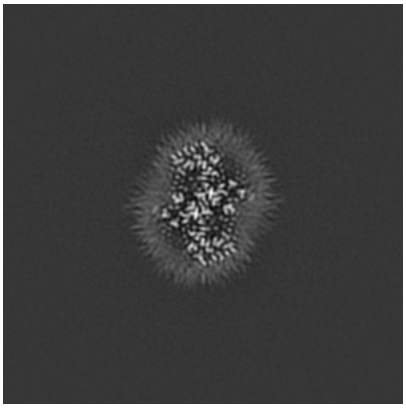
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 192



Y Index: 177

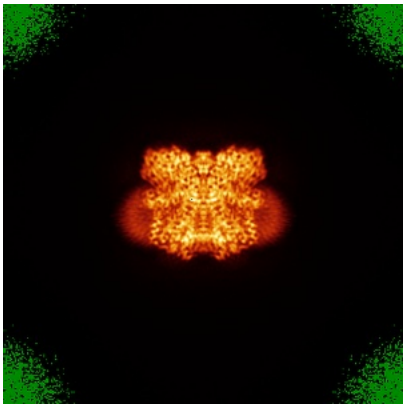


Z Index: 195

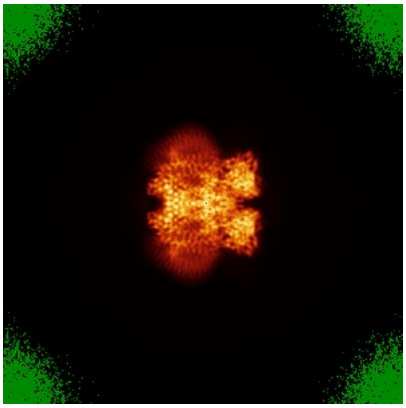
The images above show the largest variance slices of the map in three orthogonal directions.

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

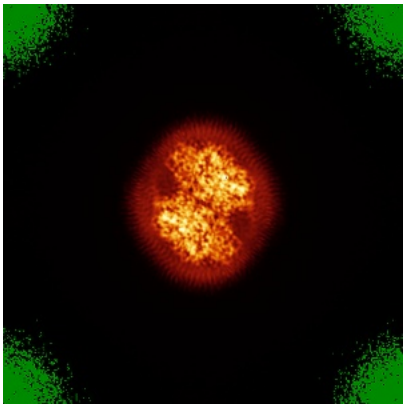
6.4.1 Primary map



X



Y

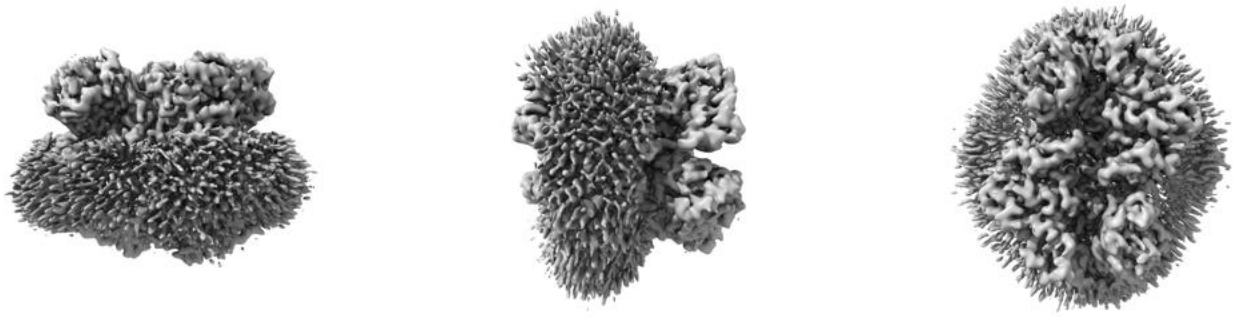


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

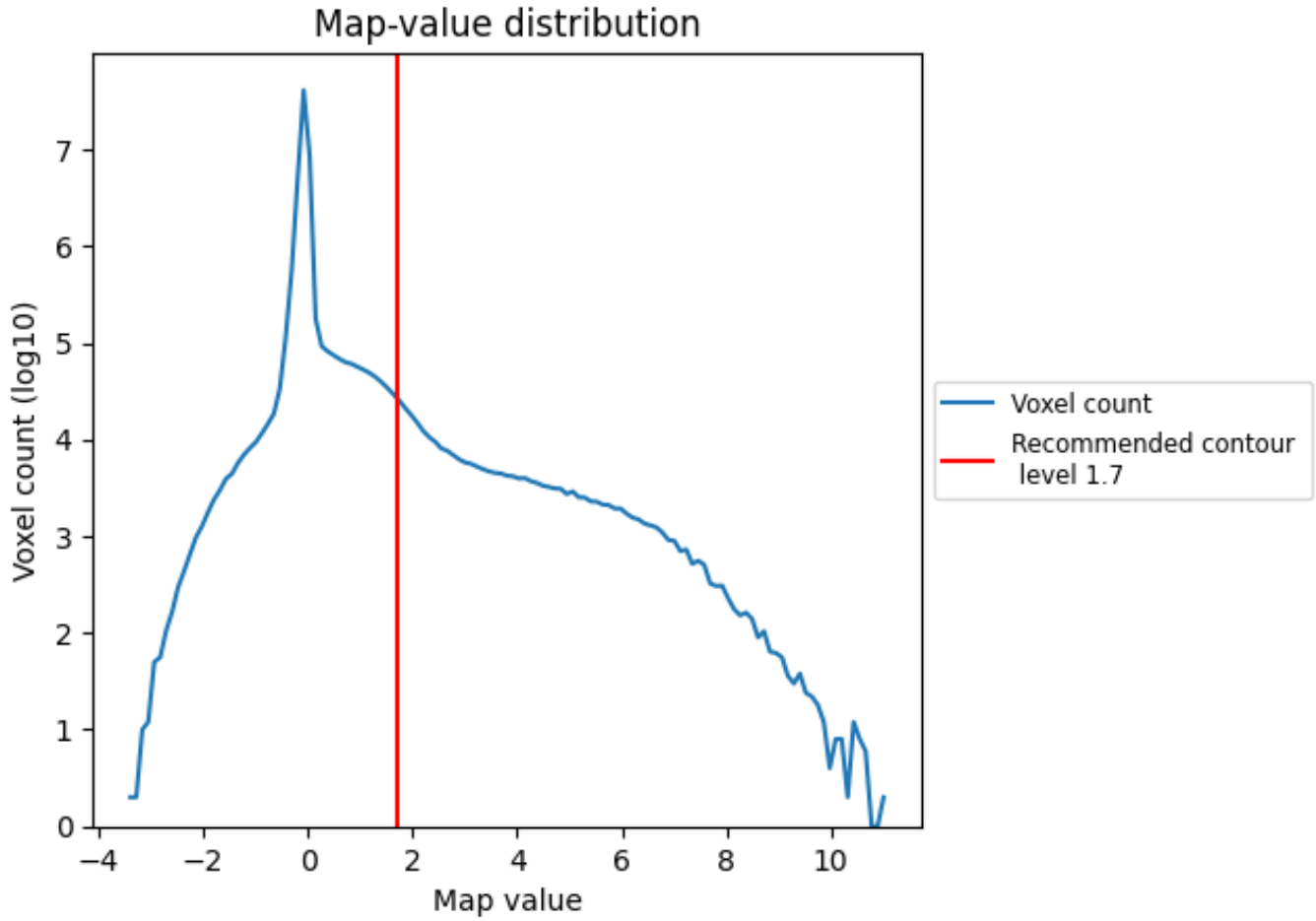
6.6 Mask visualisation (i)

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

7 Map analysis

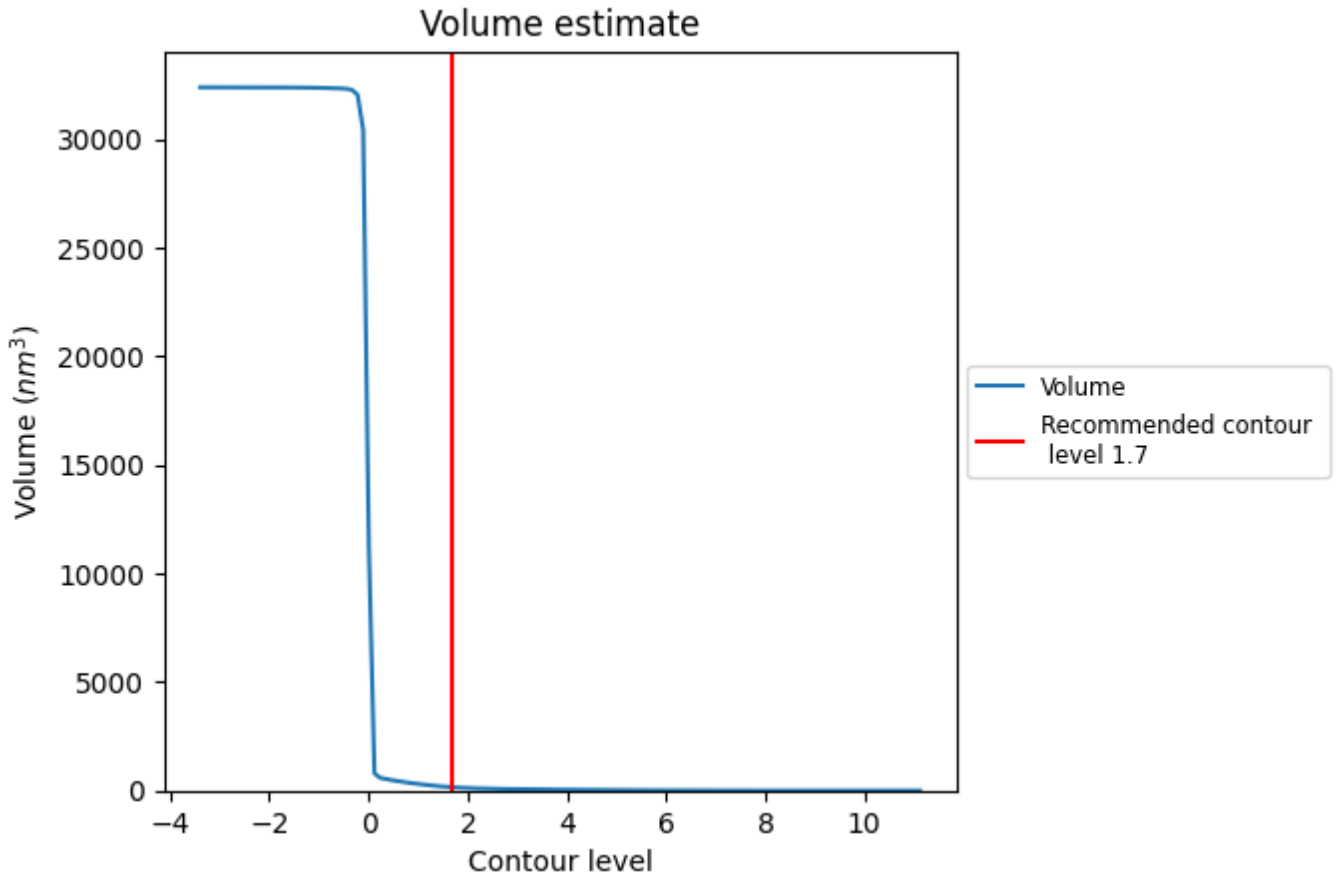
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

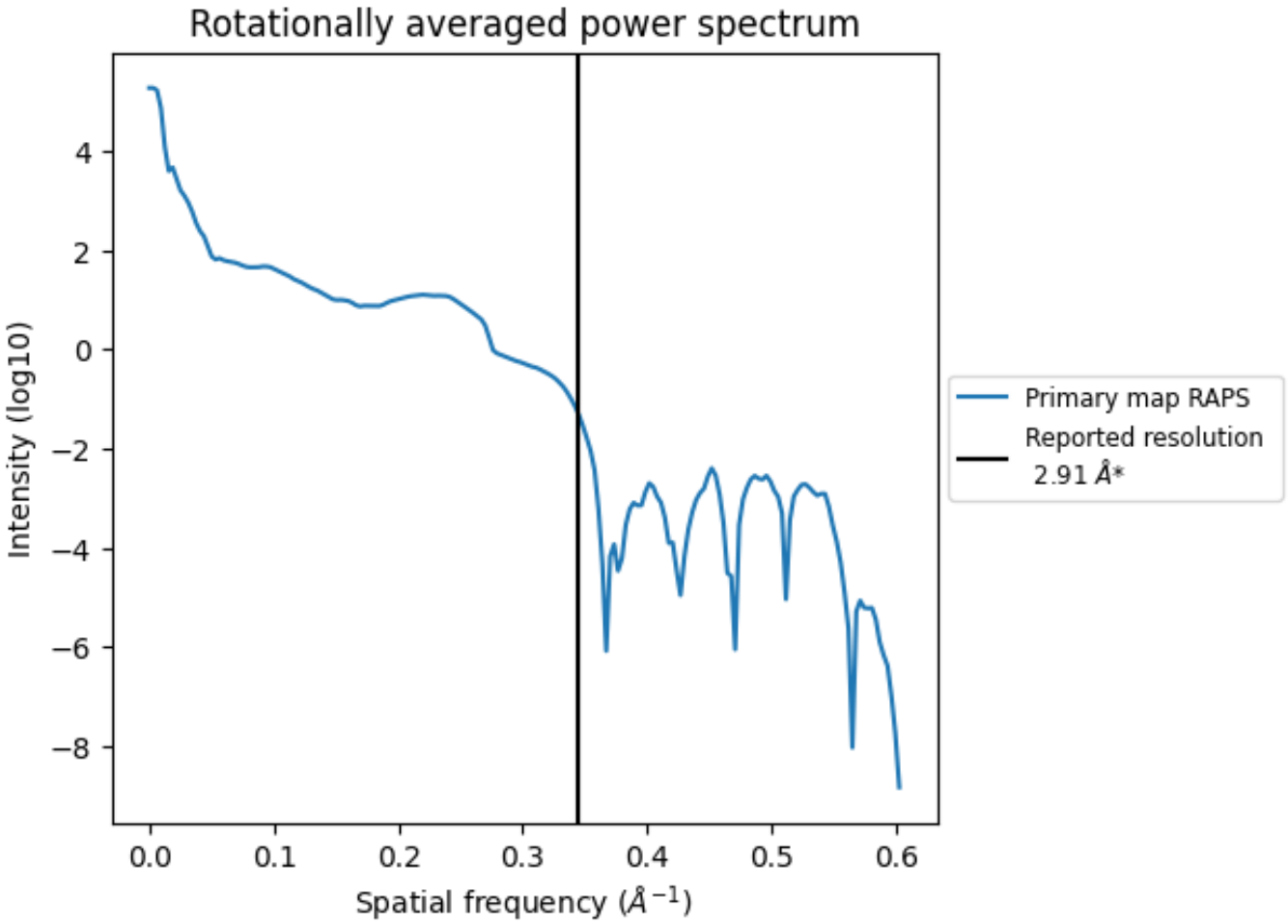
7.2 Volume estimate (i)



The volume at the recommended contour level is 151 nm^3; this corresponds to an approximate mass of 137 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 0.344 Å^{-1}

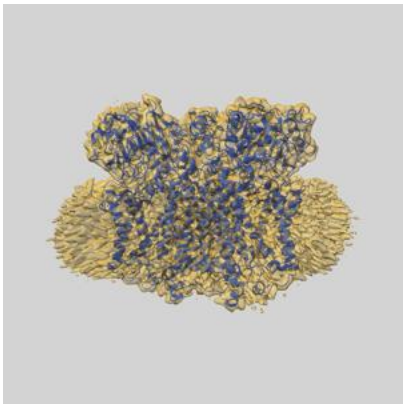
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

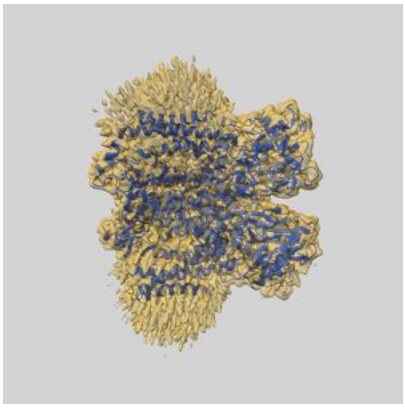
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25989 and PDB model 7TLJ. Per-residue inclusion information can be found in section 3 on page 8.

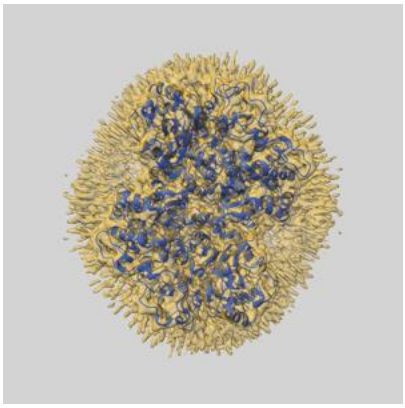
9.1 Map-model overlay



X



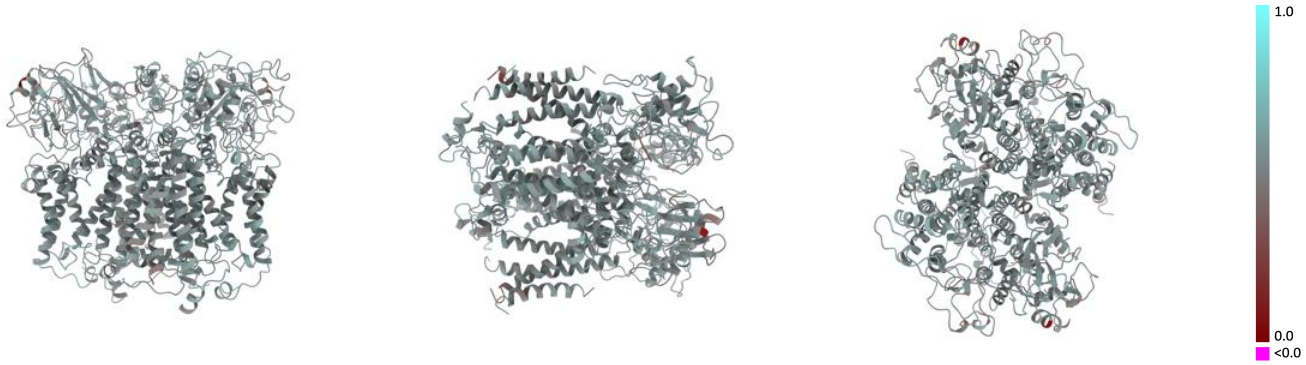
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.7 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.

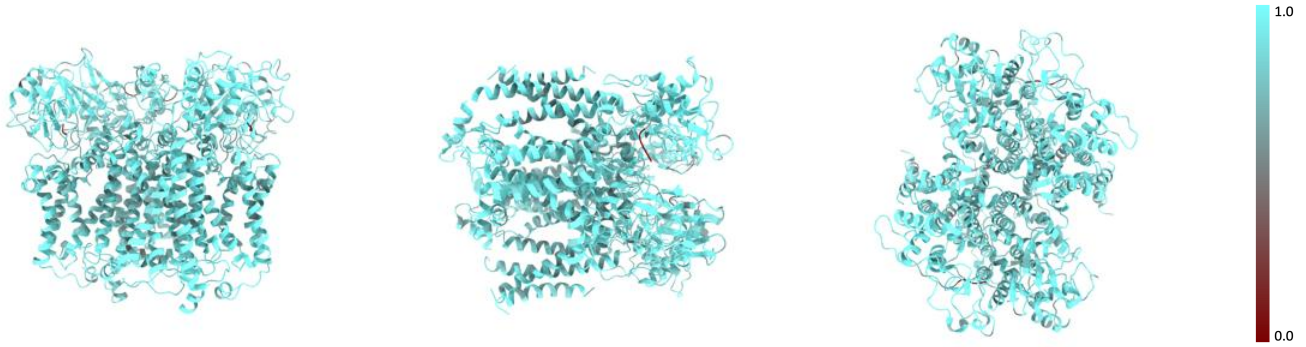
9.2 Q-score mapped to coordinate model (i)



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.

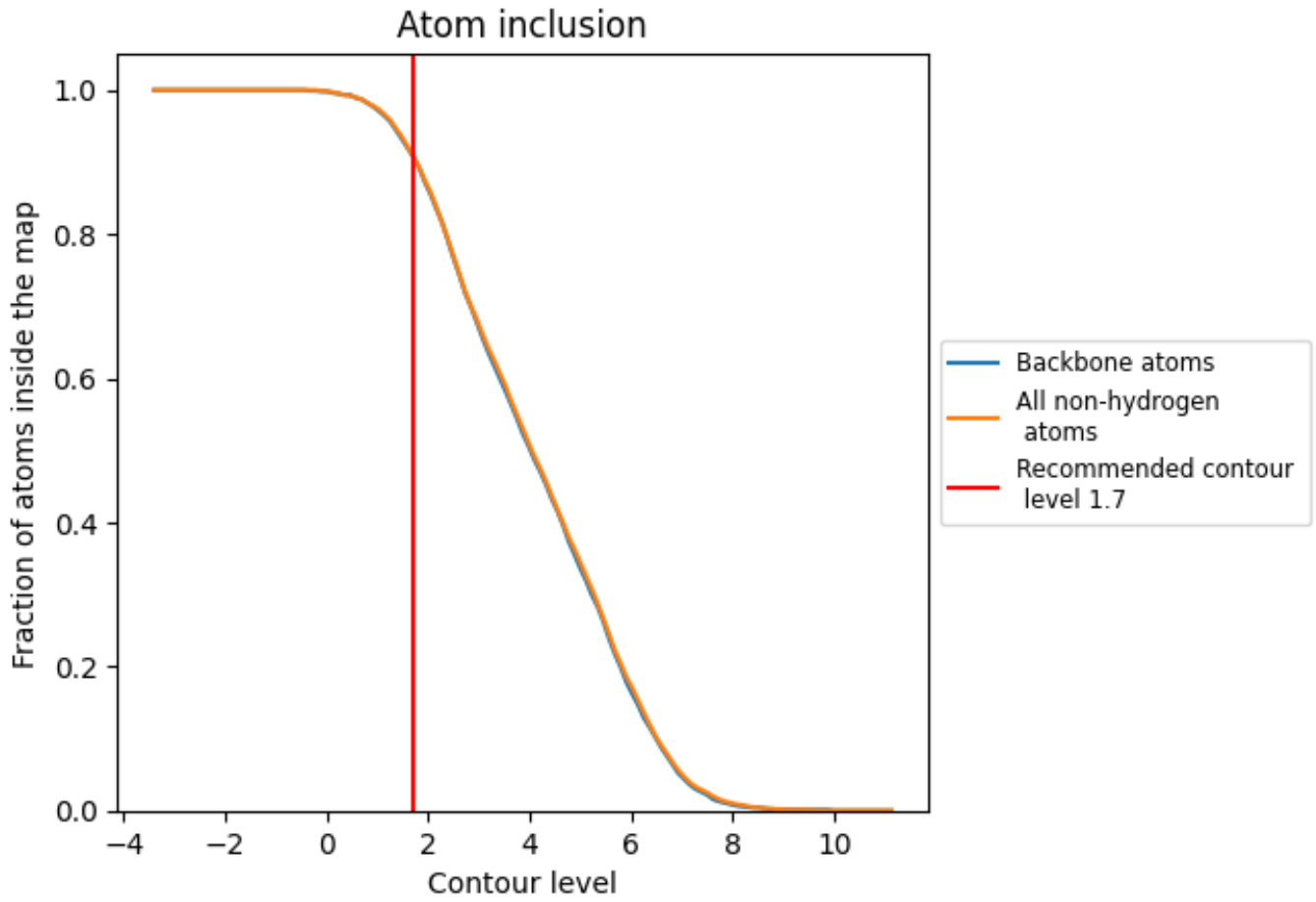
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.7).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9080	0.5320
A	0.9160	0.5430
B	0.9180	0.5290
C	0.8970	0.5130
D	0.8880	0.5000
E	0.9130	0.5430
F	0.9130	0.5250
G	0.8900	0.5140
H	0.8880	0.4980