Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 11:42 pm GMT

PDB ID	:	6FO0
EMDB ID	:	EMD-4286
Title	:	CryoEM structure of bovine cytochrome bc1 in complex with the anti-malarial compound GSK932121
Authors	:	Johnson, R.M.; Amporndanai, K.; O'Neill, P.M.; Fishwick, C.W.G.; Jamson, A.H.; Rawson, S.D.; Hasnain, S.S.; Antonyuk, S.V.; Muench, S.P.
Deposited on	:	2018-02-05
Resolution	:	4.10 Å(reported)

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

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

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

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

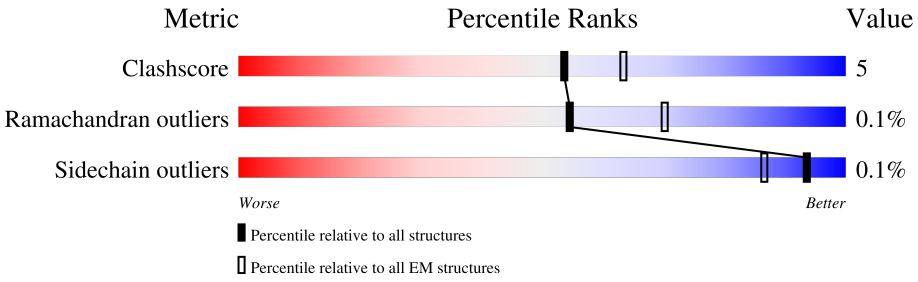
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.10 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	480	79% 14% 8%
1	N	480	79% 14% 8%
2	B	453	78% 14% 9%
2	O	453	77% 14% 9%
3	C	379	83% 14%
3	P	379	84% 13%
4	D	325	61% 12% 26%
4	Q	325	63% 11% 26%

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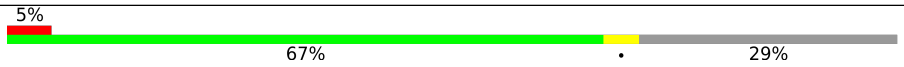
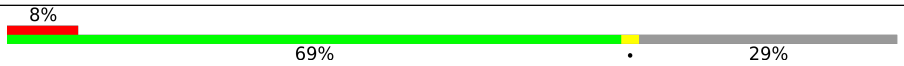
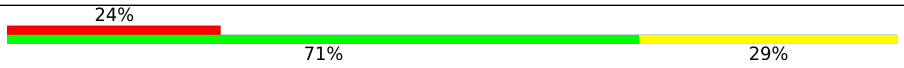
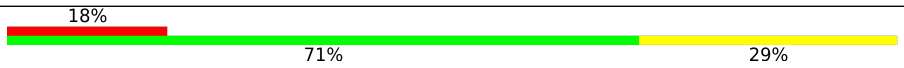
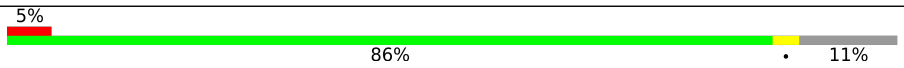
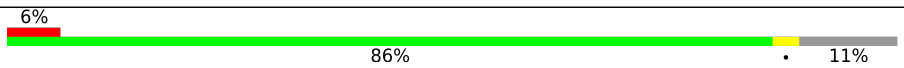
Mol	Chain	Length	Quality of chain
5	E	274	
5	R	274	
6	F	111	
6	S	111	
7	G	82	
7	T	82	
8	H	91	
8	U	91	
9	I	17	
9	V	17	
10	J	64	
10	W	64	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 61356 atoms, of which 30362 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-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	N	443	Total	C	H	N	O	S	0	0
			6753	2142	3325	603	663	20		
1	A	443	Total	C	H	N	O	S	0	0
			6753	2142	3325	603	663	20		

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	O	414	Total	C	H	N	O	S	0	0
			6206	1955	3094	549	601	7		
2	B	414	Total	C	H	N	O	S	0	0
			6206	1955	3094	549	601	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	305	GLU	GLN	conflict	UNP P23004
B	305	GLU	GLN	conflict	UNP P23004

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	P	370	Total	C	H	N	O	S	0	0
			5933	1973	2997	456	489	18		
3	C	370	Total	C	H	N	O	S	0	0
			5933	1973	2997	456	489	18		

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	Q	239	Total	C	H	N	O	S	0	0
			3751	1216	1848	327	345	15		

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Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	239	Total	C	H	N	O	S	0	0
			3751	1216	1848	327	345	15		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	R	178	Total	C	H	N	O	S	0	0
			2658	848	1311	231	260	8		
5	E	178	Total	C	H	N	O	S	0	0
			2658	848	1311	231	260	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	S	98	Total	C	H	N	O	S	0	0
			1710	547	850	154	157	2		
6	F	98	Total	C	H	N	O	S	0	0
			1710	547	850	154	157	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	56	ASP	ASN	conflict	UNP P00129
F	56	ASP	ASN	conflict	UNP P00129

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	T	74	Total	C	H	N	O	S	0	0
			1255	408	631	117	98	1		
7	G	74	Total	C	H	N	O	S	0	0
			1255	408	631	117	98	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	U	65	Total	C	H	N	O	S	0	0
			1041	321	512	96	107	5		
8	H	65	Total	C	H	N	O	S	0	0
			1041	321	512	96	107	5		

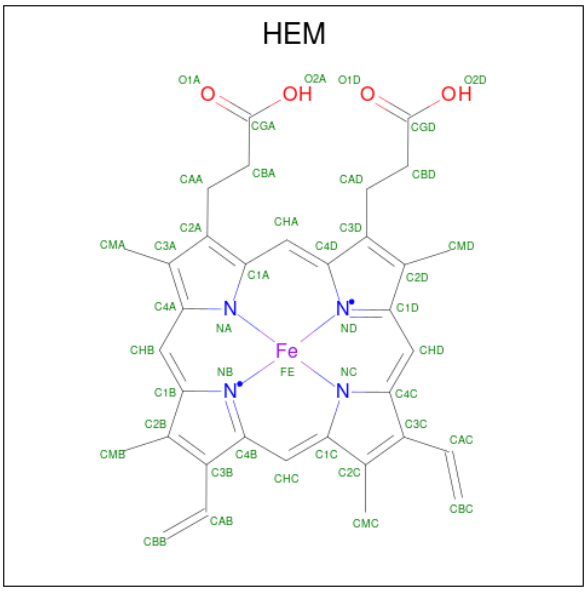
- Molecule 9 is a protein called Chain I/V.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	17	Total	C	H	N	O	0	0
			263	81	136	24	22		
9	I	17	Total	C	H	N	O	0	0
			263	81	136	24	22		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 9.

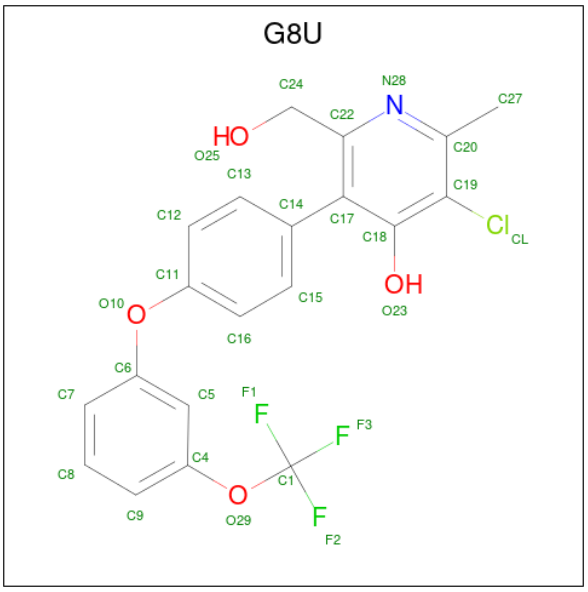
Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	57	Total	C	H	N	O	0	0
			950	312	477	82	79		
10	J	57	Total	C	H	N	O	0	0
			950	312	477	82	79		

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



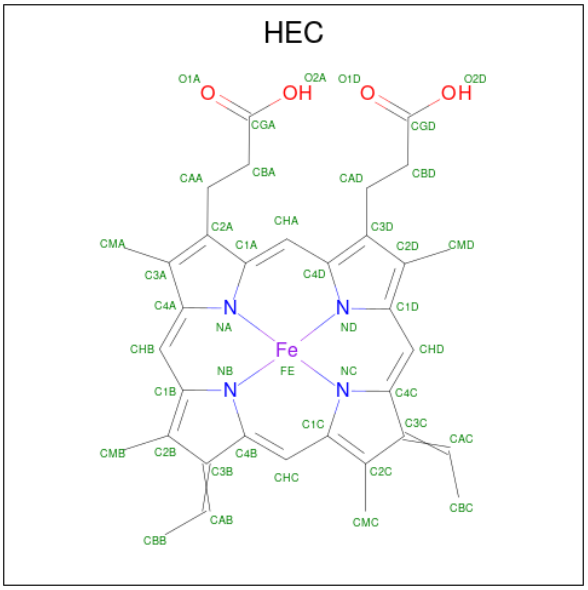
Mol	Chain	Residues	Atoms					AltConf
11	P	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
11	P	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
11	C	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
11	C	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

- Molecule 12 is 3-chloro-6-(hydroxymethyl)-2-methyl-5-{4-[3-(trifluoromethoxy)phenoxy]phenyl}pyridin-4-ol (three-letter code: G8U) (formula: $C_{20}H_{15}ClF_3NO_4$).



Mol	Chain	Residues	Atoms						AltConf
12	P	1	Total	C	Cl	F	N	O	0
			29	20	1	3	1	4	
12	C	1	Total	C	Cl	F	N	O	0
			29	20	1	3	1	4	

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



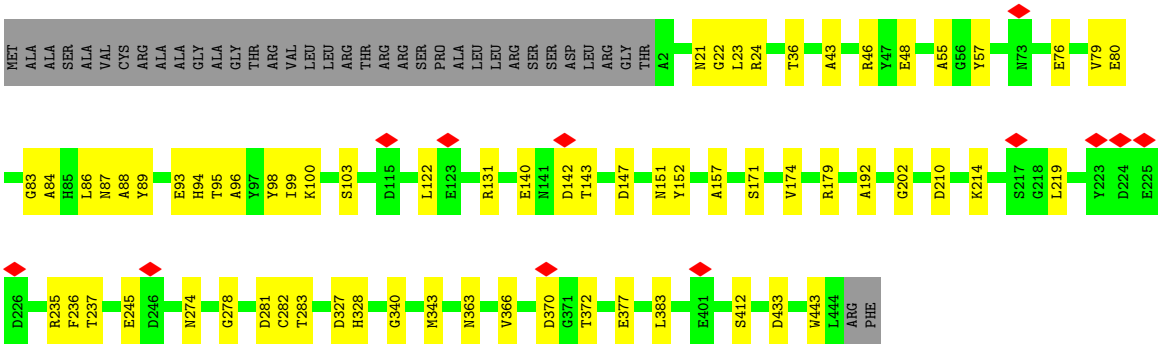
Mol	Chain	Residues	Atoms					AltConf
13	Q	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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.

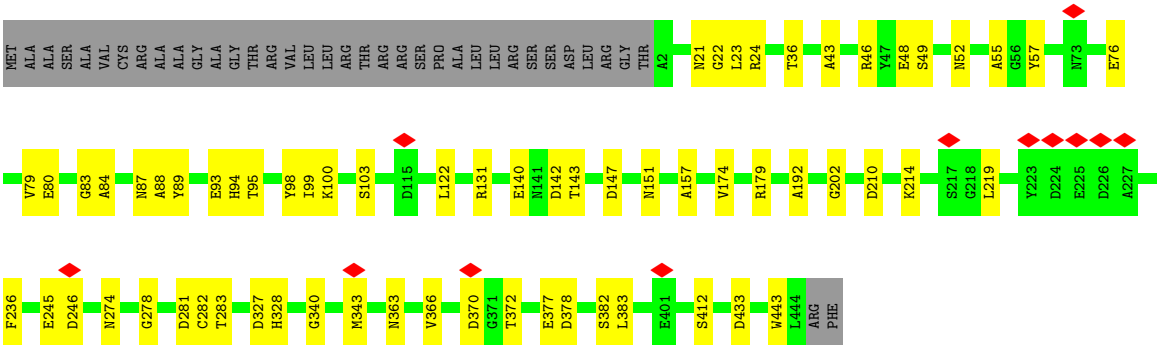
• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain N:



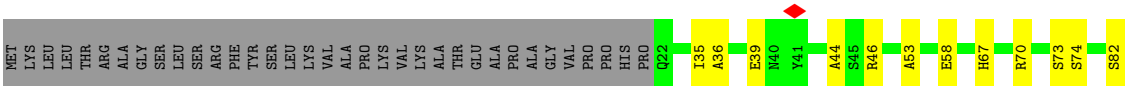
• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

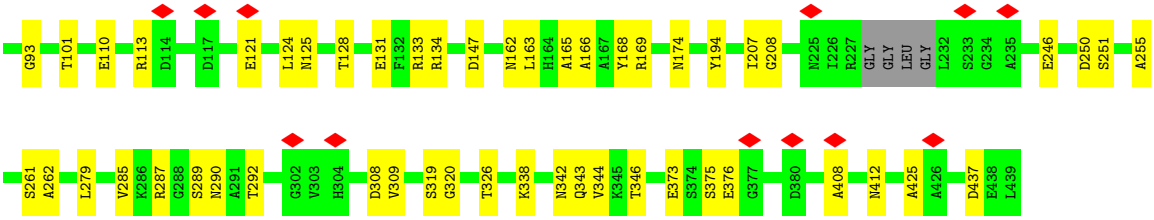
Chain A:



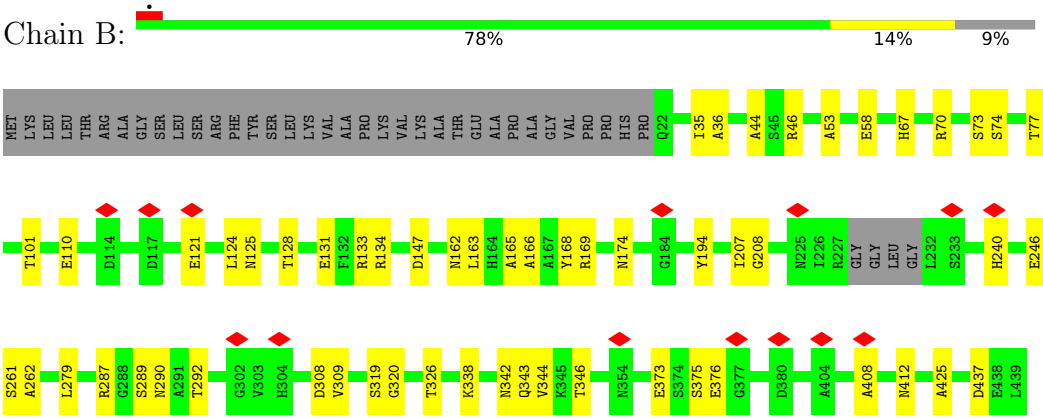
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain O:

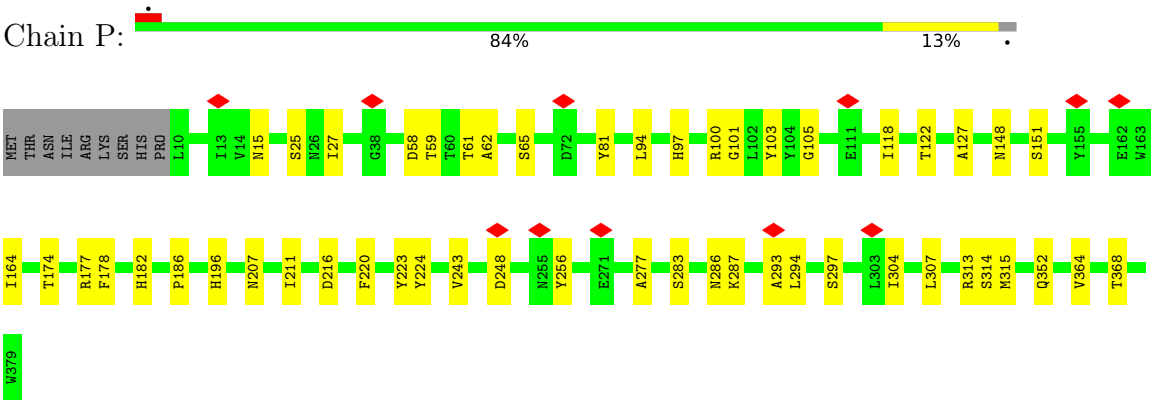




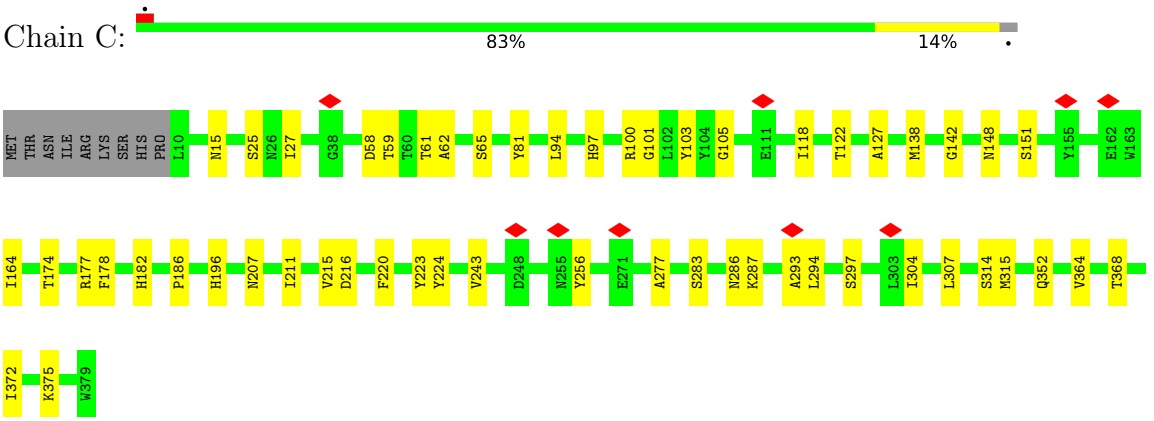
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



• Molecule 3: Cytochrome b

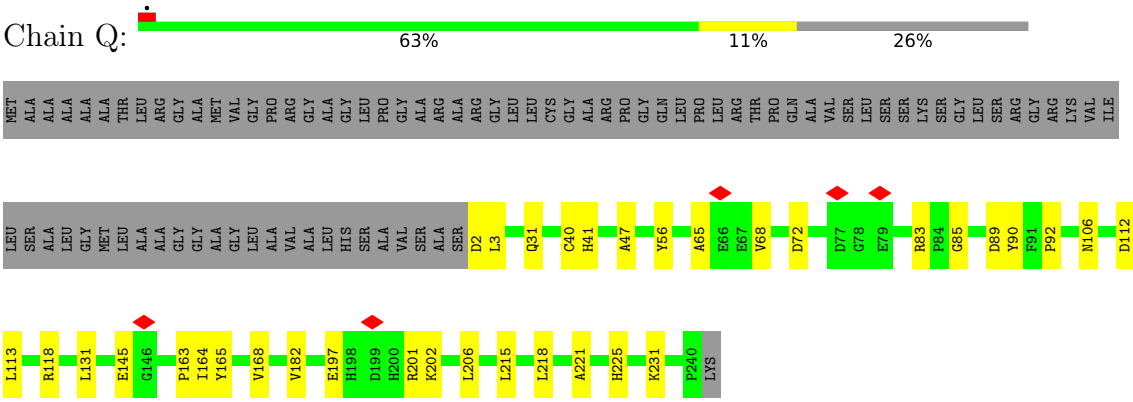


• Molecule 3: Cytochrome b



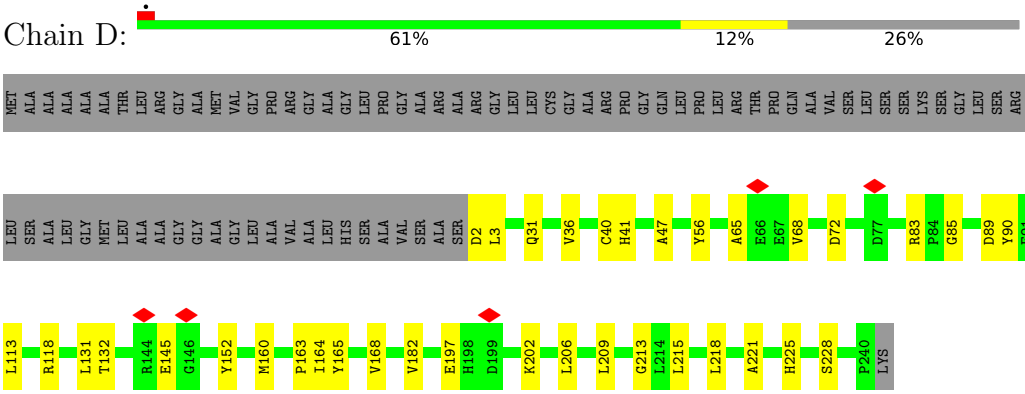
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain Q:



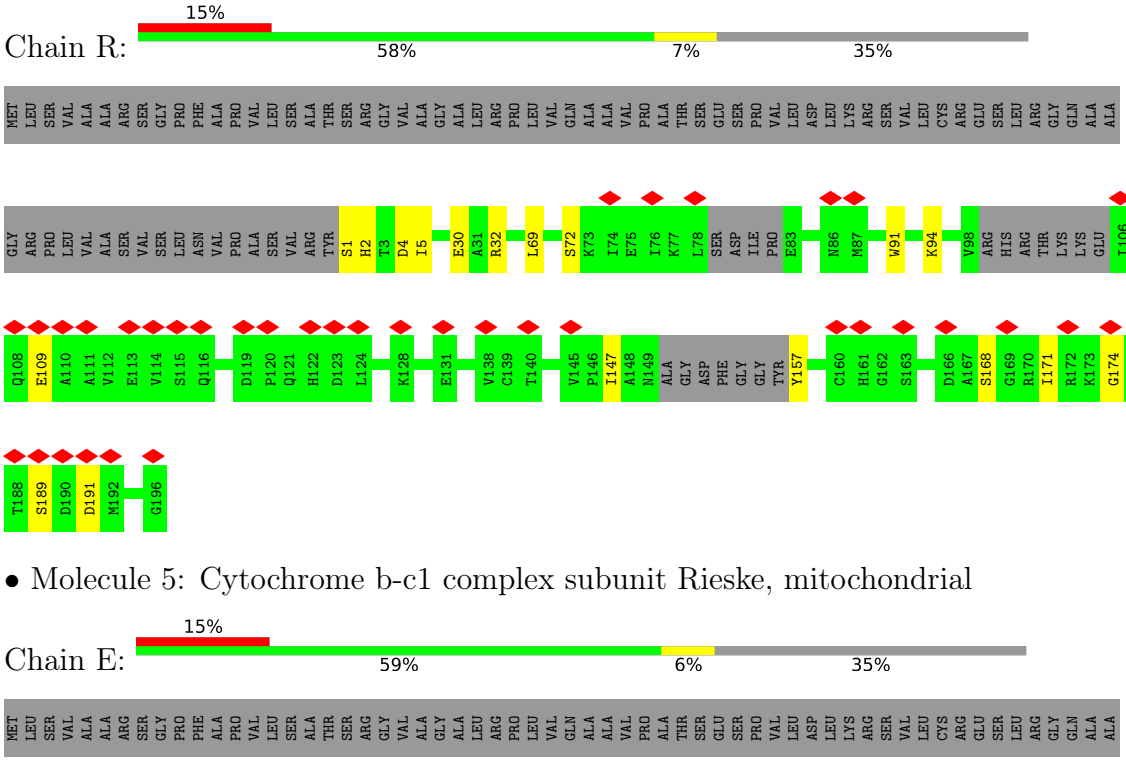
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:



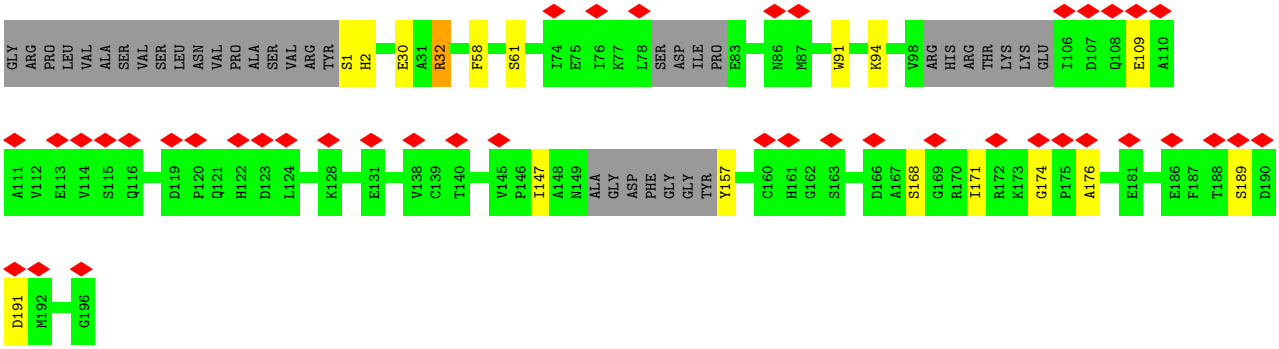
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain R:



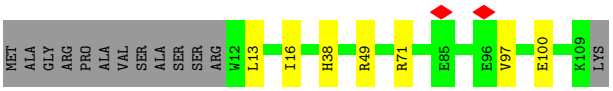
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:



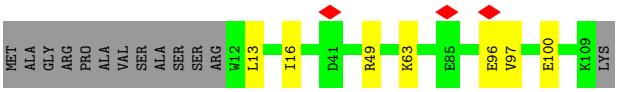
• Molecule 6: Cytochrome b-c1 complex subunit 7

Chain S:



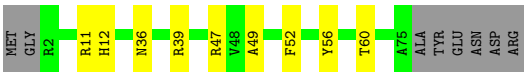
• Molecule 6: Cytochrome b-c1 complex subunit 7

Chain F:



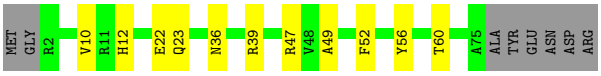
• Molecule 7: Cytochrome b-c1 complex subunit 8

Chain T:



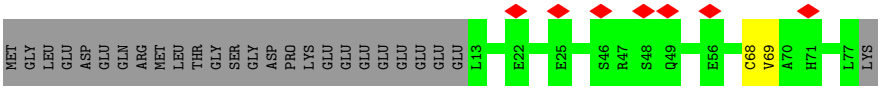
• Molecule 7: Cytochrome b-c1 complex subunit 8

Chain G:



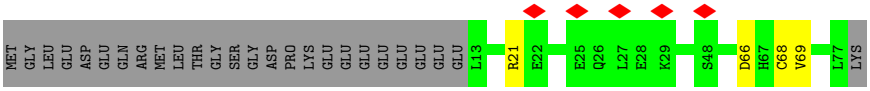
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain U:



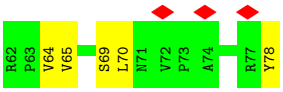
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain H:



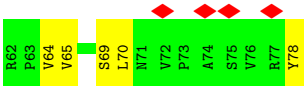
• Molecule 9: Chain I/V

Chain V:



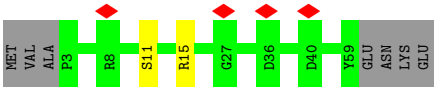
• Molecule 9: Chain I/V

Chain I:



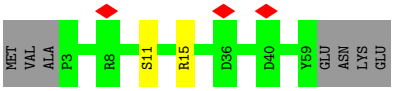
• Molecule 10: Cytochrome b-c1 complex subunit 9

Chain W:



• Molecule 10: Cytochrome b-c1 complex subunit 9

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	232910	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 ($e^-/Å^2$)	75	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	79000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.647	Depositor
Minimum map value	-0.279	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.114	Depositor
Map size (Å)	213.00002, 213.00002, 213.00002	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, HEM, G8U

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	0.53	0/3500	0.59	0/4752
1	N	0.53	0/3500	0.59	0/4752
2	B	0.52	0/3166	0.62	2/4291 (0.0%)
2	O	0.52	0/3166	0.62	2/4291 (0.0%)
3	C	0.59	0/3031	0.57	0/4150
3	P	0.59	0/3031	0.57	0/4150
4	D	0.57	0/1962	0.60	0/2665
4	Q	0.57	0/1962	0.60	0/2665
5	E	0.43	0/1373	0.59	1/1861 (0.1%)
5	R	0.43	0/1373	0.59	1/1861 (0.1%)
6	F	0.55	0/879	0.58	0/1180
6	S	0.55	0/879	0.58	0/1180
7	G	0.53	0/645	0.63	0/873
7	T	0.53	0/645	0.64	0/873
8	H	0.39	0/534	0.53	0/718
8	U	0.39	0/534	0.53	0/718
9	I	0.50	0/129	0.79	0/177
9	V	0.50	0/129	0.79	0/177
10	J	0.52	0/486	0.56	0/655
10	W	0.52	0/486	0.56	0/655
All	All	0.54	0/31410	0.59	6/42644 (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
3	C	0	1
3	P	0	1
5	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	R	0	1
All	All	0	4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	R	32	ARG	NE-CZ-NH1	5.91	123.26	120.30
2	O	70	ARG	NE-CZ-NH2	-5.91	117.35	120.30
2	B	70	ARG	NE-CZ-NH2	-5.90	117.35	120.30
5	E	32	ARG	NE-CZ-NH1	5.84	123.22	120.30
2	O	70	ARG	NE-CZ-NH1	5.27	122.93	120.30
2	B	70	ARG	NE-CZ-NH1	5.23	122.92	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	15	ASN	Peptide
5	E	174	GLY	Peptide
3	P	15	ASN	Peptide
5	R	174	GLY	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	3428	3325	3324	43	0
1	N	3428	3325	3324	46	0
2	B	3112	3094	3090	41	0
2	O	3112	3094	3090	44	0
3	C	2936	2997	2996	37	0
3	P	2936	2997	2996	36	0
4	D	1903	1848	1849	28	0
4	Q	1903	1848	1849	24	0
5	E	1347	1311	1310	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	R	1347	1311	1310	11	0
6	F	860	850	849	6	0
6	S	860	850	849	5	0
7	G	624	631	630	7	0
7	T	624	631	630	5	0
8	H	529	512	511	3	0
8	U	529	512	511	1	0
9	I	127	136	135	3	0
9	V	127	136	135	3	0
10	J	473	477	477	2	0
10	W	473	477	477	3	0
11	C	86	0	60	19	0
11	P	86	0	60	19	0
12	C	29	0	15	3	0
12	P	29	0	15	3	0
13	D	43	0	32	9	0
13	Q	43	0	32	6	0
All	All	30994	30362	30556	338	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (338) 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)
11:P:501:HEM:HBA1	11:P:501:HEM:HHA	1.65	0.79
13:D:501:HEC:HBD1	13:D:501:HEC:HHA	1.65	0.78
13:Q:501:HEC:HBD1	13:Q:501:HEC:HHA	1.65	0.78
11:C:501:HEM:HHA	11:C:501:HEM:HBA1	1.66	0.77
1:N:412:SER:OG	10:W:15:ARG:NH2	2.18	0.77
1:A:89:TYR:OH	1:A:377:GLU:OE1	2.04	0.76
1:N:89:TYR:OH	1:N:377:GLU:OE1	2.04	0.76
8:U:68:CYS:SG	8:U:69:VAL:N	2.59	0.75
8:H:68:CYS:SG	8:H:69:VAL:N	2.59	0.75
2:O:134:ARG:NH2	6:F:49:ARG:O	2.21	0.74
4:D:152:TYR:OH	8:H:66:ASP:OD2	2.06	0.74
1:N:122:LEU:O	1:N:179:ARG:NH1	2.23	0.72
4:Q:41:HIS:NE2	13:Q:501:HEC:NB	2.38	0.72
2:O:162:ASN:ND2	2:O:246:GLU:OE2	2.23	0.71
1:N:57:TYR:OH	2:O:287:ARG:NH2	2.23	0.71
2:B:162:ASN:ND2	2:B:246:GLU:OE2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:O	1:A:179:ARG:NH1	2.23	0.71
1:N:372:THR:OG1	2:O:373:GLU:OE2	2.07	0.70
1:N:80:GLU:OE1	2:O:292:THR:OG1	2.05	0.70
1:N:131:ARG:NH1	1:N:174:VAL:O	2.24	0.70
1:A:131:ARG:NH1	1:A:174:VAL:O	2.24	0.70
1:A:57:TYR:OH	2:B:287:ARG:NH2	2.25	0.69
2:B:343:GLN:O	2:B:346:THR:OG1	2.09	0.69
1:N:43:ALA:O	1:N:95:THR:OG1	2.11	0.69
1:N:142:ASP:OD1	5:R:1:SER:OG	2.11	0.68
11:C:502:HEM:HMA1	12:C:503:G8U:H15	1.75	0.68
4:Q:40:CYS:SG	13:Q:501:HEC:HAC	2.33	0.68
2:O:343:GLN:O	2:O:346:THR:OG1	2.10	0.68
1:A:36:THR:OG1	1:A:99:ILE:O	2.07	0.67
2:B:408:ALA:O	2:B:412:ASN:ND2	2.26	0.67
1:A:43:ALA:O	1:A:95:THR:OG1	2.11	0.67
1:N:87:ASN:ND2	1:N:98:TYR:OH	2.27	0.67
2:O:168:TYR:OH	2:O:320:GLY:O	2.13	0.67
11:C:502:HEM:HBC2	11:C:502:HEM:HHD	1.77	0.67
1:A:87:ASN:ND2	1:A:98:TYR:OH	2.27	0.67
3:P:174:THR:OG1	3:P:177:ARG:NH2	2.28	0.67
3:P:256:TYR:OH	4:Q:118:ARG:NH2	2.28	0.67
11:P:502:HEM:HBC2	11:P:502:HEM:HHD	1.77	0.66
3:C:174:THR:OG1	3:C:177:ARG:NH2	2.28	0.66
2:O:408:ALA:O	2:O:412:ASN:ND2	2.26	0.66
1:N:36:THR:OG1	1:N:99:ILE:O	2.06	0.66
2:B:168:TYR:OH	2:B:320:GLY:O	2.13	0.66
7:T:56:TYR:O	7:T:60:THR:OG1	2.11	0.65
1:N:366:VAL:HG11	2:O:44:ALA:HB2	1.78	0.65
6:S:49:ARG:O	2:B:134:ARG:NH2	2.30	0.65
1:A:80:GLU:OE1	2:B:292:THR:OG1	2.11	0.65
3:P:364:VAL:O	3:P:368:THR:OG1	2.12	0.64
13:Q:501:HEC:HBB3	13:Q:501:HEC:HMB1	1.80	0.64
1:A:412:SER:OG	10:J:15:ARG:NH2	2.30	0.64
1:N:370:ASP:OD2	2:O:375:SER:OG	2.14	0.64
3:P:294:LEU:O	3:P:297:SER:OG	2.08	0.63
11:P:502:HEM:HMA1	12:P:503:G8U:H15	1.80	0.63
1:N:343:MET:SD	1:N:443:TRP:N	2.72	0.62
1:A:46:ARG:NH1	1:A:93:GLU:OE2	2.32	0.62
3:P:164:ILE:O	3:P:177:ARG:NH2	2.32	0.62
3:C:256:TYR:OH	4:D:118:ARG:NH2	2.31	0.62
13:D:501:HEC:HMB1	13:D:501:HEC:HBB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:MET:SD	1:A:443:TRP:N	2.72	0.62
3:C:164:ILE:O	3:C:177:ARG:NH2	2.32	0.62
1:N:46:ARG:NH1	1:N:93:GLU:OE2	2.32	0.62
11:P:502:HEM:HBD2	11:P:502:HEM:HHA	1.81	0.62
4:Q:112:ASP:OD1	4:Q:113:LEU:N	2.32	0.61
4:D:112:ASP:OD1	4:D:113:LEU:N	2.32	0.61
1:A:142:ASP:OD1	5:E:1:SER:OG	2.18	0.61
4:D:47:ALA:HB2	4:D:90:TYR:HD1	1.65	0.60
2:O:58:GLU:O	2:O:174:ASN:ND2	2.33	0.60
7:T:36:ASN:OD1	7:T:39:ARG:NH2	2.34	0.60
2:B:58:GLU:O	2:B:174:ASN:ND2	2.33	0.60
7:G:36:ASN:OD1	7:G:39:ARG:NH2	2.34	0.60
5:R:147:ILE:O	5:R:157:TYR:N	2.34	0.60
4:Q:163:PRO:HG2	13:Q:501:HEC:HBB2	1.82	0.60
2:O:124:LEU:O	2:O:128:THR:OG1	2.13	0.60
5:E:147:ILE:O	5:E:157:TYR:N	2.34	0.60
3:C:364:VAL:O	3:C:368:THR:OG1	2.11	0.59
11:C:502:HEM:HBD2	11:C:502:HEM:HHA	1.83	0.59
3:C:207:ASN:ND2	3:C:211:ILE:O	2.36	0.59
4:Q:47:ALA:HB2	4:Q:90:TYR:HD1	1.65	0.59
1:A:246:ASP:OD2	7:G:10:VAL:N	2.35	0.59
3:P:207:ASN:ND2	3:P:211:ILE:O	2.36	0.59
1:A:23:LEU:N	1:A:192:ALA:HB1	2.18	0.58
4:D:131:LEU:HD11	13:D:501:HEC:HMB2	1.86	0.58
1:N:23:LEU:N	1:N:192:ALA:HB1	2.18	0.58
11:P:501:HEM:HMC2	11:P:501:HEM:HBC2	1.85	0.58
5:R:30:GLU:OE2	10:W:11:SER:OG	2.22	0.58
9:V:69:SER:OG	9:V:70:LEU:N	2.37	0.58
1:N:366:VAL:CG1	2:O:44:ALA:HB2	2.34	0.57
7:G:56:TYR:O	7:G:60:THR:OG1	2.11	0.57
5:R:189:SER:OG	5:R:191:ASP:OD1	2.22	0.57
9:I:69:SER:OG	9:I:70:LEU:N	2.37	0.57
1:N:76:GLU:OE2	2:O:289:SER:N	2.38	0.57
11:C:502:HEM:HBB2	11:C:502:HEM:HMB2	1.86	0.57
1:A:370:ASP:OD2	2:B:375:SER:OG	2.18	0.56
3:C:294:LEU:O	3:C:297:SER:OG	2.08	0.56
5:E:189:SER:OG	5:E:191:ASP:OD1	2.22	0.56
1:A:366:VAL:HG11	2:B:44:ALA:HB2	1.87	0.56
2:B:124:LEU:O	2:B:128:THR:OG1	2.13	0.56
11:C:501:HEM:HBC2	11:C:501:HEM:HMC2	1.87	0.56
11:P:502:HEM:HBB2	11:P:502:HEM:HMB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:48:GLU:OE2	1:N:55:ALA:N	2.39	0.56
3:P:58:ASP:OD1	3:P:59:THR:N	2.40	0.55
4:Q:221:ALA:O	4:Q:225:HIS:N	2.39	0.55
1:A:48:GLU:OE2	1:A:55:ALA:N	2.39	0.55
5:E:58:PHE:O	5:E:61:SER:OG	2.12	0.55
1:A:87:ASN:OD1	1:A:88:ALA:N	2.40	0.55
2:B:121:GLU:O	2:B:125:ASN:ND2	2.40	0.55
3:C:58:ASP:OD1	3:C:59:THR:N	2.40	0.55
4:D:40:CYS:SG	13:D:501:HEC:HAC	2.47	0.54
4:D:160:MET:SD	13:D:501:HEC:C4D	2.95	0.54
3:P:277:ALA:HB1	3:P:294:LEU:CD1	2.37	0.54
1:A:103:SER:OG	1:A:202:GLY:O	2.19	0.54
3:C:81:TYR:HB2	3:C:243:VAL:HG23	1.89	0.54
3:C:277:ALA:HB1	3:C:294:LEU:CD1	2.37	0.54
2:O:121:GLU:O	2:O:125:ASN:ND2	2.40	0.54
1:A:327:ASP:OD1	1:A:328:HIS:N	2.41	0.54
3:P:81:TYR:HB2	3:P:243:VAL:HG23	1.89	0.54
7:G:49:ALA:O	7:G:52:PHE:N	2.41	0.54
1:N:87:ASN:OD1	1:N:88:ALA:N	2.40	0.54
7:T:49:ALA:O	7:T:52:PHE:N	2.41	0.54
3:C:94:LEU:O	3:C:97:HIS:N	2.41	0.54
1:N:412:SER:O	10:W:15:ARG:NH2	2.41	0.53
3:P:277:ALA:HB1	3:P:294:LEU:HD11	1.91	0.53
4:D:221:ALA:O	4:D:225:HIS:N	2.38	0.53
5:E:109:GLU:OE2	5:E:168:SER:OG	2.23	0.53
1:N:327:ASP:OD1	1:N:328:HIS:N	2.41	0.53
3:P:94:LEU:O	3:P:97:HIS:N	2.41	0.53
2:O:250:ASP:OD1	2:O:251:SER:N	2.42	0.53
3:P:81:TYR:CB	3:P:243:VAL:HG23	2.40	0.52
2:B:46:ARG:NH1	2:B:376:GLU:OE1	2.42	0.52
3:C:148:ASN:O	3:C:151:SER:OG	2.27	0.52
3:P:25:SER:OG	3:P:216:ASP:OD2	2.16	0.52
11:P:502:HEM:HBD2	11:P:502:HEM:O2A	2.10	0.52
3:C:25:SER:OG	3:C:216:ASP:OD2	2.16	0.52
3:C:277:ALA:HB1	3:C:294:LEU:HD11	1.91	0.52
2:B:250:ASP:OD1	2:B:251:SER:N	2.42	0.52
2:O:46:ARG:NH1	2:O:376:GLU:OE1	2.42	0.52
1:A:76:GLU:OE2	2:B:289:SER:N	2.43	0.51
2:O:74:SER:O	2:O:82:SER:OG	2.11	0.51
3:P:314:SER:OG	3:P:315:MET:N	2.43	0.51
11:C:501:HEM:HBB2	11:C:501:HEM:HMB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:433:ASP:OD2	3:P:223:TYR:OH	2.28	0.51
2:O:319:SER:OG	2:O:320:GLY:N	2.43	0.51
1:N:245:GLU:OE2	7:T:11:ARG:NE	2.31	0.51
4:D:72:ASP:OD2	4:D:83:ARG:NH2	2.44	0.51
3:P:118:ILE:O	3:P:122:THR:OG1	2.18	0.51
3:P:148:ASN:O	3:P:151:SER:OG	2.27	0.51
11:P:501:HEM:HMB2	11:P:501:HEM:HBB2	1.93	0.51
4:Q:2:ASP:OD1	4:Q:3:LEU:N	2.44	0.51
3:C:81:TYR:CB	3:C:243:VAL:HG23	2.40	0.51
3:C:118:ILE:O	3:C:122:THR:OG1	2.18	0.51
2:B:319:SER:OG	2:B:320:GLY:N	2.43	0.51
3:P:178:PHE:O	3:P:182:HIS:N	2.44	0.51
4:Q:72:ASP:OD2	4:Q:83:ARG:NH2	2.44	0.51
5:R:1:SER:OG	5:R:2:HIS:N	2.44	0.51
3:C:127:ALA:CB	11:C:501:HEM:HMB1	2.41	0.50
2:O:437:ASP:OD2	2:B:169:ARG:NH2	2.44	0.50
5:R:109:GLU:OE2	5:R:168:SER:OG	2.23	0.50
3:C:314:SER:OG	3:C:315:MET:N	2.43	0.50
4:Q:215:LEU:O	4:Q:218:LEU:N	2.45	0.50
4:Q:106:ASN:ND2	4:Q:145:GLU:O	2.45	0.50
11:C:502:HEM:HBD2	11:C:502:HEM:O2A	2.12	0.50
3:P:127:ALA:CB	11:P:501:HEM:HMB1	2.42	0.50
3:C:178:PHE:O	3:C:182:HIS:N	2.44	0.50
3:C:283:SER:O	3:C:352:GLN:NE2	2.45	0.50
4:D:215:LEU:O	4:D:218:LEU:N	2.45	0.50
6:F:13:LEU:O	6:F:16:ILE:HG22	2.12	0.50
4:D:2:ASP:OD1	4:D:3:LEU:N	2.44	0.50
1:N:76:GLU:OE2	2:O:290:ASN:N	2.44	0.50
11:P:501:HEM:HBC2	11:P:501:HEM:CMC	2.42	0.50
3:P:286:ASN:OD1	3:P:287:LYS:N	2.45	0.49
3:C:127:ALA:HB2	11:C:501:HEM:HMB1	1.94	0.49
2:O:73:SER:O	2:O:74:SER:OG	2.24	0.49
2:O:279:LEU:HD11	2:O:344:VAL:HG22	1.93	0.49
6:S:13:LEU:O	6:S:16:ILE:HG22	2.12	0.49
5:E:1:SER:OG	5:E:2:HIS:N	2.43	0.49
2:B:261:SER:OG	2:B:262:ALA:N	2.45	0.49
4:D:106:ASN:ND2	4:D:145:GLU:O	2.45	0.49
3:P:283:SER:O	3:P:352:GLN:NE2	2.45	0.49
2:B:279:LEU:HD11	2:B:344:VAL:HG22	1.93	0.49
1:N:171:SER:N	5:R:4:ASP:OD1	2.43	0.49
2:O:163:LEU:HD12	2:O:425:ALA:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:261:SER:OG	2:O:262:ALA:N	2.45	0.49
3:P:248:ASP:OD1	4:Q:118:ARG:NH2	2.42	0.49
3:P:293:ALA:O	3:P:297:SER:N	2.45	0.49
1:A:366:VAL:CG1	2:B:44:ALA:HB2	2.41	0.49
2:B:131:GLU:OE1	2:B:133:ARG:NE	2.46	0.49
3:C:286:ASN:OD1	3:C:287:LYS:N	2.45	0.49
1:N:192:ALA:HB2	1:N:219:LEU:HD23	1.95	0.49
2:B:163:LEU:HD12	2:B:425:ALA:HB3	1.95	0.49
2:O:131:GLU:OE1	2:O:133:ARG:NE	2.45	0.48
3:C:101:GLY:O	3:C:105:GLY:N	2.46	0.48
3:C:293:ALA:O	3:C:297:SER:N	2.45	0.48
4:D:41:HIS:NE2	13:D:501:HEC:NB	2.61	0.48
11:C:501:HEM:HBC2	11:C:501:HEM:CMC	2.43	0.48
9:I:64:VAL:HG22	9:I:78:TYR:O	2.14	0.48
1:N:245:GLU:OE1	7:T:12:HIS:N	2.43	0.48
4:D:164:ILE:HD13	4:D:182:VAL:HG11	1.94	0.48
2:O:162:ASN:O	2:O:166:ALA:N	2.44	0.48
3:P:101:GLY:O	3:P:105:GLY:N	2.46	0.48
1:A:245:GLU:OE1	7:G:12:HIS:N	2.44	0.48
3:P:127:ALA:HB2	11:P:501:HEM:HMB1	1.95	0.48
11:P:502:HEM:HHA	11:P:502:HEM:O2A	2.14	0.48
2:B:308:ASP:OD1	2:B:309:VAL:N	2.47	0.47
3:C:186:PRO:HG2	11:C:501:HEM:HMC1	1.96	0.47
4:Q:164:ILE:HD13	4:Q:182:VAL:HG11	1.94	0.47
1:A:94:HIS:O	1:A:95:THR:OG1	2.32	0.47
1:A:192:ALA:HB2	1:A:219:LEU:HD23	1.95	0.47
1:A:79:VAL:O	1:A:83:GLY:N	2.48	0.47
1:A:433:ASP:OD2	3:C:223:TYR:OH	2.32	0.47
1:N:94:HIS:O	1:N:95:THR:OG1	2.32	0.47
4:Q:202:LYS:O	4:Q:206:LEU:N	2.48	0.47
9:V:64:VAL:HG22	9:V:78:TYR:O	2.14	0.47
1:A:340:GLY:HA2	1:A:343:MET:HE3	1.97	0.47
2:B:67:HIS:NE2	2:B:147:ASP:OD2	2.43	0.47
3:C:27:ILE:HD12	3:C:224:TYR:CZ	2.50	0.47
4:D:202:LYS:O	4:D:206:LEU:N	2.48	0.47
1:N:86:LEU:HD23	2:O:285:VAL:HG13	1.97	0.47
2:O:53:ALA:O	2:O:194:TYR:OH	2.33	0.47
11:C:501:HEM:HHA	11:C:501:HEM:CGD	2.45	0.47
1:N:21:ASN:OD1	1:N:22:GLY:N	2.49	0.46
4:D:164:ILE:CD1	4:D:182:VAL:HG11	2.45	0.46
2:B:338:LYS:O	2:B:342:ASN:ND2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:502:HEM:HHA	11:C:502:HEM:O2A	2.15	0.46
4:D:197:GLU:N	4:D:197:GLU:OE1	2.48	0.46
1:N:84:ALA:HB1	1:N:100:LYS:O	2.15	0.46
3:P:27:ILE:HD12	3:P:224:TYR:CZ	2.50	0.46
5:R:69:LEU:O	5:R:72:SER:OG	2.28	0.46
4:D:163:PRO:HG2	13:D:501:HEC:HBB2	1.97	0.46
3:P:186:PRO:HG2	11:P:501:HEM:HMC1	1.96	0.46
3:P:220:PHE:CZ	12:P:503:G8U:H13	2.51	0.46
1:N:140:GLU:O	1:N:143:THR:OG1	2.20	0.46
1:A:84:ALA:HB1	1:A:100:LYS:O	2.15	0.46
11:C:502:HEM:CMA	12:C:503:G8U:H15	2.43	0.46
1:N:363:ASN:ND2	2:O:93:GLY:O	2.48	0.46
3:P:61:THR:O	3:P:65:SER:N	2.47	0.46
2:O:338:LYS:O	2:O:342:ASN:ND2	2.49	0.46
6:S:97:VAL:O	6:S:100:GLU:N	2.49	0.46
2:B:73:SER:O	2:B:74:SER:OG	2.24	0.46
4:D:228:SER:O	7:G:23:GLN:NE2	2.49	0.46
4:Q:31:GLN:NE2	4:Q:56:TYR:OH	2.49	0.46
4:Q:197:GLU:OE1	4:Q:197:GLU:N	2.49	0.46
1:A:372:THR:OG1	2:B:373:GLU:OE2	2.15	0.46
2:B:162:ASN:O	2:B:166:ALA:N	2.44	0.46
2:B:162:ASN:HA	2:B:165:ALA:HB3	1.98	0.46
4:D:83:ARG:NH2	4:D:89:ASP:OD2	2.49	0.46
1:N:340:GLY:HA2	1:N:343:MET:HE3	1.97	0.45
1:A:274:ASN:O	1:A:278:GLY:N	2.50	0.45
4:Q:165:TYR:CE1	4:Q:168:VAL:HG23	2.52	0.45
1:A:21:ASN:OD1	1:A:22:GLY:N	2.49	0.45
1:N:79:VAL:O	1:N:83:GLY:N	2.48	0.45
2:O:279:LEU:HD11	2:O:344:VAL:CG2	2.47	0.45
4:Q:164:ILE:CD1	4:Q:182:VAL:HG11	2.45	0.45
2:B:46:ARG:NH1	2:B:110:GLU:OE2	2.49	0.45
1:A:142:ASP:OD1	5:E:2:HIS:ND1	2.44	0.45
2:B:279:LEU:HD11	2:B:344:VAL:CG2	2.47	0.45
4:D:165:TYR:CE1	4:D:168:VAL:HG23	2.51	0.45
6:F:97:VAL:O	6:F:100:GLU:N	2.48	0.45
2:B:53:ALA:O	2:B:194:TYR:OH	2.33	0.45
4:Q:131:LEU:HD11	13:Q:501:HEC:HMB2	1.98	0.45
4:D:31:GLN:NE2	4:D:56:TYR:OH	2.49	0.45
4:D:132:THR:O	8:H:21:ARG:NH2	2.49	0.45
4:Q:65:ALA:HB1	4:Q:85:GLY:C	2.37	0.45
2:B:101:THR:HG22	9:I:65:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:308:ASP:OD1	2:O:309:VAL:N	2.47	0.44
3:P:100:ARG:O	3:P:103:TYR:N	2.50	0.44
11:C:501:HEM:HBA1	11:C:501:HEM:CGD	2.47	0.44
4:D:65:ALA:HB1	4:D:85:GLY:C	2.37	0.44
1:N:103:SER:OG	1:N:202:GLY:O	2.19	0.44
4:Q:83:ARG:NH2	4:Q:89:ASP:OD2	2.49	0.44
1:N:274:ASN:O	1:N:278:GLY:N	2.49	0.44
3:P:313:ARG:HE	6:S:38:HIS:CD2	2.35	0.44
2:O:162:ASN:HA	2:O:165:ALA:HB3	1.98	0.44
1:A:140:GLU:O	1:A:143:THR:OG1	2.20	0.44
1:A:147:ASP:O	1:A:151:ASN:ND2	2.50	0.44
3:P:196:HIS:NE2	11:P:502:HEM:ND	2.66	0.44
1:N:147:ASP:O	1:N:151:ASN:ND2	2.50	0.44
1:A:157:ALA:HB1	1:A:236:PHE:CE1	2.53	0.44
3:C:196:HIS:NE2	11:C:502:HEM:ND	2.66	0.44
1:N:157:ALA:HB1	1:N:236:PHE:CE1	2.53	0.43
11:C:502:HEM:HBB2	11:C:502:HEM:CMB	2.48	0.43
5:R:171:ILE:HD13	5:R:176:ALA:HB3	2.00	0.43
2:B:255:ALA:O	2:B:326:THR:N	2.49	0.43
3:C:100:ARG:O	3:C:103:TYR:N	2.50	0.43
1:N:210:ASP:O	1:N:214:LYS:N	2.51	0.43
1:A:363:ASN:ND2	2:B:93:GLY:O	2.51	0.43
2:O:46:ARG:NH1	2:O:110:GLU:OE2	2.49	0.43
3:C:220:PHE:CZ	12:C:503:G8U:H13	2.53	0.43
5:E:30:GLU:OE2	10:J:11:SER:OG	2.12	0.43
1:N:24:ARG:NH1	1:N:383:LEU:O	2.52	0.43
2:O:133:ARG:NH1	6:F:96:GLU:OE2	2.51	0.43
1:A:281:ASP:O	1:A:283:THR:N	2.52	0.43
5:E:171:ILE:HD13	5:E:176:ALA:HB3	2.00	0.43
11:P:501:HEM:HBA1	11:P:501:HEM:CGD	2.49	0.43
11:P:501:HEM:HHA	11:P:501:HEM:CGD	2.48	0.43
3:C:61:THR:O	3:C:65:SER:N	2.47	0.43
2:O:169:ARG:NH2	2:B:437:ASP:OD2	2.52	0.43
4:D:36:VAL:HG11	13:D:501:HEC:HAB	2.00	0.43
3:P:304:ILE:O	3:P:307:LEU:N	2.47	0.42
3:C:372:ILE:O	3:C:375:LYS:N	2.50	0.42
2:O:133:ARG:NH2	6:F:96:GLU:OE2	2.51	0.42
2:O:35:ILE:HG22	2:O:36:ALA:N	2.34	0.42
5:E:91:TRP:N	5:E:94:LYS:O	2.49	0.42
2:B:35:ILE:HG22	2:B:36:ALA:N	2.34	0.42
3:C:304:ILE:O	3:C:307:LEU:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:502:HEM:HBB2	11:P:502:HEM:CMB	2.49	0.42
5:R:91:TRP:N	5:R:94:LYS:O	2.49	0.42
3:P:182:HIS:NE2	11:P:501:HEM:NB	2.68	0.42
1:A:24:ARG:NH1	1:A:383:LEU:O	2.52	0.42
1:A:49:SER:N	1:A:52:ASN:OD1	2.52	0.42
2:B:77:THR:OG1	2:B:80:ALA:O	2.25	0.42
3:C:58:ASP:O	3:C:62:ALA:HB2	2.20	0.42
3:P:58:ASP:O	3:P:62:ALA:HB2	2.20	0.42
4:Q:231:LYS:O	6:S:71:ARG:NH2	2.53	0.42
2:B:207:ILE:HG22	2:B:208:GLY:N	2.35	0.42
4:D:36:VAL:CG1	13:D:501:HEC:HAB	2.50	0.42
3:C:182:HIS:NE2	11:C:501:HEM:NB	2.68	0.42
2:O:207:ILE:HG22	2:O:208:GLY:N	2.35	0.41
4:Q:68:VAL:HG11	4:Q:92:PRO:HG2	2.02	0.41
1:N:152:TYR:CE1	5:R:5:ILE:HD13	2.55	0.41
1:A:210:ASP:O	1:A:214:LYS:N	2.51	0.41
11:P:502:HEM:CMA	12:P:503:G8U:H15	2.48	0.41
1:N:235:ARG:NH1	1:N:237:THR:OG1	2.51	0.41
1:N:281:ASP:O	1:N:283:THR:N	2.52	0.41
4:D:209:LEU:O	4:D:213:GLY:N	2.44	0.41
5:E:32:ARG:NH1	7:G:22:GLU:OE2	2.52	0.41
2:O:67:HIS:NE2	2:O:147:ASP:OD2	2.43	0.41
1:A:76:GLU:OE2	2:B:290:ASN:N	2.54	0.41
3:P:27:ILE:HD12	3:P:224:TYR:OH	2.21	0.41
4:Q:197:GLU:O	4:Q:201:ARG:N	2.48	0.41
2:O:101:THR:HG22	9:V:65:VAL:HG13	2.03	0.41
2:B:169:ARG:HE	2:B:240:HIS:HB2	1.87	0.40
4:D:68:VAL:HG11	4:D:92:PRO:HG2	2.03	0.40
1:N:95:THR:HG22	1:N:96:ALA:N	2.36	0.40
2:O:255:ALA:O	2:O:326:THR:N	2.49	0.40
1:A:378:ASP:O	1:A:382:SER:OG	2.23	0.40
3:C:215:VAL:O	6:F:63:LYS:NZ	2.44	0.40
3:C:138:MET:O	3:C:142:GLY:N	2.48	0.40
2:O:39:GLU:OE2	2:O:113:ARG:NH2	2.49	0.40
3:C:27:ILE:HD12	3:C:224:TYR:OH	2.21	0.40

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	441/480 (92%)	398 (90%)	42 (10%)	1 (0%)	47	80
1	N	441/480 (92%)	398 (90%)	42 (10%)	1 (0%)	47	80
2	B	408/453 (90%)	360 (88%)	48 (12%)	0	100	100
2	O	408/453 (90%)	360 (88%)	48 (12%)	0	100	100
3	C	368/379 (97%)	330 (90%)	38 (10%)	0	100	100
3	P	368/379 (97%)	330 (90%)	38 (10%)	0	100	100
4	D	237/325 (73%)	215 (91%)	22 (9%)	0	100	100
4	Q	237/325 (73%)	216 (91%)	21 (9%)	0	100	100
5	E	170/274 (62%)	151 (89%)	19 (11%)	0	100	100
5	R	170/274 (62%)	151 (89%)	19 (11%)	0	100	100
6	F	96/111 (86%)	91 (95%)	5 (5%)	0	100	100
6	S	96/111 (86%)	90 (94%)	6 (6%)	0	100	100
7	G	72/82 (88%)	64 (89%)	8 (11%)	0	100	100
7	T	72/82 (88%)	64 (89%)	8 (11%)	0	100	100
8	H	63/91 (69%)	58 (92%)	5 (8%)	0	100	100
8	U	63/91 (69%)	58 (92%)	5 (8%)	0	100	100
9	I	15/17 (88%)	8 (53%)	7 (47%)	0	100	100
9	V	15/17 (88%)	8 (53%)	7 (47%)	0	100	100
10	J	55/64 (86%)	53 (96%)	2 (4%)	0	100	100
10	W	55/64 (86%)	53 (96%)	2 (4%)	0	100	100
All	All	3850/4552 (85%)	3456 (90%)	392 (10%)	2 (0%)	54	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	282	CYS

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Mol	Chain	Res	Type
1	A	282	CYS

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	367/394 (93%)	367 (100%)	0	100	100
1	N	367/394 (93%)	367 (100%)	0	100	100
2	B	325/355 (92%)	325 (100%)	0	100	100
2	O	325/355 (92%)	325 (100%)	0	100	100
3	C	318/327 (97%)	318 (100%)	0	100	100
3	P	318/327 (97%)	318 (100%)	0	100	100
4	D	204/257 (79%)	204 (100%)	0	100	100
4	Q	204/257 (79%)	204 (100%)	0	100	100
5	E	147/228 (64%)	147 (100%)	0	100	100
5	R	147/228 (64%)	147 (100%)	0	100	100
6	F	90/99 (91%)	90 (100%)	0	100	100
6	S	90/99 (91%)	90 (100%)	0	100	100
7	G	66/72 (92%)	65 (98%)	1 (2%)	65	79
7	T	66/72 (92%)	65 (98%)	1 (2%)	65	79
8	H	62/85 (73%)	62 (100%)	0	100	100
8	U	62/85 (73%)	62 (100%)	0	100	100
9	I	15/15 (100%)	15 (100%)	0	100	100
9	V	15/15 (100%)	15 (100%)	0	100	100
10	J	48/54 (89%)	48 (100%)	0	100	100
10	W	48/54 (89%)	48 (100%)	0	100	100
All	All	3284/3772 (87%)	3282 (100%)	2 (0%)	93	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	T	47	ARG
7	G	47	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	252	HIS
2	O	343	GLN
4	Q	31	GLN
5	R	141	HIS
5	R	161	HIS
1	A	87	ASN
1	A	252	HIS
2	B	343	GLN
4	D	31	GLN
5	E	141	HIS
5	E	161	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)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	G8U	C	503	-	31,31,31	0.94	1 (3%)	41,45,45	1.75	6 (14%)
12	G8U	P	503	-	31,31,31	0.93	1 (3%)	41,45,45	1.73	6 (14%)
11	HEM	P	501	3	41,50,50	1.68	5 (12%)	45,82,82	1.47	10 (22%)
11	HEM	P	502	3	41,50,50	1.74	4 (9%)	45,82,82	1.47	5 (11%)
11	HEM	C	501	-	41,50,50	1.68	5 (12%)	45,82,82	1.44	8 (17%)
13	HEC	D	501	4	32,50,50	2.40	3 (9%)	24,82,82	1.70	5 (20%)
13	HEC	Q	501	4	32,50,50	2.40	3 (9%)	24,82,82	1.70	5 (20%)
11	HEM	C	502	3	41,50,50	1.73	4 (9%)	45,82,82	1.47	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
12	G8U	C	503	-	-	3/15/15/15	0/3/3/3
12	G8U	P	503	-	-	4/15/15/15	0/3/3/3
11	HEM	P	501	3	-	4/12/54/54	-
11	HEM	P	502	3	-	6/12/54/54	-
11	HEM	C	501	-	-	4/12/54/54	-
13	HEC	D	501	4	-	2/10/54/54	-
13	HEC	Q	501	4	-	2/10/54/54	-
11	HEM	C	502	3	-	6/12/54/54	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	501	HEC	C3C-C2C	-8.49	1.31	1.40
13	Q	501	HEC	C3C-C2C	-8.47	1.31	1.40
13	D	501	HEC	C2B-C3B	-7.25	1.33	1.40
13	Q	501	HEC	C2B-C3B	-7.25	1.33	1.40
11	P	502	HEM	C3C-C2C	-6.29	1.31	1.40
11	C	502	HEM	C3C-C2C	-6.29	1.31	1.40
11	C	501	HEM	C3C-C2C	-5.19	1.33	1.40
13	D	501	HEC	C3D-C2D	5.16	1.53	1.37
13	Q	501	HEC	C3D-C2D	5.14	1.52	1.37
11	P	501	HEM	C3C-C2C	-5.14	1.33	1.40
11	C	501	HEM	FE-NB	4.76	2.20	1.96
11	P	501	HEM	FE-NB	4.57	2.19	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	P	502	HEM	FE-ND	4.24	2.17	1.96
11	C	502	HEM	FE-ND	4.16	2.17	1.96
11	C	502	HEM	C3C-CAC	3.29	1.54	1.47
11	P	502	HEM	C3C-CAC	3.28	1.54	1.47
11	P	501	HEM	C3C-CAC	3.00	1.54	1.47
11	P	501	HEM	CAB-C3B	2.97	1.55	1.47
11	C	501	HEM	CAB-C3B	2.96	1.55	1.47
11	C	501	HEM	C3C-CAC	2.92	1.53	1.47
12	C	503	G8U	C19-CL	2.65	1.78	1.72
12	P	503	G8U	C19-CL	2.62	1.78	1.72
11	P	502	HEM	CAB-C3B	2.59	1.54	1.47
11	C	502	HEM	CAB-C3B	2.56	1.54	1.47
11	P	501	HEM	CHC-C4B	-2.31	1.34	1.41
11	C	501	HEM	CHC-C4B	-2.29	1.34	1.41

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	503	G8U	C27-C20-C19	-6.03	119.55	123.01
12	P	503	G8U	C27-C20-C19	-6.00	119.56	123.01
12	C	503	G8U	C14-C17-C22	-5.64	118.89	123.46
12	P	503	G8U	C14-C17-C22	-5.43	119.06	123.46
12	P	503	G8U	C20-C19-C18	-4.53	119.92	122.79
12	C	503	G8U	C20-C19-C18	-4.47	119.95	122.79
11	P	502	HEM	CAD-C3D-C4D	4.06	131.75	124.66
11	C	502	HEM	CAD-C3D-C4D	3.98	131.61	124.66
11	P	501	HEM	CMC-C2C-C3C	3.71	131.61	124.68
11	C	501	HEM	CMC-C2C-C3C	3.66	131.53	124.68
11	P	502	HEM	CAD-C3D-C2D	-3.51	121.35	127.88
11	C	502	HEM	CAD-C3D-C2D	-3.49	121.37	127.88
11	C	502	HEM	CBA-CAA-C2A	-3.46	106.72	112.62
11	P	502	HEM	CBA-CAA-C2A	-3.45	106.73	112.62
11	P	501	HEM	C4A-C3A-C2A	3.00	109.09	107.00
13	Q	501	HEC	C1D-C2D-C3D	-2.98	104.93	107.00
13	D	501	HEC	C1D-C2D-C3D	-2.91	104.97	107.00
11	P	501	HEM	C4D-ND-C1D	2.90	108.07	105.07
11	C	501	HEM	C4D-ND-C1D	2.88	108.05	105.07
11	C	501	HEM	C4A-C3A-C2A	2.88	109.00	107.00
13	D	501	HEC	CAA-CBA-CGA	-2.84	105.79	113.76
13	Q	501	HEC	CAA-CBA-CGA	-2.84	105.81	113.76
13	D	501	HEC	CMB-C2B-C1B	-2.62	124.43	128.46
11	P	501	HEM	CMA-C3A-C4A	-2.62	124.44	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Q	501	HEC	CMB-C2B-C1B	-2.62	124.44	128.46
13	D	501	HEC	C4C-C3C-C2C	2.60	109.16	106.35
13	Q	501	HEC	C4C-C3C-C2C	2.57	109.12	106.35
11	P	501	HEM	CAA-CBA-CGA	-2.47	106.85	113.76
11	C	501	HEM	CMA-C3A-C4A	-2.45	124.69	128.46
11	C	501	HEM	CBD-CAD-C3D	-2.45	105.83	112.63
11	C	501	HEM	CAA-CBA-CGA	-2.42	106.99	113.76
11	P	501	HEM	C3D-C4D-ND	-2.38	107.52	110.17
13	D	501	HEC	CAD-CBD-CGD	-2.38	107.09	113.76
13	Q	501	HEC	CAD-CBD-CGD	-2.37	107.13	113.76
11	P	501	HEM	CBD-CAD-C3D	-2.35	106.09	112.63
11	C	502	HEM	C4C-CHD-C1D	2.34	125.64	122.56
11	C	501	HEM	C3D-C4D-ND	-2.32	107.58	110.17
11	P	502	HEM	C4C-CHD-C1D	2.21	125.48	122.56
12	C	503	G8U	C20-N28-C22	2.21	121.39	118.99
11	C	502	HEM	CAA-CBA-CGA	-2.17	107.69	113.76
12	C	503	G8U	C17-C22-N28	-2.15	120.95	123.61
12	C	503	G8U	C27-C20-N28	2.15	119.82	116.49
12	P	503	G8U	C20-N28-C22	2.14	121.31	118.99
12	P	503	G8U	C17-C22-N28	-2.13	120.99	123.61
11	C	501	HEM	C3B-C2B-C1B	2.11	108.05	106.49
11	P	501	HEM	C3B-C2B-C1B	2.11	108.05	106.49
12	P	503	G8U	C27-C20-N28	2.10	119.74	116.49
11	P	502	HEM	C1D-C2D-C3D	2.06	109.12	106.96
11	P	501	HEM	CAA-C2A-C3A	-2.05	121.35	127.25
11	C	502	HEM	CHA-C4D-C3D	2.01	129.10	125.33
11	P	501	HEM	C4B-C3B-C2B	-2.01	105.52	107.11

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	P	501	HEM	C1A-C2A-CAA-CBA
11	P	501	HEM	C3A-C2A-CAA-CBA
11	P	502	HEM	C2D-C3D-CAD-CBD
11	P	502	HEM	C4D-C3D-CAD-CBD
11	C	501	HEM	C1A-C2A-CAA-CBA
11	C	501	HEM	C3A-C2A-CAA-CBA
11	C	502	HEM	C2D-C3D-CAD-CBD
11	C	502	HEM	C4D-C3D-CAD-CBD
12	P	503	G8U	F1-C1-O29-C4
12	C	503	G8U	F1-C1-O29-C4

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Mol	Chain	Res	Type	Atoms
12	C	503	G8U	F2-C1-O29-C4
13	Q	501	HEC	C2D-C3D-CAD-CBD
13	Q	501	HEC	C4D-C3D-CAD-CBD
13	D	501	HEC	C2D-C3D-CAD-CBD
13	D	501	HEC	C4D-C3D-CAD-CBD
12	P	503	G8U	F2-C1-O29-C4
12	C	503	G8U	F3-C1-O29-C4
11	P	502	HEM	C2A-CAA-CBA-CGA
11	C	502	HEM	C2A-CAA-CBA-CGA
11	P	501	HEM	C3D-CAD-CBD-CGD
11	C	501	HEM	C3D-CAD-CBD-CGD
12	P	503	G8U	F3-C1-O29-C4
11	P	501	HEM	C2A-CAA-CBA-CGA
11	P	502	HEM	C3D-CAD-CBD-CGD
11	C	502	HEM	C3D-CAD-CBD-CGD
12	P	503	G8U	N28-C22-C24-O25
11	C	502	HEM	CAA-CBA-CGA-O1A
11	C	501	HEM	C2A-CAA-CBA-CGA
11	P	502	HEM	CAA-CBA-CGA-O2A
11	C	502	HEM	CAA-CBA-CGA-O2A
11	P	502	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

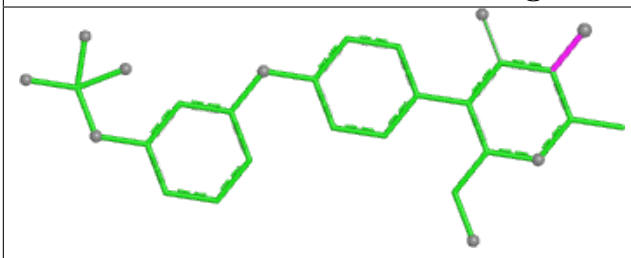
8 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	503	G8U	3	0
12	P	503	G8U	3	0
11	P	501	HEM	10	0
11	P	502	HEM	9	0
11	C	501	HEM	10	0
13	D	501	HEC	9	0
13	Q	501	HEC	6	0
11	C	502	HEM	9	0

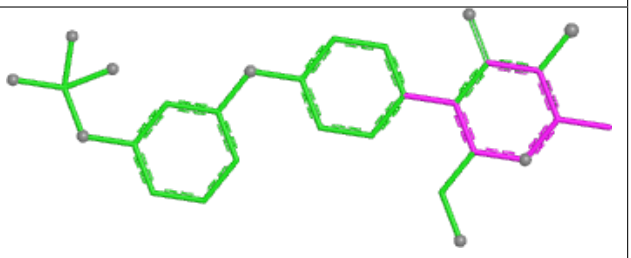
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

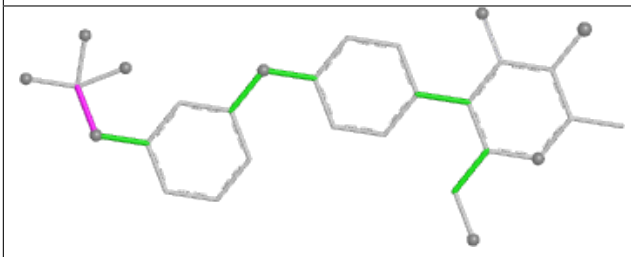
Ligand G8U C 503



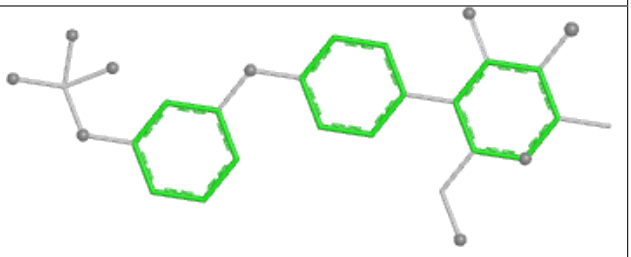
Bond lengths



Bond angles

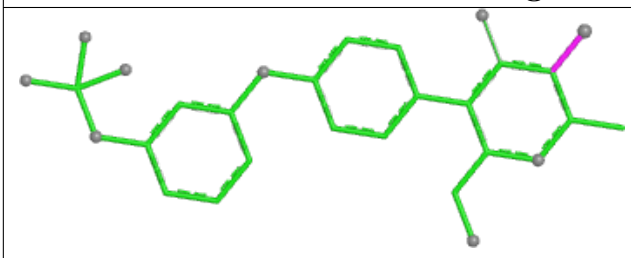


Torsions

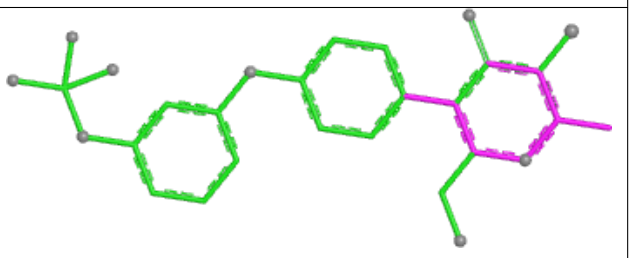


Rings

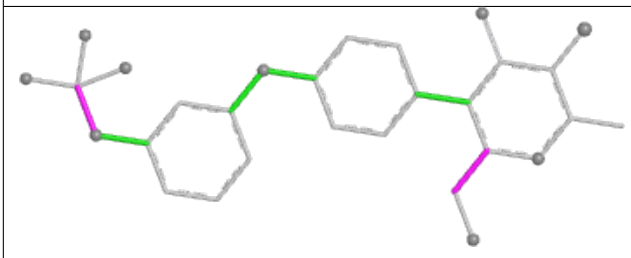
Ligand G8U P 503



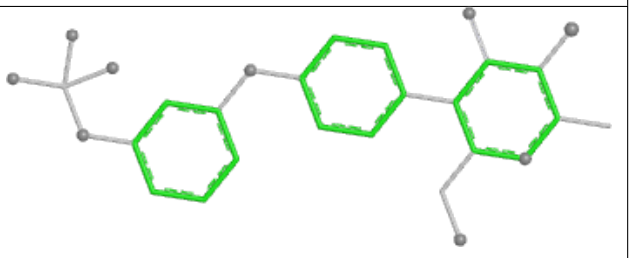
Bond lengths



Bond angles

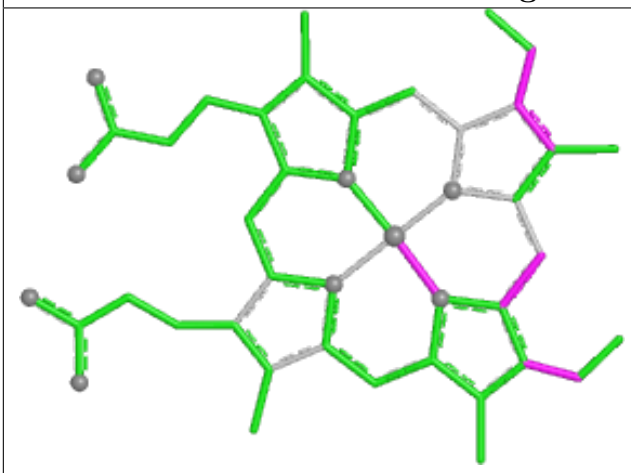


Torsions



Rings

Ligand HEM P 501



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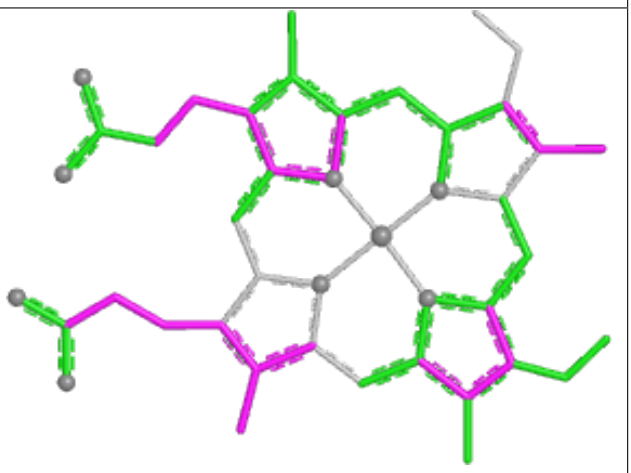
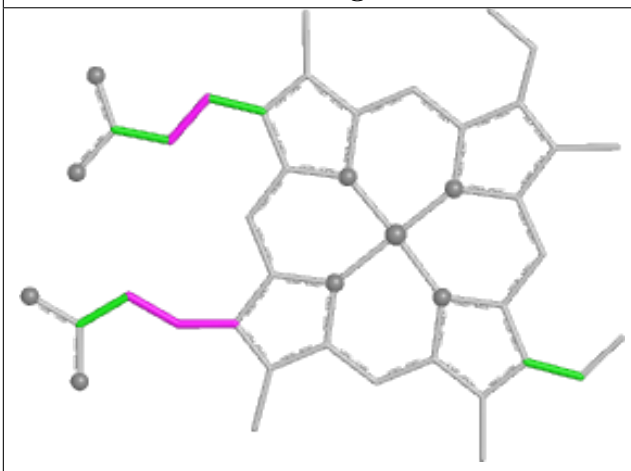
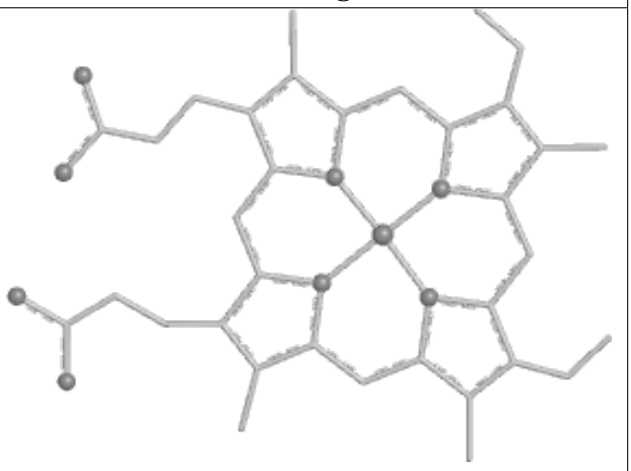


Bond angles

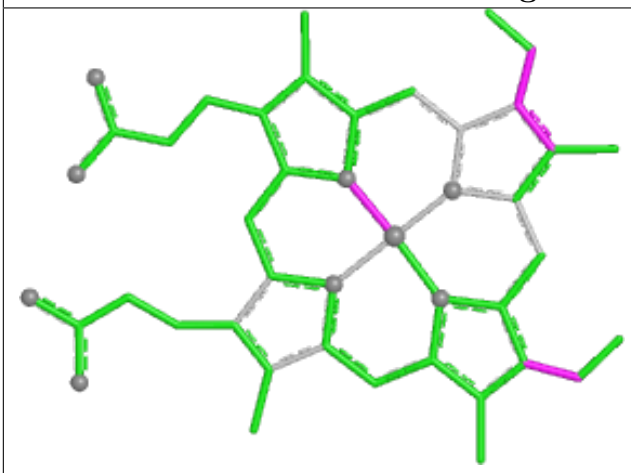


Torsions

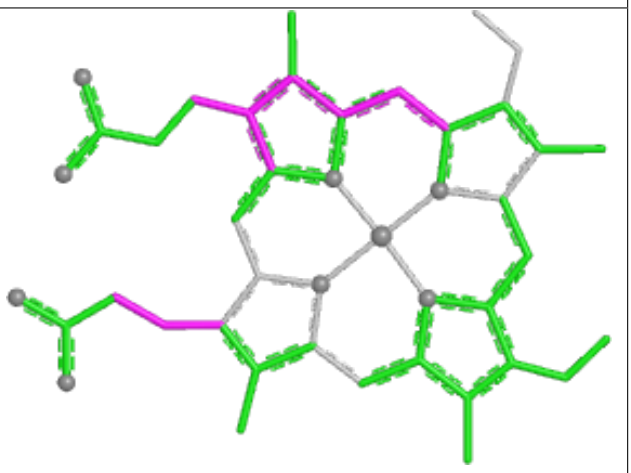


Rings

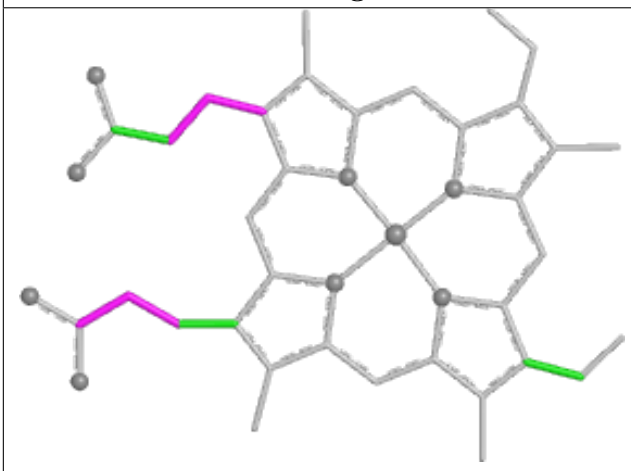
Ligand HEM P 502



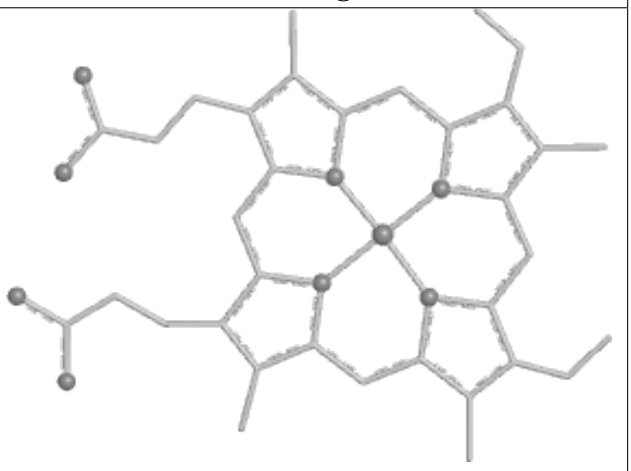
Bond lengths



Bond angles

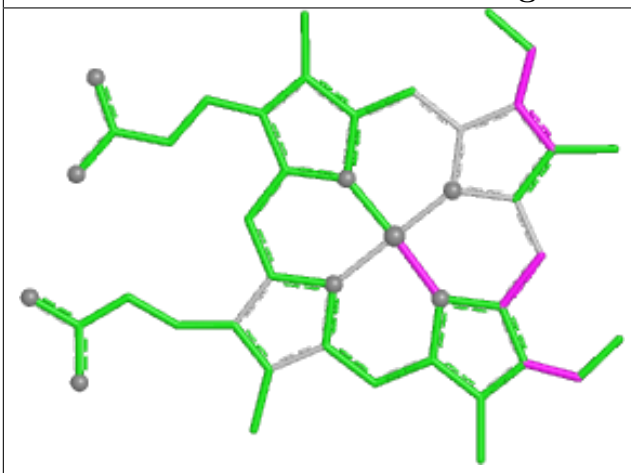


Torsions

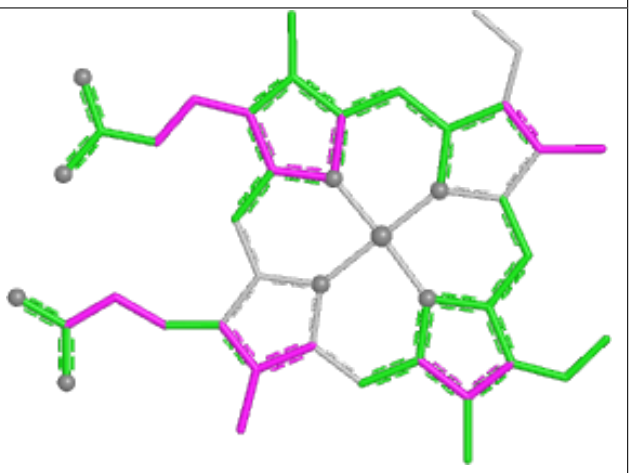


Rings

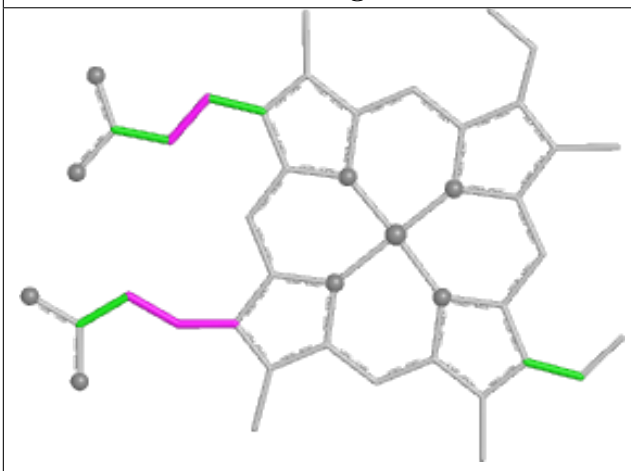
Ligand HEM C 501



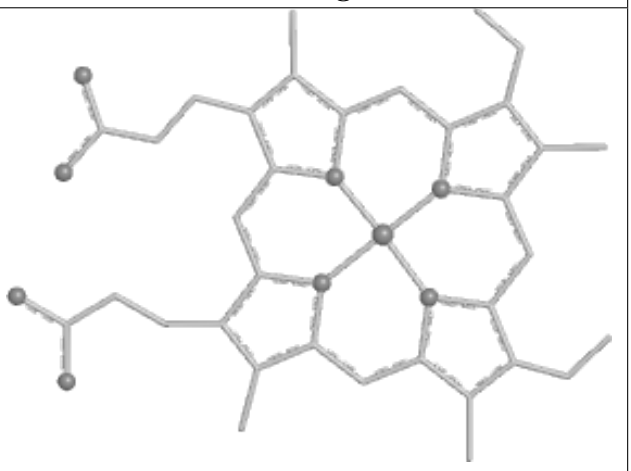
Bond lengths



Bond angles

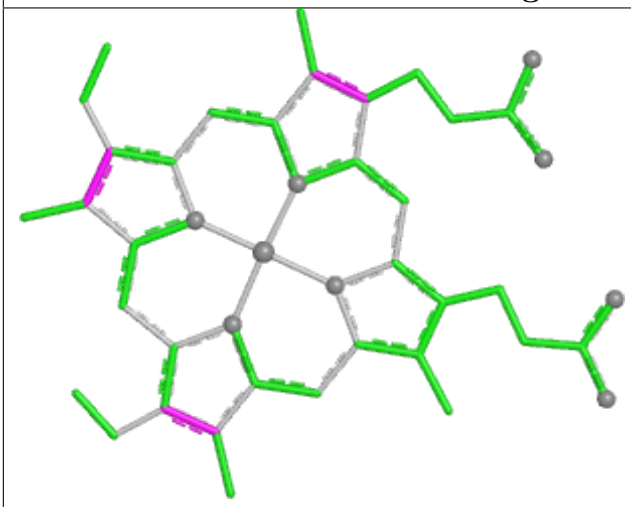


Torsions

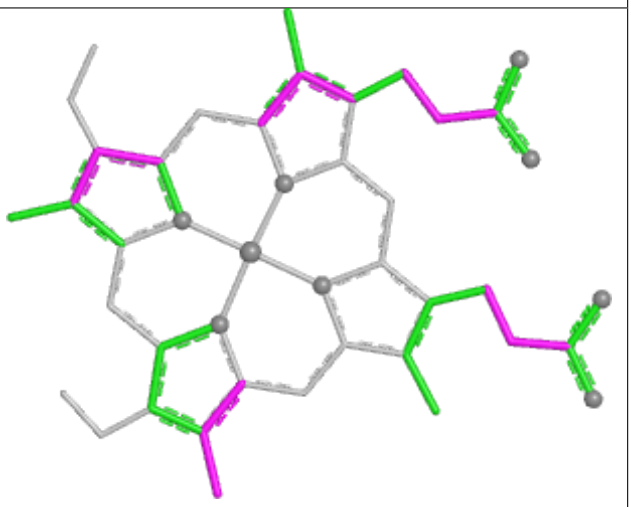


Rings

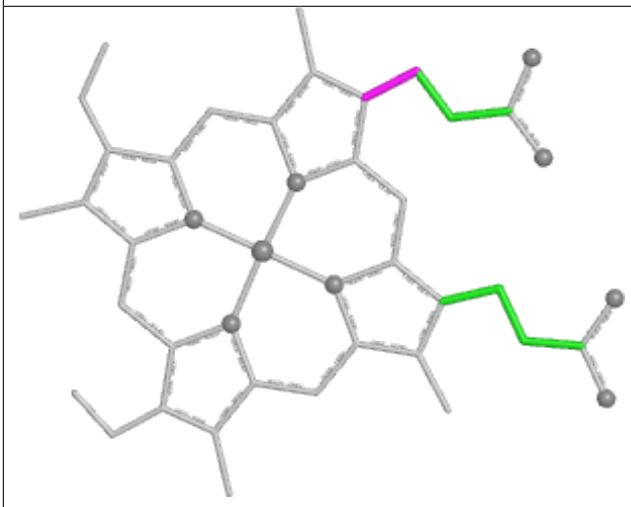
Ligand HEC D 501



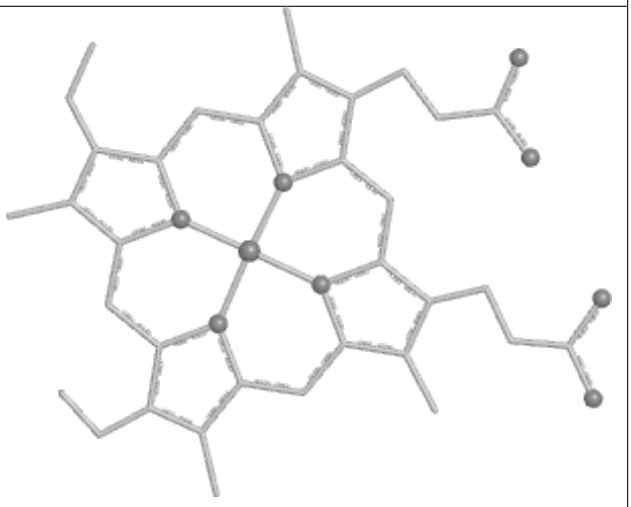
Bond lengths



Bond angles

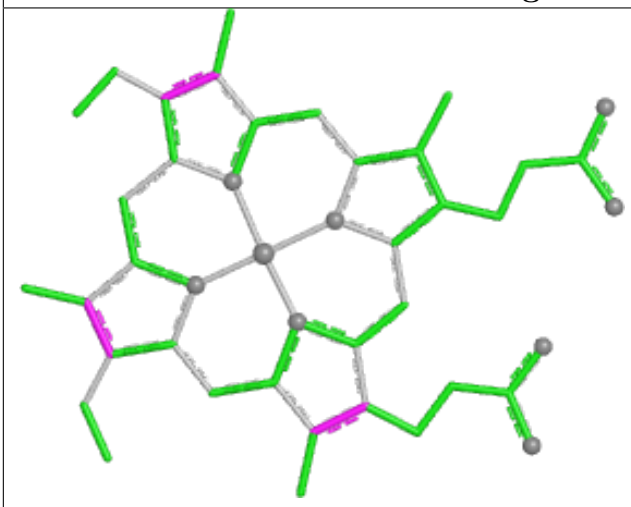


Torsions

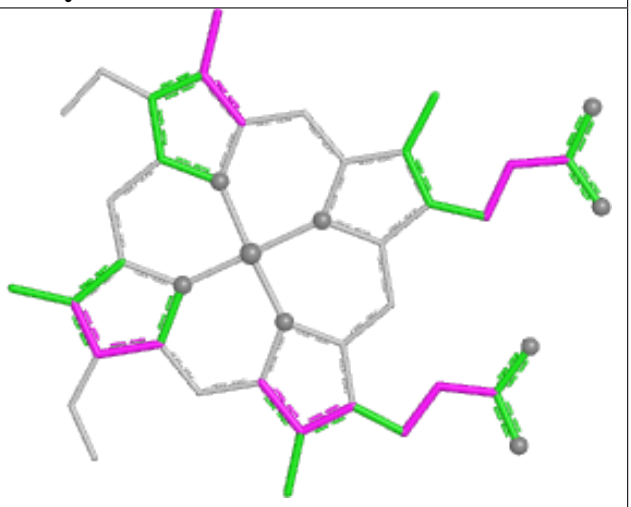


Rings

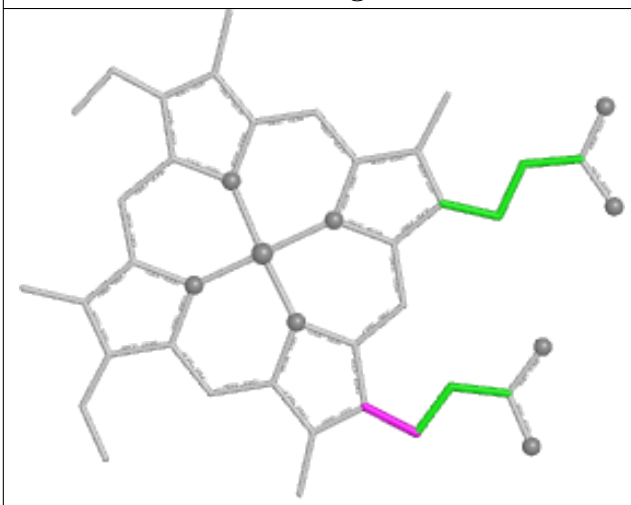
Ligand HEC Q 501



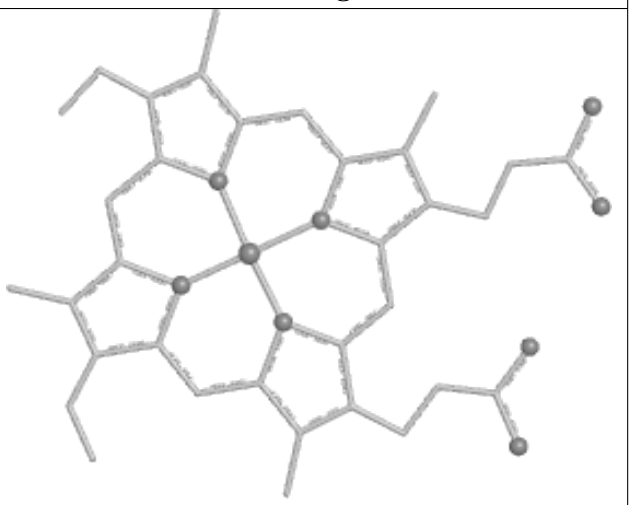
Bond lengths



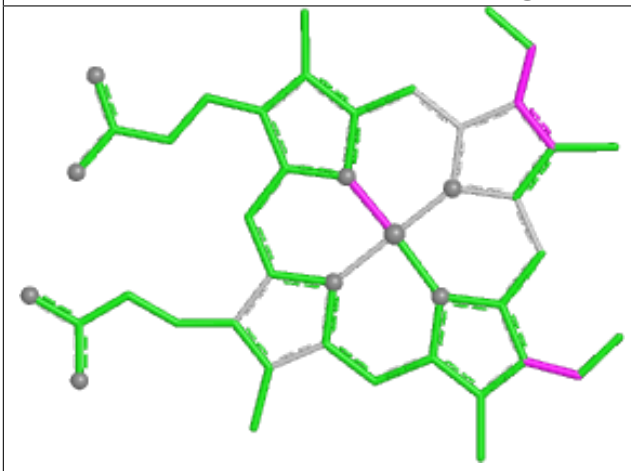
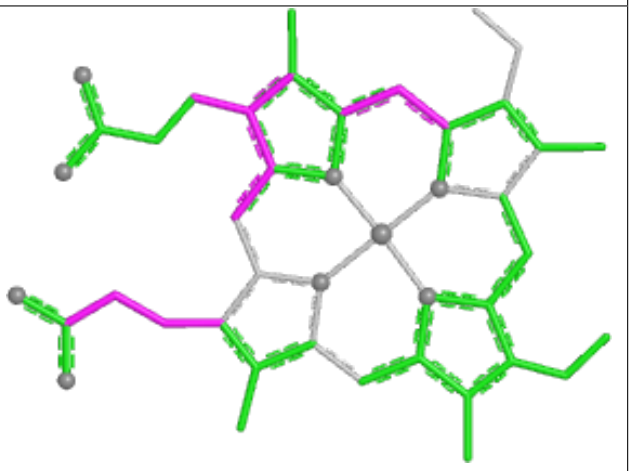
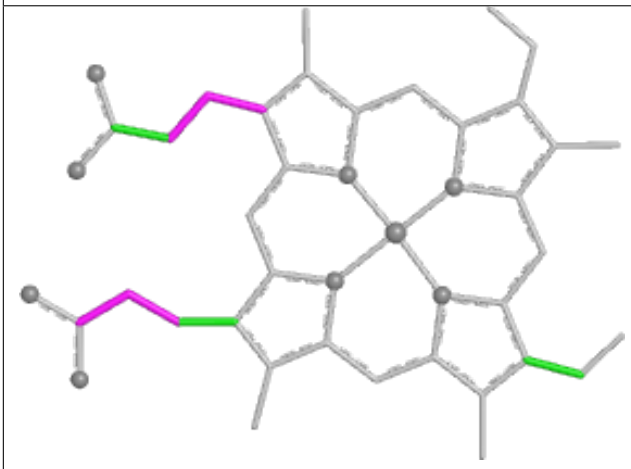
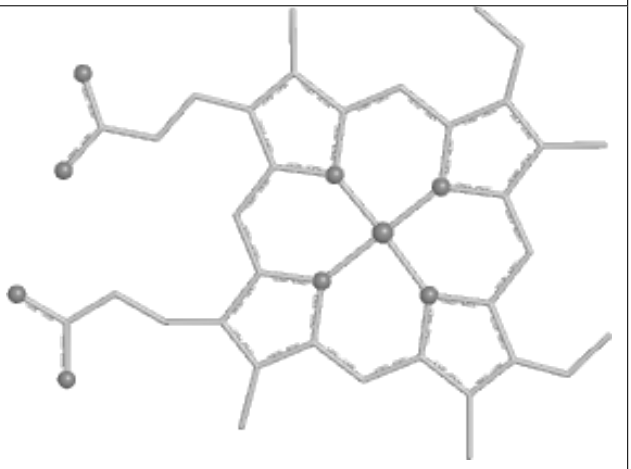
Bond angles



Torsions



Rings

Ligand HEM C 502	
	
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.

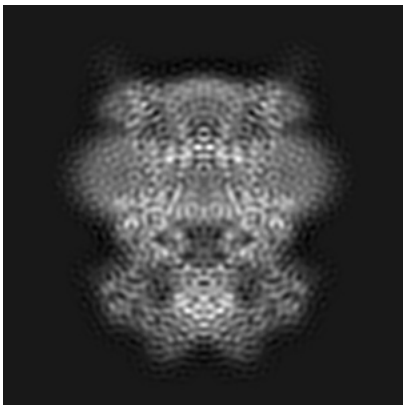
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4286. These allow visual inspection of the internal detail of the map and identification of artifacts.

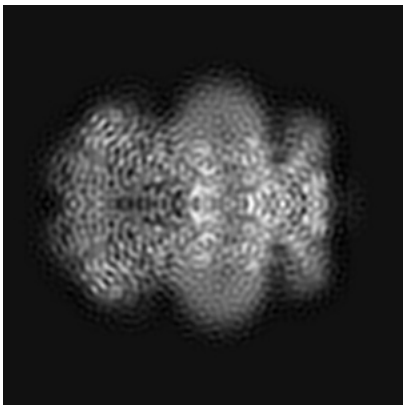
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

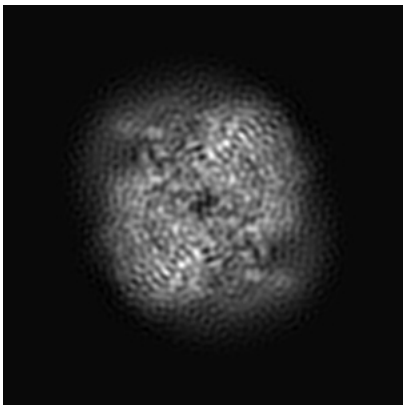
6.1.1 Primary map



X



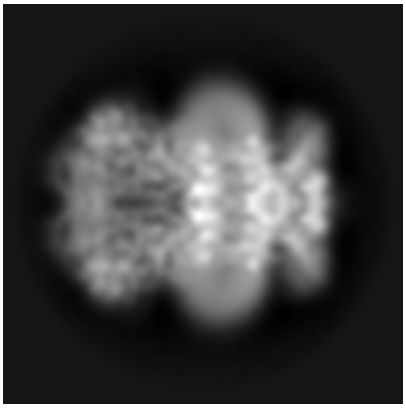
Y



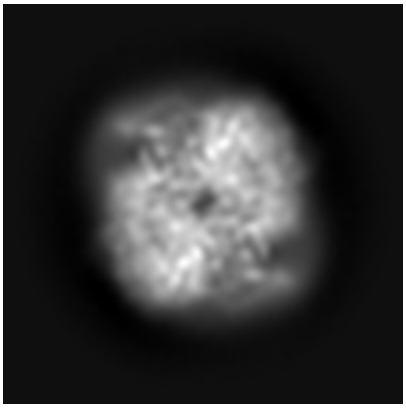
Z

6.1.2 Raw map

X



Y

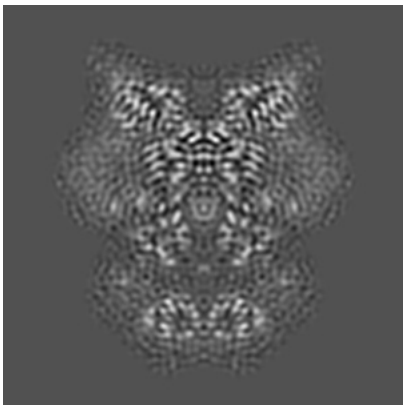


Z

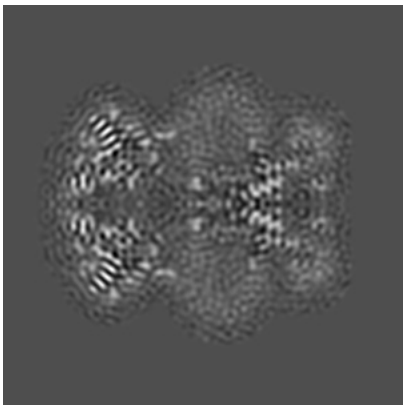
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

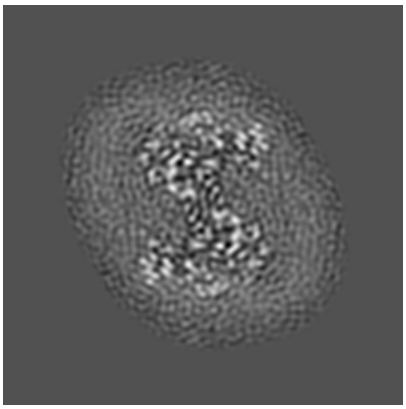
6.2.1 Primary map



X Index: 100



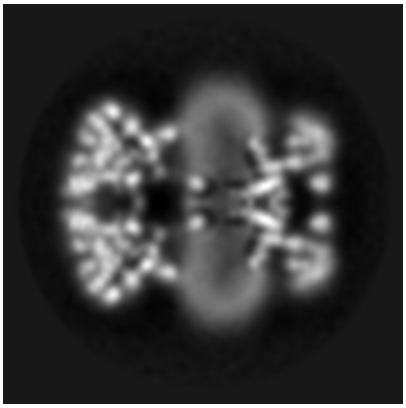
Y Index: 100



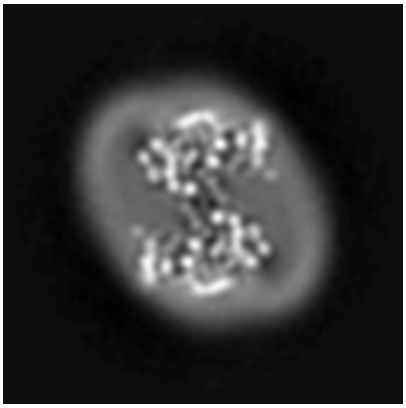
Z Index: 100

6.2.2 Raw map

X Index: 100



Y Index: 100

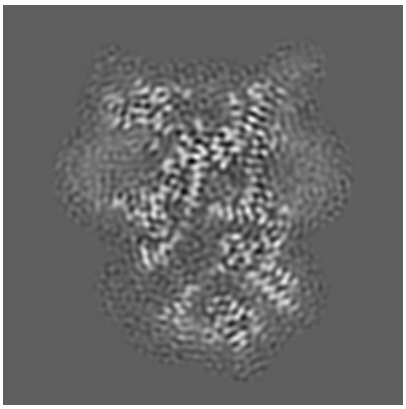


Z Index: 100

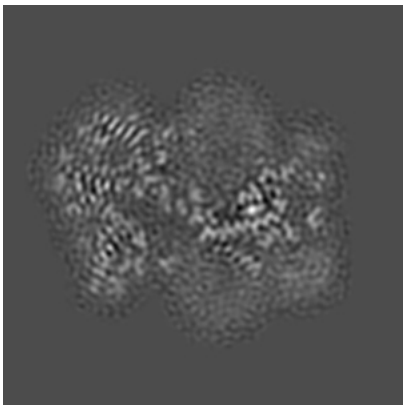
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

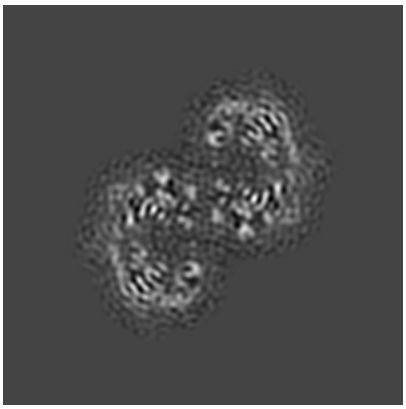
6.3.1 Primary map



X Index: 105



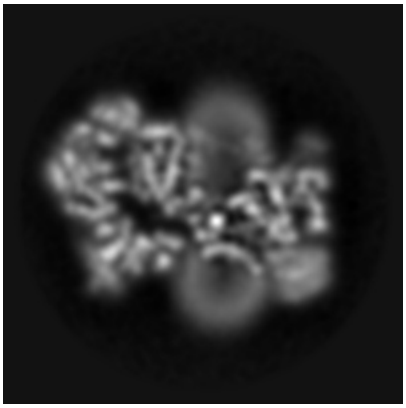
Y Index: 109



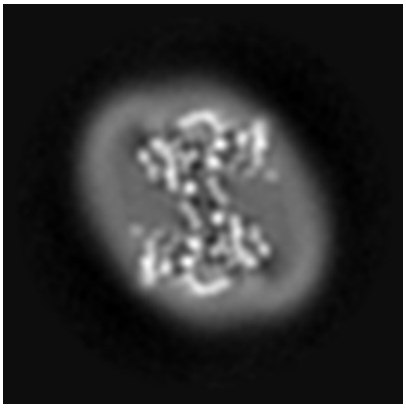
Z Index: 58

6.3.2 Raw map

X Index: 93



Y Index: 112

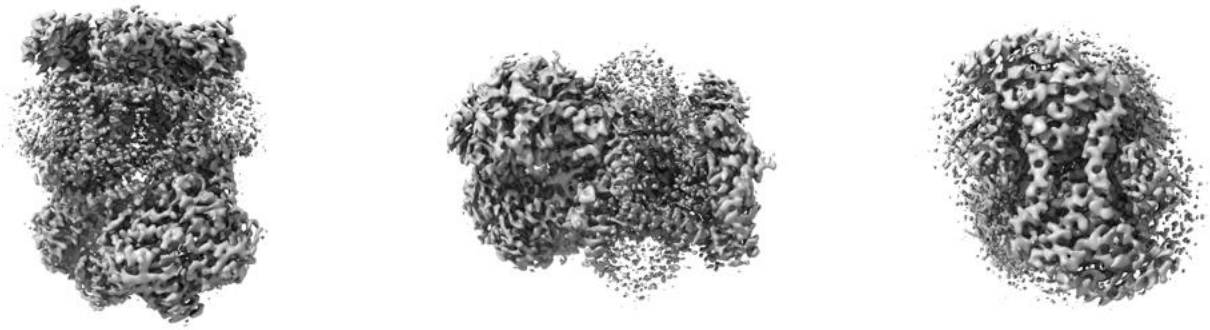


Z Index: 99

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

6.4 Orthogonal surface views (i)

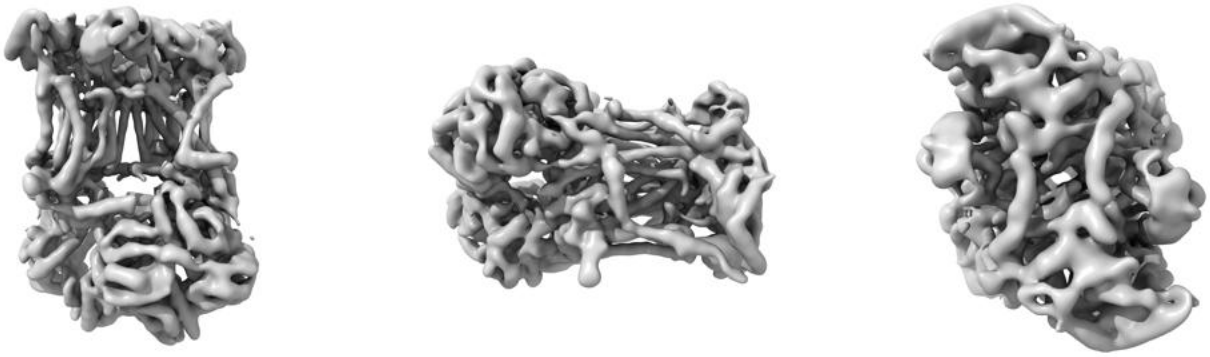
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.114. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

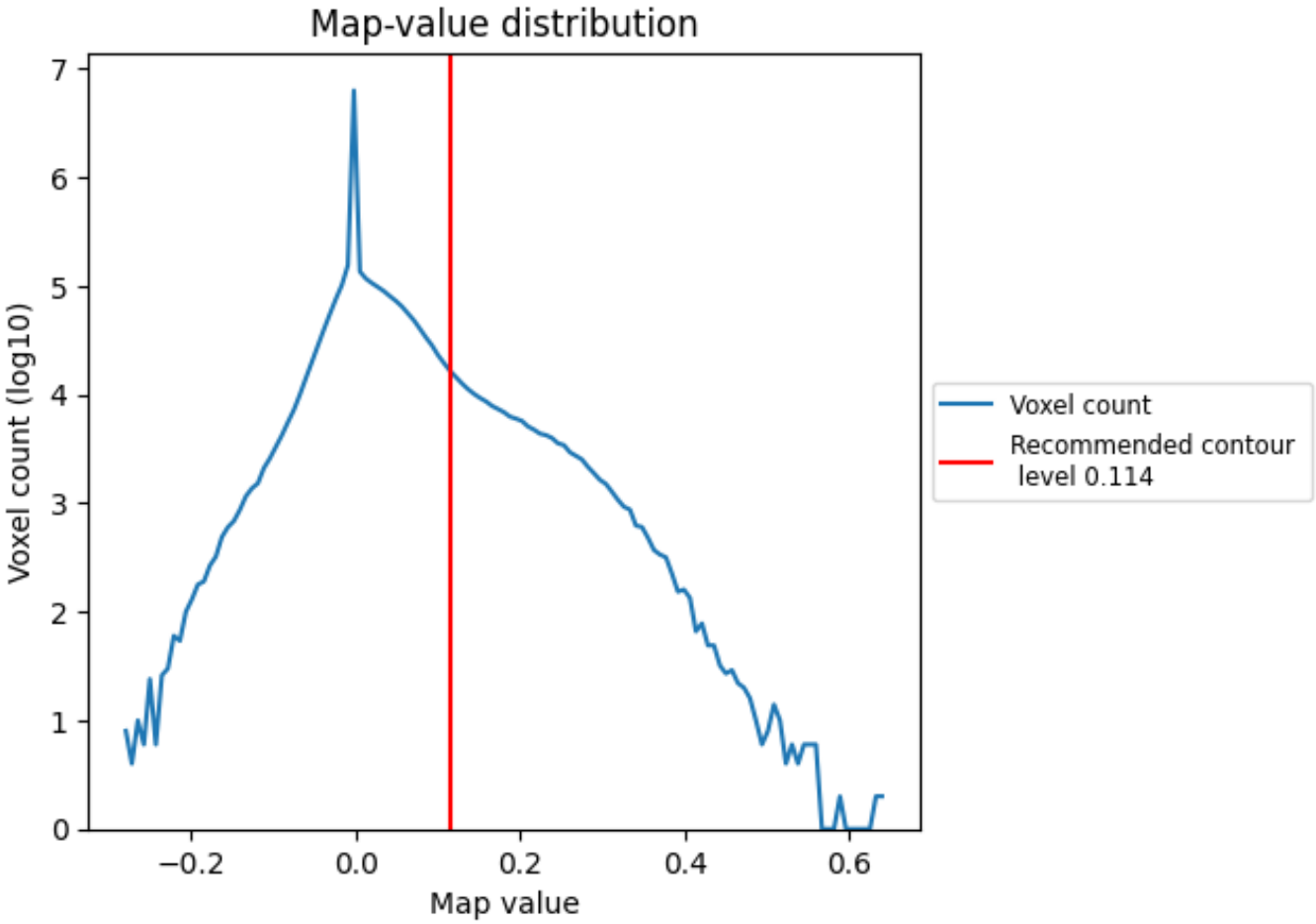
6.5 Mask visualisation (i)

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

7 Map analysis

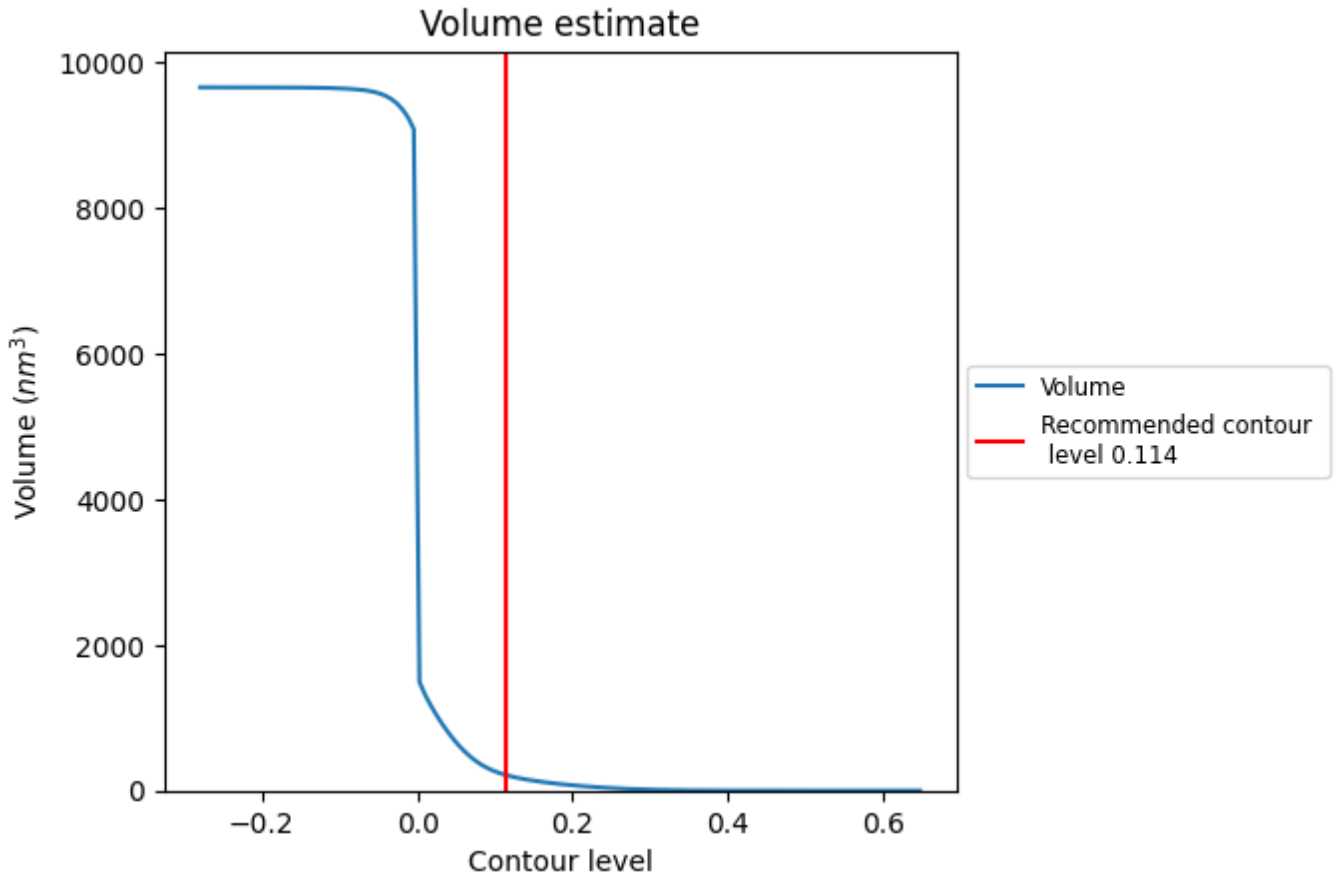
This section contains the results of statistical analysis of the map.

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.

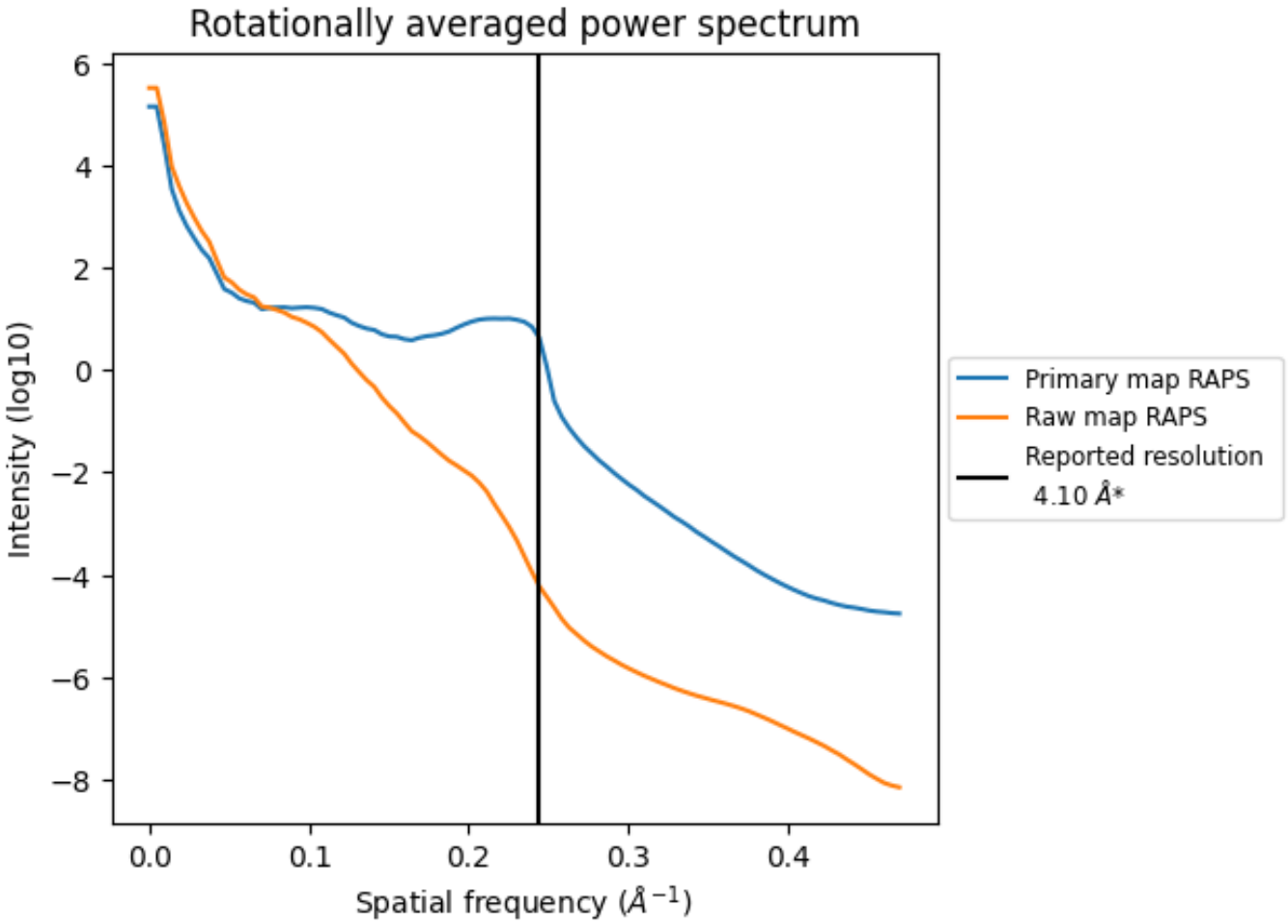
7.2 Volume estimate



The volume at the recommended contour level is 214 nm^3; this corresponds to an approximate mass of 194 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)

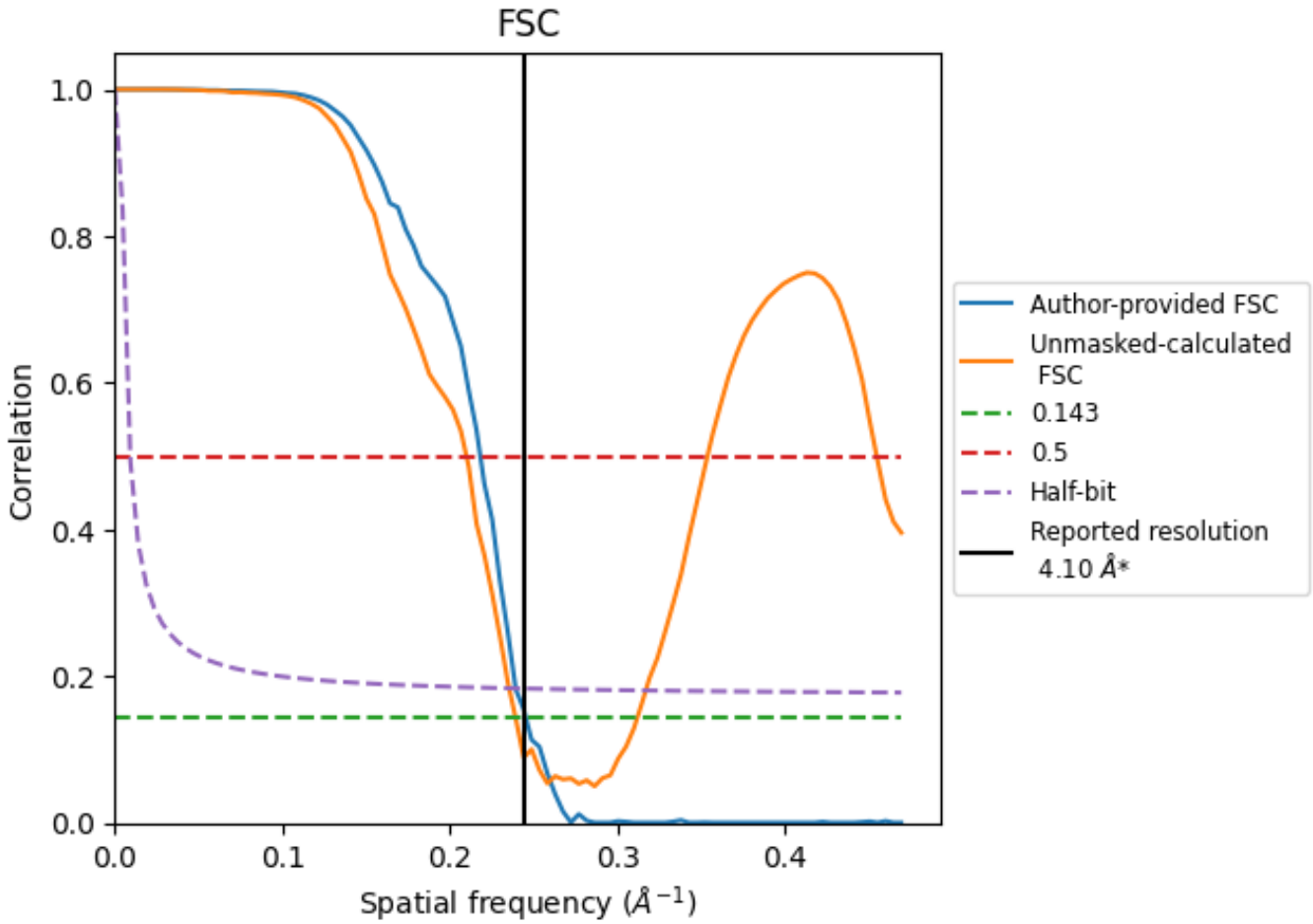


*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

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 0.244 $Å^{-1}$

8.2 Resolution estimates (i)

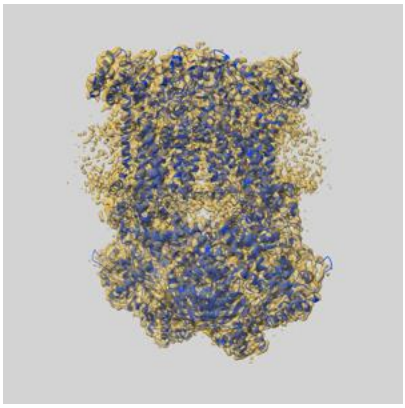
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.07	4.58	4.18
Unmasked-calculated*	4.18	4.76	4.25

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

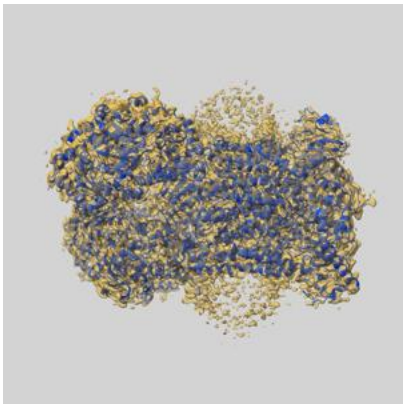
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4286 and PDB model 6FO0. Per-residue inclusion information can be found in section 3 on page 8.

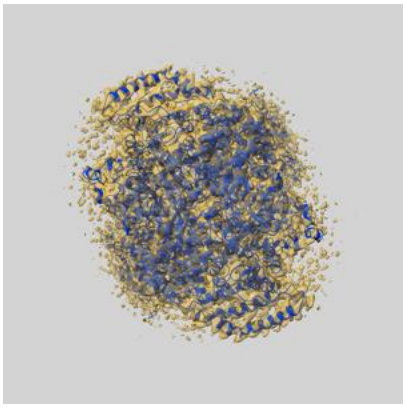
9.1 Map-model overlay



X



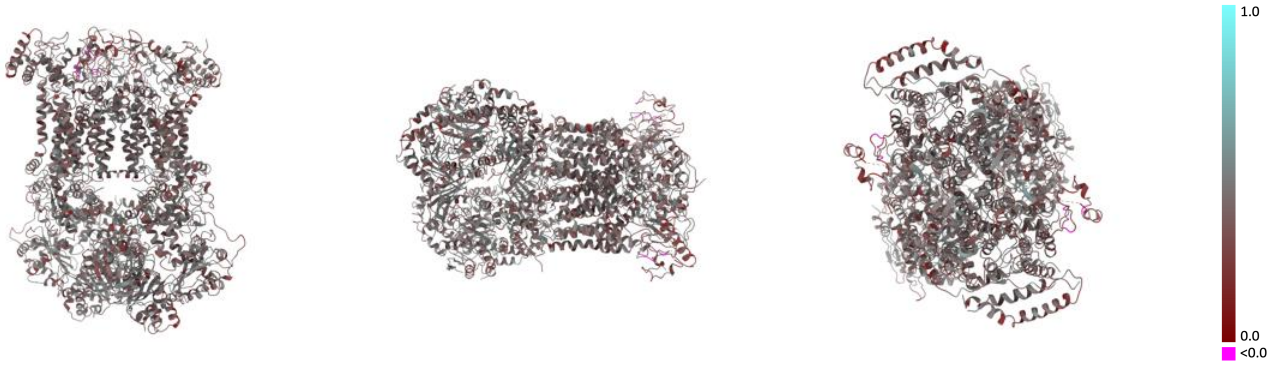
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.114 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

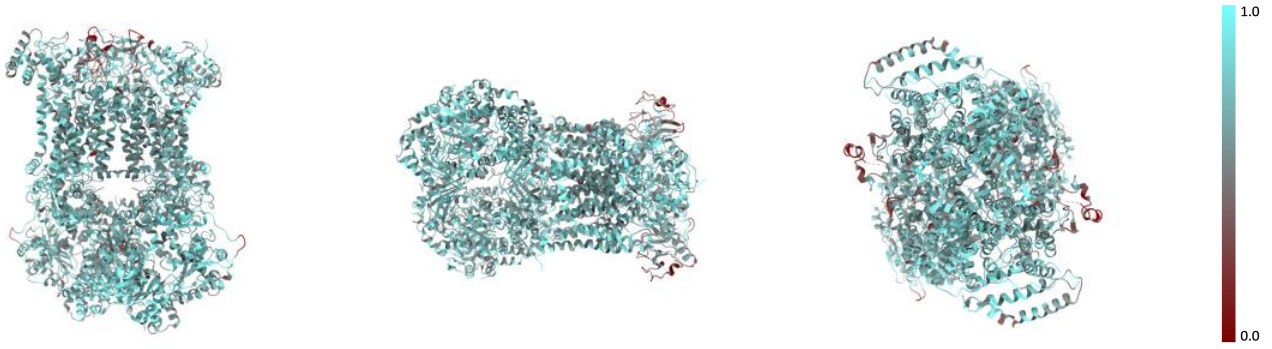
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

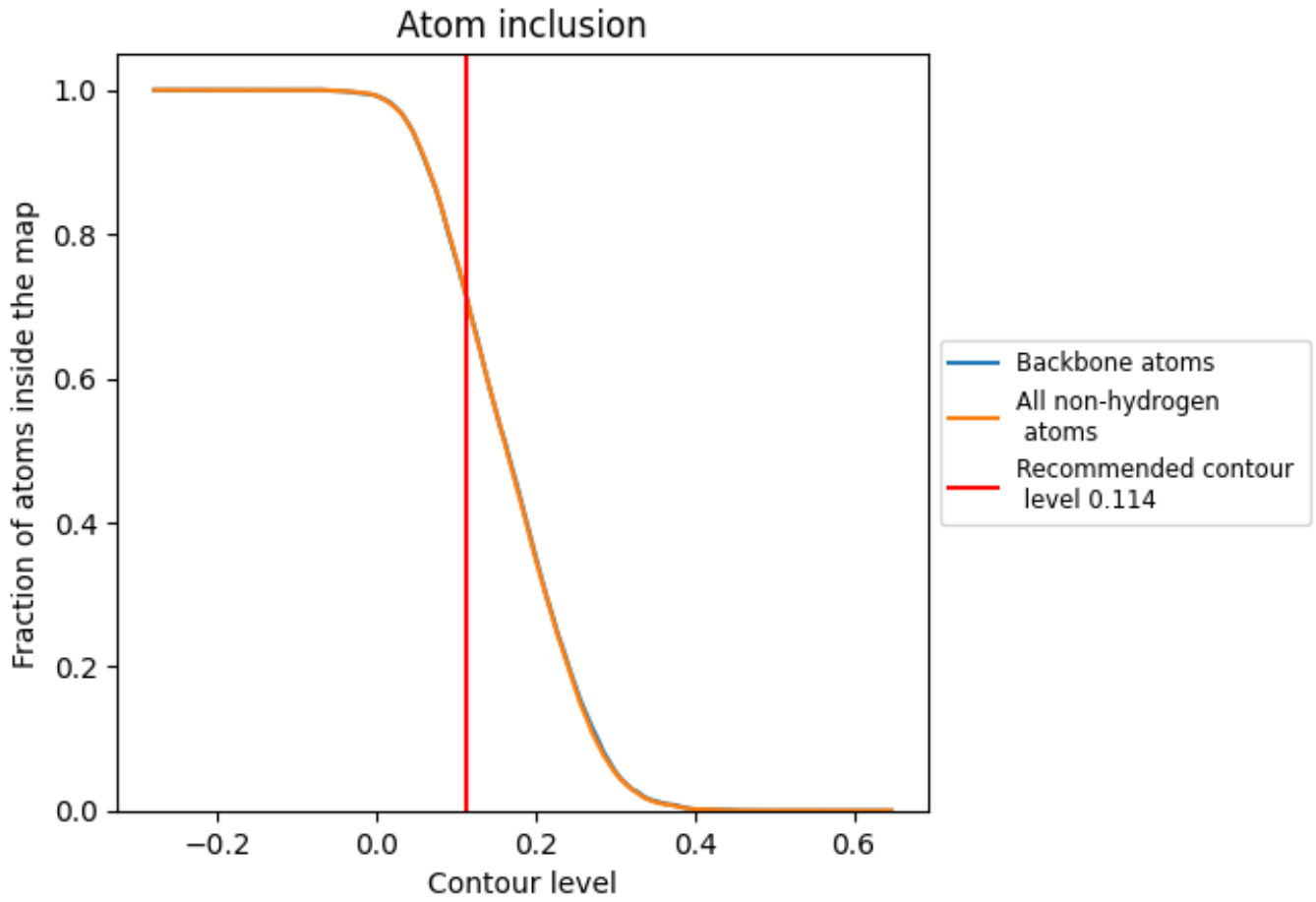
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.114).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.114) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7086	0.4070
A	0.7400	0.4170
B	0.7414	0.4210
C	0.7071	0.4110
D	0.7518	0.4170
E	0.5624	0.3480
F	0.7198	0.4130
G	0.7687	0.4120
H	0.6692	0.3570
I	0.5902	0.3800
J	0.6963	0.3980
N	0.7406	0.4160
O	0.7447	0.4200
P	0.7078	0.4110
Q	0.7550	0.4190
R	0.5639	0.3490
S	0.7246	0.4170
T	0.7754	0.4180
U	0.6576	0.3380
V	0.6230	0.3860
W	0.6638	0.3670