Full wwPDB EM Validation Report ⓘ

May 4, 2025 – 10:44 PM EDT

PDB ID	:	6CFW / pdb_00006cfw
EMDB ID	:	EMD-7468
Title	:	cryoEM structure of a respiratory membrane-bound hydrogenase
Authors	:	Li, H.L.; Yu, H.J.
Deposited on	:	2018-02-17
Resolution	:	3.70 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:

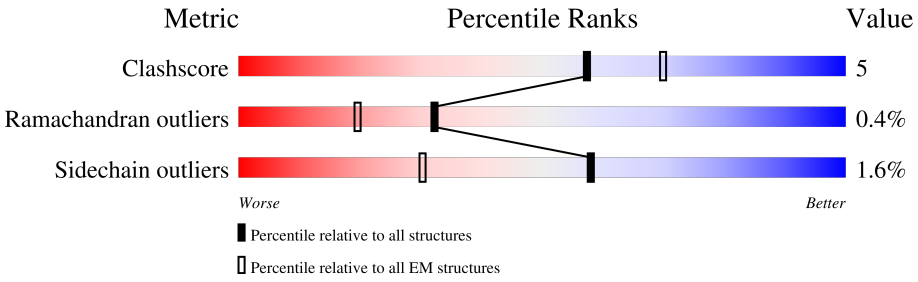
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 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	H	510	90% 9%
2	G	117	84% 13%
3	D	96	72% 9% 19%
4	I	115	37% 88% 10%
5	M	321	88% 10%
6	F	148	91% 7%
7	A	167	5% 84% 14%
8	E	99	85% 9% 6%

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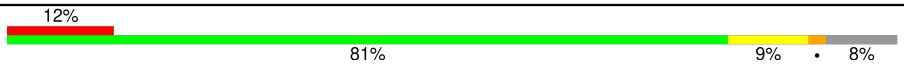
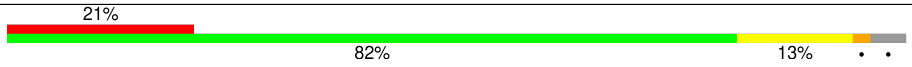
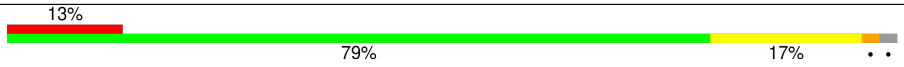
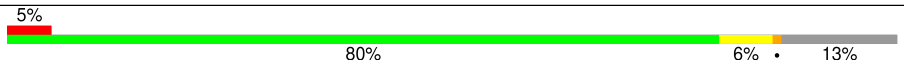
Mol	Chain	Length	Quality of chain
9	C	124	
10	B	84	
11	J	167	
12	K	173	
13	L	380	
14	N	139	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	NFU	L	401	-	-	X	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 19589 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Monovalent cation/H+ antiporter subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	H	505	3850	2580	599	648	23	0	0

- Molecule 2 is a protein called Monovalent cation/H+ antiporter subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	113	866	572	141	149	4	0	0

- Molecule 3 is a protein called MBH subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	78	579	383	89	102	5	0	0

- Molecule 4 is a protein called MBH subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	I	114	811	539	132	137	3	0	0

- Molecule 5 is a protein called Mbh13 NADH dehydrogenase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	M	317	2468	1666	384	409	9	0	0

- Molecule 6 is a protein called Monovalent cation/H+ antiporter subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	145	1073	715	178	177	3	0	0

- Molecule 7 is a protein called Monovalent cation/H+ antiporter subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	165	Total	C	N	O	S	0	0
			1314	871	212	228	3		

- Molecule 8 is a protein called MBH subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	93	Total	C	N	O	S	0	0
			732	484	114	133	1		

- Molecule 9 is a protein called Monovalent cation/H+ antiporter subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	114	Total	C	N	O	S	0	0
			870	575	147	144	4		

- Molecule 10 is a protein called Monovalent cation/H+ antiporter subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	82	Total	C	N	O	S	0	0
			622	422	94	105	1		

- Molecule 11 is a protein called Probable membrane-bound hydrogenase subunit mbhJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	143	Total	C	N	O	S	0	0
			1091	705	188	192	6		

- Molecule 12 is a protein called Membrane-bound hydrogenase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	166	Total	C	N	O	S	0	0
			1362	876	228	253	5		

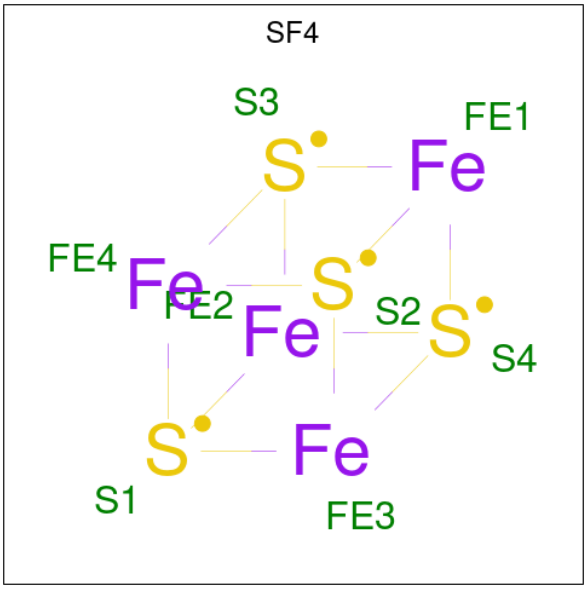
- Molecule 13 is a protein called Membrane-bound hydrogenase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	374	Total	C	N	O	S	0	0
			2965	1885	526	539	15		

- Molecule 14 is a protein called NADH-plastoquinone oxidoreductase subunit.

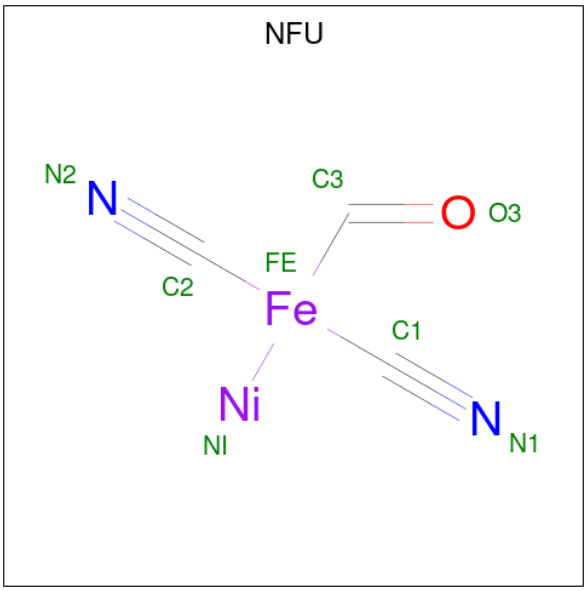
Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	121	Total	C	N	O	S	0	0
			954	622	153	168	11		

- Molecule 15 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms				AltConf
15	J	1	Total	Fe	S		0
			8	4	4		
15	N	1	Total	Fe	S		0
			8	4	4		
15	N	1	Total	Fe	S		0
			8	4	4		

- Molecule 16 is formyl[bis(hydrocyanato-1kappaC)]ironnickel(Fe-Ni) (CCD ID: NFU) (formula: C_3HFeN_2NiO).



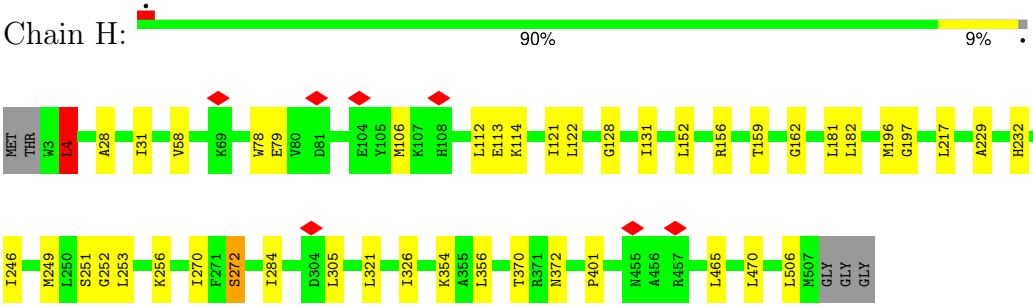
Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	N	Ni	O	
16	L	1	8	3	1	2	1	1	0

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.

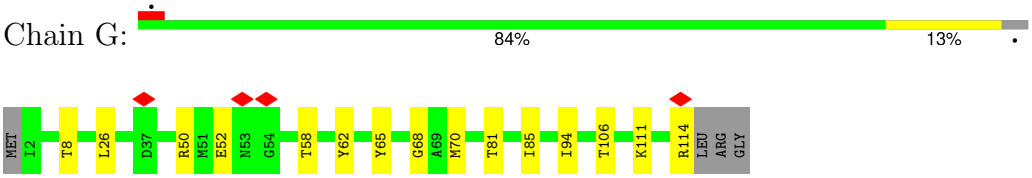
• Molecule 1: Monovalent cation/H+ antiporter subunit D

Chain H:



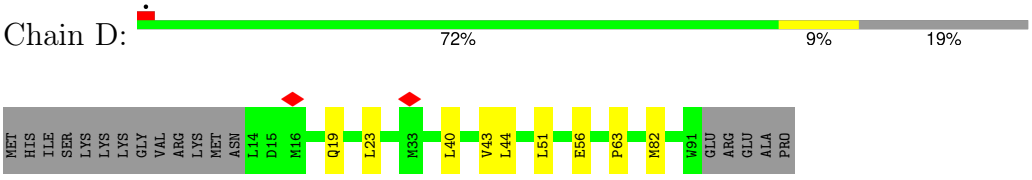
• Molecule 2: Monovalent cation/H+ antiporter subunit C

Chain G:



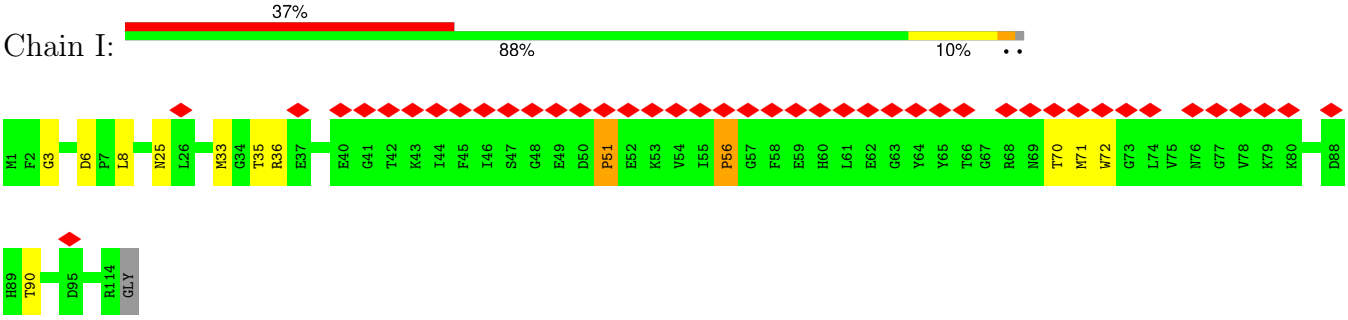
• Molecule 3: MBH subunit

Chain D:



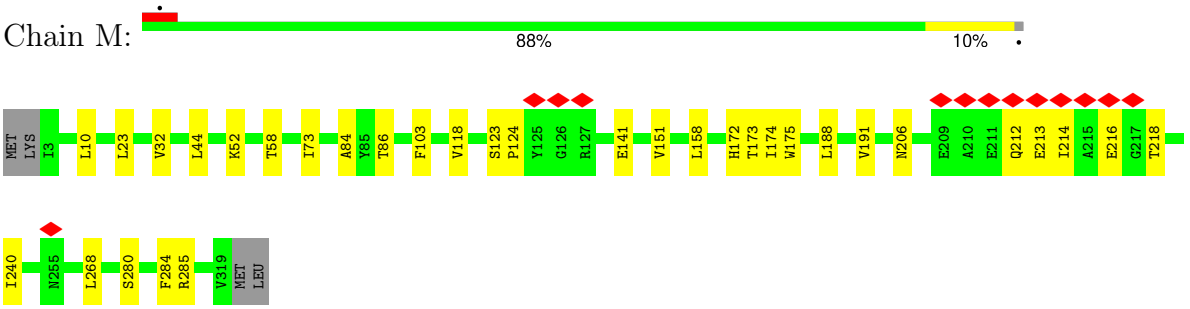
• Molecule 4: MBH subunit

Chain I:



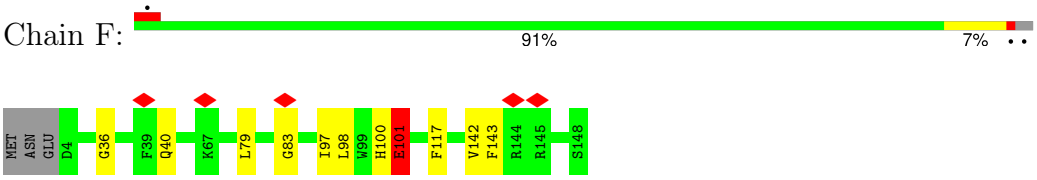
• Molecule 5: Mbh13 NADH dehydrogenase subunit

Chain M:



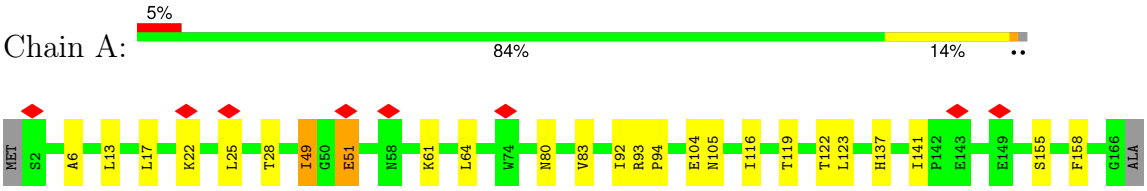
• Molecule 6: Monovalent cation/H+ antiporter subunit B

Chain F:



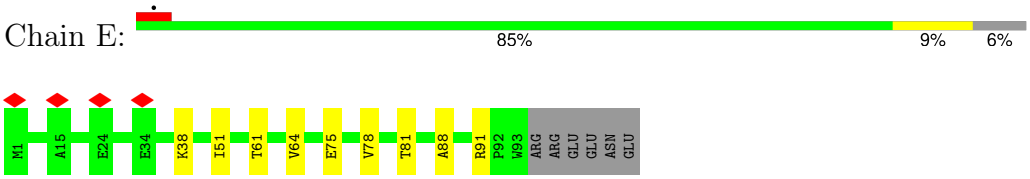
• Molecule 7: Monovalent cation/H+ antiporter subunit E

Chain A:



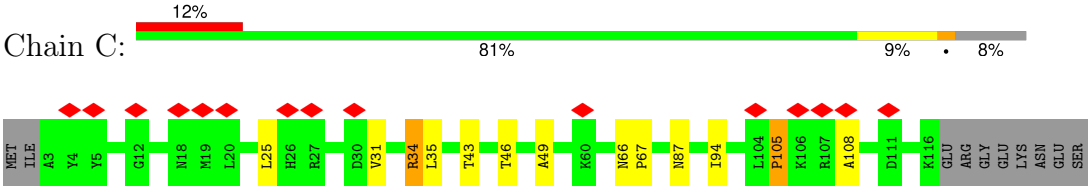
• Molecule 8: MBH subunit

Chain E:



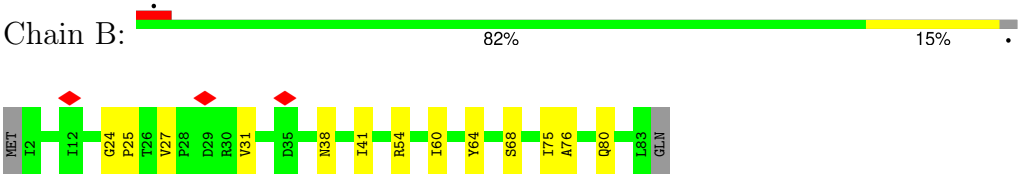
• Molecule 9: Monovalent cation/H+ antiporter subunit G

Chain C:



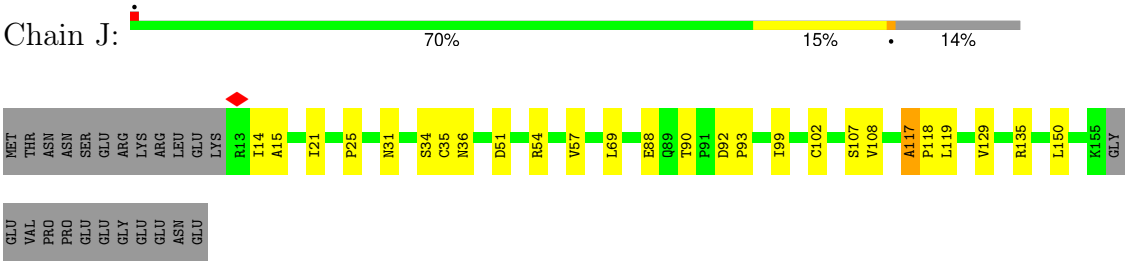
• Molecule 10: Monovalent cation/H+ antiporter subunit F

Chain B:



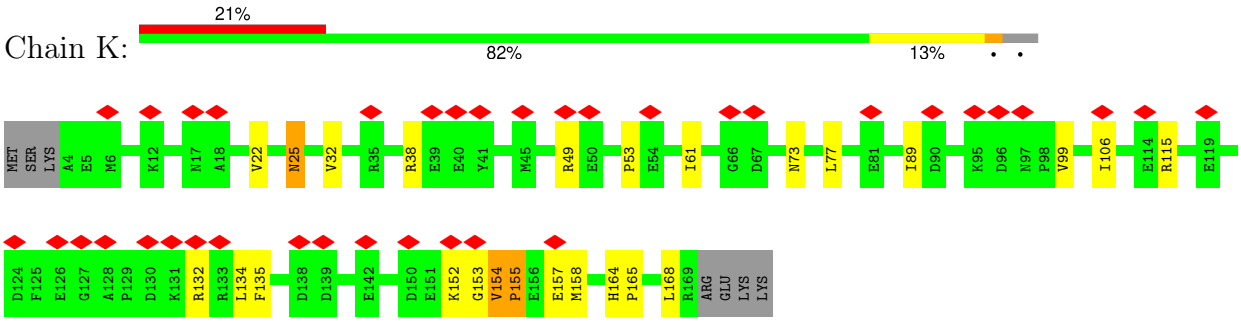
• Molecule 11: Probable membrane-bound hydrogenase subunit mbhJ

Chain J:



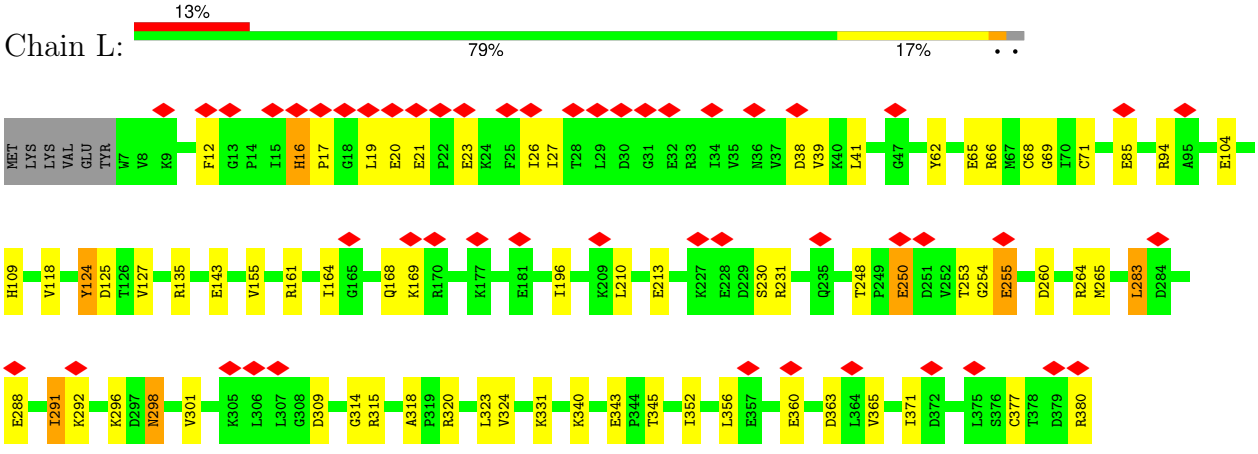
• Molecule 12: Membrane-bound hydrogenase subunit beta

Chain K:



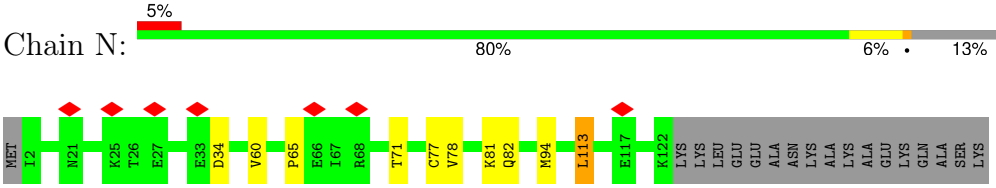
• Molecule 13: Membrane-bound hydrogenase subunit alpha

Chain L:



• Molecule 14: NADH-plastoquinone oxidoreductase subunit

Chain N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	131679	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.414	Depositor
Minimum map value	-0.113	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.048	Depositor
Map size (Å)	304.64, 304.64, 304.64	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.088, 1.088, 1.088	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, NFU

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	H	0.43	0/3945	0.68	2/5371 (0.0%)
2	G	0.44	0/881	0.67	0/1202
3	D	0.44	0/586	0.59	0/798
4	I	0.38	0/828	0.76	2/1127 (0.2%)
5	M	0.42	0/2529	0.72	1/3445 (0.0%)
6	F	0.42	0/1100	0.77	3/1489 (0.2%)
7	A	0.36	0/1354	0.72	0/1852
8	E	0.38	0/750	0.54	0/1020
9	C	0.35	0/891	0.66	0/1212
10	B	0.40	0/632	0.62	0/865
11	J	0.50	0/1118	0.79	0/1525
12	K	0.34	0/1399	0.74	2/1895 (0.1%)
13	L	0.39	0/3025	0.66	1/4094 (0.0%)
14	N	0.43	0/977	0.72	3/1330 (0.2%)
All	All	0.41	0/20015	0.70	14/27225 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	2
5	M	0	1
6	F	0	3
7	A	0	1
9	C	0	1
11	J	0	5
12	K	0	4
All	All	0	17

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	56	PRO	N-CA-CB	6.96	110.56	103.25
6	F	100	HIS	N-CA-C	-6.02	101.22	109.71
4	I	51	PRO	N-CA-CB	5.95	109.49	103.25
1	H	4	LEU	CA-CB-CG	5.56	135.77	116.30
13	L	298	ASN	N-CA-C	-5.55	106.43	113.43
5	M	206	ASN	N-CA-C	-5.51	103.71	110.65
14	N	60	VAL	N-CA-C	-5.28	107.68	113.43
12	K	134	LEU	CA-C-N	5.25	129.87	122.46
12	K	134	LEU	C-N-CA	5.25	129.87	122.46
14	N	65	PRO	CA-C-N	5.12	131.31	121.54
14	N	65	PRO	C-N-CA	5.12	131.31	121.54
1	H	401	PRO	N-CA-C	5.07	116.88	110.70
6	F	101	GLU	CA-C-N	-5.05	113.94	121.87
6	F	101	GLU	C-N-CA	-5.05	113.94	121.87

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	A	119	THR	Peptide
9	C	105	PRO	Peptide
6	F	142	VAL	Peptide
6	F	143	PHE	Peptide
6	F	97	ILE	Peptide
1	H	272	SER	Peptide
1	H	4	LEU	Peptide
11	J	102	CYS	Peptide
11	J	117	ALA	Peptide
11	J	14	ILE	Peptide
11	J	150	LEU	Mainchain
11	J	92	ASP	Peptide
12	K	153	GLY	Peptide
12	K	154	VAL	Peptide
12	K	25	ASN	Peptide
12	K	53	PRO	Peptide
5	M	141	GLU	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	H	3850	0	4047	27	0
2	G	866	0	935	11	0
3	D	579	0	625	9	0
4	I	811	0	761	9	0
5	M	2468	0	2629	27	0
6	F	1073	0	1113	4	0
7	A	1314	0	1329	13	0
8	E	732	0	730	6	0
9	C	870	0	913	7	0
10	B	622	0	679	10	0
11	J	1091	0	1127	12	0
12	K	1362	0	1331	12	0
13	L	2965	0	3003	65	0
14	N	954	0	992	6	0
15	J	8	0	0	0	0
15	N	16	0	0	0	0
16	L	8	0	0	3	0
All	All	19589	0	20214	181	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 (181) 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:H:122:LEU:HD23	1:H:249:MET:CE	1.37	1.53
1:H:122:LEU:CD2	1:H:249:MET:HE3	1.50	1.42
5:M:214:ILE:HG12	13:L:365:VAL:HG21	1.18	1.10
13:L:320:ARG:HD3	16:L:401:NFU:N1	1.66	1.08
13:L:19:LEU:HD21	13:L:21:GLU:O	1.55	1.05
13:L:19:LEU:CD2	13:L:21:GLU:O	2.11	0.99
5:M:214:ILE:CG1	13:L:365:VAL:HG21	1.97	0.93
1:H:122:LEU:CD2	1:H:249:MET:CE	2.28	0.89
13:L:16:HIS:CG	13:L:17:PRO:HD2	2.09	0.86
13:L:345:THR:HG22	13:L:345:THR:O	1.73	0.86

Continued on next page...

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:214:ILE:HG12	13:L:365:VAL:CG2	2.06	0.85
13:L:255:GLU:N	13:L:255:GLU:OE1	2.10	0.84
13:L:250:GLU:O	13:L:254:GLY:O	1.97	0.81
13:L:19:LEU:HG	13:L:21:GLU:H	1.51	0.76
5:M:214:ILE:HD11	13:L:12:PHE:CZ	2.22	0.75
5:M:214:ILE:HD12	13:L:16:HIS:CE1	2.22	0.75
11:J:36:ASN:HD21	13:L:21:GLU:HG3	1.51	0.75
7:A:49:ILE:O	7:A:49:ILE:HG12	1.88	0.73
1:H:122:LEU:HD23	1:H:249:MET:HE3	0.74	0.72
6:F:101:GLU:OE2	6:F:101:GLU:HA	1.89	0.71
5:M:214:ILE:HD12	13:L:16:HIS:ND1	2.08	0.68
4:I:70:THR:C	4:I:72:TRP:H	2.00	0.68
7:A:51:GLU:HA	7:A:51:GLU:OE1	1.92	0.67
1:H:121:ILE:HG21	8:E:81:THR:HG21	1.79	0.64
5:M:214:ILE:HD11	13:L:12:PHE:HZ	1.60	0.64
7:A:93:ARG:NH2	7:A:141:ILE:O	2.30	0.64
13:L:345:THR:O	13:L:345:THR:CG2	2.45	0.64
9:C:25:LEU:O	9:C:34:ARG:NH1	2.31	0.63
13:L:68:CYS:SG	13:L:69:GLY:N	2.72	0.63
13:L:164:ILE:O	13:L:168:GLN:NE2	2.32	0.63
5:M:214:ILE:HB	13:L:16:HIS:CE1	2.34	0.63
13:L:19:LEU:HD21	13:L:23:GLU:OE1	1.99	0.62
12:K:73:ASN:HD22	12:K:89:ILE:HD11	1.64	0.61
6:F:98:LEU:HD23	6:F:117:PHE:HB3	1.82	0.61
13:L:291:ILE:HD12	13:L:292:LYS:HB2	1.82	0.61
3:D:82:MET:HE3	10:B:75:ILE:HG12	1.80	0.61
5:M:212:GLN:HB3	5:M:216:GLU:HB2	1.80	0.61
13:L:360:GLU:HB2	13:L:363:ASP:HB2	1.83	0.61
4:I:70:THR:O	4:I:72:TRP:N	2.34	0.60
1:H:252:GLY:O	1:H:256:LYS:NZ	2.35	0.59
11:J:69:LEU:HD11	11:J:90:THR:HG21	1.83	0.59
5:M:214:ILE:HB	13:L:16:HIS:HE1	1.66	0.59
11:J:51:ASP:O	11:J:54:ARG:NH2	2.35	0.59
13:L:210:LEU:HA	13:L:213:GLU:HG2	1.84	0.58
14:N:71:THR:HG22	14:N:113:LEU:HB3	1.86	0.58
13:L:260:ASP:O	13:L:264:ARG:NH1	2.37	0.58
7:A:123:LEU:HB3	7:A:137:HIS:HB3	1.86	0.57
3:D:40:LEU:HD23	10:B:27:VAL:HG11	1.86	0.57
5:M:214:ILE:CG1	13:L:365:VAL:CG2	2.77	0.56
4:I:36:ARG:NH1	11:J:88:GLU:O	2.39	0.56
6:F:36:GLY:O	6:F:40:GLN:NE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:70:THR:C	4:I:72:TRP:N	2.63	0.56
12:K:49:ARG:NH1	12:K:106:ILE:O	2.40	0.55
1:H:122:LEU:HD23	1:H:249:MET:HE1	1.71	0.55
11:J:135:ARG:NH1	13:L:143:GLU:OE2	2.34	0.55
12:K:22:VAL:HG22	12:K:32:VAL:HG12	1.87	0.55
13:L:352:ILE:CD1	13:L:371:ILE:HG12	2.37	0.54
10:B:76:ALA:O	10:B:80:GLN:HB2	2.06	0.54
13:L:298:ASN:O	13:L:301:VAL:HG22	2.07	0.54
12:K:135:PHE:HB3	13:L:41:LEU:HD12	1.89	0.54
13:L:296:LYS:O	13:L:298:ASN:N	2.39	0.54
6:F:79:LEU:O	6:F:83:GLY:N	2.41	0.54
13:L:19:LEU:HD23	13:L:21:GLU:O	2.04	0.54
13:L:16:HIS:ND1	13:L:17:PRO:HD2	2.23	0.53
1:H:197:GLY:HA3	1:H:506:LEU:HD13	1.90	0.53
5:M:280:SER:O	5:M:284:PHE:HB3	2.07	0.53
11:J:31:ASN:ND2	13:L:20:GLU:O	2.41	0.53
3:D:51:LEU:HD11	10:B:41:ILE:HG21	1.91	0.53
7:A:92:ILE:HG22	7:A:94:PRO:HD3	1.89	0.53
9:C:35:LEU:HD11	9:C:94:ILE:HG23	1.91	0.53
9:C:105:PRO:HG2	9:C:108:ALA:HB2	1.91	0.52
13:L:343:GLU:OE1	13:L:380:ARG:NH1	2.43	0.52
1:H:239:HIS:CE1	1:H:251:SER:HB2	2.44	0.52
3:D:44:LEU:HD21	10:B:31:VAL:HG22	1.92	0.51
7:A:155:SER:HB2	7:A:158:PHE:HD2	1.74	0.51
3:D:63:PRO:HB3	10:B:60:ILE:HD11	1.91	0.51
1:H:356:LEU:HD12	1:H:470:LEU:HB3	1.93	0.51
13:L:161:ARG:HH12	14:N:81:LYS:HB3	1.76	0.50
13:L:320:ARG:CD	16:L:401:NFU:N1	2.58	0.50
11:J:25:PRO:HG2	11:J:57:VAL:HG12	1.92	0.50
13:L:230:SER:OG	13:L:315:ARG:NH1	2.45	0.50
7:A:116:ILE:O	7:A:122:THR:OG1	2.30	0.50
12:K:115:ARG:NE	12:K:132:ARG:O	2.37	0.50
14:N:81:LYS:HE2	14:N:94:MET:HG3	1.93	0.50
9:C:31:VAL:O	9:C:34:ARG:HB2	2.12	0.49
13:L:314:GLY:O	13:L:324:VAL:HA	2.13	0.49
13:L:248:THR:HG22	13:L:250:GLU:H	1.77	0.49
4:I:3:GLY:HA3	4:I:6:ASP:HB2	1.95	0.49
7:A:61:LYS:O	7:A:64:LEU:HB3	2.12	0.49
1:H:196:MET:HG2	1:H:270:ILE:HD11	1.95	0.48
9:C:43:THR:OG1	9:C:87:ASN:ND2	2.45	0.48
13:L:318:ALA:HB2	13:L:323:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:50:ARG:NH1	2:G:52:GLU:OE2	2.47	0.48
12:K:164:HIS:CD2	12:K:165:PRO:HD2	2.49	0.48
1:H:113:GLU:OE1	1:H:114:LYS:NZ	2.38	0.48
5:M:52:LYS:HB2	11:J:21:ILE:HG22	1.95	0.48
13:L:65:GLU:OE2	13:L:66:ARG:NH2	2.47	0.48
4:I:35:THR:HG22	5:M:58:THR:HB	1.95	0.48
2:G:85:ILE:HG12	8:E:78:VAL:HG11	1.95	0.48
13:L:352:ILE:CG2	13:L:356:LEU:HD23	2.43	0.47
8:E:88:ALA:O	8:E:91:ARG:NH1	2.46	0.47
13:L:26:ILE:HD11	13:L:38:ASP:HB2	1.96	0.47
13:L:309:ASP:HB2	13:L:331:LYS:HG3	1.96	0.47
2:G:114:ARG:NH1	4:I:90:THR:O	2.47	0.47
12:K:155:PRO:HB2	12:K:157:GLU:H	1.79	0.47
13:L:250:GLU:OE1	13:L:255:GLU:CB	2.63	0.47
13:L:124:TYR:HB3	13:L:127:VAL:HG12	1.97	0.47
1:H:272:SER:O	1:H:272:SER:OG	2.24	0.47
5:M:173:THR:HG23	5:M:175:TRP:H	1.80	0.47
4:I:25:ASN:ND2	5:M:73:ILE:HD11	2.30	0.46
5:M:188:LEU:HA	5:M:191:VAL:HG22	1.97	0.46
12:K:155:PRO:HG2	12:K:158:MET:H	1.79	0.46
11:J:99:ILE:HA	11:J:129:VAL:HG23	1.97	0.46
2:G:58:THR:OG1	10:B:54:ARG:NH2	2.47	0.46
7:A:80:ASN:O	7:A:83:VAL:HB	2.15	0.46
5:M:151:VAL:HG23	5:M:174:ILE:HD11	1.98	0.46
13:L:253:THR:O	13:L:253:THR:OG1	2.30	0.46
13:L:255:GLU:N	13:L:255:GLU:CD	2.73	0.45
3:D:43:VAL:HG11	3:D:82:MET:HE2	1.97	0.45
11:J:34:SER:OG	11:J:35:CYS:N	2.50	0.45
5:M:86:THR:HG22	5:M:103:PHE:HE1	1.81	0.45
13:L:118:VAL:HG11	13:L:265:MET:HE3	1.98	0.45
14:N:77:CYS:SG	14:N:78:VAL:N	2.90	0.45
5:M:123:SER:HA	5:M:124:PRO:HD3	1.77	0.45
13:L:260:ASP:OD1	13:L:260:ASP:N	2.49	0.45
1:H:229:ALA:O	1:H:232:HIS:ND1	2.48	0.45
11:J:36:ASN:HD21	13:L:21:GLU:CG	2.23	0.45
14:N:34:ASP:OD1	14:N:34:ASP:N	2.49	0.45
7:A:13:LEU:O	7:A:17:LEU:HB2	2.17	0.44
13:L:62:TYR:HE2	14:N:82:GLN:HG3	1.83	0.44
1:H:28:ALA:HA	1:H:31:ILE:HG22	1.99	0.44
1:H:106:MET:SD	1:H:156:ARG:NH1	2.90	0.44
3:D:51:LEU:HD13	10:B:64:TYR:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:66:ASN:HA	9:C:67:PRO:HD3	1.87	0.44
1:H:122:LEU:HD23	1:H:249:MET:HE2	1.71	0.44
1:H:159:THR:HG23	1:H:162:GLY:H	1.83	0.44
5:M:32:VAL:HG21	5:M:285:ARG:HH21	1.83	0.44
5:M:86:THR:HG21	5:M:240:ILE:HD12	2.00	0.44
12:K:25:ASN:ND2	13:L:85:GLU:OE2	2.47	0.44
1:H:152:LEU:HD13	1:H:246:ILE:HD12	1.99	0.44
11:J:107:SER:OG	11:J:108:VAL:N	2.50	0.43
2:G:81:THR:HG23	8:E:75:GLU:HB2	2.00	0.43
5:M:10:LEU:HD13	5:M:84:ALA:HB2	1.99	0.43
1:H:182:LEU:HD22	1:H:217:LEU:HD11	1.99	0.43
1:H:370:THR:HG22	1:H:372:ASN:H	1.83	0.43
7:A:22:LYS:HE3	7:A:28:THR:HG23	2.00	0.43
7:A:6:ALA:HB2	7:A:49:ILE:HG21	2.00	0.43
13:L:94:ARG:HH11	13:L:288:GLU:HA	1.84	0.43
2:G:62:TYR:HD2	8:E:51:ILE:HD11	1.84	0.43
10:B:38:ASN:ND2	10:B:68:SER:OG	2.51	0.43
8:E:61:THR:HA	8:E:64:VAL:HG12	1.99	0.42
1:H:284:ILE:HG23	1:H:321:LEU:HD12	2.01	0.42
3:D:19:GLN:NE2	3:D:56:GLU:OE2	2.50	0.42
10:B:24:GLY:HA2	10:B:25:PRO:HD3	1.90	0.42
4:I:33:MET:N	4:I:33:MET:SD	2.92	0.42
1:H:58:VAL:HG12	1:H:79:GLU:HG2	2.00	0.42
5:M:213:GLU:O	5:M:214:ILE:HG13	2.20	0.42
13:L:169:LYS:HG3	13:L:283:LEU:HD11	2.02	0.42
13:L:320:ARG:HB2	16:L:401:NFU:N1	2.34	0.42
2:G:106:THR:HG21	2:G:111:LYS:HE3	2.01	0.42
5:M:214:ILE:HG21	13:L:17:PRO:O	2.20	0.42
13:L:109:HIS:HD2	13:L:135:ARG:HH21	1.68	0.42
13:L:125:ASP:N	13:L:125:ASP:OD1	2.52	0.42
1:H:58:VAL:HA	1:H:78:TRP:O	2.20	0.41
2:G:50:ARG:NH2	2:G:70:MET:O	2.54	0.41
1:H:249:MET:HG3	1:H:253:LEU:HD12	2.03	0.41
1:H:354:LYS:HA	1:H:354:LYS:HD3	1.90	0.41
2:G:65:TYR:OH	2:G:68:GLY:O	2.31	0.41
12:K:168:LEU:HD13	12:K:168:LEU:HA	1.96	0.41
2:G:8:THR:HG21	3:D:23:LEU:HD12	2.02	0.41
5:M:118:VAL:HG21	5:M:218:THR:HG22	2.02	0.41
13:L:19:LEU:HG	13:L:20:GLU:N	2.35	0.41
1:H:128:GLY:HA2	1:H:131:ILE:HG22	2.03	0.41
5:M:158:LEU:HD11	5:M:172:HIS:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:46:THR:O	9:C:49:ALA:HB3	2.21	0.41
13:L:16:HIS:CG	13:L:17:PRO:CD	2.94	0.41
2:G:94:ILE:HD13	2:G:94:ILE:HA	1.95	0.40
7:A:104:GLU:HG3	7:A:105:ASN:HB2	2.02	0.40
12:K:38:ARG:HH22	12:K:99:VAL:HG23	1.85	0.40
12:K:61:ILE:HG12	13:L:340:LYS:HD3	2.03	0.40
13:L:104:GLU:OE1	13:L:231:ARG:NH1	2.54	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	H	503/510 (99%)	469 (93%)	34 (7%)	0	100 100
2	G	111/117 (95%)	102 (92%)	9 (8%)	0	100 100
3	D	76/96 (79%)	74 (97%)	2 (3%)	0	100 100
4	I	112/115 (97%)	90 (80%)	19 (17%)	3 (3%)	4 29
5	M	315/321 (98%)	275 (87%)	40 (13%)	0	100 100
6	F	143/148 (97%)	123 (86%)	20 (14%)	0	100 100
7	A	163/167 (98%)	137 (84%)	26 (16%)	0	100 100
8	E	91/99 (92%)	86 (94%)	5 (6%)	0	100 100
9	C	112/124 (90%)	100 (89%)	12 (11%)	0	100 100
10	B	80/84 (95%)	77 (96%)	3 (4%)	0	100 100
11	J	141/167 (84%)	115 (82%)	22 (16%)	4 (3%)	4 28
12	K	164/173 (95%)	140 (85%)	22 (13%)	2 (1%)	11 41
13	L	372/380 (98%)	338 (91%)	34 (9%)	0	100 100
14	N	119/139 (86%)	100 (84%)	19 (16%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2502/2640 (95%)	2226 (89%)	267 (11%)	9 (0%)	32 62

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	I	51	PRO
4	I	56	PRO
4	I	71	MET
11	J	15	ALA
11	J	117	ALA
11	J	118	PRO
12	K	154	VAL
11	J	93	PRO
12	K	155	PRO

5.3.2 Protein sidechains

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	H	401/403 (100%)	395 (98%)	6 (2%)	60 75
2	G	93/96 (97%)	92 (99%)	1 (1%)	70 80
3	D	62/78 (80%)	62 (100%)	0	100 100
4	I	69/97 (71%)	68 (99%)	1 (1%)	62 76
5	M	264/268 (98%)	261 (99%)	3 (1%)	70 80
6	F	106/109 (97%)	105 (99%)	1 (1%)	75 84
7	A	139/140 (99%)	136 (98%)	3 (2%)	47 65
8	E	74/80 (92%)	73 (99%)	1 (1%)	62 76
9	C	88/97 (91%)	87 (99%)	1 (1%)	70 80
10	B	64/66 (97%)	64 (100%)	0	100 100
11	J	121/143 (85%)	120 (99%)	1 (1%)	79 85
12	K	148/155 (96%)	146 (99%)	2 (1%)	62 76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	L	318/324 (98%)	306 (96%)	12 (4%)	28 53
14	N	110/124 (89%)	109 (99%)	1 (1%)	75 84
All	All	2057/2180 (94%)	2024 (98%)	33 (2%)	58 74

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	4	LEU
1	H	112	LEU
1	H	181	LEU
1	H	305	LEU
1	H	326	ILE
1	H	465	LEU
2	G	26	LEU
4	I	8	LEU
5	M	23	LEU
5	M	44	LEU
5	M	268	LEU
6	F	101	GLU
7	A	25	LEU
7	A	49	ILE
7	A	51	GLU
8	E	38	LYS
9	C	34	ARG
11	J	119	LEU
12	K	77	LEU
12	K	152	LYS
13	L	16	HIS
13	L	27	ILE
13	L	39	VAL
13	L	71	CYS
13	L	124	TYR
13	L	155	VAL
13	L	196	ILE
13	L	250	GLU
13	L	255	GLU
13	L	283	LEU
13	L	291	ILE
13	L	377	CYS
14	N	113	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	190	GLN
1	H	302	GLN
1	H	349	ASN
5	M	206	ASN
5	M	265	ASN
7	A	137	HIS
8	E	49	HIS
9	C	87	ASN
11	J	16	GLN
12	K	73	ASN
12	K	164	HIS
13	L	49	GLN
13	L	109	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\|>2$
15	SF4	N	202	-	0,12,12	-	-	-		
15	SF4	N	201	-	0,12,12	-	-	-		
16	NFU	L	401	13	2,7,7	1.31	0	-		
15	SF4	J	201	-	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	SF4	N	202	-	-	-	0/6/5/5
15	SF4	N	201	-	-	-	0/6/5/5
15	SF4	J	201	-	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	L	401	NFU	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

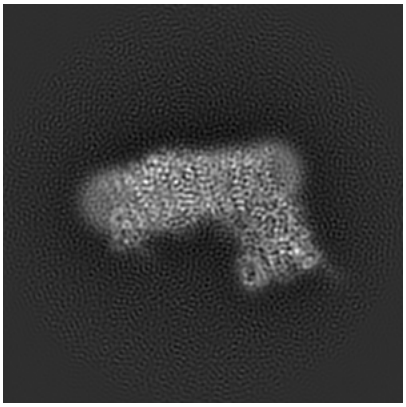
This section contains visualisations of the EMDB entry EMD-7468. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

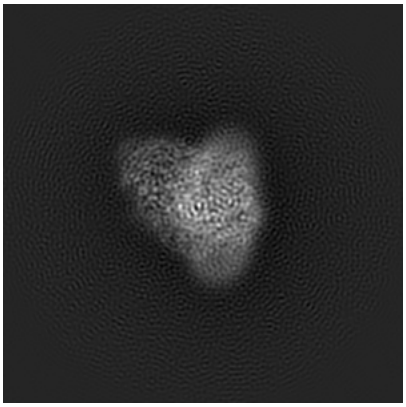
6.1 Orthogonal projections

6.1.1 Primary map

X



Y

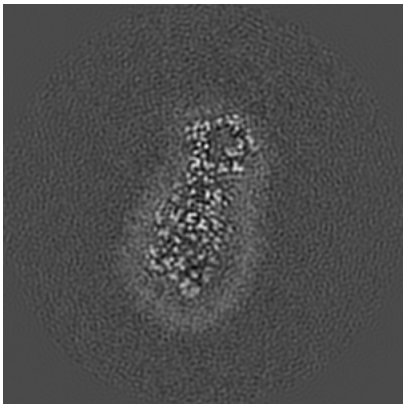


Z

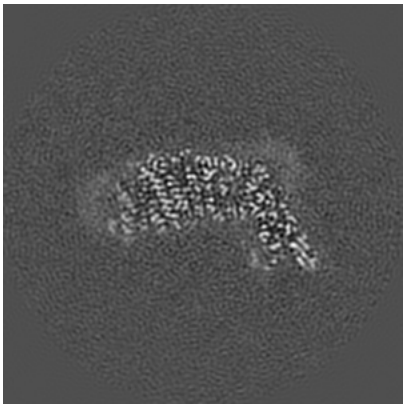
The images above show the map projected in three orthogonal directions.

6.2 Central slices

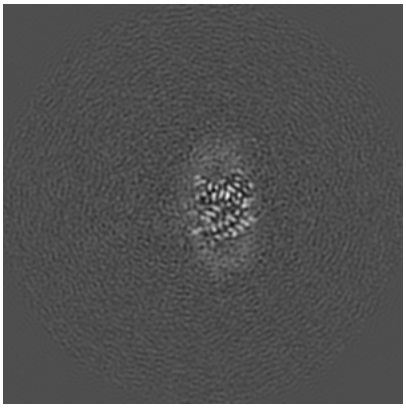
6.2.1 Primary map



X Index: 140



Y Index: 140

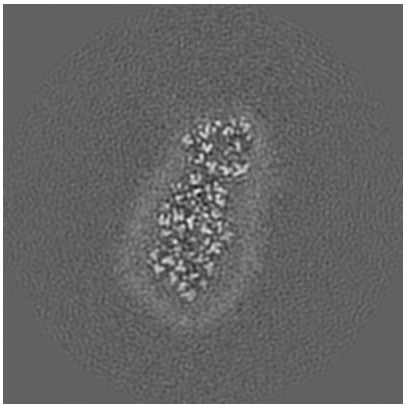


Z Index: 140

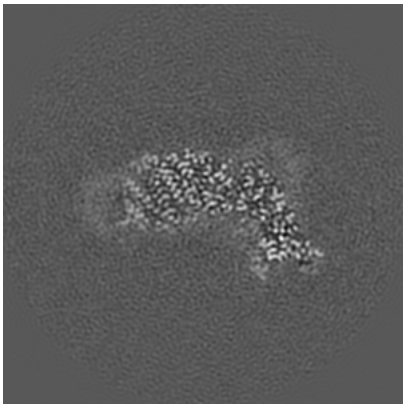
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

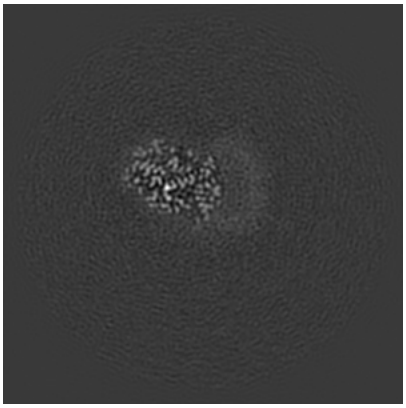
6.3.1 Primary map



X Index: 145



Y Index: 143

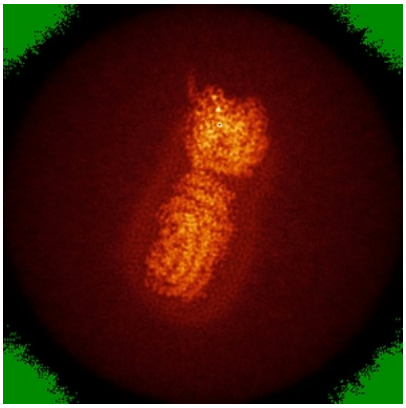


Z Index: 194

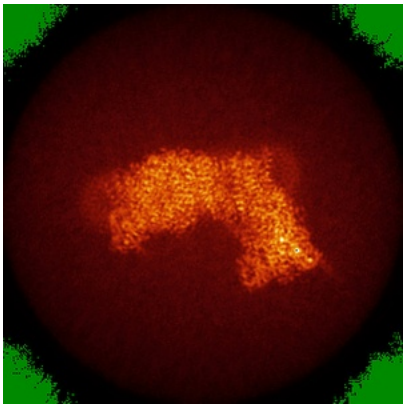
The images above show the largest variance slices of the map in three orthogonal directions.

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

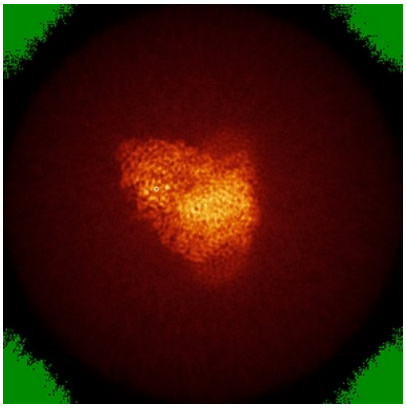
6.4.1 Primary map



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

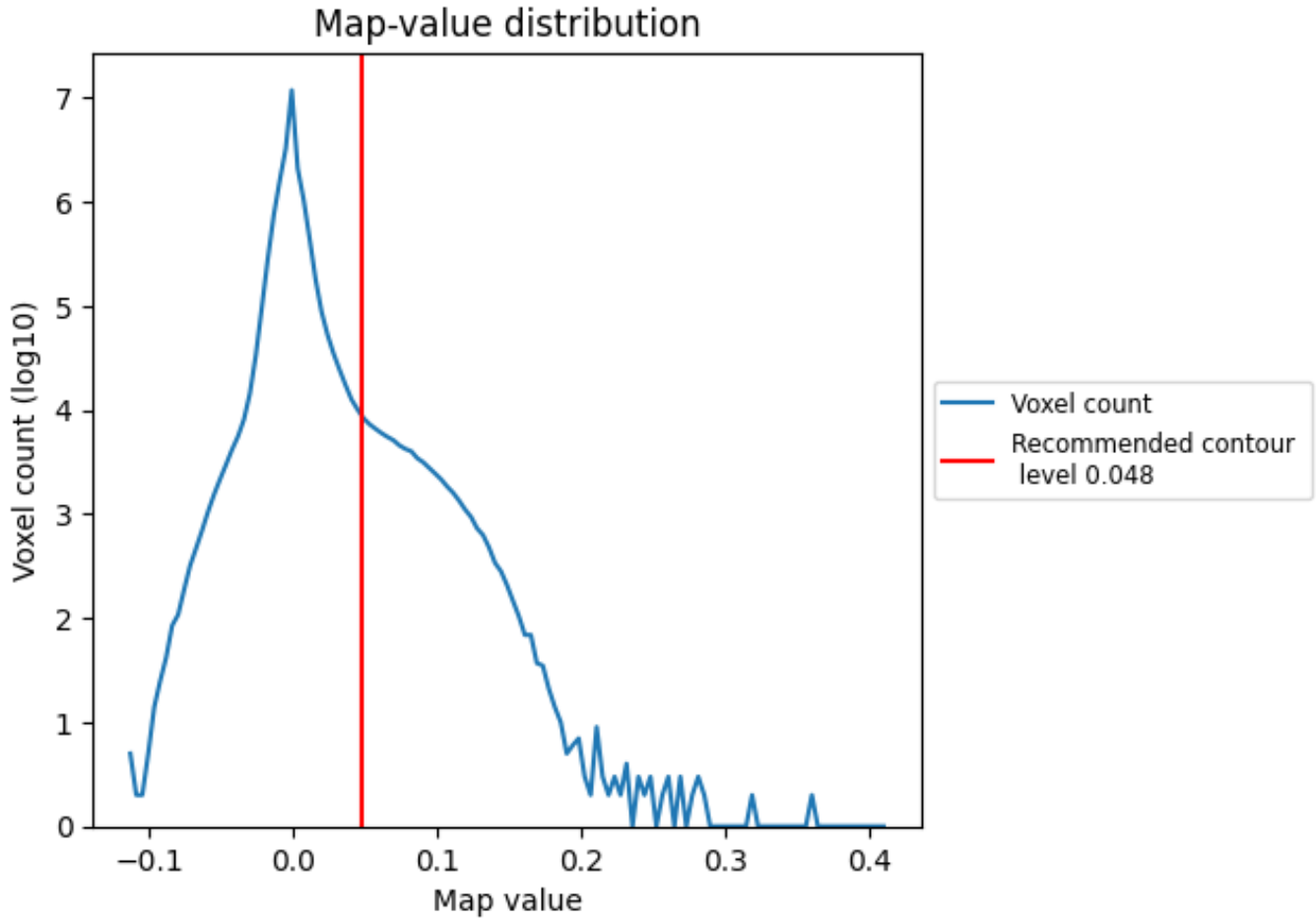
6.6 Mask visualisation (i)

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

7 Map analysis

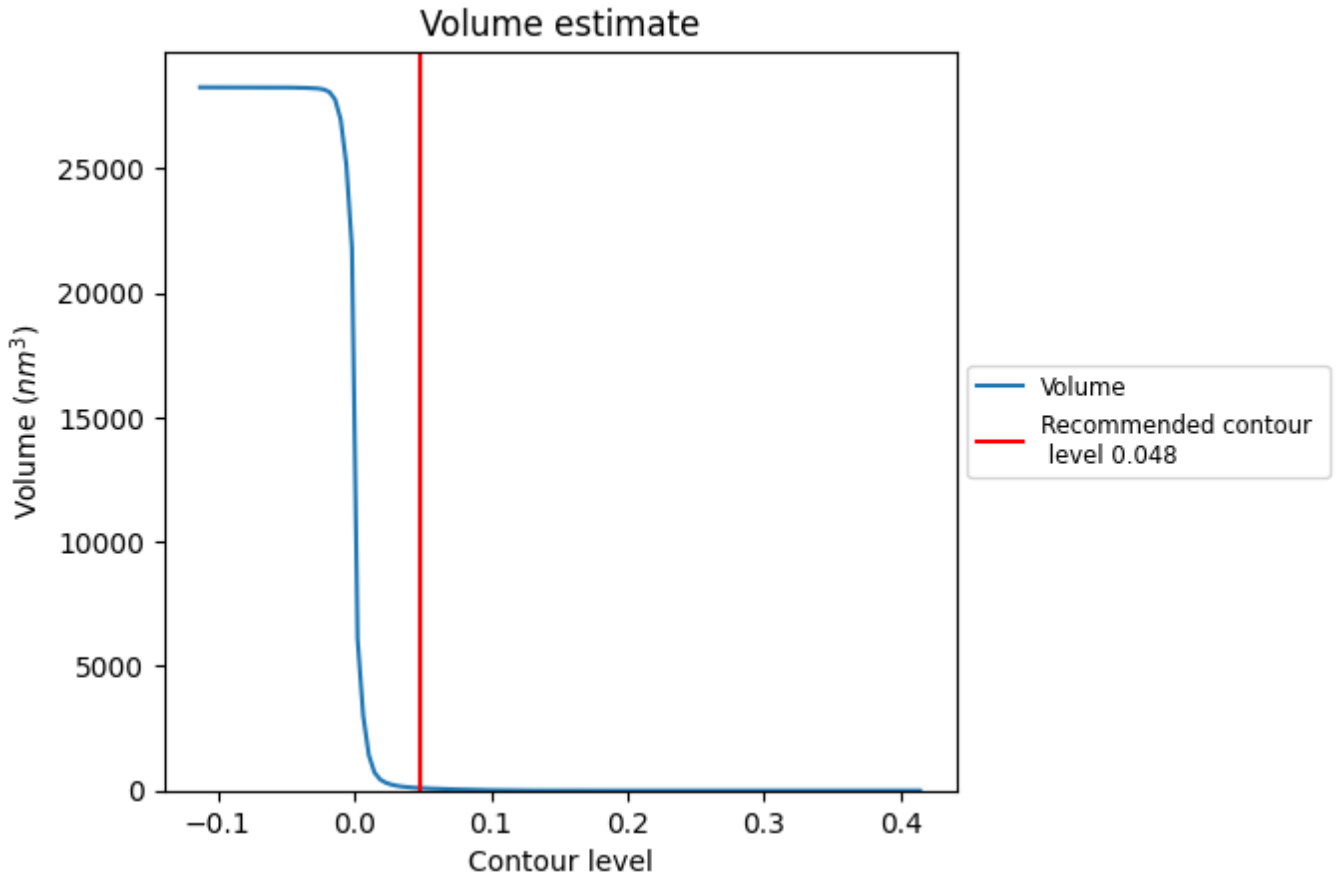
This section contains the results of statistical analysis of the map.

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.

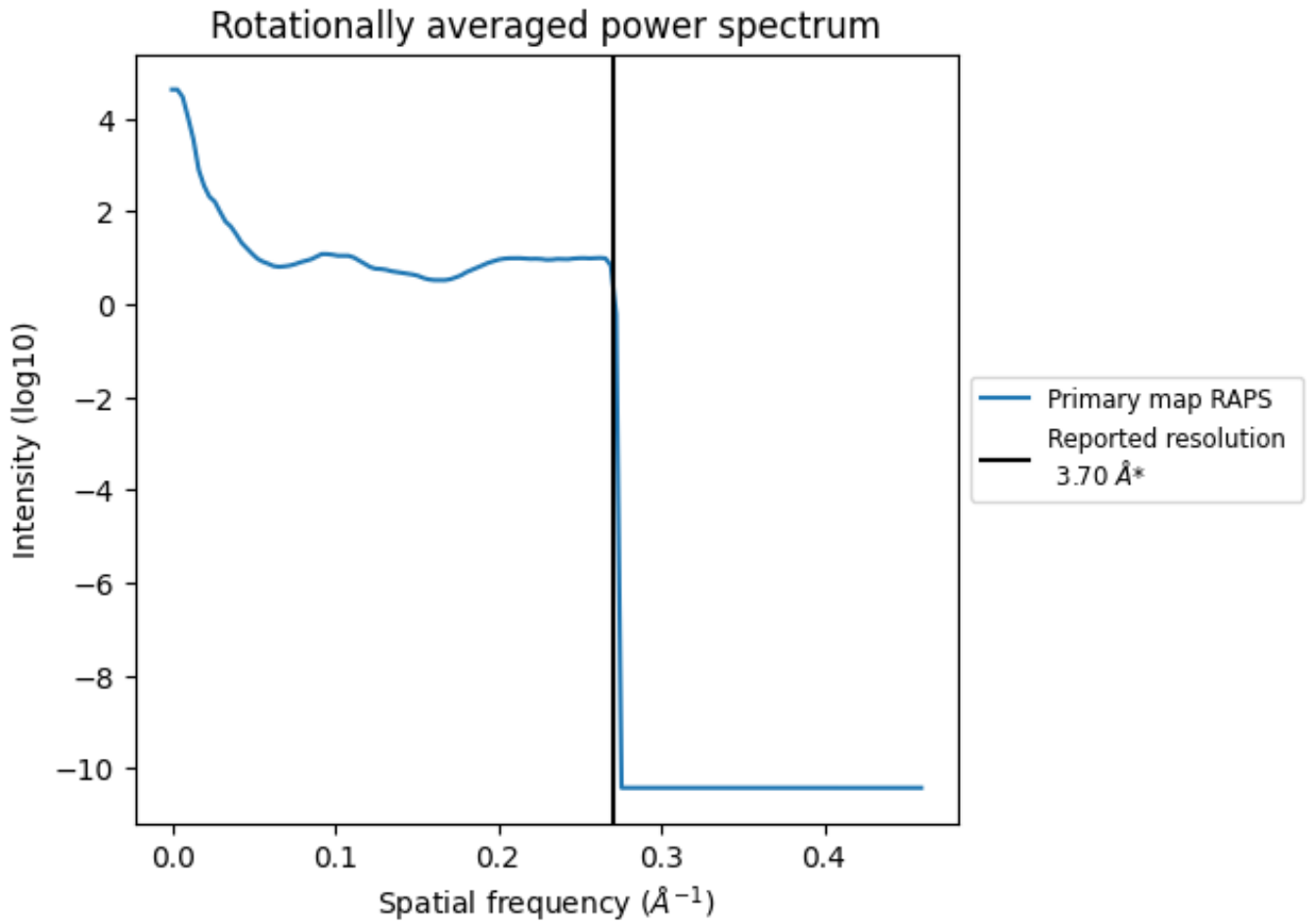
7.2 Volume estimate



The volume at the recommended contour level is 100 nm^3; this corresponds to an approximate mass of 90 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)

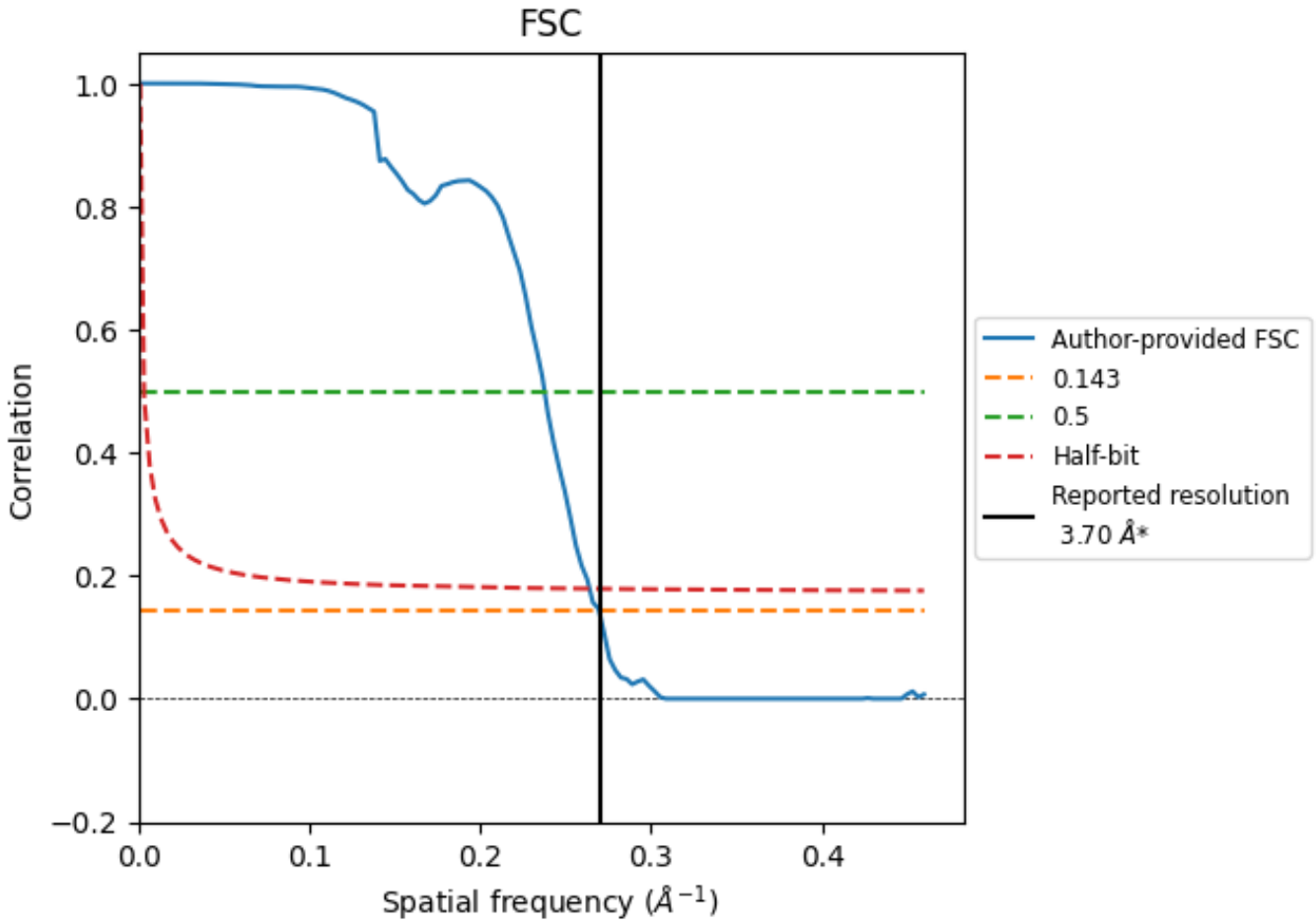


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

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 0.270 Å^{-1}

8.2 Resolution estimates (i)

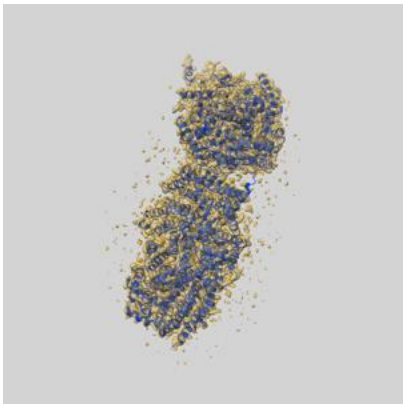
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.71	4.21	3.79
Unmasked-calculated*	-	-	-

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

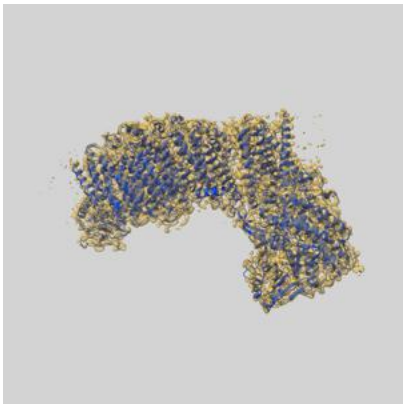
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-7468 and PDB model 6CFW. Per-residue inclusion information can be found in section 3 on page 8.

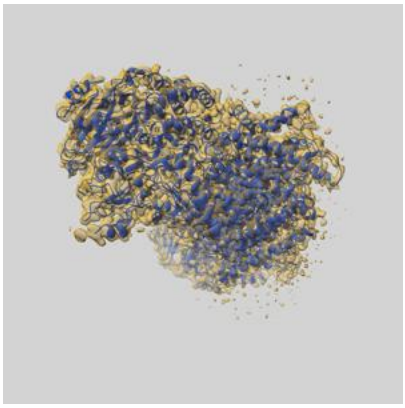
9.1 Map-model overlay



X



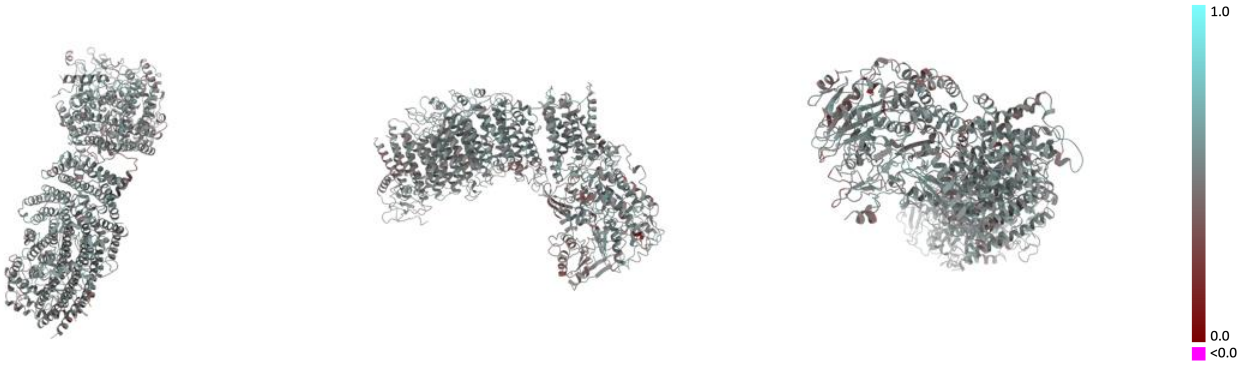
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.048 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

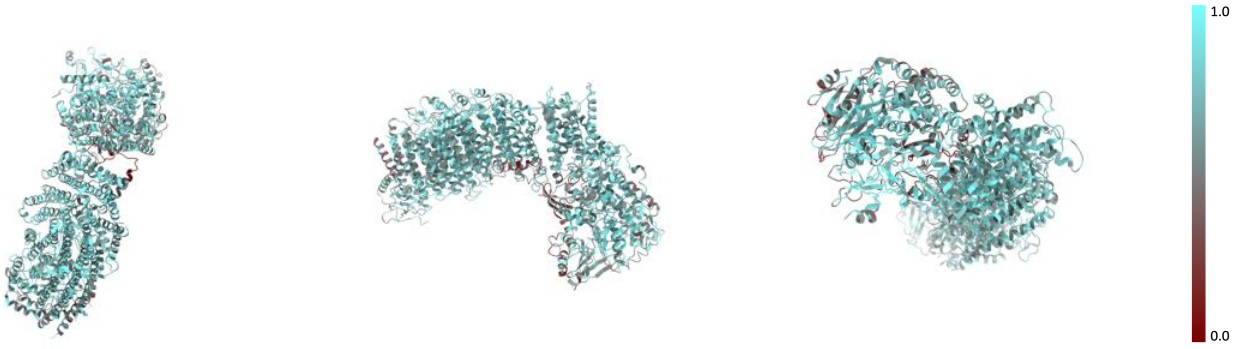
9.2 Q-score mapped to coordinate model



X Y Z

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

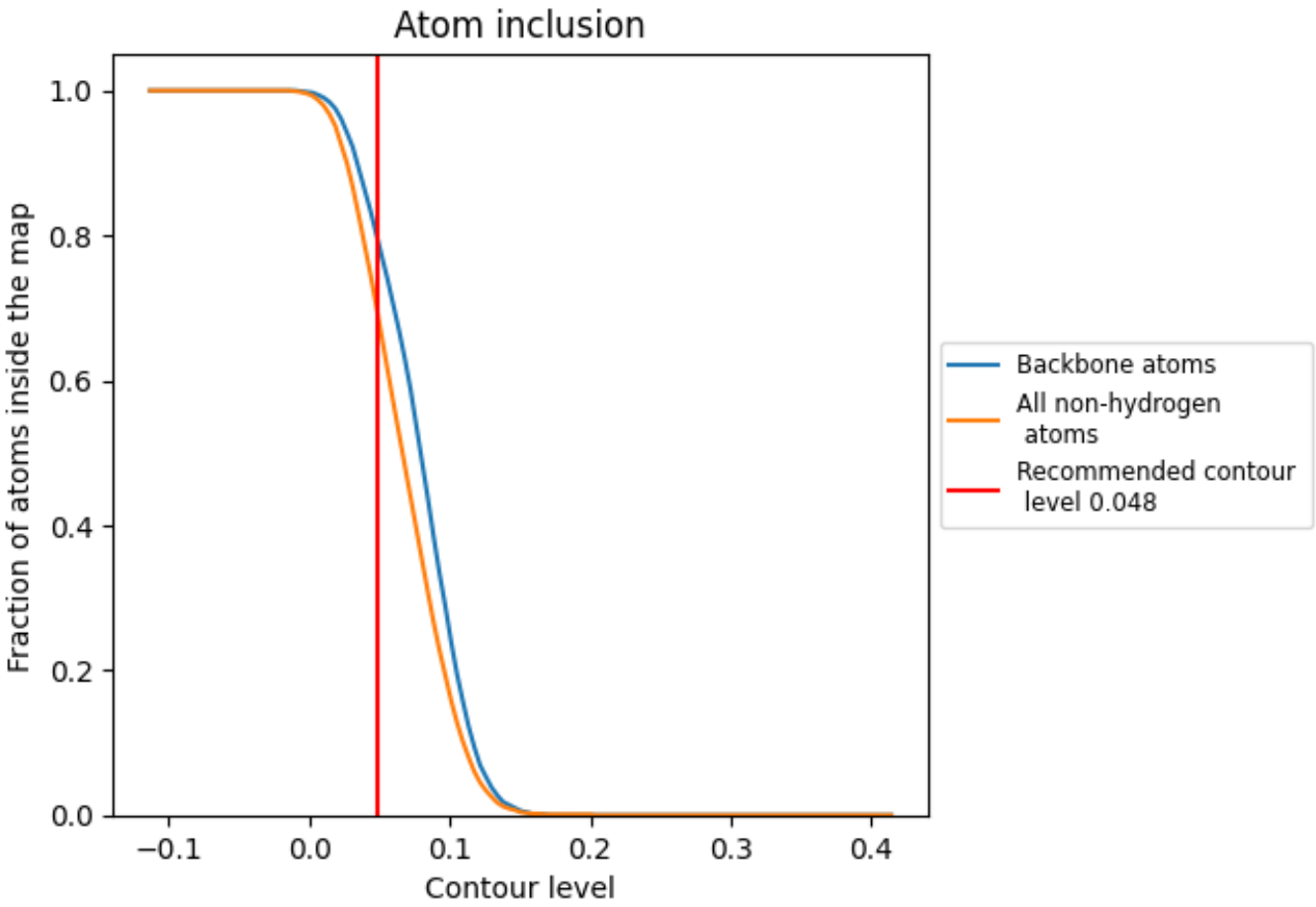
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.048).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 70% 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 (0.048) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7010	0.4990
A	0.6520	0.4720
B	0.7260	0.5020
C	0.6330	0.4720
D	0.7310	0.5070
E	0.7330	0.5090
F	0.7210	0.5080
G	0.7590	0.5080
H	0.7570	0.5230
I	0.5450	0.4630
J	0.7860	0.5280
K	0.5830	0.4510
L	0.6610	0.4920
M	0.7200	0.5080
N	0.7410	0.5020