Full wwPDB EM Validation Report (i)

Dec 17, 2022 – 05:55 pm GMT

PDB ID	:	6ZIQ
EMDB ID	:	EMD-11228
Title	:	bovine ATP synthase stator domain, state 1
Authors	:	Spikes, T.E.; Montgomery, M.G.; Walker, J.E.
Deposited on	:	2020-06-26
Resolution	:	4.33 Å(reported)
Based on initial models	:	2WSS, 2V7Q, 2CLY

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 (i) symbol.

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

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

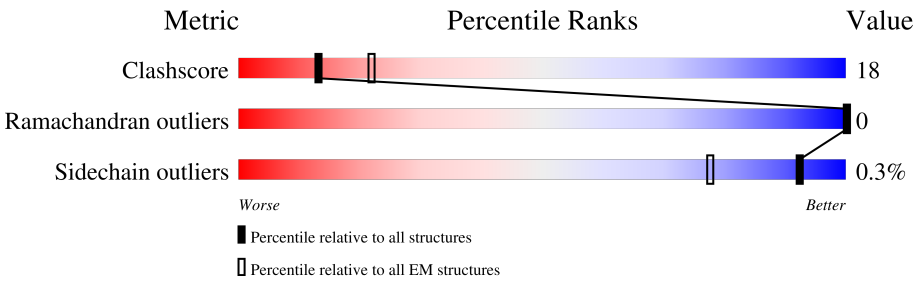
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.33 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	8	66	14% 45% 17% 38%
2	a	226	21% 100%
3	d	160	19% 96% • •
4	e	70	30% 57% • 41%
5	f	87	25% 95% 5%
6	g	102	40% 77% 23%
7	j	60	53% 80% 20%
8	k	57	58% 63% 37%

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Mol	Chain	Length	Quality of chain
9	M	75	52% 60% 31% 9%
9	N	75	51% 60% 39%
9	O	75	51% 36% 20% 41%
10	b	214	6% 97%
11	h	76	21% 82% 18%
12	S	190	21% 40% 28% 32%
13	C	510	6% 10% 7% 83%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 22312 atoms, of which 11373 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 ATP synthase protein 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	8	41	696	231	352	52	58	3	0	0

- Molecule 2 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	a	226	3611	1155	1870	276	298	12	0	0

- Molecule 3 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	d	155	2549	821	1276	207	242	3	0	0

- Molecule 4 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	e	41	687	218	352	61	55	1	0	0

- Molecule 5 is a protein called ATP synthase subunit f, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	f	83	1411	456	718	120	114	3	0	0

- Molecule 6 is a protein called ATP synthase subunit g, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	g	79	1291	420	662	100	108	1	0	0

- Molecule 7 is a protein called ATP synthase subunit ATP5MPL, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	j	48	828	267	428	66	65	2	0	0

- Molecule 8 is a protein called ATP synthase membrane subunit DAPIT, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	k	36	596	192	307	47	48	2	0	0

- Molecule 9 is a protein called ATP synthase F(0) complex subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	M	68	994	326	507	75	82	4	0	0
9	N	75	1096	356	559	83	94	4	0	0
9	O	44	707	234	364	51	55	3	0	0

- Molecule 10 is a protein called ATP synthase F(0) complex subunit B1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	b	209	3456	1095	1755	292	308	6	0	0

- Molecule 11 is a protein called ATP synthase-coupling factor 6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	h	62	1009	326	495	87	99	2	0	0

- Molecule 12 is a protein called ATP synthase subunit O, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	S	129	2048	627	1057	171	186	7	0	0

- Molecule 13 is a protein called ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	C	89	1333	409	671	115	136	2	0	0

There is a discrepancy between the modelled and reference sequences:

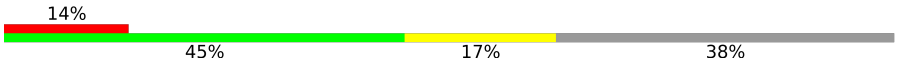
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	GLU	GLN	microheterogeneity	UNP P19483

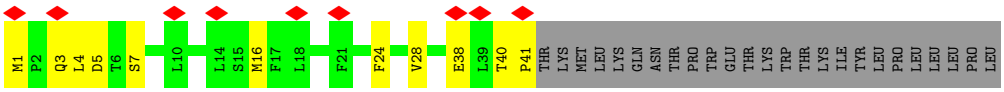
3 Residue-property plots (i)

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: ATP synthase protein 8

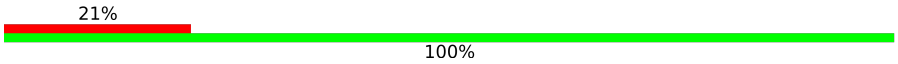
Chain 8:

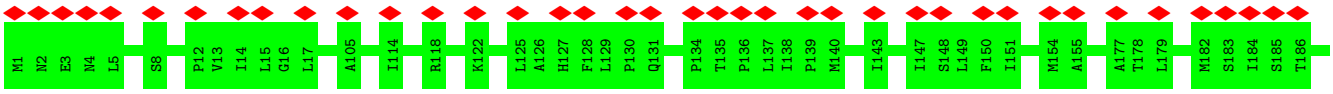


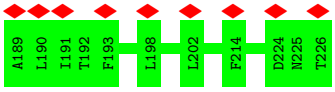


- Molecule 2: ATP synthase subunit a

Chain a:

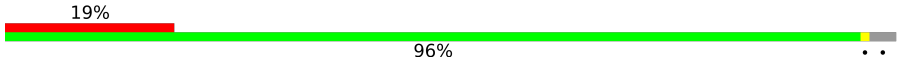


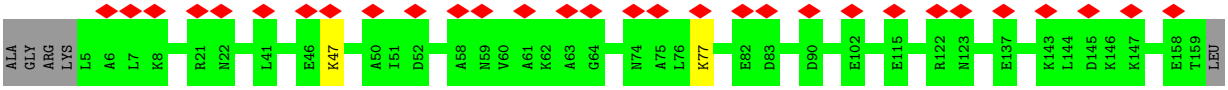




- Molecule 3: ATP synthase subunit d, mitochondrial

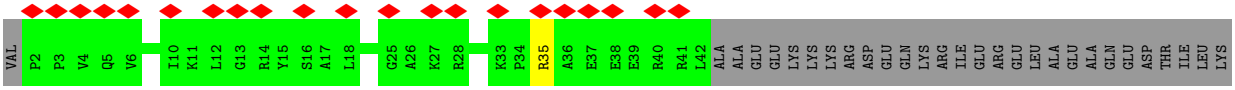
Chain d:





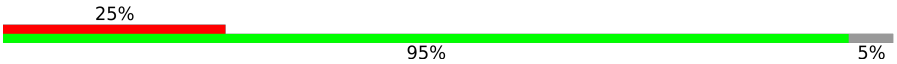
- Molecule 4: ATP synthase subunit e, mitochondrial

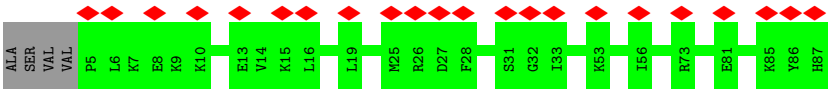
Chain e:



- Molecule 5: ATP synthase subunit f, mitochondrial

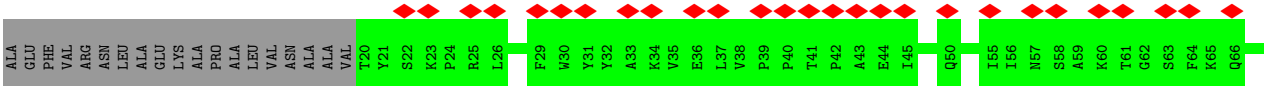
Chain f:

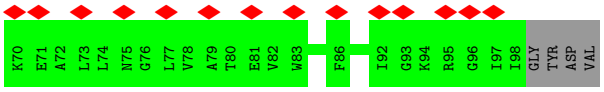




• Molecule 6: ATP synthase subunit g, mitochondrial

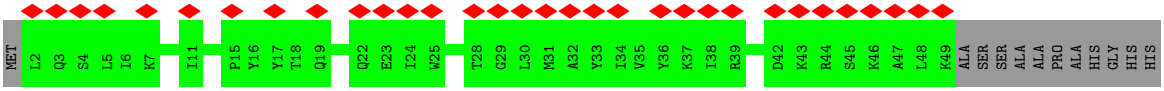
Chain g:





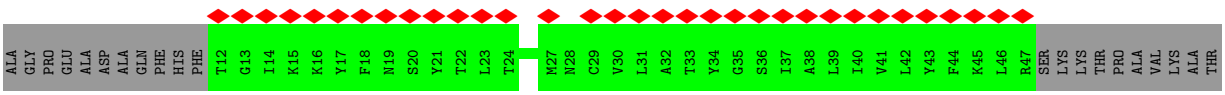
• Molecule 7: ATP synthase subunit ATP5MPL, mitochondrial

Chain j:



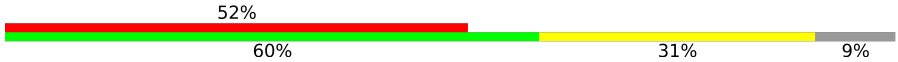
• Molecule 8: ATP synthase membrane subunit DAPIT, mitochondrial

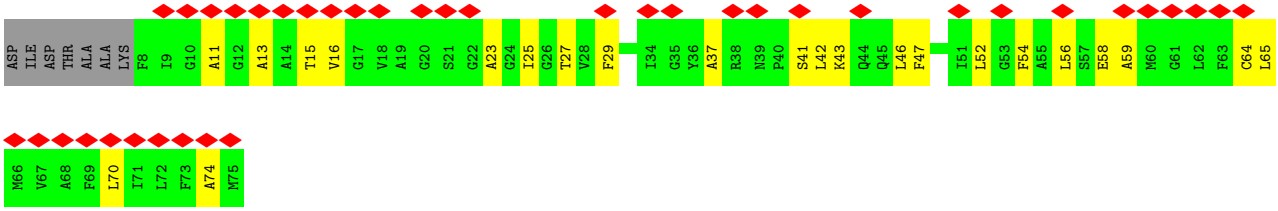
Chain k:



• Molecule 9: ATP synthase F(0) complex subunit C1, mitochondrial

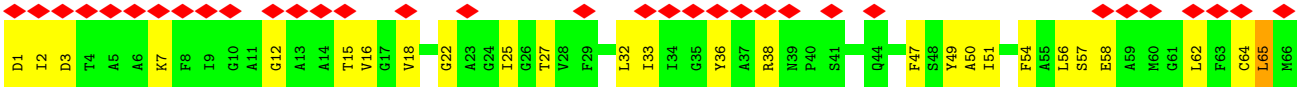
Chain M:

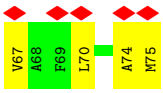




• Molecule 9: ATP synthase F(0) complex subunit C1, mitochondrial

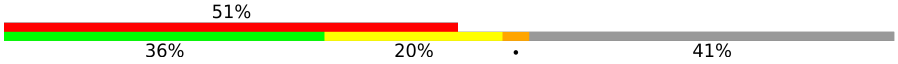
Chain N:

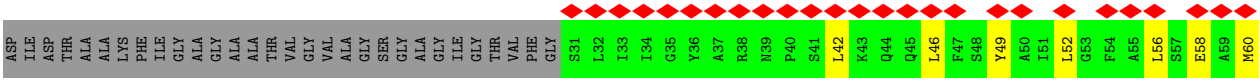


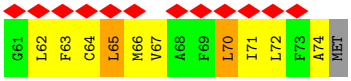


• Molecule 9: ATP synthase F(0) complex subunit C1, mitochondrial

Chain O:

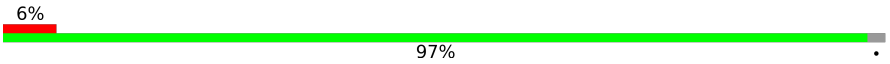


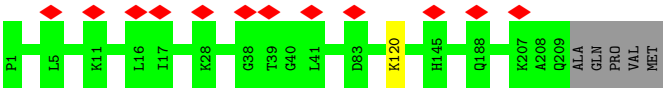




• Molecule 10: ATP synthase F(0) complex subunit B1, mitochondrial

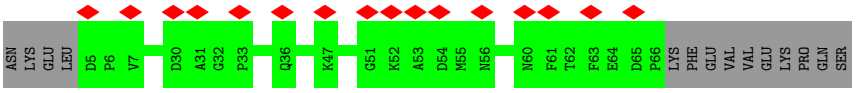
Chain b:





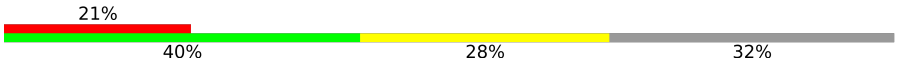
• Molecule 11: ATP synthase-coupling factor 6, mitochondrial

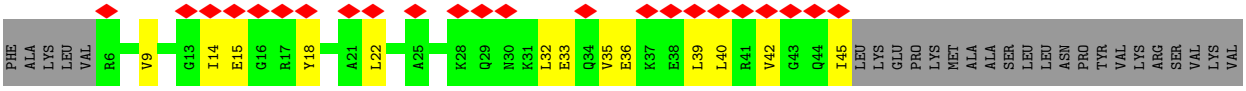
Chain h:

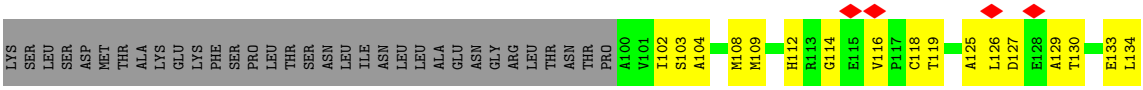


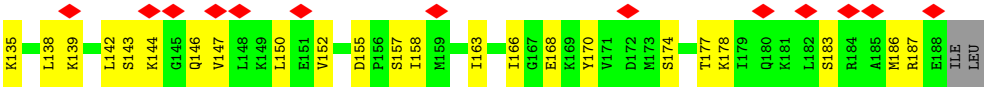
• Molecule 12: ATP synthase subunit O, mitochondrial

Chain S:



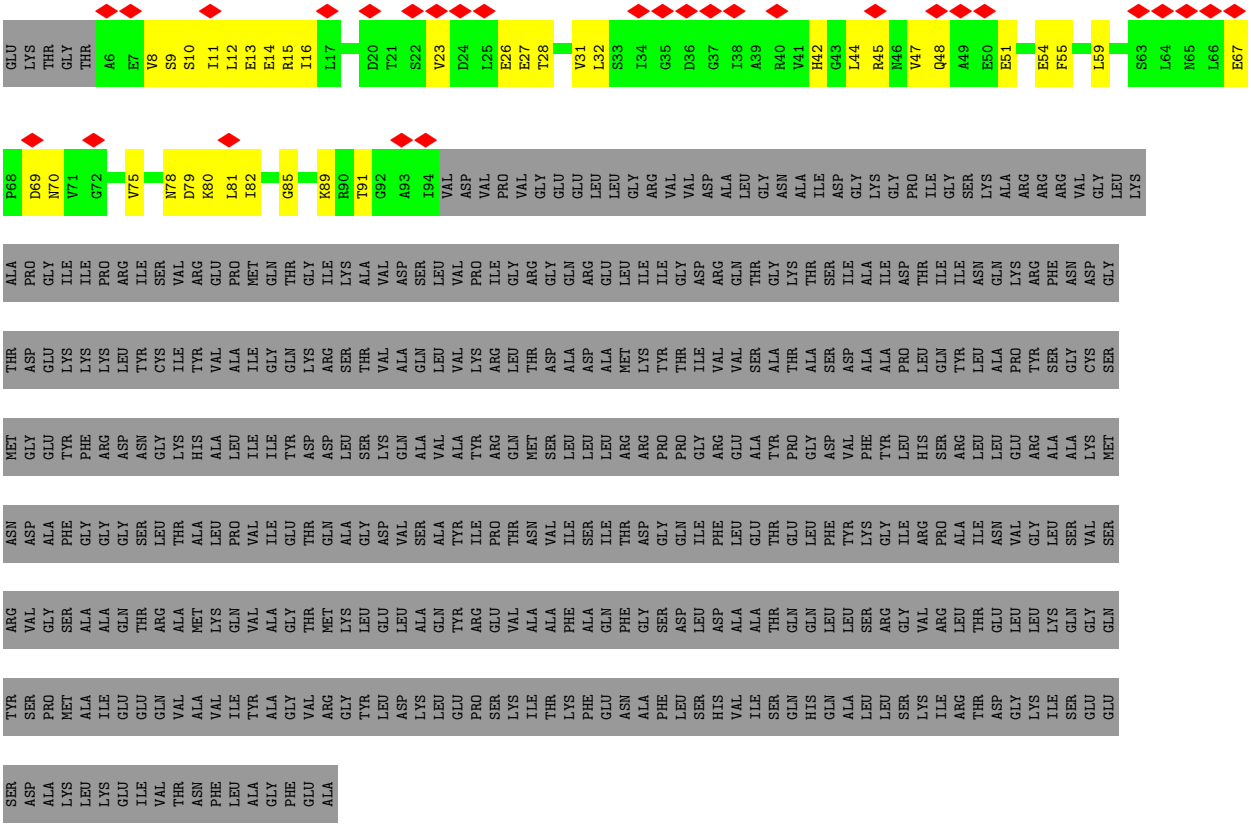






• Molecule 13: ATP synthase subunit alpha, mitochondrial

Chain C:


GLU LYS THR GLY THR A6 E7 V8 S9 S10 I11 L12 E13 E14 R15 I16 L17 D20 T21 S22 V23 D24 L25 E26 E27 T28 V31 L32 S33 I34 G35 D36 G37 I38 A39 R40 V41 H42 G43 L44 R45 M46 V47 Q48 A49 E50 E51 E54 F55 L59 S63 L64 N65 L66 E67
P68 D69 N70 V71 G72 V75 N78 D79 K80 L81 I82 G85 K89 R90 T91 G92 A93 T94 VAL ASP VAL PRO VAL GLY GLU GLU LEU LEU GLY ILE ARG VAL VAL ASP ALA LEU GLY ASN ALA ILE ASP GLY LYS GLY PRO ILE GLY SER LYS ALA ARG ARG VAL GLY LEU LYS
ALA PRO GLY ILE ILE PRO ARG ILE SER VAL ARG GLU PRO MET GLN THR GLY ILE LYS ALA VAL ASP SER LEU VAL PRO ILE GLY ARG GLY GLU GLN ARG GLU LEU LEU GLY ILE ILE GLY ASP ARG GLN THR GLY LYS THR SER ILE ASP ILE ALA ILE ASP THR ILE ILE GLY SER LYS ALA ARG PHE ASN ASP GLY
THR ASP GLU LYS LYS LYS LEU TYR CYS ILE TYR VAL ALA ILE GLY GLN LYS ARG SER THR VAL ALA GLN LEU VAL LYS ARG LEU THR ASP ALA ASP ALA MET LYS TYR THR ILE VAL VAL SER ALA THR ALA SER ASP ALA ALA PRO LEU GLN TYR LEU ALA PRO TYR SER GLY CYS SER
MET GLY GLU TYR PHE ARG ASP ASN GLY LYS HIS ALA LEU ILE ILE TYR ASP ASP LEU SER LYS GLN ALA VAL ALA TYR ARG GLN MET SER LEU LEU LEU ARG ARG PRO PRO GLY ARG GLU ALA TYR PRO GLY ASP VAL PHE TYR LEU HIS SER ARG LEU LEU GLU ARG ALA ALA LYS MET
ASN ASP ALA PHE GLY GLY GLY SER LEU THR ALA LEU PRO VAL ILE GLU THR GLN ALA GLY ASP VAL SER ALA TYR ILE PRO THR ASN VAL ILE SER ILE THR ASP GLY GLN ILE PHE LEU GLU THR GLU LEU PHE TYR LYS GLY ILE ARG PRO ALA ILE ASN VAL GLY LEU SER VAL SER
ARG VAL GLY SER ALA ALA GLN THR ARG ALA MET LYS GLN VAL ALA GLY THR MET LYS LEU GLU LEU ALA GLN TYR ARG GLU VAL ALA ALA PHE ALA GLN PHE GLY SER ASP LEU ASP ALA ALA THR GLN GLN LEU LEU SER ARG GLY VAL ARG LEU THR GLU LEU LEU LYS GLN GLY GLN
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SER ASP ALA LYS LEU LYS GLU ILE VAL THR ASN PHE LEU ALA GLY PHE GLU ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	90850	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 ($e^-/Å^2$)	4.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0187	Depositor
Map size (Å)	524.0, 524.0, 524.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: M3L

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	8	0.33	0/355	0.42	0/483
2	a	0.32	0/1779	0.50	0/2433
3	d	0.29	0/1304	0.42	0/1768
4	e	0.29	0/343	0.46	0/460
5	f	0.32	0/711	0.42	0/952
6	g	0.27	0/646	0.47	0/879
7	j	0.30	0/410	0.49	0/552
8	k	0.26	0/294	0.43	0/395
9	M	0.32	0/484	0.47	0/653
9	N	0.36	0/534	0.56	1/721 (0.1%)
9	O	0.36	0/338	0.81	6/456 (1.3%)
10	b	0.32	0/1733	0.44	0/2334
11	h	0.32	0/526	0.52	0/707
12	S	0.29	0/1000	0.46	0/1341
13	C	0.28	0/665	0.49	0/894
All	All	0.31	0/11122	0.48	7/15028 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	O	70	LEU	CB-CG-CD2	5.99	121.18	111.00
9	O	52	LEU	CB-CG-CD2	5.76	120.80	111.00
9	O	65	LEU	CB-CG-CD1	5.69	120.67	111.00
9	O	65	LEU	CB-CG-CD2	5.69	120.67	111.00
9	N	65	LEU	CB-CG-CD1	-5.44	101.75	111.00
9	O	52	LEU	CB-CG-CD1	5.40	120.18	111.00
9	O	70	LEU	CB-CG-CD1	5.33	120.06	111.00

There are no chirality outliers.

There are no planarity outliers.

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	8	344	352	352	9	0
2	a	1741	1870	1870	0	0
3	d	1273	1276	1275	0	0
4	e	335	352	352	0	0
5	f	693	718	718	0	0
6	g	629	662	662	0	0
7	j	400	428	428	0	0
8	k	289	307	307	0	0
9	M	487	507	506	21	0
9	N	537	559	558	35	0
9	O	343	364	363	22	0
10	b	1701	1755	1755	0	0
11	h	514	495	495	0	0
12	S	991	1057	1055	46	0
13	C	662	671	671	31	0
All	All	10939	11373	11367	137	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 18.

All (137) 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)
9:N:70:LEU:O	9:N:74:ALA:N	2.09	0.86
9:N:15:THR:HG1	9:O:64:CYS:HG	1.15	0.85
13:C:78:ASN:OD1	13:C:79:ASP:N	2.11	0.83
9:M:37:ALA:O	9:N:38:ARG:NH2	2.11	0.82
13:C:54:GLU:OE1	13:C:91:THR:HG23	1.82	0.80
9:M:11:ALA:O	9:M:15:THR:HG23	1.85	0.77
12:S:183:SER:O	12:S:187:ARG:NH1	2.17	0.77
12:S:33:GLU:N	12:S:33:GLU:OE1	2.17	0.76
12:S:127:ASP:O	12:S:130:THR:OG1	2.03	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:S:139:LYS:NZ	12:S:146:GLN:O	2.14	0.75
9:M:54:PHE:CZ	9:N:56:LEU:HD13	2.22	0.75
9:O:62:LEU:HD13	9:O:65:LEU:HD12	1.71	0.71
9:M:43:M3L:O	9:M:46:LEU:N	2.23	0.70
13:C:59:LEU:HD21	13:C:78:ASN:O	1.91	0.70
9:N:36:TYR:CD2	9:O:42:LEU:HD21	2.28	0.68
13:C:67:GLU:OE1	13:C:69:ASP:N	2.26	0.67
13:C:48:GLN:N	13:C:51:GLU:OE1	2.28	0.67
13:C:32:LEU:HD21	13:C:42:HIS:HB3	1.78	0.66
13:C:78:ASN:OD1	13:C:80:LYS:N	2.28	0.66
1:8:24:PHE:O	1:8:28:VAL:HG22	1.97	0.65
9:N:54:PHE:CE1	9:O:56:LEU:HD13	2.36	0.61
9:M:13:ALA:O	9:M:16:VAL:HG22	2.00	0.61
9:M:25:ILE:HD11	9:N:57:SER:HA	1.82	0.61
9:N:1:ASP:OD1	9:N:2:ILE:N	2.35	0.60
9:N:65:LEU:HD21	9:O:63:PHE:CZ	2.37	0.59
9:N:7:LYS:NZ	9:N:75:MET:SD	2.78	0.57
13:C:32:LEU:HD21	13:C:42:HIS:CB	2.34	0.57
12:S:186:MET:SD	12:S:187:ARG:NH2	2.74	0.57
13:C:79:ASP:O	13:C:82:ILE:N	2.37	0.56
13:C:10:SER:O	13:C:13:GLU:N	2.38	0.56
12:S:116:VAL:HG21	12:S:142:LEU:HD22	1.88	0.56
12:S:155:ASP:OD2	12:S:157:SER:N	2.37	0.56
9:O:66:MET:SD	9:O:67:VAL:N	2.79	0.55
12:S:125:ALA:C	12:S:126:LEU:HD22	2.27	0.55
9:O:58:GLU:O	9:O:62:LEU:HD23	2.07	0.55
1:8:1:MET:HG2	1:8:4:LEU:HD23	1.89	0.54
9:N:65:LEU:HD11	9:O:63:PHE:CE2	2.43	0.54
9:M:41:SER:C	9:M:42:LEU:HD22	2.28	0.54
12:S:36:GLU:O	12:S:40:LEU:HD23	2.08	0.53
13:C:10:SER:O	13:C:14:GLU:OE1	2.25	0.53
12:S:9:VAL:HG13	12:S:9:VAL:O	2.09	0.52
9:N:15:THR:OG1	9:O:64:CYS:SG	2.40	0.52
13:C:47:VAL:HG13	13:C:47:VAL:O	2.10	0.52
9:N:47:PHE:O	9:N:51:ILE:HD12	2.11	0.51
13:C:28:THR:HG22	13:C:89:LYS:HG3	1.92	0.51
9:M:54:PHE:CZ	9:N:56:LEU:HD22	2.45	0.51
12:S:158:ILE:HD13	12:S:163:ILE:CD1	2.41	0.51
12:S:158:ILE:HD13	12:S:163:ILE:HD13	1.92	0.51
13:C:26:GLU:O	13:C:28:THR:HG23	2.11	0.50
9:N:33:ILE:HG23	9:O:46:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:S:116:VAL:HG23	12:S:116:VAL:O	2.11	0.50
13:C:59:LEU:HD22	13:C:81:LEU:HD21	1.92	0.50
13:C:27:GLU:OE2	13:C:45:ARG:N	2.45	0.50
9:N:65:LEU:HD11	9:O:63:PHE:CZ	2.46	0.50
9:M:52:LEU:O	9:M:56:LEU:HD23	2.11	0.50
9:N:64:CYS:O	9:N:67:VAL:HG12	2.11	0.50
12:S:170:TYR:CB	13:C:28:THR:HG21	2.42	0.50
9:O:66:MET:SD	9:O:67:VAL:HG23	2.52	0.49
12:S:114:GLY:O	12:S:147:VAL:N	2.43	0.49
9:O:70:LEU:O	9:O:74:ALA:N	2.40	0.49
9:N:47:PHE:HZ	9:O:49:TYR:CE1	2.31	0.49
12:S:150:LEU:HD13	12:S:152:VAL:HG23	1.95	0.49
12:S:14:ILE:HG13	12:S:15:GLU:N	2.29	0.48
13:C:31:VAL:O	13:C:85:GLY:N	2.43	0.48
1:8:5:ASP:O	1:8:7:SER:N	2.46	0.48
1:8:1:MET:SD	9:N:70:LEU:HD22	2.54	0.48
12:S:129:ALA:O	12:S:133:GLU:OE1	2.31	0.48
9:M:54:PHE:HZ	9:N:56:LEU:HD22	1.79	0.48
9:M:41:SER:O	9:M:42:LEU:HD22	2.14	0.48
12:S:178:LYS:NZ	13:C:23:VAL:HG11	2.28	0.48
12:S:118:CYS:SG	12:S:119:THR:N	2.87	0.48
9:O:62:LEU:HA	9:O:65:LEU:HG	1.96	0.47
12:S:39:LEU:HD23	12:S:102:ILE:HA	1.96	0.47
9:M:70:LEU:O	9:M:74:ALA:N	2.47	0.47
13:C:12:LEU:HD23	13:C:15:ARG:HH21	1.80	0.47
9:M:27:THR:HA	9:N:27:THR:HG21	1.96	0.47
12:S:35:VAL:O	12:S:39:LEU:CD1	2.63	0.47
12:S:143:SER:OG	12:S:144:LYS:N	2.48	0.46
13:C:44:LEU:O	13:C:47:VAL:HG12	2.15	0.46
9:N:18:VAL:HG11	9:N:65:LEU:HD12	1.98	0.46
12:S:35:VAL:O	12:S:39:LEU:HD12	2.16	0.46
12:S:18:TYR:O	12:S:22:LEU:HD23	2.16	0.46
13:C:55:PHE:CE1	13:C:75:VAL:HG22	2.52	0.45
13:C:8:VAL:O	13:C:11:ILE:HG22	2.15	0.45
9:M:47:PHE:HE1	9:N:49:TYR:CZ	2.34	0.45
12:S:104:ALA:O	12:S:108:MET:HG3	2.16	0.45
12:S:118:CYS:SG	12:S:166:ILE:HD13	2.56	0.45
9:N:58:GLU:OE2	9:N:62:LEU:HD21	2.17	0.45
9:M:47:PHE:CE1	9:N:49:TYR:CZ	3.05	0.45
1:8:38:GLU:OE1	1:8:40:THR:N	2.50	0.45
12:S:102:ILE:HG13	12:S:103:SER:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:58:GLU:O	9:N:62:LEU:HD23	2.17	0.44
12:S:109:MET:SD	12:S:112:HIS:ND1	2.85	0.44
12:S:130:THR:O	12:S:134:LEU:HG	2.17	0.44
12:S:150:LEU:CD1	12:S:152:VAL:HG23	2.47	0.44
12:S:170:TYR:HB3	13:C:28:THR:HG21	2.00	0.44
12:S:187:ARG:HA	12:S:187:ARG:NE	2.33	0.44
9:N:2:ILE:HG23	9:N:3:ASP:N	2.33	0.44
9:O:63:PHE:C	9:O:63:PHE:CD2	2.91	0.44
9:M:54:PHE:CE2	9:N:56:LEU:HD13	2.52	0.43
12:S:135:LYS:O	12:S:139:LYS:HG2	2.18	0.43
12:S:138:LEU:HD22	12:S:166:ILE:HD11	2.00	0.43
9:O:42:LEU:O	9:O:46:LEU:HD12	2.18	0.43
12:S:42:VAL:HA	12:S:45:ILE:HD12	2.00	0.43
1:8:40:THR:HB	1:8:41:PRO:HD2	2.00	0.43
12:S:32:LEU:HA	12:S:35:VAL:HG12	2.01	0.43
9:M:64:CYS:SG	9:M:65:LEU:N	2.91	0.43
12:S:186:MET:HA	13:C:15:ARG:HD2	1.99	0.43
12:S:186:MET:HG3	13:C:16:ILE:HD11	1.99	0.43
9:M:23:ALA:O	9:M:27:THR:HG23	2.19	0.43
12:S:174:SER:OG	12:S:177:THR:HG22	2.18	0.43
9:N:32:LEU:HD12	9:N:50:ALA:CB	2.49	0.43
1:8:38:GLU:OE1	1:8:40:THR:OG1	2.30	0.42
9:O:63:PHE:CE2	9:O:67:VAL:HG21	2.53	0.42
13:C:8:VAL:HG23	13:C:9:SER:N	2.33	0.42
12:S:39:LEU:HA	12:S:42:VAL:HG22	2.01	0.42
9:M:58:GLU:O	9:M:59:ALA:C	2.58	0.42
9:N:16:VAL:O	9:N:18:VAL:N	2.52	0.42
9:N:47:PHE:O	9:N:51:ILE:CD1	2.67	0.42
13:C:27:GLU:HG2	13:C:44:LEU:HD23	2.02	0.42
9:N:12:GLY:O	9:N:15:THR:HG22	2.20	0.42
12:S:109:MET:O	12:S:112:HIS:HB3	2.20	0.42
9:O:60:MET:HA	9:O:60:MET:CE	2.50	0.41
12:S:158:ILE:HG21	12:S:163:ILE:CD1	2.49	0.41
9:M:29:PHE:CE2	9:N:56:LEU:HD12	2.56	0.41
12:S:168:GLU:O	13:C:28:THR:N	2.53	0.41
12:S:163:ILE:CG2	12:S:170:TYR:HE1	2.33	0.41
13:C:32:LEU:HD11	13:C:42:HIS:HB2	2.03	0.41
1:8:3:GLN:C	1:8:4:LEU:HD22	2.41	0.41
9:O:71:ILE:HG13	9:O:72:LEU:N	2.36	0.41
12:S:150:LEU:HD12	12:S:150:LEU:C	2.42	0.40
9:M:43:M3L:O	9:M:46:LEU:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:36:TYR:CE2	9:O:42:LEU:HD21	2.56	0.40
13:C:67:GLU:HB3	13:C:70:ASN:O	2.22	0.40
9:O:63:PHE:O	9:O:66:MET:HG3	2.21	0.40
1:8:16:MET:SD	1:8:16:MET:C	3.00	0.40
9:N:22:GLY:HA2	9:N:25:ILE:HG12	2.03	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	8	39/66 (59%)	29 (74%)	10 (26%)	0	100	100
2	a	224/226 (99%)	210 (94%)	14 (6%)	0	100	100
3	d	153/160 (96%)	134 (88%)	19 (12%)	0	100	100
4	e	39/70 (56%)	39 (100%)	0	0	100	100
5	f	81/87 (93%)	74 (91%)	7 (9%)	0	100	100
6	g	77/102 (76%)	71 (92%)	6 (8%)	0	100	100
7	j	46/60 (77%)	43 (94%)	3 (6%)	0	100	100
8	k	34/57 (60%)	32 (94%)	2 (6%)	0	100	100
9	M	65/75 (87%)	62 (95%)	3 (5%)	0	100	100
9	N	72/75 (96%)	64 (89%)	8 (11%)	0	100	100
9	O	41/75 (55%)	38 (93%)	3 (7%)	0	100	100
10	b	207/214 (97%)	196 (95%)	11 (5%)	0	100	100
11	h	60/76 (79%)	49 (82%)	11 (18%)	0	100	100
12	S	125/190 (66%)	114 (91%)	11 (9%)	0	100	100
13	C	87/510 (17%)	78 (90%)	9 (10%)	0	100	100
All	All	1350/2043 (66%)	1233 (91%)	117 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	8	41/66 (62%)	41 (100%)	0	100	100
2	a	200/200 (100%)	200 (100%)	0	100	100
3	d	139/142 (98%)	137 (99%)	2 (1%)	67	81
4	e	34/59 (58%)	33 (97%)	1 (3%)	42	64
5	f	72/75 (96%)	72 (100%)	0	100	100
6	g	67/83 (81%)	67 (100%)	0	100	100
7	j	42/49 (86%)	42 (100%)	0	100	100
8	k	31/46 (67%)	31 (100%)	0	100	100
9	M	45/50 (90%)	45 (100%)	0	100	100
9	N	50/50 (100%)	50 (100%)	0	100	100
9	O	34/50 (68%)	34 (100%)	0	100	100
10	b	186/190 (98%)	185 (100%)	1 (0%)	88	93
11	h	56/70 (80%)	56 (100%)	0	100	100
12	S	110/165 (67%)	110 (100%)	0	100	100
13	C	73/413 (18%)	73 (100%)	0	100	100
All	All	1180/1708 (69%)	1176 (100%)	4 (0%)	92	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	d	47	LYS
3	d	77	LYS
4	e	35	ARG
10	b	120	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	8	32	ASN
1	8	36	ASN
2	a	101	ASN
2	a	119	ASN
2	a	168	HIS
6	g	57	ASN
9	N	45	GLN
10	b	122	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)

3 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
9	M3L	M	43	9	10,11,12	0.42	0	9,14,16	0.40	0
9	M3L	N	43	9	10,11,12	0.51	0	9,14,16	0.65	0
9	M3L	O	43	9	10,11,12	0.55	0	9,14,16	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	M3L	M	43	9	-	2/9/10/12	-
9	M3L	N	43	9	-	6/9/10/12	-
9	M3L	O	43	9	-	1/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	M	43	M3L	N-CA-CB-CG
9	M	43	M3L	C-CA-CB-CG
9	N	43	M3L	N-CA-CB-CG
9	N	43	M3L	C-CA-CB-CG
9	O	43	M3L	CG-CD-CE-NZ
9	N	43	M3L	CD-CE-NZ-CM2
9	N	43	M3L	CD-CE-NZ-CM3
9	N	43	M3L	CD-CE-NZ-CM1
9	N	43	M3L	CE-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	43	M3L	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

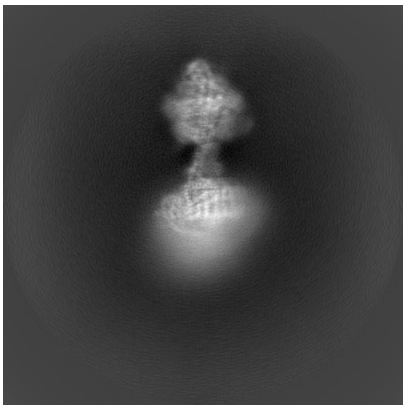
6 Map visualisation (i)

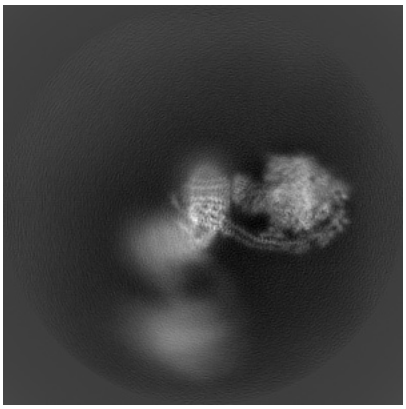
This section contains visualisations of the EMDB entry EMD-11228. These allow visual inspection of the internal detail of the map and identification of artifacts.

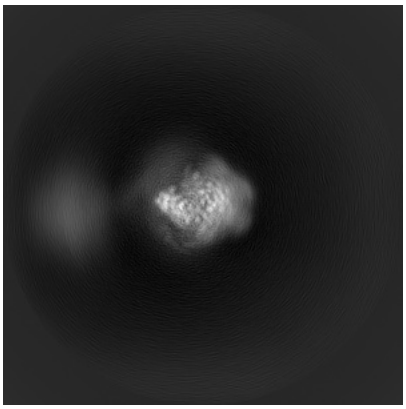
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

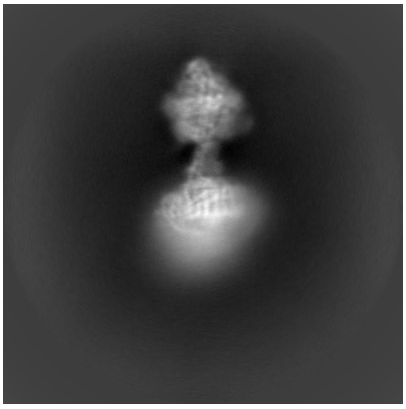
6.1.1 Primary map

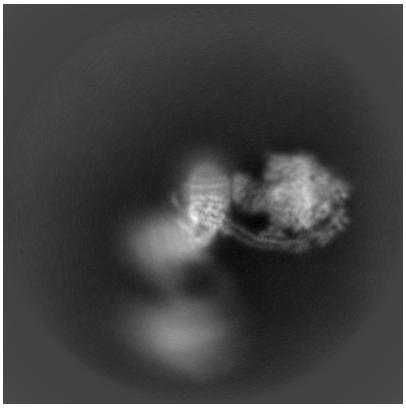

X

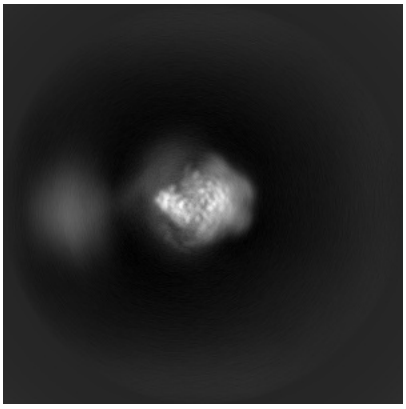

Y


Z

6.1.2 Raw map


X

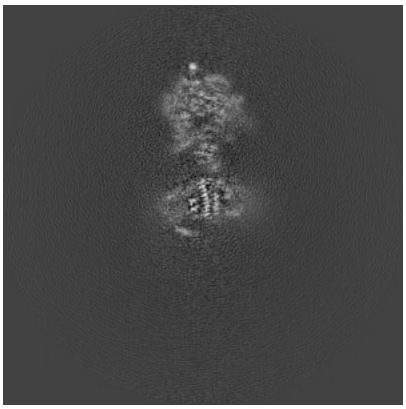

Y

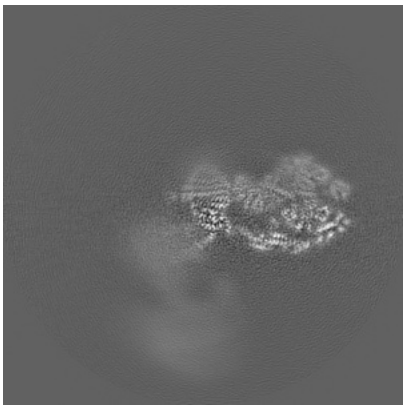

Z

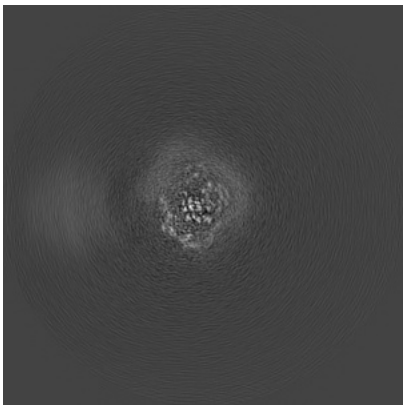
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

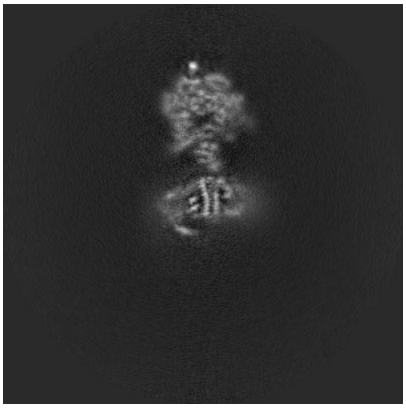
6.2.1 Primary map

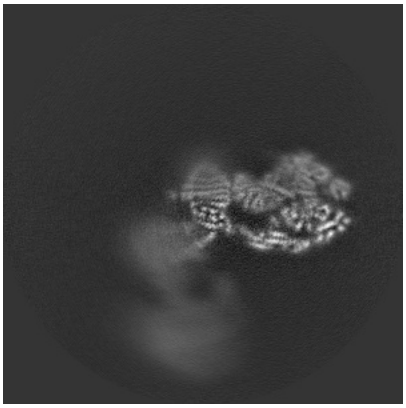

X Index: 250

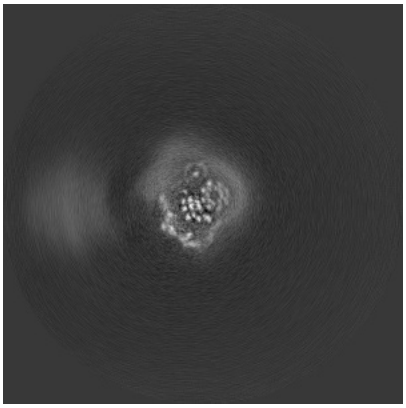

Y Index: 250


Z Index: 250

6.2.2 Raw map


X Index: 250

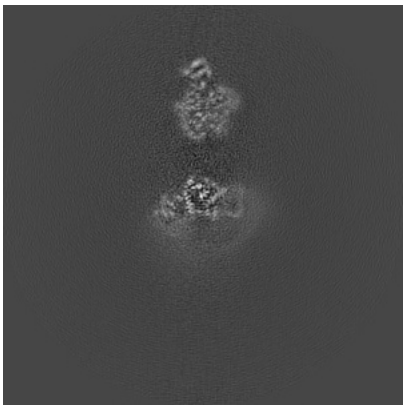

Y Index: 250

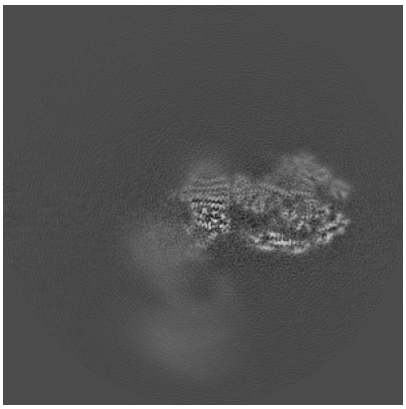

Z Index: 250

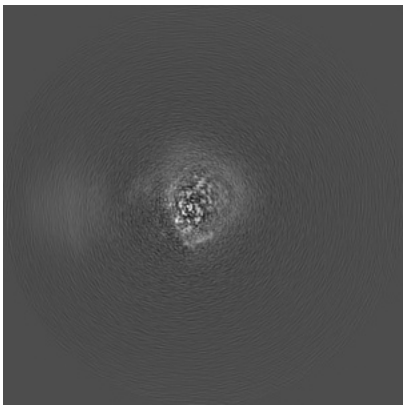
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

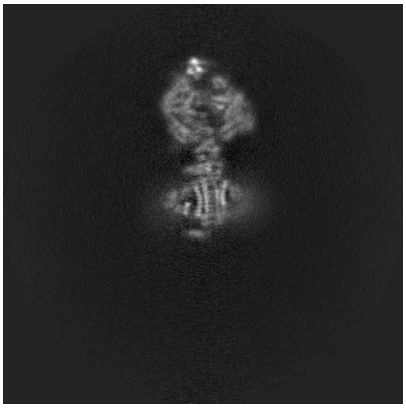
6.3.1 Primary map

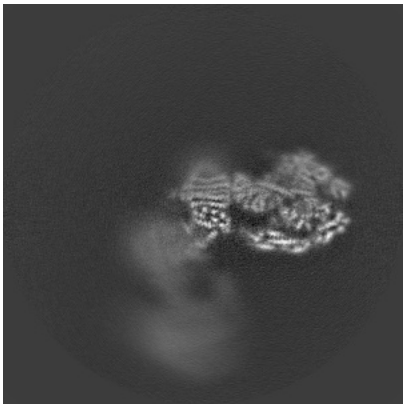

X Index: 231

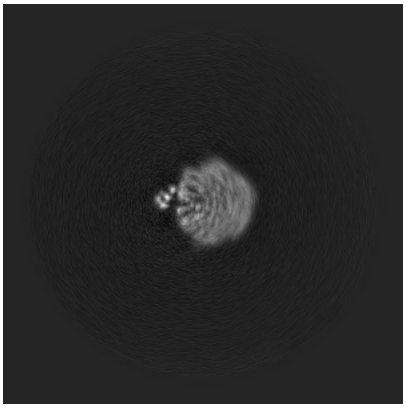

Y Index: 252


Z Index: 259

6.3.2 Raw map


X Index: 258


Y Index: 252


Z Index: 377

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 0.0187. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

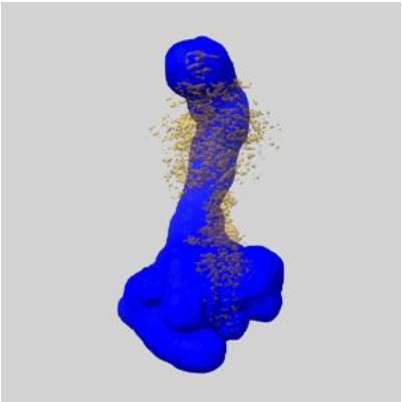
6.5 Mask visualisation (i)

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

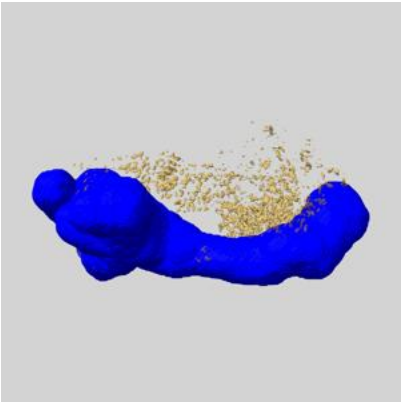
A mask typically either:

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

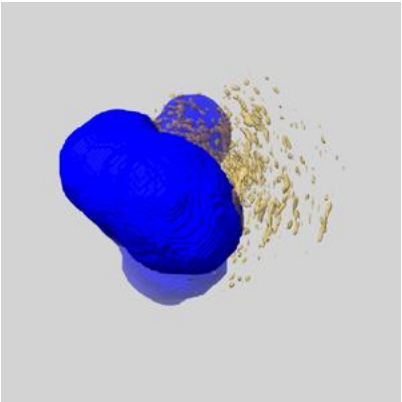
6.5.1 emd_11228_msk_1.map (i)



X



Y

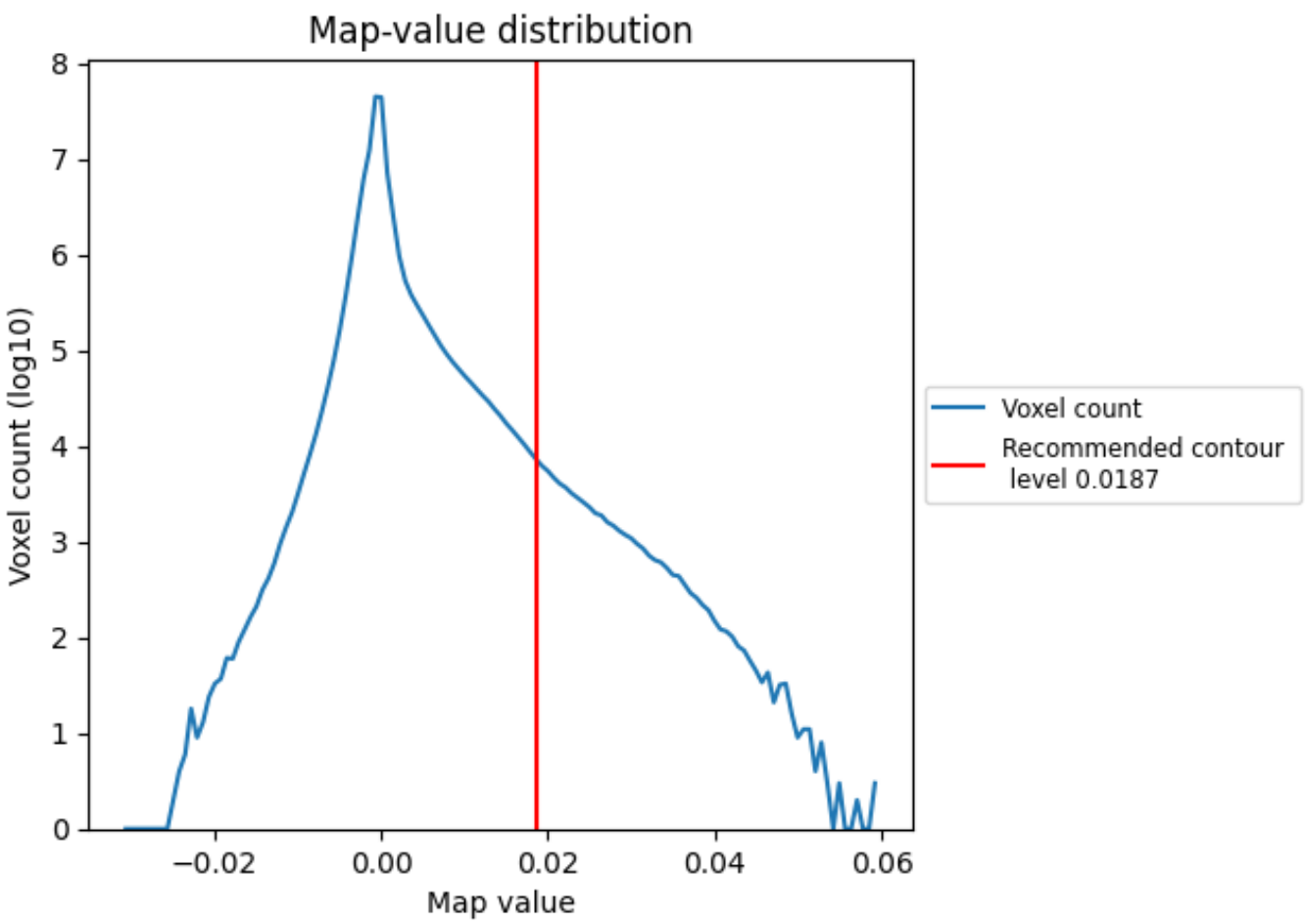


Z

7 Map analysis (i)

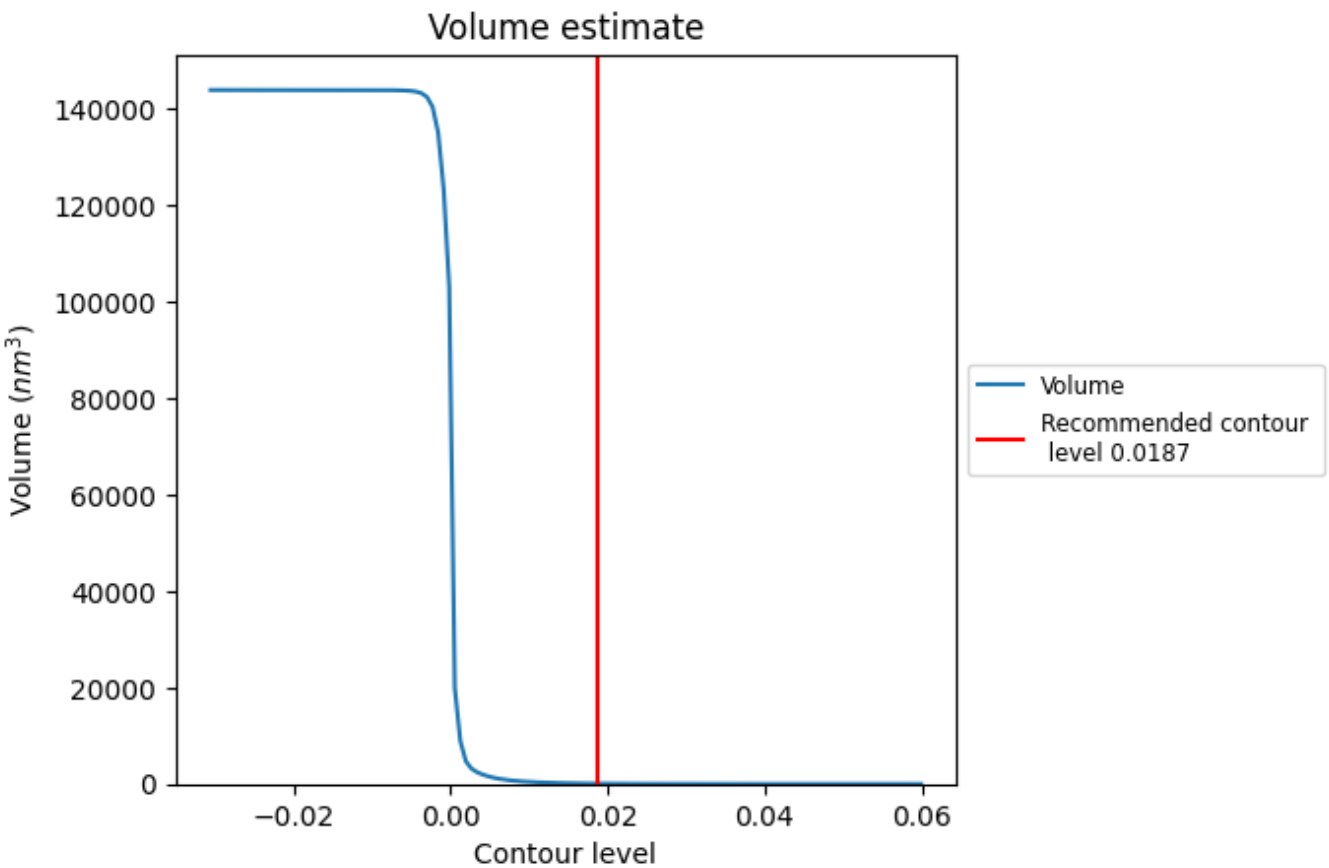
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

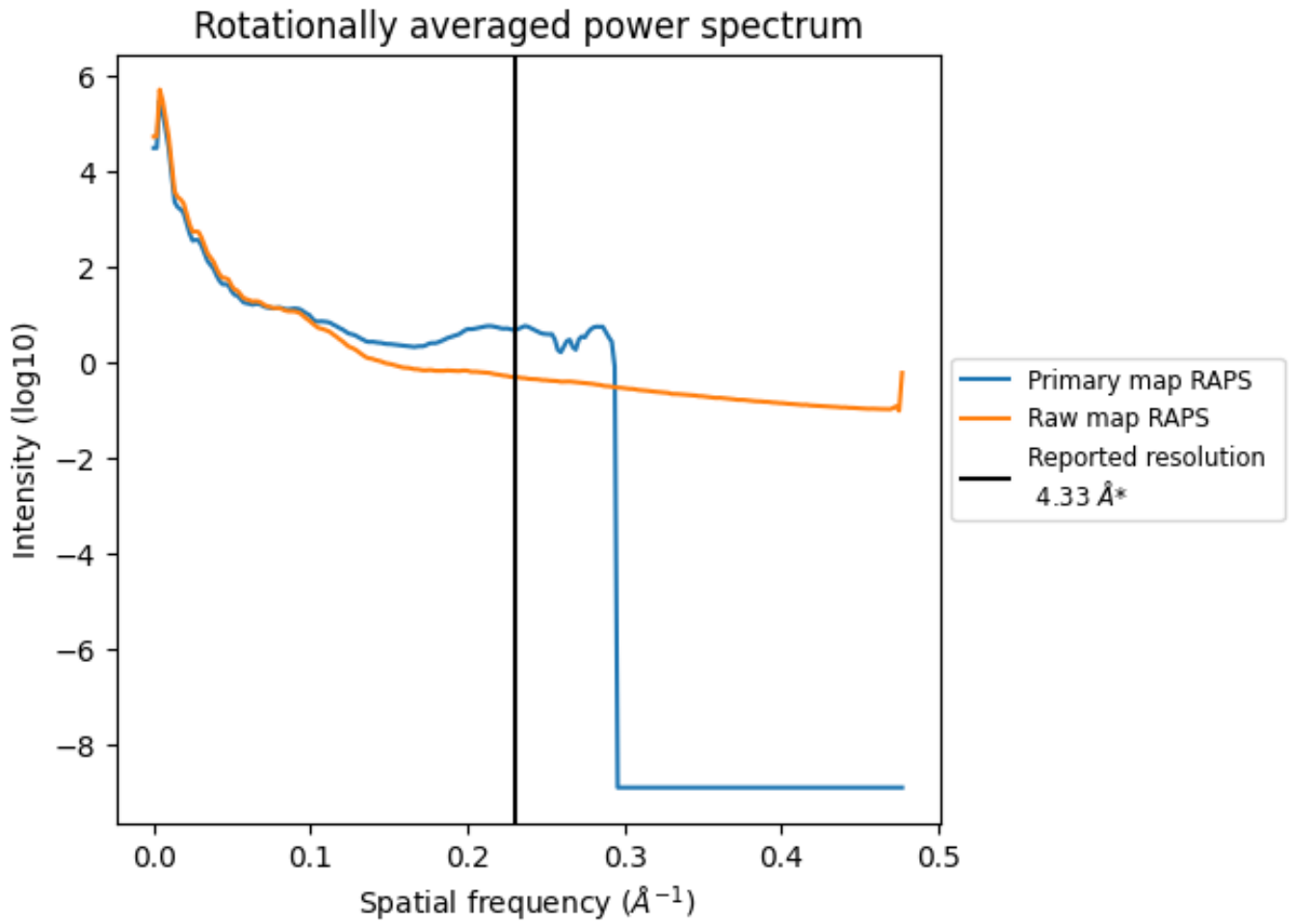
7.2 Volume estimate (i)



The volume at the recommended contour level is 68 nm^3; this corresponds to an approximate mass of 62 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)

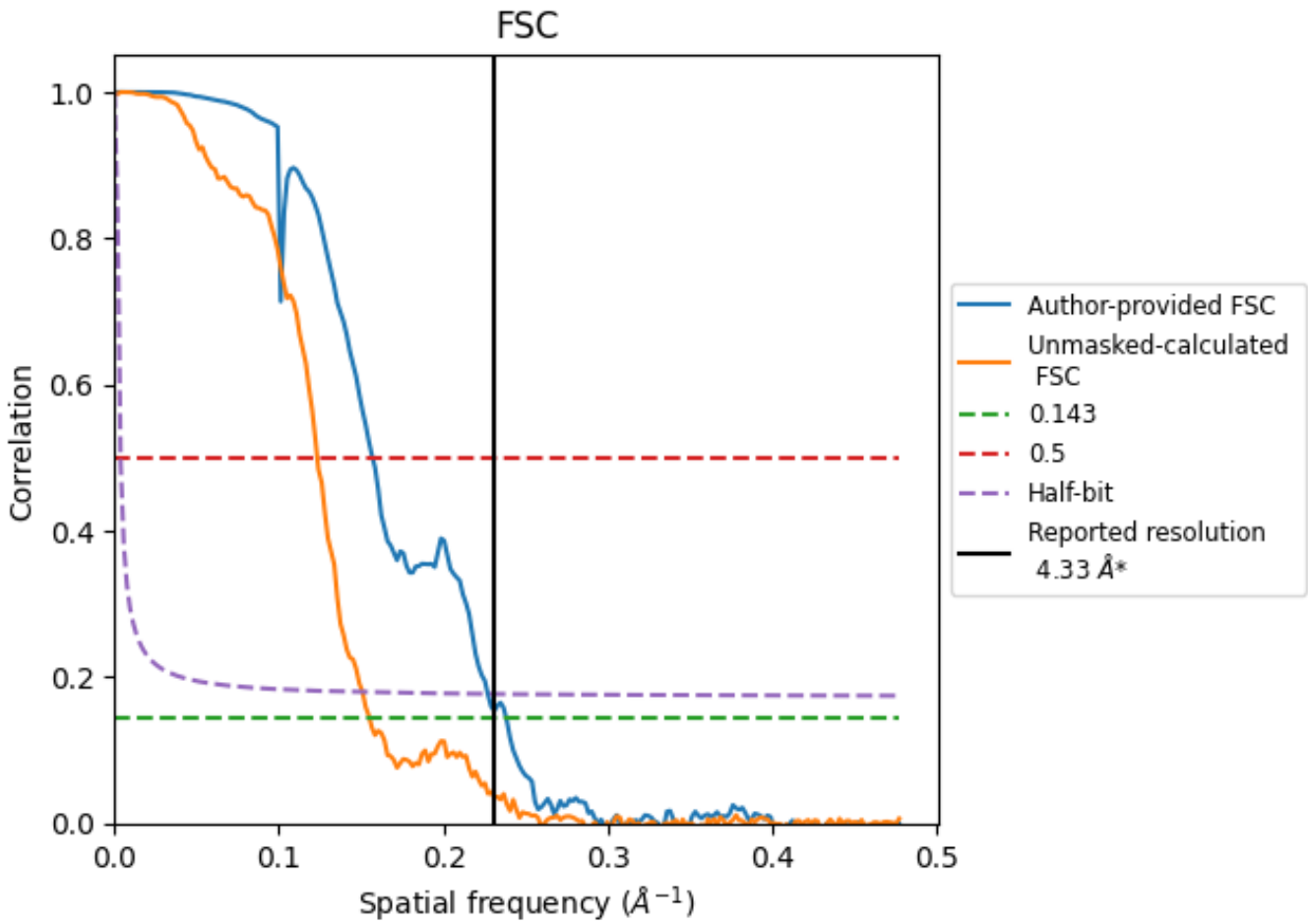


*Reported resolution corresponds to spatial frequency of 0.231 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.231 Å^{-1}

8.2 Resolution estimates (i)

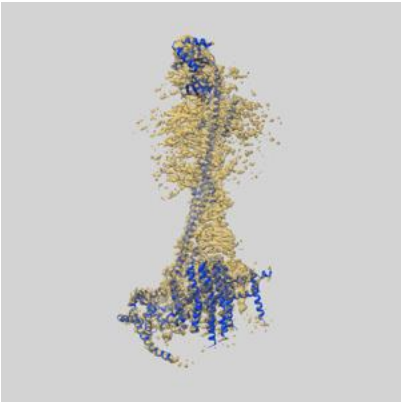
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.33	-	-
Author-provided FSC curve	4.20	6.38	4.41
Unmasked-calculated*	6.45	8.11	6.63

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.45 differs from the reported value 4.33 by more than 10 %

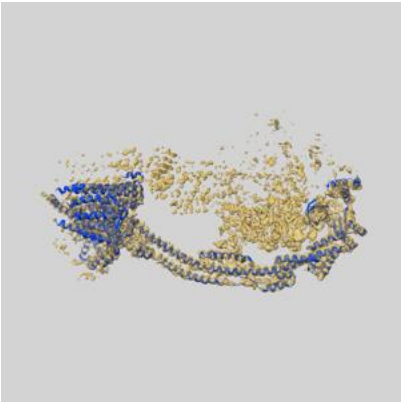
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11228 and PDB model 6ZIQ. Per-residue inclusion information can be found in section 3 on page 7.

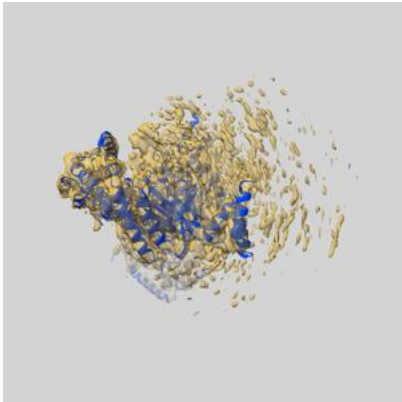
9.1 Map-model overlay (i)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0187 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

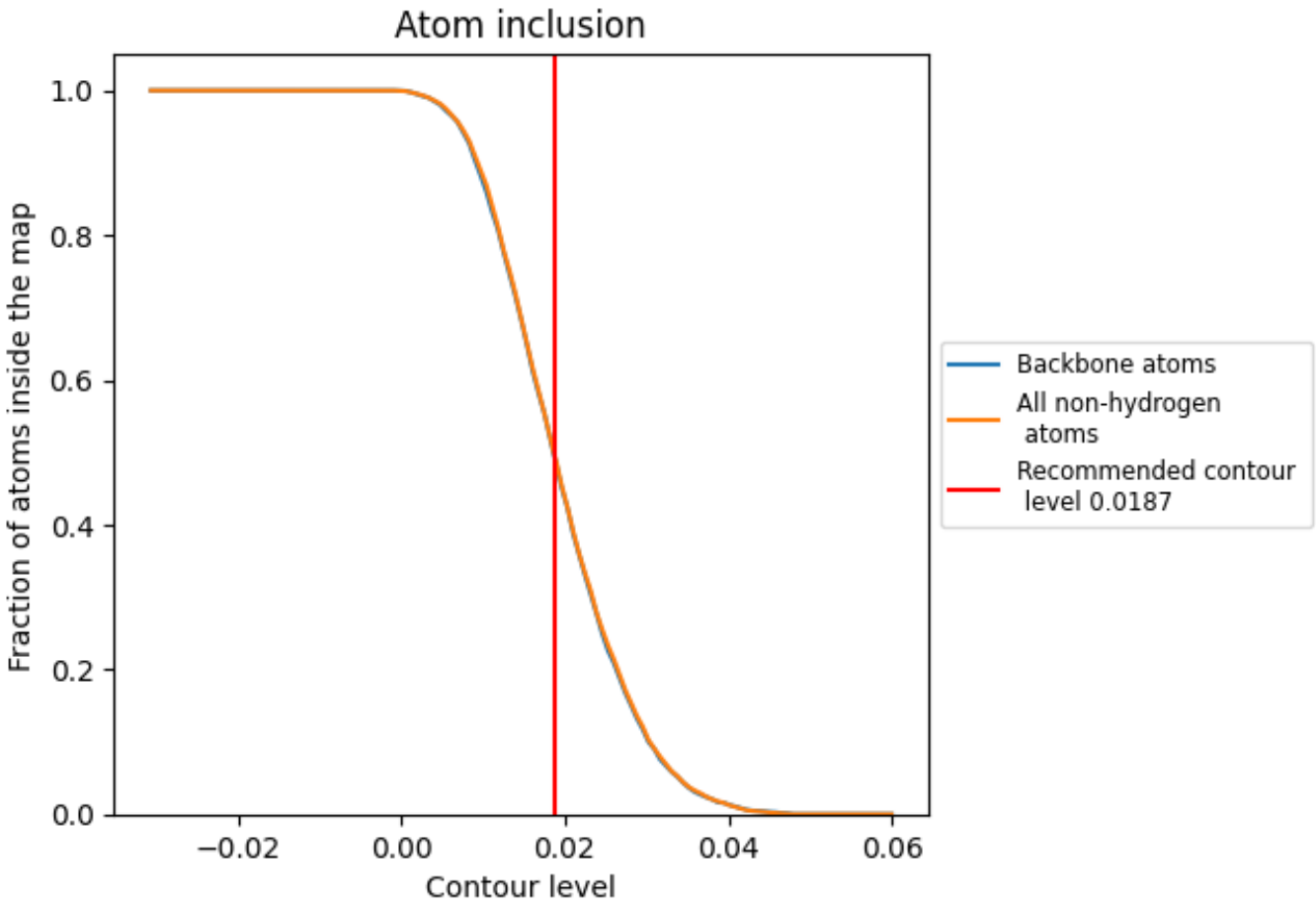
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0187).

9.4 Atom inclusion (i)



At the recommended contour level, 49% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0187) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4971	0.3850
8	0.5643	0.4680
C	0.4985	0.4010
M	0.3747	0.3840
N	0.3790	0.3810
O	0.2242	0.3610
S	0.4810	0.3240
a	0.5654	0.4300
b	0.6078	0.3970
d	0.5810	0.3970
e	0.4143	0.3410
f	0.5514	0.4200
g	0.3786	0.3380
h	0.4811	0.3010
j	0.3470	0.3870
k	0.1957	0.3220