WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Dec 18, 2022 – 11:54 pm GMT

PDB ID	:	7NJX
EMDB ID	:	EMD-12426
Title	:	Mycobacterium smegmatis ATP synthase Fo combined class 4
Authors	:	Montgomery, M.G.; Petri, J.; Spikes, T.E.; Walker, J.E.
Deposited on	:	2021-02-17
Resolution	:	4.32 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 (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:
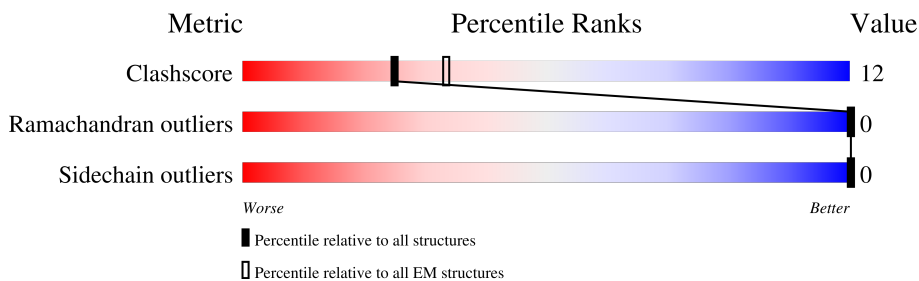
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 4.32 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.
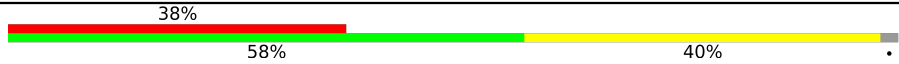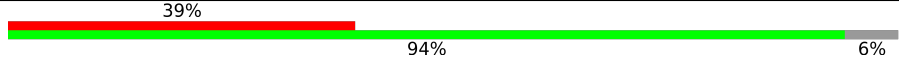
Metric	Percentile Ranks	Value
Clashscore		12
Ramachandran outliers		0
Sidechain outliers		0

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

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	L	86	47% / 66% 31% •
1	M	86	43% / 73% 24% •
1	N	86	45% / 80% 17% •
1	O	86	47% / 80% 17% •
1	P	86	36% / 81% 16% •
1	Q	86	37% / 72% 26% •
1	R	86	55% / 76% 22% •
1	S	86	58% / 63% 35% •

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Mol	Chain	Length	Quality of chain
1	T	86	38% 58% 40%
2	a	252	39% 94% 6%
3	b	180	9% 35% 65%
4	d	445	5% 14% 86%

2   Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 16426 atoms, of which 8337 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 subunit c.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	L	84	Total	C	H	N	O	S	0	0
			1192	387	603	96	104	2		
1	M	84	Total	C	H	N	O	S	0	0
			1192	387	603	96	104	2		
1	N	84	Total	C	H	N	O	S	0	0
			1192	387	603	96	104	2		
1	O	84	Total	C	H	N	O	S	0	0
			1192	387	603	96	104	2		
1	P	84	Total	C	H	N	O	S	0	0
			1192	387	603	96	104	2		
1	Q	84	Total	C	H	N	O	S	0	0
			1192	387	603	96	104	2		
1	R	84	Total	C	H	N	O	S	0	0
			1192	387	603	96	104	2		
1	S	84	Total	C	H	N	O	S	0	0
			1192	387	603	96	104	2		
1	T	84	Total	C	H	N	O	S	0	0
			1192	387	603	96	104	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	a	238	Total	C	H	N	O	S	0	0
			3767	1252	1916	292	301	6		

- Molecule 3 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	b	63	Total	C	H	N	O	S	0	0
			979	312	503	79	84	1		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	171	HIS	-	expression tag	UNP A0R204
b	172	HIS	-	expression tag	UNP A0R204
b	173	HIS	-	expression tag	UNP A0R204
b	174	HIS	-	expression tag	UNP A0R204
b	175	HIS	-	expression tag	UNP A0R204
b	176	HIS	-	expression tag	UNP A0R204
b	177	HIS	-	expression tag	UNP A0R204
b	178	HIS	-	expression tag	UNP A0R204
b	179	HIS	-	expression tag	UNP A0R204
b	180	HIS	-	expression tag	UNP A0R204

• Molecule 4 is a protein called ATP synthase subunit b-delta.

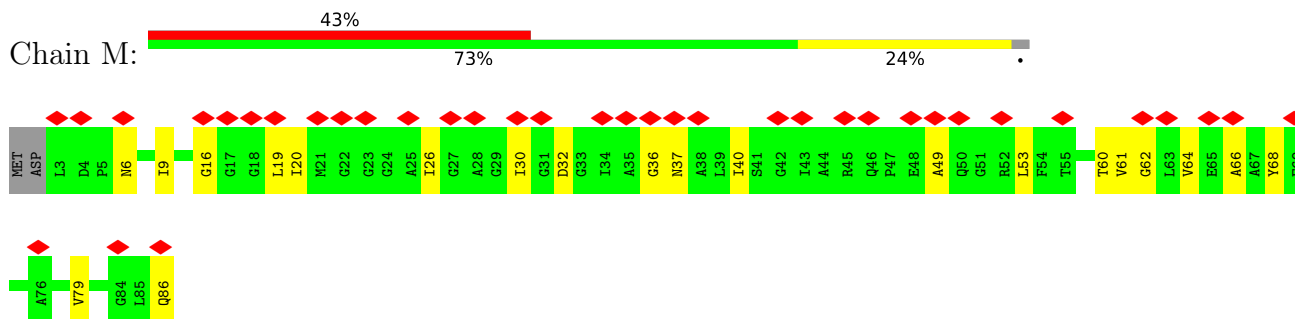| Mol	Chain	Residues	Atoms						AltConf	Trace
4	d	61	Total	C	H	N	O	S	0	0
			952	299	491	81	78	3		

3 Residue-property plots ⓘ

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.
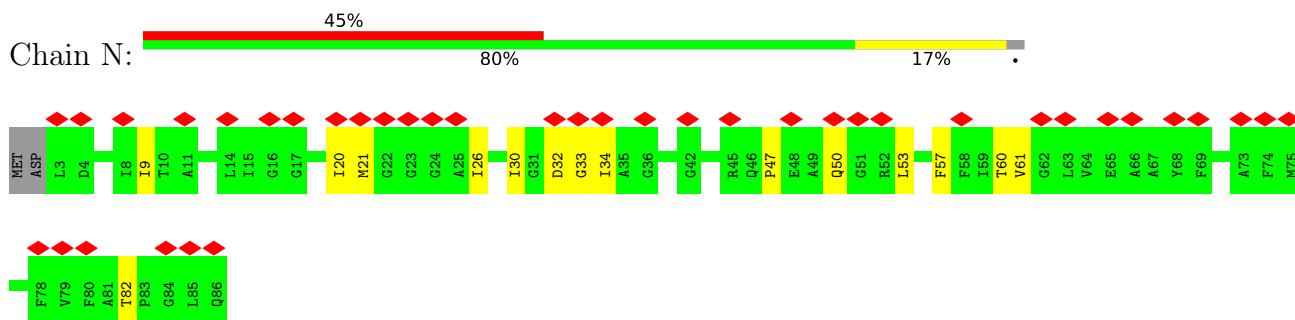
• Molecule 1: ATP synthase subunit c
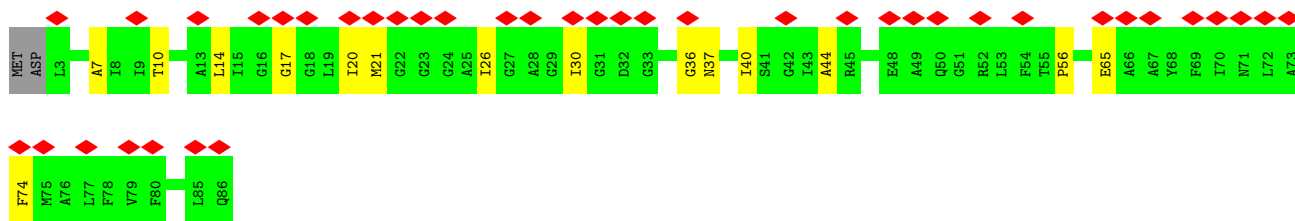

• Molecule 1: ATP synthase subunit c

• Molecule 1: ATP synthase subunit c

• Molecule 1: ATP synthase subunit c
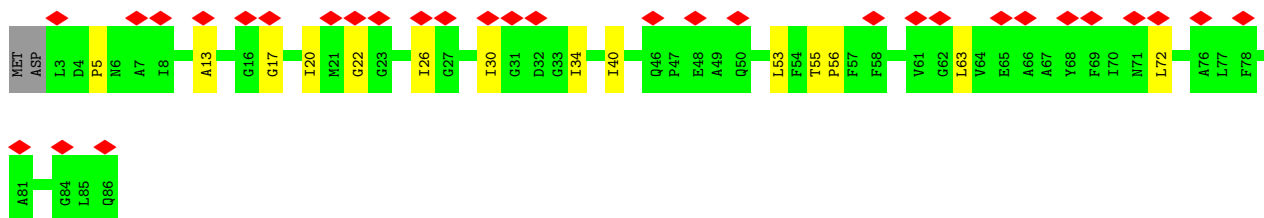
• Molecule 1: ATP synthase subunit c

Chain P:

• Molecule 1: ATP synthase subunit c

Chain Q:

• Molecule 1: ATP synthase subunit c

Chain R:

• Molecule 1: ATP synthase subunit c

Chain S:

A66 A67 Y68 F69 I70 N71 L72 A73 F74 M75 A76 L77 F78 A81 T82 P83 G84 L85 Q86
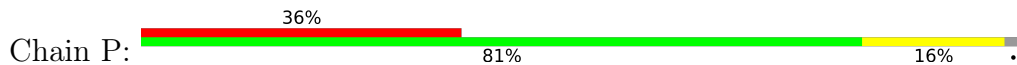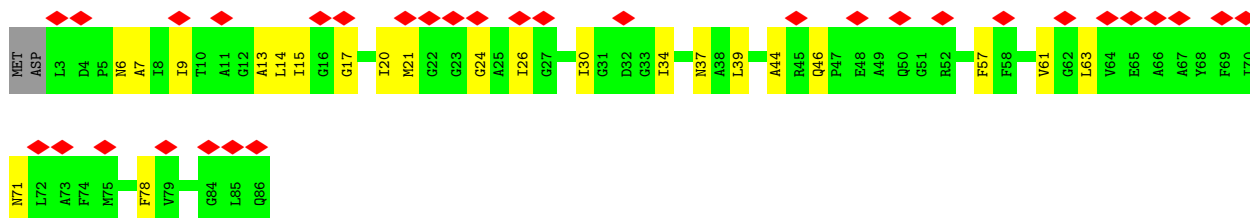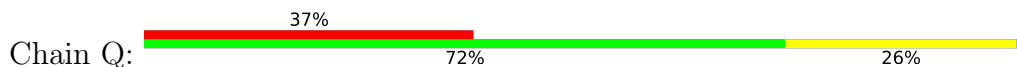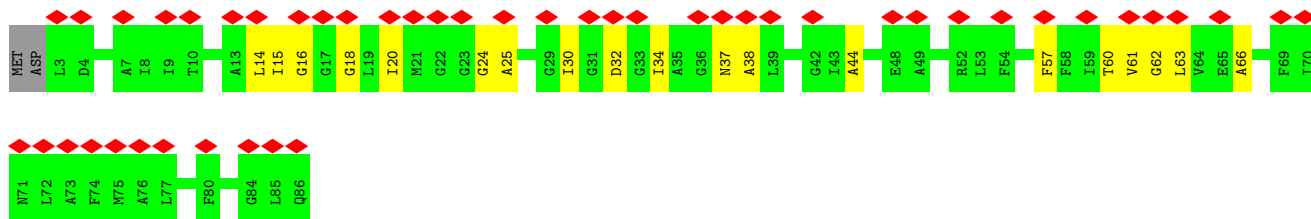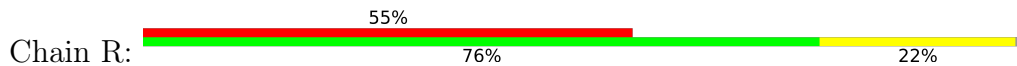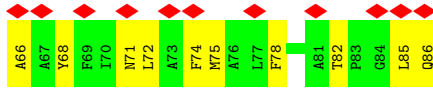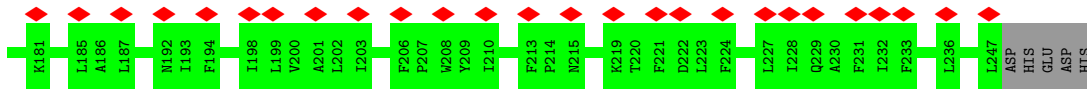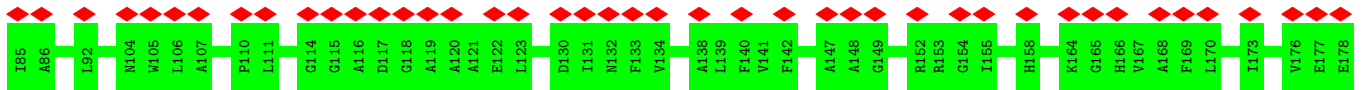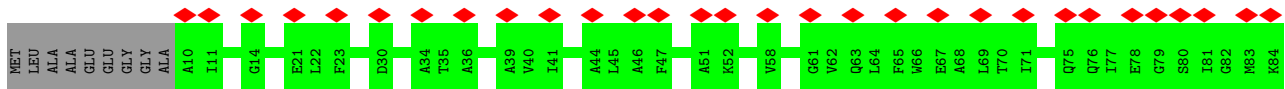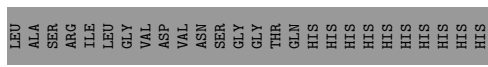
• Molecule 1: ATP synthase subunit c

Chain T:

38%
58%   40%

MET ASP L3 A7 I8 I9 T10 A11 G12 A13 L14 I15 G16 G17 G18 L19 I20 M21 G22 G23 G24 A25 I26 G29 I30 G31 D32 G33 I34 A35 G36 N37 A38 L39 I40 S41 G42 I43 A44 R45 Q46 P47 E48 R52 L53 F54 T55 P56 F57 F58 I59 T60 V61 G62 L63 V64 E65

A66 A67 Y68 F69 L72 A73 F74 M75 A76 L77 F78 V79 T82 Q86

• Molecule 2: ATP synthase subunit a

Chain a:

39%
94%   6%

MET LEU ALA ALA GLU GLU GLY ALA A10 I11 G14 E21 L22 F23 D30 A34 T35 A36 A39 V40 I41 A44 L45 A46 F47 A51 K52 V58 G61 V62 Q63 L64 F65 W66 E67 A68 L69 T70 I71 Q75 Q76 I77 E78 G79 S80 I81 G82 M83 K84

I85 A86 L92 N104 W105 L106 A107 P110 L111 G114 G115 A116 D117 G118 A119 A120 A121 E122 L123 D130 I131 N132 F133 V134 A138 L139 F140 V141 F142 A147 A148 G149 R152 R153 G154 I155 H158 K164 G165 H166 V167 A168 F169 L170 I173 V176 E177 E178

K181 L185 A186 L187 N192 I193 F194 I198 L199 V200 A201 L202 I203 F206 P207 W208 Y209 I210 F213 P214 N215 K219 T220 F221 D222 L223 F224 L227 I228 Q229 A230 F231 I232 F233 L236 L247 ASP HIS GLU ASP HIS

• Molecule 3: ATP synthase subunit b

Chain b:

9%
35%   65%

MET GLY GLU PHE SER ALA THR ILE LEU LEU ALA ALA SER GLN ALA ALA GLU GLU GLY GLY GLY S22 N23 F24 L25 I26 F31 F32 L35 I36 W48 V49 E59 R60 E61 A62 D70 E76 A79 Q82 A83 D84 TYR GLU LYS GLU MET ALA GLU GLU ALA ARG ALA

GLN ALA SER ALA LEU ARG ASP GLU ALA ARG ALA ALA GLY ARG SER VAL VAL ASP GLU LYS ARG ALA GLN ALA SER GLY GLU VAL VAL ALA GLN THR LEU THR GLN ALA ASP GLN LEU LEU SER ALA GLN GLY ASP VAL ARG SER GLY LEU GLU SER SER VAL ASP GLY LEU LEU SER ALA LYS

LEU ALA SER ARG ILE LEU GLY VAL ASP VAL ASN SER GLY GLY THR GLN HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS

• Molecule 4: ATP synthase subunit b-delta

Chain d:

5%
14%   86%

M1 S2 I3 F4 I5 G6 Q7 L8 I9 G10 F11 A12 I17 I18 V19 K20 R27 R31 N32 E35 A36 V37 R38 A39 A40 L41 E46 A47 A48 K60 A61 LEU ALA ASP ALA LYS ALA GLU GLU SER GLU LYS VAL THR GLU GLU ALA LYS GLN ASP SER GLU ARG ILE ALA

ALA GLN LEU SER GLU GLN ALA GLY SER GLU ALA GLU ARG ILE LYS ALA GLN GLY ALA GLN GLN ILE LEU GLN LEU MET ARG GLN GLN LEU ILE ARG GLN LEU ARG THR GLY LEU GLY ALA GLU ALA VAL ASN LYS ALA ALA GLU ILE VAL ARG ALA HIS VAL ALA ASP PRO GLN ALA GLN SER

ALA THR VAL ASP ARG PHE LEU SER GLU GLU LEU GLN GLN MET ALA PRO SER SER VAL VAL ILE ASP THR ALA ALA THR SER ARG GLN LEU ARG ALA ALA SER ARG GLN GLN SER LEU ALA LEU GLU VAL LYS PHE ASP SER VAL ALA GLY LEU GLU ASP ALA ALA GLY LEU THR ASN LEU ALA ASP

GLU LEU ALA SER VAL ALA LYS LEU LEU SER GLU THR ALA LEU ASN LYS HIS LEU ALA GLU PRO THR ASP ASP SER ALA PRO LYS VAL ARG LEU GLU GLU ARG SER LEU LEU SER ASP LYS VAL SER ALA THR THR LEU ASP LEU LEU ARG ALA VAL ASN SER ARG TRP SER THR GLU

SER ASN LEU ILE ASP ALA VAL GLU HIS THR ALA ARG ALA LEU ALA LEU LEU LYS ARG GLU ALA GLU ILE ALA GLY LEU VAL ASP GLU VAL GLU GLN GLN LEU PHE ARG PHE GLY VAL ARG LEU ASP ALA ILE GLU ALA LEU PRO ARG LEU SER ALA LEU LEU SER ASP TYR THR PRO ALA GLY GLY ARG VAL

ALA LEU LEU ASP LYS ALA LEU THR GLY ARG PRO GLY VAL ASN GLN THR ALA ALA LEU LEU SER GLN THR VAL GLY LEU LEU ARG GLY GLU GLU ARG ALA ASP GLU ALA VAL ILE ASP LEU ALA GLU LEU ALA VAL VAL SER ARG ALA GLY LEU VAL VAL ALA HIS VAL SER VAL SER ALA ALA ALA GLU

LEU SER ASP ALA GLN ARG THR ARG LEU THR GLU VAL LEU SER ARG ILE TYR GLY ARG PRO VAL SER VAL GLN LEU LEU HIS VAL ASP PRO GLU LEU LEU GLY LEU SER ILE THR VAL GLY ASP GLU VAL ILE ASP SER GLY SER ILE ALA SER ARG LEU ALA ALA ALA GLN THR GLY LEU PRO

ASP

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16411	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 $(e^-/\text{Å}^2)$	59.86	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.038	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0144	Depositor
Map size (Å)	415.0, 415.0, 415.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	L	0.28	0/600	0.47	0/814
1	M	0.27	0/600	0.45	0/814
1	N	0.27	0/600	0.46	0/814
1	O	0.27	0/600	0.45	0/814
1	P	0.27	0/600	0.44	0/814
1	Q	0.27	0/600	0.45	0/814
1	R	0.27	0/600	0.45	0/814
1	S	0.27	0/600	0.46	0/814
1	T	0.26	0/600	0.45	0/814
2	a	0.26	0/1905	0.43	0/2602
3	b	0.26	0/484	0.41	0/658
4	d	0.25	0/468	0.44	0/632
All	All	0.27	0/8257	0.44	0/11218

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	L	589	603	603	26	0
1	M	589	603	603	18	0
1	N	589	603	603	21	0
1	O	589	603	603	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	589	603	603	18	0
1	Q	589	603	603	23	0
1	R	589	603	603	24	0
1	S	589	603	603	30	0
1	T	589	603	603	34	0
2	a	1851	1916	1916	0	0
3	b	476	503	503	0	0
4	d	461	491	491	0	0
All	All	8089	8337	8337	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 12.

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)
1:T:78:PHE:O	1:T:82:THR:OG1	2.03	0.76
1:Q:46:GLN:NE2	1:R:44:ALA:O	2.19	0.76
1:S:71:ASN:OD1	1:T:68:TYR:OH	2.03	0.73
1:N:32:ASP:OD1	1:N:33:GLY:N	2.21	0.73
1:S:71:ASN:ND2	1:T:25:ALA:HB2	2.06	0.70
1:O:30:ILE:HG21	1:P:30:ILE:CD1	2.24	0.68
1:Q:17:GLY:HA2	1:Q:20:ILE:HD12	1.75	0.68
1:T:46:GLN:OE1	1:T:52:ARG:NH2	2.28	0.66
1:P:63:LEU:HD23	1:Q:61:VAL:HG21	1.79	0.65
1:L:67:ALA:O	1:L:70:ILE:HG22	1.98	0.64
1:O:10:THR:O	1:O:14:LEU:HD23	1.99	0.63
1:P:20:ILE:HG23	1:Q:21:MET:SD	2.40	0.62
1:S:56:PRO:O	1:S:60:THR:HG23	2.00	0.61
1:N:9:ILE:HD11	1:O:7:ALA:HA	1.81	0.61
1:O:30:ILE:HG21	1:P:30:ILE:HD13	1.83	0.61
1:L:67:ALA:O	1:L:71:ASN:ND2	2.33	0.61
1:S:10:THR:O	1:S:14:LEU:HD23	2.02	0.59
1:M:6:ASN:ND2	1:M:86:GLN:O	2.35	0.57
1:S:5:PRO:HB3	1:T:7:ALA:HB2	1.85	0.57
1:Q:63:LEU:HD22	1:R:32:ASP:OD2	2.05	0.56
1:S:6:ASN:ND2	1:S:86:GLN:O	2.38	0.56
1:R:38:ALA:HB2	1:S:37:ASN:OD1	2.04	0.56
1:S:38:ALA:HB1	1:T:40:ILE:HB	1.86	0.55
1:S:74:PHE:CE2	1:T:72:LEU:HD13	2.40	0.55
1:P:30:ILE:HG21	1:Q:30:ILE:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:34:ILE:HG22	1:O:37:ASN:HB2	1.88	0.55
1:S:38:ALA:HB2	1:T:37:ASN:OD1	2.06	0.55
1:N:20:ILE:HG23	1:O:21:MET:CE	2.38	0.54
1:L:71:ASN:OD1	1:M:68:TYR:OH	2.22	0.53
1:N:57:PHE:CZ	1:N:61:VAL:HG21	2.43	0.53
1:N:47:PRO:O	1:N:50:GLN:NE2	2.38	0.53
1:S:85:LEU:HD12	1:S:85:LEU:O	2.09	0.52
1:S:19:LEU:HD13	1:T:19:LEU:HG	1.91	0.52
1:M:30:ILE:HG21	1:N:30:ILE:HG12	1.92	0.52
1:T:56:PRO:O	1:T:60:THR:HG23	2.10	0.52
1:L:7:ALA:HA	1:T:9:ILE:HD11	1.92	0.52
1:M:49:ALA:O	1:M:53:LEU:HD23	2.09	0.52
1:M:62:GLY:O	1:M:66:ALA:N	2.33	0.52
1:L:56:PRO:O	1:L:59:ILE:HG22	2.11	0.51
1:Q:39:LEU:HD22	1:Q:57:PHE:CG	2.46	0.51
1:S:68:TYR:CZ	1:S:72:LEU:HD21	2.45	0.50
1:O:74:PHE:CE2	1:P:72:LEU:HD11	2.46	0.50
1:N:20:ILE:HG23	1:O:21:MET:HE1	1.94	0.50
1:M:79:VAL:O	1:M:79:VAL:HG12	2.12	0.49
1:Q:6:ASN:HA	1:Q:9:ILE:HD12	1.94	0.49
1:Q:20:ILE:CG1	1:R:18:GLY:HA2	2.42	0.49
1:Q:30:ILE:HG21	1:R:30:ILE:HG12	1.94	0.49
1:L:64:VAL:N	1:M:32:ASP:OD2	2.45	0.49
1:L:22:GLY:O	1:L:26:ILE:HG12	2.12	0.49
1:Q:13:ALA:HA	1:R:14:LEU:HD23	1.96	0.48
1:O:56:PRO:HG2	1:P:40:ILE:HD13	1.95	0.48
1:S:15:ILE:HB	1:T:15:ILE:CD1	2.44	0.47
1:N:57:PHE:N	1:O:40:ILE:HD11	2.30	0.47
1:M:20:ILE:HG23	1:N:21:MET:HE1	1.96	0.47
1:O:65:GLU:HA	1:O:65:GLU:OE2	2.14	0.47
1:S:60:THR:HG22	1:T:36:GLY:HA3	1.97	0.46
1:R:57:PHE:O	1:R:61:VAL:HG12	2.15	0.46
1:L:30:ILE:HG13	1:L:31:GLY:N	2.30	0.46
1:P:53:LEU:HD21	1:Q:44:ALA:HB2	1.97	0.46
1:L:26:ILE:O	1:L:30:ILE:HG12	2.16	0.46
1:R:38:ALA:HB1	1:S:40:ILE:HB	1.98	0.46
1:M:26:ILE:HG23	1:N:26:ILE:HG12	1.98	0.46
1:L:67:ALA:O	1:L:68:TYR:C	2.55	0.45
1:R:61:VAL:HG13	1:R:62:GLY:N	2.31	0.45
1:T:21:MET:HE3	1:T:72:LEU:HA	1.98	0.45
1:L:79:VAL:HG23	1:L:80:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:16:GLY:O	1:M:20:ILE:HG12	2.16	0.45
1:L:14:LEU:HD23	1:T:13:ALA:HA	1.98	0.45
1:P:34:ILE:HG22	1:Q:37:ASN:HB2	1.99	0.45
1:S:78:PHE:O	1:S:82:THR:OG1	2.23	0.45
1:T:11:ALA:O	1:T:15:ILE:HG12	2.17	0.45
1:L:37:ASN:HA	1:T:38:ALA:HB2	1.99	0.45
1:M:30:ILE:HG21	1:N:30:ILE:HG23	1.98	0.45
1:Q:20:ILE:HD11	1:Q:78:PHE:CE2	2.52	0.45
1:R:38:ALA:HB2	1:S:37:ASN:CG	2.38	0.44
1:R:63:LEU:O	1:R:66:ALA:HB3	2.17	0.44
1:L:63:LEU:O	1:L:66:ALA:HB3	2.18	0.44
1:M:60:THR:OG1	1:M:61:VAL:N	2.50	0.44
1:S:65:GLU:O	1:S:66:ALA:C	2.56	0.44
1:P:17:GLY:HA2	1:P:20:ILE:HD12	1.99	0.44
1:L:61:VAL:HG11	1:T:63:LEU:HD13	1.98	0.44
1:O:17:GLY:HA2	1:O:20:ILE:HD12	1.99	0.44
1:S:34:ILE:HG22	1:T:37:ASN:HB2	2.00	0.44
1:T:29:GLY:O	1:T:32:ASP:OD1	2.34	0.44
1:L:26:ILE:HD12	1:T:26:ILE:HG21	1.99	0.43
1:L:72:LEU:HD11	1:T:74:PHE:CZ	2.53	0.43
1:R:24:GLY:HA2	1:S:25:ALA:HB1	2.00	0.43
1:M:64:VAL:HG22	1:N:32:ASP:OD1	2.18	0.43
1:L:34:ILE:HG22	1:M:37:ASN:HB2	2.00	0.43
1:Q:24:GLY:HA2	1:R:25:ALA:HB1	2.01	0.43
1:N:53:LEU:HD21	1:O:44:ALA:HB2	2.00	0.43
1:Q:15:ILE:HG22	1:R:15:ILE:CD1	2.49	0.43
1:T:36:GLY:O	1:T:40:ILE:HG12	2.19	0.43
1:L:38:ALA:HB1	1:M:40:ILE:HB	1.99	0.43
1:T:32:ASP:OD1	1:T:33:GLY:N	2.52	0.43
1:P:22:GLY:O	1:P:26:ILE:HG12	2.19	0.43
1:R:60:THR:HG23	1:R:61:VAL:N	2.33	0.43
1:M:6:ASN:HA	1:M:9:ILE:HD12	2.01	0.42
1:R:16:GLY:O	1:R:20:ILE:HG13	2.19	0.42
1:T:55:THR:HB	1:T:56:PRO:HD3	2.01	0.42
1:L:40:ILE:HB	1:T:38:ALA:HB1	2.02	0.42
1:N:32:ASP:OD1	1:N:32:ASP:C	2.57	0.42
1:L:19:LEU:HD13	1:M:19:LEU:CD1	2.49	0.42
1:T:40:ILE:O	1:T:43:ILE:HG22	2.19	0.42
1:S:63:LEU:HD23	1:T:32:ASP:HB2	2.01	0.42
1:N:30:ILE:HG21	1:O:30:ILE:CD1	2.49	0.42
1:N:9:ILE:HG22	1:N:82:THR:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:34:ILE:HG22	1:R:37:ASN:HB2	2.01	0.42
1:S:30:ILE:HG21	1:T:30:ILE:HD13	2.02	0.42
1:P:26:ILE:HG21	1:Q:26:ILE:HD12	2.02	0.42
1:T:45:ARG:NE	1:T:45:ARG:HA	2.35	0.42
1:L:32:ASP:CB	1:T:64:VAL:HG22	2.49	0.42
1:O:26:ILE:HG21	1:P:26:ILE:HD12	2.01	0.42
1:P:13:ALA:HB2	1:Q:14:LEU:HD13	2.02	0.42
1:S:11:ALA:O	1:S:15:ILE:HG12	2.20	0.42
1:L:21:MET:HE3	1:L:72:LEU:HA	2.02	0.41
1:L:32:ASP:HB3	1:T:64:VAL:HG22	2.01	0.41
1:O:26:ILE:HB	1:P:26:ILE:CD1	2.50	0.41
1:Q:71:ASN:OD1	1:R:25:ALA:HB2	2.20	0.41
1:L:56:PRO:HA	1:L:59:ILE:HG22	2.02	0.41
1:Q:20:ILE:HG13	1:R:18:GLY:HA2	2.02	0.41
1:L:60:THR:HG21	1:M:36:GLY:HA3	2.02	0.41
1:R:34:ILE:HD13	1:S:34:ILE:HG13	2.02	0.41
1:P:26:ILE:HB	1:Q:26:ILE:CD1	2.51	0.41
1:P:55:THR:HB	1:P:56:PRO:HD3	2.03	0.41
1:N:26:ILE:HB	1:O:26:ILE:CD1	2.50	0.41
1:P:5:PRO:HB3	1:Q:7:ALA:HB2	2.03	0.41
1:S:17:GLY:HA2	1:S:75:MET:HG2	2.02	0.41
1:R:15:ILE:CG2	1:S:15:ILE:HD12	2.51	0.40
1:T:61:VAL:HG13	1:T:62:GLY:N	2.37	0.40
1:N:60:THR:HG21	1:O:36:GLY:HA3	2.03	0.40
1:N:26:ILE:HB	1:O:26:ILE:HD11	2.03	0.40
1:R:20:ILE:HG12	1:S:21:MET:HB2	2.02	0.40
1:S:9:ILE:HD12	1:T:10:THR:HB	2.02	0.40
1:N:30:ILE:HG21	1:O:30:ILE:HD12	2.04	0.40
1:R:34:ILE:HG22	1:S:37:ASN:HB2	2.04	0.40
1:R:57:PHE:HA	1:R:60:THR:HG22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	L	82/86 (95%)	75 (92%)	7 (8%)	0	100	100
1	M	82/86 (95%)	74 (90%)	8 (10%)	0	100	100
1	N	82/86 (95%)	77 (94%)	5 (6%)	0	100	100
1	O	82/86 (95%)	80 (98%)	2 (2%)	0	100	100
1	P	82/86 (95%)	78 (95%)	4 (5%)	0	100	100
1	Q	82/86 (95%)	76 (93%)	6 (7%)	0	100	100
1	R	82/86 (95%)	78 (95%)	4 (5%)	0	100	100
1	S	82/86 (95%)	79 (96%)	3 (4%)	0	100	100
1	T	82/86 (95%)	77 (94%)	5 (6%)	0	100	100
2	a	236/252 (94%)	225 (95%)	11 (5%)	0	100	100
3	b	61/180 (34%)	54 (88%)	7 (12%)	0	100	100
4	d	59/445 (13%)	58 (98%)	1 (2%)	0	100	100
All	All	1094/1651 (66%)	1031 (94%)	63 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	L	54/56 (96%)	54 (100%)	0	100	100
1	M	54/56 (96%)	54 (100%)	0	100	100
1	N	54/56 (96%)	54 (100%)	0	100	100
1	O	54/56 (96%)	54 (100%)	0	100	100
1	P	54/56 (96%)	54 (100%)	0	100	100
1	Q	54/56 (96%)	54 (100%)	0	100	100
1	R	54/56 (96%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	54/56 (96%)	54 (100%)	0	100	100
1	T	54/56 (96%)	54 (100%)	0	100	100
2	a	191/200 (96%)	191 (100%)	0	100	100
3	b	50/134 (37%)	50 (100%)	0	100	100
4	d	45/347 (13%)	45 (100%)	0	100	100
All	All	772/1185 (65%)	772 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	71	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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-12426. 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 |
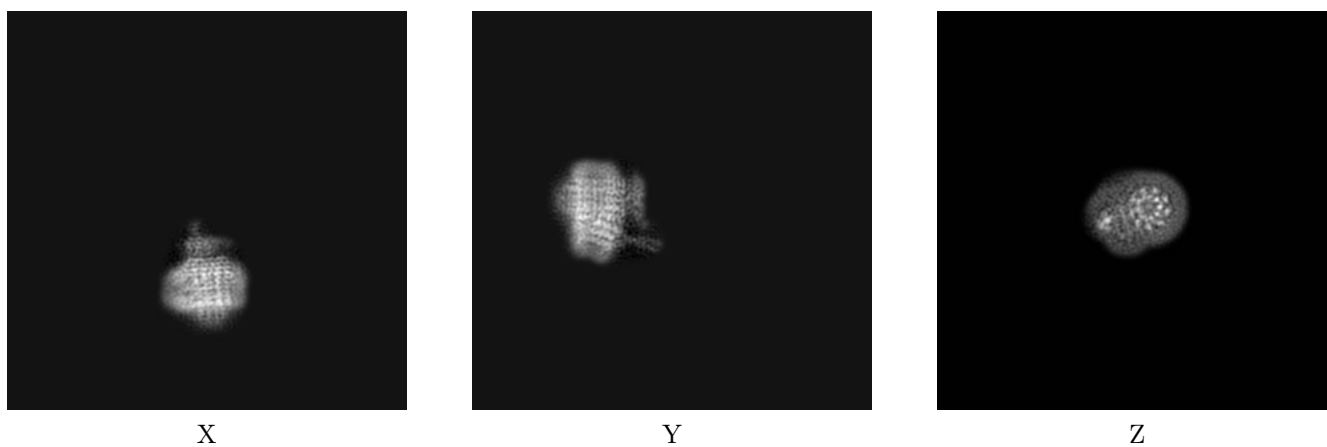
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map

| X Index: 250 | Y Index: 250 | Z Index: 250 |
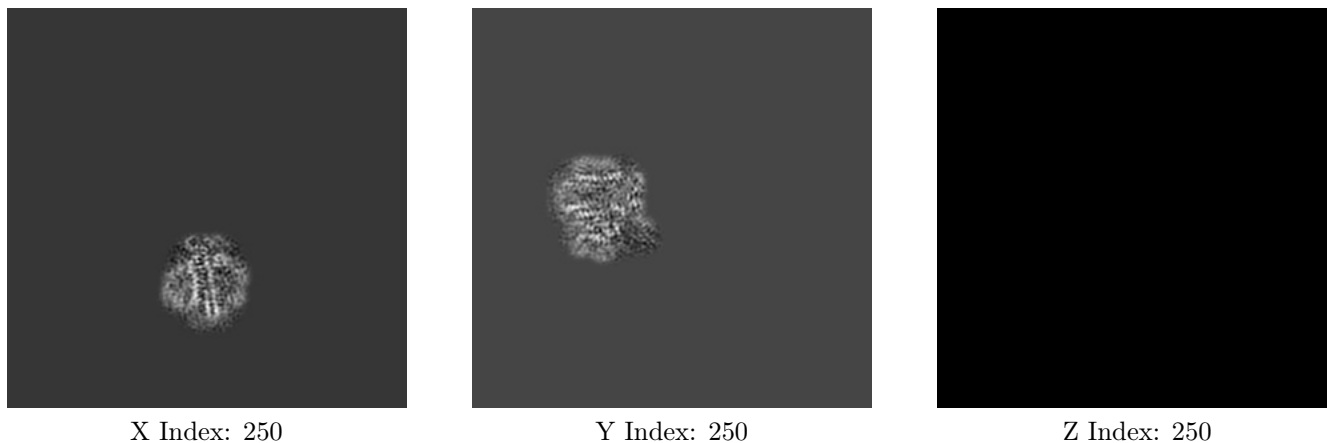
The images above show central slices of the map in three orthogonal directions.

6.3   Largest variance slices   ⓘ
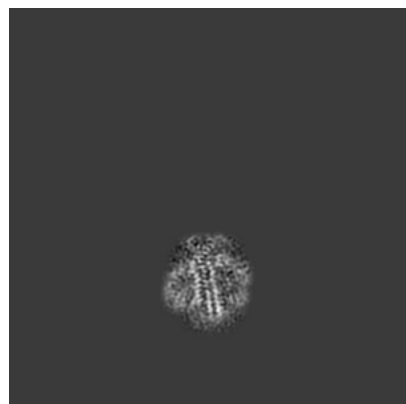
6.3.1   Primary map
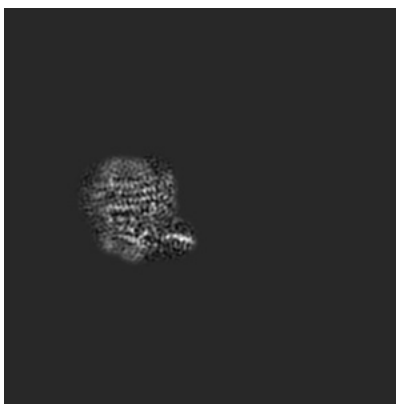
| X Index: 251 | Y Index: 236 | Z Index: 134 |
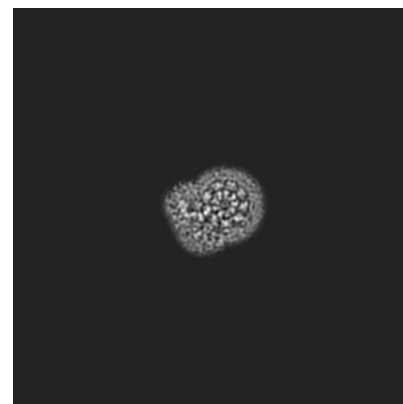
The images above show the largest variance slices of the map in three orthogonal directions.

6.4   Orthogonal surface views   ⓘ
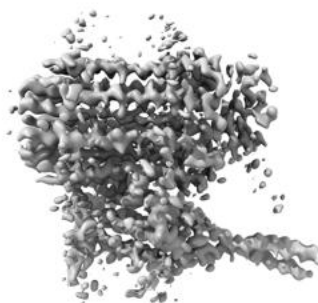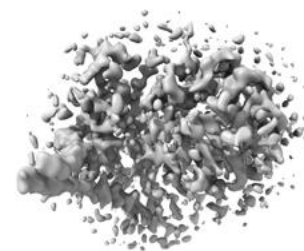
6.4.1   Primary map

| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.0144. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5　Mask visualisation　ⓘ

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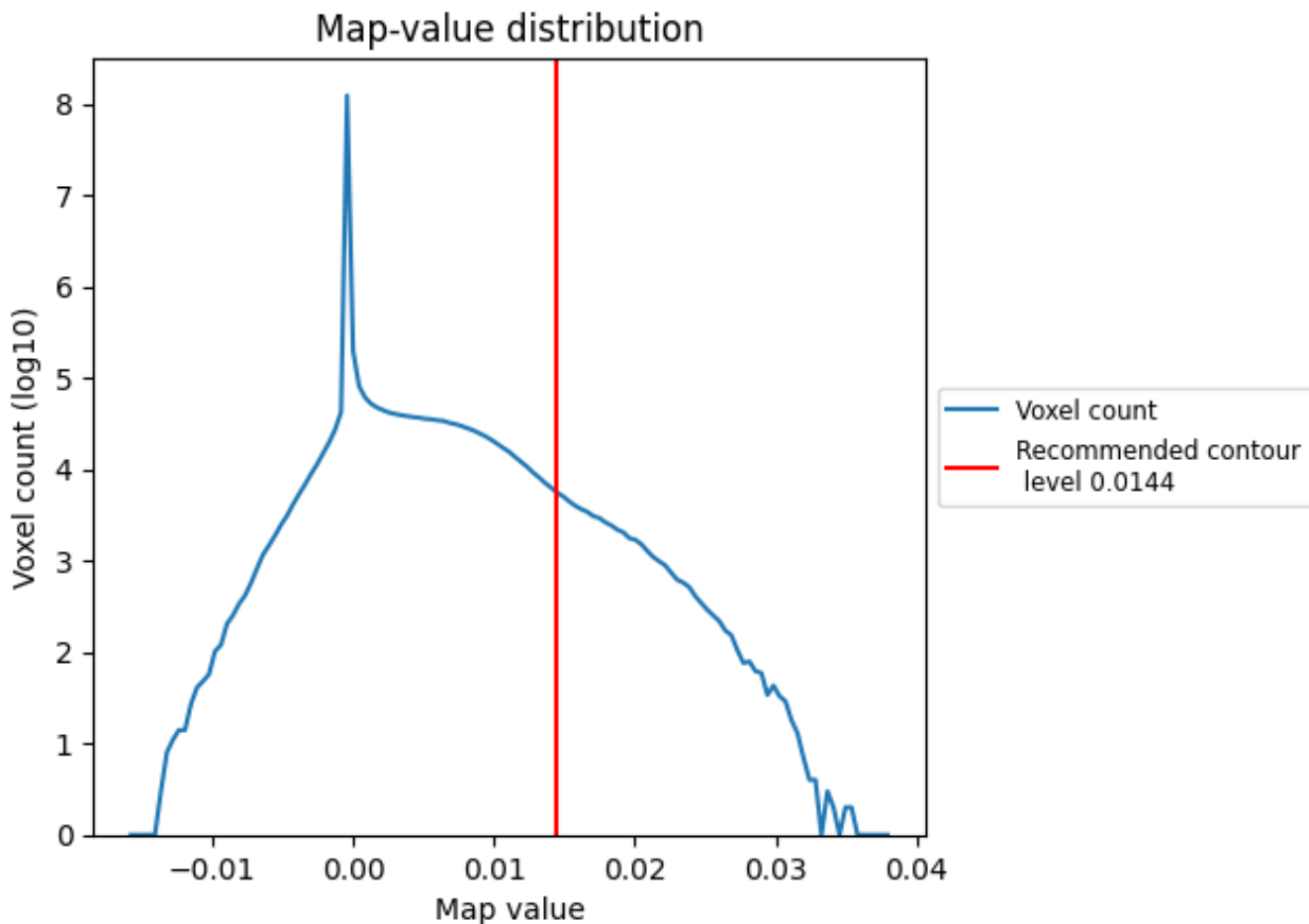
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
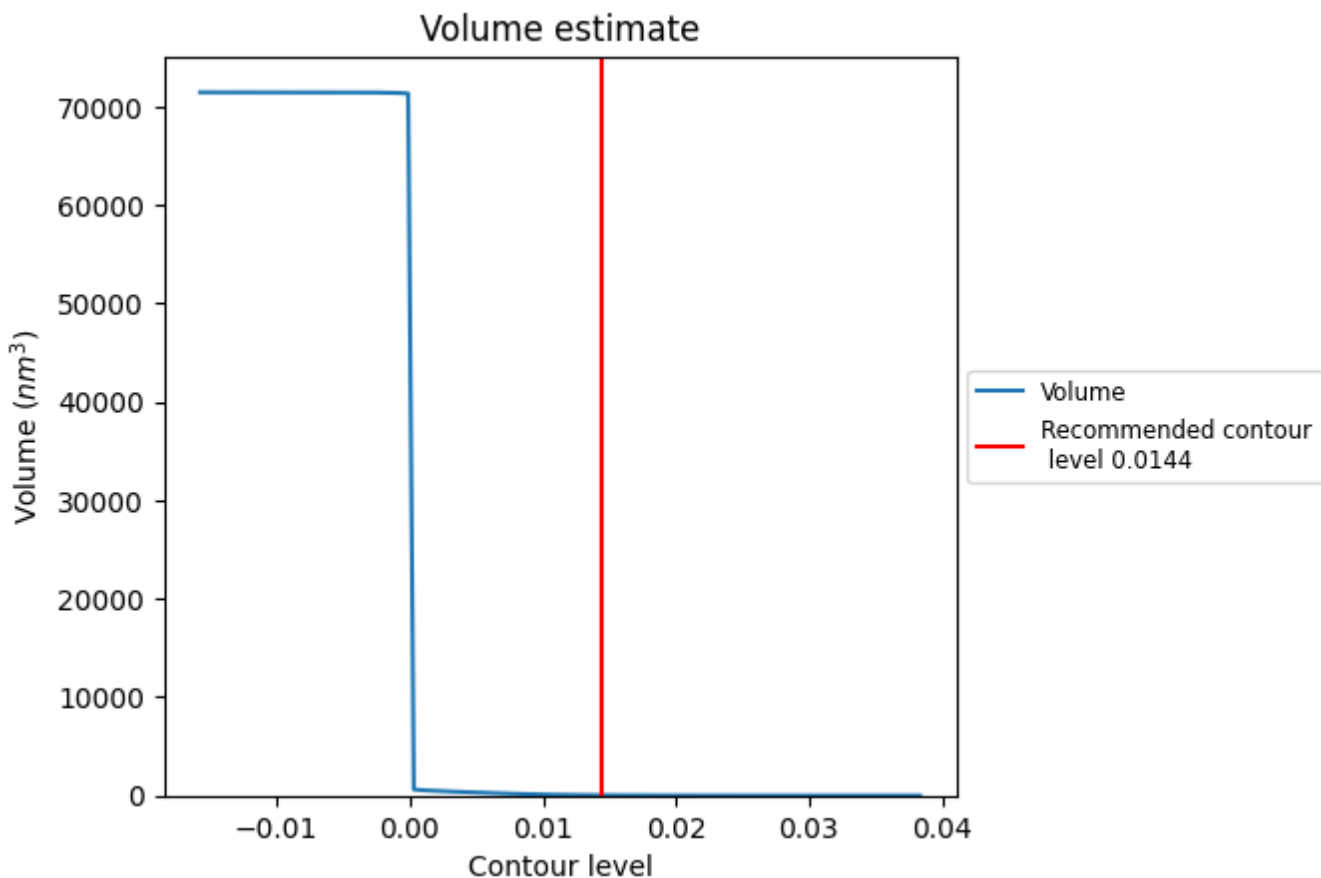
Volume estimate

The volume at the recommended contour level is 33 nm^3; this corresponds to an approximate mass of 29 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 ⓘ
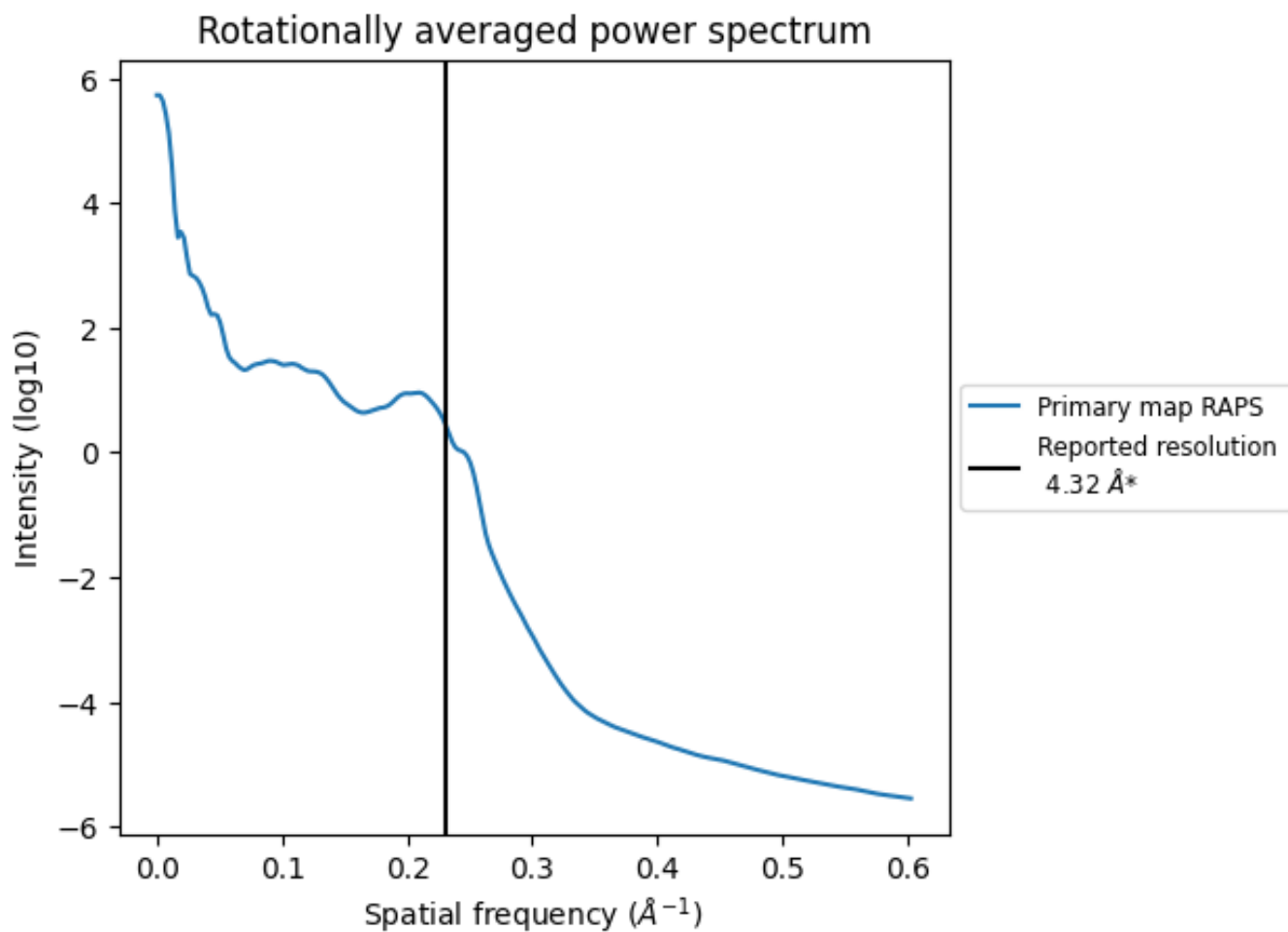
*Reported resolution corresponds to spatial frequency of 0.231 Å^{-1}

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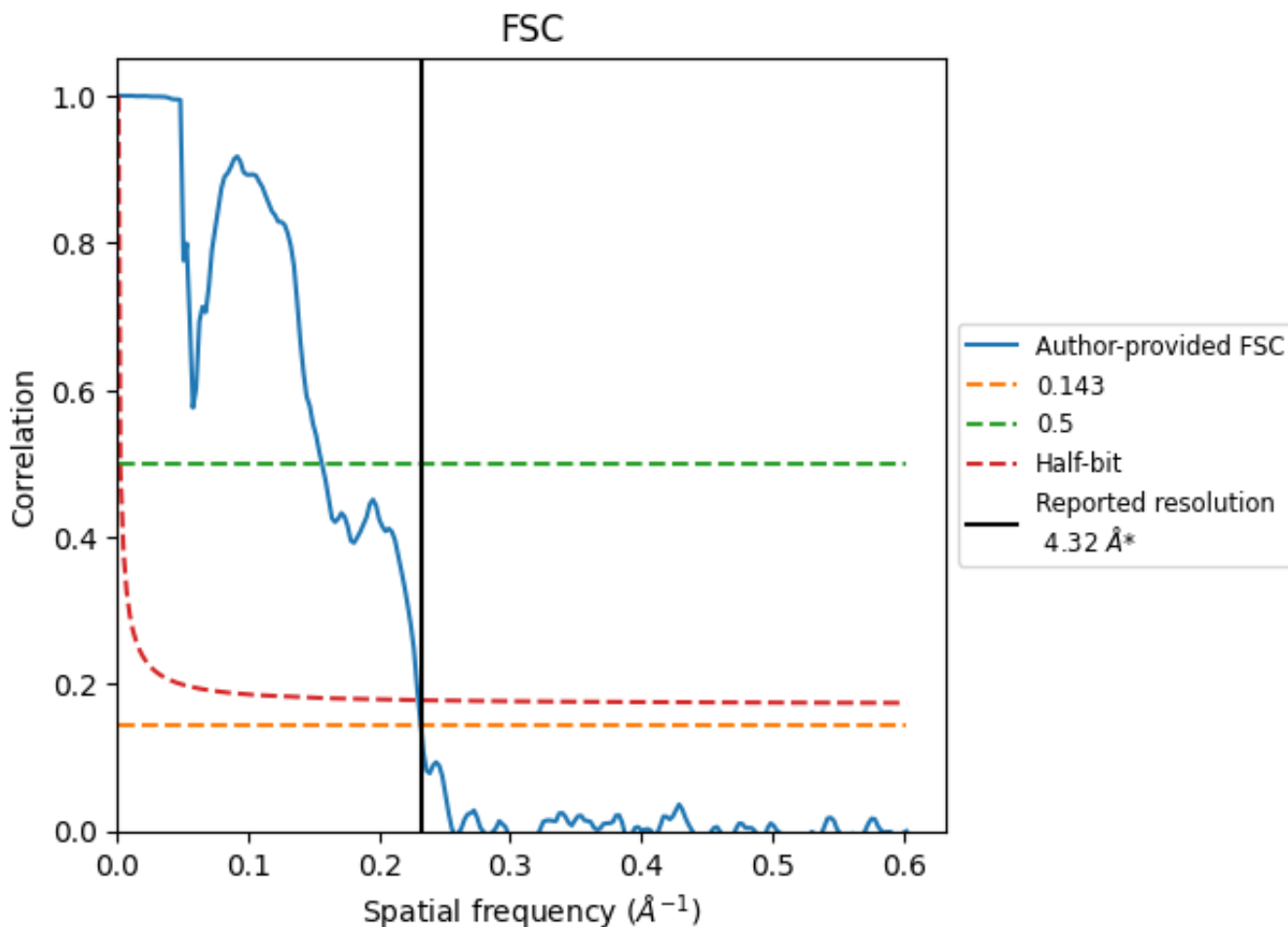
*Reported resolution corresponds to spatial frequency of 0.231 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.32	-	-
Author-provided FSC curve	4.31	6.40	4.35
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-12426 and PDB model 7NJX. Per-residue inclusion information can be found in section 3 on page 6.

## 9.1 Map-model overlay ⓘ
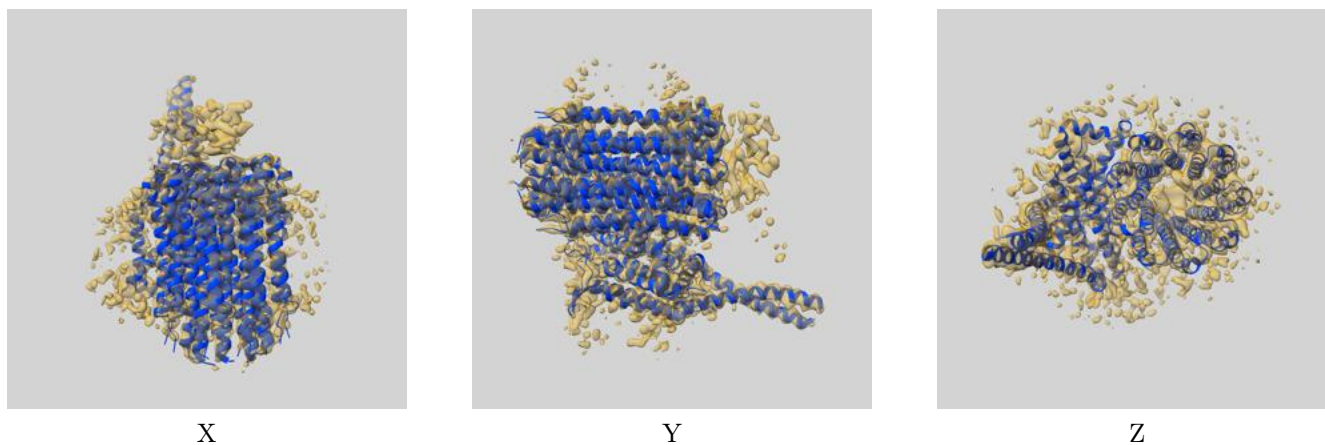
| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.0144 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
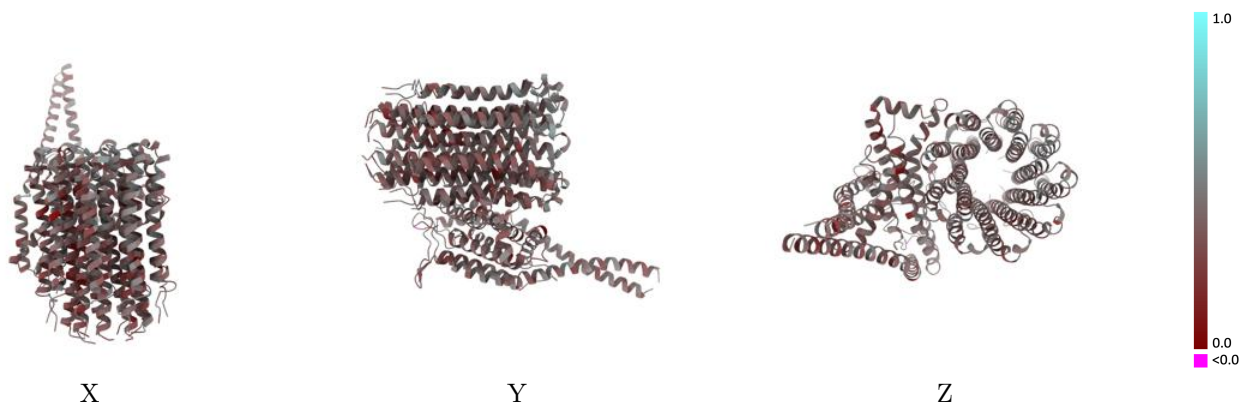
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
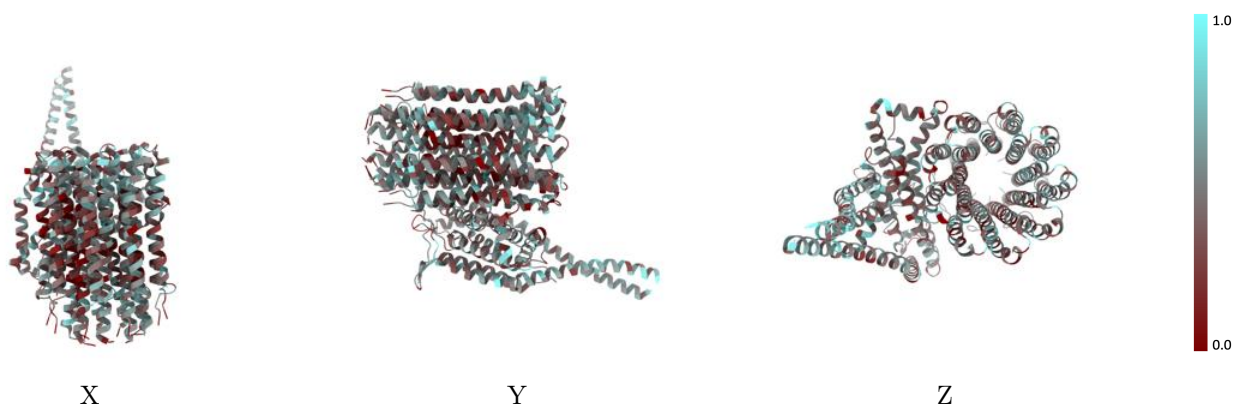
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0144).

9.4   Atom inclusion ⓘ
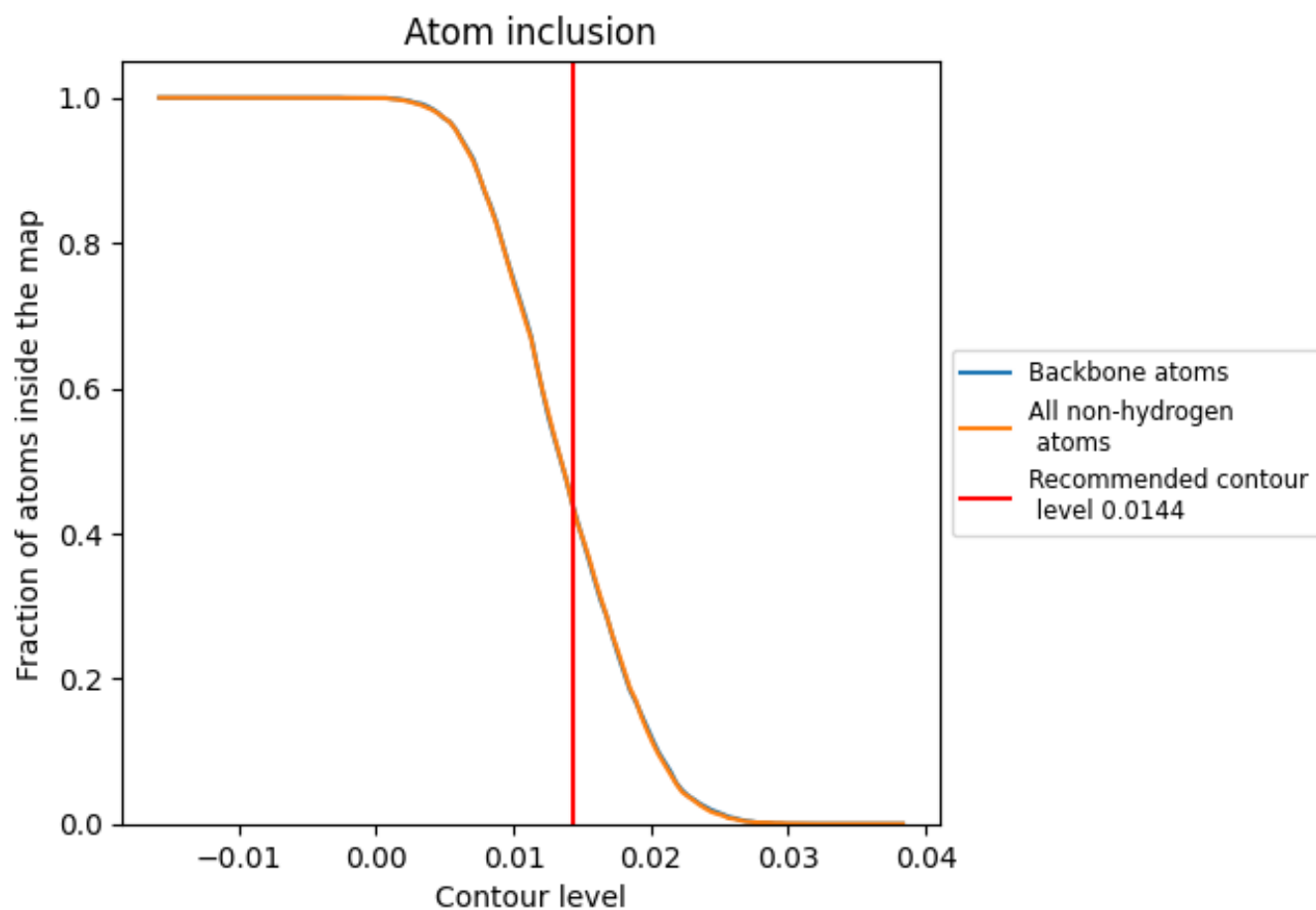
At the recommended contour level, 43% of all backbone atoms, 43% of all non-hydrogen atoms, are inside the map.

9.5　Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0144) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4329	0.3730
L	0.4332	0.3660
M	0.4332	0.3700
N	0.4092	0.3640
O	0.4384	0.3930
P	0.4709	0.4070
Q	0.4726	0.3980
R	0.3733	0.3630
S	0.3818	0.3370
T	0.4606	0.3740
a	0.4527	0.3660
b	0.5202	0.3940
d	0.4626	0.3560

1.0

0.0

<0.0