WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Jun 24, 2023 – 01:29 PM EDT

PDB ID	:	7UXA
EMDB ID	:	EMD-26856
Title	:	Human tRNA Splicing Endonuclease Complex bound to pre-tRNA-ARG
Authors	:	Stanley, R.E.; Hayne, C.K.
Deposited on	:	2022-05-05
Resolution	:	3.28 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.

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 3.28 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		7
Ramachandran outliers		0
Sidechain outliers		1.2%
RNA backbone		0.67

Worse   *Better*

■ Percentile relative to all structures
▯ Percentile relative to all EM structures
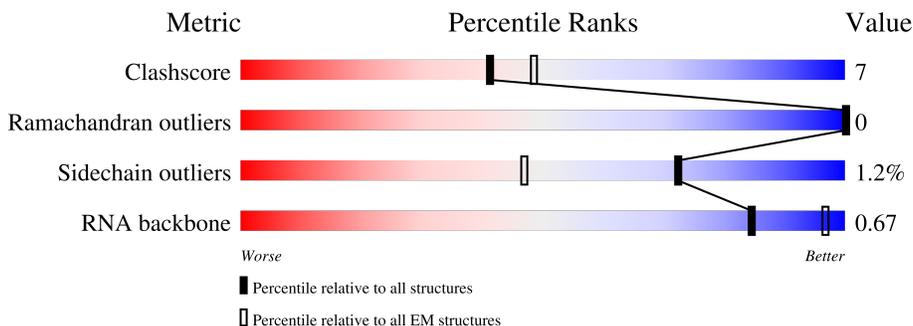
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	352	6% / 57% / 9% / 35%
2	B	183	· / 56% / 13% / 31%
3	C	483	· / 29% / 12% / 59%
4	D	551	· / 39% / 9% / 52%
5	E	88	48% / 34% / 7% / 11%

2   Entity composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 8120 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 tRNA-splicing endonuclease subunit Sen34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	230	1762	1122	326	310	4	0	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	initiating methionine	UNP Q9BSV6
A	-41	ALA	-	expression tag	UNP Q9BSV6
A	-40	SER	-	expression tag	UNP Q9BSV6
A	-39	TRP	-	expression tag	UNP Q9BSV6
A	-38	SER	-	expression tag	UNP Q9BSV6
A	-37	HIS	-	expression tag	UNP Q9BSV6
A	-36	PRO	-	expression tag	UNP Q9BSV6
A	-35	GLN	-	expression tag	UNP Q9BSV6
A	-34	PHE	-	expression tag	UNP Q9BSV6
A	-33	GLU	-	expression tag	UNP Q9BSV6
A	-32	LYS	-	expression tag	UNP Q9BSV6
A	-31	GLY	-	expression tag	UNP Q9BSV6
A	-30	GLY	-	expression tag	UNP Q9BSV6
A	-29	GLY	-	expression tag	UNP Q9BSV6
A	-28	ALA	-	expression tag	UNP Q9BSV6
A	-27	ARG	-	expression tag	UNP Q9BSV6
A	-26	GLY	-	expression tag	UNP Q9BSV6
A	-25	GLY	-	expression tag	UNP Q9BSV6
A	-24	SER	-	expression tag	UNP Q9BSV6
A	-23	GLY	-	expression tag	UNP Q9BSV6
A	-22	GLY	-	expression tag	UNP Q9BSV6
A	-21	GLY	-	expression tag	UNP Q9BSV6
A	-20	SER	-	expression tag	UNP Q9BSV6
A	-19	TRP	-	expression tag	UNP Q9BSV6
A	-18	SER	-	expression tag	UNP Q9BSV6
A	-17	HIS	-	expression tag	UNP Q9BSV6
A	-16	PRO	-	expression tag	UNP Q9BSV6
A	-15	GLN	-	expression tag	UNP Q9BSV6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	PHE	-	expression tag	UNP Q9BSV6
A	-13	GLU	-	expression tag	UNP Q9BSV6
A	-12	LYS	-	expression tag	UNP Q9BSV6
A	-11	GLY	-	expression tag	UNP Q9BSV6
A	-10	PHE	-	expression tag	UNP Q9BSV6
A	-9	ASP	-	expression tag	UNP Q9BSV6
A	-8	TYR	-	expression tag	UNP Q9BSV6
A	-7	LYS	-	expression tag	UNP Q9BSV6
A	-6	ASP	-	expression tag	UNP Q9BSV6
A	-5	ASP	-	expression tag	UNP Q9BSV6
A	-4	ASP	-	expression tag	UNP Q9BSV6
A	-3	ASP	-	expression tag	UNP Q9BSV6
A	-2	LYS	-	expression tag	UNP Q9BSV6
A	-1	GLY	-	expression tag	UNP Q9BSV6
A	0	THR	-	expression tag	UNP Q9BSV6
A	247	ALA	TYR	engineered mutation	UNP Q9BSV6
A	255	ALA	HIS	engineered mutation	UNP Q9BSV6
A	286	ALA	LYS	engineered mutation	UNP Q9BSV6

- Molecule 2 is a protein called tRNA-splicing endonuclease subunit Sen15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	126	971	626	154	184	7	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	172	GLY	-	expression tag	UNP Q8WW01
B	173	PRO	-	expression tag	UNP Q8WW01
B	174	GLU	-	expression tag	UNP Q8WW01
B	175	GLN	-	expression tag	UNP Q8WW01
B	176	LYS	-	expression tag	UNP Q8WW01
B	177	LEU	-	expression tag	UNP Q8WW01
B	178	ILE	-	expression tag	UNP Q8WW01
B	179	SER	-	expression tag	UNP Q8WW01
B	180	GLU	-	expression tag	UNP Q8WW01
B	181	GLU	-	expression tag	UNP Q8WW01
B	182	ASP	-	expression tag	UNP Q8WW01
B	183	LEU	-	expression tag	UNP Q8WW01

- Molecule 3 is a protein called tRNA-splicing endonuclease subunit Sen2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	200	Total 1615	C 1054	N 266	O 286	S 9	0	1

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	369	ALA	TYR	engineered mutation	UNP Q8NCE0
C	377	ALA	HIS	engineered mutation	UNP Q8NCE0
C	416	ALA	LYS	engineered mutation	UNP Q8NCE0
C	466	ASP	-	expression tag	UNP Q8NCE0
C	467	TYR	-	expression tag	UNP Q8NCE0
C	468	LYS	-	expression tag	UNP Q8NCE0
C	469	ASP	-	expression tag	UNP Q8NCE0
C	470	ASP	-	expression tag	UNP Q8NCE0
C	471	ASP	-	expression tag	UNP Q8NCE0
C	472	ASP	-	expression tag	UNP Q8NCE0
C	473	LYS	-	expression tag	UNP Q8NCE0
C	474	GLY	-	expression tag	UNP Q8NCE0
C	475	PHE	-	expression tag	UNP Q8NCE0
C	476	TRP	-	expression tag	UNP Q8NCE0
C	477	SER	-	expression tag	UNP Q8NCE0
C	478	HIS	-	expression tag	UNP Q8NCE0
C	479	PRO	-	expression tag	UNP Q8NCE0
C	480	GLN	-	expression tag	UNP Q8NCE0
C	481	PHE	-	expression tag	UNP Q8NCE0
C	482	GLU	-	expression tag	UNP Q8NCE0
C	483	LYS	-	expression tag	UNP Q8NCE0

- Molecule 4 is a protein called tRNA-splicing endonuclease subunit Sen54.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	264	Total 2105	C 1344	N 375	O 380	S 6	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	527	GLN	-	expression tag	UNP Q7Z6J9
D	528	ALA	-	expression tag	UNP Q7Z6J9
D	529	TYR	-	expression tag	UNP Q7Z6J9
D	530	VAL	-	expression tag	UNP Q7Z6J9
D	531	GLU	-	expression tag	UNP Q7Z6J9
D	532	GLN	-	expression tag	UNP Q7Z6J9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	533	LYS	-	expression tag	UNP Q7Z6J9
D	534	LEU	-	expression tag	UNP Q7Z6J9
D	535	ILE	-	expression tag	UNP Q7Z6J9
D	536	SER	-	expression tag	UNP Q7Z6J9
D	537	GLU	-	expression tag	UNP Q7Z6J9
D	538	GLU	-	expression tag	UNP Q7Z6J9
D	539	ASP	-	expression tag	UNP Q7Z6J9
D	540	LEU	-	expression tag	UNP Q7Z6J9
D	541	ASN	-	expression tag	UNP Q7Z6J9
D	542	SER	-	expression tag	UNP Q7Z6J9
D	543	ALA	-	expression tag	UNP Q7Z6J9
D	544	VAL	-	expression tag	UNP Q7Z6J9
D	545	ASP	-	expression tag	UNP Q7Z6J9
D	546	HIS	-	expression tag	UNP Q7Z6J9
D	547	HIS	-	expression tag	UNP Q7Z6J9
D	548	HIS	-	expression tag	UNP Q7Z6J9
D	549	HIS	-	expression tag	UNP Q7Z6J9
D	550	HIS	-	expression tag	UNP Q7Z6J9
D	551	HIS	-	expression tag	UNP Q7Z6J9

- Molecule 5 is a RNA chain called RNA (78-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	E	78	1665	744	299	545	77	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	E	2	2	2	0

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: tRNA-splicing endonuclease subunit Sen34

Chain A:

• Molecule 2: tRNA-splicing endonuclease subunit Sen15

Chain B:

• Molecule 3: tRNA-splicing endonuclease subunit Sen2

Chain C:

• Molecule 4: tRNA-splicing endonuclease subunit Sen54

Chain D:

| 39% | 9% | 52% |
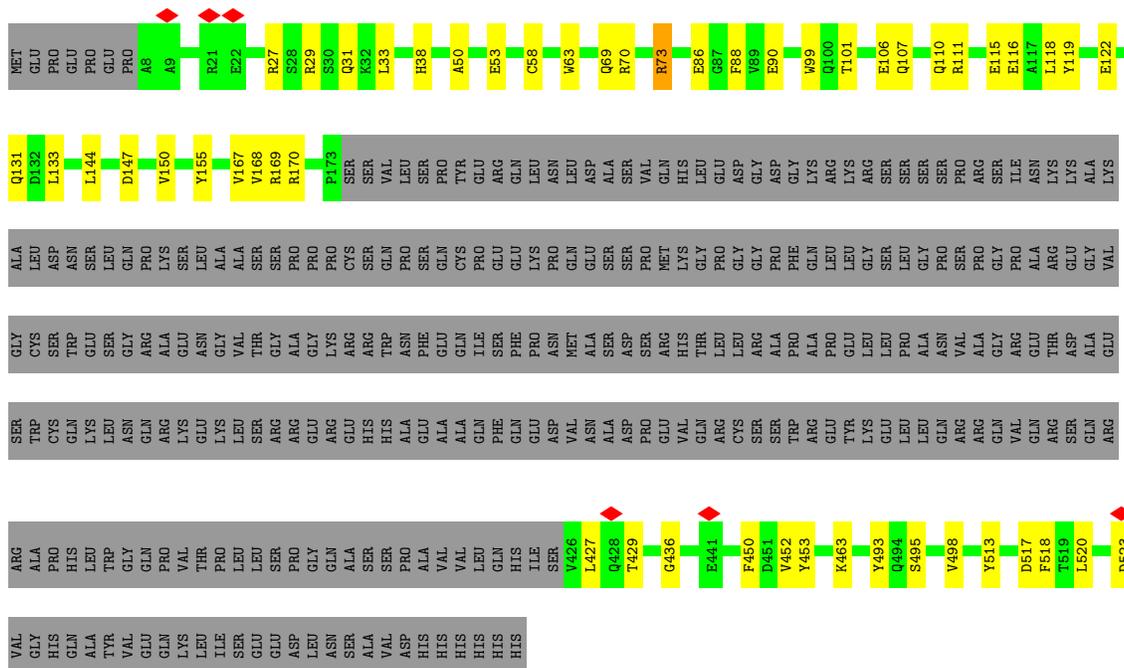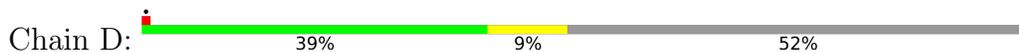
• Molecule 5: RNA (78-MER)

Chain E:

| 48% | 34% | 7% | 11% |

4   Experimental information   ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	152031	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA, FEI TITAN KRIOS	Depositor
Voltage (kV)	200, 300	Depositor
Electron dose $(e^-/\text{Å}^2)$	54, 60	Depositor
Minimum defocus (nm)	1200, 1200	Depositor
Maximum defocus (nm)	2200, 2200	Depositor
Magnification	45000, 81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.145	Depositor
Minimum map value	-1.969	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	298.24, 298.24, 298.24	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.27	0/1805	0.51	0/2459
2	B	0.26	0/993	0.44	0/1355
3	C	0.27	0/1653	0.47	0/2235
4	D	0.29	0/2157	0.49	0/2920
5	E	0.38	1/1861 (0.1%)	0.75	0/2897
All	All	0.30	1/8469 (0.0%)	0.56	0/11866

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1	G	OP3-P	-10.69	1.48	1.61

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1762	0	1772	24	0
2	B	971	0	961	15	0
3	C	1615	0	1637	36	0
4	D	2105	0	2071	39	0
5	E	1665	0	839	19	0

Continued on next page...

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	2	0	0	0	0
All	All	8120	0	7280	112	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 7.

All (112) 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)
4:D:27:ARG:NH2	5:E:17:G:OP1	2.25	0.69
2:B:145:GLU:HG2	3:C:358:VAL:HG11	1.75	0.67
3:C:347:HIS:ND1	3:C:440:MET:SD	2.68	0.67
3:C:350:ARG:NH1	3:C:354:TRP:O	2.29	0.66
3:C:329:TRP:NE1	3:C:434:MET:O	2.31	0.64
1:A:282:THR:HG21	1:A:306:TRP:HB2	1.79	0.63
4:D:167:VAL:HB	4:D:453:TYR:HB2	1.81	0.63
4:D:115:GLU:OE1	4:D:170:ARG:NH2	2.33	0.61
4:D:168:VAL:HG22	4:D:452:VAL:HG22	1.83	0.61
4:D:495:SER:OG	4:D:498:VAL:O	2.17	0.61
1:A:35:ALA:O	4:D:70:ARG:NH2	2.36	0.59
4:D:115:GLU:HB3	4:D:150:VAL:HG11	1.85	0.58
1:A:2:LEU:HB2	1:A:66:VAL:HG12	1.86	0.58
4:D:29:ARG:HH22	4:D:69:GLN:H	1.51	0.58
3:C:323:LEU:HD22	3:C:327:LYS:HD3	1.85	0.58
1:A:62:GLU:OE1	1:A:221:TYR:OH	2.20	0.58
3:C:459:ARG:NH2	5:E:11:C:O2	2.37	0.57
3:C:359:GLY:HA3	3:C:367:LEU:HG	1.87	0.56
4:D:118:LEU:HB2	4:D:144:LEU:HD12	1.87	0.56
1:A:252:LEU:HD23	4:D:58:CYS:HB3	1.88	0.54
3:C:43:GLU:HB3	3:C:45:ILE:HG12	1.90	0.54
5:E:58:A:H2'	5:E:59:A:C8	2.43	0.54
2:B:66:VAL:HG21	2:B:107:PRO:HB3	1.88	0.54
5:E:1:G:H2'	5:E:2:G:H8	1.72	0.54
3:C:70:ILE:HD11	3:C:298:GLN:HE22	1.73	0.54
3:C:349:PHE:O	3:C:354:TRP:HB2	2.08	0.53
3:C:47:ASN:HB3	3:C:335:VAL:HG21	1.91	0.53
4:D:122:GLU:OE1	4:D:155:TYR:OH	2.26	0.53
3:C:39:ILE:N	3:C:313:CYS:O	2.41	0.53
1:A:41:ARG:NH1	4:D:119:TYR:OH	2.42	0.53
1:A:298:LYS:NZ	1:A:299:VAL:O	2.43	0.52
1:A:290:LEU:O	2:B:116:HIS:NE2	2.35	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ARG:NH1	1:A:250:ASP:OD1	2.43	0.51
2:B:120:ARG:NH2	2:B:157:ASP:OD1	2.33	0.51
2:B:144:VAL:HG22	2:B:150:ILE:HG12	1.92	0.51
3:C:40:PHE:HB2	3:C:314:LEU:HA	1.93	0.51
3:C:66:PHE:HD2	3:C:307:LEU:HD11	1.77	0.50
2:B:123:LEU:HD23	2:B:157:ASP:HB2	1.95	0.49
1:A:77:ARG:HG2	4:D:131:GLN:HG3	1.95	0.49
4:D:517:ASP:OD1	4:D:518:PHE:N	2.46	0.49
1:A:28:VAL:HG21	1:A:60:LEU:HD21	1.95	0.49
4:D:31:GLN:NE2	5:E:14:A:N3	2.53	0.49
1:A:55:GLU:OE2	1:A:220:ARG:NH1	2.46	0.48
3:C:41:ARG:HG3	3:C:317:TYR:CD1	2.48	0.48
3:C:364:THR:HG22	3:C:383:ILE:HD11	1.95	0.48
3:C:371:LYS:HG2	3:C:372:GLY:H	1.79	0.48
3:C:348:TYR:HB2	4:D:427:LEU:HD13	1.95	0.48
5:E:16:U:H4'	5:E:17:G:H2'	1.96	0.47
4:D:106:GLU:HG2	4:D:107:GLN:HG3	1.96	0.47
4:D:101:THR:O	4:D:169:ARG:NH1	2.47	0.47
3:C:326:VAL:O	3:C:330:LYS:HG2	2.15	0.47
1:A:77:ARG:HA	4:D:133:LEU:HD11	1.96	0.46
2:B:127:ARG:HB2	2:B:137:MET:HG3	1.97	0.46
4:D:38:HIS:ND1	4:D:58:CYS:SG	2.85	0.46
3:C:373:PRO:HB2	3:C:374:PRO:HD3	1.96	0.46
1:A:60:LEU:HB3	1:A:66:VAL:HG22	1.98	0.46
1:A:302:THR:HG21	2:B:119:ILE:HG21	1.98	0.46
1:A:20:GLN:HA	4:D:63:TRP:CH2	2.51	0.45
3:C:454:VAL:HG11	3:C:457:ARG:HH11	1.82	0.45
3:C:346:TYR:CE1	3:C:356:PRO:HG2	2.52	0.45
2:B:80:ASN:HB2	2:B:93:VAL:HG23	1.99	0.45
5:E:3:C:H2'	5:E:4:U:H6	1.82	0.45
2:B:90:ILE:O	2:B:107:PRO:HD2	2.16	0.45
3:C:350:ARG:NH1	3:C:355:VAL:HA	2.32	0.44
3:C:354:TRP:HE1	4:D:520:LEU:HB3	1.81	0.44
5:E:53:A:H4'	5:E:54:U:O5'	2.17	0.44
4:D:73:ARG:H	4:D:73:ARG:HD3	1.83	0.44
5:E:68:G:H2'	5:E:69:U:C6	2.52	0.44
3:C:332:PHE:HA	3:C:335:VAL:HG12	1.99	0.44
4:D:90:GLU:HB2	4:D:111:ARG:HG2	1.99	0.44
3:C:439:CYS:O	3:C:443:ILE:HG12	2.17	0.44
1:A:260:ALA:HB1	1:A:291:CYS:SG	2.58	0.44
1:A:271:LEU:HD23	1:A:271:LEU:HA	1.89	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:450:LEU:HD11	4:D:513:TYR:HB3	1.99	0.44
2:B:69:ASP:OD2	2:B:152:TYR:OH	2.35	0.43
1:A:77:ARG:H	1:A:77:ARG:HD2	1.83	0.43
5:E:78:C:H2'	5:E:79:A:C8	2.54	0.43
2:B:110:ILE:HG12	3:C:360:LEU:HD13	2.01	0.43
4:D:436:GLY:HA3	4:D:493:TYR:CG	2.54	0.43
5:E:25:C:C4	5:E:26:A:N7	2.87	0.43
5:E:26:A:C5	5:E:27:U:C5	3.06	0.43
3:C:56:ASP:O	3:C:60:LEU:HG	2.18	0.42
4:D:99:TRP:CH2	4:D:110:GLN:HB3	2.54	0.42
4:D:115:GLU:HG2	4:D:116:GLU:N	2.35	0.42
2:B:84:LEU:O	2:B:88:GLN:N	2.53	0.42
1:A:6:VAL:HA	1:A:10:ARG:O	2.20	0.42
3:C:303:GLU:HG2	3:C:346:TYR:OH	2.20	0.42
4:D:70:ARG:NE	4:D:122:GLU:O	2.52	0.42
5:E:14:A:H2'	5:E:15:A:O4'	2.19	0.42
4:D:99:TRP:O	4:D:463:LYS:NZ	2.36	0.42
1:A:271:LEU:O	1:A:275:VAL:HG23	2.19	0.41
3:C:348:TYR:CE2	3:C:445:VAL:HG11	2.54	0.41
4:D:50:ALA:O	4:D:53:GLU:HG2	2.19	0.41
5:E:27:U:H2'	5:E:28:U:H6	1.84	0.41
5:E:18:G:O2'	5:E:72:G:N7	2.43	0.41
2:B:145:GLU:HG3	2:B:147:ASP:H	1.86	0.41
2:B:116:HIS:O	2:B:120:ARG:HG2	2.20	0.41
3:C:386:LEU:HD21	3:C:425:LYS:HD2	2.03	0.41
4:D:86:GLU:HB3	4:D:88:PHE:CE2	2.56	0.41
3:C:63:LYS:HD2	3:C:63:LYS:HA	1.94	0.41
3:C:353:GLY:HA3	4:D:523:ASP:HB2	2.03	0.41
4:D:147:ASP:N	4:D:147:ASP:OD1	2.54	0.41
1:A:42:GLN:OE1	4:D:33:LEU:HD11	2.21	0.40
1:A:184:LEU:HD11	4:D:27:ARG:HH11	1.86	0.40
4:D:101:THR:HB	4:D:167:VAL:HG13	2.03	0.40
1:A:35:ALA:N	4:D:122:GLU:OE2	2.54	0.40
3:C:459:ARG:HH12	5:E:24:G:H21	1.68	0.40
3:C:302:GLU:OE1	3:C:302:GLU:N	2.53	0.40
4:D:168:VAL:HG13	4:D:450:PHE:HB3	2.03	0.40
5:E:32:C:H2'	5:E:33:U:C6	2.56	0.40
5:E:71:C:H3'	5:E:72:G:H21	1.86	0.40
5:E:1:G:H2'	5:E:2:G:C8	2.55	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	A	226/352 (64%)	215 (95%)	11 (5%)	0	100	100
2	B	124/183 (68%)	122 (98%)	2 (2%)	0	100	100
3	C	196/483 (41%)	182 (93%)	14 (7%)	0	100	100
4	D	260/551 (47%)	244 (94%)	16 (6%)	0	100	100
All	All	806/1569 (51%)	763 (95%)	43 (5%)	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	A	178/272 (65%)	177 (99%)	1 (1%)	86	91
2	B	108/155 (70%)	106 (98%)	2 (2%)	57	77
3	C	175/426 (41%)	172 (98%)	3 (2%)	60	78
4	D	222/471 (47%)	220 (99%)	2 (1%)	78	87
All	All	683/1324 (52%)	675 (99%)	8 (1%)	72	83

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	PHE
2	B	42	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	46	TYR
3	C	46	ASN
3	C	397	ARG
3	C	432	LYS
4	D	73	ARG
4	D	429	THR

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

Mol	Chain	Res	Type
4	D	464	ASN

5.3.3　RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	E	76/88 (86%)	14 (18%)	0

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	E	16	U
5	E	17	G
5	E	18	G
5	E	19	A
5	E	20	U
5	E	21	A
5	E	22	G
5	E	51	C
5	E	52	A
5	E	53	A
5	E	62	U
5	E	63	U
5	E	71	C
5	E	88	G

There are no RNA pucker outliers to report.

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 ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-26856. 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
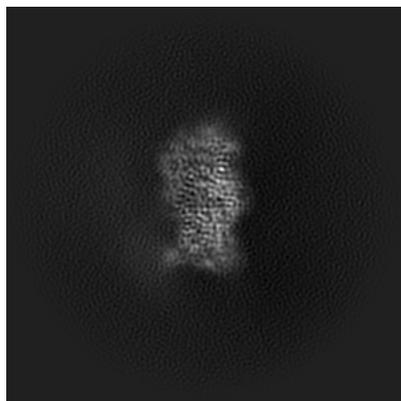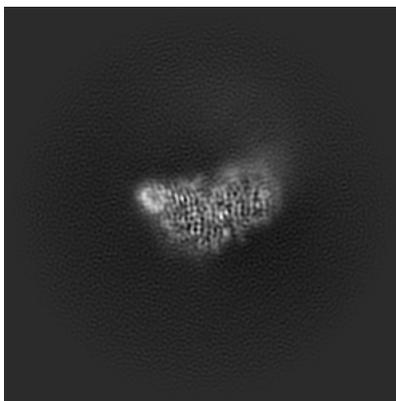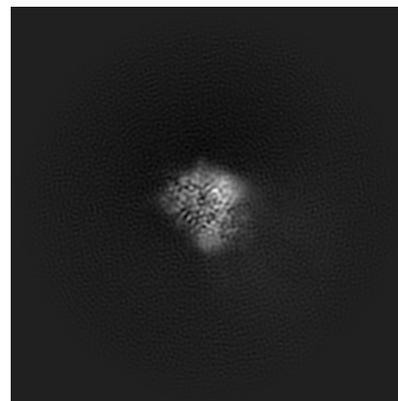
X   Y   Z

6.1.2 Raw map

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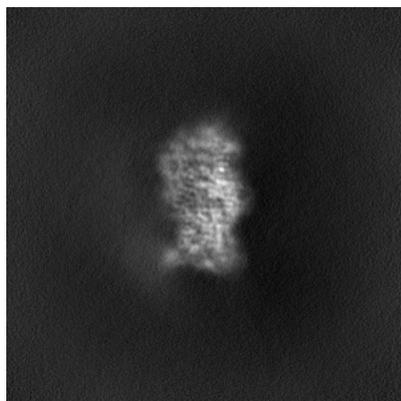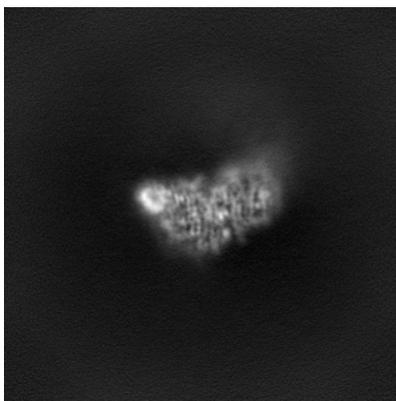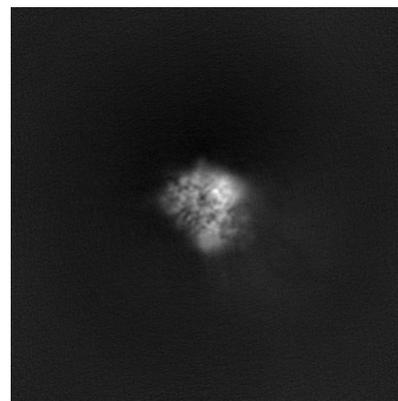
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
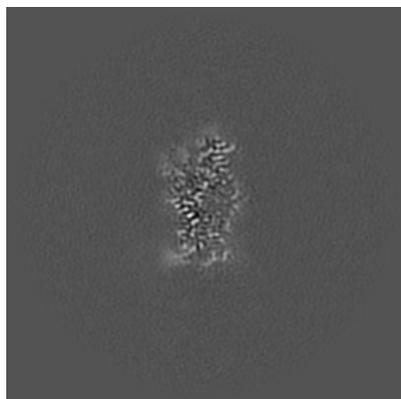
6.2.1 Primary map
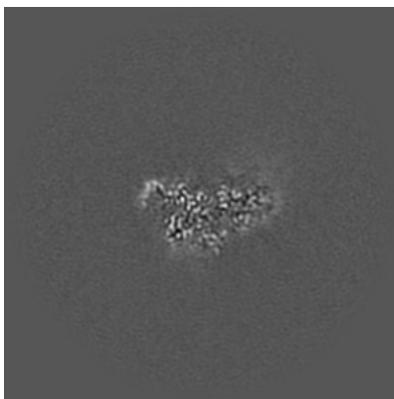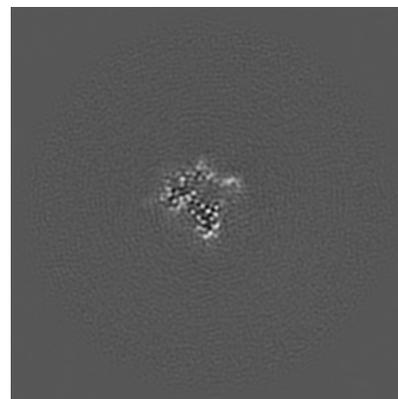
| X Index: 160 | Y Index: 160 | Z Index: 160 |

6.2.2 Raw map
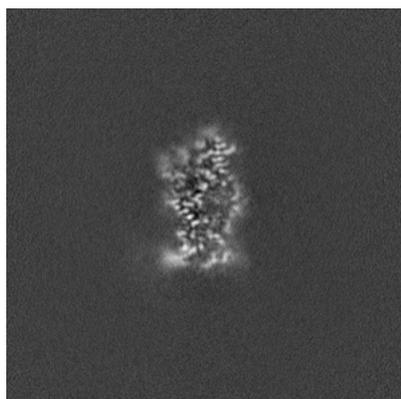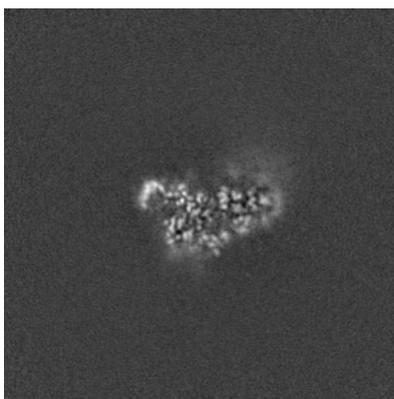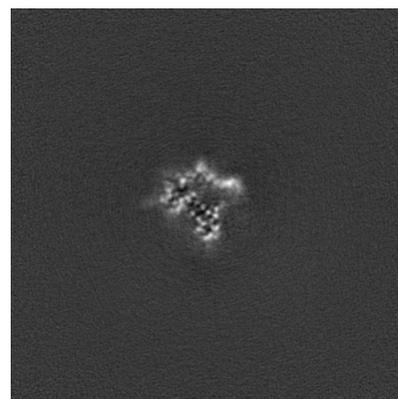
| X Index: 160 | Y Index: 160 | Z Index: 160 |

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

6.3　Largest variance slices (i)

6.3.1　Primary map
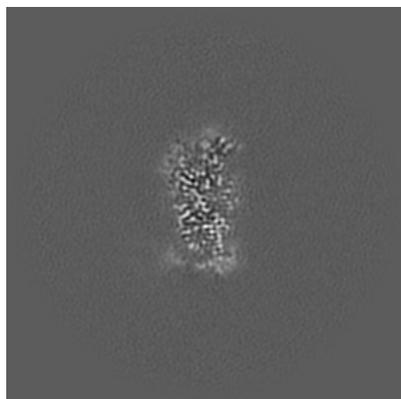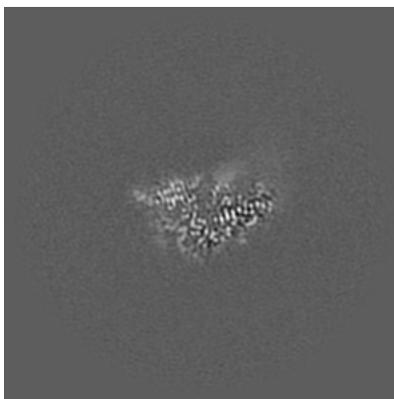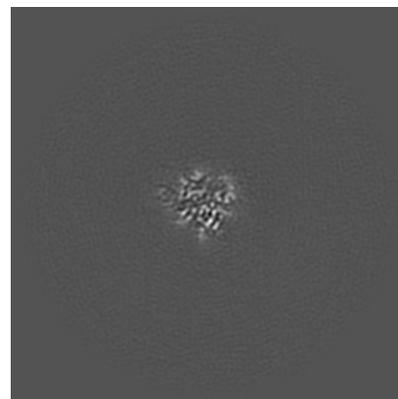
| X Index: 165 | Y Index: 170 | Z Index: 152 |

6.3.2　Raw map
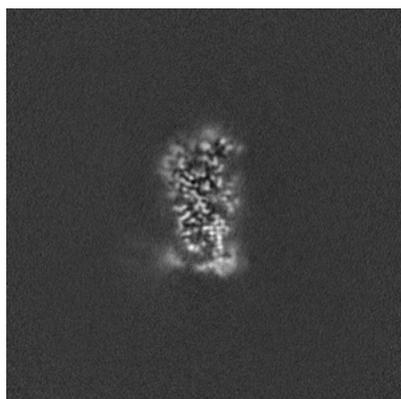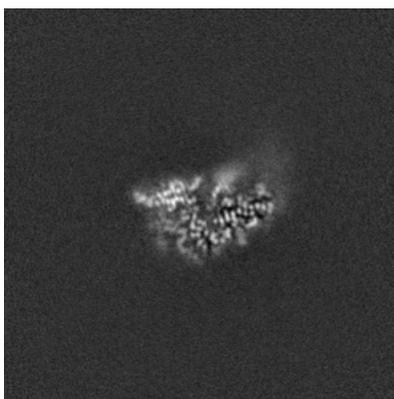
| X Index: 165 | Y Index: 170 | Z Index: 177 |

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

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

6.4.1 Primary map
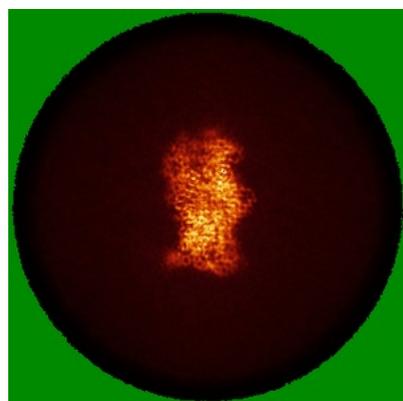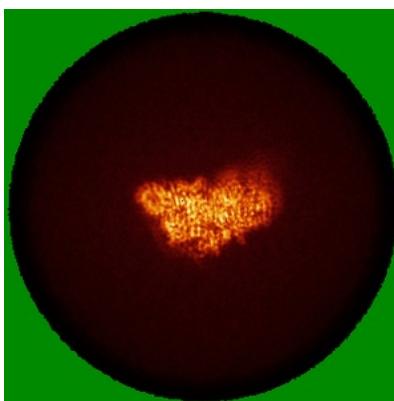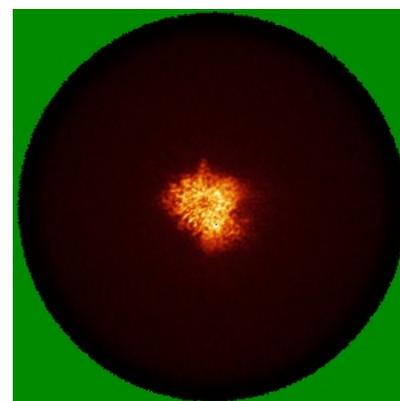
| X | Y | Z |

6.4.2 Raw map

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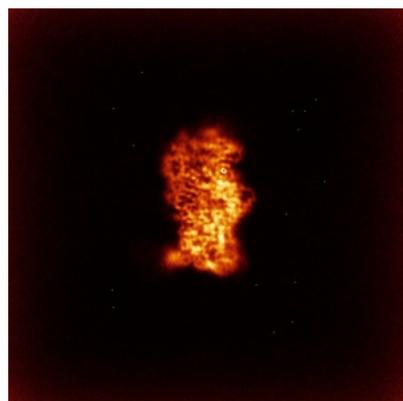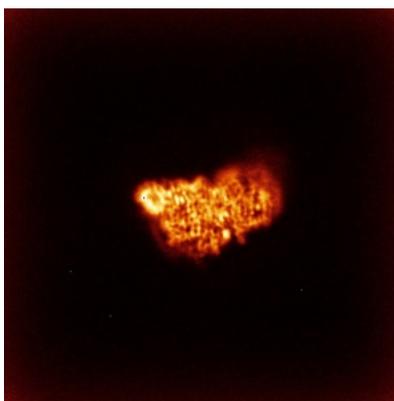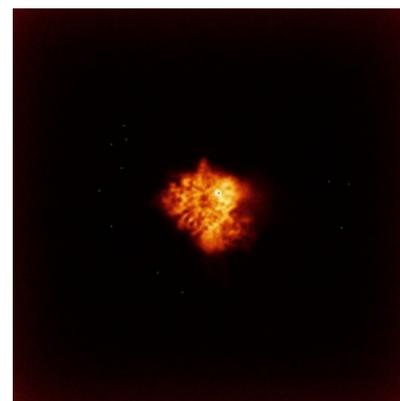
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

| X | Y | Z |
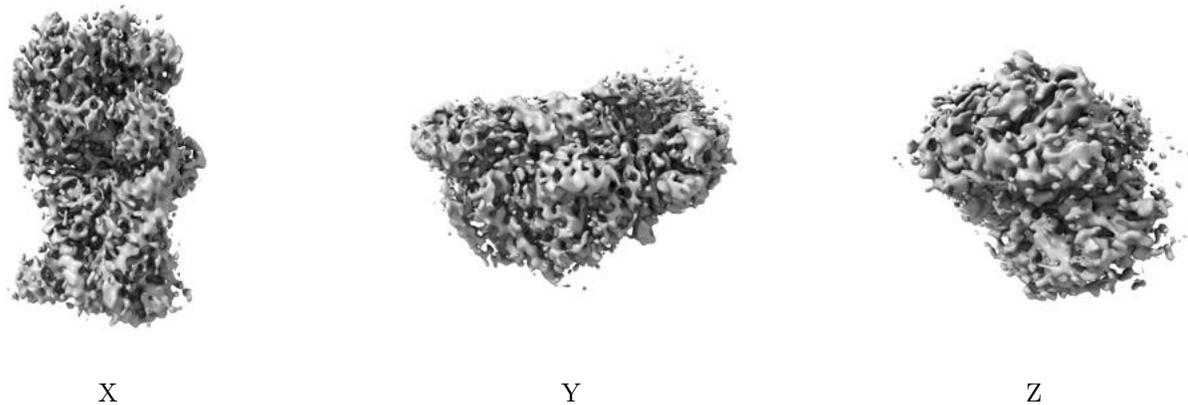
The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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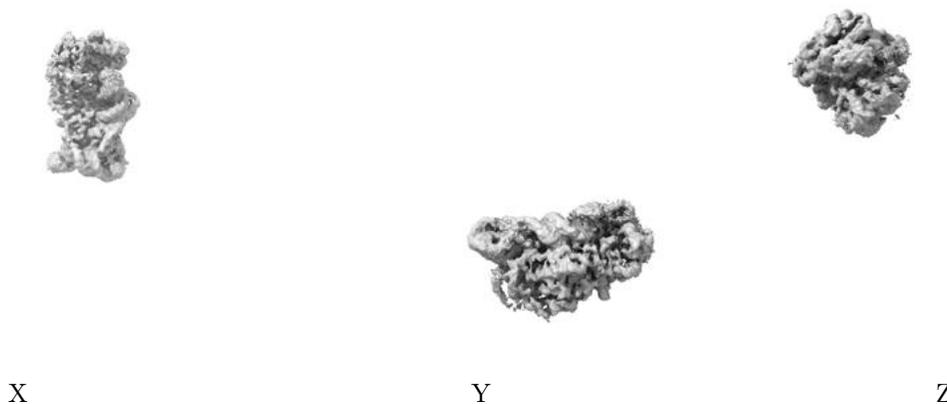
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

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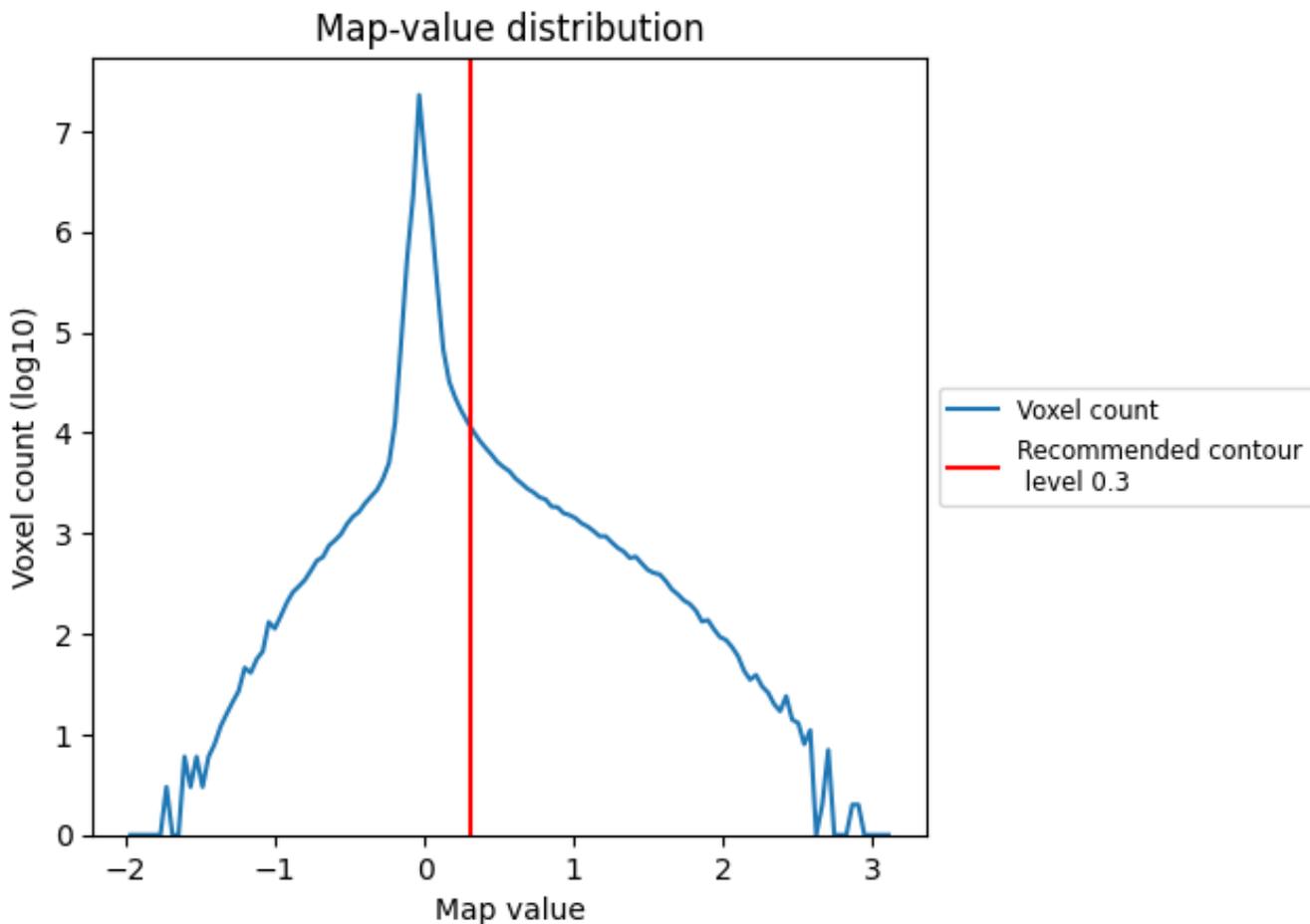
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate ⓘ
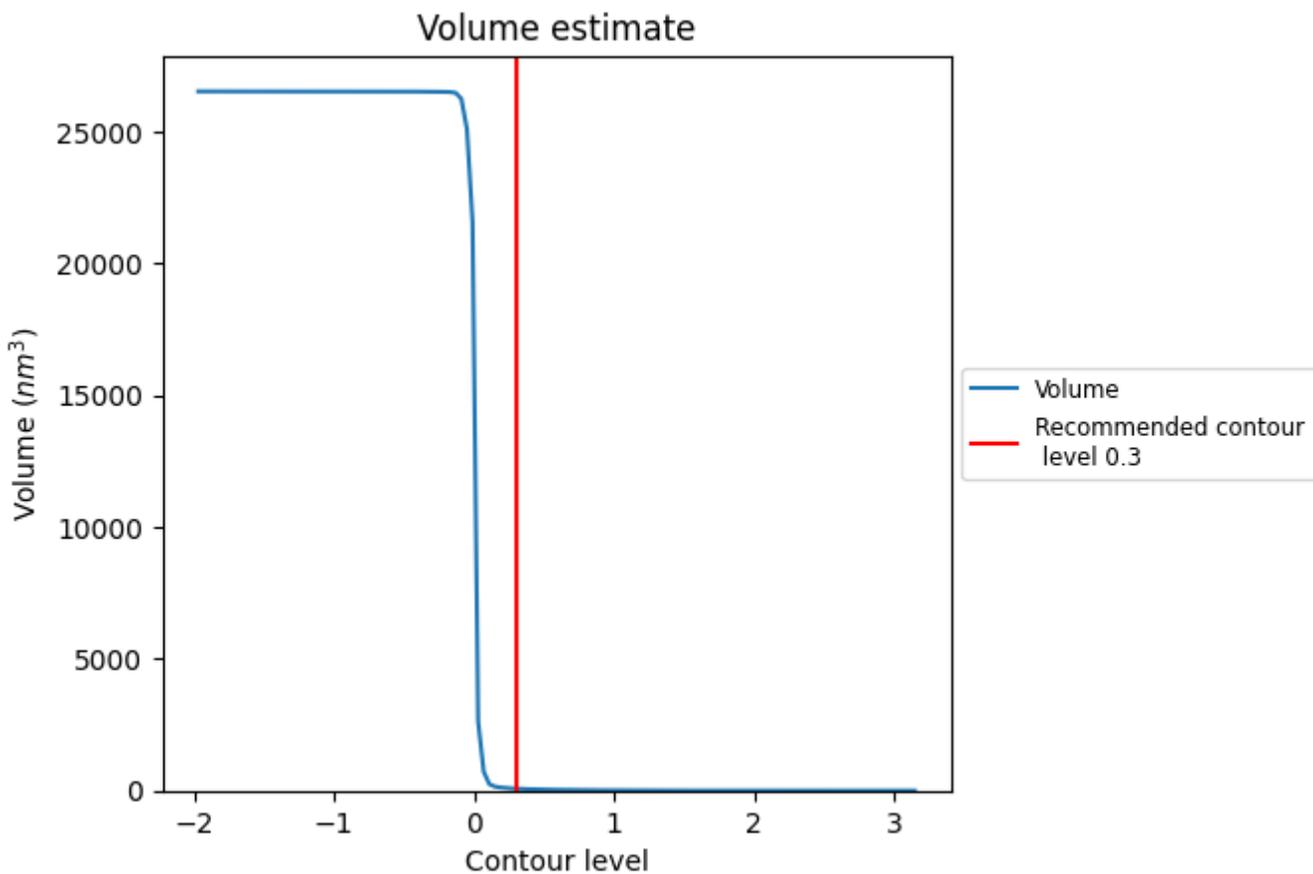
The volume at the recommended contour level is 74 nm^3; this corresponds to an approximate mass of 67 kDa.

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 ⓘ
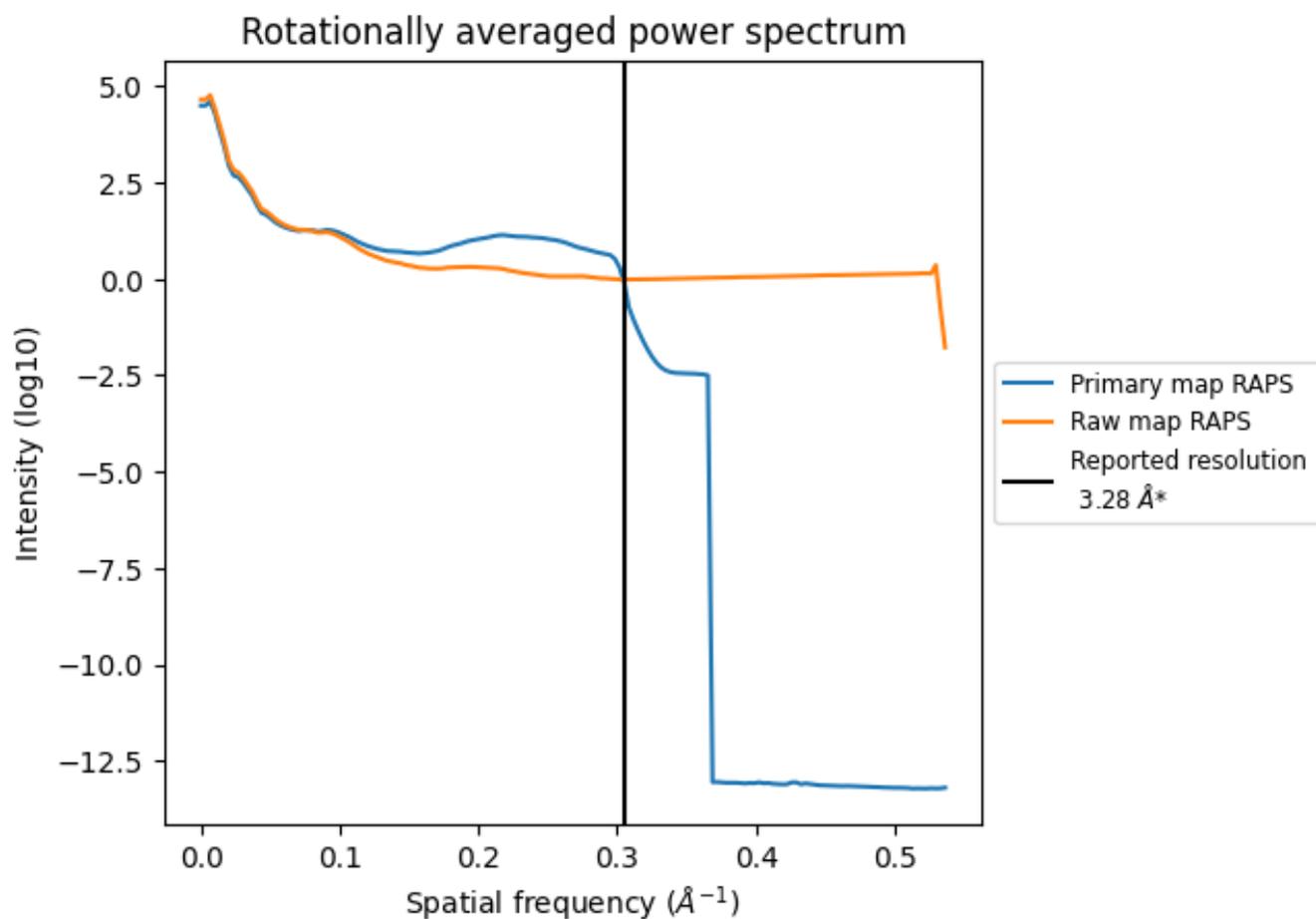
*Reported resolution corresponds to spatial frequency of 0.305 Å^{-1}

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 ⓘ
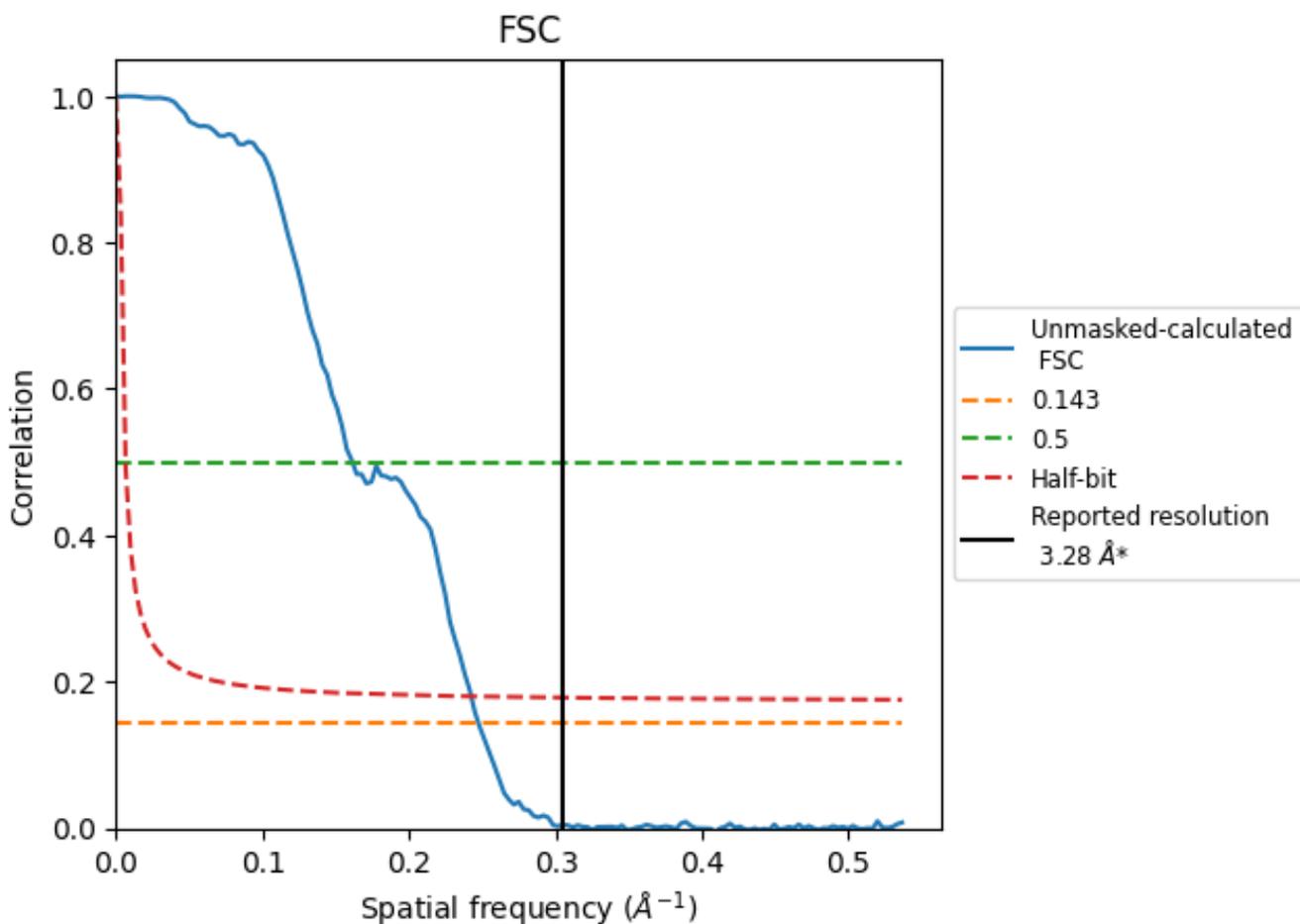
*Reported resolution corresponds to spatial frequency of 0.305 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.04	6.20	4.12

*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 4.04 differs from the reported value 3.28 by more than 10 %

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-26856 and PDB model 7UXA. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay (i)

| X | Y | Z |
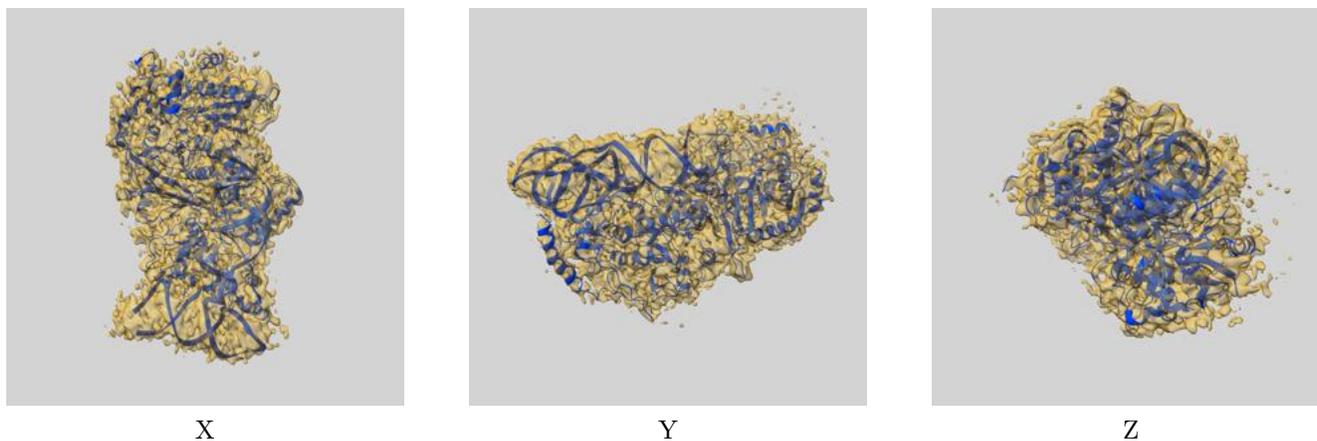
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model　ⓘ

X　　　　　　　　　　Y　　　　　　　　　　Z
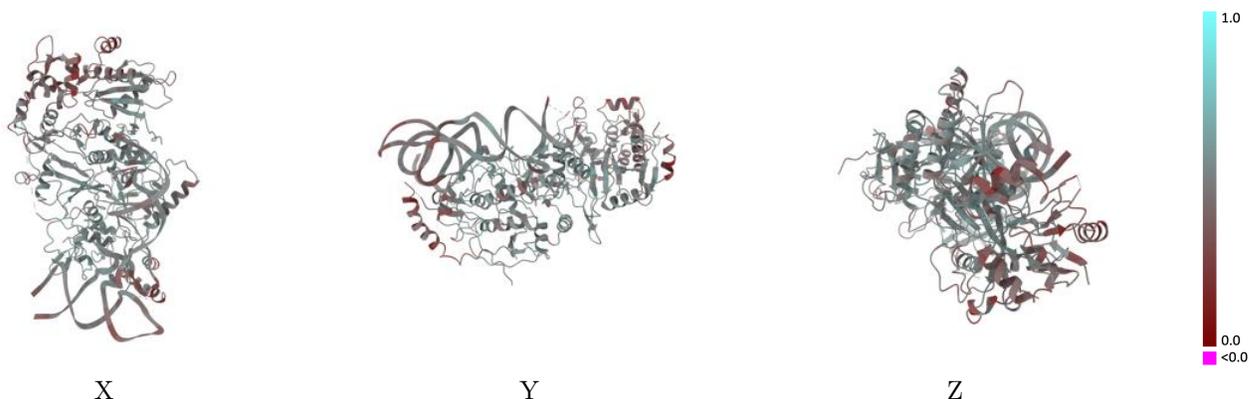
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
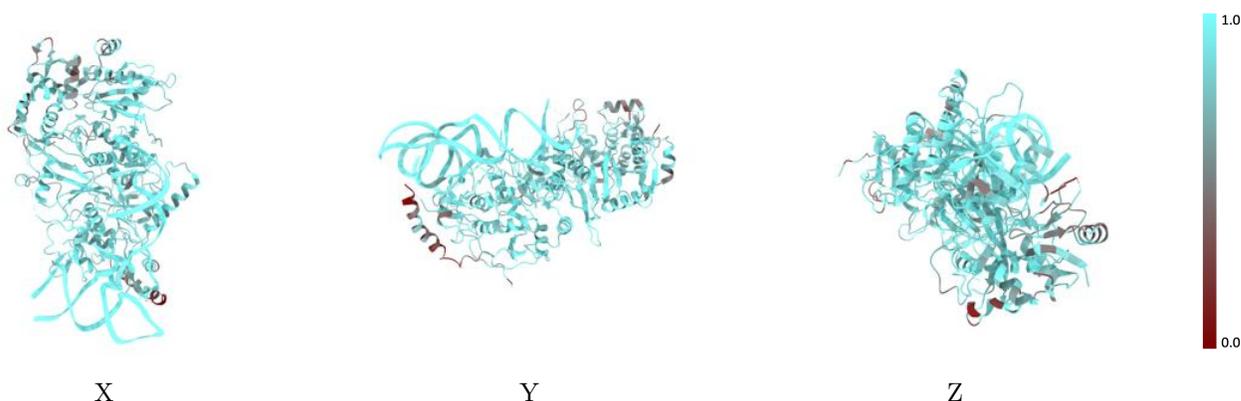
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion ⓘ
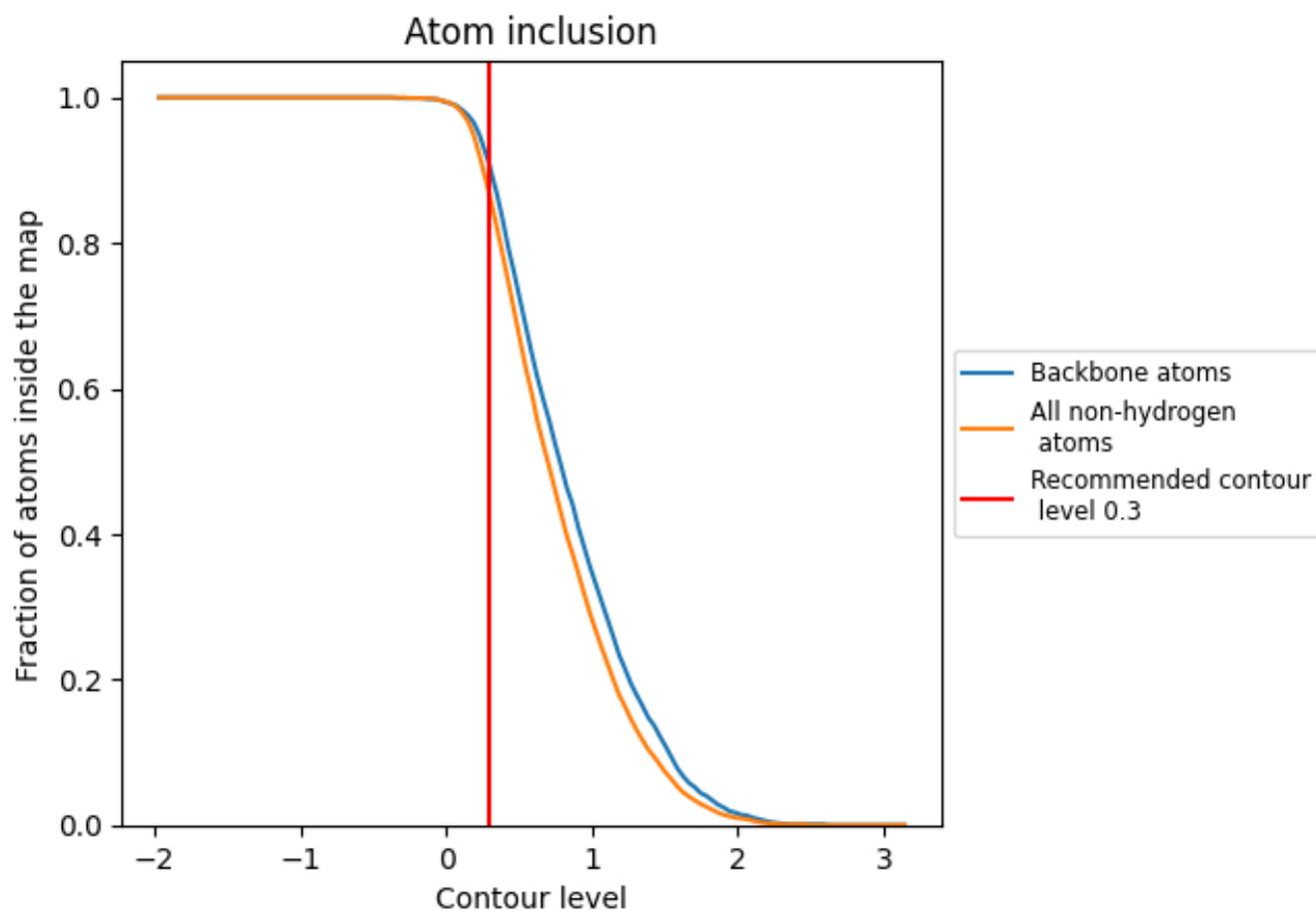
At the recommended contour level, 91% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8650	0.4720
A	0.8390	0.4890
B	0.8480	0.4550
C	0.7810	0.4350
D	0.8870	0.5050
E	0.9570	0.4600

1.0

0.0
<0.0