



wwPDB EM Validation Summary Report ⓘ

Jan 1, 2025 – 09:42 AM EST

PDB ID : 8T4S
EMDB ID : EMD-41039
Title : MERS-CoV Nsp1 protein bound to the Human 40S Ribosomal subunit
Authors : Devarkar, S.C.; Xiong, Y.
Deposited on : 2023-06-09
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

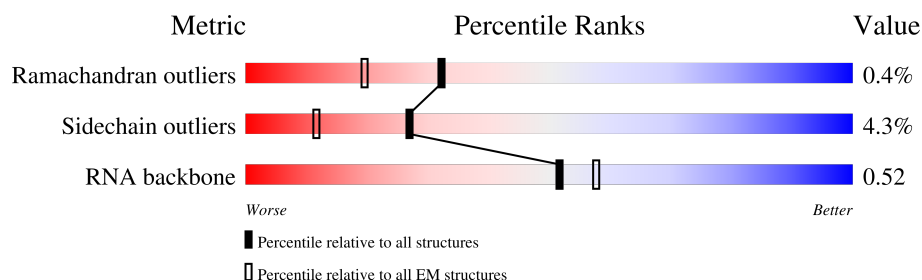
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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 2.60 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.




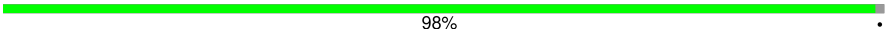




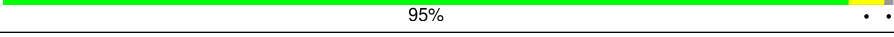

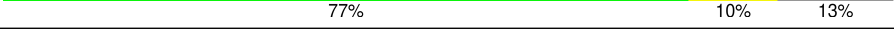

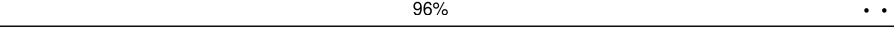
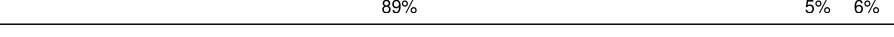
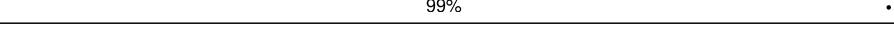
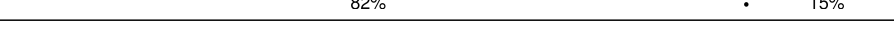
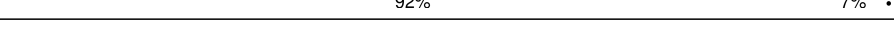
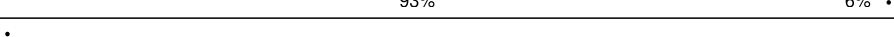
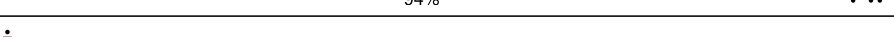

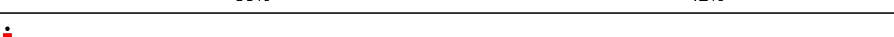






Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 $\leq 5\%$. 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	2	1869	
2	A	295	
3	B	264	
4	C	293	
5	D	243	
6	E	263	
7	F	204	
8	G	249	

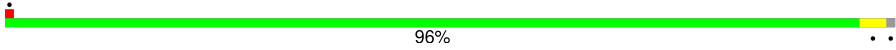


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Mol	Chain	Length	Quality of chain
9	H	194	
10	I	208	
11	J	194	
12	K	165	
13	L	158	
14	M	132	
15	N	151	
16	O	151	
17	P	145	
18	Q	146	
19	R	135	
20	S	152	
21	T	145	
22	U	119	
23	V	83	
24	W	130	
25	X	143	
26	Y	133	
27	Z	125	
28	a	115	
29	b	84	
30	c	69	
31	d	56	
32	e	133	
33	f	156	

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Mol	Chain	Length	Quality of chain
34	g	317	 96%
35	h	25	 88%12%
36	n	193	 13%87%

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 74894 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 RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1671	Total	C	N	O	P	0	0
			35677	15925	6406	11675	1671		

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	213	Total	C	N	O	S	0	0
			1686	1072	295	311	8		

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	218	Total	C	N	O	S	0	0
			1690	1094	289	297	10		

- Molecule 5 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	225	Total	C	N	O	S	0	0
			1752	1117	315	313	7		

- Molecule 6 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 7 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 8 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	230	Total	C	N	O	S	0	0
			1864	1164	373	320	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	221	ARG	LYS	variant	UNP P62753

- Molecule 9 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	186	Total	C	N	O	S	0	0
			1501	957	276	267	1		

- Molecule 10 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 11 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 12 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	97	Total	C	N	O	S	0	0
			816	533	144	133	6		

- Molecule 13 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	121	Total	C	N	O	S	0	0
			935	586	165	175	9		

- Molecule 15 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 16 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

- Molecule 17 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	126	Total	C	N	O	S	0	0
			1037	659	196	175	7		

- Molecule 18 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	138	Total	C	N	O	S	0	0
			1097	698	206	190	3		

- Molecule 19 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 20 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	143	Total	C	N	O	S	0	0
			1184	743	240	200	1		

- Molecule 21 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	144	Total	C	N	O	S	0	0
			1122	703	217	199	3		

- Molecule 22 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 23 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	82	Total	C	N	O	S	0	0
			625	384	116	120	5		

- Molecule 24 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 25 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 26 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 27 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 28 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	99	Total	C	N	O	S	0	0
			794	494	165	130	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	78	VAL	ALA	conflict	UNP P62854

- Molecule 29 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 30 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 31 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 32 is a protein called FAU ubiquitin-like and ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	56	Total	C	N	O	S	0	0
			442	273	96	72	1		

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	74	Total	C	N	O	S	0	0
			610	385	117	101	7		

- Molecule 34 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 35 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	22	Total	C	N	O	S	0	0
			213	130	57	23	3		

- Molecule 36 is a protein called Replicase polypeptide 1ab.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	n	25	Total	C	N	O	S	0	0
			206	134	32	38	2		

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	2	96	Total	Mg	0
			96	96	
37	I	1	Total	Mg	0
			1	1	

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	a	1	Total	Zn	0
			1	1	
38	d	1	Total	Zn	0
			1	1	
38	f	1	Total	Zn	0
			1	1	

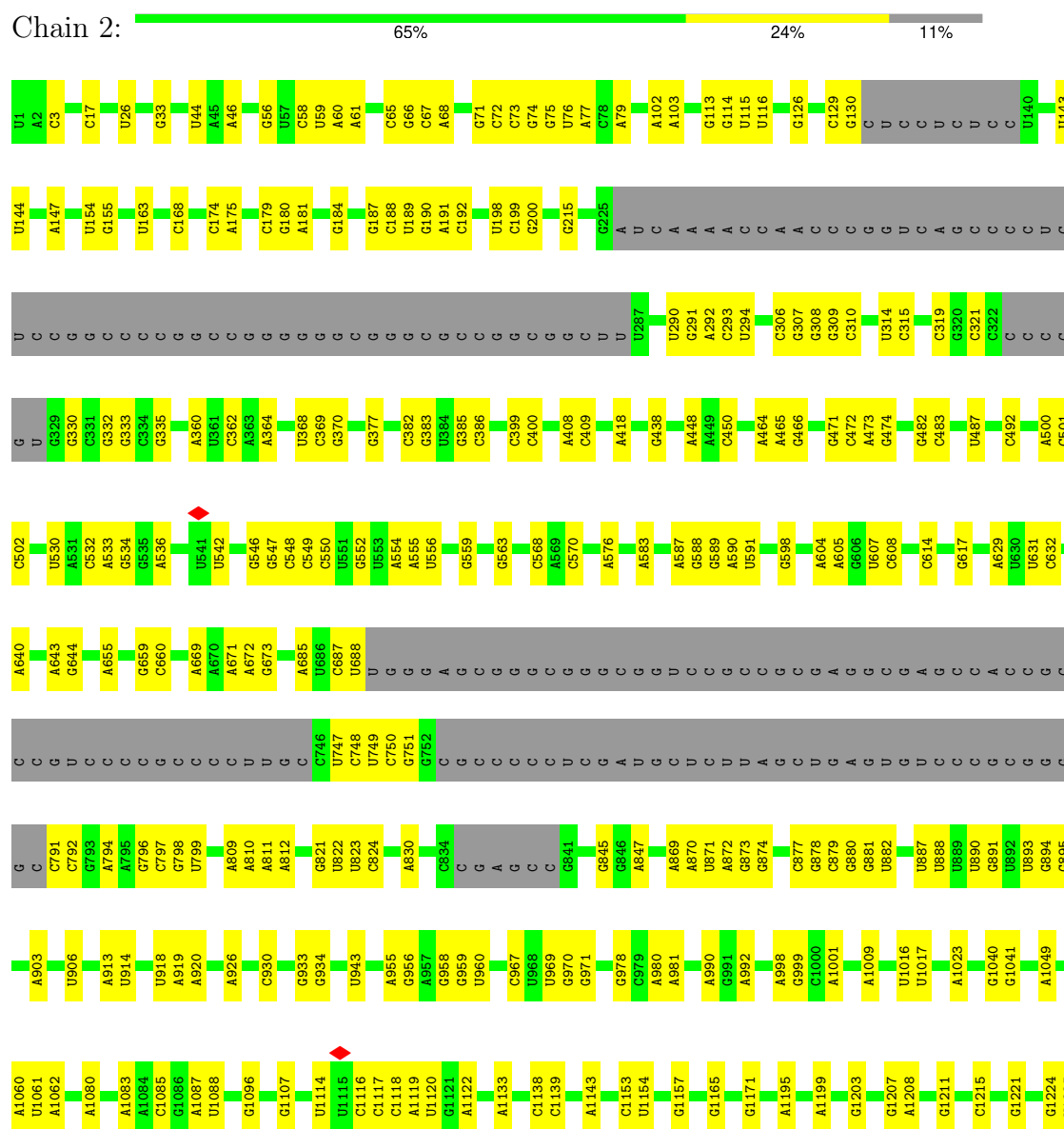
- Molecule 39 is water.

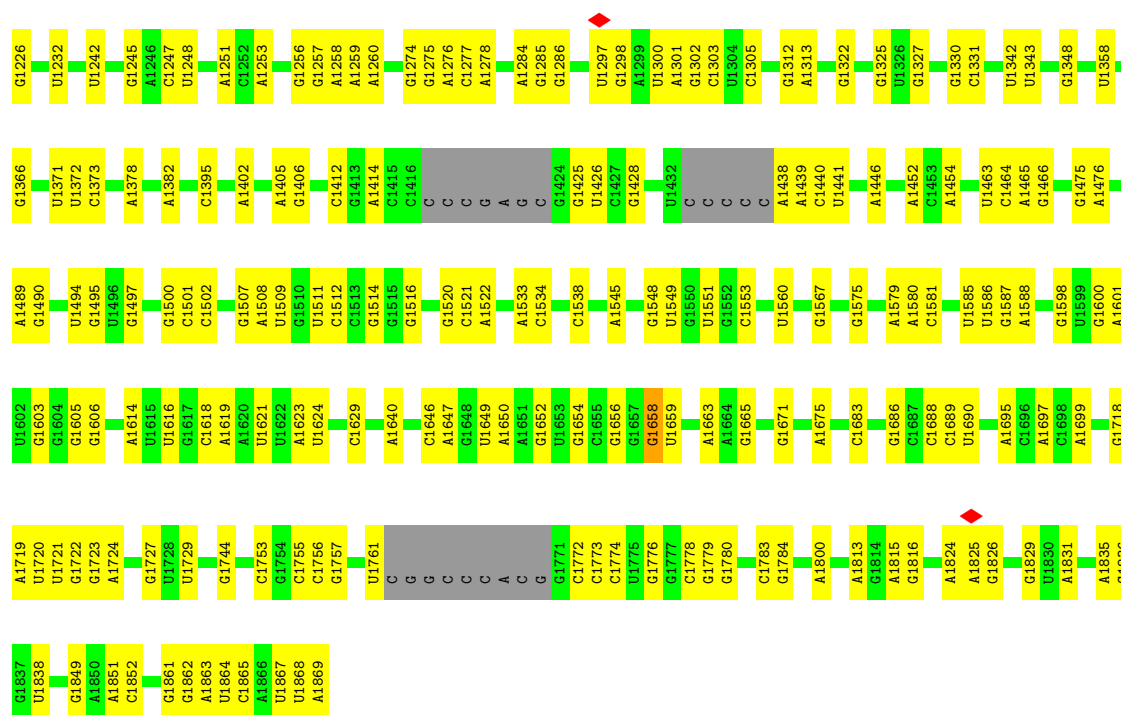
Mol	Chain	Residues	Atoms		AltConf
39	2	4	Total	O	0
			4	4	

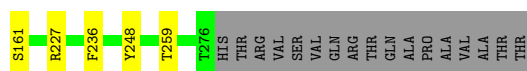
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 18S rRNA

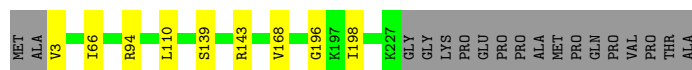






- Molecule 5: 40S ribosomal protein S3

Chain D: 89% 7%



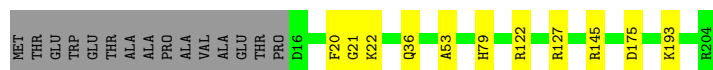
- Molecule 6: 40S ribosomal protein S4, X isoform

Chain E: 98%



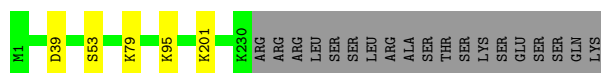
- Molecule 7: 40S ribosomal protein S5

Chain F: 87% 5% 7%



- Molecule 8: 40S ribosomal protein S6

Chain G: 90% 8%



- Molecule 9: 40S ribosomal protein S7

Chain H: 15% 91% 5%




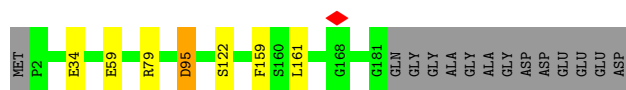
- Molecule 10: 40S ribosomal protein S8

Chain I: 98%



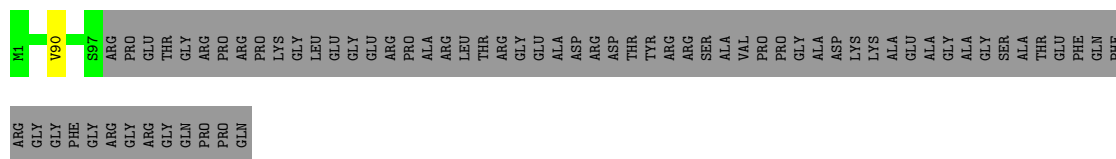
- Molecule 11: 40S ribosomal protein S9

Chain J:  89% 7%



- Molecule 12: 40S ribosomal protein S10

Chain K:  58% 41%




- Molecule 13: 40S ribosomal protein S11

Chain L:  91% 5%



- Molecule 14: 40S ribosomal protein S12

Chain M:  5% 86% 6% 8%




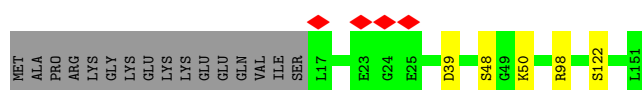
- Molecule 15: 40S ribosomal protein S13

Chain N:  95%



- Molecule 16: 40S ribosomal protein S14

Chain O:  86% 11%



- Molecule 17: 40S ribosomal protein S15

Chain P:  77% 10% 13%



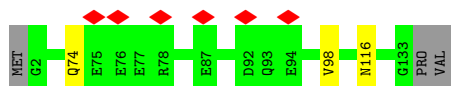
- Molecule 18: 40S ribosomal protein S16

Chain Q: 90% 5% 5%



- Molecule 19: 40S ribosomal protein S17

Chain R: 96% . .



- Molecule 20: 40S ribosomal protein S18

Chain S: 89% 5% 6%



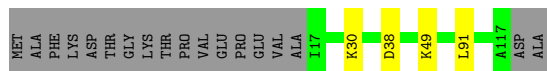
- Molecule 21: 40S ribosomal protein S19

Chain T: 99% ..



- Molecule 22: 40S ribosomal protein S20

Chain U: 82% . 15%



- Molecule 23: 40S ribosomal protein S21

Chain V: 92% 7% .



- Molecule 24: 40S ribosomal protein S15a

Chain W: 93% 6% .

A diagram showing a linear sequence of five colored blocks: MET (grey), G2 (green), F14 (yellow), R40 (yellow), and D56 (green). The blocks are connected by horizontal lines.

- Chain e:  40% 58%

[illegible]

- Chain f:

[illegible]

- Chain g:  96%

Diagram illustrating the protein structure of the T2 domain, showing residues MET, T2, D48, F113, D116, C182, T186, D234, Y246, I275, S276, T277, I314, G315, THR, and ARG. Red diamonds highlight specific residues (I275, S276, T277).

- Chain h: 88% 12%

M1	Q22	ARG	SER	LYS
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- Chain n: 13% 87%

MET	SER	PHE	VAL	ALA	GLY	VAL	THR	GLN	GLY	ALA	ARG	THR	TYR	ARG	ALA	ALA	LEU	ASN	SER	GLU	LYS	HIS	GLN	ASP	HIS	VAL	SER	LEU	THR	VAL	PRO	LEU	CYS	GLY	SER	GLY	ASN	LEU	VAL	PRO	TRP	PHE	MET	ASP	GLY	GLY	ASN	ASN	ALA	TYR	GLU	VAL	THR	
ALA	MET	LEU	LEV	LVS	GLU	PRO	LEU	TYR	VAl	PRO	ARG	ILE	LEU	ALA	HIS	THR	ARG	HIS	LEU	PRO	GLY	GLY	PRO	ARG	VAL	THR	LEU	GLU	VAL	LEU	ILE	ALA	CYS	GLY	ASN	GLU	PRO	PHE	MET	VAL	ASN	GLN	LEU	ALA	THR	SER	SER	SER	ASN	ALA	LEU	VAL	GLY	THR

LEU	GLN	GLY	LYS	PRO	ILE	GLY	MET	PHE	PHE	PRO	TYR	ASP	ILE	GLU	LEU	VAL	THR	GLY	LYS	GLN	ASN	ILE	LEU	LEU	ARG	LYS	TYR	GLY	ARG	GLY	GLY	TYR	HIS	TYR	THR	PRO	PHE	HIS	TYR	GLU	ARG	ASP	ASN	THR	SER	GLN	ILE	GLY	GLY
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	267551	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.809	Depositor
Minimum map value	-0.270	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	406.6, 406.6, 406.6	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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, ZN

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	2	0.51	0/39895	0.78	1/62174 (0.0%)
2	A	0.31	0/1723	0.52	0/2341
3	B	0.28	0/1756	0.50	0/2350
4	C	0.33	0/1726	0.50	0/2332
5	D	0.33	0/1780	0.56	0/2397
6	E	0.34	0/2118	0.55	0/2849
7	F	0.38	0/1516	0.62	0/2037
8	G	0.30	0/1887	0.58	0/2513
9	H	0.28	0/1524	0.54	0/2042
10	I	0.33	0/1711	0.57	0/2282
11	J	0.35	0/1524	0.60	1/2035 (0.0%)
12	K	0.35	0/840	0.54	0/1133
13	L	0.35	0/1250	0.57	0/1673
14	M	0.29	0/945	0.54	0/1269
15	N	0.30	0/1226	0.53	0/1649
16	O	0.28	0/1023	0.58	0/1372
17	P	0.37	0/1058	0.62	0/1414
18	Q	0.35	0/1114	0.58	0/1492
19	R	0.30	0/1082	0.56	0/1452
20	S	0.32	0/1202	0.60	0/1610
21	T	0.32	0/1142	0.52	0/1530
22	U	0.30	0/813	0.58	0/1092
23	V	0.33	0/631	0.61	1/844 (0.1%)
24	W	0.40	0/1051	0.56	0/1406
25	X	0.35	0/1116	0.59	1/1490 (0.1%)
26	Y	0.34	0/1031	0.57	0/1370
27	Z	0.31	0/580	0.58	0/780
28	a	0.30	0/807	0.55	0/1082
29	b	0.27	0/653	0.51	0/876
30	c	0.34	0/490	0.72	0/656
31	d	0.39	0/469	0.56	0/623
32	e	0.42	0/447	0.55	0/587

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	f	0.40	0/622	0.54	0/822
34	g	0.33	0/2497	0.53	0/3399
35	h	0.25	0/214	0.83	0/272
36	n	0.26	0/211	0.37	0/283
All	All	0.43	0/79674	0.69	4/115528 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1658	G	C2'-C3'-O3'	6.57	124.21	113.70
25	X	98	ASP	CB-CG-OD1	5.18	122.96	118.30
23	V	40	ASP	CB-CG-OD1	5.16	122.94	118.30
11	J	95	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
2	A	211/295 (72%)	202 (96%)	8 (4%)	1 (0%)	25	47
3	B	211/264 (80%)	205 (97%)	6 (3%)	0	100	100
4	C	216/293 (74%)	210 (97%)	6 (3%)	0	100	100
5	D	223/243 (92%)	217 (97%)	5 (2%)	1 (0%)	30	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	E	260/263 (99%)	256 (98%)	4 (2%)	0	100	100
7	F	187/204 (92%)	169 (90%)	15 (8%)	3 (2%)	8	17
8	G	228/249 (92%)	221 (97%)	7 (3%)	0	100	100
9	H	184/194 (95%)	169 (92%)	15 (8%)	0	100	100
10	I	203/208 (98%)	198 (98%)	5 (2%)	0	100	100
11	J	178/194 (92%)	170 (96%)	7 (4%)	1 (1%)	22	43
12	K	95/165 (58%)	91 (96%)	4 (4%)	0	100	100
13	L	149/158 (94%)	142 (95%)	7 (5%)	0	100	100
14	M	119/132 (90%)	99 (83%)	18 (15%)	2 (2%)	7	16
15	N	147/151 (97%)	146 (99%)	1 (1%)	0	100	100
16	O	133/151 (88%)	128 (96%)	5 (4%)	0	100	100
17	P	124/145 (86%)	113 (91%)	8 (6%)	3 (2%)	5	9
18	Q	136/146 (93%)	125 (92%)	11 (8%)	0	100	100
19	R	130/135 (96%)	126 (97%)	4 (3%)	0	100	100
20	S	141/152 (93%)	129 (92%)	11 (8%)	1 (1%)	19	38
21	T	142/145 (98%)	134 (94%)	8 (6%)	0	100	100
22	U	99/119 (83%)	94 (95%)	5 (5%)	0	100	100
23	V	80/83 (96%)	77 (96%)	3 (4%)	0	100	100
24	W	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
25	X	139/143 (97%)	135 (97%)	3 (2%)	1 (1%)	19	38
26	Y	122/133 (92%)	116 (95%)	6 (5%)	0	100	100
27	Z	70/125 (56%)	69 (99%)	1 (1%)	0	100	100
28	a	97/115 (84%)	95 (98%)	1 (1%)	1 (1%)	13	29
29	b	80/84 (95%)	75 (94%)	5 (6%)	0	100	100
30	c	60/69 (87%)	56 (93%)	4 (7%)	0	100	100
31	d	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
32	e	54/133 (41%)	50 (93%)	4 (7%)	0	100	100
33	f	72/156 (46%)	61 (85%)	8 (11%)	3 (4%)	2	3
34	g	312/317 (98%)	293 (94%)	18 (6%)	1 (0%)	37	59
35	h	20/25 (80%)	19 (95%)	1 (5%)	0	100	100
36	n	23/193 (12%)	23 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4825/5768 (84%)	4588 (95%)	219 (4%)	18 (0%)	32 52

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	M	110	VAL
33	f	88	PRO
2	A	189	ILE
11	J	161	LEU
20	S	38	ARG

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
2	A	179/243 (74%)	173 (97%)	6 (3%)	32 58
3	B	194/231 (84%)	182 (94%)	12 (6%)	15 33
4	C	184/225 (82%)	179 (97%)	5 (3%)	40 66
5	D	189/202 (94%)	181 (96%)	8 (4%)	25 50
6	E	224/225 (100%)	220 (98%)	4 (2%)	54 77
7	F	159/170 (94%)	151 (95%)	8 (5%)	20 43
8	G	200/218 (92%)	195 (98%)	5 (2%)	42 68
9	H	167/174 (96%)	158 (95%)	9 (5%)	18 39
10	I	178/180 (99%)	177 (99%)	1 (1%)	84 94
11	J	160/168 (95%)	154 (96%)	6 (4%)	28 54
12	K	88/136 (65%)	87 (99%)	1 (1%)	70 86
13	L	135/142 (95%)	127 (94%)	8 (6%)	16 35
14	M	102/108 (94%)	96 (94%)	6 (6%)	16 35
15	N	130/131 (99%)	124 (95%)	6 (5%)	23 46
16	O	105/119 (88%)	100 (95%)	5 (5%)	21 44
17	P	112/130 (86%)	100 (89%)	12 (11%)	5 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	Q	114/121 (94%)	107 (94%)	7 (6%)	15	34
19	R	119/122 (98%)	116 (98%)	3 (2%)	42	68
20	S	124/132 (94%)	118 (95%)	6 (5%)	21	44
21	T	114/115 (99%)	113 (99%)	1 (1%)	75	90
22	U	93/107 (87%)	89 (96%)	4 (4%)	25	49
23	V	66/67 (98%)	61 (92%)	5 (8%)	11	23
24	W	112/113 (99%)	104 (93%)	8 (7%)	12	26
25	X	113/115 (98%)	108 (96%)	5 (4%)	24	48
26	Y	108/115 (94%)	101 (94%)	7 (6%)	14	31
27	Z	64/103 (62%)	62 (97%)	2 (3%)	35	62
28	a	87/99 (88%)	81 (93%)	6 (7%)	13	28
29	b	74/76 (97%)	73 (99%)	1 (1%)	62	82
30	c	55/62 (89%)	51 (93%)	4 (7%)	11	25
31	d	48/49 (98%)	46 (96%)	2 (4%)	25	50
32	e	45/104 (43%)	42 (93%)	3 (7%)	13	29
33	f	67/140 (48%)	61 (91%)	6 (9%)	8	16
34	g	272/275 (99%)	264 (97%)	8 (3%)	37	64
35	h	21/24 (88%)	21 (100%)	0	100	100
36	n	22/161 (14%)	22 (100%)	0	100	100
All	All	4224/4902 (86%)	4044 (96%)	180 (4%)	27	49

5 of 180 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	S	89	ASP
26	Y	26	ASP
22	U	30	LYS
24	W	30	CYS
28	a	2	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
21	T	12	GLN

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Mol	Chain	Res	Type
30	c	29	GLN
34	g	51	ASN
31	d	10	HIS
12	K	84	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1663/1869 (88%)	433 (26%)	53 (3%)

5 of 433 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	C
1	2	17	C
1	2	26	U
1	2	33	G
1	2	44	U

5 of 53 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	958	G
1	2	1330	G
1	2	1718	G
1	2	980	A
1	2	1165	G

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 100 ligands modelled in this entry, 100 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

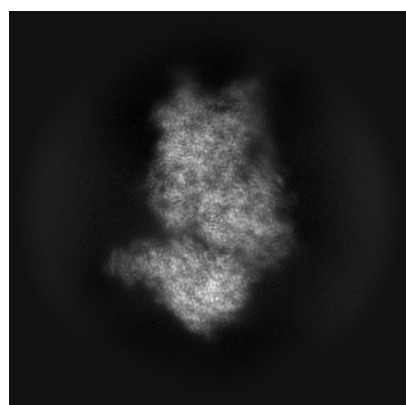
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41039. These allow visual inspection of the internal detail of the map and identification of artifacts.

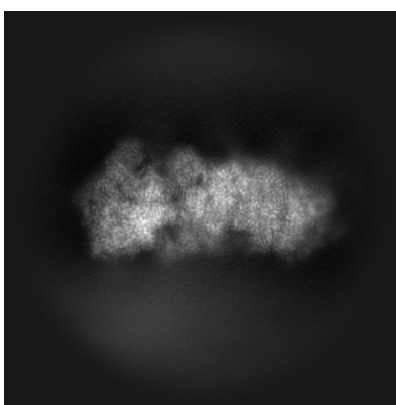
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

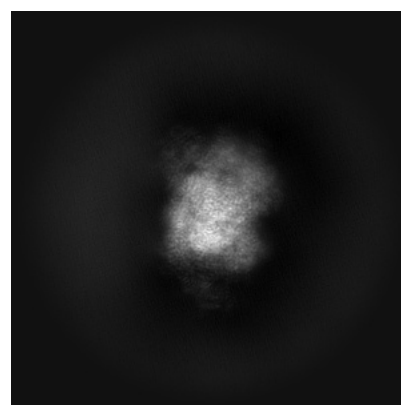
6.1.1 Primary map



X



Y

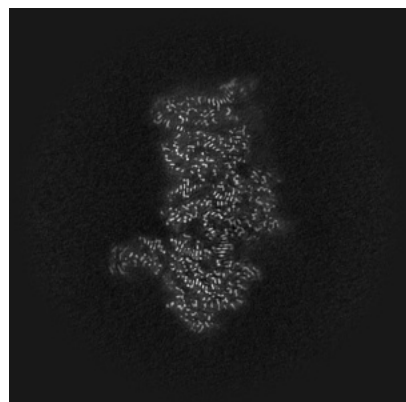


Z

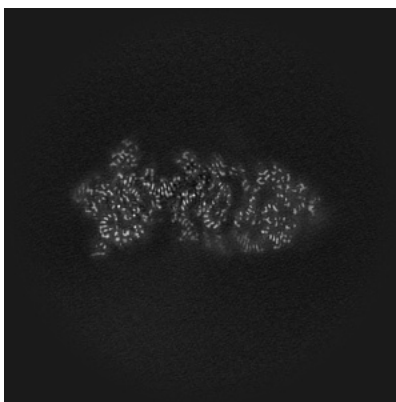
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

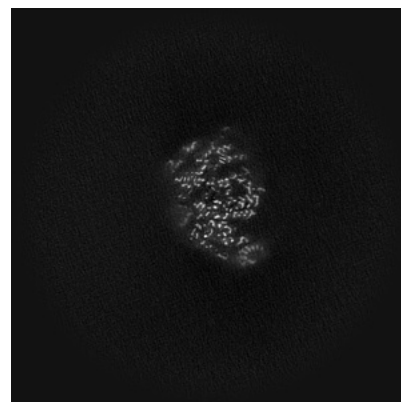
6.2.1 Primary map



X Index: 190



Y Index: 190

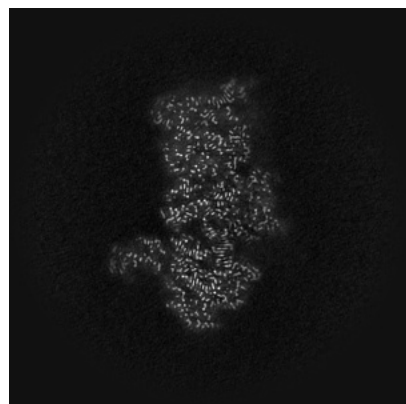


Z Index: 190

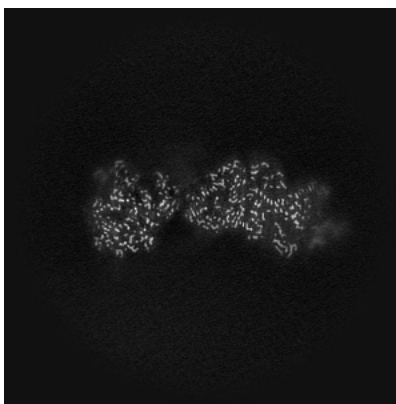
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

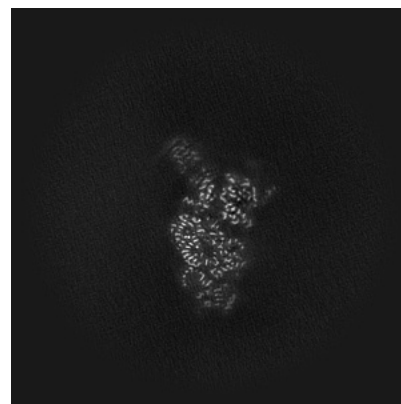
6.3.1 Primary map



X Index: 189



Y Index: 165

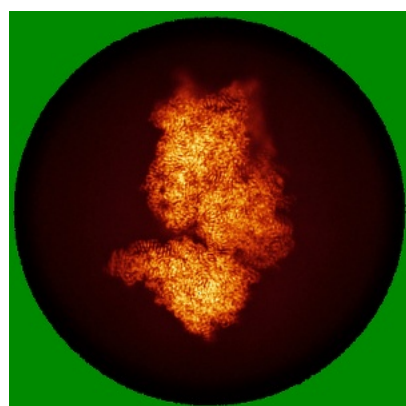


Z Index: 138

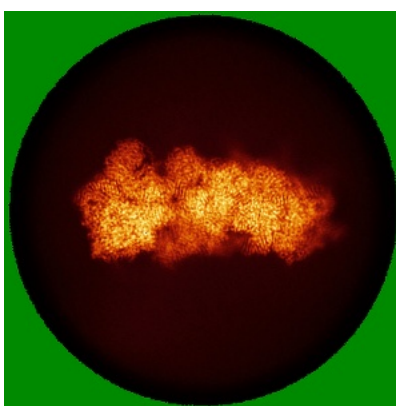
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

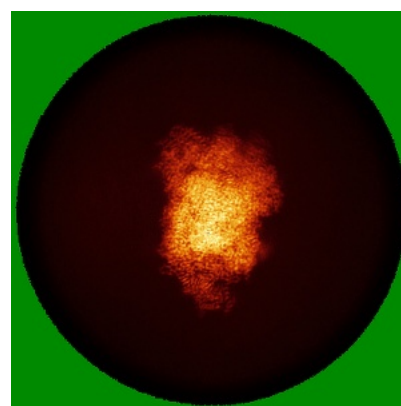
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

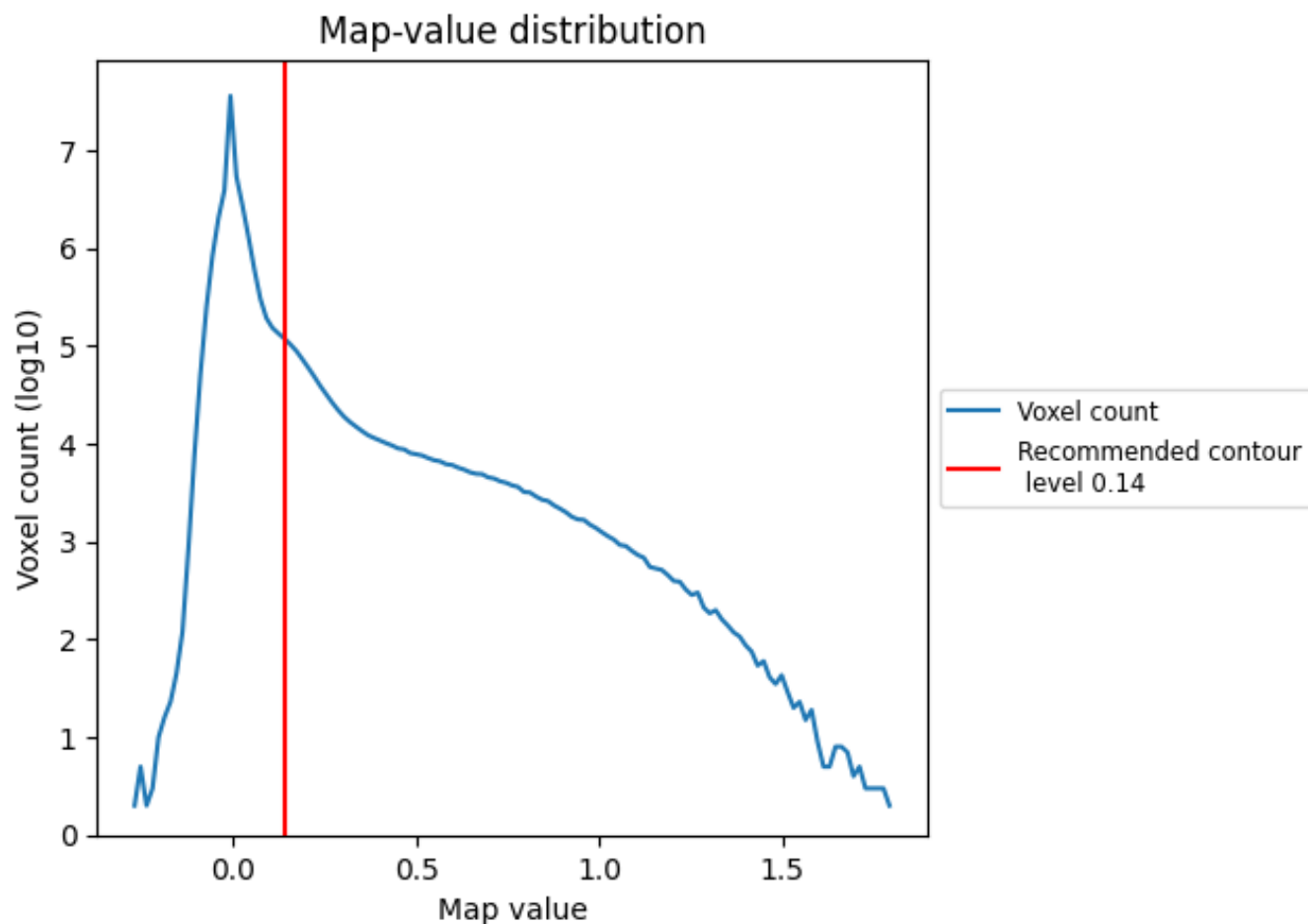
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

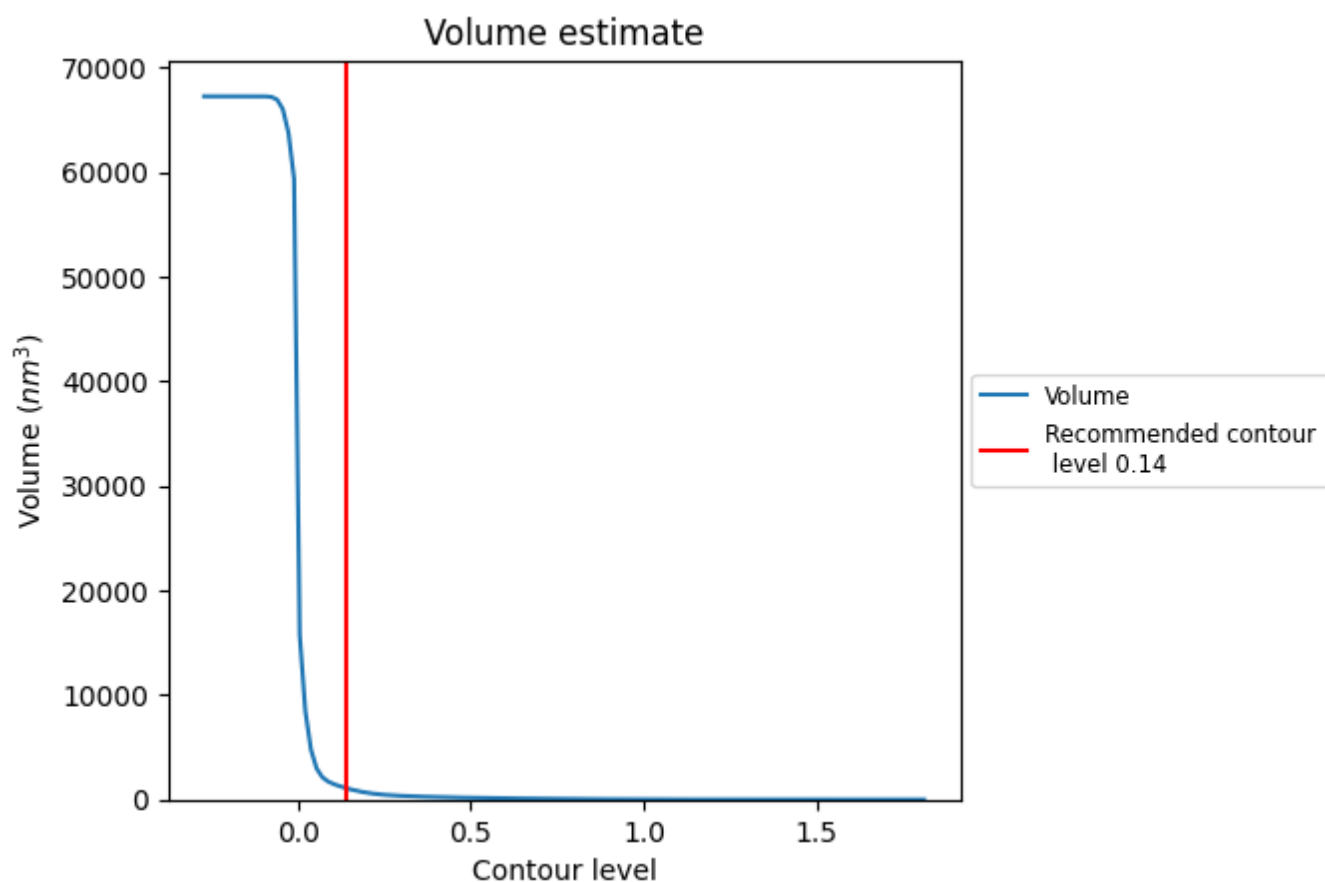
This section contains the results of statistical analysis of the map.

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.

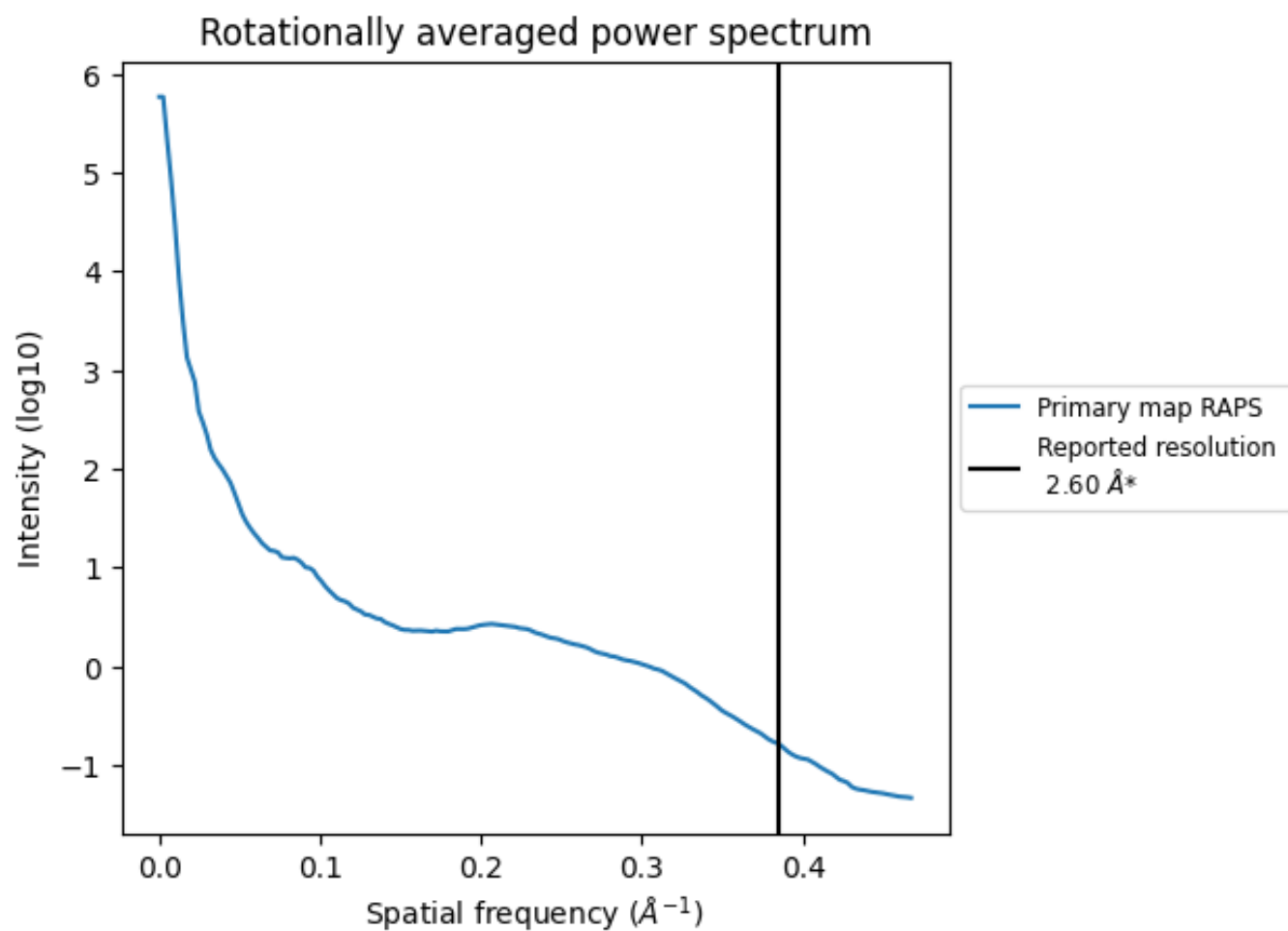
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1093 nm³; this corresponds to an approximate mass of 987 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 ⓘ

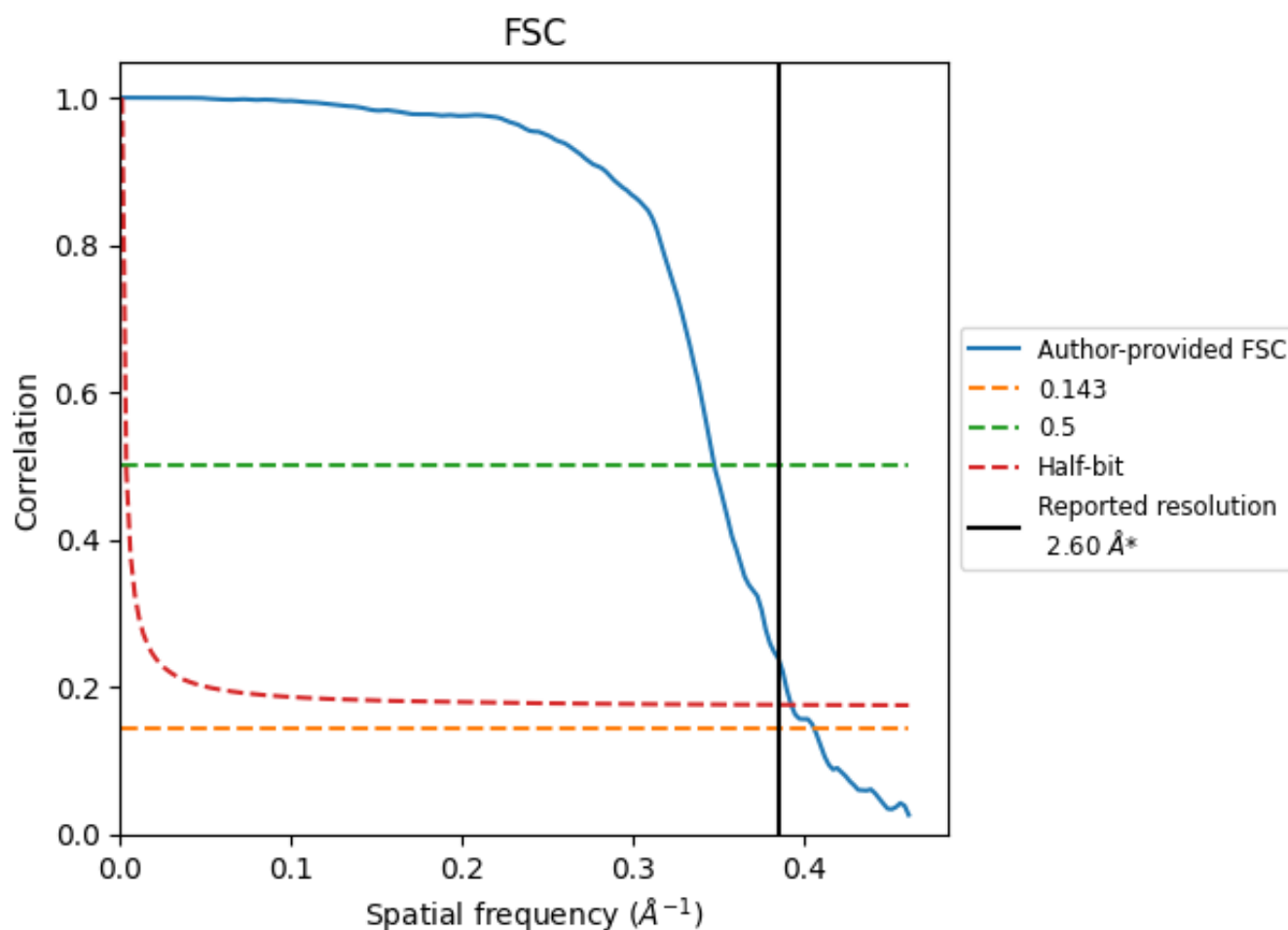


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 Å⁻¹

8.2 Resolution estimates [i](#)

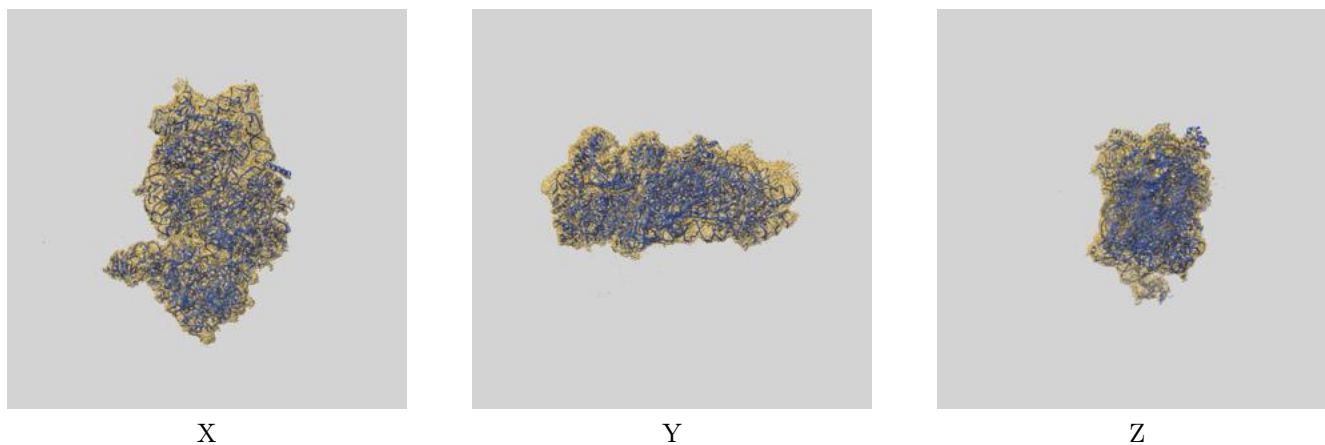
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.46	2.88	2.55
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

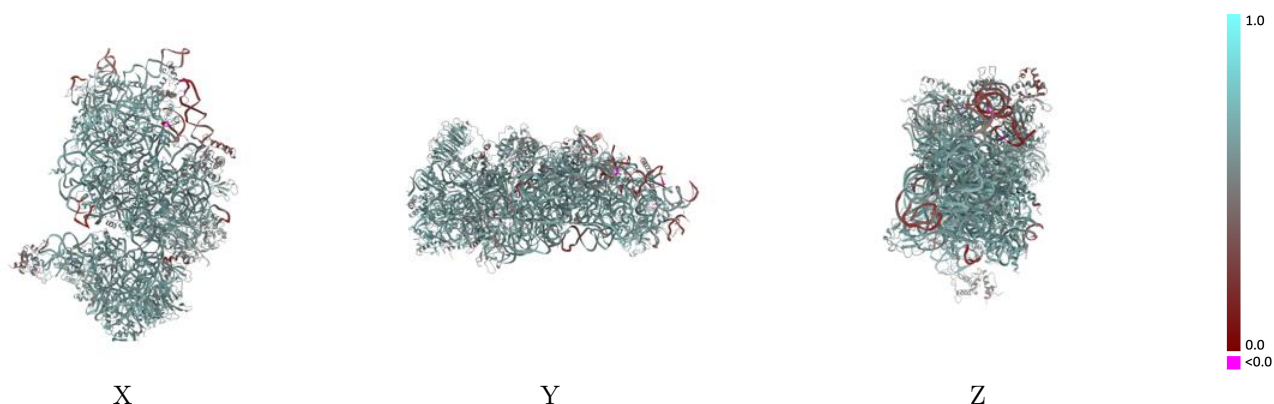
This section contains information regarding the fit between EMDB map EMD-41039 and PDB model 8T4S. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



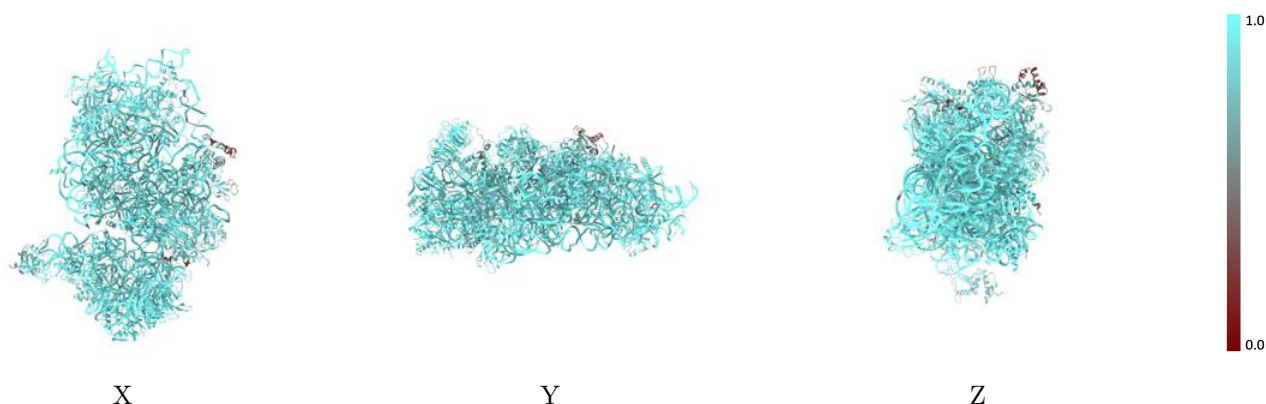
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



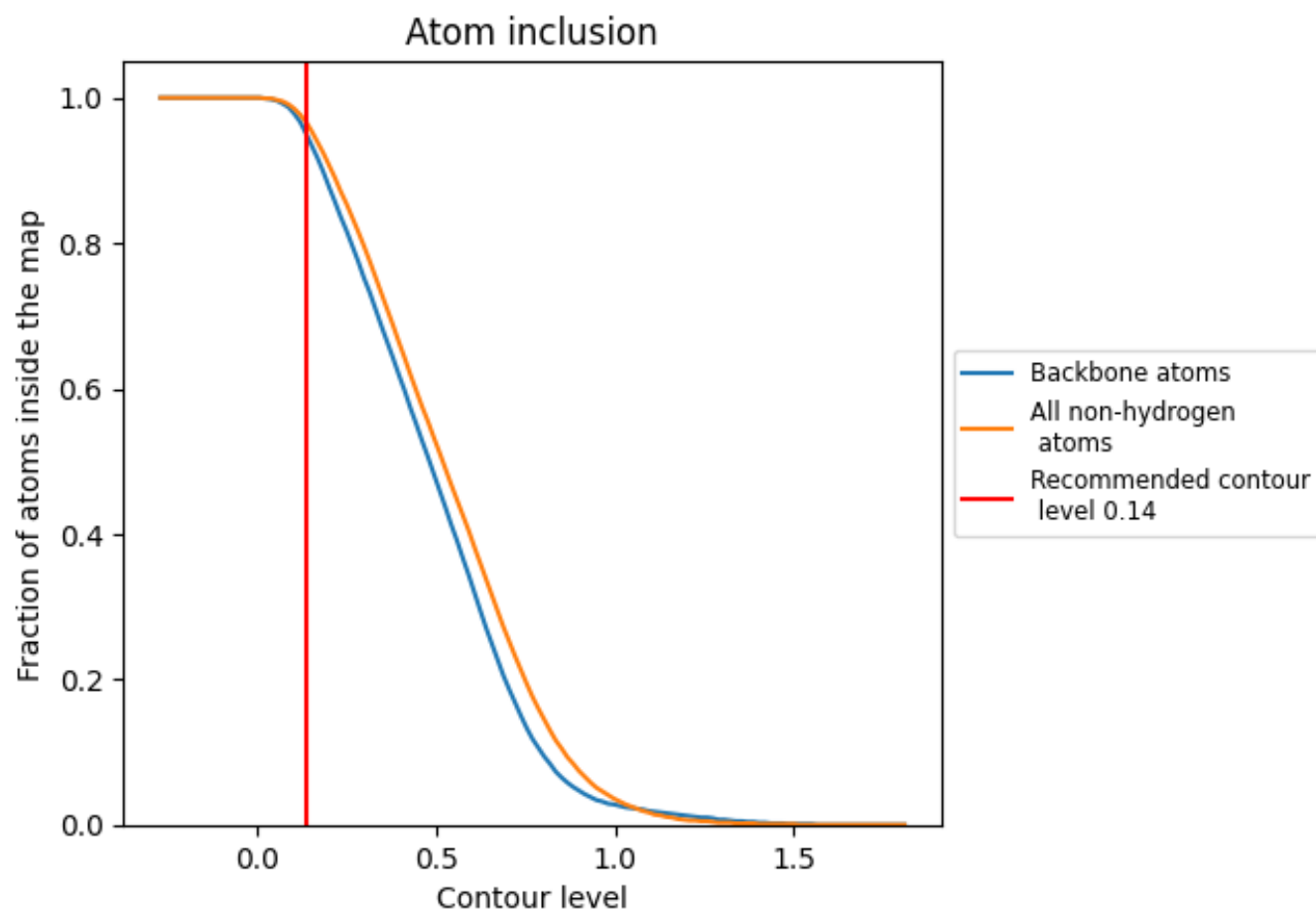
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.14).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 96% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9640	 0.5900
2	 0.9880	 0.5930
A	 0.9560	 0.5880
B	 0.9130	 0.5600
C	 0.9840	 0.6260
D	 0.9610	 0.5890
E	 0.9830	 0.6260
F	 0.9820	 0.6110
G	 0.9690	 0.5790
H	 0.7250	 0.4640
I	 0.9720	 0.6090
J	 0.9760	 0.6220
K	 0.9850	 0.6190
L	 0.9620	 0.6240
M	 0.7820	 0.4390
N	 0.9360	 0.5760
O	 0.9130	 0.5350
P	 0.9550	 0.6060
Q	 0.9980	 0.6410
R	 0.8580	 0.5380
S	 0.9640	 0.5910
T	 0.9840	 0.6230
U	 0.9540	 0.5830
V	 0.9710	 0.5890
W	 0.9810	 0.6230
X	 0.9800	 0.6220
Y	 0.9750	 0.6110
Z	 0.9720	 0.6090
a	 0.9230	 0.5900
b	 0.8380	 0.5630
c	 0.9470	 0.5570
d	 0.9840	 0.6520
e	 0.9180	 0.5820
f	 0.8490	 0.5060
g	 0.9520	 0.5840



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Chain	Atom inclusion	Q-score
h	 0.9170	 0.5610
n	 0.9360	 0.5800