W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report ⓘ

Jun 5, 2025 – 03:02 PM EDT

PDB ID	:	9NPY / pdb_00009npy
EMDB ID	:	EMD-49636
Title	:	SARS-CoV-2 nsp1 bound to the Rhinolophus lepidus 40S ribosome (local refinement of the 40S head)
Authors	:	Gen, R.; Seattle Structural Genomics Center for Infectious Disease (SSGCID); Veesler, D.
Deposited on	:	2025-03-11
Resolution	:	2.10 Å(reported)

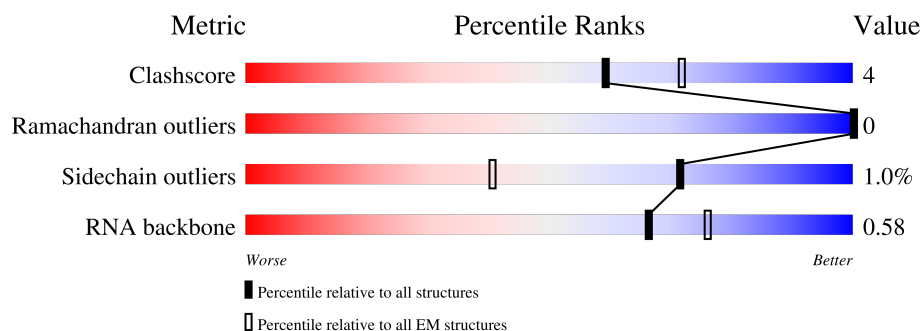The following versions of software and data (see references ⓘ) were used in the production of this report:

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

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.10 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		4
Ramachandran outliers		0
Sidechain outliers		1.0%
RNA backbone		0.58

Worse   *Better*

▍ Percentile relative to all structures

▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
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 <=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	B	243	84% 7% 9%
2	J	165	49% 9% 42%
3	L	132	8% 75% 5% • 18%
4	O	145	78% 8% 14%
5	Q	146	84% 12% • •
6	R	135	47% 5% 48%
7	S	152	86% 6% 8%

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Mol	Chain	Length	Quality of chain
8	T	145	91% 6%
9	U	119	79% 5% 16%
10	Y	125	48% 9% 43%
11	b	156	33% 63%
12	c	69	80% 10% 10%
13	d	56	93% 5%
14	i	1869	17% 7% 74%
15	E	204	83% 7% 10%
16	g	317	81% 15%

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 25171 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 40S ribosomal protein uS3, RPS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	221	Total 1601	C 1029	N 292	O 273	S 7	0	0

- Molecule 2 is a protein called 40S ribosomal protein eS10, RPS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	96	Total 776	C 513	N 135	O 122	S 6	0	0

- Molecule 3 is a protein called 40S ribosomal protein eS12, RPS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	108	Total 634	C 394	N 117	O 118	S 5	0	0

- Molecule 4 is a protein called 40S ribosomal protein uS19, RPS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	124	Total 953	C 606	N 179	O 162	S 6	0	0

- Molecule 5 is a protein called 40S ribosomal protein uS9, RPS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	140	Total 1095	C 697	N 207	O 188	S 3	0	0

- Molecule 6 is a protein called 40S ribosomal protein eS17, RPS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	70	Total 543	C 348	N 107	O 86	S 2	0	0

- Molecule 7 is a protein called 40S ribosomal protein uS13, RPS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	S	140	1072	680	217	174	1	1	0

- Molecule 8 is a protein called 40S ribosomal protein eS19, RPS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	T	141	1063	669	205	186	3	1	0

- Molecule 9 is a protein called 40S ribosomal protein uS10, RPS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	U	100	712	448	138	122	4	0	0

- Molecule 10 is a protein called 40S ribosomal protein eS25, RPS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	Y	71	537	348	100	88	1	0	0

- Molecule 11 is a protein called 40S ribosomal protein eS31, RPS27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	b	58	427	271	85	65	6	0	0

- Molecule 12 is a protein called 40S ribosomal protein eS28, RPS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	c	62	441	276	87	76	2	0	0

- Molecule 13 is a protein called 40S ribosomal protein uS14, RPS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	d	55	450	282	92	71	5	0	0

- Molecule 14 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	i	483	Total 10307	C 4607	N 1823	O 3394	P 483	0	0

- Molecule 15 is a protein called 40S ribosomal protein uS7, RPS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	184	Total 1429	C 900	N 267	O 255	S 7	0	0

- Molecule 16 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	g	307	Total 2272	C 1445	N 400	O 416	S 11	0	0

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
17	S	1	Total 1	Mg 1	0
17	T	1	Total 1	Mg 1	0
17	i	19	Total 19	Mg 19	0

- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
18	b	1	Total 1	Zn 1	0
18	d	1	Total 1	Zn 1	0

- Molecule 19 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
19	d	1	Total 1	K 1	0
19	i	7	Total 7	K 7	0
19	E	1	Total 1	K 1	0

• Molecule 20 is water.

Mol	Chain	Residues	Atoms		AltConf
20	B	11	Total 11	O 11	0
20	J	9	Total 9	O 9	0
20	O	17	Total 17	O 17	0
20	Q	42	Total 42	O 42	0
20	R	6	Total 6	O 6	0
20	S	13	Total 13	O 13	0
20	T	29	Total 29	O 29	0
20	U	12	Total 12	O 12	0
20	Y	1	Total 1	O 1	0
20	c	1	Total 1	O 1	0
20	d	19	Total 19	O 19	0
20	i	634	Total 634	O 634	0
20	E	27	Total 27	O 27	0
20	g	6	Total 6	O 6	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.
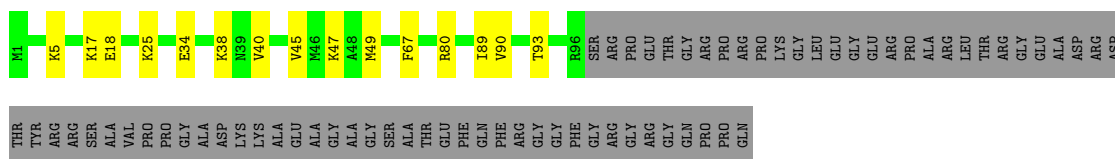
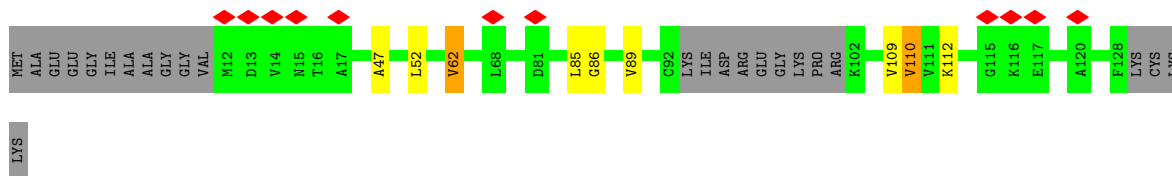• Molecule 1: 40S ribosomal protein uS3, RPS3

Chain B:
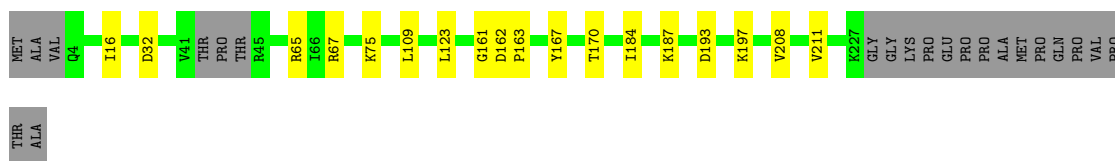
• Molecule 2: 40S ribosomal protein eS10, RPS10

Chain J:

• Molecule 3: 40S ribosomal protein eS12, RPS12

Chain L:

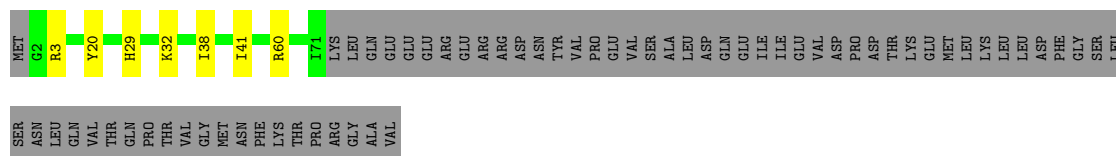• Molecule 4: 40S ribosomal protein uS19, RPS15

Chain O:

• Molecule 5: 40S ribosomal protein uS9, RPS16
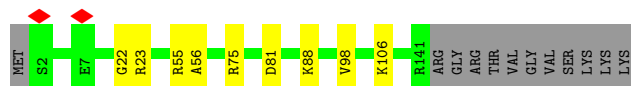
Chain Q:

84%   12%   •   •

MET PRO SER LYS GLY PRO L7 E53 L58 R62 R71 Y82 R85 S89 Q97 V100 D101 K105 D110 I111 L112 I113 Q114 L120 R126 Y141 R146

• Molecule 6: 40S ribosomal protein eS17, RPS17

Chain R:

47%   5%   48%

MET G2 R3 Y20 H29 K32 I38 I41 R60 I71 LYS LEU GLN GLU GLU GLU ARG GLU ARG ARG ASP ASN TYR VAL PRO GLU VAL SER ALA LEU ASP GLN GLU ILE ILE GLU VAL ASP PRO ASP THR LYS GLU MET LEU LYS LEU LEU ASP PHE GLY SER LEU

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

• Molecule 7: 40S ribosomal protein uS13, RPS18

Chain S:

86%   6%   8%

MET S2 E7 G22 R23 R55 A56 R75 D81 K88 V98 K106 R141 ARG GLY ARG THR VAL GLY VAL SER LYS LYS LYS

• Molecule 8: 40S ribosomal protein eS19, RPS19

Chain T:

91%   6%   •

MET PRO G3 R67 M88 R101 E108 D116 Q117 R121 Q126 R129 K143 LYS HIS

• Molecule 9: 40S ribosomal protein uS10, RPS20

Chain U:

79%   5%   16%

MET ALA PHE LYS ASP THR GLY LYS THR PRO VAL GLU PRO GLU VAL ALA I17 T25 V50 M56 K75 F80 K86 S103 I104 S105 I116 ALA ASP ALA

• Molecule 10: 40S ribosomal protein eS25, RPS25

Chain Y:

48%   9%   43%

MET PRO PRO LYS ASP ASP LYS LYS LYS LYS ASP ALA GLY LYS SER ALA LYS LYS ASP LYS ASP PRO VAL ASN LYS SER GLY LYS ALA LYS LYS LYS LYS TRP SER LYS GLY LYS VAL ARG D42 K43 L58 V62 I68 T69 V72 I79 L83 L92 V100

Y109 N112 THR LYS GLY GLY ASP ALA PRO ALA ALA GLY GLU ASP ALA
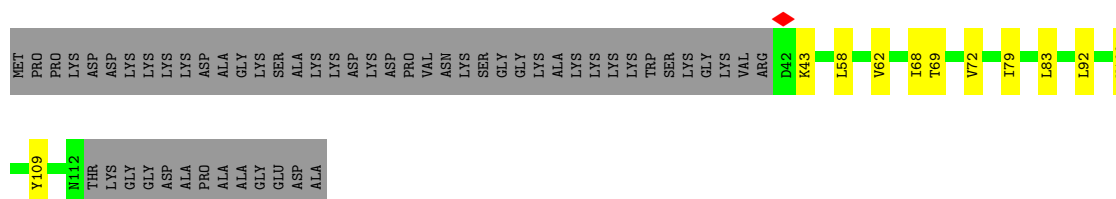
• Molecule 11: 40S ribosomal protein eS31, RPS27a

Chain b:

33%   •   63%

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

ILE GLN LYS GLU SER THR LEU HIS LEU VAL LEU ARG LEU ARG GLY GLY ALA LYS LYS ARG LYS LYS LYS SER TYR THR THR PRO K89 K90 N91 K92 H93 K99 V108 ASP GLU ASN GLY K113 M132 A133 R138 K143 Y148 C149 F150 ASN LYS PRO GLU ASP LYS

• Molecule 12: 40S ribosomal protein eS28, RPS28

Chain c:

80%   10%   10%

MET ASP THR SER ARG VAL Q7 A12 V17 Q29 V30 R31 V32 T57 R67 L68 ARG

• Molecule 13: 40S ribosomal protein uS14, RPS29

Chain d:

93%   5%   •

MET G2 L36 F52 I53 K54 L55 D56

• Molecule 14: 18S ribosomal RNA

Chain i:

17%   7%   •   74%

U A C C U G G U U G A U C C U G C C A G U A G C A U A2M U G G U U G G PSU C PSU C A A A G A U U A A G C C A U G C A U G U C U A

A G U A C G C A C G G C C G G U A C A G U G A A A C U G C G A A PSU G G C U C A2M U U A A A PSU C A C G PSU U A U G G U DMU C C PSU U

DMU G G U C C G U G G C U C U U U C U U G A C U G U G A U A2M U U C U A A2M G C U A A DMU C DMC A U G C C G

A C G G G C G C U G A C C C C U U C G G G G U C G U A PSU U U A U C A G A U C A A A A C C A A C C C G G

G U C A G C C U U C C C C U U C G G G G G G U C G G G G G G C G G G C G G U U U U G G U G A C U C U A G A U

A A C C U C G G G C C G A U C G C A C G C C C C C C G U G G C G G C G A C C A C C A U C C C A A U C G C DMU G C C C U A

U C A A C U U U C G A U G G U A G U C G C C G U G C C U A C C A U G G U G A C C A C G G G U G A C G G G G A A U C A G G

G U U C G A U DMU C C G G A G A DMG G G A G C C U G A G A A A C G G C U A C C A C A U C DMC C A A G G A2M A G G C A G C A G G C G

C G C A2M A A U U A C C C A C U C C C G A C C C G G G G A G G U A2M G U G A DMC G A A A A A U A A C A A U A C A G G A C U C U

U U C G A G G C C C U G U A A U U G G A A U G A G U C C A C PSU U U A A A A2M U C C U U A A C G A G G A2M U C C A U U G G A

• Molecule 15: 40S ribosomal protein uS7, RPS5

Chain E:

83%   7%   10%

• Molecule 16: RACK1

Chain g:

81%   15%   •

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1205667	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	30.7	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.270	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	424.448, 424.448, 424.448	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.829, 0.829, 0.829	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: B8N, K, OMG, ZN, 4AC, G7M, A2M, NMM, MG, PSU, OMC, OMU

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	B	0.19	0/1627	0.25	0/2204
2	J	0.19	0/800	0.30	0/1084
3	L	0.11	0/634	0.27	0/873
4	O	0.20	0/971	0.25	0/1307
5	Q	0.21	0/1112	0.30	0/1492
6	R	0.20	0/550	0.30	0/737
7	S	0.18	0/1092	0.27	0/1476
8	T	0.20	0/1072	0.25	0/1445
9	U	0.20	0/721	0.29	0/979
10	Y	0.13	0/543	0.25	0/734
11	b	0.12	0/436	0.27	0/583
12	c	0.18	0/443	0.28	0/598
13	d	0.22	0/461	0.31	0/613
14	i	0.28	0/11050	0.30	0/17218
15	E	0.20	0/1450	0.29	0/1954
16	g	0.18	0/2327	0.30	0/3182
All	All	0.23	0/25289	0.29	0/36479

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 ⓘ

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	B	1601	0	1600	13	0
2	J	776	0	785	11	0
3	L	634	0	501	5	0
4	O	953	0	944	7	0
5	Q	1095	0	1146	11	0
6	R	543	0	586	6	0
7	S	1072	0	1063	5	0
8	T	1063	0	1054	6	0
9	U	712	0	696	3	0
10	Y	537	0	567	7	0
11	b	427	0	376	7	0
12	c	441	0	440	4	0
13	d	450	0	436	3	0
14	i	10307	0	5217	89	0
15	E	1429	0	1457	10	0
16	g	2272	0	2126	27	0
17	S	1	0	0	0	0
17	T	1	0	0	0	0
17	i	19	0	0	0	0
18	b	1	0	0	0	0
18	d	1	0	0	0	0
19	E	1	0	0	0	0
19	d	1	0	0	0	0
19	i	7	0	0	0	0
20	B	11	0	0	0	0
20	E	27	0	0	0	0
20	J	9	0	0	0	0
20	O	17	0	0	0	0
20	Q	42	0	0	2	0
20	R	6	0	0	0	0
20	S	13	0	0	0	0
20	T	29	0	0	1	0
20	U	12	0	0	1	0
20	Y	1	0	0	0	0
20	c	1	0	0	0	0
20	d	19	0	0	1	0
20	g	6	0	0	0	0
20	i	634	0	0	0	0
All	All	25171	0	18994	187	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 4.

The worst 5 of 187 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)
16:g:73:SER:H	16:g:117:ASN:HD21	1.19	0.88
16:g:87:LEU:HB2	16:g:101:PHE:HB2	1.63	0.80
16:g:269:GLU:HG2	16:g:271:LYS:HE3	1.70	0.73
14:i:1290:G:H1	14:i:1309:U:H3	1.34	0.72
10:Y:43:LYS:HE3	14:i:1600:G:H4'	1.71	0.71

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	217/243 (89%)	217 (100%)	0	0	100	100
2	J	94/165 (57%)	93 (99%)	1 (1%)	0	100	100
3	L	104/132 (79%)	100 (96%)	4 (4%)	0	100	100
4	O	122/145 (84%)	121 (99%)	1 (1%)	0	100	100
5	Q	138/146 (94%)	136 (99%)	2 (1%)	0	100	100
6	R	68/135 (50%)	68 (100%)	0	0	100	100
7	S	139/152 (91%)	137 (99%)	2 (1%)	0	100	100
8	T	139/145 (96%)	138 (99%)	1 (1%)	0	100	100
9	U	98/119 (82%)	95 (97%)	3 (3%)	0	100	100
10	Y	69/125 (55%)	68 (99%)	1 (1%)	0	100	100
11	b	54/156 (35%)	53 (98%)	1 (2%)	0	100	100
12	c	60/69 (87%)	58 (97%)	2 (3%)	0	100	100
13	d	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
15	E	180/204 (88%)	174 (97%)	6 (3%)	0	100	100
16	g	303/317 (96%)	297 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1838/2309 (80%)	1807 (98%)	31 (2%)	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	B	152/202 (75%)	151 (99%)	1 (1%)	81	87
2	J	79/136 (58%)	78 (99%)	1 (1%)	65	72
3	L	37/108 (34%)	35 (95%)	2 (5%)	18	17
4	O	94/130 (72%)	94 (100%)	0	100	100
5	Q	111/121 (92%)	110 (99%)	1 (1%)	75	82
6	R	55/121 (46%)	55 (100%)	0	100	100
7	S	98/132 (74%)	98 (100%)	0	100	100
8	T	100/114 (88%)	100 (100%)	0	100	100
9	U	67/107 (63%)	65 (97%)	2 (3%)	36	40
10	Y	53/103 (52%)	53 (100%)	0	100	100
11	b	35/140 (25%)	35 (100%)	0	100	100
12	c	41/62 (66%)	41 (100%)	0	100	100
13	d	46/49 (94%)	46 (100%)	0	100	100
15	E	148/170 (87%)	148 (100%)	0	100	100
16	g	226/275 (82%)	220 (97%)	6 (3%)	40	44
All	All	1342/1970 (68%)	1329 (99%)	13 (1%)	71	79

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	g	15	ASN
16	g	113	PHE

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Mol	Chain	Res	Type
16	g	305	ASN
16	g	189	ILE
16	g	198	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
12	c	29	GLN
15	E	82	ASN
16	g	187	ASN
15	E	83	ASN
15	E	65	GLN

5.3.3   RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	i	482/1869 (25%)	62 (12%)	0

5 of 62 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	i	1215	C
14	i	1224	G
14	i	1227	G
14	i	1242	U
14	i	1251	A

There are no RNA pucker outliers to report.

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

20 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
14	OMC	i	1272	14	19,22,23	0.79	1 (5%)	25,31,34	1.07	3 (12%)
14	OMU	i	1326	14,17	19,22,23	0.55	0	25,31,34	1.31	5 (20%)
14	OMU	i	1442	14,17	19,22,23	0.59	0	25,31,34	1.23	4 (16%)
14	OMC	i	1391	14	19,22,23	0.76	1 (5%)	25,31,34	1.12	3 (12%)
14	OMG	i	1490	14,17	19,26,27	1.23	3 (15%)	21,38,41	0.82	1 (4%)
14	OMU	i	1288	14	19,22,23	0.75	0	25,31,34	1.30	4 (16%)
14	PSU	i	1232	14	18,21,22	4.60	8 (44%)	21,30,33	2.07	5 (23%)
14	B8N	i	1248	14	25,29,30	0.70	0	28,42,45	1.14	4 (14%)
14	A2M	i	1383	14	18,25,26	1.29	2 (11%)	20,36,39	2.09	5 (25%)
14	4AC	i	1337	14	21,24,25	3.31	10 (47%)	28,34,37	1.02	2 (7%)
14	PSU	i	1244	14	18,21,22	4.67	8 (44%)	21,30,33	1.98	5 (23%)
14	OMG	i	1328	14,19	19,26,27	1.19	2 (10%)	21,38,41	0.84	1 (4%)
14	A2M	i	1678	14	18,25,26	1.36	3 (16%)	20,36,39	1.95	7 (35%)
14	PSU	i	1367	14	18,21,22	4.66	8 (44%)	21,30,33	2.07	5 (23%)
14	PSU	i	1238	14	18,21,22	4.63	8 (44%)	21,30,33	2.03	5 (23%)
14	PSU	i	1347	14	18,21,22	4.69	8 (44%)	21,30,33	2.04	5 (23%)
14	OMG	i	1447	14	19,26,27	1.21	2 (10%)	21,38,41	0.81	1 (4%)
14	G7M	i	1639	14	20,26,27	1.15	3 (15%)	16,39,42	1.00	1 (6%)
8	NMM	T	67	8	8,11,12	2.25	1 (12%)	7,12,14	3.09	3 (42%)
14	PSU	i	1445	14	18,21,22	4.66	8 (44%)	21,30,33	2.09	6 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	OMC	i	1272	14	-	0/9/27/28	0/2/2/2
14	OMU	i	1326	14,17	-	0/9/27/28	0/2/2/2
14	OMU	i	1442	14,17	-	0/9/27/28	0/2/2/2
14	OMC	i	1391	14	-	0/9/27/28	0/2/2/2
14	OMG	i	1490	14,17	-	1/5/27/28	0/3/3/3
14	OMU	i	1288	14	-	0/9/27/28	0/2/2/2
14	PSU	i	1232	14	-	0/7/25/26	0/2/2/2
14	B8N	i	1248	14	-	2/16/34/35	0/2/2/2
14	A2M	i	1383	14	-	1/5/27/28	0/3/3/3
14	4AC	i	1337	14	-	0/11/29/30	0/2/2/2
14	PSU	i	1244	14	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	OMG	i	1328	14,19	-	1/5/27/28	0/3/3/3
14	A2M	i	1678	14	-	1/5/27/28	0/3/3/3
14	PSU	i	1367	14	-	0/7/25/26	0/2/2/2
14	PSU	i	1238	14	-	0/7/25/26	0/2/2/2
14	PSU	i	1347	14	-	0/7/25/26	0/2/2/2
14	OMG	i	1447	14	-	2/5/27/28	0/3/3/3
14	G7M	i	1639	14	-	0/3/25/26	0/3/3/3
8	NMM	T	67	8	-	1/9/11/13	-
14	PSU	i	1445	14	-	0/7/25/26	0/2/2/2

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	i	1347	PSU	C6-C5	12.43	1.49	1.35
14	i	1367	PSU	C6-C5	12.30	1.48	1.35
14	i	1244	PSU	C6-C5	12.29	1.48	1.35
14	i	1445	PSU	C6-C5	12.26	1.48	1.35
14	i	1232	PSU	C6-C5	12.23	1.48	1.35

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	T	67	NMM	NE-CZ-NH2	5.57	124.59	119.48
14	i	1445	PSU	C4-N3-C2	-5.05	119.41	126.37
14	i	1367	PSU	C4-N3-C2	-5.04	119.43	126.37
14	i	1238	PSU	C4-N3-C2	-5.03	119.44	126.37
14	i	1232	PSU	C4-N3-C2	-5.00	119.49	126.37

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	T	67	NMM	O-C-CA-CB
14	i	1328	OMG	C1'-C2'-O2'-CM2
14	i	1383	A2M	C1'-C2'-O2'-CM'
14	i	1678	A2M	C1'-C2'-O2'-CM'
14	i	1447	OMG	C3'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	i	1272	OMC	1	0
14	i	1391	OMC	1	0
14	i	1232	PSU	1	0
14	i	1383	A2M	2	0
14	i	1328	OMG	1	0
14	i	1678	A2M	2	0
14	i	1347	PSU	1	0
14	i	1447	OMG	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 32 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 ⓘ

This section contains visualisations of the EMDB entry EMD-49636. 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 ⓘ
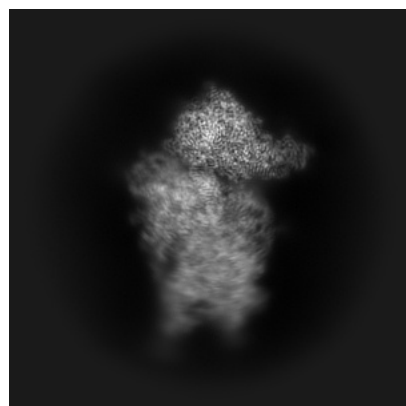
6.1.1 Primary map

X
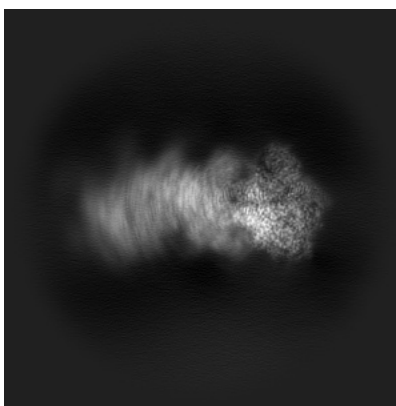
Y
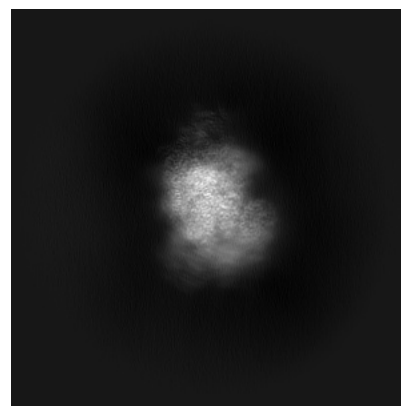
Z

6.1.2 Raw map

X

Y

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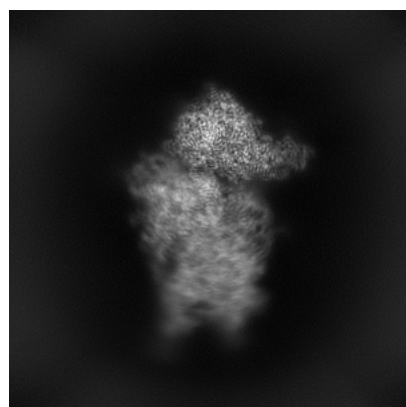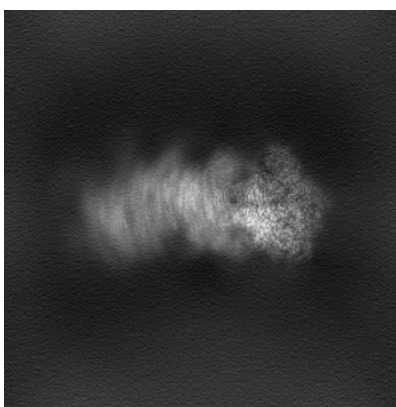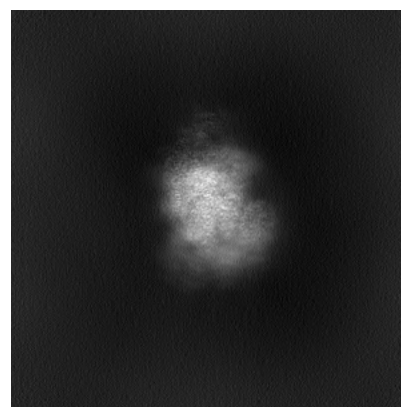
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map
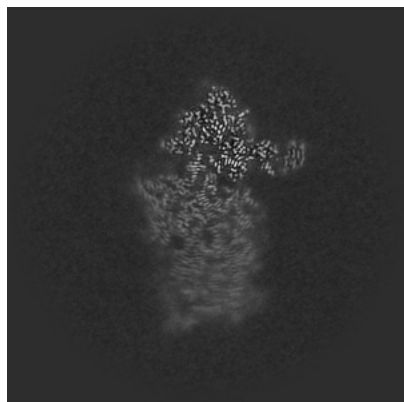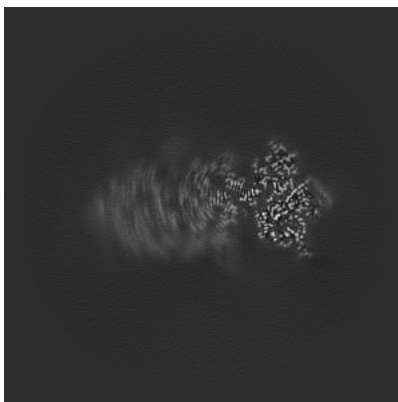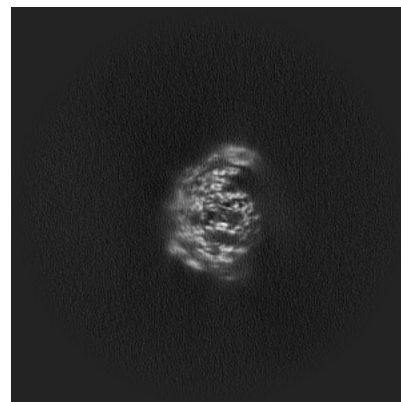
| X Index: 256 | Y Index: 256 | Z Index: 256 |

6.2.2 Raw map
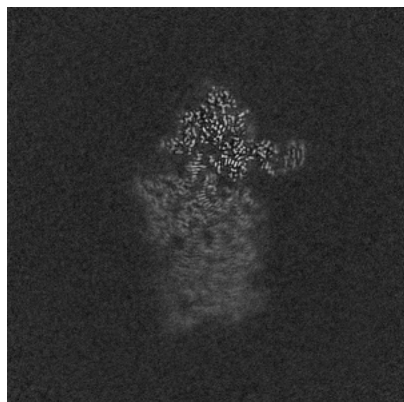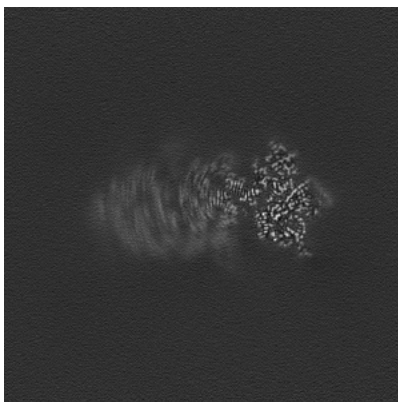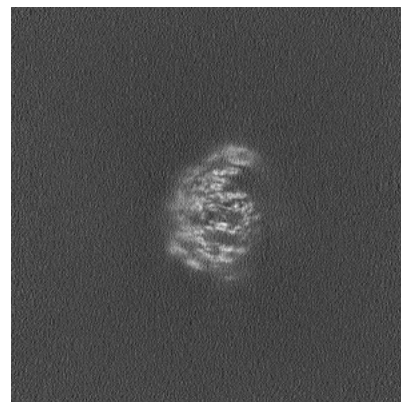
| X Index: 256 | Y Index: 256 | Z Index: 256 |

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
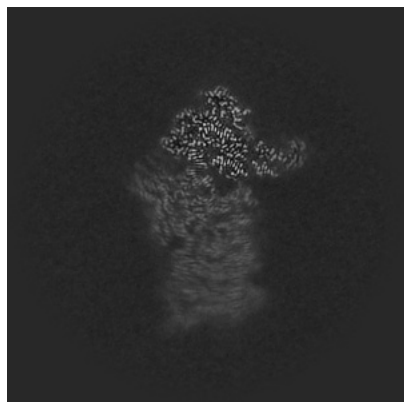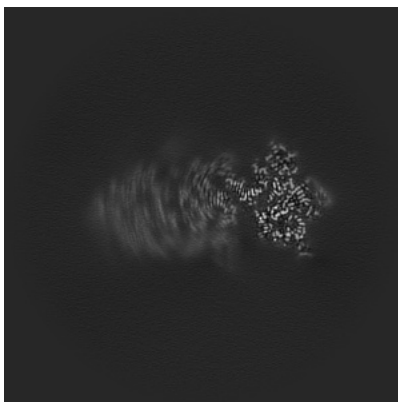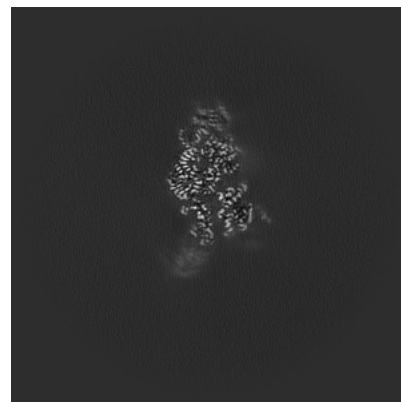
| X Index: 251 | Y Index: 257 | Z Index: 325 |

6.3.2 Raw map
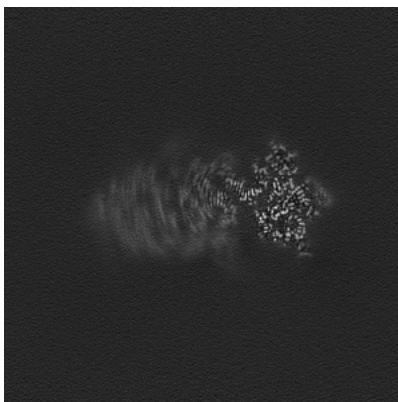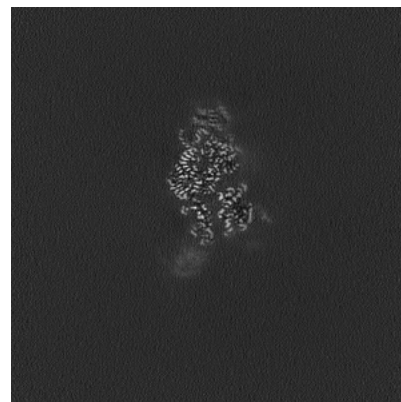
| X Index: 251 | Y Index: 257 | Z Index: 325 |

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
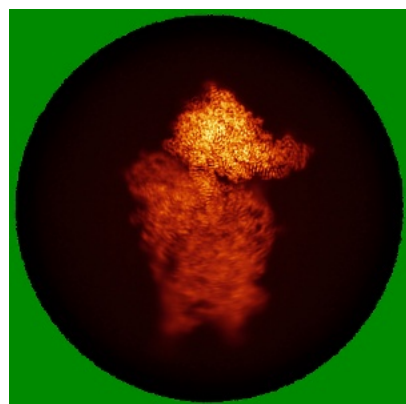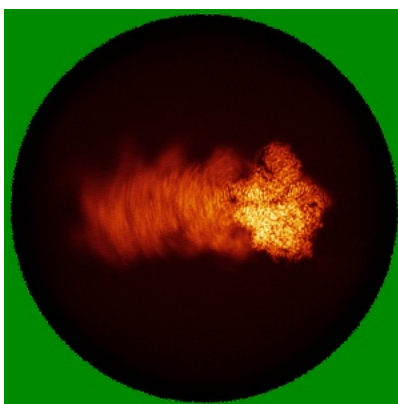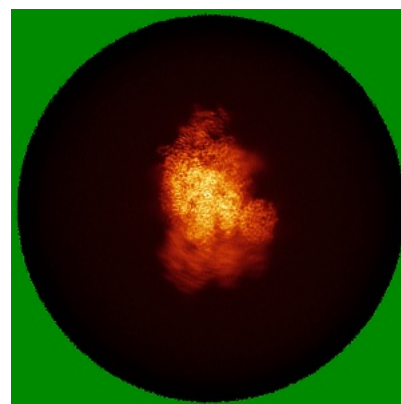
| X | Y | Z |

6.4.2 Raw map

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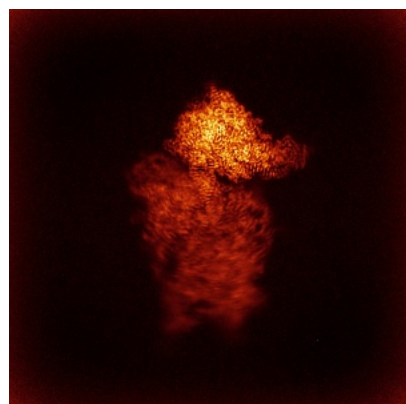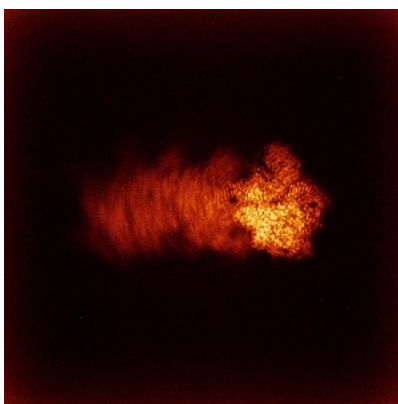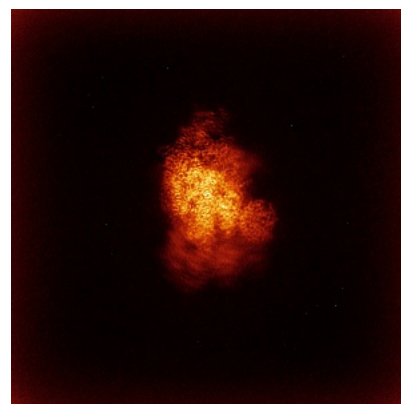
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X   Y   Z
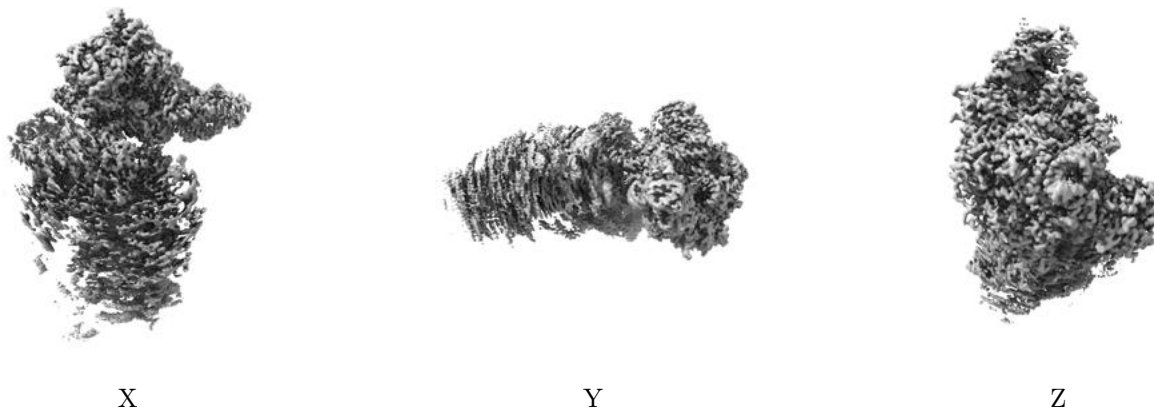
The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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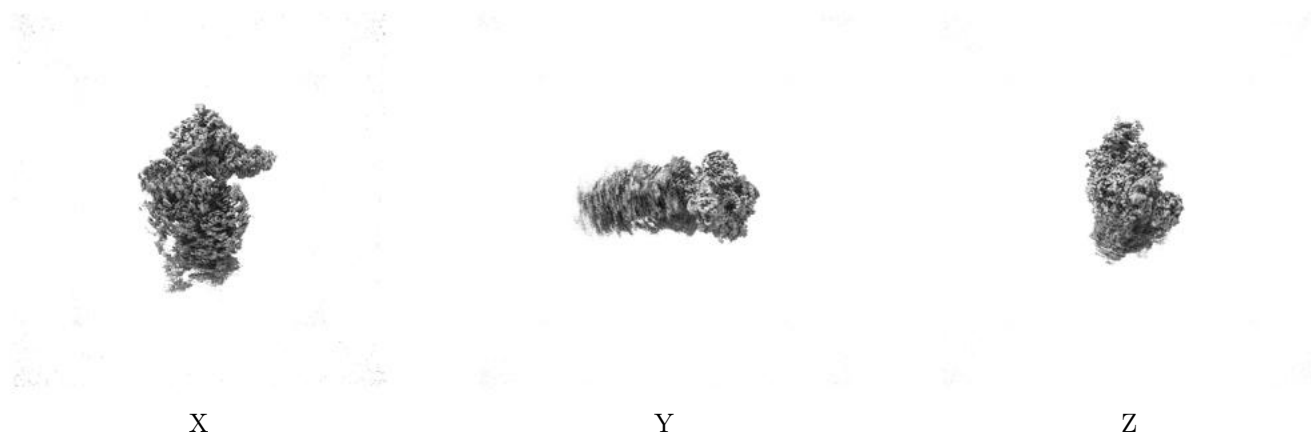
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation ⓘ

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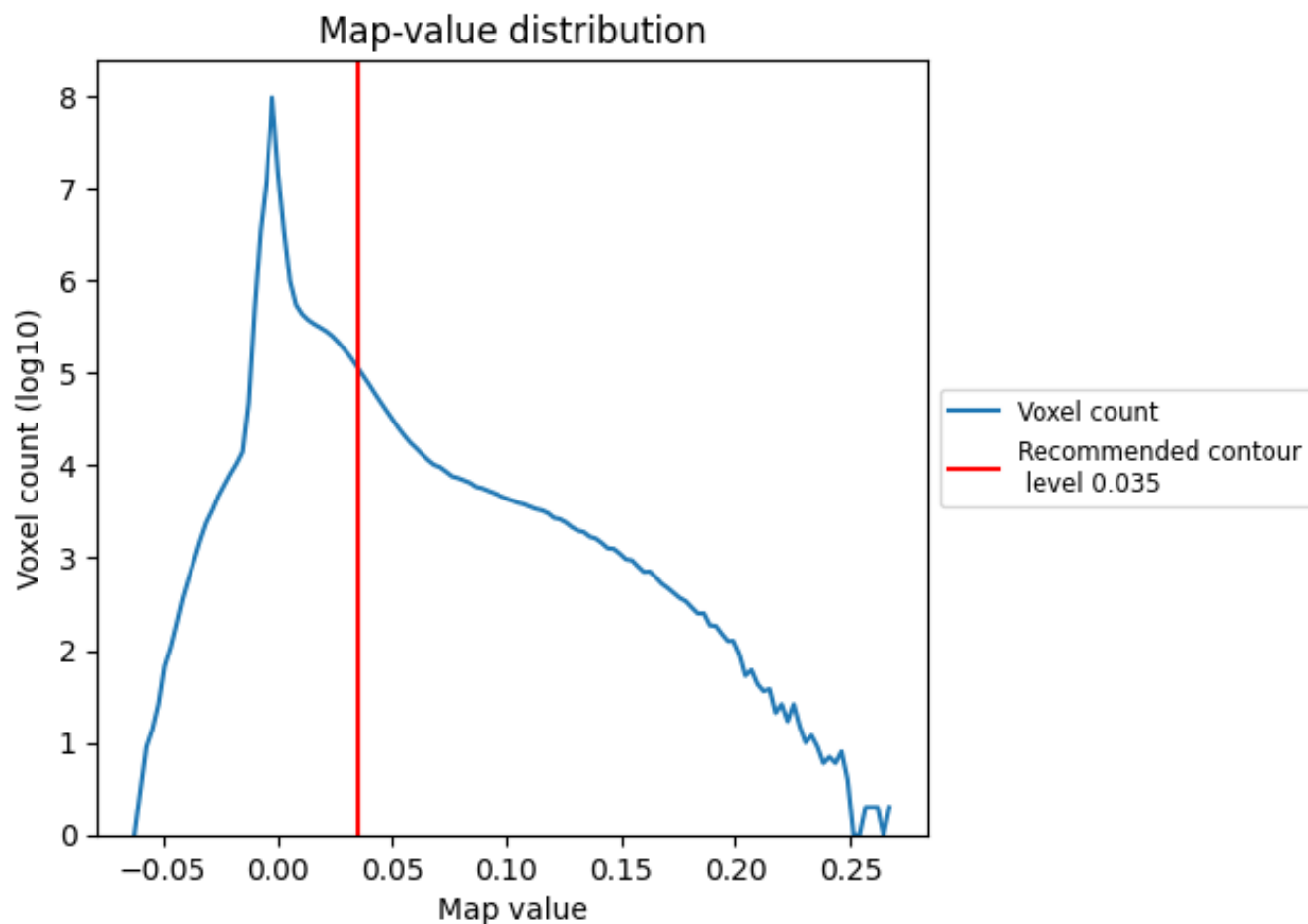
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
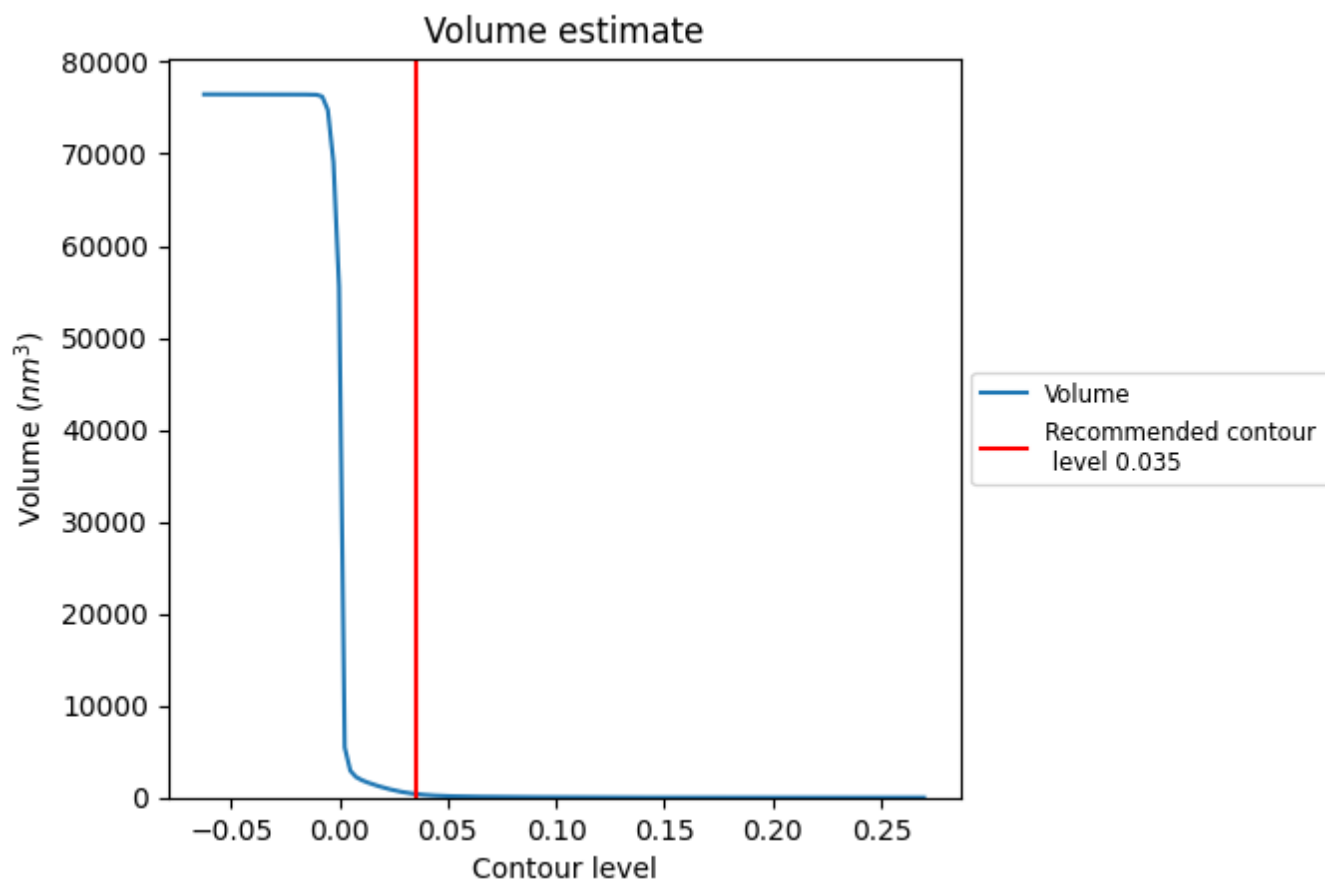
The volume at the recommended contour level is 395 nm^3; this corresponds to an approximate mass of 357 kDa.

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 ⓘ
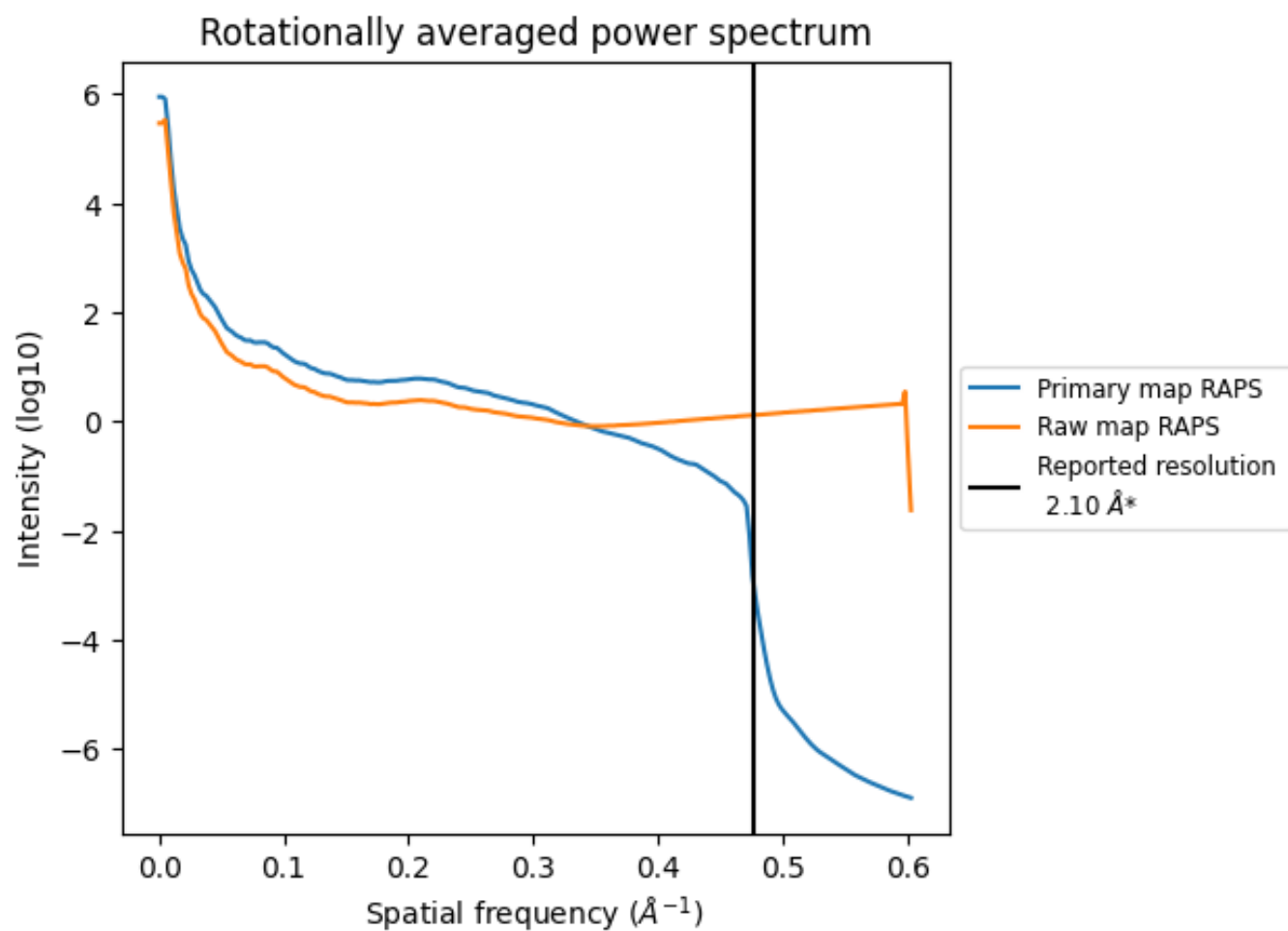
*Reported resolution corresponds to spatial frequency of 0.476 Å^{-1}

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 ⓘ
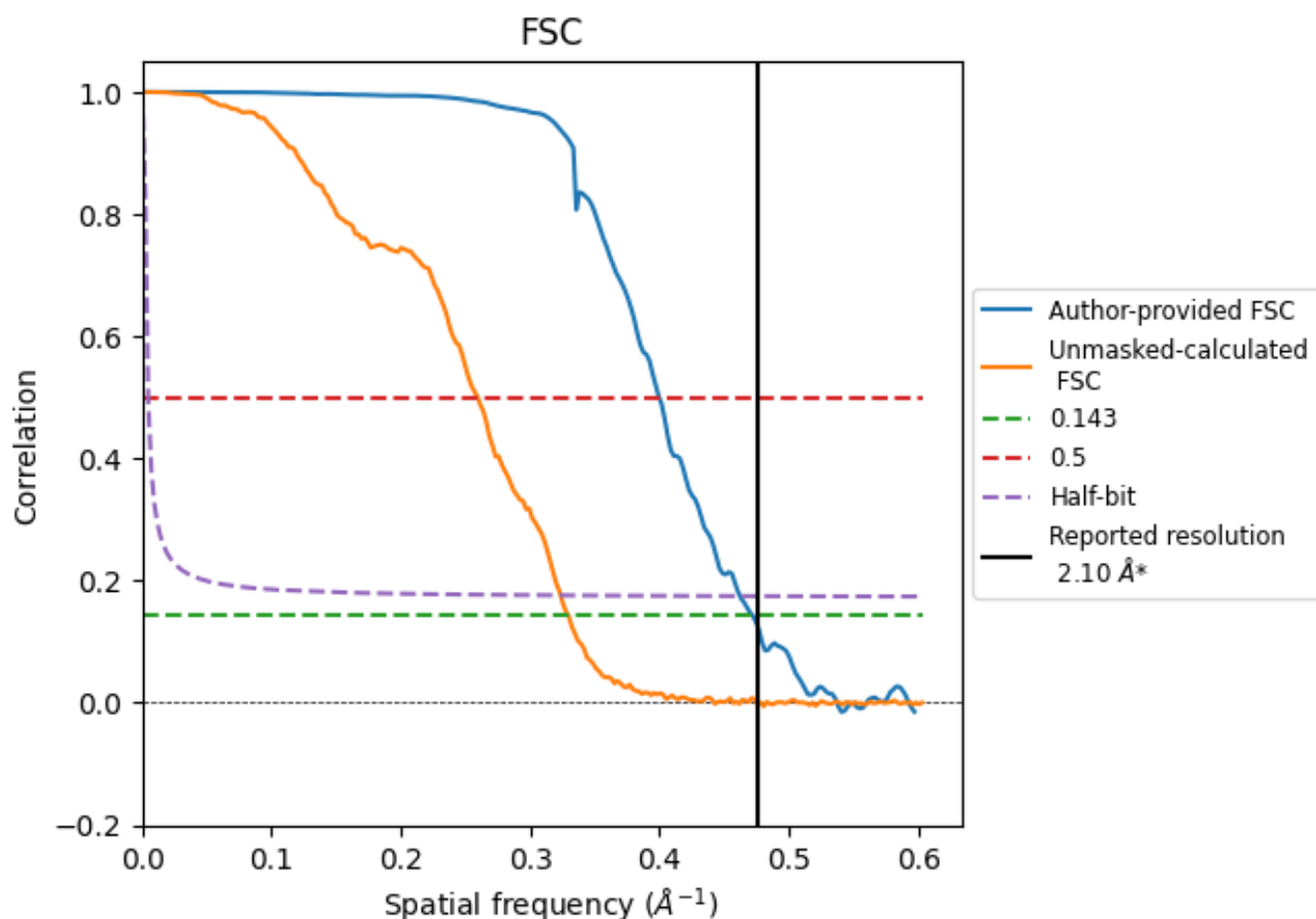
*Reported resolution corresponds to spatial frequency of 0.476 Å^{-1}

8.2   Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.12	2.50	2.16
Unmasked-calculated*	3.03	3.86	3.09

*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 3.03 differs from the reported value 2.1 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-49636 and PDB model 9NPY. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay ⓘ

X	Y	Z
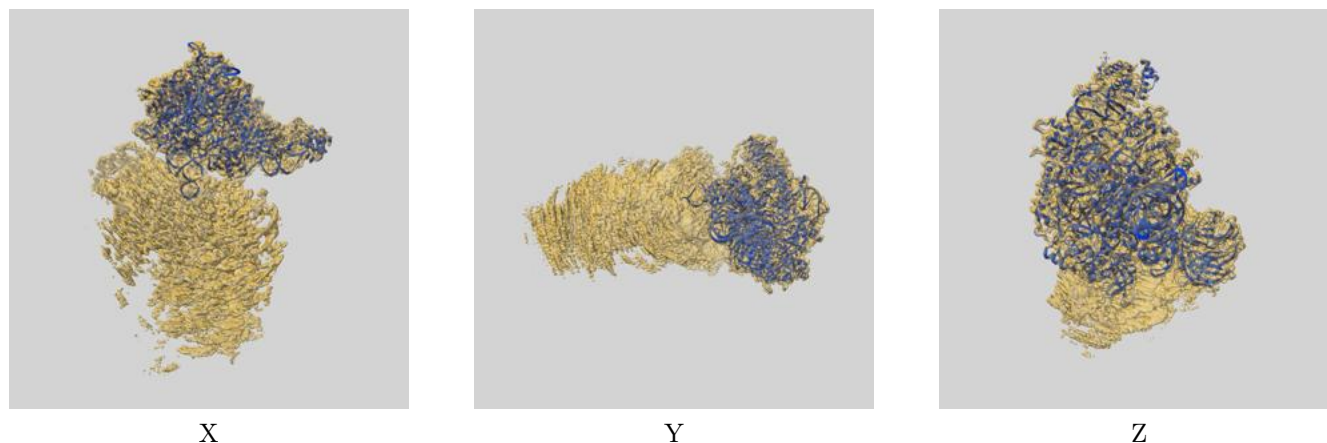
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model ⓘ
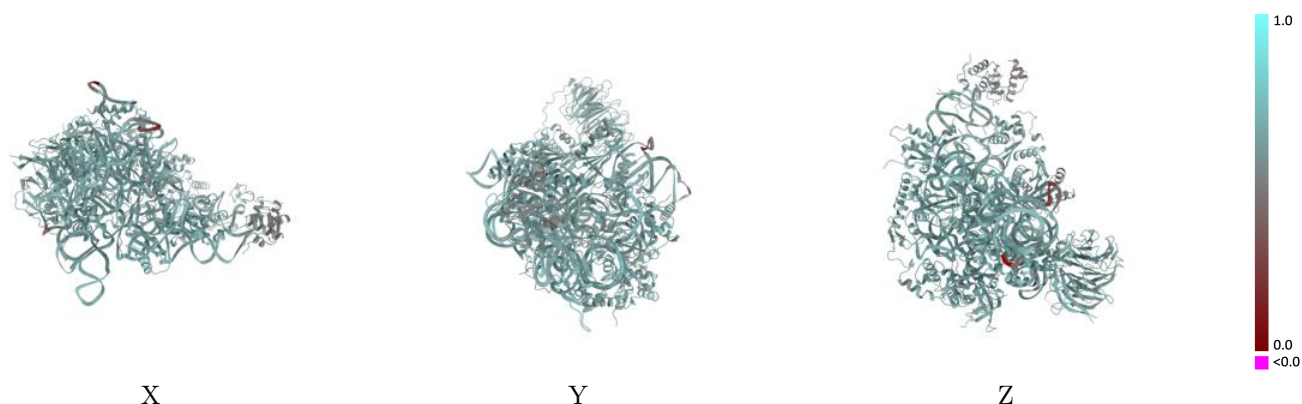
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ
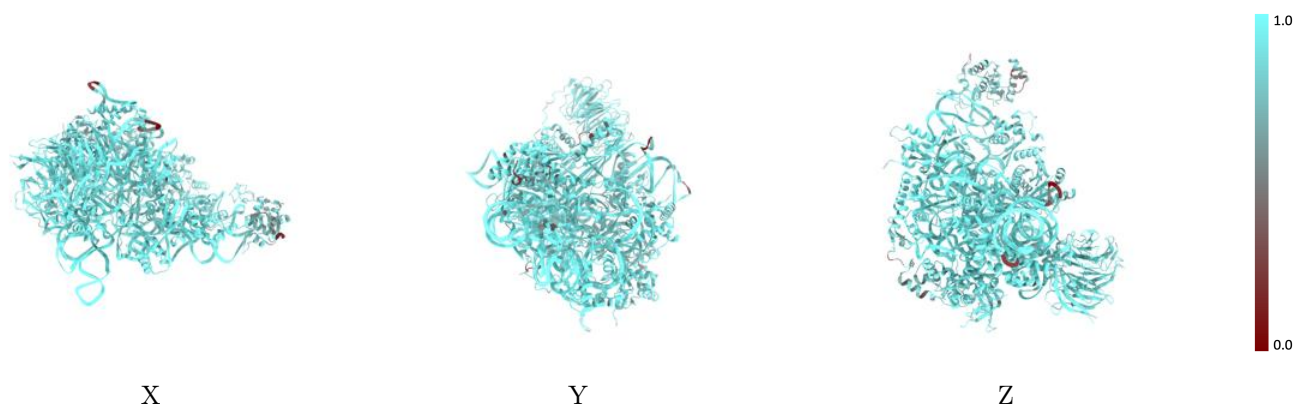
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4 Atom inclusion ⓘ
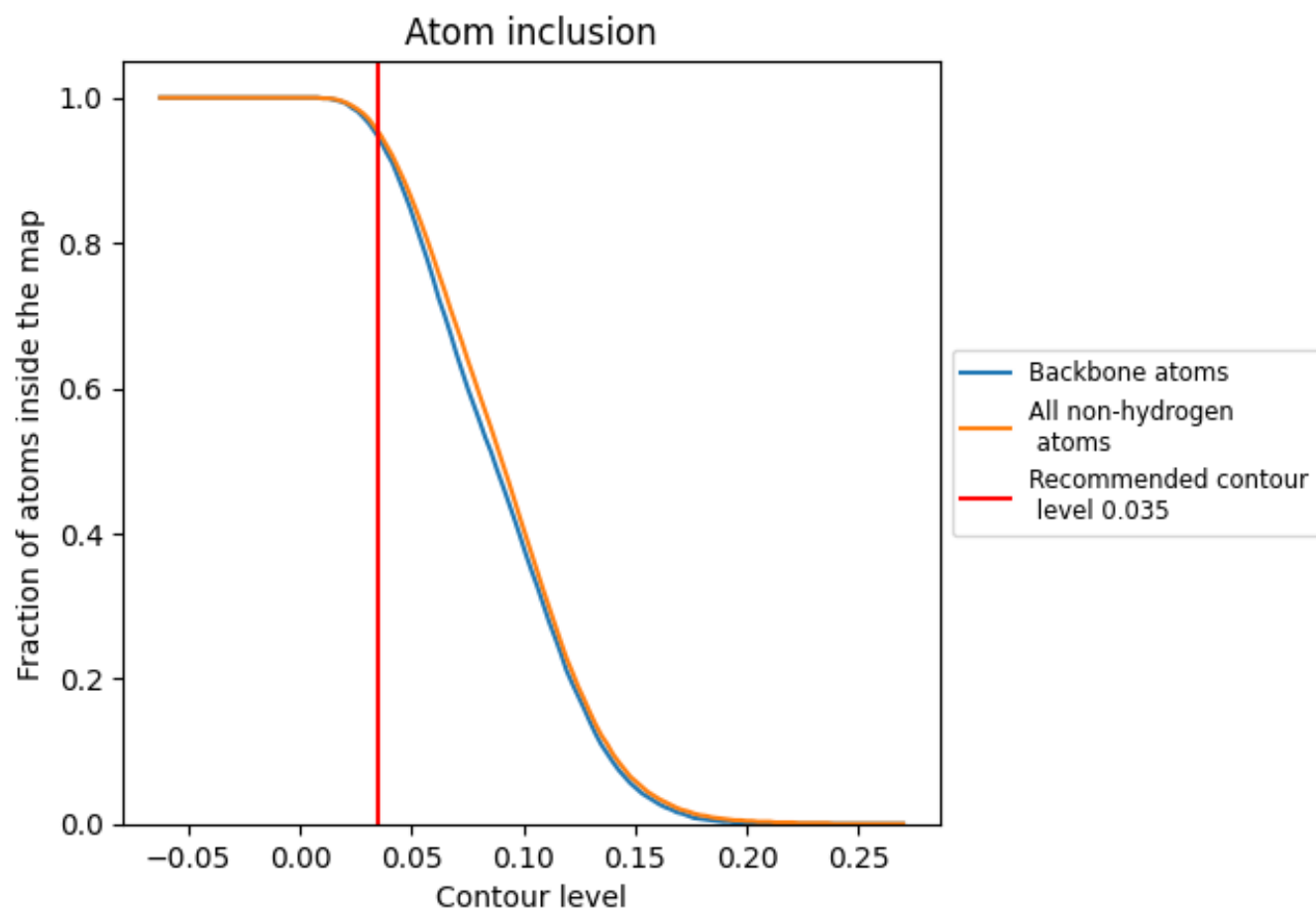
At the recommended contour level, 95% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9530	0.6380
B	0.9530	0.6390
E	0.9610	0.6500
J	0.9580	0.6390
L	0.7200	0.5130
O	0.9420	0.6420
Q	0.9790	0.6680
R	0.9600	0.6400
S	0.9250	0.6370
T	0.9880	0.6570
U	0.9280	0.6310
Y	0.7880	0.6170
b	0.8210	0.5880
c	0.9250	0.6130
d	0.9750	0.6770
g	0.9440	0.6210
i	0.9840	0.6460

1.0

0.0
<0.0