



Full wwPDB EM Validation Report ⓘ

Jul 24, 2025 – 07:52 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)

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 ⓘ 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:

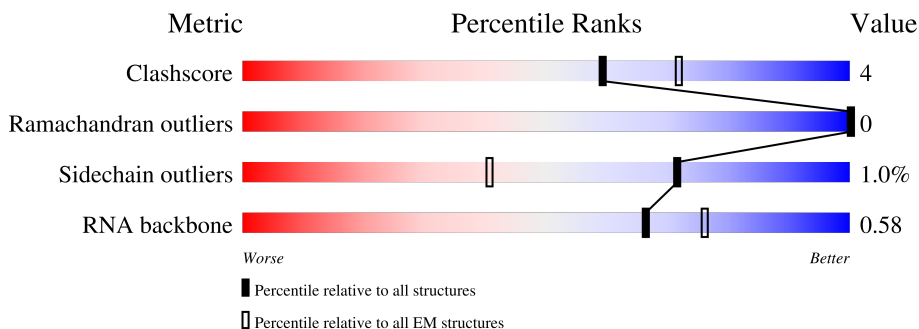
EMDB validation analysis : 0.0.1.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

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	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 $\leq 5\%$. 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	B	243	
2	J	165	
3	L	132	
4	O	145	
5	Q	146	
6	R	135	
7	S	152	

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Mol	Chain	Length	Quality of chain
8	T	145	
9	U	119	
10	Y	125	
11	b	156	
12	c	69	
13	d	56	
14	i	1869	
15	E	204	
16	g	317	

2 Entry composition

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	C	N	O	S	0	0
			1601	1029	292	273	7		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 16 is a protein called RACK1.

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

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

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

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

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

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

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

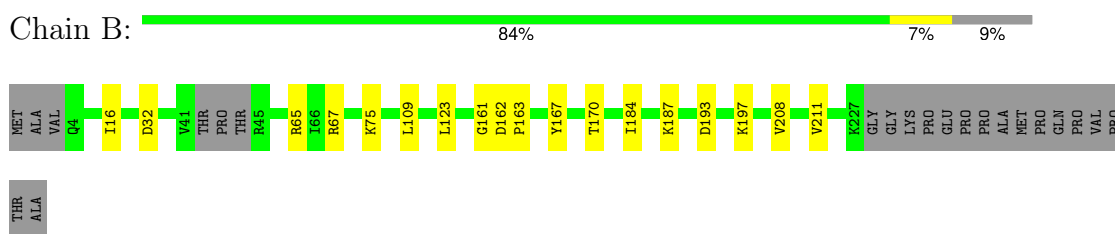
- Molecule 20 is water.

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

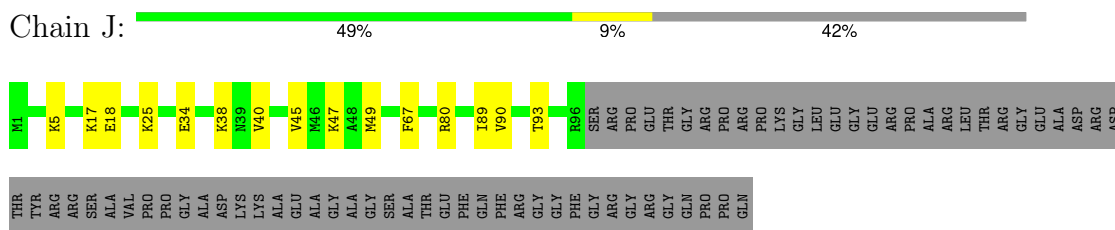
3 Residue-property plots

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.

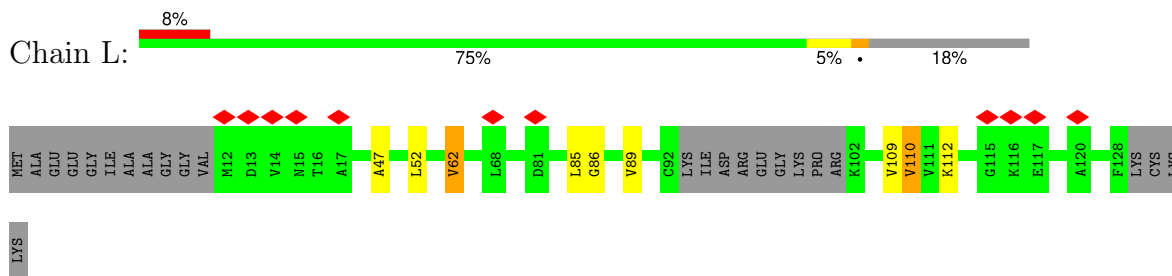
- Molecule 1: 40S ribosomal protein uS3, RPS3



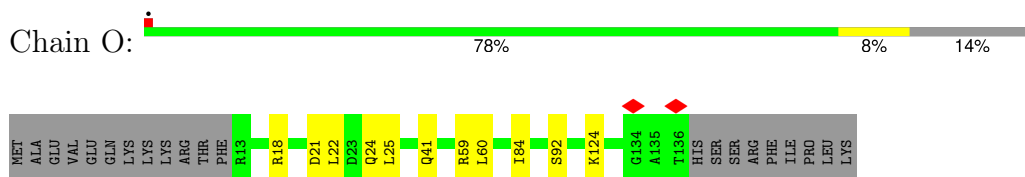
- Molecule 2: 40S ribosomal protein eS10, RPS10




- Molecule 3: 40S ribosomal protein eS12, RPS12



- Molecule 4: 40S ribosomal protein uS19, RPS15



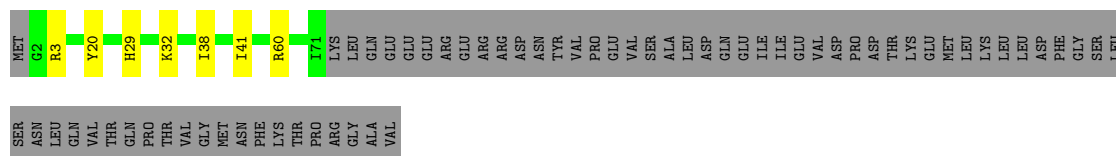
- Molecule 5: 40S ribosomal protein uS9, RPS16

Chain Q:  84% 12%




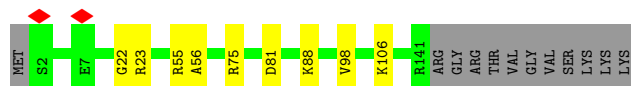
- Molecule 6: 40S ribosomal protein eS17, RPS17

Chain R:  47% 5% 48%



- Molecule 7: 40S ribosomal protein uS13, RPS18

Chain S:  86% 6% 8%




- Molecule 8: 40S ribosomal protein eS19, RPS19

Chain T:  91% 6%



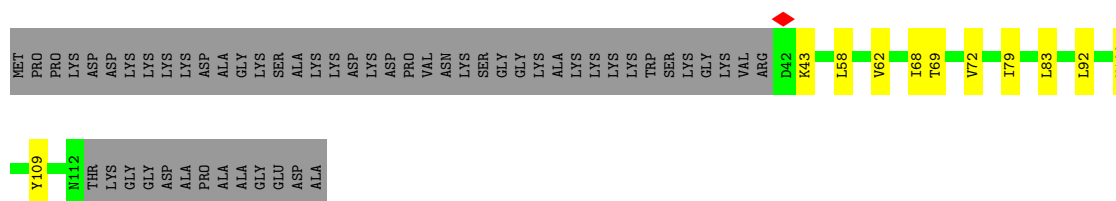
- Molecule 9: 40S ribosomal protein uS10, RPS20

Chain U:  79% 5% 16%

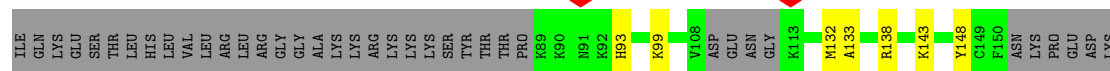


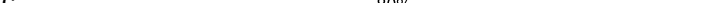
- Molecule 10: 40S ribosomal protein eS25, RPS25

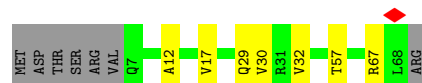
Chain Y:  48% 9% 43%



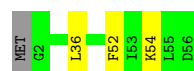
- Molecule 11: 40S ribosomal protein eS31, RPS27a



- Chain c: 



- Chain d:  93% 5%



- Chain i: 17% 7% 74%



- Molecule 15: 40S ribosomal protein uS7, RPS5

Chain E:

83%

7%

10%

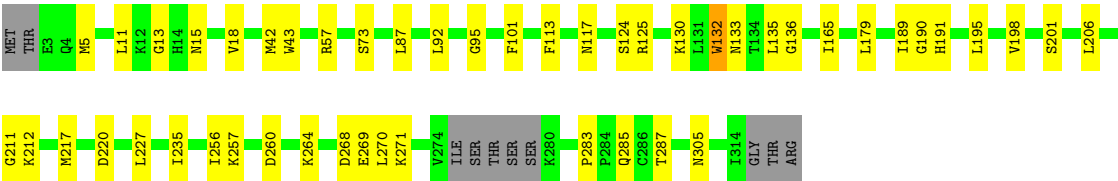


● Molecule 16: RACK1

Chain g:

81%

15%



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 (\AA)	424.448, 424.448, 424.448	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.829, 0.829, 0.829	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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.

All (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
10:Y:100:VAL:HG21	15:E:102:LEU:HD11	1.72	0.71
14:i:1228:A:H2'	14:i:1229:G:C8	2.28	0.69
12:c:29:GLN:HE22	12:c:67:ARG:HA	1.56	0.69
16:g:13:GLY:H	16:g:43:TRP:HH2	1.41	0.69
14:i:1396:A:O2'	14:i:1398:G:N7	2.26	0.68
10:Y:58:LEU:HD12	10:Y:62:VAL:HG21	1.77	0.67
16:g:256:ILE:HB	16:g:270:LEU:HB2	1.76	0.67
4:O:41:GLN:HG3	4:O:84:ILE:HD12	1.77	0.64
14:i:1588:A:H2'	14:i:1589:A:C8	2.33	0.63
1:B:16:ILE:HD11	13:d:36:LEU:HD23	1.82	0.62
14:i:1536:G:H2'	14:i:1537:A:C8	2.34	0.62
14:i:1461:G:H3'	14:i:1463:U:H3	1.65	0.62
14:i:1536:G:H2'	14:i:1537:A:H8	1.65	0.61
15:E:71:ARG:NH2	15:E:148:ASN:OD1	2.33	0.61
9:U:80:PHE:HB3	13:d:52:PHE:HB3	1.82	0.61
2:J:17:LYS:NZ	2:J:18:GLU:OE2	2.35	0.60
16:g:18:VAL:O	16:g:287:THR:OG1	2.18	0.59
5:Q:53:GLU:OE1	5:Q:85:ARG:NH2	2.29	0.59
7:S:22:GLY:HA2	7:S:56:ALA:HB3	1.83	0.59
10:Y:68:ILE:HB	10:Y:109:TYR:HB2	1.84	0.58
14:i:1354:G:N2	14:i:1357:A:OP2	2.32	0.58
15:E:63:LYS:HD3	15:E:71:ARG:HH12	1.68	0.58
8:T:121:ARG:NH1	14:i:1563:G:OP1	2.37	0.58
11:b:93:HIS:ND1	14:i:1305:C:OP2	2.35	0.57
5:Q:97:GLN:HB3	5:Q:105:LYS:HG3	1.87	0.57
7:S:98:VAL:HG11	7:S:106:LYS:HG3	1.87	0.57
14:i:1351:G:O2'	14:i:1378:A:N1	2.36	0.56
2:J:80:ARG:NH1	2:J:89:ILE:O	2.34	0.56
8:T:116:ASP:OD1	8:T:117:GLN:N	2.39	0.56
4:O:18:ARG:NH1	7:S:88:LYS:O	2.40	0.55
14:i:1407:U:H2'	14:i:1408:U:C6	2.40	0.55
1:B:170:THR:HG23	1:B:187:LYS:HG2	1.89	0.55
9:U:75:LYS:NZ	20:U:201:HOH:O	2.34	0.54
16:g:191:HIS:CG	16:g:195:LEU:HD21	2.43	0.54
14:i:1667:U:H2'	14:i:1668:U:C6	2.43	0.53
1:B:32:ASP:OD2	1:B:65:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:b:138:ARG:NH2	14:i:1292:C:N3	2.43	0.52
16:g:133:ASN:HD22	16:g:135:LEU:H	1.56	0.52
4:O:22:LEU:HA	4:O:25:LEU:HD12	1.92	0.52
16:g:268:ASP:OD1	16:g:269:GLU:N	2.43	0.52
14:i:1653:U:H2'	14:i:1654:G:C8	2.44	0.51
16:g:165:ILE:HD11	16:g:179:LEU:HD13	1.92	0.51
14:i:1382:A:H2'	14:i:1383:A2M:H8	1.93	0.51
14:i:1228:A:H2'	14:i:1229:G:H8	1.73	0.51
14:i:1413:G:H2'	14:i:1414:A:H8	1.75	0.51
14:i:1281:G:H2'	14:i:1282:A:C8	2.45	0.51
4:O:59:ARG:NH1	14:i:1299:A:OP1	2.44	0.51
11:b:133:ALA:HB1	14:i:1308:U:O2'	2.11	0.51
4:O:21:ASP:OD2	4:O:24:GLN:NE2	2.44	0.51
13:d:54:LYS:NZ	20:d:204:HOH:O	2.43	0.51
14:i:1255:G:OP1	14:i:1256:G:O2'	2.24	0.50
16:g:201:SER:HB3	16:g:206:LEU:HB2	1.93	0.50
14:i:1595:U:H2'	14:i:1596:U:C6	2.46	0.50
14:i:1678:A2M:O2'	14:i:1679:A:H5'	2.12	0.50
9:U:56:MET:HB2	9:U:86:LYS:HB3	1.92	0.50
14:i:1628:C:H2'	14:i:1629:C:C6	2.46	0.49
3:L:52:LEU:HD11	3:L:62:VAL:HG12	1.93	0.49
7:S:75:ARG:NH1	7:S:81:ASP:OD1	2.45	0.49
14:i:1374:C:H2'	14:i:1375:G:O4'	2.12	0.49
1:B:67:ARG:NE	2:J:93:THR:O	2.34	0.49
14:i:1227:G:C2	14:i:1228:A:C8	3.00	0.49
14:i:1531:A:H2'	14:i:1532:C:C6	2.48	0.49
1:B:161:GLY:HA3	14:i:1388:A:H61	1.77	0.49
14:i:1277:C:H2'	14:i:1278:A:H8	1.76	0.49
3:L:47:ALA:HB1	3:L:110:VAL:HG13	1.94	0.49
5:Q:100:VAL:HG12	5:Q:101:ASP:H	1.78	0.48
16:g:257:LYS:NZ	16:g:269:GLU:OE2	2.41	0.48
10:Y:79:ILE:HB	10:Y:83:LEU:HD23	1.96	0.48
6:R:3:ARG:HG3	14:i:1454:A:C8	2.49	0.48
2:J:25:LYS:HD3	2:J:67:PHE:HE2	1.79	0.48
8:T:126:GLN:HG3	8:T:129:ARG:HH21	1.79	0.48
5:Q:89:SER:HB3	5:Q:112:LEU:HD13	1.95	0.48
12:c:12:ALA:HB1	12:c:32:VAL:HB	1.96	0.47
7:S:23:ARG:O	7:S:55:ARG:HD2	2.14	0.47
14:i:1217:A:H2'	14:i:1218:C:C6	2.50	0.47
14:i:1597:C:H4'	14:i:1603:G:O6	2.12	0.47
11:b:132:MET:HE1	11:b:148:TYR:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ASP:OD2	1:B:197:LYS:N	2.47	0.47
16:g:190:GLY:HA3	16:g:217:MET:HE1	1.96	0.47
14:i:1395:C:O2'	14:i:1396:A:H5'	2.15	0.47
6:R:20:TYR:CD1	6:R:38:ILE:HD12	2.50	0.47
11:b:143:LYS:NZ	14:i:1311:C:OP1	2.41	0.47
16:g:195:LEU:HA	16:g:211:GLY:HA3	1.97	0.47
11:b:138:ARG:NE	14:i:1292:C:O2	2.39	0.47
14:i:1328:OMG:H1'	14:i:1328:OMG:HM23	1.69	0.47
16:g:283:PRO:O	16:g:285:GLN:NE2	2.45	0.46
14:i:1223:A:H2'	14:i:1224:G:O4'	2.15	0.46
14:i:1562:C:H2'	14:i:1563:G:H8	1.81	0.46
16:g:212:LYS:HA	16:g:235:ILE:HG23	1.97	0.46
14:i:1403:C:N3	14:i:1434:C:N4	2.64	0.46
14:i:1406:G:H2'	14:i:1407:U:C6	2.50	0.46
3:L:47:ALA:HA	3:L:112:LYS:HA	1.97	0.46
14:i:1643:U:H2'	14:i:1644:C:C6	2.50	0.46
14:i:1365:G:H2'	14:i:1366:G:C8	2.50	0.46
14:i:1673:U:O2'	15:E:84:GLY:O	2.29	0.46
5:Q:126:ARG:NH1	20:Q:203:HOH:O	2.49	0.46
14:i:1214:A:H2'	14:i:1217:A:N7	2.31	0.46
16:g:5:MET:HB2	16:g:270:LEU:HD21	1.98	0.46
1:B:163:PRO:O	1:B:167:TYR:HB2	2.17	0.45
8:T:101:ARG:NH1	20:T:301:HOH:O	2.38	0.45
14:i:1405:A:H2'	14:i:1406:G:O4'	2.17	0.45
14:i:1550:G:H3'	14:i:1579:A:H61	1.80	0.45
14:i:1281:G:H2'	14:i:1282:A:H8	1.81	0.45
14:i:1387:G:H2'	14:i:1388:A:O4'	2.17	0.45
15:E:19:LEU:HD21	15:E:69:VAL:HG11	1.98	0.45
4:O:124:LYS:HD3	14:i:1239:U:H5''	1.98	0.45
16:g:11:LEU:HB3	16:g:43:TRP:CZ3	2.52	0.45
14:i:1390:U:H2'	14:i:1391:OMC:C6	2.51	0.45
15:E:40:ALA:HB1	15:E:45:TYR:CG	2.51	0.44
16:g:130:LYS:HD3	16:g:132:TRP:CZ2	2.52	0.44
3:L:85:LEU:HD21	3:L:109:VAL:HG23	2.00	0.44
2:J:47:LYS:HA	2:J:47:LYS:HD3	1.79	0.44
14:i:1408:U:H2'	14:i:1409:A:C8	2.53	0.44
2:J:5:LYS:HD2	14:i:1313:A:OP1	2.18	0.44
5:Q:82:TYR:O	5:Q:85:ARG:HG2	2.17	0.44
14:i:1232:PSU:H2'	14:i:1233:G:C8	2.52	0.44
14:i:1356:G:H2'	14:i:1357:A:C8	2.53	0.44
5:Q:110:ASP:O	5:Q:114:GLN:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:88:MET:HE3	14:i:1665:G:C8	2.53	0.43
10:Y:92:LEU:HD22	10:Y:109:TYR:HE1	1.83	0.43
1:B:211:VAL:O	6:R:20:TYR:OH	2.33	0.43
10:Y:69:THR:H	10:Y:72:VAL:HG12	1.83	0.43
14:i:1617:G:N1	14:i:1620:A:OP2	2.51	0.43
14:i:1589:A:H2'	14:i:1590:C:C6	2.54	0.43
16:g:257:LYS:HG2	16:g:269:GLU:OE1	2.18	0.43
6:R:60:ARG:NH1	14:i:1464:C:H4'	2.34	0.43
16:g:57:ARG:HD3	16:g:95:GLY:HA3	2.01	0.43
2:J:5:LYS:HB2	2:J:5:LYS:HE3	1.79	0.43
14:i:1292:C:C2	14:i:1293:A:C8	3.07	0.43
14:i:1420:G:O2'	14:i:1421:A:OP1	2.31	0.43
12:c:17:VAL:HA	12:c:30:VAL:HG12	2.00	0.42
14:i:1365:G:H2'	14:i:1366:G:H8	1.82	0.42
2:J:38:LYS:HB3	2:J:40:VAL:HG23	2.01	0.42
5:Q:113:ILE:HG12	5:Q:120:LEU:HD12	2.01	0.42
14:i:1616:U:H2'	14:i:1617:G:O4'	2.20	0.42
3:L:86:GLY:HA2	3:L:89:VAL:HG22	2.01	0.42
14:i:1278:A:H2'	14:i:1279:C:C6	2.54	0.42
5:Q:58:LEU:HB3	5:Q:62:ARG:HG3	2.00	0.42
14:i:1491:G:H2'	14:i:1492:U:C6	2.55	0.42
16:g:13:GLY:N	16:g:43:TRP:HH2	2.11	0.42
16:g:42:MET:HE2	16:g:92:LEU:HD22	2.01	0.42
16:g:124:SER:OG	16:g:125:ARG:N	2.50	0.42
16:g:260:ASP:O	16:g:264:LYS:N	2.50	0.42
2:J:25:LYS:HD3	2:J:67:PHE:CE2	2.55	0.42
14:i:1408:U:H2'	14:i:1409:A:H8	1.85	0.42
14:i:1413:G:H2'	14:i:1414:A:C8	2.55	0.41
14:i:1448:A:H2'	14:i:1449:G:O4'	2.20	0.41
14:i:1563:G:H2'	14:i:1564:C:H6	1.85	0.41
1:B:75:LYS:NZ	2:J:34:GLU:OE2	2.41	0.41
4:O:60:LEU:HD22	4:O:92:SER:HB3	2.01	0.41
6:R:29:HIS:HA	6:R:32:LYS:HE2	2.03	0.41
15:E:125:SER:OG	15:E:136:ARG:NH1	2.53	0.41
5:Q:141:TYR:OH	14:i:1668:U:OP2	2.35	0.41
14:i:1383:A2M:H1'	14:i:1383:A2M:HM'3	1.64	0.41
15:E:102:LEU:HD23	15:E:102:LEU:HA	1.89	0.41
1:B:32:ASP:OD1	1:B:32:ASP:N	2.53	0.41
14:i:1347:PSU:H2'	14:i:1348:G:N3	2.36	0.41
14:i:1410:C:H2'	14:i:1411:G:H8	1.85	0.41
14:i:1511:U:H2'	14:i:1512:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:i:1513:C:H2'	14:i:1514:G:H8	1.86	0.41
15:E:201:LYS:HG3	15:E:204:ARG:NH2	2.36	0.41
2:J:45:VAL:O	2:J:49:MET:HG2	2.20	0.41
16:g:220:ASP:HB2	16:g:227:LEU:HD21	2.03	0.41
14:i:1220:A:H2'	14:i:1221:G:O4'	2.21	0.41
14:i:1497:G:H4'	14:i:1498:A:H5'	2.03	0.41
14:i:1520:G:H2'	14:i:1520:G:N3	2.36	0.41
14:i:1606:G:N2	14:i:1632:G:H1'	2.35	0.41
1:B:162:ASP:HB3	14:i:1389:C:O2'	2.21	0.41
14:i:1678:A2M:HM'3	14:i:1678:A2M:H1'	1.49	0.41
12:c:57:THR:HG21	15:E:122:ARG:HD2	2.03	0.41
14:i:1272:OMC:H1'	14:i:1272:OMC:HM23	1.80	0.41
14:i:1417:C:O2'	14:i:1419:C:N3	2.48	0.41
14:i:1447:OMG:H1'	14:i:1447:OMG:HM23	1.84	0.41
14:i:1221:G:H2'	14:i:1222:G:C8	2.55	0.40
16:g:101:PHE:CD2	16:g:136:GLY:HA2	2.57	0.40
5:Q:71:ARG:NH1	20:Q:202:HOH:O	2.36	0.40
14:i:1217:A:H2'	14:i:1218:C:H6	1.86	0.40
8:T:108:GLU:OE2	8:T:121:ARG:NE	2.33	0.40
14:i:1265:A:H5'	14:i:1266:C:OP2	2.22	0.40
1:B:109:LEU:HD12	1:B:184:ILE:HD11	2.03	0.40
1:B:208:VAL:HG13	6:R:41:ILE:HG12	2.03	0.40
11:b:99:LYS:HD2	14:i:1286:G:OP1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	217/243 (89%)	217 (100%)	0	0	100	100
2	J	94/165 (57%)	93 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	123	LEU
2	J	90	VAL
3	L	62	VAL
3	L	110	VAL
5	Q	100	VAL
9	U	25	THR
9	U	50	VAL
16	g	15	ASN
16	g	113	PHE
16	g	132	TRP
16	g	189	ILE
16	g	198	VAL
16	g	305	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	74	GLN
2	J	42	ASN
2	J	61	GLN
4	O	24	GLN
4	O	54	HIS
4	O	104	GLN
5	Q	8	GLN
5	Q	86	GLN
7	S	73	ASN

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Mol	Chain	Res	Type
8	T	12	GLN
8	T	63	HIS
8	T	142	ASN
9	U	81	GLN
10	Y	112	ASN
12	c	29	GLN
12	c	45	ASN
15	E	65	GLN
15	E	82	ASN
15	E	83	ASN
16	g	117	ASN
16	g	187	ASN

5.3.3 RNA ⓘ

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

All (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
14	i	1253	A
14	i	1256	G
14	i	1257	G
14	i	1259	A
14	i	1260	A
14	i	1274	G
14	i	1275	G
14	i	1282	A
14	i	1293	A
14	i	1302	G
14	i	1303	C
14	i	1308	U
14	i	1309	U
14	i	1312	G
14	i	1320	G

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Mol	Chain	Res	Type
14	i	1342	U
14	i	1348	G
14	i	1358	U
14	i	1371	U
14	i	1372	U
14	i	1373	C
14	i	1378	A
14	i	1382	A
14	i	1397	U
14	i	1405	A
14	i	1406	G
14	i	1419	C
14	i	1420	G
14	i	1421	A
14	i	1423	C
14	i	1434	C
14	i	1435	C
14	i	1438	A
14	i	1439	A
14	i	1454	A
14	i	1463	U
14	i	1466	G
14	i	1489	A
14	i	1490	OMG
14	i	1497	G
14	i	1508	A
14	i	1521	C
14	i	1522	A
14	i	1533	A
14	i	1553	C
14	i	1570	G
14	i	1575	G
14	i	1578	U
14	i	1580	A
14	i	1588	A
14	i	1601	A
14	i	1621	U
14	i	1623	A
14	i	1654	G
14	i	1664	A
14	i	1665	G
14	i	1671	G

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

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	G7M	i	1639	14	-	0/3/25/26	0/3/3/3
14	PSU	i	1244	14	-	0/7/25/26	0/2/2/2
14	A2M	i	1383	14	-	1/5/27/28	0/3/3/3
14	B8N	i	1248	14	-	2/16/34/35	0/2/2/2
14	OMC	i	1391	14	-	0/9/27/28	0/2/2/2
14	A2M	i	1678	14	-	1/5/27/28	0/3/3/3
14	OMG	i	1490	17,14	-	1/5/27/28	0/3/3/3
14	PSU	i	1445	14	-	0/7/25/26	0/2/2/2
14	OMC	i	1272	14	-	0/9/27/28	0/2/2/2
14	PSU	i	1238	14	-	0/7/25/26	0/2/2/2
14	4AC	i	1337	14	-	0/11/29/30	0/2/2/2
8	NMM	T	67	8	-	1/9/11/13	-
14	OMG	i	1447	14	-	2/5/27/28	0/3/3/3
14	PSU	i	1367	14	-	0/7/25/26	0/2/2/2
14	OMU	i	1326	17,14	-	0/9/27/28	0/2/2/2
14	OMG	i	1328	19,14	-	1/5/27/28	0/3/3/3
14	PSU	i	1232	14	-	0/7/25/26	0/2/2/2
14	OMU	i	1442	17,14	-	0/9/27/28	0/2/2/2
14	PSU	i	1347	14	-	0/7/25/26	0/2/2/2
14	OMU	i	1288	14	-	0/9/27/28	0/2/2/2

All (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
14	i	1238	PSU	C6-C5	12.18	1.48	1.35
14	i	1445	PSU	C2-N1	9.67	1.49	1.36
14	i	1347	PSU	C2-N1	9.66	1.49	1.36
14	i	1367	PSU	C2-N1	9.64	1.49	1.36
14	i	1244	PSU	C2-N1	9.63	1.49	1.36
14	i	1238	PSU	C2-N1	9.59	1.49	1.36
14	i	1232	PSU	C2-N1	9.38	1.48	1.36
14	i	1244	PSU	C2-N3	8.28	1.51	1.37
14	i	1367	PSU	C2-N3	8.26	1.51	1.37
14	i	1347	PSU	C2-N3	8.23	1.51	1.37
14	i	1445	PSU	C2-N3	8.20	1.51	1.37
14	i	1238	PSU	C2-N3	8.15	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	i	1232	PSU	C2-N3	8.11	1.50	1.37
14	i	1337	4AC	C4-N3	7.04	1.44	1.32
14	i	1337	4AC	C6-C5	6.28	1.49	1.35
14	i	1337	4AC	C2-N3	6.02	1.48	1.36
8	T	67	NMM	CZ-NH2	5.98	1.48	1.34
14	i	1347	PSU	C6-N1	5.71	1.45	1.36
14	i	1244	PSU	C6-N1	5.63	1.45	1.36
14	i	1445	PSU	C6-N1	5.58	1.45	1.36
14	i	1238	PSU	C6-N1	5.57	1.45	1.36
14	i	1367	PSU	C6-N1	5.55	1.45	1.36
14	i	1232	PSU	C6-N1	5.42	1.45	1.36
14	i	1337	4AC	C4-N4	4.96	1.47	1.39
14	i	1337	4AC	C7-N4	4.91	1.47	1.37
14	i	1367	PSU	C4-N3	4.03	1.46	1.38
14	i	1244	PSU	C4-N3	4.03	1.46	1.38
14	i	1445	PSU	C4-N3	4.01	1.46	1.38
14	i	1347	PSU	C4-N3	3.98	1.46	1.38
14	i	1238	PSU	C4-N3	3.93	1.46	1.38
14	i	1337	4AC	C5-C4	3.89	1.49	1.41
14	i	1232	PSU	C4-N3	3.84	1.46	1.38
14	i	1337	4AC	C2-N1	3.67	1.47	1.40
14	i	1232	PSU	O4-C4	-3.52	1.16	1.23
14	i	1445	PSU	O4-C4	-3.46	1.17	1.23
14	i	1244	PSU	O4-C4	-3.46	1.17	1.23
14	i	1383	A2M	O5'-C5'	-3.45	1.34	1.44
14	i	1238	PSU	O4-C4	-3.42	1.17	1.23
14	i	1678	A2M	O5'-C5'	-3.42	1.34	1.44
14	i	1367	PSU	O4-C4	-3.40	1.17	1.23
14	i	1347	PSU	O4-C4	-3.35	1.17	1.23
14	i	1490	OMG	C8-N7	-3.13	1.29	1.34
14	i	1447	OMG	C8-N7	-3.10	1.30	1.34
14	i	1328	OMG	C8-N7	-3.09	1.30	1.34
14	i	1337	4AC	C6-N1	3.05	1.45	1.38
14	i	1337	4AC	O2-C2	-3.03	1.18	1.23
14	i	1639	G7M	C8-N9	2.83	1.38	1.33
14	i	1490	OMG	C5-C6	-2.82	1.41	1.47
14	i	1232	PSU	O2-C2	-2.81	1.17	1.23
14	i	1238	PSU	O2-C2	-2.76	1.17	1.23
14	i	1244	PSU	C1'-C5	2.74	1.56	1.50
14	i	1445	PSU	O2-C2	-2.71	1.17	1.23
14	i	1244	PSU	O2-C2	-2.70	1.17	1.23
14	i	1447	OMG	C5-C6	-2.70	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	i	1367	PSU	O2-C2	-2.68	1.17	1.23
14	i	1347	PSU	O2-C2	-2.68	1.17	1.23
14	i	1445	PSU	C1'-C5	2.67	1.56	1.50
14	i	1347	PSU	C1'-C5	2.66	1.56	1.50
14	i	1328	OMG	C5-C6	-2.59	1.42	1.47
14	i	1367	PSU	C1'-C5	2.59	1.56	1.50
14	i	1238	PSU	C1'-C5	2.57	1.56	1.50
14	i	1232	PSU	C1'-C5	2.52	1.56	1.50
14	i	1383	A2M	C1'-N9	-2.51	1.43	1.49
14	i	1678	A2M	O4'-C4'	-2.36	1.39	1.45
14	i	1678	A2M	C1'-N9	-2.31	1.44	1.49
14	i	1639	G7M	C6-N1	2.28	1.41	1.37
14	i	1337	4AC	O7-C7	-2.26	1.18	1.23
14	i	1272	OMC	C4-N4	2.18	1.39	1.33
14	i	1639	G7M	C2-N2	2.13	1.39	1.34
14	i	1391	OMC	C4-N4	2.13	1.39	1.33
14	i	1490	OMG	C5-C4	-2.01	1.38	1.43

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
14	i	1347	PSU	C4-N3-C2	-4.96	119.54	126.37
14	i	1383	A2M	C4'-O4'-C1'	-4.91	105.43	109.92
14	i	1244	PSU	C4-N3-C2	-4.90	119.62	126.37
14	i	1232	PSU	N1-C2-N3	4.70	120.12	115.17
14	i	1367	PSU	N1-C2-N3	4.64	120.07	115.17
14	i	1445	PSU	N1-C2-N3	4.61	120.03	115.17
14	i	1347	PSU	N1-C2-N3	4.58	120.00	115.17
14	i	1238	PSU	N1-C2-N3	4.51	119.93	115.17
8	T	67	NMM	CD-NE-CZ	4.47	131.65	123.46
14	i	1244	PSU	N1-C2-N3	4.42	119.83	115.17
14	i	1383	A2M	C3'-C2'-C1'	-3.68	95.76	102.81
14	i	1383	A2M	C1'-N9-C4	-3.67	120.19	126.64
14	i	1383	A2M	O3'-C3'-C2'	3.66	121.43	111.19
14	i	1678	A2M	C4'-O4'-C1'	-3.59	106.64	109.92
8	T	67	NMM	NH2-CZ-NH1	-3.46	112.24	120.15
14	i	1678	A2M	C1'-N9-C4	-3.42	120.64	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	i	1445	PSU	C6-C5-C4	3.42	120.48	118.17
14	i	1367	PSU	C6-C5-C4	3.30	120.40	118.17
14	i	1232	PSU	C6-N1-C2	-3.28	119.65	122.69
14	i	1238	PSU	C6-C5-C4	3.26	120.38	118.17
14	i	1445	PSU	C6-N1-C2	-3.25	119.68	122.69
14	i	1347	PSU	C6-N1-C2	-3.23	119.69	122.69
14	i	1678	A2M	C2'-C1'-N9	3.23	119.73	112.56
14	i	1347	PSU	C6-C5-C4	3.22	120.34	118.17
14	i	1367	PSU	C6-N1-C2	-3.19	119.73	122.69
14	i	1232	PSU	C6-C5-C4	3.17	120.31	118.17
14	i	1244	PSU	C6-N1-C2	-3.10	119.81	122.69
14	i	1391	OMC	C5-C4-N3	3.08	126.50	121.32
14	i	1238	PSU	C6-N1-C2	-3.03	119.88	122.69
14	i	1272	OMC	C5-C4-N3	3.00	126.38	121.32
14	i	1326	OMU	C4-N3-C2	-2.93	122.97	126.61
14	i	1244	PSU	C6-C5-C4	2.88	120.12	118.17
14	i	1248	B8N	C31-N3-C4	2.87	121.24	117.18
14	i	1678	A2M	O3'-C3'-C2'	2.86	119.19	111.19
14	i	1442	OMU	C4-N3-C2	-2.82	123.12	126.61
14	i	1367	PSU	O2-C2-N1	-2.79	119.91	122.79
14	i	1244	PSU	O2-C2-N1	-2.74	119.96	122.79
14	i	1678	A2M	O4'-C1'-C2'	2.74	111.28	106.61
14	i	1232	PSU	O2-C2-N1	-2.73	119.97	122.79
14	i	1288	OMU	C4-N3-C2	-2.69	123.27	126.61
14	i	1639	G7M	N1-C2-N3	2.61	128.09	123.32
14	i	1678	A2M	C3'-C2'-C1'	-2.60	97.83	102.81
14	i	1445	PSU	O2-C2-N1	-2.60	120.11	122.79
14	i	1248	B8N	C4-N3-C2	-2.59	122.43	125.62
14	i	1391	OMC	C4-N3-C2	-2.59	116.19	120.26
14	i	1272	OMC	C4-N3-C2	-2.55	116.24	120.26
14	i	1238	PSU	O2-C2-N1	-2.55	120.16	122.79
14	i	1337	4AC	C6-C5-C4	2.51	120.03	117.00
14	i	1347	PSU	O2-C2-N1	-2.51	120.20	122.79
14	i	1328	OMG	O6-C6-C5	2.45	129.19	124.32
14	i	1383	A2M	C4-C5-N7	2.42	111.90	109.34
14	i	1288	OMU	CM2-O2'-C2'	-2.42	108.27	114.47
14	i	1678	A2M	C4-C5-N7	2.41	111.89	109.34
14	i	1490	OMG	O6-C6-C5	2.40	129.09	124.32
14	i	1442	OMU	O4-C4-N3	-2.40	115.79	119.27
14	i	1248	B8N	C32-C33-C34	-2.36	104.18	110.45
14	i	1447	OMG	O6-C6-C5	2.32	128.92	124.32
14	i	1288	OMU	O4-C4-N3	-2.31	115.92	119.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	i	1326	OMU	O4-C4-N3	-2.30	115.93	119.27
14	i	1288	OMU	C6-C5-C4	2.30	122.47	119.53
14	i	1326	OMU	CM2-O2'-C2'	-2.30	108.57	114.47
14	i	1326	OMU	C6-C5-C4	2.22	122.37	119.53
14	i	1442	OMU	C6-C5-C4	2.18	122.31	119.53
14	i	1248	B8N	O4'-C1'-C2'	2.14	108.11	105.15
14	i	1445	PSU	O4'-C1'-C2'	2.09	108.05	105.15
14	i	1391	OMC	C5-C6-N1	-2.06	118.49	121.84
14	i	1337	4AC	C5-C4-N3	-2.05	119.39	122.60
14	i	1442	OMU	N3-C2-N1	2.04	117.55	114.89
14	i	1326	OMU	N3-C2-N1	2.03	117.54	114.89
14	i	1272	OMC	C5-C6-N1	-2.02	118.55	121.84

There are no chirality outliers.

All (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'
14	i	1447	OMG	O4'-C4'-C5'-O5'
14	i	1248	B8N	N34-C33-C34-O36
14	i	1248	B8N	N34-C33-C34-O35
14	i	1490	OMG	C4'-C5'-O5'-P

There are no ring outliers.

8 monomers are involved in 10 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

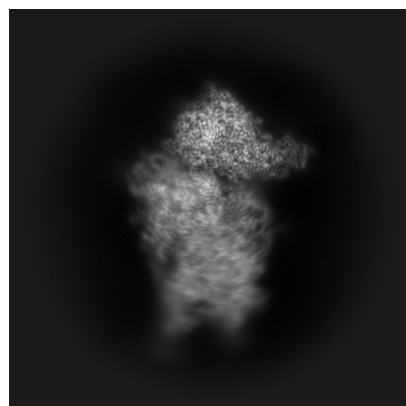
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49636. These allow visual inspection of the internal detail of the map and identification of artifacts.

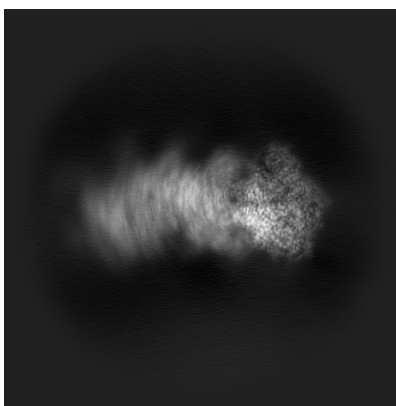
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

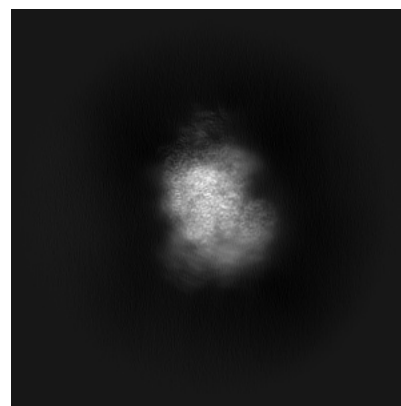
6.1.1 Primary map



X

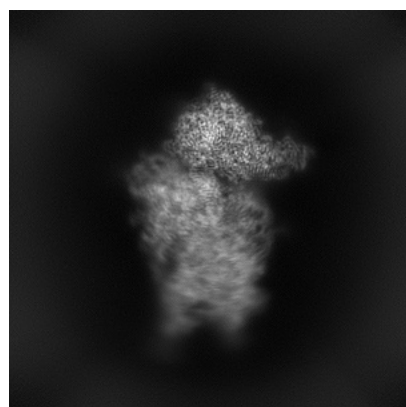


Y

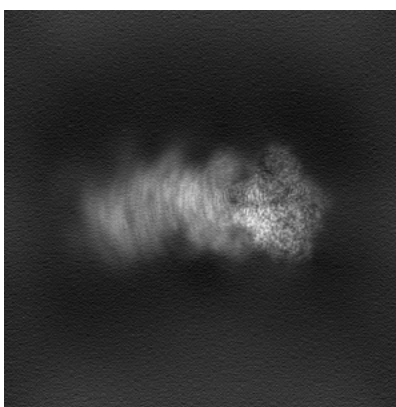


Z

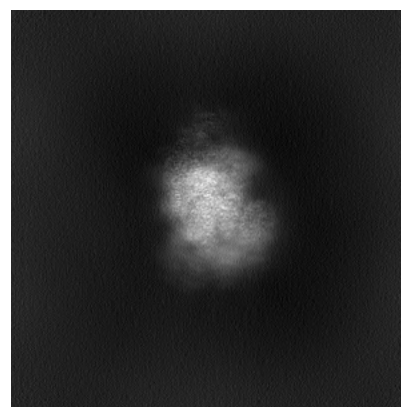
6.1.2 Raw map



X



Y

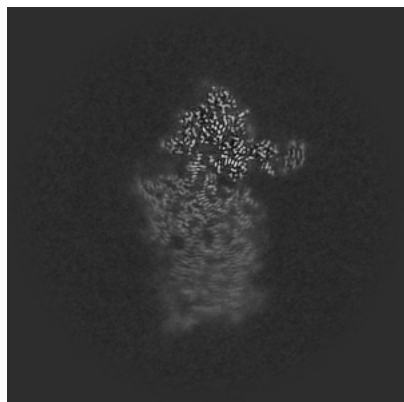


Z

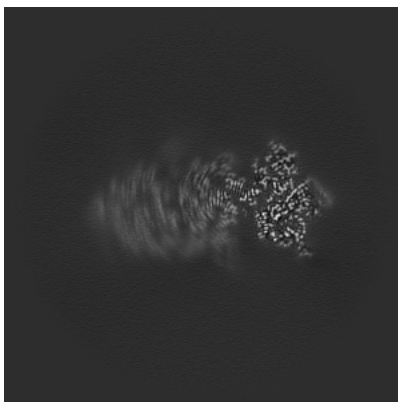
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

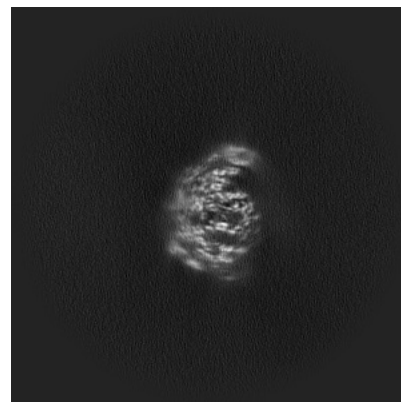
6.2.1 Primary map



X Index: 256

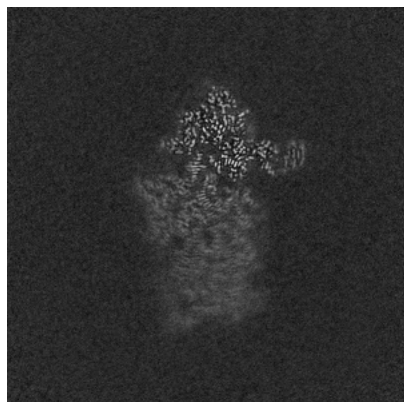


Y Index: 256

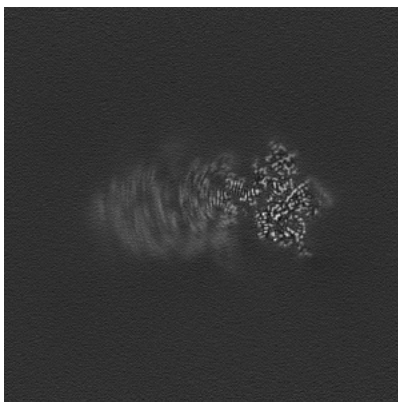


Z Index: 256

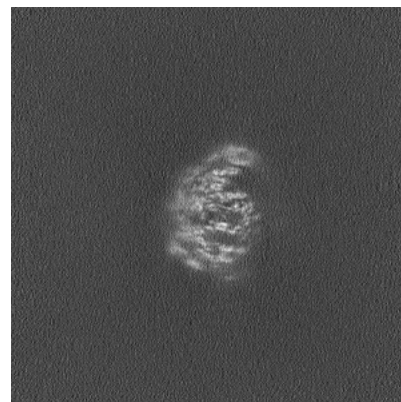
6.2.2 Raw map



X Index: 256



Y Index: 256

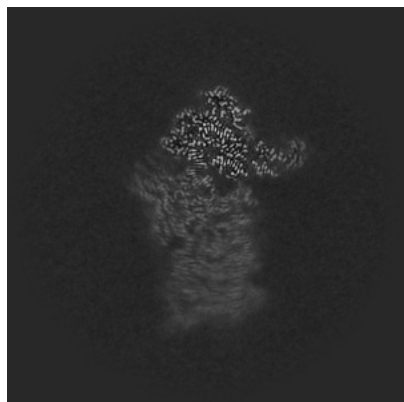


Z Index: 256

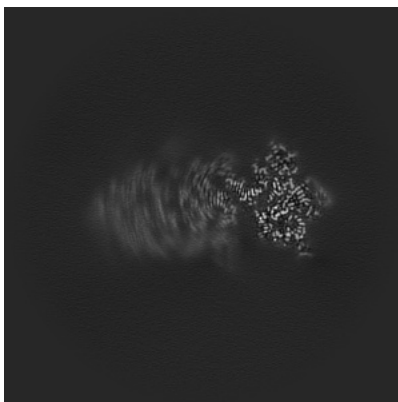
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

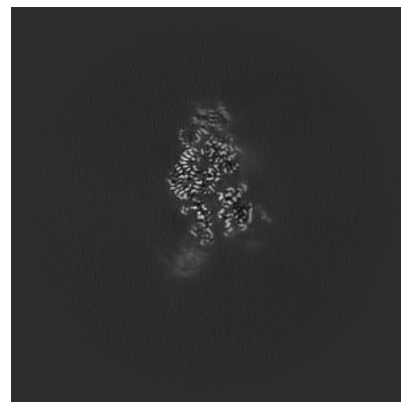
6.3.1 Primary map



X Index: 251



Y Index: 257

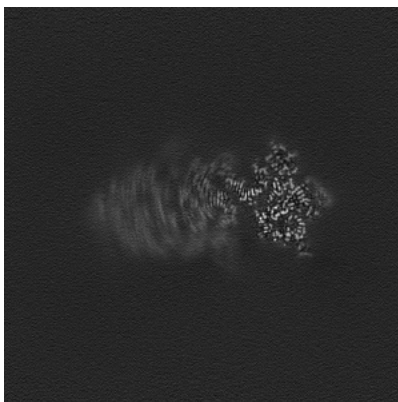


Z Index: 325

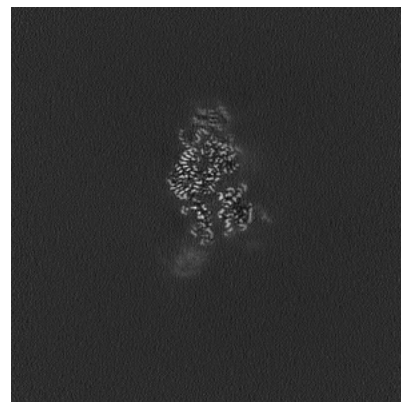
6.3.2 Raw map



X Index: 251



Y Index: 257

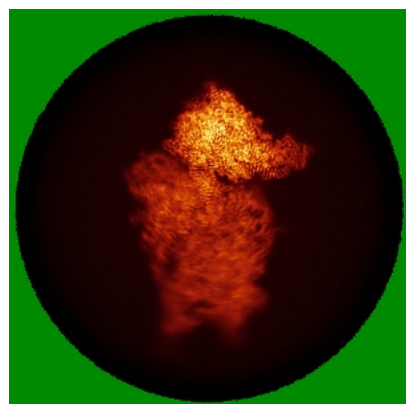


Z Index: 325

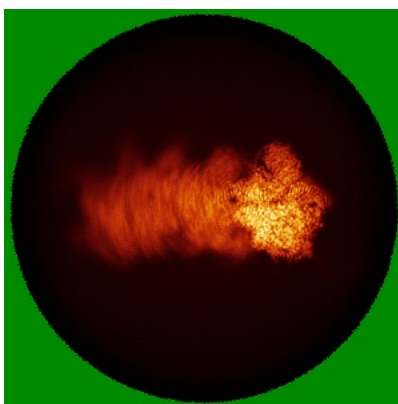
The images above show the largest variance slices of the map in three orthogonal directions.

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

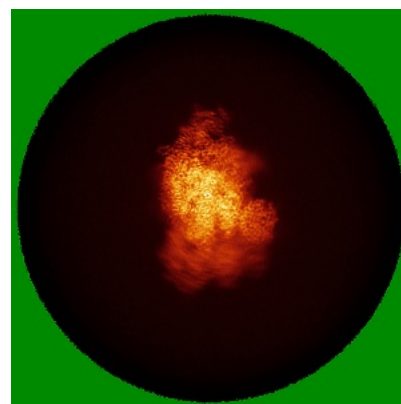
6.4.1 Primary map



X

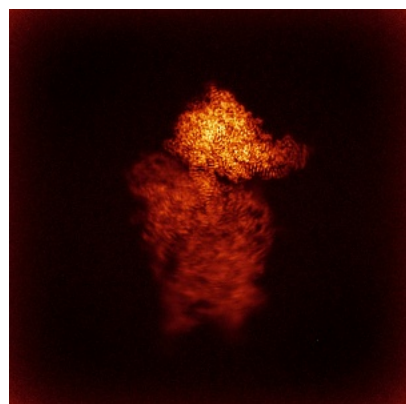


Y

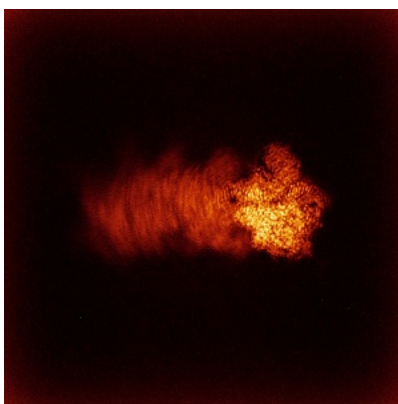


Z

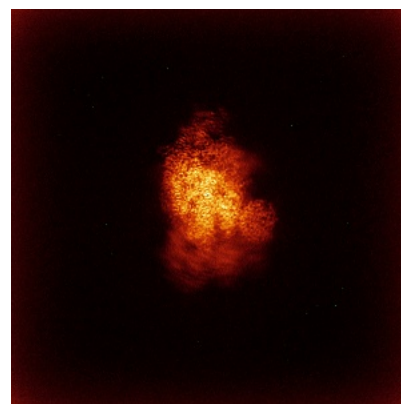
6.4.2 Raw map



X



Y

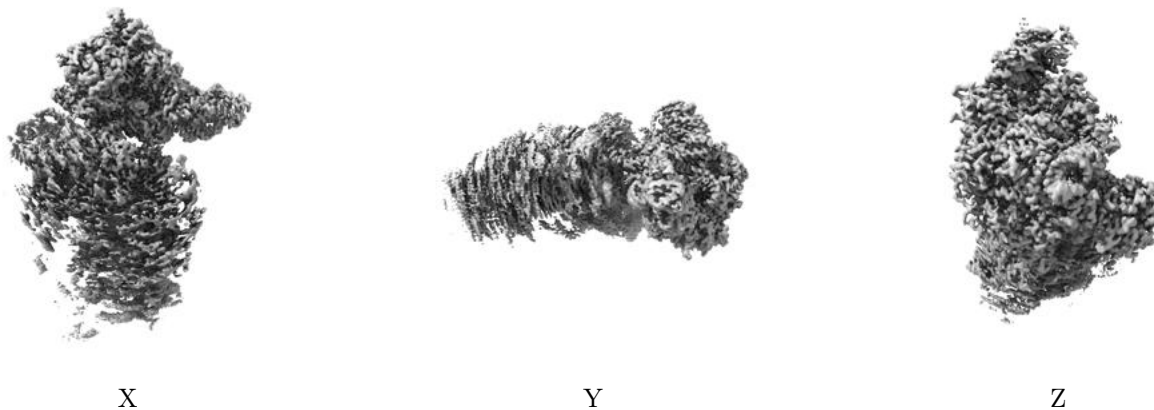


Z

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.

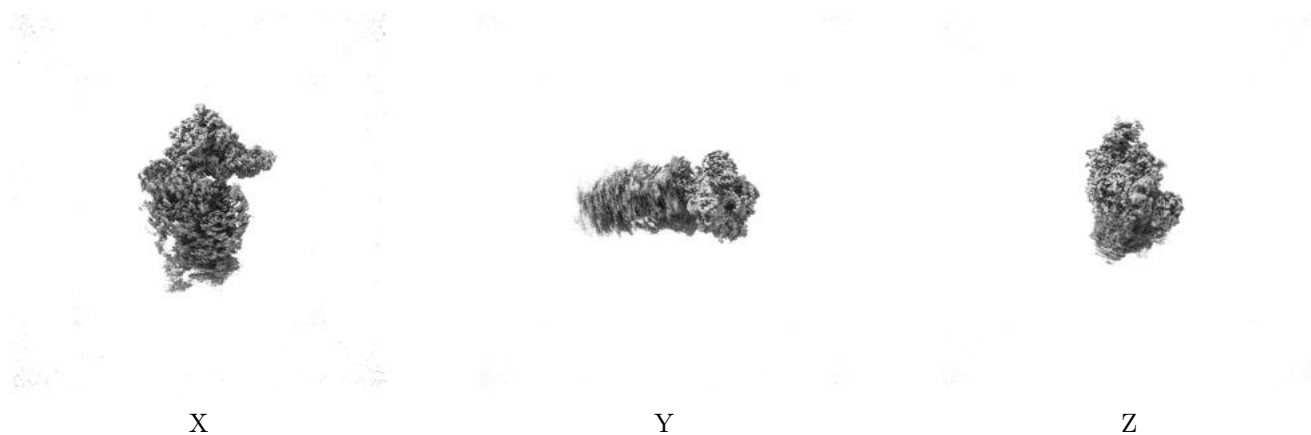
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

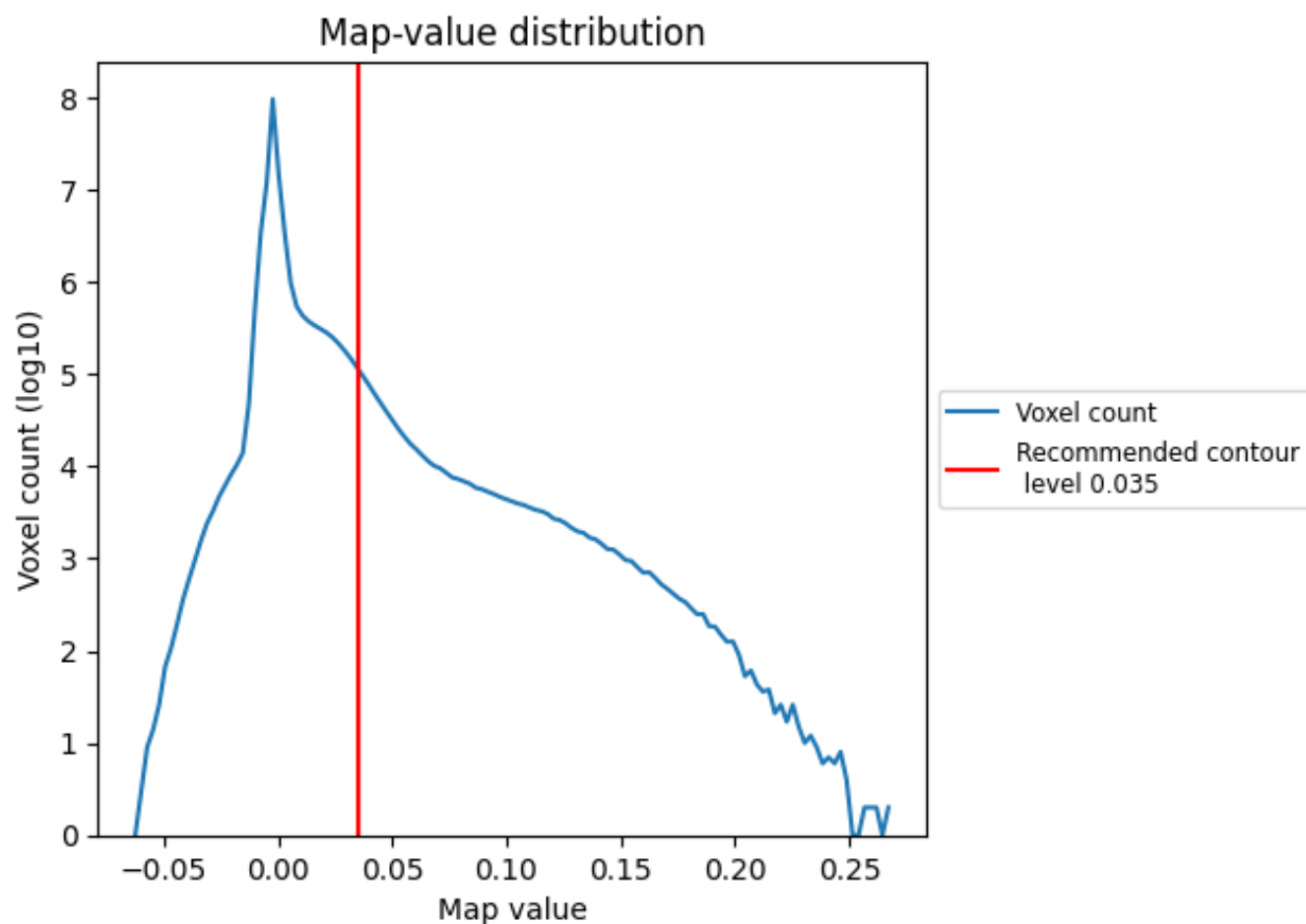
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

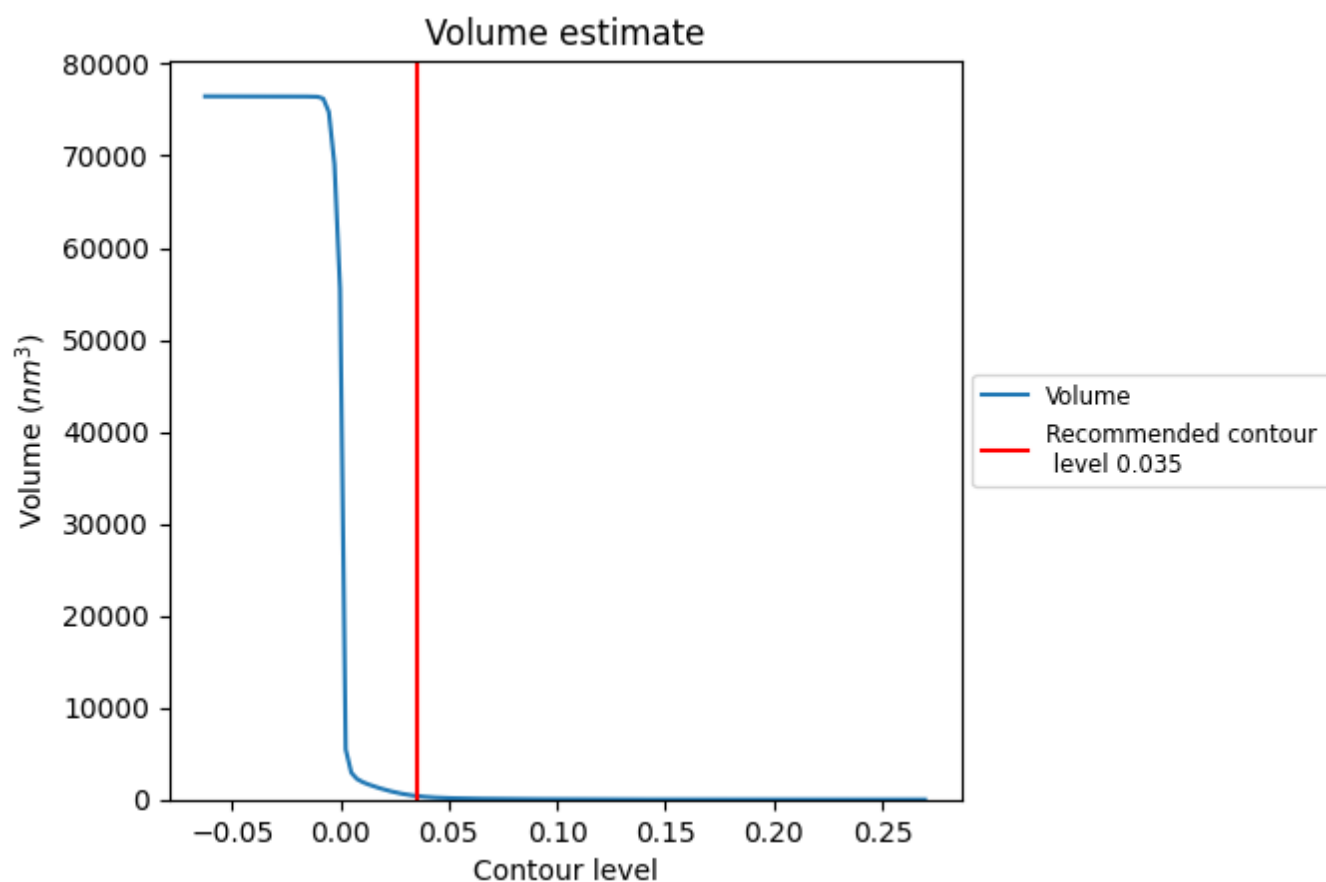
This section contains the results of statistical analysis of the map.

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.

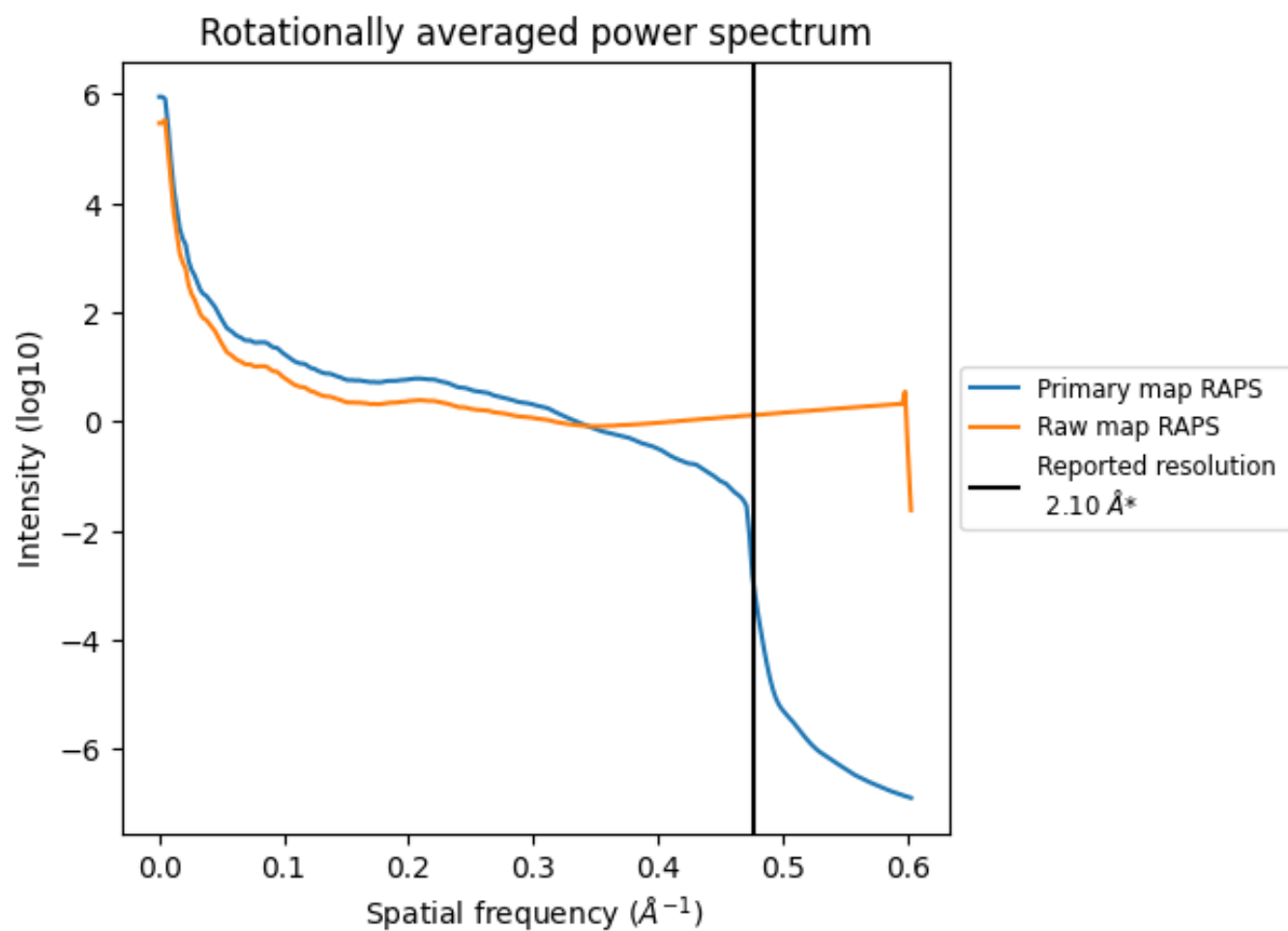
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 395 nm³; 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 ⓘ

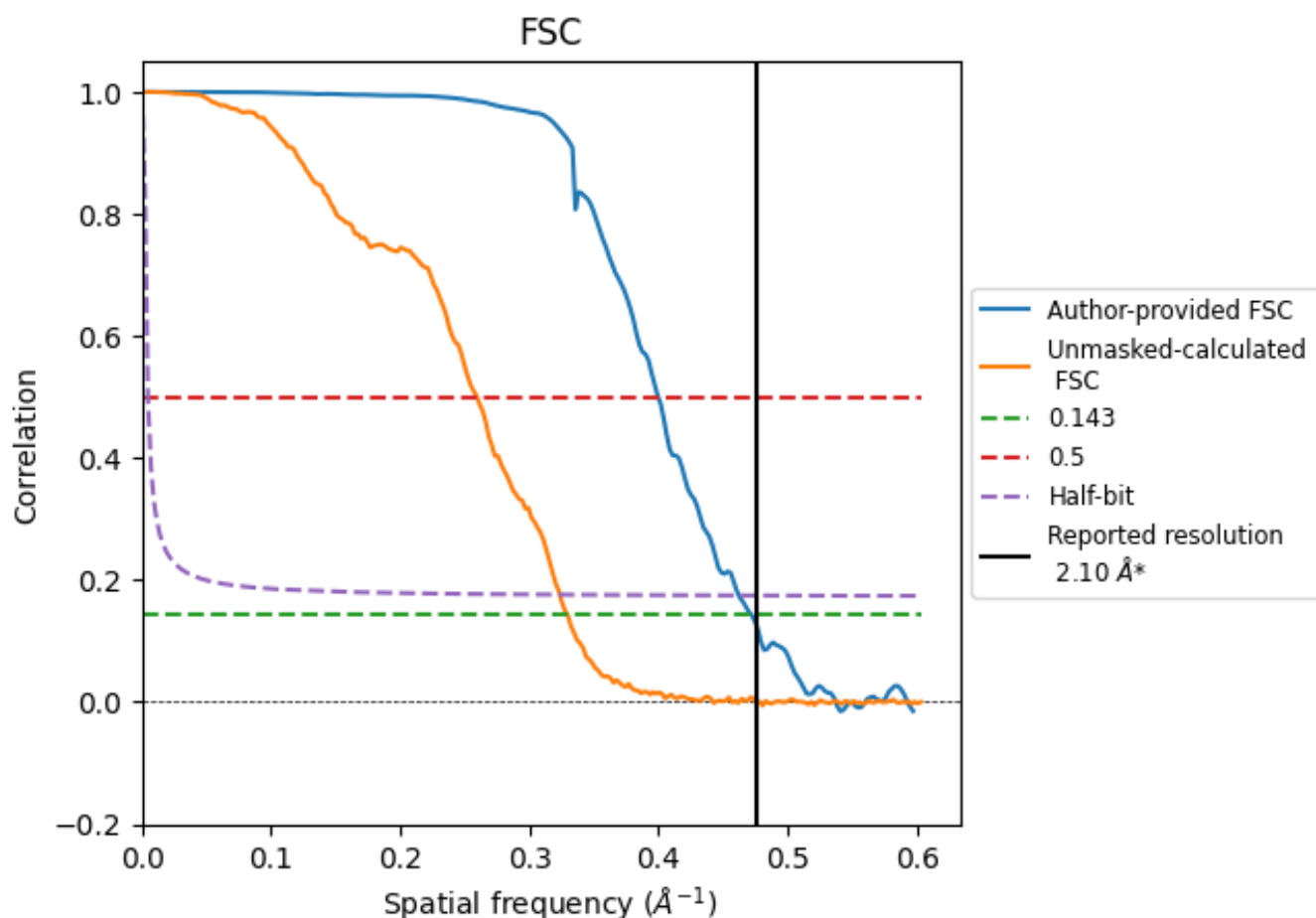


*Reported resolution corresponds to spatial frequency of 0.476 \AA^{-1}

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 0.476 \AA^{-1}

8.2 Resolution estimates [i](#)

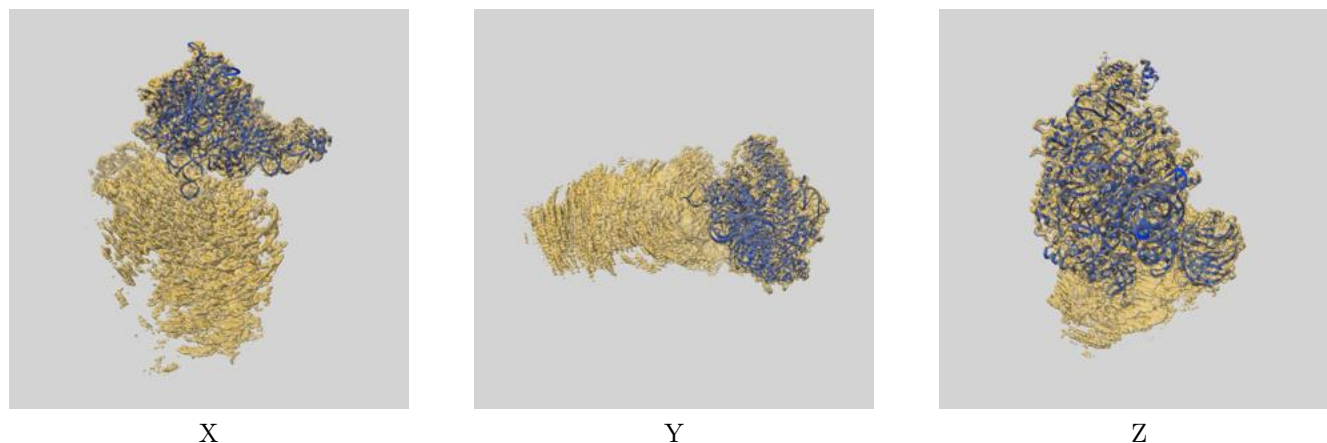
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.12	2.50	2.16
Unmasked-calculated*	3.03	3.86	3.09

*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 [i](#)

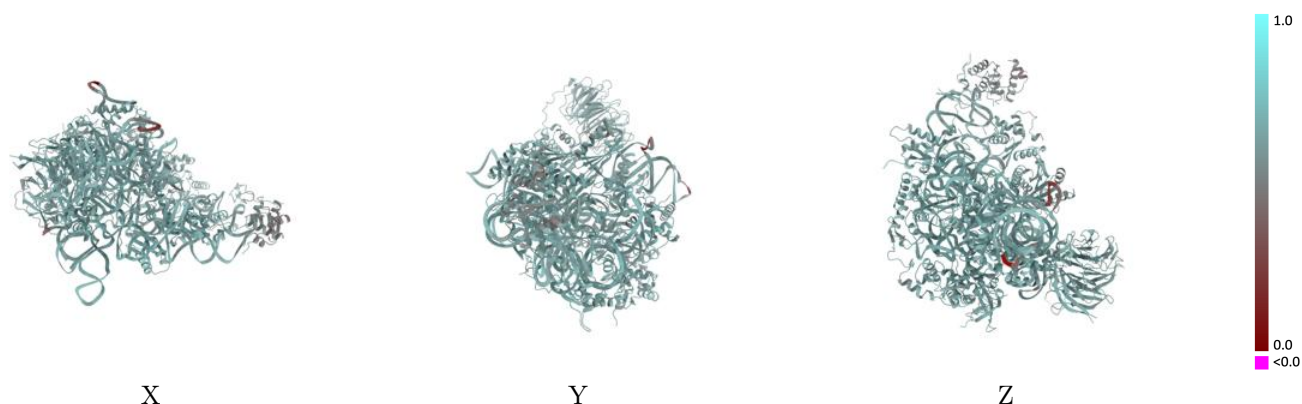
This section contains information regarding the fit between EMDB map EMD-49636 and PDB model 9NPY. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



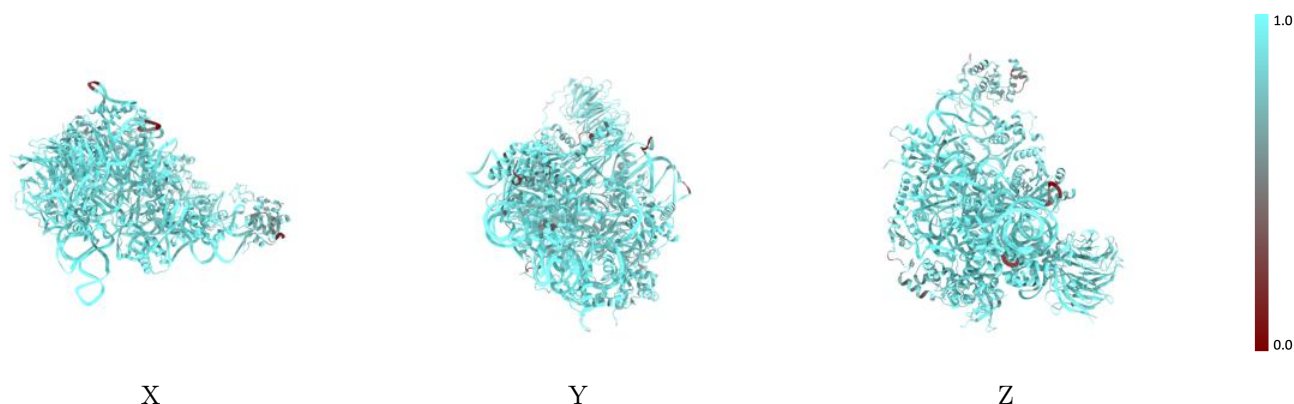
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



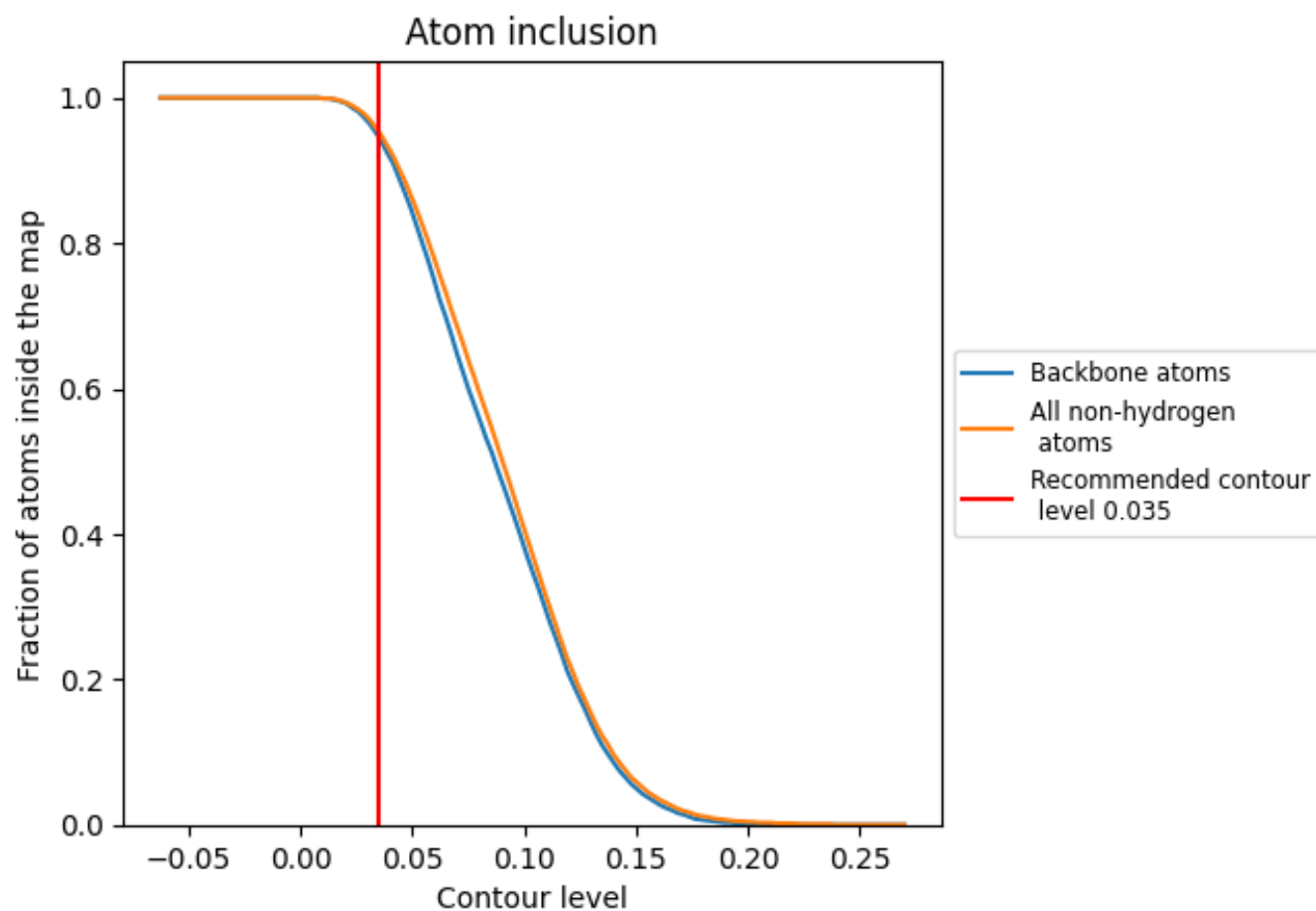
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



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.

9.5 Map-model fit summary ⓘ

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

1.0

0.0

<0.0