



## wwPDB EM Validation Summary Report ⓘ

Mar 18, 2024 – 03:56 PM JST

PDB ID : 8JIW  
EMDB ID : EMD-36332  
Title : Atomic structure of wheat ribosome reveals unique features of the plant ribosomes  
Authors : Mishra, R.K.; Sharma, P.; Hussain, T.  
Deposited on : 2023-05-28  
Resolution : 2.88 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

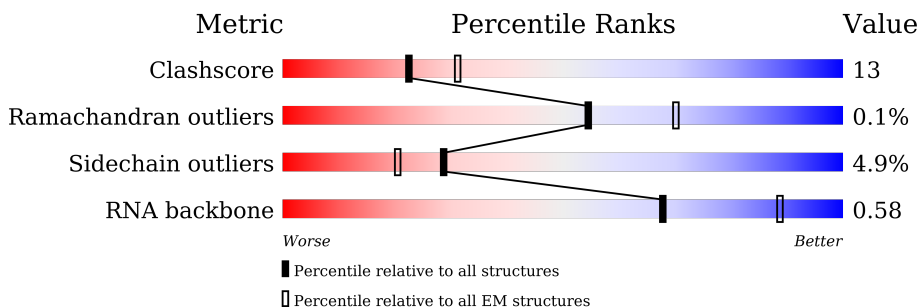
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.88 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	Ad	1811	 69% 17% 13%
2	BA	304	 35% 27% 36%
3	BB	263	 54% 25% 19%
4	BC	279	 54% 24% 21%
5	BE	265	 71% 29%
6	BG	250	 63% 27% 8%
7	BH	192	 64% 28% 5%

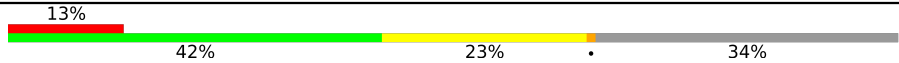
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Mol	Chain	Length	Quality of chain
8	BI	224	
9	BJ	195	
10	BL	161	
11	BN	151	
12	BO	151	
13	BR	143	
14	BV	82	
15	BW	130	
16	BX	142	
17	BY	137	
18	Ba	139	
19	Bb	86	
20	Be	62	
21	Cn	25	
22	BD	227	
23	BF	200	
24	BK	188	
25	BP	153	
26	BQ	149	
27	BS	152	
28	BT	155	
29	BU	117	
30	Bc	65	
31	Bd	56	
32	Bg	335	

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Mol	Chain	Length	Quality of chain
33	BZ	98	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment (13%), a green segment (42%), a yellow segment (23%), and a grey segment (34%). The segments are stacked from left to right in the order: red, green, yellow, grey.</p>

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 68755 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
			Total	C	N	O	P		
1	Ad	1571	33567	15010	6022	10964	1571	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	BA	195	1554	987	276	279	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	BB	213	1740	1109	313	309	9	0	0

- Molecule 4 is a protein called S5 DRBM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	BC	220	1703	1096	303	295	9	0	0

- Molecule 5 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	BE	263	2088	1334	391	356	7	0	0

- Molecule 6 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	BG	229	1847	1152	365	322	8	0	0

- Molecule 7 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	BH	182	1368	879	240	248	1	0	0

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	BI	186	1504	932	301	267	4	0	0

- Molecule 9 is a protein called 30S ribosomal protein S4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	BJ	183	1504	952	300	248	4	0	0

- Molecule 10 is a protein called 40S ribosomal protein S11 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	BL	152	1207	766	230	205	6	0	0

- Molecule 11 is a protein called Ribosomal protein S13/S15 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	BN	149	1191	763	223	203	2	0	0

- Molecule 12 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	BO	130	983	603	195	181	4	0	0

- Molecule 13 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	BR	119	969	604	182	177	6	0	0

- Molecule 14 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	BV	81	636	393	118	122	3	0	0

- Molecule 15 is a protein called 30S ribosomal protein S8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	BW	129	1032	659	188	180	5	0	0

- Molecule 16 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	BX	139	1077	684	208	182	3	0	0

- Molecule 17 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	BY	124	1011	645	196	168	2	0	0

- Molecule 18 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Ba	98	791	487	172	125	7	0	0

- Molecule 19 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Bb	86	663	416	120	119	8	0	0

- Molecule 20 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	Be	47	376	230	86	60	0	0

- Molecule 21 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Cn	25	Total	C	N	O	S	0	0
			237	145	62	27	3		

- Molecule 22 is a protein called KH type-2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BD	208	Total	C	N	O	S	0	0
			1623	1030	295	289	9		

- Molecule 23 is a protein called Ribosomal protein S7 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BF	178	Total	C	N	O	S	0	0
			1416	888	263	258	7		

- Molecule 24 is a protein called Plectin/S10 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BK	82	Total	C	N	O	S	0	0
			711	467	118	123	3		

- Molecule 25 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BP	70	Total	C	N	O	S	0	0
			567	363	110	89	5		

- Molecule 26 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BQ	139	Total	C	N	O	S	0	0
			1108	704	213	186	5		

- Molecule 27 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BS	100	Total	C	N	O	S	0	0
			822	510	173	134	5		

- Molecule 28 is a protein called 40S ribosomal protein S19.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	BT	137	Total	C	N	O	S	0	0
			1081	680	205	192	4		

- Molecule 29 is a protein called Ribosomal protein S10 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BU	101	Total	C	N	O	S	0	0
			793	495	148	146	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Bc	61	Total	C	N	O	S	0	0
			489	301	100	86	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Bd	50	Total	C	N	O	S	0	0
			403	250	82	65	6		

- Molecule 32 is a protein called Mitogen-activated protein kinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bg	271	Total	C	N	O	S	0	0
			2086	1325	363	389	9		

- Molecule 33 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BZ	65	Total	C	N	O	S	0	0
			521	330	94	96	1		

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
34	Ad	14	Total	K	0
			14	14	
34	BT	1	Total	K	0
			1	1	
34	Bd	1	Total	K	0
			1	1	

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	Ad	69	Total 69	Mg 69	0
35	BS	1	Total 1	Mg 1	0

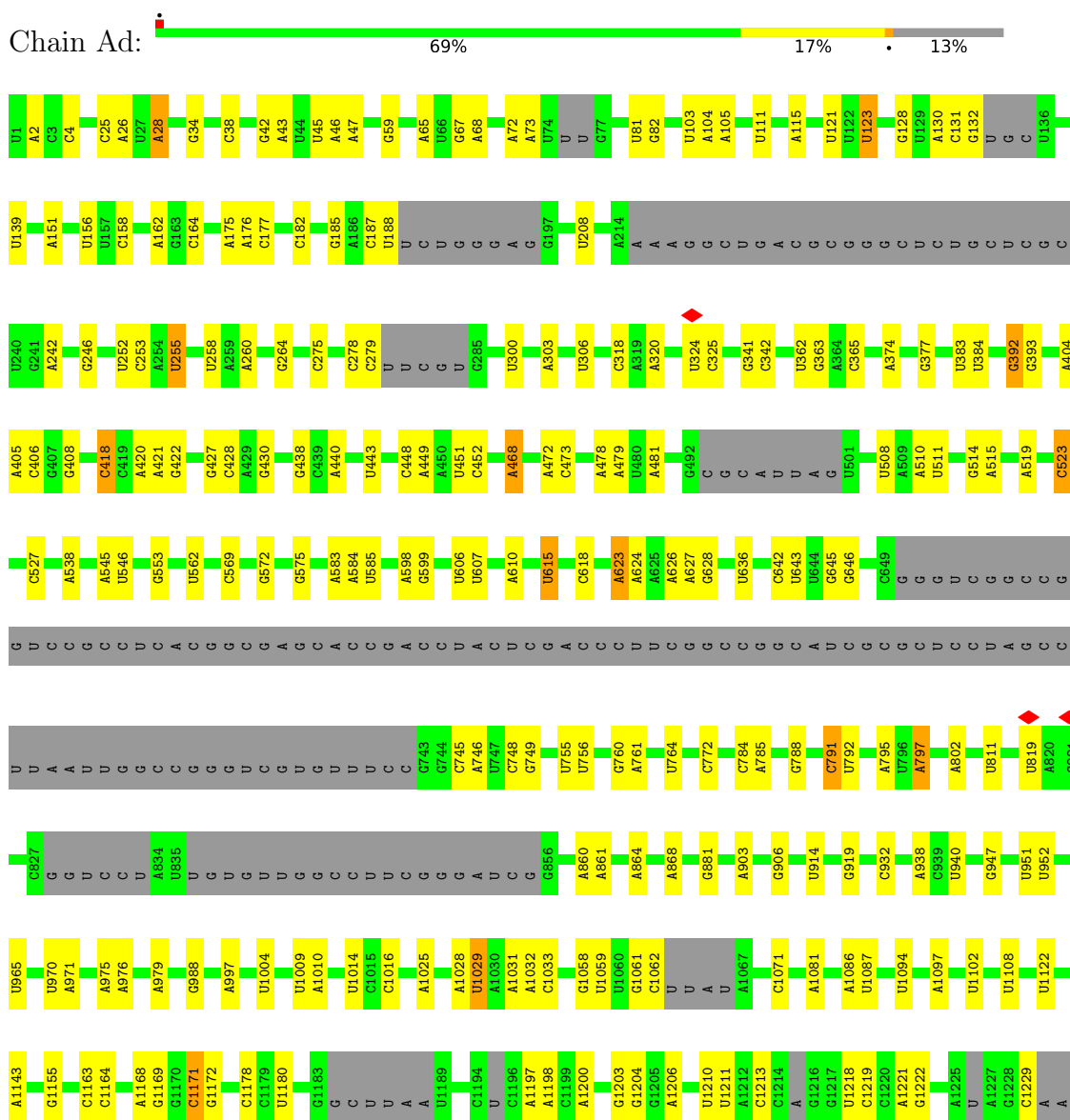
- Molecule 36 is ZINC ION (three-letter code: ZN) (formula: Zn).

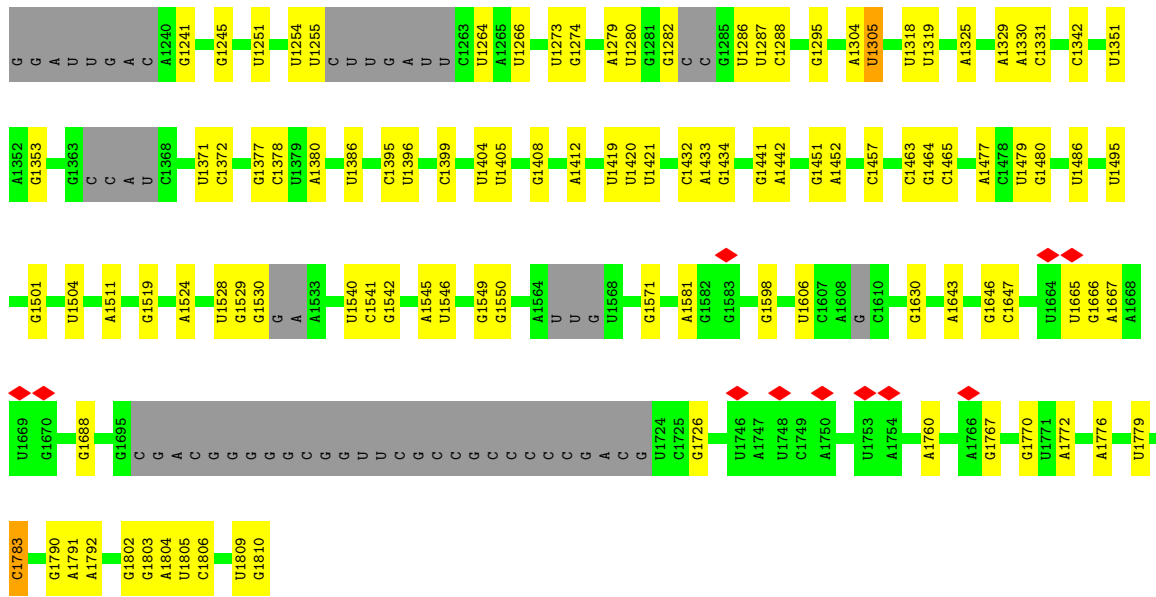
Mol	Chain	Residues	Atoms		AltConf
36	Bd	1	Total 1	Zn 1	0

### 3 Residue-property plots [i](#)

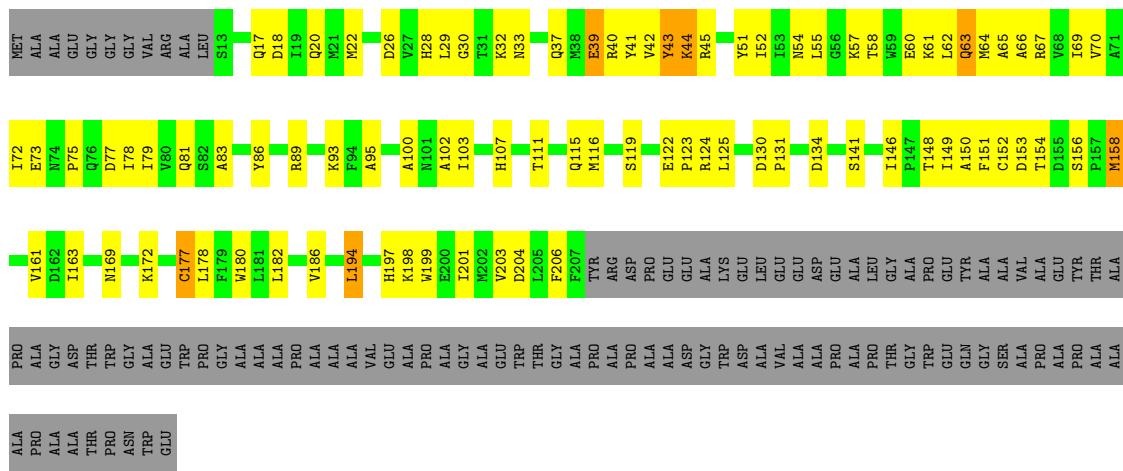
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

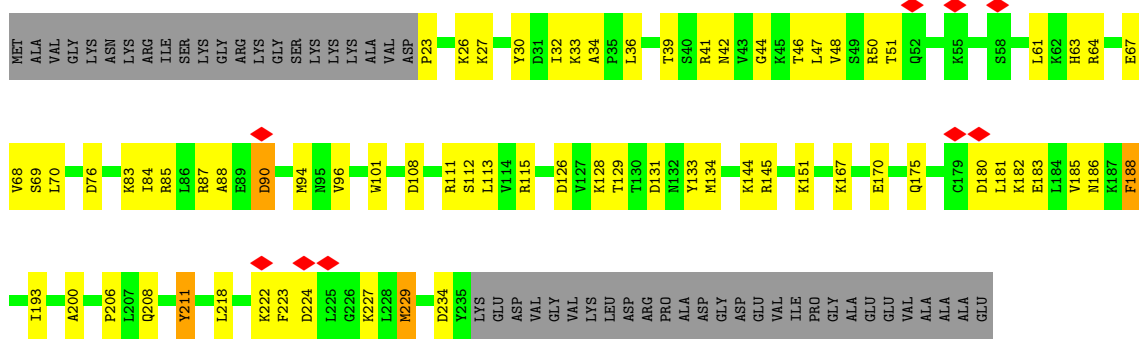




• Molecule 2: 40S ribosomal protein SA



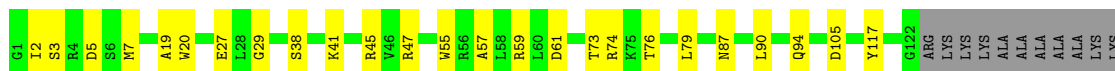
• Molecule 3: 40S ribosomal protein S3a



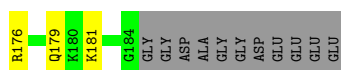
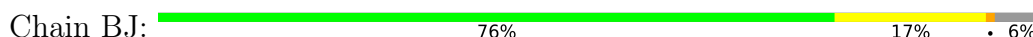




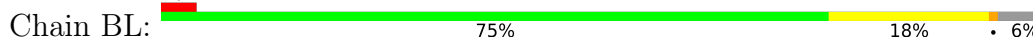
• Molecule 8: 40S ribosomal protein S8



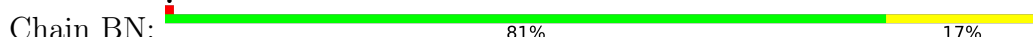
• Molecule 9: 30S ribosomal protein S4, chloroplastic



• Molecule 10: 40S ribosomal protein S11 N-terminal domain-containing protein



• Molecule 11: Ribosomal protein S13/S15 N-terminal domain-containing protein



• Molecule 12: 40S ribosomal protein S14





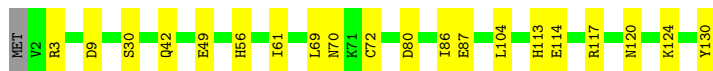
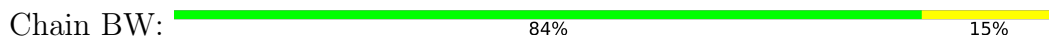
• Molecule 13: 40S ribosomal protein S17



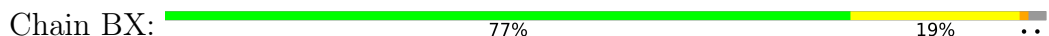
• Molecule 14: 40S ribosomal protein S21



• Molecule 15: 30S ribosomal protein S8, chloroplastic



• Molecule 16: 40S ribosomal protein S23

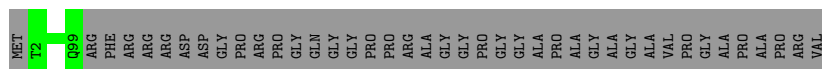


• Molecule 17: 40S ribosomal protein S24

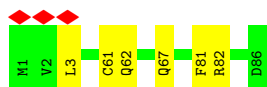


• Molecule 18: 40S ribosomal protein S26

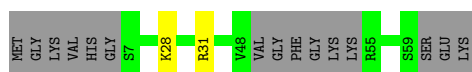




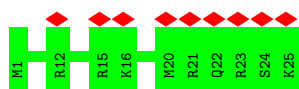
• Molecule 19: 40S ribosomal protein S27



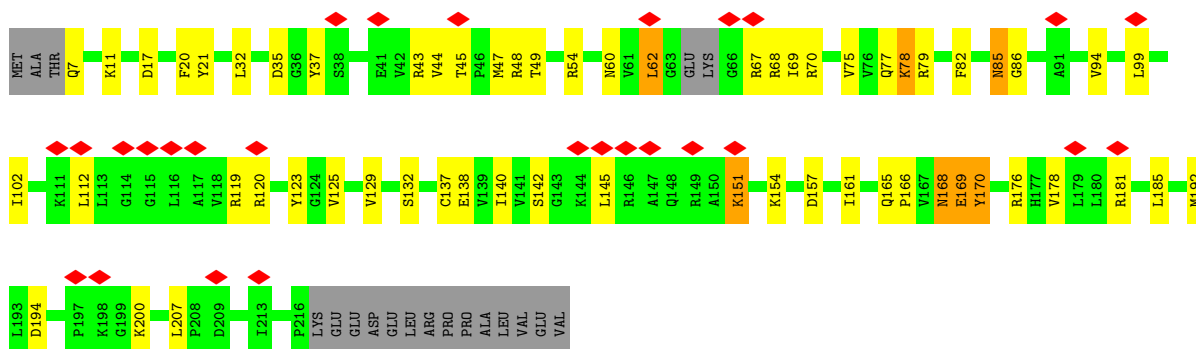
• Molecule 20: 40S ribosomal protein S30



• Molecule 21: 60S ribosomal protein L41



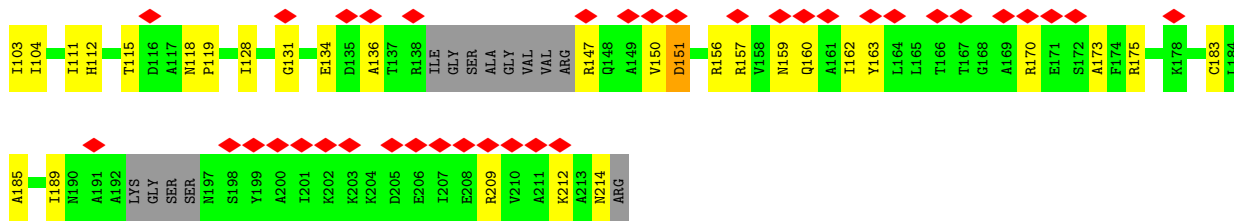
• Molecule 22: KH type-2 domain-containing protein



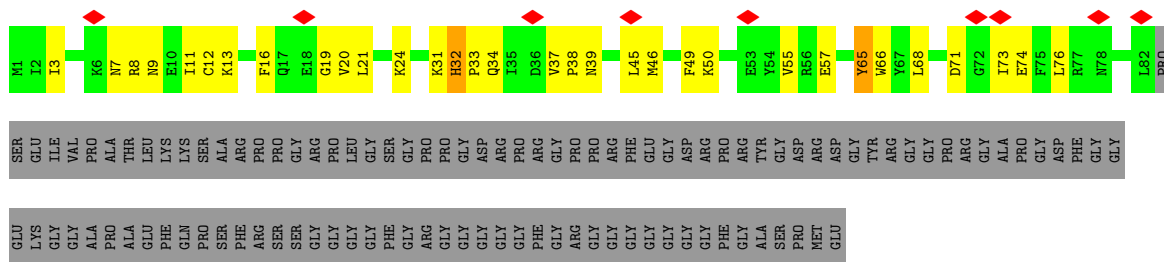
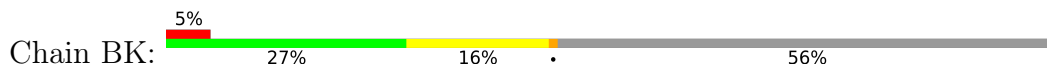
• Molecule 23: Ribosomal protein S7 domain-containing protein



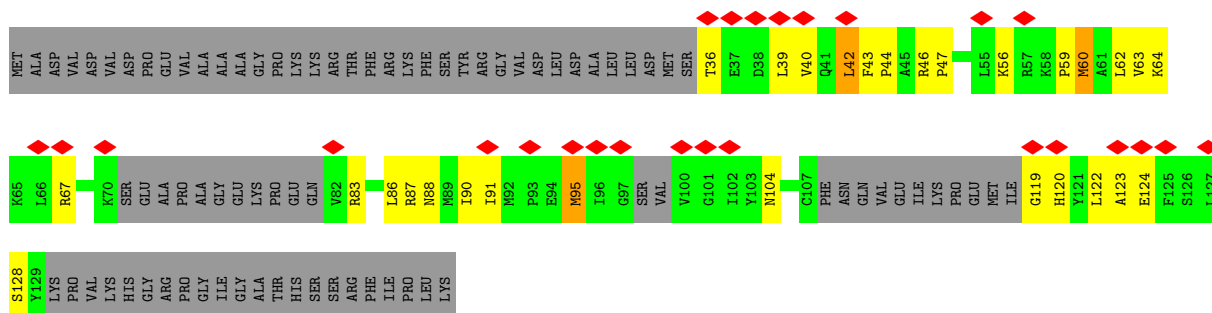
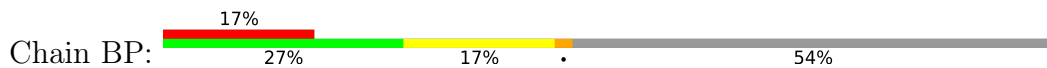




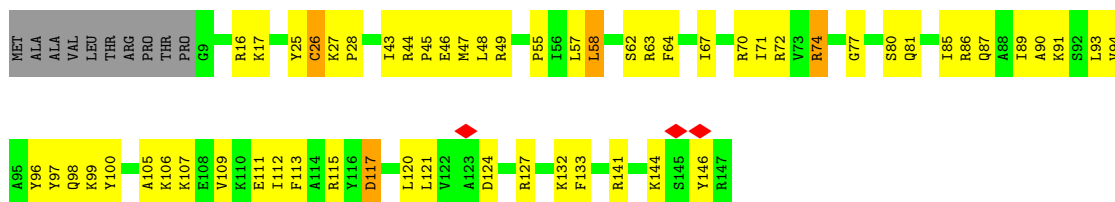
• Molecule 24: Plectin/S10 N-terminal domain-containing protein



• Molecule 25: 40S ribosomal protein S15

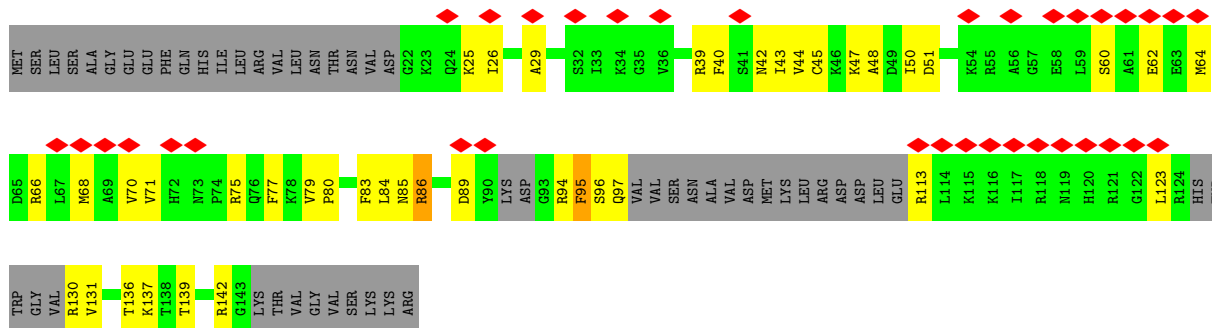


• Molecule 26: 40S ribosomal protein S16

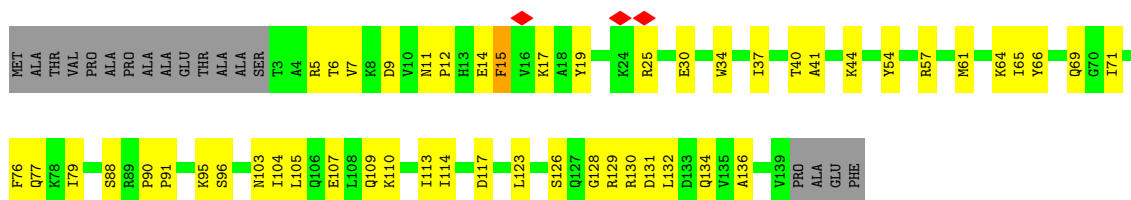


• Molecule 27: 40S ribosomal protein S18

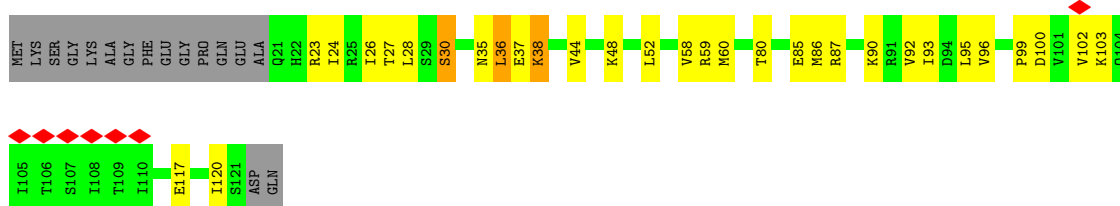




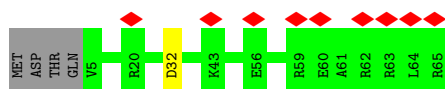
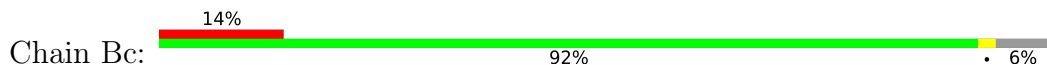
• Molecule 28: 40S ribosomal protein S19



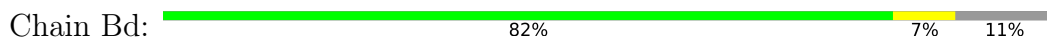
• Molecule 29: Ribosomal protein S10 domain-containing protein



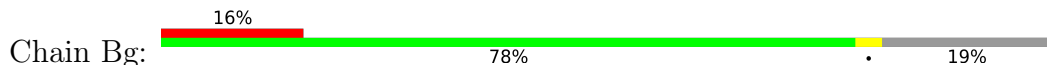
• Molecule 30: 40S ribosomal protein S28

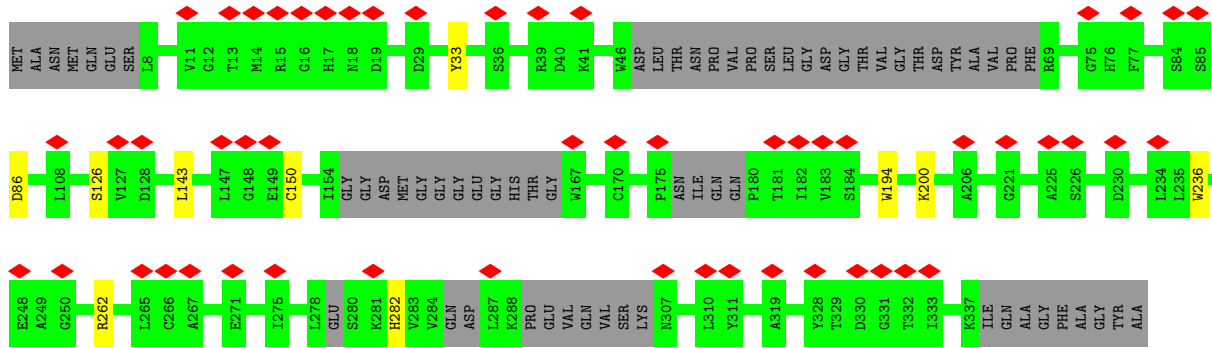


• Molecule 31: 40S ribosomal protein S29

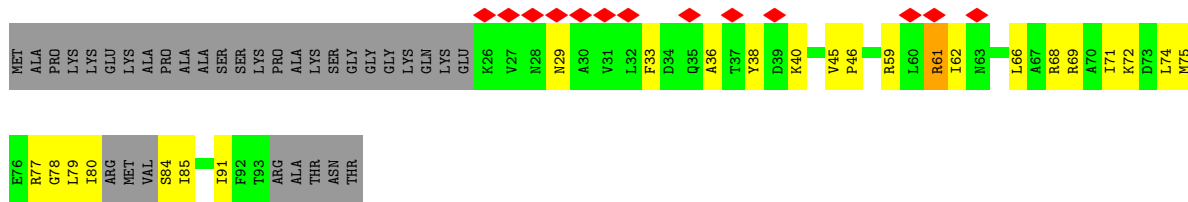


• Molecule 32: Mitogen-activated protein kinase





• Molecule 33: 40S ribosomal protein S25



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105563	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	44.60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	4.553	Depositor
Minimum map value	-1.846	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.119	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	449.40002, 449.40002, 449.40002	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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, OMU, K, MG, A2M, MA6, OMG, ZN, OMC

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	Ad	0.30	0/36448	0.80	35/56766 (0.1%)
2	BA	0.29	0/1587	0.60	1/2147 (0.0%)
3	BB	0.26	0/1770	0.56	0/2378
4	BC	0.29	0/1740	0.52	0/2351
5	BE	0.28	0/2129	0.55	0/2855
6	BG	0.28	0/1867	0.62	1/2480 (0.0%)
7	BH	0.27	0/1394	0.56	0/1894
8	BI	0.27	0/1526	0.56	0/2038
9	BJ	0.28	0/1532	0.56	0/2050
10	BL	0.29	0/1233	0.52	0/1652
11	BN	0.25	0/1215	0.49	0/1634
12	BO	0.27	0/996	0.61	0/1336
13	BR	0.26	0/979	0.64	0/1306
14	BV	0.27	0/645	0.54	0/867
15	BW	0.29	0/1050	0.53	0/1405
16	BX	0.28	0/1096	0.52	0/1460
17	BY	0.28	0/1025	0.57	1/1359 (0.1%)
18	Ba	0.28	0/806	0.59	0/1077
19	Bb	0.26	0/674	0.54	0/905
20	Be	0.24	0/380	0.56	0/502
21	Cn	0.24	0/238	0.66	0/300
22	BD	0.26	0/1647	0.56	0/2215
23	BF	0.24	0/1435	0.51	0/1932
24	BK	0.25	0/730	0.49	0/983
25	BP	0.26	0/575	0.59	0/762
26	BQ	0.53	2/1126 (0.2%)	0.80	4/1502 (0.3%)
27	BS	0.24	0/831	0.57	0/1095
28	BT	0.26	0/1103	0.56	0/1482
29	BU	0.24	0/802	0.54	0/1081
30	Bc	0.24	0/490	0.65	0/652
31	Bd	0.26	0/413	0.56	0/549
32	Bg	0.24	0/2129	0.50	0/2889

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	BZ	0.24	0/526	0.56	0/706
All	All	0.29	2/72137 (0.0%)	0.70	42/104610 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	BA	0	1
7	BH	0	1
13	BR	0	2
19	Bb	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BQ	45	PRO	CG-CD	-12.96	1.07	1.50
26	BQ	45	PRO	N-CD	7.33	1.58	1.47

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BQ	45	PRO	N-CD-CG	-14.74	81.09	103.20
26	BQ	45	PRO	CA-N-CD	-11.06	96.01	111.50
1	Ad	1395	C	C2-N1-C1'	7.71	127.28	118.80
1	Ad	1218	U	C2-N1-C1'	7.37	126.54	117.70
1	Ad	1071	C	N3-C2-O2	-7.12	116.91	121.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	BA	43	TYR	Peptide
7	BH	103	ARG	Peptide
13	BR	73	LEU	Peptide
13	BR	74	GLN	Peptide
19	Bb	62	GLN	Peptide

## 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	Ad	33567	0	16962	0	0
2	BA	1554	0	1565	64	0
3	BB	1740	0	1806	48	0
4	BC	1703	0	1790	49	0
5	BE	2088	0	2189	52	0
6	BG	1847	0	1989	47	0
7	BH	1368	0	1304	47	0
8	BI	1504	0	1548	25	0
9	BJ	1504	0	1571	22	0
10	BL	1207	0	1262	18	0
11	BN	1191	0	1284	13	0
12	BO	983	0	1012	20	0
13	BR	969	0	1013	41	0
14	BV	636	0	626	21	0
15	BW	1032	0	1068	12	0
16	BX	1077	0	1140	15	0
17	BY	1011	0	1095	15	0
18	Ba	791	0	815	0	0
19	Bb	663	0	683	0	0
20	Be	376	0	406	0	0
21	Cn	237	0	289	0	0
22	BD	1623	0	1696	32	0
23	BF	1416	0	1454	41	0
24	BK	711	0	712	28	0
25	BP	567	0	597	19	0
26	BQ	1108	0	1171	44	0
27	BS	822	0	862	30	0
28	BT	1081	0	1101	41	0
29	BU	793	0	851	25	0
30	Bc	489	0	532	0	0
31	Bd	403	0	394	0	0
32	Bg	2086	0	2057	0	0
33	BZ	521	0	548	18	0
34	Ad	14	0	0	0	0
34	BT	1	0	0	0	0
34	Bd	1	0	0	0	0
35	Ad	69	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	BS	1	0	0	0	0
36	Bd	1	0	0	0	0
All	All	68755	0	53392	747	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 13.

The worst 5 of 747 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)
13:BR:10:LYS:HG2	13:BR:53:PHE:HE1	1.36	0.89
5:BE:87:MET:HE1	5:BE:123:LEU:HB2	1.62	0.81
12:BO:95:ILE:HD13	12:BO:126:ILE:HG23	1.66	0.77
7:BH:99:ARG:HD2	7:BH:122:VAL:HG13	1.69	0.74
27:BS:80:PRO:HG3	28:BT:37:ILE:HG12	1.70	0.74

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	
2	BA	193/304 (64%)	173 (90%)	20 (10%)	0	100	100
3	BB	211/263 (80%)	185 (88%)	26 (12%)	0	100	100
4	BC	218/279 (78%)	198 (91%)	20 (9%)	0	100	100
5	BE	261/265 (98%)	225 (86%)	35 (13%)	1 (0%)	34	64
6	BG	227/250 (91%)	195 (86%)	32 (14%)	0	100	100
7	BH	180/192 (94%)	145 (81%)	34 (19%)	1 (1%)	25	55
8	BI	182/224 (81%)	175 (96%)	7 (4%)	0	100	100
9	BJ	181/195 (93%)	177 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	BL	150/161 (93%)	138 (92%)	12 (8%)	0	100	100
11	BN	147/151 (97%)	145 (99%)	2 (1%)	0	100	100
12	BO	128/151 (85%)	120 (94%)	8 (6%)	0	100	100
13	BR	117/143 (82%)	102 (87%)	14 (12%)	1 (1%)	17	45
14	BV	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
15	BW	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
16	BX	137/142 (96%)	130 (95%)	7 (5%)	0	100	100
17	BY	122/137 (89%)	120 (98%)	2 (2%)	0	100	100
18	Ba	96/139 (69%)	96 (100%)	0	0	100	100
19	Bb	84/86 (98%)	74 (88%)	10 (12%)	0	100	100
20	Be	43/62 (69%)	43 (100%)	0	0	100	100
21	Cn	23/25 (92%)	23 (100%)	0	0	100	100
22	BD	204/227 (90%)	198 (97%)	6 (3%)	0	100	100
23	BF	172/200 (86%)	160 (93%)	12 (7%)	0	100	100
24	BK	80/188 (43%)	80 (100%)	0	0	100	100
25	BP	62/153 (40%)	56 (90%)	6 (10%)	0	100	100
26	BQ	137/149 (92%)	132 (96%)	5 (4%)	0	100	100
27	BS	92/152 (60%)	85 (92%)	7 (8%)	0	100	100
28	BT	135/155 (87%)	131 (97%)	4 (3%)	0	100	100
29	BU	99/117 (85%)	96 (97%)	3 (3%)	0	100	100
30	Bc	59/65 (91%)	58 (98%)	1 (2%)	0	100	100
31	Bd	48/56 (86%)	45 (94%)	3 (6%)	0	100	100
32	Bg	257/335 (77%)	247 (96%)	10 (4%)	0	100	100
33	BZ	61/98 (62%)	58 (95%)	3 (5%)	0	100	100
All	All	4312/5276 (82%)	4007 (93%)	302 (7%)	3 (0%)	54	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	BE	261	ALA
7	BH	66	PRO
13	BR	71	LEU

### 5.3.2 Protein sidechains [i](#)

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	BA	167/228 (73%)	157 (94%)	10 (6%)	19	46
3	BB	191/228 (84%)	181 (95%)	10 (5%)	23	53
4	BC	185/221 (84%)	172 (93%)	13 (7%)	15	39
5	BE	223/224 (100%)	217 (97%)	6 (3%)	44	75
6	BG	201/215 (94%)	194 (96%)	7 (4%)	36	68
7	BH	134/171 (78%)	123 (92%)	11 (8%)	11	31
8	BI	159/180 (88%)	154 (97%)	5 (3%)	40	72
9	BJ	155/162 (96%)	150 (97%)	5 (3%)	39	71
10	BL	131/137 (96%)	125 (95%)	6 (5%)	27	58
11	BN	130/131 (99%)	127 (98%)	3 (2%)	50	79
12	BO	102/121 (84%)	95 (93%)	7 (7%)	15	39
13	BR	107/124 (86%)	98 (92%)	9 (8%)	11	30
14	BV	67/68 (98%)	63 (94%)	4 (6%)	19	46
15	BW	111/112 (99%)	110 (99%)	1 (1%)	78	92
16	BX	110/113 (97%)	105 (96%)	5 (4%)	27	59
17	BY	107/116 (92%)	103 (96%)	4 (4%)	34	66
18	Ba	85/108 (79%)	85 (100%)	0	100	100
19	Bb	78/78 (100%)	73 (94%)	5 (6%)	17	43
20	Be	38/49 (78%)	36 (95%)	2 (5%)	22	52
21	Cn	24/24 (100%)	24 (100%)	0	100	100
22	BD	174/192 (91%)	158 (91%)	16 (9%)	9	25
23	BF	153/169 (90%)	143 (94%)	10 (6%)	17	42
24	BK	78/143 (54%)	75 (96%)	3 (4%)	33	65
25	BP	59/130 (45%)	54 (92%)	5 (8%)	10	29
26	BQ	111/120 (92%)	105 (95%)	6 (5%)	22	51
27	BS	86/133 (65%)	81 (94%)	5 (6%)	20	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	BT	113/124 (91%)	106 (94%)	7 (6%)	18	45
29	BU	95/106 (90%)	92 (97%)	3 (3%)	39	71
30	Bc	54/58 (93%)	53 (98%)	1 (2%)	57	82
31	Bd	43/48 (90%)	39 (91%)	4 (9%)	9	25
32	Bg	229/278 (82%)	219 (96%)	10 (4%)	28	59
33	BZ	59/83 (71%)	56 (95%)	3 (5%)	24	53
All	All	3759/4394 (86%)	3573 (95%)	186 (5%)	29	55

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	BD	17	ASP
25	BP	60	MET
22	BD	47	MET
23	BF	60	LEU
26	BQ	74	ARG

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

Mol	Chain	Res	Type
13	BR	42	GLN
14	BV	3	ASN
28	BT	134	GLN
23	BF	94	ASN
8	BI	151	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Ad	1546/1811 (85%)	281 (18%)	0

5 of 281 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Ad	2	A
1	Ad	4	C
1	Ad	25	C
1	Ad	26	A

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Mol	Chain	Res	Type
1	Ad	28	A2M

There are no RNA pucker outliers to report.

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

46 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
1	PSU	Ad	451	1	18,21,22	4.38	7 (38%)	22,30,33	1.70	4 (18%)
1	MA6	Ad	1791	1	19,26,27	1.00	1 (5%)	18,38,41	4.73	3 (16%)
1	PSU	Ad	258	1	18,21,22	4.38	7 (38%)	22,30,33	1.75	5 (22%)
1	PSU	Ad	1004	1	18,21,22	4.45	7 (38%)	22,30,33	1.72	4 (18%)
1	PSU	Ad	585	1	18,21,22	4.44	7 (38%)	22,30,33	1.75	5 (22%)
1	PSU	Ad	1108	1	18,21,22	4.40	7 (38%)	22,30,33	1.79	4 (18%)
1	A2M	Ad	545	1	18,25,26	4.22	7 (38%)	18,36,39	2.32	4 (22%)
1	OMG	Ad	246	1	18,26,27	2.59	8 (44%)	19,38,41	1.51	4 (21%)
1	OMC	Ad	38	1	19,22,23	3.13	8 (42%)	26,31,34	1.07	2 (7%)
1	PSU	Ad	111	34,1	18,21,22	4.38	7 (38%)	22,30,33	1.76	5 (22%)
1	PSU	Ad	255	35,1	18,21,22	4.42	7 (38%)	22,30,33	1.69	4 (18%)
1	PSU	Ad	755	1	18,21,22	4.42	7 (38%)	22,30,33	1.87	4 (18%)
1	PSU	Ad	764	1	18,21,22	4.39	7 (38%)	22,30,33	1.88	5 (22%)
1	PSU	Ad	952	1	18,21,22	4.44	7 (38%)	22,30,33	1.71	4 (18%)
1	A2M	Ad	28	35,1	18,25,26	4.21	7 (38%)	18,36,39	2.42	5 (27%)
1	A2M	Ad	802	1	18,25,26	4.21	7 (38%)	18,36,39	2.24	4 (22%)
1	A2M	Ad	979	1	18,25,26	4.27	8 (44%)	18,36,39	2.61	5 (27%)
1	PSU	Ad	914	1	18,21,22	4.46	7 (38%)	22,30,33	1.69	3 (13%)
1	PSU	Ad	103	1	18,21,22	4.37	7 (38%)	22,30,33	1.87	5 (22%)
1	OMC	Ad	1647	1	19,22,23	3.14	8 (42%)	26,31,34	1.09	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	A2M	Ad	623	35,1	18,25,26	4.14	7 (38%)	18,36,39	2.24	4 (22%)
1	OMU	Ad	1014	1	19,22,23	3.27	7 (36%)	26,31,34	1.68	5 (19%)
1	OMG	Ad	392	1	18,26,27	2.54	8 (44%)	19,38,41	1.56	4 (21%)
1	OMG	Ad	599	1	18,26,27	2.55	8 (44%)	19,38,41	1.50	4 (21%)
1	PSU	Ad	811	1	18,21,22	4.42	7 (38%)	22,30,33	1.76	5 (22%)
1	OMU	Ad	615	1	19,22,23	3.27	8 (42%)	26,31,34	1.87	6 (23%)
1	A2M	Ad	440	1	18,25,26	4.16	7 (38%)	18,36,39	2.30	4 (22%)
1	PSU	Ad	1122	1	18,21,22	4.45	7 (38%)	22,30,33	1.72	4 (18%)
1	PSU	Ad	300	1	18,21,22	4.42	7 (38%)	22,30,33	1.76	5 (22%)
1	PSU	Ad	362	1	18,21,22	4.37	7 (38%)	22,30,33	1.75	4 (18%)
1	PSU	Ad	951	1	18,21,22	4.43	7 (38%)	22,30,33	1.72	5 (22%)
1	PSU	Ad	1029	1	18,21,22	4.42	7 (38%)	22,30,33	1.76	3 (13%)
1	PSU	Ad	383	35,1	18,21,22	4.39	7 (38%)	22,30,33	1.78	5 (22%)
1	A2M	Ad	1760	1	18,25,26	4.28	7 (38%)	18,36,39	2.34	4 (22%)
1	OMC	Ad	473	1	19,22,23	3.09	8 (42%)	26,31,34	0.74	0
1	MA6	Ad	1792	1	19,26,27	1.03	1 (5%)	18,38,41	5.00	3 (16%)
1	A2M	Ad	797	1	18,25,26	4.28	7 (38%)	18,36,39	2.41	4 (22%)
1	OMC	Ad	418	1	19,22,23	3.13	8 (42%)	26,31,34	1.32	4 (15%)
1	OMU	Ad	123	1	19,22,23	3.29	7 (36%)	26,31,34	1.72	5 (19%)
1	A2M	Ad	468	1	18,25,26	4.23	7 (38%)	18,36,39	2.27	4 (22%)
1	PSU	Ad	306	1	18,21,22	4.34	7 (38%)	22,30,33	1.71	4 (18%)
1	PSU	Ad	606	1	18,21,22	4.37	7 (38%)	22,30,33	1.70	5 (22%)
1	PSU	Ad	636	1	18,21,22	4.42	7 (38%)	22,30,33	1.72	3 (13%)
1	PSU	Ad	121	1	18,21,22	4.38	7 (38%)	22,30,33	1.73	4 (18%)
1	A2M	Ad	162	1	18,25,26	4.23	8 (44%)	18,36,39	2.26	4 (22%)
1	PSU	Ad	208	1	18,21,22	4.41	7 (38%)	22,30,33	1.76	5 (22%)

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
1	PSU	Ad	451	1	-	2/7/25/26	0/2/2/2
1	MA6	Ad	1791	1	-	2/7/29/30	0/3/3/3
1	PSU	Ad	258	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	Ad	1004	1	-	3/7/25/26	0/2/2/2
1	PSU	Ad	585	1	-	0/7/25/26	0/2/2/2
1	PSU	Ad	1108	1	-	2/7/25/26	0/2/2/2
1	A2M	Ad	545	1	-	1/5/27/28	0/3/3/3
1	OMG	Ad	246	1	-	3/5/27/28	0/3/3/3
1	OMC	Ad	38	1	-	3/9/27/28	0/2/2/2
1	PSU	Ad	111	34,1	-	2/7/25/26	0/2/2/2
1	PSU	Ad	255	35,1	-	3/7/25/26	0/2/2/2
1	PSU	Ad	755	1	-	4/7/25/26	0/2/2/2
1	PSU	Ad	764	1	-	0/7/25/26	0/2/2/2
1	PSU	Ad	952	1	-	2/7/25/26	0/2/2/2
1	A2M	Ad	28	35,1	-	2/5/27/28	0/3/3/3
1	A2M	Ad	802	1	-	0/5/27/28	0/3/3/3
1	A2M	Ad	979	1	-	0/5/27/28	0/3/3/3
1	PSU	Ad	914	1	-	2/7/25/26	0/2/2/2
1	PSU	Ad	103	1	-	0/7/25/26	0/2/2/2
1	OMC	Ad	1647	1	-	4/9/27/28	0/2/2/2
1	A2M	Ad	623	35,1	-	3/5/27/28	0/3/3/3
1	OMU	Ad	1014	1	-	0/9/27/28	0/2/2/2
1	OMG	Ad	392	1	-	0/5/27/28	0/3/3/3
1	OMG	Ad	599	1	-	4/5/27/28	0/3/3/3
1	PSU	Ad	811	1	-	2/7/25/26	0/2/2/2
1	OMU	Ad	615	1	-	4/9/27/28	0/2/2/2
1	A2M	Ad	440	1	-	1/5/27/28	0/3/3/3
1	PSU	Ad	1122	1	-	2/7/25/26	0/2/2/2
1	PSU	Ad	300	1	-	2/7/25/26	0/2/2/2
1	PSU	Ad	362	1	-	2/7/25/26	0/2/2/2
1	PSU	Ad	951	1	-	2/7/25/26	0/2/2/2
1	PSU	Ad	1029	1	-	7/7/25/26	0/2/2/2
1	PSU	Ad	383	35,1	-	2/7/25/26	0/2/2/2
1	A2M	Ad	1760	1	-	1/5/27/28	0/3/3/3
1	OMC	Ad	473	1	-	0/9/27/28	0/2/2/2
1	MA6	Ad	1792	1	-	6/7/29/30	0/3/3/3
1	A2M	Ad	797	1	-	2/5/27/28	0/3/3/3
1	OMC	Ad	418	1	-	6/9/27/28	0/2/2/2
1	OMU	Ad	123	1	-	3/9/27/28	0/2/2/2

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	Ad	468	1	-	2/5/27/28	0/3/3/3
1	PSU	Ad	306	1	-	2/7/25/26	0/2/2/2
1	PSU	Ad	606	1	-	1/7/25/26	0/2/2/2
1	PSU	Ad	636	1	-	3/7/25/26	0/2/2/2
1	PSU	Ad	121	1	-	5/7/25/26	0/2/2/2
1	A2M	Ad	162	1	-	1/5/27/28	0/3/3/3
1	PSU	Ad	208	1	-	3/7/25/26	0/2/2/2

The worst 5 of 320 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Ad	797	A2M	O4'-C1'	15.40	1.62	1.41
1	Ad	979	A2M	O4'-C1'	15.38	1.62	1.41
1	Ad	1760	A2M	O4'-C1'	15.37	1.62	1.41
1	Ad	162	A2M	O4'-C1'	15.19	1.62	1.41
1	Ad	468	A2M	O4'-C1'	15.17	1.62	1.41

The worst 5 of 188 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ad	1792	MA6	C1'-N9-C4	14.83	152.70	126.64
1	Ad	1791	MA6	N1-C6-N6	-14.23	102.08	117.06
1	Ad	1792	MA6	N1-C6-N6	-13.93	102.39	117.06
1	Ad	1791	MA6	C1'-N9-C4	12.67	148.90	126.64
1	Ad	979	A2M	C1'-N9-C4	6.50	138.06	126.64

There are no chirality outliers.

5 of 103 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	Ad	28	A2M	C3'-C4'-C5'-O5'
1	Ad	38	OMC	O4'-C1'-N1-C2
1	Ad	38	OMC	O4'-C1'-N1-C6
1	Ad	38	OMC	C1'-C2'-O2'-CM2
1	Ad	111	PSU	O4'-C1'-C5-C4

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 87 ligands modelled in this entry, 87 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.



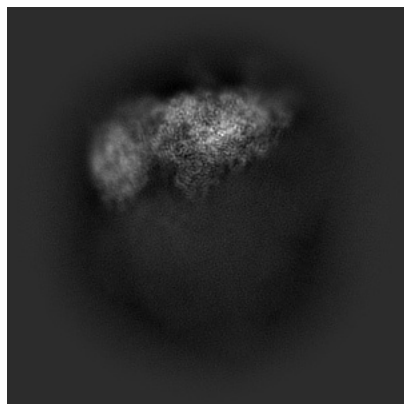
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36332. These allow visual inspection of the internal detail of the map and identification of artifacts.

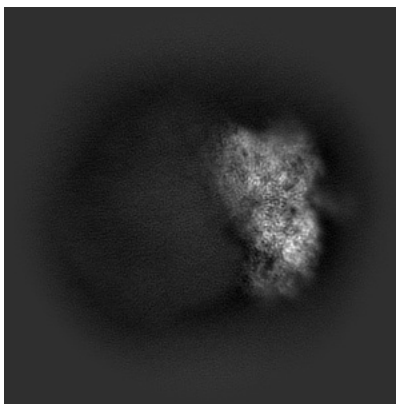
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

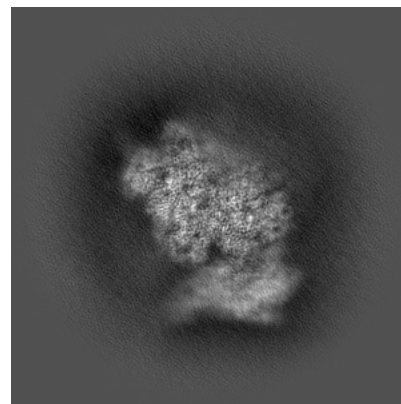
#### 6.1.1 Primary map



X

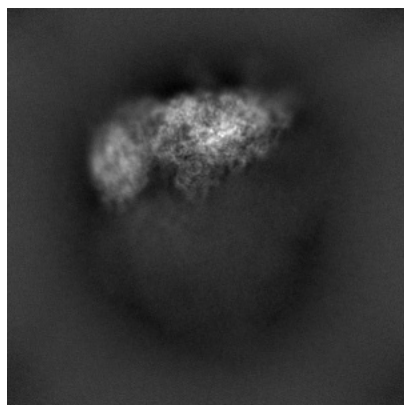


Y

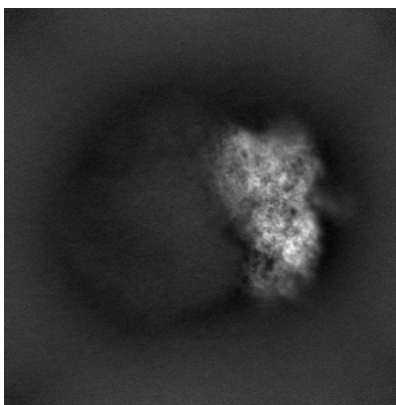


Z

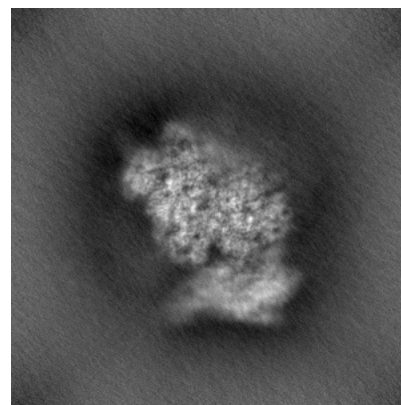
#### 6.1.2 Raw map



X



Y

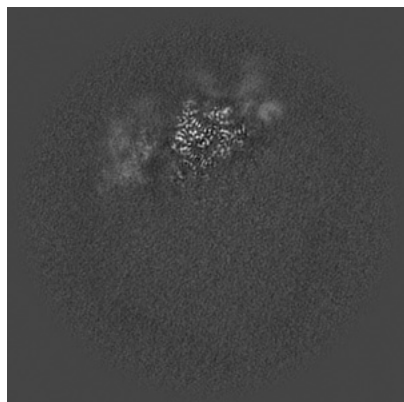


Z

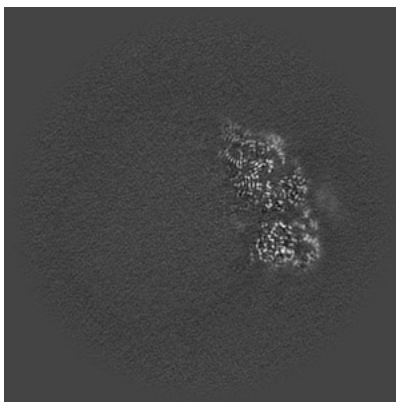
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

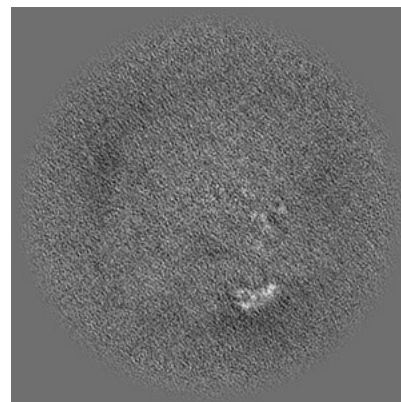
### 6.2.1 Primary map



X Index: 210

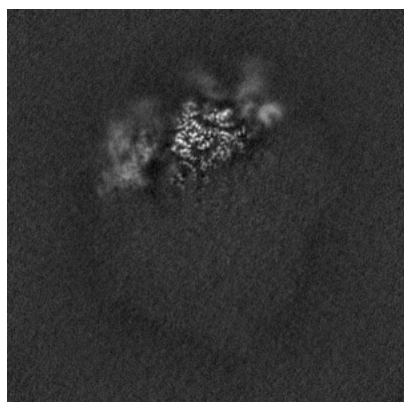


Y Index: 210

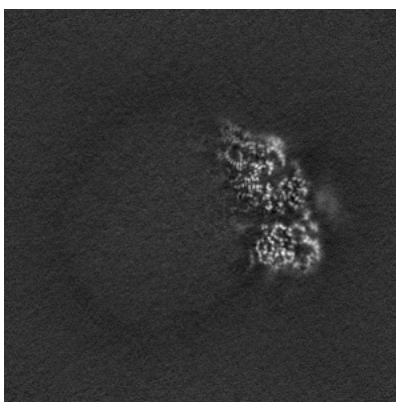


Z Index: 210

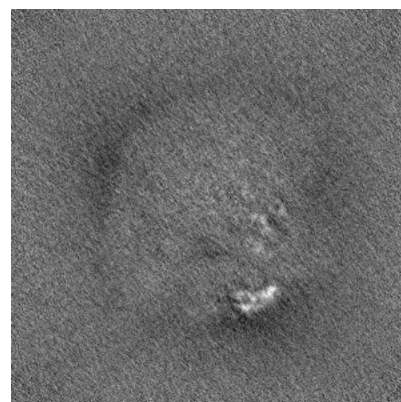
### 6.2.2 Raw map



X Index: 210



Y Index: 210

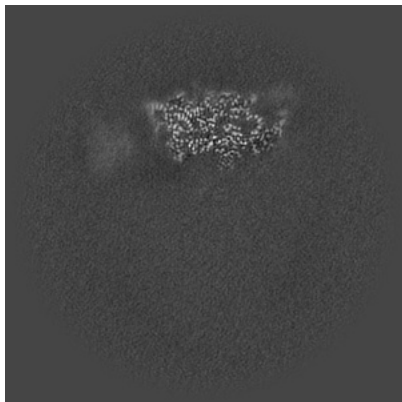


Z Index: 210

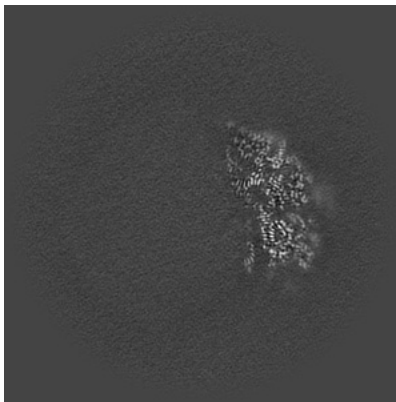
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

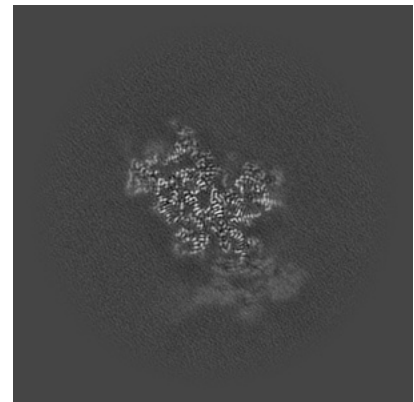
### 6.3.1 Primary map



X Index: 178

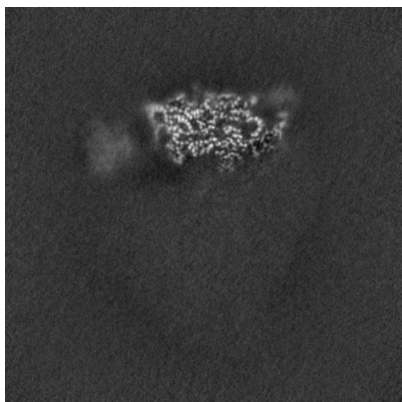


Y Index: 215

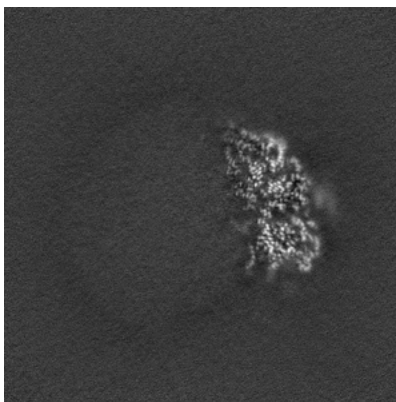


Z Index: 290

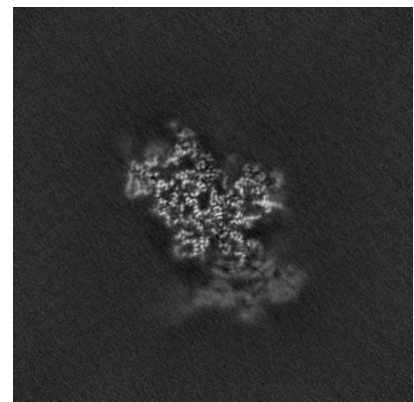
### 6.3.2 Raw map



X Index: 178



Y Index: 213

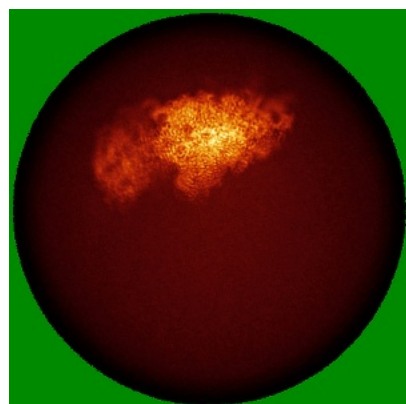


Z Index: 290

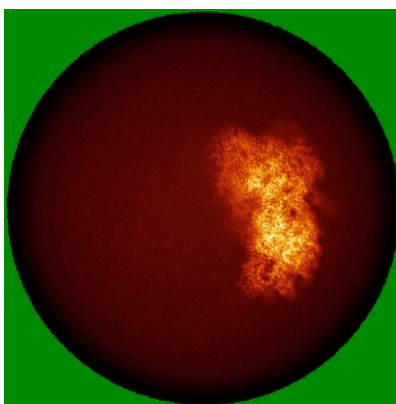
The images above show the largest variance slices of the map in three orthogonal directions.

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

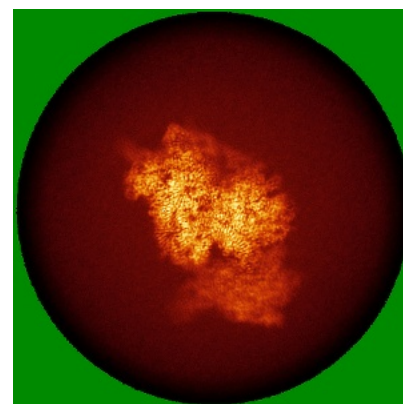
### 6.4.1 Primary map



X

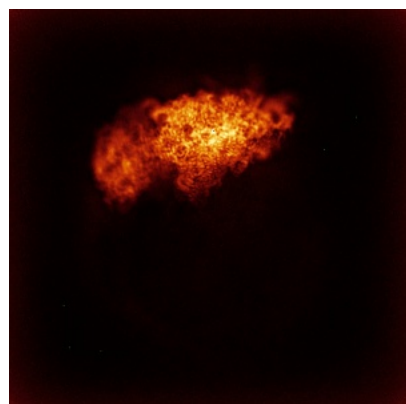


Y

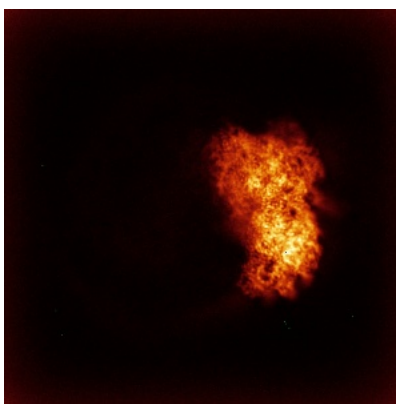


Z

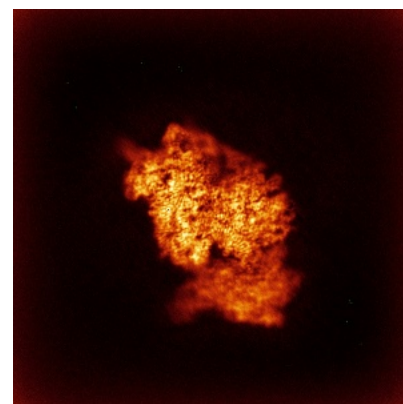
### 6.4.2 Raw map



X



Y



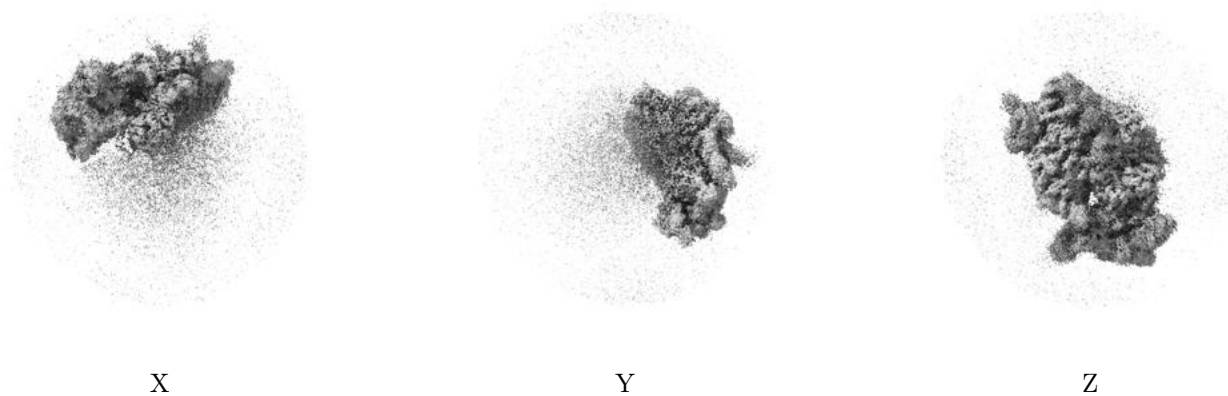
Z

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.



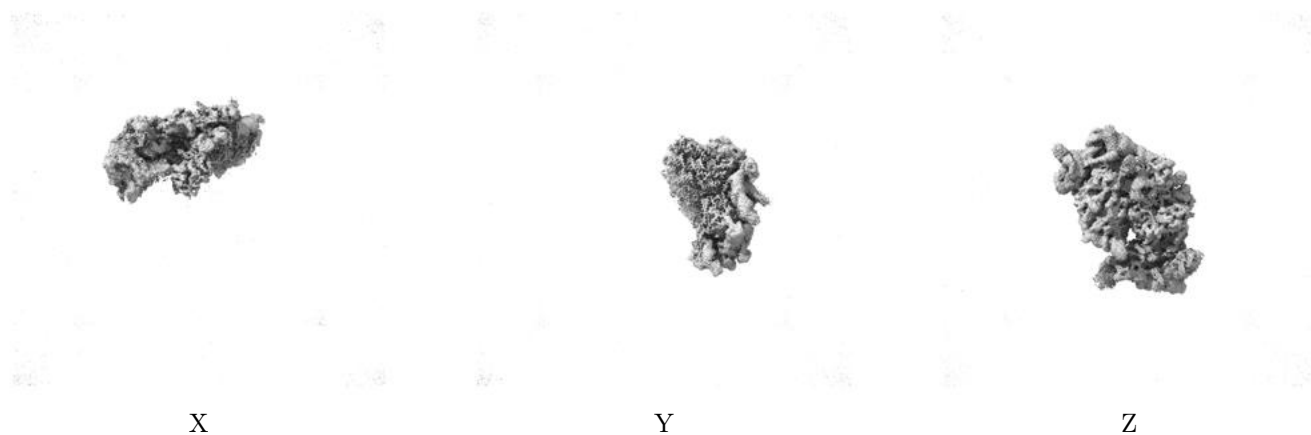
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. 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.

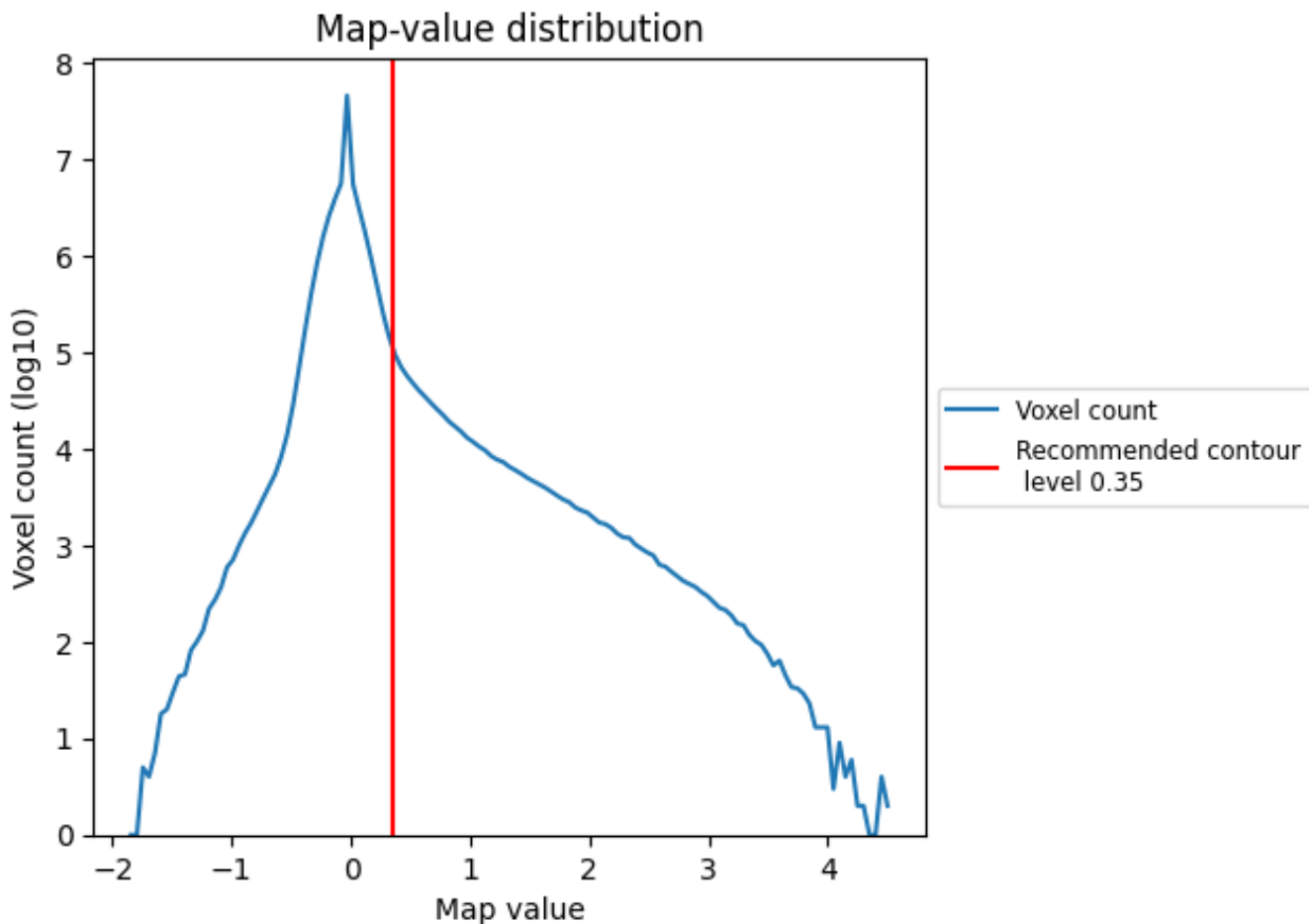
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

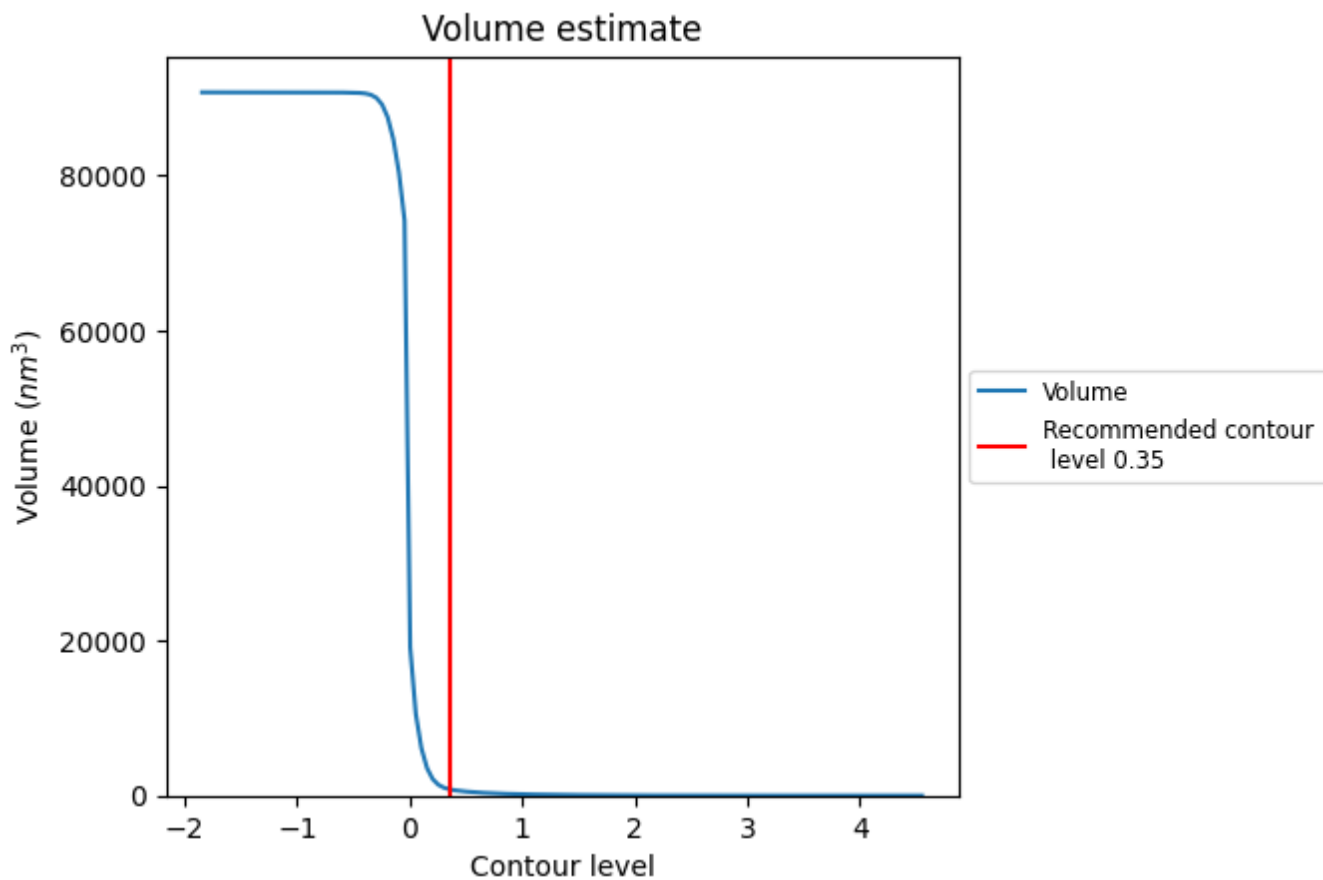
This section contains the results of statistical analysis of the map.

### 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.

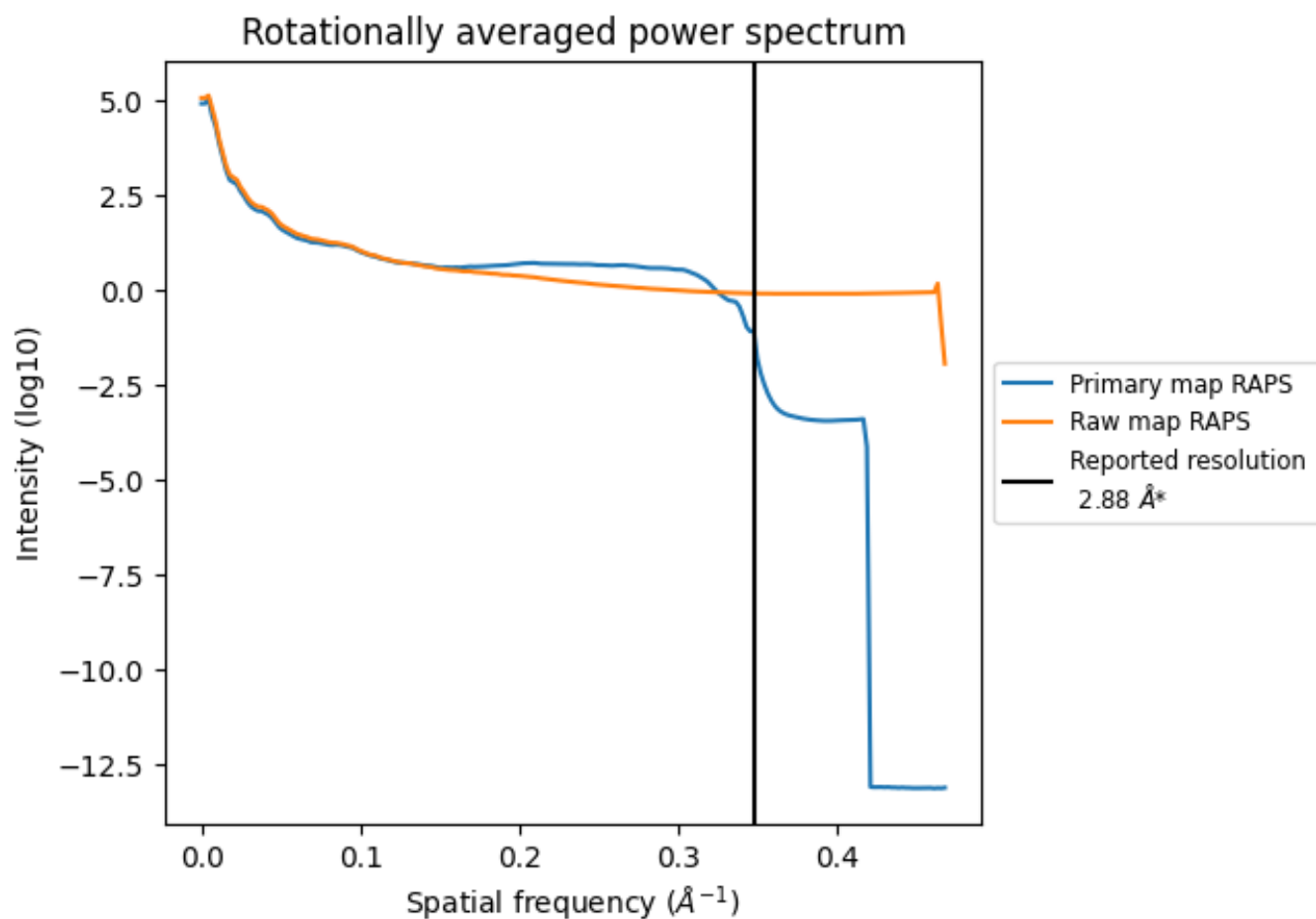
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 824 nm<sup>3</sup>; this corresponds to an approximate mass of 744 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 i



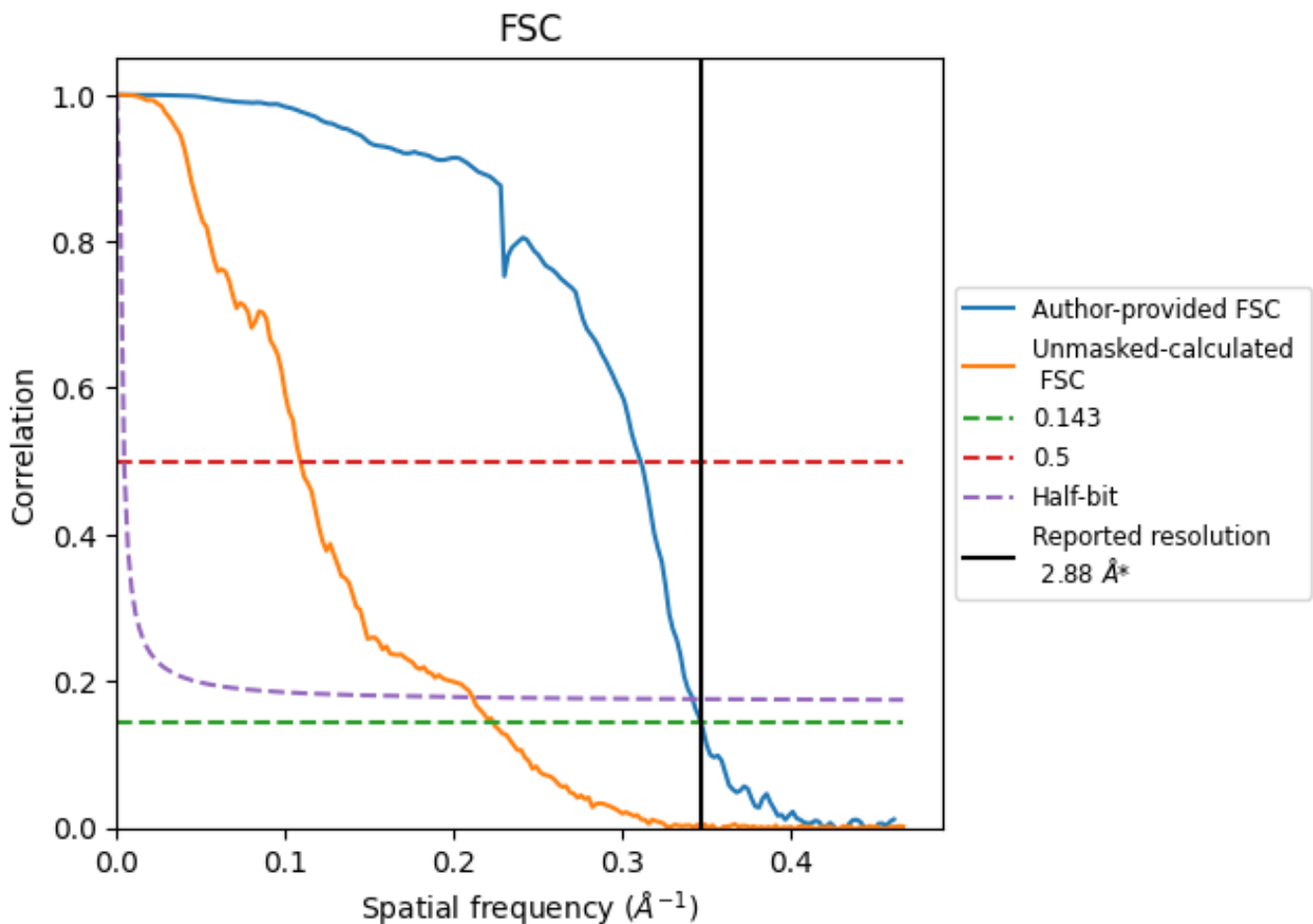
\*Reported resolution corresponds to spatial frequency of 0.347 Å<sup>-1</sup>



## 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 0.347  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

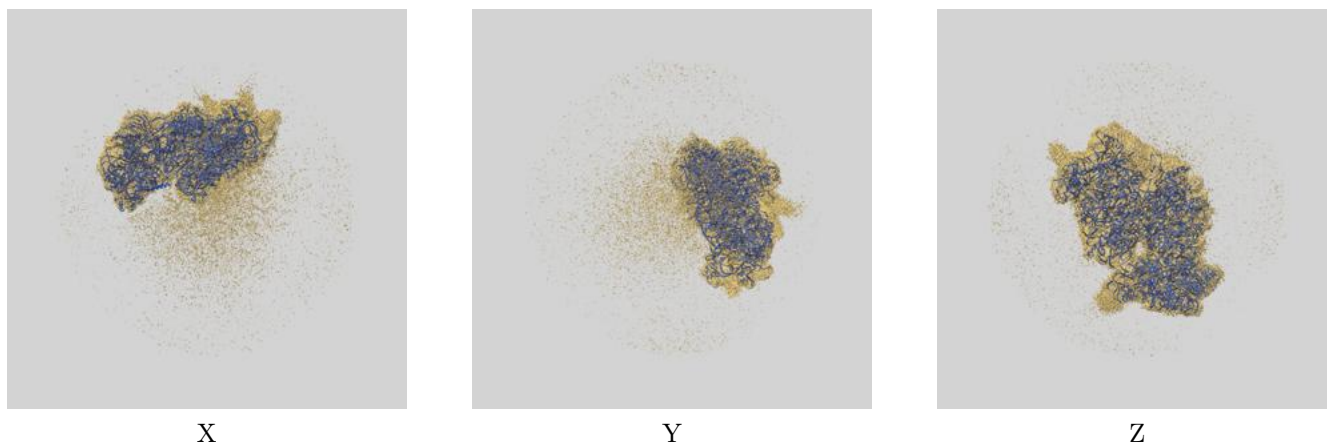
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	2.88	3.21	2.92
Unmasked-calculated*	4.47	9.16	4.73

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.47 differs from the reported value 2.88 by more than 10 %

## 9 Map-model fit [i](#)

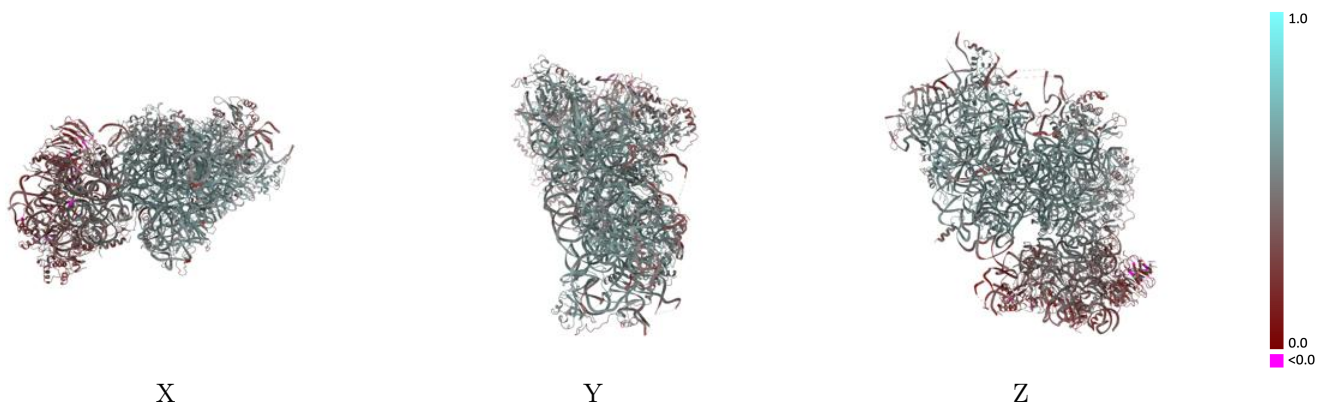
This section contains information regarding the fit between EMDB map EMD-36332 and PDB model 8JIW. Per-residue inclusion information can be found in section 3 on page 11.

### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.35 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](#)



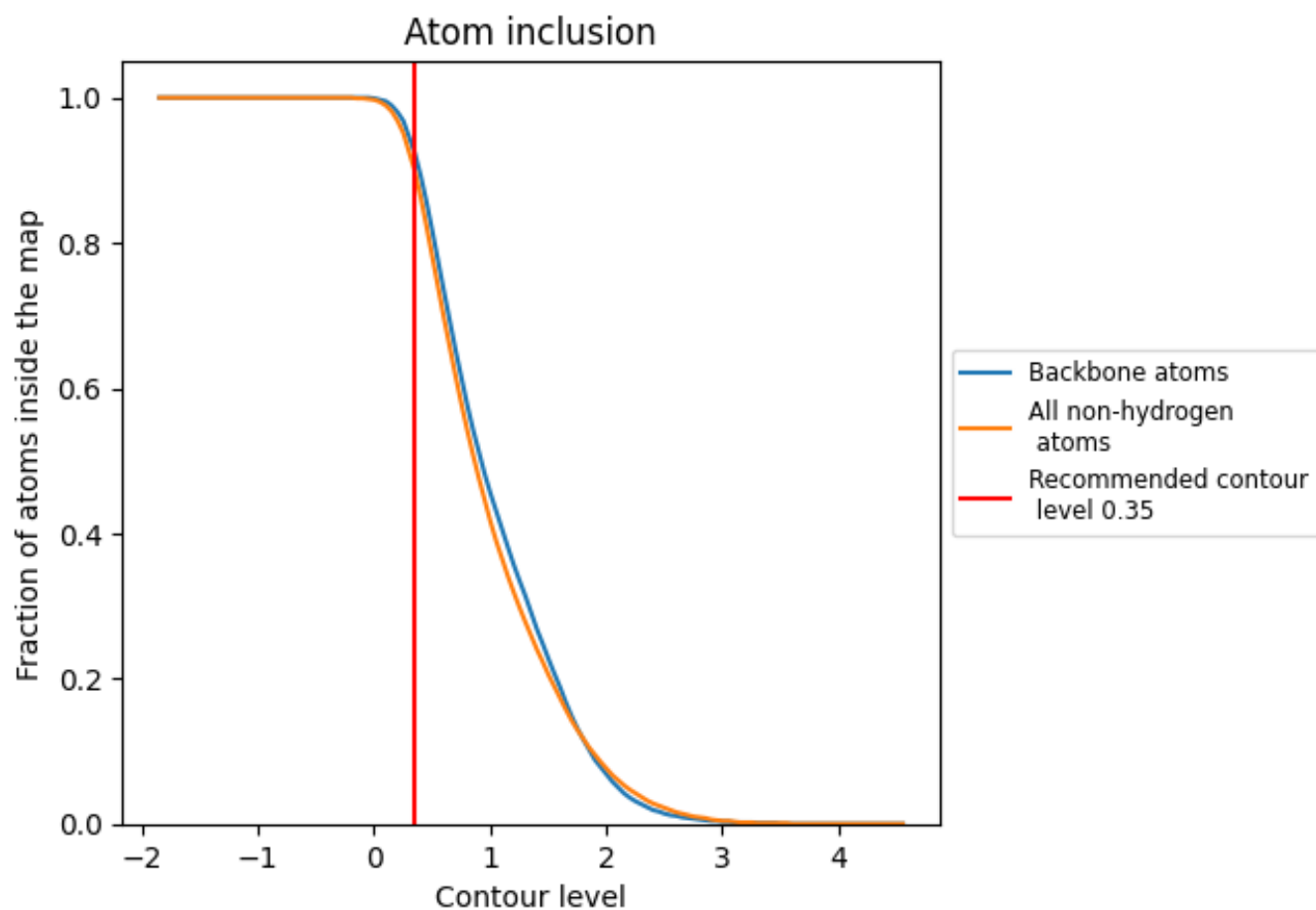
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).





































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 90% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9000	 0.4810
Ad	 0.9460	 0.5000
BA	 0.9430	 0.4900
BB	 0.8350	 0.5090
BC	 0.9530	 0.5430
BD	 0.7110	 0.3660
BE	 0.9640	 0.5440
BF	 0.6800	 0.3890
BG	 0.9350	 0.4900
BH	 0.8950	 0.4310
BI	 0.8830	 0.5570
BJ	 0.9730	 0.5350
BK	 0.7860	 0.2760
BL	 0.8910	 0.5620
BN	 0.8530	 0.5470
BO	 0.9150	 0.5340
BP	 0.5790	 0.2930
BQ	 0.8710	 0.3750
BR	 0.8000	 0.3710
BS	 0.5590	 0.3180
BT	 0.9070	 0.3450
BU	 0.8100	 0.3630
BV	 0.9600	 0.5290
BW	 0.9740	 0.5760
BX	 0.9420	 0.5790
BY	 0.9640	 0.5400
BZ	 0.6780	 0.3030
Ba	 0.9650	 0.5610
Bb	 0.9210	 0.4830
Bc	 0.7630	 0.4290
Bd	 0.8480	 0.4010
Be	 0.9810	 0.5560
Bg	 0.6490	 0.2840
Cn	 0.5870	 0.5650

