



## Full wwPDB EM Validation Report ⓘ

Apr 2, 2022 – 03:23 am BST

PDB ID : 7Q4P  
EMDB ID : EMD-13812  
Title : U2 snRNP after ATP-dependent remodelling  
Authors : Tholen, J.; Galej, W.P.  
Deposited on : 2021-11-01  
Resolution : 2.20 Å(reported)  
Based on initial models : 7ABH, 7Q3L

This is a Full wwPDB EM Validation 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.

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

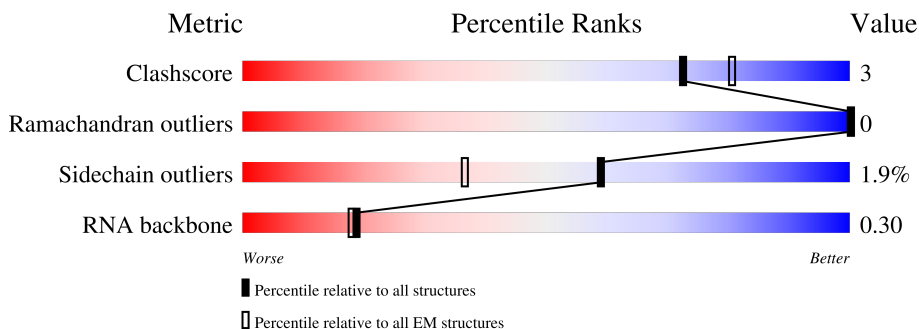
EMDB validation analysis : 0.0.0.dev97  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

# 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 2.20 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	1	464	8% 92%
2	2	188	10% 9% 5% 76%
3	9	501	18% 80%
4	A	1304	17% 81%
5	B	895	12% 87%
6	C	1217	65% 7% 28%
7	E	86	70% 5% 26%

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Mol	Chain	Length	Quality of chain
8	G	110	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a small red segment at the beginning, a large green segment labeled '67%', a small yellow segment labeled '8%', and a grey segment at the end labeled '25%'.</p>

## 2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 13451 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 Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	38	308	193	56	56	3	0	0

- Molecule 2 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	45	952	430	155	322	45	0	0

- Molecule 3 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	9	101	838	534	149	151	4	0	0

- Molecule 4 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	254	2043	1316	350	364	13	0	0

- Molecule 5 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	117	985	639	175	169	2	0	0

- Molecule 6 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	878	6926	4409	1181	1305	31	1	0

- Molecule 7 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	E	64	Total	C	N	O	S	0	0
			524	333	90	96	5		

- Molecule 8 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	G	83	Total	C	N	O	S	0	0
			629	386	112	118	13		

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
9	1	1	Total	Zn	0
			1	1	
9	9	1	Total	Zn	0
			1	1	
9	G	3	Total	Zn	0
			3	3	

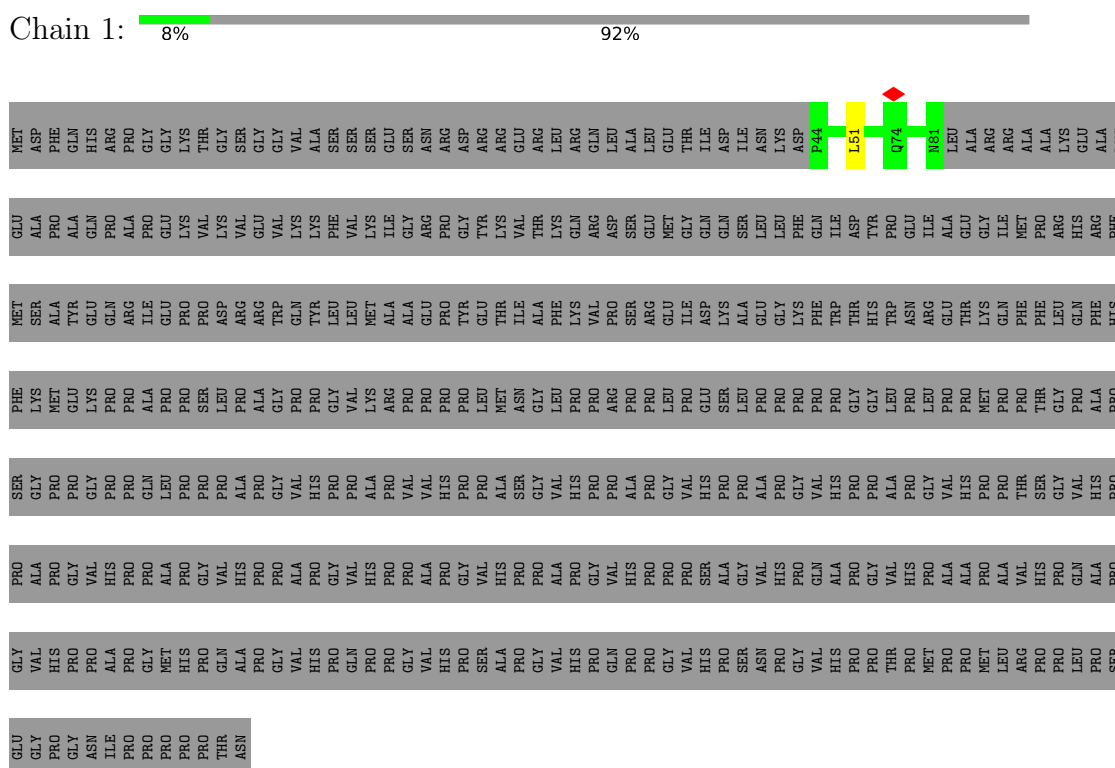
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
10	2	4	Total	O	0
			4	4	
10	A	46	Total	O	0
			46	46	
10	B	19	Total	O	0
			19	19	
10	C	148	Total	O	0
			148	148	
10	E	18	Total	O	0
			18	18	
10	G	6	Total	O	0
			6	6	

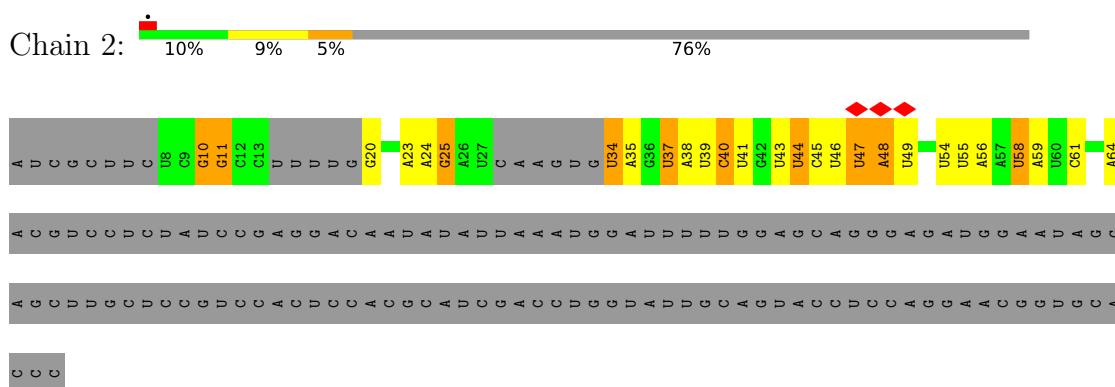
### 3 Residue-property plots

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: Splicing factor 3A subunit 2



- Molecule 2: U2 snRNA

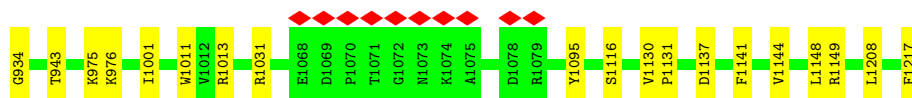




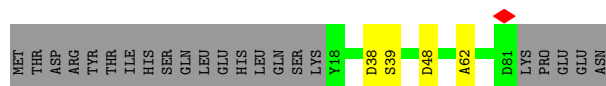








- Molecule 7: Splicing factor 3B subunit 5



- Molecule 8: PHD finger-like domain-containing protein 5A



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	158286	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	53.45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.044	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00711	Depositor
Map size (Å)	409.59998, 409.59998, 409.59998	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.64, 0.64, 0.64	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: ZN, OMU, PSU, OMC, OMG

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	1	0.28	0/316	0.60	0/423
2	2	0.68	0/733	1.16	10/1136 (0.9%)
3	9	0.34	0/864	0.75	0/1172
4	A	0.45	0/2090	0.90	2/2839 (0.1%)
5	B	0.37	0/1013	0.86	4/1366 (0.3%)
6	C	0.50	0/7076	0.96	16/9594 (0.2%)
7	E	0.41	0/540	0.85	0/731
8	G	0.41	0/637	0.83	0/855
All	All	0.47	0/13269	0.93	32/18116 (0.2%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1031	ARG	NE-CZ-NH1	-8.00	116.30	120.30
6	C	429	ARG	NE-CZ-NH1	-7.49	116.56	120.30
6	C	34	ARG	N-CA-C	-7.37	91.11	111.00
6	C	857	ALA	C-N-CA	-6.78	108.06	122.30
2	2	44	PSU	P-O3'-C3'	-6.66	111.71	119.70
5	B	471	ARG	NE-CZ-NH2	-6.43	117.08	120.30
5	B	512	GLN	CB-CA-C	6.38	123.17	110.40
2	2	54	PSU	P-O3'-C3'	-6.35	112.08	119.70
6	C	1095	TYR	CB-CG-CD2	-6.32	117.21	121.00
6	C	926	TYR	CB-CA-C	-6.13	98.13	110.40
6	C	867	ARG	NE-CZ-NH1	-6.05	117.27	120.30
2	2	56	A	P-O3'-C3'	-6.02	112.48	119.70
6	C	86	ARG	NE-CZ-NH2	-6.00	117.30	120.30
6	C	114	ARG	NE-CZ-NH2	-5.97	117.31	120.30
6	C	268	ARG	CB-CG-CD	-5.90	96.25	111.60
2	2	61	OMC	P-O3'-C3'	-5.81	112.73	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	429	ARG	NE-CZ-NH2	5.72	123.16	120.30
6	C	1149	ARG	NE-CZ-NH1	-5.71	117.45	120.30
2	2	20	G	P-O3'-C3'	-5.66	112.91	119.70
4	A	1109	ARG	CG-CD-NE	5.46	123.25	111.80
6	C	1095	TYR	CB-CG-CD1	5.34	124.20	121.00
2	2	35	A	P-O3'-C3'	-5.31	113.33	119.70
4	A	1286	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	2	55	U	P-O3'-C3'	-5.16	113.51	119.70
2	2	58	PSU	P-O3'-C3'	-5.14	113.53	119.70
5	B	471	ARG	CD-NE-CZ	5.11	130.76	123.60
5	B	471	ARG	CG-CD-NE	5.10	122.50	111.80
6	C	285	MET	N-CA-CB	-5.08	101.46	110.60
6	C	1013	ARG	NE-CZ-NH1	-5.05	117.78	120.30
2	2	34	PSU	P-O3'-C3'	-5.03	113.66	119.70
6	C	322	VAL	C-N-CA	5.02	134.25	121.70
2	2	47	OMU	P-O3'-C3'	-5.00	113.70	119.70

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	1	308	0	292	1	0
2	2	952	0	492	2	0
3	9	838	0	791	7	0
4	A	2043	0	2053	20	0
5	B	985	0	985	7	0
6	C	6926	0	6849	54	0
7	E	524	0	487	3	0
8	G	629	0	613	4	0
9	1	1	0	0	0	0
9	9	1	0	0	0	0
9	G	3	0	0	0	0
10	2	4	0	0	0	0
10	A	46	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	19	0	0	0	0
10	C	148	0	0	0	0
10	E	18	0	0	0	0
10	G	6	0	0	0	0
All	All	13451	0	12562	88	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 3.

All (88) 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)
6:C:19:HIS:CE1	6:C:342:LEU:HG	2.11	0.86
6:C:239:PRO:HG2	6:C:299:PHE:CG	2.21	0.76
3:9:486:VAL:HG21	6:C:976:LYS:HE2	1.69	0.75
6:C:789:VAL:HG21	6:C:893:VAL:HG23	1.72	0.71
6:C:19:HIS:HE1	6:C:342:LEU:HG	1.55	0.71
5:B:531:THR:HG21	5:B:571:LEU:HD12	1.73	0.70
6:C:19:HIS:NE2	6:C:340:CYS:HB3	2.08	0.68
6:C:19:HIS:CD2	6:C:340:CYS:HB3	2.30	0.67
6:C:274:ARG:HD2	6:C:389:PRO:HG3	1.78	0.65
4:A:1156:GLU:O	8:G:38:ARG:NH1	2.29	0.65
3:9:454:ASP:CG	5:B:463:ALA:HB1	2.20	0.61
6:C:239:PRO:HG2	6:C:299:PHE:CD2	2.35	0.60
6:C:789:VAL:CG2	6:C:893:VAL:HG23	2.32	0.59
3:9:484:GLY:HA3	6:C:975:LYS:HG3	1.85	0.58
6:C:288:VAL:HG12	7:E:62:ALA:HB3	1.84	0.58
6:C:930:LEU:HG	6:C:934:GLY:HA2	1.86	0.58
6:C:304:GLN:HE21	6:C:333:VAL:HG23	1.70	0.57
8:G:60:ILE:HA	8:G:88:ILE:HD12	1.87	0.56
6:C:308:GLY:HA3	6:C:333:VAL:O	2.06	0.56
1:1:51:LEU:HD22	4:A:1141:LEU:HD12	1.86	0.56
6:C:310:ILE:HD11	6:C:333:VAL:HG21	1.86	0.56
6:C:289:CYS:SG	6:C:336:ALA:HB3	2.47	0.55
6:C:1141:PHE:HE1	6:C:1208:LEU:HD23	1.73	0.55
6:C:1001:ILE:HD12	6:C:1011:TRP:CD1	2.43	0.54
5:B:471:ARG:HG3	5:B:471:ARG:HH11	1.73	0.54
6:C:291:ALA:HB2	6:C:339:MET:O	2.08	0.53
4:A:1192:VAL:O	4:A:1196:SER:HB2	2.09	0.53
6:C:19:HIS:NE2	6:C:340:CYS:CB	2.71	0.53
6:C:304:GLN:NE2	6:C:334:PRO:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1210:HIS:ND1	5:B:585:THR:HG22	2.23	0.52
6:C:249:LEU:HB3	6:C:256:ILE:HD11	1.92	0.52
4:A:1166:ILE:HD11	4:A:1199:VAL:HG11	1.90	0.52
4:A:1094:LEU:HD11	4:A:1116:ILE:HG23	1.92	0.52
4:A:1108:ASN:O	4:A:1112:THR:HG23	2.11	0.50
6:C:289:CYS:SG	6:C:339:MET:HG3	2.50	0.50
6:C:245:PRO:HD3	6:C:317:THR:HG21	1.92	0.50
6:C:238:VAL:CG1	6:C:315:LEU:HD12	2.42	0.50
6:C:293:HIS:NE2	6:C:343:LYS:HA	2.26	0.50
8:G:23:CYS:SG	8:G:25:LYS:HG2	2.52	0.50
6:C:270:PRO:HG2	6:C:379:LEU:HD22	1.93	0.49
6:C:238:VAL:HG11	6:C:315:LEU:HD12	1.94	0.49
4:A:1213:ASN:HD22	5:B:585:THR:HG23	1.76	0.49
3:9:401:GLY:O	3:9:418:GLY:HA2	2.13	0.49
5:B:525:PRO:HG2	5:B:528:ILE:HD12	1.95	0.49
6:C:245:PRO:HG3	6:C:322:VAL:HG22	1.94	0.49
3:9:420:LYS:HG3	3:9:424:ARG:HE	1.77	0.48
6:C:943:THR:HG23	6:C:976:LYS:HD2	1.94	0.48
4:A:1066:LEU:HD22	4:A:1111:CYS:HB3	1.95	0.48
6:C:19:HIS:CE1	6:C:340:CYS:HB3	2.48	0.48
3:9:422:PHE:HA	3:9:425:HIS:HD2	1.78	0.48
4:A:1098:LEU:HD22	4:A:1135:GLU:HG3	1.95	0.48
8:G:38:ARG:HE	8:G:73:LYS:HD2	1.79	0.48
6:C:274:ARG:HG2	6:C:387:PHE:CZ	2.50	0.47
6:C:302:LEU:HD12	6:C:341:VAL:HG22	1.97	0.47
6:C:223:LYS:HD3	6:C:224:TYR:CE1	2.50	0.47
5:B:531:THR:HG21	5:B:571:LEU:CD1	2.41	0.47
6:C:12:THR:O	6:C:34:ARG:NH1	2.47	0.47
6:C:304:GLN:HE21	6:C:333:VAL:CG2	2.29	0.45
6:C:306:GLU:O	6:C:335:VAL:HG21	2.16	0.45
4:A:1253:GLY:HA3	4:A:1265:TYR:CD2	2.52	0.45
4:A:1170:THR:N	4:A:1171:PRO:HD2	2.32	0.45
6:C:304:GLN:NE2	6:C:333:VAL:HG23	2.31	0.44
3:9:422:PHE:O	3:9:425:HIS:CD2	2.71	0.44
6:C:310:ILE:HG12	6:C:339:MET:SD	2.57	0.43
4:A:1281:ILE:HD11	7:E:38:ASP:HB3	2.00	0.43
4:A:1160:GLU:O	4:A:1163:LYS:HG2	2.17	0.43
4:A:1109:ARG:O	4:A:1113:THR:HG23	2.17	0.43
6:C:68:PHE:HB3	6:C:123:VAL:HG11	2.00	0.43
4:A:1177:LEU:HB3	4:A:1214:TYR:HB3	2.01	0.43
4:A:1109:ARG:HD2	4:A:1142:ASN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1281:ILE:HD12	7:E:39:SER:HA	2.02	0.42
6:C:126:LYS:HD2	6:C:177:PHE:CZ	2.54	0.42
2:2:48:A:H62	2:2:64:A:H61	1.67	0.42
6:C:68:PHE:CB	6:C:123:VAL:HG11	2.49	0.42
6:C:1116:SER:HB3	6:C:1130:VAL:HG12	2.00	0.42
4:A:1129:LEU:O	4:A:1133:MET:HG2	2.19	0.42
2:2:58:PSU:H2'	2:2:59:A:O4'	2.20	0.41
6:C:274:ARG:HD2	6:C:389:PRO:CG	2.47	0.41
6:C:298:MET:HE2	6:C:298:MET:HB2	1.80	0.41
6:C:407:ILE:HG23	6:C:425:VAL:HG13	2.03	0.41
4:A:1188:ALA:O	4:A:1192:VAL:HG23	2.21	0.41
6:C:181:MET:HE3	6:C:181:MET:HB3	1.82	0.41
6:C:308:GLY:CA	6:C:333:VAL:O	2.68	0.41
6:C:272:PRO:HD3	6:C:327:LEU:CD2	2.51	0.40
6:C:1144:VAL:HG12	6:C:1148:LEU:HD12	2.04	0.40
6:C:1130:VAL:HA	6:C:1131:PRO:HD3	1.91	0.40
6:C:239:PRO:HB2	6:C:299:PHE:CE1	2.56	0.40
6:C:893:VAL:HG22	6:C:905:VAL:HG22	2.03	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	1	36/464 (8%)	35 (97%)	1 (3%)	0	100	100
3	9	99/501 (20%)	97 (98%)	2 (2%)	0	100	100
4	A	252/1304 (19%)	252 (100%)	0	0	100	100
5	B	111/895 (12%)	110 (99%)	1 (1%)	0	100	100
6	C	871/1217 (72%)	842 (97%)	29 (3%)	0	100	100
7	E	62/86 (72%)	62 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	G	81/110 (74%)	75 (93%)	6 (7%)	0	100	100
All	All	1512/4577 (33%)	1473 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
1	1	34/382 (9%)	34 (100%)	0	100	100
3	9	87/446 (20%)	87 (100%)	0	100	100
4	A	220/1104 (20%)	217 (99%)	3 (1%)	67	80
5	B	106/776 (14%)	105 (99%)	1 (1%)	78	88
6	C	758/1051 (72%)	741 (98%)	17 (2%)	52	65
7	E	55/77 (71%)	54 (98%)	1 (2%)	59	72
8	G	71/95 (75%)	68 (96%)	3 (4%)	30	38
All	All	1331/3931 (34%)	1306 (98%)	25 (2%)	59	71

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	1195	MET
4	A	1209	ASN
4	A	1277	GLN
5	B	597	PHE
6	C	19	HIS
6	C	33	SER
6	C	65	LEU
6	C	82	SER
6	C	181	MET
6	C	221	VAL
6	C	295	THR
6	C	296	LYS

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Mol	Chain	Res	Type
6	C	297	SER
6	C	298	MET
6	C	342	LEU
6	C	390	ARG
6	C	429	ARG
6	C	435	LEU
6	C	929	LYS
6	C	1137	ASP
6	C	1217	PHE
7	E	48	ASP
8	G	12	ARG
8	G	34	ASP
8	G	83	ASP

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

Mol	Chain	Res	Type
7	E	36	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	43/188 (22%)	13 (30%)	3 (6%)

All (13) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	10	OMG
2	2	11	OMG
2	2	24	A
2	2	25	OMG
2	2	37	PSU
2	2	38	A
2	2	40	OMC
2	2	44	PSU
2	2	45	C
2	2	46	U
2	2	47	OMU
2	2	48	A
2	2	49	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	23	A
2	2	34	PSU
2	2	37	PSU

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

14 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
2	PSU	2	37	2	17,21,22	1.45	2 (11%)	20,30,33	3.29	8 (40%)
2	OMC	2	40	2	15,22,23	0.74	1 (6%)	17,31,34	1.46	2 (11%)
2	PSU	2	43	2	17,21,22	1.44	2 (11%)	20,30,33	3.27	7 (35%)
2	PSU	2	58	2	17,21,22	1.42	2 (11%)	20,30,33	3.30	8 (40%)
2	PSU	2	41	2	17,21,22	1.51	2 (11%)	20,30,33	3.24	7 (35%)
2	OMG	2	10	2	18,26,27	1.40	3 (16%)	20,38,41	2.17	6 (30%)
2	OMG	2	11	2	18,26,27	1.46	3 (16%)	20,38,41	2.22	6 (30%)
2	PSU	2	34	2	17,21,22	1.44	2 (11%)	20,30,33	3.30	8 (40%)
2	PSU	2	39	2	17,21,22	1.48	2 (11%)	20,30,33	3.32	8 (40%)
2	PSU	2	44	2	17,21,22	1.41	2 (11%)	20,30,33	3.24	7 (35%)
2	OMC	2	61	2	15,22,23	0.75	1 (6%)	17,31,34	1.45	2 (11%)
2	OMU	2	47	2	14,22,23	1.12	1 (7%)	14,31,34	1.24	1 (7%)
2	OMG	2	25	2	18,26,27	1.45	3 (16%)	20,38,41	2.26	6 (30%)
2	PSU	2	54	2	17,21,22	1.41	2 (11%)	20,30,33	3.21	7 (35%)

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
2	PSU	2	37	2	-	2/7/25/26	0/2/2/2
2	OMC	2	40	2	-	2/7/27/28	0/2/2/2
2	PSU	2	43	2	-	0/7/25/26	0/2/2/2
2	PSU	2	58	2	-	2/7/25/26	0/2/2/2
2	PSU	2	41	2	-	2/7/25/26	0/2/2/2
2	OMG	2	10	2	-	2/5/27/28	0/3/3/3
2	OMG	2	11	2	-	2/5/27/28	0/3/3/3
2	PSU	2	34	2	-	1/7/25/26	0/2/2/2
2	PSU	2	39	2	-	2/7/25/26	0/2/2/2
2	PSU	2	44	2	-	1/7/25/26	0/2/2/2
2	OMC	2	61	2	-	2/7/27/28	0/2/2/2
2	OMU	2	47	2	-	4/7/27/28	0/2/2/2
2	OMG	2	25	2	-	1/5/27/28	0/3/3/3
2	PSU	2	54	2	-	2/7/25/26	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	11	OMG	C5-C6	4.63	1.49	1.41
2	2	25	OMG	C5-C6	4.59	1.49	1.41
2	2	10	OMG	C5-C6	4.39	1.48	1.41
2	2	34	PSU	C5-C4	4.17	1.50	1.41
2	2	41	PSU	C5-C4	4.17	1.50	1.41
2	2	39	PSU	C5-C4	4.15	1.50	1.41
2	2	58	PSU	C5-C4	4.14	1.50	1.41
2	2	54	PSU	C5-C4	4.11	1.50	1.41
2	2	44	PSU	C5-C4	4.03	1.50	1.41
2	2	43	PSU	C5-C4	4.03	1.50	1.41
2	2	37	PSU	C5-C4	4.01	1.50	1.41
2	2	41	PSU	C5-C1'	-3.51	1.49	1.52
2	2	37	PSU	C5-C1'	-3.26	1.49	1.52
2	2	47	OMU	C4-N3	3.24	1.38	1.33
2	2	39	PSU	C5-C1'	-3.24	1.49	1.52
2	2	43	PSU	C5-C1'	-3.06	1.49	1.52
2	2	34	PSU	C5-C1'	-2.84	1.49	1.52
2	2	44	PSU	C5-C1'	-2.81	1.49	1.52
2	2	25	OMG	C5-C4	2.74	1.48	1.40
2	2	11	OMG	C5-C4	2.74	1.48	1.40
2	2	54	PSU	C5-C1'	-2.72	1.49	1.52
2	2	10	OMG	C5-C4	2.68	1.48	1.40
2	2	58	PSU	C5-C1'	-2.60	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	61	OMC	O4'-C1'	2.23	1.44	1.41
2	2	40	OMC	O4'-C1'	2.21	1.44	1.41
2	2	25	OMG	O4'-C1'	2.09	1.44	1.41
2	2	11	OMG	O4'-C1'	2.09	1.44	1.41
2	2	10	OMG	O4'-C1'	2.07	1.44	1.41

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	58	PSU	N3-C2-N1	-8.72	121.50	128.43
2	2	39	PSU	N3-C2-N1	-8.66	121.55	128.43
2	2	44	PSU	N3-C2-N1	-8.65	121.55	128.43
2	2	34	PSU	N3-C2-N1	-8.65	121.56	128.43
2	2	54	PSU	N3-C2-N1	-8.64	121.56	128.43
2	2	41	PSU	N3-C2-N1	-8.59	121.60	128.43
2	2	43	PSU	N3-C2-N1	-8.57	121.61	128.43
2	2	37	PSU	N3-C2-N1	-8.53	121.65	128.43
2	2	39	PSU	C2-N3-C4	7.22	121.24	115.14
2	2	44	PSU	C2-N3-C4	7.20	121.22	115.14
2	2	54	PSU	C2-N3-C4	7.13	121.16	115.14
2	2	34	PSU	C2-N3-C4	7.06	121.11	115.14
2	2	41	PSU	C2-N3-C4	7.06	121.10	115.14
2	2	58	PSU	C2-N3-C4	6.98	121.03	115.14
2	2	43	PSU	C2-N3-C4	6.93	120.99	115.14
2	2	37	PSU	C2-N3-C4	6.78	120.87	115.14
2	2	25	OMG	C2-N3-C4	5.61	121.76	115.36
2	2	11	OMG	C2-N3-C4	5.41	121.54	115.36
2	2	41	PSU	C5-C4-N3	-5.39	118.42	125.36
2	2	39	PSU	C5-C4-N3	-5.35	118.47	125.36
2	2	10	OMG	C2-N3-C4	5.29	121.39	115.36
2	2	44	PSU	C5-C4-N3	-5.25	118.59	125.36
2	2	54	PSU	C5-C4-N3	-5.23	118.63	125.36
2	2	43	PSU	C5-C4-N3	-5.19	118.67	125.36
2	2	34	PSU	C5-C4-N3	-5.16	118.71	125.36
2	2	37	PSU	C5-C4-N3	-5.15	118.72	125.36
2	2	58	PSU	C5-C4-N3	-4.94	118.99	125.36
2	2	61	OMC	C4-N3-C2	4.70	121.11	116.34
2	2	40	OMC	C4-N3-C2	4.66	121.06	116.34
2	2	37	PSU	C6-N1-C2	4.16	122.22	115.36
2	2	58	PSU	C6-N1-C2	4.13	122.18	115.36
2	2	41	PSU	C6-N1-C2	4.09	122.11	115.36
2	2	34	PSU	C6-N1-C2	4.09	122.11	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	43	PSU	C6-N1-C2	4.09	122.11	115.36
2	2	39	PSU	C6-N1-C2	4.05	122.04	115.36
2	2	44	PSU	C6-N1-C2	4.02	121.98	115.36
2	2	54	PSU	C6-N1-C2	4.02	121.98	115.36
2	2	11	OMG	C2-N1-C6	4.01	122.30	115.93
2	2	10	OMG	C2-N1-C6	3.94	122.20	115.93
2	2	25	OMG	C2-N1-C6	3.92	122.16	115.93
2	2	37	PSU	C5-C6-N1	-3.90	119.65	124.44
2	2	47	OMU	C5-C4-N3	-3.89	114.75	123.31
2	2	58	PSU	C5-C1'-C2'	-3.85	108.45	115.32
2	2	11	OMG	C5-C6-N1	-3.81	118.21	123.43
2	2	25	OMG	C5-C6-N1	-3.77	118.28	123.43
2	2	37	PSU	C3'-C2'-C1'	3.76	106.26	101.93
2	2	10	OMG	C5-C6-N1	-3.74	118.31	123.43
2	2	41	PSU	C5-C6-N1	-3.74	119.84	124.44
2	2	34	PSU	C3'-C2'-C1'	3.74	106.24	101.93
2	2	43	PSU	C5-C6-N1	-3.69	119.91	124.44
2	2	11	OMG	C4-C5-C6	-3.66	117.31	120.80
2	2	10	OMG	C4-C5-C6	-3.61	117.35	120.80
2	2	39	PSU	C5-C6-N1	-3.59	120.03	124.44
2	2	43	PSU	C3'-C2'-C1'	3.56	106.04	101.93
2	2	44	PSU	C5-C6-N1	-3.56	120.07	124.44
2	2	34	PSU	C5-C6-N1	-3.55	120.08	124.44
2	2	58	PSU	C5-C6-N1	-3.52	120.12	124.44
2	2	11	OMG	N3-C2-N1	-3.52	122.53	127.22
2	2	25	OMG	N3-C2-N1	-3.50	122.56	127.22
2	2	10	OMG	N3-C2-N1	-3.49	122.57	127.22
2	2	25	OMG	C4-C5-C6	-3.44	117.52	120.80
2	2	54	PSU	C5-C6-N1	-3.40	120.26	124.44
2	2	39	PSU	C3'-C2'-C1'	3.29	105.73	101.93
2	2	41	PSU	C3'-C2'-C1'	3.28	105.72	101.93
2	2	44	PSU	C5-C1'-C2'	-3.20	109.61	115.32
2	2	39	PSU	C5-C1'-C2'	-3.12	109.76	115.32
2	2	58	PSU	O4'-C1'-C5	3.08	114.70	109.93
2	2	37	PSU	C5-C1'-C2'	-2.92	110.11	115.32
2	2	54	PSU	C5-C1'-C2'	-2.74	110.44	115.32
2	2	34	PSU	C5-C1'-C2'	-2.71	110.49	115.32
2	2	11	OMG	C4-C5-N7	-2.68	106.61	109.40
2	2	39	PSU	O4'-C1'-C5	2.63	114.01	109.93
2	2	43	PSU	C5-C1'-C2'	-2.56	110.74	115.32
2	2	58	PSU	C3'-C2'-C1'	2.56	104.88	101.93
2	2	25	OMG	C4-C5-N7	-2.55	106.74	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	54	PSU	C3'-C2'-C1'	2.47	104.79	101.93
2	2	44	PSU	C3'-C2'-C1'	2.37	104.66	101.93
2	2	10	OMG	C4-C5-N7	-2.29	107.01	109.40
2	2	40	OMC	N4-C4-N3	2.22	119.99	116.49
2	2	41	PSU	C5-C1'-C2'	-2.22	111.36	115.32
2	2	61	OMC	N4-C4-N3	2.20	119.97	116.49
2	2	34	PSU	C4'-O4'-C1'	2.14	112.06	109.42
2	2	37	PSU	O4'-C1'-C5	2.12	113.22	109.93

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2	11	OMG	O4'-C4'-C5'-O5'
2	2	39	PSU	O4'-C1'-C5-C4
2	2	39	PSU	O4'-C1'-C5-C6
2	2	40	OMC	C3'-C4'-C5'-O5'
2	2	41	PSU	O4'-C1'-C5-C4
2	2	41	PSU	O4'-C1'-C5-C6
2	2	47	OMU	C3'-C4'-C5'-O5'
2	2	47	OMU	O4'-C4'-C5'-O5'
2	2	58	PSU	O4'-C1'-C5-C4
2	2	11	OMG	C3'-C4'-C5'-O5'
2	2	40	OMC	O4'-C4'-C5'-O5'
2	2	54	PSU	C3'-C4'-C5'-O5'
2	2	44	PSU	C3'-C4'-C5'-O5'
2	2	58	PSU	O4'-C1'-C5-C6
2	2	47	OMU	C3'-C2'-O2'-CM2
2	2	47	OMU	C1'-C2'-O2'-CM2
2	2	61	OMC	O4'-C4'-C5'-O5'
2	2	10	OMG	C4'-C5'-O5'-P
2	2	34	PSU	C4'-C5'-O5'-P
2	2	37	PSU	O4'-C4'-C5'-O5'
2	2	10	OMG	C3'-C2'-O2'-CM2
2	2	54	PSU	O4'-C4'-C5'-O5'
2	2	37	PSU	C3'-C4'-C5'-O5'
2	2	25	OMG	C3'-C2'-O2'-CM2
2	2	61	OMC	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	58	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 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.



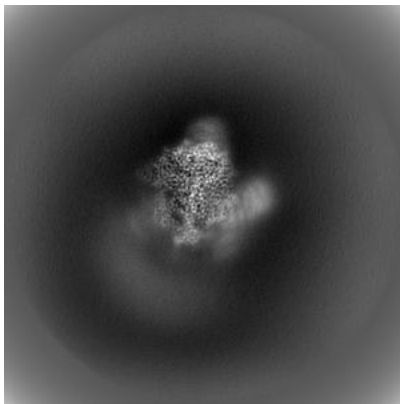
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13812. These allow visual inspection of the internal detail of the map and identification of artifacts.

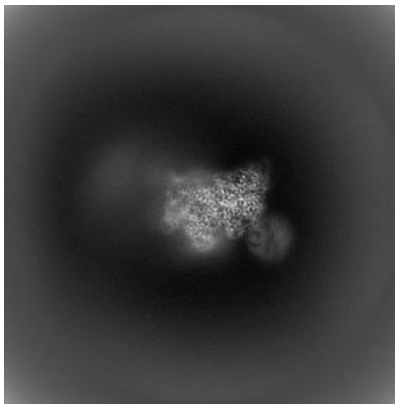
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

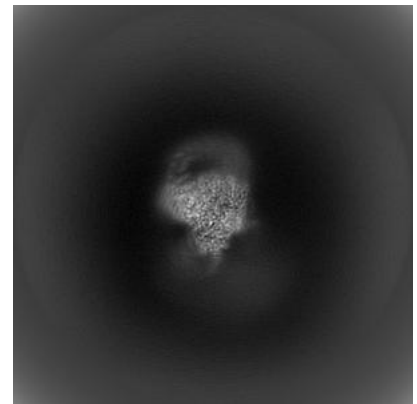
#### 6.1.1 Primary map



X

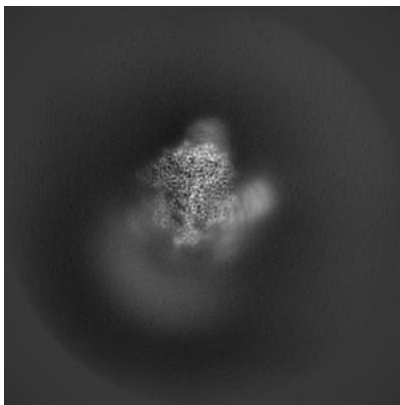


Y

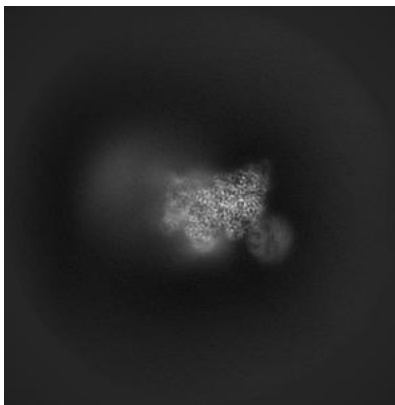


Z

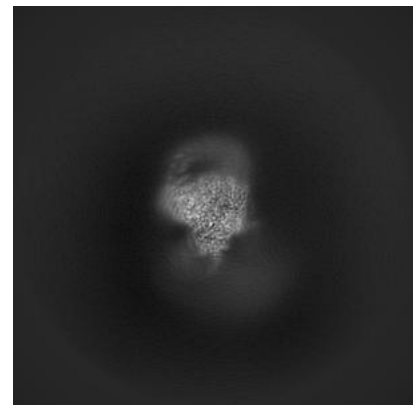
#### 6.1.2 Raw map



X



Y

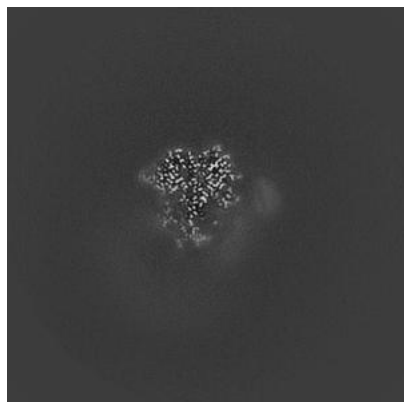


Z

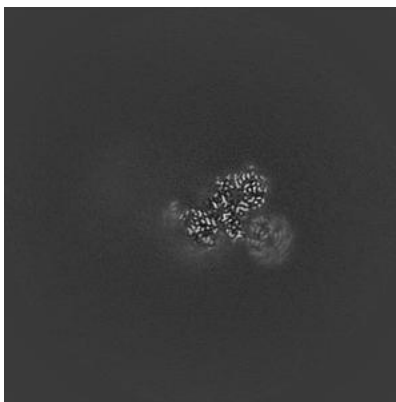
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

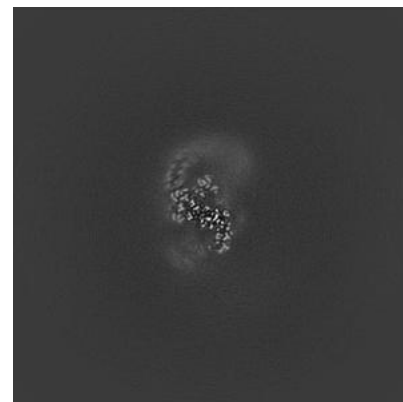
### 6.2.1 Primary map



X Index: 320

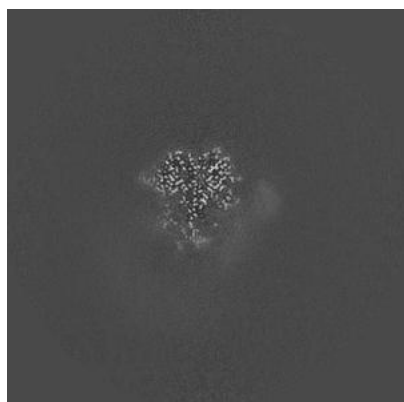


Y Index: 320

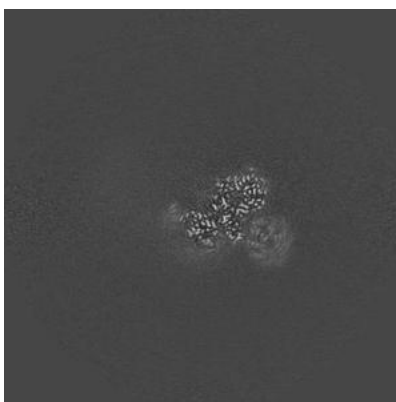


Z Index: 320

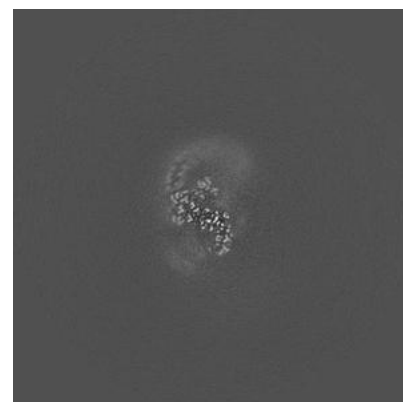
### 6.2.2 Raw map



X Index: 320



Y Index: 320

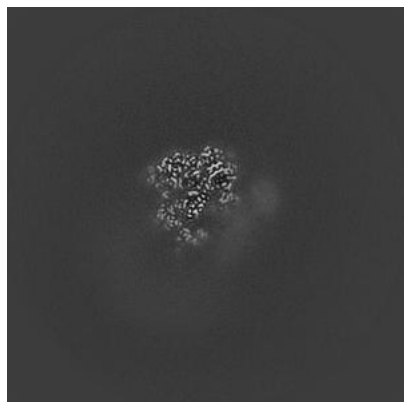


Z Index: 320

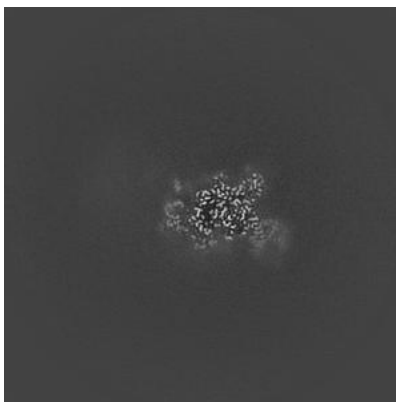
The images above show central slices of the map in three orthogonal directions.

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

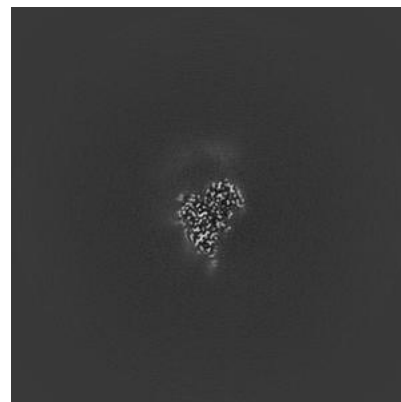
### 6.3.1 Primary map



X Index: 328

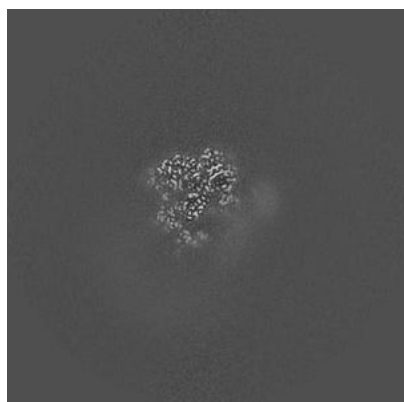


Y Index: 306

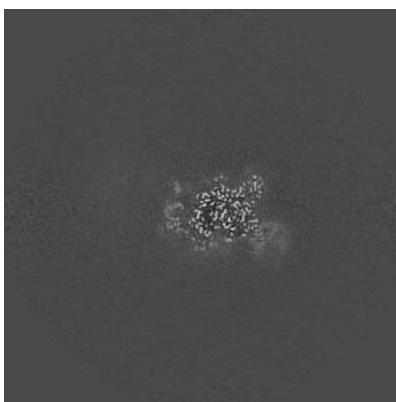


Z Index: 360

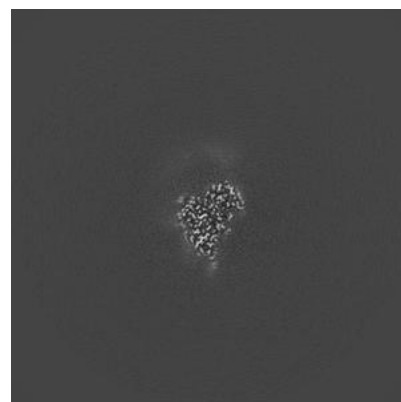
### 6.3.2 Raw map



X Index: 328



Y Index: 306



Z Index: 360

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

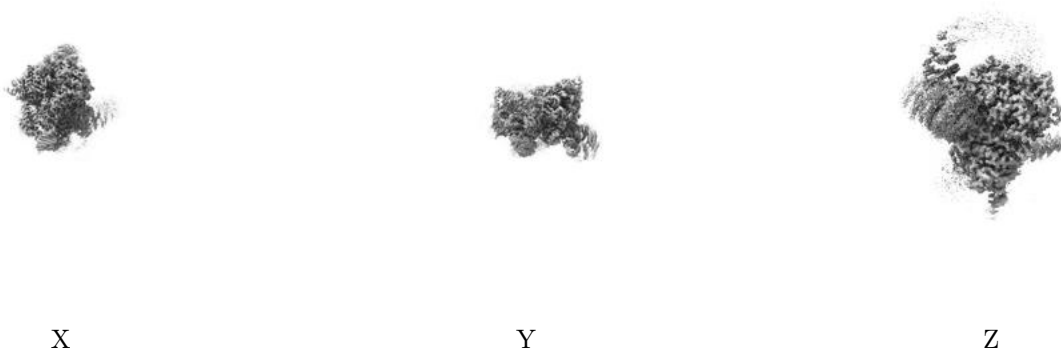
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00711. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

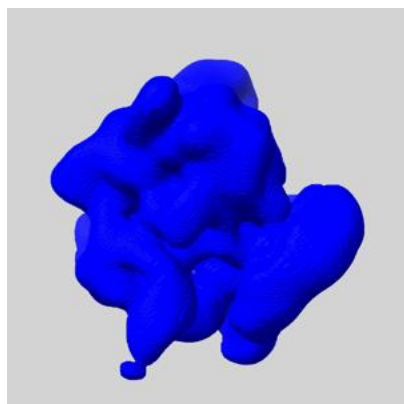
## 6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

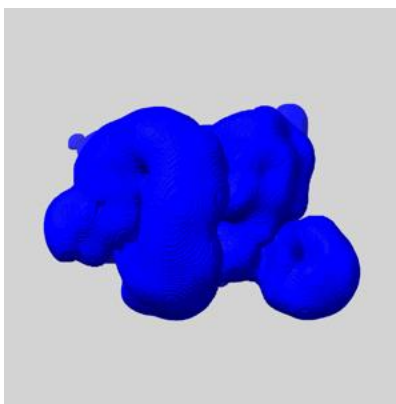
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

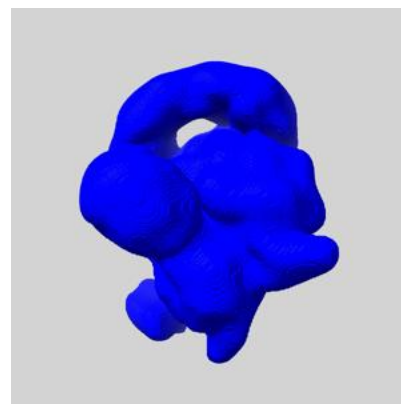
### 6.5.1 emd\_13812\_msk\_1.map [i](#)



X



Y

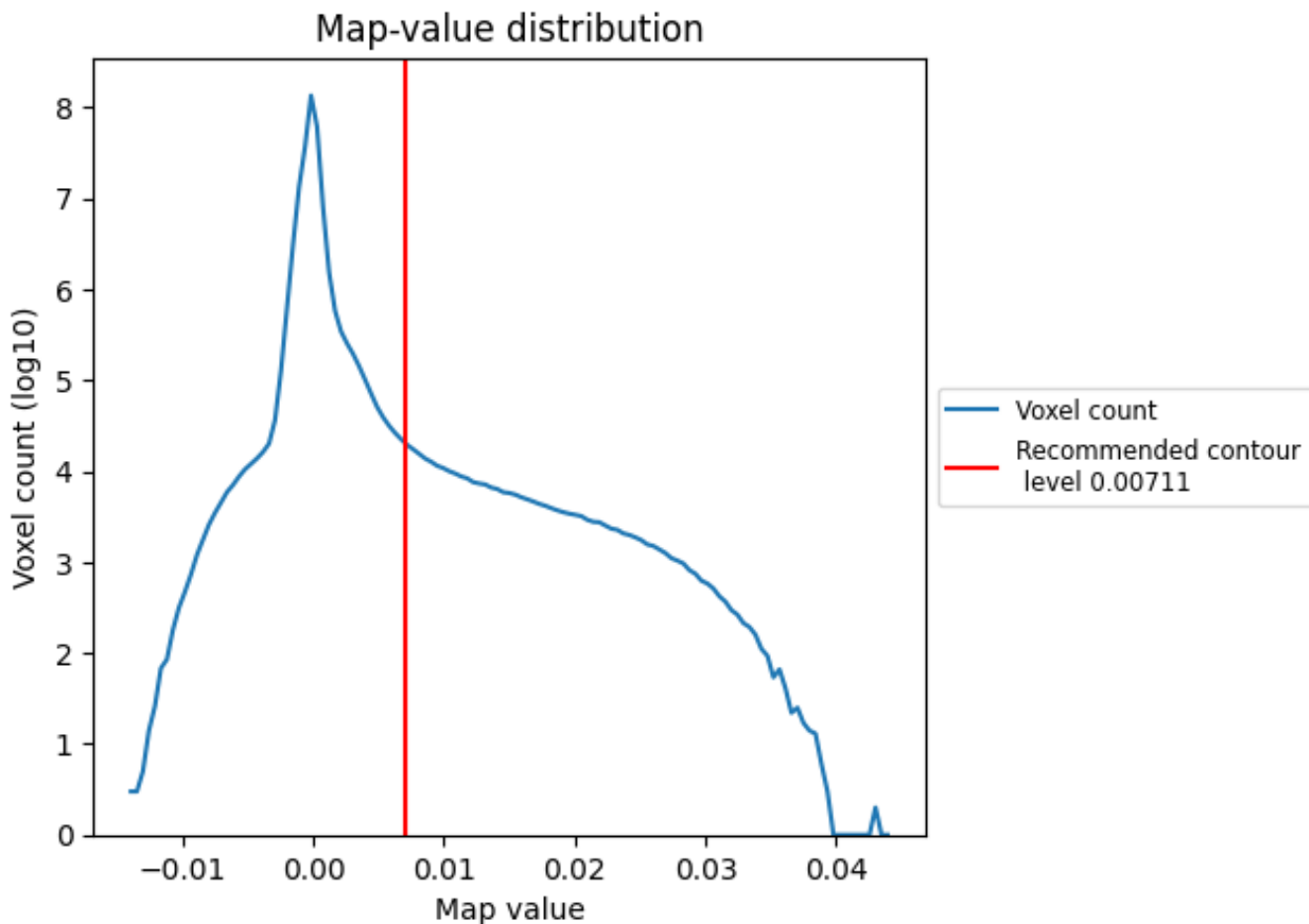


Z

## 7 Map analysis [i](#)

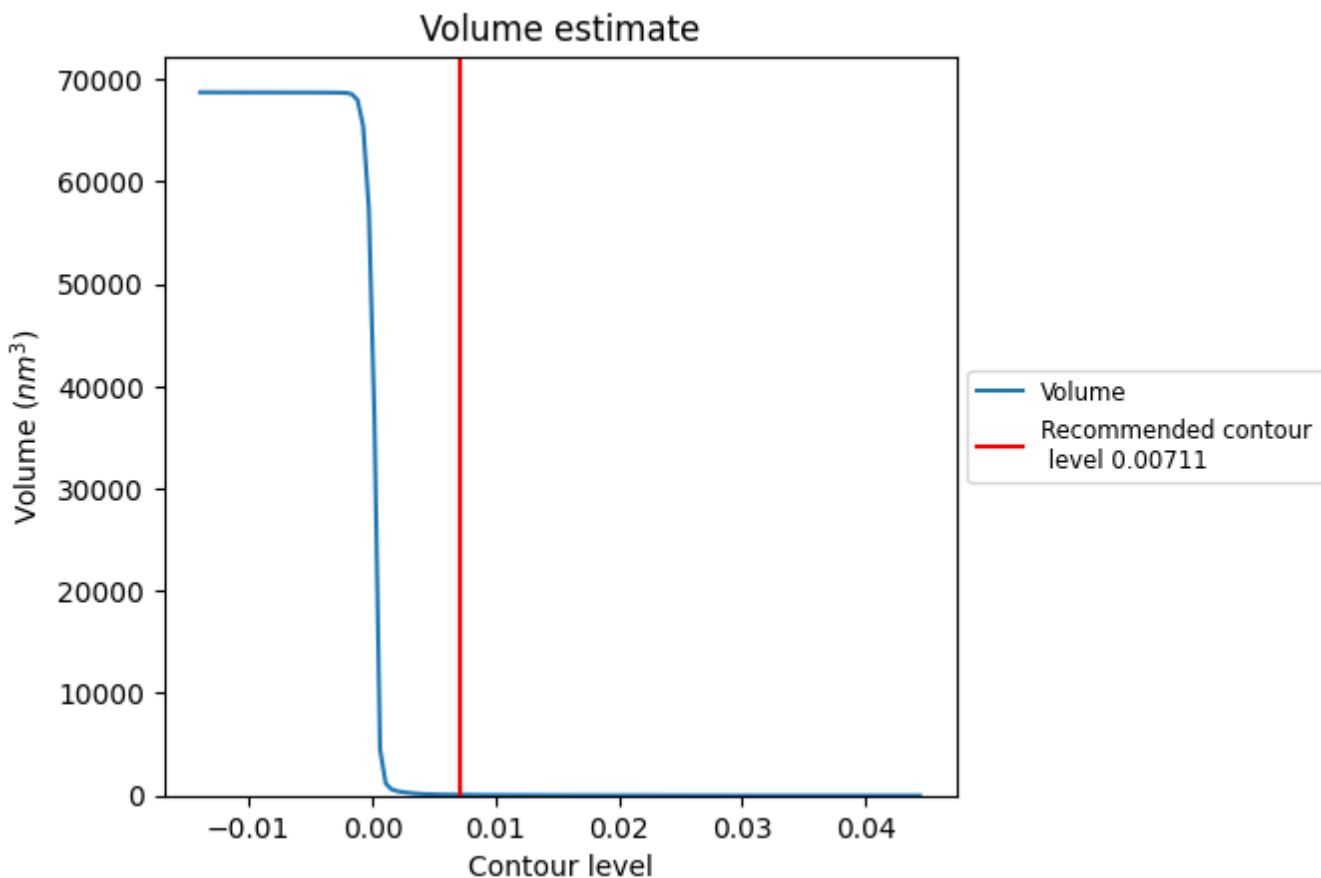
This section contains the results of statistical analysis of the map.

### 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.

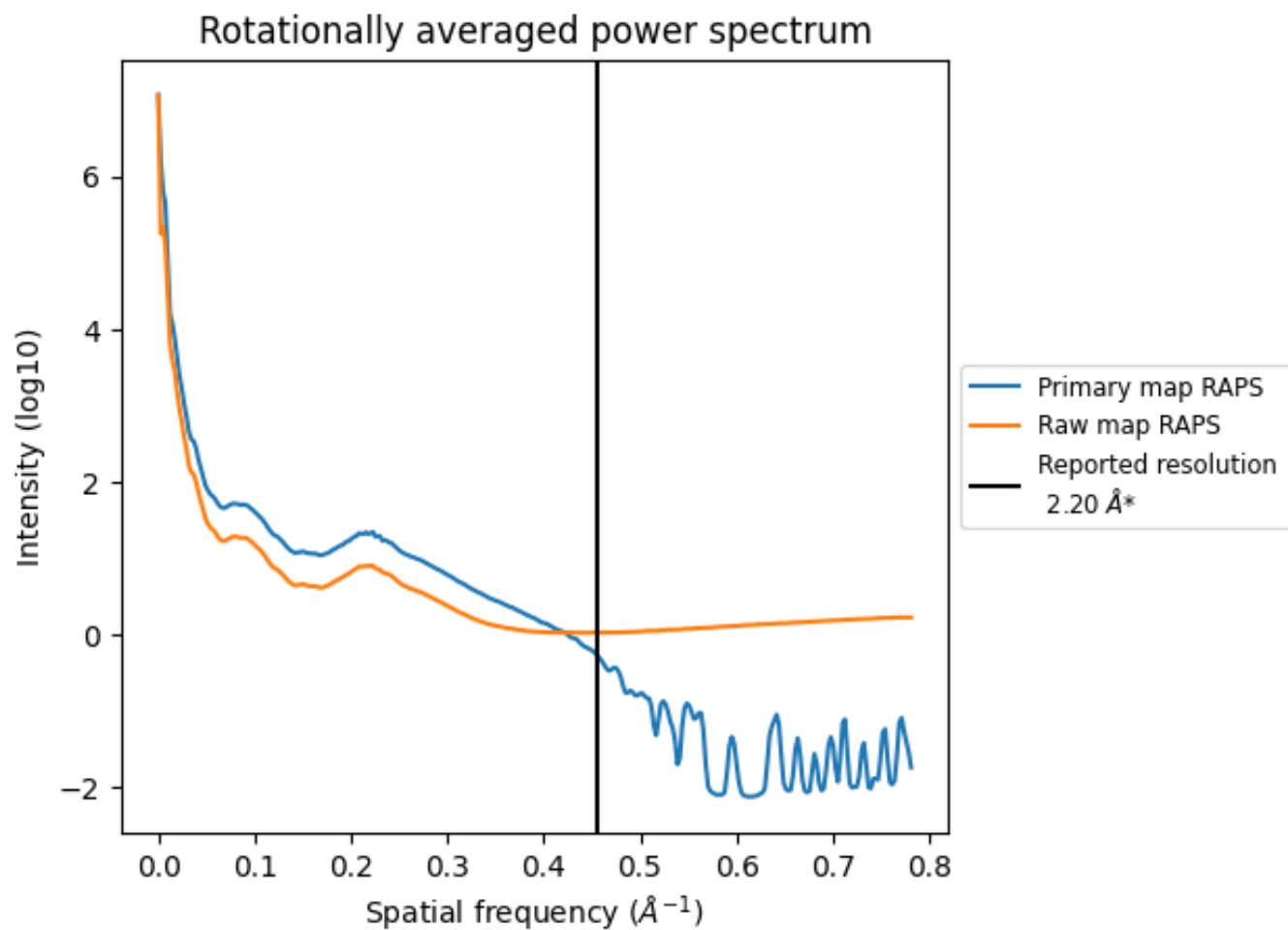
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 72 nm<sup>3</sup>; this corresponds to an approximate mass of 65 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 [\(i\)](#)



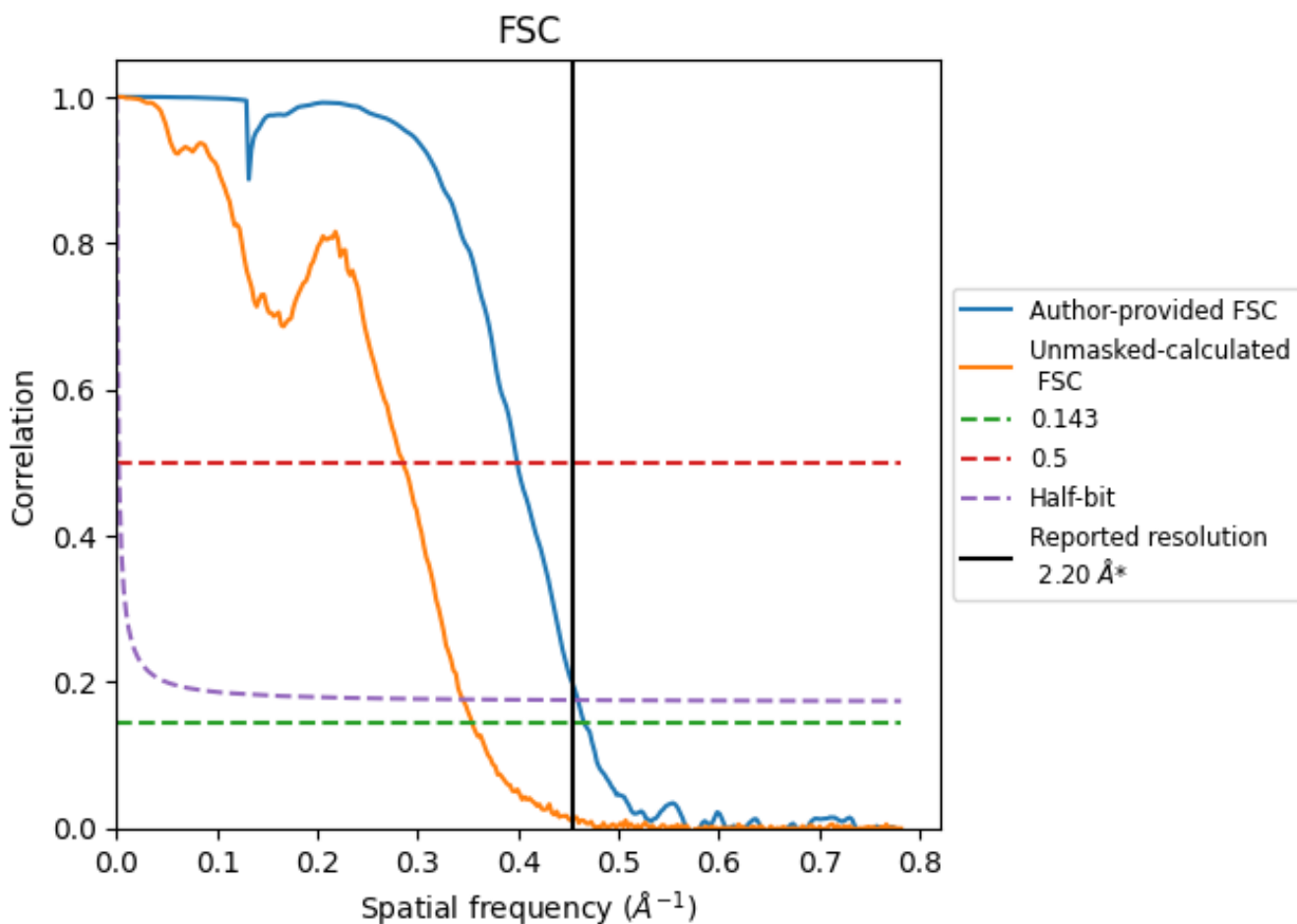
\*Reported resolution corresponds to spatial frequency of 0.455 Å<sup>-1</sup>



## 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  $0.455 \text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

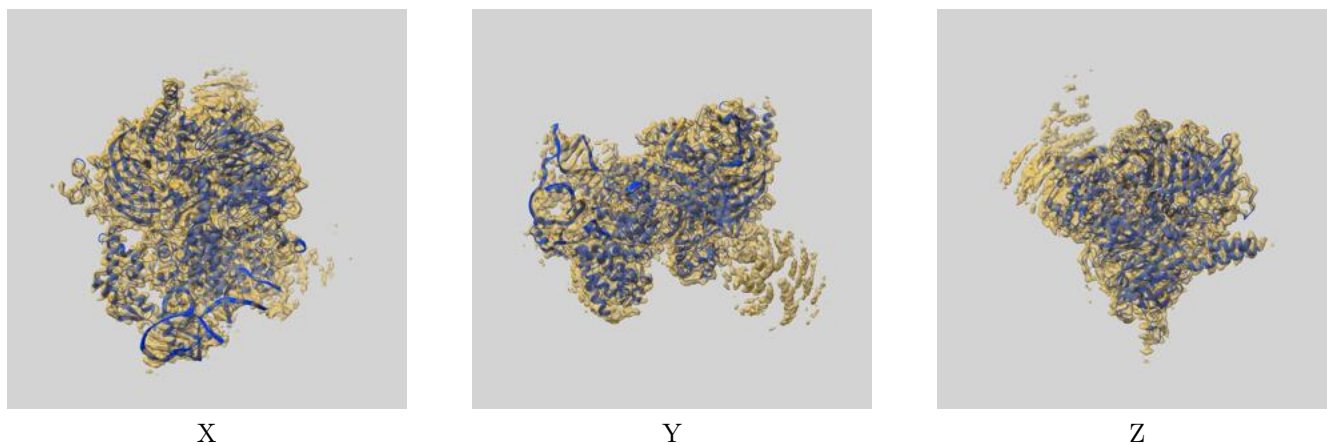
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.15	2.51	2.18
Unmasked-calculated*	2.82	3.51	2.90

\*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 2.82 differs from the reported value 2.2 by more than 10 %

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

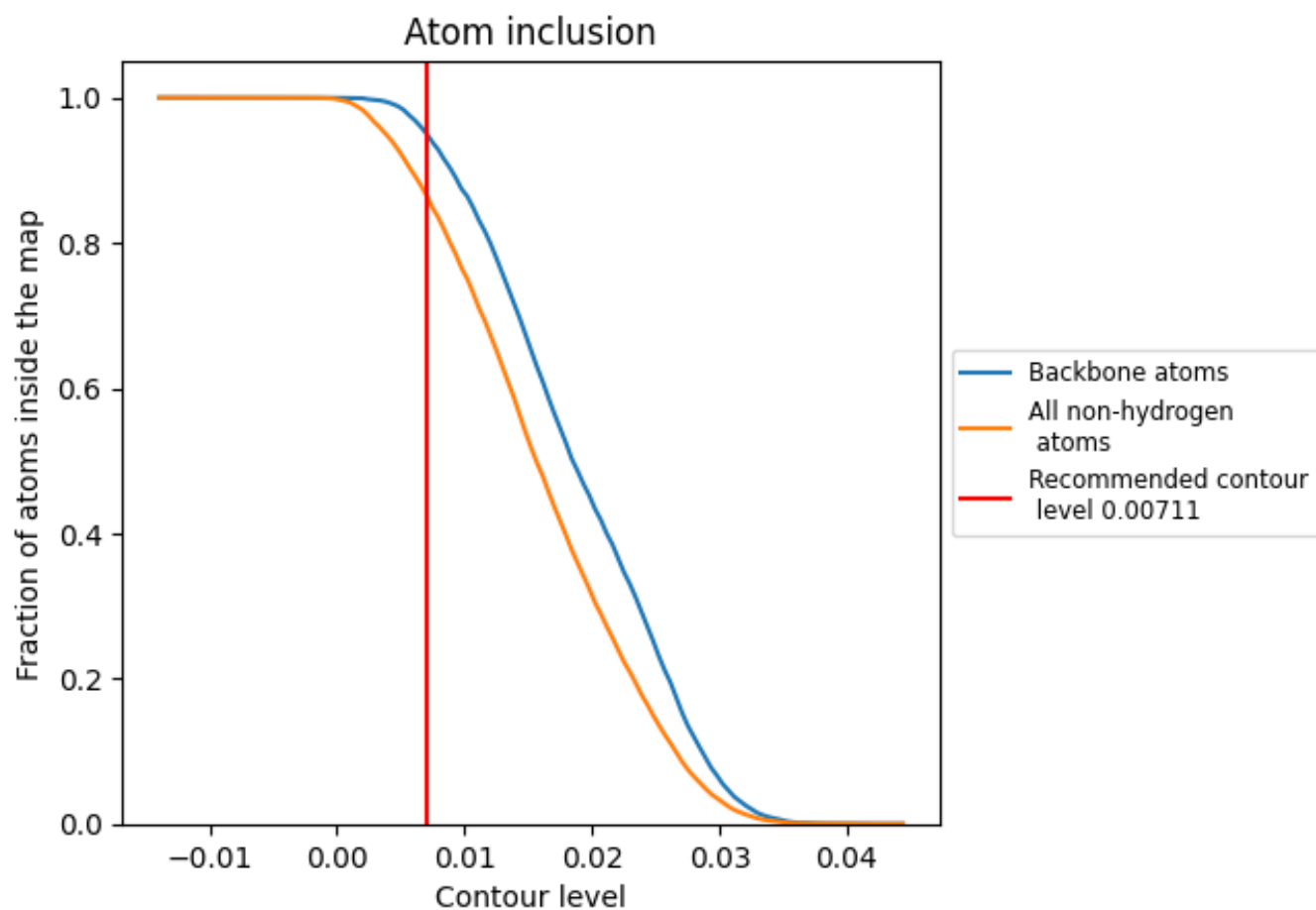
This section contains information regarding the fit between EMDB map EMD-13812 and PDB model 7Q4P. Per-residue inclusion information can be found in section 3 on page 6.

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



The images above show the 3D surface view of the map at the recommended contour level 0.00711 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 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.