



wwPDB EM Validation Summary Report ⓘ

Mar 19, 2024 – 03:40 PM JST

PDB ID : 5ZWN
EMDB ID : EMD-6973
Title : Cryo-EM structure of the yeast pre-B complex at an average resolution of 3.3 angstrom (Part II: U1 snRNP region)
Authors : Bai, R.; Wan, R.; Yan, C.; Lei, J.; Shi, Y.
Deposited on : 2018-05-16
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

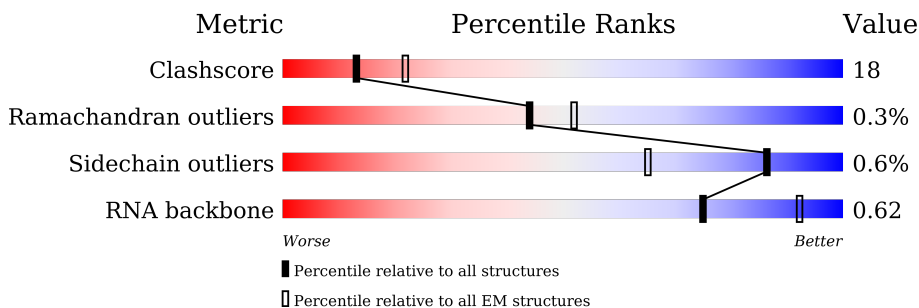
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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.







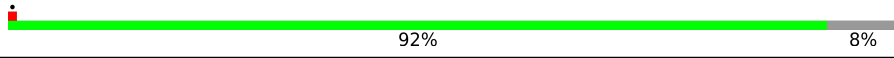
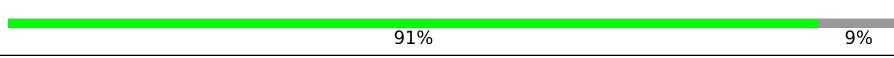
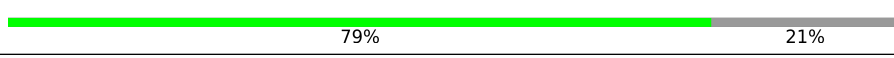

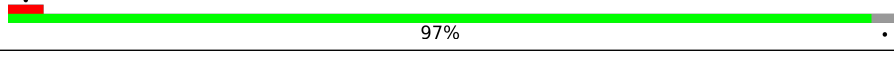
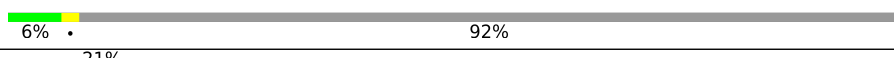
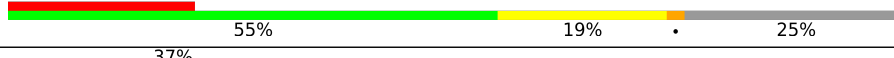
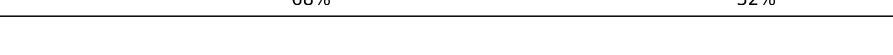

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 ≥ 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	G	22	
2	P	568	
3	Q	300	
4	R	231	
5	S	298	
6	T	544	
7	U	629	

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Mol	Chain	Length	Quality of chain
8	V	523	
9	W	492	
10	a	196	
11	b	146	
12	c	110	
13	d	101	
14	e	94	
15	f	86	
16	g	77	
17	X	619	
18	Y	261	
19	x	49	
20	y	588	

2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 33559 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 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	G	22	477	215	95	145	22	0	0

- Molecule 2 is a RNA chain called U1 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	P	480	10138	4535	1715	3408	480	0	0

- Molecule 3 is a protein called U1 small nuclear ribonucleoprotein 70 kDa homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Q	186	1219	752	232	233	2	0	0

- Molecule 4 is a protein called U1 small nuclear ribonucleoprotein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	R	184	1492	930	289	268	5	0	0

- Molecule 5 is a protein called U1 small nuclear ribonucleoprotein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	S	131	1045	665	191	186	3	0	0

- Molecule 6 is a protein called U1 small nuclear ribonucleoprotein component PRP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	T	539	4540	2976	716	829	19	0	0

- Molecule 7 is a protein called Pre-mRNA-processing factor 39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	U	583	3940	2498	684	751	7	0	0

- Molecule 8 is a protein called Protein NAM8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	V	187	1414	889	244	271	10	0	0

- Molecule 9 is a protein called 56 kDa U1 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	W	229	1841	1202	300	328	11	0	0

- Molecule 10 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	a	124	1009	637	191	178	3	0	0

- Molecule 11 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	b	119	917	575	163	176	3	0	0

- Molecule 12 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	c	101	785	504	149	128	4	0	0

- Molecule 13 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	d	92	704	448	126	127	3	0	0

- Molecule 14 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	e	74	Total	C	N	O	S	0	0
			526	346	87	90	3		

- Molecule 15 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	f	68	Total	C	N	O	S	0	0
			518	337	96	84	1		

- Molecule 16 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	g	75	Total	C	N	O	S	0	0
			552	350	98	103	1		

- Molecule 17 is a protein called U1 small nuclear ribonucleoprotein component SNU71.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	X	49	Total	C	N	O	0	0
			395	252	68	75		

- Molecule 18 is a protein called Protein LUC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	196	Total	C	N	O	S	0	0
			1400	874	258	257	11		

- Molecule 19 is a protein called U1 snRNP.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	x	49	Total	C	N	O	0	0
			245	147	49	49		

- Molecule 20 is a protein called Pre-mRNA-splicing ATP-dependent RNA helicase PRP28.

Mol	Chain	Residues	Atoms		AltConf	Trace
20	y	399	Total	C	0	399
			399	399		

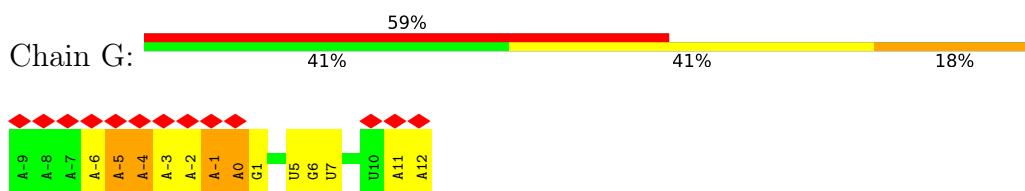
- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
21	R	1	Total 1	Zn 1	0
21	Y	2	Total 2	Zn 2	0

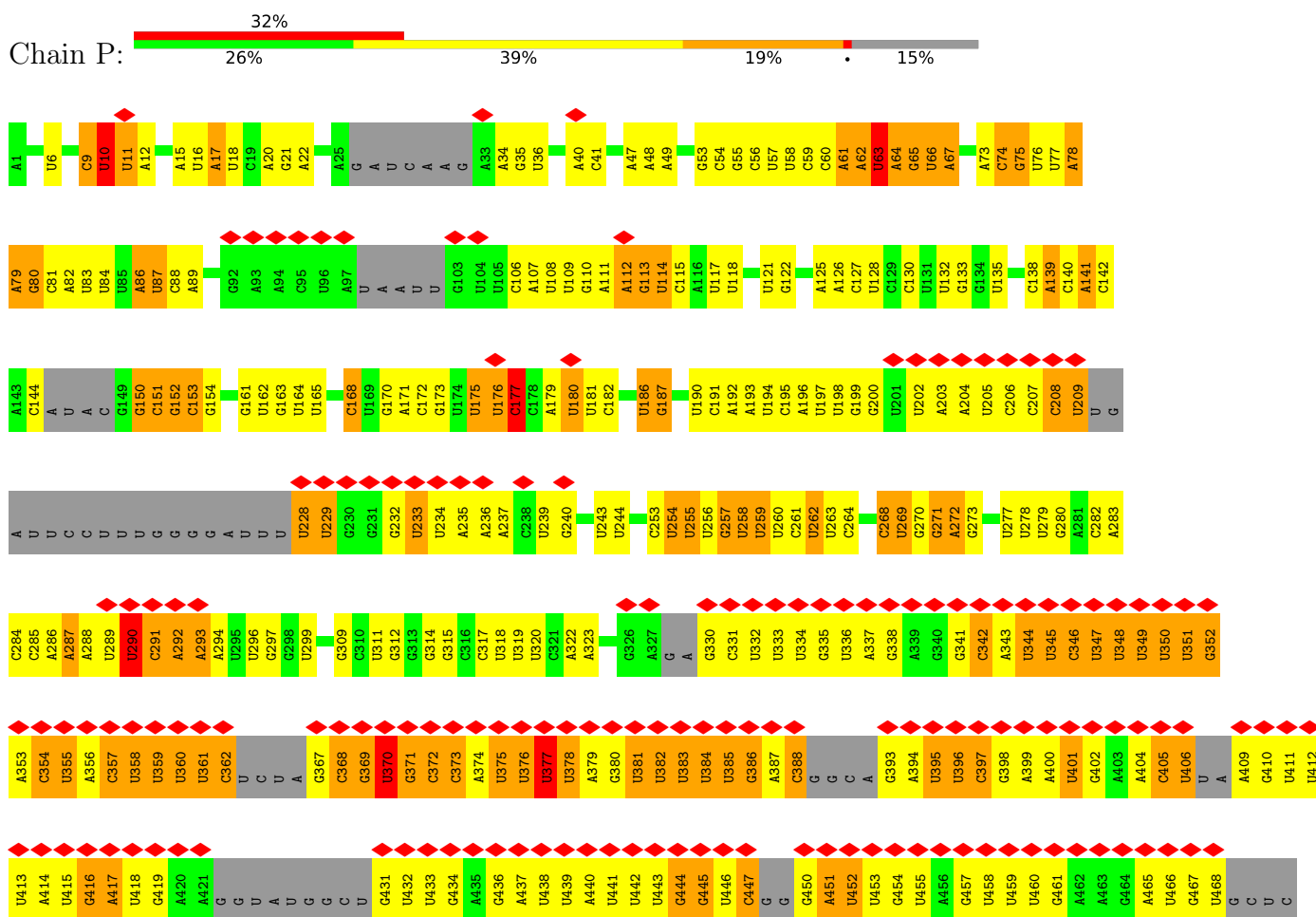
3 Residue-property plots

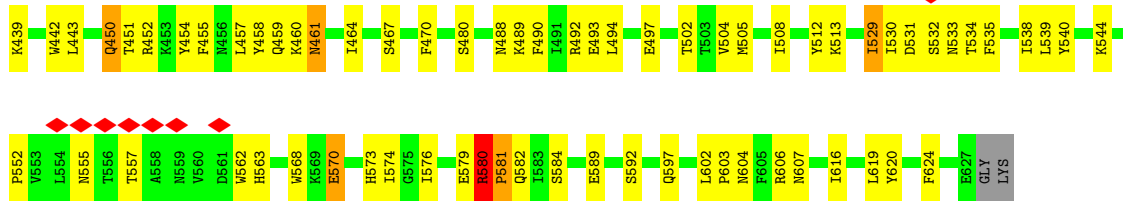
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



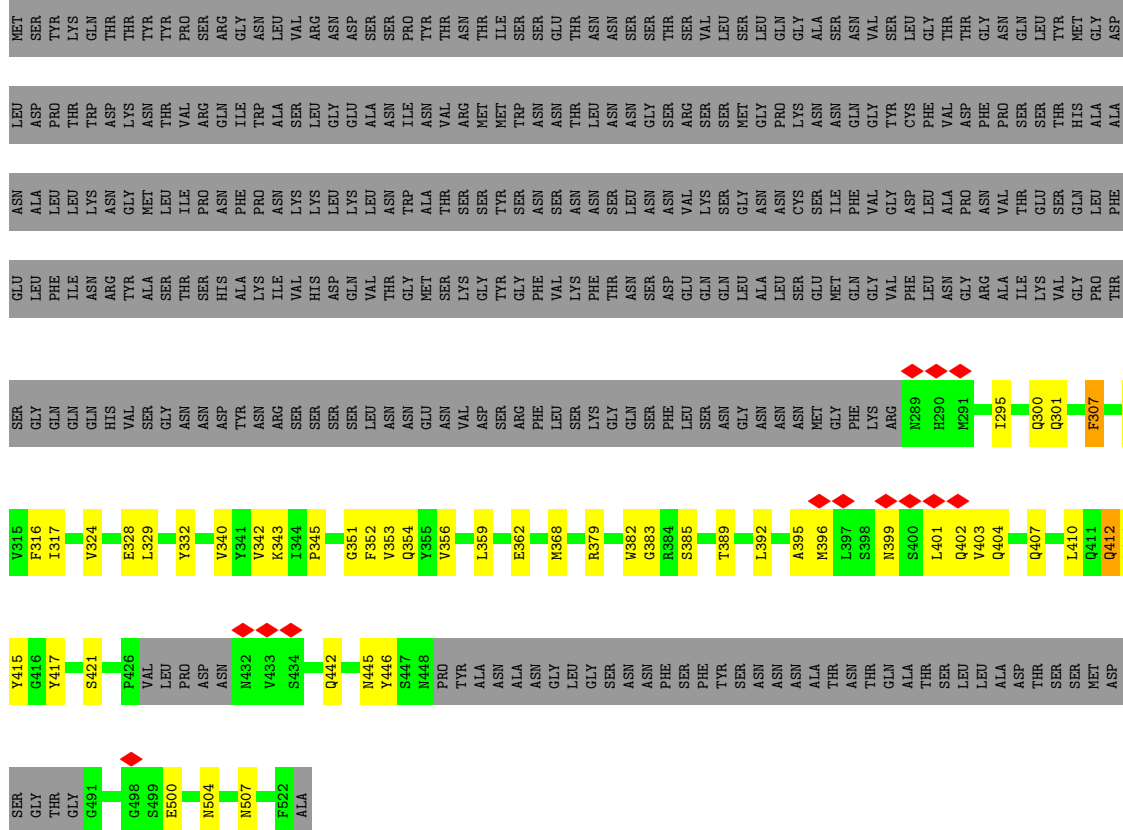
- Molecule 2: U1 snRNA





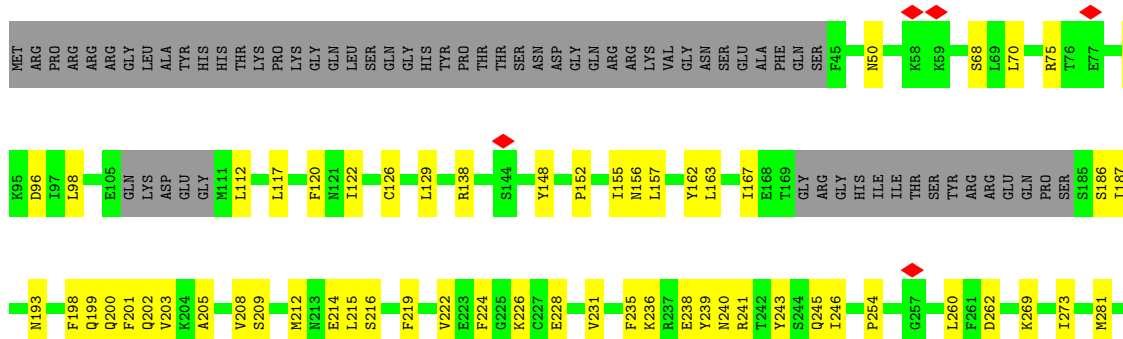
- Molecule 8: Protein NAM8

Chain V: 26% 9% 64%



- Molecule 9: 56 kDa U1 small nuclear ribonucleoprotein component

Chain W: 34% 12% 53%



Q481	L482	F483	R484	T485	M486	K487	V488	Q489	I490	M491	I492	A493	T494	N495	V496	A497	A498	R499	G500	L501	D502	I503	P504	N505	V506	S507	L508	V509	V510	N511	F512	Q513	K516	K517	M518	D519	D520	Y521	I522	H523	R524	I525	G526	R527	T528	G529	R530	A531	A532	N533	E534	G535	T536	A537	V538	S539	F540	V541
S542	A543	A544	E545	D546	E547	S548	L549	I550	R551	E552	L553	Y554	K555	Y556	V557	R558	K559	H560	D561	P562	L563	N564	S565	N566	I567	F568	S569	E570	A571	V572	K573	N574	K575	Y576	N577	V578	GLY	LYS	GLN	LEU	SER	ASN	GLU	ILE	ILE	TYR												

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	500657	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.347	Depositor
Minimum map value	-0.196	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.045	Depositor
Map size (\AA)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.338, 1.338, 1.338	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

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	G	0.23	0/537	0.81	0/835
2	P	0.62	42/11309 (0.4%)	0.98	13/17577 (0.1%)
3	Q	0.27	0/1237	0.51	1/1691 (0.1%)
4	R	0.27	0/1522	0.47	0/2047
5	S	0.27	0/1059	0.54	1/1422 (0.1%)
6	T	0.29	0/4654	0.48	0/6289
7	U	0.28	1/4002 (0.0%)	0.46	1/5497 (0.0%)
8	V	0.28	0/1441	0.51	0/1957
9	W	0.28	0/1882	0.46	0/2537
10	a	0.27	0/1016	0.57	1/1355 (0.1%)
11	b	0.25	0/926	0.53	0/1257
12	c	0.26	0/799	0.50	0/1078
13	d	0.29	0/716	0.51	0/970
14	e	0.26	0/535	0.48	0/730
15	f	0.27	0/529	0.49	0/715
16	g	0.27	0/557	0.54	0/756
17	X	0.29	0/403	0.45	0/543
18	Y	0.29	0/1417	0.55	1/1907 (0.1%)
19	x	0.28	0/244	0.30	0/340
All	All	0.42	43/34785 (0.1%)	0.71	18/49503 (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
3	Q	0	2
4	R	0	1
8	V	0	2
18	Y	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	7

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	346	C	C1'-N1	7.15	1.59	1.48
2	P	496	C	C1'-N1	7.10	1.59	1.48
2	P	361	U	C1'-N1	6.89	1.59	1.48
2	P	209	U	C1'-N1	6.87	1.59	1.48
2	P	381	U	C1'-N1	6.70	1.58	1.48

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	66	GLY	N-CA-C	8.13	133.42	113.10
2	P	208	C	OP2-P-O3'	7.44	121.56	105.20
2	P	361	U	OP2-P-O3'	7.21	121.05	105.20
2	P	360	U	OP2-P-O3'	7.14	120.92	105.20
2	P	360	U	O3'-P-O5'	-6.82	91.03	104.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	Q	97	ASP	Peptide
3	Q	98	PRO	Peptide
4	R	167	ARG	Peptide
8	V	412	GLN	Peptide
8	V	413	PRO	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	G	477	0	238	7	0
2	P	10138	0	5108	534	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	1219	0	943	20	0
4	R	1492	0	1493	51	0
5	S	1045	0	1093	22	0
6	T	4540	0	4531	144	0
7	U	3940	0	3175	108	0
8	V	1414	0	1363	54	0
9	W	1841	0	1813	51	0
10	a	1009	0	1100	0	0
11	b	917	0	961	0	0
12	c	785	0	802	0	0
13	d	704	0	735	0	0
14	e	526	0	515	0	0
15	f	518	0	502	0	0
16	g	552	0	553	0	0
17	X	395	0	391	12	0
18	Y	1400	0	1254	53	0
19	x	245	0	244	0	0
20	y	399	0	0	0	0
21	R	1	0	0	0	0
21	Y	2	0	0	0	0
All	All	33559	0	26814	959	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 18.

The worst 5 of 959 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)
2:P:445:G:O2'	2:P:446:U:H5'	1.48	1.11
2:P:234:U:H2'	2:P:235:A:C8	1.84	1.11
2:P:382:U:C2'	2:P:383:U:H5'	1.83	1.08
2:P:445:G:O2'	2:P:446:U:C5'	2.01	1.08
2:P:415:U:H5''	2:P:416:G:OP1	1.53	1.07

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	
3	Q	182/300 (61%)	168 (92%)	12 (7%)	2 (1%)	14	44
4	R	180/231 (78%)	169 (94%)	10 (6%)	1 (1%)	25	57
5	S	125/298 (42%)	118 (94%)	6 (5%)	1 (1%)	19	51
6	T	537/544 (99%)	515 (96%)	22 (4%)	0	100	100
7	U	579/629 (92%)	544 (94%)	32 (6%)	3 (0%)	29	61
8	V	181/523 (35%)	165 (91%)	16 (9%)	0	100	100
9	W	223/492 (45%)	213 (96%)	10 (4%)	0	100	100
10	a	120/196 (61%)	113 (94%)	7 (6%)	0	100	100
11	b	117/146 (80%)	108 (92%)	9 (8%)	0	100	100
12	c	99/110 (90%)	94 (95%)	5 (5%)	0	100	100
13	d	90/101 (89%)	85 (94%)	5 (6%)	0	100	100
14	e	70/94 (74%)	67 (96%)	3 (4%)	0	100	100
15	f	64/86 (74%)	61 (95%)	3 (5%)	0	100	100
16	g	73/77 (95%)	66 (90%)	7 (10%)	0	100	100
17	X	47/619 (8%)	47 (100%)	0	0	100	100
18	Y	190/261 (73%)	170 (90%)	18 (10%)	2 (1%)	14	44
19	x	47/49 (96%)	47 (100%)	0	0	100	100
All	All	2924/4756 (62%)	2750 (94%)	165 (6%)	9 (0%)	44	72

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Q	98	PRO
4	R	169	ASN
3	Q	97	ASP
7	U	132	SER
18	Y	44	ILE

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	
3	Q	84/265 (32%)	84 (100%)	0	100	100
4	R	165/214 (77%)	165 (100%)	0	100	100
5	S	114/273 (42%)	114 (100%)	0	100	100
6	T	509/519 (98%)	508 (100%)	1 (0%)	93	98
7	U	301/603 (50%)	295 (98%)	6 (2%)	55	77
8	V	154/451 (34%)	153 (99%)	1 (1%)	86	94
9	W	199/448 (44%)	199 (100%)	0	100	100
10	a	113/176 (64%)	112 (99%)	1 (1%)	78	90
11	b	106/129 (82%)	106 (100%)	0	100	100
12	c	82/103 (80%)	82 (100%)	0	100	100
13	d	79/89 (89%)	79 (100%)	0	100	100
14	e	52/83 (63%)	52 (100%)	0	100	100
15	f	51/77 (66%)	51 (100%)	0	100	100
16	g	56/66 (85%)	56 (100%)	0	100	100
17	X	45/567 (8%)	45 (100%)	0	100	100
18	Y	121/234 (52%)	117 (97%)	4 (3%)	38	66
All	All	2231/4297 (52%)	2218 (99%)	13 (1%)	86	94

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

Mol	Chain	Res	Type
8	V	307	PHE
10	a	82	LEU
18	Y	204	CYS
18	Y	72	HIS
18	Y	201	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
11	b	30	GLN
15	f	50	ASN
12	c	50	ASN
12	c	66	ASN
18	Y	76	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	G	21/22 (95%)	8 (38%)	1 (4%)
2	P	467/568 (82%)	104 (22%)	22 (4%)
All	All	488/590 (82%)	112 (22%)	23 (4%)

5 of 112 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	G	-6	A
1	G	-5	A
1	G	-4	A
1	G	-2	A
1	G	-1	A

5 of 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	P	268	C
2	P	369	G
2	P	279	U
2	P	370	U
2	P	86	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

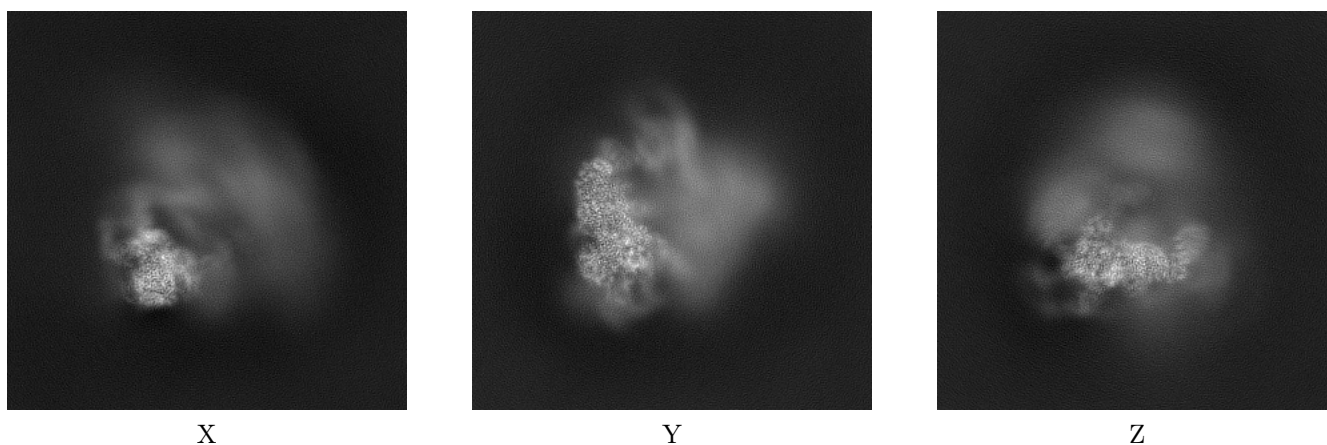
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6973. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

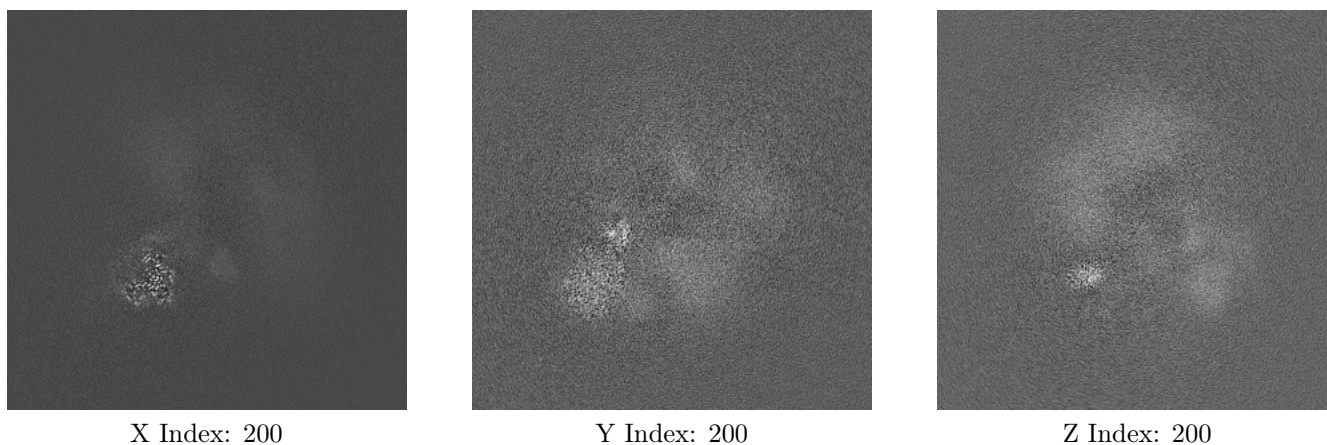
6.1.1 Primary map



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

6.2 Central slices [i](#)

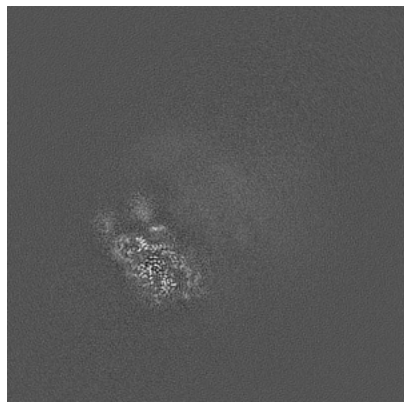
6.2.1 Primary map



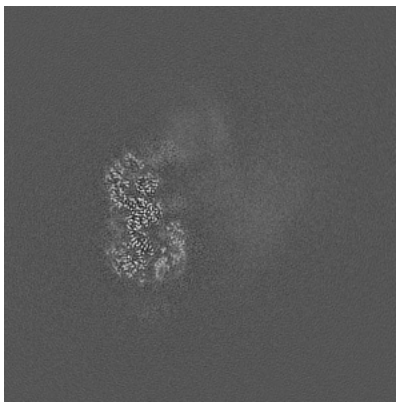
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

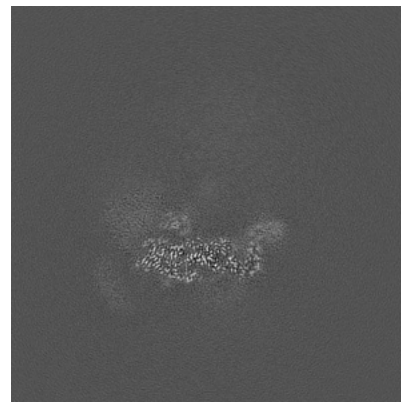
6.3.1 Primary map



X Index: 156



Y Index: 149

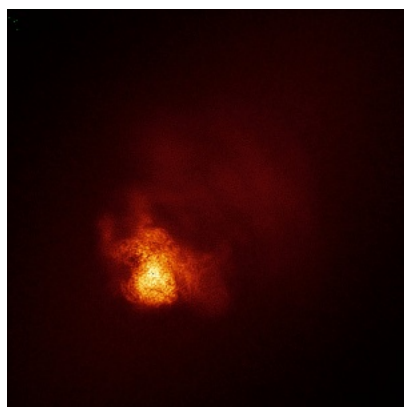


Z Index: 132

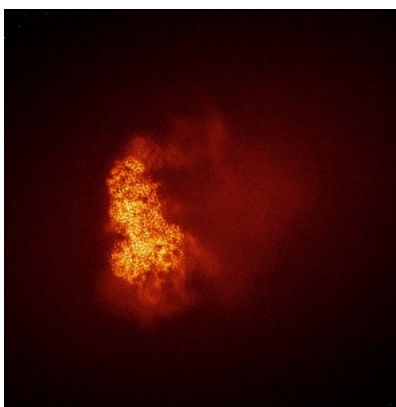
The images above show the largest variance slices of the map in three orthogonal directions.

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

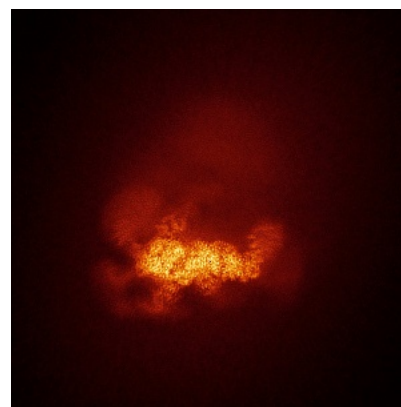
6.4.1 Primary map



X



Y

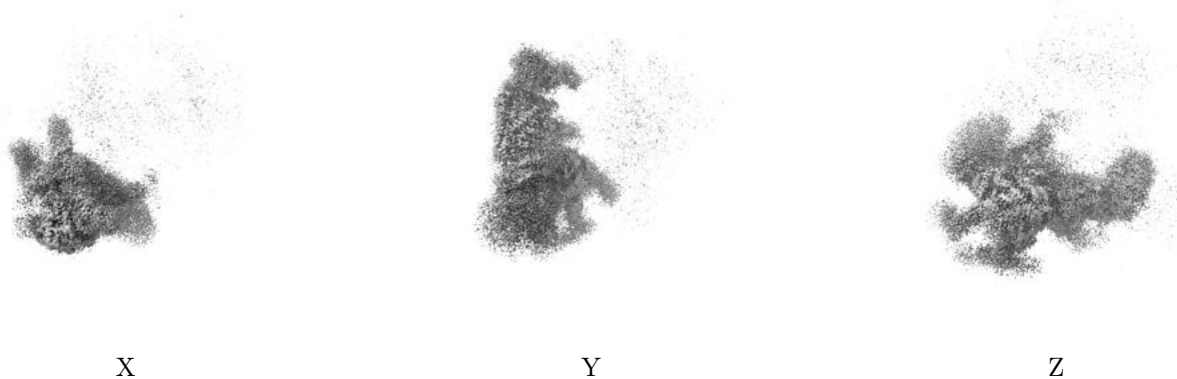


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

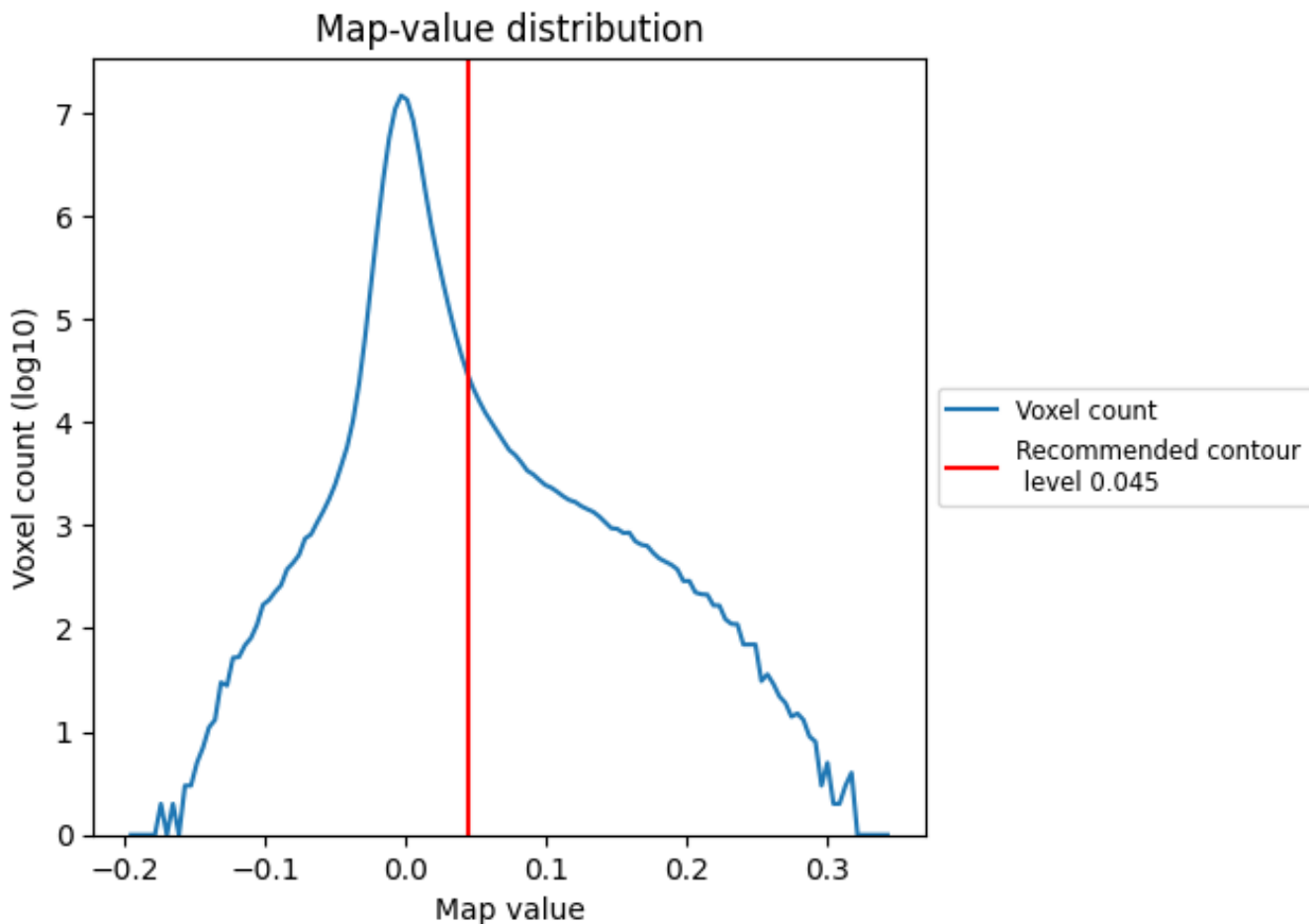
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

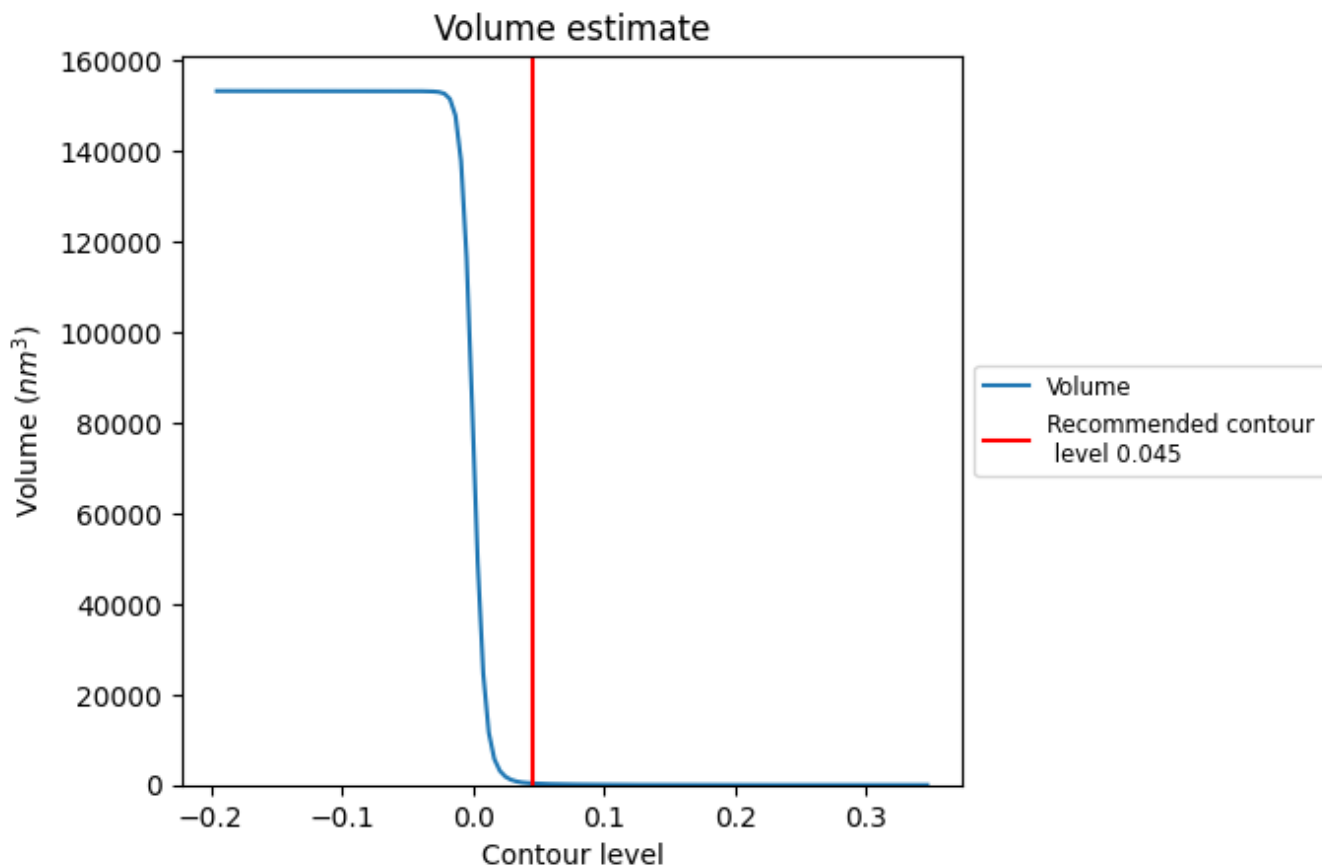
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

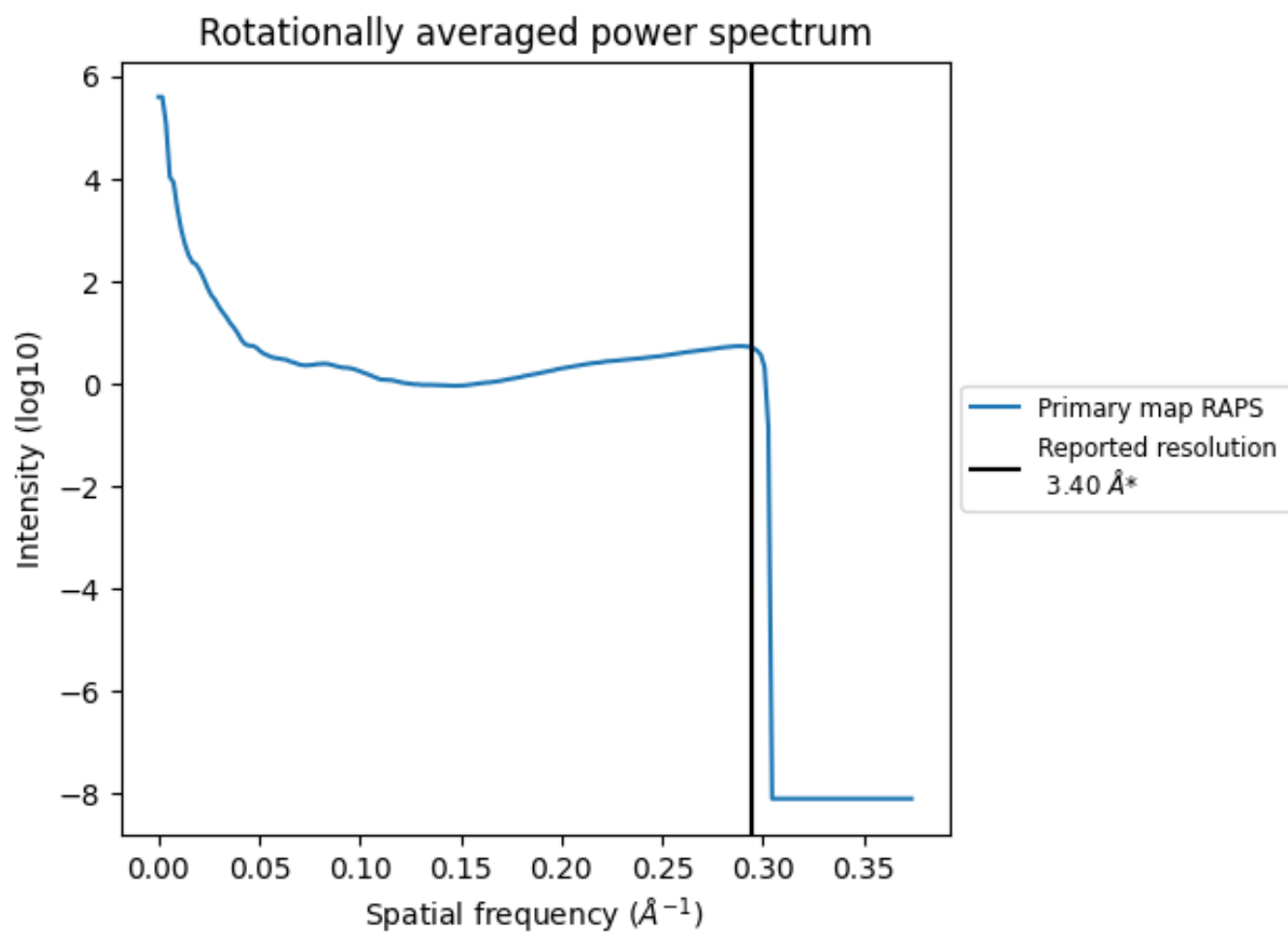
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 352 nm^3 ; this corresponds to an approximate mass of 318 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 0.294 \AA^{-1}

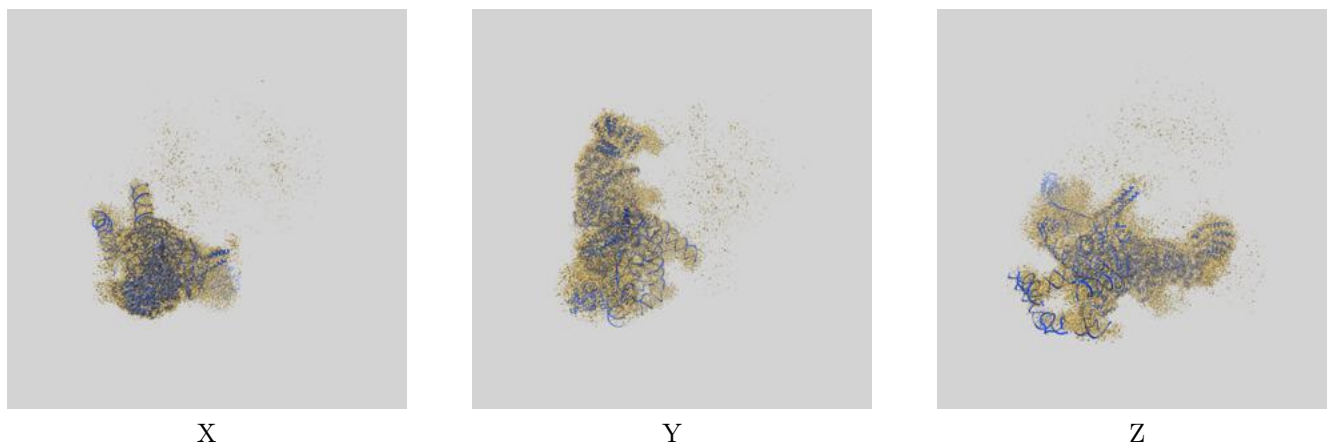
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

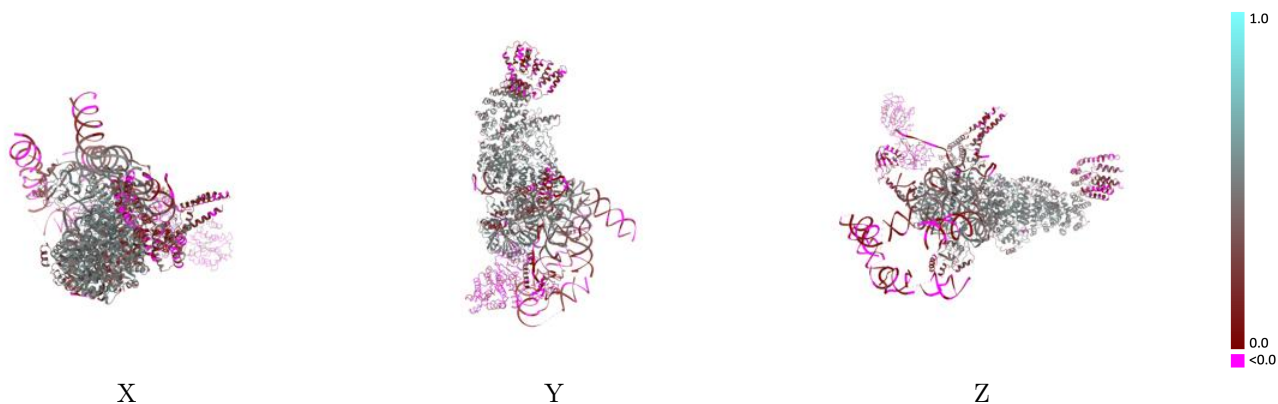
This section contains information regarding the fit between EMDB map EMD-6973 and PDB model 5ZWN. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



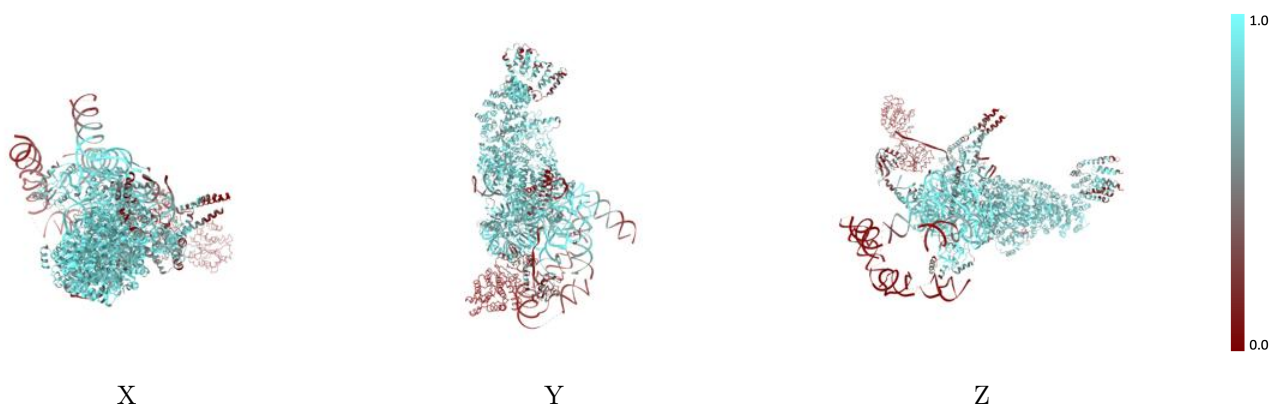
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



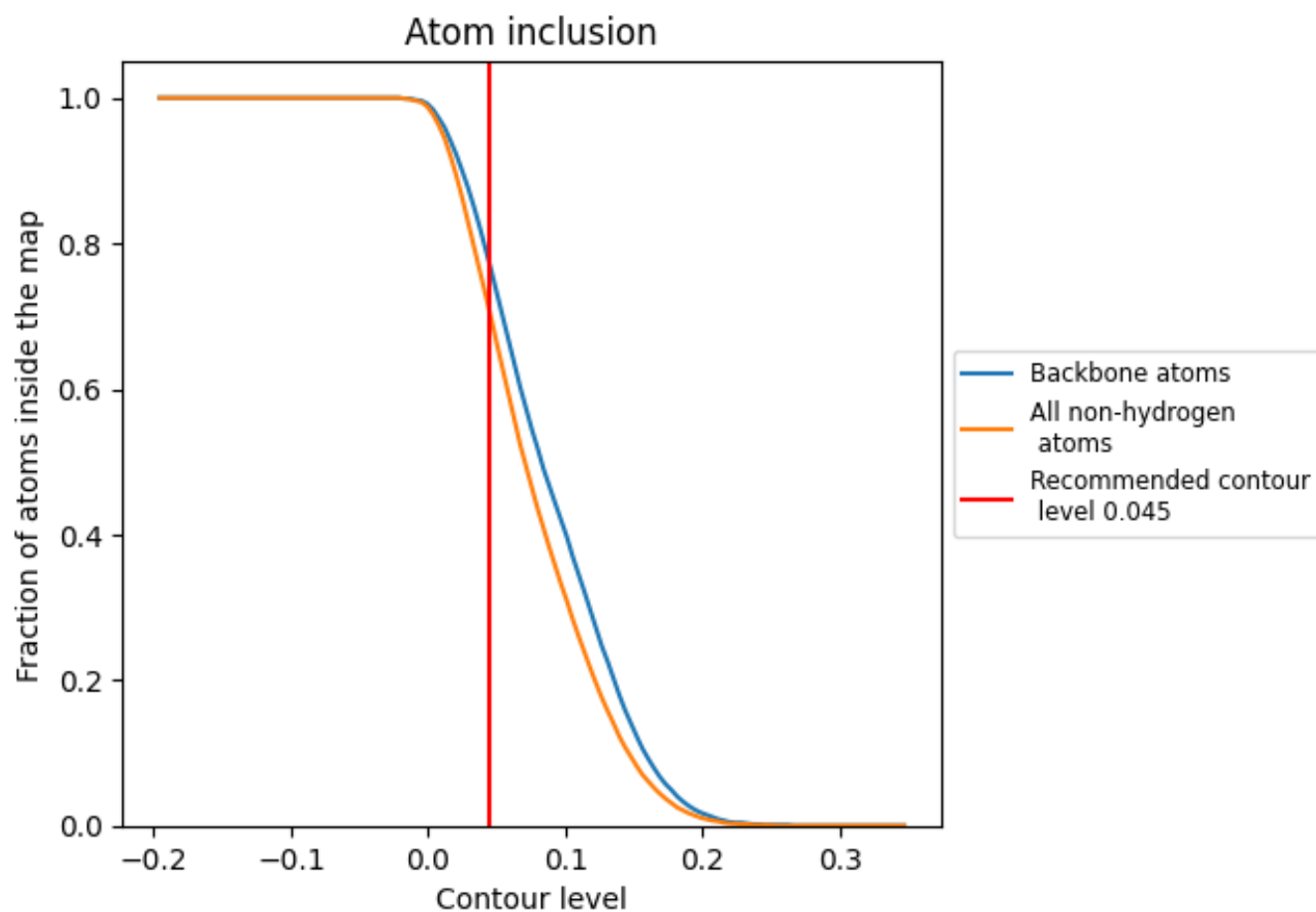
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 70% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7050	 0.3560
G	 0.3920	 0.1480
P	 0.5770	 0.2450
Q	 0.5660	 0.2580
R	 0.7850	 0.4510
S	 0.6590	 0.2830
T	 0.8670	 0.5010
U	 0.7550	 0.3460
V	 0.8010	 0.4510
W	 0.8170	 0.4520
X	 0.8180	 0.4560
Y	 0.6070	 0.2700
a	 0.7800	 0.4500
b	 0.8010	 0.4510
c	 0.8840	 0.4770
d	 0.8570	 0.5130
e	 0.8780	 0.4940
f	 0.9150	 0.5100
g	 0.8290	 0.4790
x	 0.5920	 0.2520
y	 0.0380	 -0.0240

