



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 03:57 PM UTC

PDB ID : 8YNY / pdb_00008yny
EMDB ID : EMD-39431
Title : Structure of Cas9-sgRNA ribonucleoprotein bound to nucleosome
Authors : Nagamura, R.; Kujirai, T.; Kusakizako, T.; Hirano, H.; Kurumizaka, H.; Nureki, O.
Deposited on : 2024-03-12
Resolution : 4.52 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

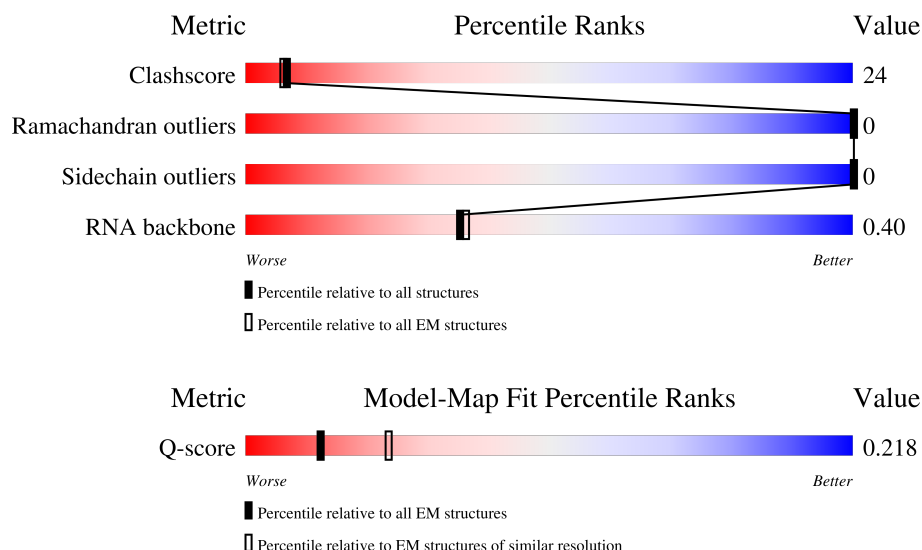
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.52 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.



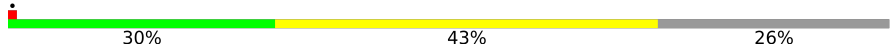
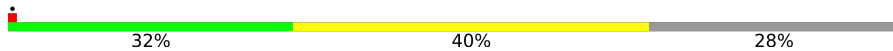
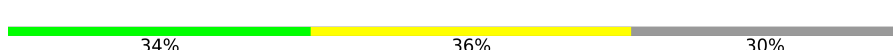
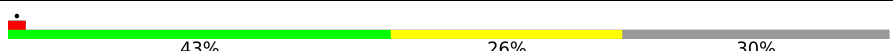
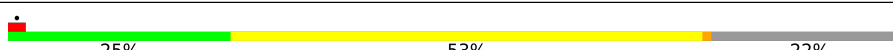
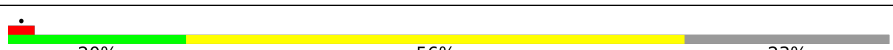
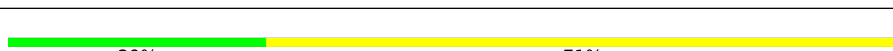
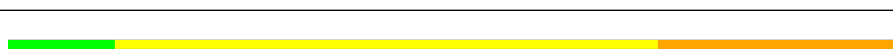
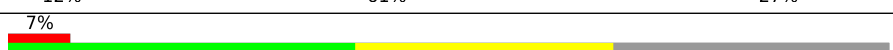
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2506 (4.02 - 5.02)

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	A	139	7% 35% 31% 35%
1	E	139	39% 26% 35%
2	B	106	5% 35% 42% 24%

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Mol	Chain	Length	Quality of chain
2	F	106	
3	C	133	
3	G	133	
4	D	129	
4	H	129	
5	I	175	
6	J	176	
7	K	17	
8	W	97	
9	X	1368	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21387 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 Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	91	Total	C	N	O	S	0	0
			743	468	141	130	4		
1	E	90	Total	C	N	O	S	0	0
			738	465	140	129	4		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P68431
A	-2	SER	-	expression tag	UNP P68431
A	-1	HIS	-	expression tag	UNP P68431
E	-3	GLY	-	expression tag	UNP P68431
E	-2	SER	-	expression tag	UNP P68431
E	-1	HIS	-	expression tag	UNP P68431

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	81	Total	C	N	O	S	0	0
			646	407	126	112	1		
2	F	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P62805
B	-2	SER	-	expression tag	UNP P62805
B	-1	HIS	-	expression tag	UNP P62805
F	-3	GLY	-	expression tag	UNP P62805
F	-2	SER	-	expression tag	UNP P62805
F	-1	HIS	-	expression tag	UNP P62805

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	96	Total	C	N	O	0	0
			743	466	146	131		
3	G	96	Total	C	N	O	0	0
			741	465	146	130		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP P04908
C	-2	SER	-	expression tag	UNP P04908
C	-1	HIS	-	expression tag	UNP P04908
G	-3	GLY	-	expression tag	UNP P04908
G	-2	SER	-	expression tag	UNP P04908
G	-1	HIS	-	expression tag	UNP P04908

- Molecule 4 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	90	Total	C	N	O	S	0	0
			699	441	123	133	2		
4	H	90	Total	C	N	O	S	0	0
			699	441	123	133	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP P06899
D	-5	SER	-	expression tag	UNP P06899
D	-4	HIS	-	expression tag	UNP P06899
H	-6	GLY	-	expression tag	UNP P06899
H	-5	SER	-	expression tag	UNP P06899
H	-4	HIS	-	expression tag	UNP P06899

- Molecule 5 is a DNA chain called DNA (175-mer).

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	137	Total	C	N	O P	0	0
			2794	1324	512	821 137		

- Molecule 6 is a DNA chain called DNA (176-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	135	Total	C	N	O	P	0	0
			2783	1314	525	809	135		

- Molecule 7 is a DNA chain called DNA (17-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	17	Total	C	N	O	P	0	0
			351	166	65	103	17		

- Molecule 8 is a RNA chain called RNA (97-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	W	97	Total	C	N	O	P	0	0
			2072	927	376	672	97		

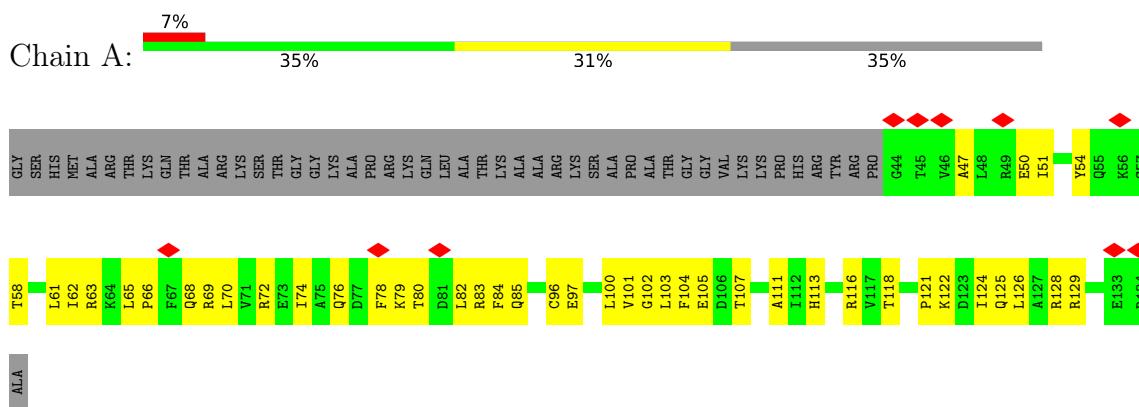
- Molecule 9 is a protein called CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	X	941	Total	C	N	O	S	0	0
			7759	4972	1352	1419	16		

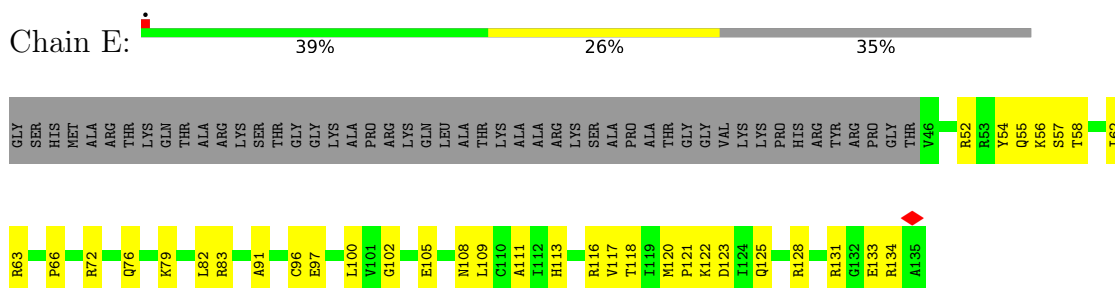
3 Residue-property plots [i](#)

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.

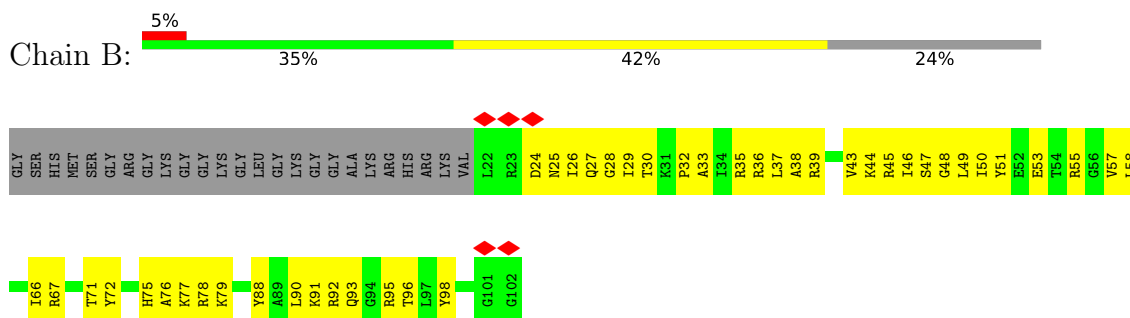
• Molecule 1: Histone H3.1



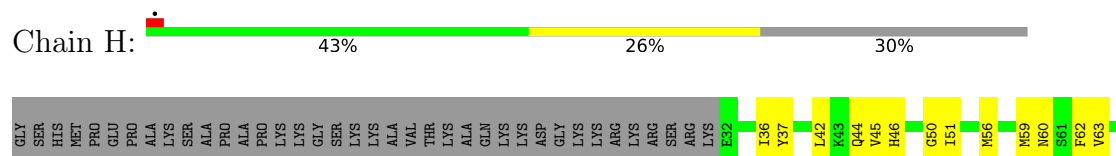
• Molecule 1: Histone H3.1



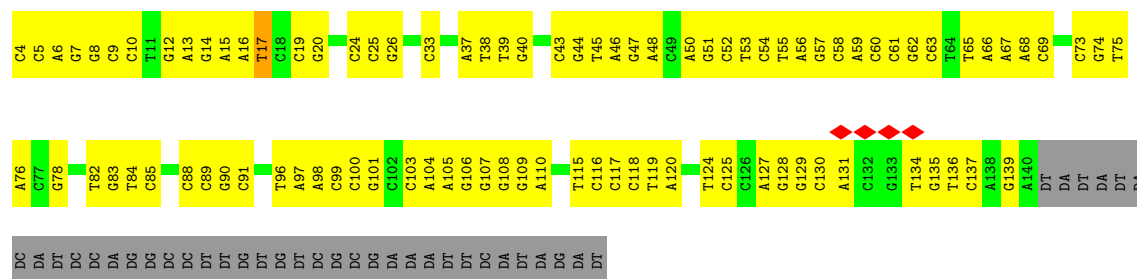
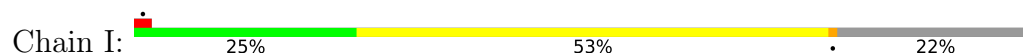
• Molecule 2: Histone H4



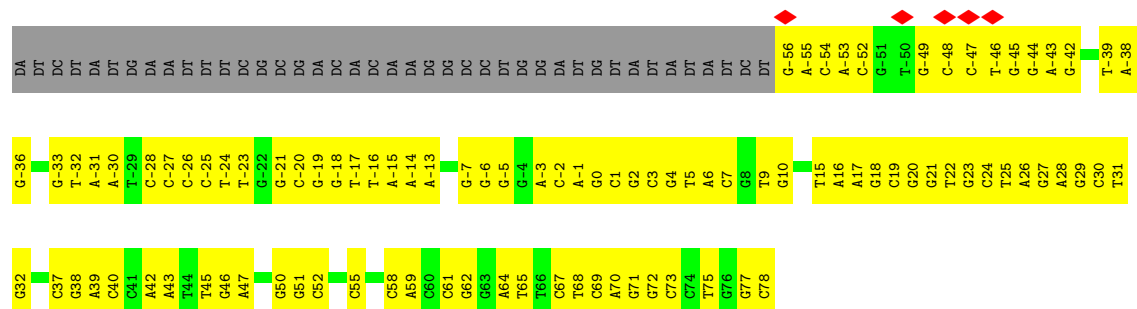
• Molecule 2: Histone H4



- Molecule 5: DNA (175-mer)



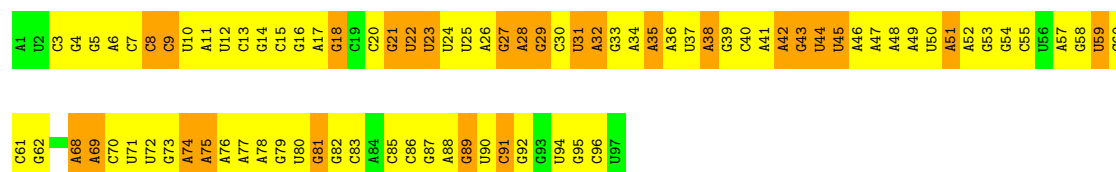
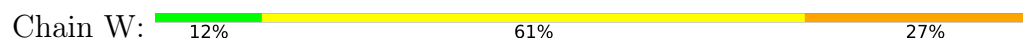
- Molecule 6: DNA (176-mer)



- Molecule 7: DNA (17-mer)



- Molecule 8: RNA (97-mer)



- Molecule 9: CRISPR-associated endonuclease Cas9/Csn1





N1308	K1222	L1144	GLY
I1309	K1223	V1146	GLU
I1310	N1224	V1147	THR
H1311	E1225	A1147	GLY
L1312	L1226		GLU
F1313		E1150	I1E
T1314	Y1232	K1151	
L1315	V1233	G1152	W1073
T1316	N1234	K1153	D1075
N1317	F1235		
L1318		S1154	
G1319	L1238	K1155	R1078
A1320	H1241	K1156	D1079
F1321	T1242	L1157	
A1322	GLU	K1161	V1083
A1323	LVS		R1084
F1324	LEU	T1166	V1085
K1325	LVS	I1167	L1087
Y1326	GLY	I1168	S1088
F1327	SER	M1169	M1089
D1328	PRO	E1170	G1090
	GLU	R1171	Q1091
	ASP		V1092
I1331	ASN	F1174	M1093
D1332	E1253	I1094	I1094
K1334	Q1254	N1177	V1095
R1335	K1255		K1096
Y1336	Q1256	D1180	K1097
		F1181	T1098
E1341	V1259	K1188	S1106
	E1260		K1107
T1346	Q1261		
L1347	H1262	K1191	F1108
I1348		K1192	S1109
	Y1285	D1193	I1110
S1351	L1266	L1194	L1111
I1352		I1195	P1112
T1353	T1269	K1196	K1113
K1354	E1271	K1197	
L1355	Q1272	L1198	A1121
E1357	T1273	P1199	
T1358	T1273	K1200	D1125
R1359	F1276	F1204	W1126
	S1277	E1205	D1127
		L1206	P1128
	V1280	E1207	K1129
	I1281	M1208	K1130
		G1209	I1131
	M1286	R1210	G1132
	L1287	G1133	
		PHE	
	Y1294	K1211	D1135
		R1212	S1136
		M1213	F1137
	K1300	L1214	T1138
		A1215	V1139
	Q1305	S1216	A1140
	A1306		Y1141
	E1307	E1219	S1142
		L1220	Y1143

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88012	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 ($e^-/\text{\AA}^2$)	54.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.728	Depositor
Minimum map value	-0.205	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.094	Depositor
Recommended contour level	0.517	Depositor
Map size ($\text{\AA}$)	304.5, 304.5, 304.5	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.5225, 1.5225, 1.5225	Depositor

5 Model quality

5.1 Standard geometry

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	A	0.16	0/751	0.35	0/1006
1	E	0.17	0/746	0.35	0/998
2	B	0.18	0/653	0.30	0/873
2	F	0.20	0/626	0.38	0/837
3	C	0.20	0/752	0.37	0/1015
3	G	0.15	0/750	0.30	0/1011
4	D	0.29	0/710	0.42	0/957
4	H	0.17	0/710	0.36	0/957
5	I	0.34	0/3131	0.64	1/4826 (0.0%)
6	J	0.36	0/3125	0.64	1/4825 (0.0%)
7	K	0.25	0/393	0.42	0/605
8	W	0.21	0/2319	0.37	0/3612
9	X	0.13	0/7900	0.29	0/10605
All	All	0.23	0/22566	0.45	2/32127 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	17	DT	O3'-P-O5'	-5.69	95.46	104.00
6	J	20	DG	O3'-P-O5'	-5.29	96.07	104.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	743	0	782	57	0
1	E	738	0	777	66	0
2	B	646	0	687	52	0
2	F	619	0	659	56	0
3	C	743	0	784	97	0
3	G	741	0	785	46	0
4	D	699	0	714	70	0
4	H	699	0	714	48	0
5	I	2794	0	1535	113	0
6	J	2783	0	1512	119	0
7	K	351	0	192	19	0
8	W	2072	0	1045	117	0
9	X	7759	0	7901	320	0
All	All	21387	0	18087	957	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 24.

The worst 5 of 957 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)
1:A:58:THR:CG2	3:G:81:ARG:HD3	1.48	1.40
9:X:5:TYR:CE1	9:X:22:THR:HG22	1.56	1.38
3:C:25:PHE:HE2	3:C:30:VAL:CG2	1.38	1.36
3:C:25:PHE:CE2	3:C:30:VAL:CG2	2.25	1.19
9:X:5:TYR:CE1	9:X:22:THR:CG2	2.30	1.14

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	A	89/139 (64%)	89 (100%)	0	0	100	100
1	E	88/139 (63%)	86 (98%)	2 (2%)	0	100	100
2	B	79/106 (74%)	77 (98%)	2 (2%)	0	100	100
2	F	76/106 (72%)	74 (97%)	2 (3%)	0	100	100
3	C	94/133 (71%)	91 (97%)	3 (3%)	0	100	100
3	G	94/133 (71%)	94 (100%)	0	0	100	100
4	D	88/129 (68%)	85 (97%)	3 (3%)	0	100	100
4	H	88/129 (68%)	85 (97%)	3 (3%)	0	100	100
9	X	913/1368 (67%)	884 (97%)	29 (3%)	0	100	100
All	All	1609/2382 (68%)	1565 (97%)	44 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	X	797/1227 (65%)	797 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
9	X	1234	ASN
9	X	1256	GLN
9	X	723	HIS
9	X	739	GLN
9	X	940	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	W	96/97 (98%)	27 (28%)	4 (4%)

5 of 27 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	W	9	C
8	W	18	G
8	W	21	G
8	W	22	U
8	W	23	U

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	W	8	C
8	W	27	G
8	W	42	A
8	W	68	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

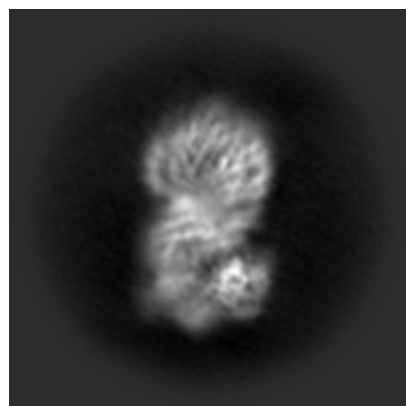
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39431. These allow visual inspection of the internal detail of the map and identification of artifacts.

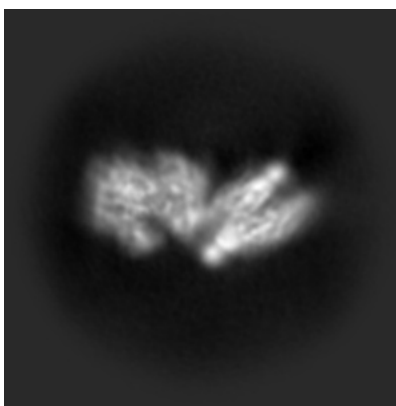
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

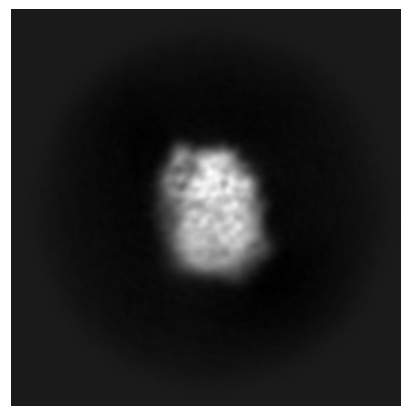
6.1.1 Primary map



X

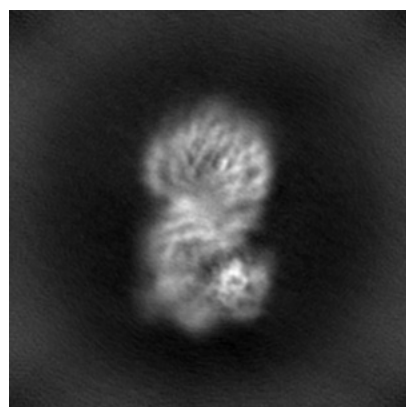


Y

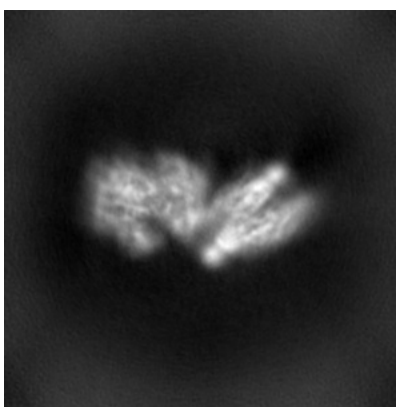


Z

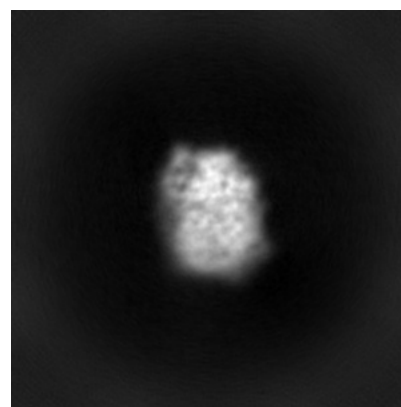
6.1.2 Raw map



X



Y

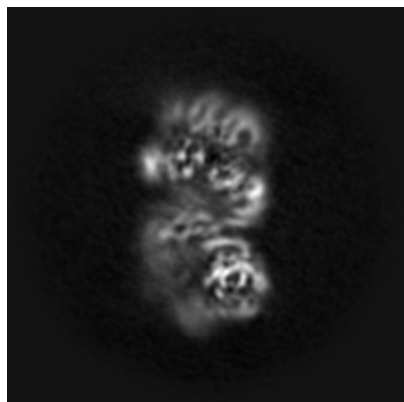


Z

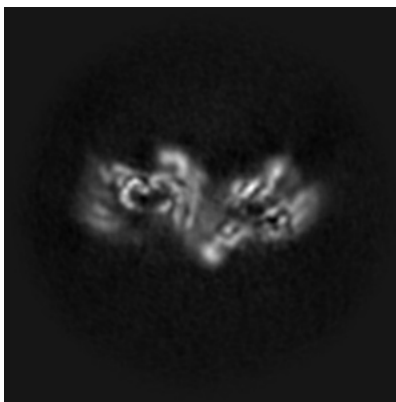
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

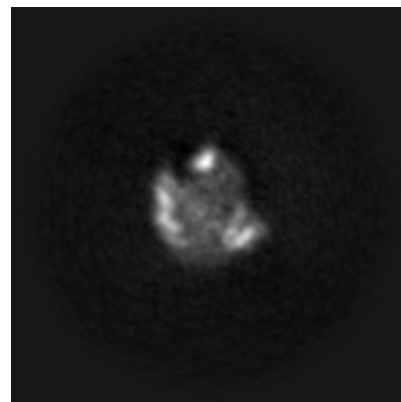
6.2.1 Primary map



X Index: 100

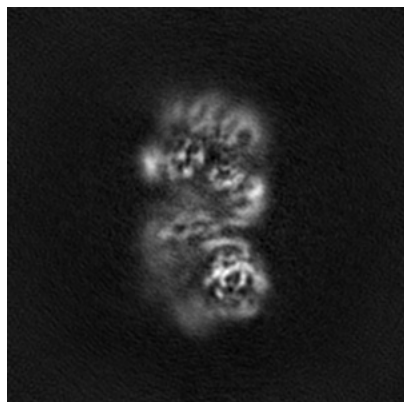


Y Index: 100

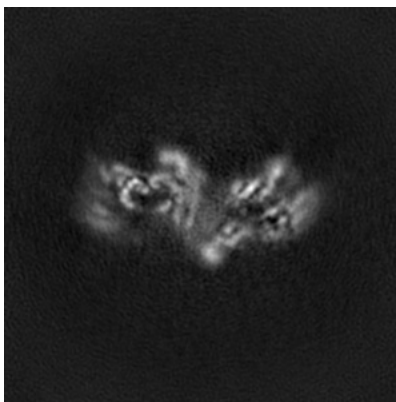


Z Index: 100

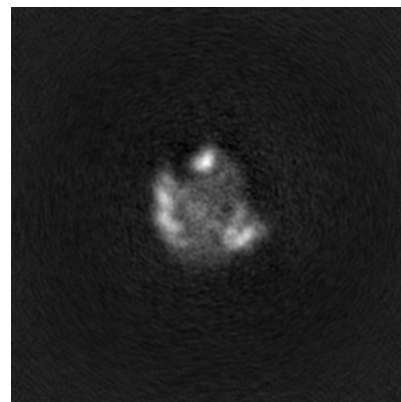
6.2.2 Raw map



X Index: 100



Y Index: 100

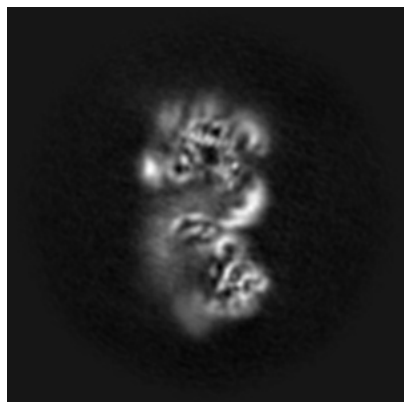


Z Index: 100

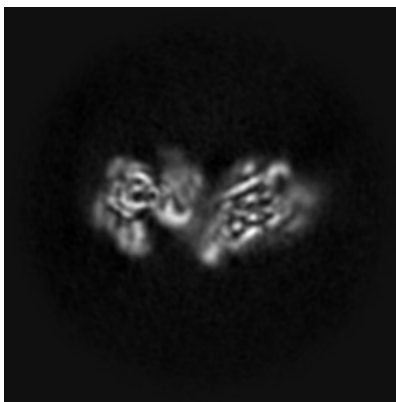
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

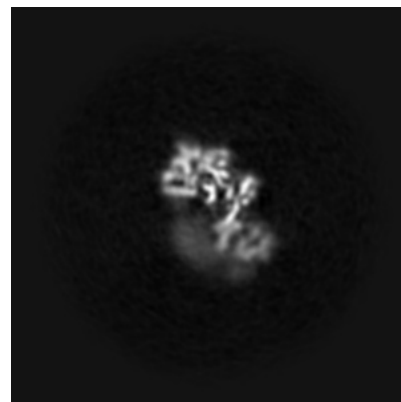
6.3.1 Primary map



X Index: 97

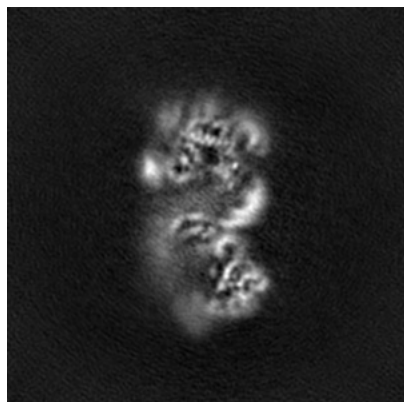


Y Index: 107

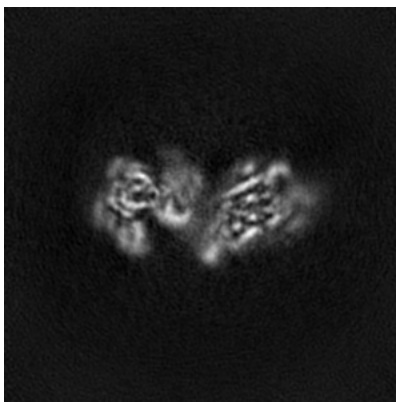


Z Index: 66

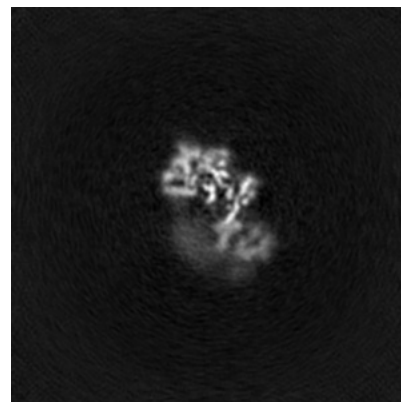
6.3.2 Raw map



X Index: 97



Y Index: 107

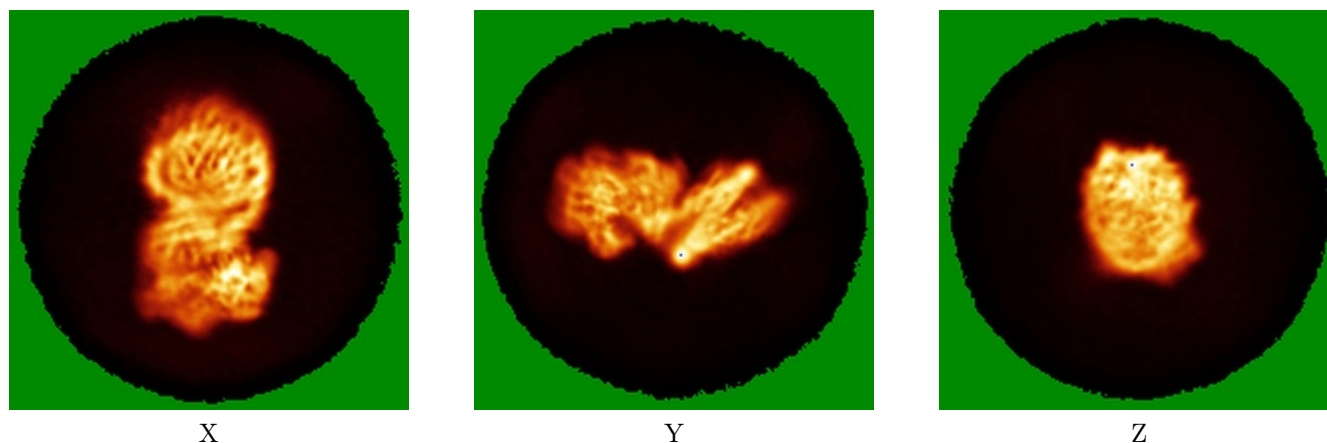


Z Index: 66

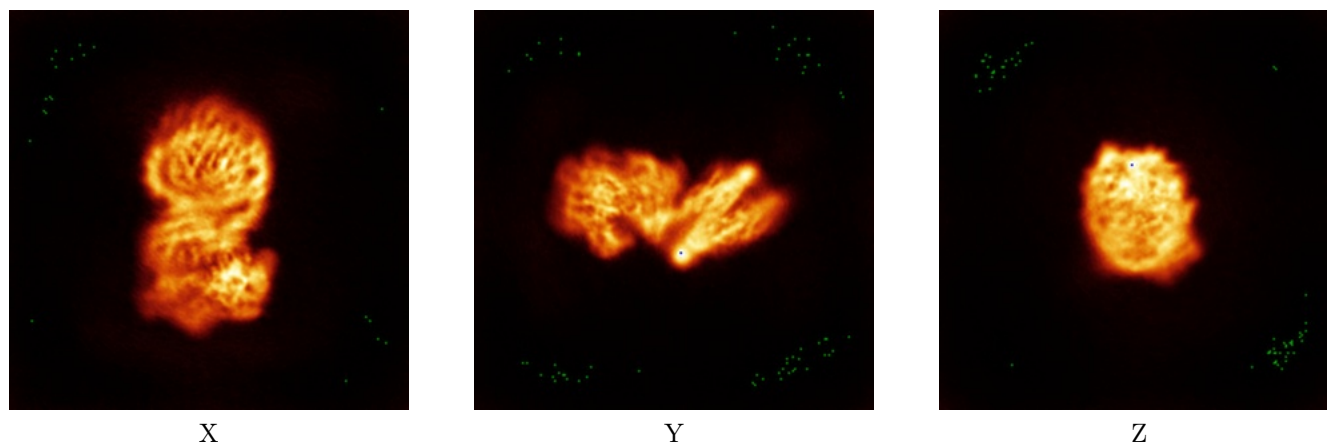
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

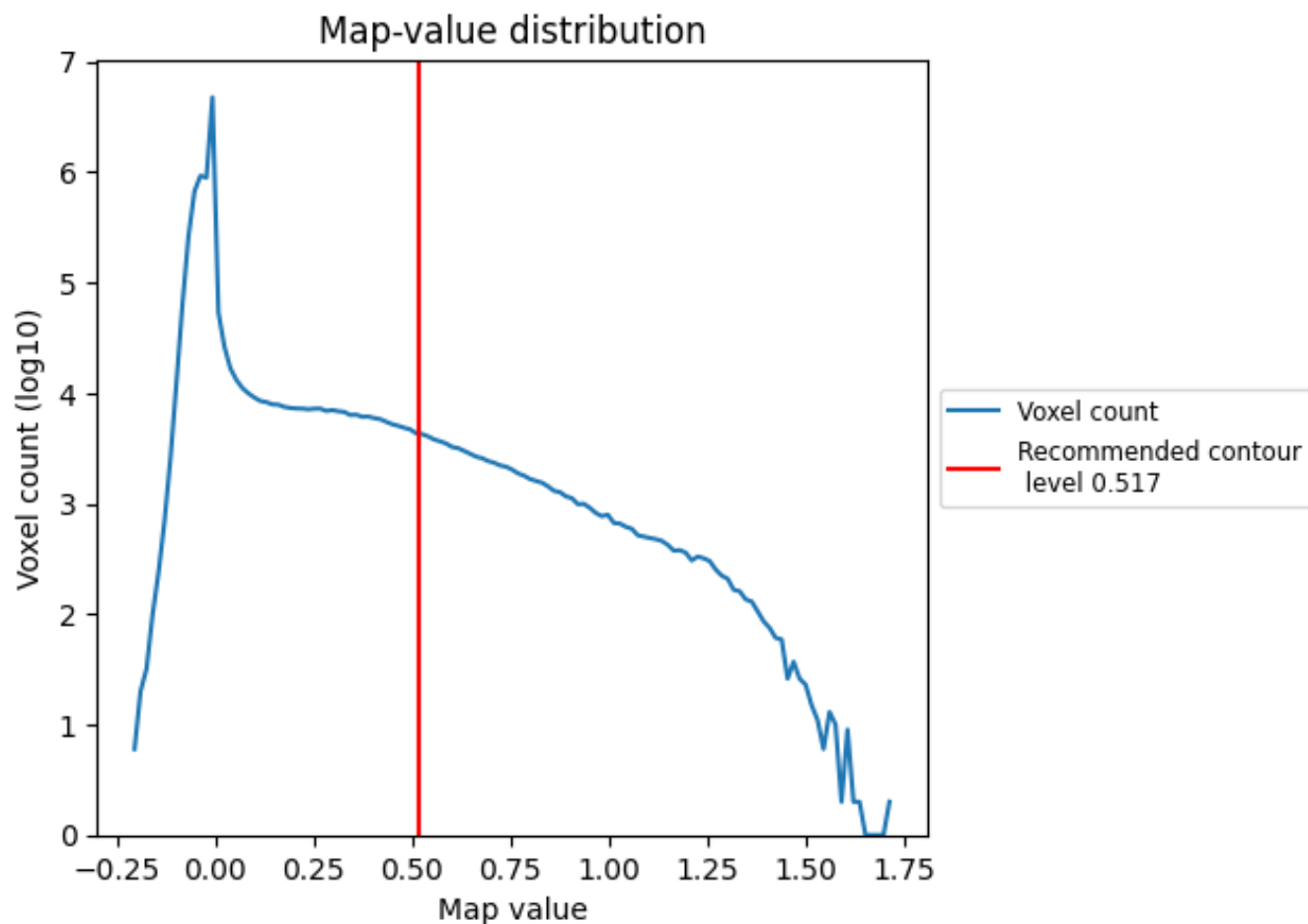
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

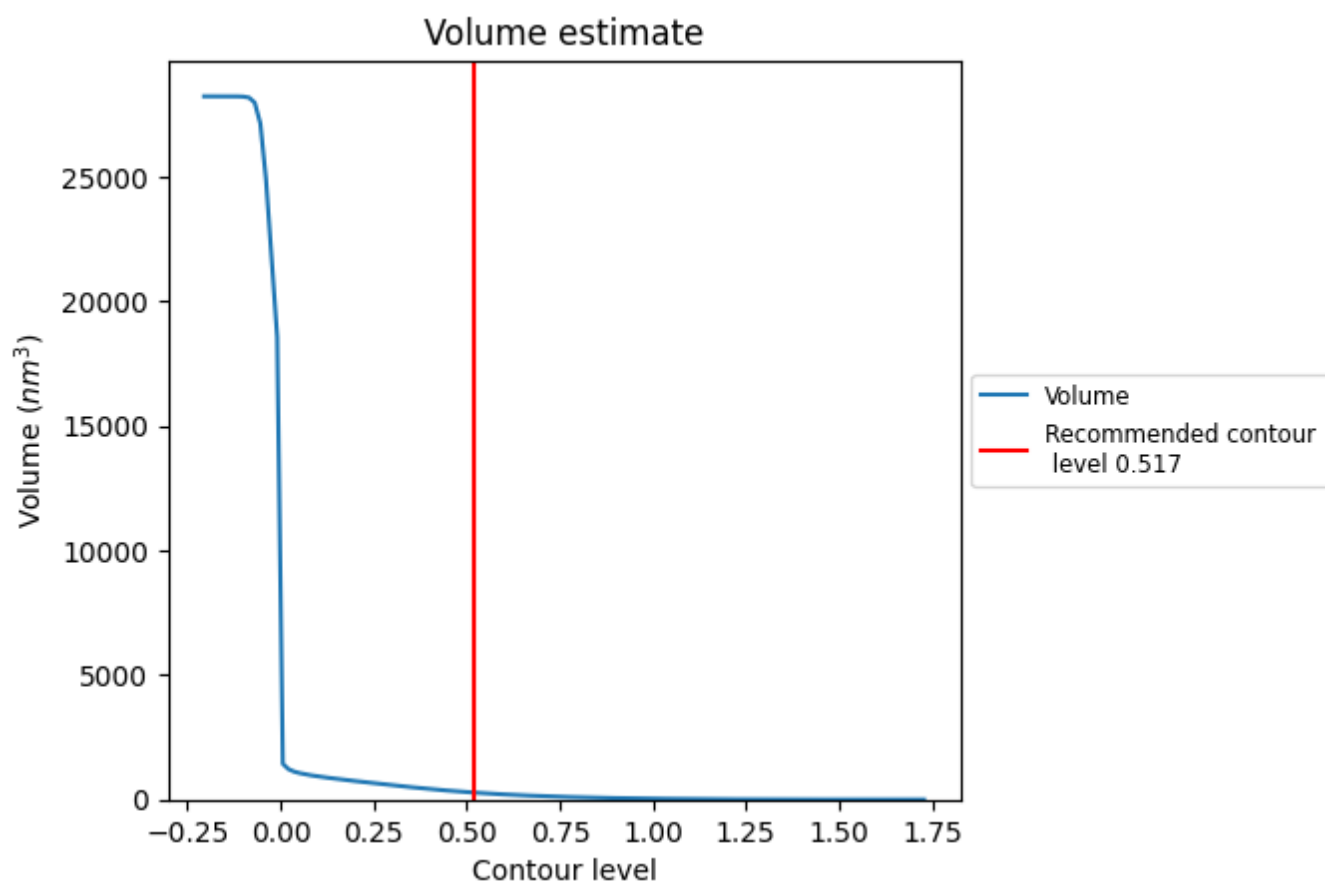
This section contains the results of statistical analysis of the map.

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.

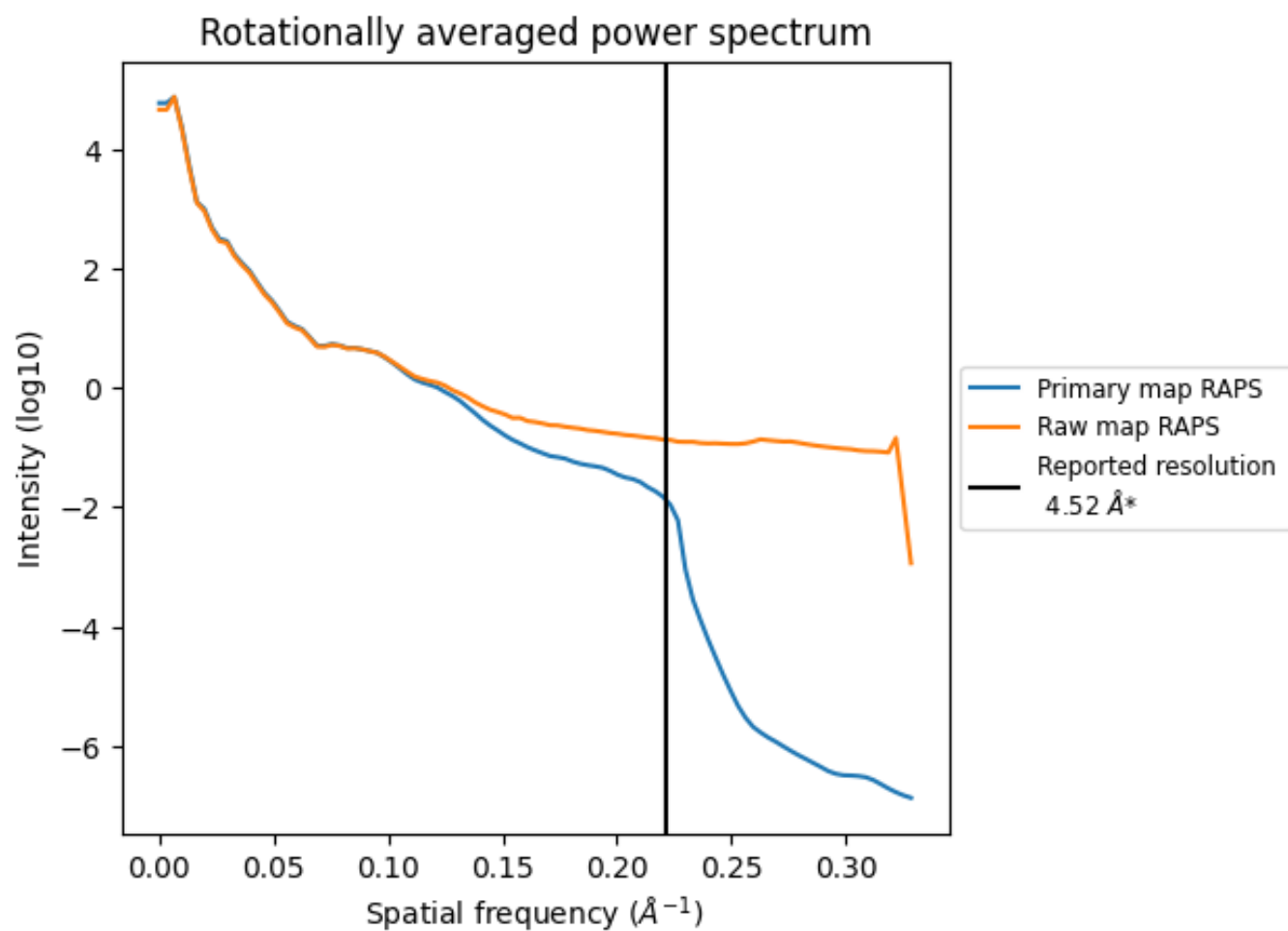
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 283 nm³; this corresponds to an approximate mass of 255 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

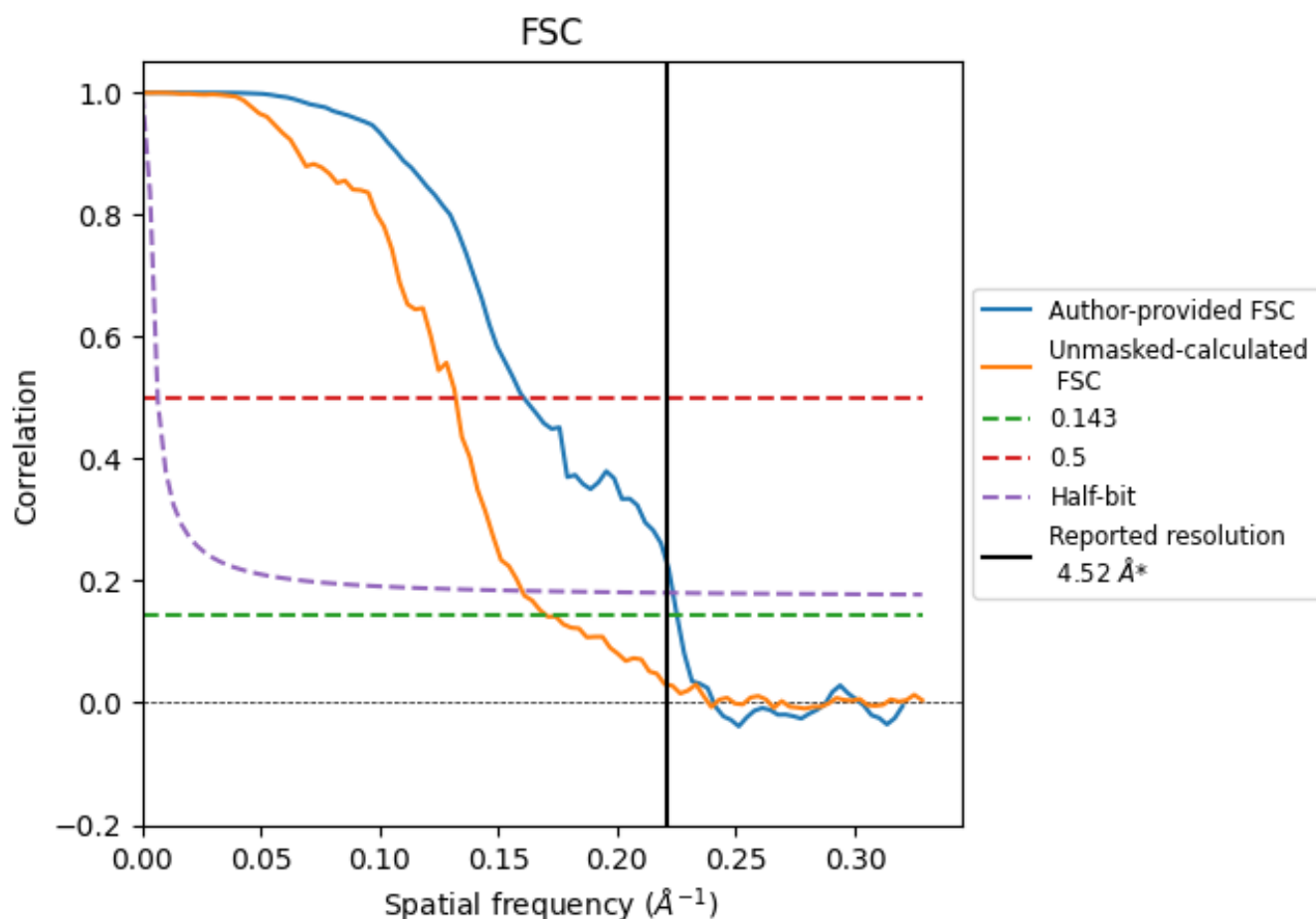


*Reported resolution corresponds to spatial frequency of 0.221 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.221 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.52	-	-
Author-provided FSC curve	4.44	6.23	4.47
Unmasked-calculated*	5.88	7.58	6.25

*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 5.88 differs from the reported value 4.52 by more than 10 %

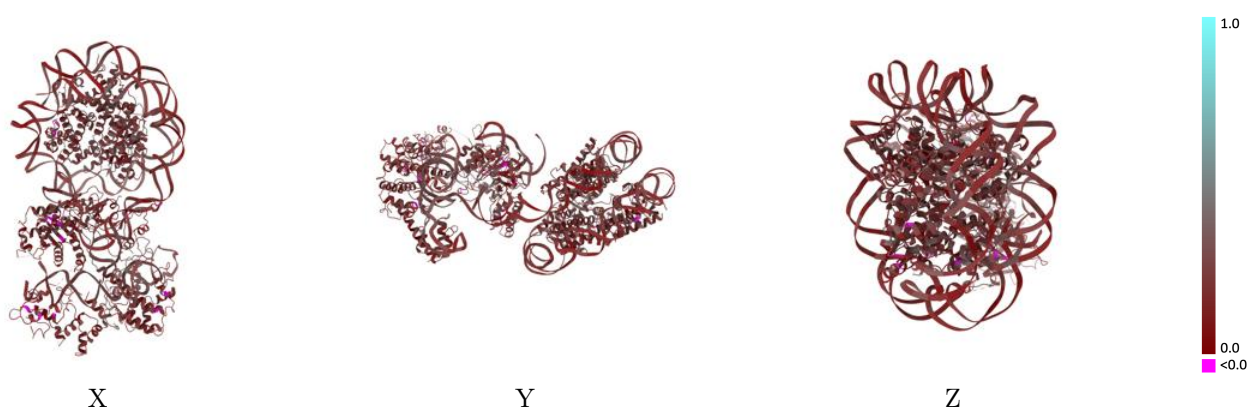
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-39431 and PDB model 8YNY. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

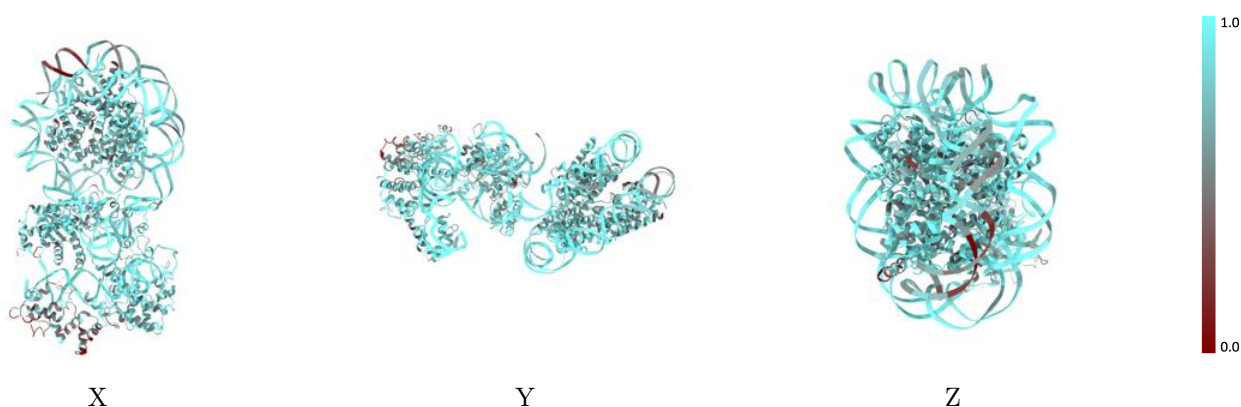
This section was not generated.

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



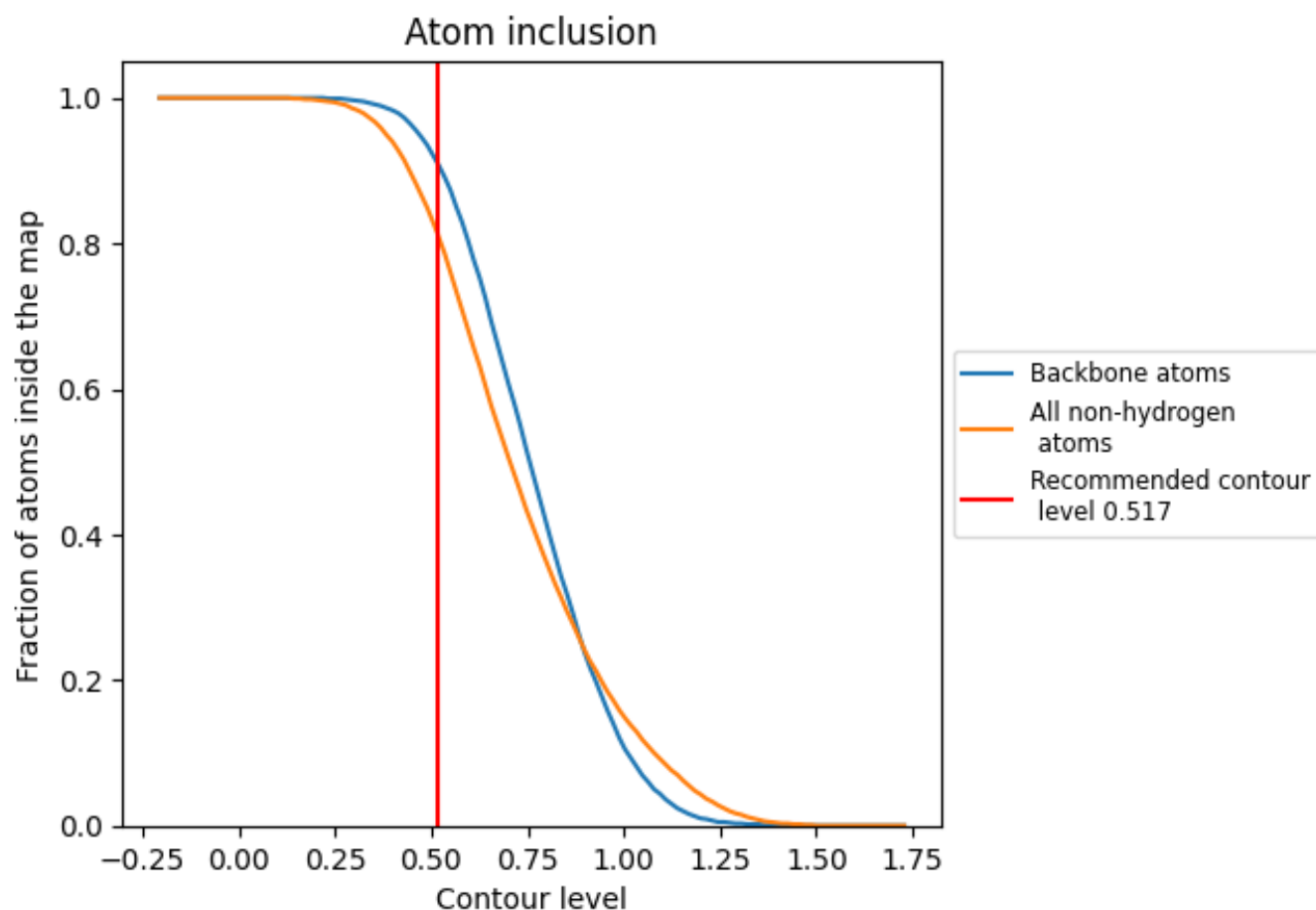
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.517).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 81% 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 (0.517) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8130	 0.2180
A	 0.7740	 0.2070
B	 0.7770	 0.2230
C	 0.8110	 0.2350
D	 0.8160	 0.2520
E	 0.8340	 0.2180
F	 0.8660	 0.2260
G	 0.7390	 0.2270
H	 0.7720	 0.2260
I	 0.8360	 0.2060
J	 0.8500	 0.1970
K	 0.9430	 0.2760
W	 0.9610	 0.2720
X	 0.7540	 0.2070

