



wwPDB EM Validation Summary Report ⓘ

Mar 14, 2026 – 04:47 AM UTC

PDB ID : 8PBL / pdb_00008pbl
EMDB ID : EMD-17586
Title : E. coli RNA polymerase elongation complex stalled at thymine dimer lesion
Authors : Woodgate, J.; Zenkin, N.
Deposited on : 2023-06-09
Resolution : 2.87 Å(reported)
Based on initial models : 8FVR, 1SL2

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:

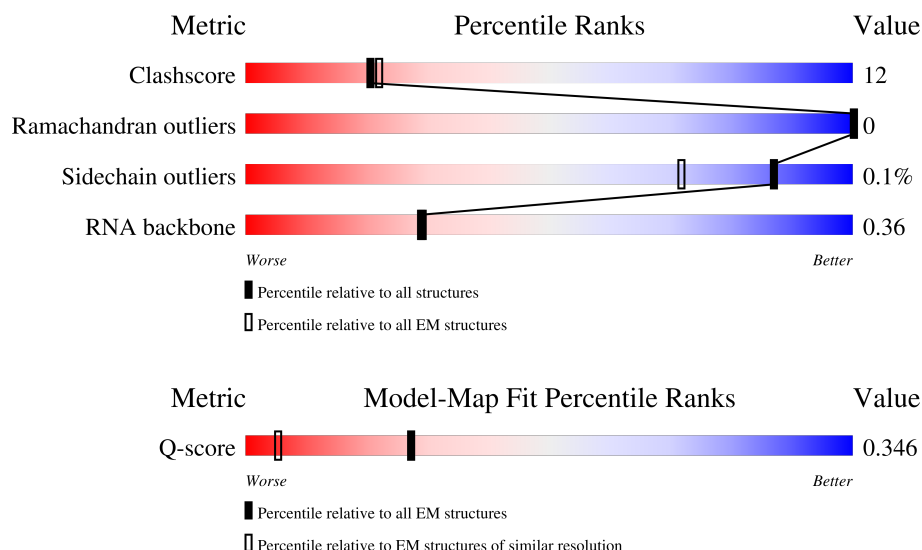
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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 2.87 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.



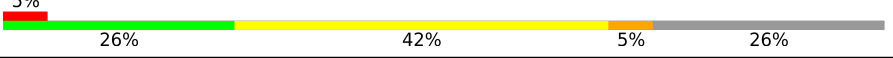
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12062 (2.37 - 3.37)

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	49	
2	B	49	
3	D	239	

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Mol	Chain	Length	Quality of chain
3	E	239	
4	F	1342	
5	G	1407	
6	H	91	
7	R	19	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 26261 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 DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	27	Total	C	N	O	P	0	0
			557	264	111	156	26		

- Molecule 2 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	27	Total	C	N	O	P	0	0
			563	270	96	170	27		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	229	Total	C	N	O	S	0	0
			1779	1108	316	349	6		
3	E	220	Total	C	N	O	S	0	0
			1695	1057	299	333	6		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	236	VAL	-	expression tag	UNP A0A5B9AW69
D	237	LEU	-	expression tag	UNP A0A5B9AW69
D	238	PHE	-	expression tag	UNP A0A5B9AW69
D	239	GLN	-	expression tag	UNP A0A5B9AW69
E	236	VAL	-	expression tag	UNP A0A5B9AW69
E	237	LEU	-	expression tag	UNP A0A5B9AW69
E	238	PHE	-	expression tag	UNP A0A5B9AW69
E	239	GLN	-	expression tag	UNP A0A5B9AW69

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	1319	Total	C	N	O	S	3	0
			10427	6544	1820	2019	44		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	1330	Total	C	N	O	S	0	0
			10352	6506	1846	1950	50		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	73	Total	C	N	O	S	0	0
			582	355	111	115	1		

- Molecule 7 is a RNA chain called mRNA.

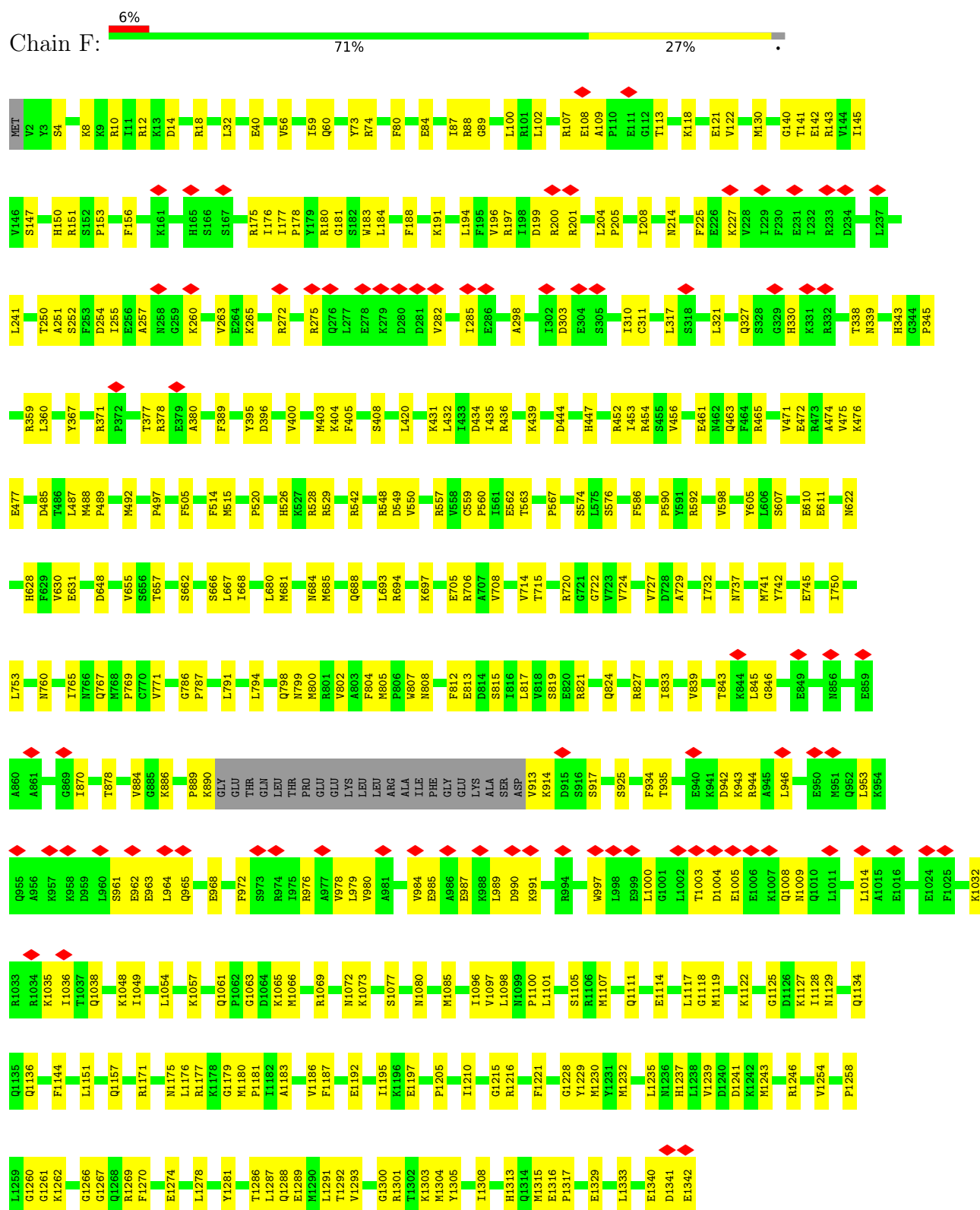
Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	14	Total	C	N	O	P	0	0
			303	135	57	97	14		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
8	G	2	Total	Zn	0
			2	2	

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	R	1	Total	Mg	0
			1	1	

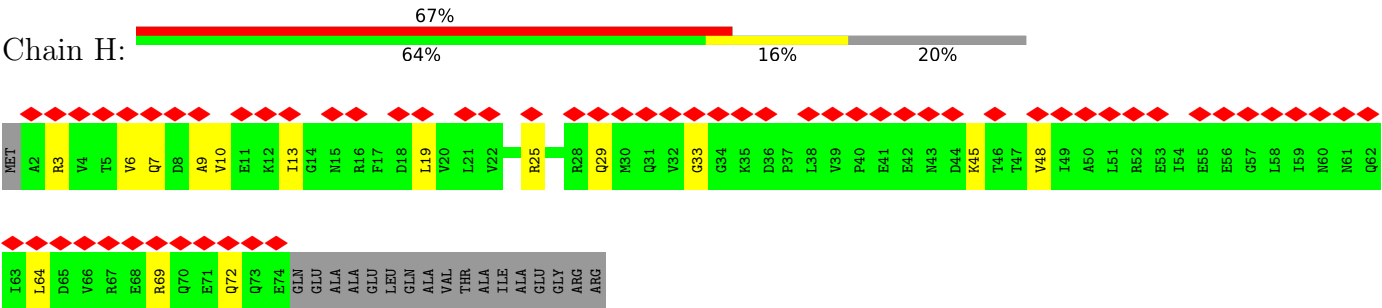


• Molecule 5: DNA-directed RNA polymerase subunit beta'

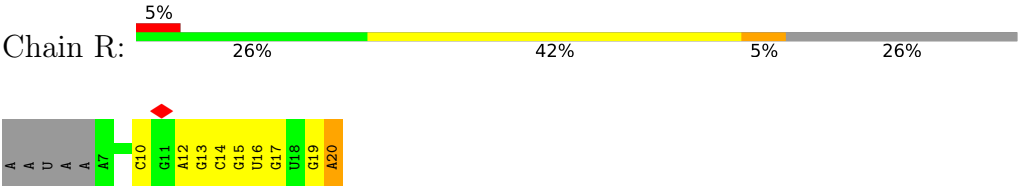


L1356	E1146	I1233	L1074	R978	S887	F773	T674	M485	R362	R259	R123	MET
H1366	A1147	V1237	K1079	N979	G893	T776	A675	S486	L363	T260	L287	LYS
R1373	R1149	Q1238	P1150	E981	V894	K789	G677	T487	H364	A261	L126	ASP
ALA	P1151	Y1241	V1081	R990	G900	G794	V682	K570	G367	T262	D129	LEU
ALA	E1152	V1246	D1082	E993	R901	L800	I685	V574	K370	S263	L132	PHE
GLY	A1154	K1247	Q1084	D902	L903	L800	I685	L579	M371	L265	R133	LEU
ALA	E1158	D1250	G1085	V1002	L903	L800	I685	Y589	A373	N266	D134	LYS
PRO	G1161	K1251	D1086	L1003	H907	V803	M697	S590	L374	R275	V138	GLN
ALA	F1165	V1255	D1087	A1004	T908	A804	M698	I591	K378	R278	V146	THR
PRO	I1173	I1256	D1088	K1005	T909	Q805	D699	Q594	P379	E148	I147	LYS
GLN	R1174	V1257	L1089	E1009	E925	D806	N700	S503	E402	R281	I147	THR
VAL	R1175	R1258	T1090	G1014	G924	L807	Q702	Q504	L282	L282	G149	GLU
ALA	V1176	Q1259	P1091	D1021	E925	D813	T703	V507	A286	A286	G150	D18
ASP	T1177	R1263	D1094	P1021	P926	C814	E704	L508	I291	I291	L154	I22
ALA	T1178	K1262	M1025	M1025	T931	E818	V706	G509	I416	I416	E155	A23
ALA	P1179	F1274	M1025	M1025	N932	M822	I707	L510	R417	R417	L156	L24
ASP	VAL	E1278	Y1099	I1028	ARG	V825	E713	M513	L423	L423	Q157	A25
GLY	ASP	G1279	F1100	I1028	THR	V825	E714	T514	M424	M424	Q158	S26
LEU	GLY	V1280	L1101	R1036	PHE	G829	K715	R515	R425	R425	E162	M29
GLU	SER	E1281	D1184	F1037	ILE	G829	K716	D516	L429	L429	L166	I30
LEU	D1186	L1292	K1104	T1038	GLY	R836	V717	R610	H430	H430	I44	T43
ASN	Y1186	L1292	A1105	T1038	GLY	R836	Y723	K615	R431	R431	L169	I44
ALA	E1187	K1297	I1106	D1039	ALA	R838	M724	P616	L432	L432	E211	P51
GLY	K1192	V1298	L1109	M1040	SER	D847	S728	F620	P439	P439	R311	P51
LEU	H1193	G1299	E1110	I1041	ARG	V848	R731	I624	V440	V440	G313	D54
GLY	R1194	D1305	D1111	D1042	ALA	K850	G732	I624	I442	I442	R314	G55
SER	Q1195	G1308	G1112	G1043	ALA	T856	S733	A633	E443	E443	K219	L56
ASP	L1196	I1309	V1113	Q1044	GLU	L857	A734	I221	G444	G444	R220	R60
ASN	F1199	F1319	Q1114	T1045	S946	V858	A735	A446	K445	K445	K222	G83
E1202	E1202	E1327	I1115	T1047	Q951	H861	Q736	I447	I447	I447	P227	R77
R1203	R1203	T1328	S1117	R1048	L960	L864	I737	Q448	Q448	Q448	P234	L78
I1210	I1210	E1334	G1118	Q1049	S961	H865	R738	A459	A459	A459	M237	K79
D1212	D1212	A1335	D1119	T1050	S961	H865	Q739	D462	D462	D462	I238	G82
P1214	P1214	G1336	R1123	D1051	R962	E866	A741	G463	G463	G463	L239	R98
E1215	E1215	V1337	I1124	E1052	R962	Q867	M743	S539	S539	S539	P243	R99
A1216	A1216	D1342	Q1126	T1054	S965	W868	G745	G540	M466	M466	V244	M102
D1219	D1219	G1346	GLU	G1055	V966	C969	L746	S543	A467	A467	L245	T111
R1222	R1222	K1348	SER	L1056	V967	D870	L746	A546	V468	V468	P246	A112
L1223	L1223	E1349	GLY	S1057	N968	L871	L746	A546	L472	L472	P247	H113
V1226	V1226	N1350	THR	L1057	S970	L872	P750	A546	T473	T473	R250	I114
I1230	I1230	V1351	LYS	L1057	G971	V877	P758	K549	A476	A476	V253	W115
			ASP	L1057	K972	D878	I759	E662	E479	E479	P254	F116
			THR	L1057	L973	R883	P763	E663	A482	A482	L255	L117
			THR	E1066	V974	S885	R764	Q667	E554	E554	D256	K118
			G1136	T1067	T975	V886						
			P1139	T1068	T976							
			D1143	A1069	S977							
			L1144	G1070								
			F1145	G1071								
				K1072								
				D1073								

● Molecule 6: DNA-directed RNA polymerase subunit omega



● Molecule 7: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	131098	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	240000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.026	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.00102	Depositor
Map size (Å)	287.0, 287.0, 287.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.574, 0.574, 0.574	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, MG, TTD

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	0.18	0/626	0.36	0/963
2	B	0.51	2/583 (0.3%)	1.02	4/894 (0.4%)
3	D	0.16	0/1801	0.35	0/2440
3	E	0.15	0/1714	0.39	0/2322
4	F	0.18	0/10602	0.39	1/14303 (0.0%)
5	G	0.17	0/10508	0.40	2/14185 (0.0%)
6	H	0.10	0/584	0.32	0/786
7	R	0.14	0/339	0.24	0/527
All	All	0.18	2/26757 (0.0%)	0.42	7/36420 (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
5	G	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	13	DA	O4'-C1'	6.96	1.55	1.41
2	B	13	DA	C5'-C4'	5.88	1.64	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	13	DA	C5'-C4'-C3'	-21.72	82.32	114.90
2	B	13	DA	C4'-C3'-O3'	11.84	127.76	110.00
2	B	13	DA	C5'-C4'-O4'	-7.44	98.24	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	13	DA	C1'-O4'-C4'	-6.16	100.47	109.70
5	G	504	GLN	CB-CA-C	-5.53	109.71	117.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	G	901	ARG	Sidechain

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	557	0	304	21	0
2	B	563	0	318	30	0
3	D	1779	0	1806	23	0
3	E	1695	0	1726	35	0
4	F	10427	0	10455	271	0
5	G	10352	0	10575	306	0
6	H	582	0	593	10	0
7	R	303	0	152	7	0
8	G	2	0	0	0	0
9	R	1	0	0	0	0
All	All	26261	0	25929	628	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 12.

The worst 5 of 628 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)
3:E:47:LEU:HD12	3:E:183:ILE:CD1	1.54	1.35
3:E:47:LEU:CD1	3:E:183:ILE:HD12	1.67	1.24
4:F:1333:LEU:HD21	5:G:115:TRP:CH2	1.76	1.19
3:D:43:LEU:O	3:D:47:LEU:HD13	1.47	1.13
3:E:47:LEU:CD1	3:E:183:ILE:CD1	2.26	1.13

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	D	227/239 (95%)	225 (99%)	2 (1%)	0	100	100
3	E	216/239 (90%)	209 (97%)	7 (3%)	0	100	100
4	F	1318/1342 (98%)	1278 (97%)	40 (3%)	0	100	100
5	G	1322/1407 (94%)	1281 (97%)	41 (3%)	0	100	100
6	H	71/91 (78%)	69 (97%)	2 (3%)	0	100	100
All	All	3154/3318 (95%)	3062 (97%)	92 (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	
3	D	197/206 (96%)	197 (100%)	0	100	100
3	E	188/206 (91%)	188 (100%)	0	100	100
4	F	1141/1157 (99%)	1140 (100%)	1 (0%)	88	97
5	G	1116/1168 (96%)	1114 (100%)	2 (0%)	87	96
6	H	63/75 (84%)	63 (100%)	0	100	100
All	All	2705/2812 (96%)	2702 (100%)	3 (0%)	87	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	327	GLN
5	G	901	ARG
5	G	951	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
5	G	771	GLN
5	G	865	HIS
5	G	1367	GLN
4	F	1061	GLN
4	F	952	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	R	13/19 (68%)	3 (23%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	R	10	C
7	R	19	G
7	R	20	A

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	TTD	B	14	2	42,45,46	1.38	9 (21%)	61,74,77	2.64	22 (36%)

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	TTD	B	14	2	-	12/22/109/110	0/5/6/6

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	14	TTD	C5-C6	3.63	1.59	1.55
2	B	14	TTD	C2T-N3T	-3.19	1.32	1.38
2	B	14	TTD	C2-N3	-2.79	1.33	1.38
2	B	14	TTD	C6T-C6	2.69	1.64	1.56
2	B	14	TTD	C1R-N1T	-2.61	1.42	1.45

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	14	TTD	C2R-C1R-N1T	-7.63	105.28	115.59
2	B	14	TTD	O3'-C3'-C2R	-7.58	84.52	110.88
2	B	14	TTD	C6T-C6-N1	4.87	136.70	118.51
2	B	14	TTD	C5T-C5-C4	4.63	127.88	112.84
2	B	14	TTD	O4R-C1R-N1T	4.59	114.09	108.65

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	14	TTD	O4'-C1'-N1-C2
2	B	14	TTD	C5R-O5R-PB-O4P
2	B	14	TTD	O4'-C1'-N1-C6
2	B	14	TTD	O4R-C4'-C5R-O5R
2	B	14	TTD	C2'-C1'-N1-C6

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	14	TTD	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

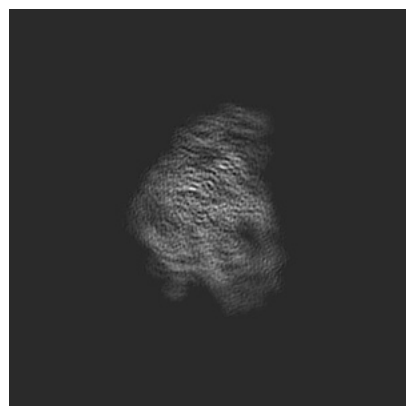
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17586. These allow visual inspection of the internal detail of the map and identification of artifacts.

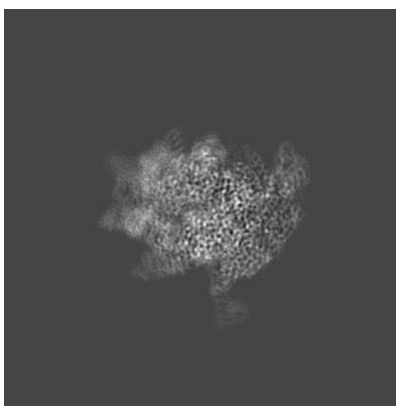
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

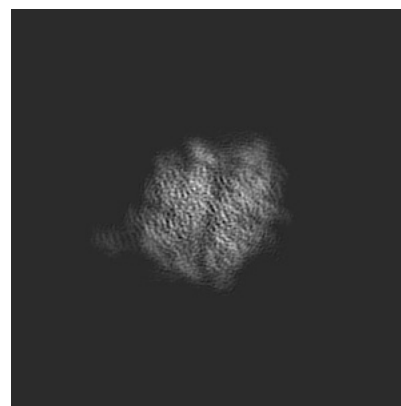
6.1.1 Primary map



X

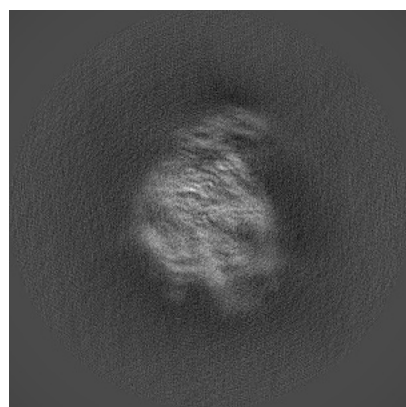


Y

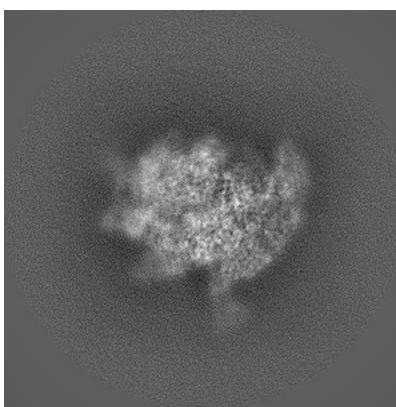


Z

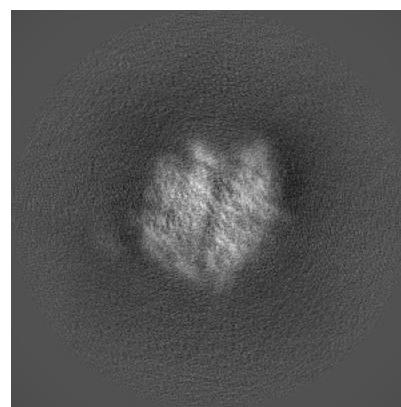
6.1.2 Raw map



X



Y

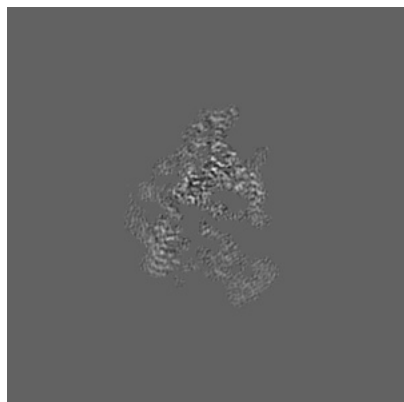


Z

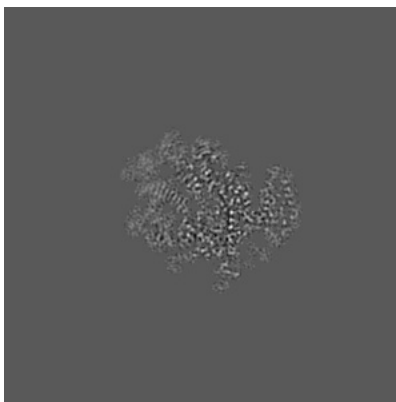
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

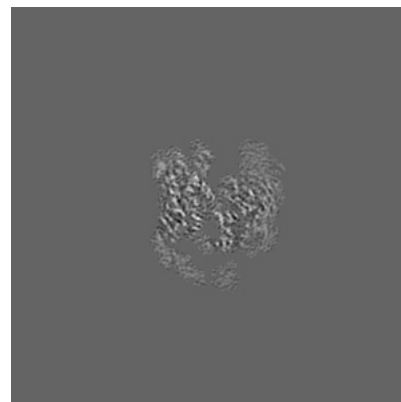
6.2.1 Primary map



X Index: 250

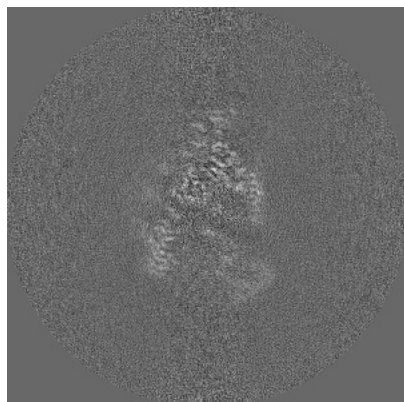


Y Index: 250

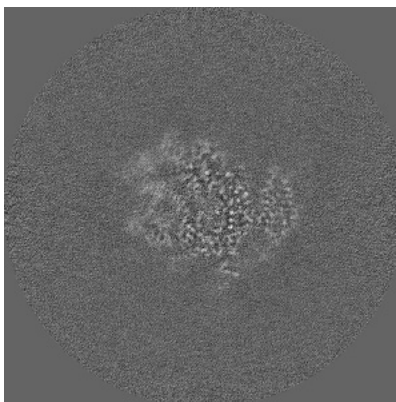


Z Index: 250

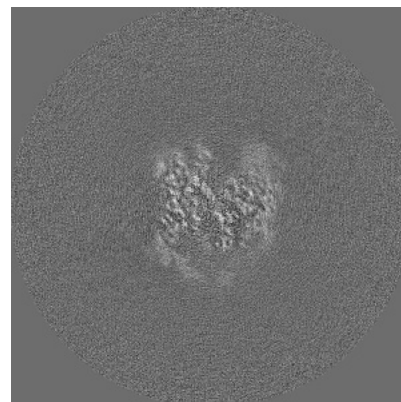
6.2.2 Raw map



X Index: 250



Y Index: 250

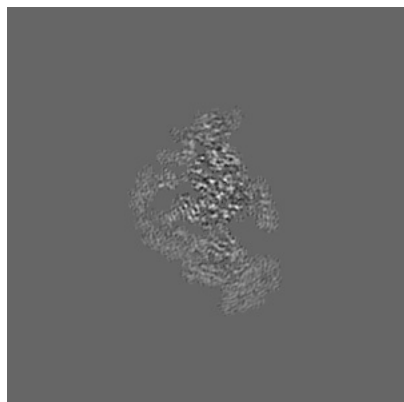


Z Index: 250

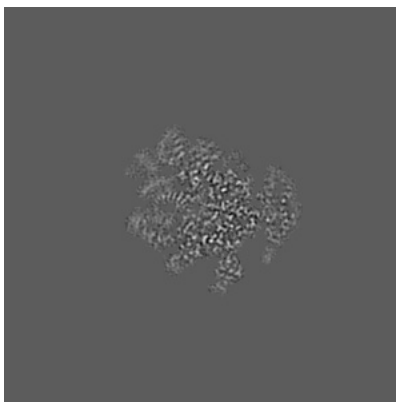
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

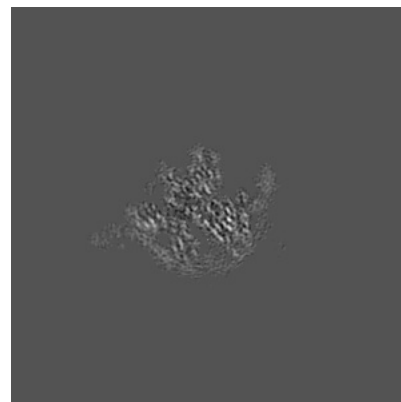
6.3.1 Primary map



X Index: 230

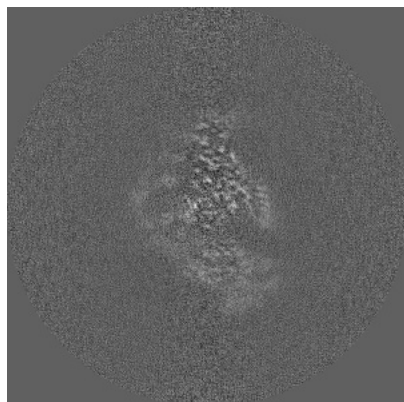


Y Index: 245

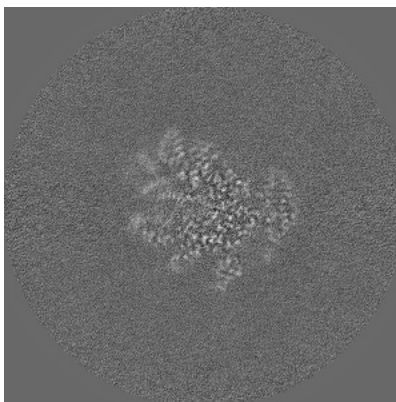


Z Index: 275

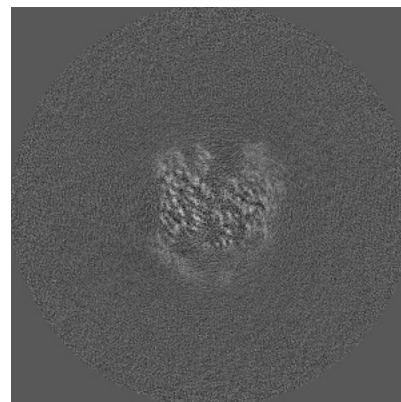
6.3.2 Raw map



X Index: 233



Y Index: 245

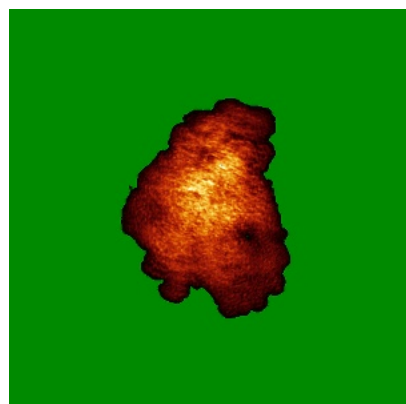


Z Index: 251

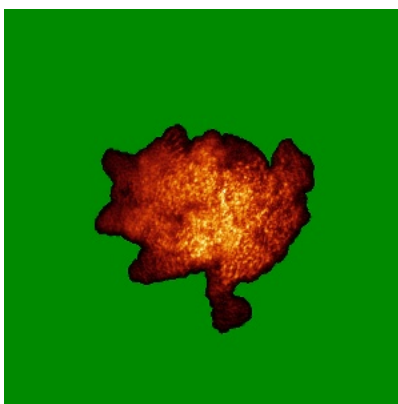
The images above show the largest variance slices of the map in three orthogonal directions.

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

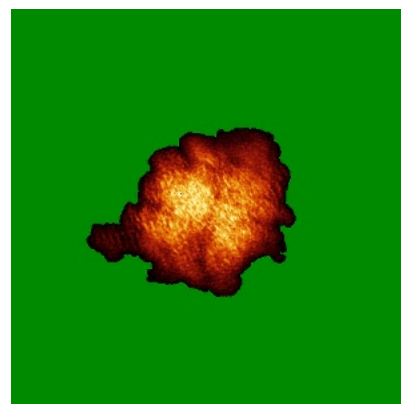
6.4.1 Primary map



X

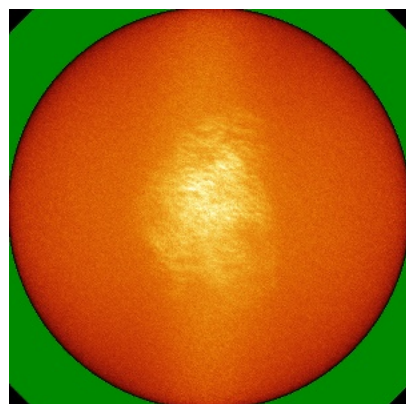


Y

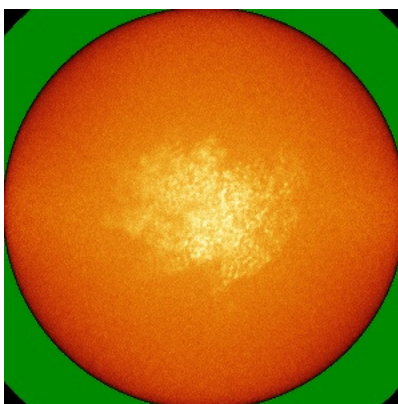


Z

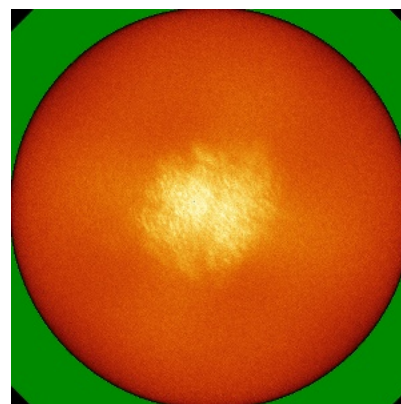
6.4.2 Raw map



X



Y

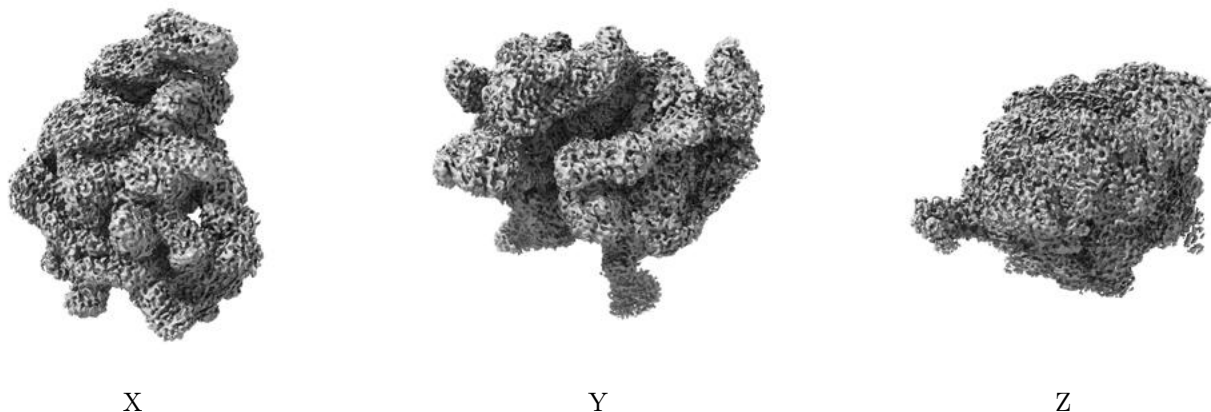


Z

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

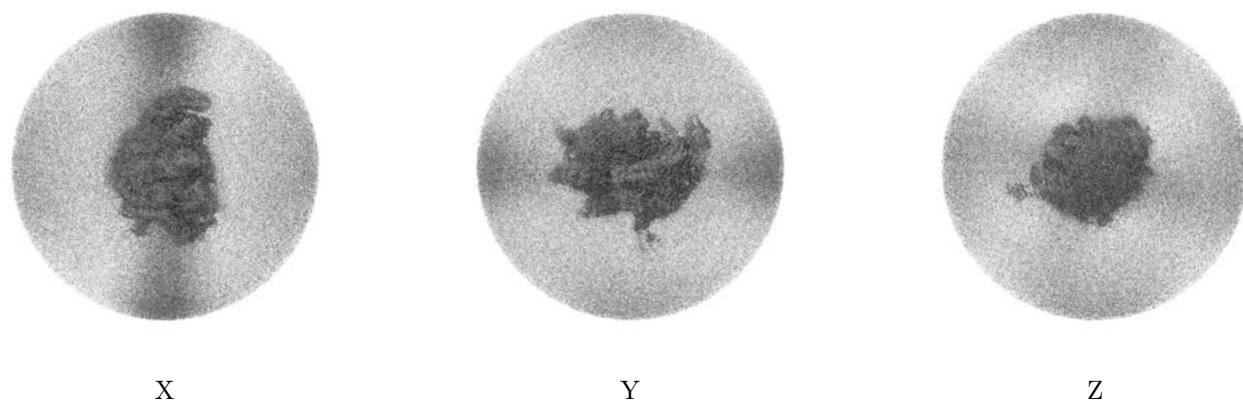
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00102. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

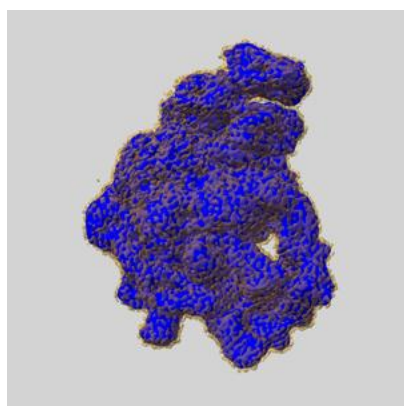
6.6 Mask visualisation [i](#)

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

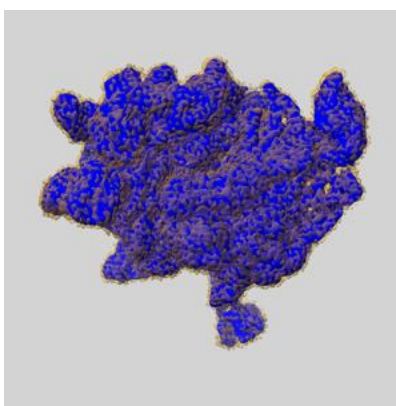
A mask typically either:

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

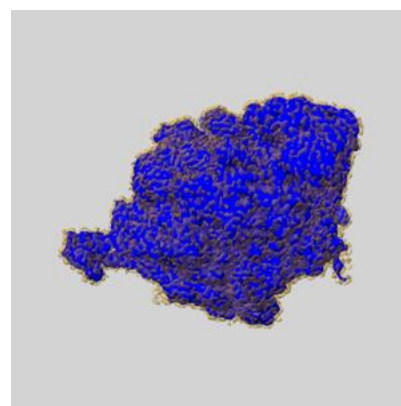
6.6.1 emd_17586_msk_1.map [i](#)



X



Y

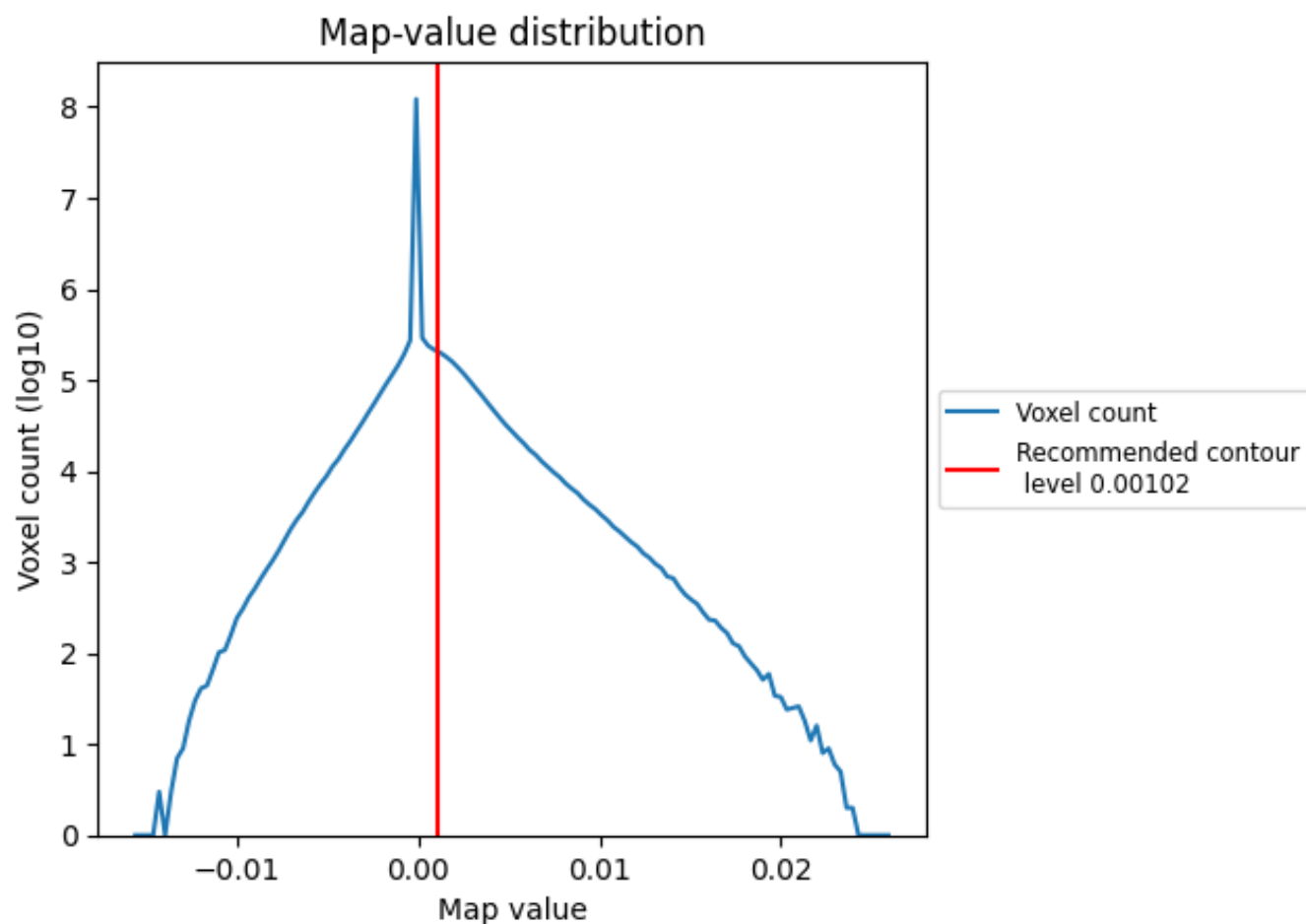


Z

7 Map analysis [i](#)

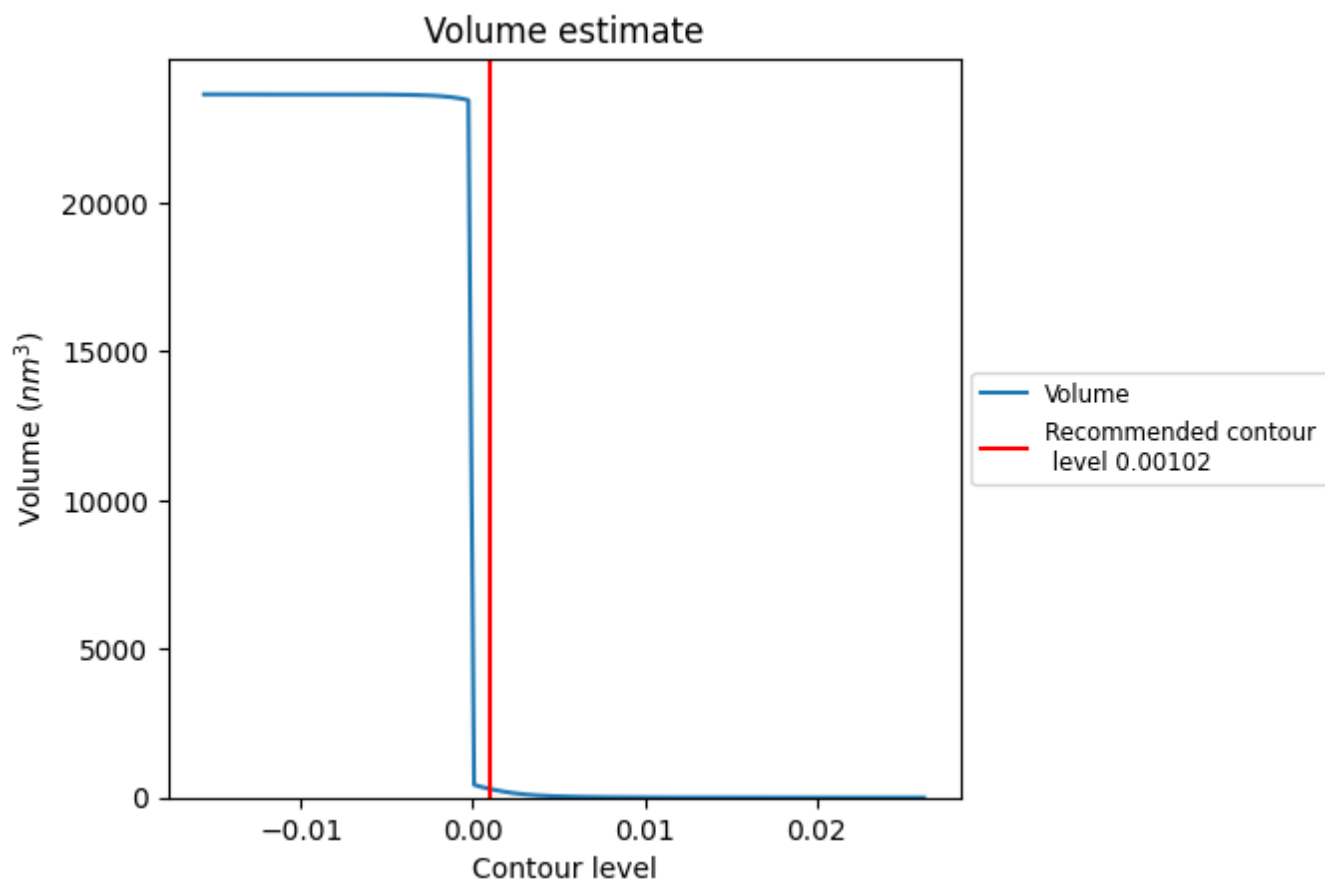
This section contains the results of statistical analysis of the map.

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.

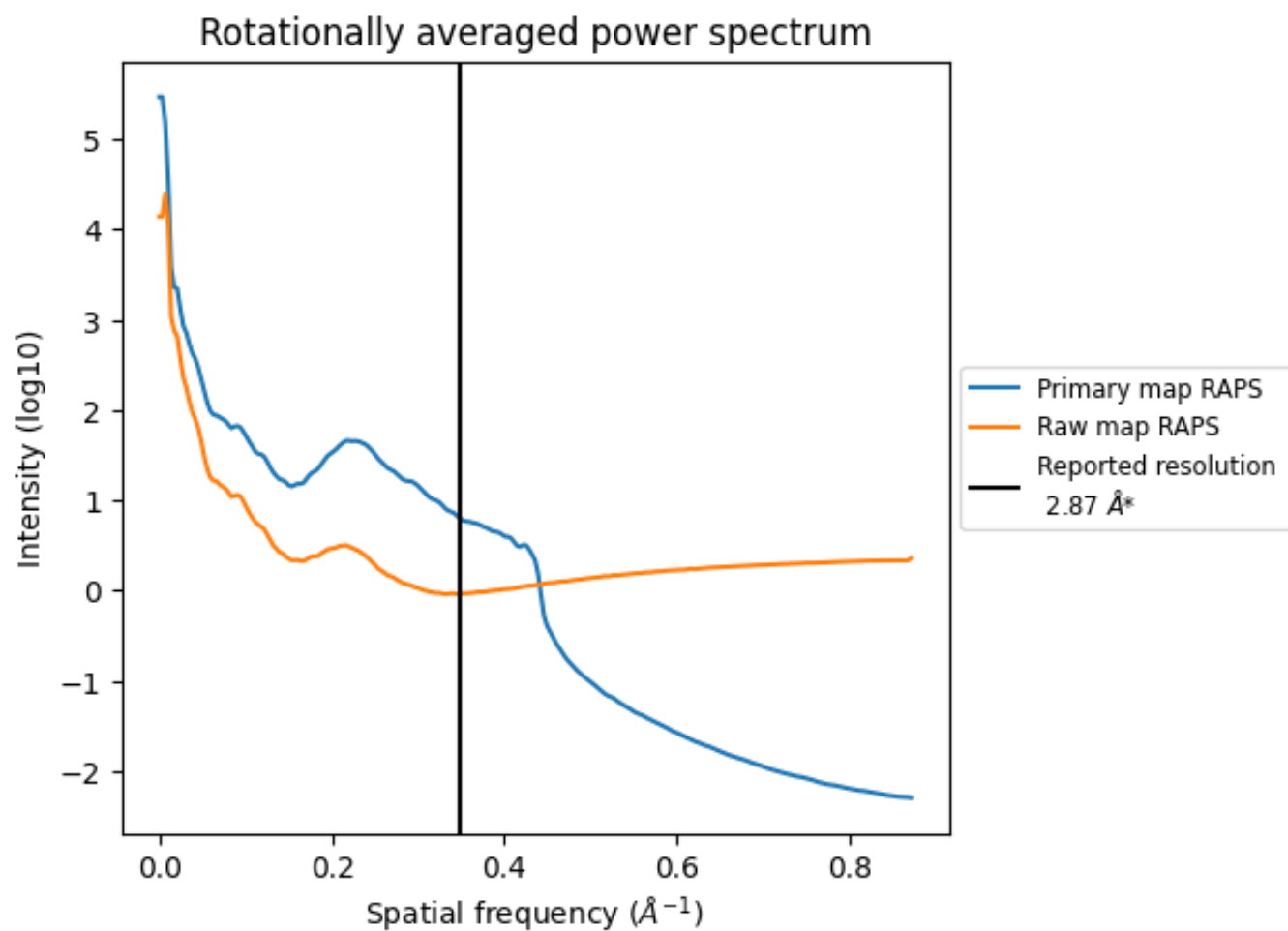
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 288 nm^3 ; this corresponds to an approximate mass of 260 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](#)

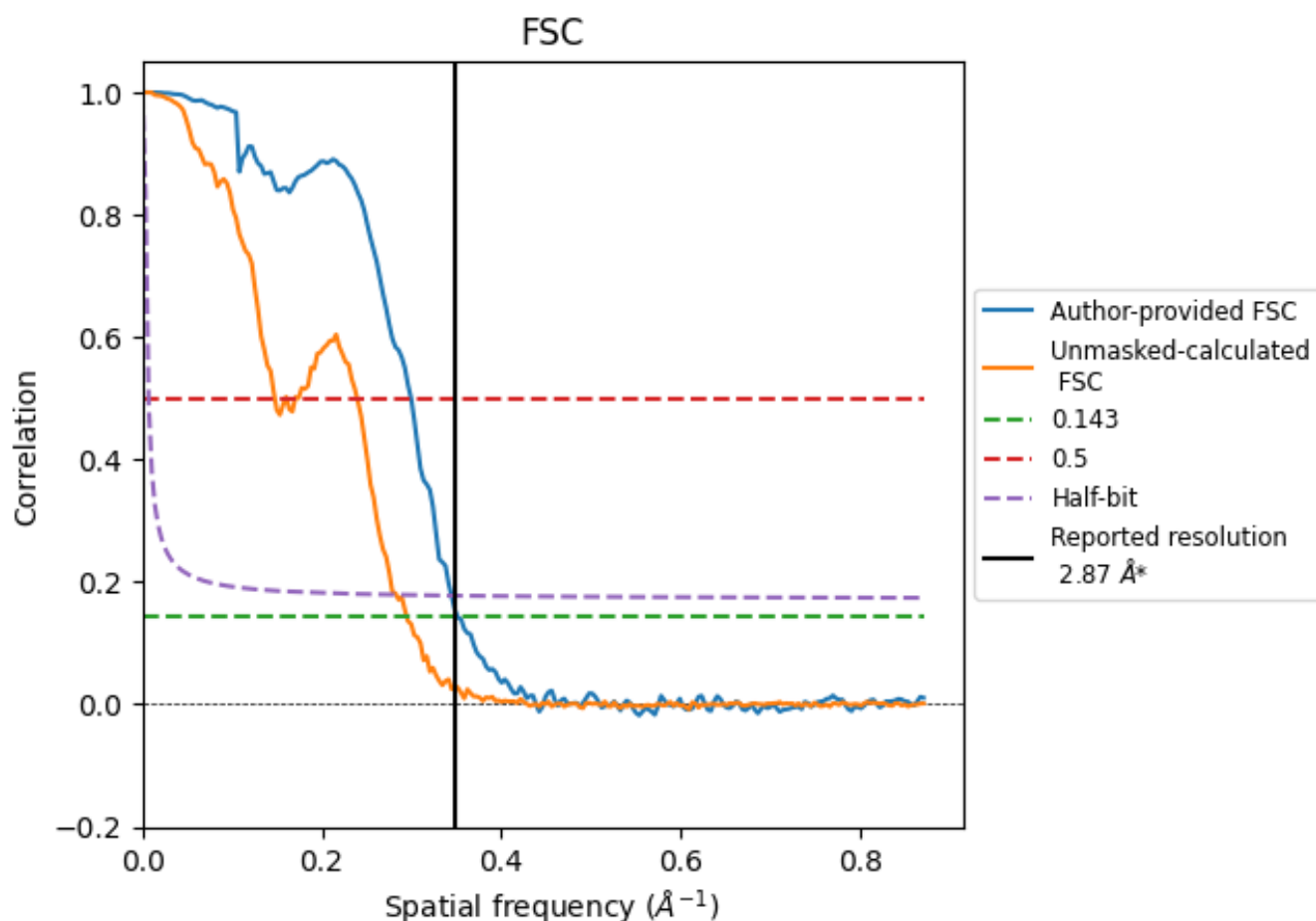


*Reported resolution corresponds to spatial frequency of 0.348 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.348 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

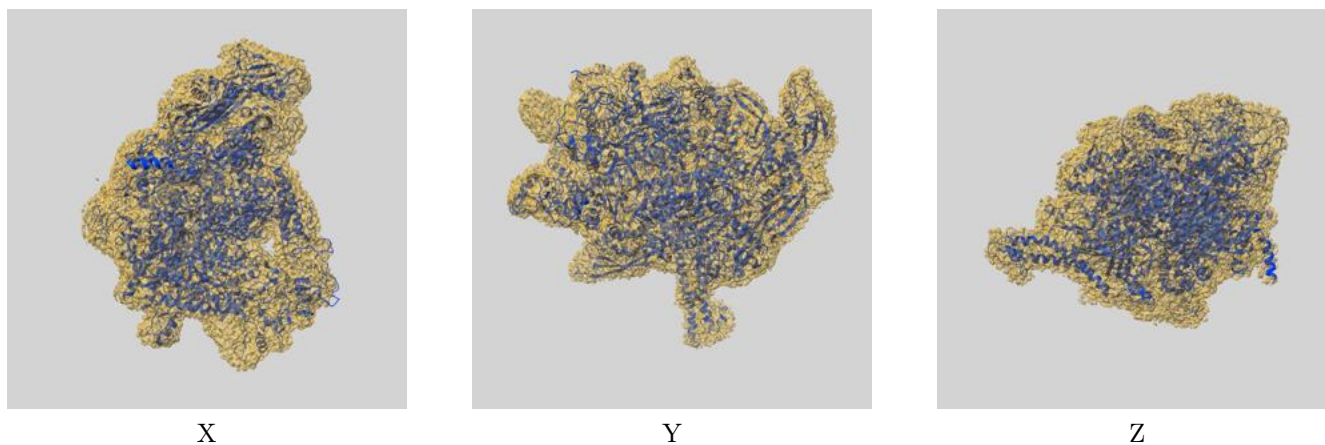
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	2.84	3.34	2.90
Unmasked-calculated*	3.39	6.78	3.53

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.39 differs from the reported value 2.87 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17586 and PDB model 8PBL. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



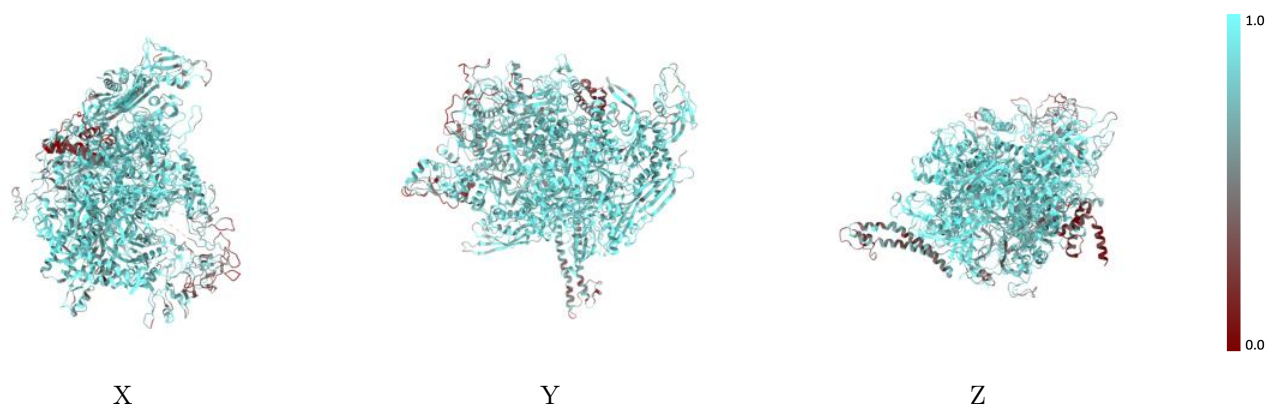
The images above show the 3D surface view of the map at the recommended contour level 0.00102 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



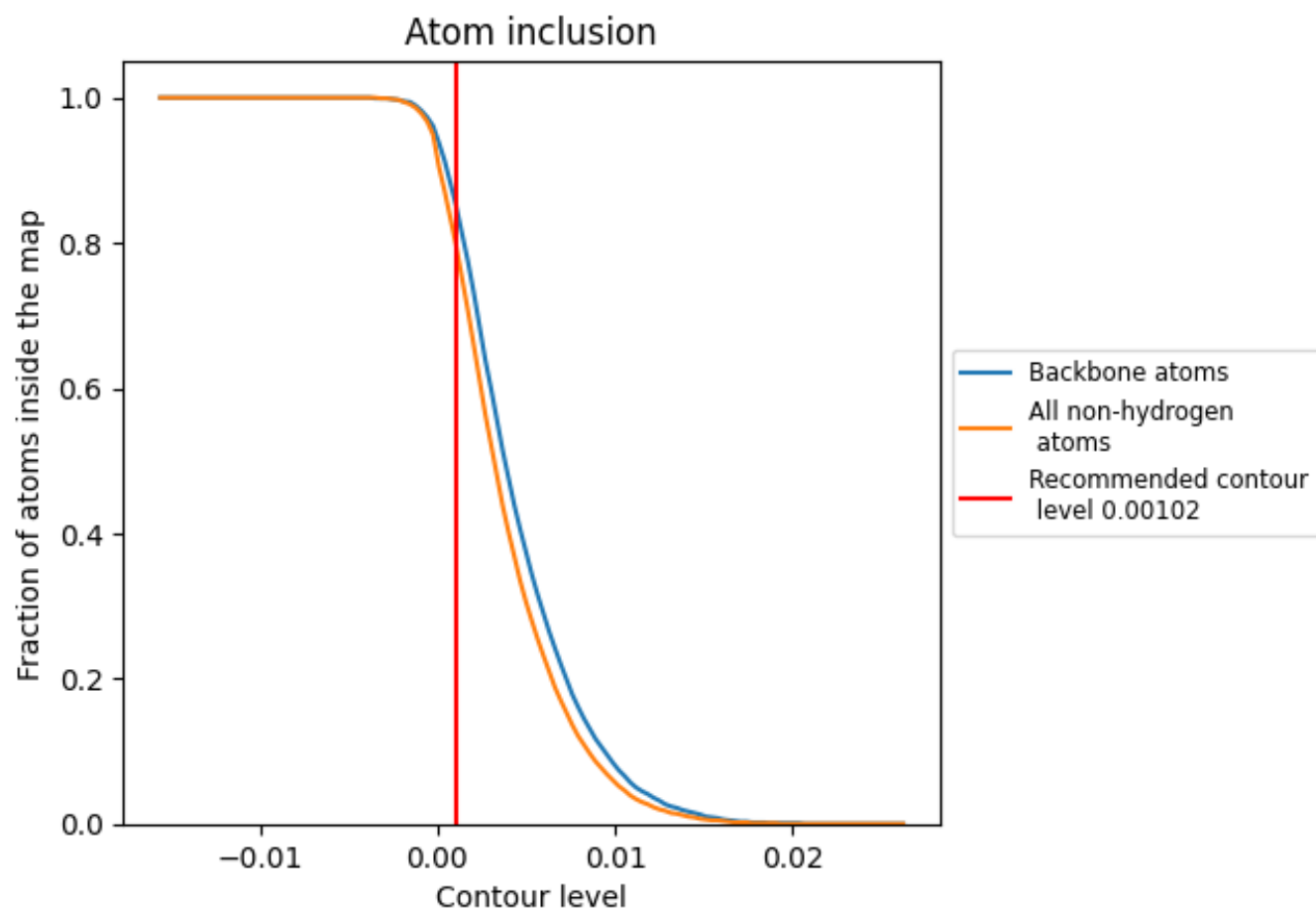
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00102).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 80% 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 (0.00102) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8000	0.3460
A	0.7790	0.2090
B	0.8770	0.3560
D	0.8450	0.4290
E	0.7590	0.3170
F	0.8250	0.3710
G	0.8030	0.3360
H	0.2280	0.0400
R	0.8090	0.3460

1.0

0.0

<0.0