wwPDB EM Validation Summary Report

Mar 14, 2026 – 03:28 AM UTC

PDB ID	:	7Z8S / pdb_00007z8s
EMDB ID	:	EMD-14562
Title	:	Mot1:TBP:DNA - post hydrolysis state
Authors	:	Woike, S.; Eustermann, S.; Jung, J.; Wenzl, S.J.; Hagemann, G.; Bartho, J.D.; Lammens, K.; Butryn, A.; Herzog, F.; Hopfner, K.-P.
Deposited on	:	2022-03-18
Resolution	:	3.90 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:

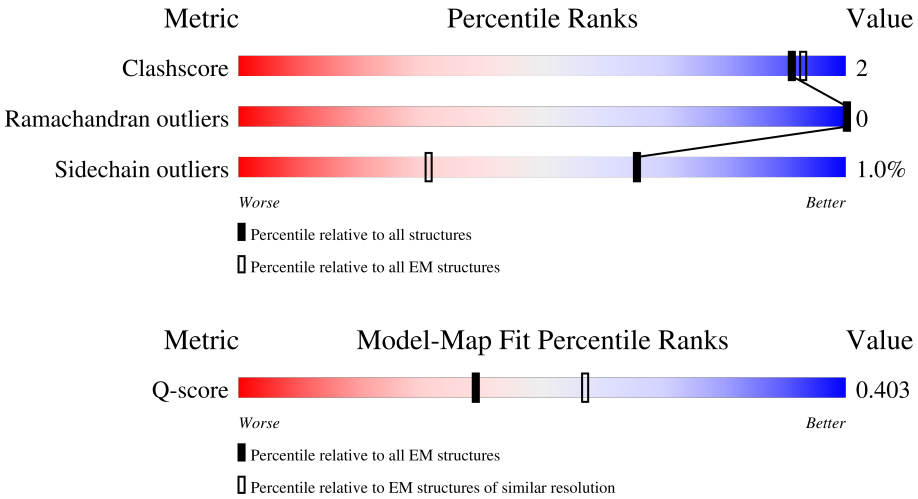
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & 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 3.90 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	-
Q-score	-	25397	8855 (3.40 - 4.40)

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 <=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	36	56% 97%
2	B	36	53% 97%
3	D	276	61% 36%
4	E	1897	75% 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 29271 atoms, of which 14473 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 DNA (36-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	A	36	1144	348	400	147	213	36	0	0

- Molecule 2 is a DNA chain called DNA (36-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
2	B	36	1135	345	403	132	219	36	0	0

- Molecule 3 is a protein called Putative tata-box binding protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	D	178	2907	919	1490	245	247	6	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	initiating methionine	UNP G0SAL6
D	-19	GLY	-	expression tag	UNP G0SAL6
D	-18	SER	-	expression tag	UNP G0SAL6
D	-17	SER	-	expression tag	UNP G0SAL6
D	-16	HIS	-	expression tag	UNP G0SAL6
D	-15	HIS	-	expression tag	UNP G0SAL6
D	-14	HIS	-	expression tag	UNP G0SAL6
D	-13	HIS	-	expression tag	UNP G0SAL6
D	-12	HIS	-	expression tag	UNP G0SAL6
D	-11	HIS	-	expression tag	UNP G0SAL6
D	-10	SER	-	expression tag	UNP G0SAL6
D	-9	SER	-	expression tag	UNP G0SAL6
D	-8	GLY	-	expression tag	UNP G0SAL6
D	-7	GLU	-	expression tag	UNP G0SAL6
D	-6	ASN	-	expression tag	UNP G0SAL6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	LEU	-	expression tag	UNP G0SAL6
D	-4	TYR	-	expression tag	UNP G0SAL6
D	-3	PHE	-	expression tag	UNP G0SAL6
D	-2	GLN	-	expression tag	UNP G0SAL6
D	-1	GLY	-	expression tag	UNP G0SAL6
D	0	HIS	-	expression tag	UNP G0SAL6

- Molecule 4 is a protein called Helicase-like protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	1514	Total	C	H	N	O	S	0	0
			24085	7559	12180	2090	2192	64		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1887	ALA	-	expression tag	UNP G0S6C0
E	1888	ALA	-	expression tag	UNP G0S6C0
E	1889	ALA	-	expression tag	UNP G0S6C0
E	1890	TRP	-	expression tag	UNP G0S6C0
E	1891	SER	-	expression tag	UNP G0S6C0
E	1892	HIS	-	expression tag	UNP G0S6C0
E	1893	PRO	-	expression tag	UNP G0S6C0
E	1894	GLN	-	expression tag	UNP G0S6C0
E	1895	PHE	-	expression tag	UNP G0S6C0
E	1896	GLU	-	expression tag	UNP G0S6C0
E	1897	LYS	-	expression tag	UNP G0S6C0

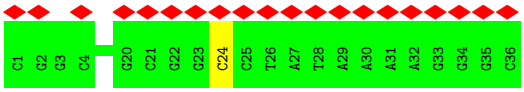
3 Residue-property plots (i)

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: DNA (36-MER)

Chain A:

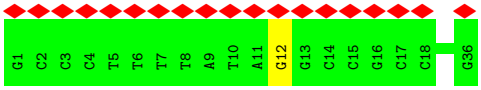




• Molecule 2: DNA (36-MER)

Chain B:

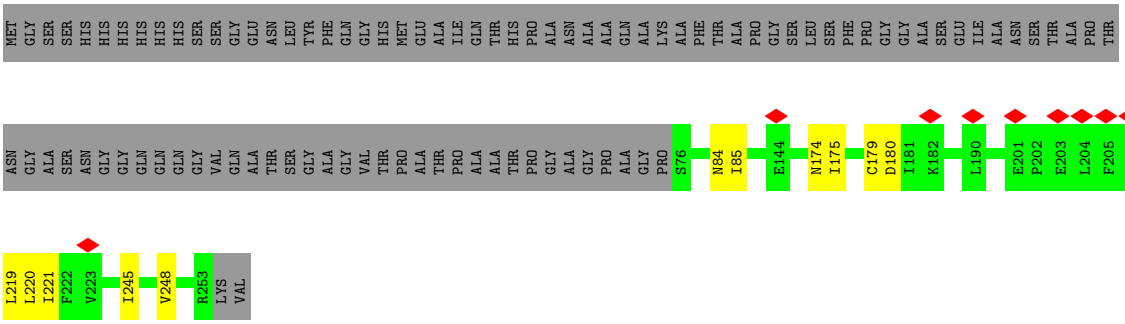




• Molecule 3: Putative tata-box binding protein

Chain D:

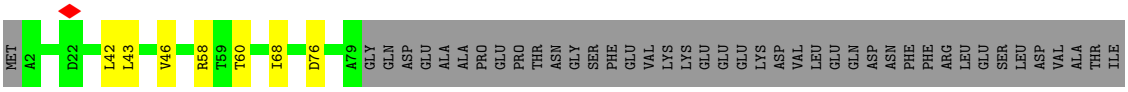


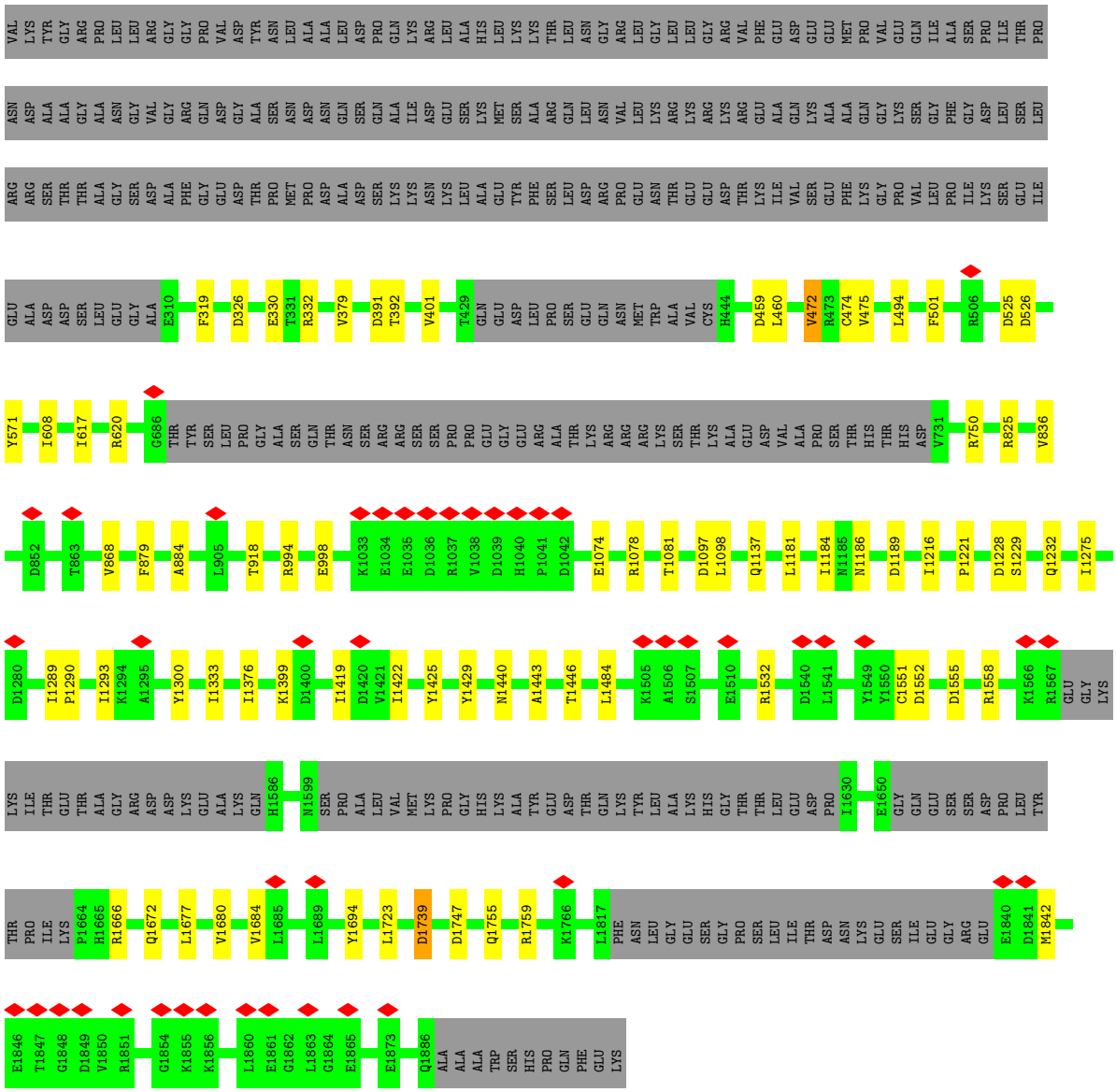


• Molecule 4: Helicase-like protein

Chain E:






VAL LYS TYR GLY ARG PRO LEU LEU ARG GLY GLY PRO VAL ASP TYR ASN LEU ALA ALA LEU ASP PRO GLN LYS ARG LEU ALA HIS LEU LYS LYS THR LEU ASN GLY ARG LEU GLY LEU LEU GLY ARG VAL PHE GLU ASP GLU GLU MET PRO VAL GLU GLN ILE ALA SER PRO ILE THR PRO
ASN ASP ALA ALA GLY ALA ASN GLY VAL GLY ARG GLN ASP GLY ALA SER ASN ASP ASN GLN SER GLN ALA ILE ASP GLU SER LYS MET SER ALA ARG GLN LEU ASP ARG PRO GLU ASN THR GLU GLU ASP THR LYS ILE VAL SER GLU PHE LYS GLY PRO VAL LEU PRO ILE LYS SER GLU ILE
ARG ARG SER THR THR ALA GLY SER ASP ALA PHE GLY GLU ASP THR PRO MET PRO ASP ALA ASP SER LYS LYS ASN LYS LEU ALA GLU TYR PHE SER LEU ASP ARG PRO GLU ASN THR GLU GLU ASP THR LYS ILE VAL SER GLU PHE LYS GLY PRO VAL LEU PRO ILE LYS SER GLU ILE
GLU ALA ASP ASP SER LEU GLU GLY ALA E310 F319 D326 E330 T331 R332 V379 D391 T392 V401 T429 GLN GLU ASP LEU PRO SER GLU GLN ASN MET TRP ALA VAL CYS H444 D459 L460 V472 R473 C474 V475 L494 F501 R506 D525 D526
Y571 I608 I617 R620 G686 THR TYR SER LEU PRO GLY ALA SER GLN THR ASN SER ARG ARG SER SER PRO PRO GLU GLY GLU ARG ALA THR LYS ARG ARG ARG LYS SER SER THR LYS ALA GLU ASP VAL ALA PRO SER THR HIS THR HIS ASP V731 R750 R825 V836
D852 T863 V868 F879 A884 L905 T918 R994 E998 K1033 E1034 E1035 D1036 R1037 V1038 D1039 H1040 P1041 D1042 E1074 R1078 T1081 D1097 L1098 Q1137 L1181 I1184 N1185 N1186 D1189 I1216 P1221 D1228 S1229 Q1232 I1275
D1280 I1289 P1290 I1293 K1294 A1295 Y1300 I1333 I1376 K1399 D1400 I1419 D1420 V1421 I1422 Y1425 Y1429 N1440 A1443 T1446 L1484 K1505 A1506 S1507 E1510 R1532 D1540 L1541 Y1549 Y1550 C1551 D1552 D1555 R1558 K1566 R1567 GLU GLY LYS
LYS ILE THR GLU THR ALA GLY ARG ASP ASP LYS GLU ALA LYS GLN H1586 N1599 SER PRO ALA LEU VAL MET LYS PRO GLY HIS LYS ALA TYR GLU ASP THR GLN LYS TYR LEU ALA LYS HIS GLY THR THR LEU GLU ASP PRO I1630 E1650 GLY GLN GLU SER SER ASP PRO LEU TYR
THR PRO ILE LYS P1664 H1665 R1666 Q1672 L1677 V1680 V1684 L1685 L1689 Y1694 L1723 D1739 D1747 Q1755 R1759 K1766 L1817 PHE ASN LEU GLY GLU SER GLY PRO SER LEU ILE THR ASP ASN LYS GLU SER ILE GLU GLU GLY ARG GLU E1840 D1841 M1842
E1846 T1847 G1848 D1849 V1850 R1851 G1854 K1855 K1856 L1860 E1861 G1862 L1863 G1864 E1865 E1873 Q1886 ALA ALA ALA TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	118973	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.098	Depositor
Minimum map value	-0.056	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	338.88, 338.88, 338.88	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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	0.26	0/836	0.44	0/1289
2	B	0.28	0/818	0.50	0/1259
3	D	0.19	0/1444	0.41	0/1945
4	E	0.18	0/12118	0.42	2/16413 (0.0%)
All	All	0.19	0/15216	0.43	2/20906 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	46	VAL	CA-C-N	5.10	123.45	120.24
4	E	46	VAL	C-N-CA	5.10	123.45	120.24

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	744	400	400	1	0
2	B	732	403	403	1	0
3	D	1417	1490	1489	5	0
4	E	11905	12180	12166	40	0
All	All	14798	14473	14458	46	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 2.

The worst 5 of 46 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)
4:E:472:VAL:HG21	4:E:501:PHE:CE1	2.34	0.63
4:E:571:TYR:CE1	4:E:608:ILE:HD13	2.35	0.61
4:E:1289:ILE:HD12	4:E:1290:PRO:HD2	1.83	0.59
4:E:58:ARG:NH2	4:E:330:GLU:OE1	2.35	0.59
4:E:1672:GLN:NE2	4:E:1747:ASP:OD2	2.36	0.58

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	176/276 (64%)	172 (98%)	4 (2%)	0	100	100
4	E	1498/1897 (79%)	1469 (98%)	29 (2%)	0	100	100
All	All	1674/2173 (77%)	1641 (98%)	33 (2%)	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	154/219 (70%)	153 (99%)	1 (1%)	78	80
4	E	1299/1620 (80%)	1285 (99%)	14 (1%)	65	74
All	All	1453/1839 (79%)	1438 (99%)	15 (1%)	65	75

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	825	ARG
4	E	1694	TYR
4	E	918	THR
4	E	1739	ASP
4	E	1429	TYR

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

Mol	Chain	Res	Type
4	E	1426	ASN
4	E	1548	ASN
4	E	1770	ASN
4	E	1557	GLN
4	E	853	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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.

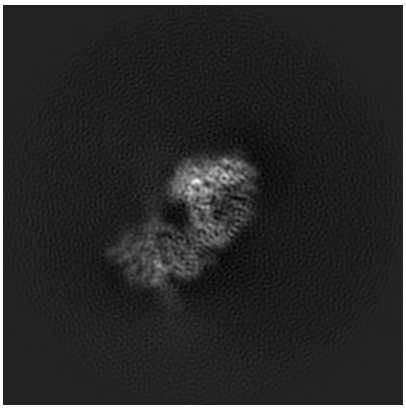
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14562. These allow visual inspection of the internal detail of the map and identification of artifacts.

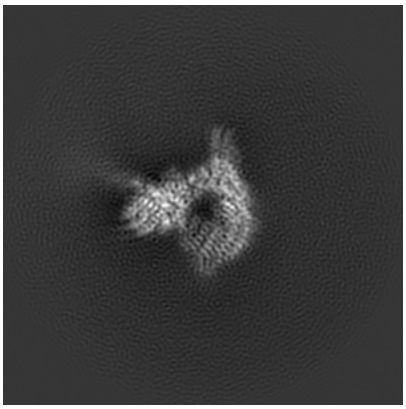
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

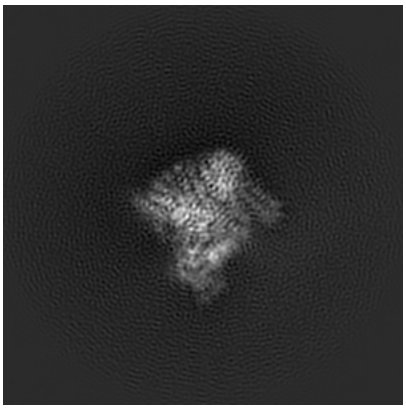
6.1.1 Primary map



X

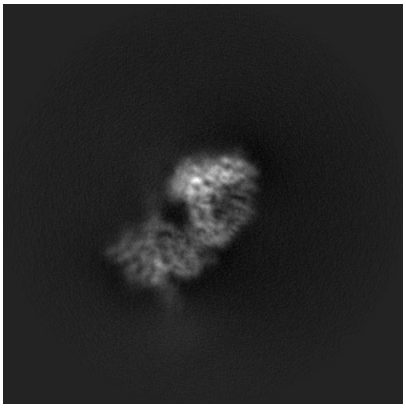


Y

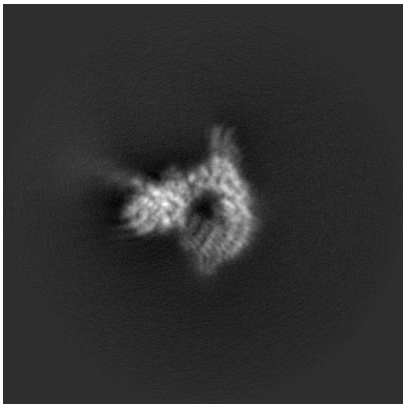


Z

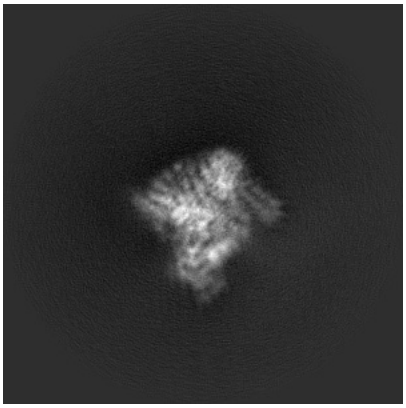
6.1.2 Raw map



X



Y

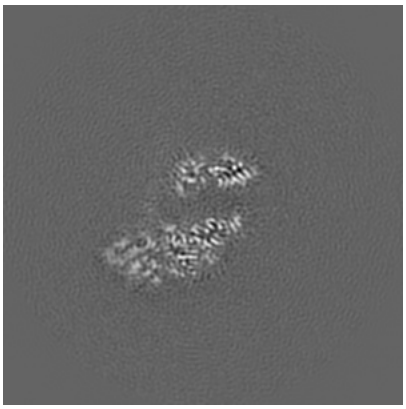


Z

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

6.2 Central slices (i)

6.2.1 Primary map



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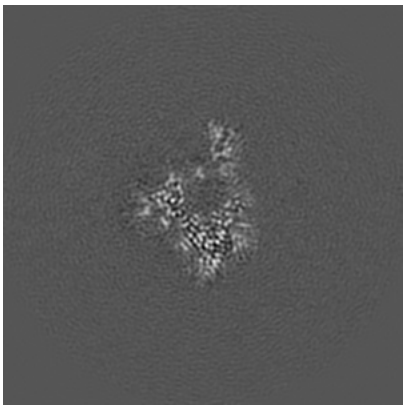

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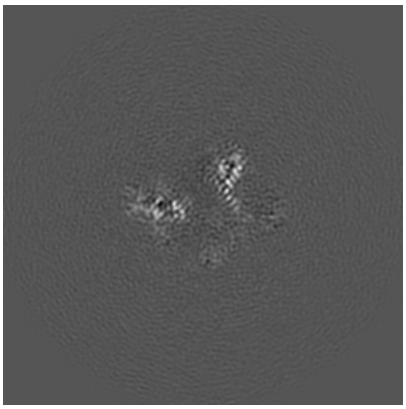
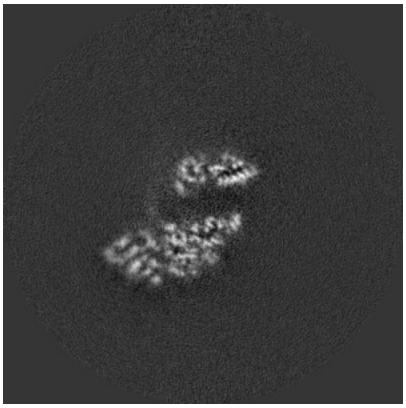


Z Index: 160

6.2.2 Raw map



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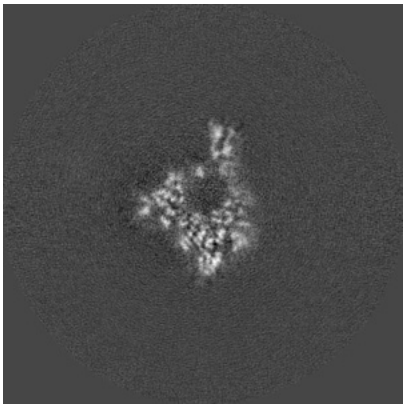
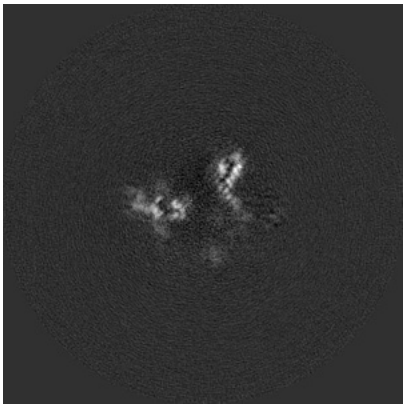


Y Index: 160

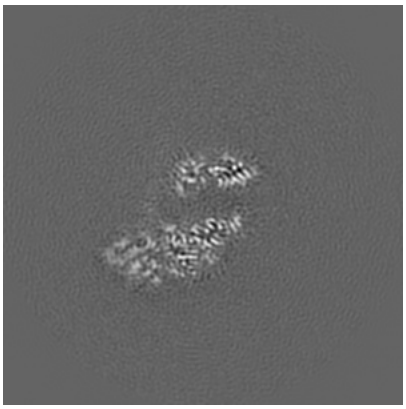


Z Index: 160

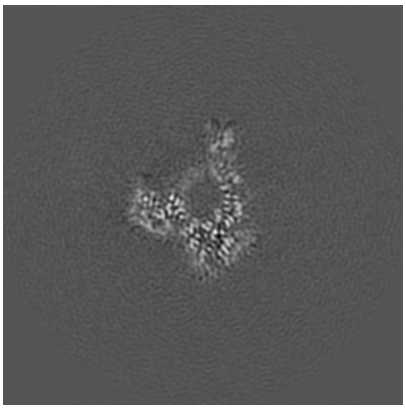
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

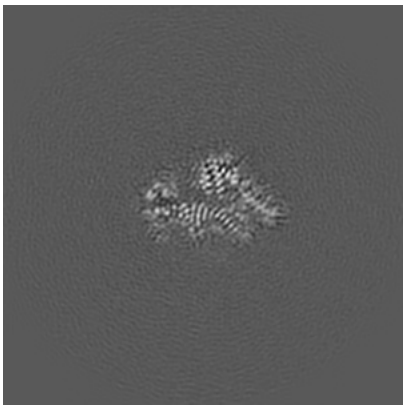
6.3.1 Primary map



X Index: 160

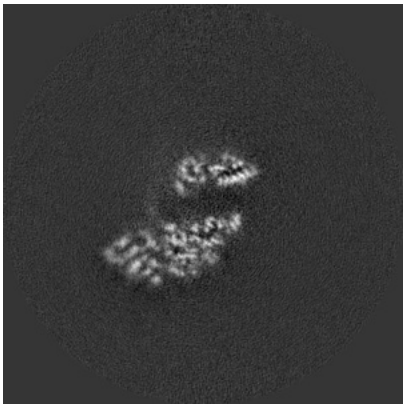


Y Index: 154

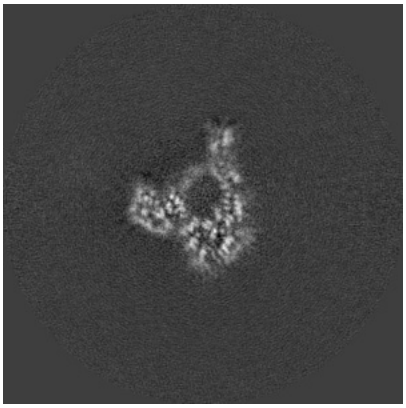


Z Index: 178

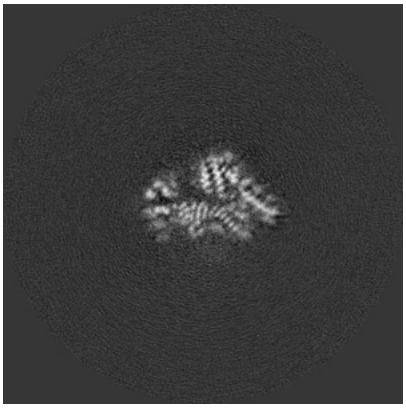
6.3.2 Raw map



X Index: 160



Y Index: 154

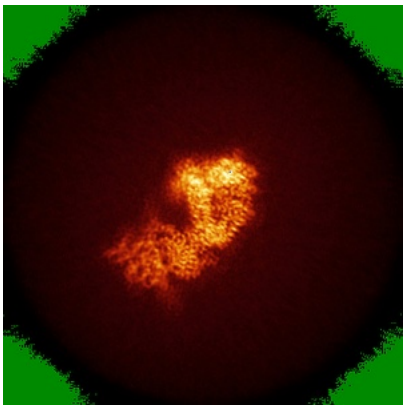


Z Index: 178

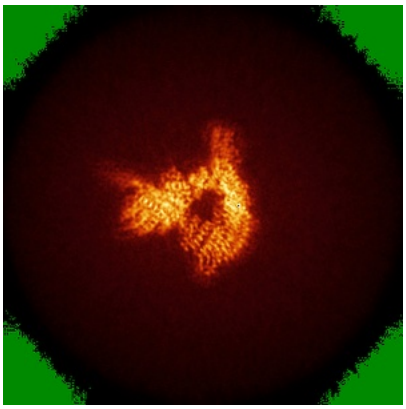
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

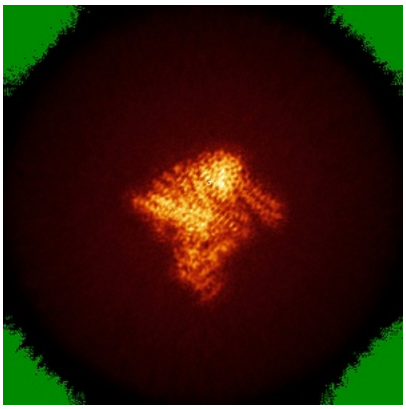
6.4.1 Primary map



X

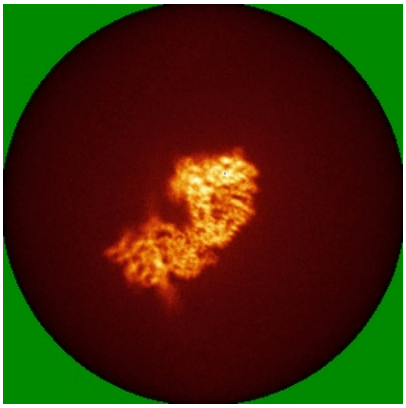


Y

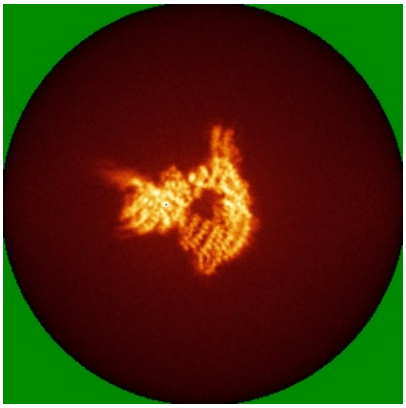


Z

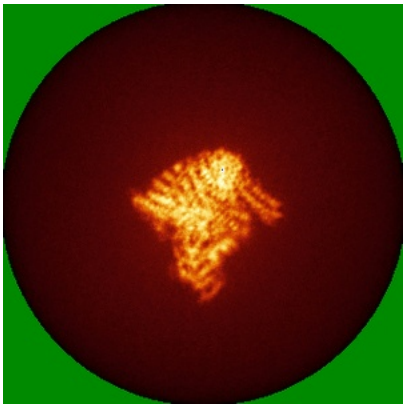
6.4.2 Raw map



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)

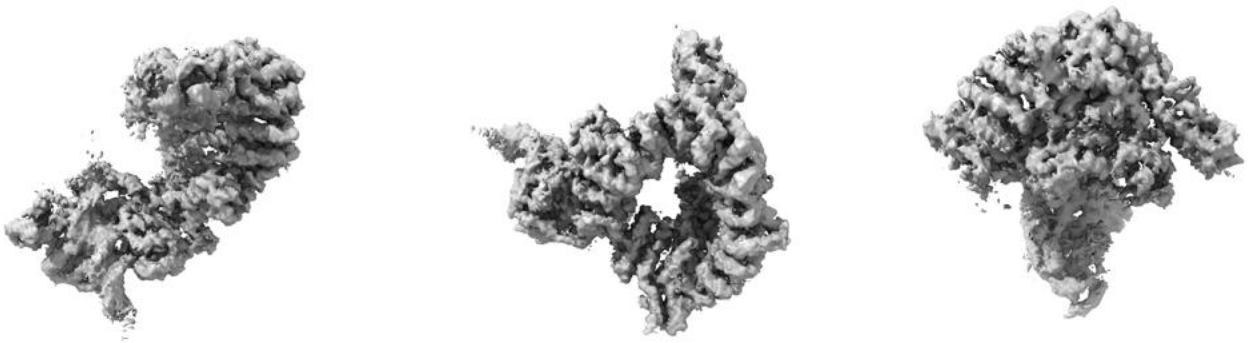
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. 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



X Y Z

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.

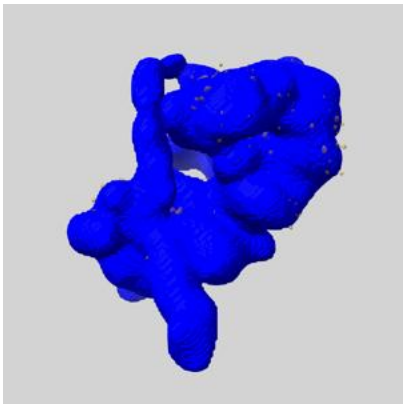
6.6 Mask visualisation

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

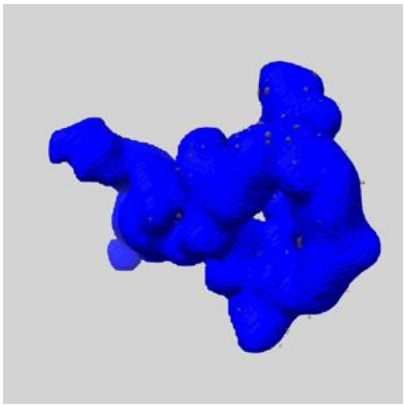
A mask typically either:

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

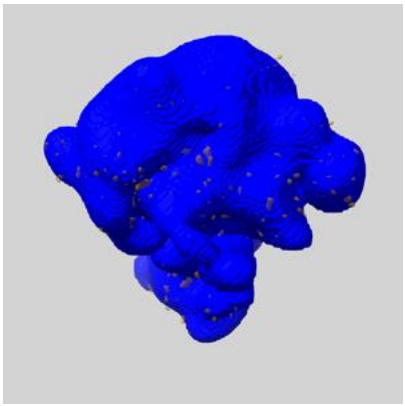
6.6.1 emd_14562_msk_1.map



X



Y

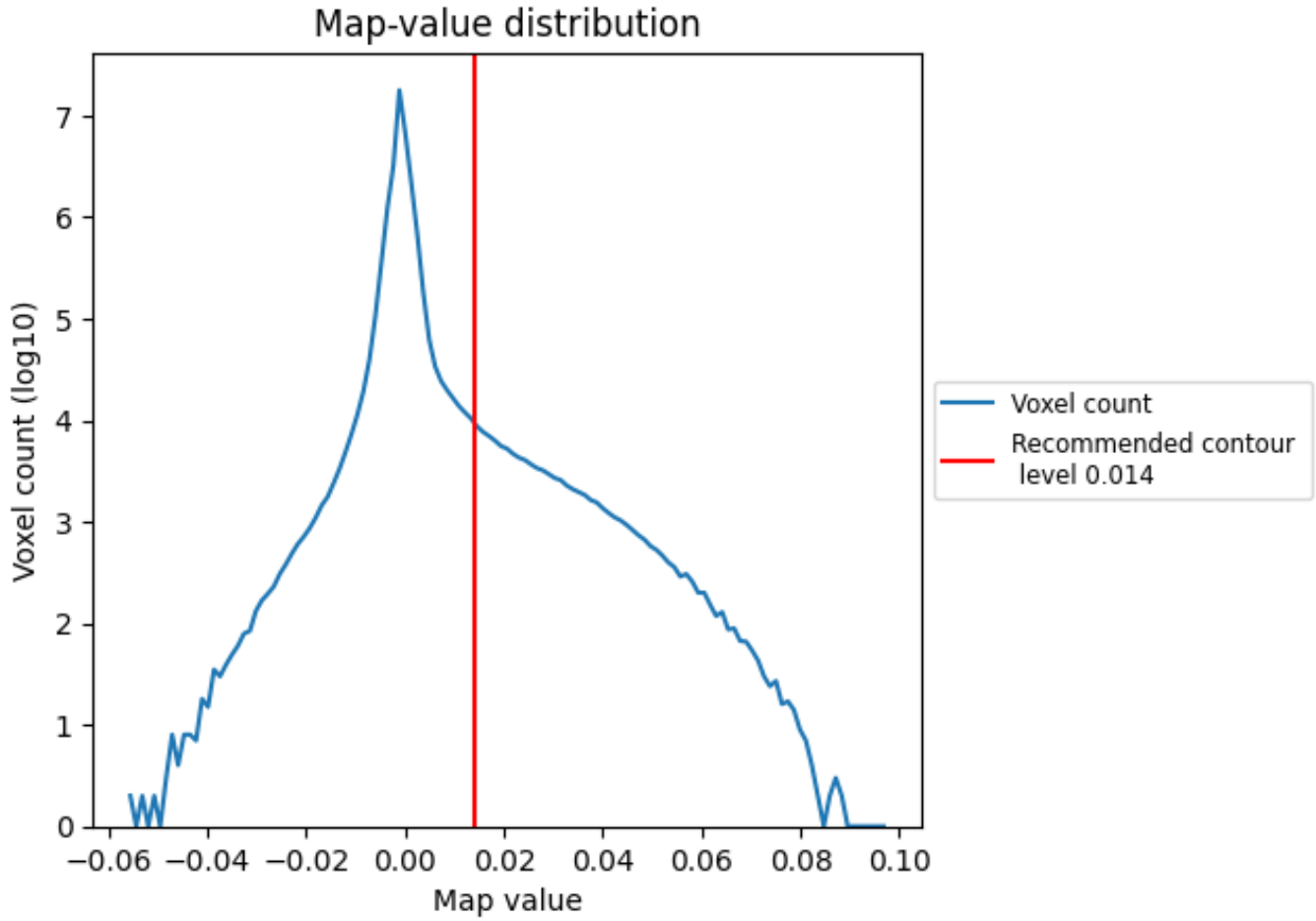


Z

7 Map analysis

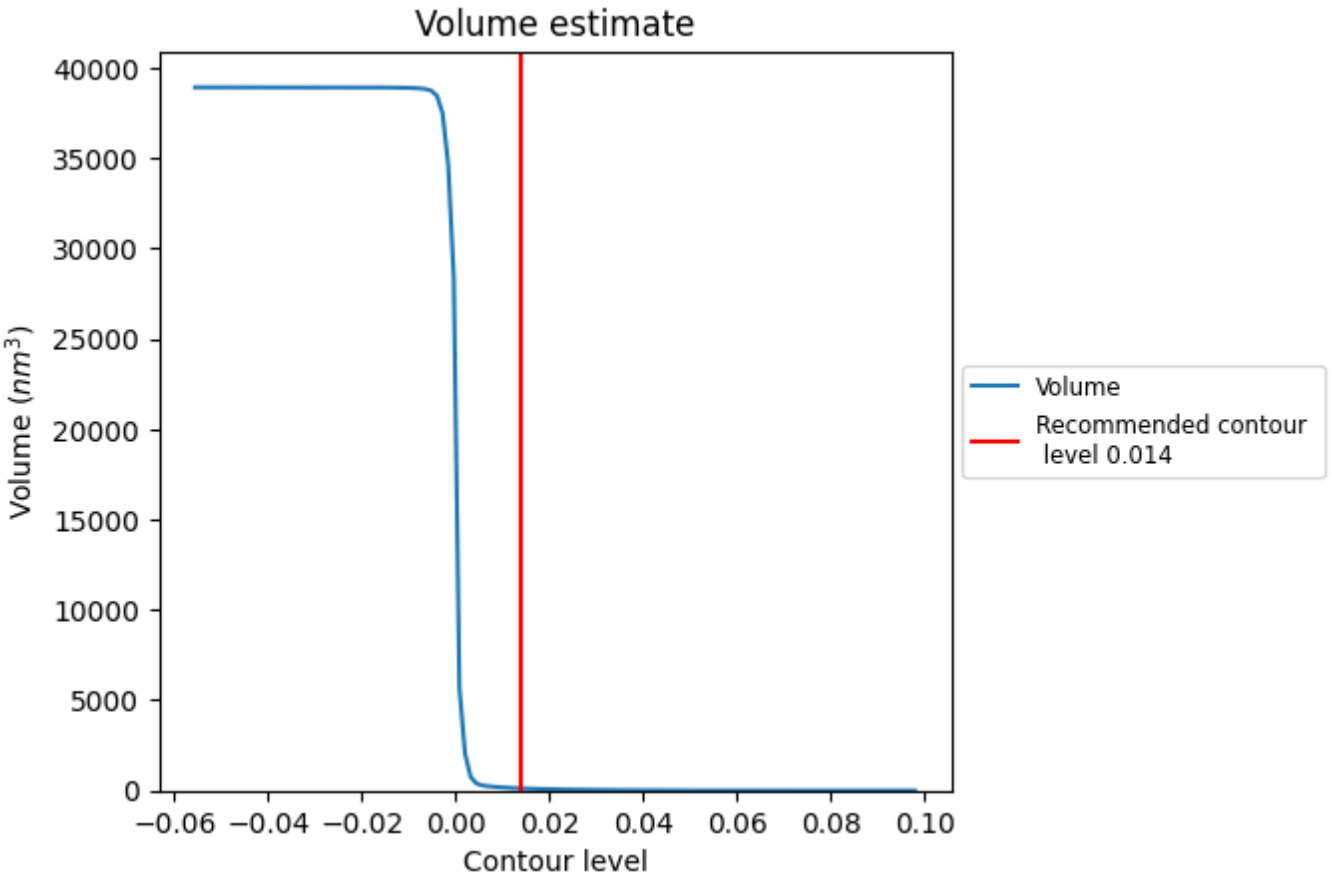
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

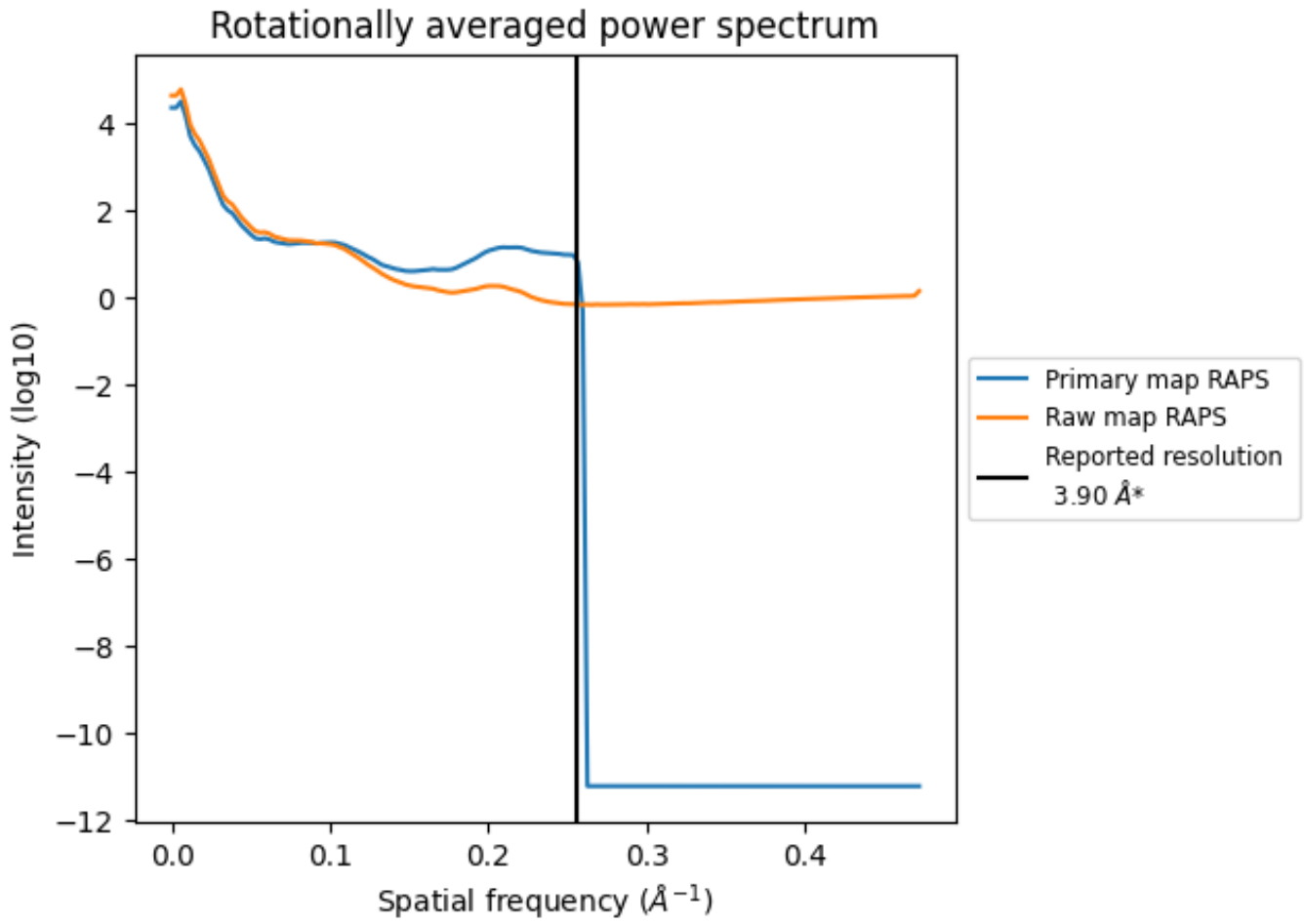
7.2 Volume estimate (i)



The volume at the recommended contour level is 120 nm^3; this corresponds to an approximate mass of 108 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)

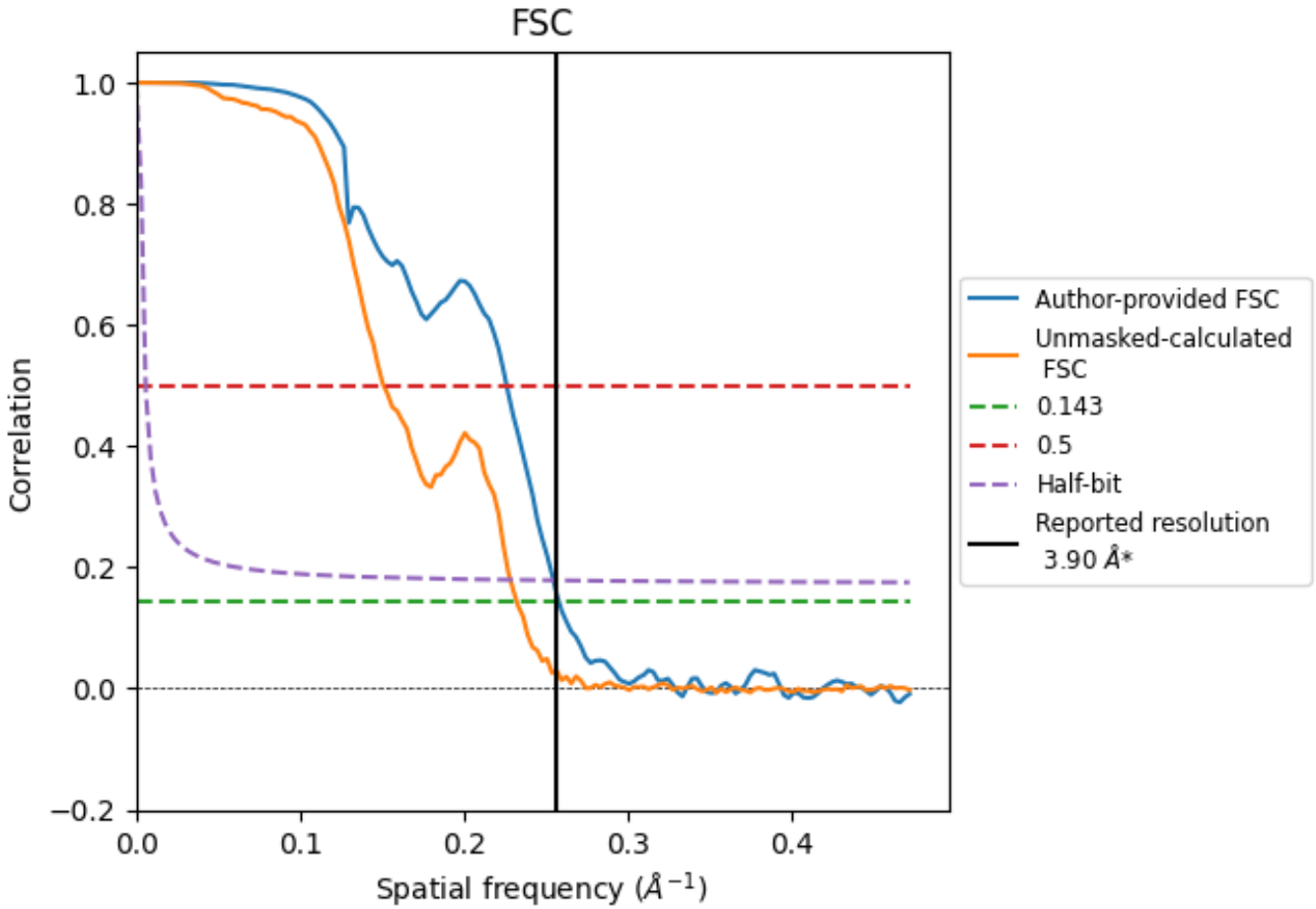


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2 Resolution estimates (i)

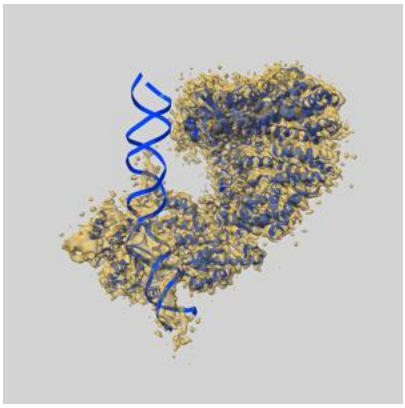
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.87	4.42	3.93
Unmasked-calculated*	4.30	6.62	4.38

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.30 differs from the reported value 3.9 by more than 10 %

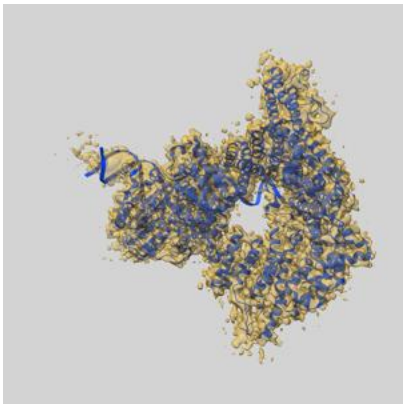
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14562 and PDB model 7Z8S. Per-residue inclusion information can be found in section 3 on page 5.

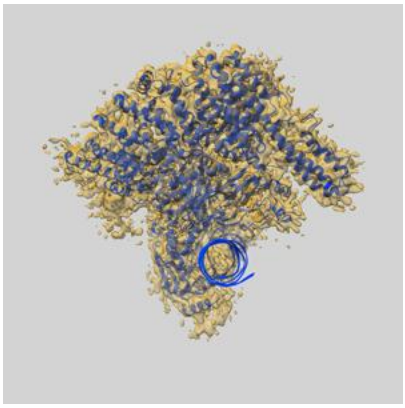
9.1 Map-model overlay



X



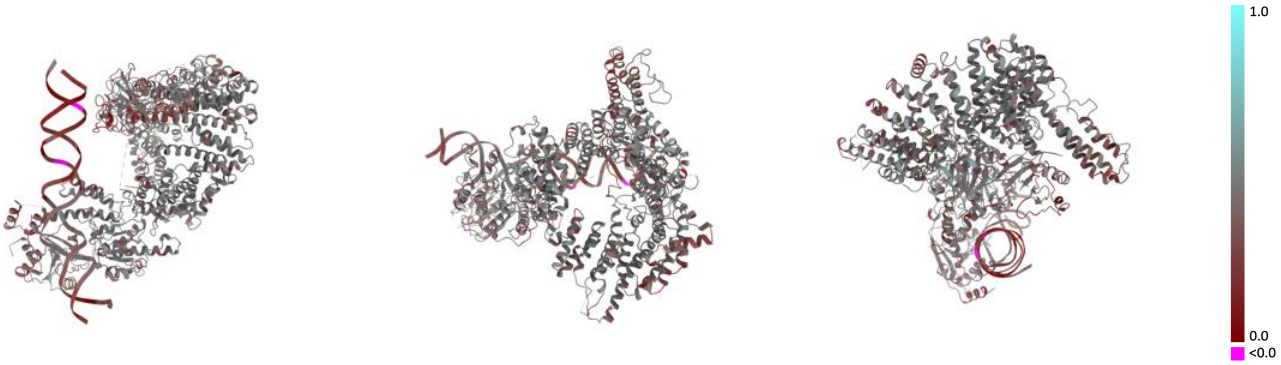
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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.

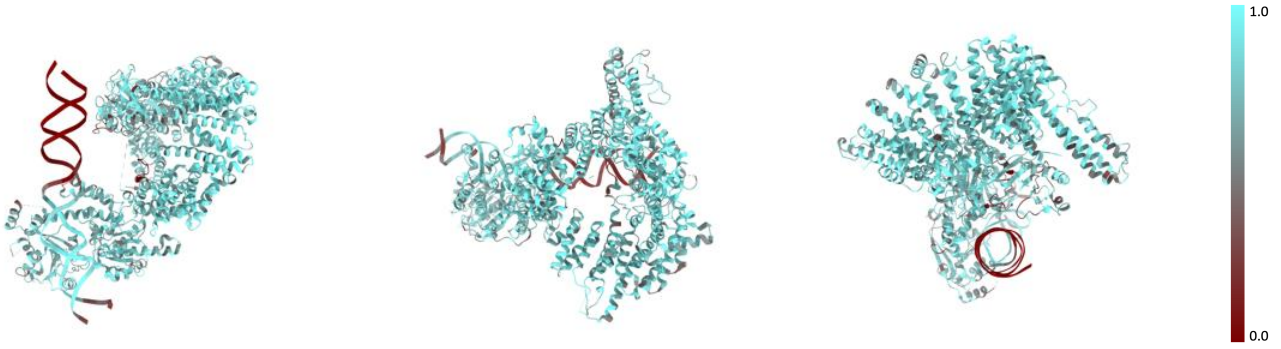
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

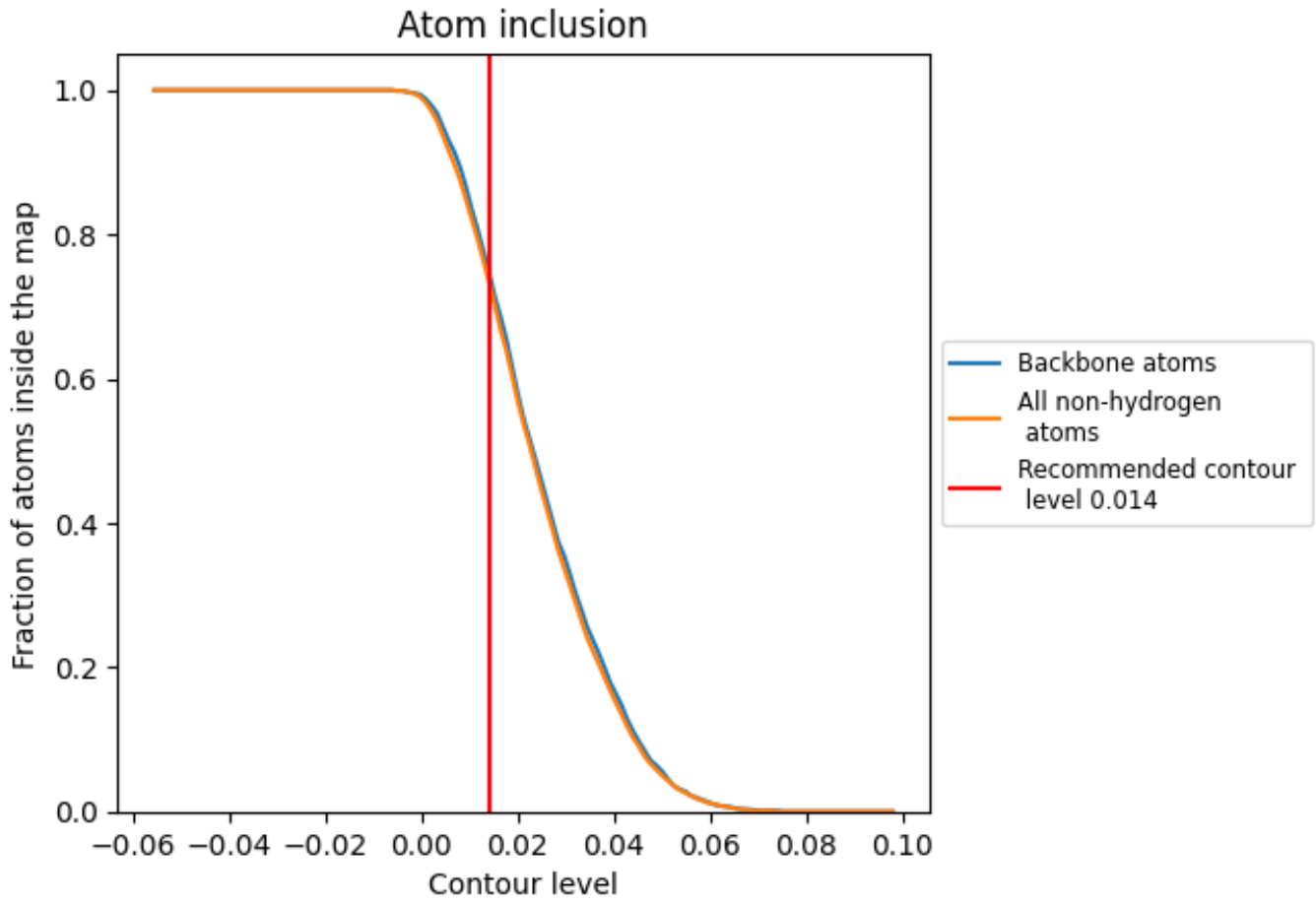
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 74% 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 (0.014) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.7360	0.4030
A	0.3860	0.2400
B	0.4330	0.2530
D	0.7570	0.4040
E	0.8020	0.4230