



wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 02:42 pm BST

PDB ID : 6HV8
EMDB ID : EMD-0287
Title : Cryo-EM structure of *S. cerevisiae* Polymerase epsilon deltacat mutant
Authors : Goswami, P.; Purkiss, A.; Cheung, A.; Costa, A.
Deposited on : 2018-10-10
Resolution : 4.40 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

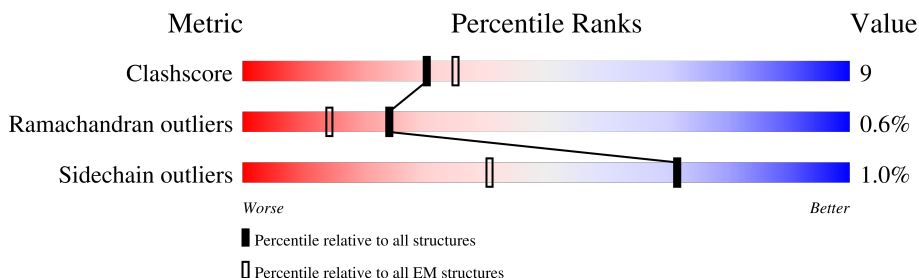
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	B	689	
2	A	914	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9206 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 DNA polymerase epsilon subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	410	Total	C	N	O	S	0	0
			3256	2085	554	603	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	266	ASN	MET	conflict	UNP P24482

- Molecule 2 is a protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	774	Total	C	N	O	S	0	0
			5948	3819	992	1104	33		

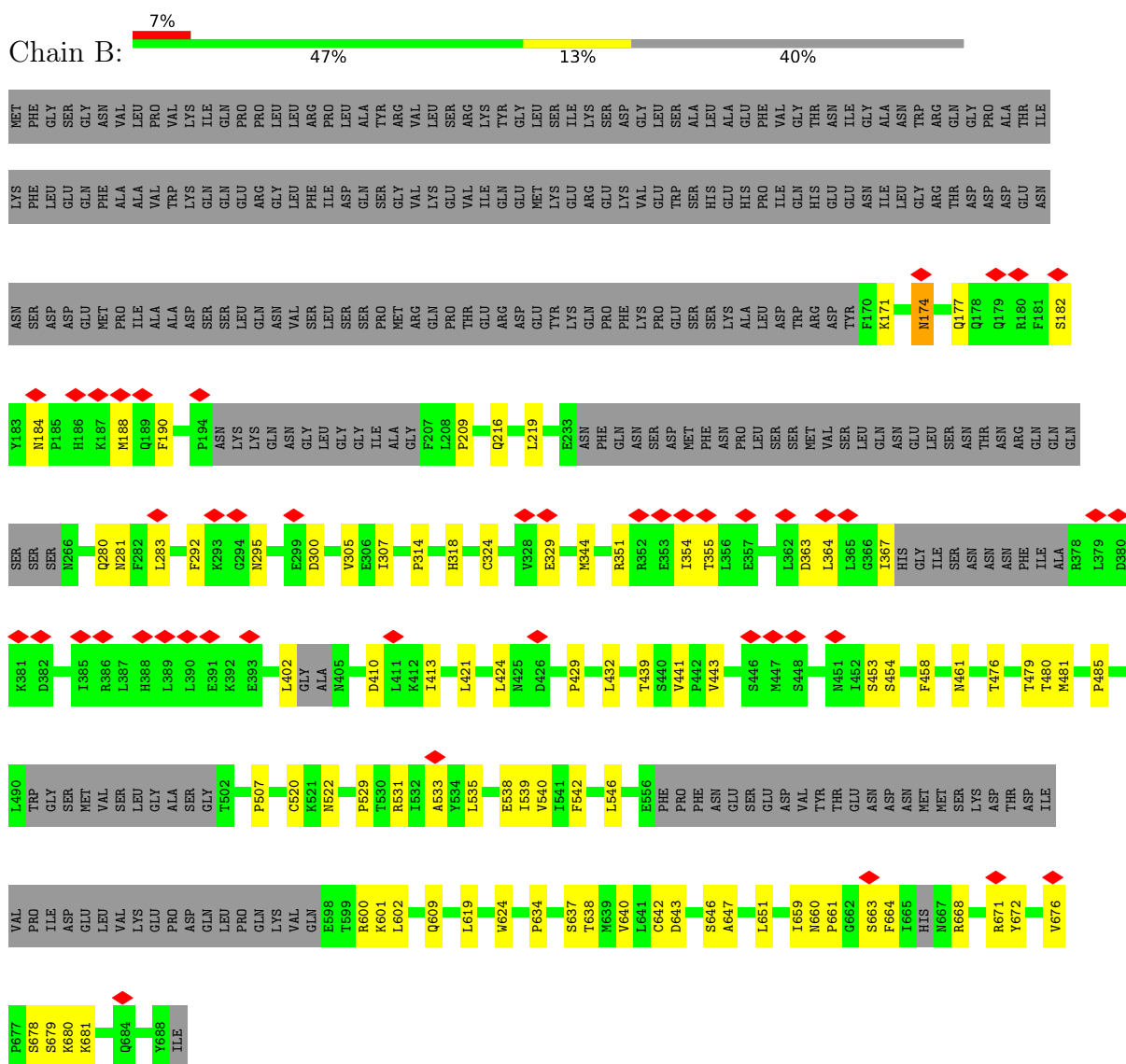
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Zn	0
			2	2	

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: DNA polymerase epsilon subunit B



• Molecule 2: DNA polymerase epsilon catalytic subunit A



ILE	L2058	C2059	H2060	W2061	M2062	L2063	L2064	S2065	K2066	S2067	T2068	E2071	ARG	THR	LEU	ARG	LYS	GLU	THR	LEU	LEU	LYS	ILE	PHE	GLU	LEU	ARG	GLN	ASP	PHE	ALA	LYS	VAL	ALA	GLU	PHE	LYS	ASP	PRO	SER	LEU	S2100	L2101	V2102	C2108	C2111	S2115	D2118	F2119	C2120	K2121	ALA	ALA	PRO	GLU	SER																																																																				
F2128	S2129	L2146	K2149	L2158	R2163	C2164	S2165	R2166	C2167	H2168	D2173	S2176	A2182	G2183	A2184	W2185	L2189	P2190	R2191	T2221	V1836	T1840	E1850	Y1860	A1861	D1862	R1863	N1864	Q1865	I1866	L1867	I1868	K1869	T1870	Y1873	S1874	P1875	Y1879	M1886	R1890	T1891	N1892	P1893	M1894	F1895	S1896	Y1897	L1898	D1899	Y1905	W1906	L1909	I1910	W1911	M1912	D1913	K1914	F1915	N1916	F1917	S2043	H2044	L2045	N2046	V2047	K2048	N2049	P2050	K2056	S2057																																																						
L1649	N1657	I1660	C1661	L1662	L1663	R1664	L1665	D1666	S1667	M1668	L1675	R1678	I1685	V1686	L1687	W1688	W1689	N1690	L1695	P1696	G1699	G1700	I1701	Q1702	N1703	ASP	PHE	ASP	LEU	ASN	THR	SER	W1711	I1712	W1713	S1716	E1717	F1718	P1719	K1720	I1721	V1726	Y1727	D1728	N1729	V1730	V1731	L1732	D1733	D1737	N1742	F1743	I1744	L1745	T1746	S1747	ALA	LEU	ILE	ASN	ASP	ALA	GLU	GLY	SER	ASP	VAL	ASN	ASN	ASN	MET	GLY	ILE	ASP	LYS	ASP	ALA	VAL	ILE	ASN	SER	PRO	THR	GLN	ARG	PRO	THR	GLN	ILE	VAL	ASN	VAL	LYS	LYS	GLN	ASP	K1993	E1994	D1995	S1996	V1997	E1998	D2029	P2030	A2034	ASP	TYR	VAL	ILE	PRO	VAL	LEU	PRO	GLY	S2043	H2044	L2045	N2046	V2047	K2048	N2049	P2050	K2056	S2057
I1552	K1553	E1559	T1564	K1568	L1569	Y1570	R1571	R1572	Q1575	L1580	K1581	G1585	L1586	L1589	L1590	L1591	L1592	Q1593	S1594	P1595	F1596	T1597	T1598	K1599	L1600	T1603	L1606	L1607	N1608	P1611	I1612	V1613	K1614	L1615	S1616	L1617	N1618	E1619	V1620	L1621	L1622	Q1628	P1629	T1630	L1640	I1646																																																																														
GLU	MET	LYS	ASP	L1468	E1472	N1473	E1474	L1475	Y1476	L1477	M1482	G1485	H1489	T1492	S1493	I1494	G1495	Y1496	E1497	F1498	K1503	T1508	L1512	V1513	L1514	K1515	P1516	Q1519	E1522	I1523	M1524	A1525	S1526	S1527	I1531	Y1532	K1533	F1536	K1540	I1543	E1544	V1549	L1550	D1551																																																																																
S1390	N1391	P1392	ALA	GLY	GLY	GLN	LEU	PHE	LYS	ILE	THR	LEU	PRO	E1404	F1407	K1411	C1414	T1415	E1421	N1422	V1423	L1424	G1425	G1429	T1430	I1431	T1432	P1433	ASP	LEU	ALA	SER	VAL	THR	PHE	ARG	SER	LYS	ALA	MET	GLY	ALA	LEU	LYS	GLY	ILE	GLN	GLN	GLY	PHE																																																																										
S1308	M1309	I1310	R1311	K1312	Q1313	A1314	E1315	S1316	Y1317	A1318	I1319	N1320	T1321	W1322	L1325	S1330	G1331	V1335	L1336	E1337	V1338	F1339	V1340	T1341	I1342	N1343	G1344	I1349	T1350	F1351	H1352	Y1358	M1359	K1362	P1367	L1368	I1371	K1372	N1373	C1374	L1375	I1376	A1381	S1382	M1385	N1386	P1387	K1388	T1389																																																																											

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	161376	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.290	Depositor
Minimum map value	-0.158	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.0576	Depositor
Map size (Å)	200.56001, 200.56001, 200.56001	wwPDB
Map dimensions	184, 184, 184	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality

5.1 Standard geometry

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	B	0.44	0/3318	0.71	1/4493 (0.0%)
2	A	0.45	0/6061	0.85	17/8223 (0.2%)
All	All	0.45	0/9379	0.80	18/12716 (0.1%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1687	LEU	CA-CB-CG	7.72	133.06	115.30
2	A	1622	LEU	CA-CB-CG	7.21	131.88	115.30
2	A	2030	PRO	N-CA-CB	6.60	111.22	103.30
2	A	2063	LEU	CA-CB-CG	6.26	129.71	115.30
1	B	300	ASP	CB-CG-OD1	6.04	123.73	118.30

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	B	3256	0	3258	51	0
2	A	5948	0	5712	110	0
3	A	2	0	0	0	0
All	All	9206	0	8970	160	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 9.

The worst 5 of 160 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:B:182:SER:O	1:B:190:PHE:HA	1.76	0.85
2:A:2068:THR:HA	2:A:2071:GLU:HB3	1.59	0.84
2:A:1906:TRP:HB3	2:A:1909:LEU:HD11	1.69	0.74
2:A:1879:TYR:OH	2:A:1886:MET:SD	2.49	0.69
2:A:1712:ILE:HG12	2:A:1712:ILE:O	1.96	0.65

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	B	394/689 (57%)	339 (86%)	53 (14%)	2 (0%)	25	63
2	A	754/914 (82%)	548 (73%)	201 (27%)	5 (1%)	19	56
All	All	1148/1603 (72%)	887 (77%)	254 (22%)	7 (1%)	24	59

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	1657	ASN
2	A	1712	ILE
1	B	443	VAL
1	B	535	LEU
2	A	1668	MET

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	
1	B	368/629 (58%)	367 (100%)	1 (0%)	91	92
2	A	627/837 (75%)	618 (99%)	9 (1%)	62	76
All	All	995/1466 (68%)	985 (99%)	10 (1%)	71	81

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	1668	MET
2	A	1794	MET
2	A	2062	MET
2	A	1325	LEU
2	A	1411	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	1742	ASN
2	A	1657	ASN
2	A	1608	ASN
2	A	1373	ASN
2	A	1609	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

Of 2 ligands modelled in this entry, 2 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2060:HIS	C	2061:VAL	N	14.34
1	B	280:GLN	C	281:ASN	N	5.02

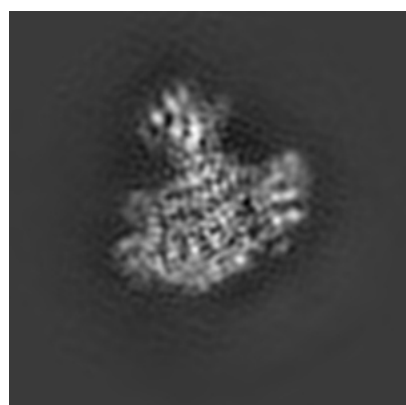
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0287. These allow visual inspection of the internal detail of the map and identification of artifacts.

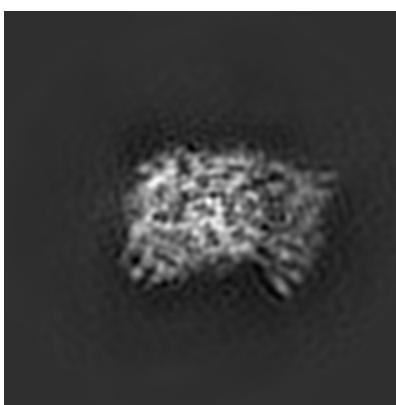
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

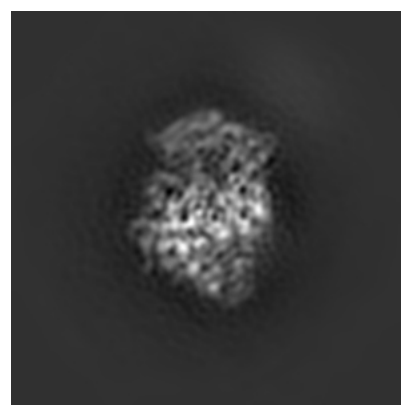
6.1.1 Primary map



X



Y

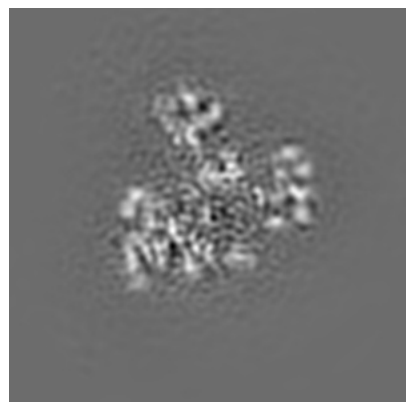


Z

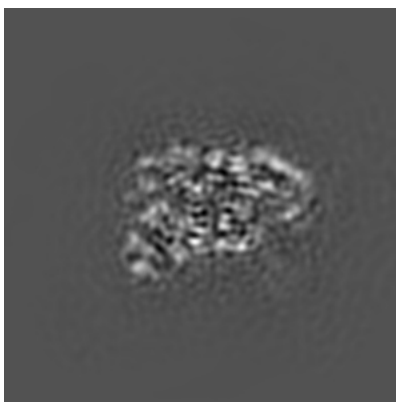
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

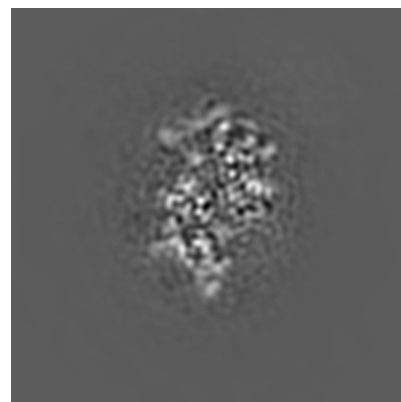
6.2.1 Primary map



X Index: 92



Y Index: 92

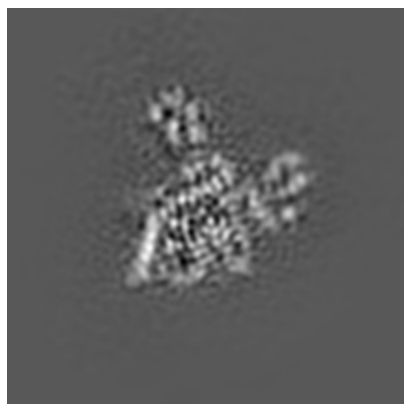


Z Index: 92

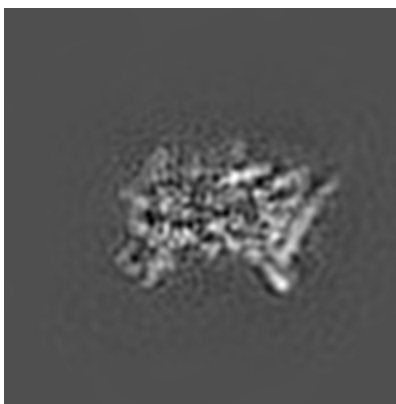
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

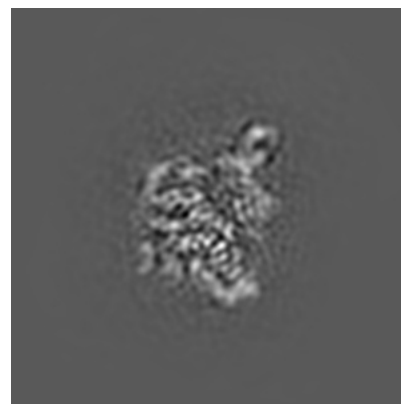
6.3.1 Primary map



X Index: 84



Y Index: 85

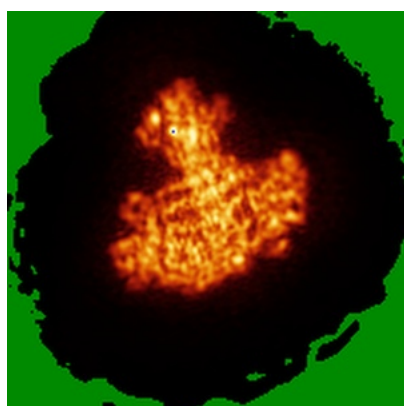


Z Index: 76

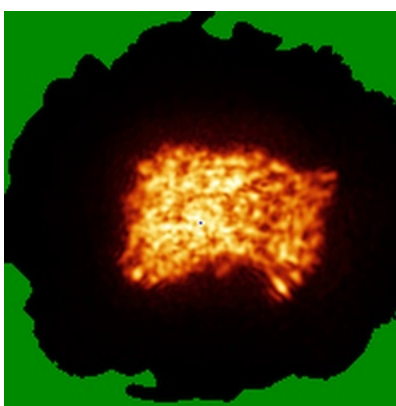
The images above show the largest variance slices of the map in three orthogonal directions.

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

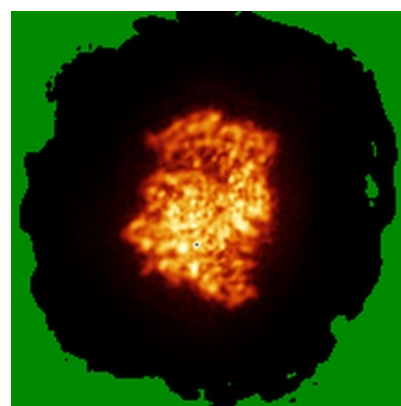
6.4.1 Primary map



X



Y

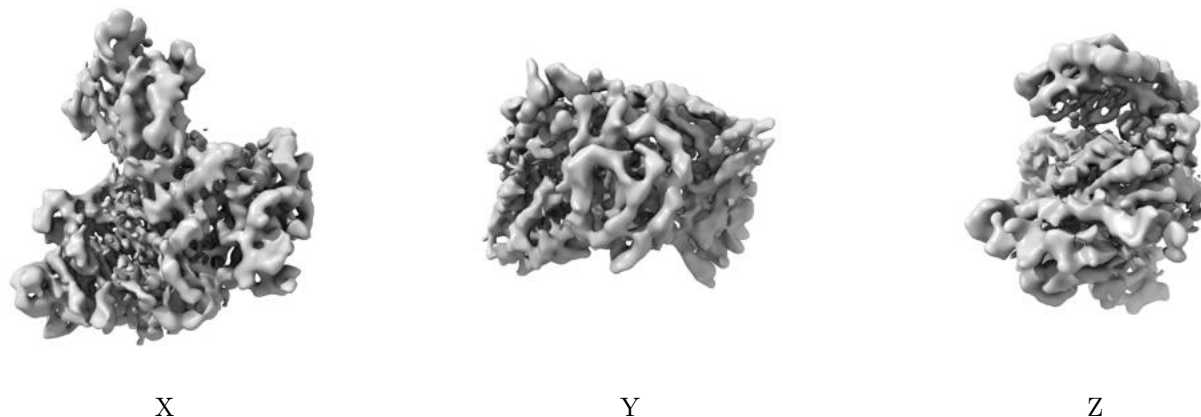


Z

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 0.0576. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

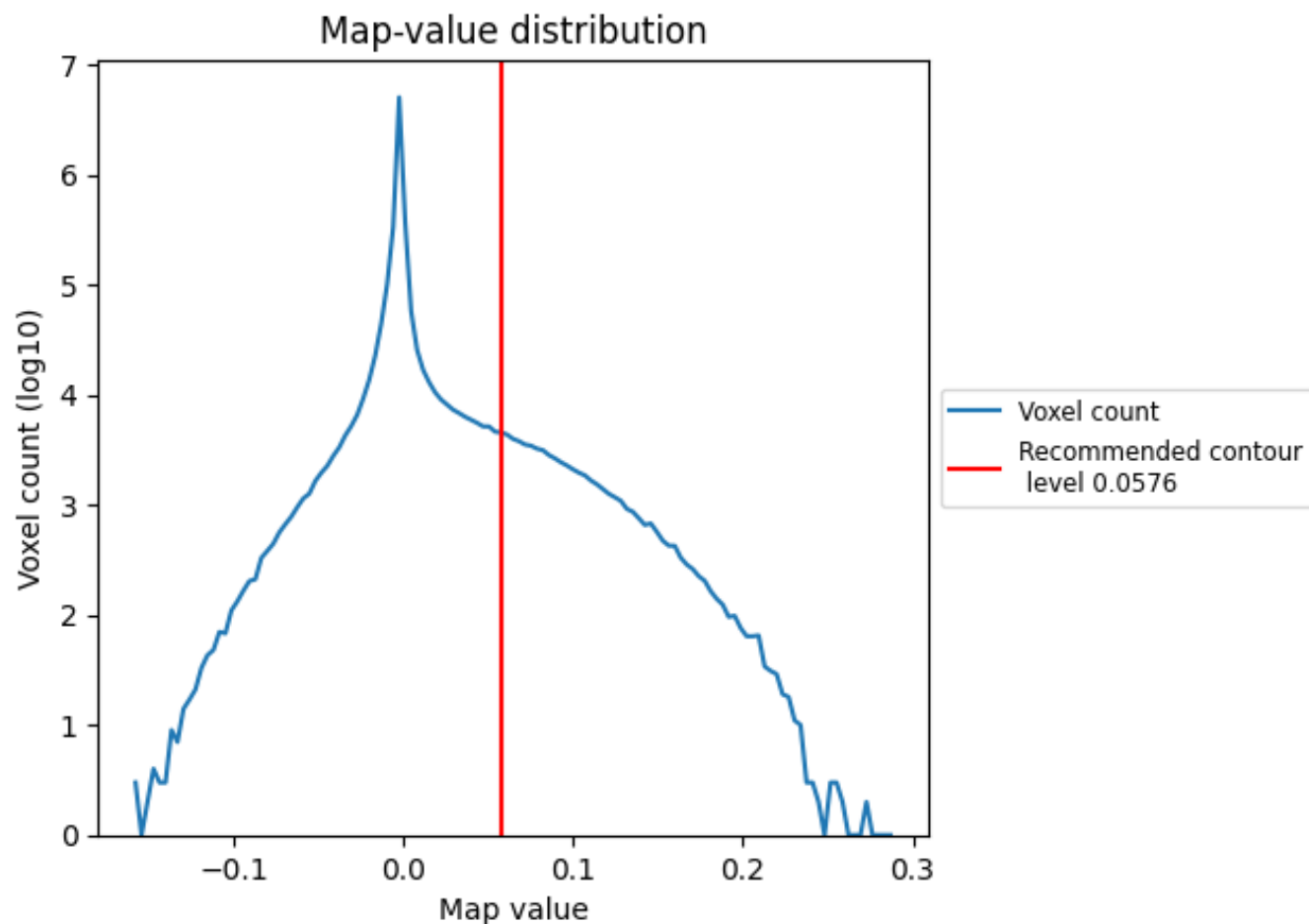
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

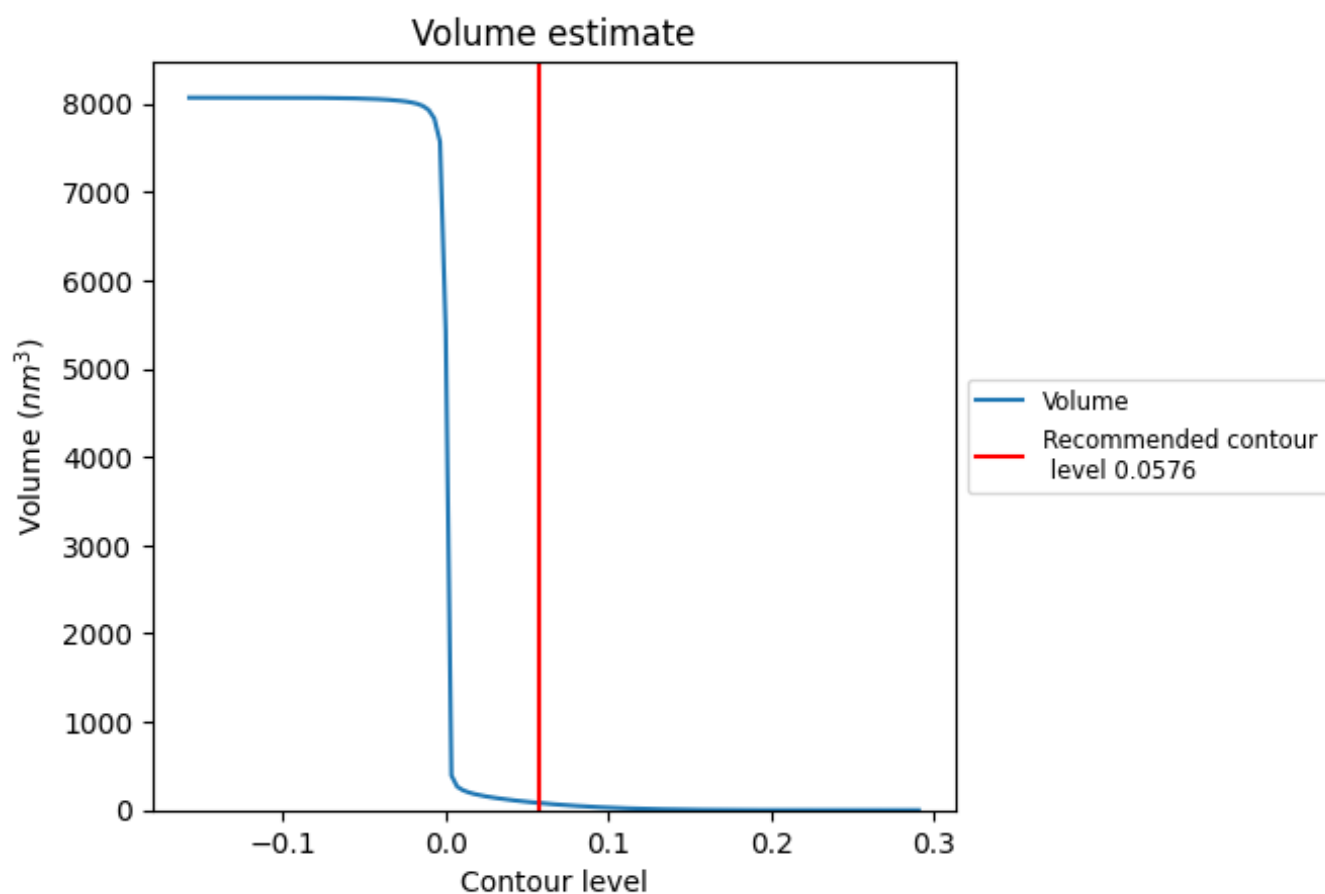
This section contains the results of statistical analysis of the map.

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.

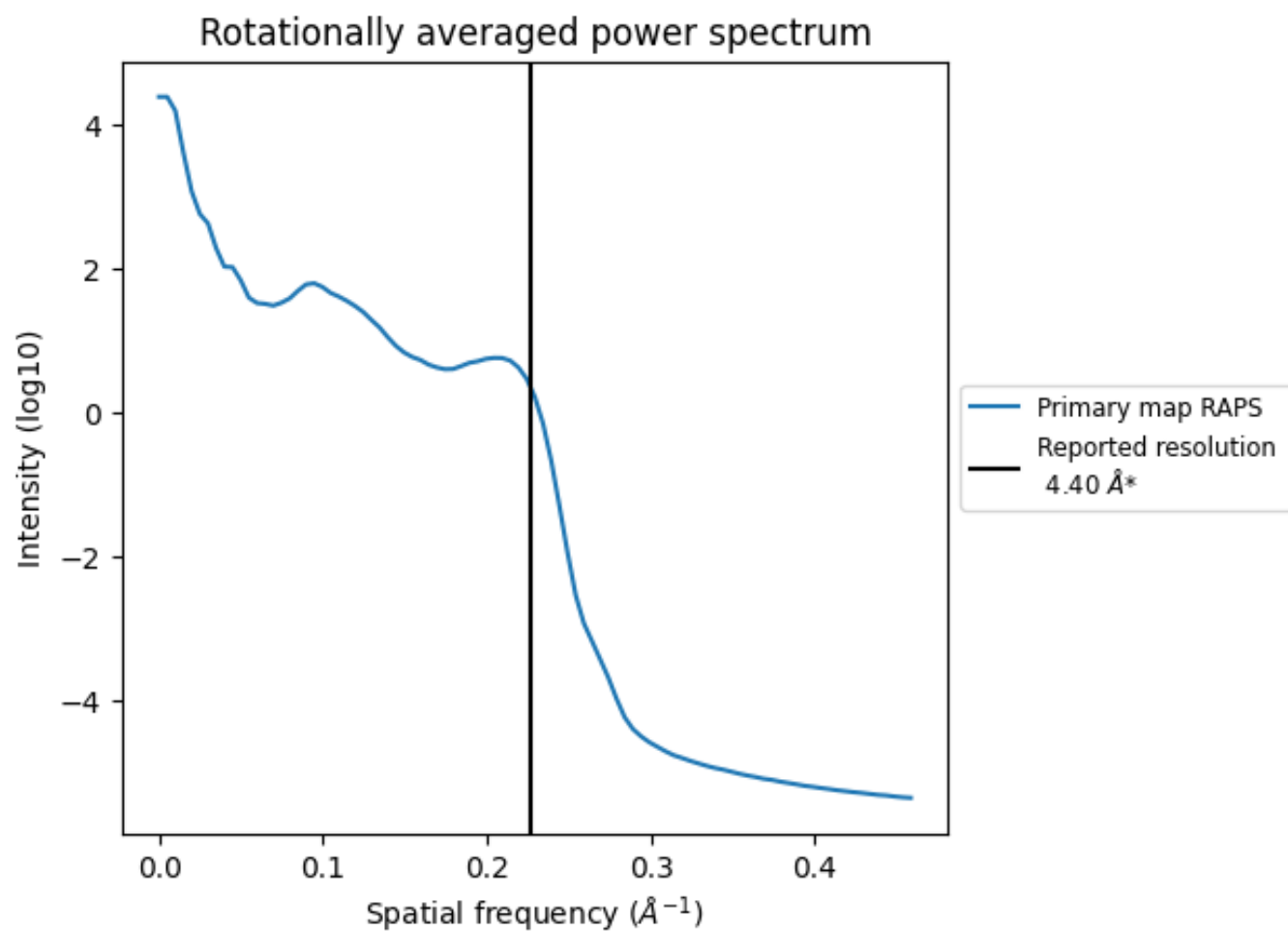
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 81 nm³; this corresponds to an approximate mass of 73 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 0.227 Å⁻¹

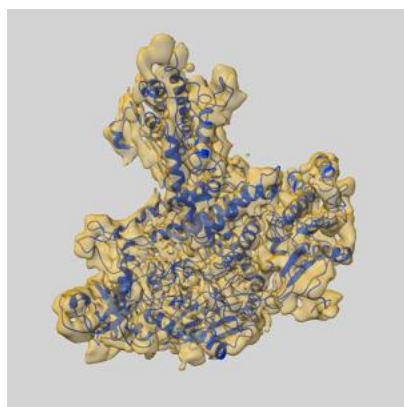
8 Fourier-Shell correlation

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

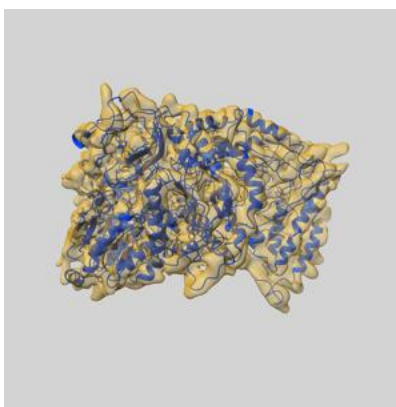
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0287 and PDB model 6HV8. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

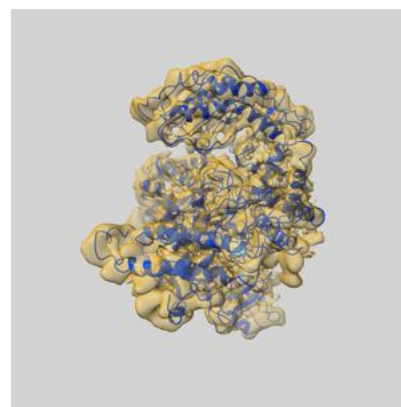
9.1 Map-model overlay [i](#)



X



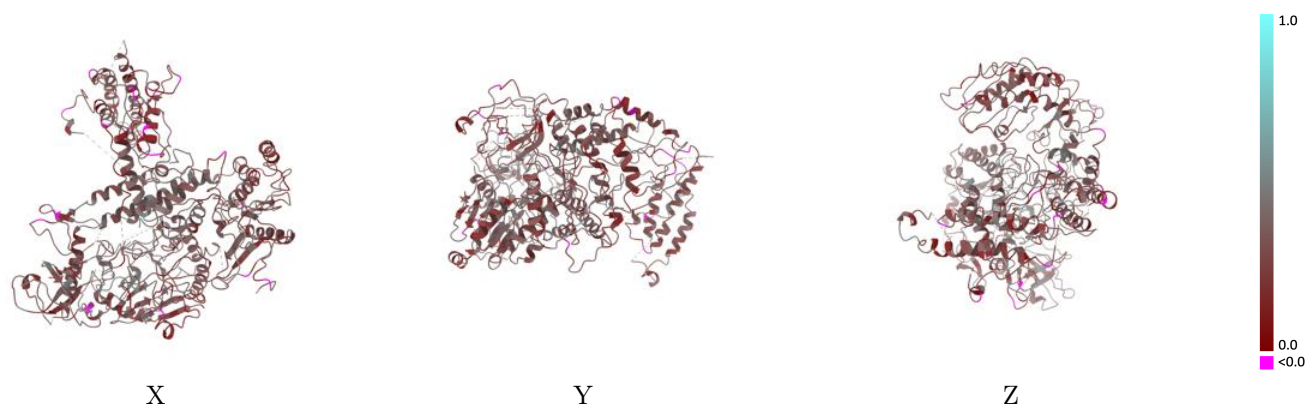
Y



Z

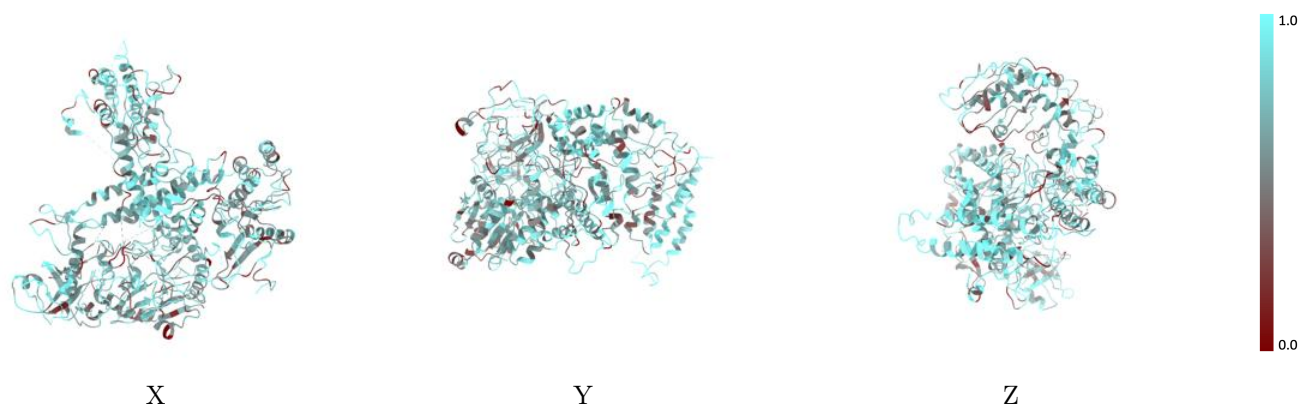
The images above show the 3D surface view of the map at the recommended contour level 0.0576 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



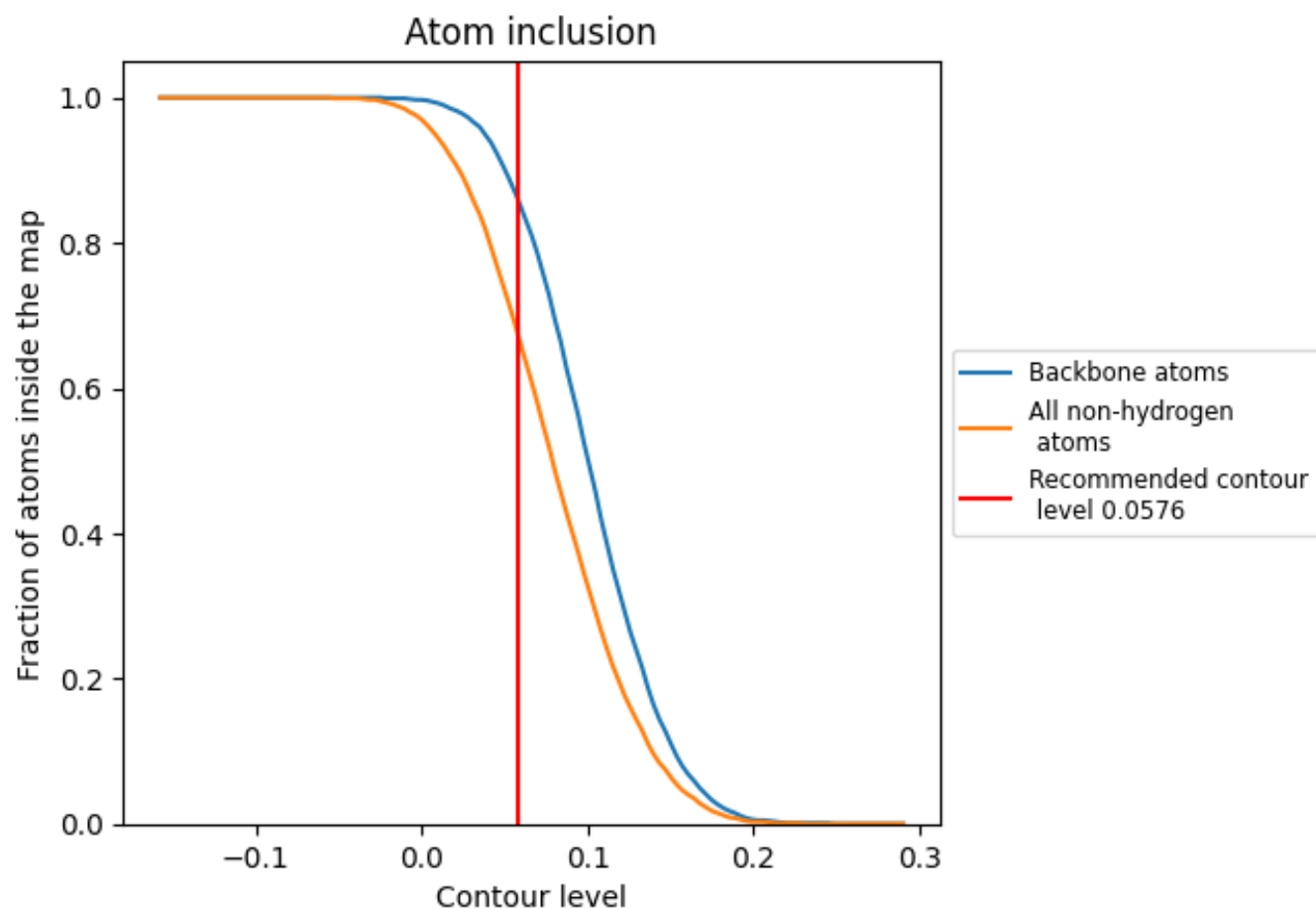
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0576).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 68% 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 (0.0576) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6780	<div></div> 0.3150
A	<div></div> 0.6750	<div></div> 0.3050
B	<div></div> 0.6840	<div></div> 0.3320

