



wwPDB EM Validation Summary Report ⓘ

Apr 25, 2026 – 09:56 PM EDT

PDB ID : 9PVP / pdb_00009pvp
EMDB ID : EMD-71895
Title : Cryo-EM structure of receptor tyrosine kinase ROS1 extracellular domain
Authors : Li, H.; Klein, D.
Deposited on : 2025-08-03
Resolution : 4.57 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
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

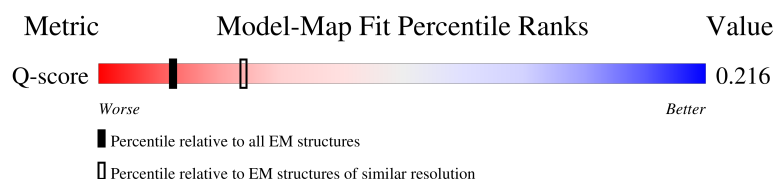
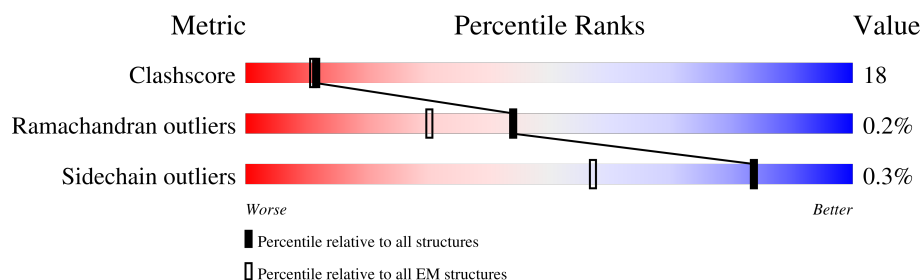
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.57 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	2418 (4.07 - 5.07)

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	1854	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13753 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 Proto-oncogene tyrosine-protein kinase ROS.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1715	Total	C	N	O	S	0	0
			13599	8740	2229	2570	60		

There are 34 discrepancies between the modelled and reference sequences:

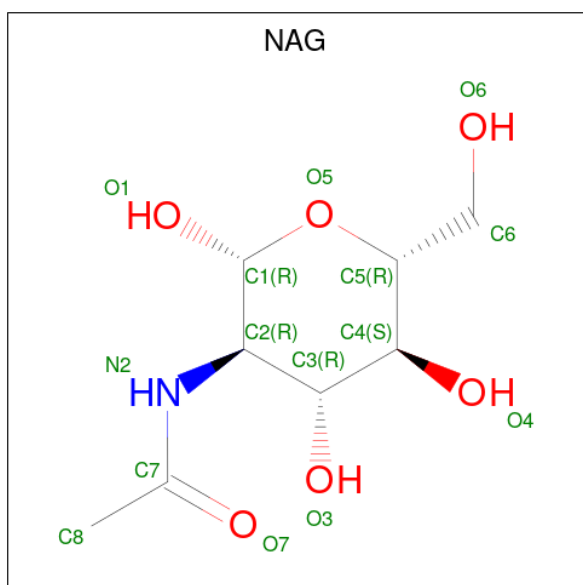
Chain	Residue	Modelled	Actual	Comment	Reference
A	1848	GLY	-	expression tag	UNP Q78DX7
A	1849	GLY	-	expression tag	UNP Q78DX7
A	1850	GLY	-	expression tag	UNP Q78DX7
A	1851	SER	-	expression tag	UNP Q78DX7
A	1852	SER	-	expression tag	UNP Q78DX7
A	1853	ALA	-	expression tag	UNP Q78DX7
A	1854	TRP	-	expression tag	UNP Q78DX7
A	1855	SER	-	expression tag	UNP Q78DX7
A	1856	HIS	-	expression tag	UNP Q78DX7
A	1857	PRO	-	expression tag	UNP Q78DX7
A	1858	GLN	-	expression tag	UNP Q78DX7
A	1859	PHE	-	expression tag	UNP Q78DX7
A	1860	GLU	-	expression tag	UNP Q78DX7
A	1861	LYS	-	expression tag	UNP Q78DX7
A	1862	GLY	-	expression tag	UNP Q78DX7
A	1863	GLY	-	expression tag	UNP Q78DX7
A	1864	GLY	-	expression tag	UNP Q78DX7
A	1865	SER	-	expression tag	UNP Q78DX7
A	1866	GLY	-	expression tag	UNP Q78DX7
A	1867	GLY	-	expression tag	UNP Q78DX7
A	1868	GLY	-	expression tag	UNP Q78DX7
A	1869	SER	-	expression tag	UNP Q78DX7
A	1870	GLY	-	expression tag	UNP Q78DX7
A	1871	GLY	-	expression tag	UNP Q78DX7
A	1872	SER	-	expression tag	UNP Q78DX7
A	1873	ALA	-	expression tag	UNP Q78DX7
A	1874	TRP	-	expression tag	UNP Q78DX7
A	1875	SER	-	expression tag	UNP Q78DX7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1876	HIS	-	expression tag	UNP Q78DX7
A	1877	PRO	-	expression tag	UNP Q78DX7
A	1878	GLN	-	expression tag	UNP Q78DX7
A	1879	PHE	-	expression tag	UNP Q78DX7
A	1880	GLU	-	expression tag	UNP Q78DX7
A	1881	LYS	-	expression tag	UNP Q78DX7

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	

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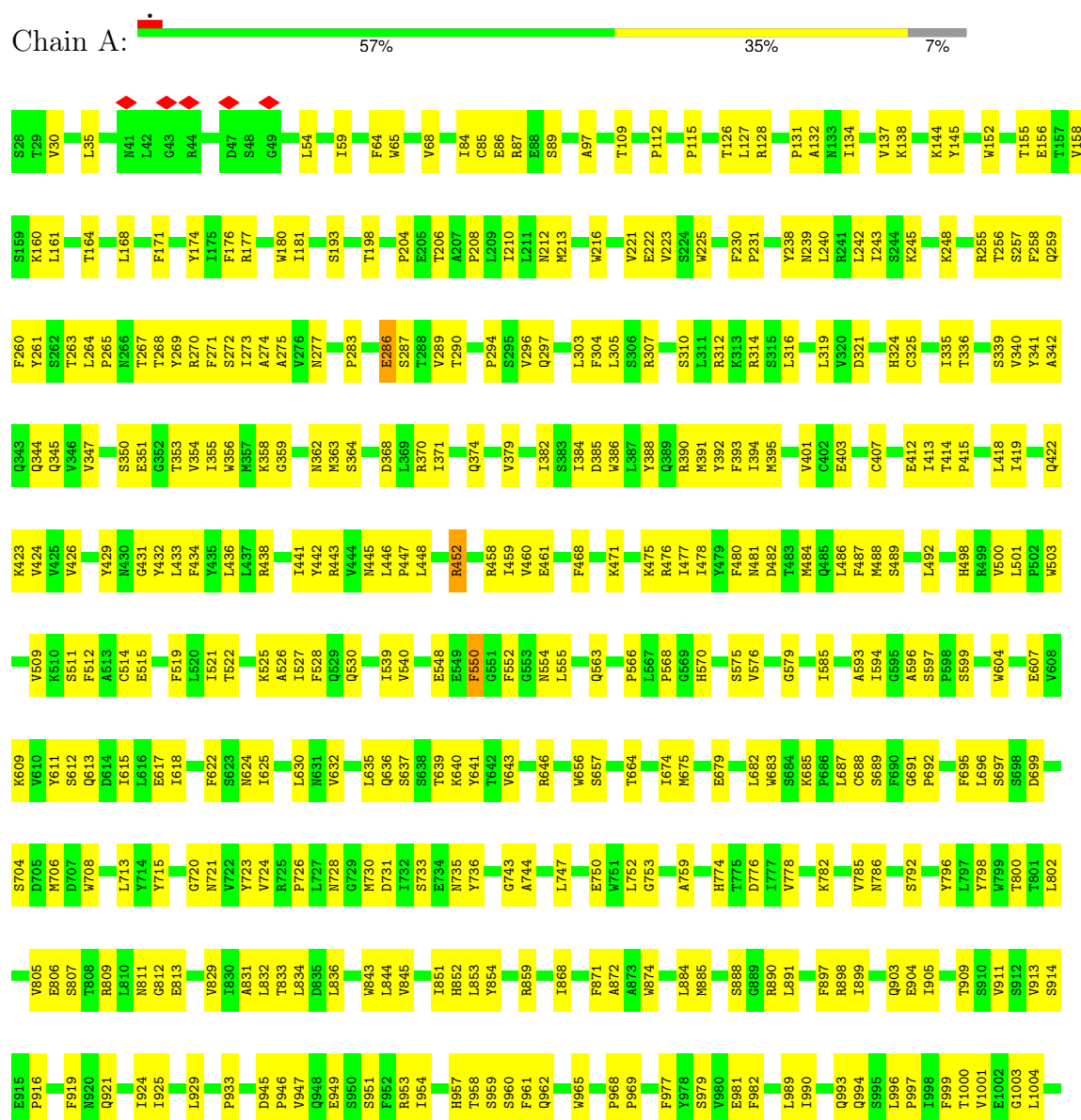
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Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	

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: Proto-oncogene tyrosine-protein kinase ROS



TRP	SER	N1719	P1633	Y1529	K1436	W1346	T1245	Q1167	G1089	L1009
SER	ARG	V1724	E1634	S1530	S1443	I1347	Q1246	N1168	T1090	F1010
HIS	TRP		E1635	E1531	D1444		V1250	V1169	M1011	L1012
PRO	GLN		M1636	E1534	T1454	T1350	D1251	V1170	L1017	
PHE	VAL		W1637	H1535	R1352	K1351	H1254	W1172	F1018	
GLU	PHE		C1638	L1536	Q1353	Q1353	K1255	F1174	Y1019	
LYS	ASN			I1542	T1456	E1354	V1256	S1175		
GLY	GLY		S1641	Q1543	S1457	I1355	K1257	L1176	Q1024	
GLY	SER			G1544	L1458	W1356	S1258			
CYS	CYS		M1648	Q1545	T1459	A1357	P1259	V1180		
SER	SER		E1653	T1546	L1462	M1358	S1181	S1107	L1028	
ILE	PRO			K1547	P1463	D1359	T1182		S1029	
GLY	GLY		A1657	S1548	P1464		V1183	Q1110	F1030	
GLY	THR		L1658		V1465	G1362	T1269	L1111	R1031	
GLY	TRP		V1659	P1551	L1466	C1363	T1270	E1112	A1032	
ARG	ARG		P1660	A1553	V1471	Q1364	T1271	E1117	P1033	
SER	SER		E1661	V1554	H1472	C1365	I1272	Y1118	E1034	
LYS	LYS		M1662	C1555	G1473	V1368	S1273	V1119	V1036	
LEU	LEU		T1663	H1556		I1369	Y1277	V1120	P1037	
GLY	GLY		S1664	I1557	T1480	M1370	P1278	A1121	S1038	
GLY	GLY		L1665	M1558	Y1481	L1374	L1279	F1122	P1040	
THR	PHE		Q1666		L1482		L1280	Q1123	E1041	
PHE	GLN		L1667	L1567	M1486	K1377	T1286	V1124	H1042	
GLN	PHE		D1668	F1570	E1487	R1378	E1287	R1125	F1043	
ARG	ARG		W1669	W1571	A1488	T1383	D1290	V1126		
ALA	ALA		L1677	P1577	A1491	V1384	H1293	F1127	F1045	
VAL	VAL		T1678			D1385	Q1306	L1201	F1046	
ALA	ALA			P1580	R1496		H1307	L1202	I1047	
ASN	ASN		W1681	K1581	R1497	I1389	Q1294	P1132	L1048	
GLU	GLU		F1682	S1582	H1498	T1295	M1295	G1133	S1049	
ILE	ILE		E1683	V1583	K1499	W1390	F1296	P1134	S1050	
GLY	ASP		L1684	V1584	I1392	I1391	Y1297	F1135	G1051	
LEU	ASN		Q1685	R1585	M1500	M1393		V1139	R1052	
GLY	GLY		K1686	T1586	L1501		Q1306		Y1053	
GLU	SER		W1687	Q1587	E1502	K1396	H1307	S1144	V1060	
TYR	ARG		K1688	M1590	S1503	D1397	F1214	E1145	V1061	
GLU	LEU		M1689	S1591	Q1504		V1219	I1146	E1062	
ILE	MET		M1690	Y1592	E1505	I1401	A1225	K1147	F1063	
SER	TYR		E1691	P1600	N1506	Q1403	V1227	C1149	R1064	
GLU	THR		F1692		V1507		D1228	P1150	W1066	
ASP	LEU		Y1693		A1508		W1229	Y1151	K1067	
THR	GLU		H1694	F1606	R1509	S1413	I1230	I1153		
VAL	VAL		V1695	L1613	P1515	R1419	G1318	S1154	M1072	
LEU	LEU		K1696		S1517	G1319	C1322	L1155	G1073	
VAL	LYS		G1619		M1518	H1422		L1156	K1077	
GLU	GLY		G1620		Y1519	I1423		G1157	F1078	
ASP	ILE		G1621		M1520	L1424		H1233	E1079	
GLY	SER		Q1622		I1521	Y1425		K1159		
GLY	ASN					S1427		I1160	Y1082	
ASP	ASP		Q1701		A1524	G1333		V1161	H1083	
GLY	GLY				V1525	A1334		F1162	I1084	
GLY	GLY		C1707		W1526	M1335		L1163	S1085	
SER	SER				M1626	A1429		D1164		
SER	GLN		D1711		N1527	L1430		M1165		
ALA	ALA		L1712		Y1528			D1166	S1088	
			Q1713							
			P1714							
			Y1715							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23490	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.895	Depositor
Minimum map value	-0.387	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.0857	Depositor
Map size (Å)	499.19998, 499.19998, 499.19998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	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: NAG

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	2/13982 (0.0%)	0.39	4/19068 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1259	PRO	CG-CD	-11.01	1.13	1.50
1	A	1259	PRO	N-CD	5.86	1.55	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1259	PRO	CA-N-CD	-12.84	94.03	112.00
1	A	1259	PRO	N-CD-CG	-12.42	84.56	103.20
1	A	1259	PRO	CA-CB-CG	-7.61	90.04	104.50
1	A	1311	PRO	CA-N-CD	-5.40	104.44	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13599	0	13278	480	0
2	A	154	0	141	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13753	0	13419	480	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

The worst 5 of 480 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:1034:GLU:HB3	1:A:1073:GLY:HA2	1.54	0.90
1:A:1147:LYS:NZ	1:A:1149:CYS:SG	2.53	0.81
1:A:1250:VAL:HG22	1:A:1259:PRO:HD3	1.65	0.77
1:A:385:ASP:HB2	1:A:392:TYR:HE1	1.49	0.75
1:A:1358:MET:HE2	1:A:1365:CYS:HB3	1.69	0.72

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	1713/1854 (92%)	1612 (94%)	98 (6%)	3 (0%)	43 77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1352	ARG
1	A	452	ARG
1	A	550	PHE

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
1	A	1531/1642 (93%)	1526 (100%)	5 (0%)	86 84

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	286	GLU
1	A	1151	TYR
1	A	1528	TYR
1	A	1542	ILE
1	A	1636	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1167	GLN
1	A	1325	ASN
1	A	1708	ASN
1	A	1522	GLN
1	A	921	GLN

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

11 ligands are 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	NAG	A	1905	1	14,14,15	0.20	0	17,19,21	0.42	0
2	NAG	A	1904	1	14,14,15	0.34	0	17,19,21	0.44	0
2	NAG	A	1906	1	14,14,15	0.41	0	17,19,21	0.60	0
2	NAG	A	1901	-	14,14,15	0.22	0	17,19,21	0.42	0
2	NAG	A	1911	-	14,14,15	0.22	0	17,19,21	0.42	0
2	NAG	A	1903	1	14,14,15	0.21	0	17,19,21	0.43	0
2	NAG	A	1908	1	14,14,15	0.33	0	17,19,21	0.54	0
2	NAG	A	1902	-	14,14,15	0.20	0	17,19,21	0.44	0
2	NAG	A	1907	-	14,14,15	0.22	0	17,19,21	0.43	0
2	NAG	A	1909	-	14,14,15	0.22	0	17,19,21	0.41	0
2	NAG	A	1910	1	14,14,15	0.25	0	17,19,21	0.53	0

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	NAG	A	1905	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1904	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1906	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1901	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1911	-	-	2/6/23/26	0/1/1/1
2	NAG	A	1903	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1908	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1902	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1907	-	-	2/6/23/26	0/1/1/1
2	NAG	A	1909	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1910	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1908	NAG	C4-C5-C6-O6
2	A	1905	NAG	C4-C5-C6-O6
2	A	1908	NAG	O5-C5-C6-O6
2	A	1903	NAG	O5-C5-C6-O6
2	A	1905	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1911	NAG	1	0
2	A	1908	NAG	1	0

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.

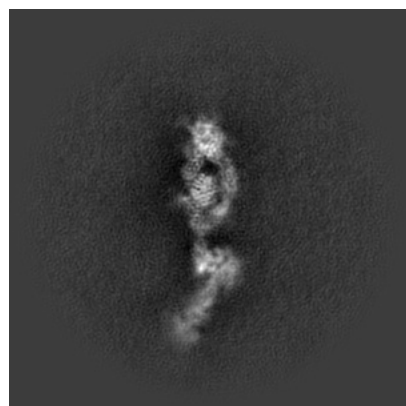
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71895. These allow visual inspection of the internal detail of the map and identification of artifacts.

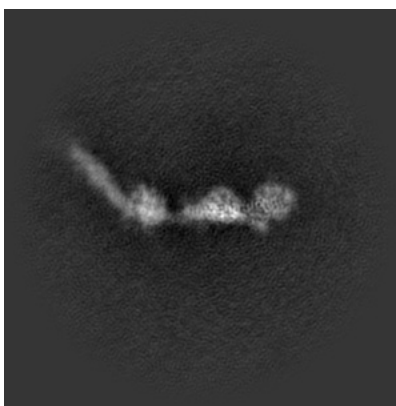
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

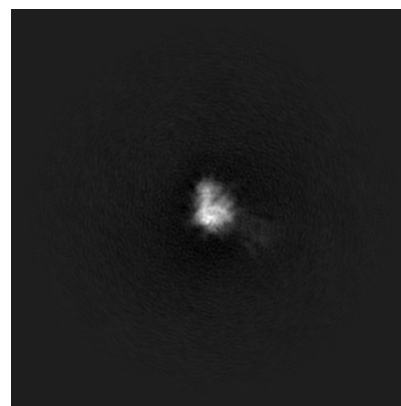
6.1.1 Primary map



X

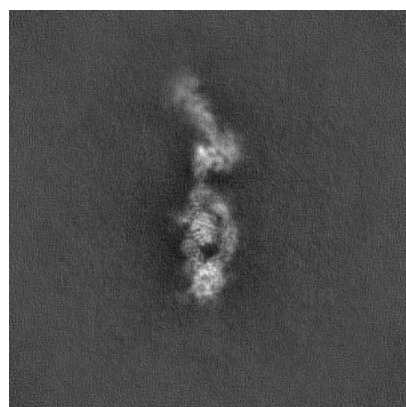


Y

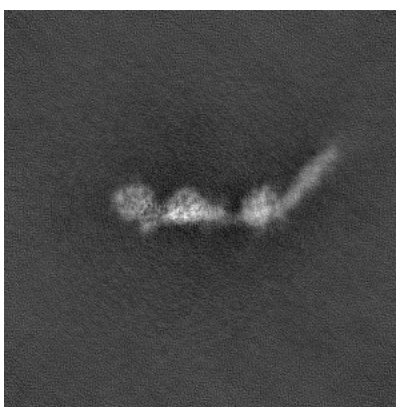


Z

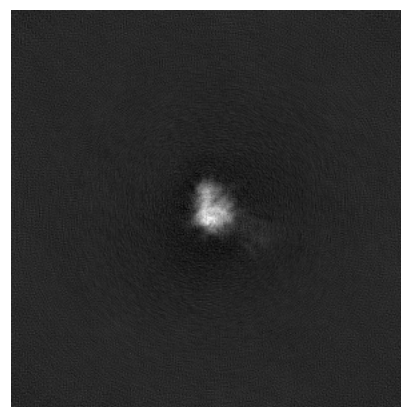
6.1.2 Raw map



X



Y

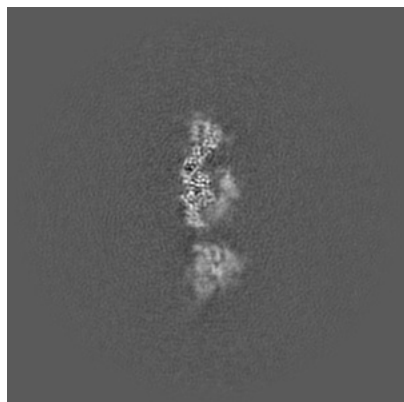


Z

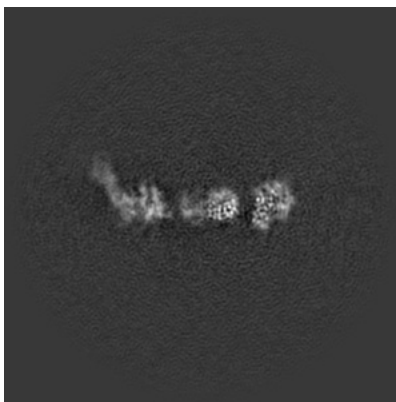
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

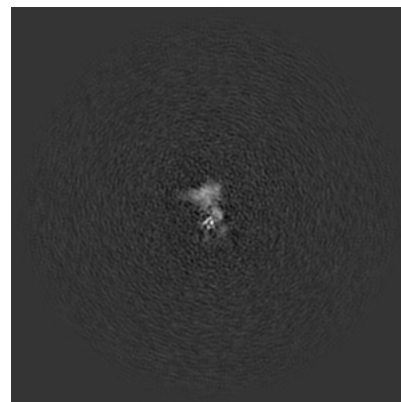
6.2.1 Primary map



X Index: 192

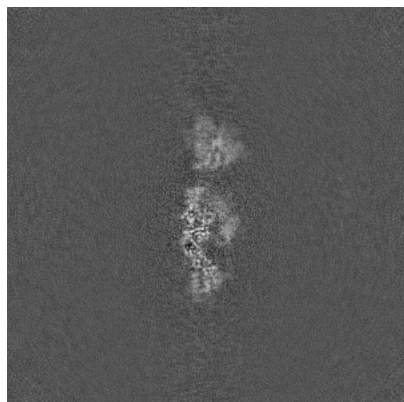


Y Index: 192

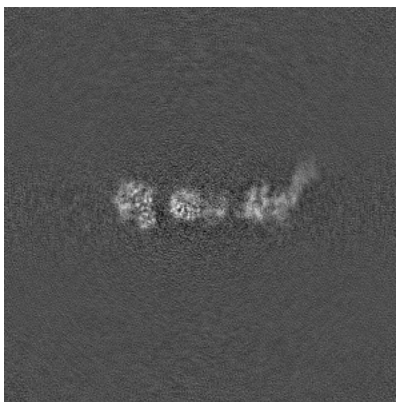


Z Index: 192

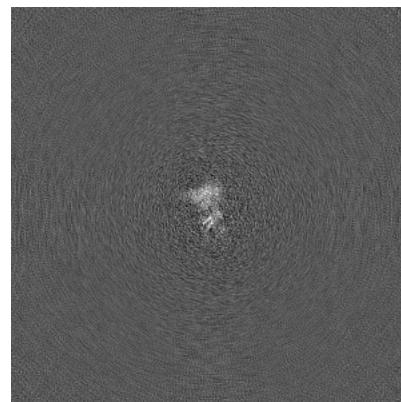
6.2.2 Raw map



X Index: 192



Y Index: 192

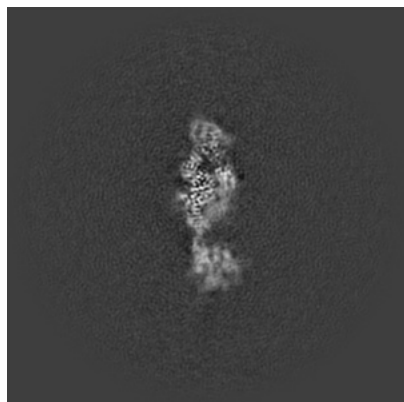


Z Index: 192

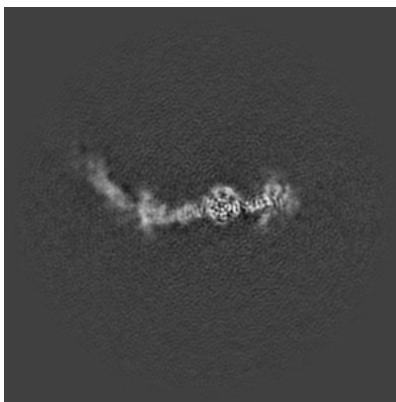
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

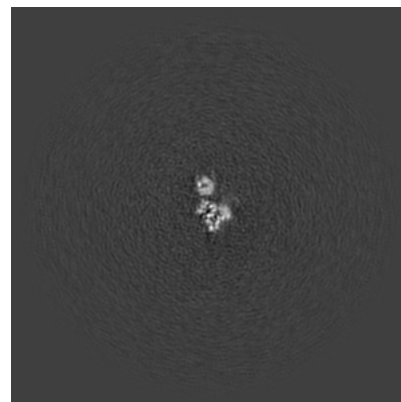
6.3.1 Primary map



X Index: 188

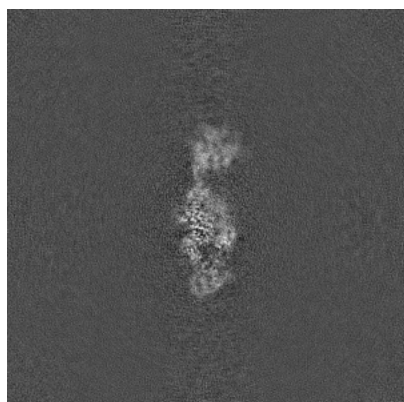


Y Index: 184

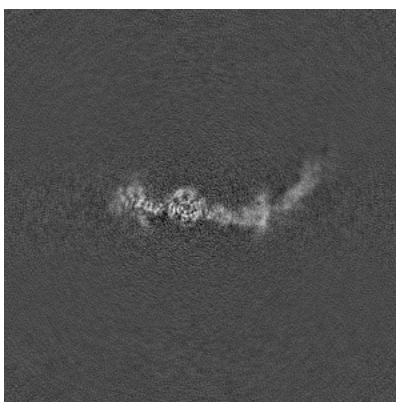


Z Index: 216

6.3.2 Raw map



X Index: 188



Y Index: 184

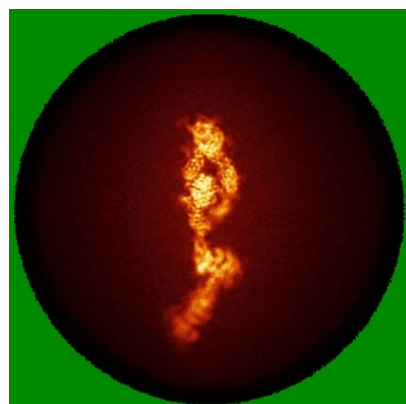


Z Index: 167

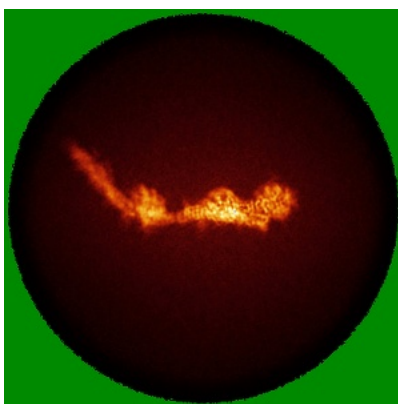
The images above show the largest variance slices of the map in three orthogonal directions.

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

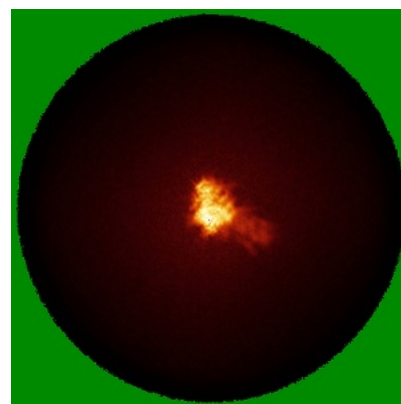
6.4.1 Primary map



X

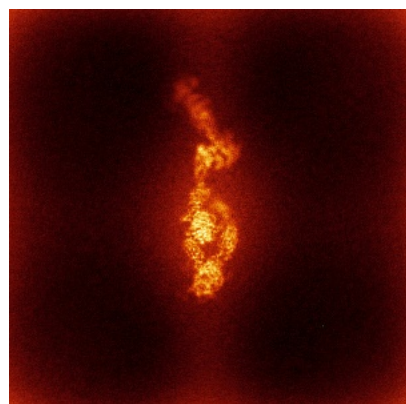


Y

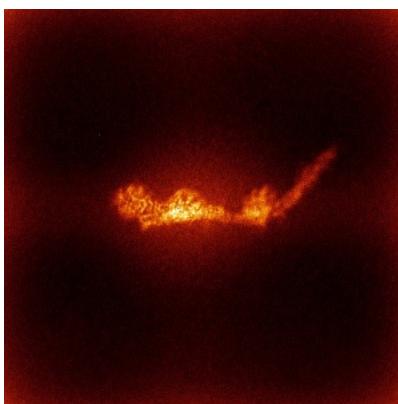


Z

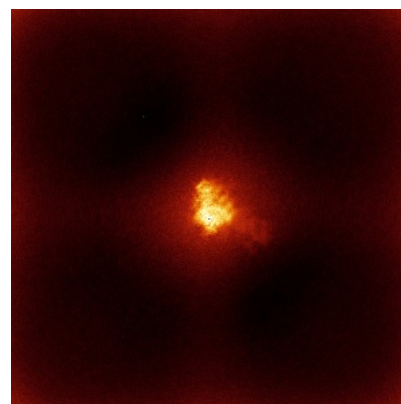
6.4.2 Raw map



X



Y

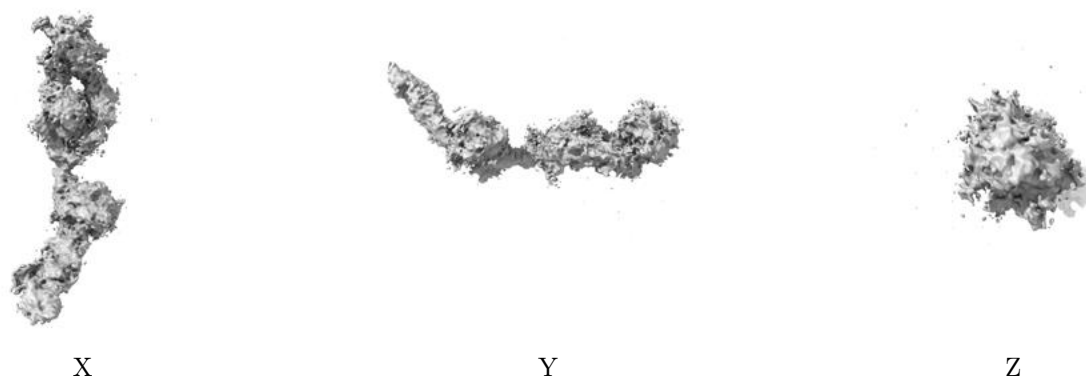


Z

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.

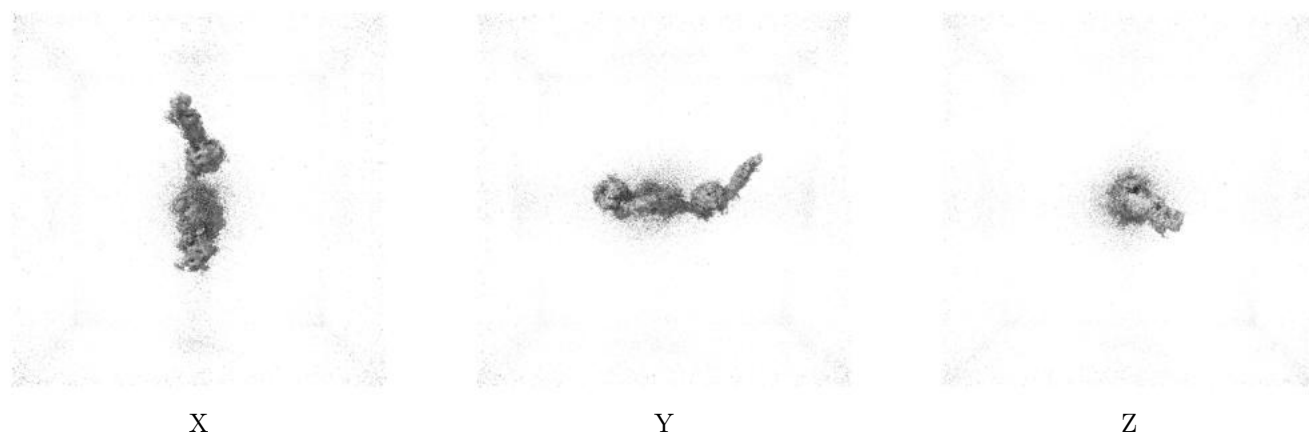
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0857. 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.

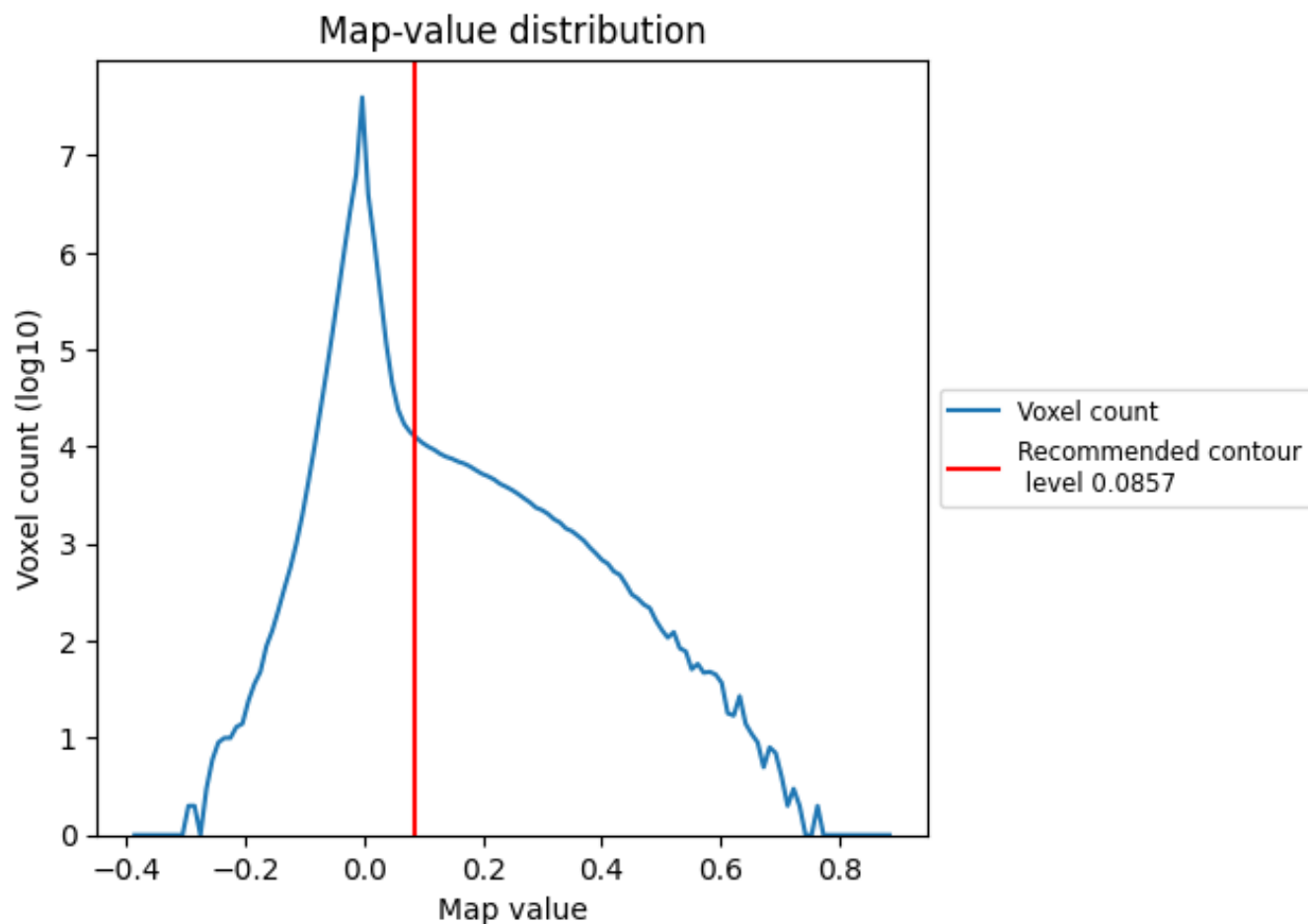
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

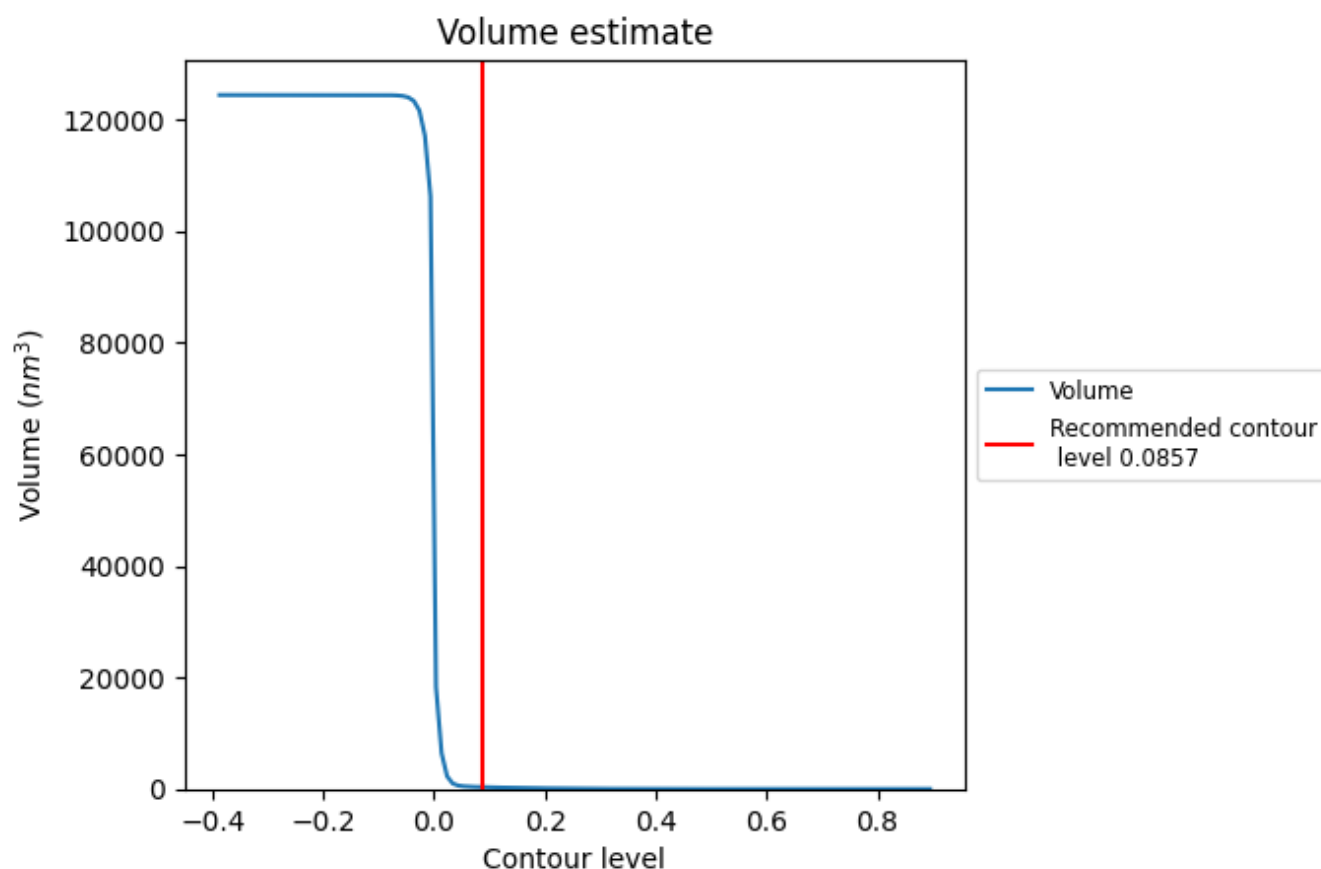
This section contains the results of statistical analysis of the map.

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.

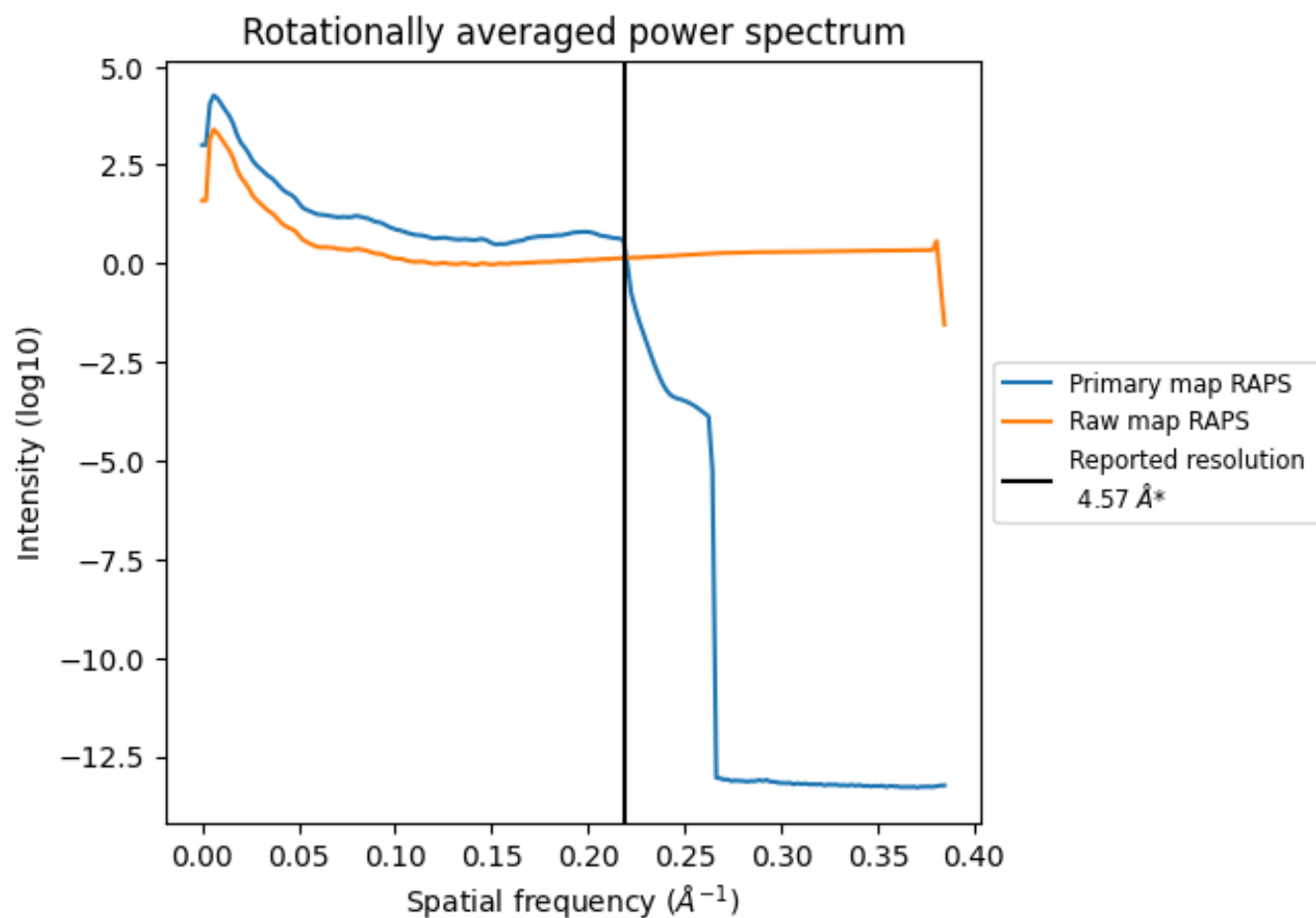
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 334 nm³; this corresponds to an approximate mass of 301 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 ⓘ

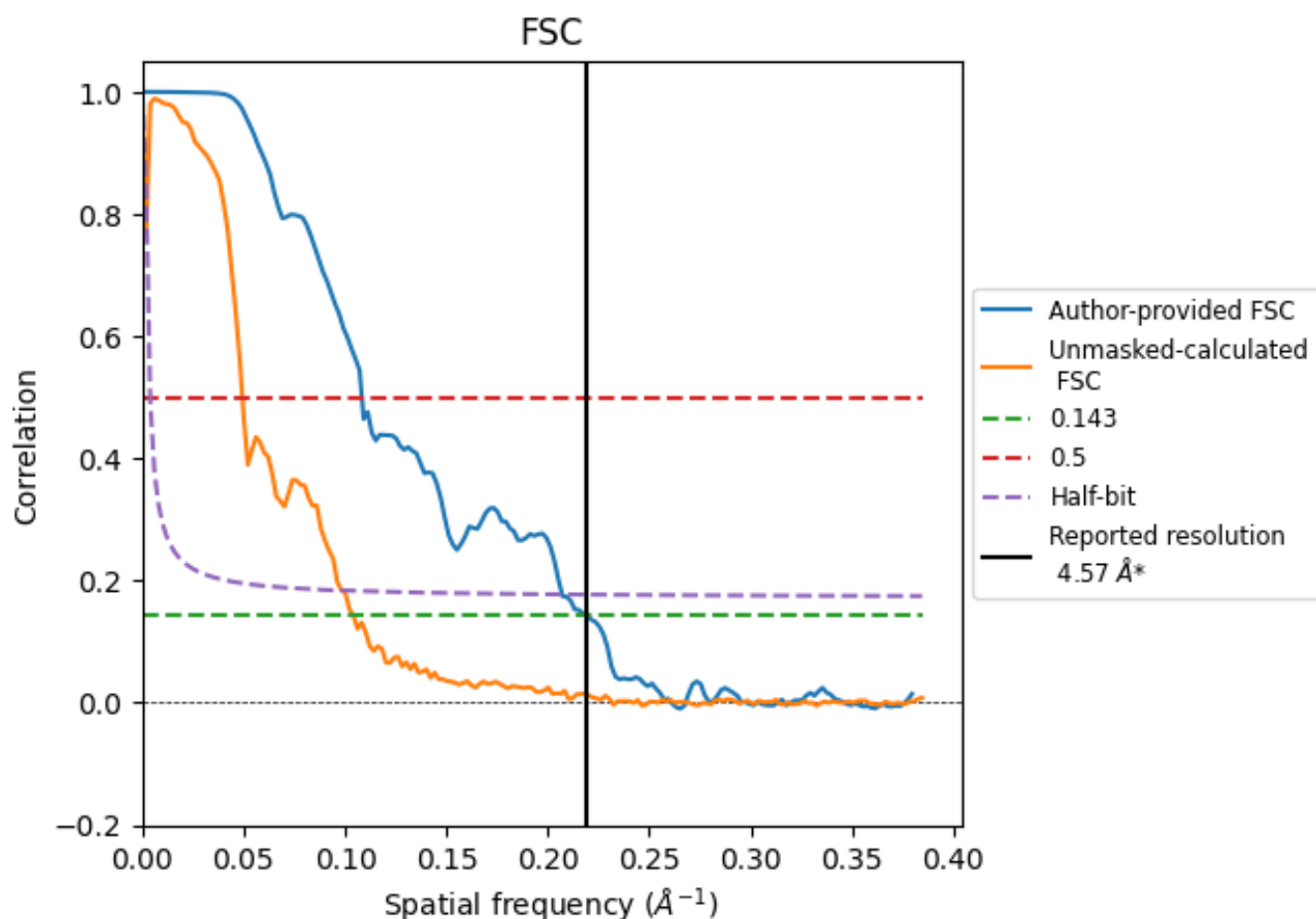


*Reported resolution corresponds to spatial frequency of 0.219 $\text{\AA}^{-1}$

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 0.219 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

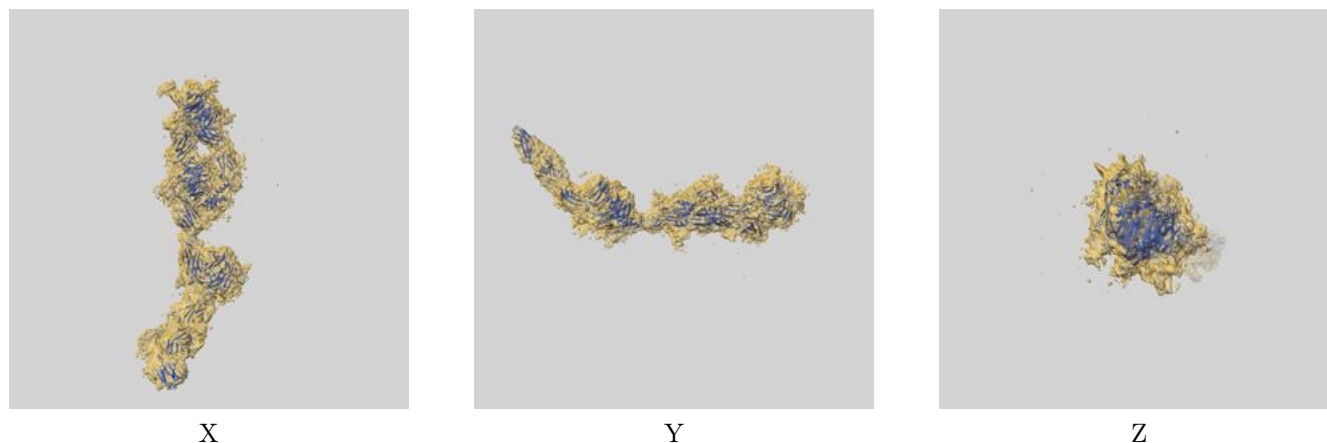
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.57	-	-
Author-provided FSC curve	4.57	9.23	4.83
Unmasked-calculated*	9.62	20.24	454.55

*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 9.62 differs from the reported value 4.57 by more than 10 %

9 Map-model fit [i](#)

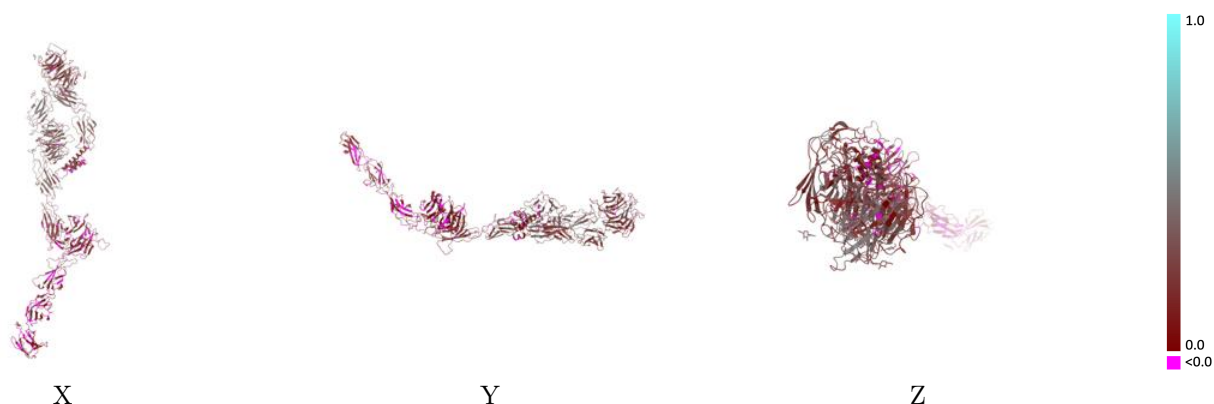
This section contains information regarding the fit between EMDB map EMD-71895 and PDB model 9PVP. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



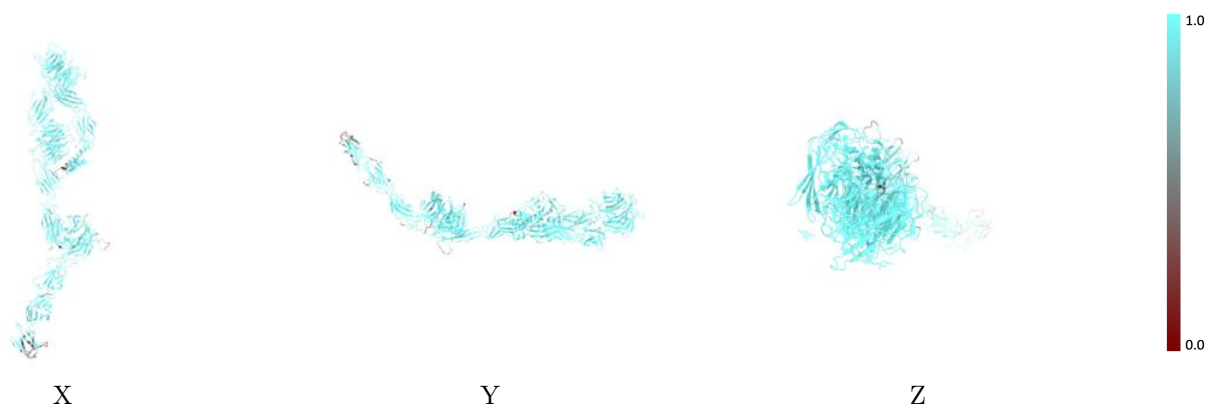
The images above show the 3D surface view of the map at the recommended contour level 0.0857 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



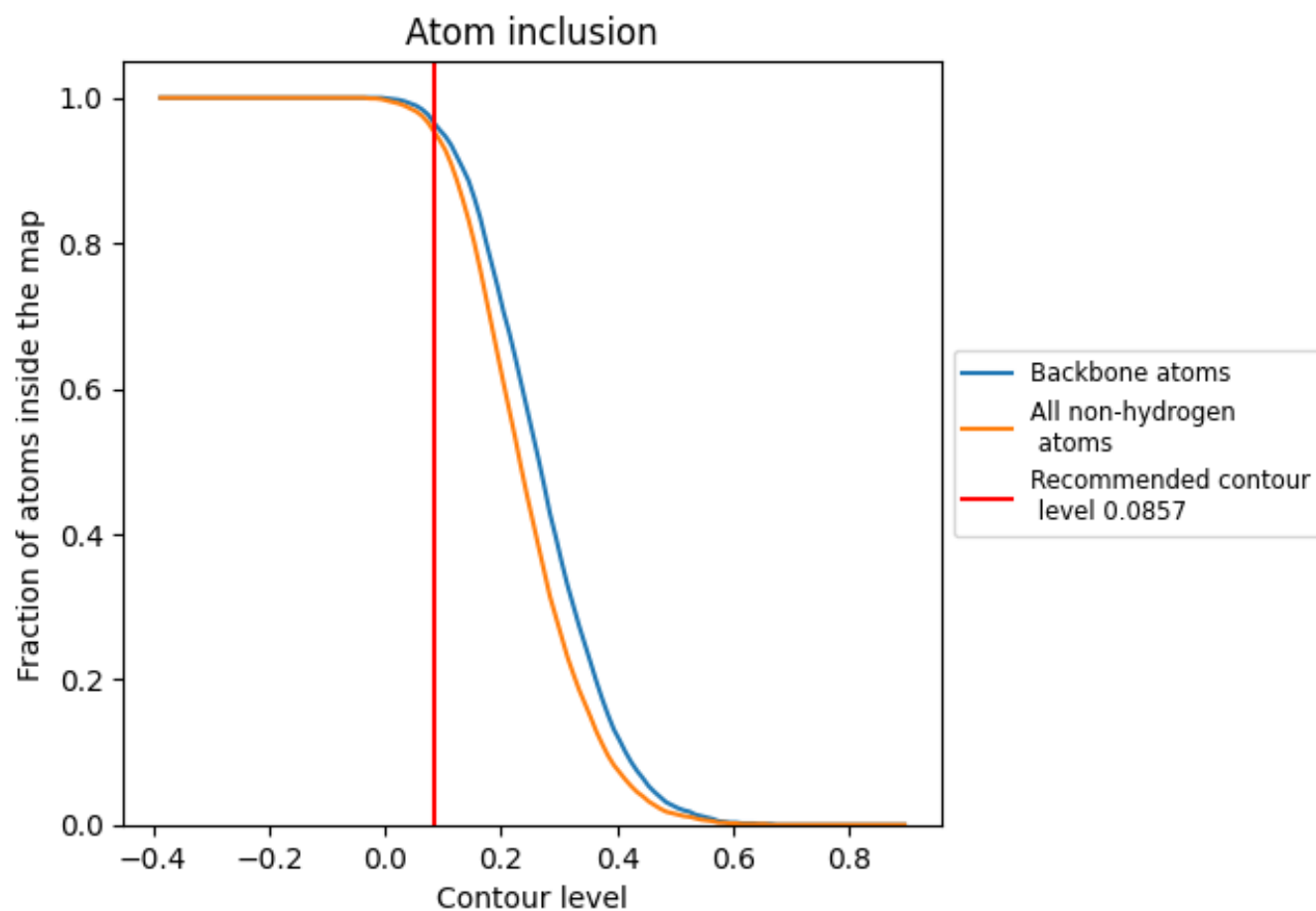
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0857).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.0857) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9520	0.2160
A	0.9520	0.2160

