



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 12:42 PM UTC

PDB ID : 6KWX / pdb_00006kwx
EMDB ID : EMD-0780
Title : cryo-EM structure of human PA200
Authors : Ouyang, S.; Hongxin, G.
Deposited on : 2019-09-09
Resolution : 3.75 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:

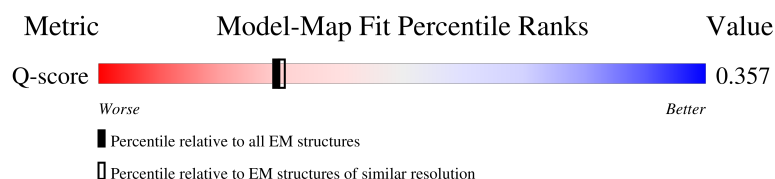
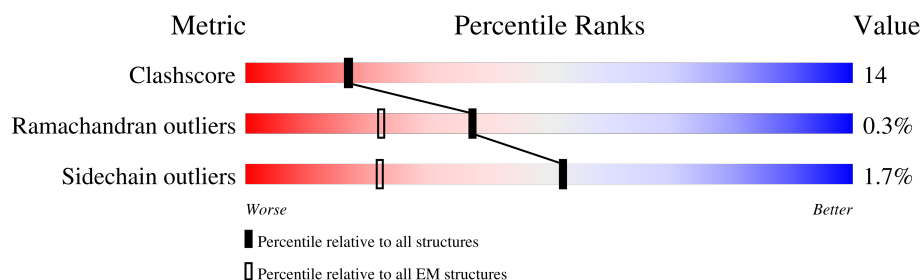
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.75 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	10301 (3.25 - 4.25)

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	1878	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IHP	A	1902	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14227 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 Proteasome activator complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1751	Total	C	N	O	S	0	0
			14147	9105	2414	2549	79		

There are 37 discrepancies between the modelled and reference sequences:

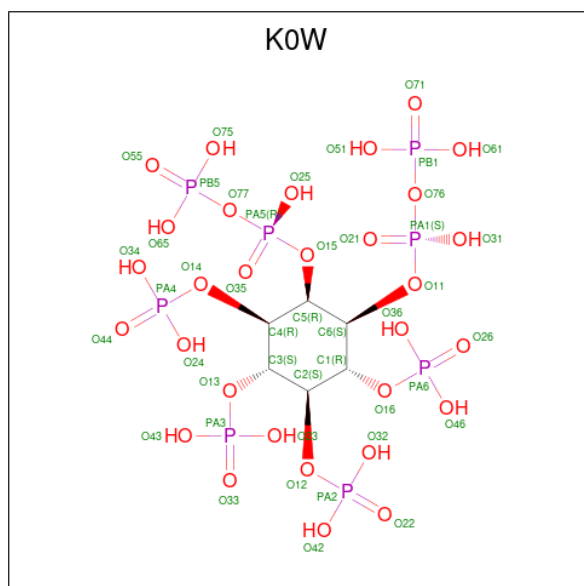
Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	MET	-	initiating methionine	UNP Q14997
A	-33	GLY	-	expression tag	UNP Q14997
A	-32	THR	-	expression tag	UNP Q14997
A	-31	THR	-	expression tag	UNP Q14997
A	-30	ARG	-	expression tag	UNP Q14997
A	-29	SER	-	expression tag	UNP Q14997
A	-28	THR	-	expression tag	UNP Q14997
A	-27	MET	-	expression tag	UNP Q14997
A	-26	SER	-	expression tag	UNP Q14997
A	-25	TYR	-	expression tag	UNP Q14997
A	-24	TYR	-	expression tag	UNP Q14997
A	-23	HIS	-	expression tag	UNP Q14997
A	-22	HIS	-	expression tag	UNP Q14997
A	-21	HIS	-	expression tag	UNP Q14997
A	-20	HIS	-	expression tag	UNP Q14997
A	-19	HIS	-	expression tag	UNP Q14997
A	-18	HIS	-	expression tag	UNP Q14997
A	-17	ASP	-	expression tag	UNP Q14997
A	-16	TYR	-	expression tag	UNP Q14997
A	-15	ASP	-	expression tag	UNP Q14997
A	-14	ILE	-	expression tag	UNP Q14997
A	-13	PRO	-	expression tag	UNP Q14997
A	-12	THR	-	expression tag	UNP Q14997
A	-11	THR	-	expression tag	UNP Q14997
A	-10	GLU	-	expression tag	UNP Q14997
A	-9	ASN	-	expression tag	UNP Q14997
A	-8	LEU	-	expression tag	UNP Q14997
A	-7	TYR	-	expression tag	UNP Q14997

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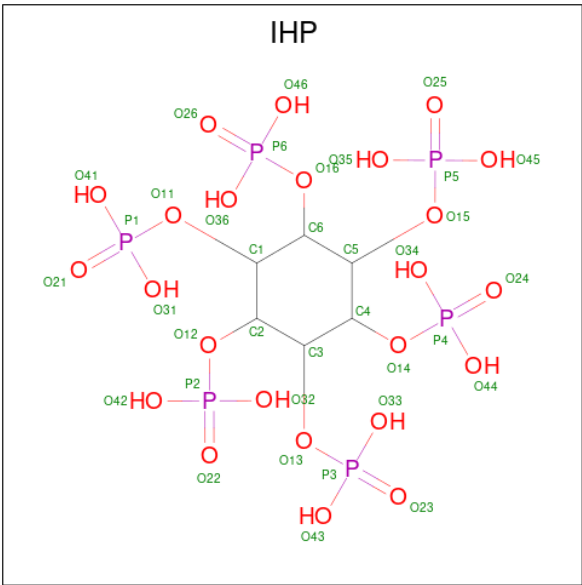
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	PHE	-	expression tag	UNP Q14997
A	-5	GLN	-	expression tag	UNP Q14997
A	-4	GLY	-	expression tag	UNP Q14997
A	-3	ALA	-	expression tag	UNP Q14997
A	-2	MET	-	expression tag	UNP Q14997
A	-1	ASP	-	expression tag	UNP Q14997
A	0	PRO	-	expression tag	UNP Q14997
A	821	ILE	LEU	conflict	UNP Q14997
A	822	LEU	ILE	conflict	UNP Q14997

- Molecule 2 is [(1 {S},2 {R},3 {R},4 {S},5 {S},6 {R})-2-[oxidanyl(phosphonooxy)phosphoryl]oxy-3,4,5,6-tetraphosphonooxy-cyclohexyl] phosphono hydrogen phosphate (CCD ID: K0W) (formula: C₆H₂₀O₃₀P₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	P	0
			44	6	30	8	

- Molecule 3 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆) (labeled as "Ligand of Interest" by depositor).

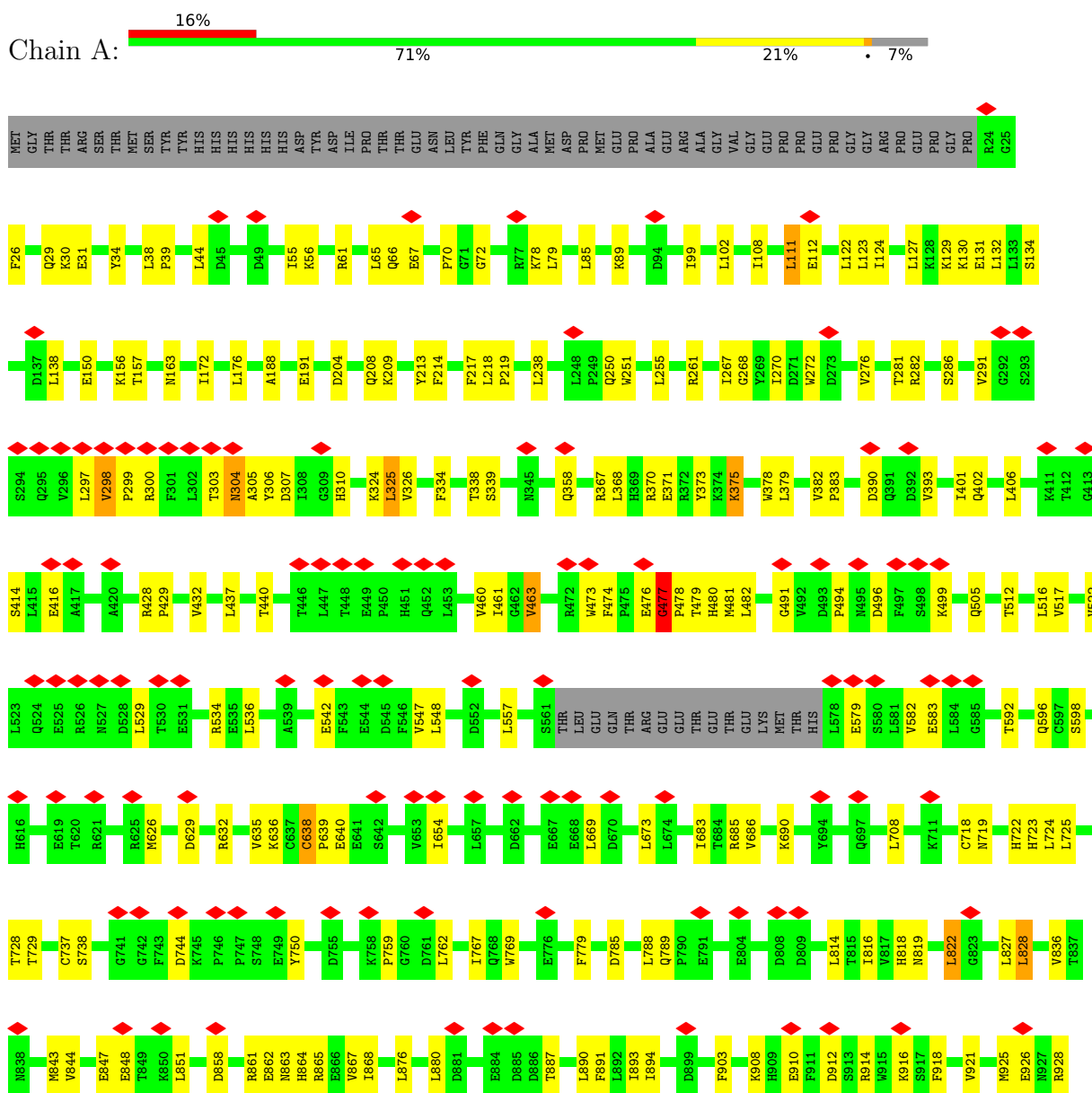


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
3	A	1	36	6	24	6	0

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: Proteasome activator complex subunit 4



H1791	L1792	M1793	D1794	P1795	Q1796	P1797	I1798	E1799	M1800	T1801	V1802	K1803	K1804	T1805	L1806	S1807	M1808	F1809	R1810	T1811	T1812	H1813	HIS	ASP	ASN	TRP	GLN	GLU	LYS	GLN	PHE	THR	ASP	ASP	GLN	LEU	LEU	VAL	THR	ASP	LEU	LEU	VAL	SER	PRO	CYS	TYR	TYR	ALA								
Q1730	L1731	C1732	K1733	T1734	K1735	L1736	P1737	K1738	LYS	ARG	LYS	ASP	PRO	GLY	SER	VAL	GLY	ASP	THR	ILE	PRO	S1753	A1754	E1755	L1756	V1757	K1758	R1759	H1760	A1761	G1762	V1763	L1764	G1765	L1766	G1767	A1768	C1769	V1770	L1771	S1772	S1773	D1776	V1777	P1778	T1779	V1780	M1781	P1782	Q1783	M1784	L1785	M1786	N1787	L1788	S1789	A1790
T1663	Y1664	L1665	Q1666	T1667	M1668	V1669	F1670	V1671	N1672	L1673	F1674	L1677	E1680	D1681	A1682	D1685	I1686	R1687	V1688	I1691	S1692	L1693	L1694	E1695	D1696	E1697	Q1698	V1701	R1702	E1703	M1704	A1705	A1706	T1707	T1708	L1709	L1712	L1713	Q1714	C1715	M1716	T1719	M1720	D1721	S1722	P1723	M1724	Q1725	I1726	F1727	E1728	A1729					
K1572	L1573	L1574	K1575	L1576	L1578	L1581	M1582	R1587	A1592	E1595	L1600	F1603	F1604	K1605	I1606	A1607	P1608	V1609	E1610	M1611	D1612	D1613	S1614	Y1615	D1616	E1617	L1618	K1619	R1620	D1621	A1622	K1623	L1624	L1628	Q1631	Q1638	K1647	Q1648	T1649	A1650	R1651	S1652	S1653	R1658	Y1659	T1660	V1661	L1662									
P1480	E1481	L1482	R1485	L1486	L1490	K1493	L1494	V1497	Y1498	K1499	M1500	V1501	R1502	I1505	G1506	S1507	V1508	T1510	Y1511	I1512	F1513	M1514	I1515	D1516	I1537	K1540	L1541	V1547	D1548	E1549	E1550	I1551	Q1552	M1553	H1554	V1555	MET	GLU	GLU	ASN	GLY	ILE	GLY	GLU	D1565	E1566	R1567	I1571									
I1382	I1383	A1384	G1385	W1393	K1397	V1398	W1402	C1406	L1409	A1412	N1415	E1419	C1427	I1428	C1432	E1433	S1434	R1435	K1439	L1440	L1443	F1444	E1445	L1446	L1447	L1448	E1449	S1450	P1451	L1452	S1453	G1454	E1455	G1456	G1457	D1461	A1462	L1468	Q1469	Q1475	W1476	V1477	R1478	V1479													
V1269	E1270	K1271	T1272	H1273	W1274	M1282	V1285	Y1286	E1290	L1295	R1299	E1300	D1301	Q1306	Q1307	I1308	K1317	Q1321	L1322	I1323	L1326	S1327	L1328	E1329	D1330	R1331	K1332	G1333	K1334	D1335	R1341	G1347	R1350	M1351	L1357	L1360	H1363	D1370	S1371	H1372	A1380	E1381															
K1135	D1138	R1141	M1142	L1146	V1147	D1148	D1152	G1153	V1154	E1155	Q1156	R1157	K1162	F1163	E1164	G1168	G1169	L1170	R1176	D1177	D1178	L1181	P1182	L1183	I1186	R1187	E1191	N1192	L1193	M1194	H1195	D1196	K1213	K1216	I1224	C1227	E1228	P1235	T1236	Q1237	E1262																
H1035	S1036	A1041	H1044	V1050	Q1051	T1052	W1053	P1054	A1055	I1056	V1057	S1062	Q1063	A1064	M1065	S1066	L1067	V1073	R1074	D1077	D1078	L1079	A1080	E1081	K1082	R1085	Q1086	G1091	I1096	S1099	Q1109	K1111	N1112	P1113	N1116	Q1117	L1120	E1123	K1124	I1125	I1129	K1130	R1131														
L929	K932	K933	Q934	H935	I936	L939	L940	T941	D942	R943	E949	L950	R951	T952	L953	G957	C958	Y959	Y960	K961	K962	I963	D966	H967	I968	R969	D970	L971	L972	R973	L974	S980	R983	H984	K985	F990	D1003	I1004	L1009	E1010	D1015	R1016	V1019	T1020	G1033	M1034											

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	18.901	Depositor
Minimum map value	-11.801	Depositor
Average map value	-0.010	Depositor
Map value standard deviation	1.005	Depositor
Recommended contour level	4	Depositor
Map size ($\text{\AA}$)	208.0, 208.0, 208.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	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: KOW, IHP

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	0.46	0/14476	0.87	31/19631 (0.2%)

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	THR	N-CA-C	12.07	124.44	111.28
1	A	1270	GLU	N-CA-C	10.47	122.77	111.36
1	A	1112	ASN	CA-C-N	9.49	131.70	119.84
1	A	1112	ASN	C-N-CA	9.49	131.70	119.84
1	A	1125	ILE	N-CA-C	-8.99	103.92	112.83

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	14147	0	14364	397	0
2	A	44	0	0	14	0
3	A	36	0	6	11	0
All	All	14227	0	14370	397	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 14.

The worst 5 of 397 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:972:LEU:HD11	1:A:1004:ILE:CD1	1.30	1.60
1:A:972:LEU:CD1	1:A:1004:ILE:HD11	1.34	1.53
1:A:300:ARG:NH1	1:A:1631:GLN:HG2	1.26	1.49
1:A:298:VAL:CG2	1:A:299:PRO:HD3	1.57	1.33
1:A:324:LYS:O	1:A:326:VAL:N	1.63	1.31

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	1743/1878 (93%)	1580 (91%)	157 (9%)	6 (0%)	36 66

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	LEU
1	A	477	GLY
1	A	962	LYS
1	A	1113	PRO
1	A	1480	PRO

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	1593/1705 (93%)	1566 (98%)	27 (2%)	53 67

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1020	THR
1	A	1397	LYS
1	A	1672	ASN
1	A	1295	LEU
1	A	1428	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1116	ASN
1	A	1363	HIS
1	A	1132	GLN
1	A	1292	GLN
1	A	1474	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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
3	IHP	A	1902	-	36,36,36	0.73	0	60,60,60	0.97	0
2	K0W	A	1901	-	42,44,44	1.77	7 (16%)	68,74,74	1.15	6 (8%)

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
3	IHP	A	1902	-	-	2/30/54/54	0/1/1/1
2	K0W	A	1901	-	-	10/42/66/66	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1901	K0W	PA5-O77	5.78	1.65	1.59
2	A	1901	K0W	PA1-O76	5.29	1.65	1.59
2	A	1901	K0W	PA3-O13	3.55	1.65	1.59
2	A	1901	K0W	PA6-O16	3.02	1.64	1.59
2	A	1901	K0W	PA4-O14	2.86	1.64	1.59

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1901	K0W	C5-C6-C1	3.35	117.78	110.43
2	A	1901	K0W	C5-C4-C3	2.78	116.52	110.43
2	A	1901	K0W	C4-C3-C2	2.60	116.12	110.43
2	A	1901	K0W	C6-C1-C2	2.36	115.61	110.43
2	A	1901	K0W	PA6-O16-C1	-2.06	117.92	123.43

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1901	K0W	C4-C3-O13-PA3

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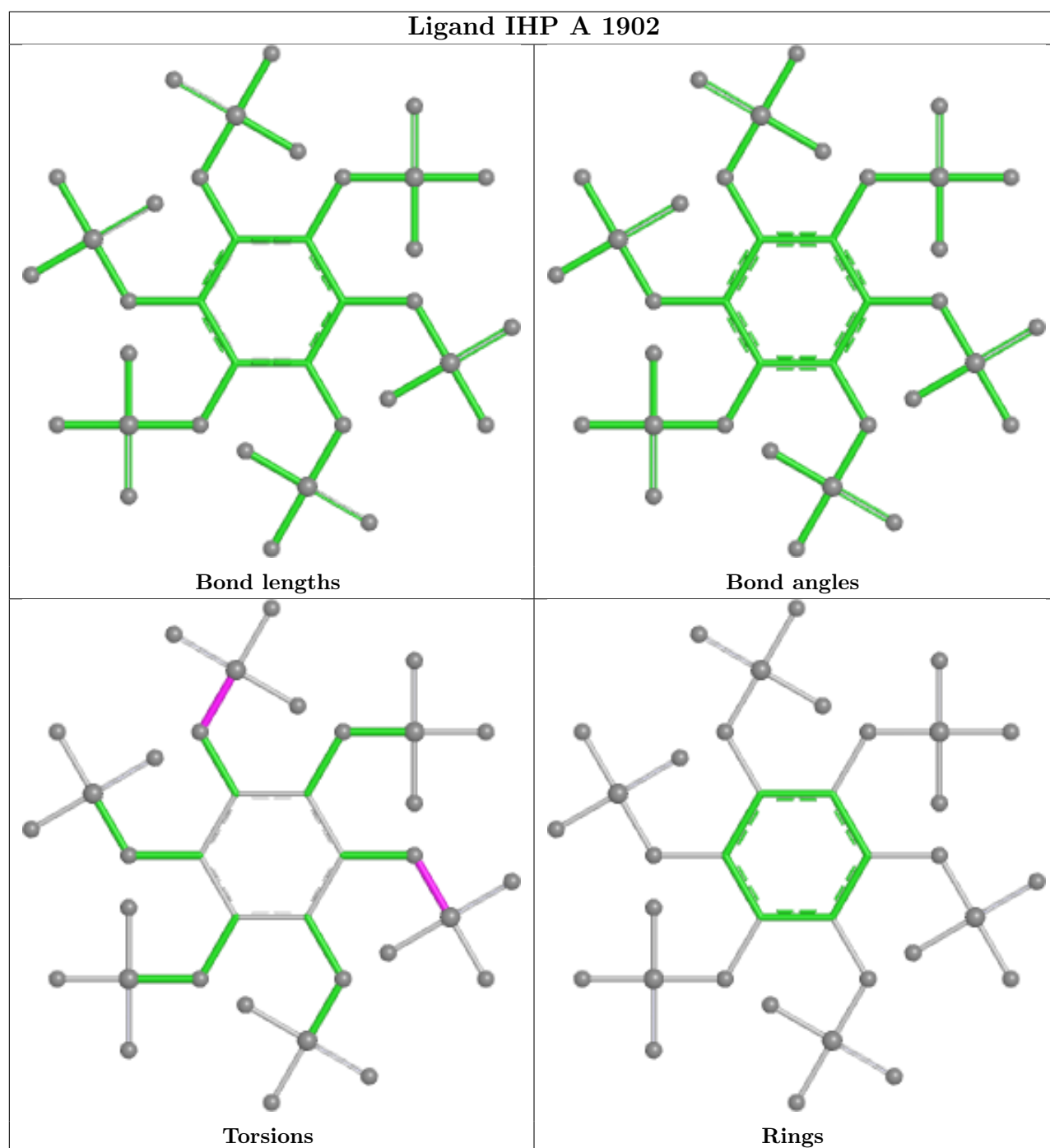
Mol	Chain	Res	Type	Atoms
2	A	1901	K0W	C6-O11-PA1-O76
2	A	1901	K0W	C3-O13-PA3-O23
3	A	1902	IHP	C3-O13-P3-O43
2	A	1901	K0W	C2-C3-O13-PA3

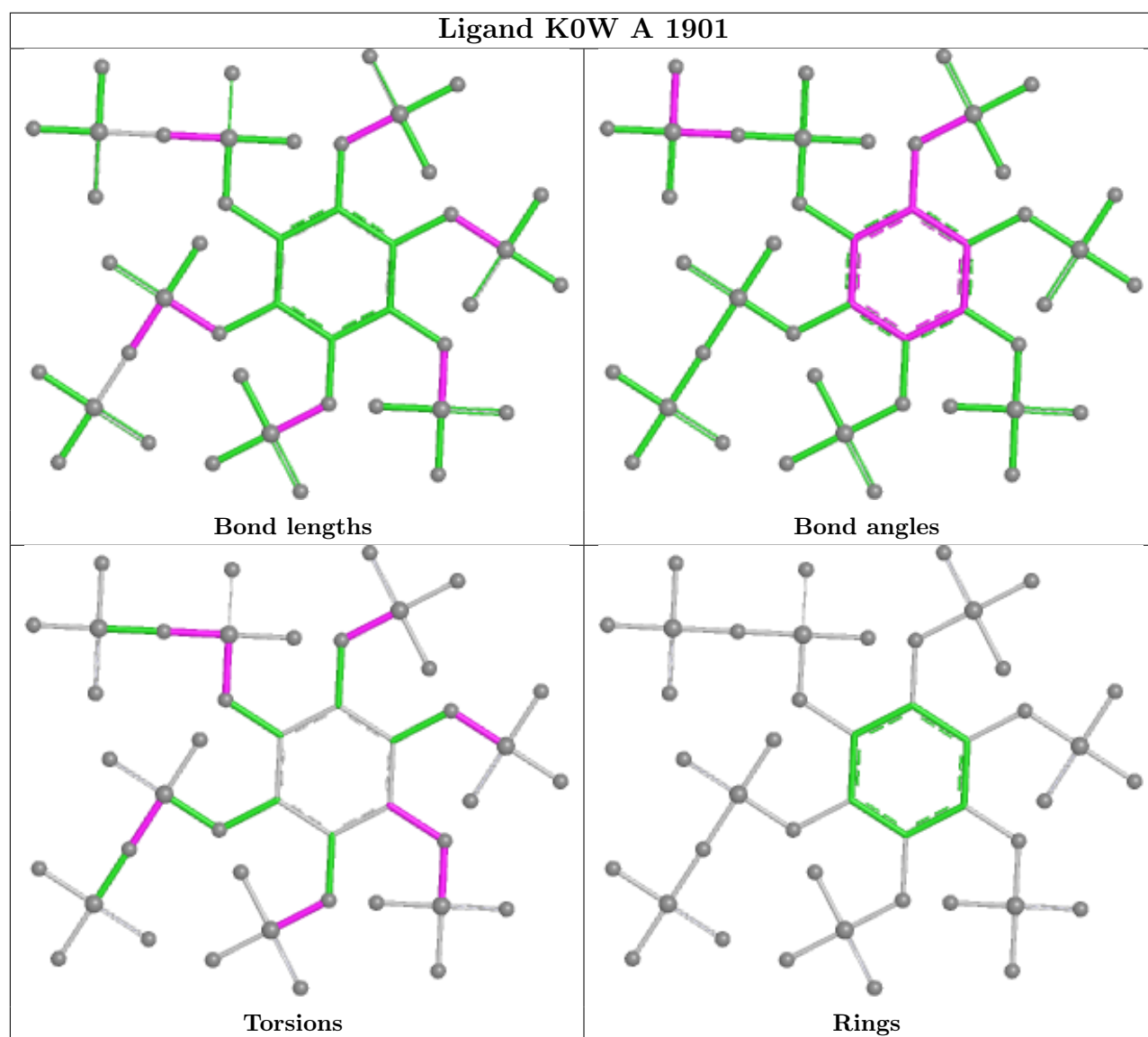
There are no ring outliers.

2 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1902	IHP	11	0
2	A	1901	K0W	14	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

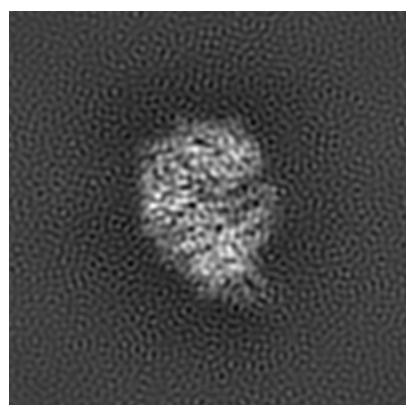
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0780. These allow visual inspection of the internal detail of the map and identification of artifacts.

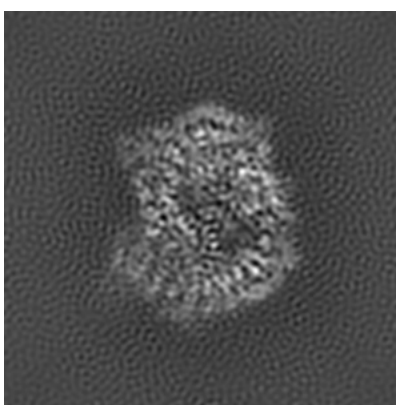
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

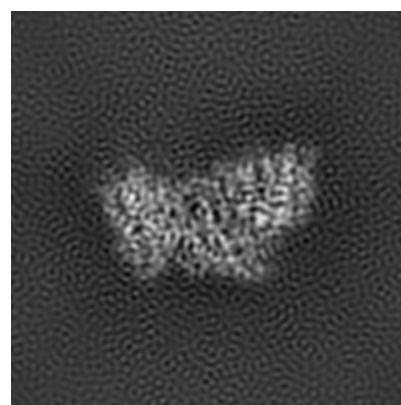
6.1.1 Primary map



X



Y

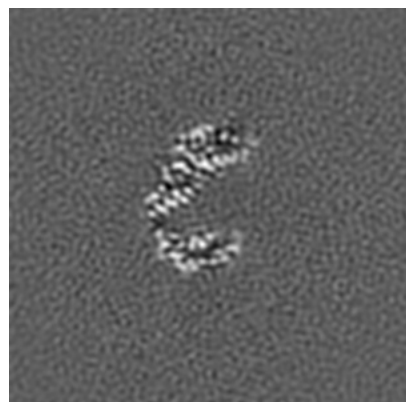


Z

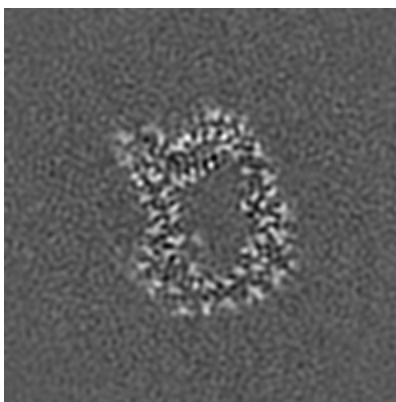
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

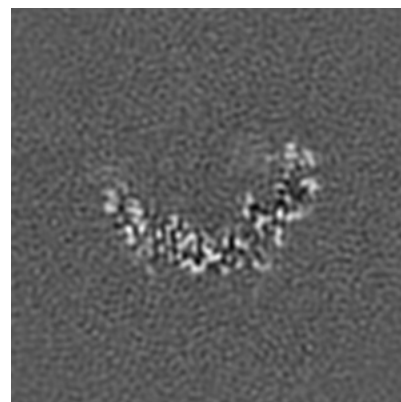
6.2.1 Primary map



X Index: 100



Y Index: 100

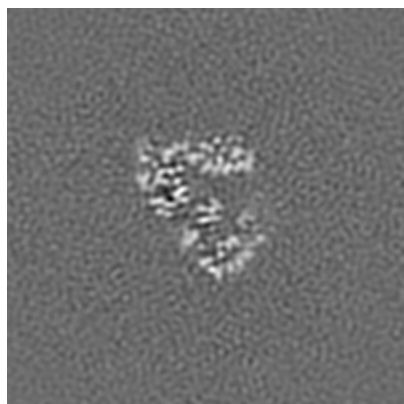


Z Index: 100

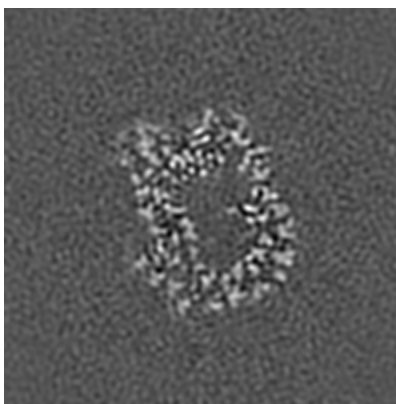
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

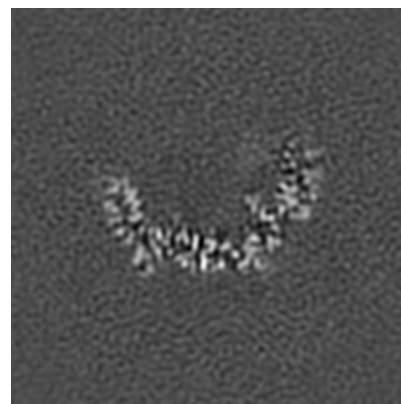
6.3.1 Primary map



X Index: 118



Y Index: 97

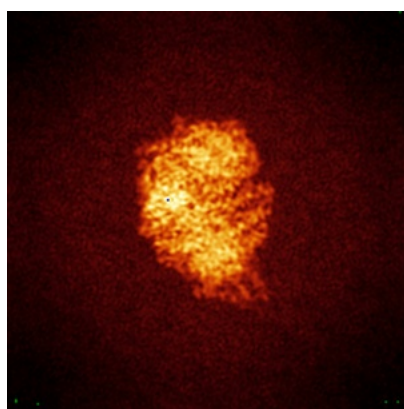


Z Index: 102

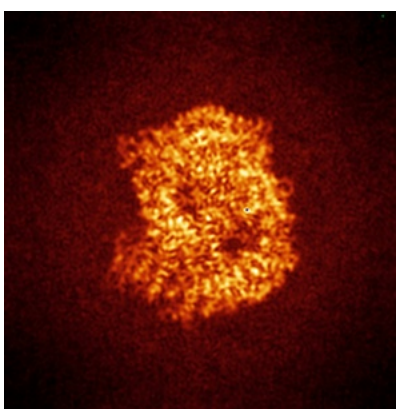
The images above show the largest variance slices of the map in three orthogonal directions.

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

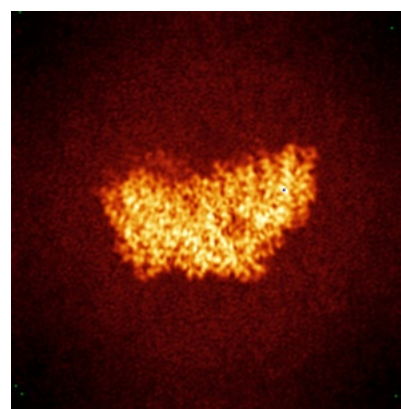
6.4.1 Primary map



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

This section was not generated.

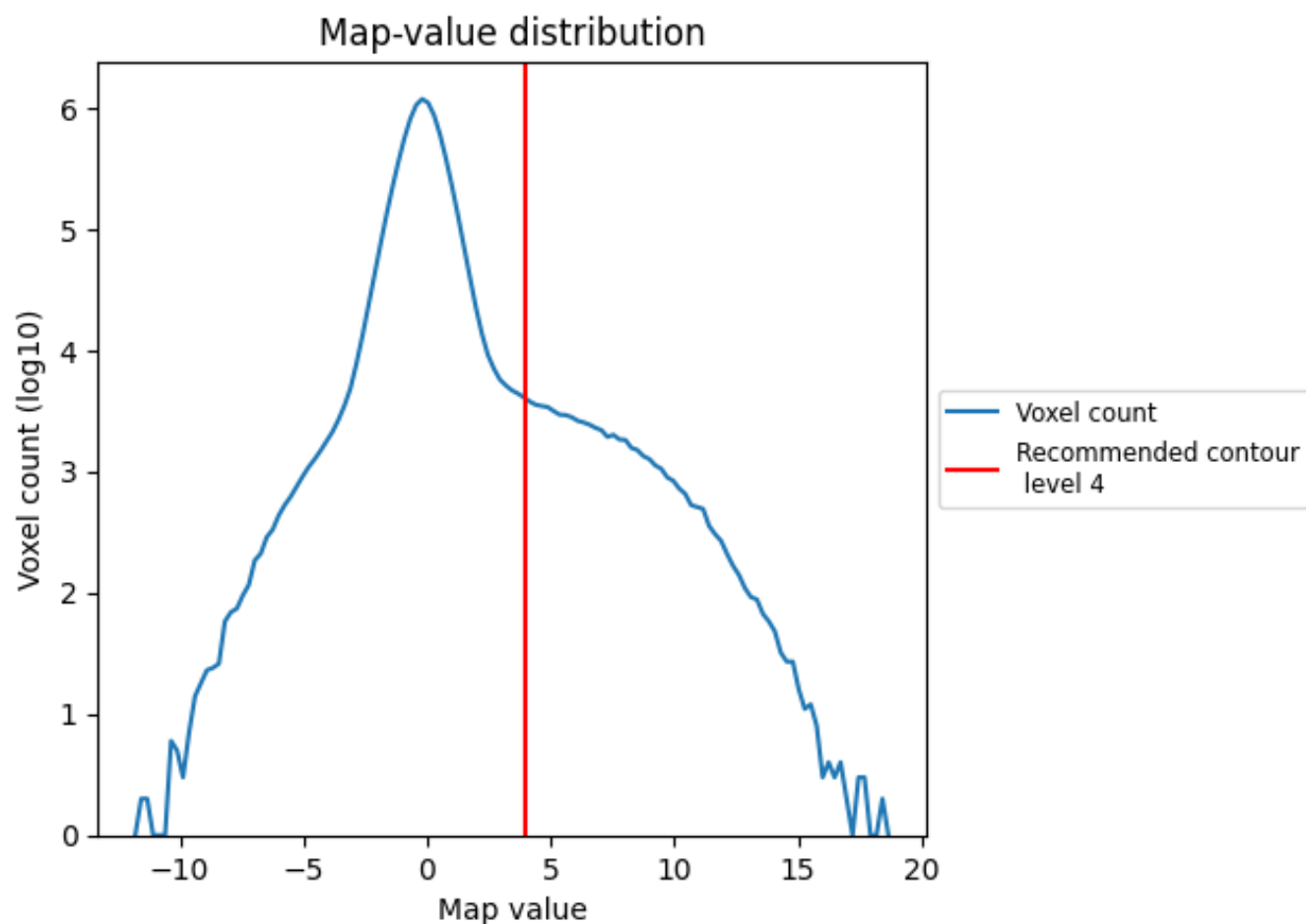
6.6 Mask visualisation

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

7 Map analysis [i](#)

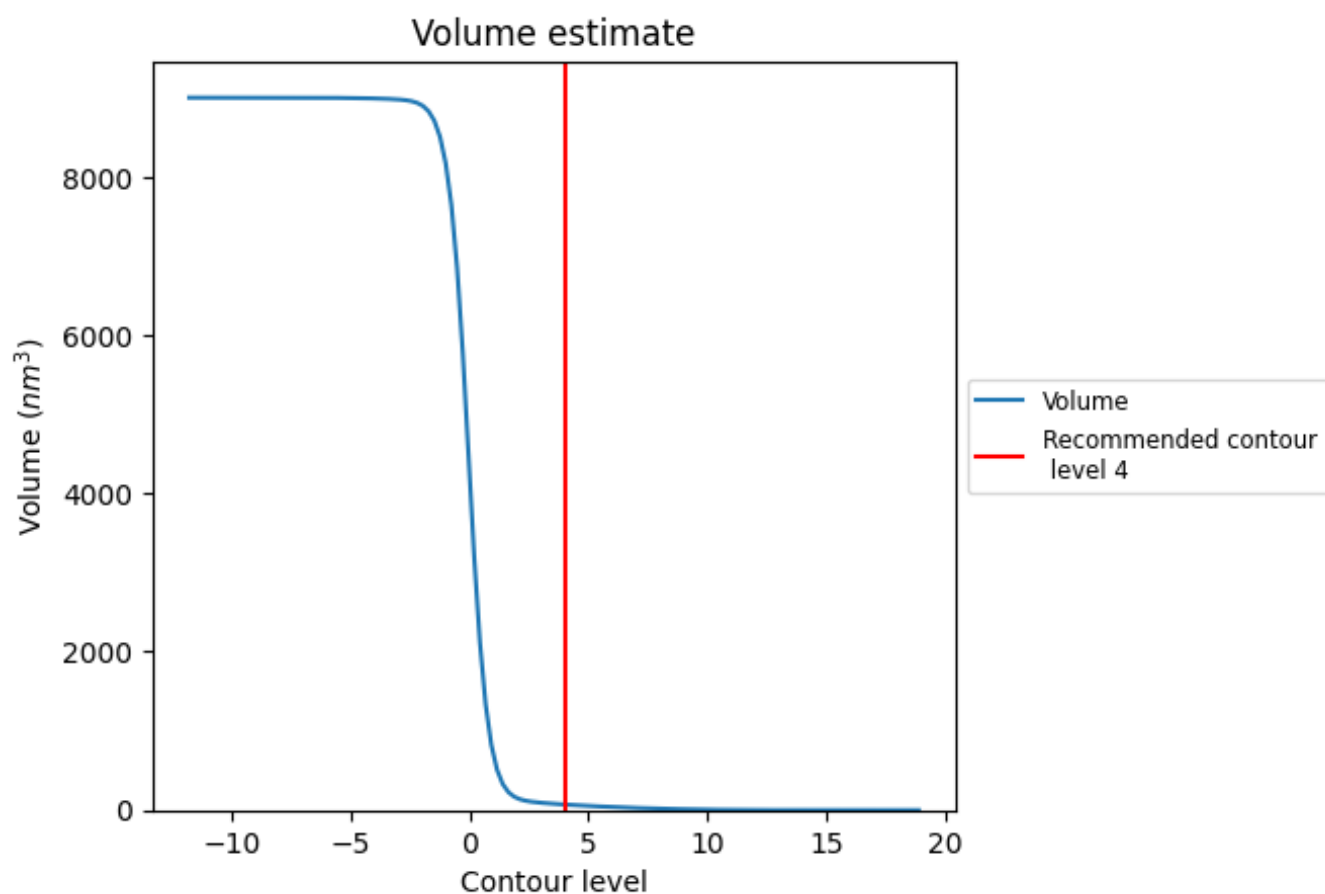
This section contains the results of statistical analysis of the map.

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.

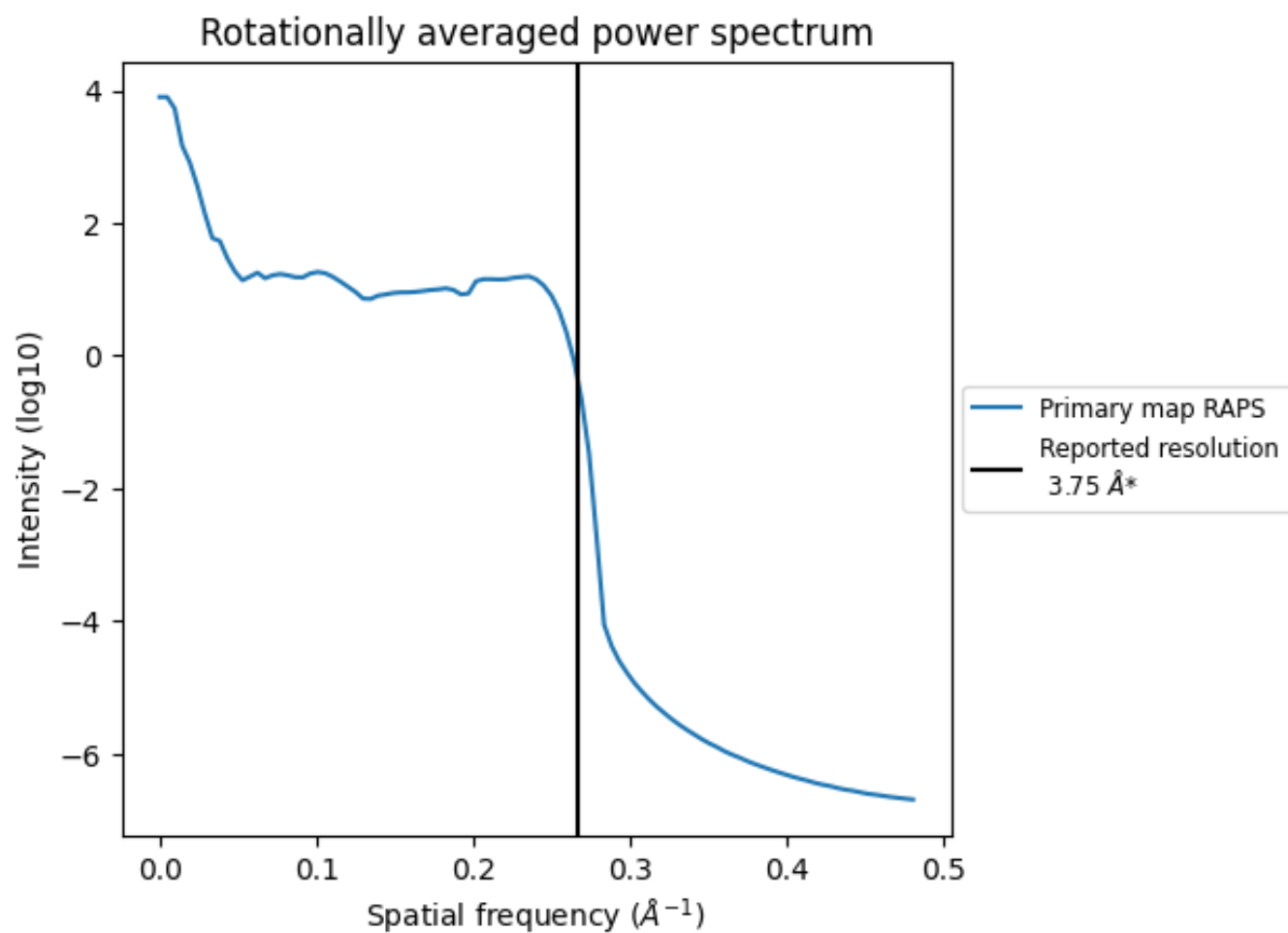
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 71 nm³; this corresponds to an approximate mass of 64 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](#)

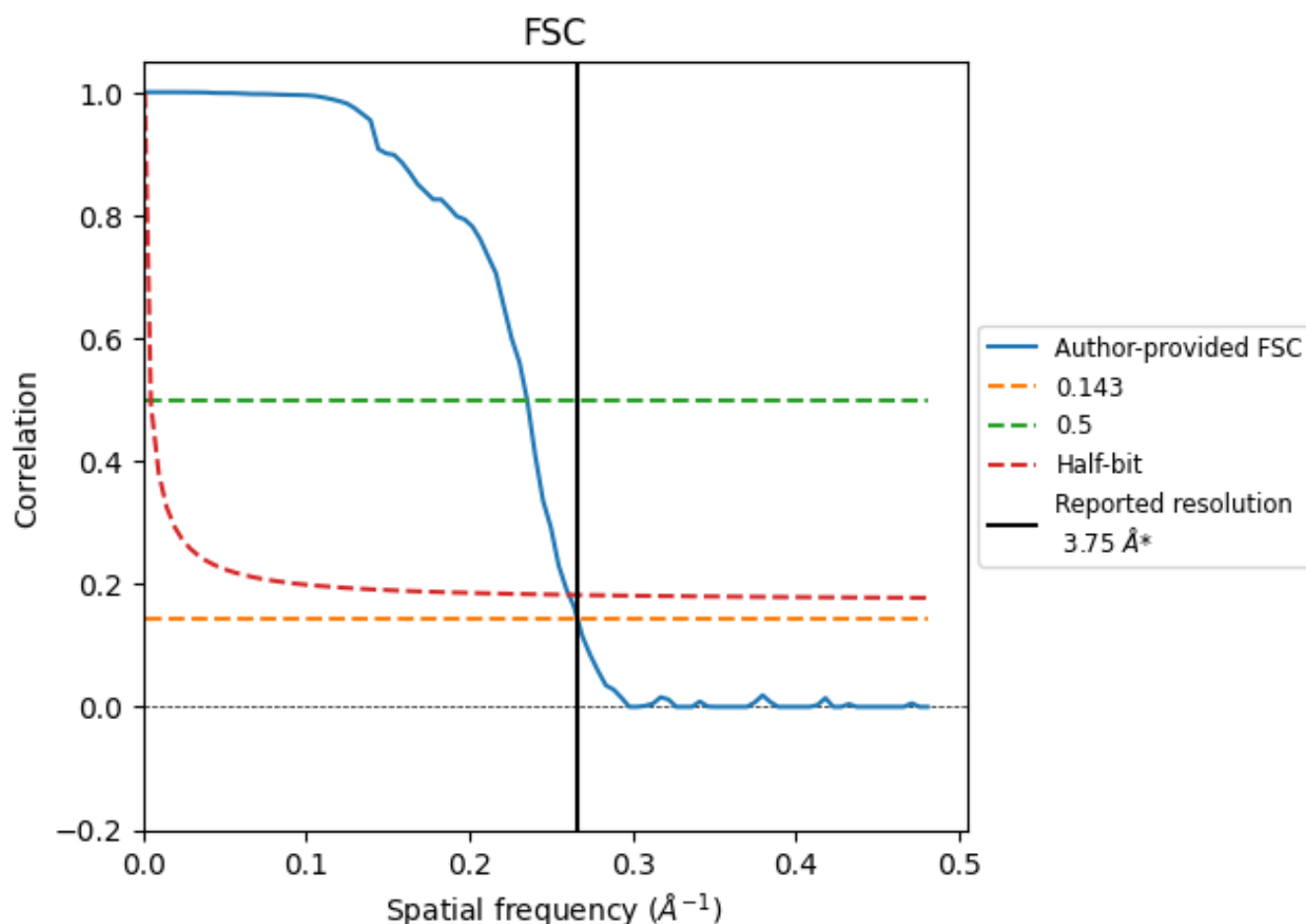


*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

8.2 Resolution estimates [i](#)

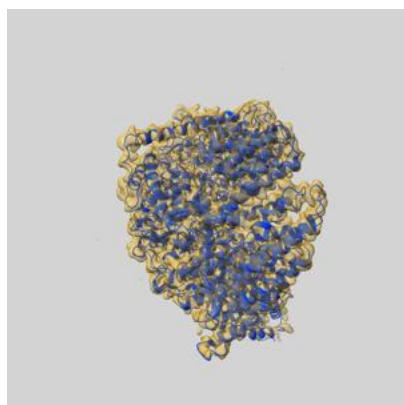
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.75	-	-
Author-provided FSC curve	3.75	4.25	3.83
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

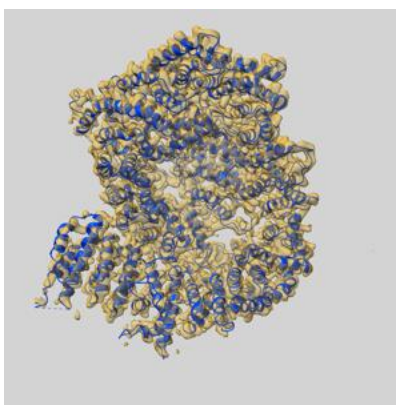
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0780 and PDB model 6KWX. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

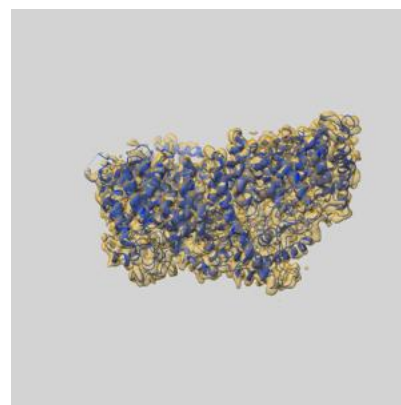
9.1 Map-model overlay [i](#)



X



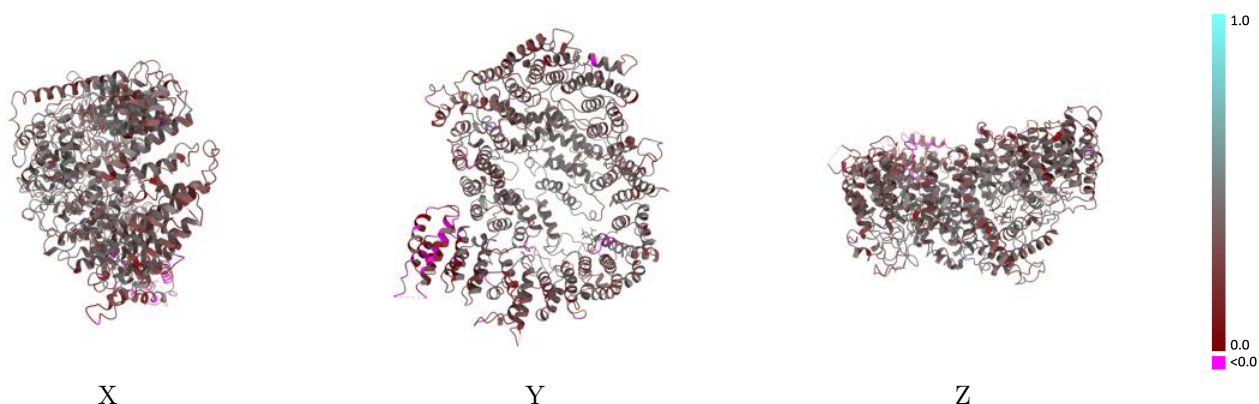
Y



Z

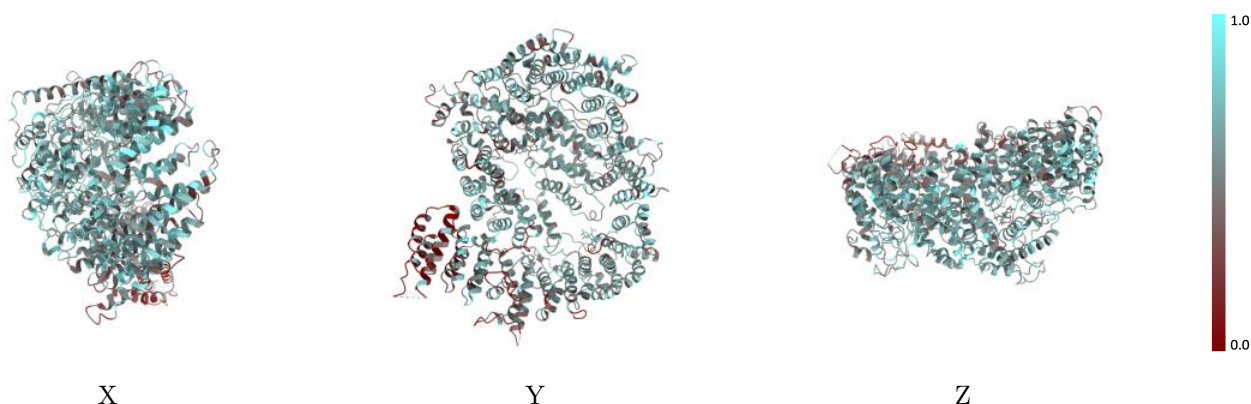
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



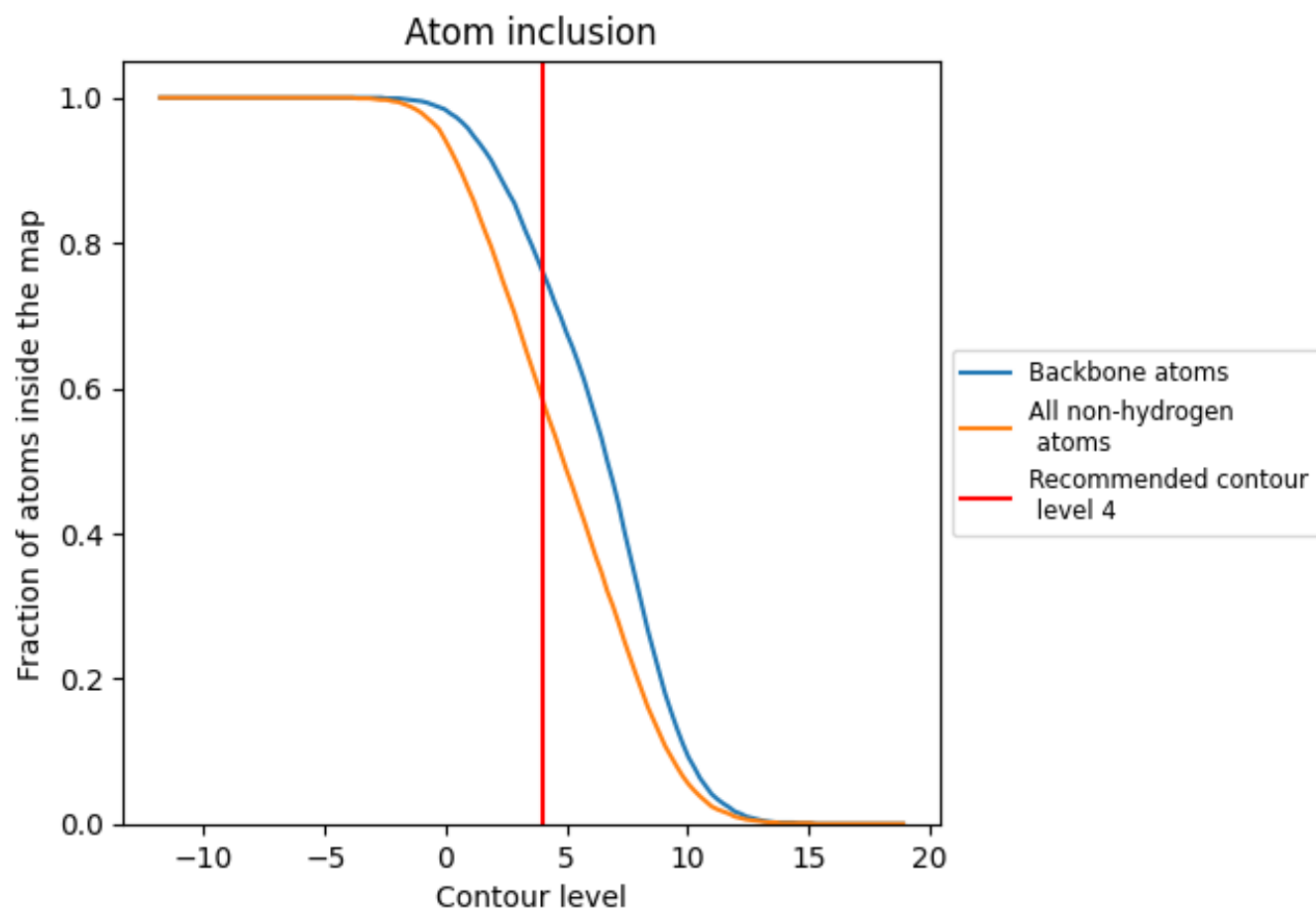
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4).

9.4 Atom inclusion ⓘ



At the recommended contour level, 76% of all backbone atoms, 58% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5840	0.3570
A	0.5840	0.3570

