



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 12:21 PM UTC

PDB ID : 7OTV / pdb_00007otv
EMDB ID : EMD-13067
Title : DNA-PKcs in complex with wortmannin
Authors : Liang, S.; Thomas, S.E.; Blundell, T.L.
Deposited on : 2021-06-10
Resolution : 3.24 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

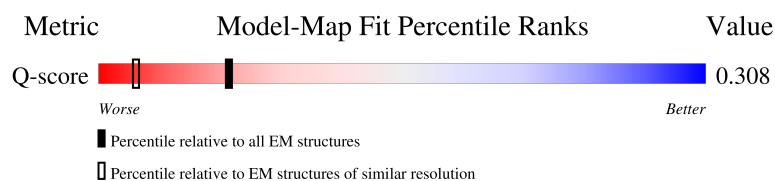
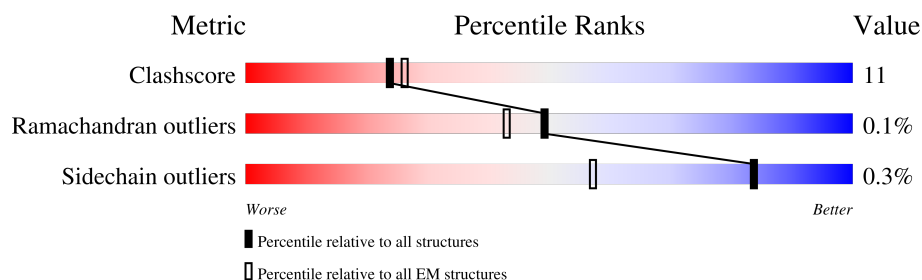
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.24 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	14594 (2.74 - 3.74)

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	4148	

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
2	KWT	A	6101	-	-	X	-

2 Entry composition [i](#)

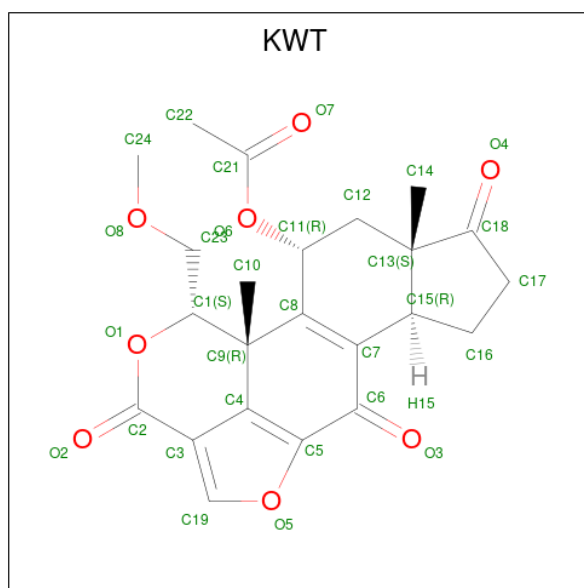
There are 2 unique types of molecules in this entry. The entry contains 29041 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-PKcs.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3656	29010	18609	4903	5307	191	0	0

- Molecule 2 is (1S,6BR,9AS,11R,11BR)-9A,11B-DIMETHYL-1-[(METHYLOXY)METHYL]-3,6,9-TRIOXO-1,6,6B,7,8,9,9A,10,11,11B-DECAHYDRO-3H-FURO[4, 3,2-DE]INDENO[4,5-H][2]BENZOPYRAN-11-YL ACETATE (CCD ID: KWT) (formula: C₂₃H₂₄O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
2	A	1	31	23	8	0

3 Residue-property plots

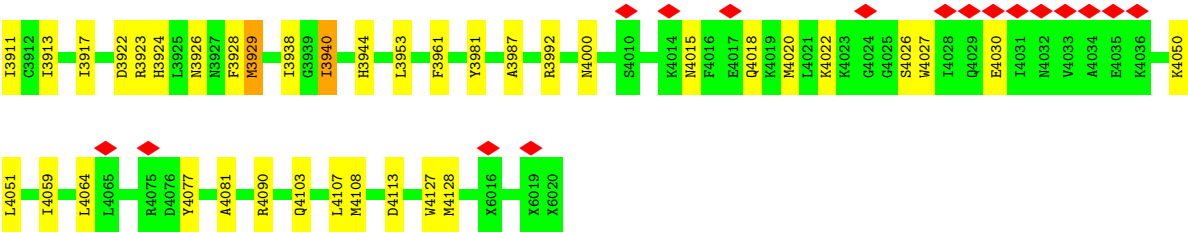
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-PKcs



P967	L1163	S1300	L1395	F1519	A1634	R1787	Y1874	Q1964	SER	H2091	E2180	N2270
D975	L1168	M1303	V1398	C1525	K1635	R1788	K1875	F1965	TYR	E2092	Q2181	S2271
Y976	L1178	H1304	L1402	E1526	D1636	G1789	M1880	S1968	LEU	C2093	I2182	V2272
L991	R1178	A1308	M1403	R1527	E1640	S1790	E1969	K1970	ALA	L2097	H2183	L2276
F995	E1182	A1309	L1406	T1641	K1642	T1793	L1884	P1971	SER	H2103	M2185	L2277
D1005	C1183	E1310	P1410	L1528	I1652	Q1794	V1795	L1884	THR	H2104	V2186	N2280
T1006	H1185	K1311	L1424	L1532	I1657	G1796	P1885	P1971	LEU	H2105	V2187	N2281
L1009	I1188	C1312	T1424	L1538	S1657	L1797	D1888	N1974	GLU	L2108	E2188	A2282
E1011	E1189	PHE	S1427	A1541	S1664	E1799	V1889	L1975	MET	L2109	I2189	N2283
L1010	L1190	GLY	L1431	SER	D1685	Y1802	H1890	N1980	SER	PRO	L2199	D2289
E1011	L1190	GLY	L1431	LEU	D1685	E1803	K1891	L1981	GLN	PRO	A2200	T2201
D1015	V1195	T1315	C1432	SER	K1689	R1806	E1893	L1984	PHE	GLY	V2205	C2292
G1016	P1204	A1317	Q1442	GLN	G1690	L1812	K1894	K1985	ASP	GLY	P2206	T2294
I1017	L2008	A1318	R1445	S1549	V1693	S1813	S1895	K1985	SER	GLY	K2207	Q2295
V1018	L1208	G1319	S1446	V1550	L1696	F1814	T1896	ARG	VAL	GLY	D2208	E2298
D1019	L1212	M1320	R1447	F1553	T1700	R1815	Q1898	TYR	GLN	PRO	E2209	V2299
P1020	L1212	T1322	L1448	F1553	G1705	S1816	V1899	PHE	TYR	GLY	V2210	L2211
V1021	V1217	S1323	V1452	E1557	G1710	Q1817	F1900	ARG	VAL	GLY	S2212	A2212
R1026	S1218	P1324	V1458	E1557	R1711	S1818	H1901	TYR	VAL	GLY	W2125	R2213
G1030	F1219	Q1325	L1458	V1560	R1715	F1820	H1901	GLY	VAL	GLY	L2133	F2218
I1033	N1221	K1334	I1467	L1562	E1715	R1822	G1902	GLY	VAL	GLY	L2137	I2219
L1037	T1223	V1339	I1467	L1562	I1718	S1823	C1904	LEU	VAL	GLY	V2138	M2220
R1062	E1225	R1340	S1470	L1567	I1722	L1824	T1905	PRO	PRO	GLY	P2139	H2221
A1081	Q1231	T1351	Q1471	E1570	F1722	L1827	E1907	MET	GLU	ARG	F2145	G2222
F1082	S1233	S1352	T1473	L1571	I1718	L1828	E1907	GLY	GLU	ARG	K2148	L2236
N1083	G1234	P1353	D1474	K1573	F1722	L1836	T1912	LYS	ILE	ARG	W2152	L2235
N1084	L1235	L1358	L1475	N1574	Q1725	R1837	I1916	LYS	ILE	ARG	E2155	T2240
I1085	L1236	L1359	H1476	L1575	S1726	E1838	Y1920	LYS	ILE	ARG	E2155	L2241
Y1086	T1240	M1365	S1477	S1586	G1732	V1845	E1925	ALA	ARG	GLN	R2158	C2244
E1087	L1241	T1366	V1479	S1586	T1733	D1846	E1930	ALA	GLY	THR	W2164	W2245
E1088	L1242	M1369	E1482	N1589	P1734	L1849	M1931	ALA	GLY	THR	L2165	L2249
E1097	L1269	L1372	L1483	T1590	R1735	S1853	Q1932	ALA	GLY	THR	S2166	L2249
L1104	L1261	V1373	S1485	K1591	Q1754	R1854	Q1932	ALA	GLY	THR	P2167	P2252
M1108	E1265	Q1374	L1486	M1592	M1757	F1855	L1933	ALA	GLY	THR	L2168	Y2253
I1124	C1266	T1375	D1495	L1597	L1758	T1856	E1935	ALA	GLY	THR	L2169	K2254
Q1125	C1267	C1377	E1496	Q1614	L1759	T1856	R1936	ALA	GLY	THR	Q2170	L2255
Q1126	L1268	E1378	R1497	K1617	E1760	K1857	R1937	ALA	GLY	THR	L2171	L2256
D1129	T1269	L1381	Q1498	L1618	E1764	L1858	R1938	ALA	GLY	THR	S2174	K2259
R1151	A1286	I1382	C1499	I1622	E1769	E1859	Y1940	ALA	GLY	THR	E2175	F2260
P1158	L1290	I1386	L1503	K1627	Q1770	S1861	Y1945	ALA	GLY	THR	W2176	S2261
P1159	F1296	V1389	L1505	W1632	F1782	D1864	I1949	ALA	GLY	THR	N2177	G2262
		Q1390	S1506	W1633	I1785	I1867	V1955	ALA	GLY	THR	G2178	K2268
		M1392	L1514		A1786	K1870	Q1963	ALA	GLY	THR	G2179	D2269





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64179	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 ($e^-/\text{\AA}^2$)	47.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.589	Depositor
Minimum map value	-1.600	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.22	Depositor
Map size (Å)	339.04, 339.04, 339.04	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.304, 1.304, 1.304	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: KWT

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	0/29502	0.40	1/39893 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	3483	MET	N-CA-C	8.43	121.23	111.11

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	29010	0	29193	603	0
2	A	31	0	23	23	0
All	All	29041	0	29216	603	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 11.

The worst 5 of 603 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:3809:THR:CB	1:A:3929:MET:CE	2.16	1.22
1:A:3809:THR:CB	1:A:3929:MET:HE3	1.72	1.14
1:A:3809:THR:HB	1:A:3929:MET:HE3	1.14	1.14
1:A:3751:LEU:HD13	2:A:6101:KWT:H143	1.15	1.09
1:A:3809:THR:CG2	1:A:3929:MET:HE1	1.87	1.04

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	3602/4148 (87%)	3293 (91%)	305 (8%)	4 (0%)	48	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3481	SER
1	A	2787	HIS
1	A	3406	ALA
1	A	1968	SER

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	3196/3671 (87%)	3185 (100%)	11 (0%)	86	87

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3753	LYS
1	A	3806	LEU
1	A	3940	ILE
1	A	3929	MET
1	A	3729	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2422	GLN
1	A	3787	GLN
1	A	2784	GLN
1	A	3470	GLN
1	A	2553	HIS

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 ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	KWT	A	6101	-	32,35,35	16.94	12 (37%)	35,57,57	8.69	12 (34%)

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	KWT	A	6101	-	-	0/7/75/75	0/5/5/5

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	6101	KWT	O5-C19	94.60	3.09	1.37
2	A	6101	KWT	C11-C8	9.40	1.61	1.51
2	A	6101	KWT	C15-C7	5.22	1.59	1.52
2	A	6101	KWT	C5-C4	4.80	1.42	1.34
2	A	6101	KWT	O1-C2	4.51	1.43	1.35

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	6101	KWT	O5-C19-C3	-37.69	72.73	111.19
2	A	6101	KWT	C19-O5-C5	-25.14	81.37	105.21
2	A	6101	KWT	O5-C5-C4	21.52	123.27	110.22
2	A	6101	KWT	C9-C4-C5	-5.28	117.45	125.96
2	A	6101	KWT	C11-O6-C21	4.11	123.10	117.00

There are no chirality outliers.

There are no torsion outliers.

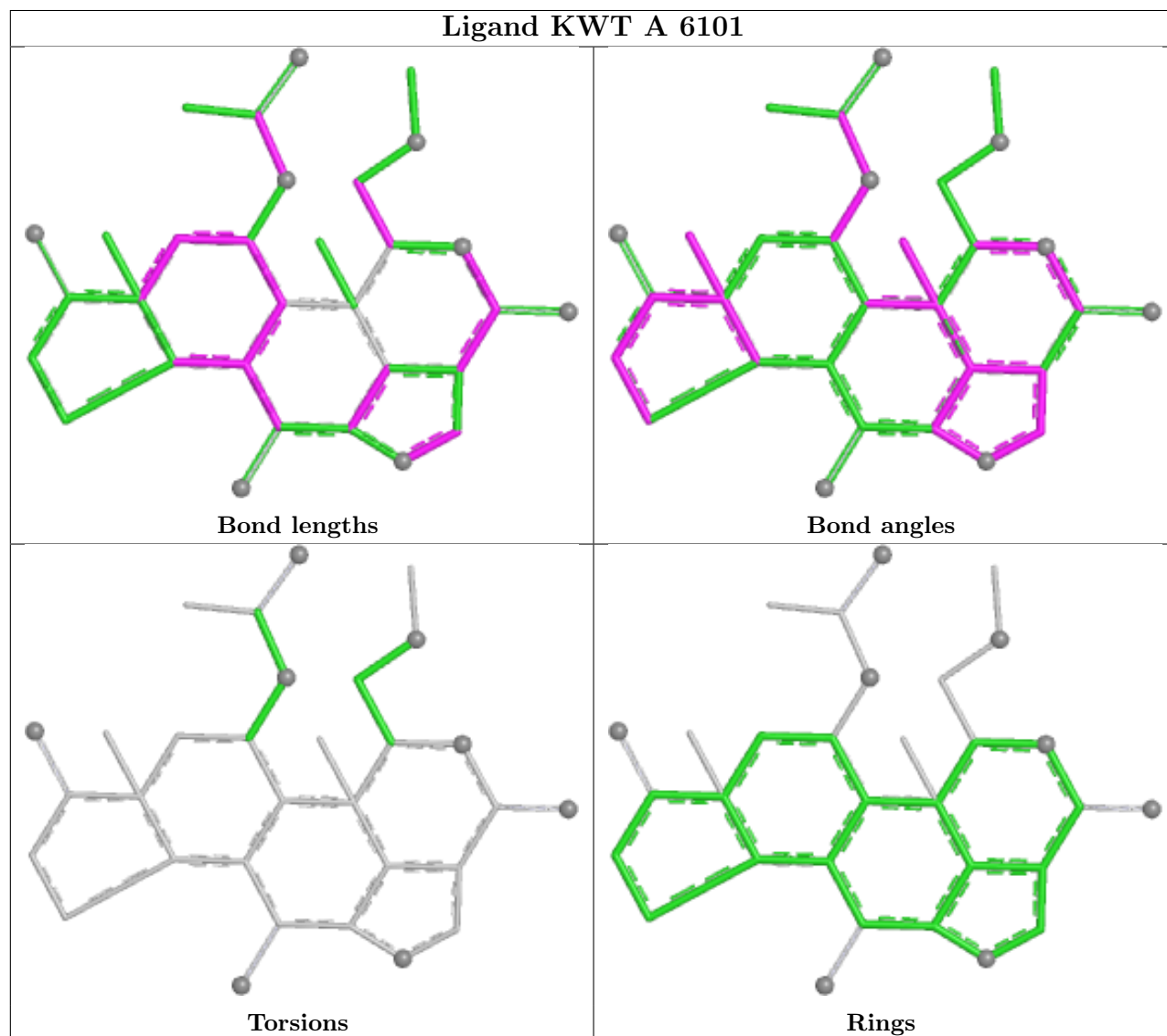
There are no ring outliers.

1 monomer is involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	6101	KWT	23	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	4128:MET	C	6001:UNK	N	84.17

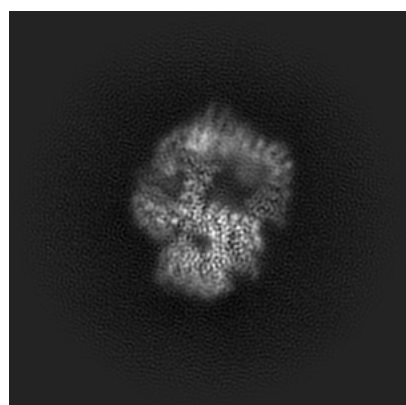
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13067. These allow visual inspection of the internal detail of the map and identification of artifacts.

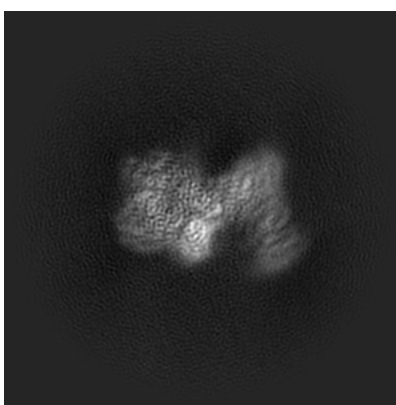
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

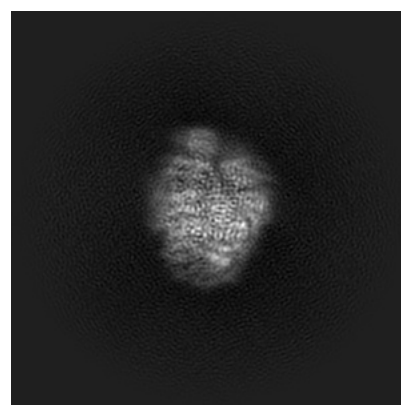
6.1.1 Primary map



X



Y

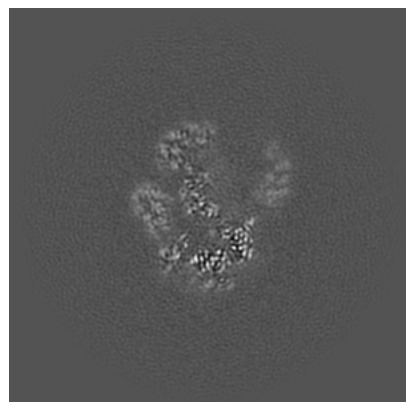


Z

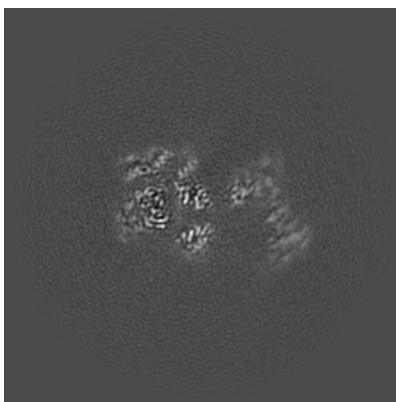
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

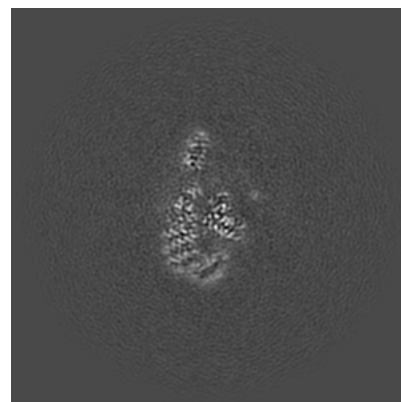
6.2.1 Primary map



X Index: 130



Y Index: 130

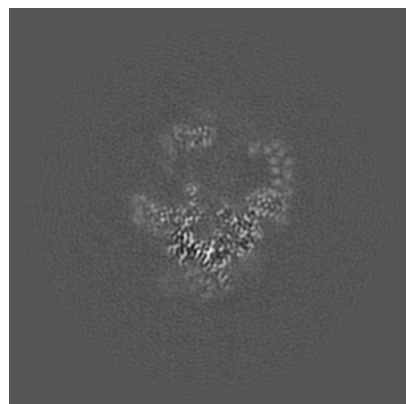


Z Index: 130

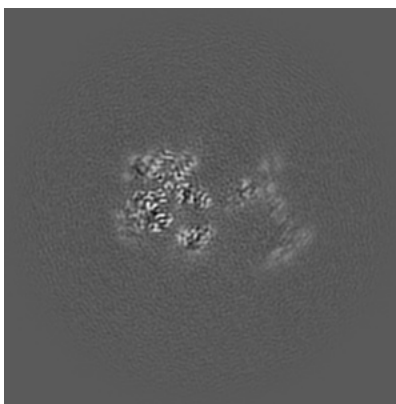
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

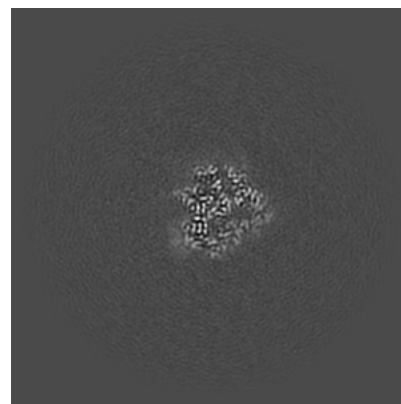
6.3.1 Primary map



X Index: 121



Y Index: 132

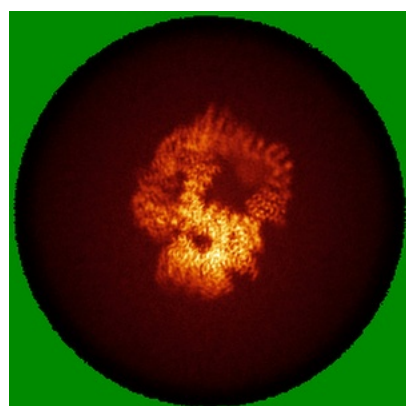


Z Index: 101

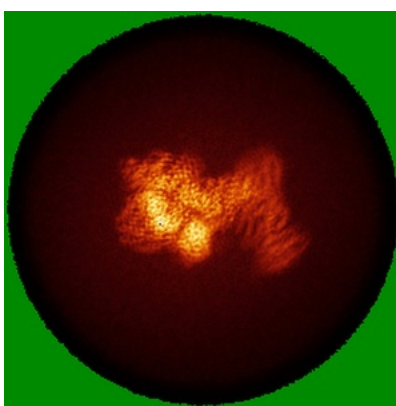
The images above show the largest variance slices of the map in three orthogonal directions.

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

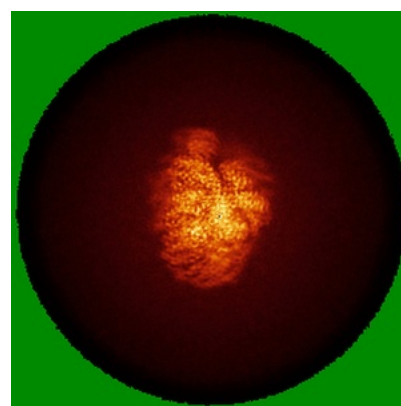
6.4.1 Primary map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.22. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

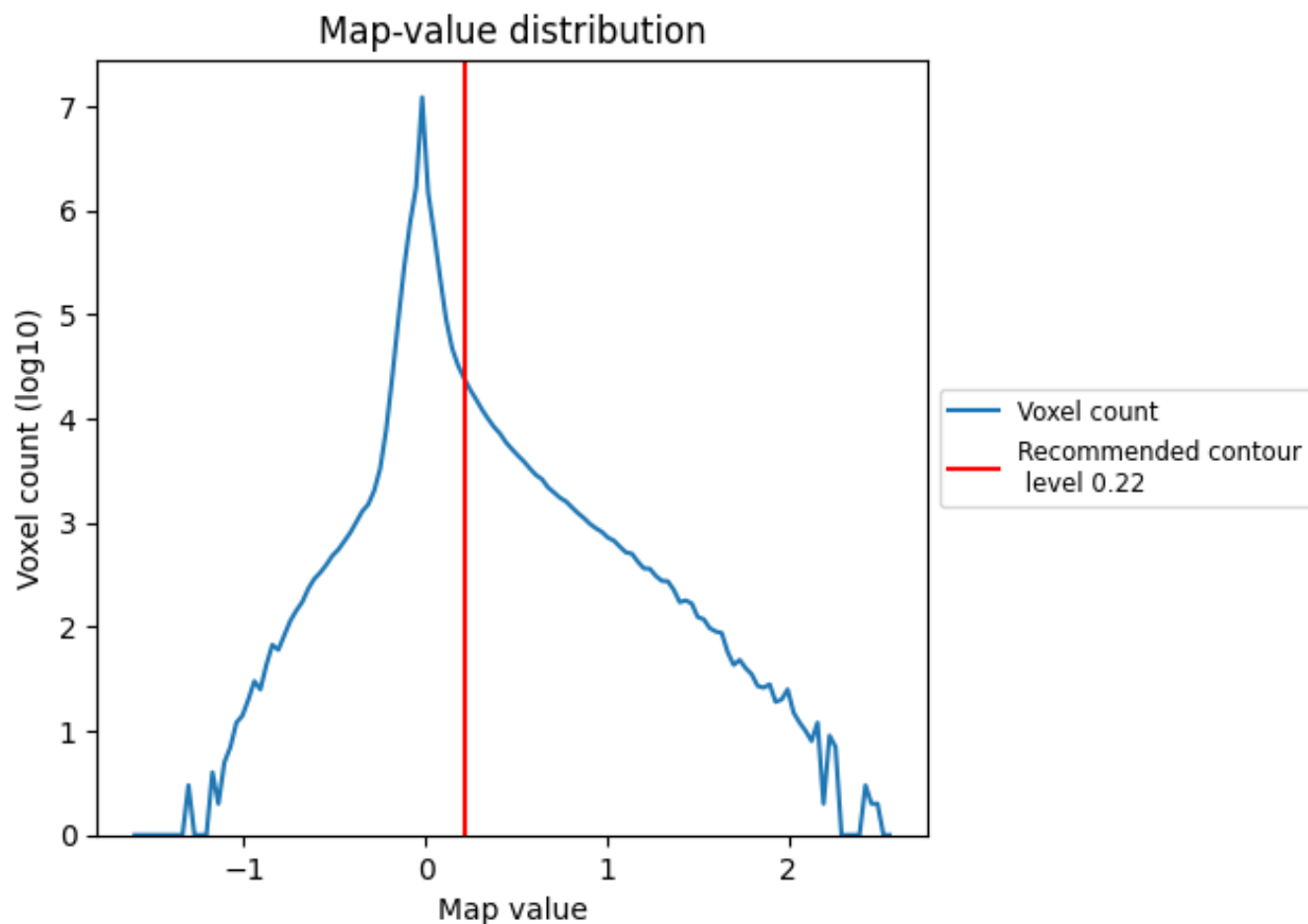
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

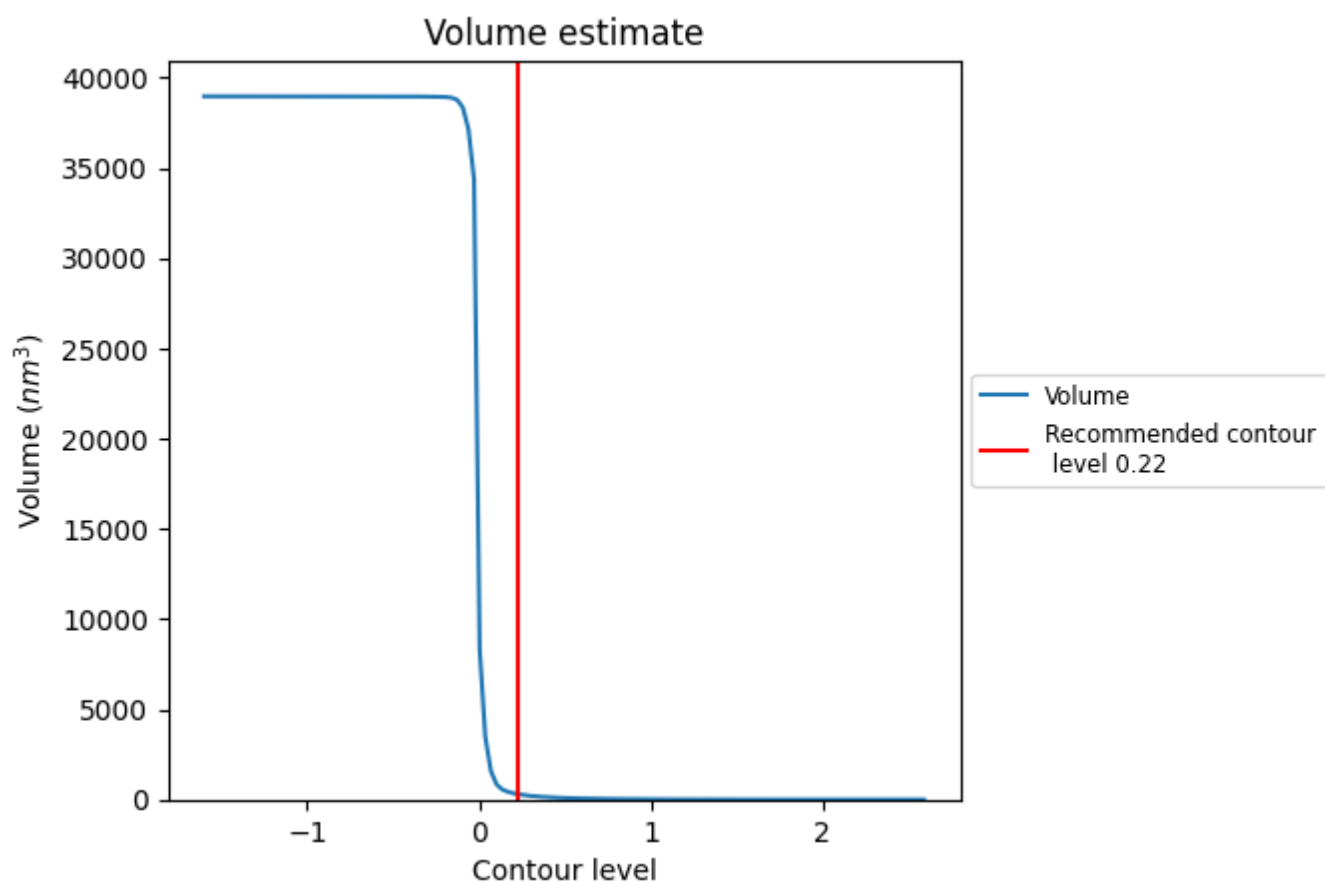
This section contains the results of statistical analysis of the map.

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.

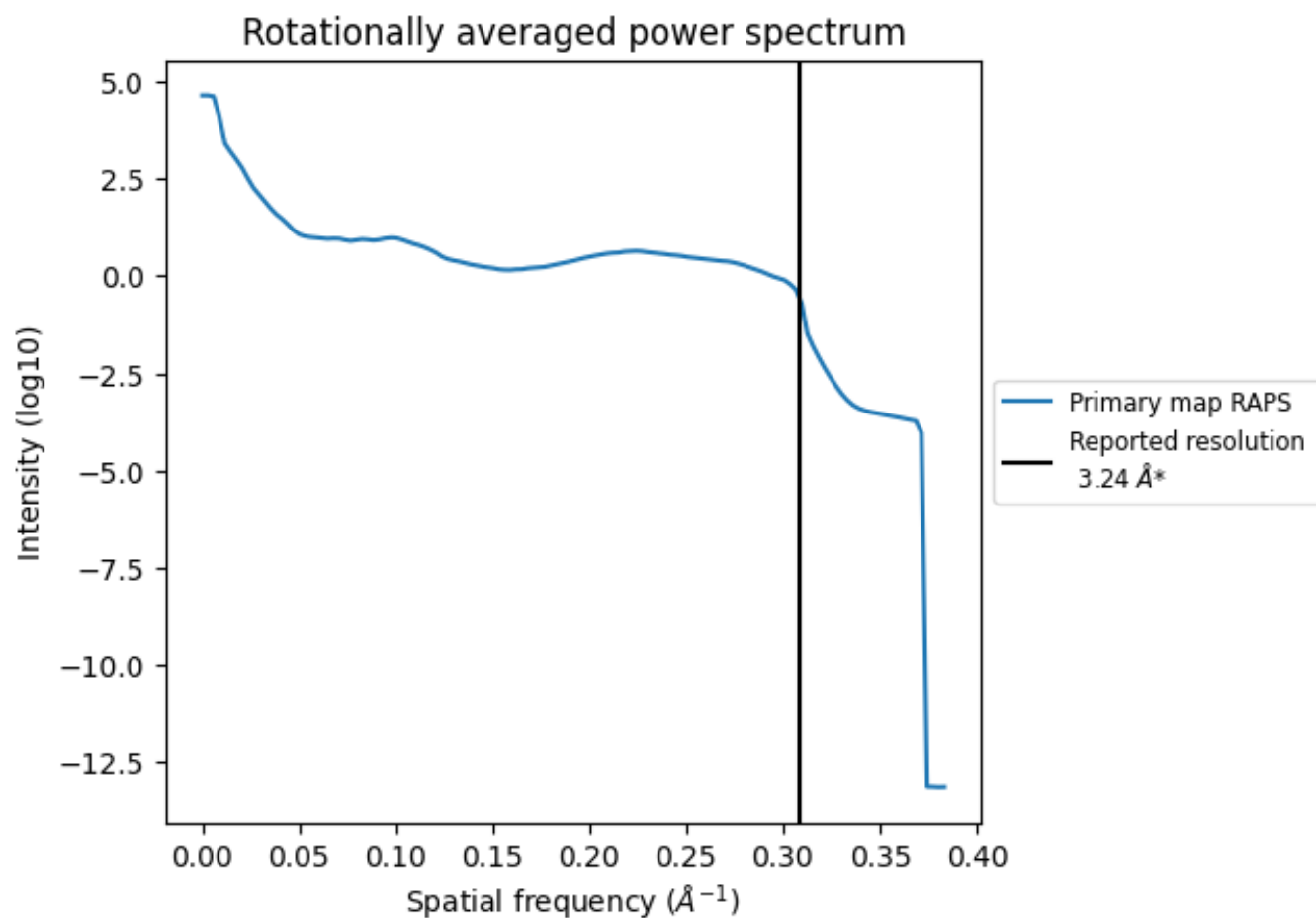
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 311 nm³; this corresponds to an approximate mass of 281 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 0.309 Å⁻¹

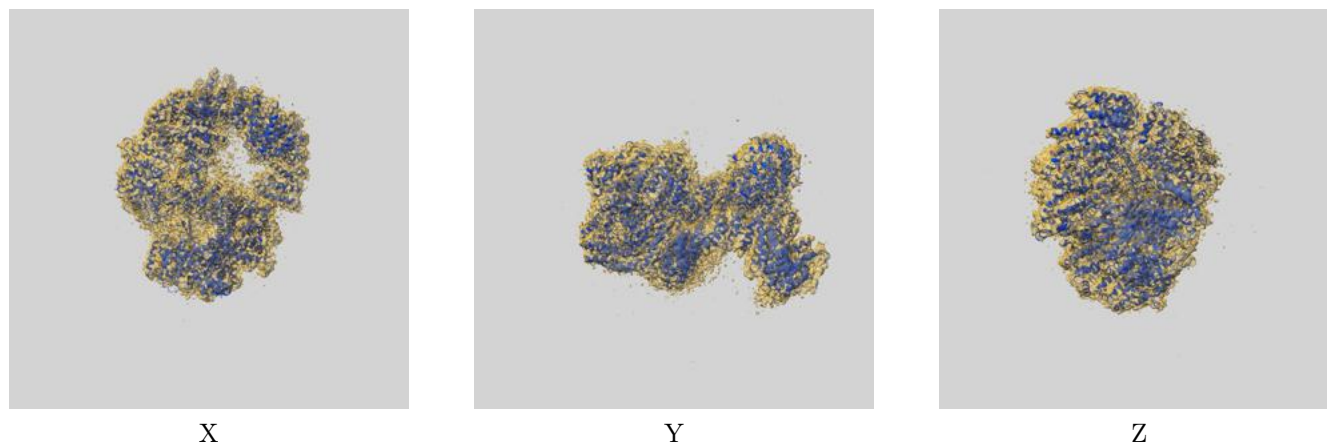
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

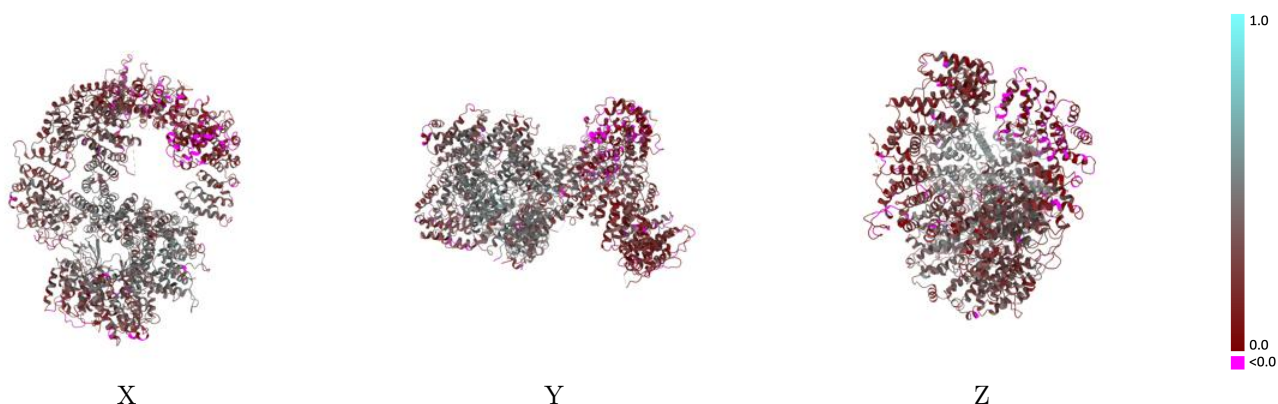
This section contains information regarding the fit between EMDB map EMD-13067 and PDB model 7OTV. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



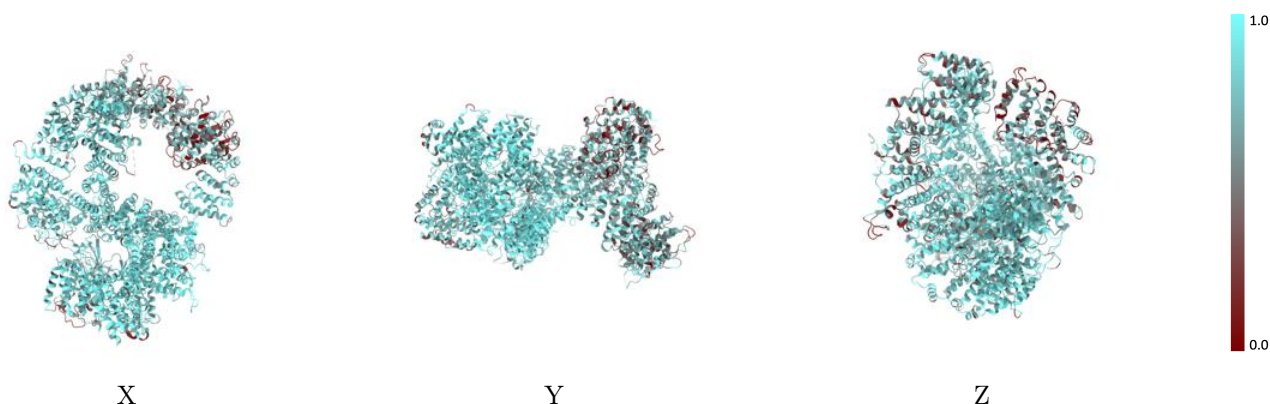
The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



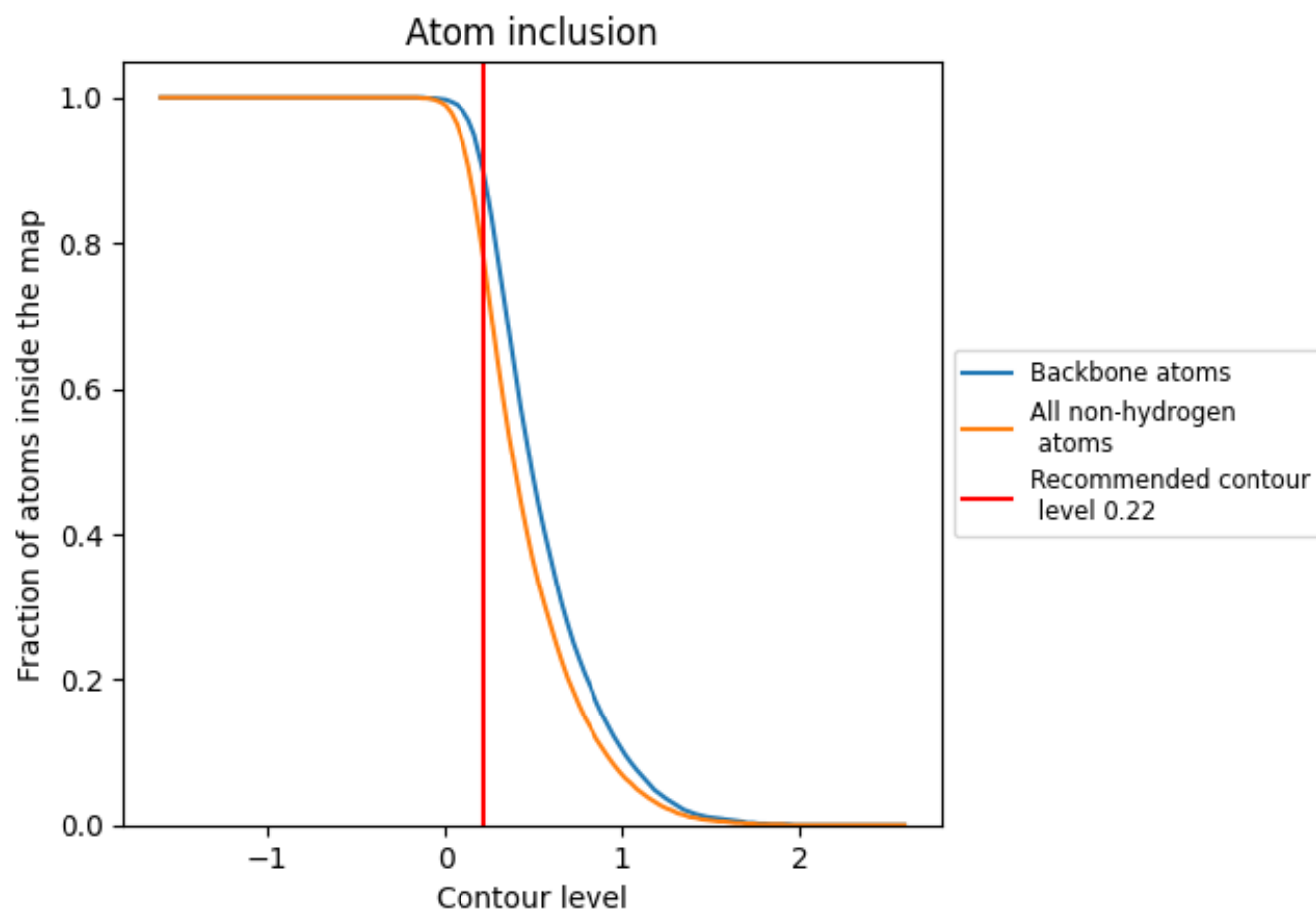
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.22).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 78% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7790	0.3080
A	0.7790	0.3080

