



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 11:24 AM UTC

PDB ID : 9CHO / pdb_00009cho
EMDB ID : EMD-45591
Title : Autoinhibited full-length LRRK2(I2020T) on microtubules with MLI-2
Authors : Chen, S.; Villa, E.; Leschziner, A.E.
Deposited on : 2024-07-01
Resolution : 7.80 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

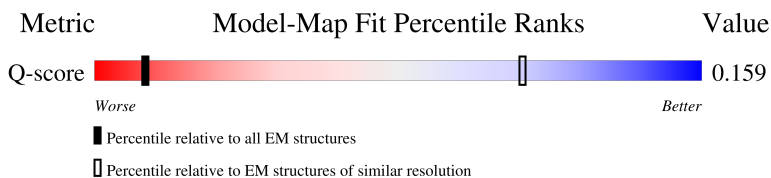
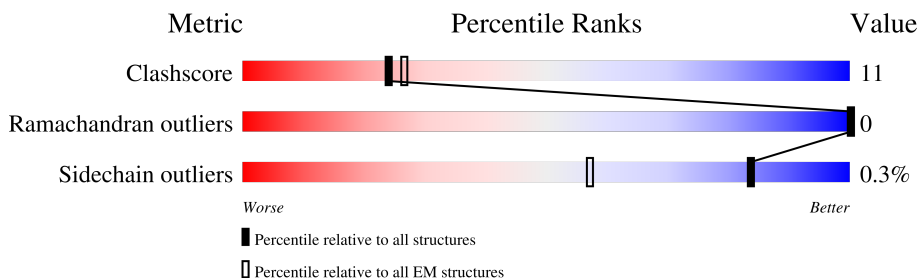
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.80 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	370 (7.30 - 8.30)

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	1985	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 26795 atoms, of which 12678 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.

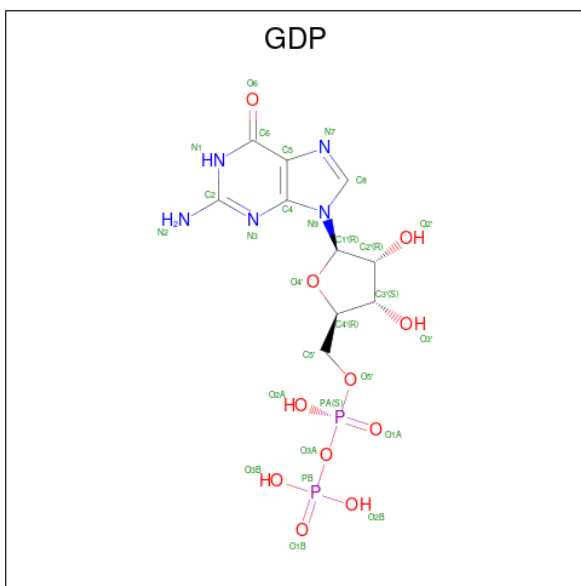
- Molecule 1 is a protein called Leucine-rich repeat serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
1	A	1792	26702	9000	12641	2421	2553	0	0

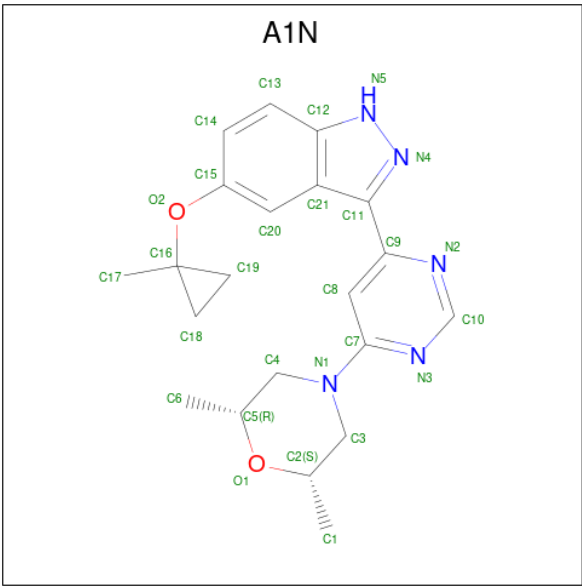
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2020	THR	ILE	engineered mutation	UNP Q5S007

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂) (labeled as "Ligand of Interest" by depositor).



of Interest" by depositor).

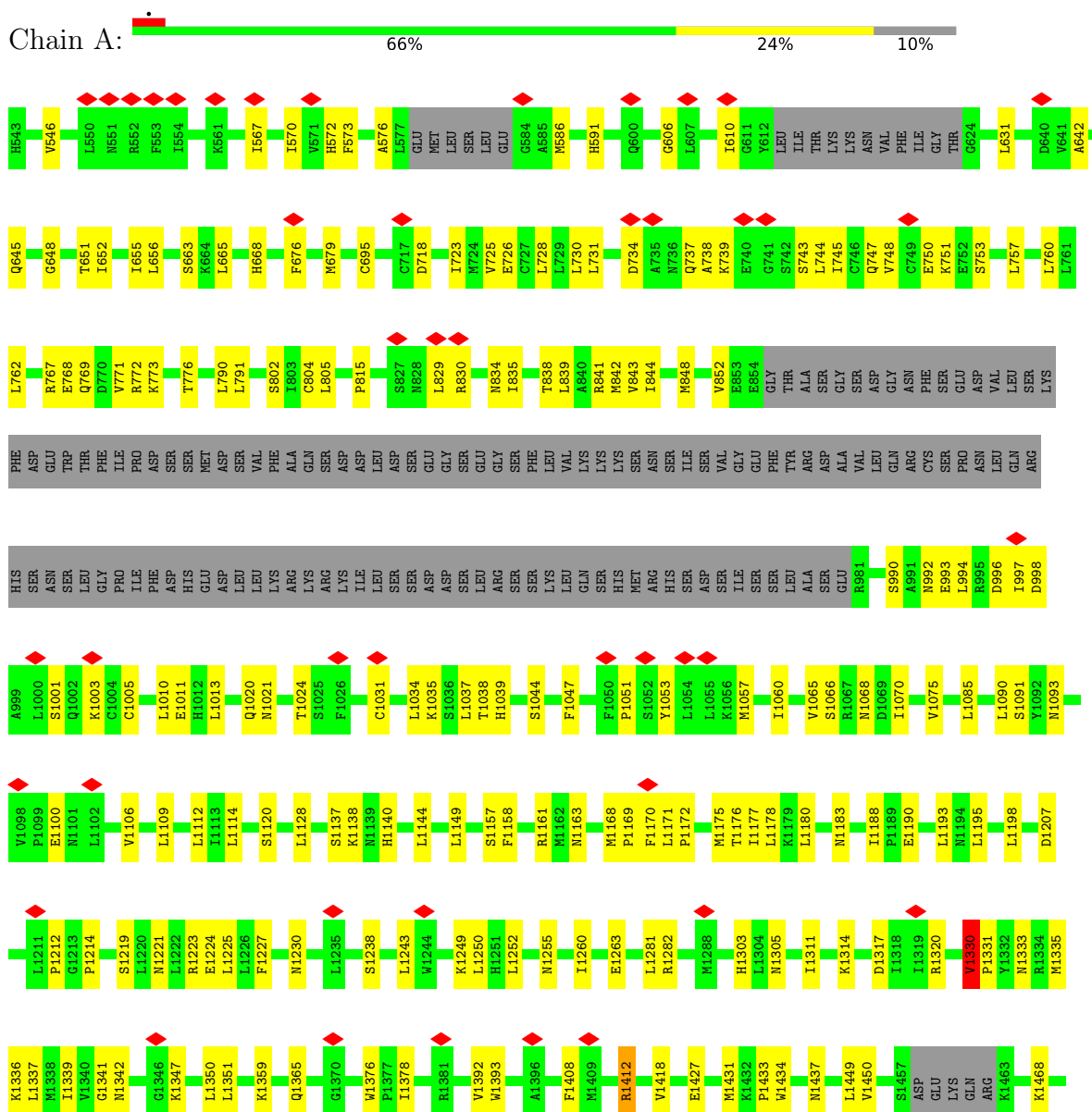


Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
3	A	1	53	21	25	5	2	0

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: Leucine-rich repeat serine/threonine-protein kinase 2



L2444	L2445	T2354	T2355	T2356	V2359	L2363	Y2364	L2365	N2369	V2372	V2375	W2376	D2377	K2378	K2379	K2382	D2388	C2389	V2390	H2391	F2392	L2393	R2394	K2402	R2413	V2414	L2417	C2418	L2419	Q2420	T2423	A2424	L2425	V2426	T2427	G2428	G2430	H2433	T2434	L2435	L2436	L2437	D2438	T2441	R2442	R2443							
T2267	A2268	D2269	G2270	K2271	L2272	A2273	L2274	V2280	A2285	A2286	P2287	L2288	K2289	I2290	L2291	N2292	L2293	G2294	N2295	T2298	P2299	L2300	S2306	E2311	R2312	N2313	V2314	W2315	W2316	G2317	G2318	C2319	G2320	T2321	K2322	L2323	F2324	D2329	F2330	T2331	L2332	L2336	E2337	T2338	R2339	Y2346	A2347	A2348	F2349	S2350	L2364	V2365	G2266
F2181	L2182	D2183	L2184	Y2189	T2190	E2193	V2194	A2195	D2196	L2204	V2205	H2206	L2207	P2208	K2211	E2212	W2214	I2215	V2216	G2217	G2218	V2226	I2227	N2228	T2229	G2232	K2233	K2234	R2235	L2238	E2239	K2240	M2241	T2242	V2245	S2252	F2253	S2254	K2255	Q2256	S2257	K2258	Q2259	K2260	L2263	L2264	V2265	G2266					
GLY	ILE	LYS	THR	SER	GLU	G2034	R2045	GLY	ASN	VAL	ILE	TYR	ASN	Y2064	D2065	T2069	R2072	E2085	D2094	F2095	V2096	S2125	A2126	Q2127	V2128	I2131	K2148	I2151	V2152	E2153	A2157	T2158	H2159	S2162	R2163	N2164	L2169	H2173	T2174	D2175	Q2178	L2179	S2180										
N1909	LYS	H1911	R1915	C1925	H1926	H1929	P1930	S1931	L1932	R1941	P1942	R1943	M1944	L1945	V1946	E1948	L1949	L1958	S1965	R1968	R1973	D1980	G1981	L1982	H1986	Y1992	K1996	P1997	H1998	L2002	Y2006	D2017	Y2018	G2019	THR	ALA	GLN	TYR	CYS	CYS	ARG	MET											
D1782	H1783	I1784	M1788	S1688	E1689	I1692	R1693	L1694	Y1695	M1702	G1703	F1704	M1705	L1708	I1709	G1624	M1710	L1713	P1717	L1720	SER	GLY	ARG	GLU	ARG	A1726	W1734	R1735	Q1736	G1737	I1738	Y1739	L1740	P1744	C1748	L1749	V1750	G1751	S1752	E1760	L1763	T1766	V1668	C1770	Q1779	V1780	V1781						
Y1596	P1600	K1601	W1602	K1605	Q1609	V1613	K1614	V1615	E1616	H1621	P1622	K1623	G1624	I1625	D1630	VAL	GLU	LYS	PHE	LEU	SER	ARG	LYS	LYS	PHE	P1642	Q1648	Y1649	F1650	K1651	E1654	Q1657	I1658	A1659	LEU	PRO	ILE	GLY	GLU	TYR	LEU	L1668	V1669	P1670	L1673	P1683							

4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	60556	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 ($e^-/\text{\AA}^2$)	120	Depositor
Minimum defocus (nm)	3500	Depositor
Maximum defocus (nm)	5500	Depositor
Magnification	42000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.085	Depositor
Minimum map value	-2.635	Depositor
Average map value	0.185	Depositor
Map value standard deviation	0.233	Depositor
Recommended contour level	1	Depositor
Map size (Å)	414.912, 414.912, 414.912	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.161, 2.161, 2.161	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: GDP, A1N

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	0.47	1/14323 (0.0%)	0.90	45/19372 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1943	ARG	CZ-NH1	-11.30	1.17	1.32

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1305	ASN	N-CA-C	-9.01	97.15	110.48
1	A	1493	GLU	N-CA-C	8.75	123.46	111.39
1	A	1412	ARG	CA-CB-CG	8.48	131.05	114.10
1	A	802	SER	CA-C-N	7.62	130.20	122.96
1	A	802	SER	C-N-CA	7.62	130.20	122.96

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1330	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	A	1408	PHE	Sidechain
1	A	1596	TYR	Sidechain
1	A	1941	ARG	Sidechain
1	A	1965	SER	Mainchain

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	14061	12641	14329	307	0
2	A	28	12	12	0	0
3	A	28	25	0	2	0
All	All	14117	12678	14341	307	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 307 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:1412:ARG:HG3	1:A:1518:VAL:HG11	1.51	0.93
1:A:815:PRO:HB2	1:A:1005:CYS:SG	2.12	0.89
1:A:631:LEU:HD21	1:A:652:ILE:HD11	1.60	0.83
1:A:1949:LEU:HD11	3:A:2701:A1N:C6	2.09	0.81
1:A:665:LEU:O	1:A:668:HIS:HB3	1.81	0.80

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	1770/1985 (89%)	1545 (87%)	225 (13%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1563/1790 (87%)	1558 (100%)	5 (0%)	86	86

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

Mol	Chain	Res	Type
1	A	546	VAL
1	A	1333	ASN
1	A	1958	LEU
1	A	1973	ARG
1	A	2096	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2178	GLN
1	A	2433	HIS
1	A	2510	HIS
1	A	2468	ASN
1	A	1230	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A1N	A	2701	-	29,32,32	5.02	16 (55%)	40,48,48	4.49	14 (35%)
2	GDP	A	2601	-	29,30,30	0.86	1 (3%)	45,47,47	1.06	3 (6%)

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	A1N	A	2701	-	-	2/12/29/29	0/5/5/5
2	GDP	A	2601	-	-	3/16/32/32	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2701	A1N	C11-N4	-19.56	1.14	1.33
3	A	2701	A1N	C20-C21	-6.61	1.29	1.39
3	A	2701	A1N	O1-C2	-6.54	1.33	1.44
3	A	2701	A1N	C21-C11	-6.39	1.31	1.47
3	A	2701	A1N	O1-C5	-6.33	1.33	1.44

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2701	A1N	C21-C11-N4	23.72	123.90	110.36
3	A	2701	A1N	C10-N3-C7	7.31	121.08	114.95
3	A	2701	A1N	C21-C12-N5	-6.84	101.68	106.59
3	A	2701	A1N	N3-C10-N2	-4.37	121.97	128.58
3	A	2701	A1N	C11-C9-N2	4.31	123.13	116.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

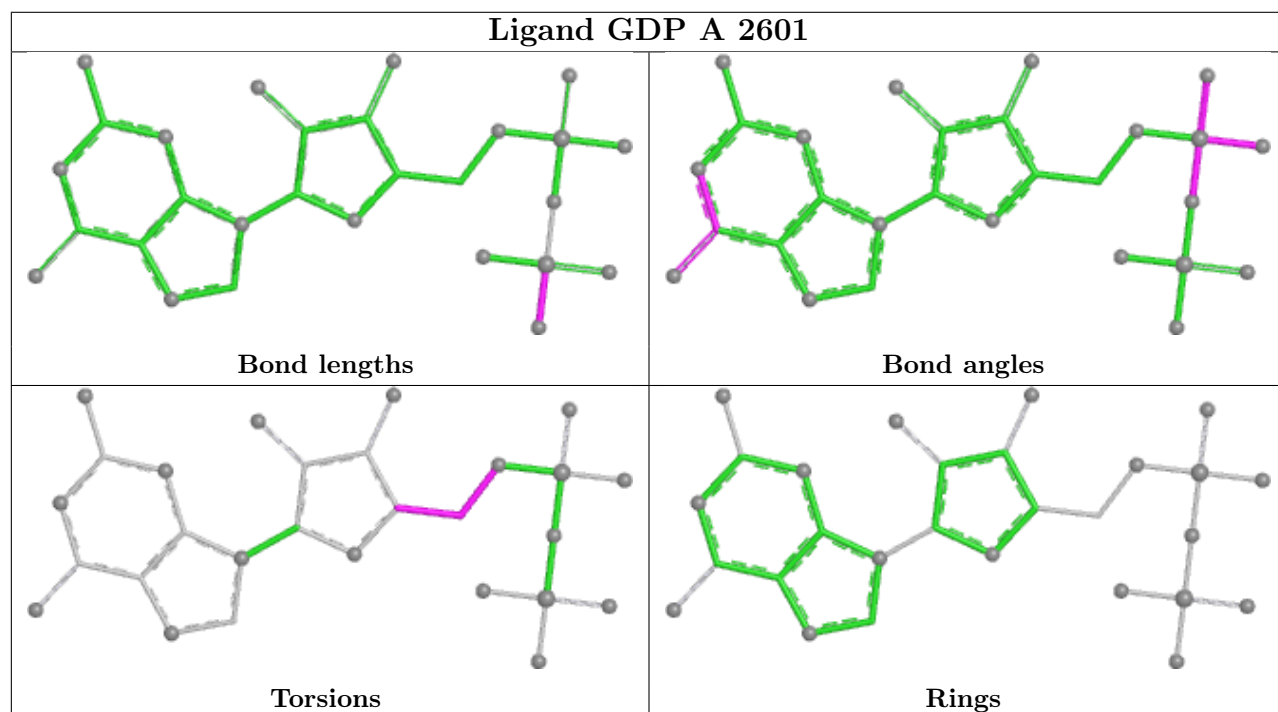
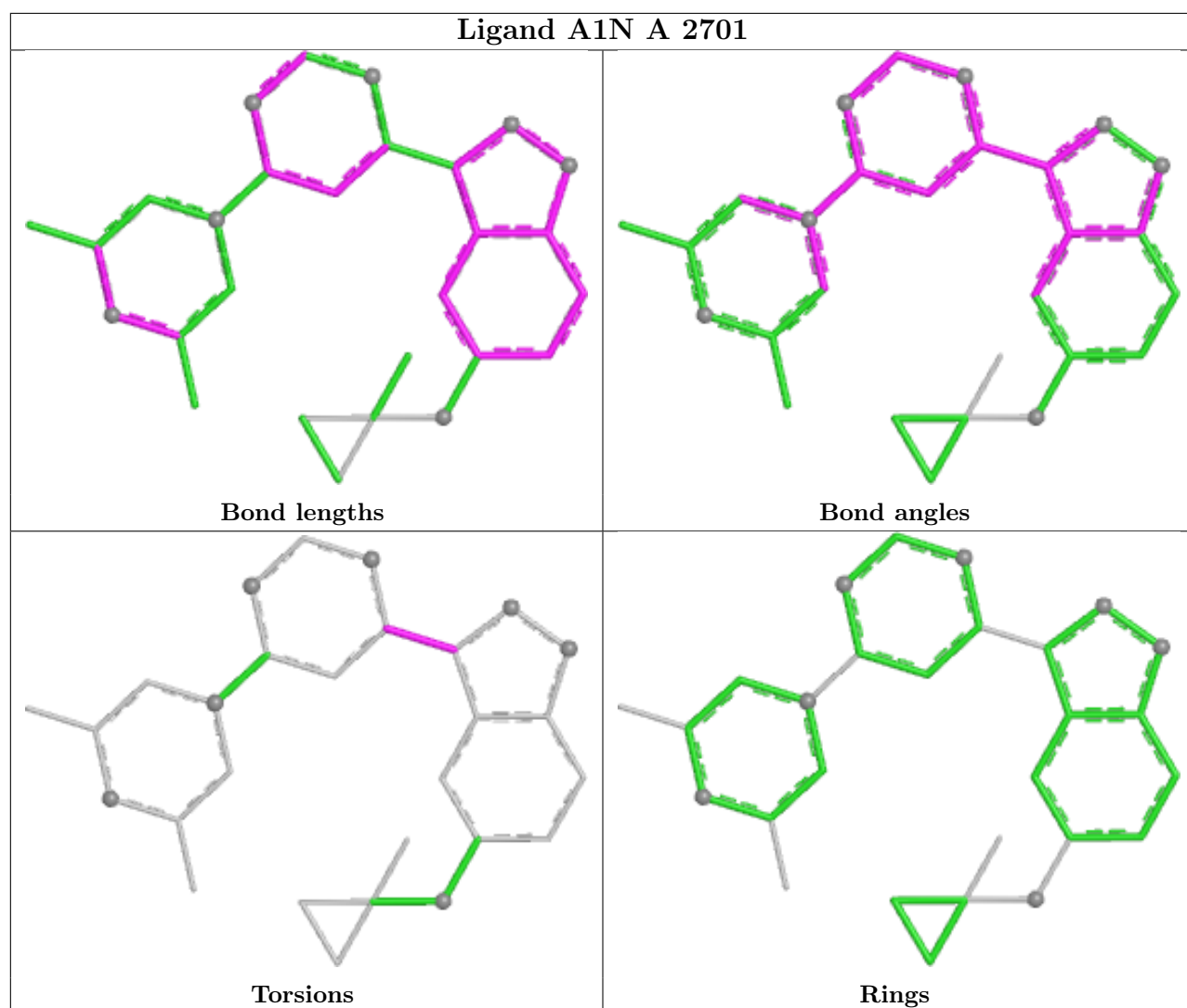
Mol	Chain	Res	Type	Atoms
2	A	2601	GDP	C3'-C4'-C5'-O5'
2	A	2601	GDP	O4'-C4'-C5'-O5'
3	A	2701	A1N	C21-C11-C9-C8
3	A	2701	A1N	C21-C11-C9-N2
2	A	2601	GDP	C4'-C5'-O5'-PA

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2701	A1N	2	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.

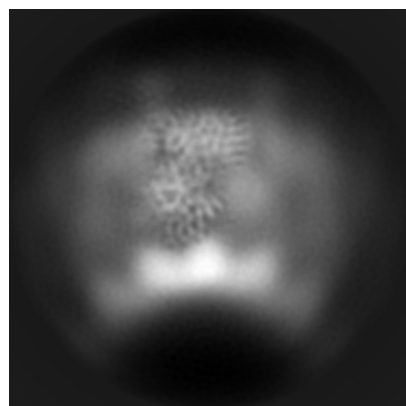
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45591. These allow visual inspection of the internal detail of the map and identification of artifacts.

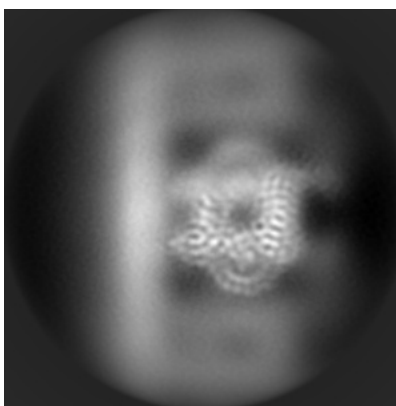
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

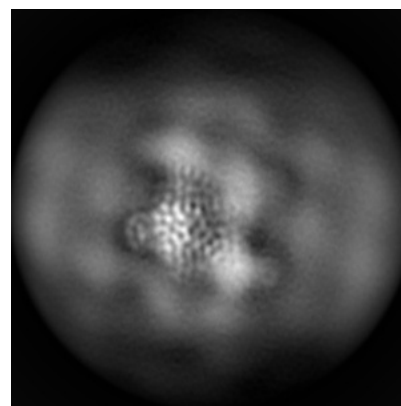
6.1.1 Primary map



X

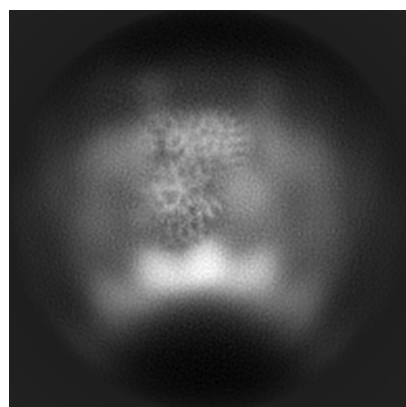


Y

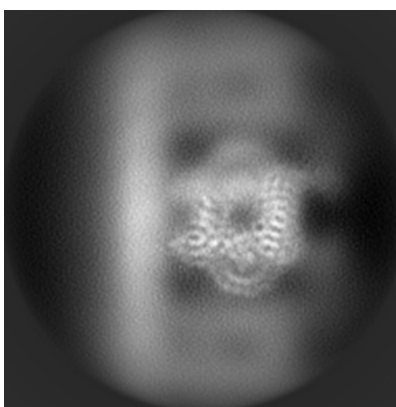


Z

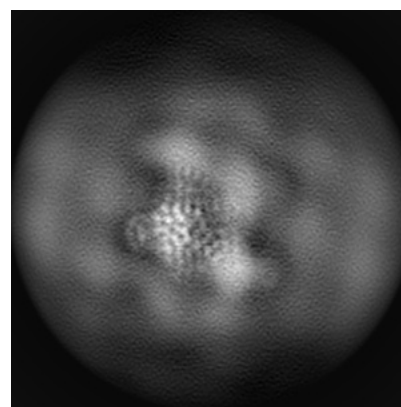
6.1.2 Raw map



X



Y

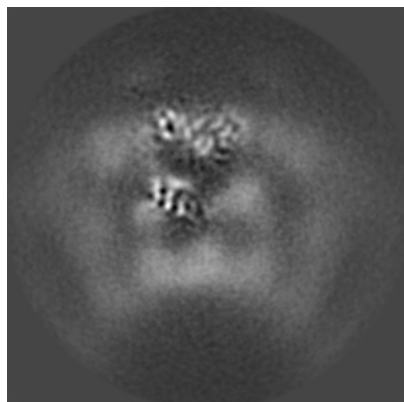


Z

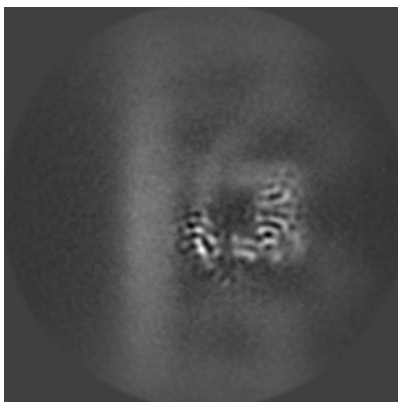
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

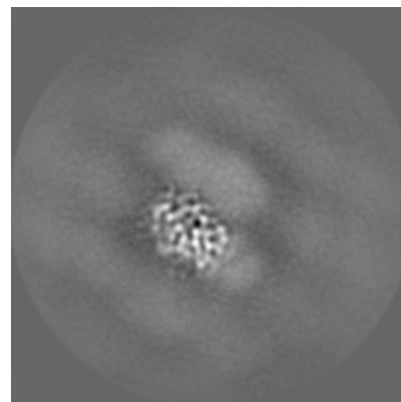
6.2.1 Primary map



X Index: 96

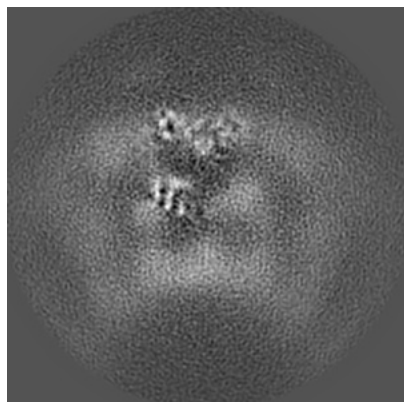


Y Index: 96

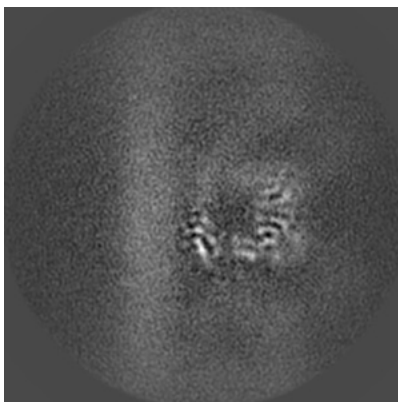


Z Index: 96

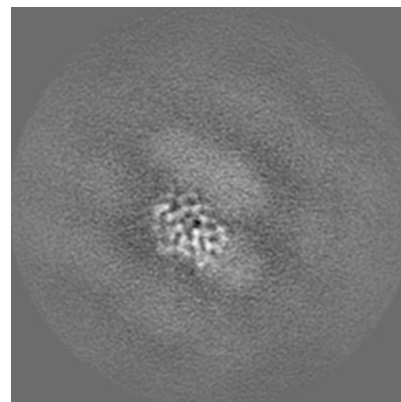
6.2.2 Raw map



X Index: 96



Y Index: 96

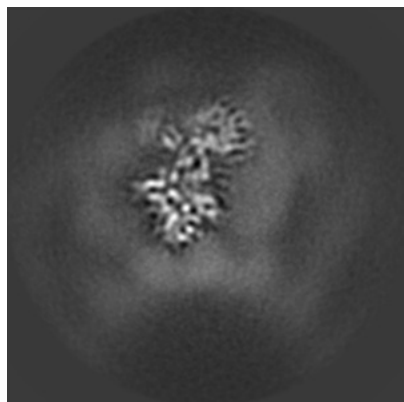


Z Index: 96

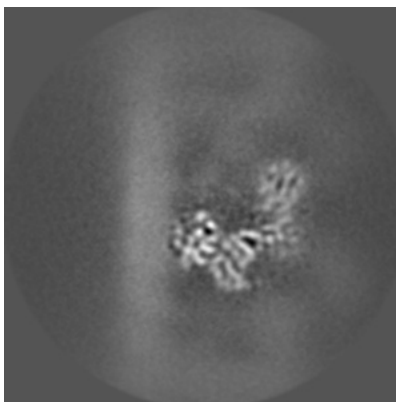
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

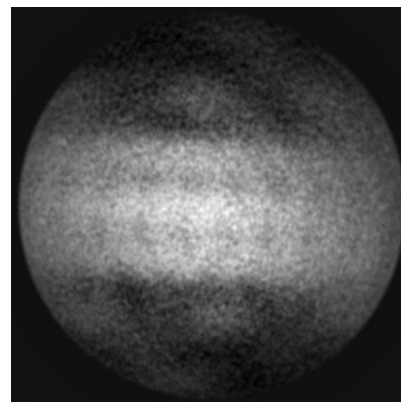
6.3.1 Primary map



X Index: 80

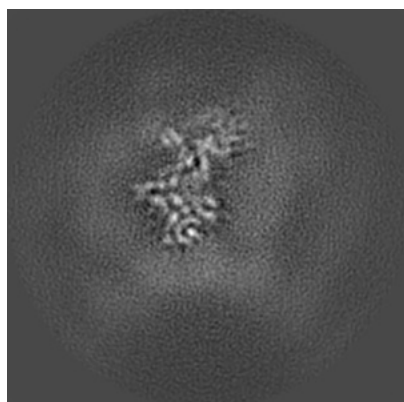


Y Index: 91

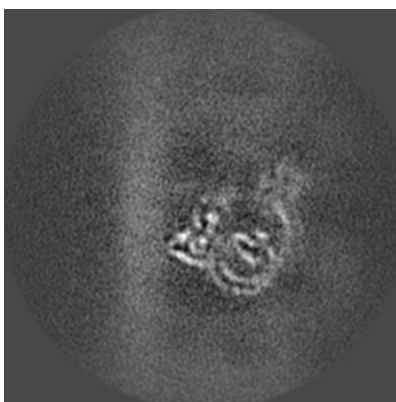


Z Index: 66

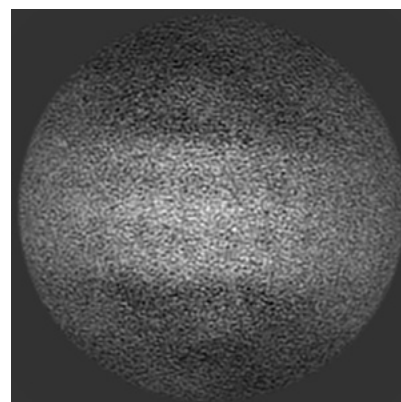
6.3.2 Raw map



X Index: 79



Y Index: 86

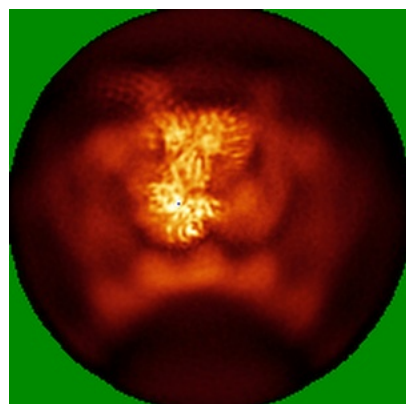


Z Index: 66

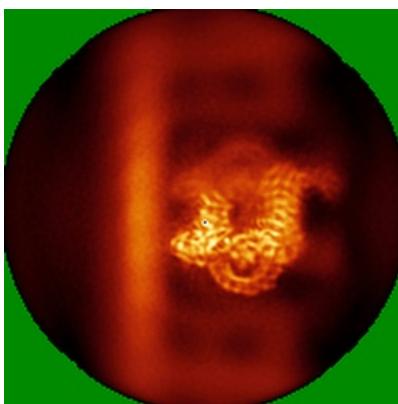
The images above show the largest variance slices of the map in three orthogonal directions.

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

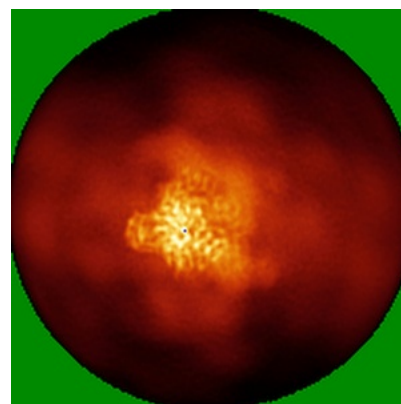
6.4.1 Primary map



X

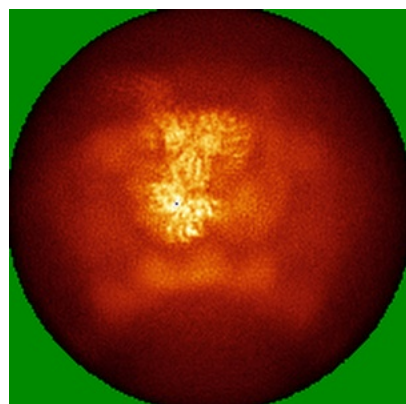


Y

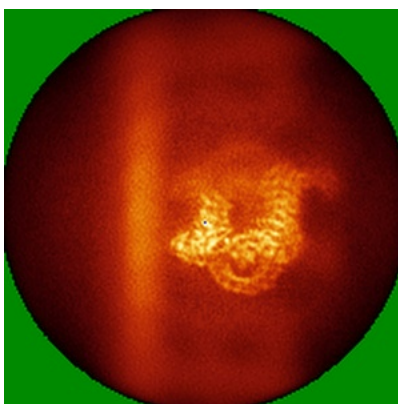


Z

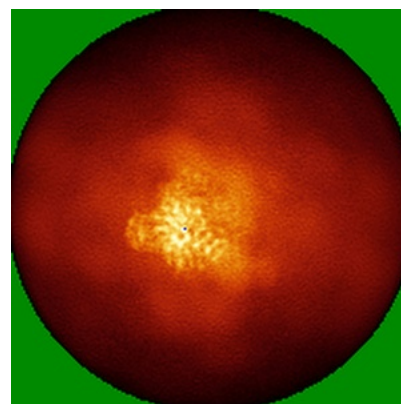
6.4.2 Raw map



X



Y

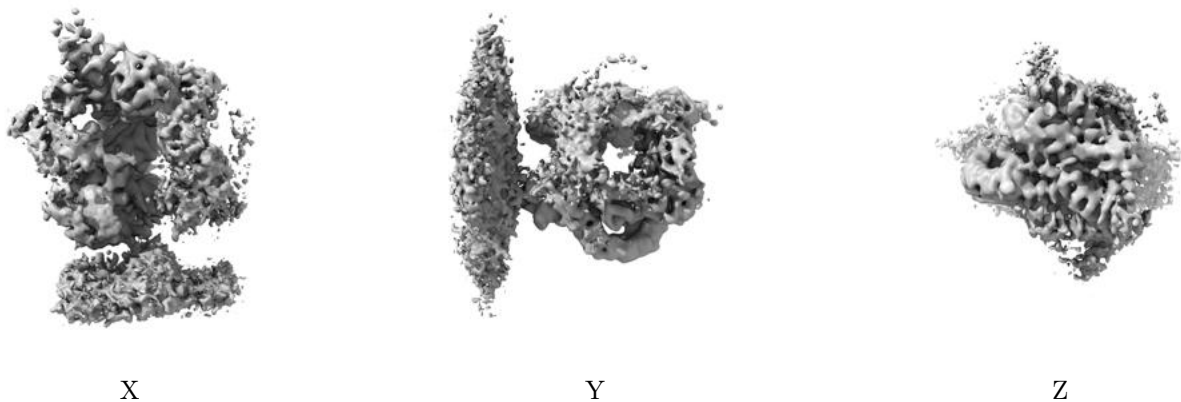


Z

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.

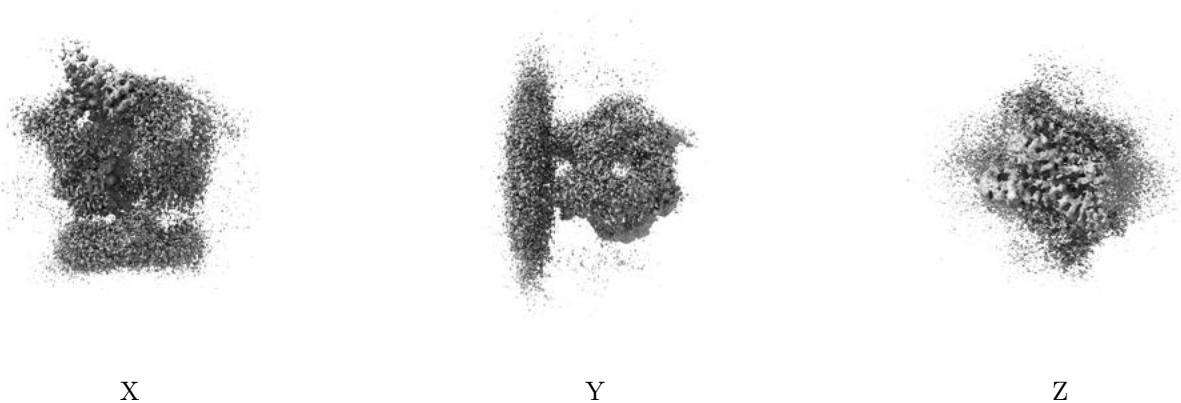
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. 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.

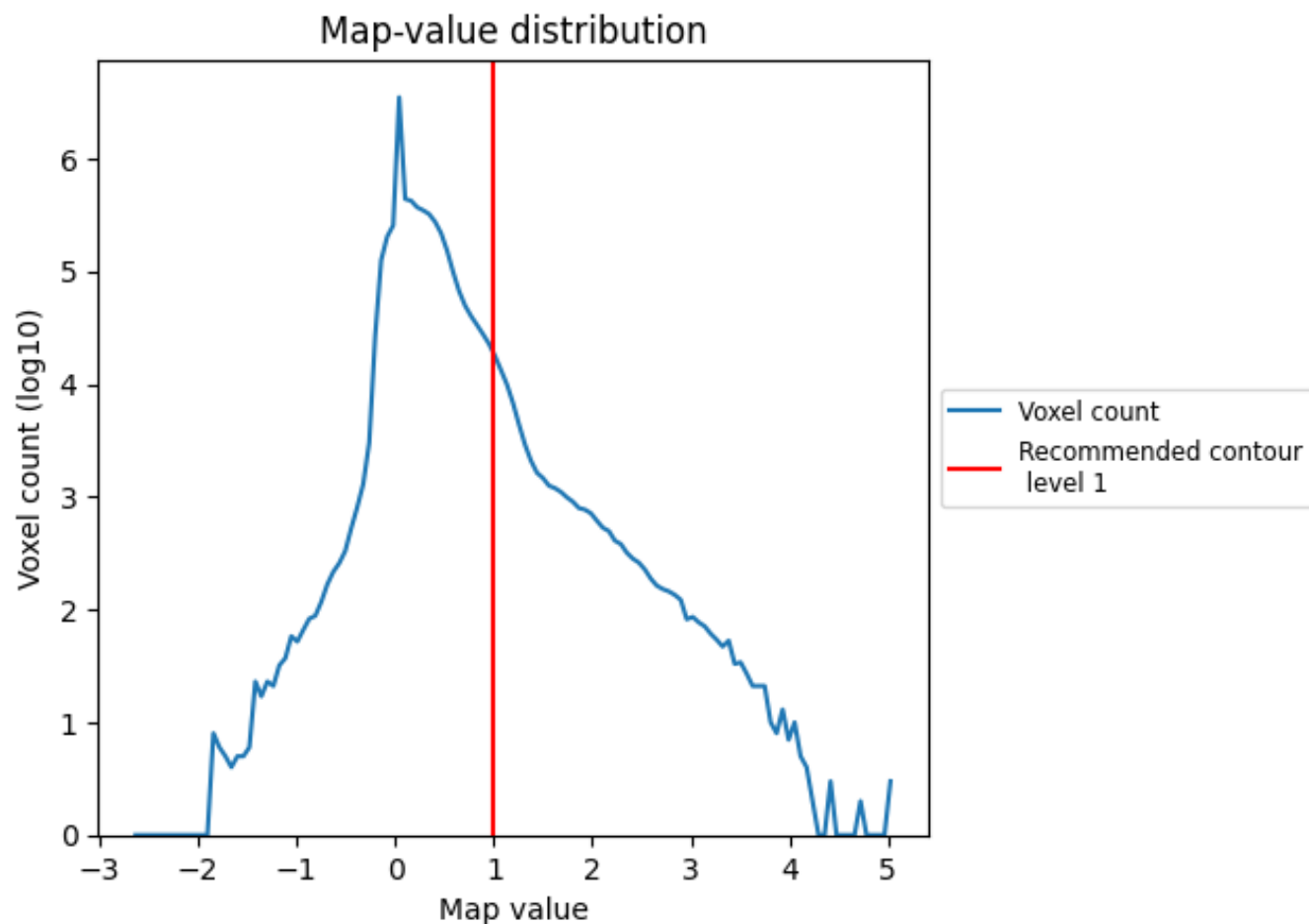
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

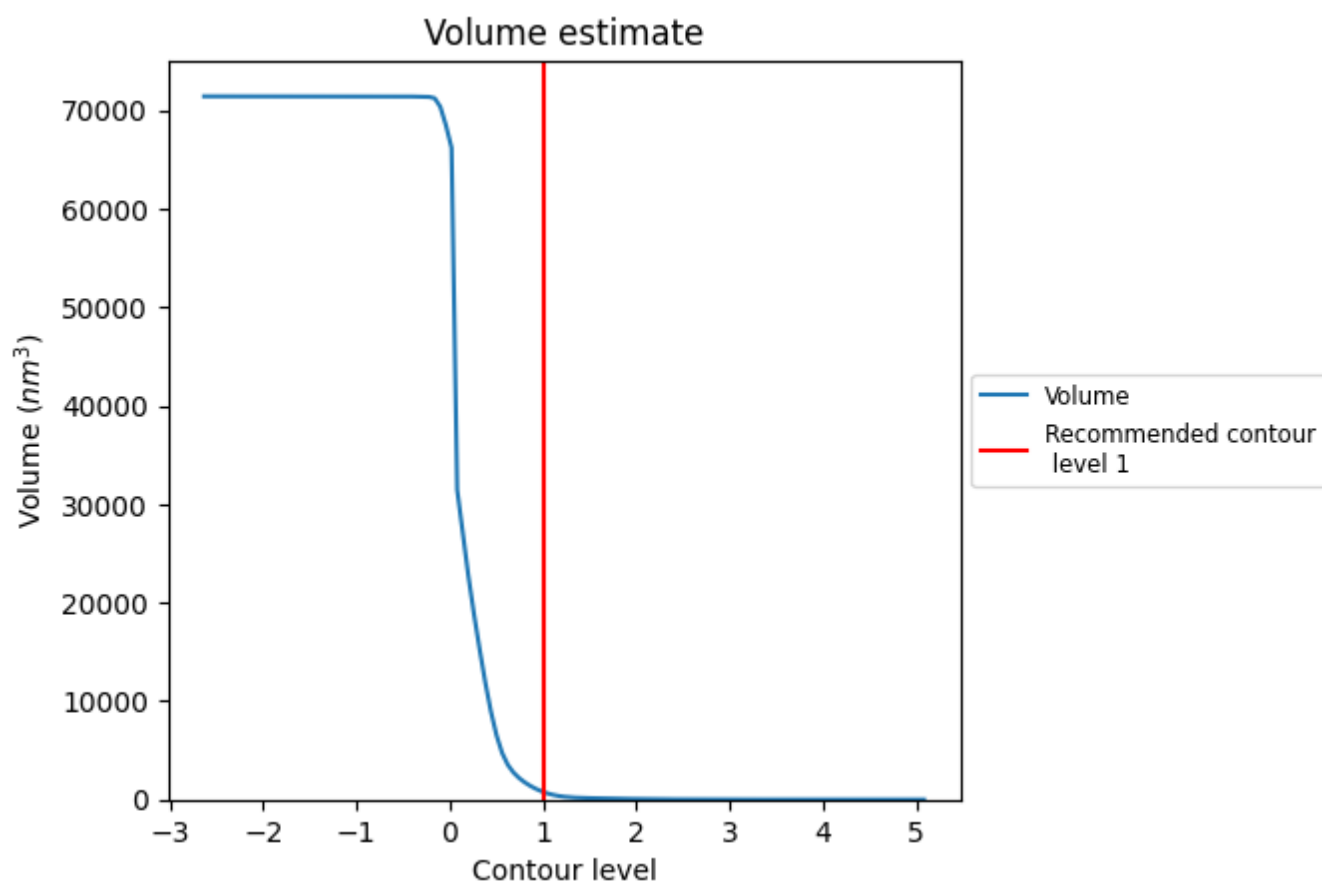
This section contains the results of statistical analysis of the map.

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.

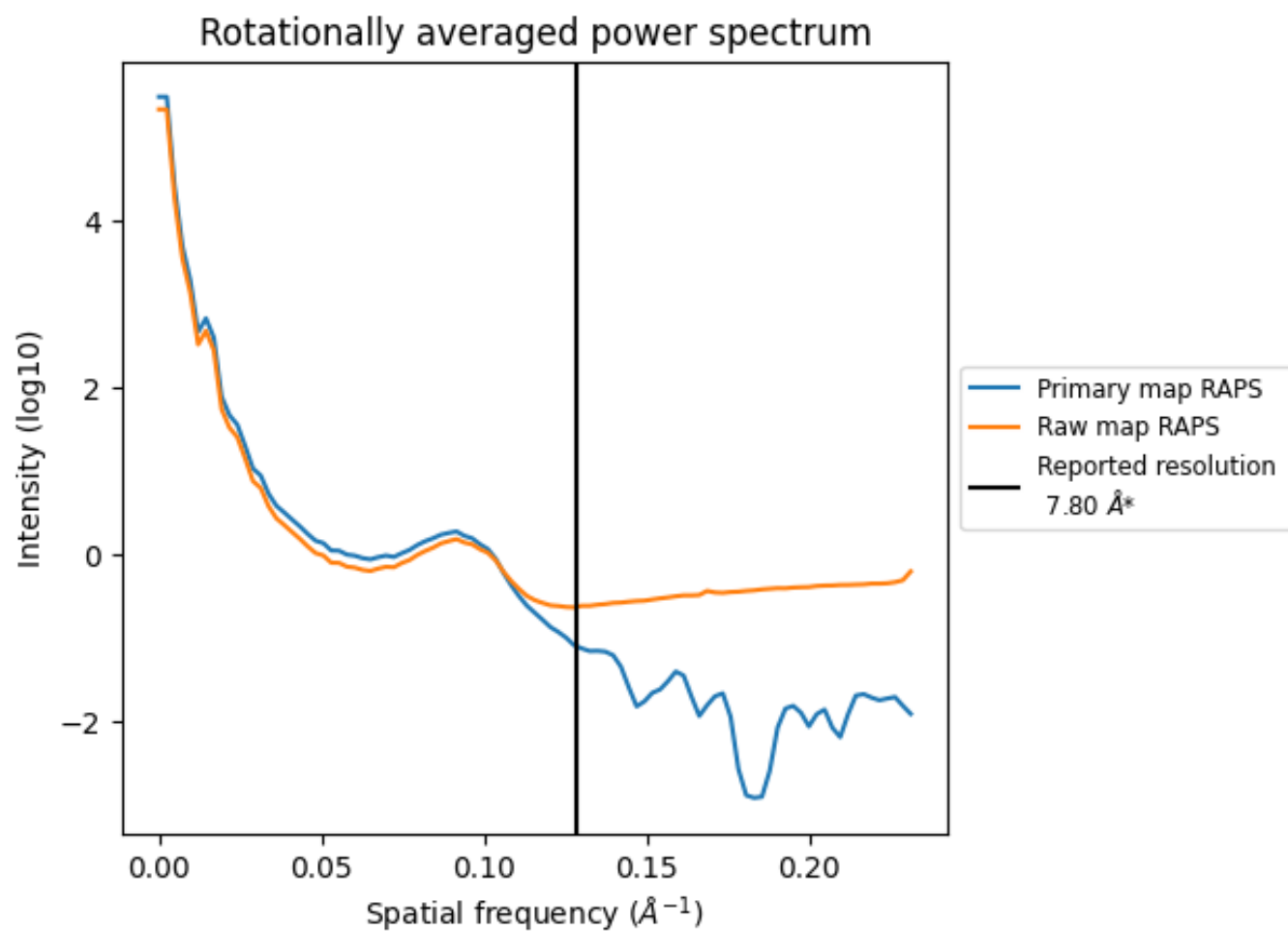
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 785 nm³; this corresponds to an approximate mass of 710 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 ⓘ

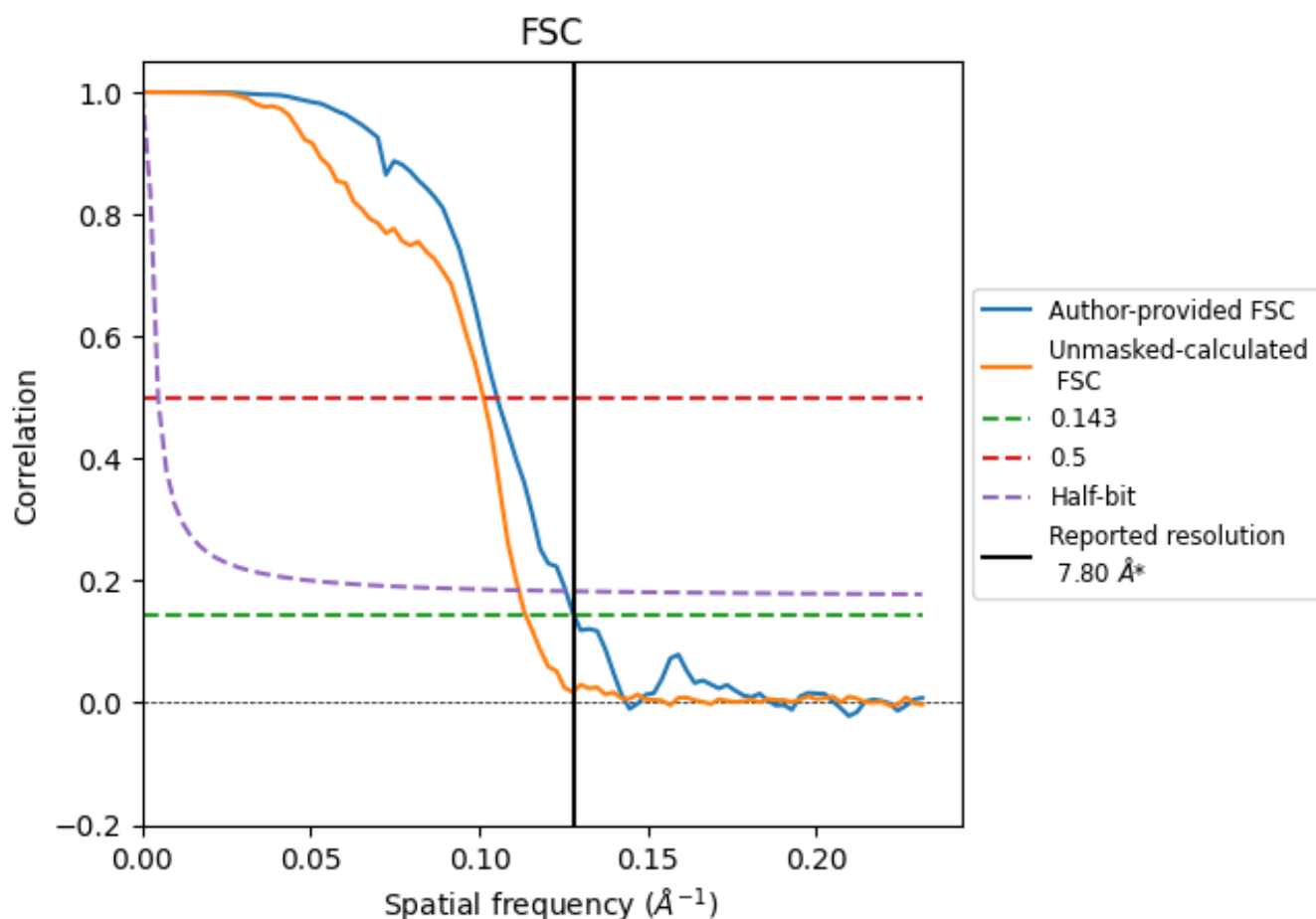


*Reported resolution corresponds to spatial frequency of 0.128 Å⁻¹

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 0.128 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.80	-	-
Author-provided FSC curve	7.80	9.50	7.96
Unmasked-calculated*	8.79	9.87	8.95

*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 8.79 differs from the reported value 7.8 by more than 10 %

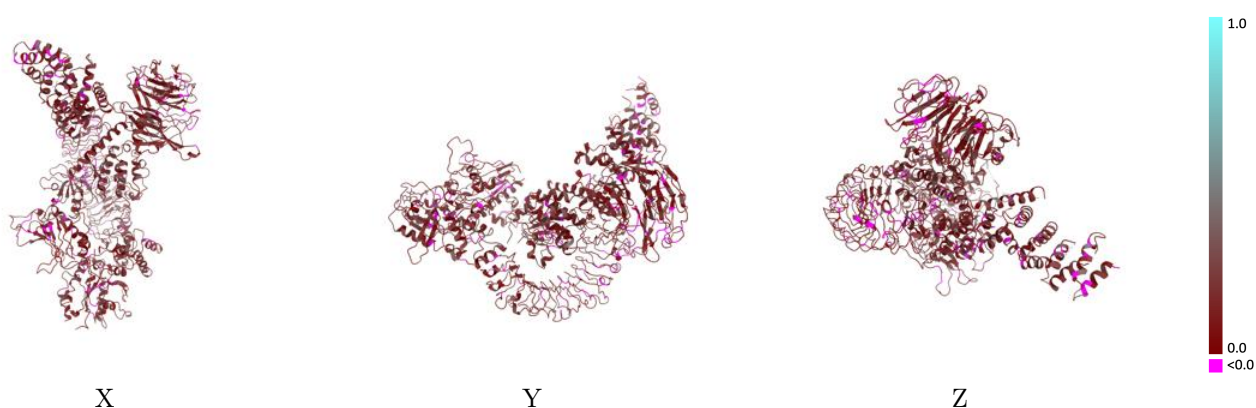
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-45591 and PDB model 9CHO. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

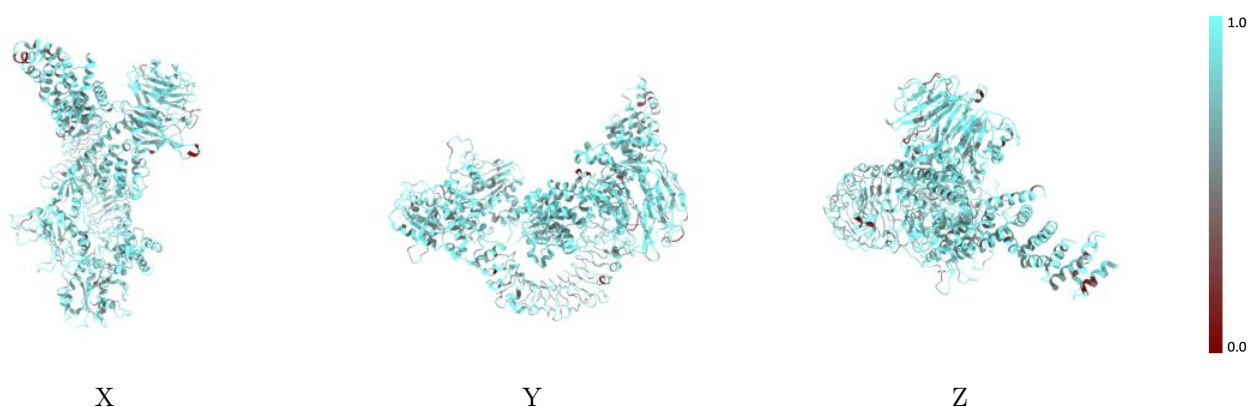
This section was not generated.

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



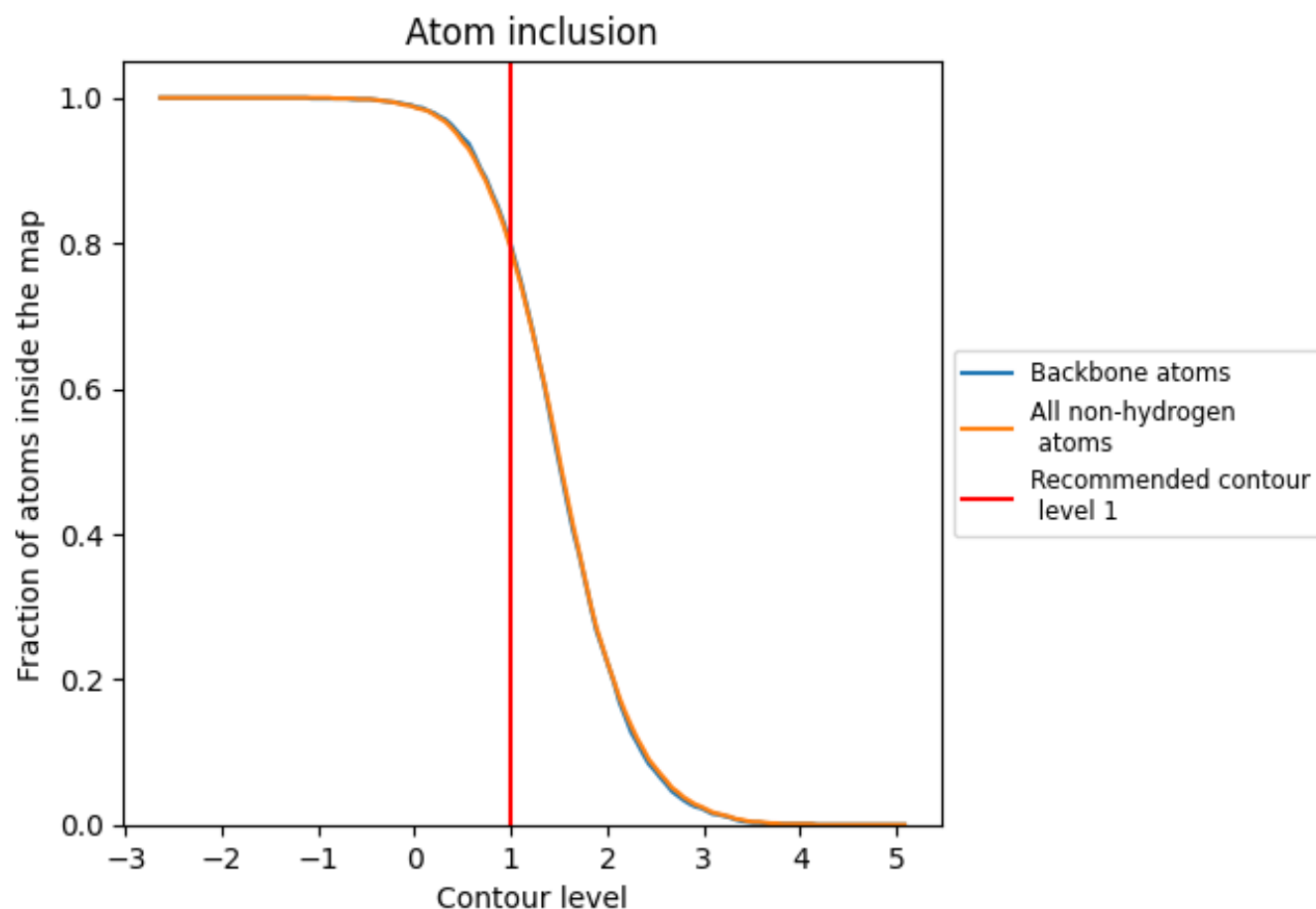
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 79% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7930	0.1590
A	0.8030	0.1590

