



wwPDB EM Validation Summary Report ⓘ

Aug 15, 2026 – 01:03 PM EDT

PDB ID : 9YCD / pdb_00009ycd
EMDB ID : EMD-72768
Title : Leucine Rich Repeat Kinase 2 R1441C mutant (active)
Authors : Villagran Suarez, A.; Bodrug, T.; Leschziner, A.
Deposited on : 2025-09-18
Resolution : 3.63 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.dev133
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) : 2.50

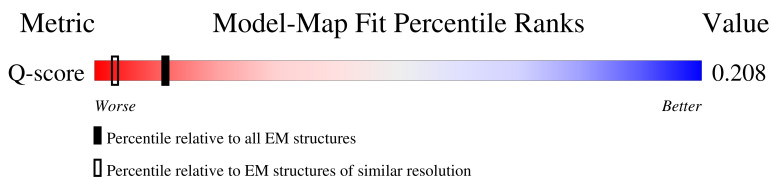
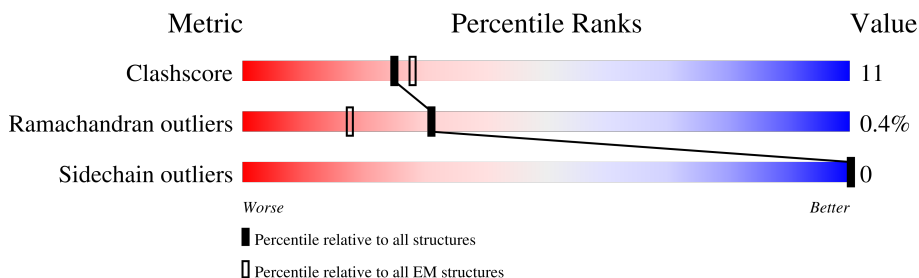
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.63 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	11696 (3.13 - 4.13)

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	2527	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 8602 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.

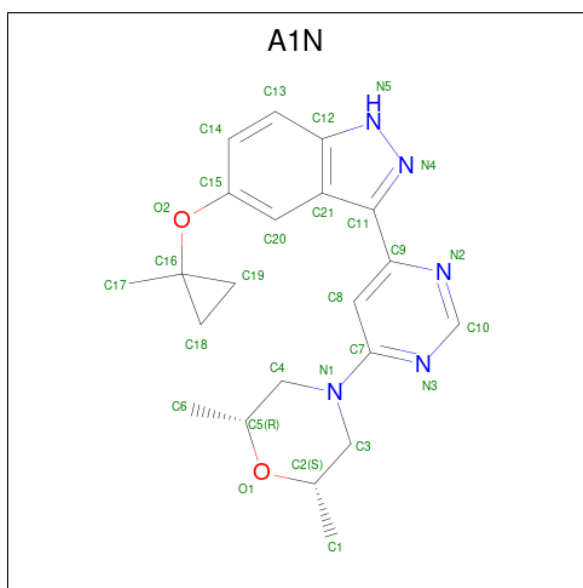
- Molecule 1 is a protein called Leucine-rich repeat serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1117	Total	C	N	O	S	3	0
			8574	5492	1485	1545	52		

There is a discrepancy between the modelled and reference sequences:

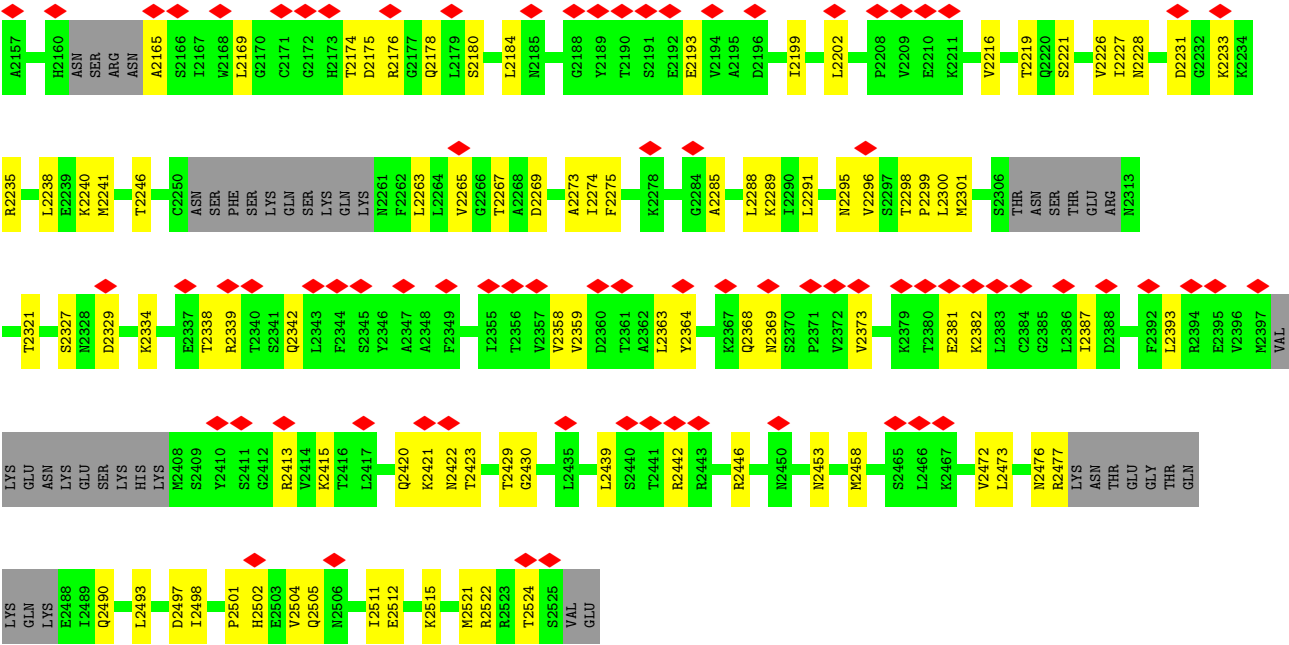
Chain	Residue	Modelled	Actual	Comment	Reference
A	1441	CYS	ARG	engineered mutation	UNP Q5S007

- Molecule 2 is (2 {R},6 {S})-2,6-dimethyl-4-[6-[5-(1-methylcyclopropyl)oxy-1 {H}-indazol-3-yl]pyrimidin-4-yl]morpholine (CCD ID: A1N) (formula: C₂₁H₂₅N₅O₂).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			28	21	5	2	

V2056	P1942	K1824	N1730	P1642	Q1516	K1423	PHE	PRO	LEU	TLE	LYS	ASN	ASN	SER	SER	ARG
Y2057	R1943	L1827	R1731	K1643	L1517	K1424	LEU	PRO	ASP	SER	CYS	ALA	ALA	PHE	PHE	VAL
S2058	M1944	D1828	M1732	K1643	VAL	Q1425	GLN	GLU	MET	SER	ILE	THR	THR	LEU	LEU	THR
F2059	L1945	D1829	Y1733	M1646	GLY	A1426	ARG	GLY	SER	SER	LEU	THR	THR	LEU	LEU	THR
L2063	V1946	L1830	Q1736	K1646	Q1521	E1427	LEU	CYS	ASN	GLU	LYS	GLN	PHE	LYS	LYS	TYR
L1965	M1831	M1831	G1737	Y1649	D1525	V1428	LYS	GLU	ILE	ASN	ASN	GLN	GLN	GLN	GLN	GLN
L1969	K1832	K1833	Y1738	F1650	D1525	D1429	LYS	GLU	ILE	PHE	ASN	GLN	GLN	GLN	GLN	GLN
L2067	K1833	K1833	Y1739	F1651	E1529	A1430	ALA	ASN	GLN	LEU	LEU	GLN	GLN	GLN	GLN	GLN
T1969	L1840	L1840	L1740	L1652	Y1530	T1438	PRO	THR	TYR	GLU	ALA	GLN	GLN	GLN	GLN	GLN
T2069	L1970	L1970	N1741	L1653	E1531	K1439	VAL	THR	LEU	GLU	ALA	GLN	GLN	GLN	GLN	GLN
Q1971	V1841	V1841	W1742	E1654	E1531	K1439	TYR	SER	PRO	CYS	TYR	ASN	ASN	ASN	ASN	ASN
H1972	N1842	N1842	W1742	E1655	E1532	K1439	ARG	ASP	GLY	PRO	ASN	THR	THR	THR	THR	THR
R1973	F1656	F1656	C1748	F1656	I1533	L1449	ARG	ASP	PRO	LYS	GLN	GLN	GLN	GLN	GLN	GLN
L1973	Q1657	Q1657	L1749	Q1657	I1534	V1450	LYS	VAL	ALA	VAL	LEU	LEU	LEU	LEU	LEU	LEU
L1976	D1844	D1844	V1750	I1658	I1535	V1450	LEU	VAL	ALA	VAL	LEU	LEU	LEU	LEU	LEU	LEU
H1977	Q1845	Q1845	G1751	A1659	R1538	D1455	M1338	TYR	TRP	SER	VAL	THR	THR	THR	THR	THR
H1977	PRO	PRO	G1751	A1659	R1538	D1455	M1338	ASN	ASN	LYS	VAL	THR	THR	THR	THR	THR
V1978	ARG	ARG	S1752	F1661	R1550	V1456	I1339	LEU	ASN	SER	PRO	HIS	HIS	HIS	HIS	HIS
H1986	THR	THR	H1758	I1662	R1552	S1457	V1340	GLU	LEU	ALA	GLU	GLU	GLU	GLU	GLU	GLU
M1989	I1850	I1850	P1759	GLY	R1551	ASP	S1345	ARG	ASN	ALA	ASP	ASP	ASP	ASP	ASP	ASP
M1989	P1857	P1857	E1760	GLU	R1552	GLU	V1340	SER	LEU	ALA	ASP	ASP	ASP	ASP	ASP	ASP
I1990	D1858	D1858	S1761	GLU	R1552	GLU	V1340	ARG	ASN	ALA	ASP	ASP	ASP	ASP	ASP	ASP
I1991	L1859	L1859	F1762	GLU	R1552	GLU	V1340	ASN	ASN	ALA	ASP	ASP	ASP	ASP	ASP	ASP
Y1992	L1860	L1860	K1763	GLU	R1552	GLU	V1340	ASN	ASN	ALA	ASP	ASP	ASP	ASP	ASP	ASP
R1993	L1861	L1861	I1765	GLU	R1552	GLU	V1340	ASN	ASN	ALA	ASP	ASP	ASP	ASP	ASP	ASP
D1994	L1864	L1864	C1774	H1684	Q1555	R1462	LYS	PRO	LEU	ALA	VAL	VAL	VAL	VAL	VAL	VAL
L1995	P1865	P1865	V1780	C1685	Q1555	R1462	LYS	PRO	LEU	ALA	VAL	VAL	VAL	VAL	VAL	VAL
P1997	R1866	R1866	V1781	E1686	Q1555	R1462	LYS	PRO	LEU	ALA	VAL	VAL	VAL	VAL	VAL	VAL
P2007	L1885	L1885	D1782	E1689	Q1555	R1462	LYS	PRO	LEU	ALA	VAL	VAL	VAL	VAL	VAL	VAL
T2020	S1889	S1889	D1785	I1692	Q1555	R1462	LYS	PRO	LEU	ALA	VAL	VAL	VAL	VAL	VAL	VAL
Q2022	F1890	F1890	S1786	R1693	Q1555	R1462	LYS	PRO	LEU	ALA	VAL	VAL	VAL	VAL	VAL	VAL
Y2023	L1887	L1887	L1787	L1694	Q1555	R1462	LYS	PRO	LEU	ALA	VAL	VAL	VAL	VAL	VAL	VAL
C2024	V1893	V1893	E1790	M1697	Q1555	R1462	LYS	PRO	LEU	ALA	VAL	VAL	VAL	VAL	VAL	VAL
C2025	Y1894	Y1894	E1790	P1701	Q1555	R1462	LYS	PRO	LEU	ALA	VAL	VAL	VAL	VAL	VAL	VAL
T2031	R1895	R1895	G1794	P1701	Q1555	R1462	LYS	PRO	LEU	ALA	VAL	VAL	VAL	VAL	VAL	VAL
S2032	E1902	E1902	I1798	F1704	P1600	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
E2033	V1905	V1905	ASP	W1705	L1603	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
G2034	K1906	K1906	ILE	S1706	L1603	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
T2035	I1907	I1907	CYS	W1706	L1603	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
F2038	T1912	T1912	GLY	I1709	K1605	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
P2041	S1913	S1913	GLY	M1710	K1605	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
E2042	L1914	L1914	GLY	R1711	K1605	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
V2043	R1915	R1915	GLY	L1712	K1605	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
A2044	E1920	E1920	GLY	L1713	K1605	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
R2045	L1921	L1921	GLY	L1713	K1605	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
G2046	L1927	L1927	GLY	L1713	K1605	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
N2047	H1928	H1928	GLY	L1713	K1605	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
Y2050	I1940	I1940	GLY	L1713	K1605	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
N2051	R1941	R1941	GLY	L1713	K1605	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
Q2052	L1941	L1941	GLY	L1713	K1605	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
V2128	V2128	V2128	ASP	F1704	P1600	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
F2129	F2129	F2129	ASP	W1705	L1603	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
I2131	I2131	I2131	ASP	S1706	L1603	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
L2132	L2132	L2132	ASP	W1706	L1603	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
N2133	N2133	N2133	ASP	I1709	K1605	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
L2137	L2137	L2137	ASP	M1710	K1605	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
R2142	R2142	R2142	ASP	R1711	K1605	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
L2146	L2146	L2146	ASP	L1712	K1605	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
P2147	P2147	P2147	ASP	L1713	K1605	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
K2148	K2148	K2148	ASP	L1713	K1605	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
N2149	N2149	N2149	ASP	L1713	K1605	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
V2150	V2150	V2150	ASP	L1713	K1605	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
I2151	I2151	I2151	ASP	L1713	K1605	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
M2155	M2155	M2155	ASP	L1713	K1605	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP
V2156	V2156	V2156	ASP	L1713	K1605	K1496	LYS	TRP	TRP	LYS	ASP	ASP	ASP	ASP	ASP	ASP



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63806	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.816	Depositor
Minimum map value	-0.563	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.0691	Depositor
Map size (Å)	304.0, 304.0, 304.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	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: 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	0.18	0/8729	0.54	2/11831 (0.0%)

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	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2020	ILE	N-CA-C	-6.92	107.14	113.71
1	A	1366	SER	CB-CA-C	-5.48	110.24	116.54

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1649	TYR	Peptide
1	A	1650	PHE	Peptide
1	A	1941	ARG	Peptide

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	8574	0	8472	180	0
2	A	28	0	0	0	0
All	All	8602	0	8472	180	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 180 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:1721:SER:HG	1:A:1726:ALA:N	1.71	0.89
1:A:1418:VAL:HA	1:A:1450:VAL:O	1.93	0.69
1:A:2104:TRP:NE1	1:A:2137:LEU:O	2.26	0.68
1:A:1860:ILE:HA	1:A:1940:ILE:HG12	1.79	0.65
1:A:1740:LEU:HB3	1:A:1742:TRP:HE1	1.62	0.64

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	1090/2527 (43%)	964 (88%)	122 (11%)	4 (0%)	30 59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1816	PHE
1	A	1843	PRO
1	A	1572	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1345	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	897/2281 (39%)	897 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2047	ASN
1	A	2313	ASN
1	A	2510	HIS
1	A	2453	ASN
1	A	1977	HIS

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

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	A1N	A	2601	-	29,32,32	0.98	0	40,48,48	1.47	4 (10%)

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	A1N	A	2601	-	-	6/12/29/29	0/5/5/5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2601	A1N	C5-O1-C2	4.57	118.89	112.12
2	A	2601	A1N	O1-C2-C1	4.06	114.48	106.88
2	A	2601	A1N	O1-C5-C6	3.74	113.88	106.88
2	A	2601	A1N	C10-N3-C7	3.30	117.72	114.95

There are no chirality outliers.

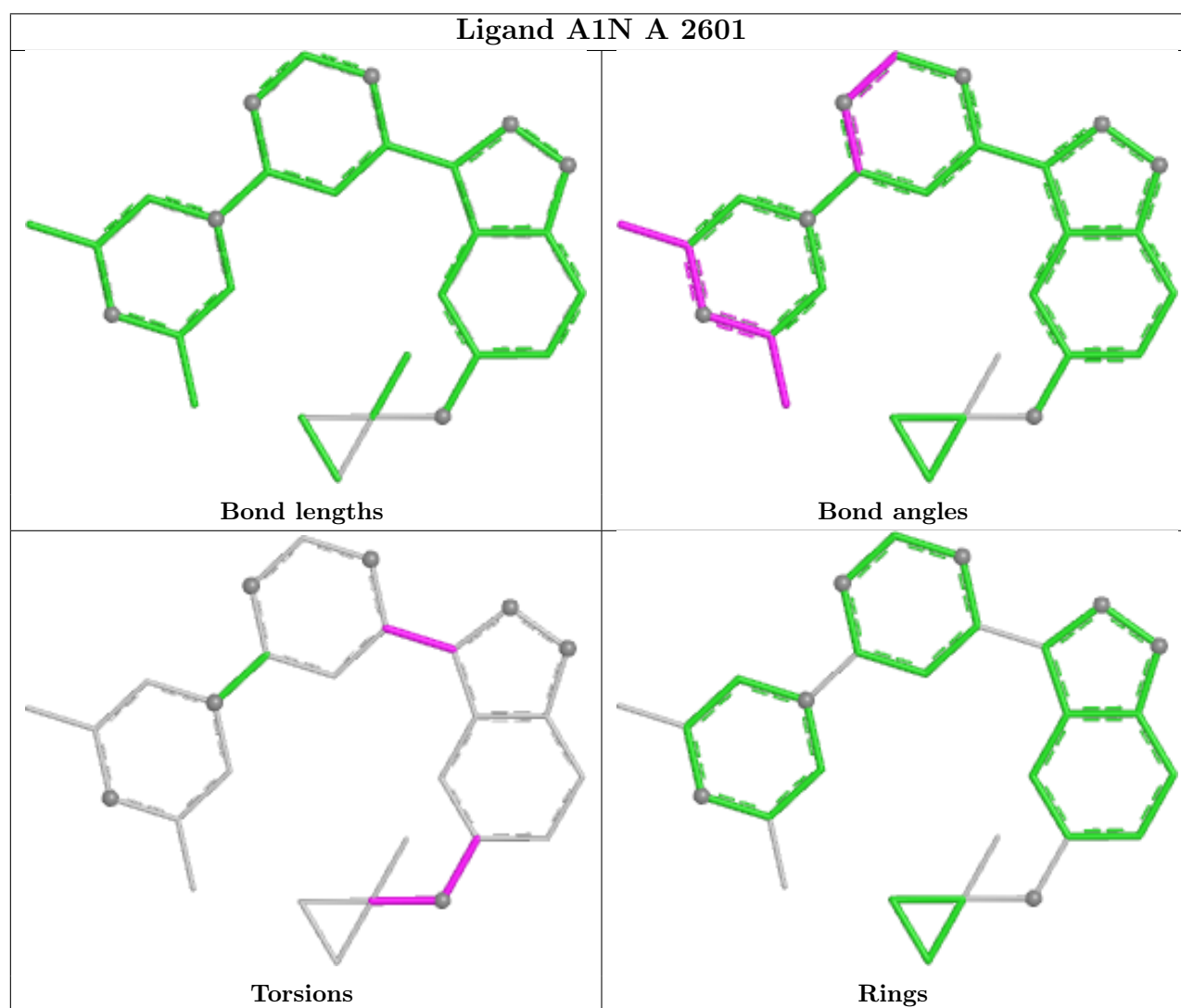
5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2601	A1N	C21-C11-C9-N2
2	A	2601	A1N	C21-C11-C9-C8
2	A	2601	A1N	C20-C15-O2-C16
2	A	2601	A1N	C14-C15-O2-C16
2	A	2601	A1N	C18-C16-O2-C15

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no chain breaks in this entry.

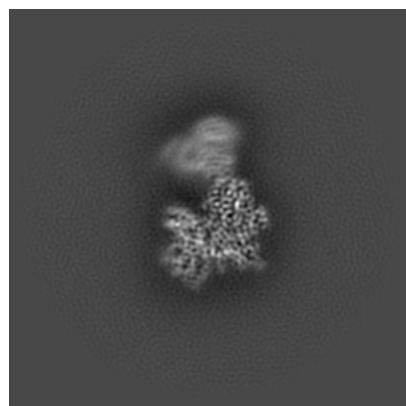
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72768. These allow visual inspection of the internal detail of the map and identification of artifacts.

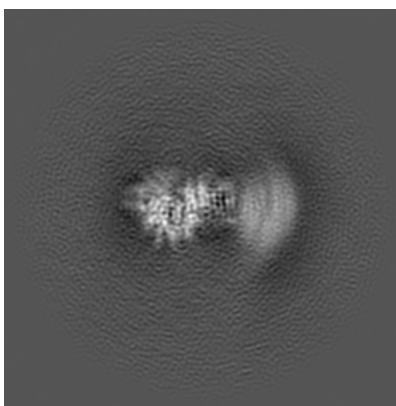
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

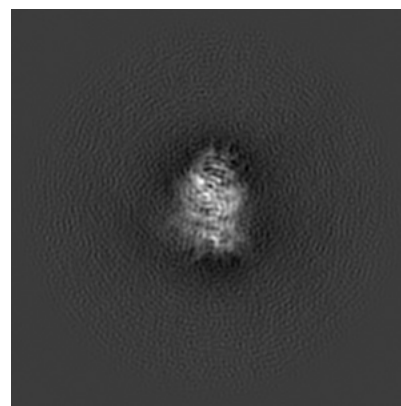
6.1.1 Primary map



X

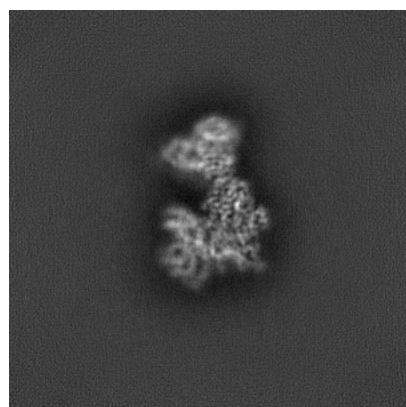


Y

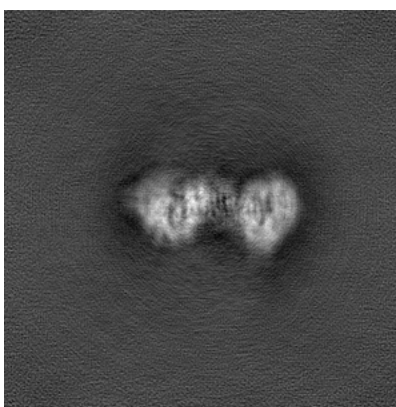


Z

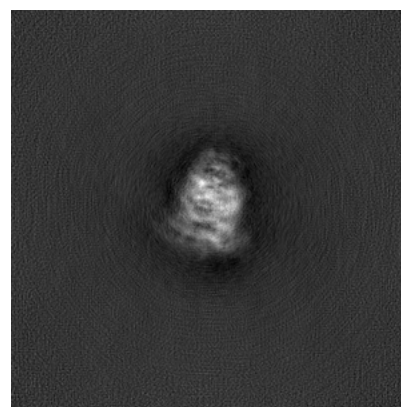
6.1.2 Raw map



X



Y

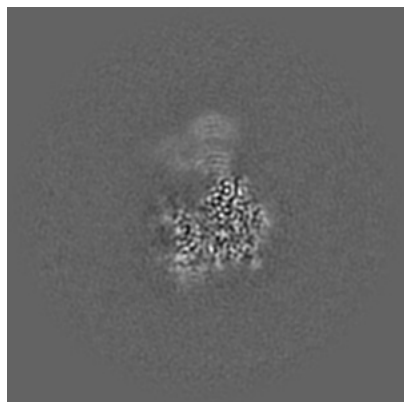


Z

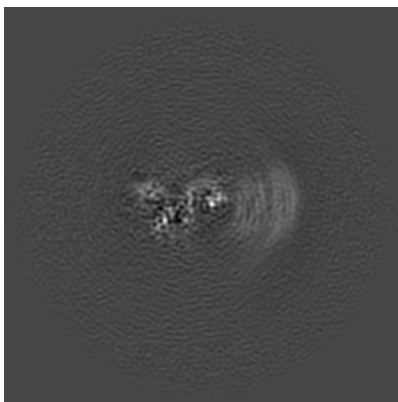
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

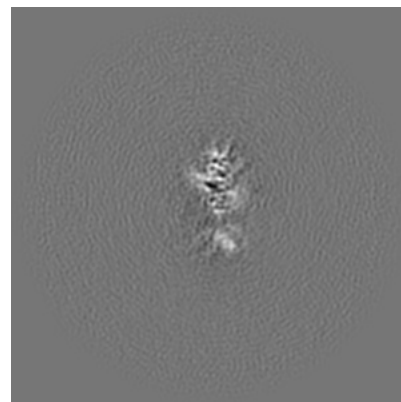
6.2.1 Primary map



X Index: 160

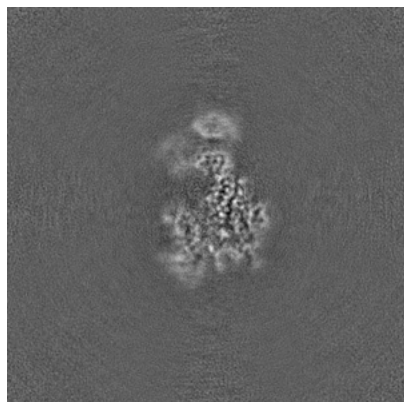


Y Index: 160

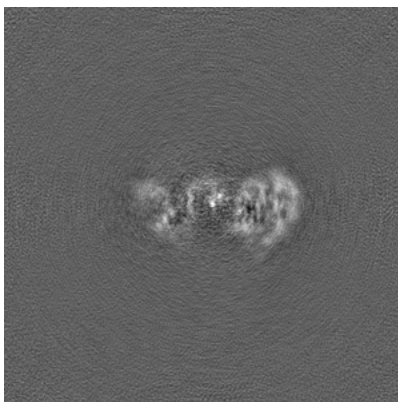


Z Index: 160

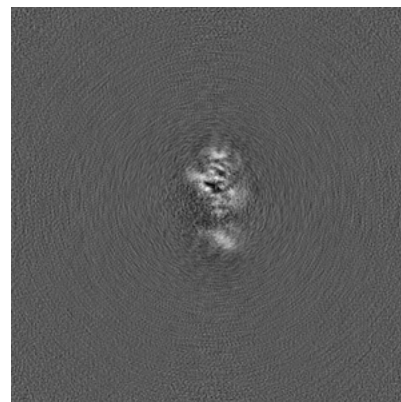
6.2.2 Raw map



X Index: 160



Y Index: 160

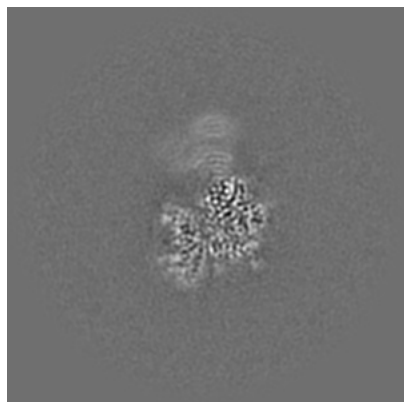


Z Index: 160

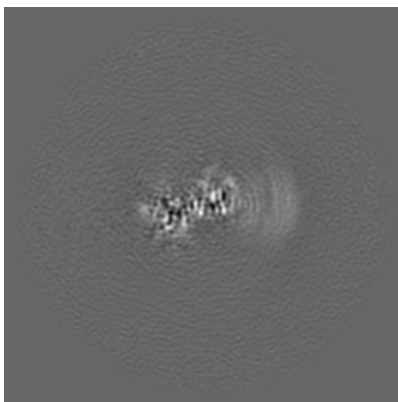
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

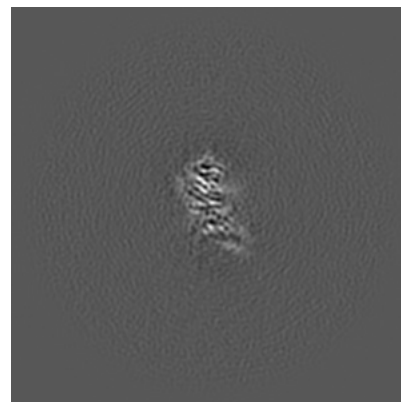
6.3.1 Primary map



X Index: 162

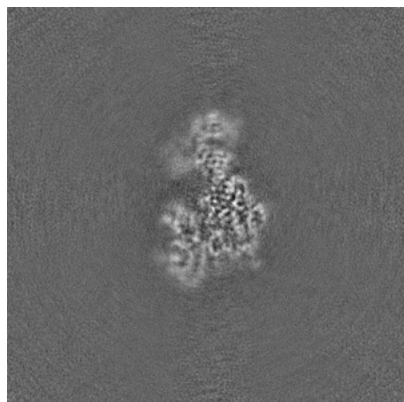


Y Index: 170

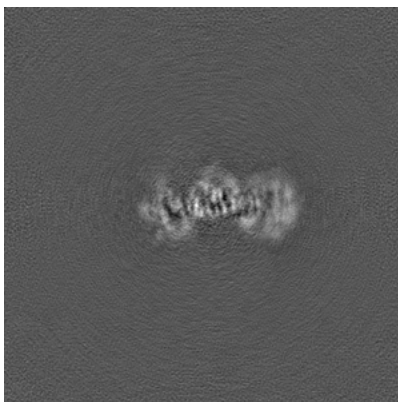


Z Index: 126

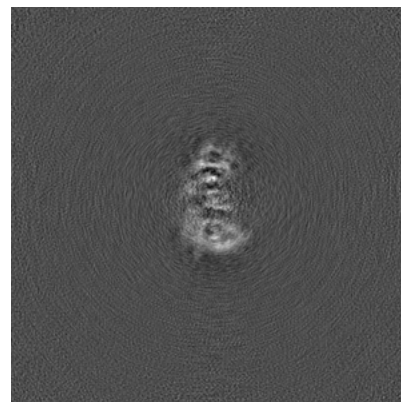
6.3.2 Raw map



X Index: 163



Y Index: 171

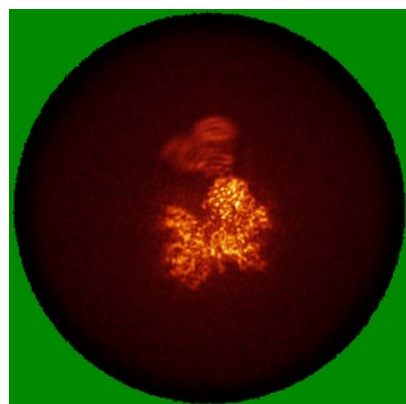


Z Index: 148

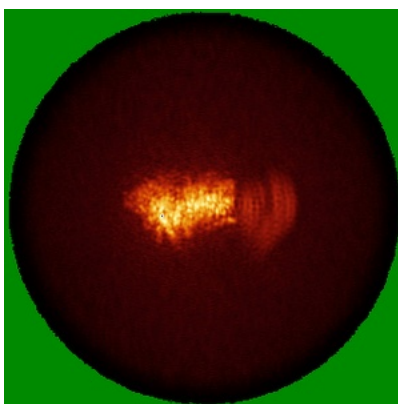
The images above show the largest variance slices of the map in three orthogonal directions.

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

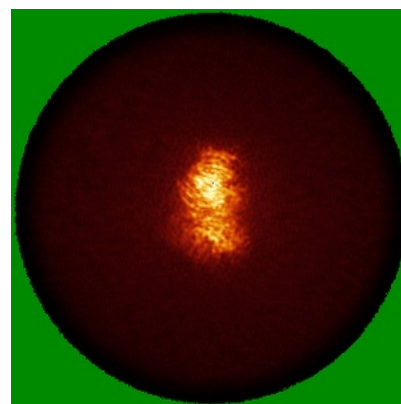
6.4.1 Primary map



X

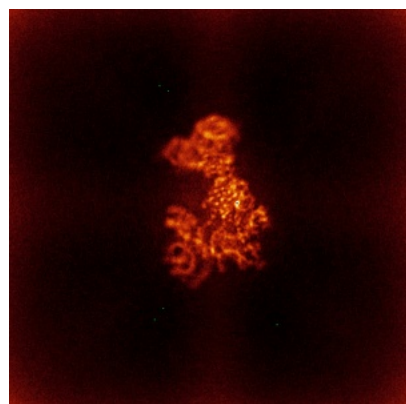


Y

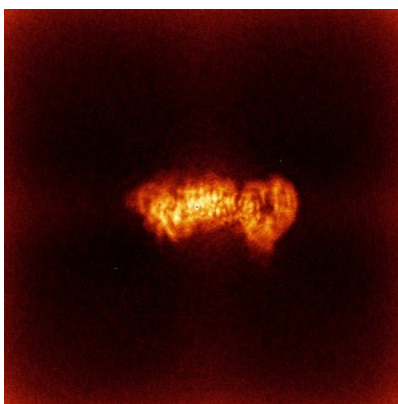


Z

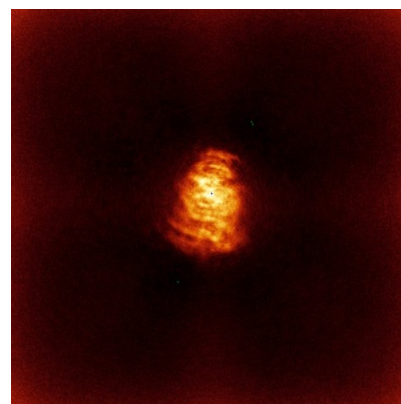
6.4.2 Raw map



X



Y

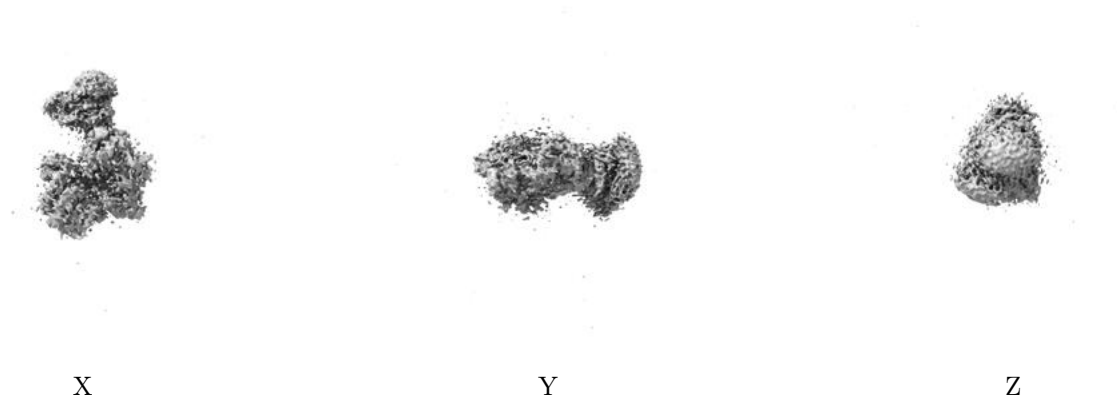


Z

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.

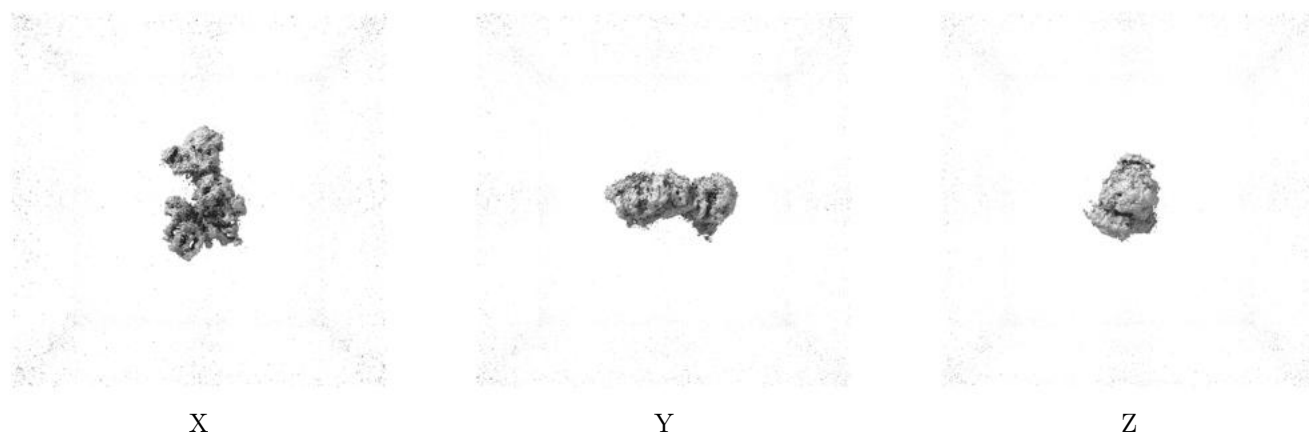
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0691. 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.

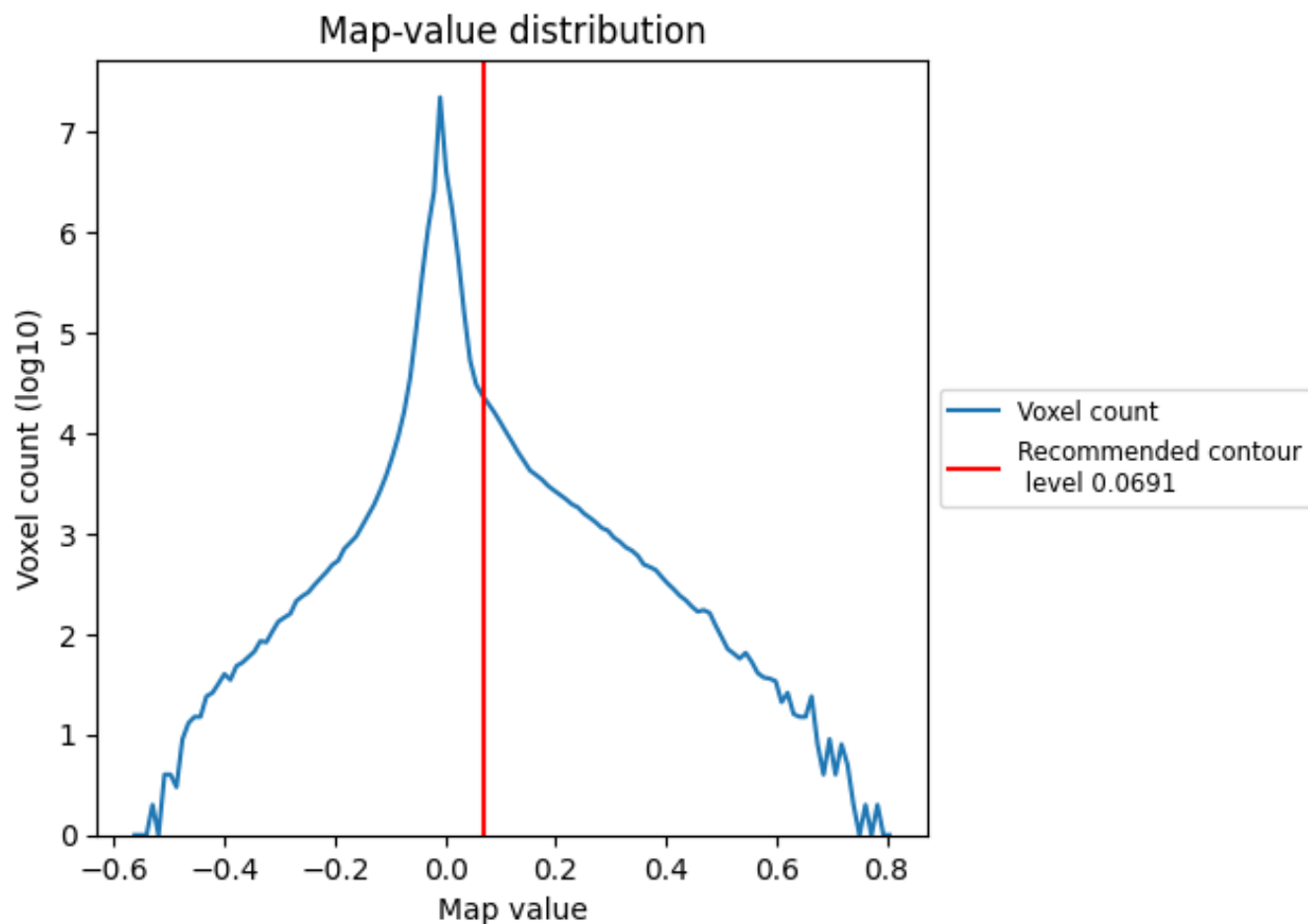
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

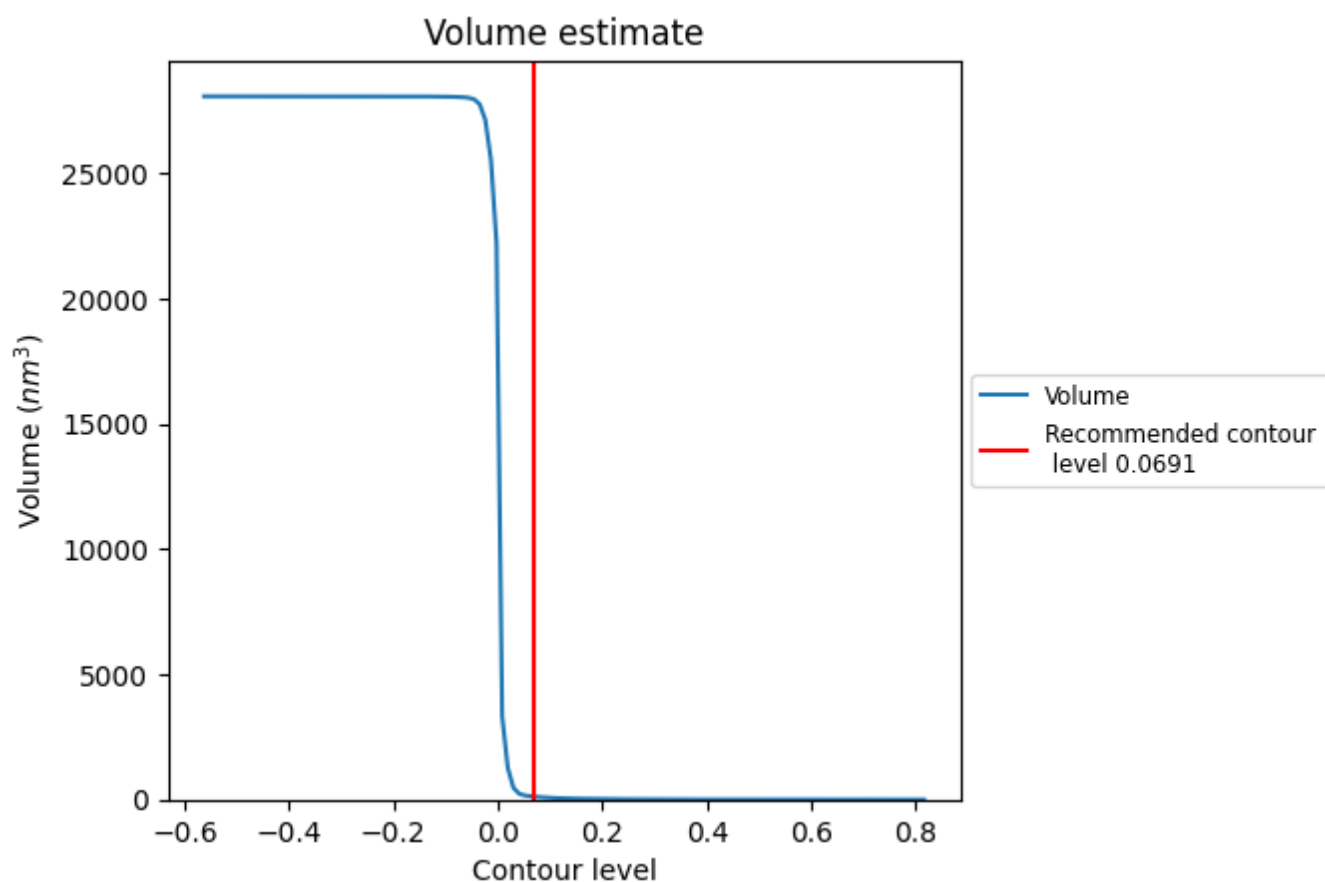
This section contains the results of statistical analysis of the map.

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.

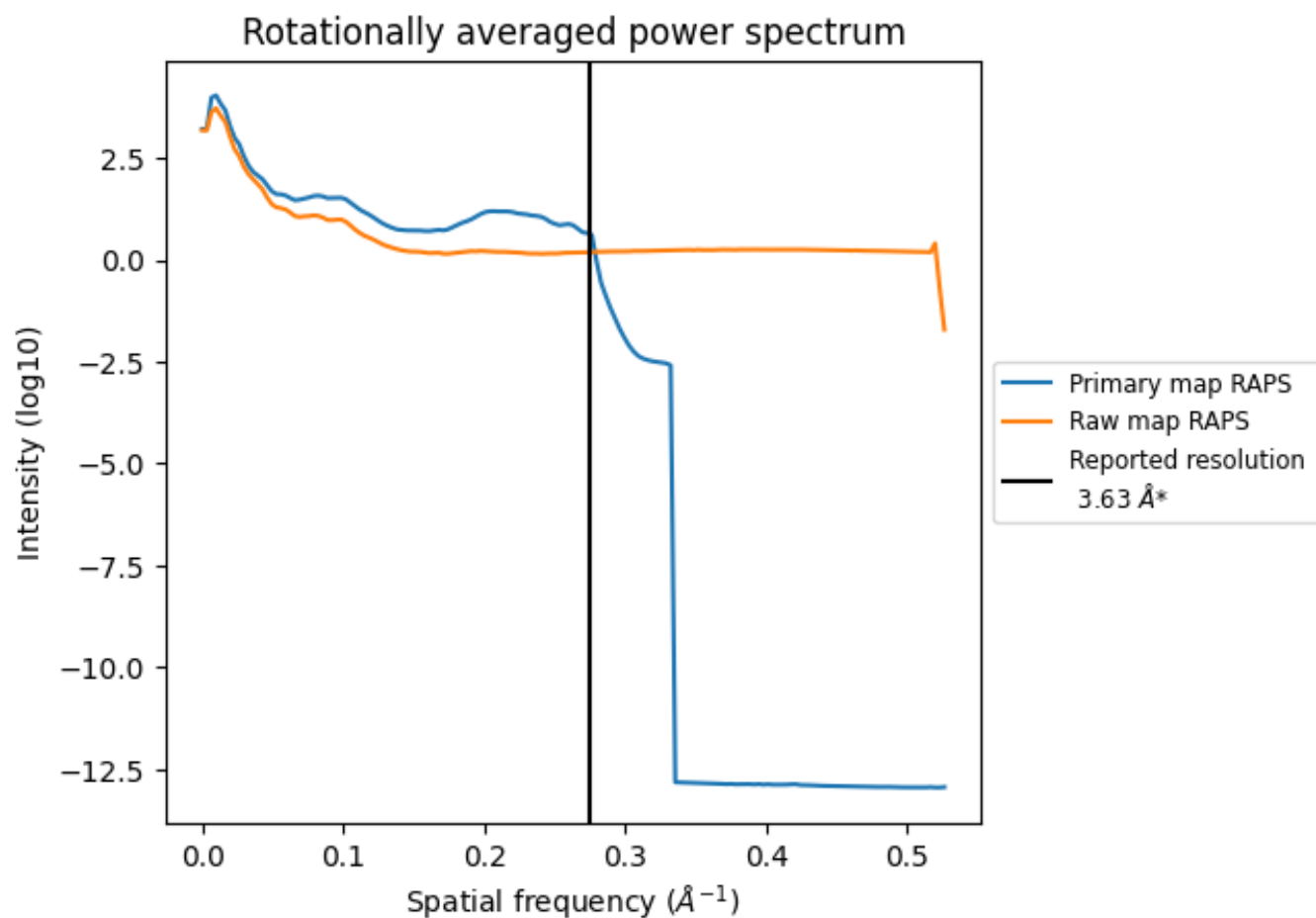
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 119 nm^3 ; this corresponds to an approximate mass of 107 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 ⓘ

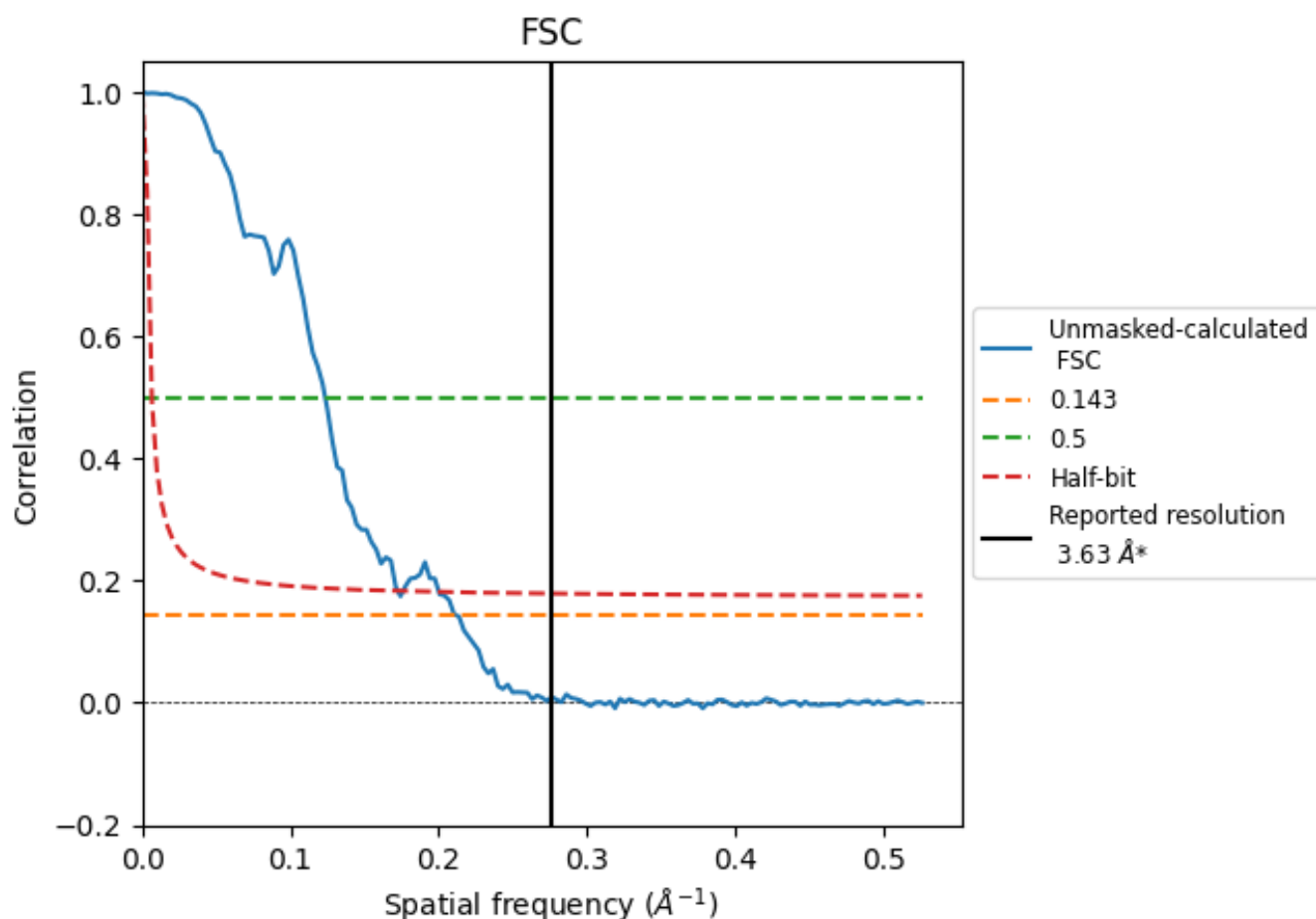


*Reported resolution corresponds to spatial frequency of 0.275 Å⁻¹

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 0.275 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

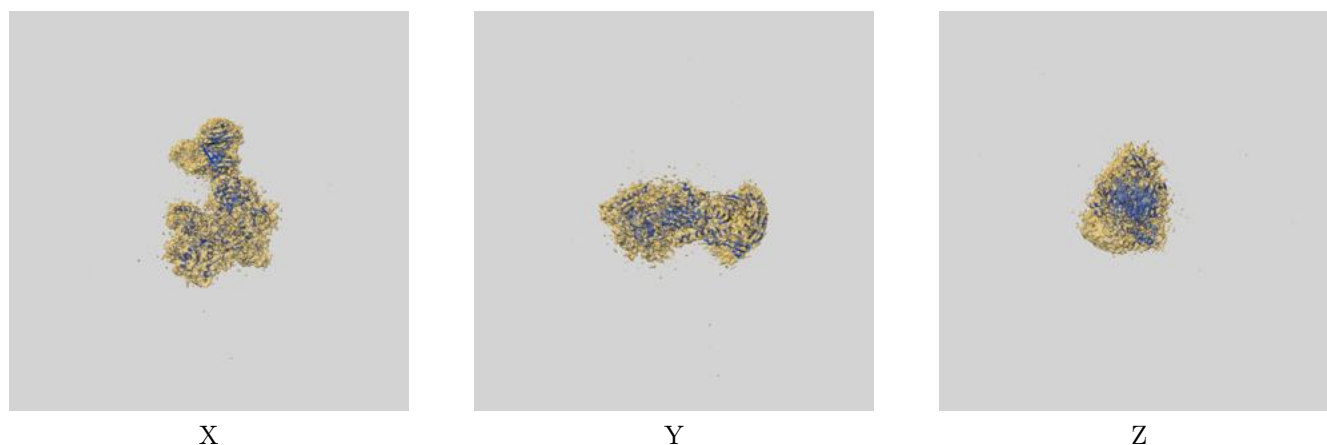
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.63	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.72	8.10	5.80

*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 4.72 differs from the reported value 3.63 by more than 10 %

9 Map-model fit [i](#)

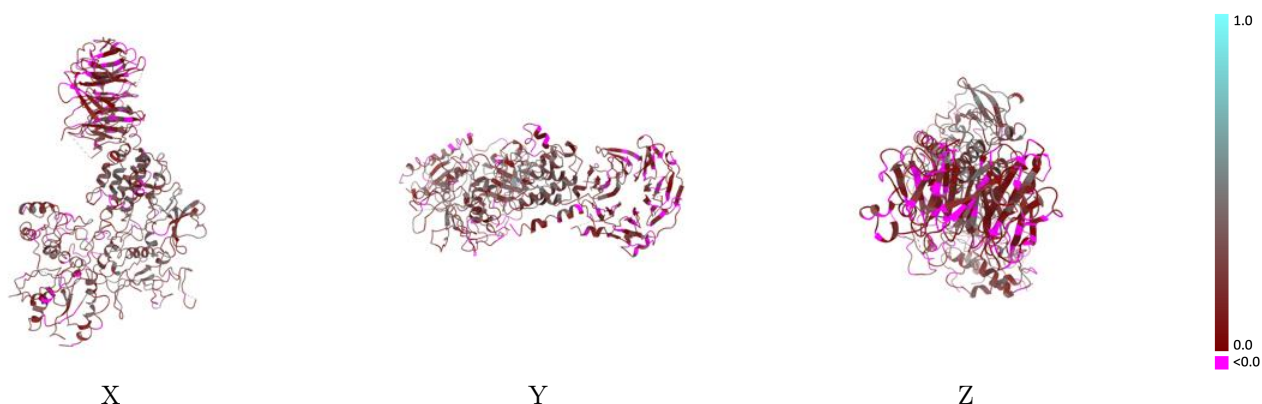
This section contains information regarding the fit between EMDB map EMD-72768 and PDB model 9YCD. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



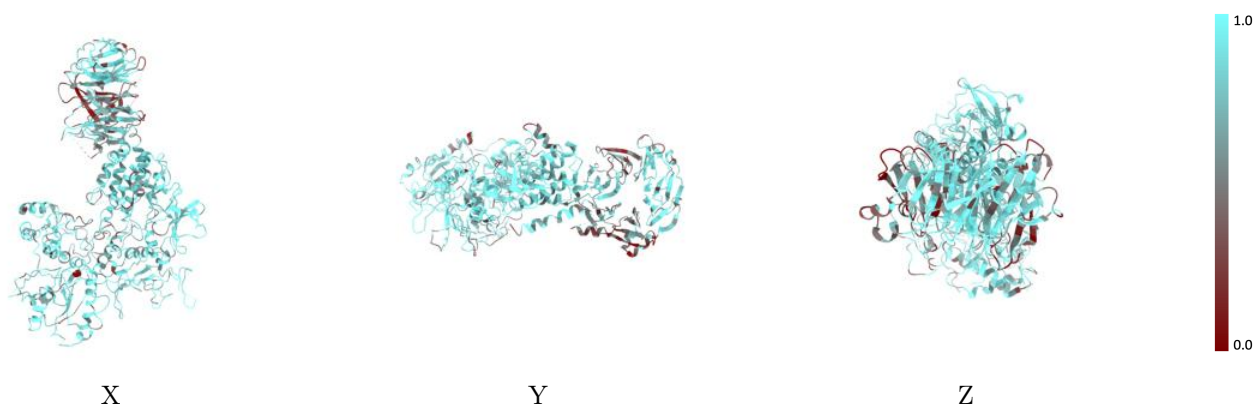
The images above show the 3D surface view of the map at the recommended contour level 0.0691 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



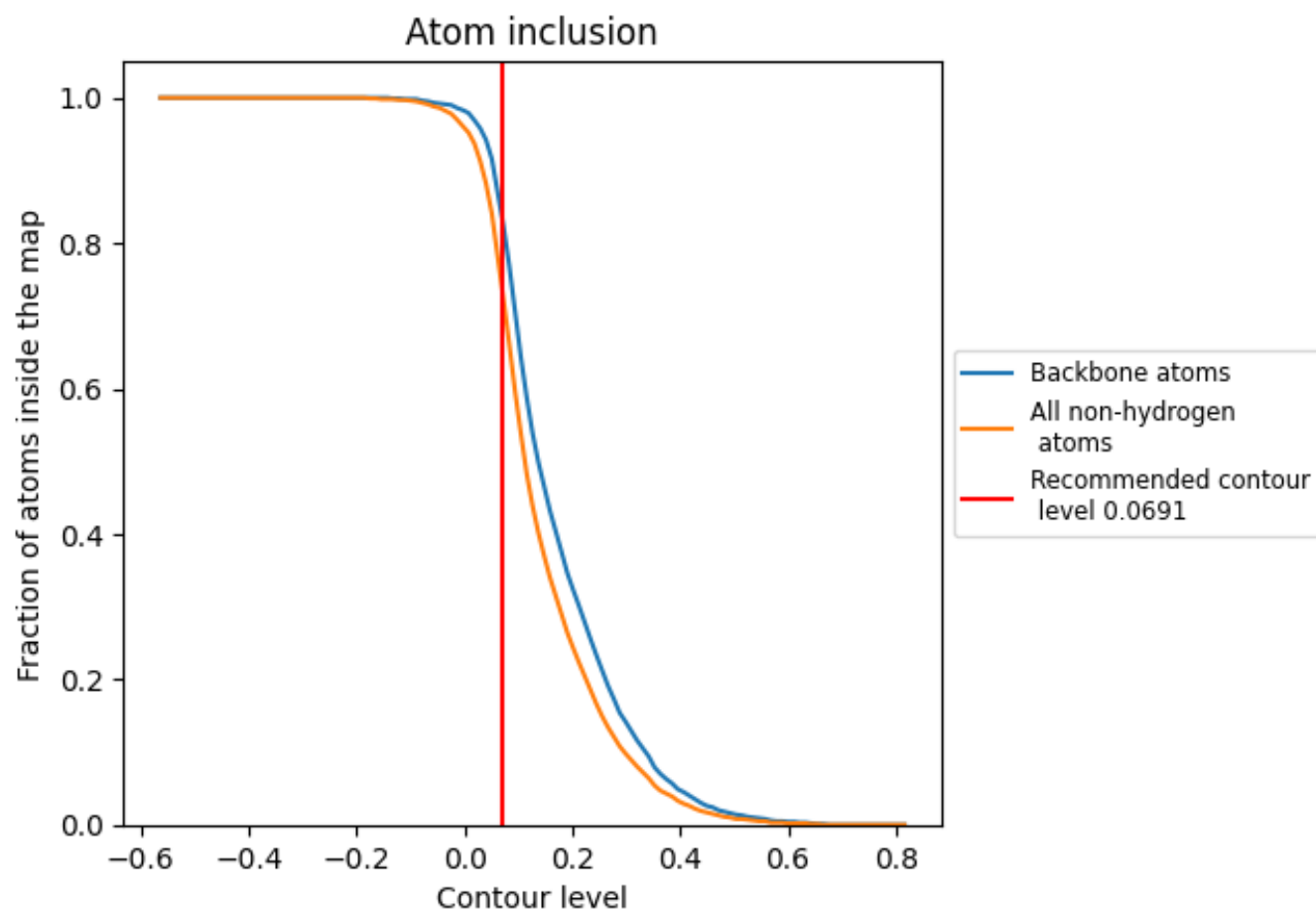
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0691).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 74% 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 (0.0691) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7430	0.2080
A	0.7430	0.2080

