



Full wwPDB EM Validation Report ⓘ

Aug 10, 2026 – 02:38 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 Full wwPDB EM Validation 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

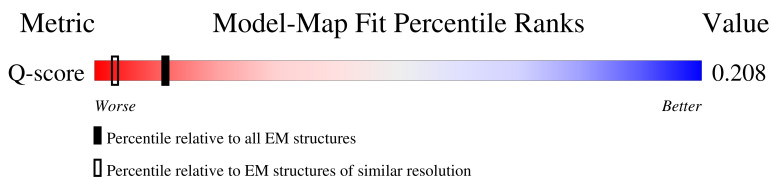
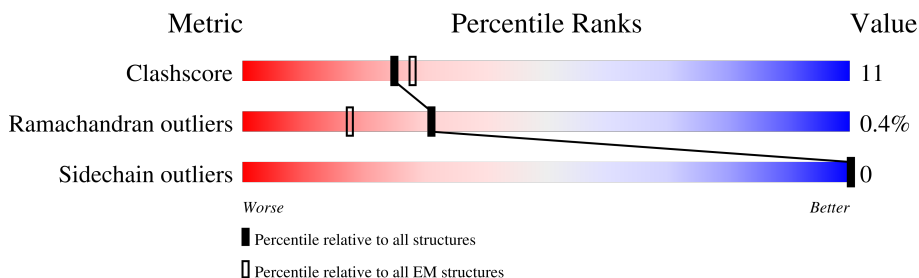
1 Overall quality at a glance

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.

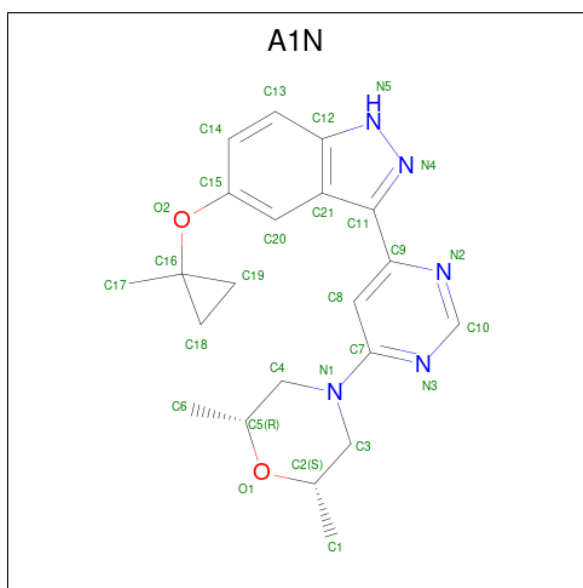
- Molecule 1 is a protein called Leucine-rich repeat serine/threonine-protein kinase 2.

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:

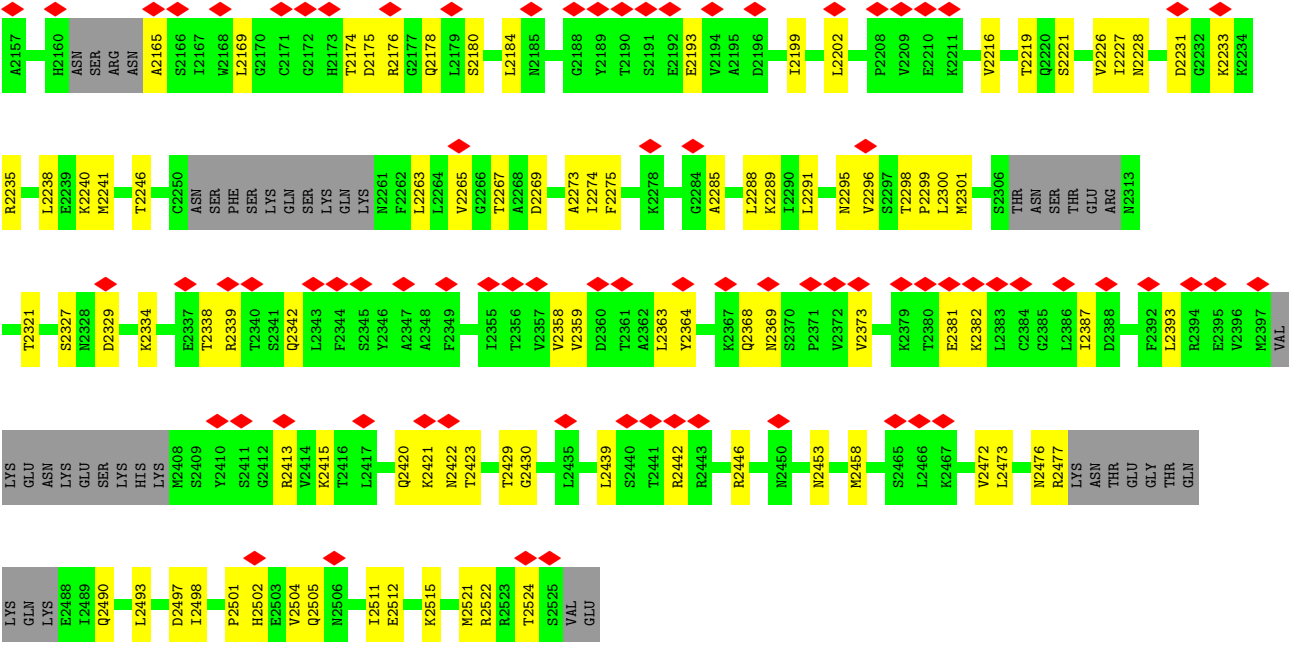
Chain	Residue	Modelled	Actual	Comment	Reference
A	1441	CYS	ARG	engineered mutation	UNP Q5S007

- 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	M1730	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	MET
S2058	M1944	D1828	M1732	K1643	VAL	Q1425	GLN	GLU	MET	SER	PRO	THR	THR	LEU	LEU	VAL
F2059	L1945	D1829	Y1733	M1646	GLY	E1426	ARG	GLY	SER	SER	LEU	THR	THR	GLN	GLN	ILE
L2063	V1946	L1830	Q1736	Y1649	Q1521	E1427	LEU	CYS	ASN	ASN	LEU	PRO	PHE	LYS	LYS	TYR
L1965	M1831	L1831	G1737	F1650	D1525	V1428	LYS	GLU	ILE	ASP	GLN	GLN	GLN	HIS	GLN	GLN
L1969	K1832	K1833	Y1738	K1651	E1529	D1429	LYS	GLU	ASP	ASP	GLN	GLN	GLN	MET	MET	SER
L2068	K1833	K1833	Y1739	F1651	E1530	A1430	ALA	ASN	GLN	GLN	GLN	GLN	GLN	ASN	ASN	ASN
L1970	L1840	L1840	L1740	L1652	E1531	T1438	VAL	LEU	TYR	LEU	ALA	ALA	ALA	ILE	ILE	ALA
Q1971	L1841	L1841	N1741	E1654	E1531	K1439	TYR	SER	PRO	GLY	TYR	TYR	TYR	ASP	VAL	VAL
H1972	N1842	N1842	W1742	E1655	I1532	L1449	ARG	ASP	PRO	GLY	ASN	ASN	THR	ILE	GLY	GLY
R1973	L1843	L1843	C1748	F1656	I1533	V1450	MET	VAL	PRO	ALA	LEU	LEU	LEU	SER	GLY	GLY
L1974	D1844	D1844	L1749	Q1657	I1534	D1455	LYS	VAL	HIS	ALA	SER	SER	SER	THR	THR	ALA
Q1945	Q1845	Q1845	V1750	I1658	L1535	V1456	LEU	TRP	TRP	LEU	LEU	LEU	LEU	TYR	TYR	ALA
PRO	PRO	PRO	G1751	A1659	R1538	S1457	M1338	ASN	LYS	LYS	PRO	HIS	HIS	ASP	ASP	SER
ARG	ARG	ARG	S1752	F1661	R1550	ASP	I1339	LEU	SER	SER	GLU	GLU	GLU	ALA	ALA	GLY
THR	THR	THR	H1758	I1662	R1552	GLY	V1340	GLU	LEU	ALA	ASP	ASP	ASP	LEU	LEU	SER
I1850	I1850	I1850	P1759	GLY	R1552	LYS	S1345	ARG	ASN	ARG	ASN	ASN	ASN	VAL	VAL	ASP
P1857	P1857	P1857	E1760	GLU	Q1555	GLN	T1357	SER	PRO	PHE	LEU	LEU	LEU	GLY	GLY	GLY
D1858	D1858	D1858	S1761	GLU	Q1555	R1462	LYS	GLY	LEU	ALA	VAL	VAL	VAL	ASP	ASP	ASP
L1859	L1859	L1859	F1762	R1677	Q1561	T1469	LYS	GLY	LEU	ALA	GLY	GLY	GLY	ASP	ASP	ASN
L1860	L1860	L1860	K1763	H1684	E1566	K1471	D1361	ASN	PHE	THR	THR	THR	THR	LEU	LEU	ASN
L1861	L1861	L1861	I1765	C1685	A1572	E1472	L1362	GLY	GLY	PRO	GLY	GLY	GLY	LEU	LEU	GLN
L1864	L1864	L1864	C1774	E1686	L1583	N1475	G1363	LEU	GLN	PHE	GLY	GLY	GLY	SER	SER	SER
P1865	P1865	P1865	V1780	E1689	L1583	K1476	M1364	LEU	ILE	LEU	GLN	GLN	GLN	ARG	ARG	LYS
R1866	R1866	R1866	G1781	E1689	L1583	R1477	Q1365	SER	ILE	PRO	ILE	ILE	ILE	ASN	PHE	PHE
L1885	L1885	L1885	D1782	E1689	L1583	R1477	S1366	LYS	ILE	PRO	ILE	ILE	ILE	ASN	ASN	ASN
S1889	S1889	S1889	D1785	I1692	D1587	A1481	D1372	GLY	LEU	LEU	LEU	LEU	LEU	GLY	GLY	VAL
F1890	F1890	F1890	S1786	R1693	D1587	T1482	V1373	ASN	ASP	ASP	GLY	GLY	GLY	ASN	ASN	ASN
L1787	L1787	L1787	L1787	L1694	Q1591	R1483	D1372	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL
E1790	E1790	E1790	M1697	L1592	Q1591	D1484	W1376	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL
R1893	R1893	R1893	P1701	S1593	L1592	Y1485	F1377	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL
Y1894	Y1894	Y1894	P1701	D1594	S1593	F1486	I1378	LEU	ALA	SER	ILE	ILE	ILE	ASP	ASP	ASP
R1895	R1895	R1895	F1704	P1600	D1594	F1487	Q1379	TYR	TYR	GLN	ASN	ASN	ASN	HIS	HIS	SER
E1902	E1902	E1902	W1705	P1600	P1600	V1488	I1380	TRP	LEU	ASN	LYS	LYS	LYS	GLY	GLY	MET
V1905	V1905	V1905	S1706	L1603	L1603	N1489	R1381	SER	TRP	ASP	CYS	CYS	CYS	ASP	ASP	ASP
K1906	K1906	K1906	W1706	C1604	C1604	PHE	ASP	ASN	SER	PHE	VAL	VAL	VAL	LEU	LEU	SER
I1907	I1907	I1907	I1709	K1605	K1605	A1490	LYS	ASN	ARG	ARG	ARG	ARG	ARG	LEU	LEU	VAL
T1912	T1912	T1912	M1710	G1605	G1605	K1496	R1386	LYS	VAL	ILE	LYS	LYS	LYS	ARG	ARG	ALA
S1913	S1913	S1913	R1711	I1610	I1610	L1497	D1387	ASN	GLU	ILE	LEU	LEU	LEU	VAL	VAL	GLN
L1914	L1914	L1914	L1712	L1611	L1611	A1498	I1388	GLY	LEU	GLY	LEU	LEU	LEU	ARG	ARG	ALA
R1915	R1915	R1915	L1713	L1611	L1611	L1500	W1389	ILE	LEU	ALA	LEU	LEU	LEU	ASP	ASP	GLN
T1806	T1806	T1806	S1716	G1617	G1617	R1501	L1390	LYS	TRP	PRO	GLY	GLY	GLY	ILE	ILE	SER
W1811	W1811	W1811	Y1716	H1621	H1621	T1504	W1393	ASN	LEU	LEU	LEU	LEU	LEU	GLY	GLY	ASN
A1812	A1812	A1812	S1721	H1621	H1621	E1507	W1393	LYS	ALA	LEU	ASN	ASN	ASN	LEU	LEU	LYS
L1813	L1813	L1813	G1722	P1622	P1622	E1507	A1413	ASP	VAL	PRO	VAL	VAL	VAL	ASP	ASP	GLY
F1816	F1816	F1816	R1723	I1626	I1626	F1511	A1413	ILE	ASP	HIS	LEU	LEU	LEU	GLY	GLY	GLY
H1822	H1822	H1822	GLU	I1626	I1626	R1514	V1418	THR	ILE	LEU	LEU	LEU	LEU	ASP	ASP	SER
Q1823	Q1823	Q1823	ARG	K1633	K1633	D1515	D1420	VAL	GLU	ARG	ASN	ASN	ASN	LEU	LEU	GLY
L1940	L1940	L1940	A1726	K1633	K1633	R1514	Y1419	THR	GLU	THR	LEU	LEU	LEU	SER	SER	SER
R1941	R1941	R1941	L1727	K1637	K1637	D1515	D1420	VAL	ILE	VAL	GLN	GLN	GLN	ARG	ARG	ARG



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

5.1 Standard geometry

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

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.

All (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
1:A:1740:LEU:HB2	1:A:1748:CYS:HB3	1.79	0.64
1:A:1693:ARG:O	1:A:1764:LYS:HA	1.97	0.64
1:A:2512:GLU:OE1	1:A:2515:LYS:NZ	2.30	0.64
1:A:2358:VAL:HB	1:A:2364:TYR:HB2	1.79	0.63
1:A:2146:LEU:O	1:A:2490:GLN:NE2	2.29	0.63
1:A:1976:LEU:HD21	1:A:2511:ILE:HD11	1.81	0.62
1:A:2246:THR:OG1	1:A:2300:LEU:O	2.15	0.62
1:A:1750:VAL:HG22	1:A:1765:ILE:HG12	1.81	0.62
1:A:1864:LEU:O	1:A:1866:ARG:NH2	2.33	0.61
1:A:1730:ASN:HB2	1:A:1741:ASN:HB3	1.83	0.61
1:A:2453:ASN:ND2	1:A:2477:ARG:O	2.35	0.60
1:A:2174:THR:OG1	1:A:2176:ARG:NH1	2.34	0.60
1:A:1481:ALA:O	1:A:1483:ARG:NH1	2.34	0.59
1:A:2263:LEU:HB3	1:A:2275:PHE:HB2	1.83	0.59
1:A:1701:PRO:HG2	1:A:1704:PHE:HB2	1.84	0.59
1:A:2051:ASN:OD1	1:A:2052:GLN:N	2.35	0.59
1:A:2373:VAL:HB	1:A:2387:ILE:HB	1.85	0.59
1:A:1529:GLU:HA	1:A:1532:LYS:HD3	1.85	0.58
1:A:1813:LEU:HD12	1:A:1822:HIS:HB3	1.86	0.58
1:A:1498:ALA:O	1:A:1501:ARG:HB2	2.05	0.57
1:A:1489:ASN:ND2	1:A:1490:ALA:H	2.00	0.57
1:A:1677:ARG:NH2	1:A:1752:SER:O	2.37	0.57
1:A:2321:THR:O	1:A:2338:THR:OG1	2.22	0.57
1:A:1928:HIS:HD2	1:A:2521:MET:HG3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1449:LEU:HB2	1:A:1482:ILE:HD11	1.87	0.56
1:A:2147:PRO:HG2	1:A:2150:VAL:HG21	1.88	0.56
1:A:1812:ALA:HB2	1:A:1827:LEU:HD12	1.86	0.56
1:A:1652:LEU:HA	1:A:1655:LYS:HB3	1.87	0.56
1:A:1713:LEU:HA	1:A:1716:SER:HB2	1.87	0.56
1:A:1840:LEU:HG	1:A:1841:VAL:HG23	1.88	0.56
1:A:2067:LEU:HD13	1:A:2104:TRP:HE3	1.71	0.56
1:A:1497:LEU:O	1:A:1500:LEU:HB3	2.06	0.56
1:A:1677:ARG:NH2	1:A:1736:GLN:O	2.38	0.55
1:A:1692:ILE:HB	1:A:1813:LEU:HB2	1.88	0.55
1:A:1785:ASP:HB3	1:A:1915[B]:ARG:HE	1.71	0.55
1:A:1912:THR:OG1	1:A:1913:SER:N	2.39	0.55
1:A:2129:PHE:O	1:A:2133:ASN:HB2	2.07	0.55
1:A:1552:ARG:HA	1:A:1555:GLN:HG2	1.89	0.55
1:A:1654:GLU:O	1:A:1657:GLN:NE2	2.40	0.55
1:A:1830:LEU:HA	1:A:1833:LYS:HE3	1.87	0.55
1:A:2274:ILE:HB	1:A:2289:LYS:HG2	1.89	0.55
1:A:1861:LEU:HD13	1:A:1940:ILE:HD13	1.89	0.54
1:A:1913:SER:O	1:A:1943:ARG:NH2	2.37	0.53
1:A:2043:VAL:HG22	1:A:2050:TYR:CZ	2.44	0.53
1:A:2265:VAL:HB	1:A:2273:ALA:HB3	1.89	0.53
1:A:1711:ARG:HG3	1:A:1787:LEU:HD21	1.92	0.52
1:A:1905:VAL:HG12	1:A:1946:VAL:HG23	1.92	0.52
1:A:2269:ASP:HA	1:A:2296:VAL:HA	1.92	0.52
1:A:2387:ILE:HA	1:A:2442:ARG:HH21	1.73	0.52
1:A:1907:ILE:HD12	1:A:1944:MET:HB3	1.90	0.52
1:A:1969:THR:O	1:A:1973:ARG:HG2	2.10	0.52
1:A:1697:MET:O	1:A:1761:SER:OG	2.24	0.52
1:A:1709:ILE:HG13	1:A:1738:ILE:HD11	1.93	0.52
1:A:1811:TRP:HZ2	1:A:1824:LYS:HG2	1.75	0.51
1:A:1372:ASP:OD1	1:A:1373:VAL:N	2.43	0.51
1:A:1864:LEU:HD12	1:A:1865:PRO:HD2	1.92	0.51
1:A:2423:THR:HG23	1:A:2439:LEU:HB2	1.91	0.51
1:A:1955:LEU:HD21	1:A:2066:ILE:HD12	1.92	0.51
1:A:1978:VAL:HG13	1:A:2059:PHE:HE1	1.76	0.51
1:A:1782:ASP:HB2	1:A:1915[A]:ARG:HH22	1.75	0.51
1:A:1654:GLU:HB2	1:A:1660:LEU:HD21	1.91	0.51
1:A:1971:GLN:HG2	1:A:2066:ILE:HG12	1.92	0.50
1:A:2267:THR:OG1	1:A:2269:ASP:OD1	2.29	0.50
1:A:1859:LEU:HA	1:A:1914:LEU:HD21	1.94	0.50
1:A:1864:LEU:HD13	1:A:1921:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1895:ARG:NE	1:A:1902:GLU:OE2	2.44	0.50
1:A:1373:VAL:HG23	1:A:1393:TRP:HA	1.94	0.49
1:A:1971:GLN:NE2	1:A:2066:ILE:HG23	2.27	0.49
1:A:1733:TYR:HD1	1:A:1738:ILE:HD12	1.78	0.49
1:A:2169:LEU:HB3	1:A:2180:SER:HB2	1.95	0.49
1:A:2199:ILE:HA	1:A:2219:THR:HA	1.94	0.49
1:A:1841:VAL:O	1:A:1850:ILE:N	2.46	0.48
1:A:2453:ASN:HD22	1:A:2477:ARG:HB3	1.78	0.48
1:A:1550:ARG:HE	1:A:1594:ASP:HA	1.78	0.48
1:A:1583:LEU:HD23	1:A:1600:PRO:HG3	1.96	0.48
1:A:1684:HIS:CE1	1:A:1686:GLU:HB3	2.48	0.48
1:A:2155:MET:HA	1:A:2202:LEU:HD12	1.95	0.48
1:A:1489:ASN:HD22	1:A:1490:ALA:H	1.62	0.48
1:A:2274:ILE:O	1:A:2288:LEU:N	2.47	0.48
1:A:1993:ARG:NH1	1:A:2022:GLN:OE1	2.38	0.47
1:A:1705:TRP:HE3	1:A:1709:ILE:HD11	1.80	0.47
1:A:2106:MET:HA	1:A:2109:LYS:HD3	1.96	0.47
1:A:2221:SER:O	1:A:2240:LYS:NZ	2.43	0.47
1:A:1377:PRO:HA	1:A:1390:LEU:H	1.80	0.47
1:A:1997:PRO:HG2	1:A:2073:ILE:HD11	1.96	0.47
1:A:2069:THR:OG1	1:A:2070:GLY:N	2.40	0.47
1:A:2155:MET:HE2	1:A:2493:LEU:HD21	1.97	0.47
1:A:2076:GLY:HA3	1:A:2083:PHE:HD1	1.80	0.47
1:A:2128:VAL:HA	1:A:2131:ILE:HD12	1.97	0.47
1:A:2175:ASP:OD1	1:A:2176:ARG:N	2.48	0.47
1:A:2216:VAL:HG22	1:A:2226:VAL:HG22	1.97	0.47
1:A:2415:LYS:HE2	1:A:2430:GLY:HA2	1.97	0.47
1:A:1927:LEU:HA	1:A:2522:ARG:HH12	1.79	0.46
1:A:2041:PRO:HD3	1:A:2057:TYR:HE2	1.81	0.46
1:A:2142:ARG:NH1	1:A:2184:LEU:O	2.36	0.46
1:A:2327:SER:OG	1:A:2329:ASP:OD1	2.32	0.46
1:A:2476:ASN:HB3	1:A:2490:GLN:HB3	1.95	0.46
1:A:2334:LYS:HE2	1:A:2381:GLU:HG3	1.97	0.46
1:A:1920:GLU:HG2	1:A:1945:LEU:HD11	1.97	0.46
1:A:1994:ASP:OD1	1:A:2035:THR:N	2.48	0.46
1:A:1439:LYS:HZ1	1:A:1477:ARG:HH11	1.63	0.46
1:A:2497:ASP:OD1	1:A:2498:ILE:N	2.49	0.46
1:A:2289:LYS:HE2	1:A:2291:LEU:HD21	1.97	0.45
1:A:2458:MET:HG2	1:A:2472:VAL:HG22	1.98	0.45
1:A:2521:MET:HA	1:A:2524:THR:HG22	1.97	0.45
1:A:1928:HIS:O	1:A:2522:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1530:LEU:HA	1:A:1533:ILE:HG22	1.98	0.45
1:A:2063:LEU:HA	1:A:2066:ILE:HG22	1.99	0.45
1:A:2369:ASN:HA	1:A:2413:ARG:HG3	1.99	0.45
1:A:1340:VAL:HG21	1:A:1438:ILE:HD11	1.99	0.45
1:A:1535:LEU:HA	1:A:1538:ARG:HH11	1.82	0.45
1:A:1993:ARG:NH2	1:A:2033:GLU:OE1	2.49	0.45
1:A:2155:MET:HE1	1:A:2473:LEU:HB2	1.99	0.44
1:A:1811:TRP:CZ2	1:A:1824:LYS:HG2	2.52	0.44
1:A:2420:GLN:NE2	1:A:2498:ILE:HG13	2.32	0.44
1:A:2241:MET:HG2	1:A:2267:THR:HG21	2.00	0.44
1:A:1489:ASN:HD21	1:A:1497:LEU:HD13	1.82	0.44
1:A:2421:LYS:HE2	1:A:2421:LYS:HB2	1.82	0.44
1:A:1552:ARG:HG3	1:A:1555:GLN:HE21	1.81	0.44
1:A:1860:ILE:HB	1:A:1940:ILE:HG21	1.99	0.44
1:A:1986:HIS:ND1	1:A:2052:GLN:OE1	2.44	0.44
1:A:1790:GLU:HA	1:A:2031:THR:HG23	2.00	0.44
1:A:1971:GLN:HE21	1:A:2066:ILE:HG23	1.83	0.44
1:A:2382:LYS:HE3	1:A:2382:LYS:HA	1.99	0.44
1:A:2041:PRO:HD3	1:A:2057:TYR:CE2	2.52	0.43
1:A:1425:GLN:HE22	1:A:1469:ILE:HD12	1.83	0.43
1:A:2393:LEU:HD11	1:A:2429:THR:HG21	2.01	0.43
1:A:2107:VAL:HG22	1:A:2137:LEU:HD23	2.01	0.43
1:A:1885:LEU:HB2	1:A:1893:VAL:HG13	2.01	0.43
1:A:1993:ARG:NH1	1:A:2031:THR:OG1	2.38	0.43
1:A:2233:LYS:H	1:A:2233:LYS:HG2	1.59	0.43
1:A:1829:ASP:C	1:A:1831:MET:H	2.27	0.42
1:A:1959:LEU:HD22	1:A:2069:THR:HA	2.01	0.42
1:A:2165:ALA:HB1	1:A:2184:LEU:HD12	2.01	0.42
1:A:2295:ASN:H	1:A:2298:THR:HG1	1.64	0.42
1:A:1989:MET:HB2	1:A:2025:CYS:HB2	2.01	0.42
1:A:1991:ILE:HG12	1:A:1993:ARG:HB3	2.02	0.42
1:A:2227:ILE:HG23	1:A:2235:ARG:HG2	2.00	0.42
1:A:2502:HIS:HA	1:A:2505:GLN:NE2	2.34	0.42
1:A:1689:GLU:N	1:A:1689:GLU:OE1	2.51	0.42
1:A:1423:LYS:HB2	1:A:1427:GLU:HB2	2.01	0.42
1:A:1653:LEU:HD12	1:A:1658:ILE:HB	2.02	0.42
1:A:1732:MET:SD	1:A:1739:TYR:HB3	2.60	0.42
1:A:1942:PRO:HB2	1:A:1944:MET:HG2	2.01	0.42
1:A:1488:VAL:HG21	1:A:1496:ALA:HB3	2.01	0.42
1:A:1694:LEU:HA	1:A:1763:LEU:O	2.20	0.42
1:A:2299:PRO:HG2	1:A:2301:MET:SD	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1345:SER:H	1:A:1420:ASP:HB2	1.84	0.42
1:A:1710:ASN:C	1:A:1710:ASN:HD22	2.28	0.42
1:A:2422:ASN:HD21	1:A:2501:PRO:HB2	1.85	0.41
1:A:1425:GLN:HA	1:A:1428:VAL:HG12	2.01	0.41
1:A:2035:THR:HB	1:A:2038:PHE:HB2	2.03	0.41
1:A:2339:ARG:NH1	1:A:2342:GLN:OE1	2.44	0.41
1:A:1455:ASP:OD1	1:A:1456:VAL:N	2.54	0.41
1:A:1750:VAL:HG21	1:A:1780:VAL:HG11	2.03	0.41
1:A:2238:LEU:HD22	1:A:2285:ALA:HB3	2.01	0.41
1:A:1583:LEU:HD21	1:A:1603:LEU:HG	2.03	0.41
1:A:1711:ARG:NH2	1:A:2023:TYR:O	2.53	0.41
1:A:1504:ILE:HA	1:A:1507:GLU:HG2	2.02	0.41
1:A:1774:CYS:HB3	1:A:1857:PRO:HG3	2.02	0.41
1:A:2178:GLN:HG3	1:A:2193:GLU:HA	2.02	0.41
1:A:1471:LYS:O	1:A:1475:ASN:ND2	2.54	0.41
1:A:1758:HIS:O	1:A:1758:HIS:ND1	2.52	0.41
1:A:2359:VAL:HA	1:A:2363:LEU:HD13	2.02	0.41
1:A:2056:VAL:O	1:A:2059:PHE:HB3	2.21	0.41
1:A:2446:ARG:HG3	1:A:2504:VAL:HG21	2.03	0.40
1:A:1970:LEU:HD12	1:A:2007:PRO:HG3	2.02	0.40
1:A:2368:GLN:OE1	1:A:2369:ASN:N	2.53	0.40
1:A:1376:TRP:NE1	1:A:1378:ILE:HD11	2.36	0.40
1:A:1760:GLU:OE1	1:A:1760:GLU:N	2.51	0.40
1:A:2110:LEU:HD13	1:A:2131:ILE:HG21	2.03	0.40
1:A:2228:ASN:HB3	1:A:2231:ASP:HB3	2.03	0.40
1:A:2502:HIS:HA	1:A:2505:GLN:HE22	1.86	0.40

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
1	A	1345	SER

5.3.2 Protein sidechains ⓘ

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. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1425	GLN
1	A	1657	GLN
1	A	1977	HIS
1	A	2047	ASN
1	A	2313	ASN
1	A	2453	ASN
1	A	2510	HIS

5.3.3 RNA ⓘ

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](#)

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.

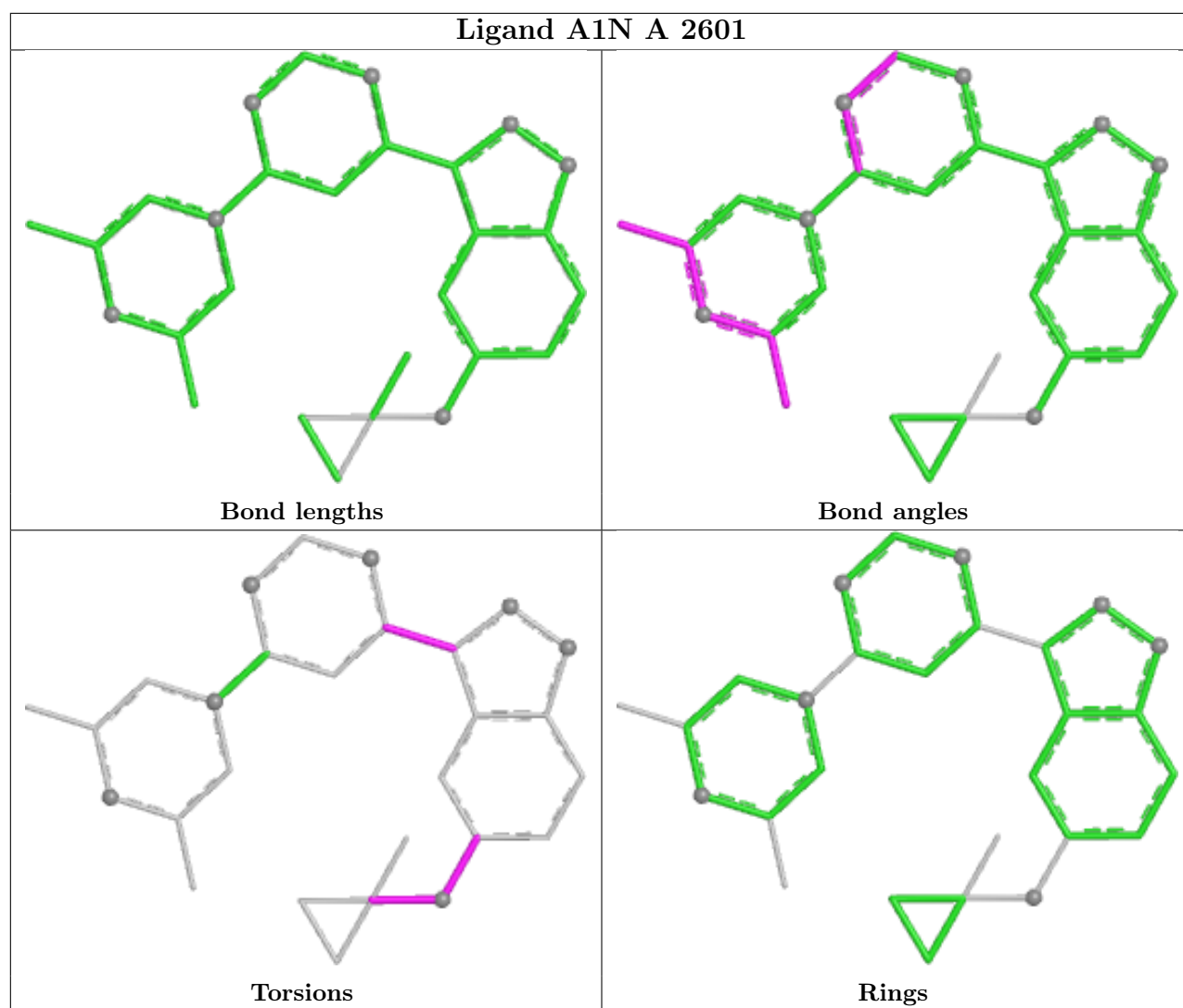
All (6) torsion outliers are listed below:

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
2	A	2601	A1N	C19-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 [i](#)

There are no chain breaks in this entry.

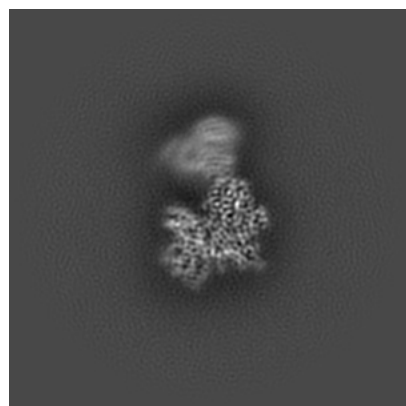
6 Map visualisation [i](#)

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.

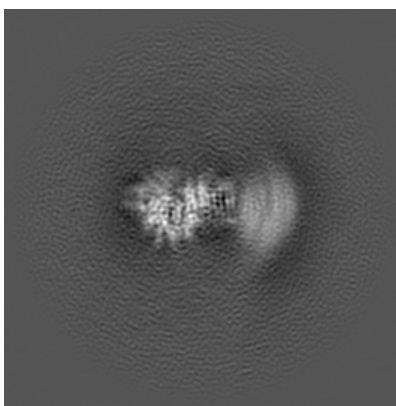
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

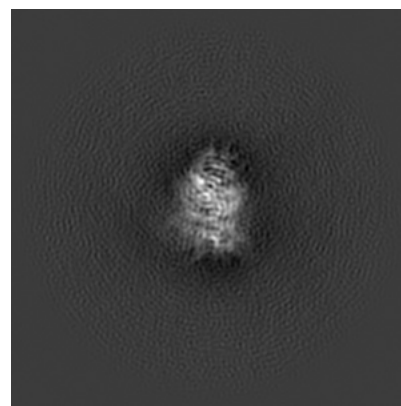
6.1.1 Primary map



X

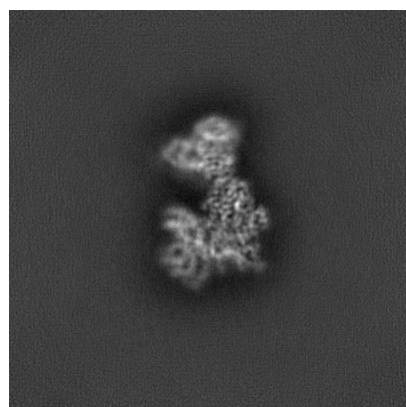


Y

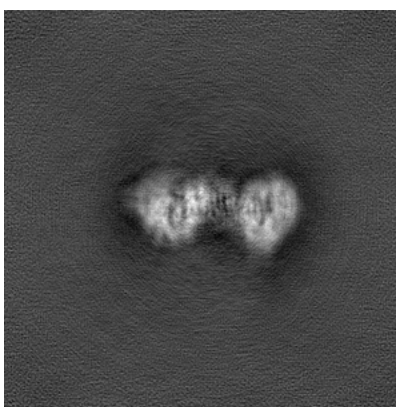


Z

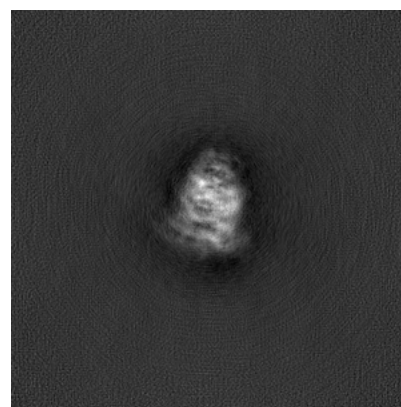
6.1.2 Raw map



X



Y

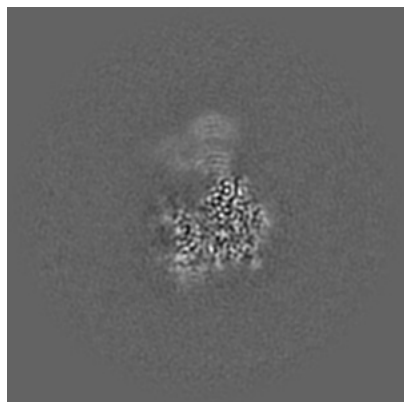


Z

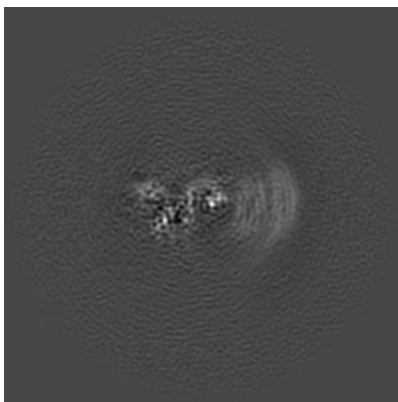
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

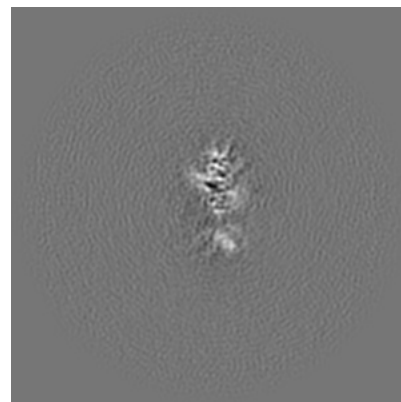
6.2.1 Primary map



X Index: 160

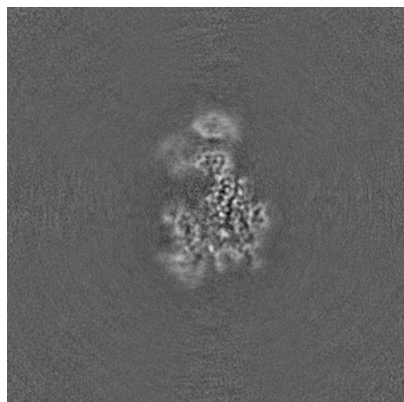


Y Index: 160

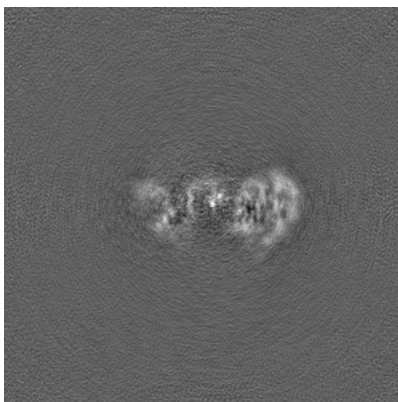


Z Index: 160

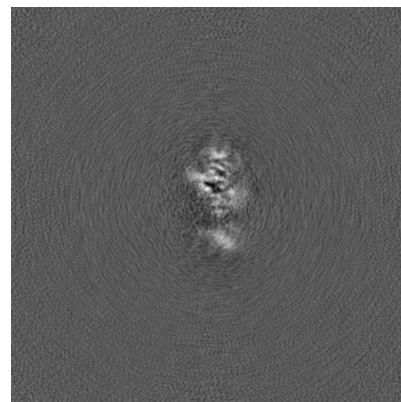
6.2.2 Raw map



X Index: 160



Y Index: 160

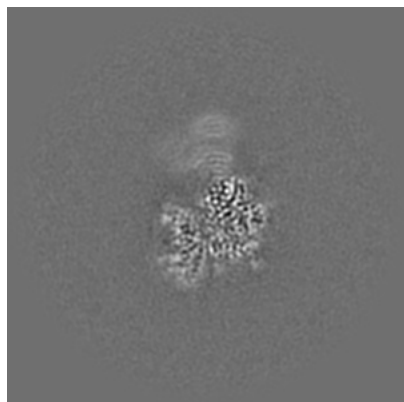


Z Index: 160

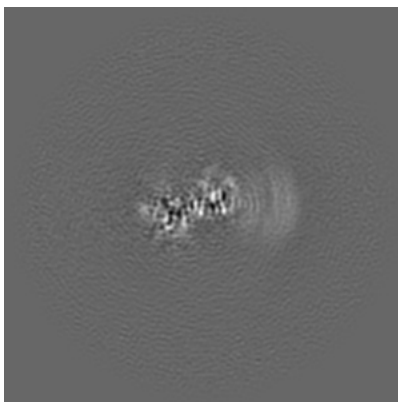
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

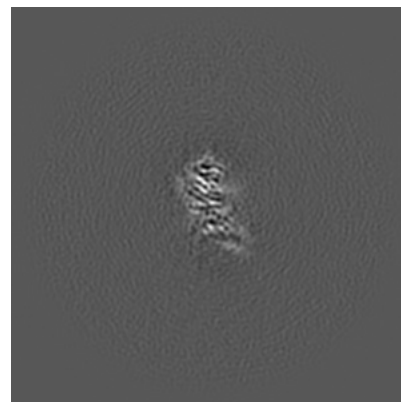
6.3.1 Primary map



X Index: 162

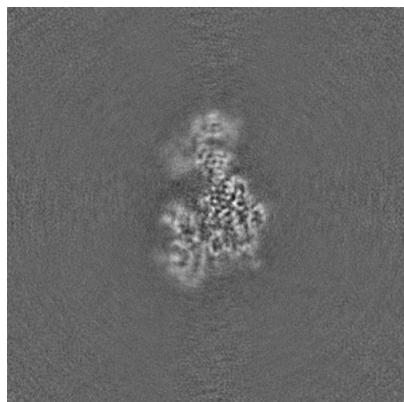


Y Index: 170

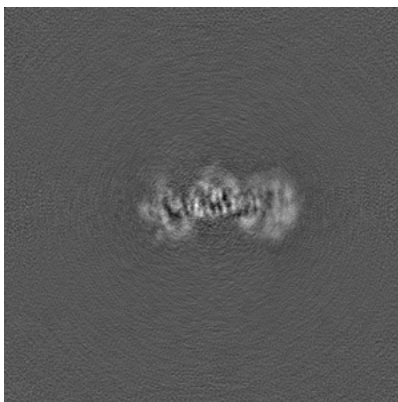


Z Index: 126

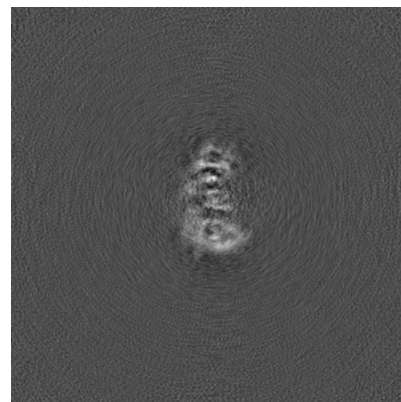
6.3.2 Raw map



X Index: 163



Y Index: 171

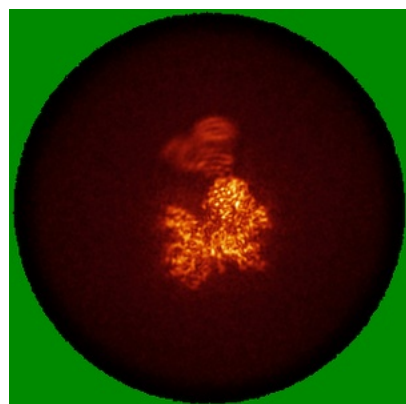


Z Index: 148

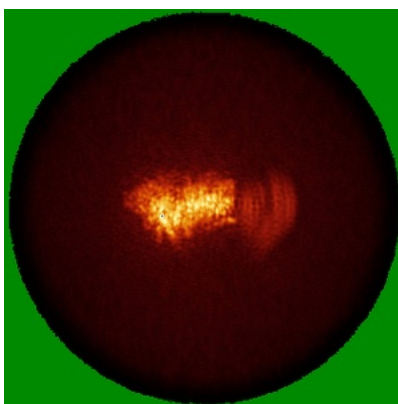
The images above show the largest variance slices of the map in three orthogonal directions.

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

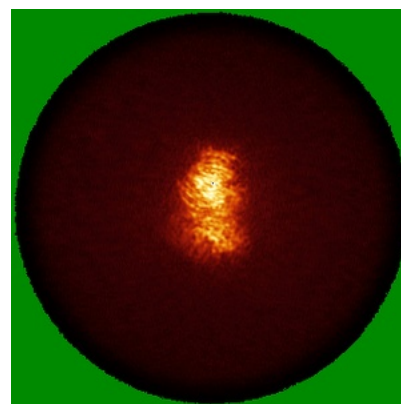
6.4.1 Primary map



X

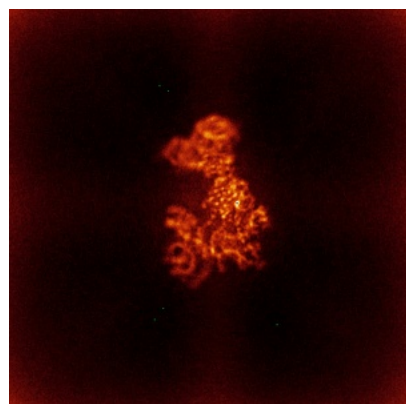


Y

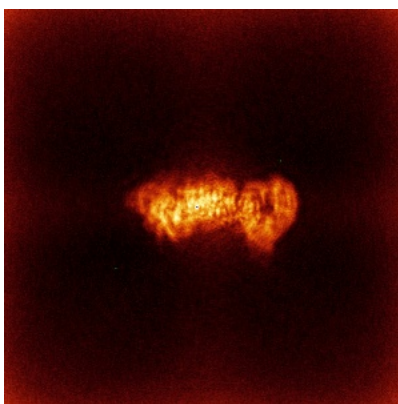


Z

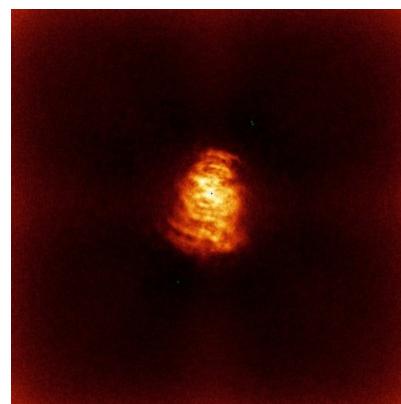
6.4.2 Raw map



X



Y

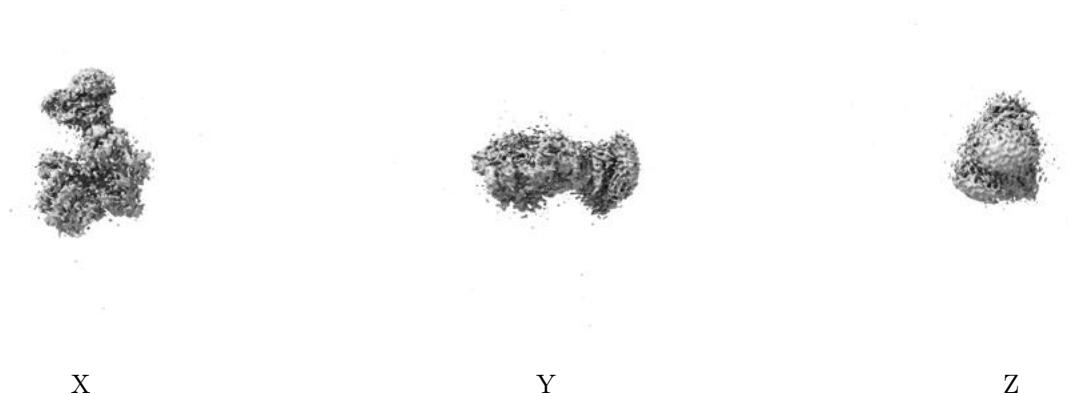


Z

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.

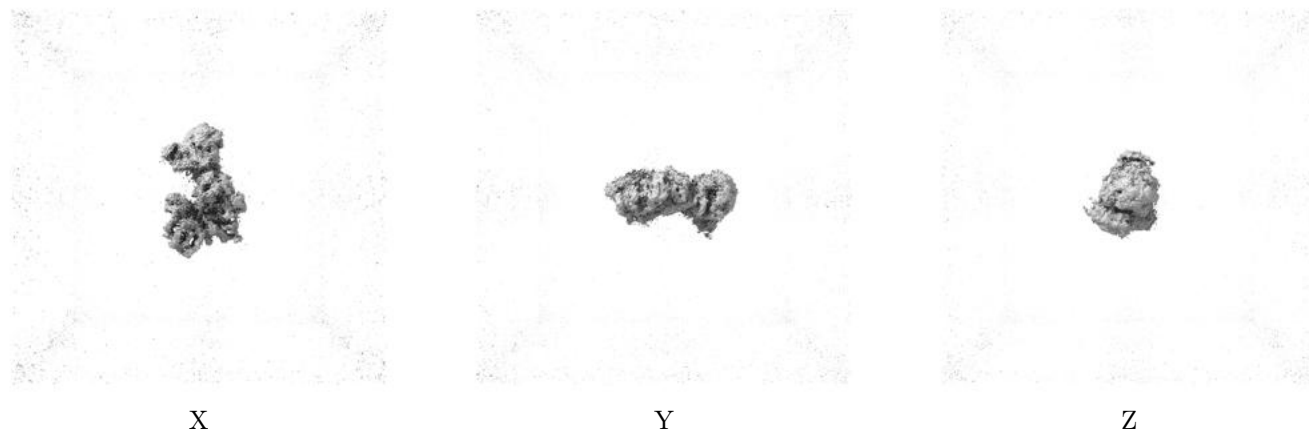
6.5 Orthogonal surface views [i](#)

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.

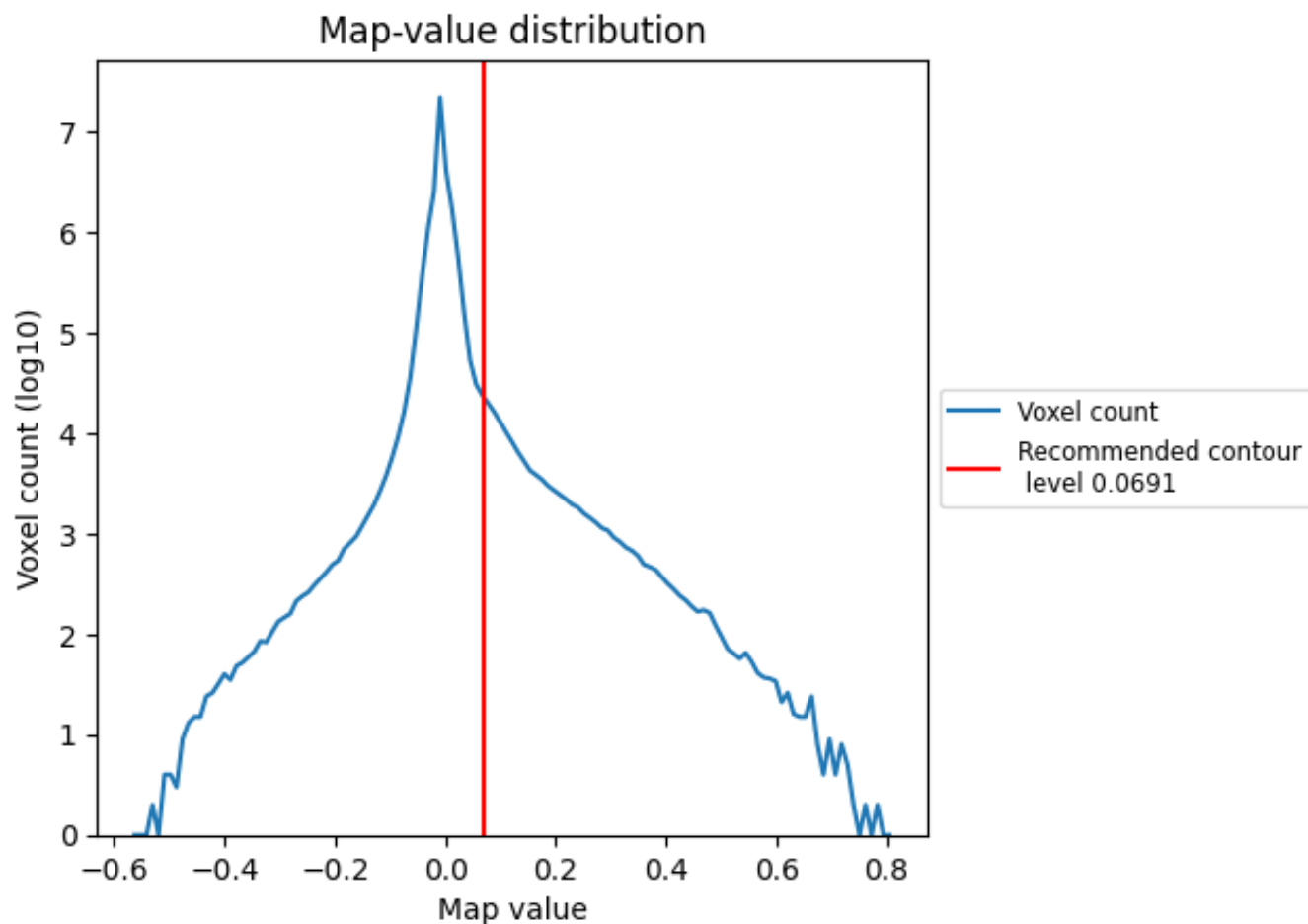
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

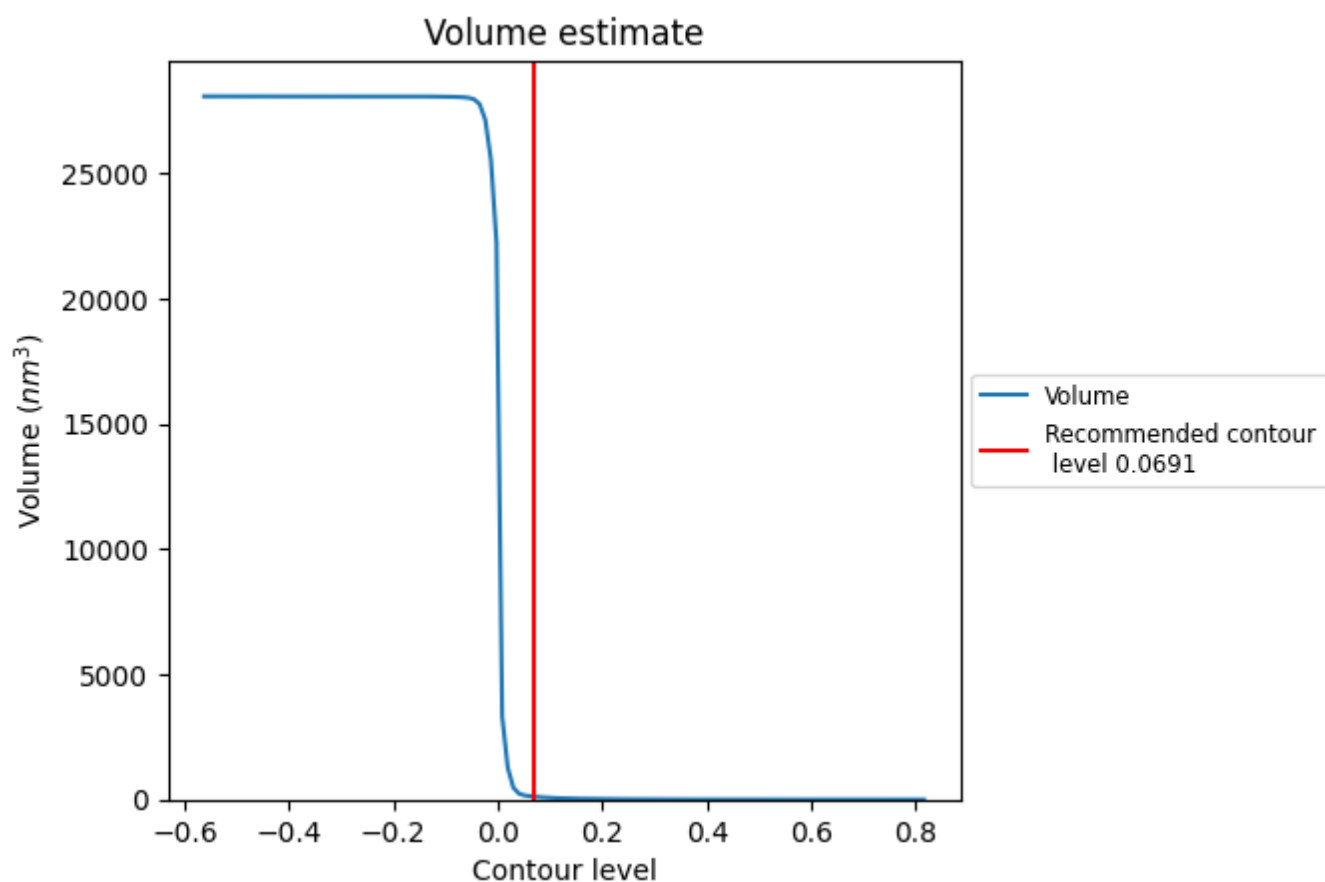
This section contains the results of statistical analysis of the map.

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.

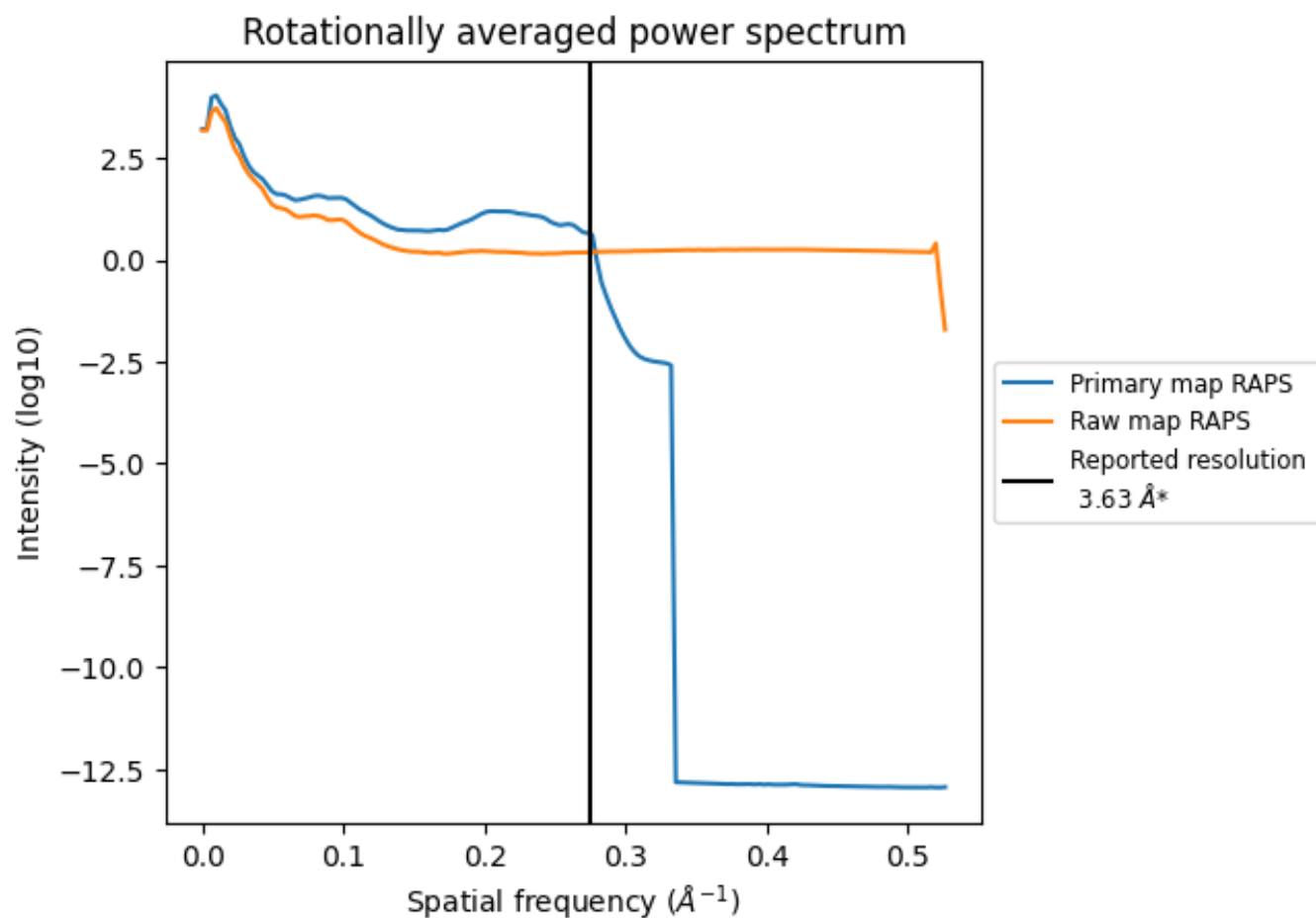
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 119 nm³; 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 ⓘ

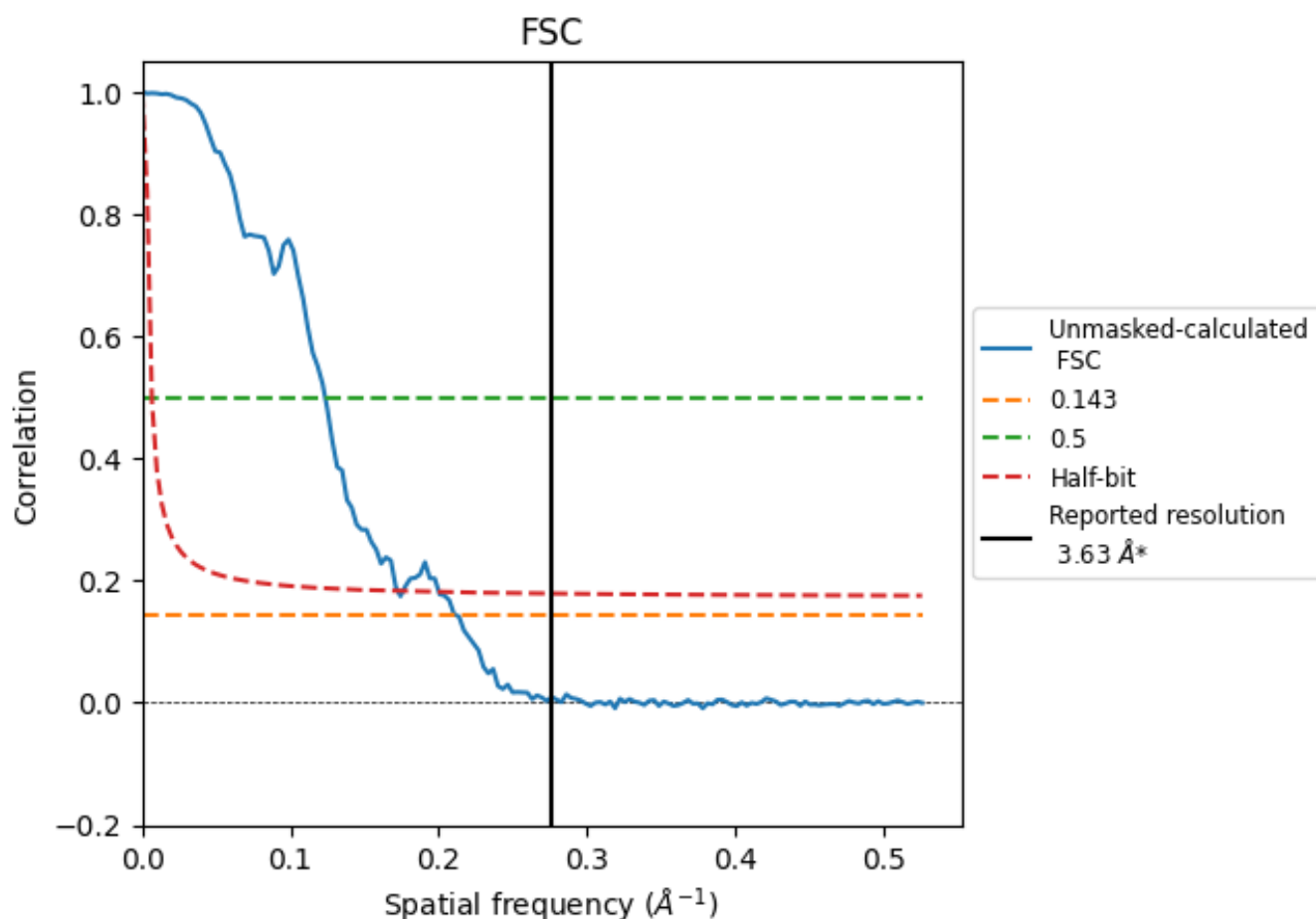


*Reported resolution corresponds to spatial frequency of 0.275 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.275 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

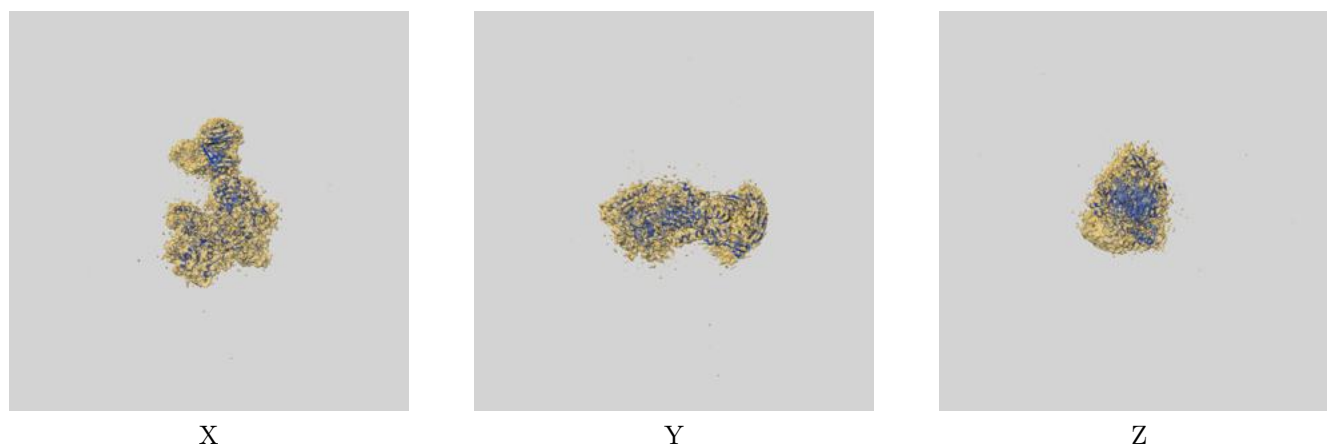
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.63	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.72	8.10	5.80

*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](#)

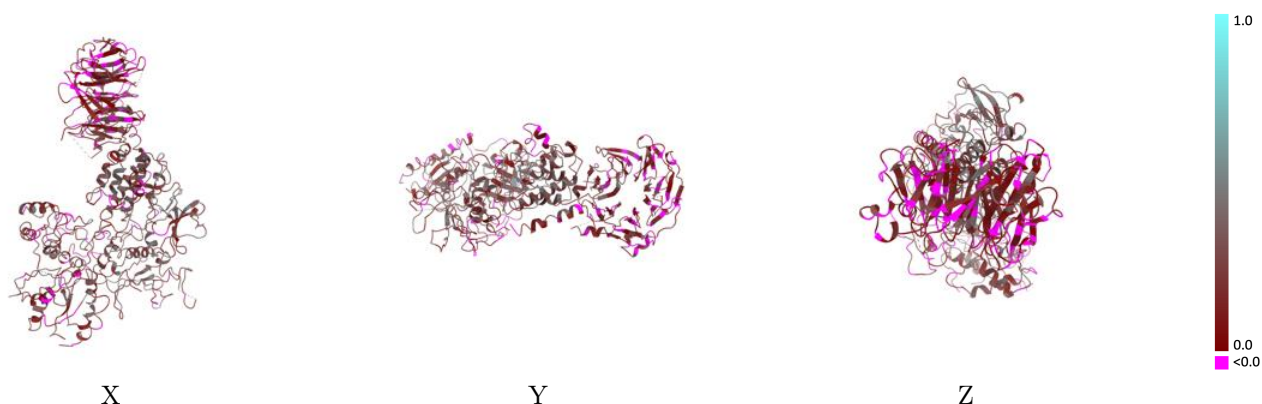
This section contains information regarding the fit between EMDB map EMD-72768 and PDB model 9YCD. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



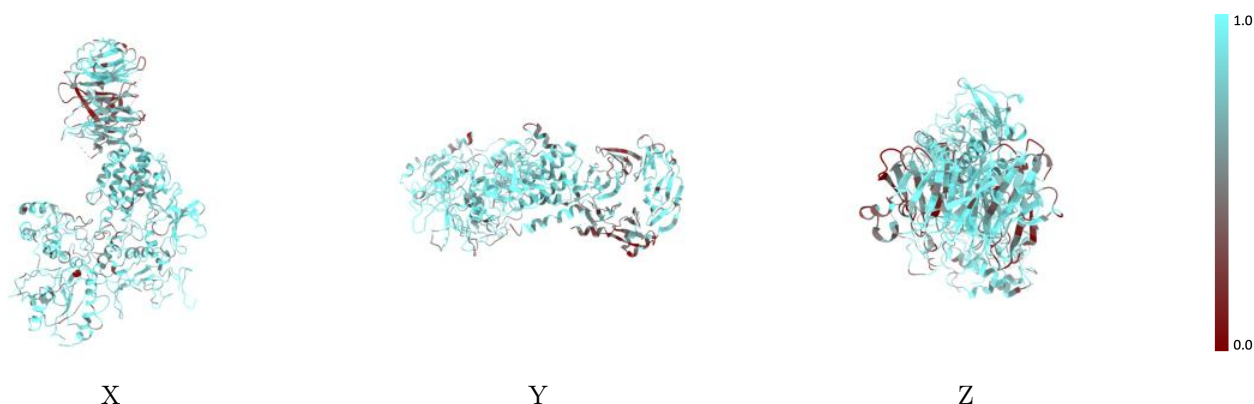
The images above show the 3D surface view of the map at the recommended contour level 0.0691 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



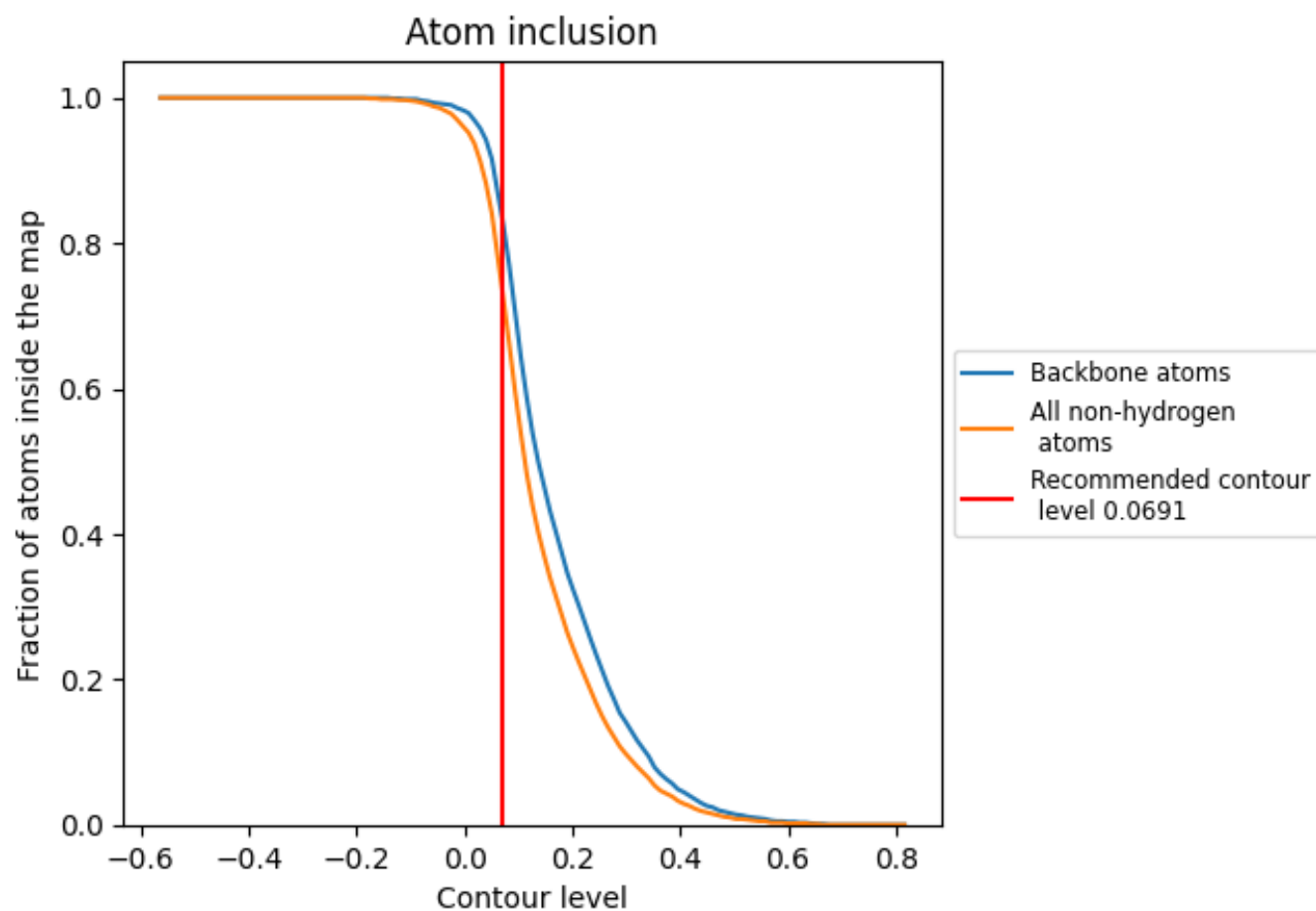
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

