



Full wwPDB EM Validation Report ⓘ

Aug 10, 2026 – 03:05 PM EDT

PDB ID : 9Y7I / pdb_00009y7i
EMDB ID : EMD-72656
Title : Leucine Rich Repeat Kinase 2 bound to GMP-PNP (active)
Authors : Villagran Suarez, A.; Bodrug, T.; Leschziner, A.
Deposited on : 2025-09-10
Resolution : 3.73 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

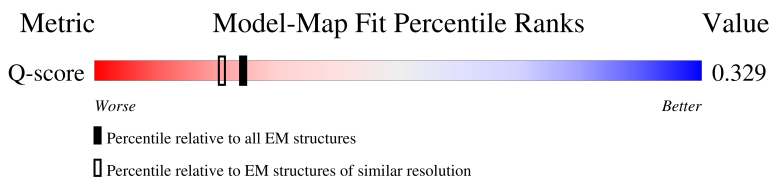
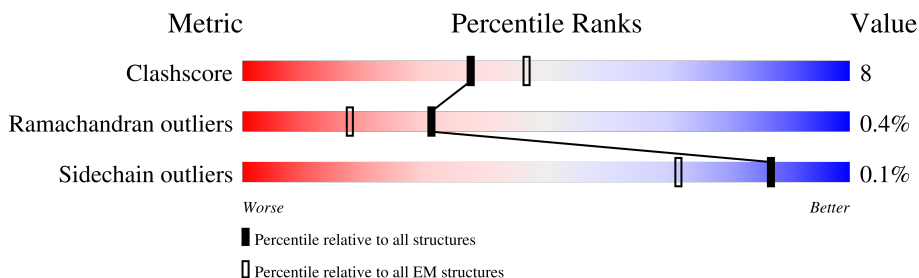
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.73 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	10415 (3.23 - 4.23)

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](#)

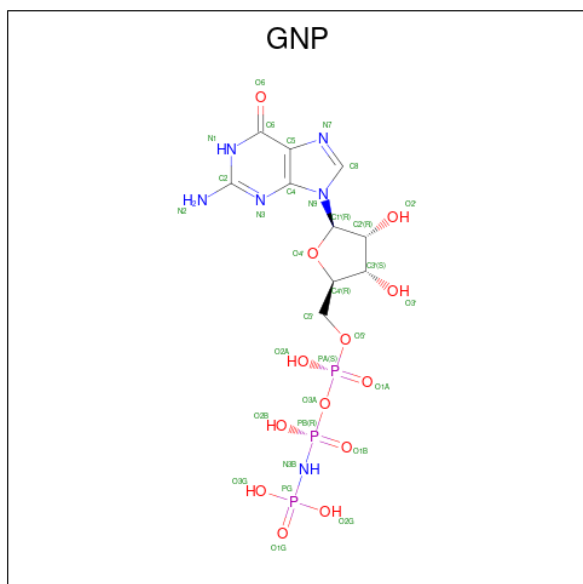
There are 3 unique types of molecules in this entry. The entry contains 8192 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

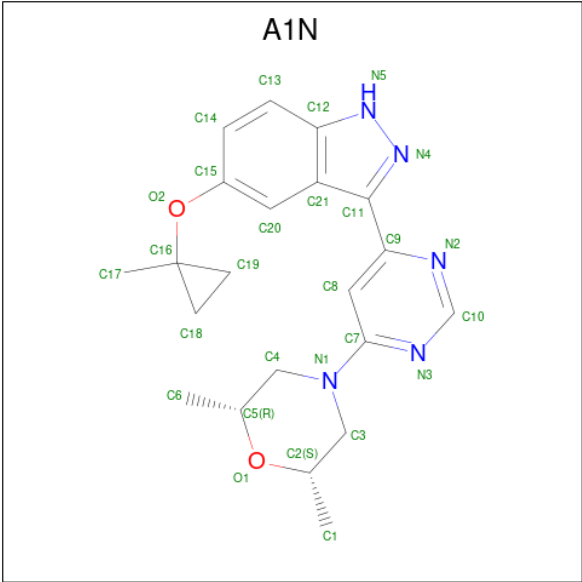
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1101	8132	5209	1401	1475	47	4	0

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



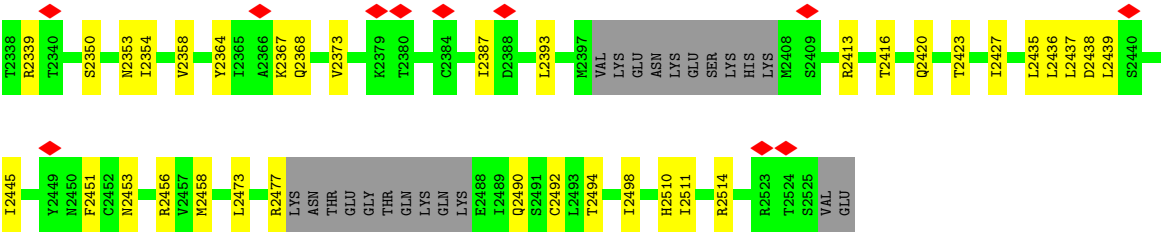
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	32	10	6	13	3	0

- Molecule 3 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: $C_{21}H_{25}N_5O_2$).



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

K2233	K2234	K2235	H2236	K2240	M2241	T2242	V2245	T2246	C2250	ASN	SER	SER	PHE	LYS	GLN	SER	LYS	ARG	ASN	GLN	LYS	N2261	F2262	L2263	G2266	V2280	K2281	L2282	A2285	I2293	L2300	S2306	THR	ASN	SER	THR	GLU	ARG	N2313	V2314	M2315	G2318	C2319	F2324	S2325	F2326	L2335	I2336	E2337
12111	K2112	K2116	R2122	T2141	R2142	L2145	L2146	V2152	A2157	H2160	ASN	SER	ARG	ASN	A2185	G2177	L2182	N2185	T2186	E2187	G2188	A2195	A2203	L2204	V2205	E2210	K2211	E2212	S2213	W2214	L2215	V2216	S2217	G2218	S2221	G2222	L2225	V2226	E2098	S2325	G2100	C2101	A2102	V2107	E2108				
F2003	N2008	L2015	A2016	Q2022	C2025	R2026	M2027	G2028	I2029	E2033	G2034	T2035	H2047	V2048	I2049	Y2050	N2051	Q2052	Q2053	A2054	L2063	Y2064	D2065	I2066	T2069	R2072	L2077	K2078	F2079	P2080	N2081	E2085	L2086	E2087	I2089	P2095	E2098	S2325	G2100	C2101	A2102	V2107	E2108						
D1844	Q1845	PRO	ARG	THR	I1850	L1861	A1862	D1863	E1874	E1899	V1905	N1909	K1910	R1915	R1918	Y2050	N2051	Q2052	Q2053	A2054	L2063	Y2064	D2065	I2066	T2069	R2072	L2077	K2078	F2079	P2080	N2081	E2085	L2086	E2087	I2089	P2095	E2098	S2325	G2100	C2101	A2102	V2107	E2108						
L1727	M1730	R1731	W1734	R1735	Q1736	G1737	L1740	M1741	W1742	S1743	P1744	E1745	A1746	Y1747	S1752	L1763	K1764	I1765	T1766	V1767	P1768	R1771	L1776	I1798	ASP	ILE	CYS	GLY	GLU	GLY	S1946	M1947	E1948	S1951	Q1971	H1972	R1973	L1976	H1977	D1980	L1985	M1989	I1990	R1993	D1994	N1999	V2000		
L1449	V1450	G1451	S1457	ASP	GLU	LYS	R1462	A1481	I1482	R1483	D1484	Y1485	H1486	F1487	T1491	E1492	GLU	SER	ASP	GLY	A1496	I1509	K1512	I1513	R1514	D1515	V1518	V1519	G1520	GLN	ILE	PRO	ASP	G1526	K1539	N1540	V1541	E1566	A1589	I1590	L1595	K1614	V1615	GLY	CYS	PRO			
PHE	LEU	GLN	ARG	LEU	LYS	VAL	P1331	L1337	M1342	Q1353	K1358	LYS	SER	ASP	GLY	ASP	GLU	ASP	GLY	M1364	Q1365	S1366	A1367	I1371	R1381	D1382	K1383	R1384	K1385	R1386	V1392	F1395	F1401	Y1415	L1416	A1417	V1418	Q1425	L1435	F1436	N1437	I1438	R1441	V1447	I1448				
LEU	ASP	MET	SER	GLY	ASN	ASP	ILE	TYR	TRP	LYS	SER	LEU	ASN	GLY	PRO	ALA	VAL	TRP	TRP	LYS	PHE	ALA	ALA	ALA	PRO	PRO	ILE	LEU	ASP	LEU	GLY	ALA	TYR	TRP	SER	VAL	VAL	GLY	ILE	LEU	ASN	ASP	ILE	ILE					
PRO	PRO	GLU	ILE	CYS	LEU	GLU	ASN	THR	SER	VAL	ASP	VAL	TRP	LYS	ASN	GLU	LEU	ARG	GLU	PRO	ASN	GLU	PHE	GLY	LYS	TRP	LEU	PRO	LEU	ASP	GLU	LEU	HIS	ASN	ASN	ASP	ASP	VAL	SER	ARG	VAL	VAL	GLY	ILE	ILE				
THR	VAL	ILE	LYS	GLN	THR	GLY	VAL	THR	GLY	ASP	VAL	VAL	TRP	LYS	ASN	GLU	LEU	ARG	GLU	PRO	ASN	GLU	PHE	GLY	LYS	TRP	LEU	PRO	LEU	ASP	GLU	LEU	HIS	ASN	ASN	ASP	ASP	VAL	SER	ARG	VAL	VAL	GLY	ILE	ILE				
ARG	MET	VAL	ILE	LYS	THR	GLN	MET	LYS	ASP	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
ARG	MET	VAL	ILE	LYS	THR	GLN	MET	LYS	ASP	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO	PHE	ASP	GLY	ALA	ASN	GLN	LYS	GLU	MET	ASP	LEU	VAL	VAL	VAL				
SER	PHE	LEU	VAL	LYS	GLN	LYS	LYS	THR	GLY	VAL	VAL	GLY	GLU	GLY	ALA	SER	GLY	SER	ASP	ALA	SER	ASP	VAL	ASN	GLY	LEU	ARG	GLY	PRO	ILE	PRO																		



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94877	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56.68	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	0.758	Depositor
Minimum map value	-0.447	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.0899	Depositor
Map size (Å)	269.28, 269.28, 269.28	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.935, 0.935, 0.935	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, GNP

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	0.21	0/8271	0.57	2/11247 (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	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2107	VAL	N-CA-C	-8.02	105.67	113.53
1	A	1989	MET	N-CA-CB	-6.02	107.31	114.17

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	8132	0	7660	119	0
2	A	32	0	13	0	0
3	A	28	0	0	0	0
All	All	8192	0	7673	119	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 8.

All (119) 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:1415:TYR:O	1:A:1447:VAL:HA	1.69	0.92
1:A:2205:VAL:HB	1:A:2214:TRP:O	1.87	0.74
1:A:2315:MET:HB2	1:A:2326:PHE:HB2	1.76	0.68
1:A:1730:ASN:HB2	1:A:1741:ASN:HB3	1.75	0.67
1:A:2065:ASP:OD1	1:A:2072:ARG:NH1	2.29	0.66
1:A:1771:ARG:NH1	1:A:1771:ARG:O	2.30	0.63
1:A:1812:ALA:HB2	1:A:1827:LEU:HD12	1.81	0.63
1:A:2358:VAL:HB	1:A:2364:TYR:HB2	1.80	0.63
1:A:1905:VAL:HG12	1:A:1946:VAL:HG22	1.79	0.63
1:A:2101:CYS:SG	1:A:2102:ALA:N	2.72	0.62
1:A:1993:ARG:NH1	1:A:2033:GLU:O	2.32	0.62
1:A:2063:LEU:HA	1:A:2066:ILE:HG22	1.84	0.60
1:A:2216:VAL:HG23	1:A:2226:VAL:HG22	1.83	0.60
1:A:2205:VAL:HG11	1:A:2280:VAL:HG21	1.83	0.59
1:A:1716:SER:OG	1:A:1731:ARG:NH1	2.36	0.58
1:A:1861:LEU:HD13	1:A:1940:ILE:HD13	1.85	0.58
1:A:2420:GLN:NE2	1:A:2498:ILE:O	2.36	0.57
1:A:1693:ARG:HB2	1:A:1765:ILE:HB	1.87	0.57
1:A:2146:LEU:O	1:A:2490:GLN:NE2	2.34	0.57
1:A:1337:LEU:HD22	1:A:1392:VAL:HG12	1.87	0.56
1:A:1971:GLN:HG3	1:A:2066:ILE:HG12	1.88	0.56
1:A:1418:VAL:HG12	1:A:1450:VAL:HB	1.87	0.56
1:A:2221:SER:O	1:A:2240:LYS:NZ	2.39	0.55
1:A:1415:TYR:HD1	1:A:1438:ILE:HD11	1.72	0.55
1:A:1677:ARG:HH12	1:A:1752:SER:H	1.54	0.54
1:A:2177:GLY:HA3	1:A:2195:ALA:HB3	1.90	0.54
1:A:1668:LEU:HD22	1:A:1713:LEU:HD22	1.89	0.54
1:A:1451:GLY:H	1:A:1487:PHE:HB2	1.73	0.53
1:A:1691:ILE:O	1:A:1766:THR:HA	2.08	0.53
1:A:1840:LEU:HG	1:A:1841:VAL:HG23	1.91	0.52
1:A:2350:SER:O	1:A:2367:LYS:NZ	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1693:ARG:O	1:A:1764:LYS:HA	2.11	0.51
1:A:1371:ILE:HG22	1:A:1395:PHE:HA	1.92	0.51
1:A:1951:SER:OG	1:A:2003:PHE:O	2.29	0.51
1:A:1935:LEU:HD12	1:A:1947:MET:HB3	1.92	0.51
1:A:2141:THR:HG22	1:A:2142:ARG:HG3	1.93	0.50
1:A:1999:ASN:ND2	1:A:2016:ALA:O	2.36	0.50
1:A:2436:LEU:HB2	1:A:2445:ILE:HB	1.94	0.50
1:A:2000:VAL:HG12	1:A:2015:ILE:HG22	1.94	0.50
1:A:1595:LEU:HD22	1:A:1648:GLN:HB3	1.93	0.49
1:A:2453:ASN:ND2	1:A:2477:ARG:O	2.42	0.49
1:A:2022:GLN:N	1:A:2022:GLN:OE1	2.44	0.49
1:A:1934:SER:OG	1:A:1948:GLU:OE2	2.27	0.48
1:A:2152:VAL:O	1:A:2456:ARG:NH1	2.46	0.48
1:A:2423:THR:HB	1:A:2439:LEU:HB2	1.95	0.48
1:A:2368:GLN:OE1	1:A:2413:ARG:NH1	2.43	0.48
1:A:1657:GLN:O	1:A:1659:ALA:N	2.47	0.48
1:A:2145:LEU:HD13	1:A:2492:CYS:HB3	1.96	0.47
1:A:1874:GLU:HG3	1:A:1899:GLU:HA	1.96	0.47
1:A:1747:TYR:HB2	1:A:1768:PRO:HD3	1.97	0.47
1:A:1830:LEU:H	1:A:1833:LYS:HG3	1.79	0.47
1:A:2393:LEU:HD21	1:A:2435:LEU:HD21	1.97	0.47
1:A:2236:HIS:NE2	1:A:2280:VAL:O	2.41	0.47
1:A:1589:ALA:HB3	1:A:2050:TYR:HA	1.96	0.46
1:A:1985:LEU:HD22	1:A:1990:ILE:HD11	1.97	0.46
1:A:1740:LEU:HB3	1:A:1742:TRP:HZ3	1.81	0.46
1:A:2182:LEU:HA	1:A:2188:GLY:O	2.15	0.46
1:A:1994:ASP:OD1	1:A:2035:THR:OG1	2.34	0.46
1:A:2028:GLY:HA3	1:A:2049:ILE:HG22	1.98	0.46
1:A:2282:LEU:HB2	1:A:2285:ALA:HB2	1.98	0.46
1:A:1712:LEU:HD13	1:A:1715:ILE:HD11	1.97	0.46
1:A:1973:ARG:O	1:A:1977:HIS:ND1	2.36	0.46
1:A:2246:THR:OG1	1:A:2266:GLY:O	2.32	0.46
1:A:1661:PRO:O	1:A:2026:ARG:NH1	2.49	0.46
1:A:2112:LYS:O	1:A:2116:LYS:NZ	2.40	0.46
1:A:2225:LEU:HD11	1:A:2235:ARG:HB3	1.98	0.46
1:A:2213:SER:OG	1:A:2229:THR:OG1	2.26	0.45
1:A:1909:ASN:OD1	1:A:1910:LYS:N	2.49	0.45
1:A:2008:ASN:HA	1:A:2510:HIS:HE1	1.81	0.45
1:A:1689:GLU:N	1:A:1689:GLU:OE1	2.50	0.45
1:A:1976:LEU:HD21	1:A:2511:ILE:HD11	1.99	0.45
1:A:1693:ARG:HA	1:A:1693:ARG:HD2	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2054:ALA:HA	1:A:2122:ARG:NH2	2.32	0.45
1:A:1435:LEU:HA	1:A:1438:ILE:HG22	1.99	0.45
1:A:1764:LYS:HE2	1:A:1764:LYS:HB3	1.77	0.45
1:A:2427:ILE:HB	1:A:2435:LEU:HB2	1.99	0.44
1:A:1937:ALA:HB3	1:A:1946:VAL:HB	1.98	0.44
1:A:1673:LEU:HD23	1:A:1673:LEU:HA	1.89	0.44
1:A:1441[A]:ARG:HD2	1:A:1441[A]:ARG:HA	1.50	0.44
1:A:2053:GLN:HE21	1:A:2122:ARG:HB3	1.83	0.44
1:A:2222:GLY:HA2	1:A:2245:VAL:HG23	2.00	0.44
1:A:2427:ILE:HD13	1:A:2437:LEU:HD23	2.00	0.44
1:A:1812:ALA:HB3	1:A:1825:ILE:HG23	2.00	0.44
1:A:2337:GLU:HG3	1:A:2339:ARG:H	1.83	0.43
1:A:2438:ASP:HB2	1:A:2445:ILE:HD11	1.99	0.43
1:A:1416:LEU:HG	1:A:1448:ILE:HB	2.01	0.43
1:A:2324:PHE:HB3	1:A:2335:LEU:HD12	2.00	0.43
1:A:2098:GLU:HG3	1:A:2099:TYR:CD1	2.54	0.43
1:A:2142:ARG:NH2	1:A:2187:GLU:OE2	2.51	0.43
1:A:2300:LEU:HD13	1:A:2319:CYS:HB2	2.01	0.43
1:A:2108:GLU:HA	1:A:2111:ILE:HG12	2.01	0.42
1:A:1863:ASP:OD1	1:A:1863:ASP:N	2.48	0.42
1:A:1695:TYR:HB2	1:A:1763:LEU:HB3	2.01	0.42
1:A:2353:ASN:OD1	1:A:2353:ASN:N	2.53	0.42
1:A:2416:THR:HG21	1:A:2458:MET:H	1.83	0.42
1:A:1734:TRP:CD1	1:A:1736:GLN:H	2.37	0.42
1:A:1915:ARG:HA	1:A:1915:ARG:HD2	1.88	0.42
1:A:2051:ASN:OD1	1:A:2052:GLN:N	2.43	0.42
1:A:1940:ILE:HG23	1:A:1941:ARG:HD2	2.02	0.42
1:A:2420:GLN:NE2	1:A:2498:ILE:HG13	2.35	0.42
1:A:1980:ASP:OD2	1:A:2514:ARG:NH2	2.48	0.41
1:A:1734:TRP:HD1	1:A:1736:GLN:H	1.67	0.41
1:A:2022:GLN:HE21	1:A:2029:ILE:HD13	1.85	0.41
1:A:2354:ILE:HD13	1:A:2367:LYS:HG2	2.02	0.41
1:A:1353:GLN:HG2	1:A:1491:THR:HA	2.02	0.41
1:A:1924:LEU:HD12	1:A:1935:LEU:HB2	2.02	0.41
1:A:2203:ALA:HB3	1:A:2216:VAL:HG12	2.01	0.41
1:A:1814:TYR:HE1	1:A:1825:ILE:HB	1.84	0.41
1:A:2216:VAL:HG11	1:A:2263:LEU:HD11	2.02	0.41
1:A:1692:ILE:HG23	1:A:1764:LYS:HG3	2.03	0.41
1:A:1743:SER:O	1:A:1745:GLU:N	2.53	0.41
1:A:1863:ASP:OD2	1:A:1918:ARG:NH2	2.48	0.41
1:A:2152:VAL:HG13	1:A:2473:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2373:VAL:HB	1:A:2387:ILE:HB	2.03	0.41
1:A:1481:ALA:HB1	1:A:1483:ARG:HG2	2.03	0.41
1:A:1675:ASP:HA	1:A:1735:ARG:HB2	2.03	0.40
1:A:1985:LEU:HD23	1:A:1985:LEU:HA	1.95	0.40
1:A:2064:TYR:CE1	1:A:2095:PRO:HG3	2.57	0.40
1:A:2451:PHE:HE1	1:A:2494:THR:HG21	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	1073/2527 (42%)	957 (89%)	112 (10%)	4 (0%)	30 60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1843	PRO
1	A	1425	GLN
1	A	1658	ILE
1	A	1657	GLN

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	782/2281 (34%)	780 (100%)	2 (0%)	86	83

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1441[A]	ARG
1	A	1441[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1779	GLN
1	A	1783	HIS
1	A	1919	GLN

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	2602	-	29,32,32	1.02	1 (3%)	40,48,48	1.55	6 (15%)
2	GNP	A	2601	-	34,34,34	1.32	5 (14%)	47,54,54	0.82	2 (4%)

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	2602	-	-	6/12/29/29	0/5/5/5
2	GNP	A	2601	-	-	4/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2601	GNP	PB-O3A	4.76	1.65	1.59
2	A	2601	GNP	PG-N3B	3.07	1.71	1.63
2	A	2601	GNP	PB-O1B	2.90	1.50	1.46
2	A	2601	GNP	PG-O1G	2.79	1.50	1.46
2	A	2601	GNP	PB-O2B	-2.25	1.50	1.56
3	A	2602	A1N	N5-N4	-2.02	1.31	1.36

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2602	A1N	C5-O1-C2	4.65	119.01	112.12
3	A	2602	A1N	O1-C5-C6	4.05	114.47	106.88
3	A	2602	A1N	C10-N3-C7	3.95	118.26	114.95
3	A	2602	A1N	O1-C2-C1	3.76	113.92	106.88
2	A	2601	GNP	O1B-PB-N3B	-2.86	107.56	111.77
3	A	2602	A1N	C13-C14-C15	2.44	122.52	119.73
2	A	2601	GNP	O3A-PB-N3B	2.30	112.96	106.59
3	A	2602	A1N	O2-C15-C20	2.02	126.54	119.16

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2601	GNP	PB-N3B-PG-O1G
2	A	2601	GNP	PG-N3B-PB-O1B

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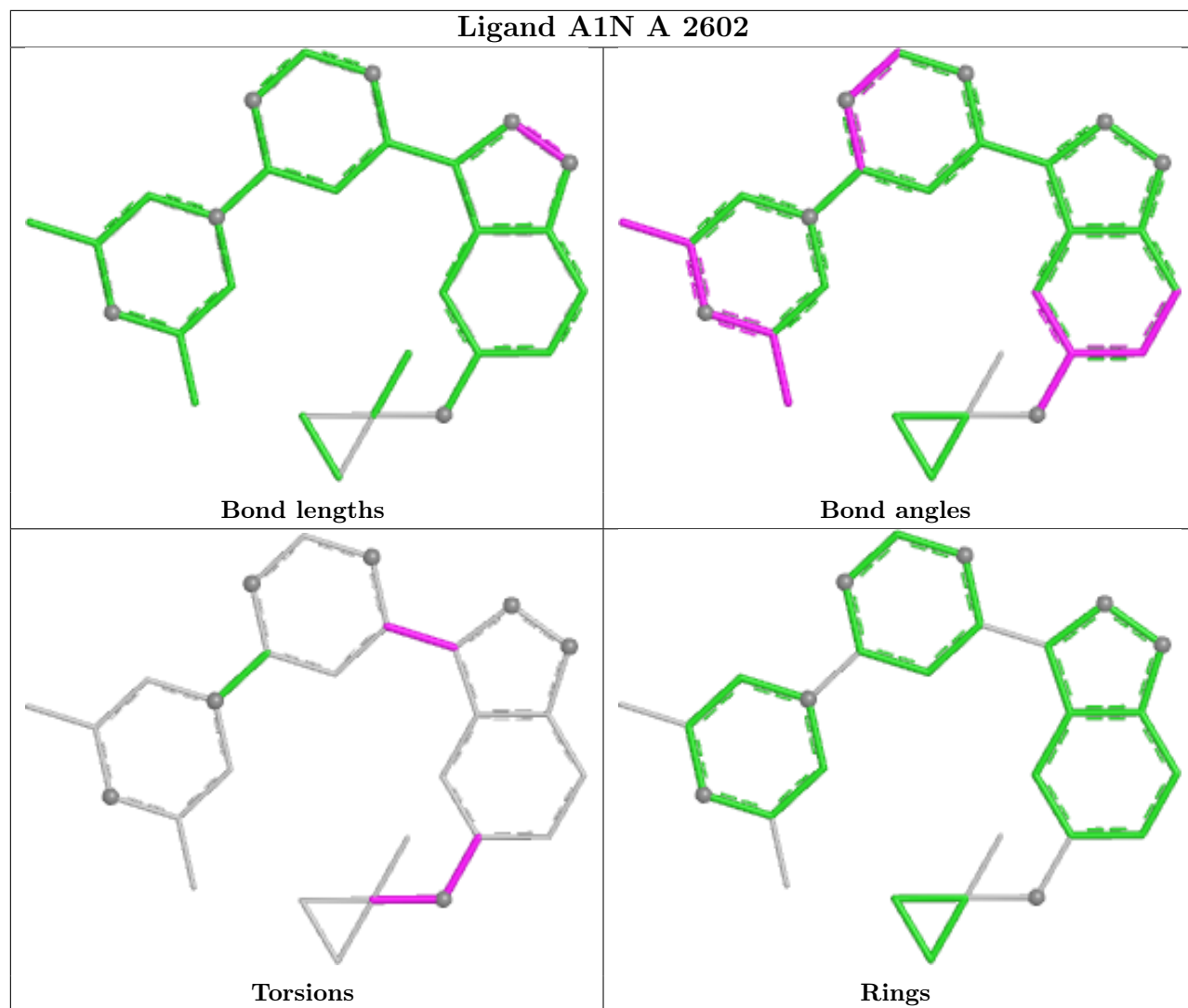
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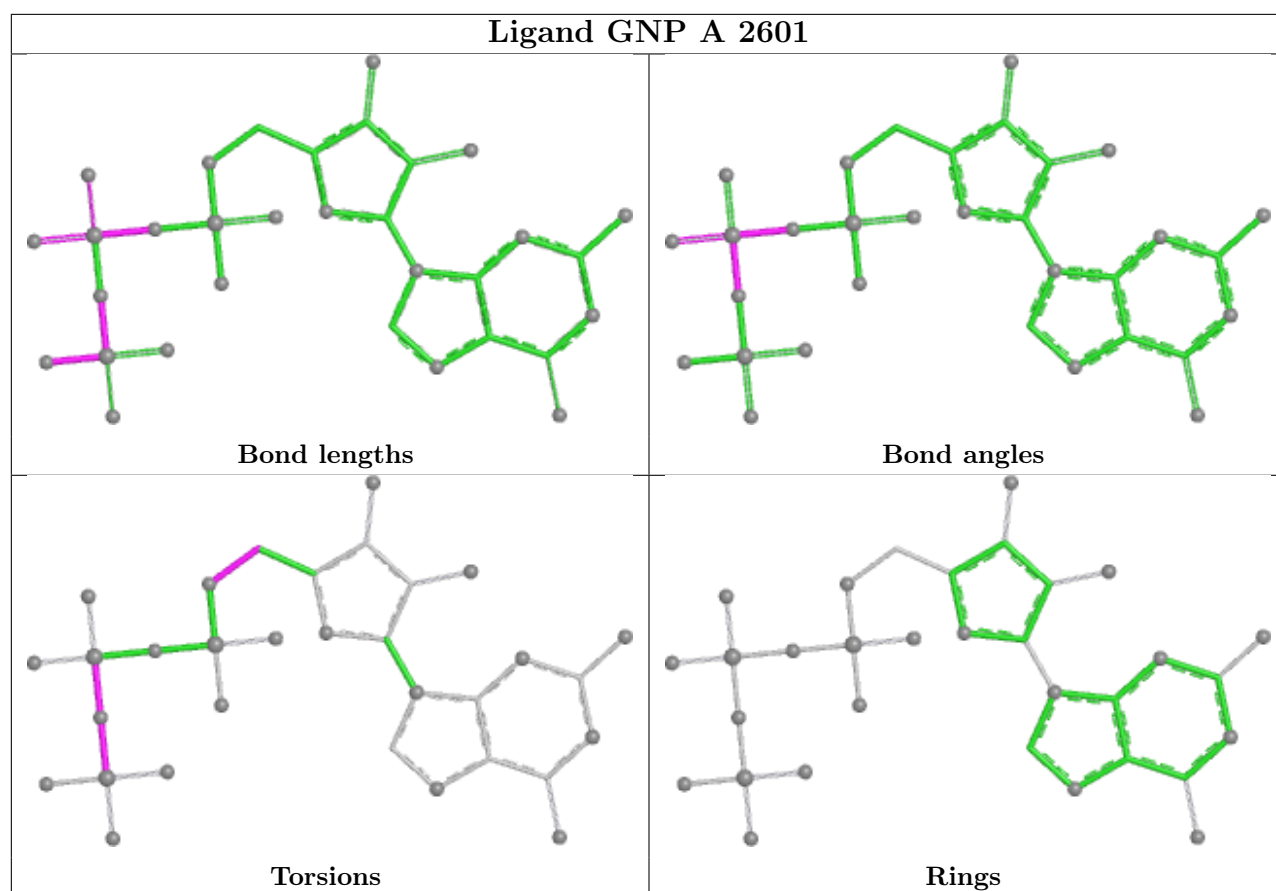
Mol	Chain	Res	Type	Atoms
2	A	2601	GNP	PG-N3B-PB-O3A
3	A	2602	A1N	C19-C16-O2-C15
3	A	2602	A1N	C21-C11-C9-N2
3	A	2602	A1N	C21-C11-C9-C8
3	A	2602	A1N	C18-C16-O2-C15
3	A	2602	A1N	C20-C15-O2-C16
2	A	2601	GNP	C4'-C5'-O5'-PA
3	A	2602	A1N	C14-C15-O2-C16

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.

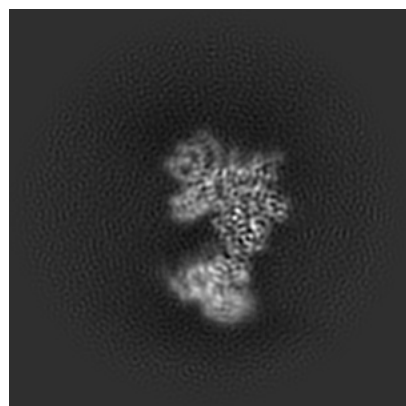
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72656. These allow visual inspection of the internal detail of the map and identification of artifacts.

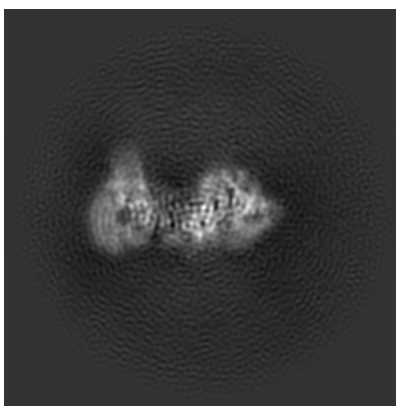
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

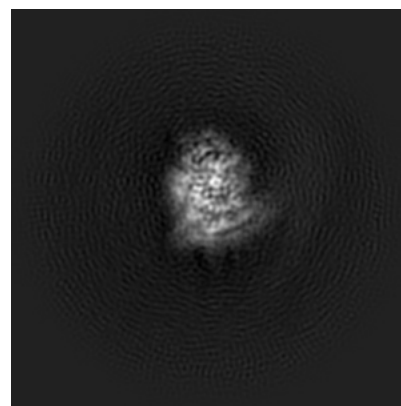
6.1.1 Primary map



X

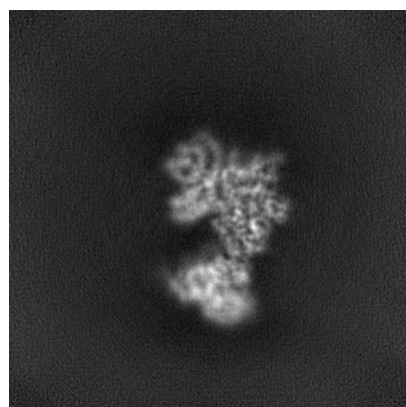


Y

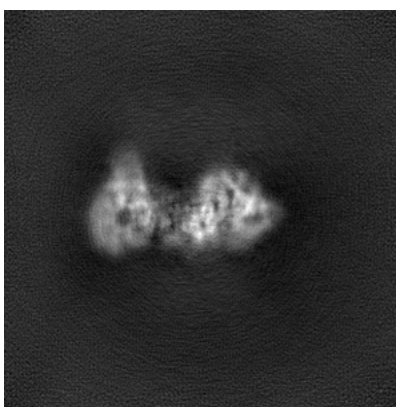


Z

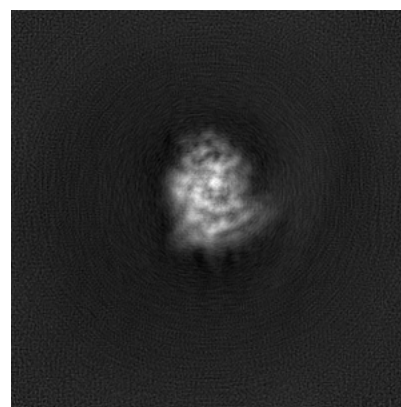
6.1.2 Raw map



X



Y

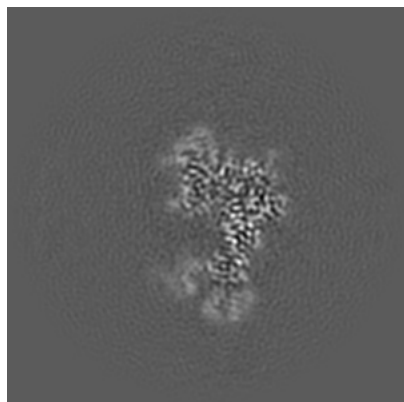


Z

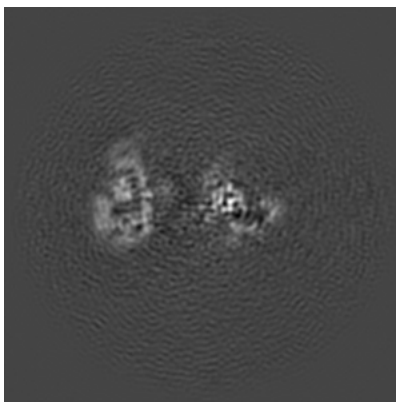
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

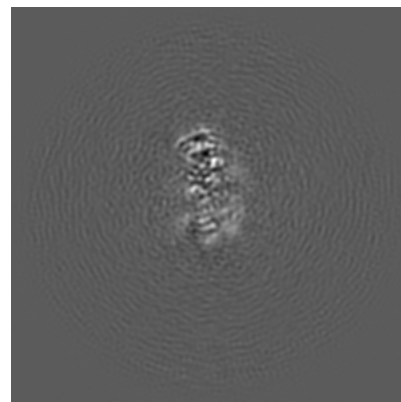
6.2.1 Primary map



X Index: 144

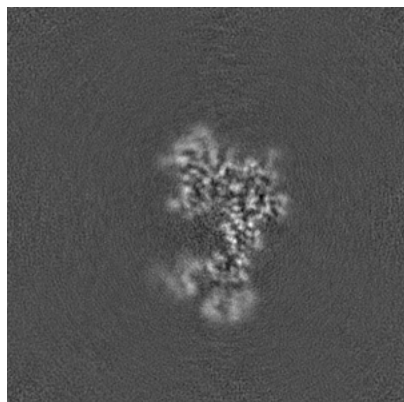


Y Index: 144

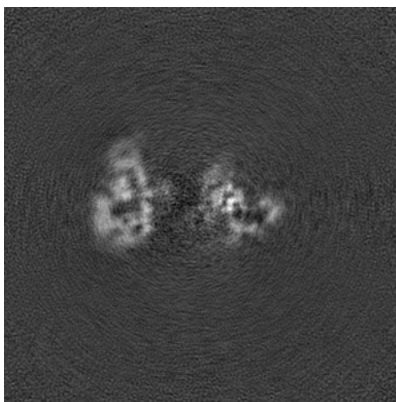


Z Index: 144

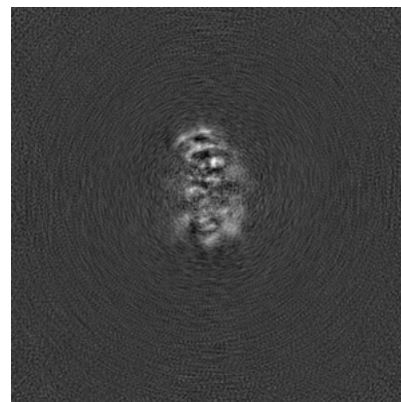
6.2.2 Raw map



X Index: 144



Y Index: 144

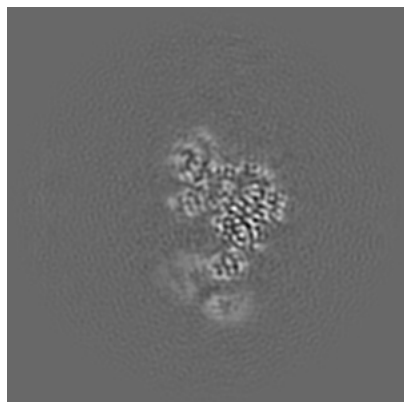


Z Index: 144

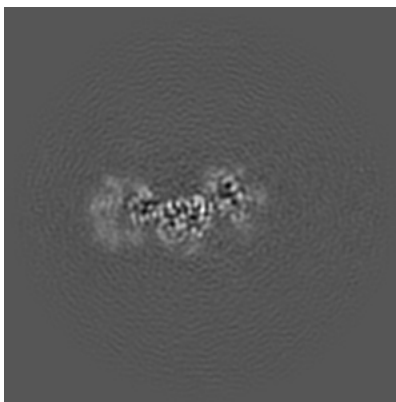
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

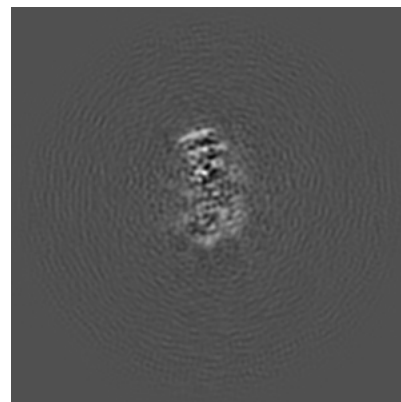
6.3.1 Primary map



X Index: 140

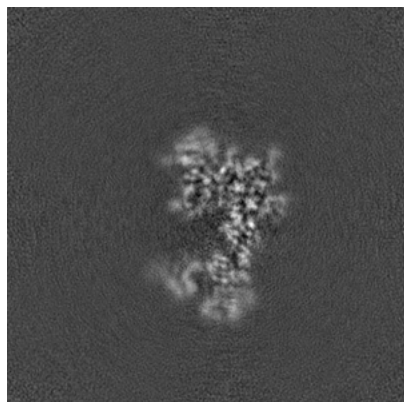


Y Index: 164

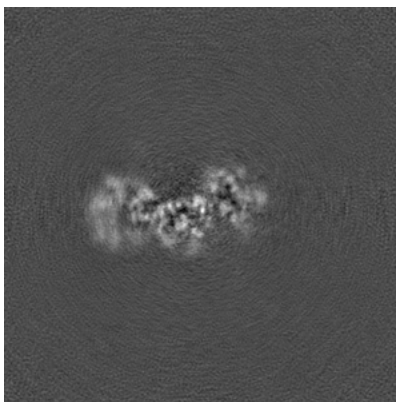


Z Index: 146

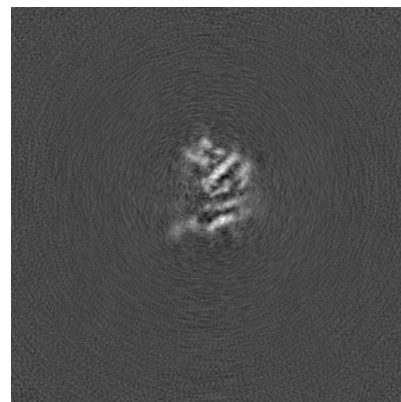
6.3.2 Raw map



X Index: 146



Y Index: 163

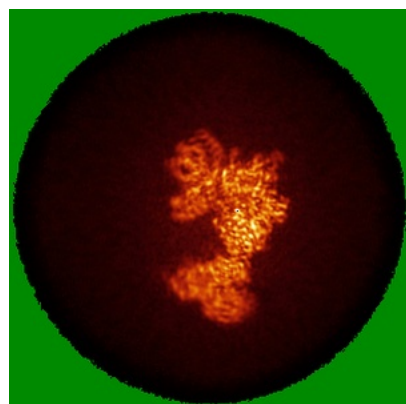


Z Index: 157

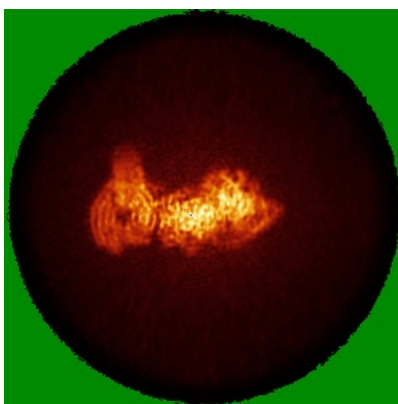
The images above show the largest variance slices of the map in three orthogonal directions.

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

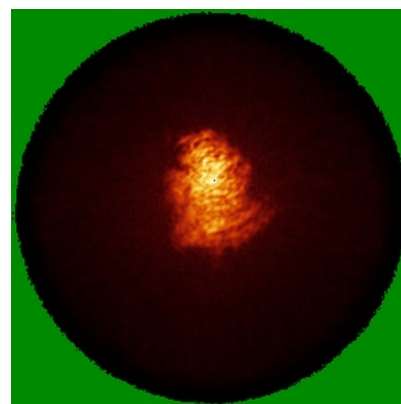
6.4.1 Primary map



X

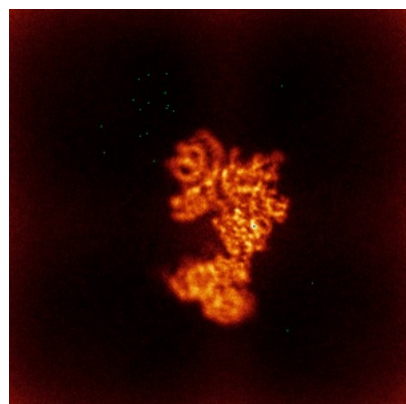


Y

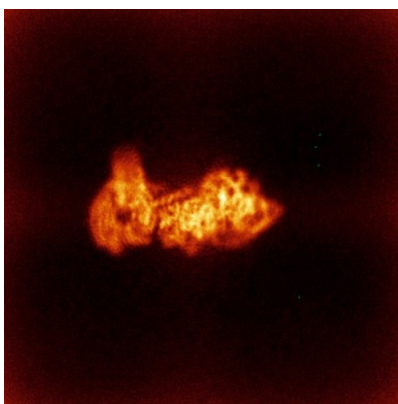


Z

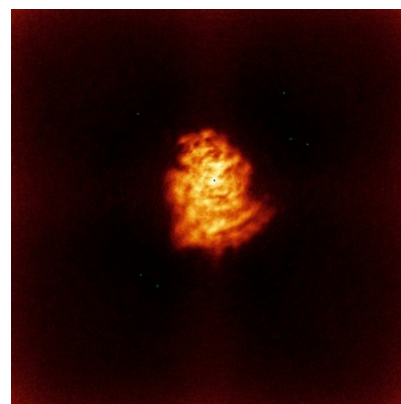
6.4.2 Raw map



X



Y

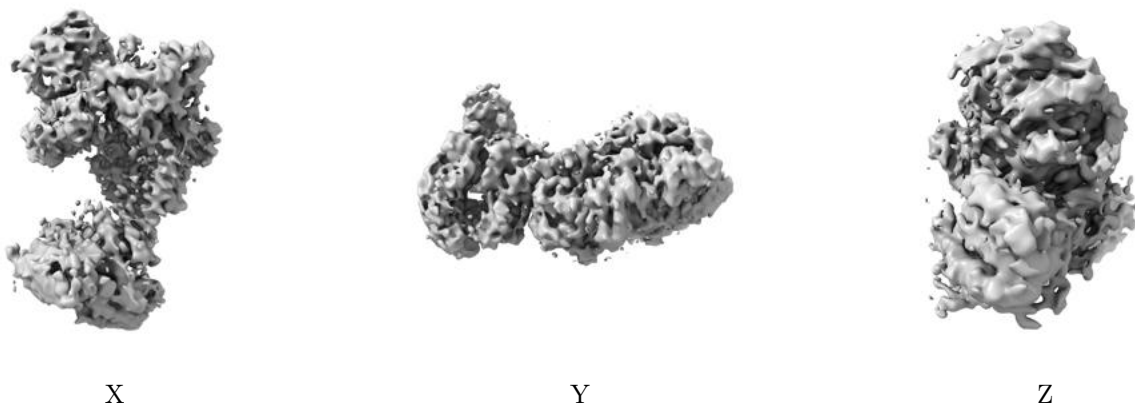


Z

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.

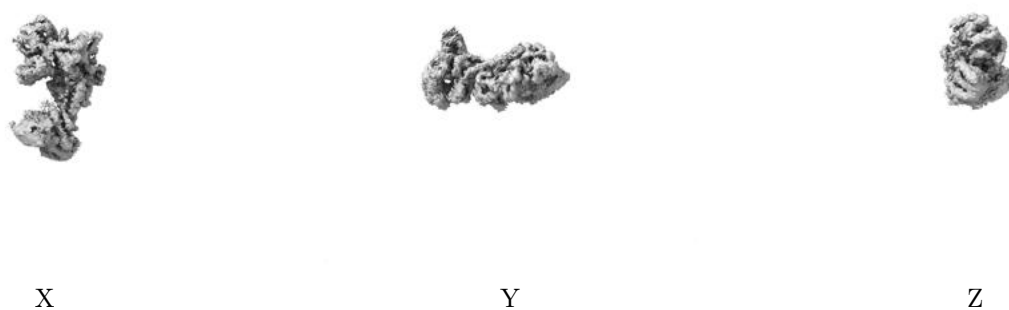
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0899. 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.

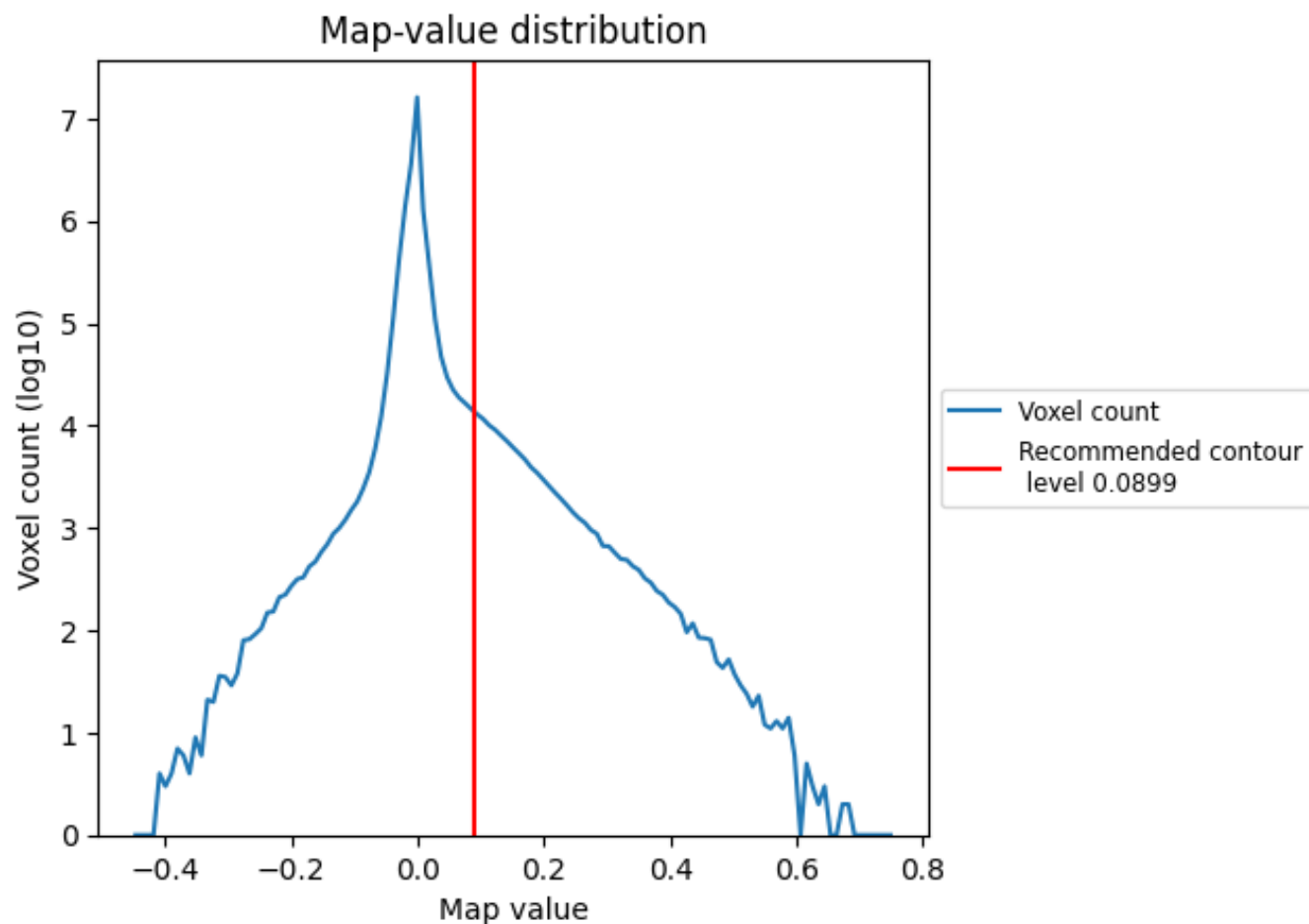
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

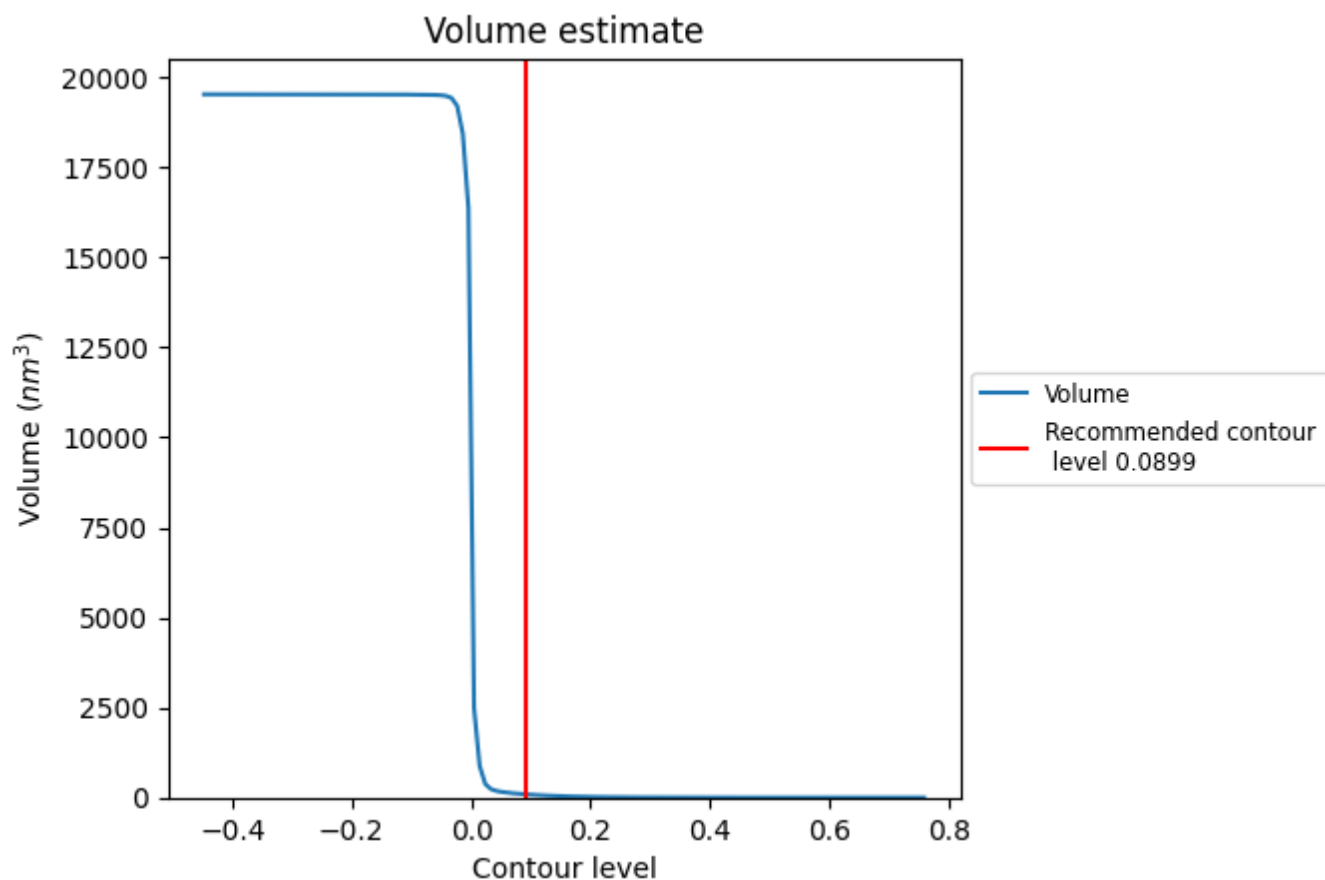
This section contains the results of statistical analysis of the map.

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.

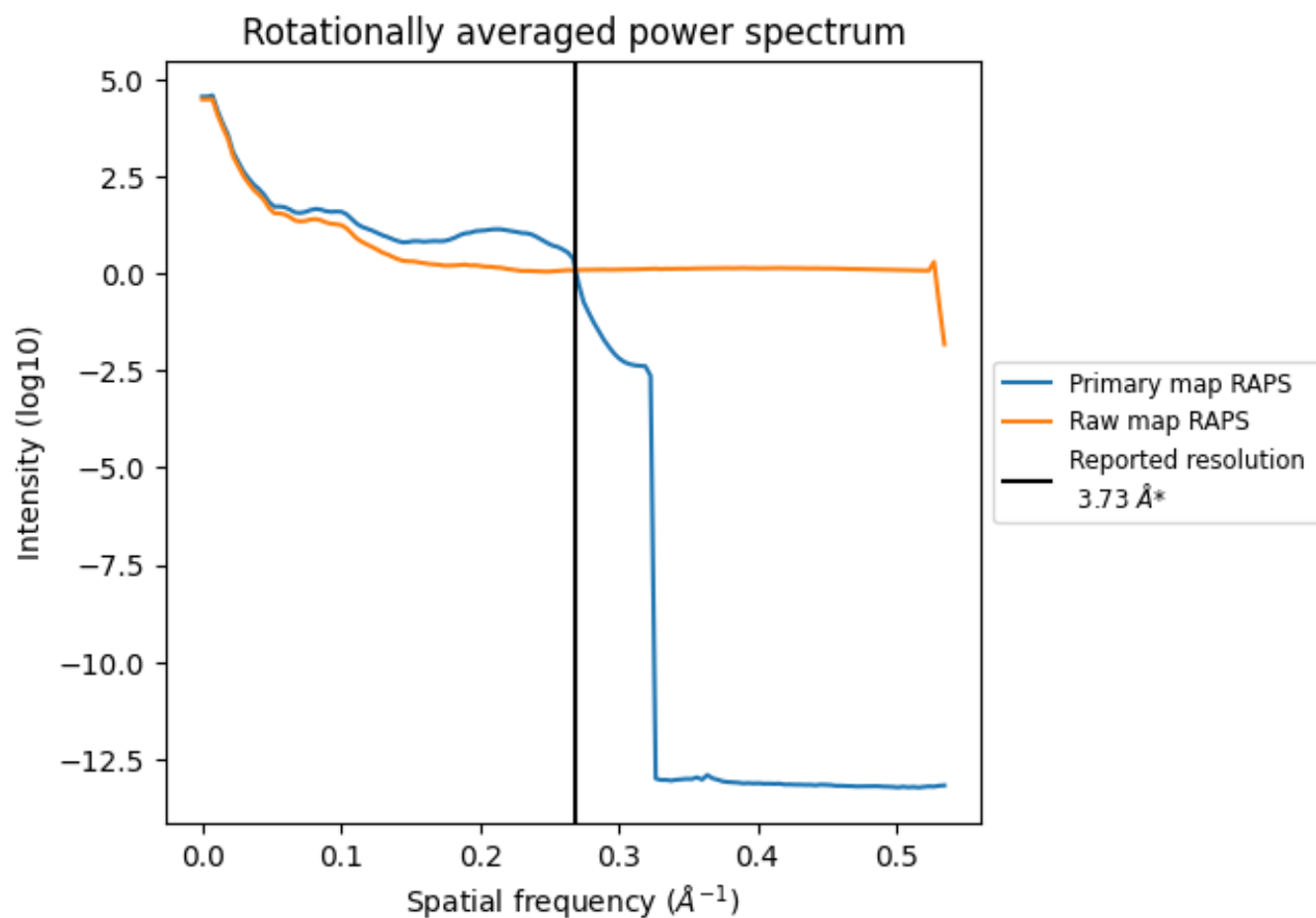
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 91 nm^3 ; this corresponds to an approximate mass of 82 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 ⓘ

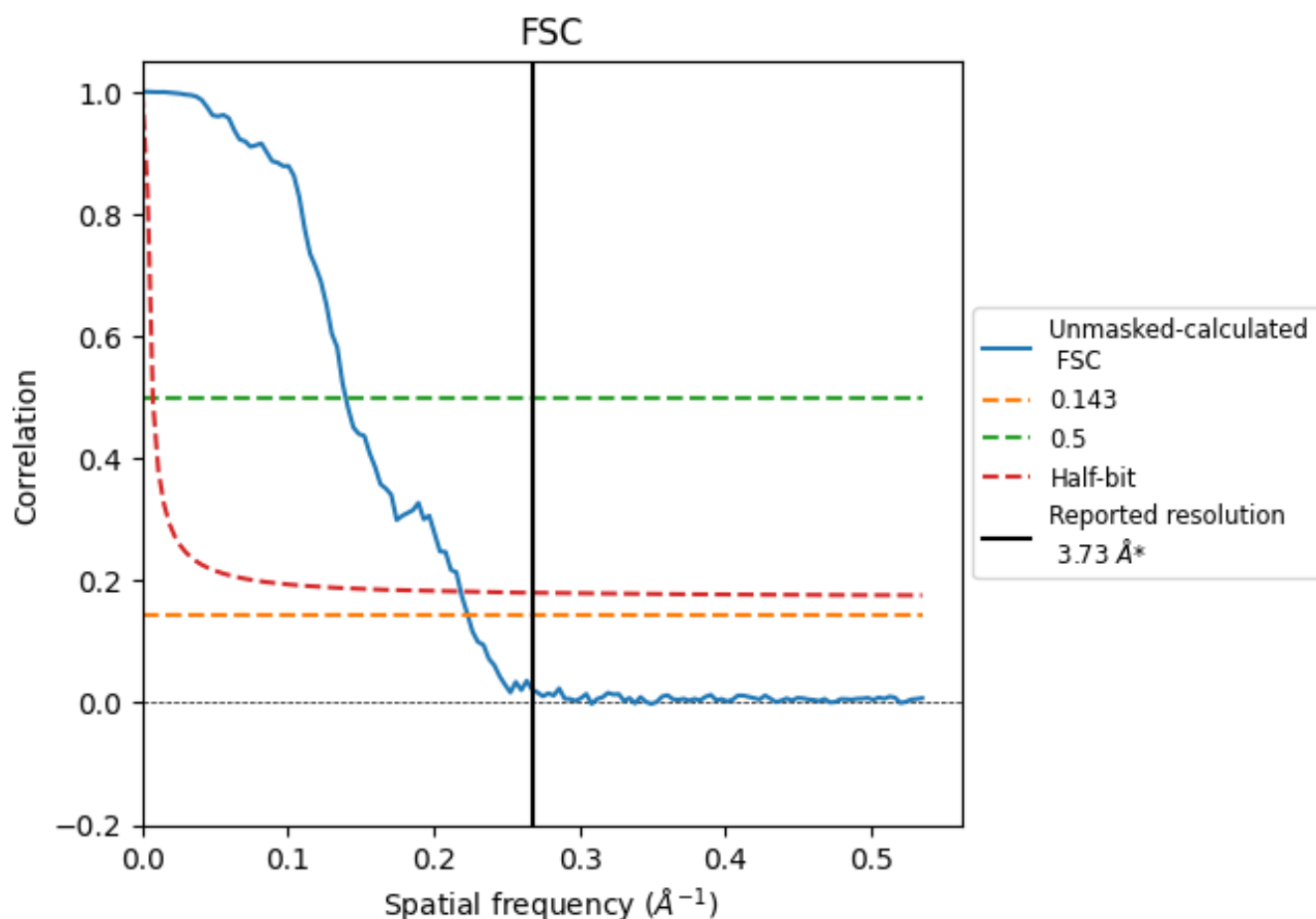


*Reported resolution corresponds to spatial frequency of 0.268 Å⁻¹

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 0.268 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

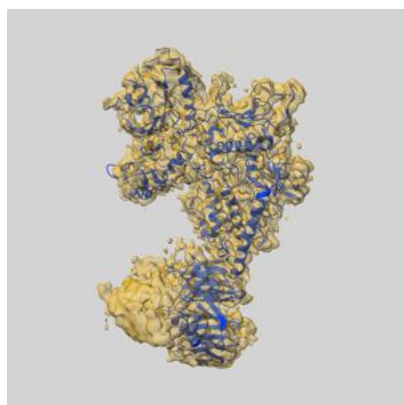
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.73	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.48	7.17	4.58

*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 4.48 differs from the reported value 3.73 by more than 10 %

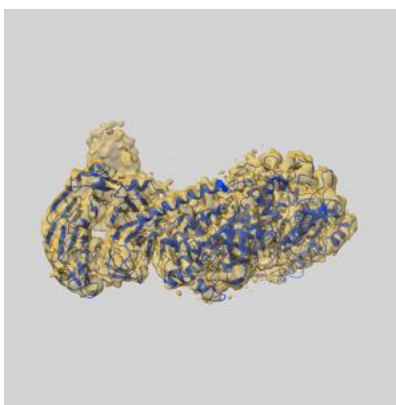
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72656 and PDB model 9Y7I. Per-residue inclusion information can be found in section 3 on page 5.

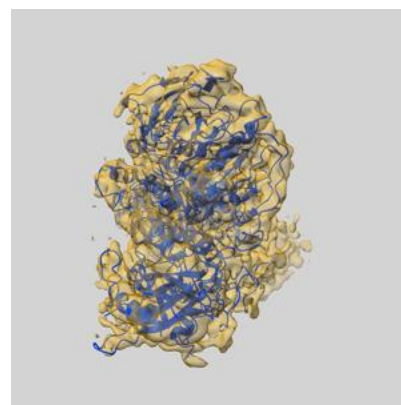
9.1 Map-model overlay [i](#)



X



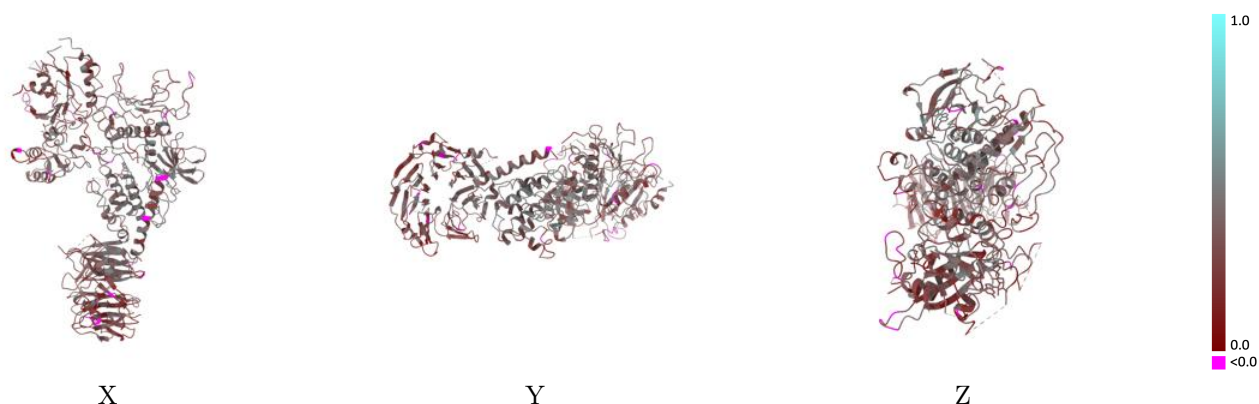
Y



Z

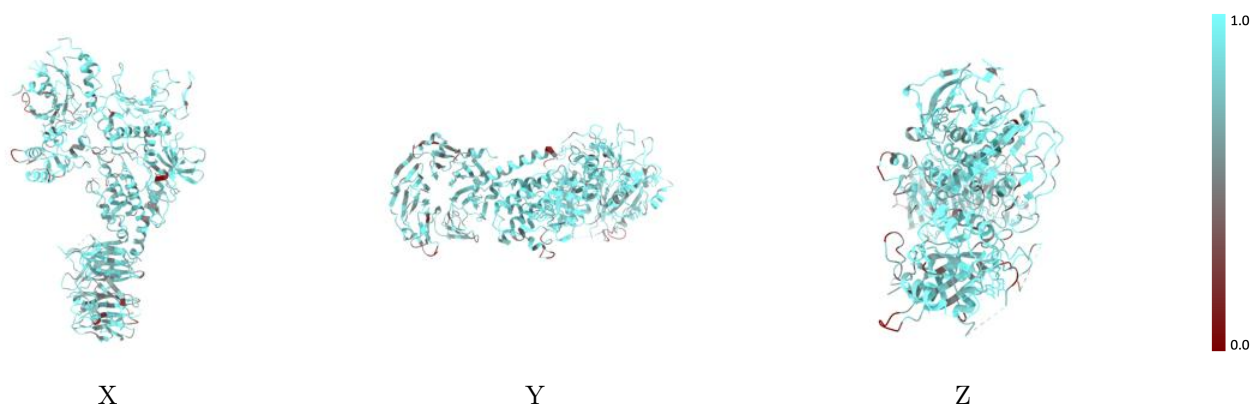
The images above show the 3D surface view of the map at the recommended contour level 0.0899 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



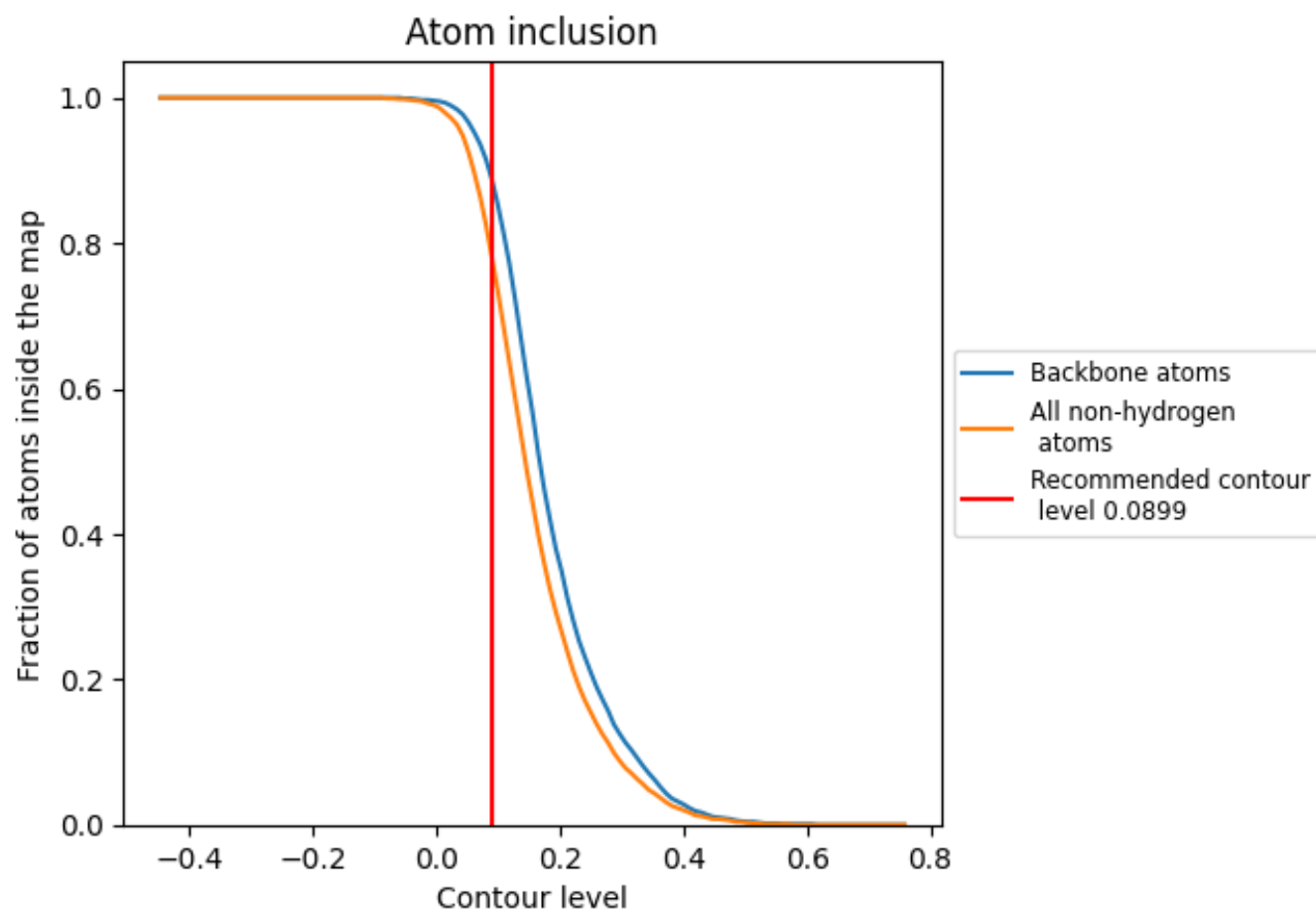
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0899).

9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0899) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7790	0.3290
A	0.7790	0.3290

