



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 03:48 PM UTC

PDB ID : 8U8B / pdb_00008u8b
EMDB ID : EMD-42020
Title : Cryo-EM structure of LRRK2 bound to type II inhibitor rebastinib
Authors : Zhu, H.; Sun, J.
Deposited on : 2023-09-16
Resolution : 3.70 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

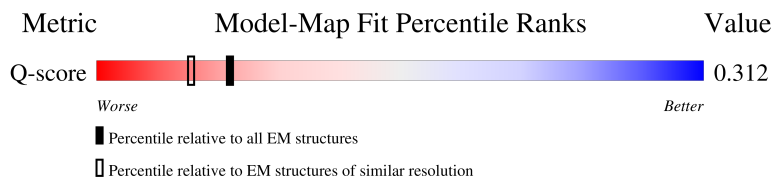
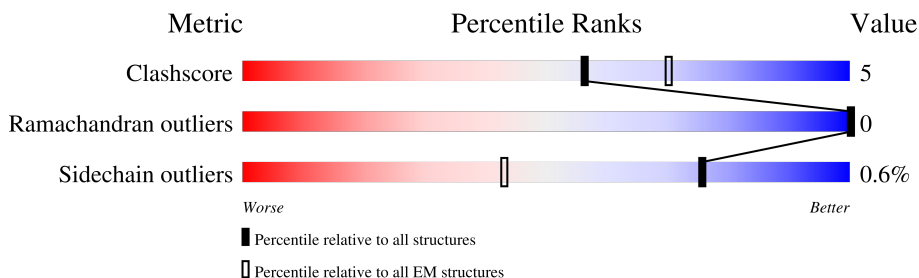
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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	24% 60% 8% 32%
1	B	2527	23% 60% 8% 32%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 24694 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.

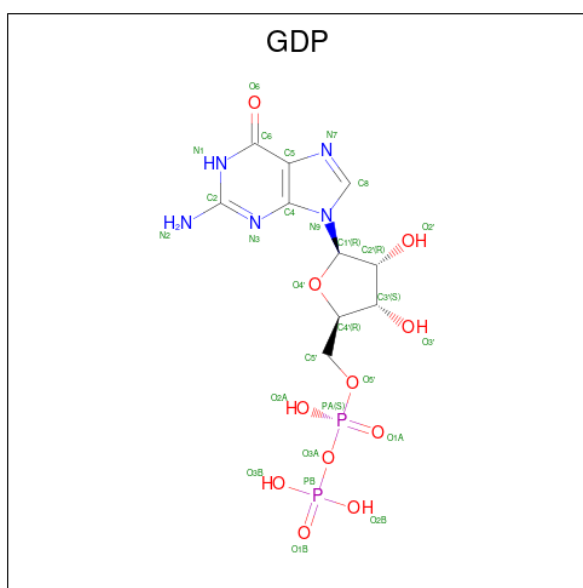
- Molecule 1 is a protein called Leucine-rich repeat serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1712	Total	C	N	O	S	0	0
			12278	7922	2090	2194	72		
1	B	1712	Total	C	N	O	S	0	0
			12278	7922	2090	2194	72		

There are 6 discrepancies between the modelled and reference sequences:

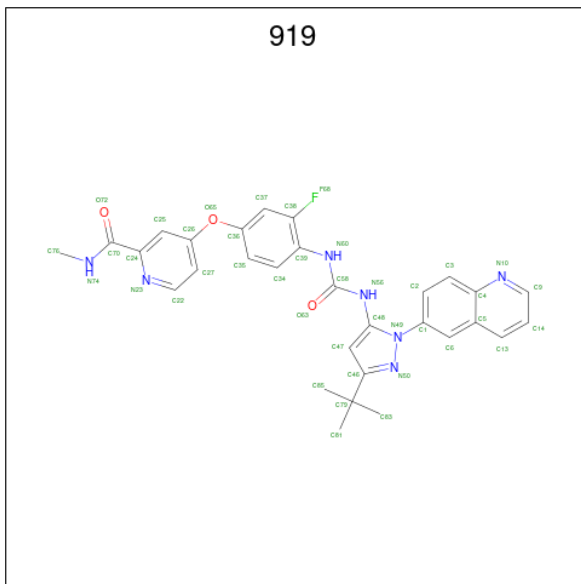
Chain	Residue	Modelled	Actual	Comment	Reference
A	50	HIS	ARG	conflict	UNP Q5S007
A	1647	THR	SER	conflict	UNP Q5S007
A	2397	THR	MET	conflict	UNP Q5S007
B	50	HIS	ARG	conflict	UNP Q5S007
B	1647	THR	SER	conflict	UNP Q5S007
B	2397	THR	MET	conflict	UNP Q5S007

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

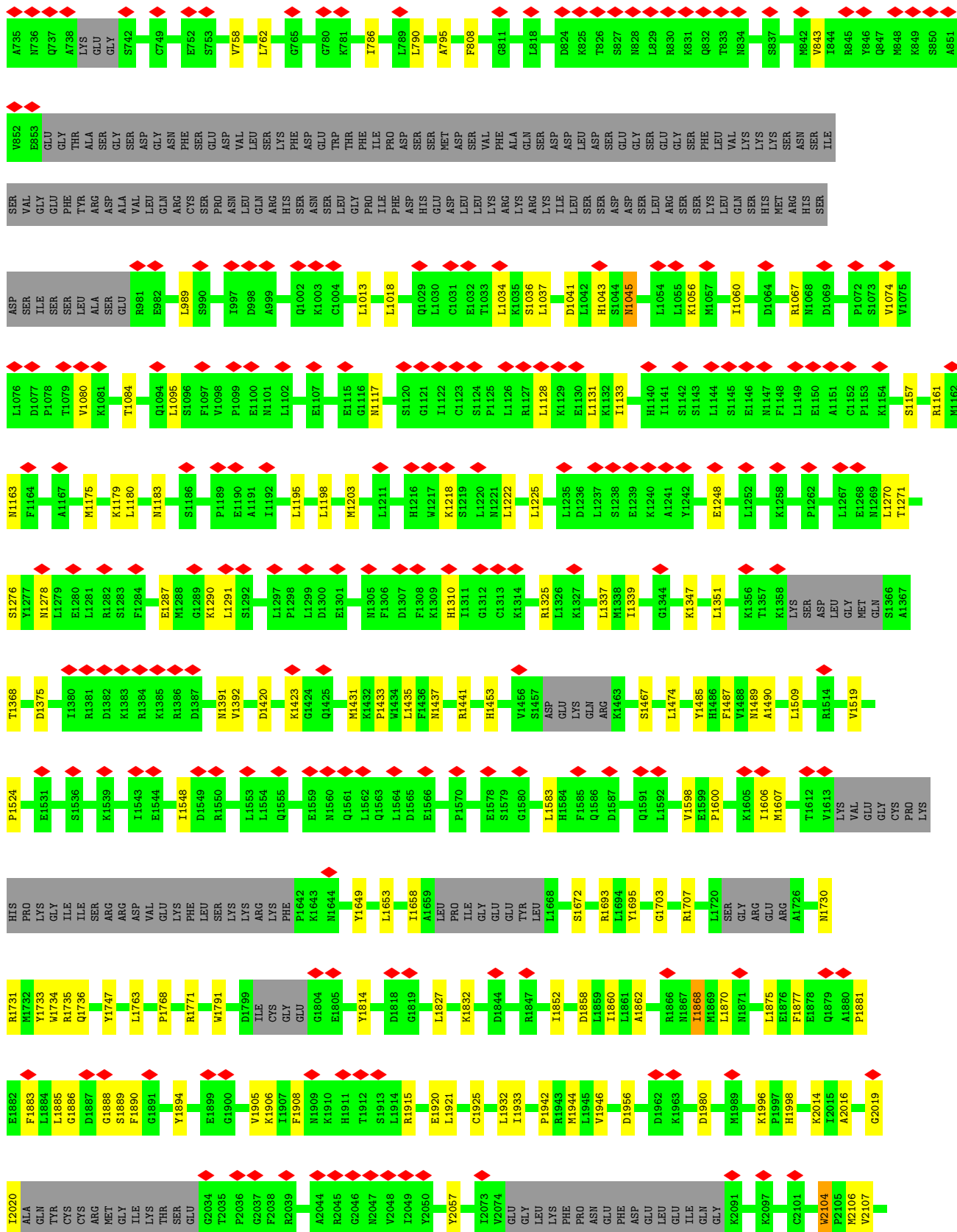


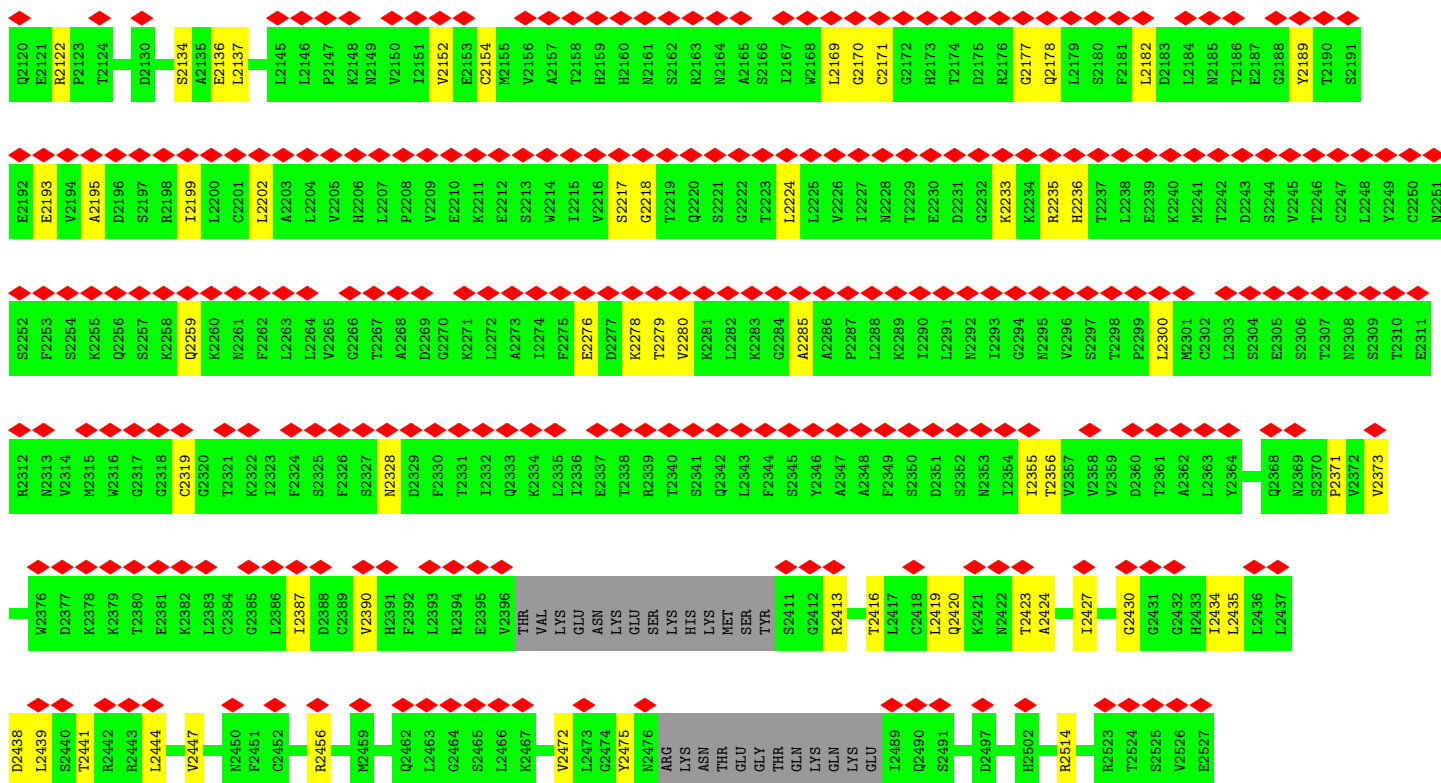
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			28	10	5	11	2	
2	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 3 is 4-[4-({[3-tert-butyl-1-(quinolin-6-yl)-1H-pyrazol-5-yl]carbamoyl}amino)-3-fluorophenoxy]-N-methylpyridine-2-carboxamide (CCD ID: 919) (formula: C₃₀H₂₈FN₇O₃) (labeled as "Ligand of Interest" by depositor).

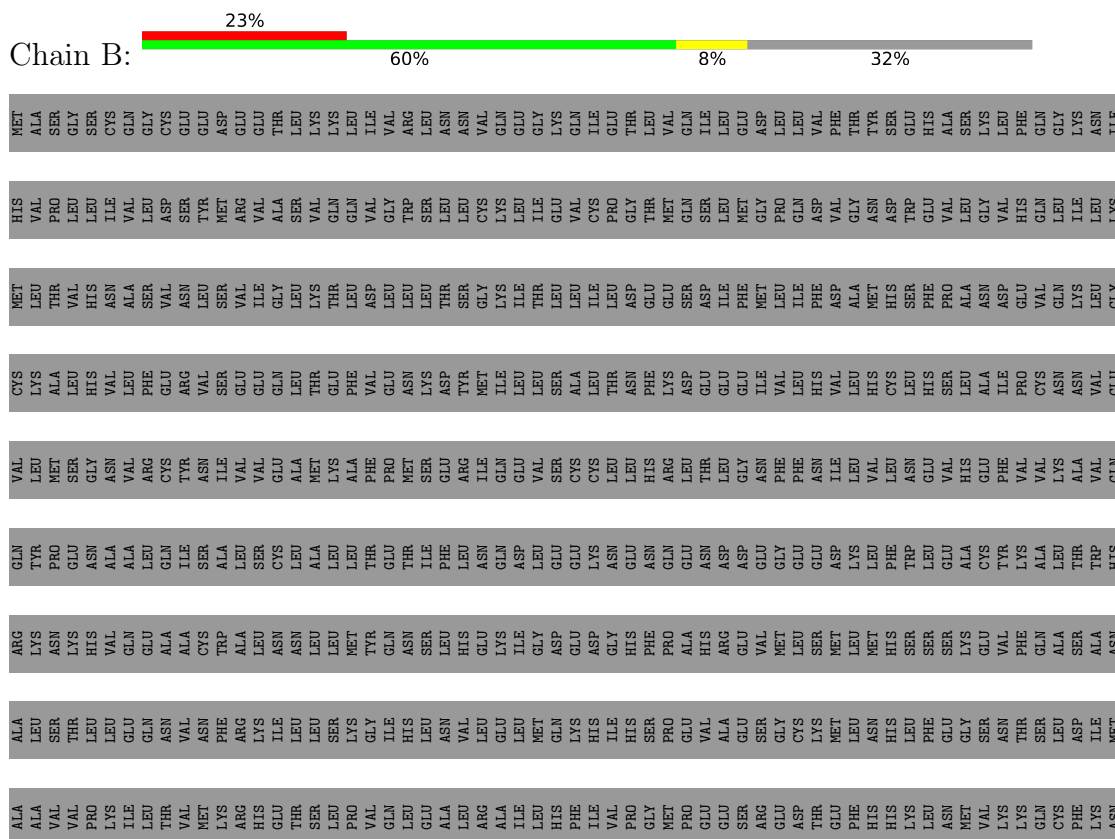


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	F	N	O	0
			41	30	1	7	3	
3	B	1	Total	C	F	N	O	0
			41	30	1	7	3	

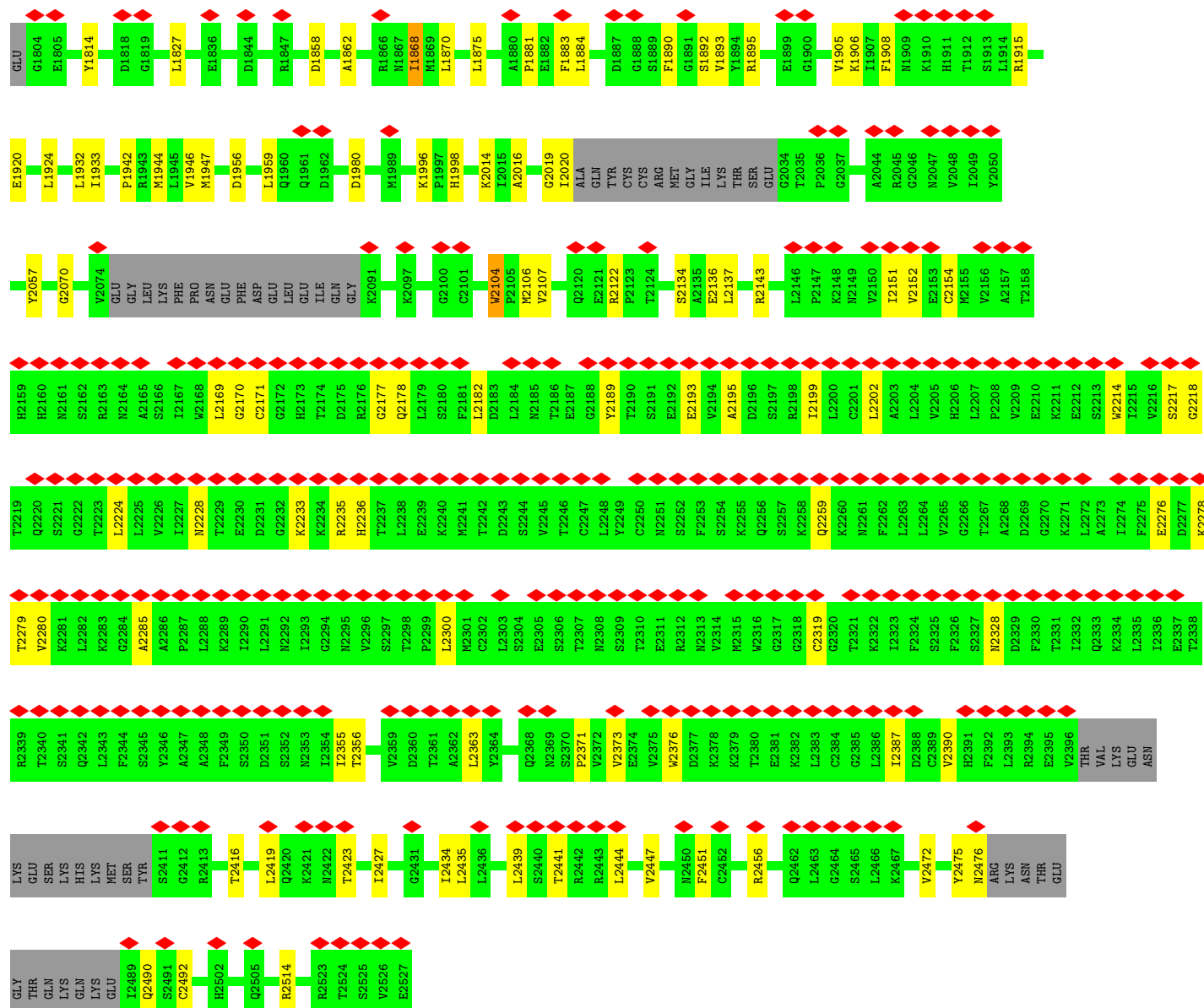




- Molecule 1: Leucine-rich repeat serine/threonine-protein kinase 2



ASP	ILE	HIS	LYS	LEU	VAL	LEU	ALA	ALA	ASN	ARG	PHE	ILE	GLY	ASN	PRO	G558	I559	Q560	K561	C562	G563	L564	K565	V566	I567	S568	S569	I570	V571	H572	F573	P574	D575	A576	L577	GLU	MET	LEU	LEU	LEU	GLU	G584	A585	M586	D587	S588	V589	L593	Q594	M595	Y596	F597	D598	D599	Q600	E601	I602								
Q603	C604	L605	S608	L609	I610	G611	Y612	LEU	ILE	THR	LYS	LYS	ASN	VAL	PHE	ILE	G623	G624	Q625	H626	L627	I630	S633	S634	L635	Y636	G637	F638	K639	D640	V641	A642	E643	T646	F649	I652	I655	L656	K657	L658	S659	A660	S661	F662	S663	K664	V667	H668	H669	S670															
F671	D672	L673	V674	I675	F676	H677	S680	S681	N682	I683	M684	E685	Q686	K687	D688	Q689	Q690	F691	L692	N693	L694	C695	C696	K697	C698	F699	A700	A703	M704	D705	D706	Y707	L708	K709	N710	L713	E714	N715	A716	C717	D718	Q719	N720	N721	S722	E726	L729	L730	Q732	A733	D734	N735													
Q737	A738	LYS	GLU	GLY	S742	C749	E750	K751	E752	V753	L762	G765	R772	T776	I777	S778	I779	G780	K781	G782	D783	I786	L790	A795	N801	F808	G811	L818	D824	K825	T826	S827	N828	L829	R830	K831	Q832	T833	N834	S837	M842	I844																							
R846	Y846	Q847	M848	K849	S850	A851	V852	E853	GLU	GLY	THR	ARG	ALA	SER	GLY	SER	ASP	GLY	ASN	PHE	SER	PRO	ASN	GLU	VAL	SER	LEU	HIS	SER	LYS	ASN	PHE	ASP	LEU	GLY	TRP	PHE	ILE	PRO	ASP	HIS	GLU	ASP	LEU	LEU	LYS	MET	ASP	VAL	PHE	ALA	GLN	SER	ASP	ASP	LEU	SER	GLU	GLY	SER	GLU	GLY	PHE	LEU	VAL
LYS	LYS	LYS	SER	ASN	SER	ILE	SER	VAL	GLY	ILE	PHE	TYR	ARG	ASP	ALA	VAL	GLN	ARG	CYS	SER	PRO	ASN	GLU	GLN	ARG	HIS	SER	LYS	ASN	PHE	SER	LEU	GLY	PRO	ILE	PHE	ILE	ASP	HIS	GLU	ASP	LEU	LEU	LYS	MET	ASP	VAL	PHE	ALA	GLN	SER	ASP	ASP	LEU	SER	GLU	GLY	SER	GLU	GLY	PHE	LEU	VAL		
GLN	SER	HIS	MET	ARG	HIS	SER	ASP	SER	ILE	SER	SER	LEU	ALA	SER	GLU	R881	D988	A989	Q1002	K1003	C1004	E1011	K1015	L1023	Q1029	L1034	L1037	D1041	L1042	H1043	N1044	N1045	T1048	L1054	L1055	K1056	R1067	N1068	D1069	P1072	S1073	V1074	V1075	L1076	D1077	P1078																			
T1079	V1080	K1081	L1085	N1093	Q1094	S1096	F1097	V1098	P1099	L1102	E1107	K1108	L1109	N1117	K1118	I1119	S1120	G1121	I1122	C1123	S1124	R1127	L1128	K1129	L1130	L1131	K1132	I1133	N1139	H1140	I1141	S1142	S1143	L1144	S1145	E1146	N1147	F1148	L1149	E1150	A1151	C1152	P1153	K1154	S1157	R1161	M1162	N1163	F1164																
A1167	S1174	M1175	K1179	N1183	C1187	T1188	P1189	E1190	A1191	I1192	L1195	L1198	L1201	D1202	H1216	W1217	K1218	S1219	L1220	N1221	L1222	L1225	L1235	D1236	L1237	S1238	E1239	K1240	A1241	Y1242	L1243	E1248	L1252	L1257	P1262	E1263	C1266	L1270	D1274	V1275	S1276																								
Y1277	N1278	R1282	K1290	L1291	D1300	F1306	D1307	F1308	K1309	H1310	C1313	K1314	A1315	K1316	R1320	Q1323	L1326	K1327	L1337	M1338	I1339	K1347	L1351	K1356	T1357	K1358	LYS	SER	ASP	LEU	GLY	MET	S1366	A1367	T1368	D1375	I1380	R1381	D1382	K1383	R1384	K1385	R1386	D1387																					
L1388	M1391	V1392	E1400	D1420	K1423	M1431	K1432	P1433	W1434	L1435	F1436	N1437	R1441	H1453	L1454	D1455	V1456	S1457	ASP	GLU	LYS	GLN	ARG	K1463	S1467	K1471	L1474	Y1485	H1486	F1487	V1488	N1489	A1490	D1495	L1509	V1519	E1529	S1536	H1540	I1543																									
I1548	D1549	Q1555	E1559	N1560	Q1561	L1562	Q1563	L1564	E1578	L1583	Q1586	D1587	L1592	V1598	E1599	P1600	T1606	M1607	T1612	V1613	VAL	GLU	GLY	CYS	PRO	LYS	HIS	PRO	LYS	LYS	GLY	ILE	SER	ARG	ASP	VAL	GLU	PHE	SER	LYS	LYS	ARG	PHE	P1642	K1643																				
N1644	L1653	I1658	A1659	PRO	ILE	GLY	GLU	GLU	TYR	L1668	S1672	L1673	H1684	R1693	L1694	Y1695	G1703	R1707	R1711	L1720	SER	GLY	ARG	GLU	ARG	A1726	W1734	R1735	Q1736	P1744	Y1747	L1763	P1768	R1771	W1791	I1798	D1799	ILE	CYS	GLY																									



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75005	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	67.53	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.862	Depositor
Minimum map value	-2.223	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.8	Depositor
Map size ($\text{\AA}$)	498.04803, 498.04803, 498.04803	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.297, 1.297, 1.297	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 919

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	0.14	0/12507	0.41	0/17088
1	B	0.15	0/12507	0.42	0/17088
All	All	0.15	0/25014	0.42	0/34176

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2104	TRP	Peptide
1	B	2104	TRP	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	12278	0	11696	122	0
1	B	12278	0	11696	115	0
2	A	28	0	12	1	0
2	B	28	0	12	1	0
3	A	41	0	28	3	0
3	B	41	0	28	3	0
All	All	24694	0	23472	237	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 5.

The worst 5 of 237 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:B:1933:ILE:HD13	1:B:2014:LYS:HD2	1.77	0.67
1:B:1161:ARG:O	1:B:1163:ASN:ND2	2.28	0.67
1:A:1933:ILE:HD13	1:A:2014:LYS:HD2	1.77	0.66
1:B:2427:ILE:HB	1:B:2435:LEU:HB2	1.78	0.66
1:A:1161:ARG:O	1:A:1163:ASN:ND2	2.29	0.65

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	1066/2527 (42%)	984 (92%)	82 (8%)	0	100	100
1	B	1682/2527 (67%)	1559 (93%)	123 (7%)	0	100	100
All	All	2748/5054 (54%)	2543 (92%)	205 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	1202/2281 (53%)	1195 (99%)	7 (1%)	78	79
1	B	1202/2281 (53%)	1194 (99%)	8 (1%)	76	77
All	All	2404/4562 (53%)	2389 (99%)	15 (1%)	76	79

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1310	HIS
1	B	1915	ARG
1	B	1485	TYR
1	B	2020	ILE
1	B	1892	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1045	ASN
1	B	1229	HIS
1	B	1093	ASN
1	B	1710	ASN
1	A	1425	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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$
2	GDP	B	2601	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	6 (13%)
2	GDP	A	2601	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	6 (13%)
3	919	A	2602	-	45,45,45	2.15	7 (15%)	64,65,65	2.10	18 (28%)
3	919	B	2602	-	45,45,45	2.15	8 (17%)	64,65,65	2.08	18 (28%)

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	GDP	B	2601	-	-	2/16/32/32	0/3/3/3
2	GDP	A	2601	-	-	2/16/32/32	0/3/3/3
3	919	A	2602	-	-	4/28/28/28	0/5/5/5
3	919	B	2602	-	-	4/28/28/28	0/5/5/5

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2602	919	C70-N74	8.92	1.45	1.33
3	B	2602	919	C70-N74	8.85	1.45	1.33
3	A	2602	919	C48-N56	5.37	1.47	1.39
3	B	2602	919	C48-N56	5.35	1.47	1.39
3	A	2602	919	C58-N60	4.44	1.47	1.37

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2602	919	C24-C70-N74	8.09	121.10	115.56
3	A	2602	919	C24-C70-N74	8.03	121.06	115.56
2	A	2601	GDP	C5-C4-N3	-6.28	118.40	128.39
2	B	2601	GDP	C5-C4-N3	-6.27	118.41	128.39
2	A	2601	GDP	C2-N3-C4	5.09	121.06	112.30

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

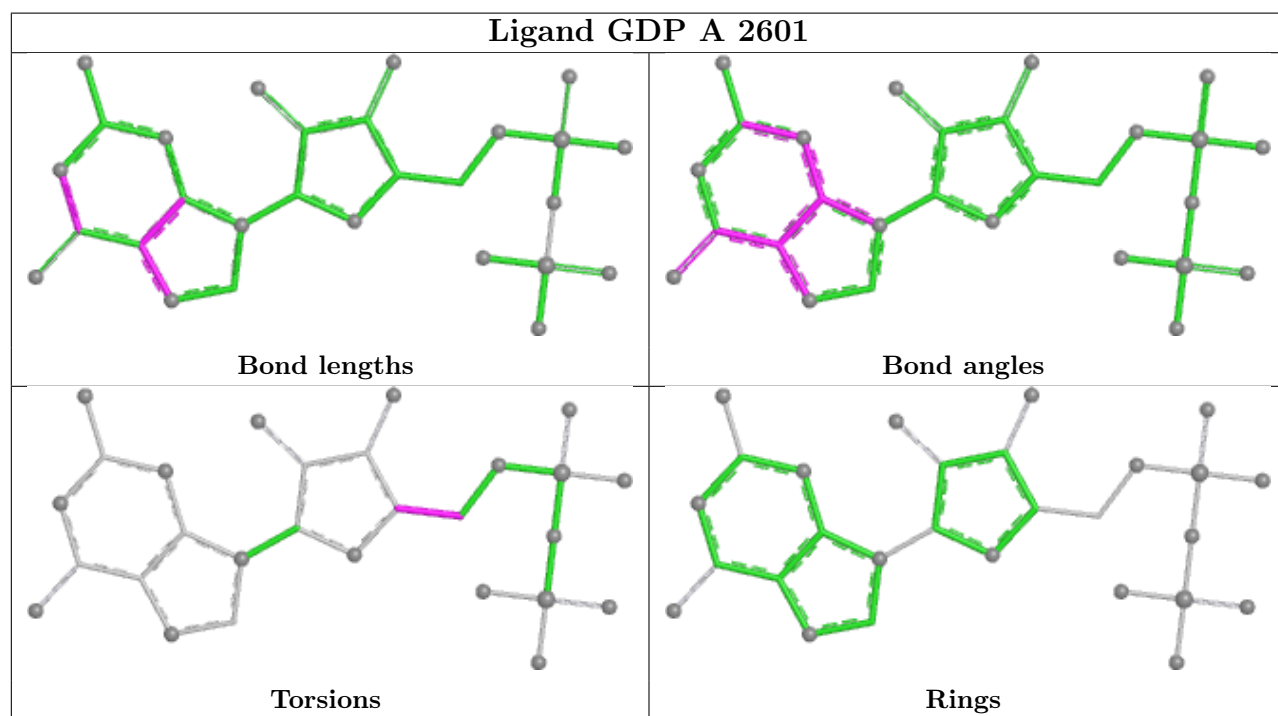
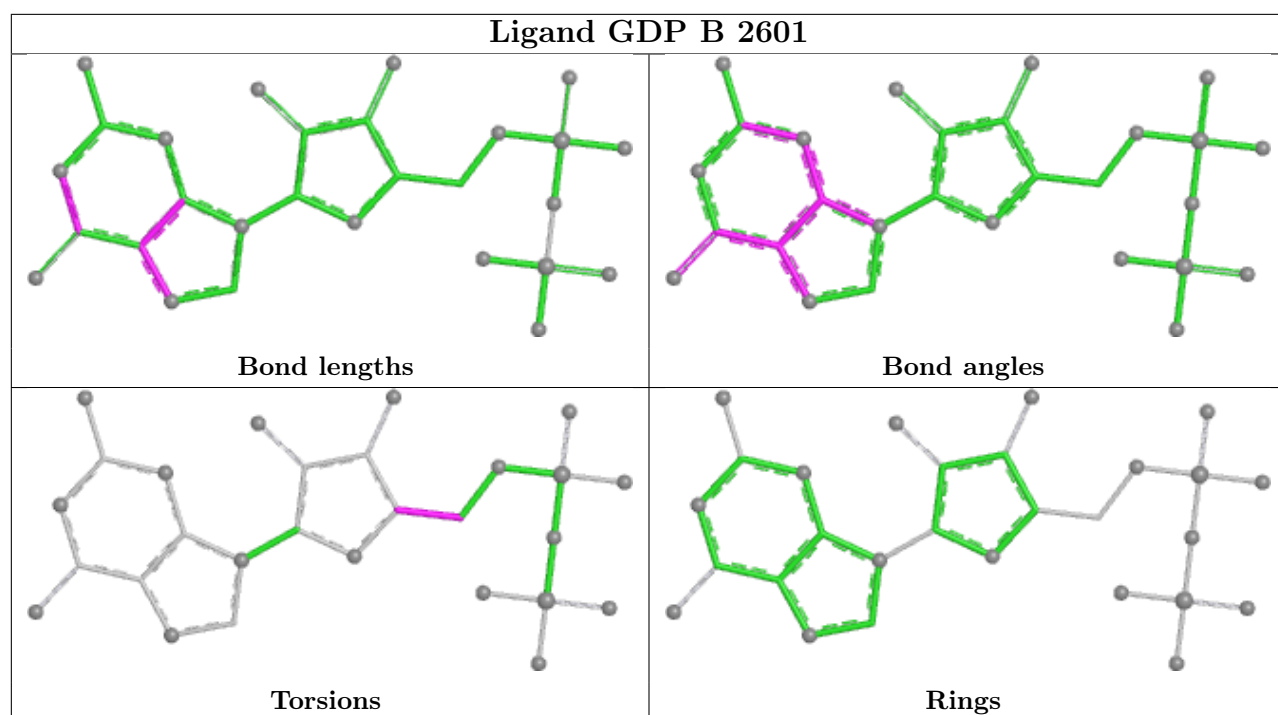
Mol	Chain	Res	Type	Atoms
2	A	2601	GDP	C3'-C4'-C5'-O5'
2	B	2601	GDP	C3'-C4'-C5'-O5'
3	B	2602	919	C2-C1-N49-N50
3	A	2602	919	C2-C1-N49-N50
3	B	2602	919	C6-C1-N49-N50

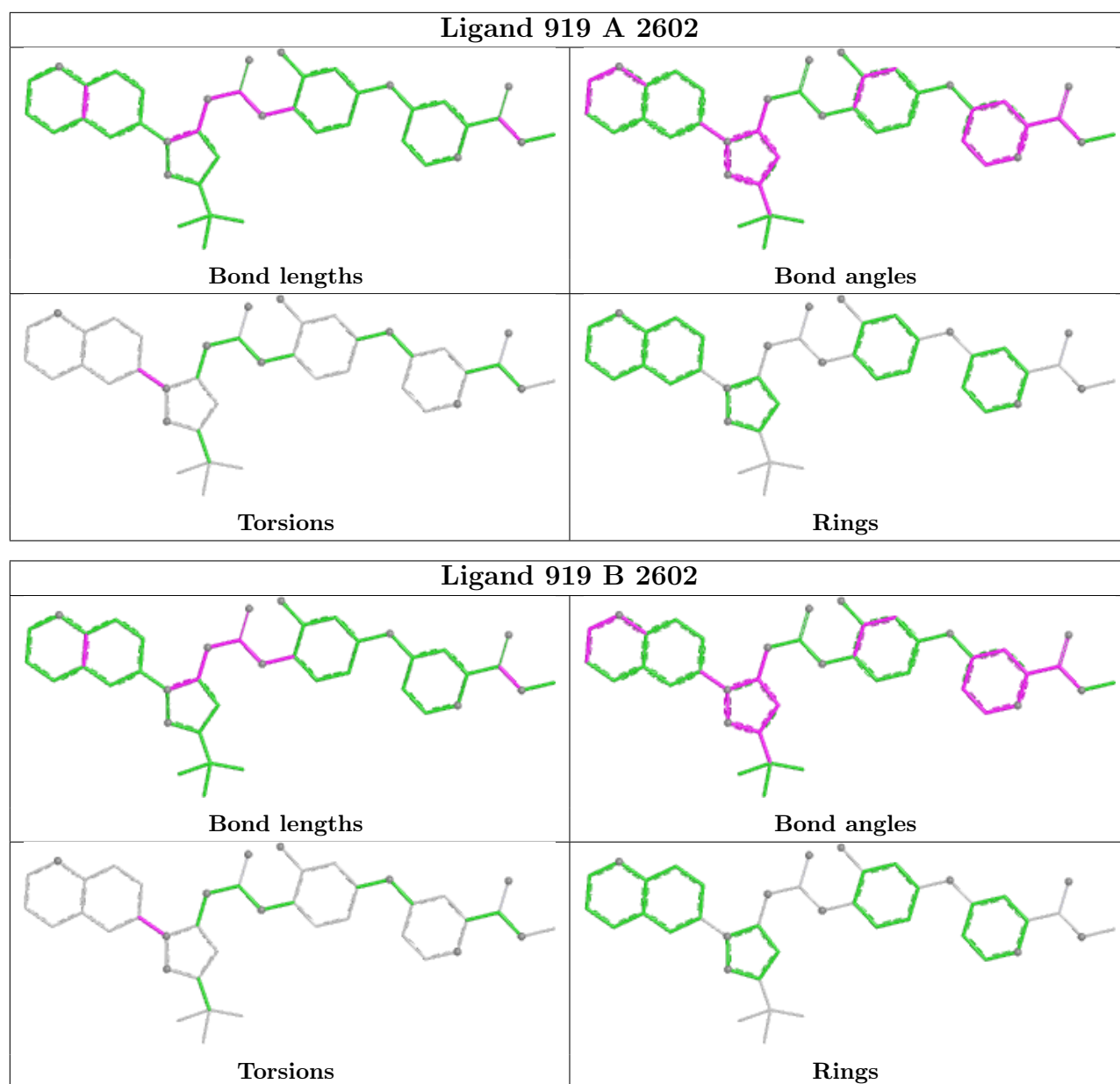
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2601	GDP	1	0
2	A	2601	GDP	1	0
3	A	2602	919	3	0
3	B	2602	919	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

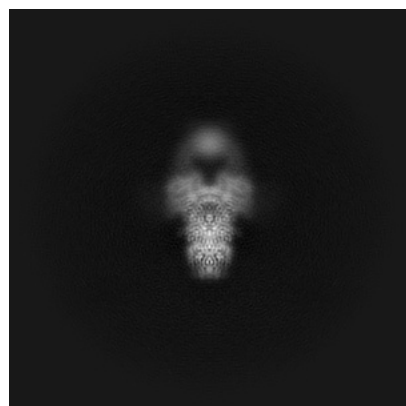
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42020. These allow visual inspection of the internal detail of the map and identification of artifacts.

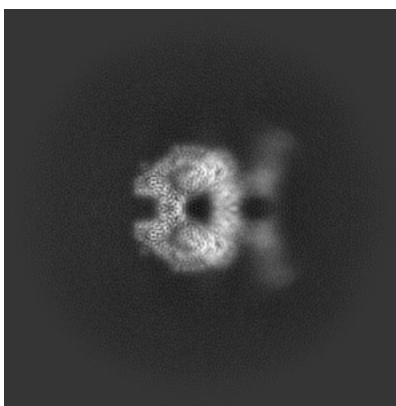
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

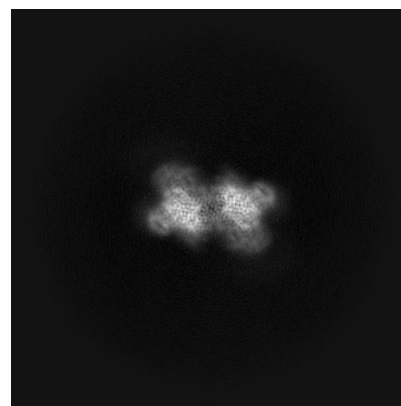
6.1.1 Primary map



X

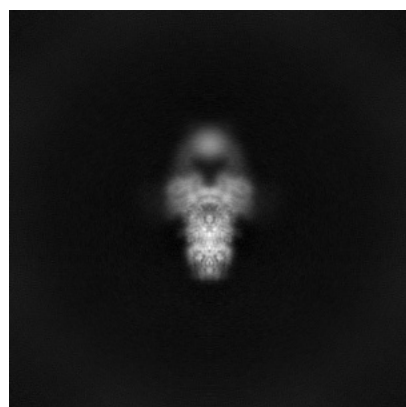


Y

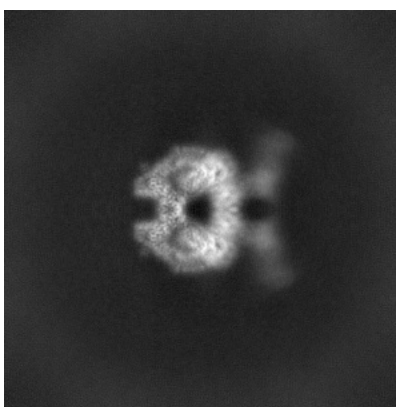


Z

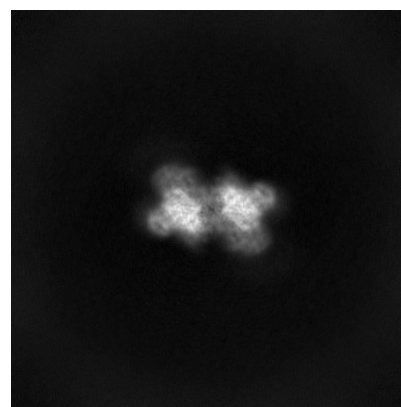
6.1.2 Raw map



X



Y

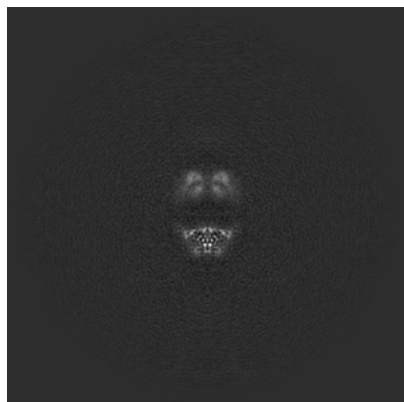


Z

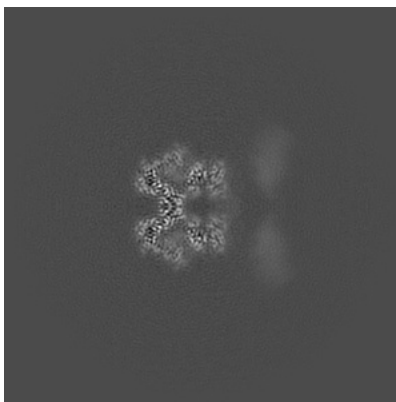
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

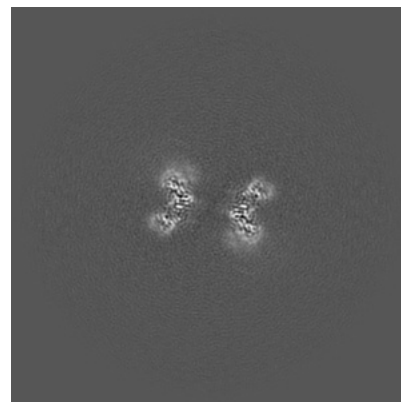
6.2.1 Primary map



X Index: 192

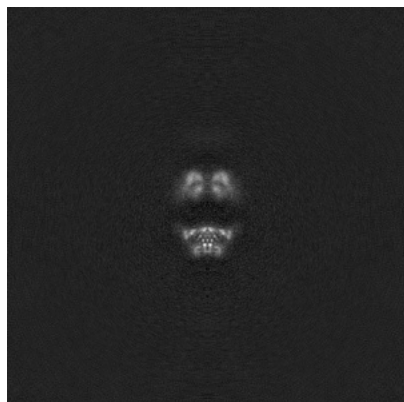


Y Index: 192

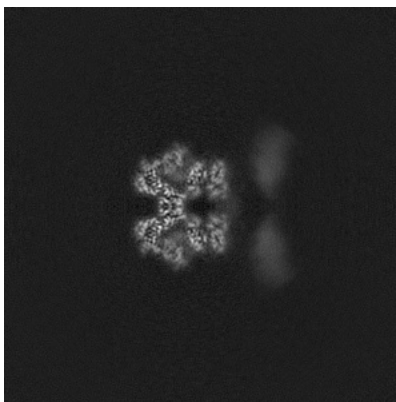


Z Index: 192

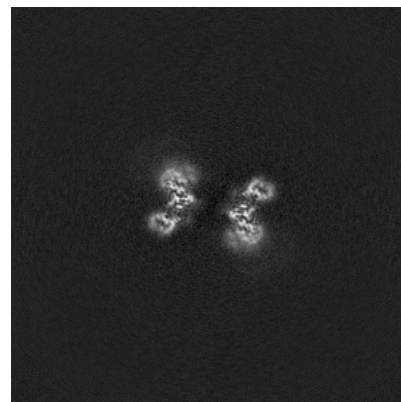
6.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

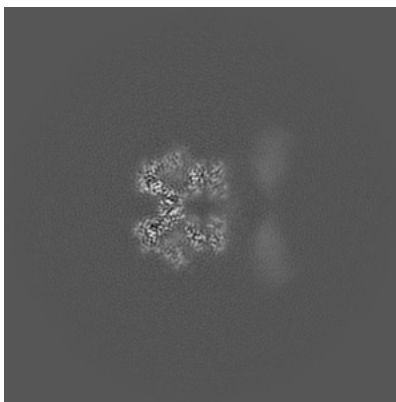
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

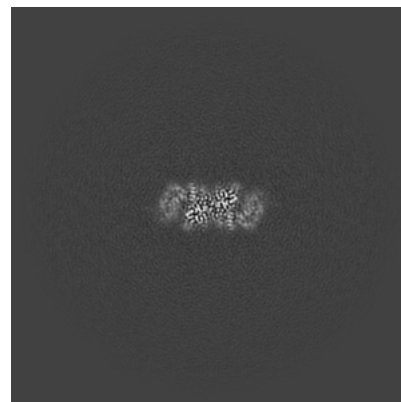
6.3.1 Primary map



X Index: 170

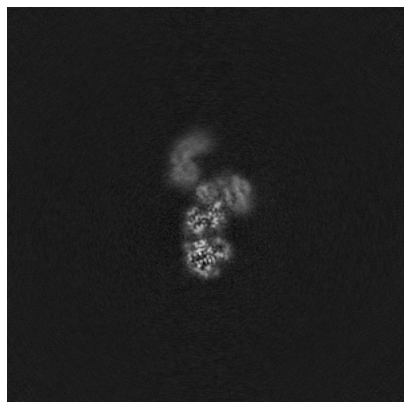


Y Index: 191

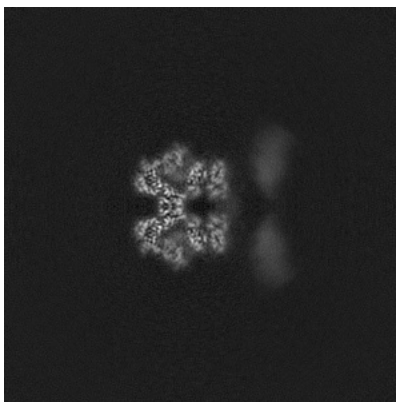


Z Index: 154

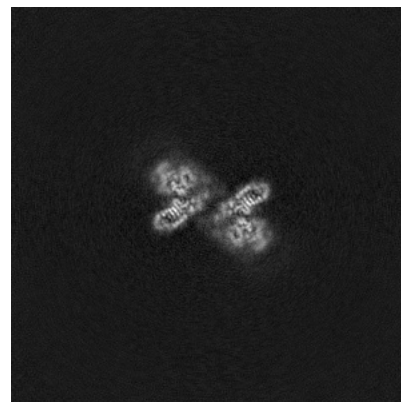
6.3.2 Raw map



X Index: 170



Y Index: 192

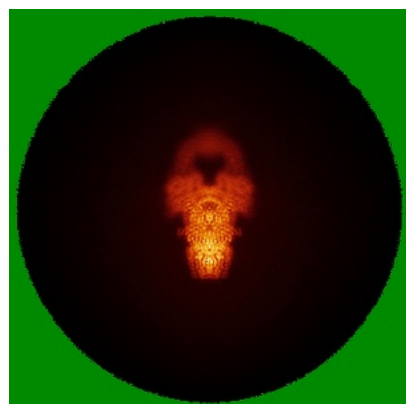


Z Index: 200

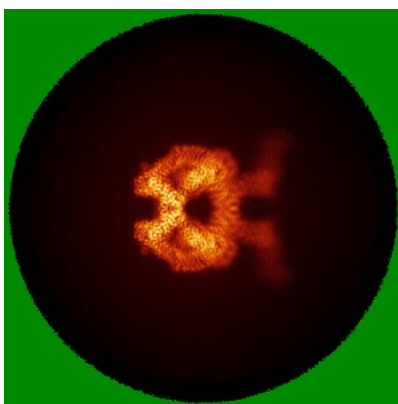
The images above show the largest variance slices of the map in three orthogonal directions.

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

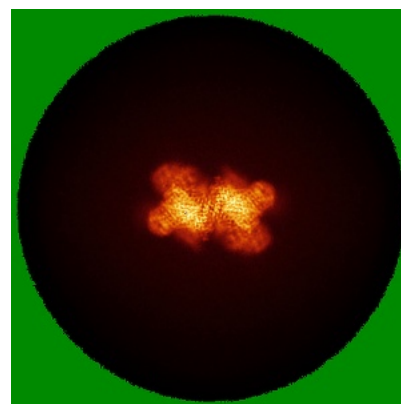
6.4.1 Primary map



X



Y

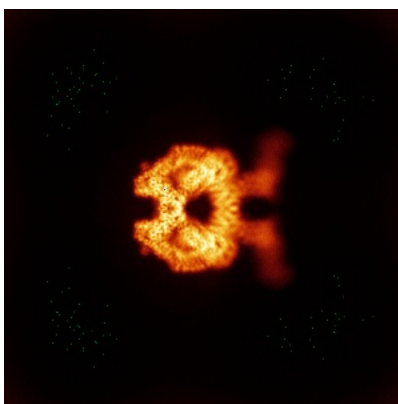


Z

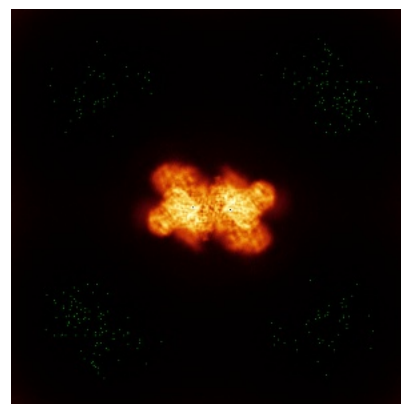
6.4.2 Raw map



X



Y

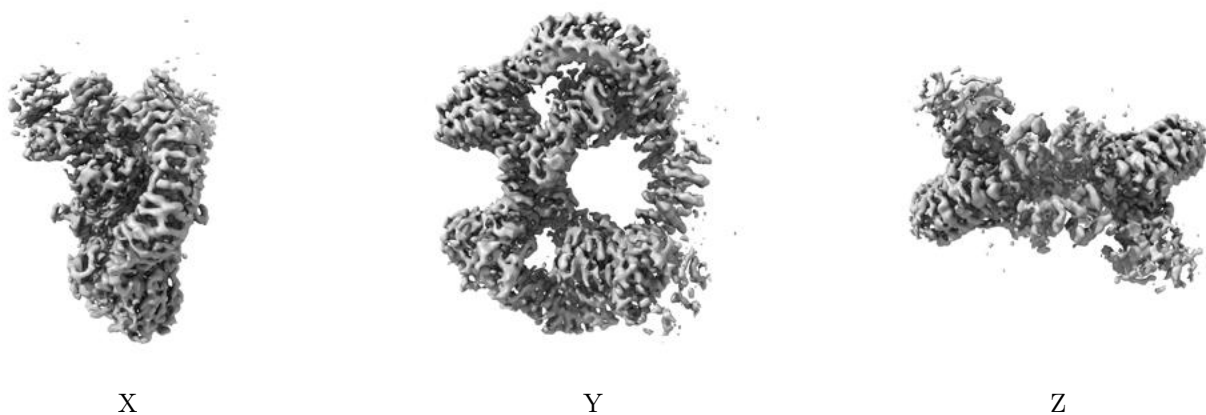


Z

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.

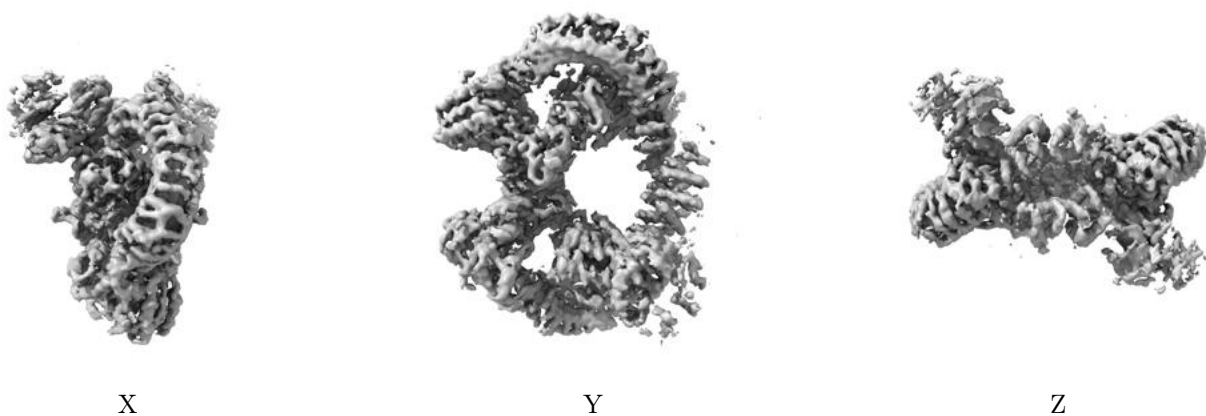
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.8. 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.

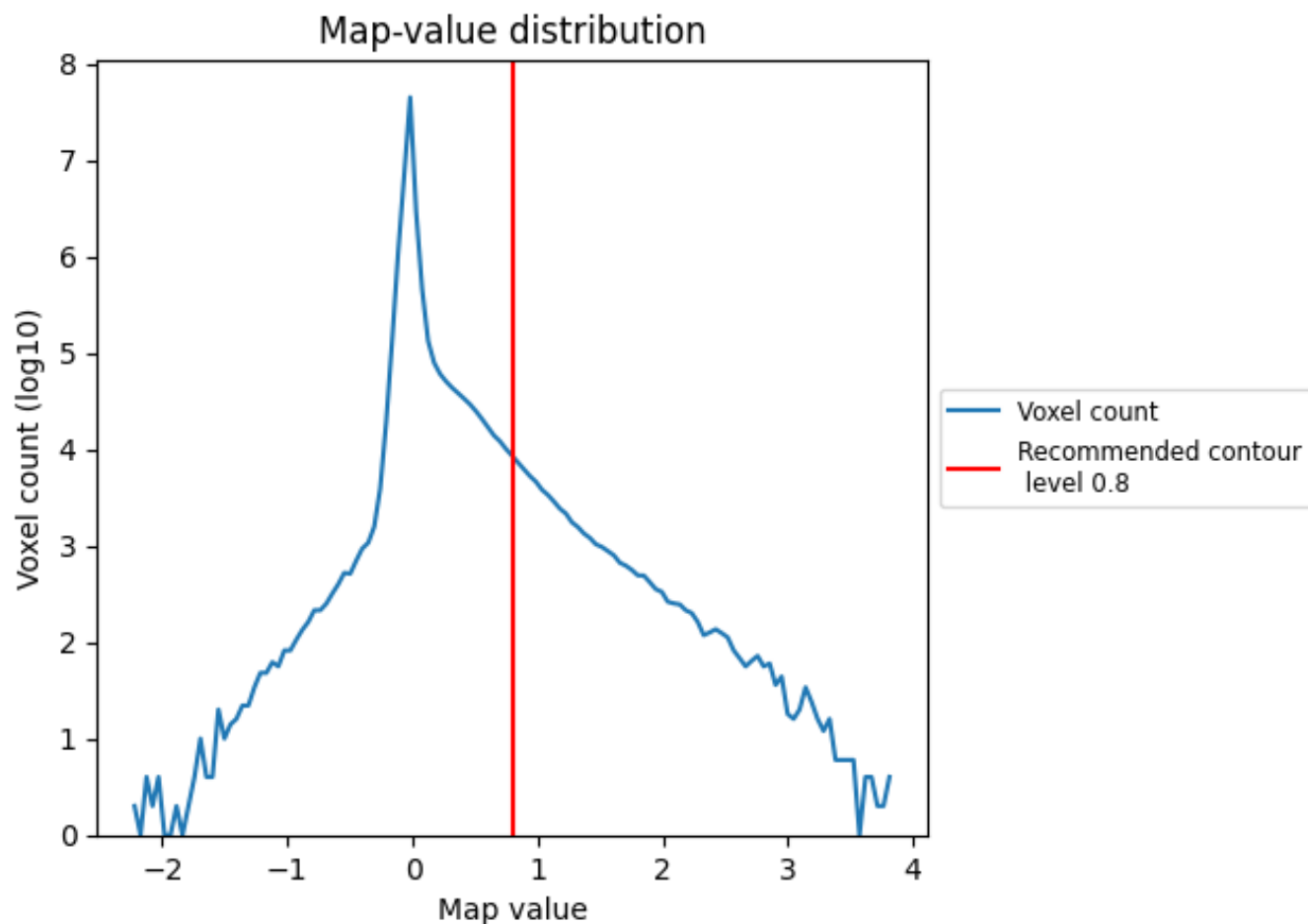
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

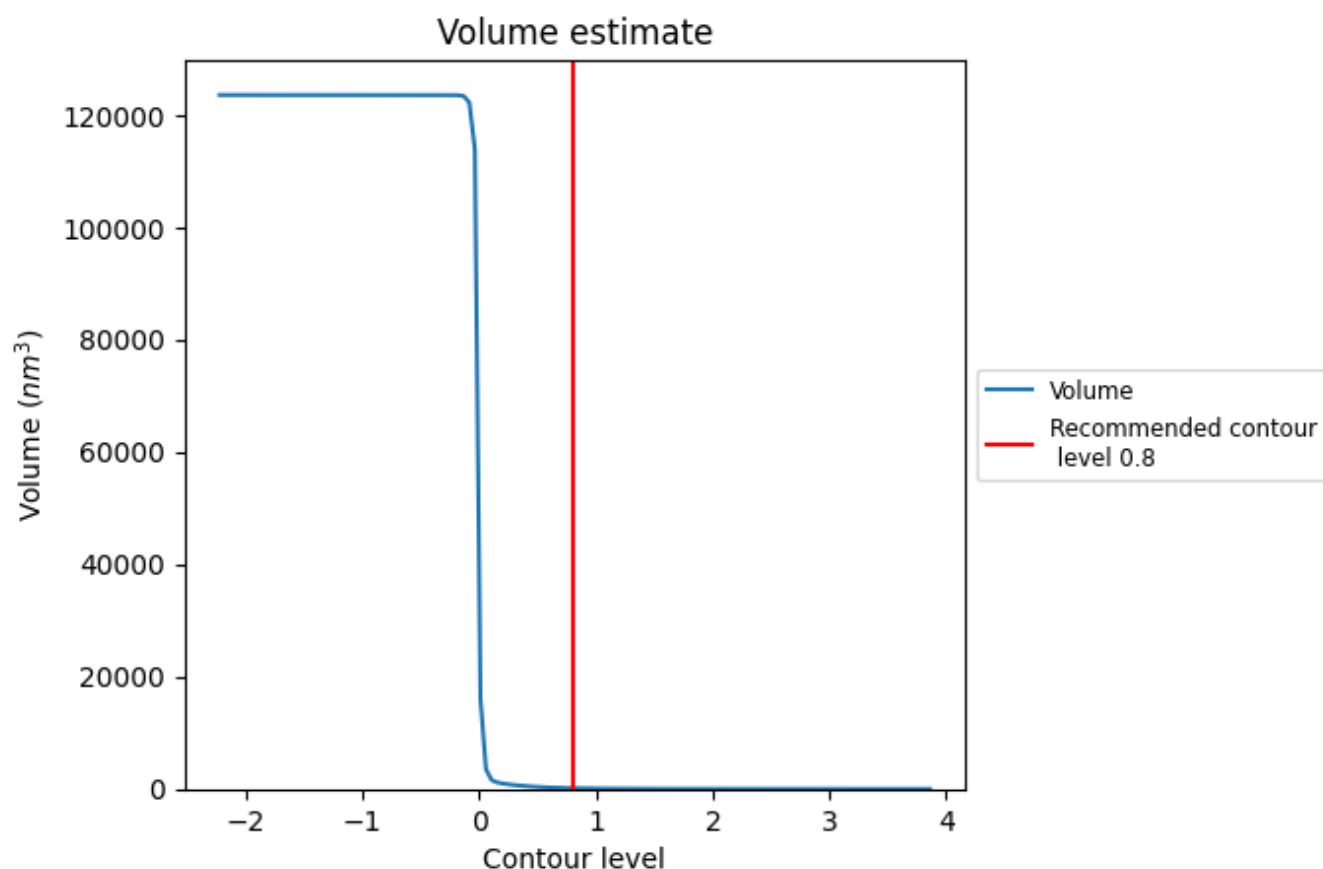
This section contains the results of statistical analysis of the map.

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.

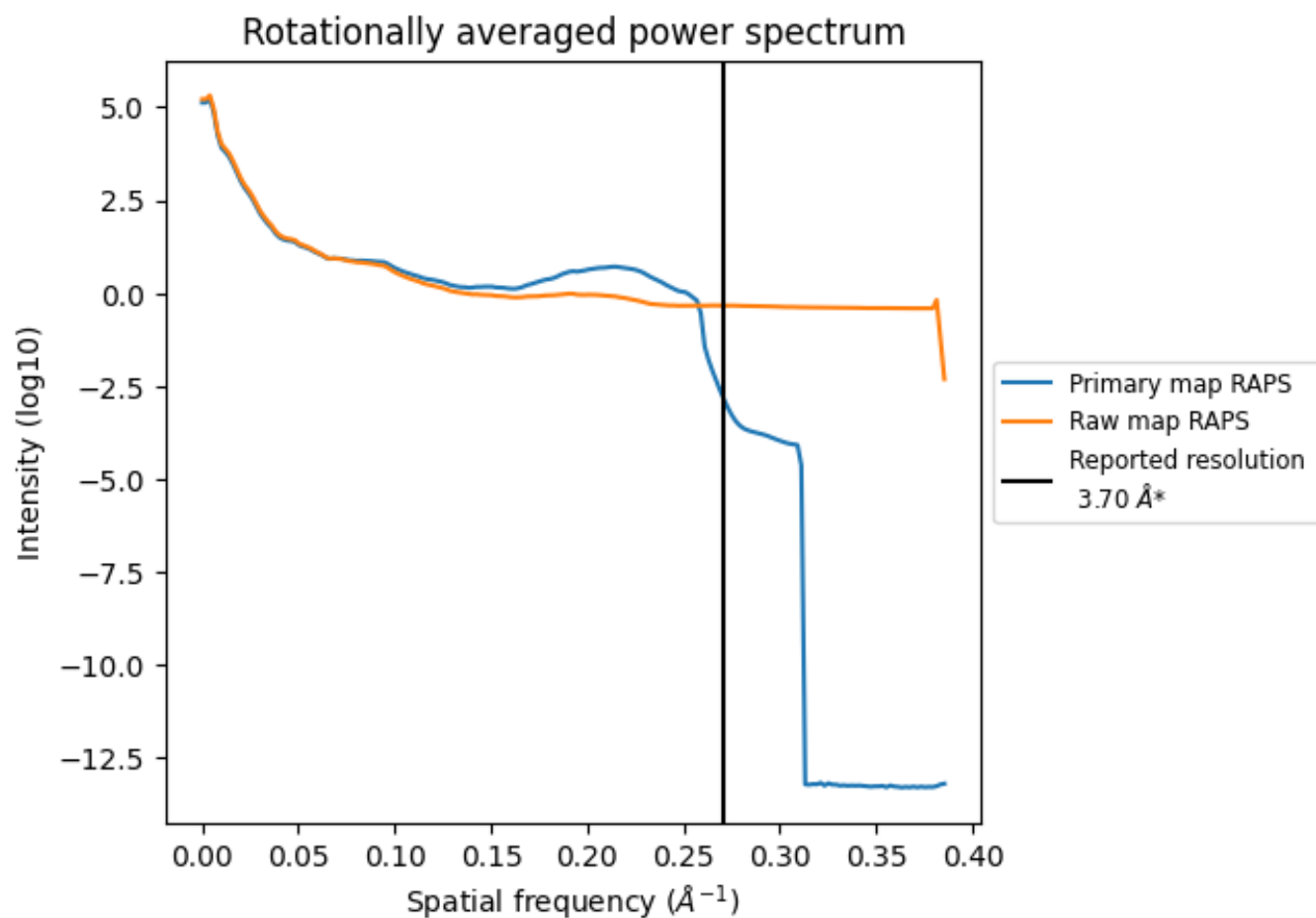
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 135 nm³; this corresponds to an approximate mass of 122 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 ⓘ

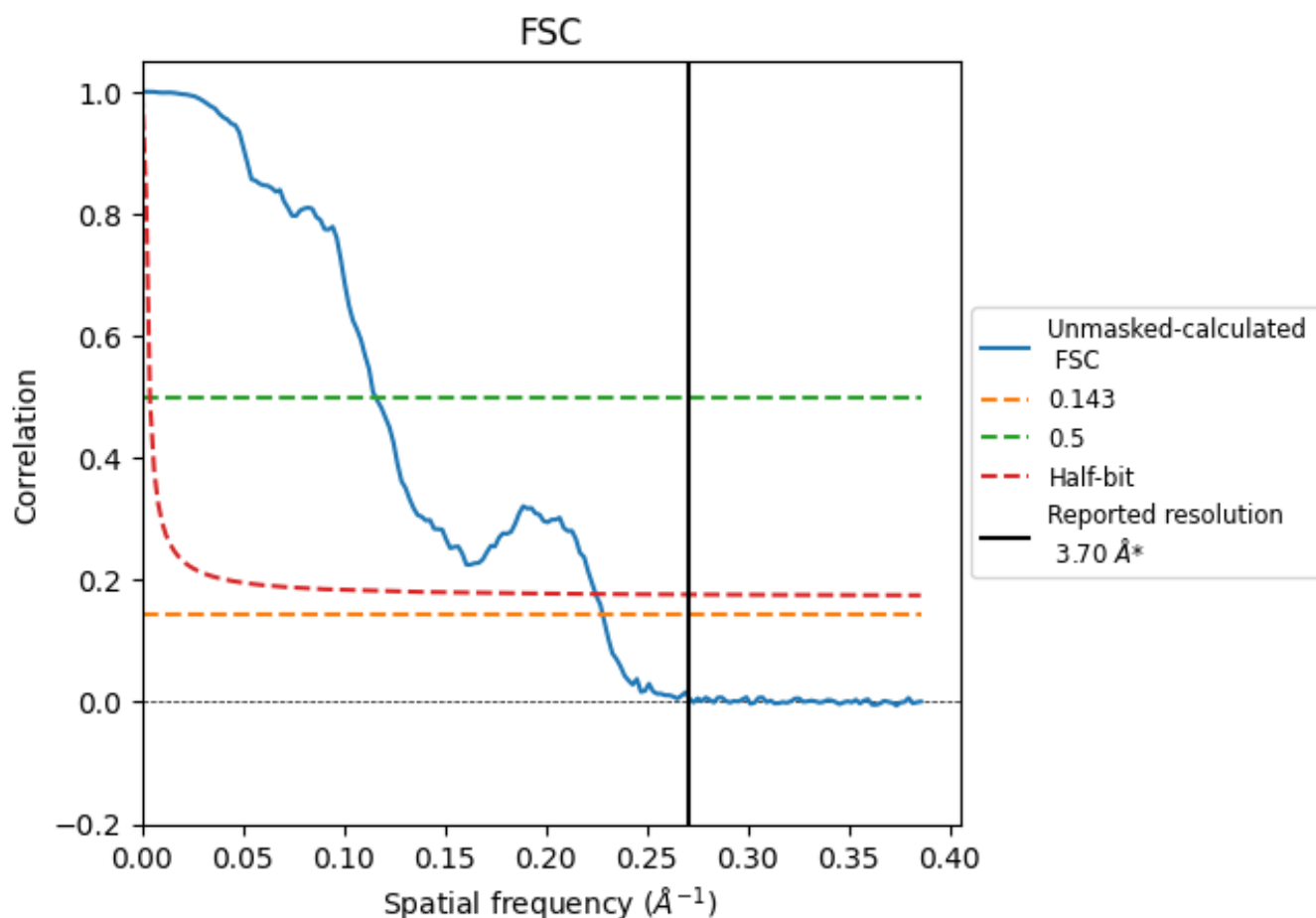


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

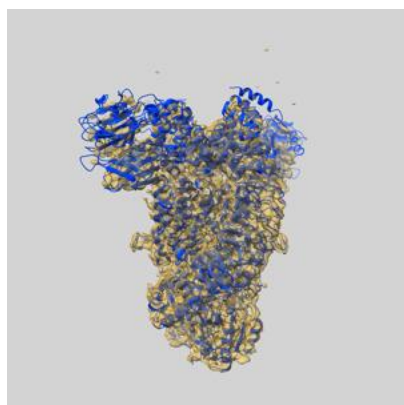
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.38	8.66	4.45

*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 4.38 differs from the reported value 3.7 by more than 10 %

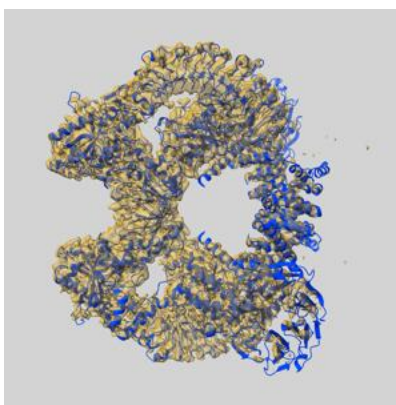
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42020 and PDB model 8U8B. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

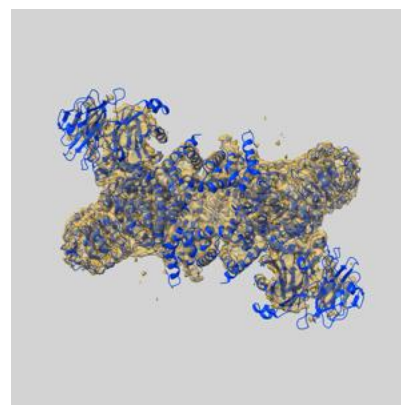
9.1 Map-model overlay [i](#)



X



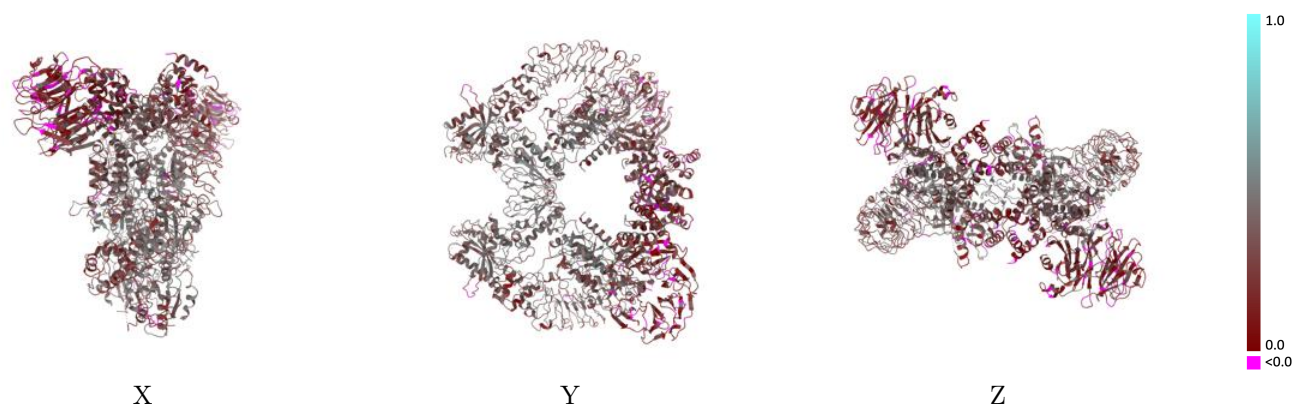
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8 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](#)

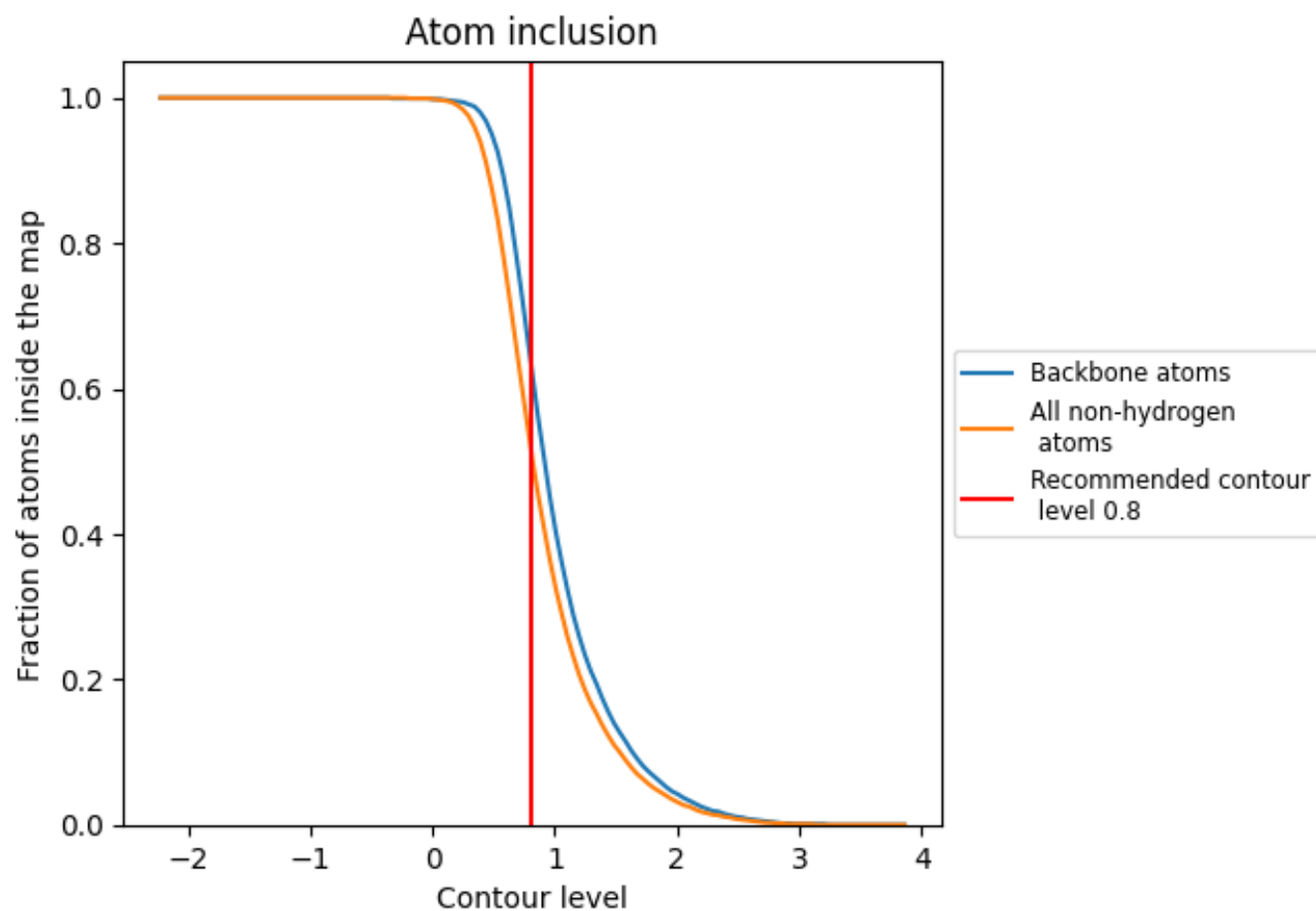


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 52% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5230	0.3120
A	0.5210	0.3060
B	0.5250	0.3170

