



wwPDB EM Validation Summary Report ⓘ

Nov 11, 2024 – 08:18 AM JST

PDB ID : 5YKE
EMDB ID : EMD-6831
Title : Structure of pancreatic ATP-sensitive potassium channel bound with glibenclamide and ATPgammaS (focused refinement on TM at 4.11Å)
Authors : Chen, L.; Wu, J.X.
Deposited on : 2017-10-14
Resolution : 4.11 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

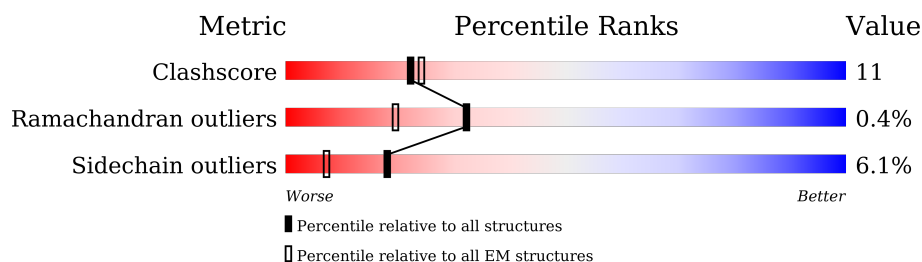
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.11 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	390	 20% 13% 66%
1	C	390	 19% 13% 66%
1	E	390	 20% 13% 66%
1	G	390	 20% 13% 66%
2	B	1582	 7% 40% 12% 47%
2	D	1582	 7% 40% 12% 47%
2	F	1582	 7% 40% 12% 47%
2	H	1582	 7% 40% 12% 47%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30636 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.

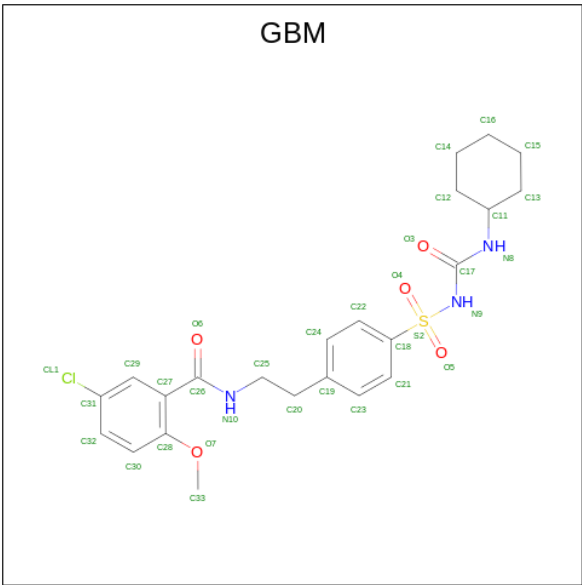
- Molecule 1 is a protein called ATP-sensitive inward rectifier potassium channel 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	133	Total	C	N	O	S	0	0
			1028	681	174	163	10		
1	C	133	Total	C	N	O	S	0	0
			1028	681	174	163	10		
1	E	133	Total	C	N	O	S	0	0
			1028	681	174	163	10		
1	G	133	Total	C	N	O	S	0	0
			1028	681	174	163	10		

- Molecule 2 is a protein called ATP-binding cassette sub-family C member 8 isoform X2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	845	Total	C	N	O	S	0	0
			6598	4345	1102	1115	36		
2	D	845	Total	C	N	O	S	0	0
			6598	4345	1102	1115	36		
2	F	845	Total	C	N	O	S	0	0
			6598	4345	1102	1115	36		
2	H	845	Total	C	N	O	S	0	0
			6598	4345	1102	1115	36		

- Molecule 3 is 5-chloro-N-(2-{4-[(cyclohexylcarbamoyl)sulfamoyl]phenyl}ethyl)-2-methoxybenzamide (three-letter code: GBM) (formula: C₂₃H₂₈ClN₃O₅S).

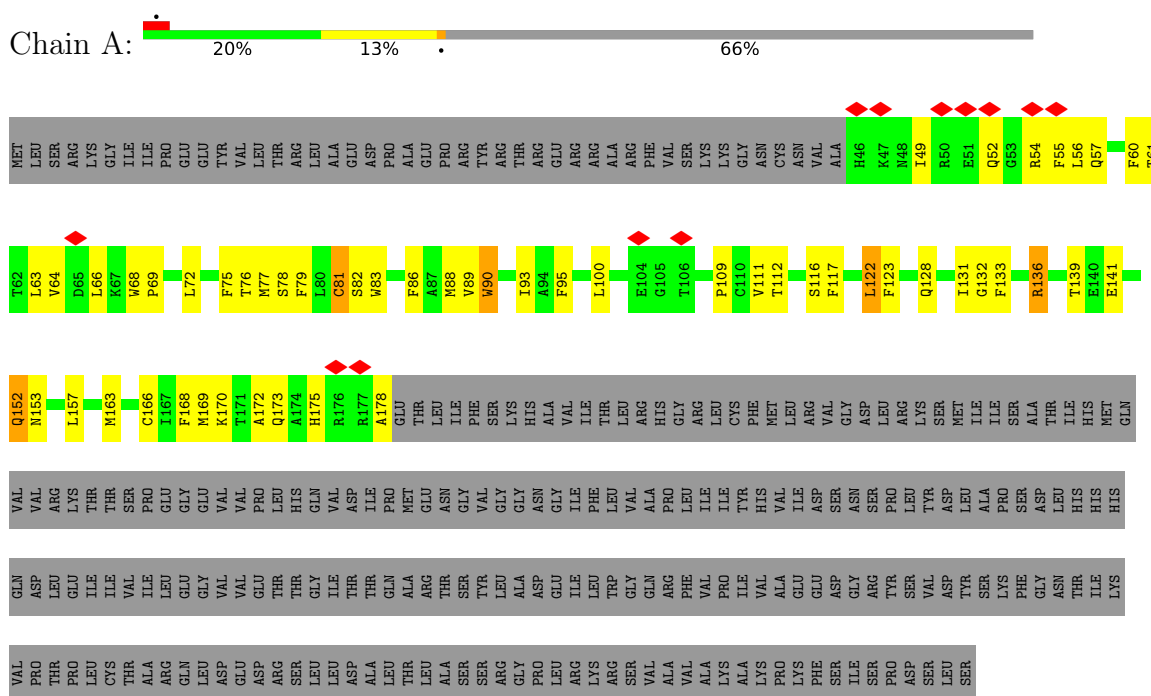


Mol	Chain	Residues	Atoms						AltConf
3	B	1	Total 33	C 23	Cl 1	N 3	O 5	S 1	0
3	D	1	Total 33	C 23	Cl 1	N 3	O 5	S 1	0
3	F	1	Total 33	C 23	Cl 1	N 3	O 5	S 1	0
3	H	1	Total 33	C 23	Cl 1	N 3	O 5	S 1	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

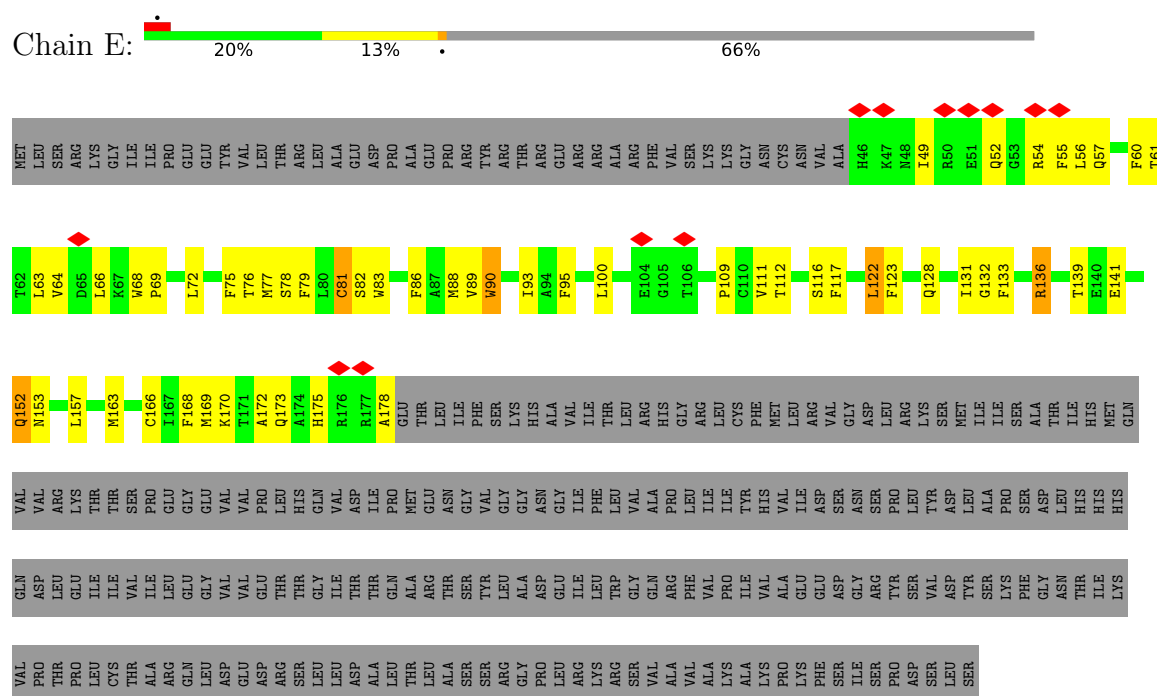
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



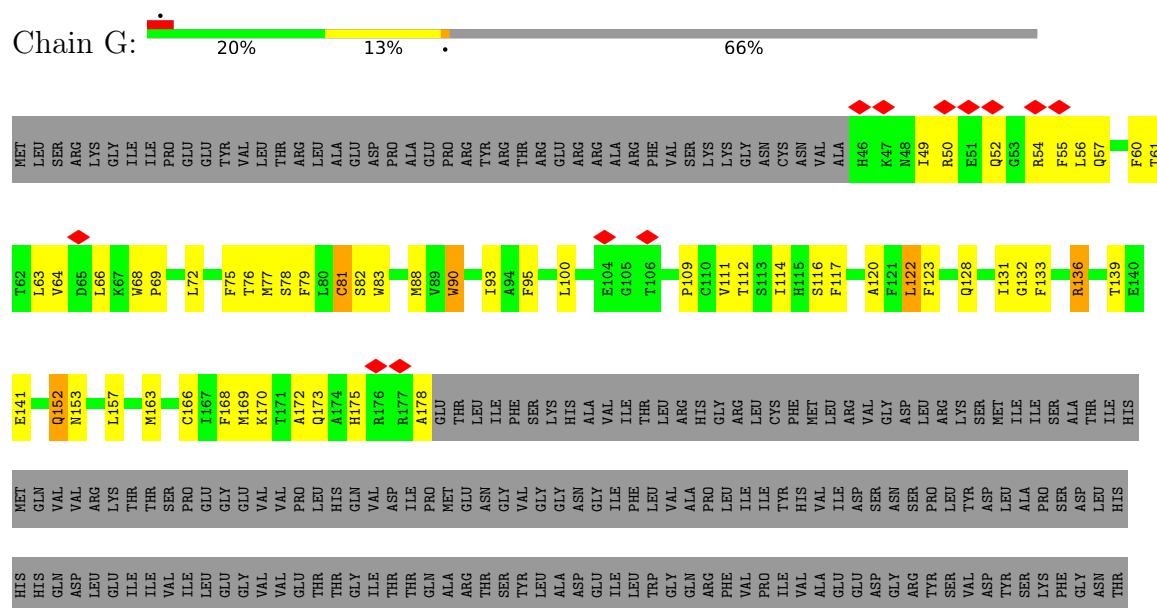
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



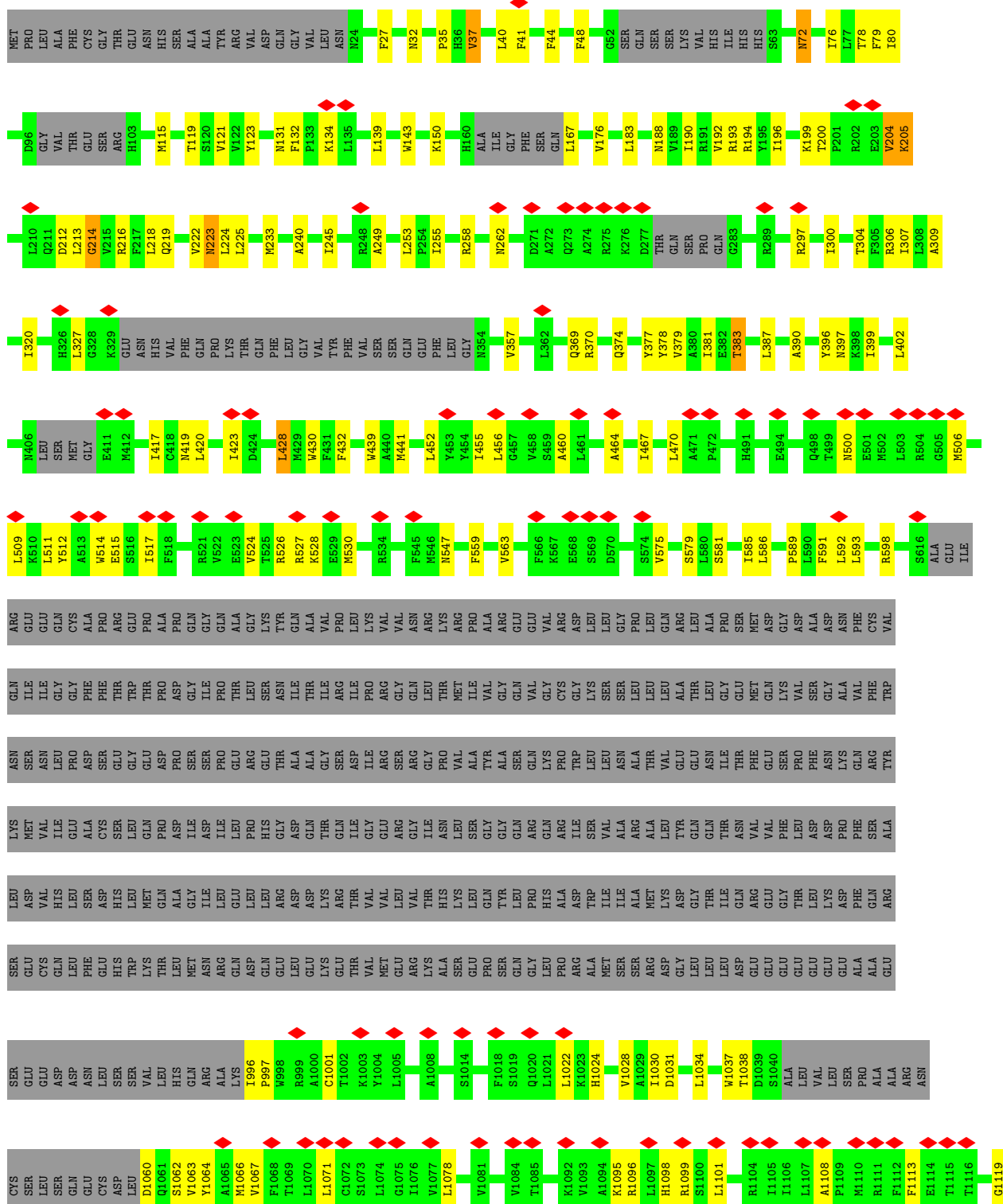
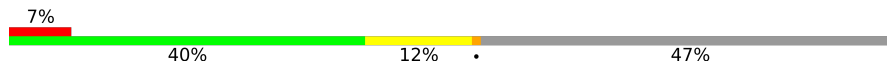
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



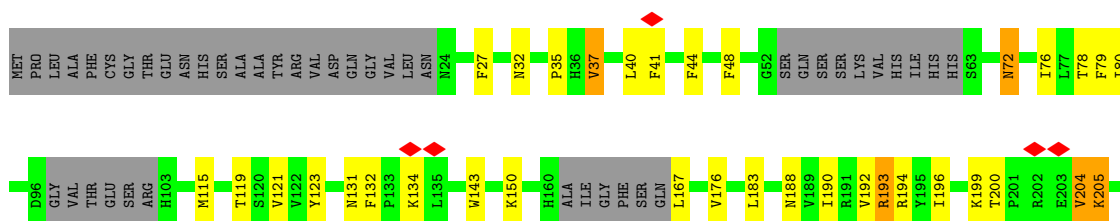
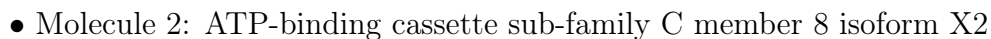
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



Chain B:











ASN	LEU	SER	SER	VAL	LEU	HIS	GLN	ARG	ALA	LYS	1996	P997	R998	R999	A1000	C1001	T1002	K1003	Y1004	L1005	A1008	S1014	F1018	S1019	Q1020	L1021	L1022	K1023	H1024	Y1028	A1029	I1030	L1034	W1037	T1038	D1039	S1040	ALA	LEU	VAL	LEU	SER	PRO	ALA	ALA	ARG	ASN	CYS	SER	LEU	GLN	GLU				
CYS	ASP	LEU	D1060	Q1061	S1062	V1063	Y1064	A1065	M1066	V1067	F1068	T1069	L1070	L1071	C1072	S1073	L1074	G1075	I1076	V1077	L1078	V1081	V1084	T1085	K1086	L1087	H1088	R1089	S1100	L1101	R1104	I1105	I1106	L1107	A1108	P1109	M1110	R1111	F1112	F1113	E1114	T1115	T1116	G1119	S1120	I1121	L1122	N1123	R1124	F1125						
S1126	S1127	D1128	C1129	M1130	T1131	I1132	I1136	L1140	R1145	S1152	A1153	T1155	V1156	I1157	S1158	Y1159	V1160	L1165	V1166	A1167	L1168	L1169	P1170	L1171	V1174	R1187	Q1190	T1195	L1198	P1199	L1200	F1204	A1205	E1206	R1215	A1216	F1217	R1218	Y1219	Q1224	L1227	Y1230														
S1238	L1239	F1240	L1241	T1242	M1245	R1246	W1247	R1251	M1252	E1253	Y1254	N1270	S1271	E1275	L1276	L1280	L1289	S1292	L1295	M1296	R1300	M1305	E1306	I1307	Q1308	L1309	V1312	H1316	A1317	L1318	L1319	K1320	T1321	GLU	ALA	GLU	SER	PHE	TYR	GLU	GLY	LEU	PHE	ALA	PRO	SER	LEU	ILE								
PRO	LYS	ASN	TRP	PRO	GLY	ASP	GLN	GLY	LYS	ILE	GLN	ASN	LEU	SER	VAL	LYS	ARG	TYR	ASP	SER	SER	LEU	LYS	ARG	PRO	VAL	LEU	ILE	GLY	ILE	ILE	GLY	CYS	GLY	ARG	THR	GLY	SER	GLY	LYS	LYS	SER	GLU	SER	PHE	TYR	GLU	GLY	LEU	PHE	ALA	PRO	SER	LEU	ILE	
VAL	ASP	MET	PHE	GLU	GLY	ARG	ILE	ILE	ILE	ASP	GLY	ILE	ASP	ILE	ALA	LEU	LEU	PRO	LEU	HIS	THR	GLY	ARG	GLY	ASN	ARG	LEU	PRO	VAL	ILE	ILE	THR	PHE	GLY	THR	LYS	LYS	CYS	SER	ALA	ASP	GLN	THR	ALA	THR	TRP	GLU	ALA	ARG	LEU						
GLU	ILE	ALA	GLN	LEU	LYS	LEU	VAL	VAL	VAL	LYS	ALA	THR	PRO	GLY	ASP	THR	ALA	ILE	THR	ILE	GLY	GLN	ARG	GLN	ARG	GLN	ARG	GLY	ALA	PHE	VAL	ARG	LYS	THR	ASP	SER	ILE	LYS	PHE	PRO	GLU	GLU	ILE	LYS	MET	ASP	GLU	THR	THR	LEU	VAL	PHE	ALA			
THR	GLU	ASN	ILE	GLN	GLN	LYS	VAL	THR	THR	ALA	PHE	ALA	ASP	ARG	THR	VAL	VAL	THR	ILE	THR	ALA	HIS	ARG	VAL	VAL	HIS	THR	ILE	LEU	GLN	SER	GLY	ALA	ASP	LEU	VAL	VAL	PRO	PHE	LYS	ILE	GLU	THR	THR	LEU	ASP	GLU	SER	GLN	GLY	THR	VAL	PHE	ALA		
SER	PHE	VAL	ARG	ALA	ASP	LYS																																																		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	74633	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.130	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	329.15997, 329.15997, 329.15997	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	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: GBM

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	0.42	0/1055	0.58	0/1434
1	C	0.42	0/1055	0.58	0/1434
1	E	0.42	0/1055	0.58	0/1434
1	G	0.42	0/1055	0.58	0/1434
2	B	0.29	0/6738	0.45	0/9165
2	D	0.29	0/6738	0.45	0/9165
2	F	0.29	0/6738	0.45	0/9165
2	H	0.29	0/6738	0.45	0/9165
All	All	0.31	0/31172	0.47	0/42396

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1028	0	1046	42	0
1	C	1028	0	1046	43	0
1	E	1028	0	1046	42	0
1	G	1028	0	1046	43	0
2	B	6598	0	6827	142	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	6598	0	6827	145	0
2	F	6598	0	6827	145	0
2	H	6598	0	6827	142	0
3	B	33	0	28	4	0
3	D	33	0	28	3	0
3	F	33	0	28	3	0
3	H	33	0	28	3	0
All	All	30636	0	31604	698	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 698 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)
2:D:1125:PHE:HA	2:D:1129:CYS:SG	1.95	1.07
2:F:1125:PHE:HA	2:F:1129:CYS:SG	1.95	1.06
2:H:1125:PHE:HA	2:H:1129:CYS:SG	1.95	1.06
2:B:1125:PHE:HA	2:B:1129:CYS:SG	1.95	1.06
2:H:1124:ARG:HD2	2:H:1318:LEU:HD12	1.41	1.03

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	131/390 (34%)	121 (92%)	10 (8%)	0	100	100
1	C	131/390 (34%)	121 (92%)	10 (8%)	0	100	100
1	E	131/390 (34%)	121 (92%)	10 (8%)	0	100	100
1	G	131/390 (34%)	121 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	827/1582 (52%)	798 (96%)	25 (3%)	4 (0%)	25	62
2	D	827/1582 (52%)	798 (96%)	25 (3%)	4 (0%)	25	62
2	F	827/1582 (52%)	798 (96%)	25 (3%)	4 (0%)	25	62
2	H	827/1582 (52%)	798 (96%)	25 (3%)	4 (0%)	25	62
All	All	3832/7888 (49%)	3676 (96%)	140 (4%)	16 (0%)	32	67

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	199	LYS
2	D	199	LYS
2	F	199	LYS
2	H	199	LYS
2	B	212	ASP

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	108/339 (32%)	95 (88%)	13 (12%)	4	18
1	C	108/339 (32%)	95 (88%)	13 (12%)	4	18
1	E	108/339 (32%)	95 (88%)	13 (12%)	4	18
1	G	108/339 (32%)	95 (88%)	13 (12%)	4	18
2	B	708/1371 (52%)	671 (95%)	37 (5%)	19	43
2	D	708/1371 (52%)	671 (95%)	37 (5%)	19	43
2	F	708/1371 (52%)	671 (95%)	37 (5%)	19	43
2	H	708/1371 (52%)	671 (95%)	37 (5%)	19	43
All	All	3264/6840 (48%)	3064 (94%)	200 (6%)	18	39

5 of 200 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	119	THR
2	F	1238	SER
2	H	1318	LEU
2	F	193	ARG
2	F	430	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	1135	HIS
1	E	128	GLN
2	H	485	GLN
1	G	128	GLN
1	G	152	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](#)

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
3	GBM	H	2001	-	35,35,35	2.03	4 (11%)	48,48,48	1.87	7 (14%)
3	GBM	B	2001	-	35,35,35	2.03	4 (11%)	48,48,48	1.87	7 (14%)
3	GBM	D	2001	-	35,35,35	2.03	4 (11%)	48,48,48	1.87	7 (14%)
3	GBM	F	2001	-	35,35,35	2.03	4 (11%)	48,48,48	1.87	7 (14%)

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	GBM	H	2001	-	-	8/27/35/35	0/3/3/3
3	GBM	B	2001	-	-	8/27/35/35	0/3/3/3
3	GBM	D	2001	-	-	8/27/35/35	0/3/3/3
3	GBM	F	2001	-	-	8/27/35/35	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	GBM	C18-S2	-10.16	1.60	1.76
3	D	2001	GBM	C18-S2	-10.16	1.60	1.76
3	F	2001	GBM	C18-S2	-10.16	1.60	1.76
3	H	2001	GBM	C18-S2	-10.16	1.60	1.76
3	B	2001	GBM	C27-C28	4.65	1.49	1.40

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001	GBM	O5-S2-O4	-9.72	107.60	119.55
3	D	2001	GBM	O5-S2-O4	-9.72	107.60	119.55
3	F	2001	GBM	O5-S2-O4	-9.72	107.60	119.55
3	H	2001	GBM	O5-S2-O4	-9.72	107.60	119.55
3	B	2001	GBM	O7-C28-C27	3.76	122.02	116.55

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2001	GBM	C27-C26-N10-C25
3	D	2001	GBM	C27-C26-N10-C25

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Mol	Chain	Res	Type	Atoms
3	F	2001	GBM	C27-C26-N10-C25
3	H	2001	GBM	C27-C26-N10-C25
3	B	2001	GBM	O6-C26-N10-C25

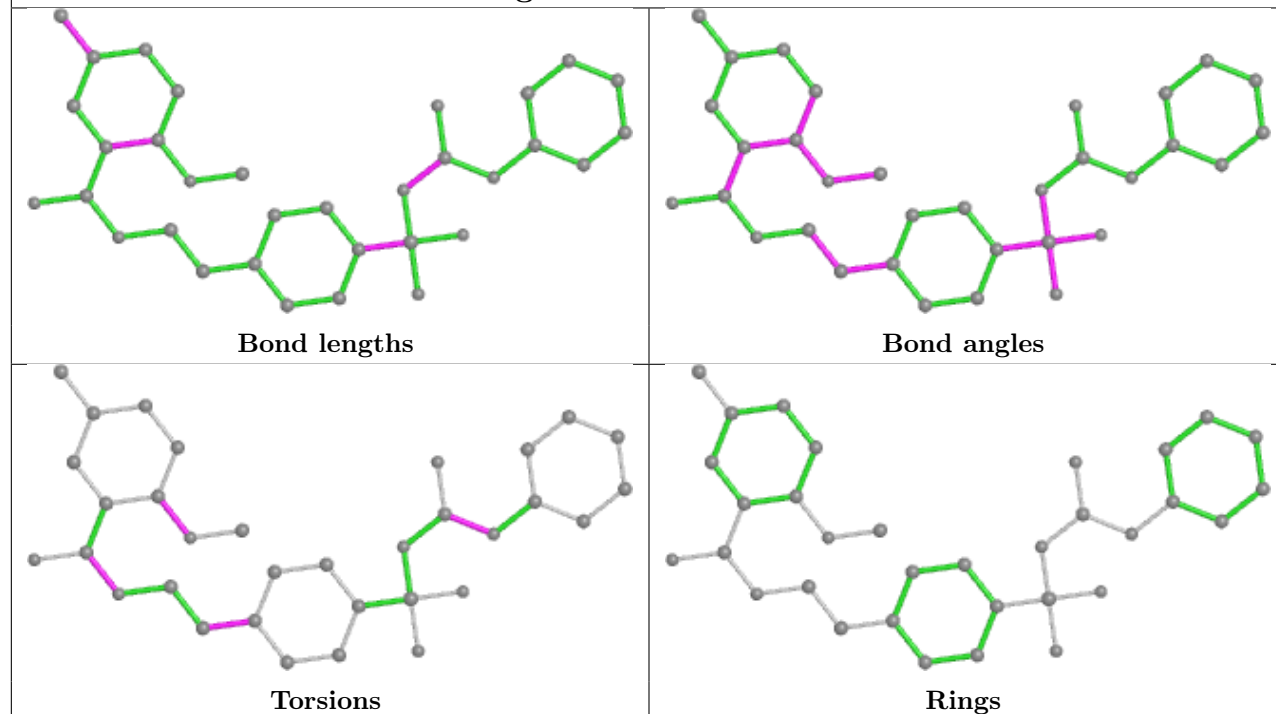
There are no ring outliers.

4 monomers are involved in 13 short contacts:

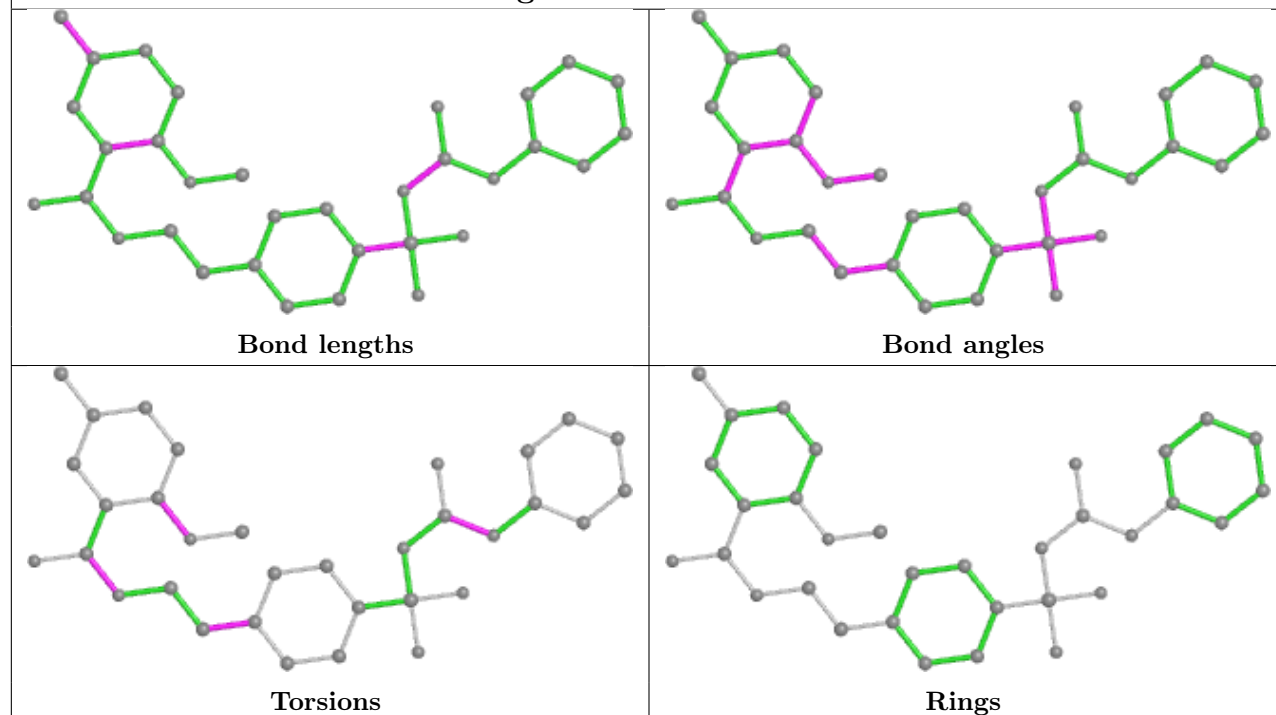
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	2001	GBM	3	0
3	B	2001	GBM	4	0
3	D	2001	GBM	3	0
3	F	2001	GBM	3	0

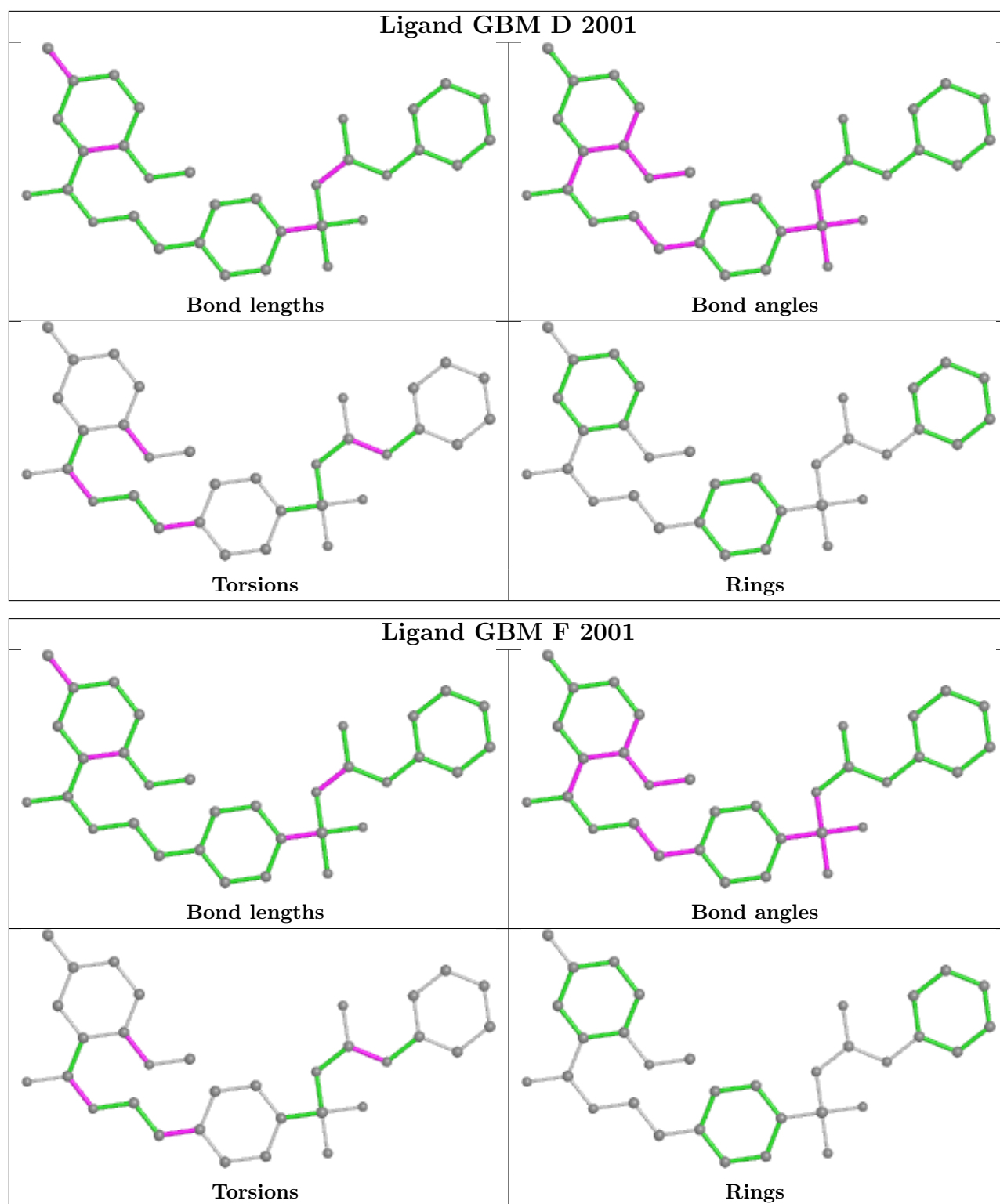
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand GBM H 2001



Ligand GBM B 2001





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

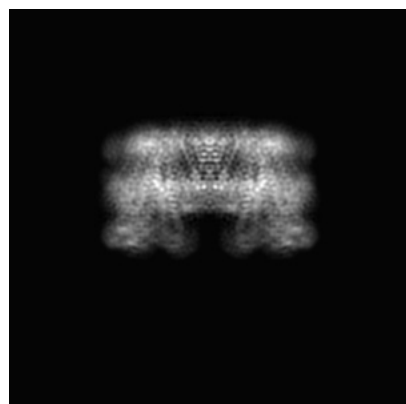
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6831. These allow visual inspection of the internal detail of the map and identification of artifacts.

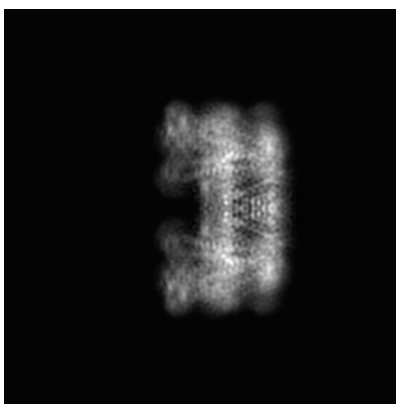
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

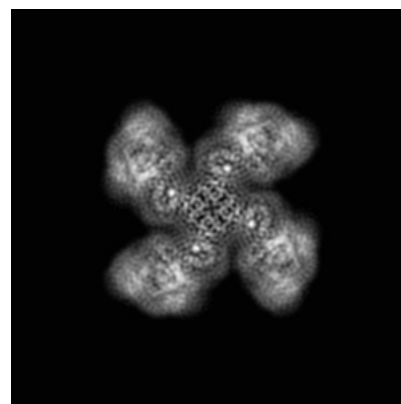
6.1.1 Primary map



X

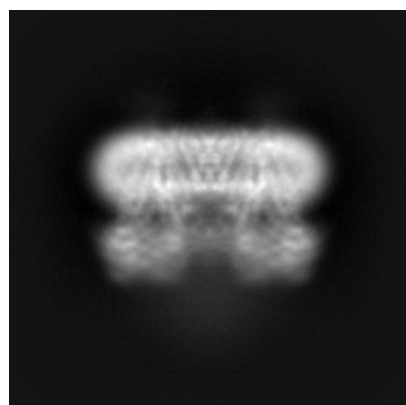


Y

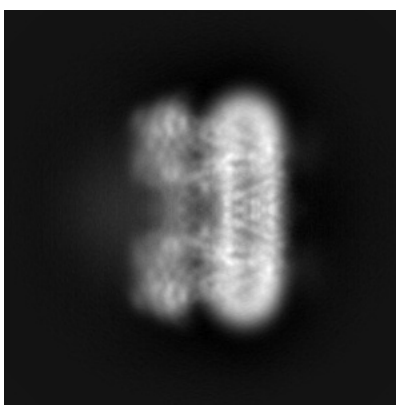


Z

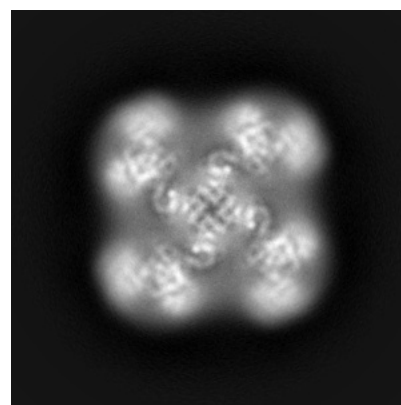
6.1.2 Raw map



X



Y

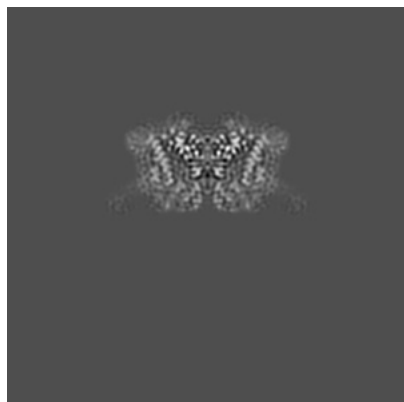


Z

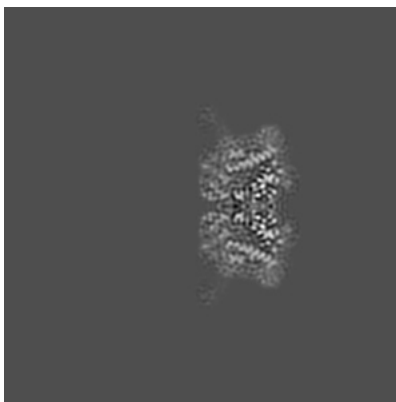
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

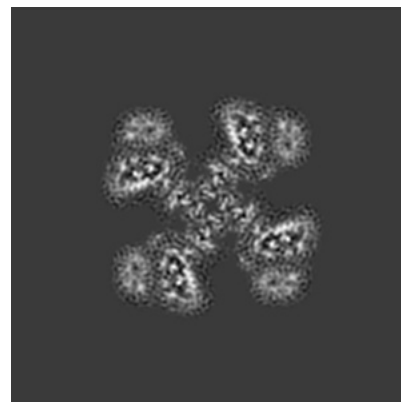
6.2.1 Primary map



X Index: 156

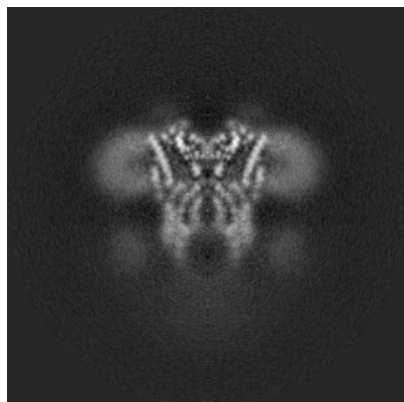


Y Index: 156

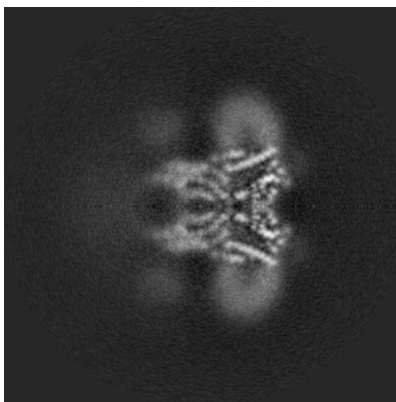


Z Index: 156

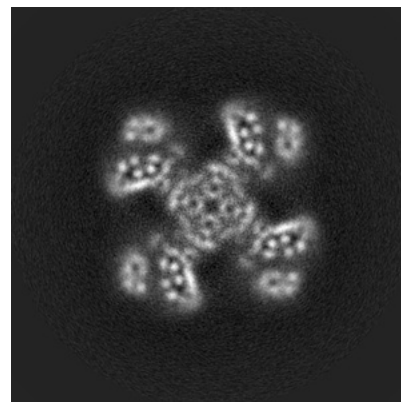
6.2.2 Raw map



X Index: 156



Y Index: 156

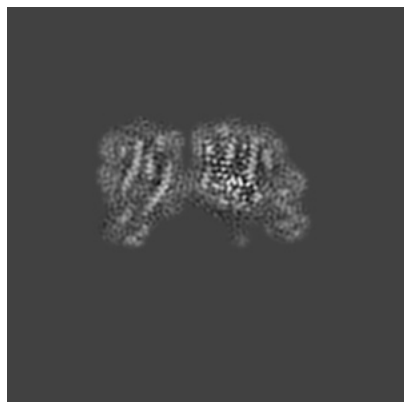


Z Index: 156

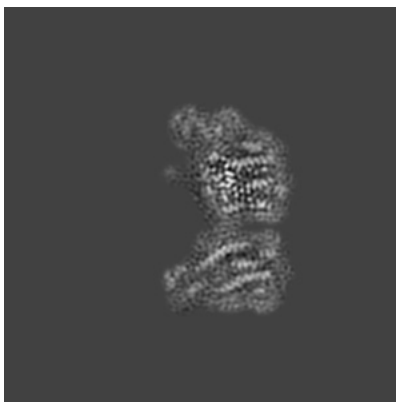
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

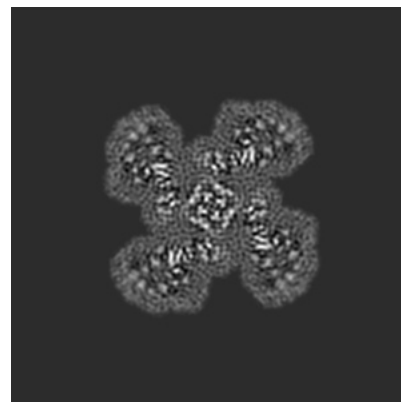
6.3.1 Primary map



X Index: 117

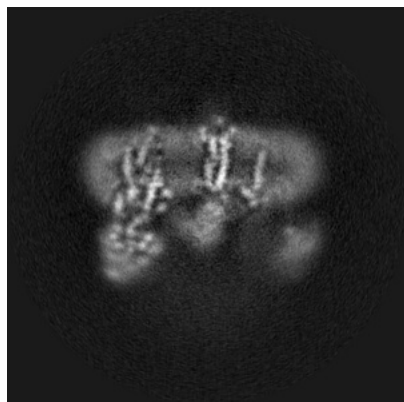


Y Index: 195

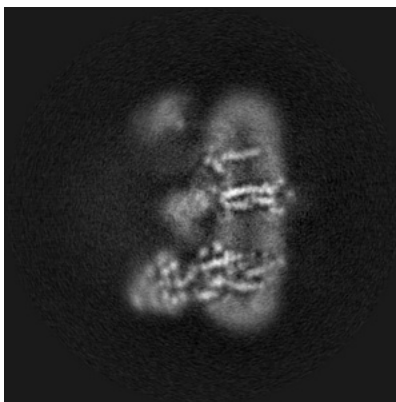


Z Index: 173

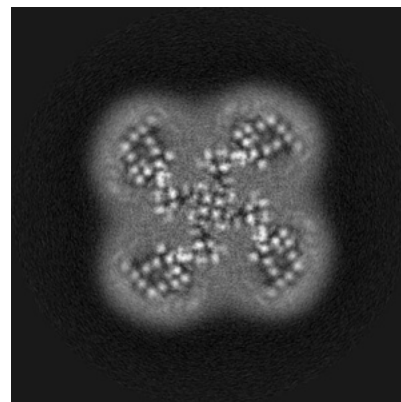
6.3.2 Raw map



X Index: 125



Y Index: 187

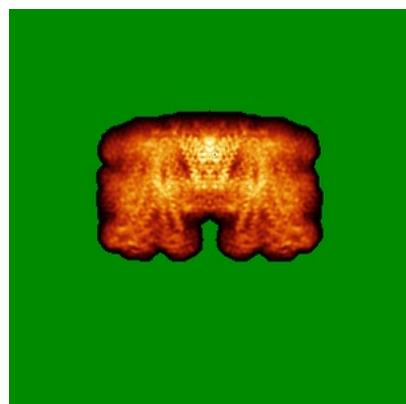


Z Index: 175

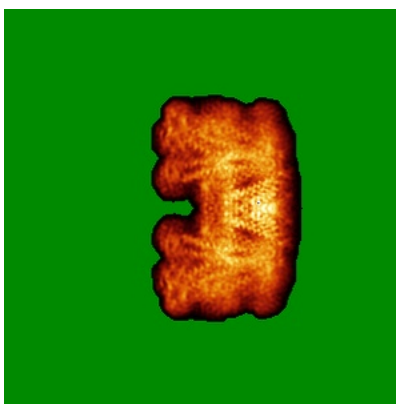
The images above show the largest variance slices of the map in three orthogonal directions.

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

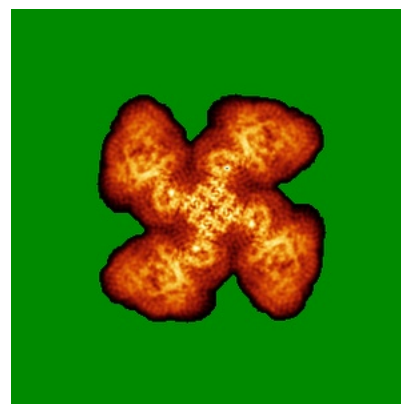
6.4.1 Primary map



X



Y

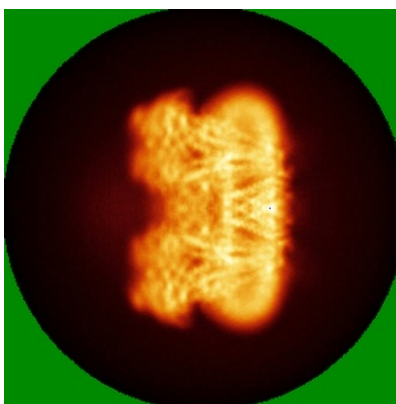


Z

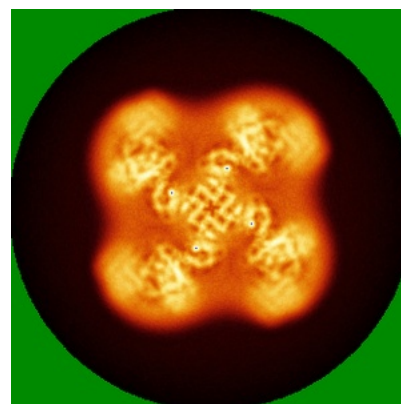
6.4.2 Raw map



X



Y

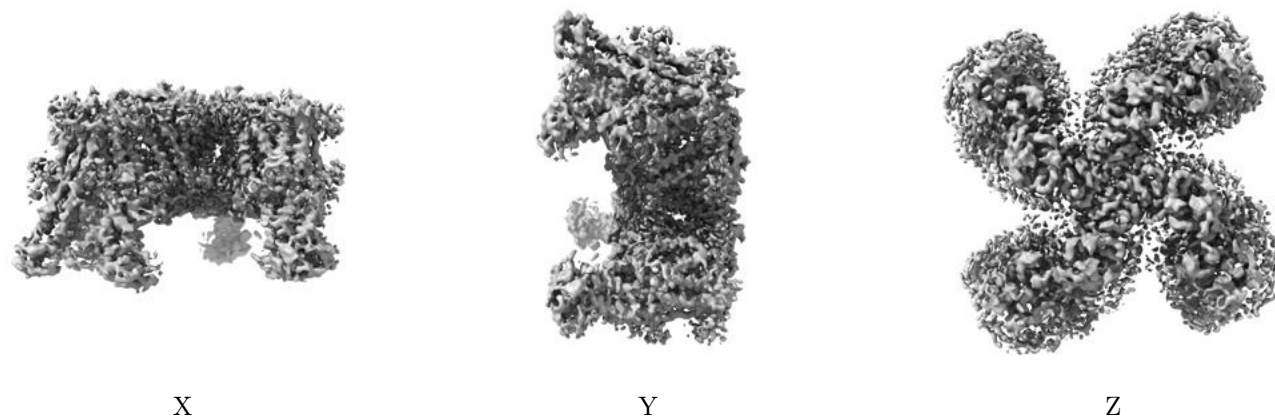


Z

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.

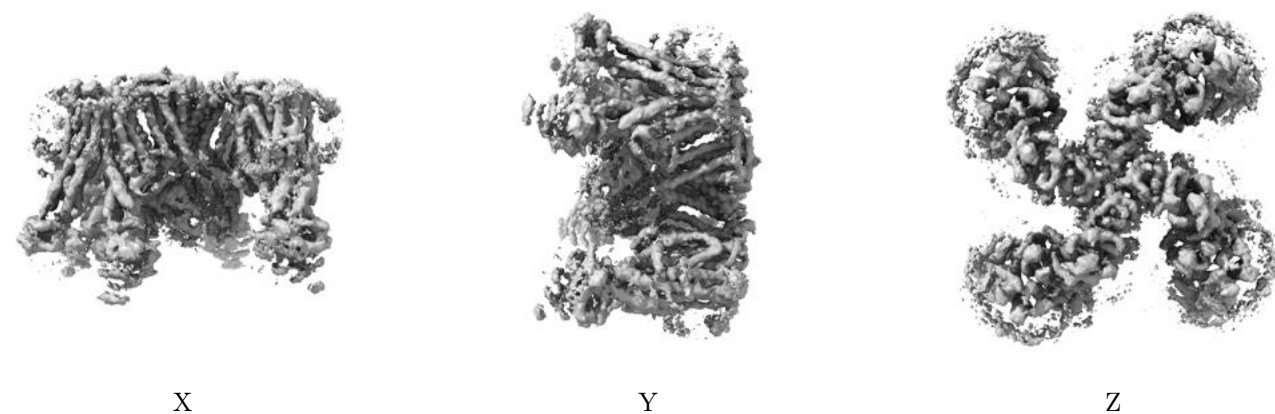
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.028. 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.

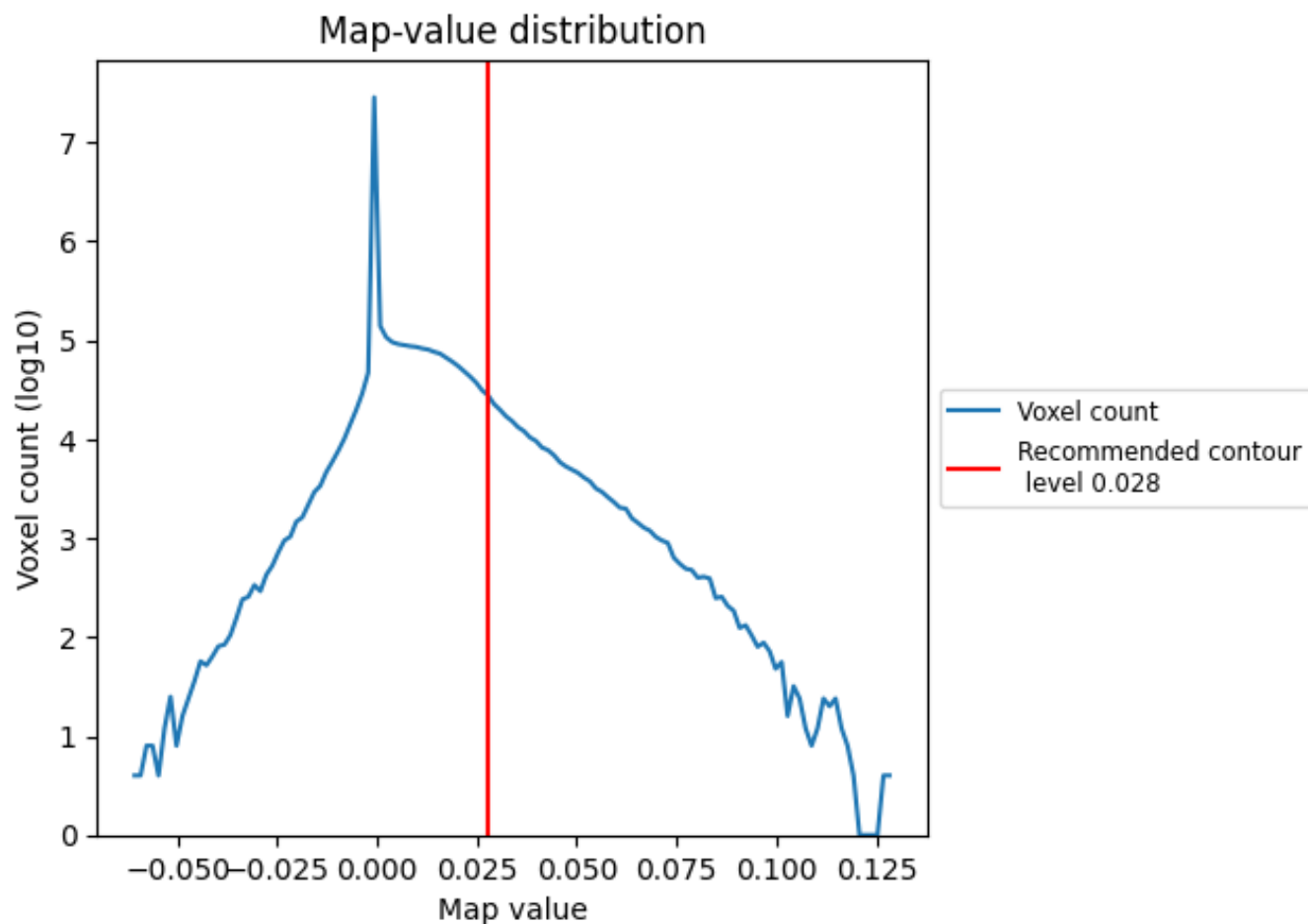
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

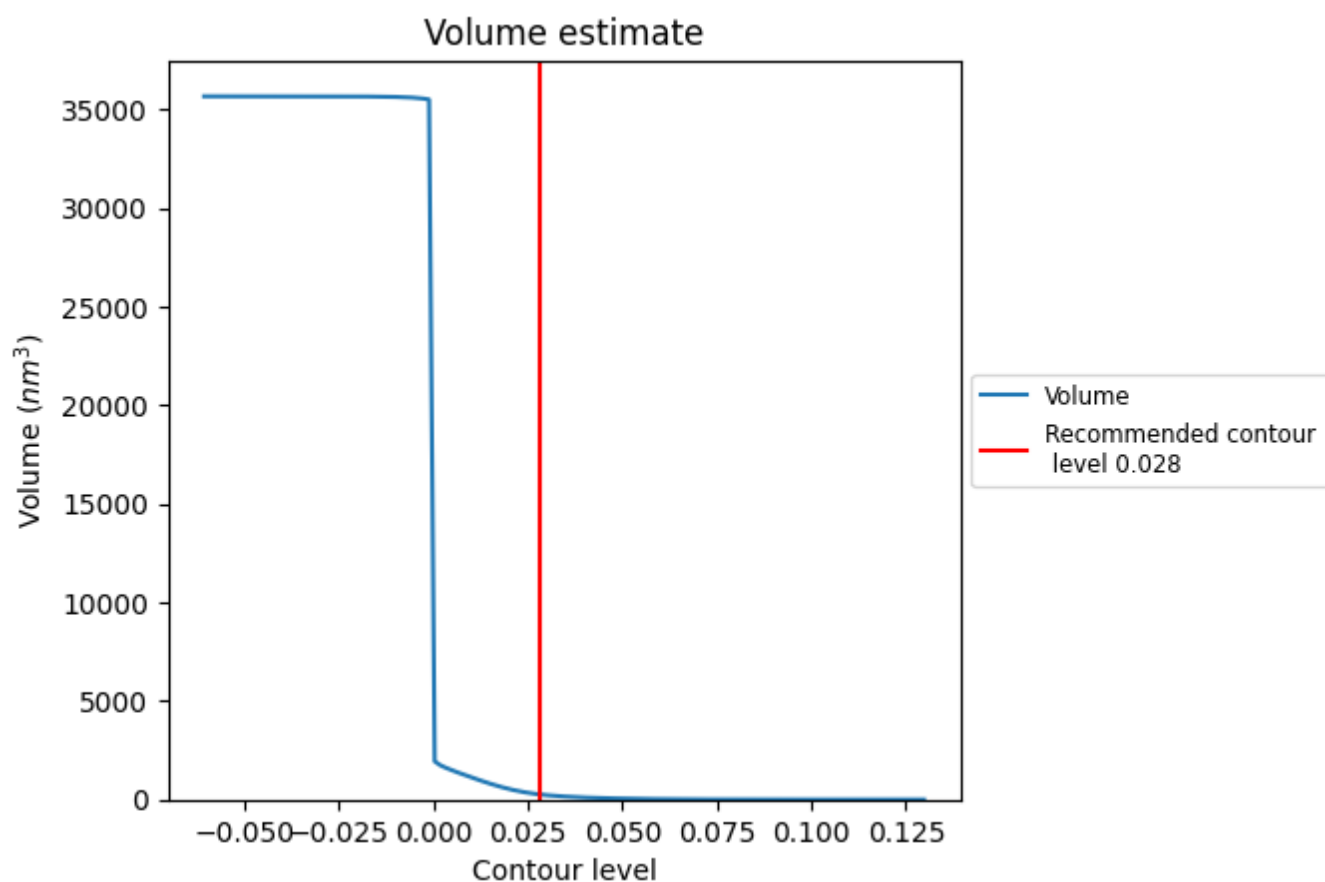
This section contains the results of statistical analysis of the map.

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.

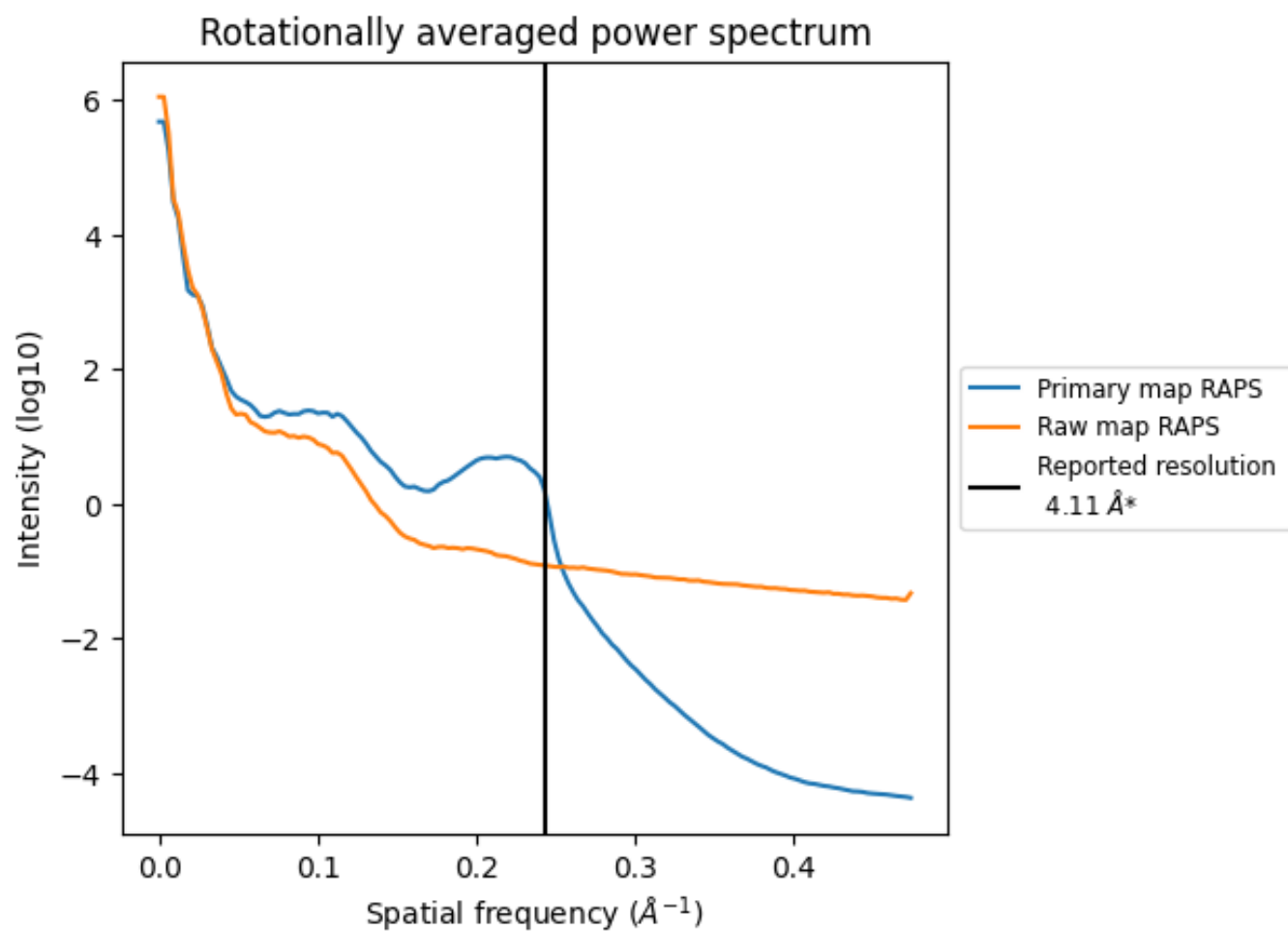
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 264 nm³; this corresponds to an approximate mass of 238 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 ⓘ

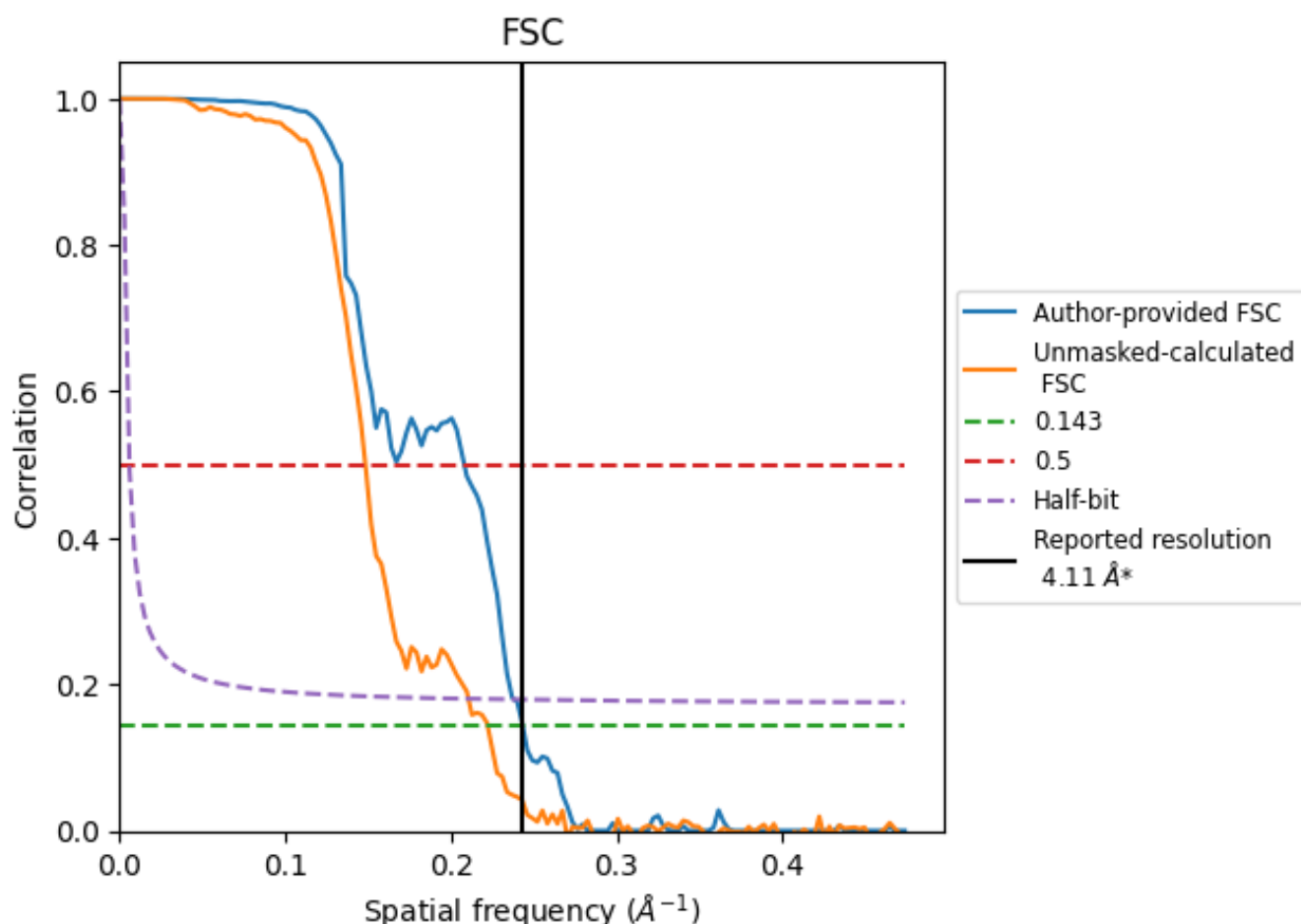


*Reported resolution corresponds to spatial frequency of 0.243 Å⁻¹

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 0.243 Å⁻¹

8.2 Resolution estimates [i](#)

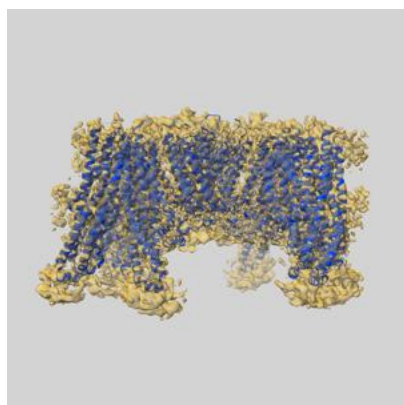
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.11	-	-
Author-provided FSC curve	4.11	4.81	4.19
Unmasked-calculated*	4.50	6.74	4.75

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

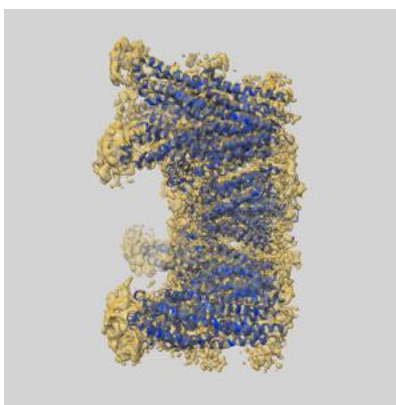
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6831 and PDB model 5YKE. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

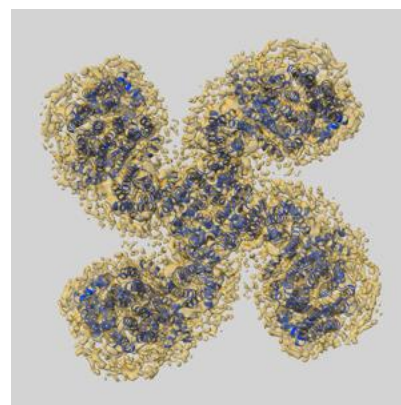
9.1 Map-model overlay [i](#)



X



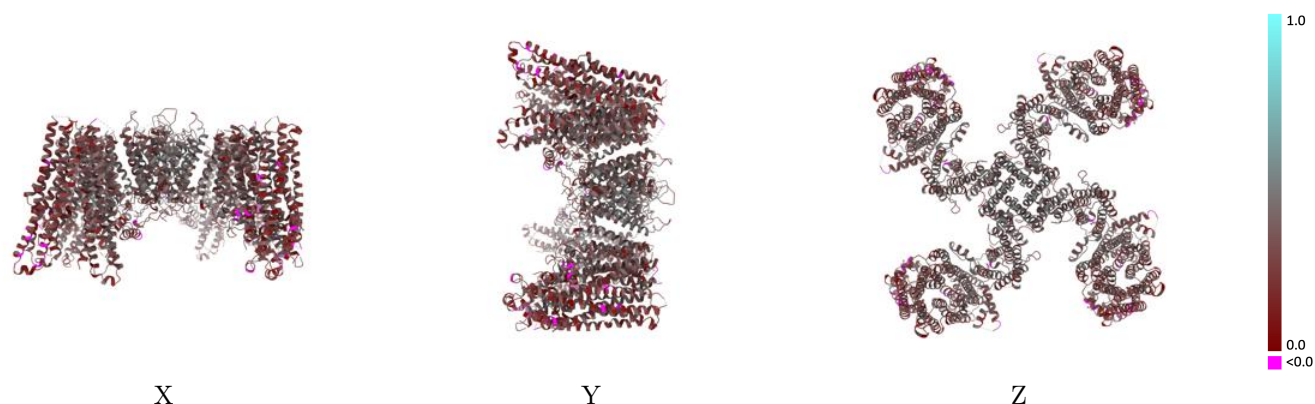
Y



Z

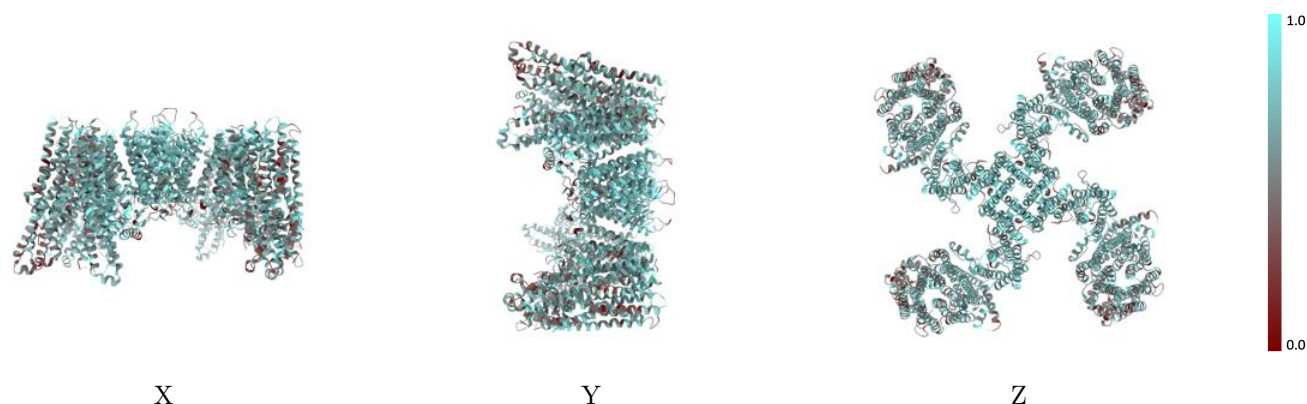
The images above show the 3D surface view of the map at the recommended contour level 0.028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



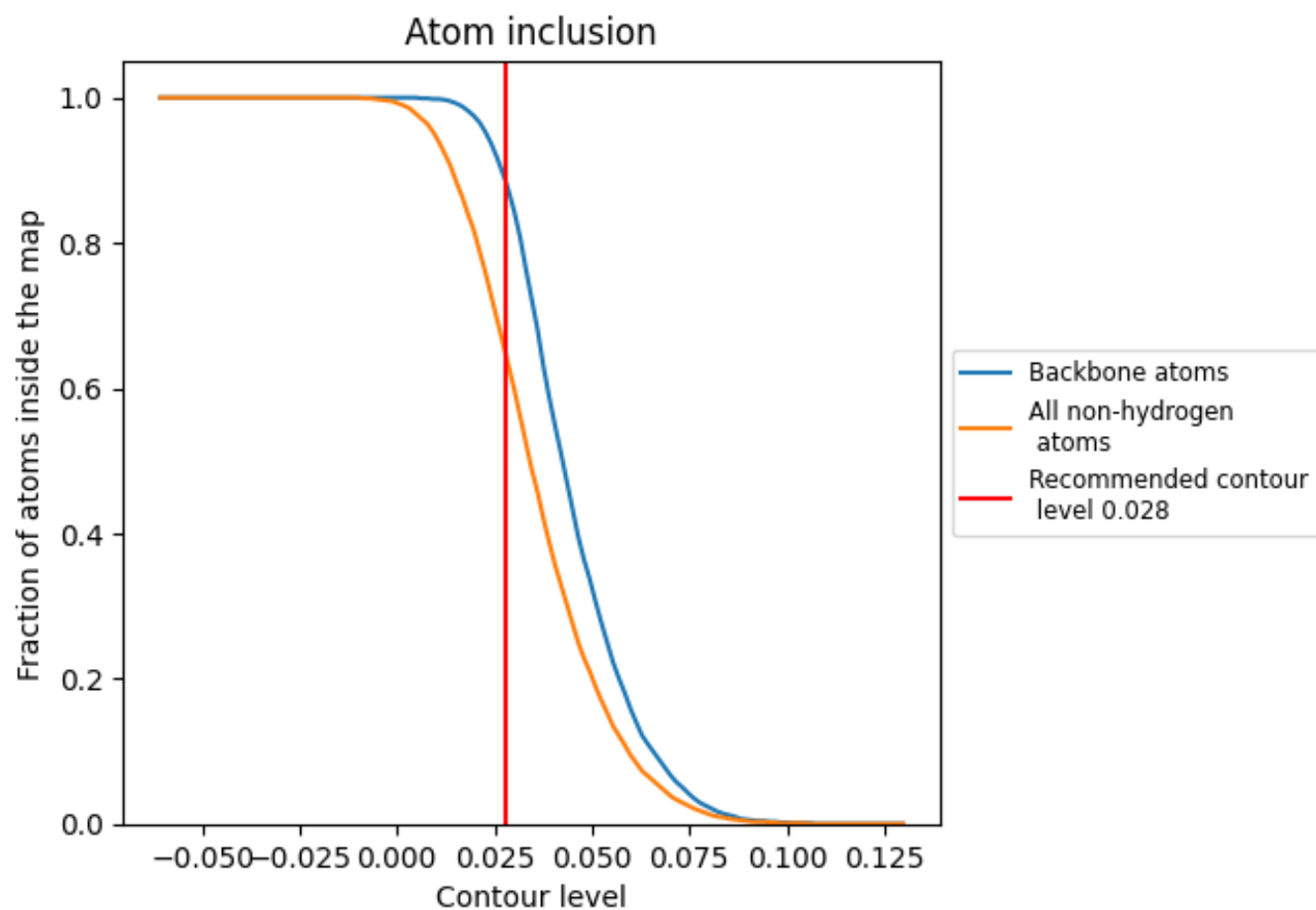
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.028).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 64% 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 (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6450	<div></div> 0.3180
A	<div></div> 0.7230	<div></div> 0.3950
B	<div></div> 0.6330	<div></div> 0.3060
C	<div></div> 0.7230	<div></div> 0.3930
D	<div></div> 0.6330	<div></div> 0.3070
E	<div></div> 0.7230	<div></div> 0.3950
F	<div></div> 0.6330	<div></div> 0.3070
G	<div></div> 0.7230	<div></div> 0.3950
H	<div></div> 0.6330	<div></div> 0.3060

1.0

0.0

<0.0