



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 04:27 PM UTC

PDB ID : 9IS8 / pdb_00009is8
EMDB ID : EMD-60834
Title : Cryo-EM structure of AKT1-AtKC1(G315D)
Authors : Dongliang, L.; Zijie, Z.; Yannan, Q.; Yuyue, T.; Huaizong, S.
Deposited on : 2024-07-17
Resolution : 2.77 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

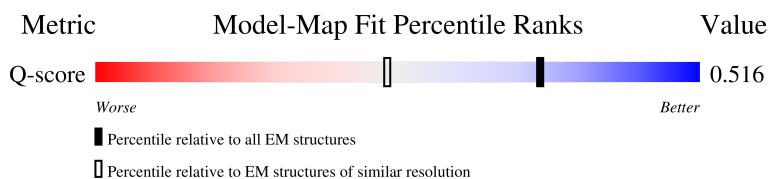
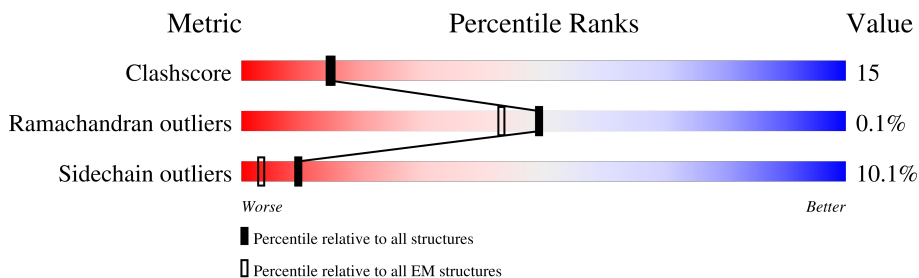
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.77 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	10695 (2.27 - 3.27)

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	885	9% 33% 15% • 50%
1	C	885	10% 33% 15% • 50%
1	D	885	15% 30% 18% • 50%
2	B	710	15% 41% 22% • 33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14809 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 Potassium channel AKT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	441	Total	C	N	O	S	0	0
			3599	2341	608	630	20		
1	C	441	Total	C	N	O	S	0	0
			3599	2341	608	630	20		
1	D	440	Total	C	N	O	S	0	0
			3591	2335	607	629	20		

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	858	LEU	-	expression tag	UNP Q38998
A	859	GLU	-	expression tag	UNP Q38998
A	860	GLY	-	expression tag	UNP Q38998
A	861	SER	-	expression tag	UNP Q38998
A	862	ASP	-	expression tag	UNP Q38998
A	863	GLU	-	expression tag	UNP Q38998
A	864	VAL	-	expression tag	UNP Q38998
A	865	ASP	-	expression tag	UNP Q38998
A	866	ALA	-	expression tag	UNP Q38998
A	867	GLY	-	expression tag	UNP Q38998
A	868	SER	-	expression tag	UNP Q38998
A	869	ALA	-	expression tag	UNP Q38998
A	870	ALA	-	expression tag	UNP Q38998
A	871	ALA	-	expression tag	UNP Q38998
A	872	SER	-	expression tag	UNP Q38998
A	873	GLY	-	expression tag	UNP Q38998
A	874	GLY	-	expression tag	UNP Q38998
A	875	SER	-	expression tag	UNP Q38998
A	876	GLY	-	expression tag	UNP Q38998
A	877	SER	-	expression tag	UNP Q38998
A	878	ASP	-	expression tag	UNP Q38998
A	879	TYR	-	expression tag	UNP Q38998
A	880	LYS	-	expression tag	UNP Q38998
A	881	ASP	-	expression tag	UNP Q38998

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	882	ASP	-	expression tag	UNP Q38998
A	883	ASP	-	expression tag	UNP Q38998
A	884	ASP	-	expression tag	UNP Q38998
A	885	LYS	-	expression tag	UNP Q38998
C	858	LEU	-	expression tag	UNP Q38998
C	859	GLU	-	expression tag	UNP Q38998
C	860	GLY	-	expression tag	UNP Q38998
C	861	SER	-	expression tag	UNP Q38998
C	862	ASP	-	expression tag	UNP Q38998
C	863	GLU	-	expression tag	UNP Q38998
C	864	VAL	-	expression tag	UNP Q38998
C	865	ASP	-	expression tag	UNP Q38998
C	866	ALA	-	expression tag	UNP Q38998
C	867	GLY	-	expression tag	UNP Q38998
C	868	SER	-	expression tag	UNP Q38998
C	869	ALA	-	expression tag	UNP Q38998
C	870	ALA	-	expression tag	UNP Q38998
C	871	ALA	-	expression tag	UNP Q38998
C	872	SER	-	expression tag	UNP Q38998
C	873	GLY	-	expression tag	UNP Q38998
C	874	GLY	-	expression tag	UNP Q38998
C	875	SER	-	expression tag	UNP Q38998
C	876	GLY	-	expression tag	UNP Q38998
C	877	SER	-	expression tag	UNP Q38998
C	878	ASP	-	expression tag	UNP Q38998
C	879	TYR	-	expression tag	UNP Q38998
C	880	LYS	-	expression tag	UNP Q38998
C	881	ASP	-	expression tag	UNP Q38998
C	882	ASP	-	expression tag	UNP Q38998
C	883	ASP	-	expression tag	UNP Q38998
C	884	ASP	-	expression tag	UNP Q38998
C	885	LYS	-	expression tag	UNP Q38998
D	858	LEU	-	expression tag	UNP Q38998
D	859	GLU	-	expression tag	UNP Q38998
D	860	GLY	-	expression tag	UNP Q38998
D	861	SER	-	expression tag	UNP Q38998
D	862	ASP	-	expression tag	UNP Q38998
D	863	GLU	-	expression tag	UNP Q38998
D	864	VAL	-	expression tag	UNP Q38998
D	865	ASP	-	expression tag	UNP Q38998
D	866	ALA	-	expression tag	UNP Q38998
D	867	GLY	-	expression tag	UNP Q38998

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	868	SER	-	expression tag	UNP Q38998
D	869	ALA	-	expression tag	UNP Q38998
D	870	ALA	-	expression tag	UNP Q38998
D	871	ALA	-	expression tag	UNP Q38998
D	872	SER	-	expression tag	UNP Q38998
D	873	GLY	-	expression tag	UNP Q38998
D	874	GLY	-	expression tag	UNP Q38998
D	875	SER	-	expression tag	UNP Q38998
D	876	GLY	-	expression tag	UNP Q38998
D	877	SER	-	expression tag	UNP Q38998
D	878	ASP	-	expression tag	UNP Q38998
D	879	TYR	-	expression tag	UNP Q38998
D	880	LYS	-	expression tag	UNP Q38998
D	881	ASP	-	expression tag	UNP Q38998
D	882	ASP	-	expression tag	UNP Q38998
D	883	ASP	-	expression tag	UNP Q38998
D	884	ASP	-	expression tag	UNP Q38998
D	885	LYS	-	expression tag	UNP Q38998

- Molecule 2 is a protein called Potassium channel KAT3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	474	Total	C	N	O	S	0	0
			3861	2533	636	676	16		

There are 49 discrepancies between the modelled and reference sequences:

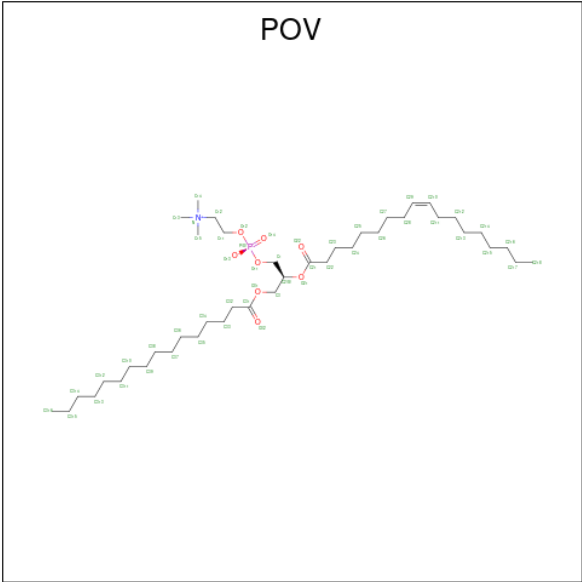
Chain	Residue	Modelled	Actual	Comment	Reference
B	315	ASP	GLY	engineered mutation	UNP P92960
B	663	LEU	-	expression tag	UNP P92960
B	664	GLU	-	expression tag	UNP P92960
B	665	GLY	-	expression tag	UNP P92960
B	666	SER	-	expression tag	UNP P92960
B	667	ASP	-	expression tag	UNP P92960
B	668	GLU	-	expression tag	UNP P92960
B	669	VAL	-	expression tag	UNP P92960
B	670	ASP	-	expression tag	UNP P92960
B	671	ALA	-	expression tag	UNP P92960
B	672	GLY	-	expression tag	UNP P92960
B	673	SER	-	expression tag	UNP P92960
B	674	ALA	-	expression tag	UNP P92960
B	675	ALA	-	expression tag	UNP P92960

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	676	ALA	-	expression tag	UNP P92960
B	677	SER	-	expression tag	UNP P92960
B	678	GLY	-	expression tag	UNP P92960
B	679	GLY	-	expression tag	UNP P92960
B	680	SER	-	expression tag	UNP P92960
B	681	GLY	-	expression tag	UNP P92960
B	682	SER	-	expression tag	UNP P92960
B	683	TRP	-	expression tag	UNP P92960
B	684	SER	-	expression tag	UNP P92960
B	685	HIS	-	expression tag	UNP P92960
B	686	PRO	-	expression tag	UNP P92960
B	687	GLN	-	expression tag	UNP P92960
B	688	PHE	-	expression tag	UNP P92960
B	689	GLU	-	expression tag	UNP P92960
B	690	LYS	-	expression tag	UNP P92960
B	691	GLY	-	expression tag	UNP P92960
B	692	GLY	-	expression tag	UNP P92960
B	693	GLY	-	expression tag	UNP P92960
B	694	ALA	-	expression tag	UNP P92960
B	695	ARG	-	expression tag	UNP P92960
B	696	GLY	-	expression tag	UNP P92960
B	697	GLY	-	expression tag	UNP P92960
B	698	SER	-	expression tag	UNP P92960
B	699	GLY	-	expression tag	UNP P92960
B	700	GLY	-	expression tag	UNP P92960
B	701	GLY	-	expression tag	UNP P92960
B	702	SER	-	expression tag	UNP P92960
B	703	TRP	-	expression tag	UNP P92960
B	704	SER	-	expression tag	UNP P92960
B	705	HIS	-	expression tag	UNP P92960
B	706	PRO	-	expression tag	UNP P92960
B	707	GLN	-	expression tag	UNP P92960
B	708	PHE	-	expression tag	UNP P92960
B	709	GLU	-	expression tag	UNP P92960
B	710	LYS	-	expression tag	UNP P92960

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			39	30	8	1	
3	B	1	Total	C	O	P	0
			39	30	8	1	
3	C	1	Total	C	O	P	0
			39	30	8	1	
3	D	1	Total	C	O	P	0
			39	30	8	1	

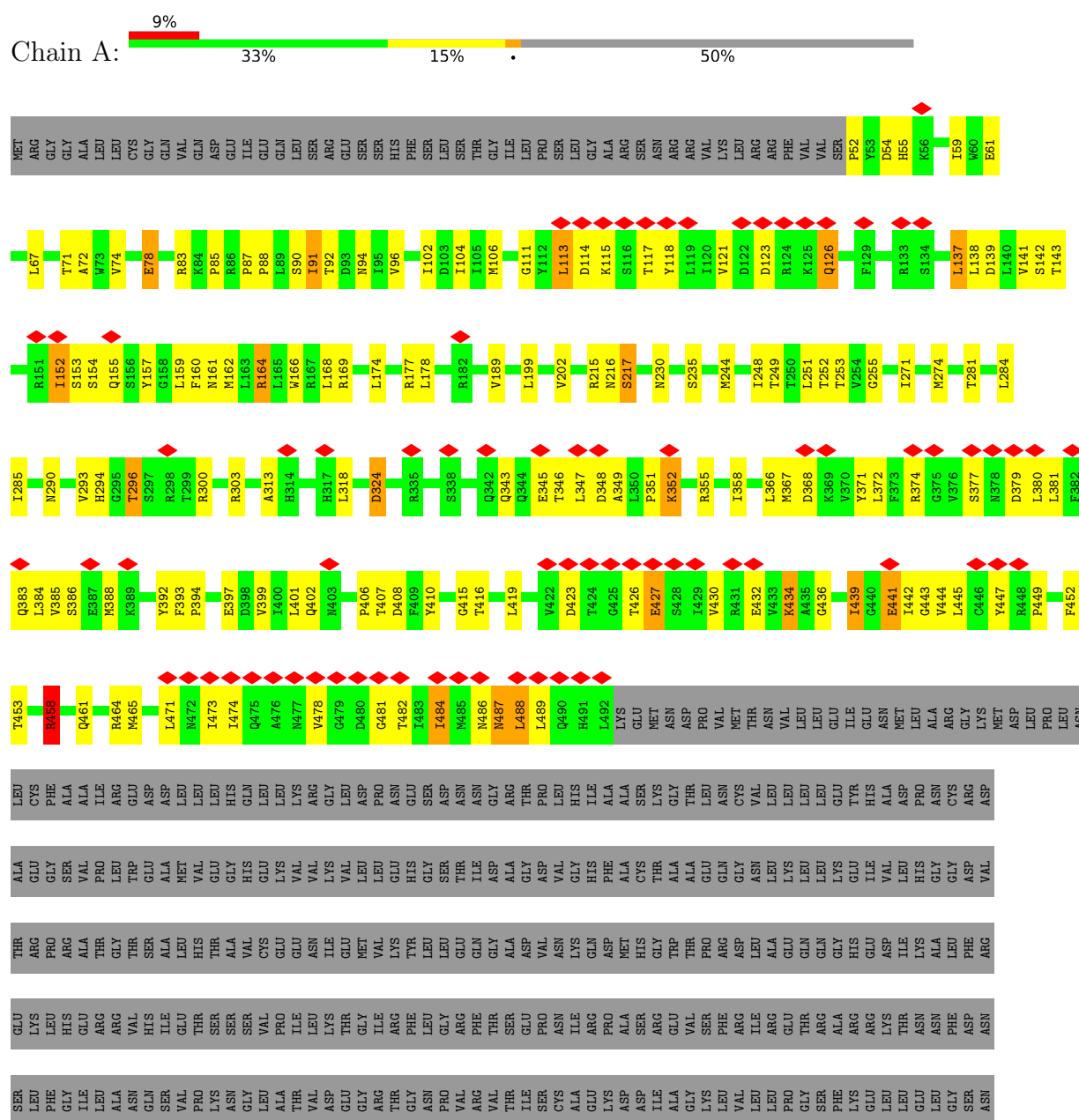
- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
4	C	2	Total	K	0
			2	2	
4	D	1	Total	K	0
			1	1	

3 Residue-property plots

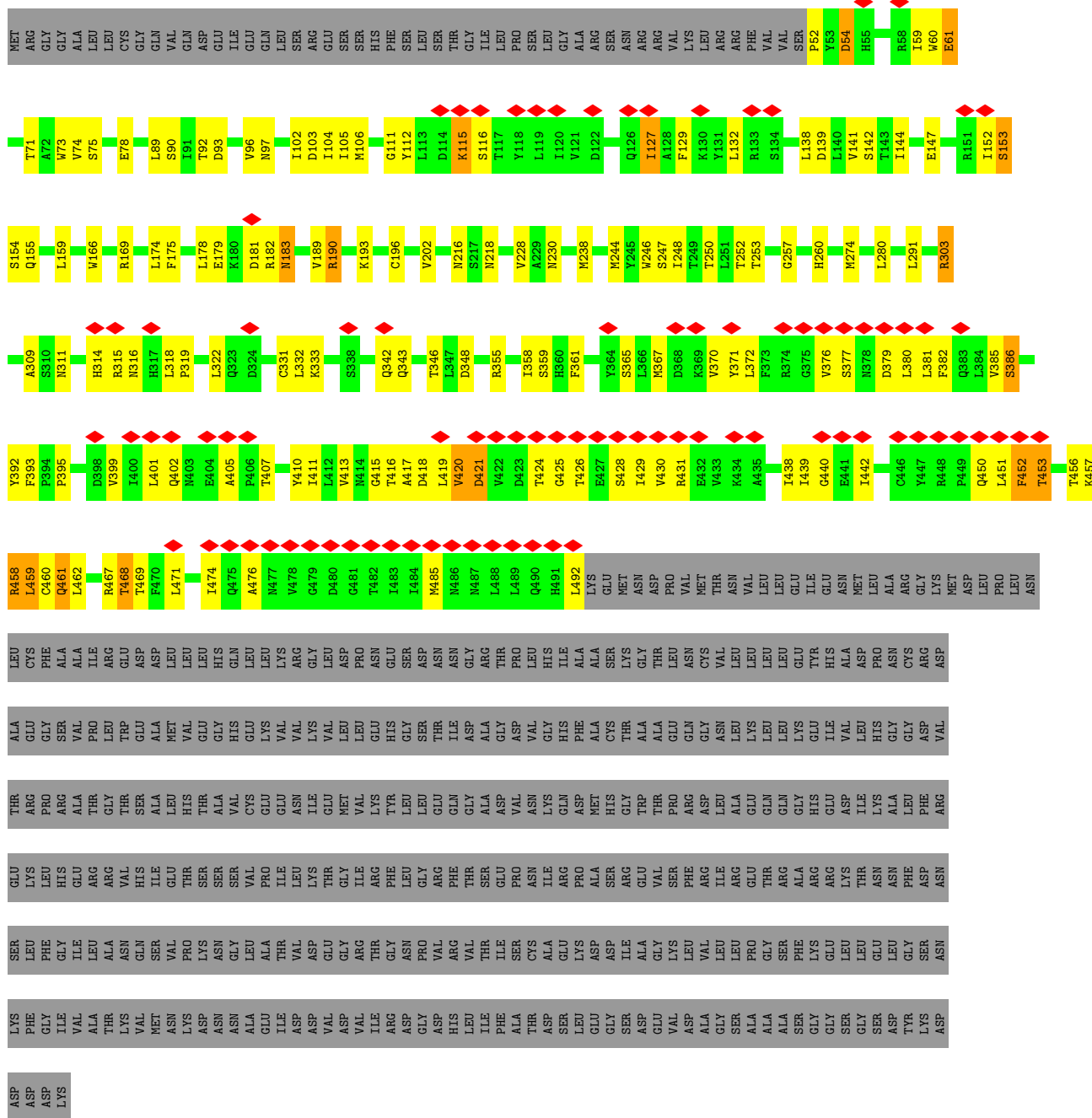
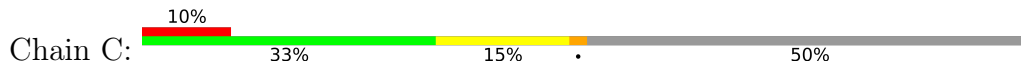
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Potassium channel AKT1

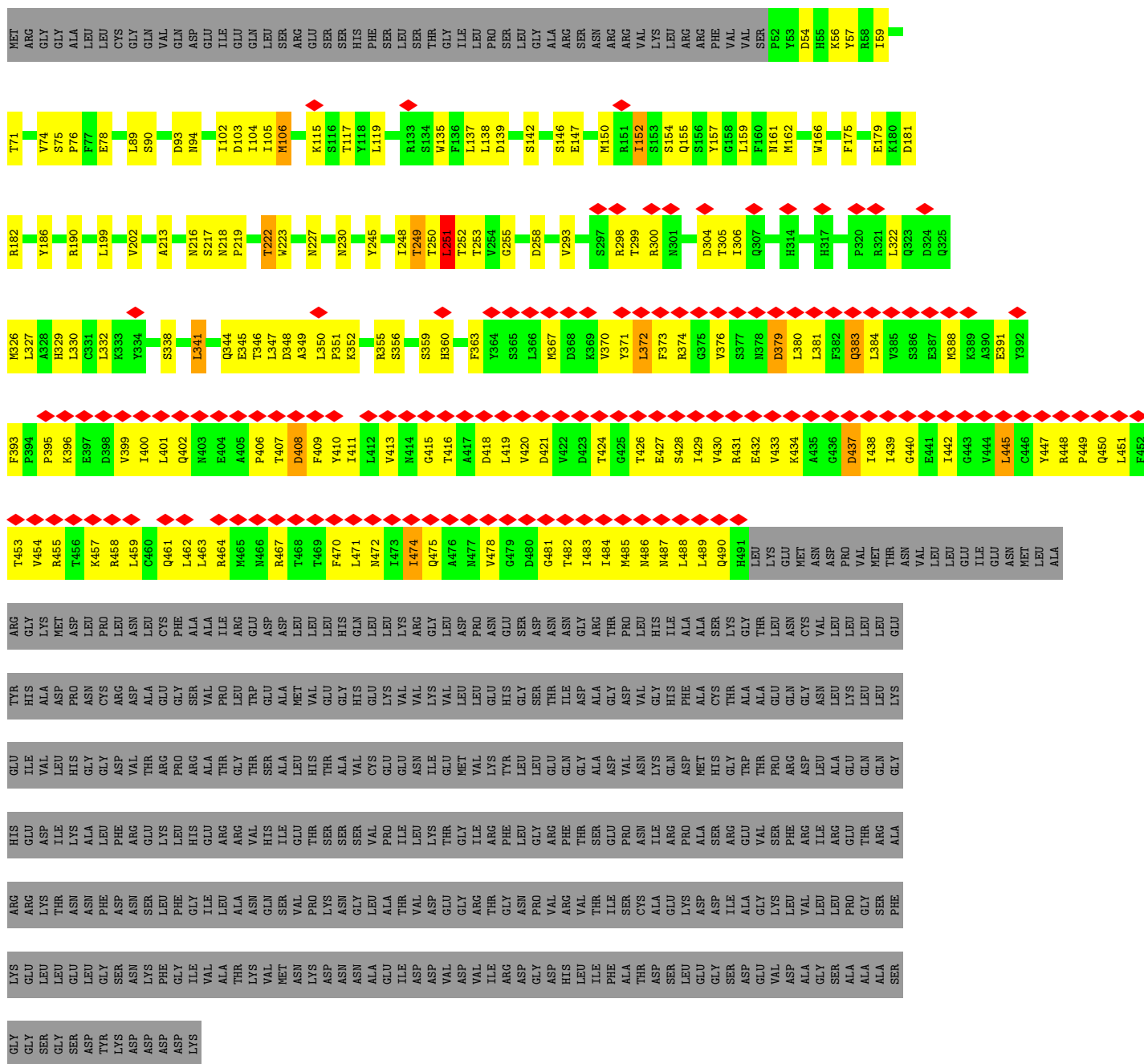


[illegible]

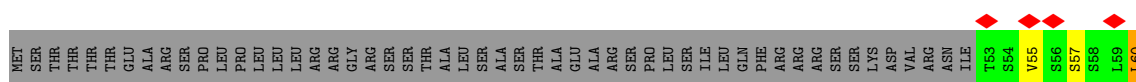
- Molecule 1: Potassium channel AKT1

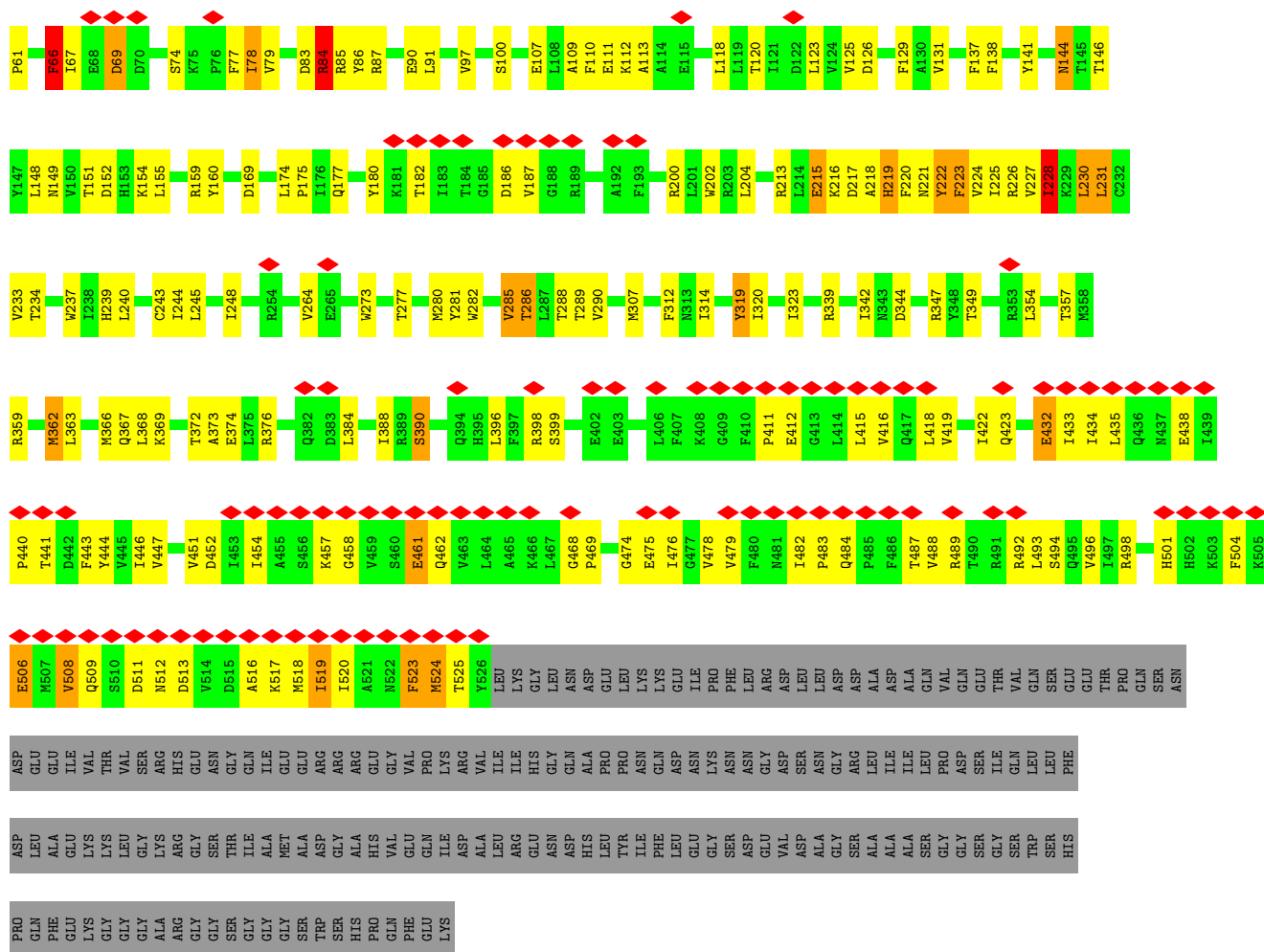


- Molecule 1: Potassium channel AKT1



Chain B: 15% 41% 22% 22%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	649659	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	8.860	Depositor
Minimum map value	-5.951	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.160	Depositor
Recommended contour level	0.642	Depositor
Map size (Å)	258.552, 258.552, 258.552	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0773, 1.0773, 1.0773	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: K, POV

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	0.43	1/3689 (0.0%)	0.53	1/5010 (0.0%)
1	C	0.38	0/3689	0.54	1/5010 (0.0%)
1	D	0.43	3/3681 (0.1%)	0.55	4/4999 (0.1%)
2	B	0.59	6/3958 (0.2%)	0.77	12/5368 (0.2%)
All	All	0.47	10/15017 (0.1%)	0.61	18/20387 (0.1%)

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	C	0	1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	458	ARG	C-O	-10.47	1.12	1.23
2	B	215	GLU	C-O	-7.36	1.13	1.23
2	B	217	ASP	C-O	-7.34	1.15	1.23
1	D	250	THR	C-O	-6.93	1.14	1.23
1	D	251	LEU	C-O	-6.07	1.17	1.24

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	222	TYR	CB-CA-C	-9.63	95.68	110.90
1	A	78	GLU	CB-CA-C	-9.26	96.27	110.90
1	D	250	THR	CA-CB-OG1	-8.60	96.70	109.60
2	B	216	LYS	N-CA-C	-7.21	105.02	113.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	217	ASP	CA-C-O	-6.59	113.23	120.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	303	ARG	Sidechain

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	3599	0	3614	93	0
1	C	3599	0	3614	130	0
1	D	3591	0	3602	125	0
2	B	3861	0	3907	130	0
3	A	39	0	52	0	0
3	B	39	0	52	0	0
3	C	39	0	52	9	0
3	D	39	0	52	3	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
All	All	14809	0	14945	448	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 15.

The worst 5 of 448 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:B:479:VAL:HG11	2:B:523:PHE:CE2	1.49	1.47
2:B:479:VAL:CG1	2:B:523:PHE:HE2	1.61	1.13
1:C:458:ARG:HG2	1:D:117:THR:HG21	1.26	1.12
1:A:458:ARG:HH21	1:A:458:ARG:HB3	1.24	1.01
1:C:395:PRO:HB3	1:C:458:ARG:O	1.64	0.96

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	439/885 (50%)	396 (90%)	43 (10%)	0	100	100
1	C	439/885 (50%)	393 (90%)	46 (10%)	0	100	100
1	D	438/885 (50%)	403 (92%)	35 (8%)	0	100	100
2	B	472/710 (66%)	429 (91%)	41 (9%)	2 (0%)	30	57
All	All	1788/3365 (53%)	1621 (91%)	165 (9%)	2 (0%)	49	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	85	ARG
2	B	60	LEU

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	392/766 (51%)	353 (90%)	39 (10%)	7	22
1	C	392/766 (51%)	354 (90%)	38 (10%)	8	23
1	D	391/766 (51%)	356 (91%)	35 (9%)	9	26
2	B	420/615 (68%)	371 (88%)	49 (12%)	5	15
All	All	1595/2913 (55%)	1434 (90%)	161 (10%)	9	21

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	386	SER
1	D	341	LEU
1	C	453	THR
1	D	105	ILE
1	D	391	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	277	ASN
1	D	294	HIS
1	D	487	ASN
2	B	495	GLN
2	B	423	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](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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	POV	B	801	-	38,38,51	0.57	0	41,43,59	0.71	2 (4%)
3	POV	C	901	-	38,38,51	1.10	2 (5%)	41,43,59	1.38	5 (12%)
3	POV	D	901	-	38,38,51	0.57	0	41,43,59	0.89	3 (7%)
3	POV	A	901	-	38,38,51	1.35	7 (18%)	41,43,59	1.27	6 (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	POV	B	801	-	-	21/40/40/55	-
3	POV	C	901	-	-	19/40/40/55	-
3	POV	D	901	-	-	26/40/40/55	-
3	POV	A	901	-	-	21/40/40/55	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	POV	C313-C312	-3.44	1.34	1.51
3	C	901	POV	O22-C21	-3.10	1.13	1.22
3	A	901	POV	C27-C28	-2.76	1.40	1.52
3	A	901	POV	O22-C21	-2.75	1.14	1.22
3	A	901	POV	C23-C22	-2.46	1.43	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	901	POV	O21-C21-C22	5.28	122.89	111.48
3	A	901	POV	O11-P-O14	3.49	115.87	106.44
3	D	901	POV	O21-C21-C22	3.35	118.72	111.48
3	A	901	POV	O21-C21-C22	3.28	118.58	111.48
3	A	901	POV	O12-P-O11	-2.79	99.38	106.67

There are no chirality outliers.

5 of 87 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	POV	C1-O11-P-O12
3	A	901	POV	C1-O11-P-O13

Continued on next page...

Continued from previous page...

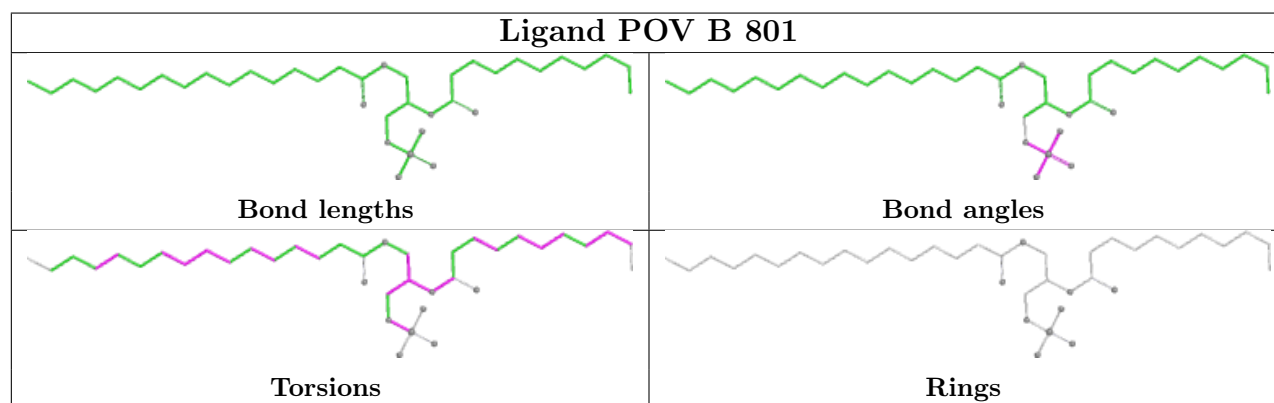
Mol	Chain	Res	Type	Atoms
3	A	901	POV	C1-O11-P-O14
3	B	801	POV	C1-O11-P-O12
3	B	801	POV	C1-O11-P-O13

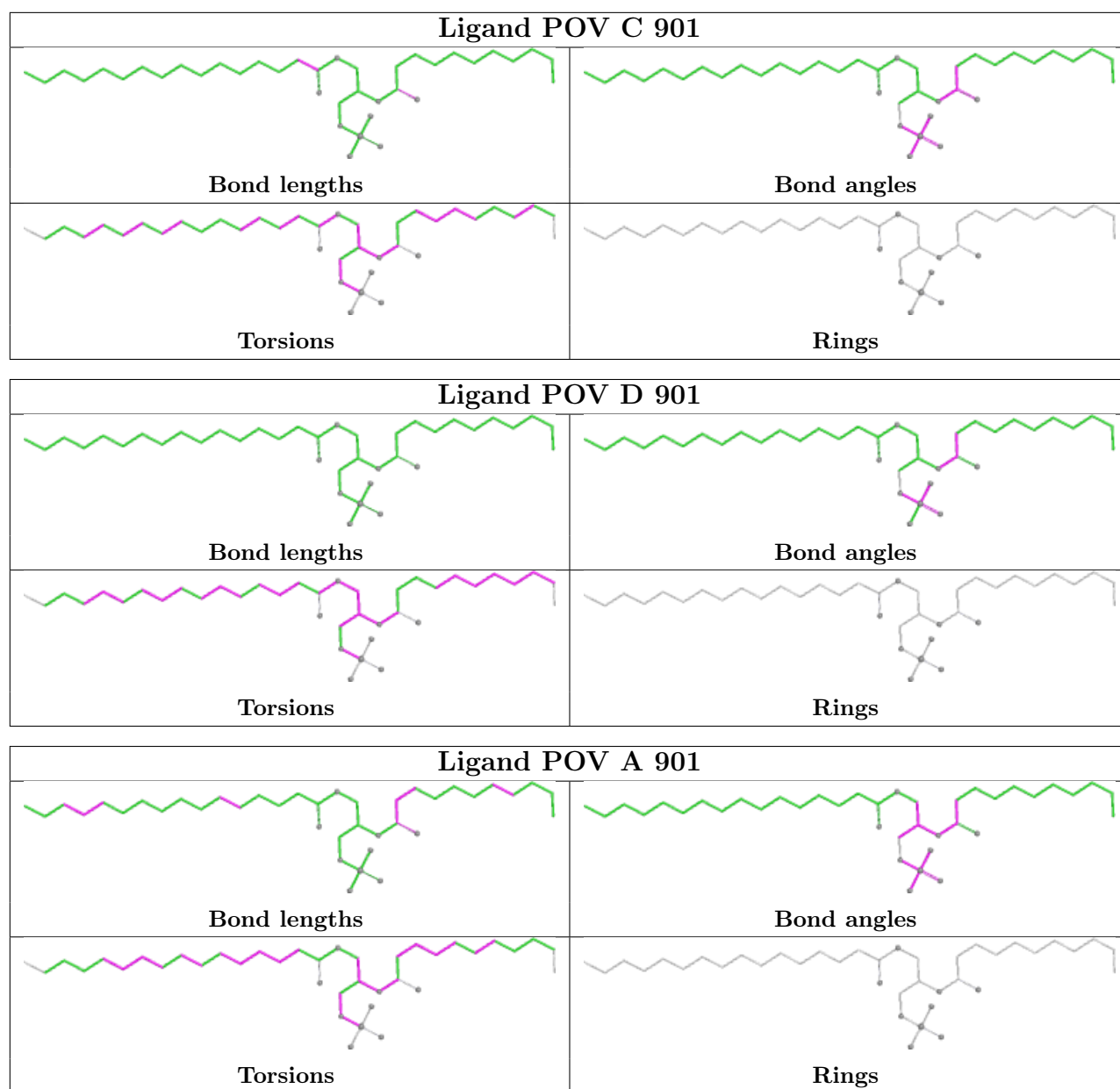
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	901	POV	9	0
3	D	901	POV	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.

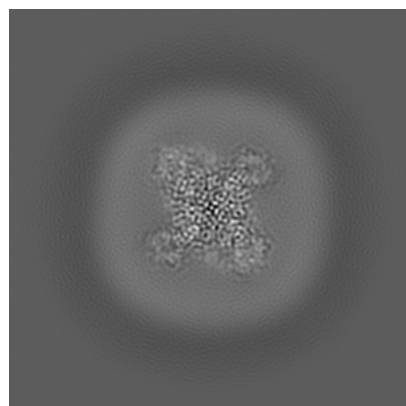
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60834. These allow visual inspection of the internal detail of the map and identification of artifacts.

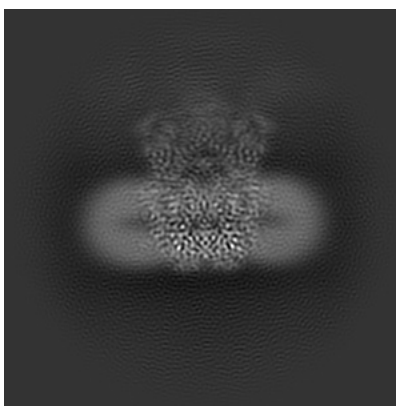
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

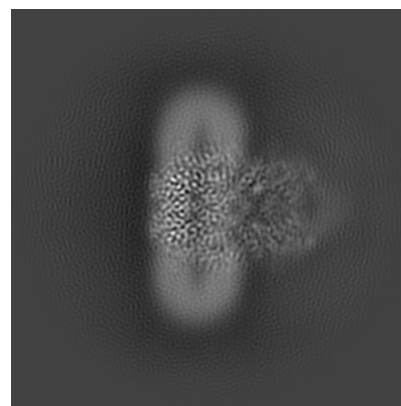
6.1.1 Primary map



X

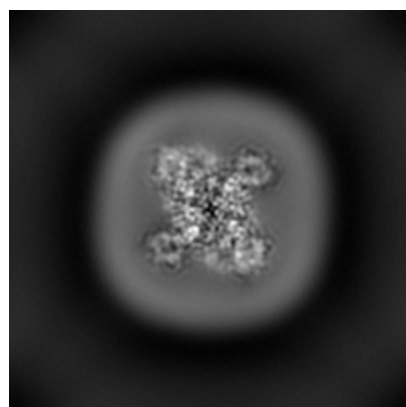


Y

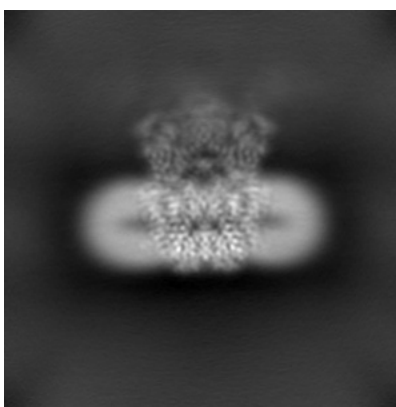


Z

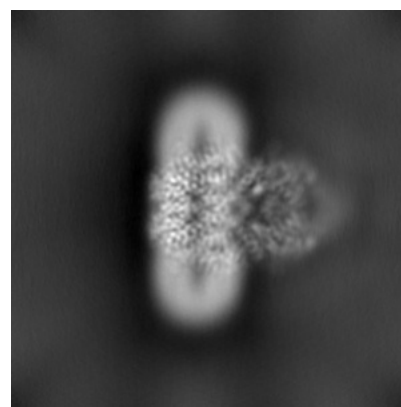
6.1.2 Raw map



X



Y

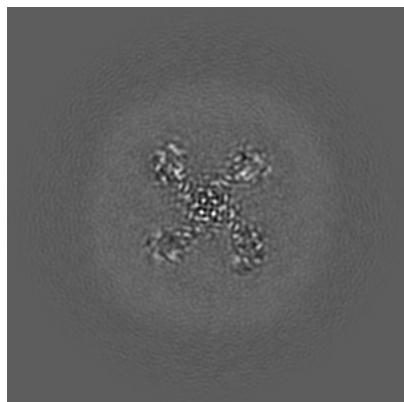


Z

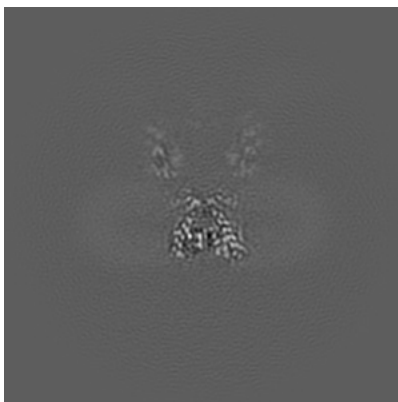
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

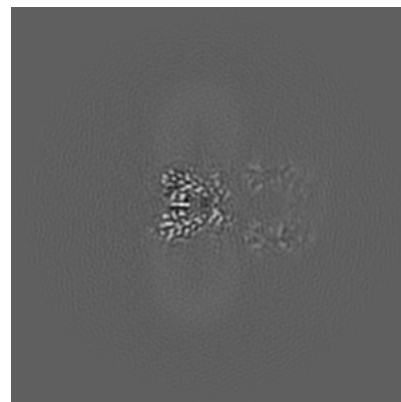
6.2.1 Primary map



X Index: 120

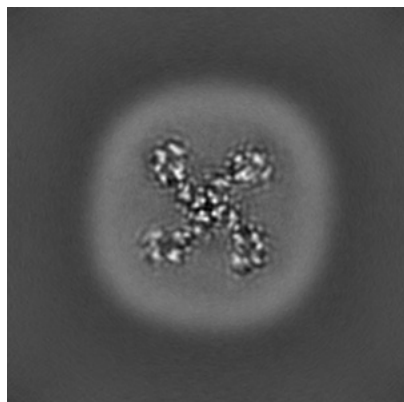


Y Index: 120

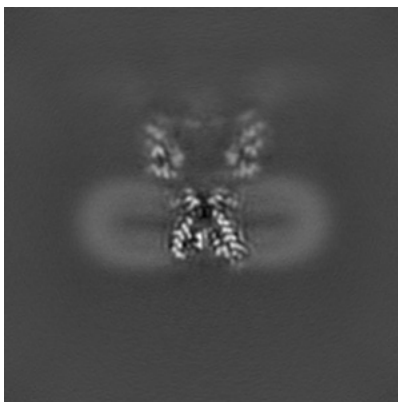


Z Index: 120

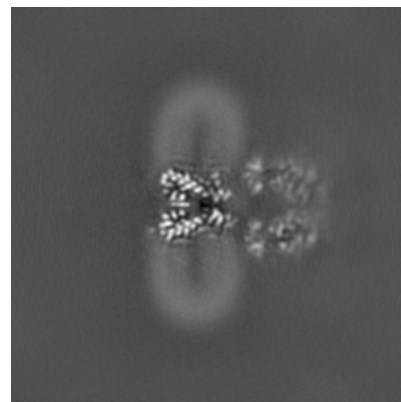
6.2.2 Raw map



X Index: 120



Y Index: 120

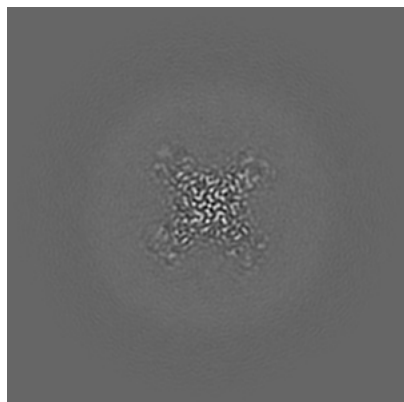


Z Index: 120

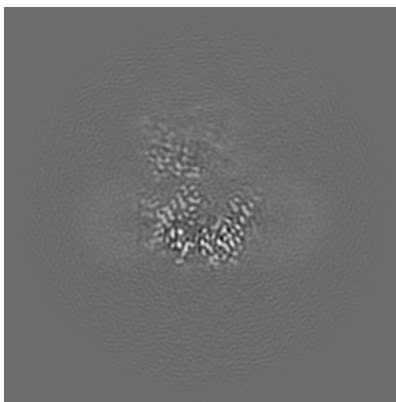
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

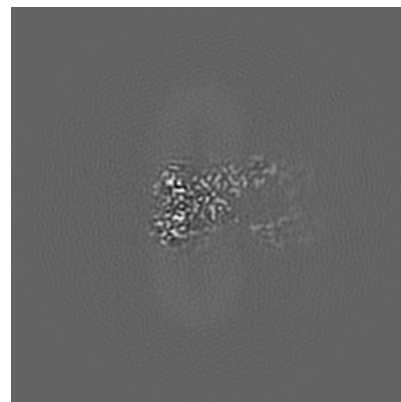
6.3.1 Primary map



X Index: 102

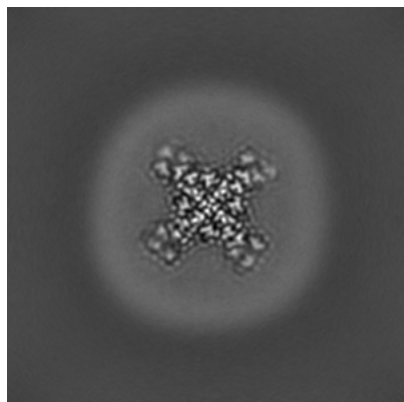


Y Index: 137

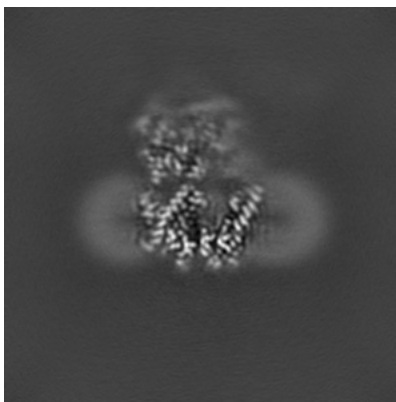


Z Index: 112

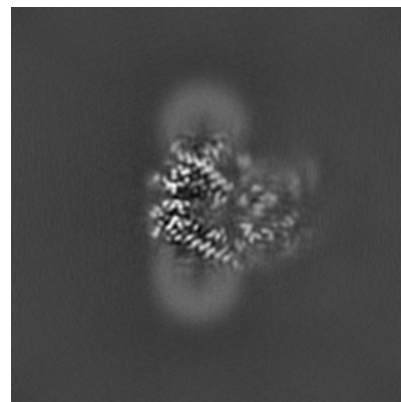
6.3.2 Raw map



X Index: 101



Y Index: 138

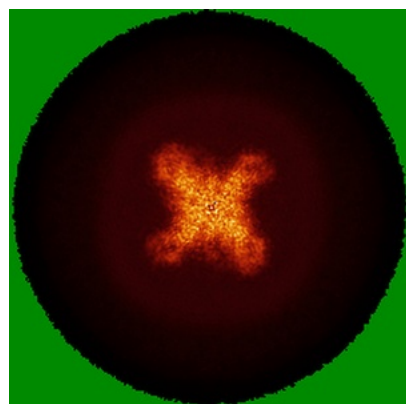


Z Index: 137

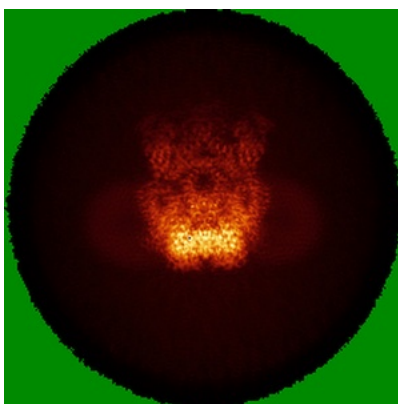
The images above show the largest variance slices of the map in three orthogonal directions.

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

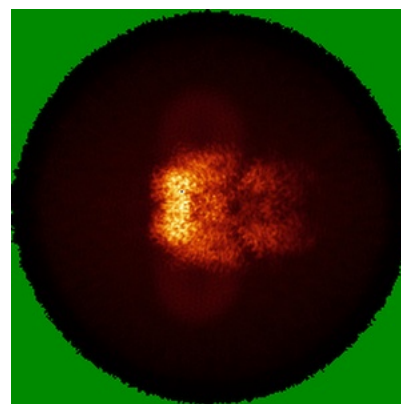
6.4.1 Primary map



X

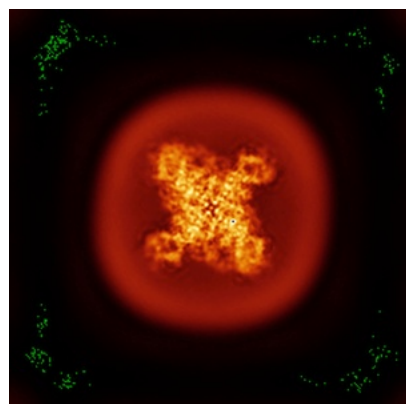


Y

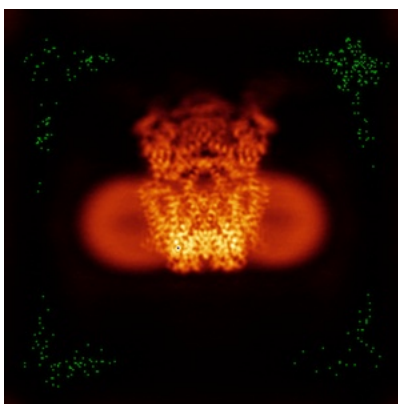


Z

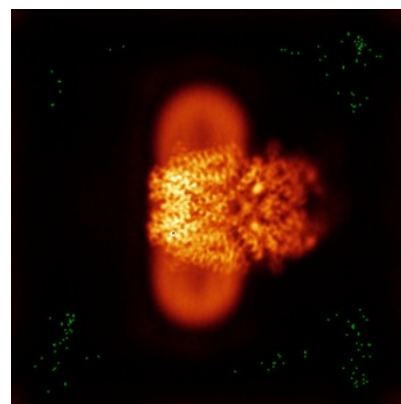
6.4.2 Raw map



X



Y

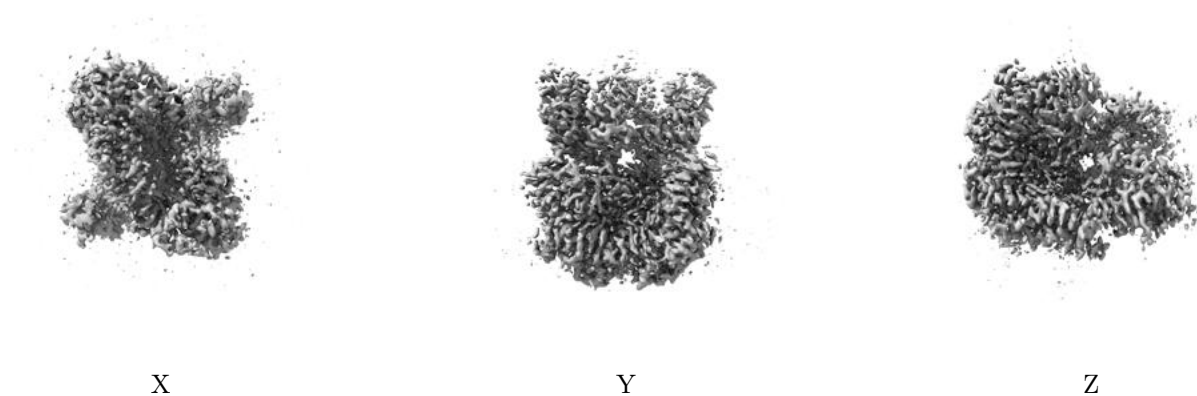


Z

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.

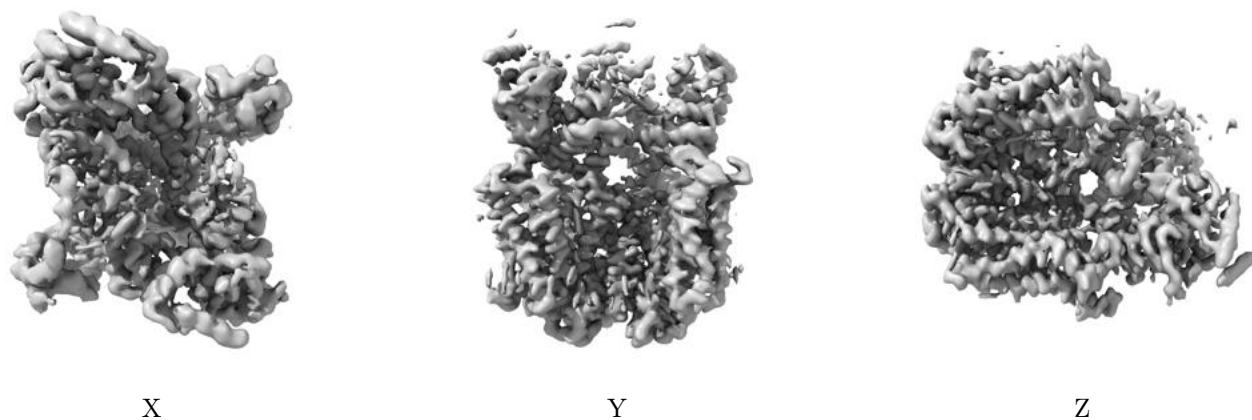
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.642. 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.

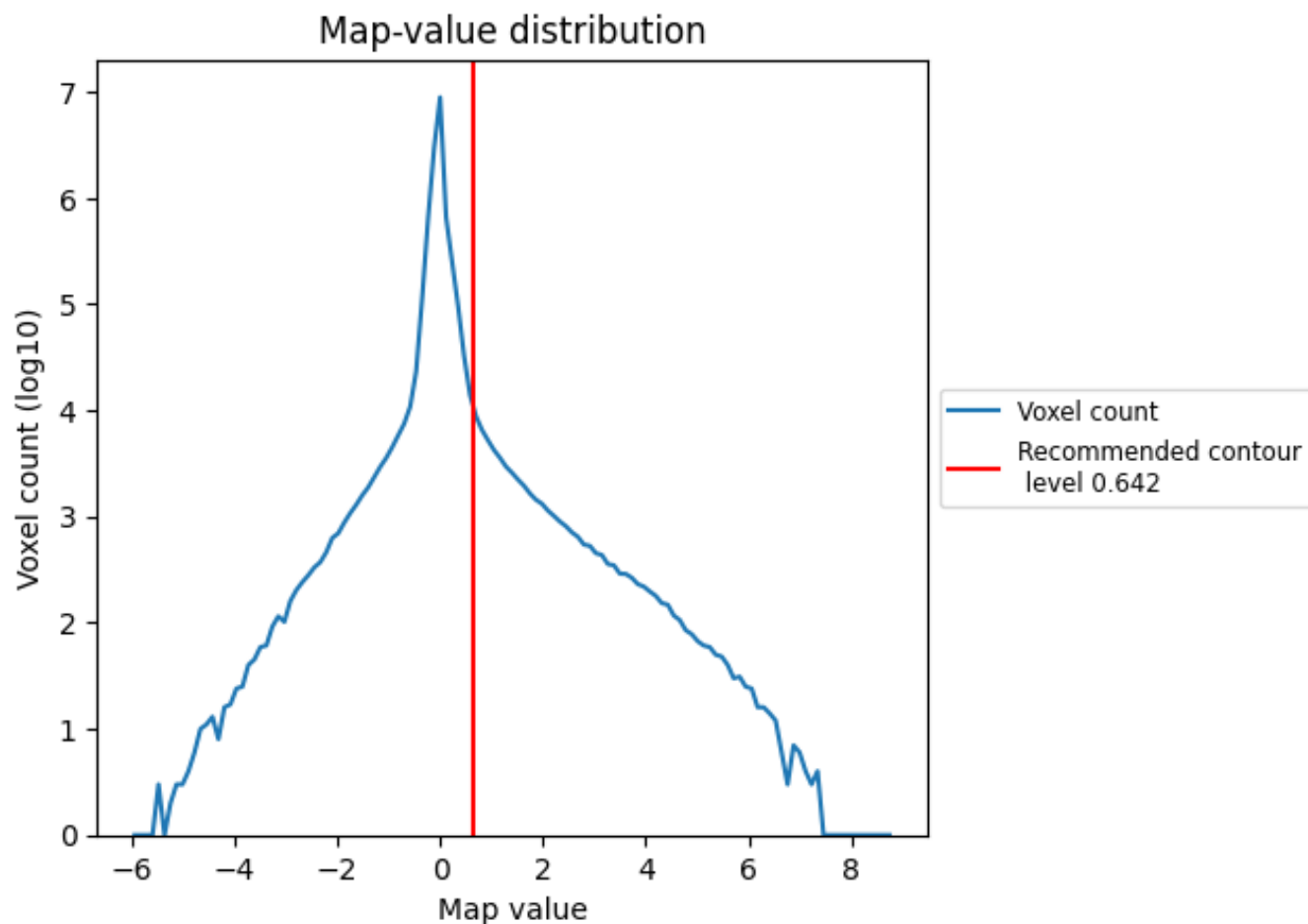
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

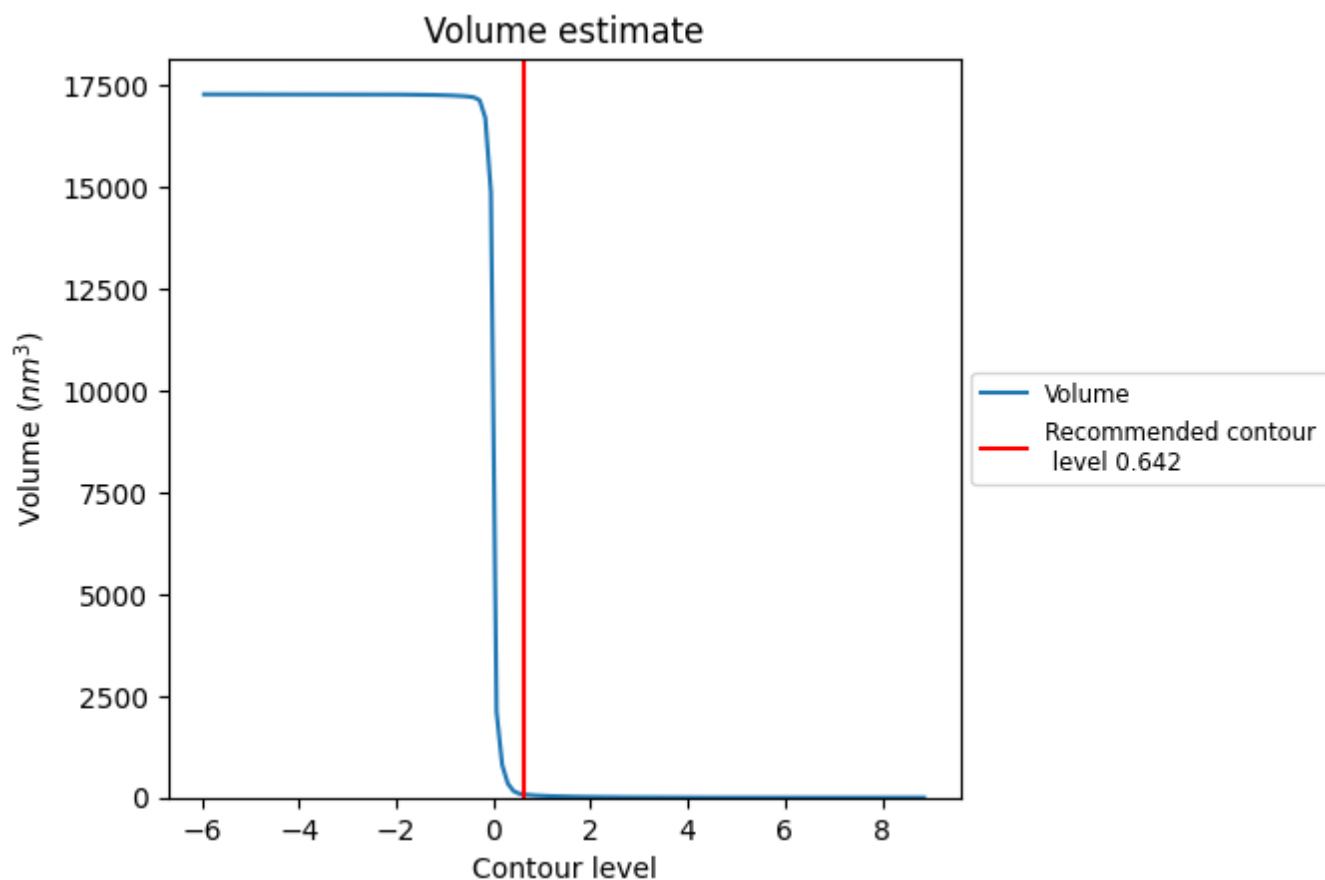
This section contains the results of statistical analysis of the map.

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.

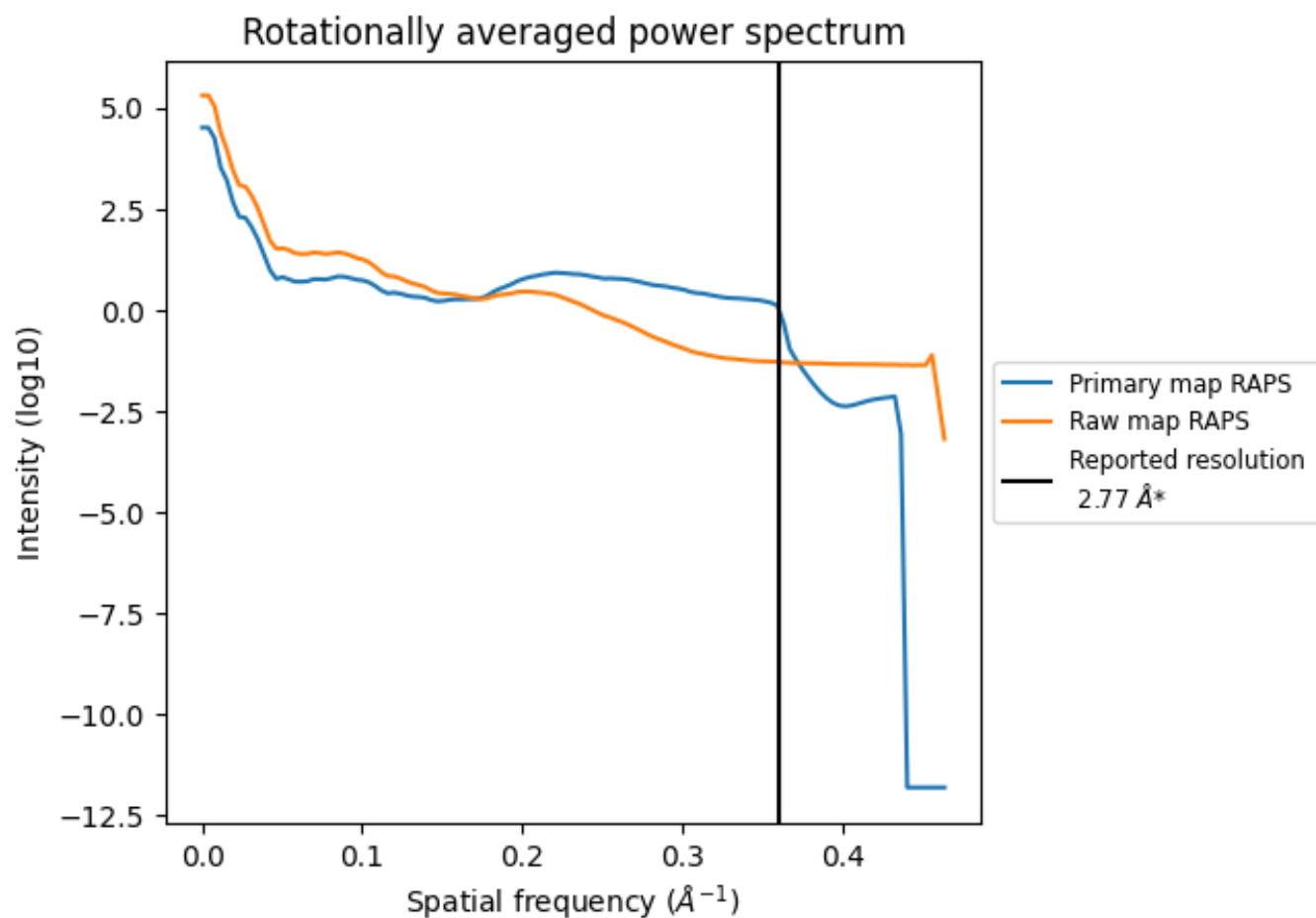
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 74 nm^3 ; this corresponds to an approximate mass of 67 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 ⓘ

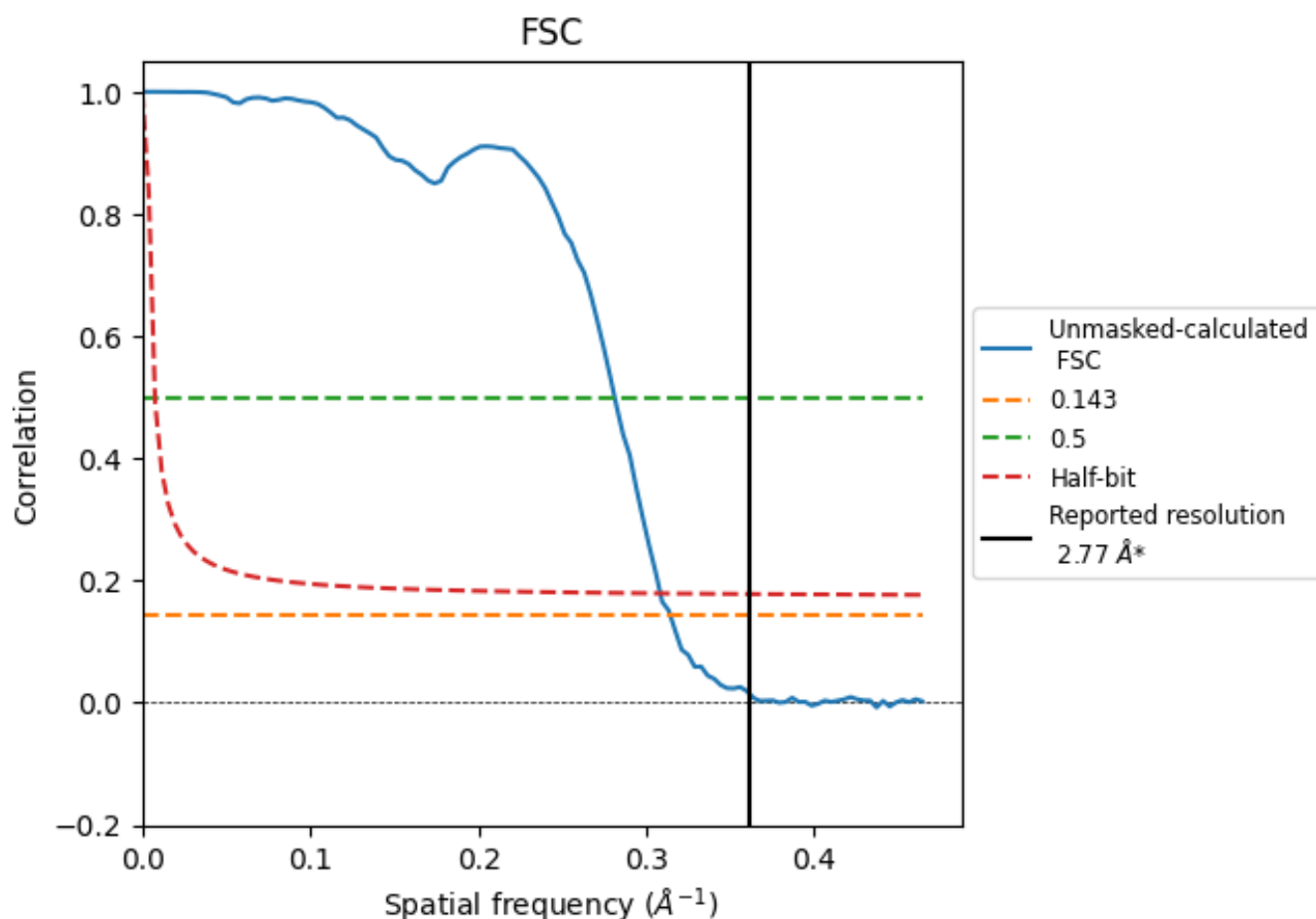


*Reported resolution corresponds to spatial frequency of 0.361 Å⁻¹

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 0.361 Å⁻¹

8.2 Resolution estimates [i](#)

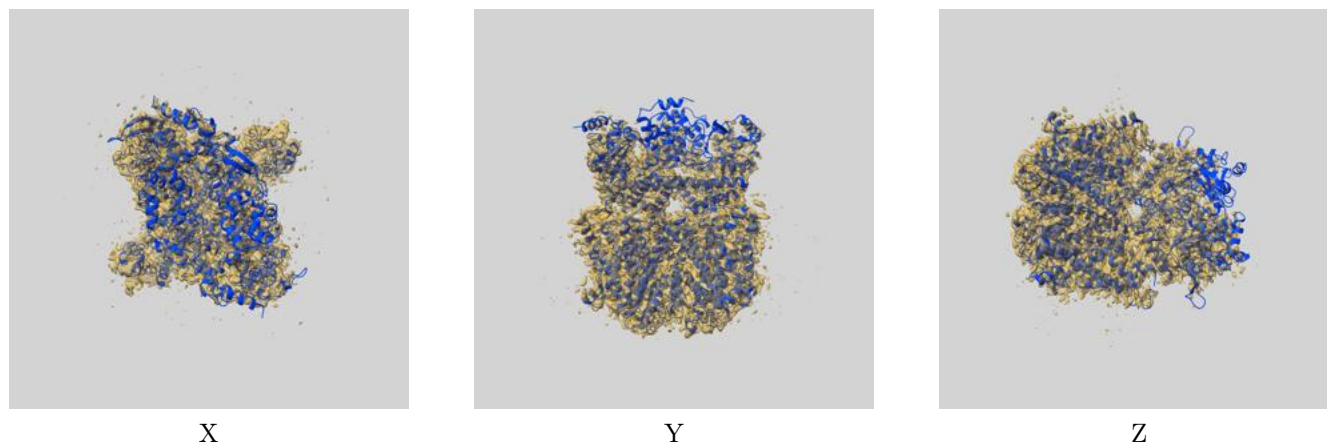
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.77	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.18	3.56	3.24

*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 3.18 differs from the reported value 2.77 by more than 10 %

9 Map-model fit [i](#)

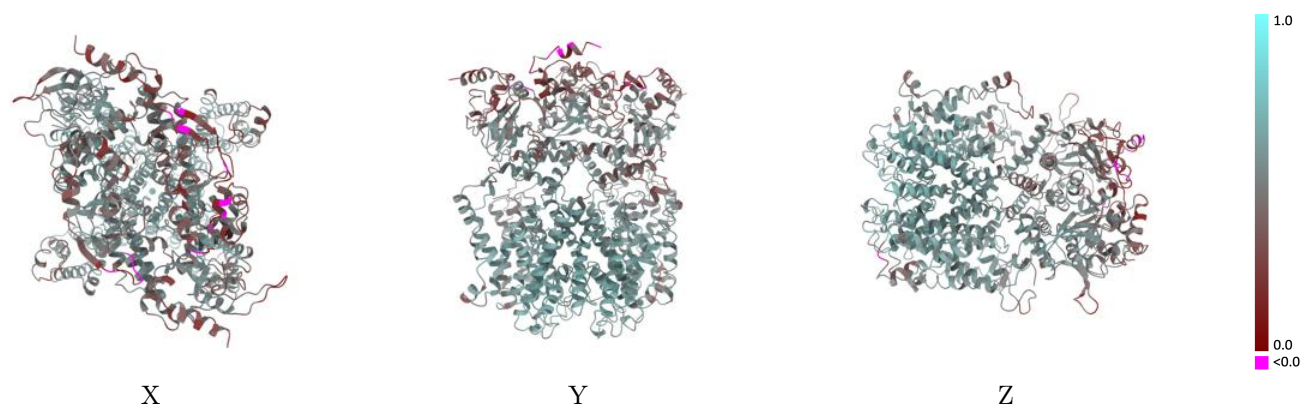
This section contains information regarding the fit between EMDB map EMD-60834 and PDB model 9IS8. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



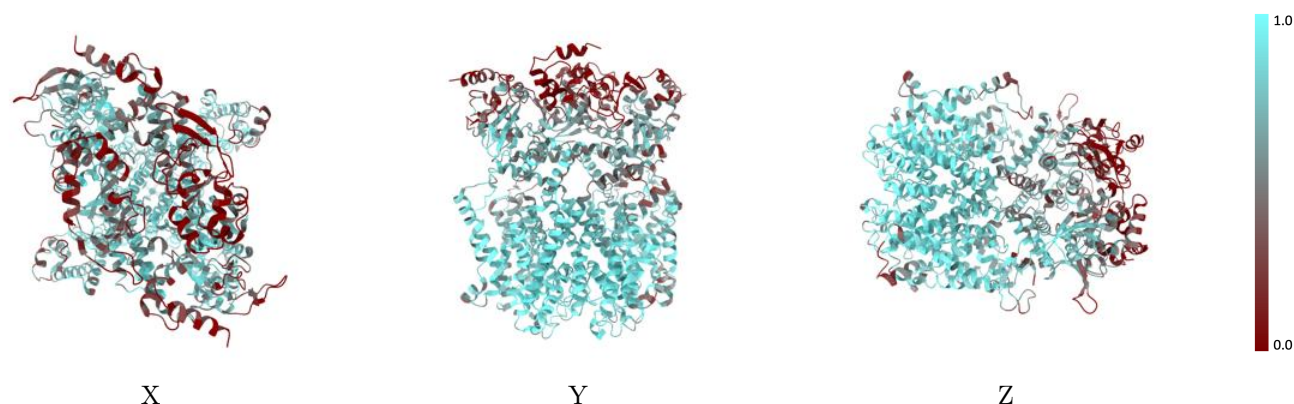
The images above show the 3D surface view of the map at the recommended contour level 0.642 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



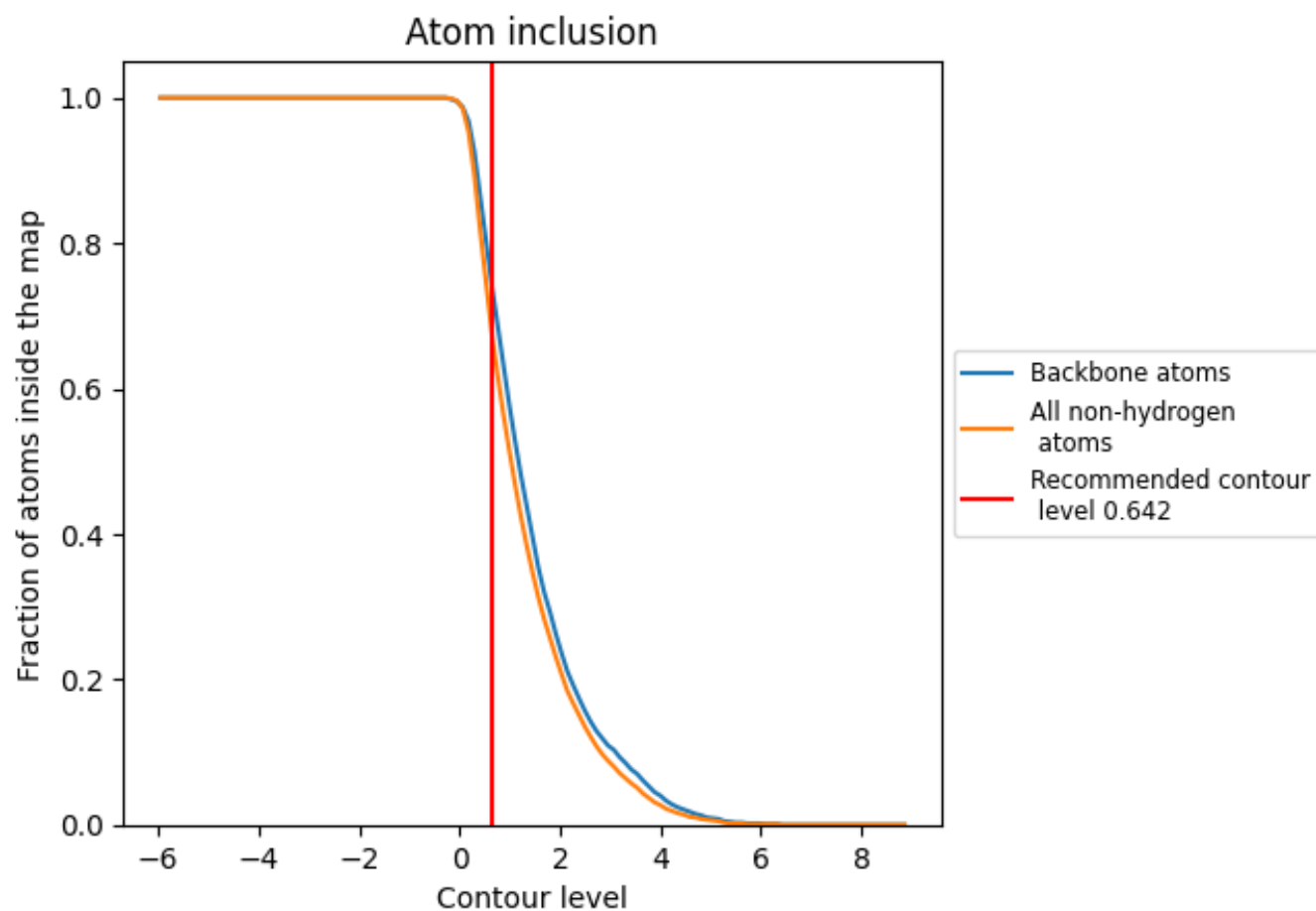
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.642).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 68% 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 (0.642) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6770	0.5160
A	0.7140	0.5290
B	0.6800	0.5250
C	0.7020	0.5200
D	0.6120	0.4880

