wwPDB EM Validation Summary Report (i)

May 12, 2025 – 04:10 PM JST

PDB ID	:	7WM2 / pdb_00007wm2
EMDB ID	:	EMD-32598
Title	:	Cryo-EM structure of AKT1
Authors	:	Dongliang, L.; Zijie, Z.; Yannan, Q.; Yuyue, T.; Huaizong, S.
Deposited on	:	2022-01-14
Resolution	:	2.69 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 (i) 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 (i)) were used in the production of this report:

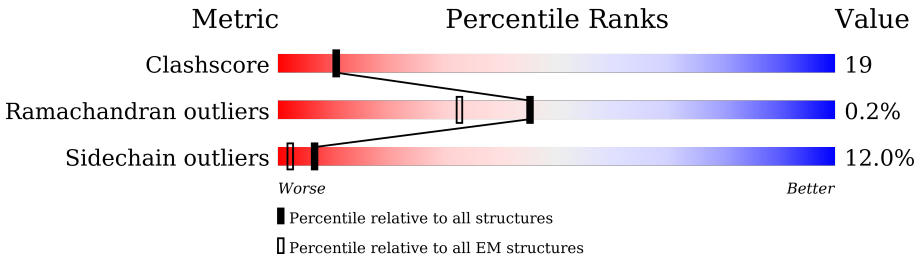
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.69 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 <=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	895	5% 32% 16% • 47%
1	B	895	7% 32% 16% • • 48%
1	C	895	6% 32% 17% • 47%
1	D	895	7% 34% 16% • 48%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15485 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	470	Total	C	N	O	S	0	0
			3837	2491	651	672	23		
1	B	469	Total	C	N	O	S	0	0
			3826	2485	647	671	23		
1	C	470	Total	C	N	O	S	0	0
			3837	2491	651	672	23		
1	D	469	Total	C	N	O	S	0	0
			3826	2485	647	671	23		

There are 152 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	ASP	-	expression tag	UNP Q38998
A	877	TYR	-	expression tag	UNP Q38998
A	878	LYS	-	expression tag	UNP Q38998
A	879	ASP	-	expression tag	UNP Q38998

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Chain	Residue	Modelled	Actual	Comment	Reference
A	880	ASP	-	expression tag	UNP Q38998
A	881	ASP	-	expression tag	UNP Q38998
A	882	ASP	-	expression tag	UNP Q38998
A	883	LYS	-	expression tag	UNP Q38998
A	884	GLY	-	expression tag	UNP Q38998
A	885	SER	-	expression tag	UNP Q38998
A	886	HIS	-	expression tag	UNP Q38998
A	887	HIS	-	expression tag	UNP Q38998
A	888	HIS	-	expression tag	UNP Q38998
A	889	HIS	-	expression tag	UNP Q38998
A	890	HIS	-	expression tag	UNP Q38998
A	891	HIS	-	expression tag	UNP Q38998
A	892	HIS	-	expression tag	UNP Q38998
A	893	HIS	-	expression tag	UNP Q38998
A	894	HIS	-	expression tag	UNP Q38998
A	895	HIS	-	expression tag	UNP Q38998
B	858	LEU	-	expression tag	UNP Q38998
B	859	GLU	-	expression tag	UNP Q38998
B	860	GLY	-	expression tag	UNP Q38998
B	861	SER	-	expression tag	UNP Q38998
B	862	ASP	-	expression tag	UNP Q38998
B	863	GLU	-	expression tag	UNP Q38998
B	864	VAL	-	expression tag	UNP Q38998
B	865	ASP	-	expression tag	UNP Q38998
B	866	ALA	-	expression tag	UNP Q38998
B	867	GLY	-	expression tag	UNP Q38998
B	868	SER	-	expression tag	UNP Q38998
B	869	ALA	-	expression tag	UNP Q38998
B	870	ALA	-	expression tag	UNP Q38998
B	871	ALA	-	expression tag	UNP Q38998
B	872	SER	-	expression tag	UNP Q38998
B	873	GLY	-	expression tag	UNP Q38998
B	874	GLY	-	expression tag	UNP Q38998
B	875	SER	-	expression tag	UNP Q38998
B	876	ASP	-	expression tag	UNP Q38998
B	877	TYR	-	expression tag	UNP Q38998
B	878	LYS	-	expression tag	UNP Q38998
B	879	ASP	-	expression tag	UNP Q38998
B	880	ASP	-	expression tag	UNP Q38998
B	881	ASP	-	expression tag	UNP Q38998
B	882	ASP	-	expression tag	UNP Q38998
B	883	LYS	-	expression tag	UNP Q38998

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Chain	Residue	Modelled	Actual	Comment	Reference
B	884	GLY	-	expression tag	UNP Q38998
B	885	SER	-	expression tag	UNP Q38998
B	886	HIS	-	expression tag	UNP Q38998
B	887	HIS	-	expression tag	UNP Q38998
B	888	HIS	-	expression tag	UNP Q38998
B	889	HIS	-	expression tag	UNP Q38998
B	890	HIS	-	expression tag	UNP Q38998
B	891	HIS	-	expression tag	UNP Q38998
B	892	HIS	-	expression tag	UNP Q38998
B	893	HIS	-	expression tag	UNP Q38998
B	894	HIS	-	expression tag	UNP Q38998
B	895	HIS	-	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	ASP	-	expression tag	UNP Q38998
C	877	TYR	-	expression tag	UNP Q38998
C	878	LYS	-	expression tag	UNP Q38998
C	879	ASP	-	expression tag	UNP Q38998
C	880	ASP	-	expression tag	UNP Q38998
C	881	ASP	-	expression tag	UNP Q38998
C	882	ASP	-	expression tag	UNP Q38998
C	883	LYS	-	expression tag	UNP Q38998
C	884	GLY	-	expression tag	UNP Q38998
C	885	SER	-	expression tag	UNP Q38998
C	886	HIS	-	expression tag	UNP Q38998
C	887	HIS	-	expression tag	UNP Q38998

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Chain	Residue	Modelled	Actual	Comment	Reference
C	888	HIS	-	expression tag	UNP Q38998
C	889	HIS	-	expression tag	UNP Q38998
C	890	HIS	-	expression tag	UNP Q38998
C	891	HIS	-	expression tag	UNP Q38998
C	892	HIS	-	expression tag	UNP Q38998
C	893	HIS	-	expression tag	UNP Q38998
C	894	HIS	-	expression tag	UNP Q38998
C	895	HIS	-	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
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	ASP	-	expression tag	UNP Q38998
D	877	TYR	-	expression tag	UNP Q38998
D	878	LYS	-	expression tag	UNP Q38998
D	879	ASP	-	expression tag	UNP Q38998
D	880	ASP	-	expression tag	UNP Q38998
D	881	ASP	-	expression tag	UNP Q38998
D	882	ASP	-	expression tag	UNP Q38998
D	883	LYS	-	expression tag	UNP Q38998
D	884	GLY	-	expression tag	UNP Q38998
D	885	SER	-	expression tag	UNP Q38998
D	886	HIS	-	expression tag	UNP Q38998
D	887	HIS	-	expression tag	UNP Q38998
D	888	HIS	-	expression tag	UNP Q38998
D	889	HIS	-	expression tag	UNP Q38998
D	890	HIS	-	expression tag	UNP Q38998
D	891	HIS	-	expression tag	UNP Q38998

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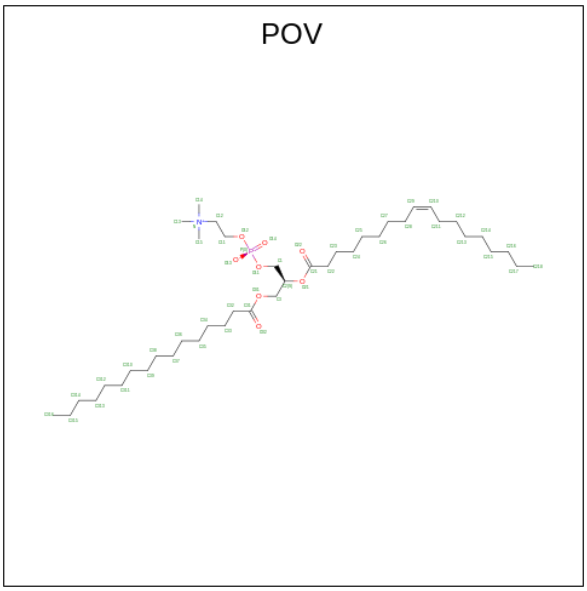
Chain	Residue	Modelled	Actual	Comment	Reference
D	892	HIS	-	expression tag	UNP Q38998
D	893	HIS	-	expression tag	UNP Q38998
D	894	HIS	-	expression tag	UNP Q38998
D	895	HIS	-	expression tag	UNP Q38998

- Molecule 2 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: $C_{42}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

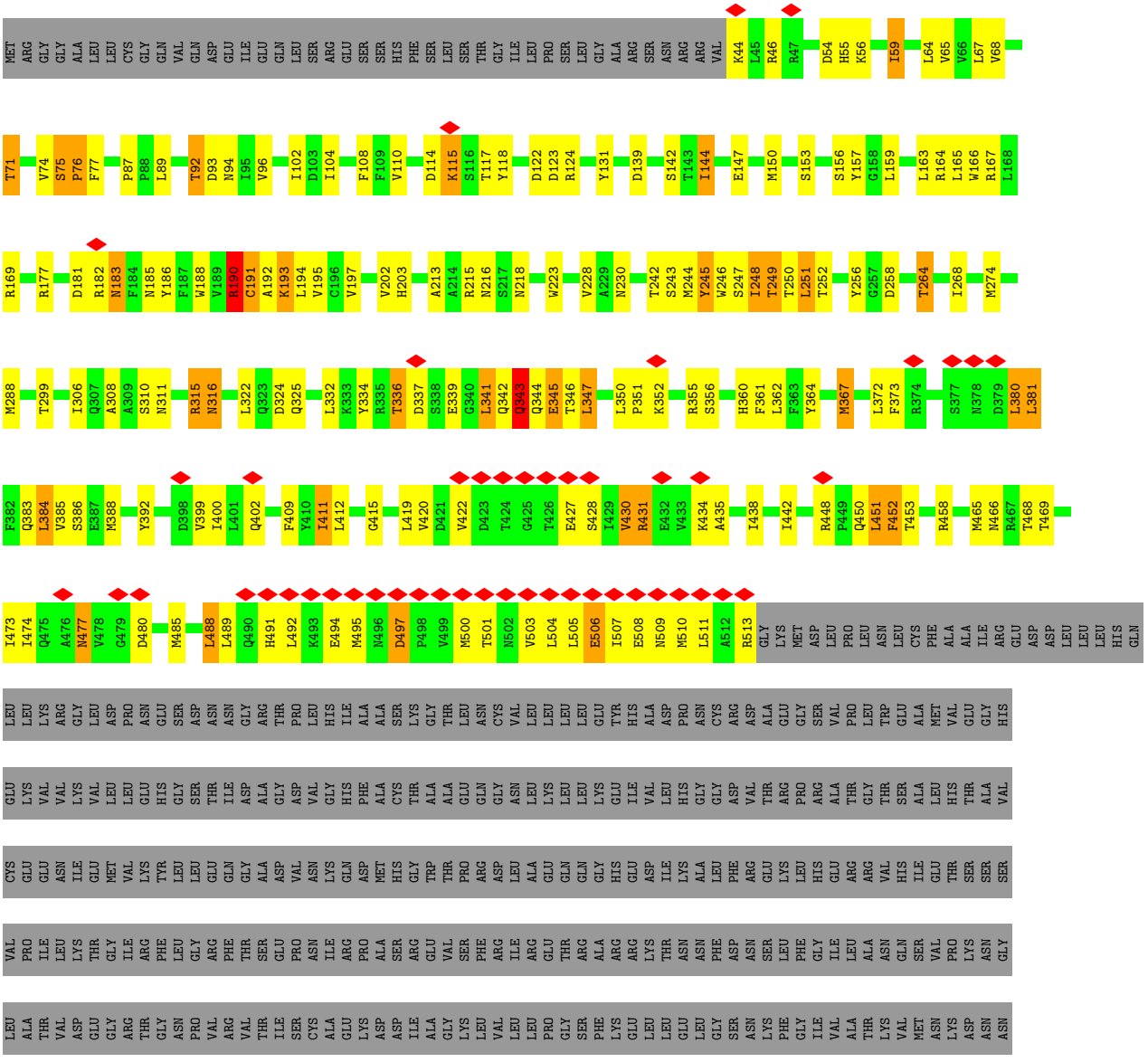
Mol	Chain	Residues	Atoms		AltConf
3	A	3	Total	K	0
			3	3	

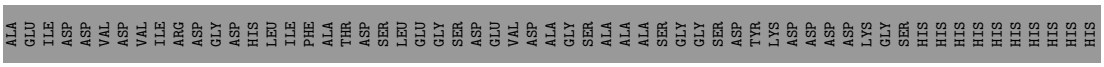
3 Residue-property plots (i)

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

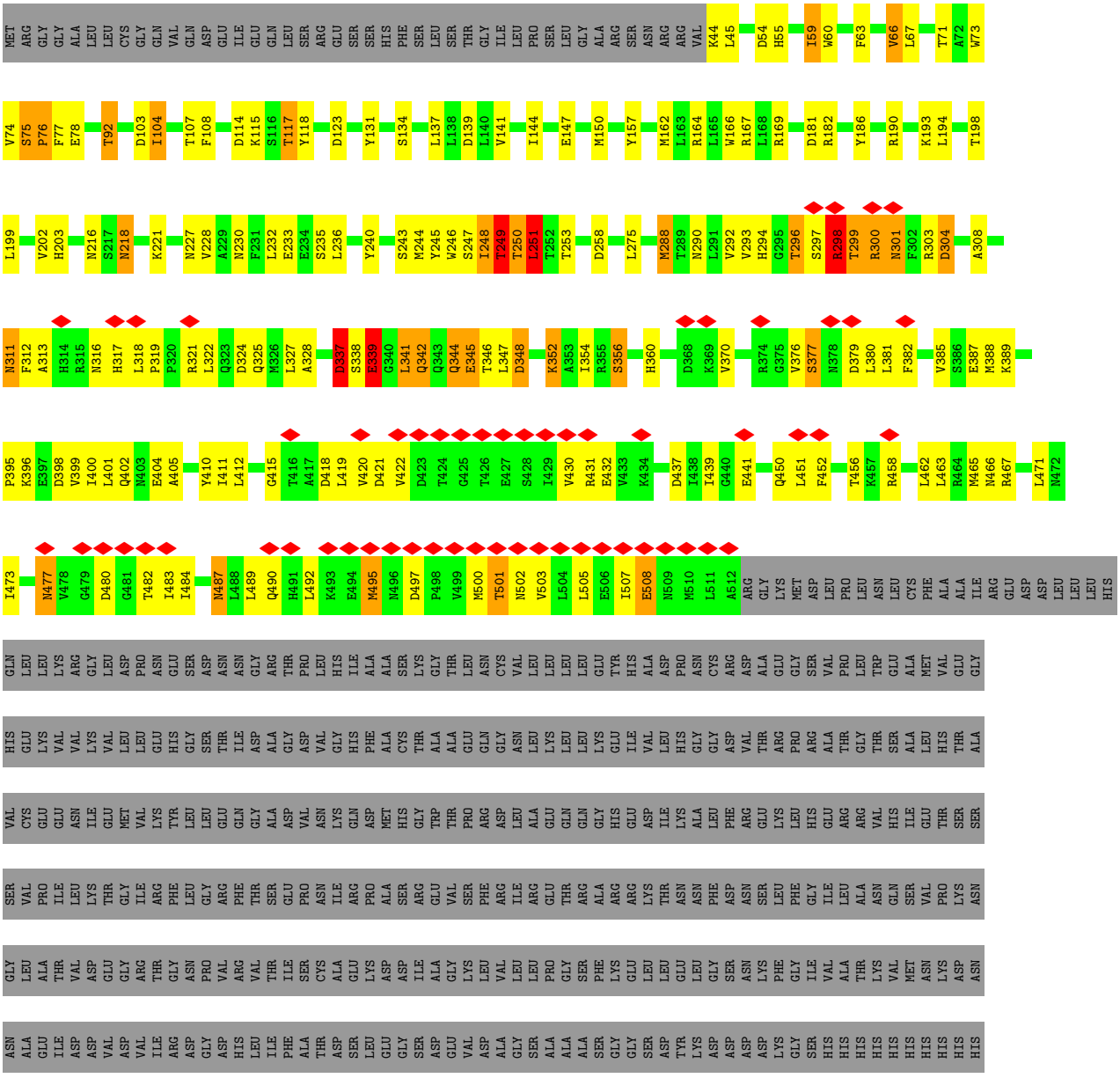
Chain A:





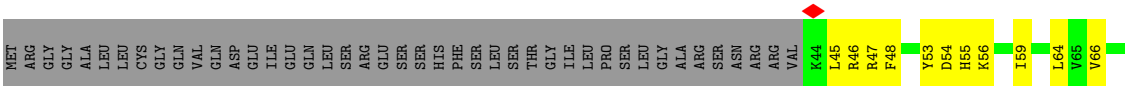
• Molecule 1: Potassium channel AKT1

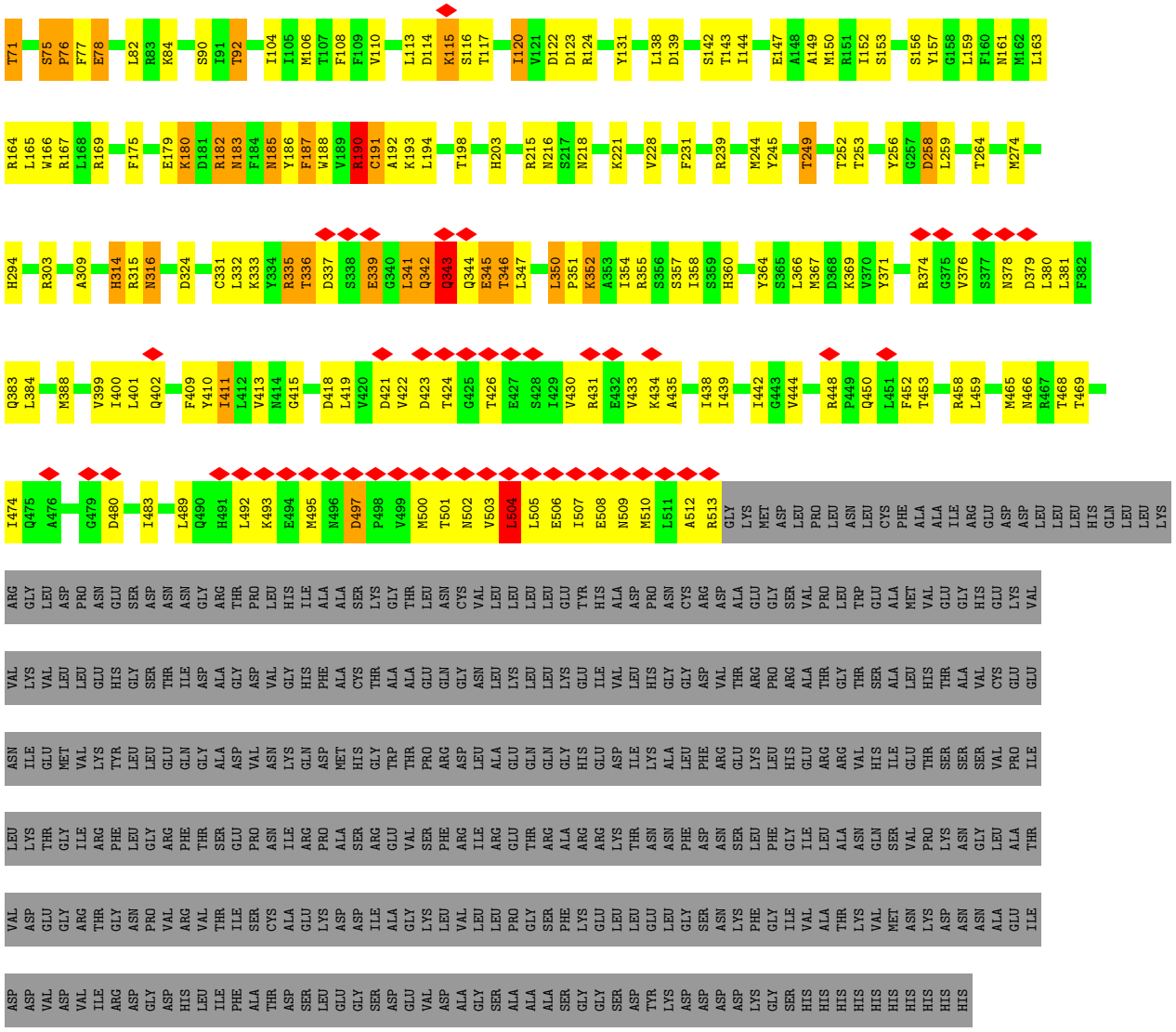
Chain B:



• Molecule 1: Potassium channel AKT1

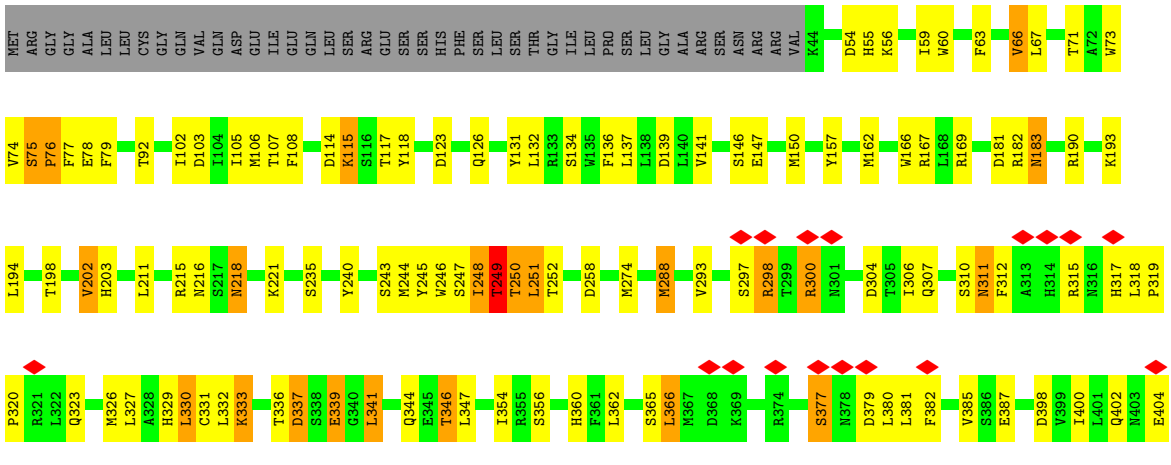
Chain C:

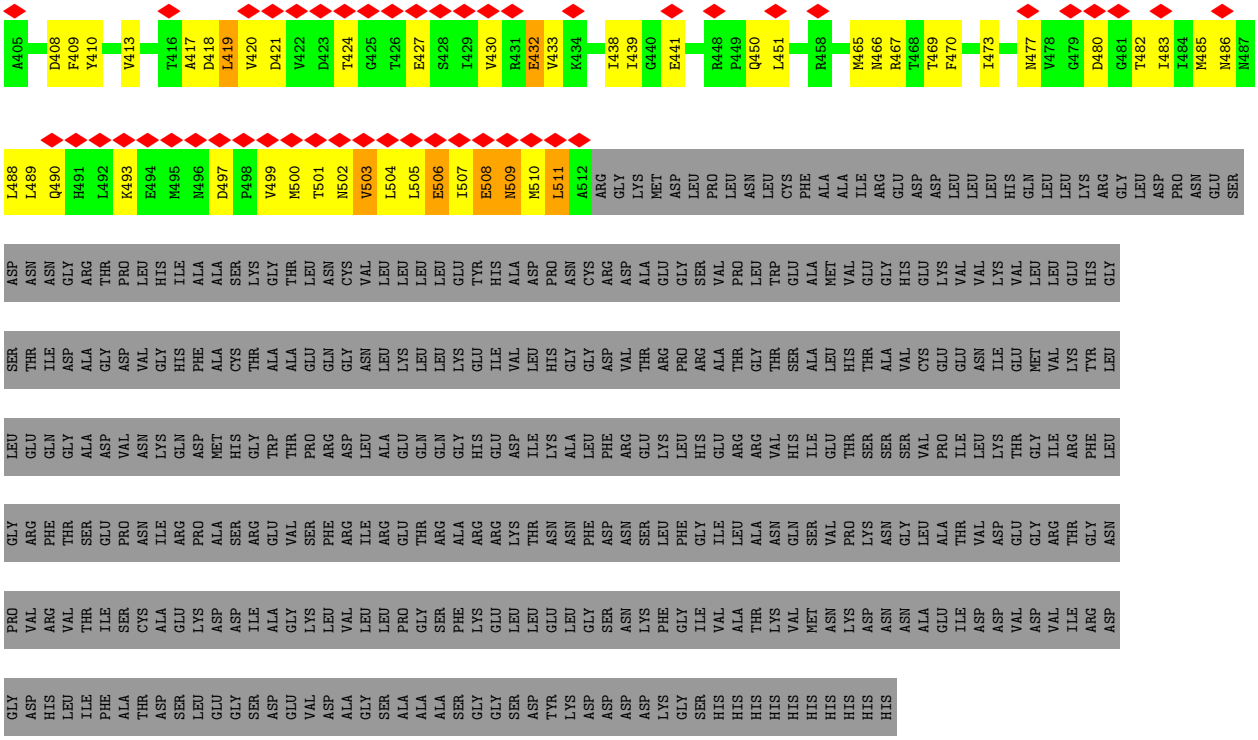




• Molecule 1: Potassium channel AKT1

Chain D:




A405 D408 F409 Y410 V413 T416 A417 D418 L419 V420 D421 V422 D423 T424 G425 T426 E427 S428 I429 V430 R431 E432 V433 K434 I438 I439 G440 E441 R448 P449 Q450 L451 R458 M465 N466 R467 T468 T469 F470 I473 N477 V478 G479 D480 G481 T482 I483 I484 M485 N486 N487
L488 L489 Q490 H491 L492 K493 E494 M495 N496 D497 P498 V499 M500 T501 N502 V503 L504 L505 E506 I507 E508 N509 M510 L511 A512 ARG GLY LYS MET ASP LEU PRO LEU ASN LEU CYS PHE ALA ALA ILE ARG GLU ASP ASP LEU LEU LEU HIS GLN LEU LEU LYS ARG GLY LEU ASP PRO ASN GLU SER
ASP ASN ASN GLY ARG THR PRO LEU HIS ILE ALA ALA ALA SER LYS GLY THR LEU ASN CYS VAL LEU LEU LEU LEU LEU GLU TYR HIS ALA ASP PRO ASN CYS ARG ASP ALA GLU GLY SER VAL PRO LEU TRP GLU ALA MET VAL GLU GLY HIS GLU LYS VAL VAL LYS VAL LEU LEU GLU HIS GLY
SER THR ILE ASP ALA GLY ASP VAL GLY HIS PHE ALA CYS THR ALA ALA GLU GLN GLY ASN LEU LYS GLU LEU LEU LYS GLU ILE VAL LEU HIS GLY GLY ASP VAL THR ARG PRO ARG ALA THR GLY THR SER ALA LEU HIS THR ALA VAL CYS GLU GLU ASN ILE GLU MET VAL LYS TYR LEU
LEU GLU GLN GLY ALA ASP VAL ASN LYS GLN ASP MET HIS GLY TRP THR PRO ARG ASP LEU ALA GLU GLN GLN GLY HIS GLU ASP ILE LYS ALA LEU PHE ARG GLU LYS LEU HIS GLU ARG ARG VAL HIS ILE GLU THR SER SER SER VAL PRO ILE LEU LYS THR GLY ILE ARG PHE LEU
GLY ARG PHE THR SER GLU PRO ASN ILE ARG PRO ALA SER ARG GLU VAL SER PHE ARG ILE ARG GLU THR ARG ALA ARG ARG LYS THR ASN ASN PHE ASP ASN SER LEU PHE GLY ILE LEU ALA ASN GLN SER VAL PRO LYS ASN GLY LEU ALA ALA THR VAL ASP GLU GLY ARG THR GLY ASN
PRO VAL ARG VAL THR ILE SER CYS ALA GLU LYS ASP ASP ILE ALA GLY LYS LEU VAL LEU LEU PRO GLY SER PHE LYS GLU LEU LEU GLU LEU GLY SER ASN LYS PHE GLY ILE VAL ALA THR LYS VAL MET ASN LYS ASP ASN ASN ALA GLU ILE ASP ASP VAL ASP VAL ILE ARG ASP
GLY ASP HIS LEU ILE PHE ALA THR ASP SER LEU GLU GLY SER ASP GLU VAL ASP ALA GLY SER ALA ALA ALA SER GLY GLY SER ASP TYR LYS ASP ASP ASP LYS GLY SER HIS HIS HIS HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	399278	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	9.181	Depositor
Minimum map value	-4.910	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.159	Depositor
Recommended contour level	0.436	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

5.1 Standard geometry

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

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	0.63	13/3929 (0.3%)	0.65	6/5333 (0.1%)
1	B	0.67	12/3918 (0.3%)	0.73	10/5319 (0.2%)
1	C	0.58	5/3929 (0.1%)	0.66	5/5333 (0.1%)
1	D	0.63	10/3918 (0.3%)	0.63	5/5319 (0.1%)
All	All	0.63	40/15694 (0.3%)	0.67	26/21304 (0.1%)

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	76	PRO	C-O	-8.42	1.13	1.24
1	A	76	PRO	C-O	-8.29	1.13	1.24
1	D	76	PRO	C-O	-8.26	1.13	1.24
1	B	76	PRO	C-O	-8.18	1.13	1.24
1	A	250	THR	C-O	-8.04	1.14	1.24

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	344	GLN	N-CA-C	-7.56	104.96	114.56
1	B	250	THR	CA-CB-OG1	-6.87	99.30	109.60
1	C	187	PHE	N-CA-C	-6.40	104.38	111.36
1	B	339	GLU	CB-CA-C	-6.20	100.50	110.79
1	B	303	ARG	CB-CG-CD	-6.11	97.24	111.30

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	3837	0	3869	150	0
1	B	3826	0	3855	146	0
1	C	3837	0	3869	190	0
1	D	3826	0	3856	139	0
2	A	39	0	52	0	0
2	B	39	0	52	1	0
2	C	39	0	52	5	0
2	D	39	0	52	2	0
3	A	3	0	0	0	0
All	All	15485	0	15657	579	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 19.

The worst 5 of 579 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:D:202:VAL:CG2	1:D:251:LEU:HD12	1.76	1.15
1:B:202:VAL:CG2	1:B:251:LEU:HD12	1.78	1.14
1:B:202:VAL:HG23	1:B:251:LEU:HD12	1.30	1.14
1:B:312:PHE:HB2	1:C:343:GLN:CG	1.82	1.09
1:D:202:VAL:HG23	1:D:251:LEU:HD12	1.31	1.08

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	468/895 (52%)	435 (93%)	32 (7%)	1 (0%)	44 68
1	B	467/895 (52%)	449 (96%)	18 (4%)	0	100 100
1	C	468/895 (52%)	431 (92%)	35 (8%)	2 (0%)	30 55
1	D	467/895 (52%)	442 (95%)	25 (5%)	0	100 100
All	All	1870/3580 (52%)	1757 (94%)	110 (6%)	3 (0%)	45 68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	343	GLN
1	A	343	GLN
1	C	504	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	420/776 (54%)	367 (87%)	53 (13%)	3 9
1	B	419/776 (54%)	367 (88%)	52 (12%)	4 9
1	C	420/776 (54%)	368 (88%)	52 (12%)	4 9
1	D	419/776 (54%)	374 (89%)	45 (11%)	5 13
All	All	1678/3104 (54%)	1476 (88%)	202 (12%)	6 10

5 of 202 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	115	LYS
1	C	350	LEU
1	D	508	GLU
1	C	143	THR
1	C	258	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	260	HIS
1	C	450	GLN
1	D	509	ASN
1	C	294	HIS
1	C	323	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	$\#\|Z\| > 2$
2	POV	D	901	-	38,38,51	0.54	0	42,43,59	0.87	3 (7%)
2	POV	C	901	-	38,38,51	0.51	0	42,43,59	0.68	2 (4%)
2	POV	B	901	-	38,38,51	0.57	0	42,43,59	0.83	1 (2%)
2	POV	A	901	-	38,38,51	0.55	0	42,43,59	0.69	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	D	901	-	-	25/40/40/55	-
2	POV	C	901	-	-	20/40/40/55	-
2	POV	B	901	-	-	18/40/40/55	-
2	POV	A	901	-	-	19/40/40/55	-

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	901	POV	O21-C21-C22	3.35	118.71	111.50
2	C	901	POV	O13-P-O14	2.65	121.04	110.68
2	A	901	POV	O13-P-O14	2.62	120.95	110.68
2	B	901	POV	O13-P-O14	2.57	120.74	110.68
2	D	901	POV	O13-P-O14	2.47	120.34	110.68

There are no chirality outliers.

5 of 82 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	POV	C1-C2-O21-C21
2	B	901	POV	C1-O11-P-O12
2	B	901	POV	C1-O11-P-O13
2	B	901	POV	C211-C210-C29-C28
2	C	901	POV	C22-C21-O21-C2

There are no ring outliers.

3 monomers are involved in 8 short contacts:

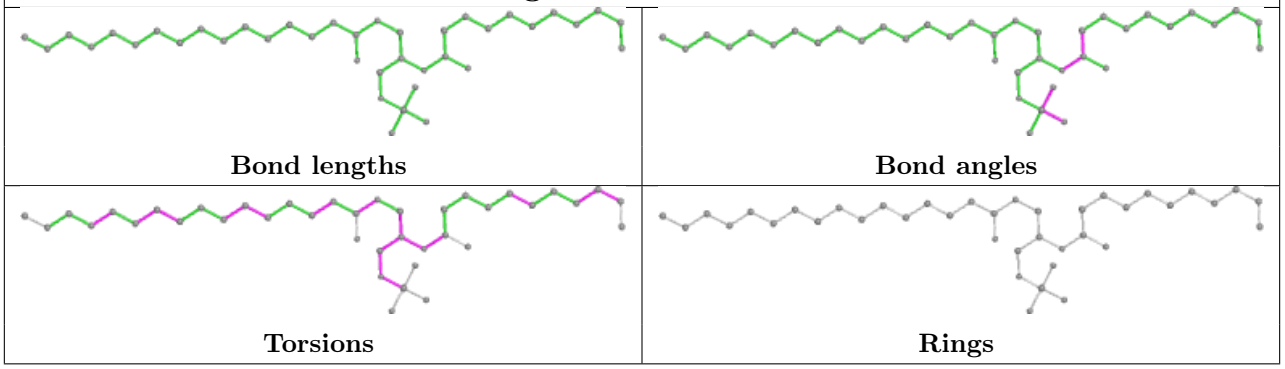
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	901	POV	2	0
2	C	901	POV	5	0
2	B	901	POV	1	0

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 then 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

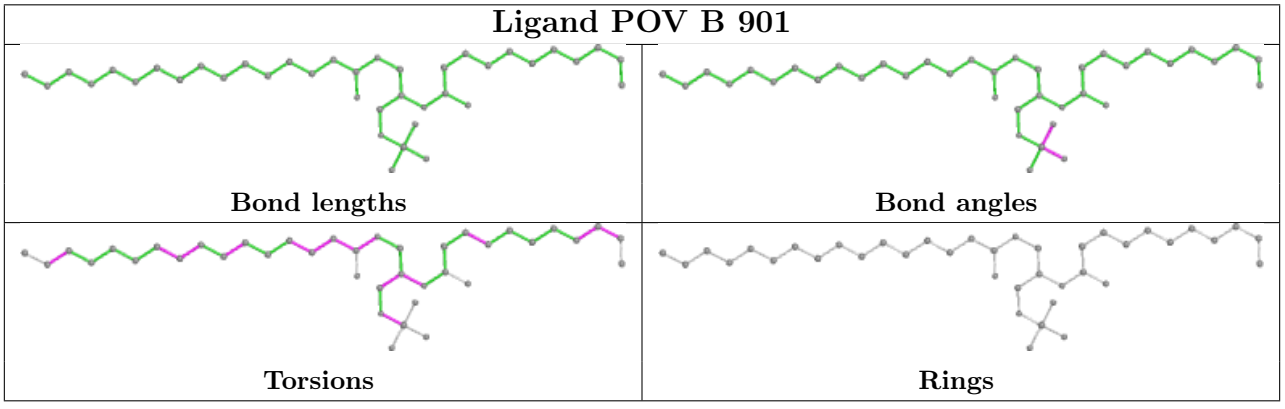
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand POV D 901

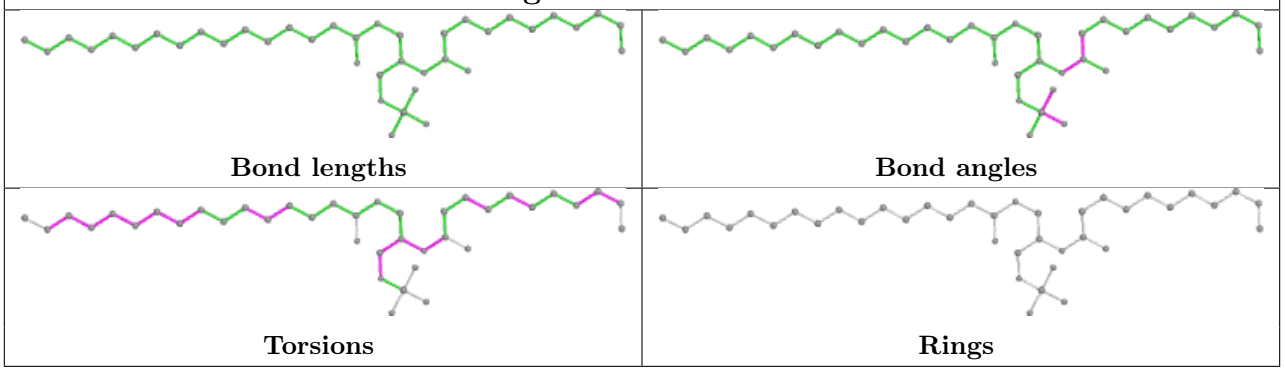
Ligand POV C 901



Ligand POV B 901



Ligand POV A 901



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.

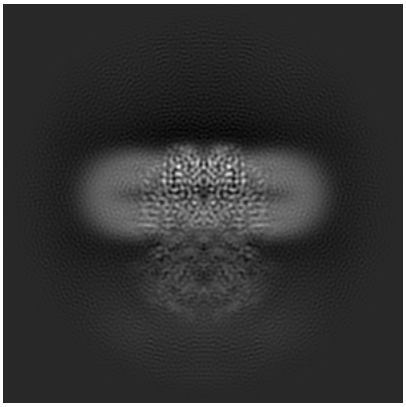
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32598. These allow visual inspection of the internal detail of the map and identification of artifacts.

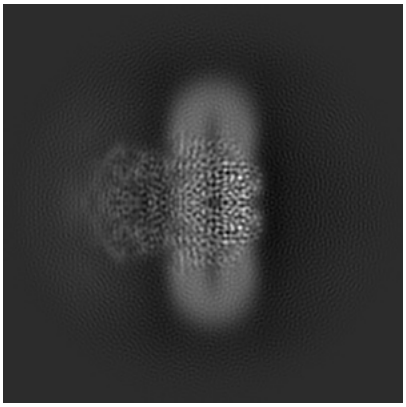
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

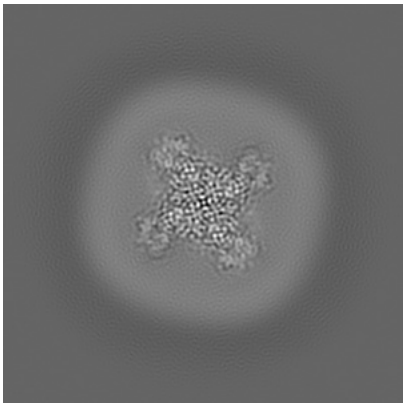
6.1.1 Primary map



X



Y

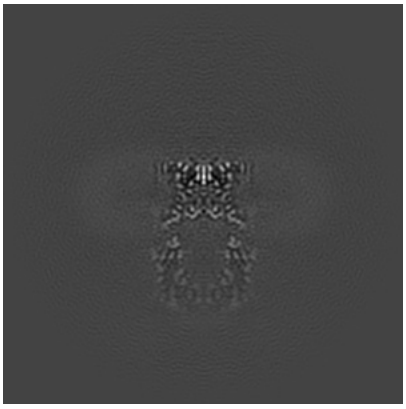


Z

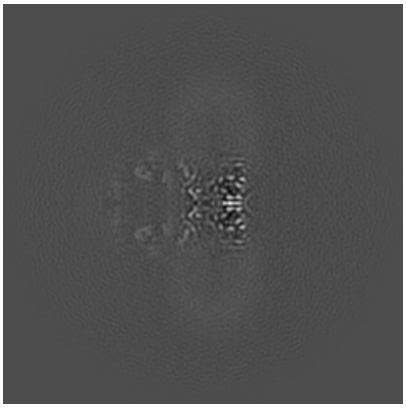
The images above show the map projected in three orthogonal directions.

6.2 Central slices

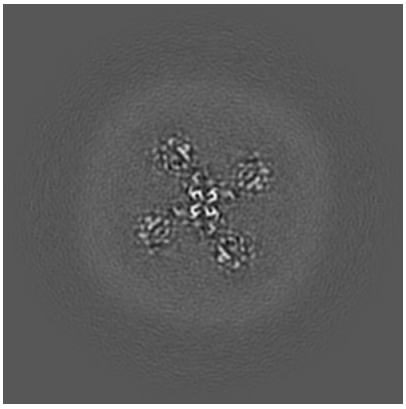
6.2.1 Primary map



X Index: 120



Y Index: 120

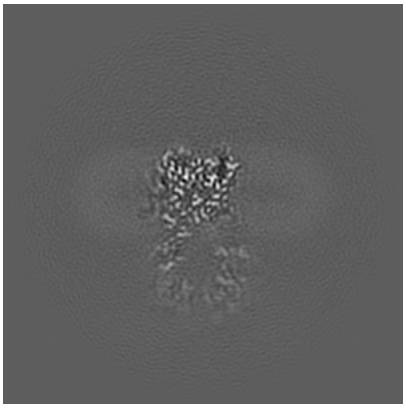


Z Index: 120

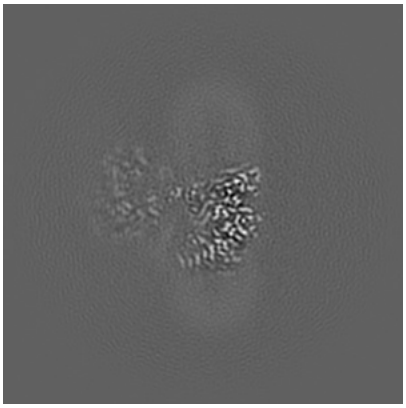
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

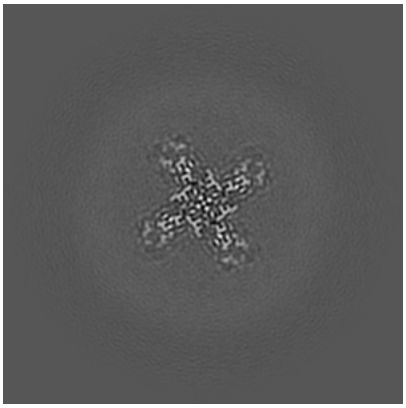
6.3.1 Primary map



X Index: 126



Y Index: 108

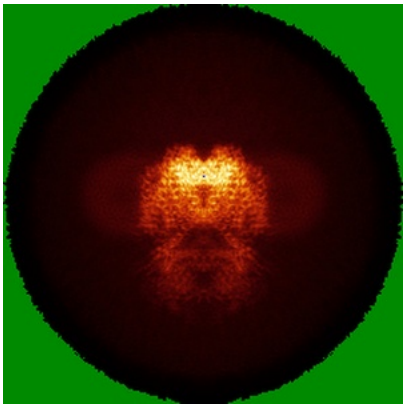


Z Index: 133

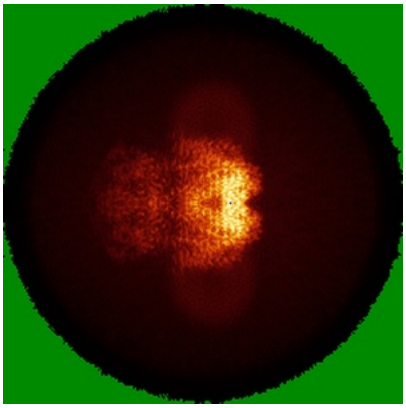
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

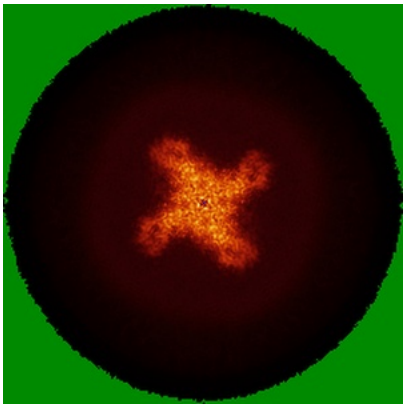
6.4.1 Primary map



X



Y



Z

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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.436. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

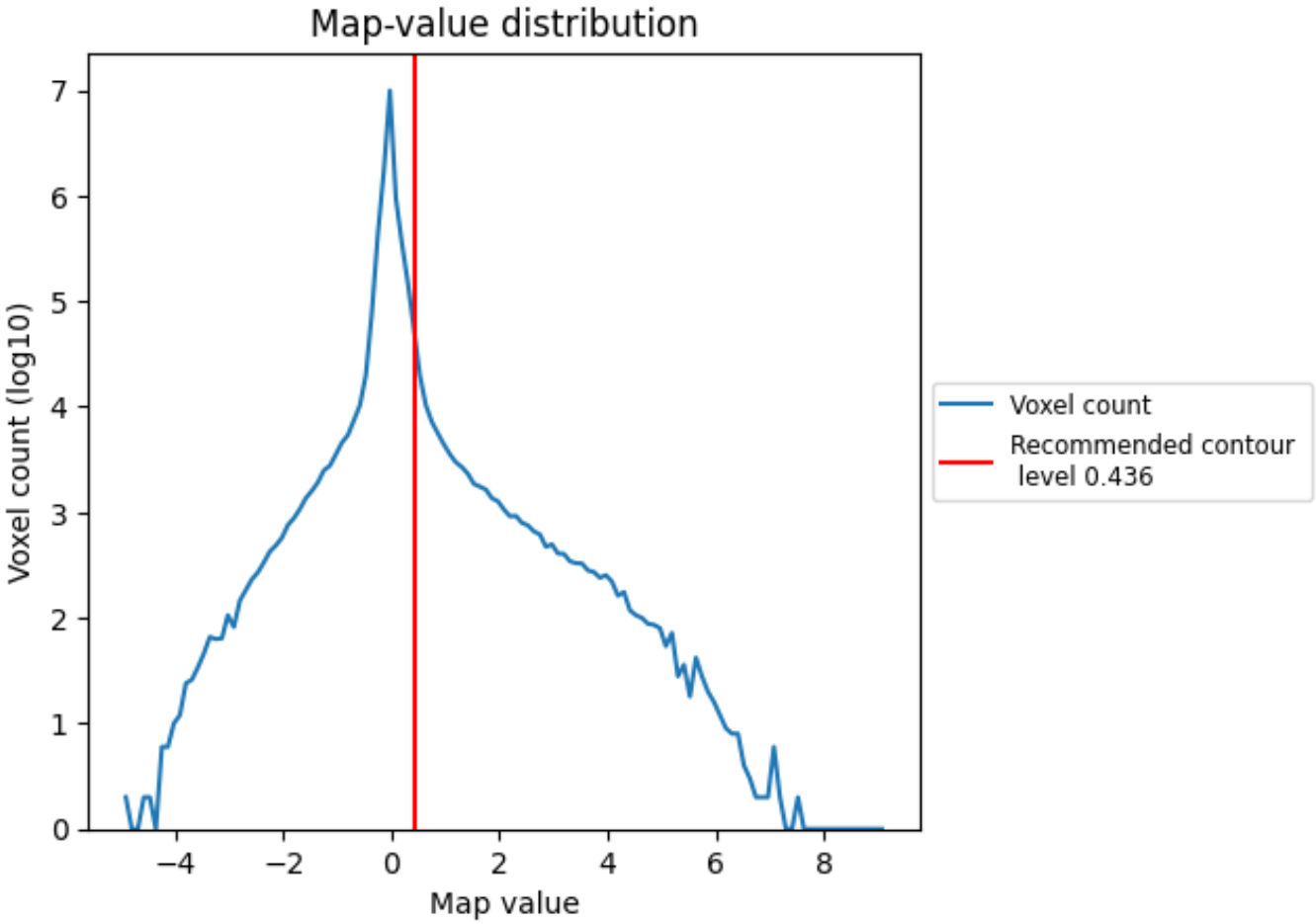
6.6 Mask visualisation (i)

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

7 Map analysis

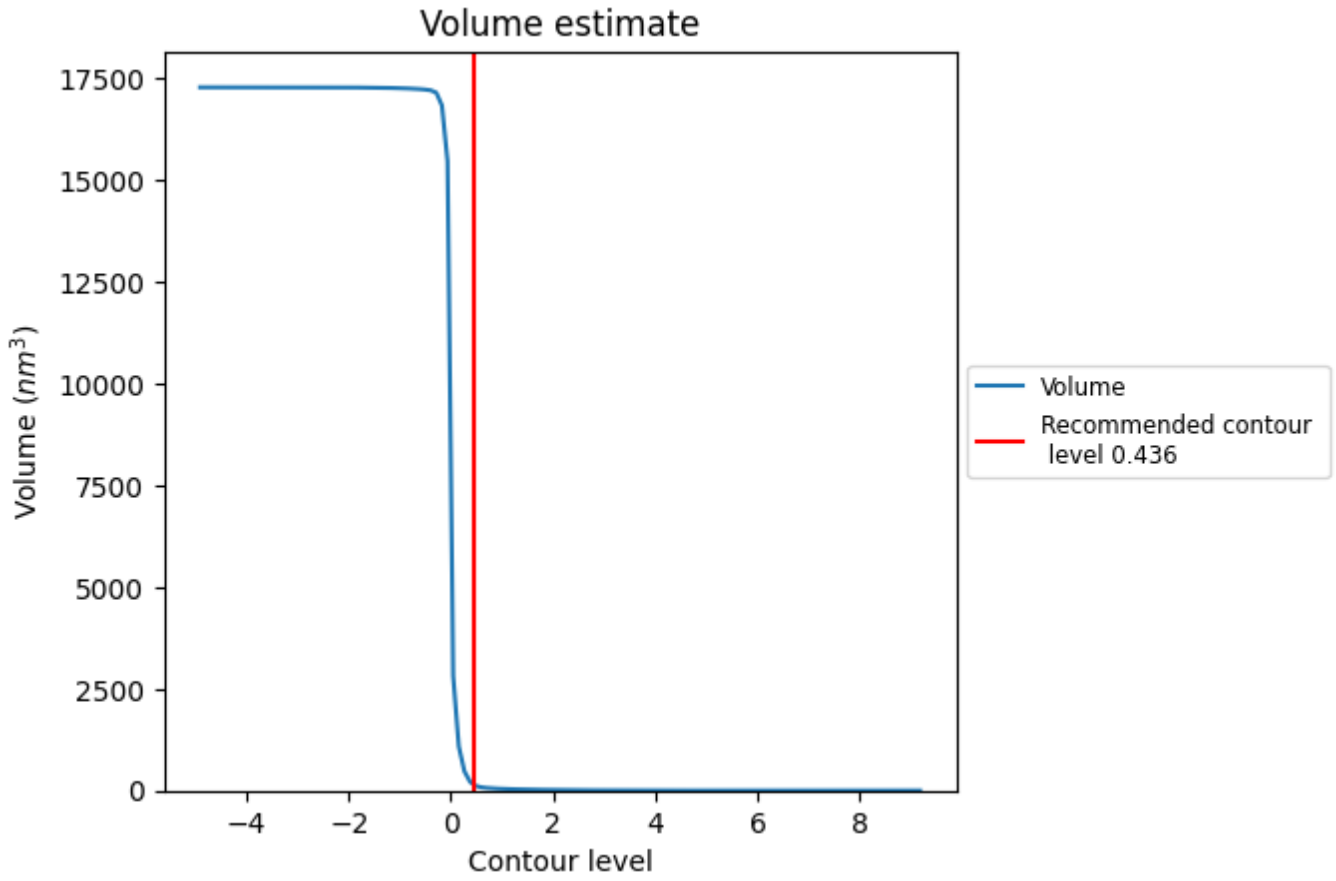
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

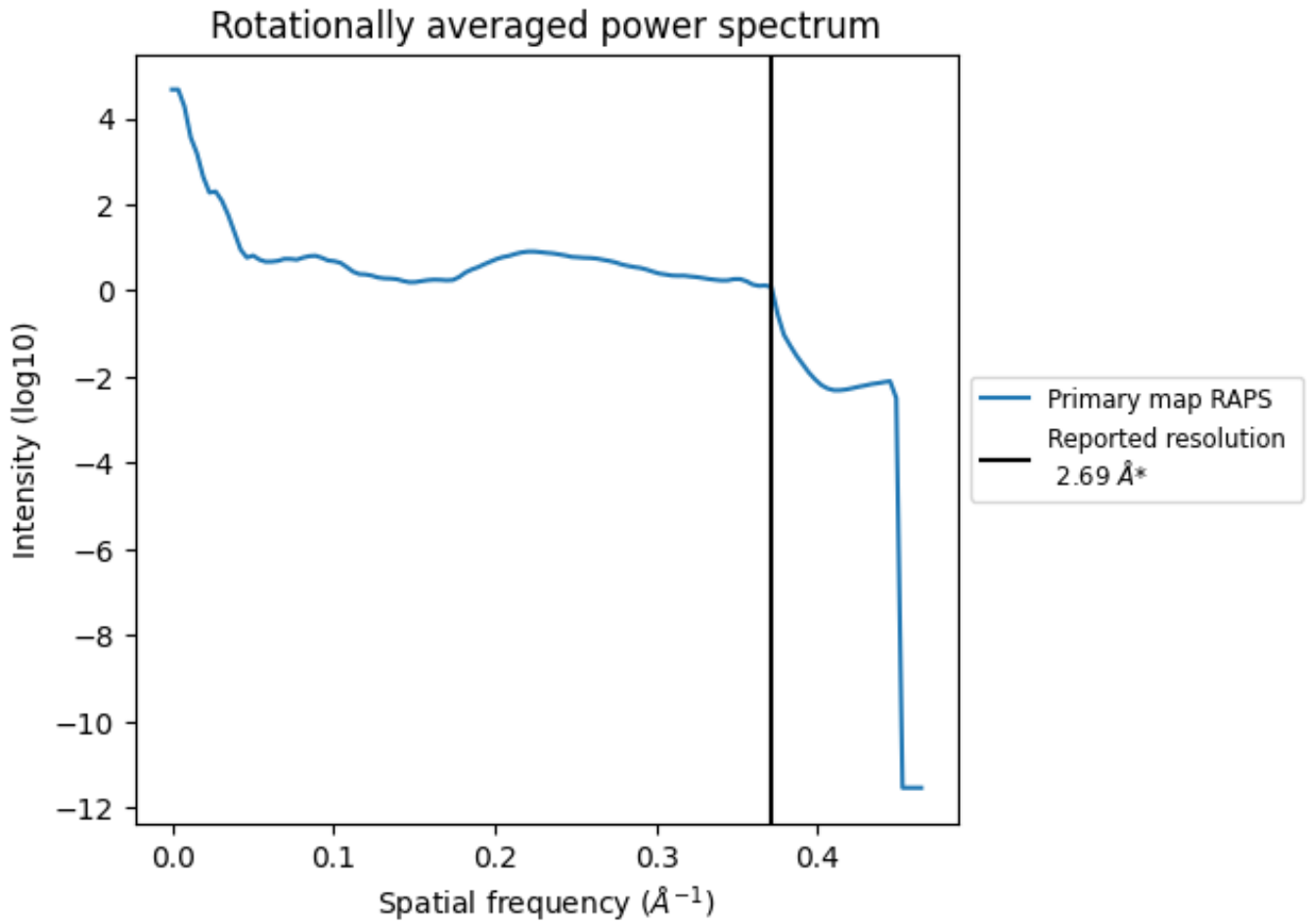
7.2 Volume estimate (i)



The volume at the recommended contour level is 159 nm^3; this corresponds to an approximate mass of 144 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 (i)



*Reported resolution corresponds to spatial frequency of 0.372 $Å^{-1}$

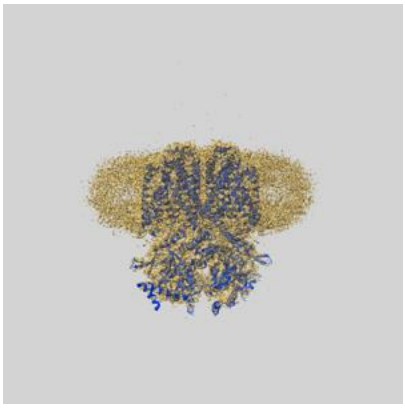
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

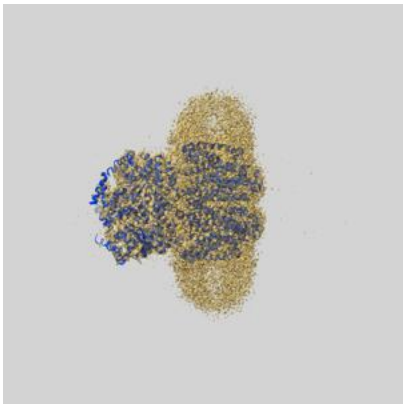
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32598 and PDB model 7WM2. Per-residue inclusion information can be found in section 3 on page 8.

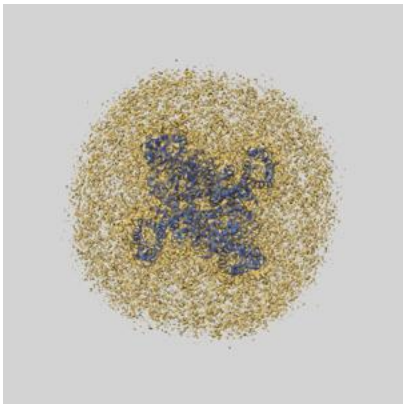
9.1 Map-model overlay



X



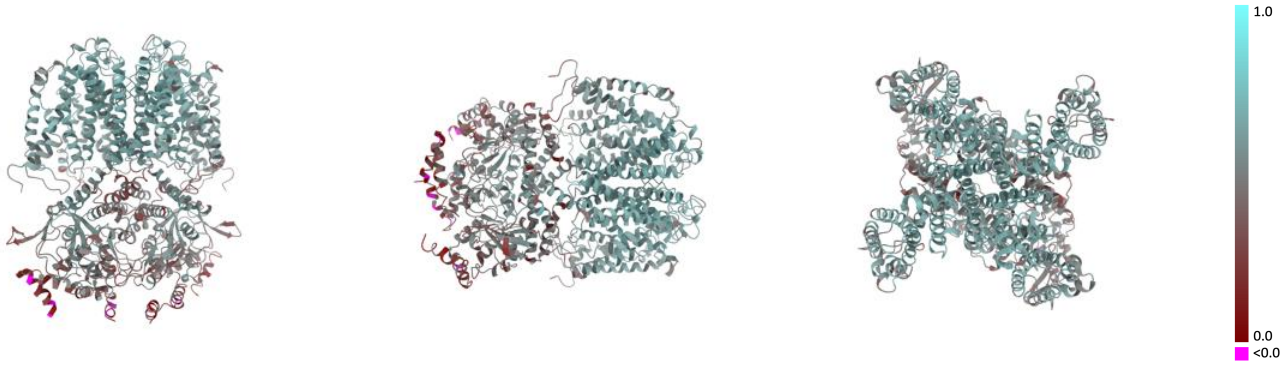
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.436 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.

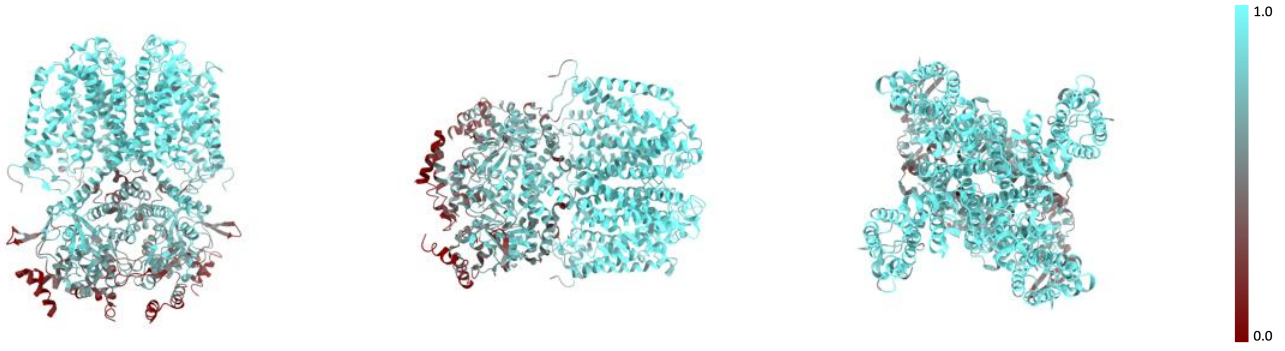
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

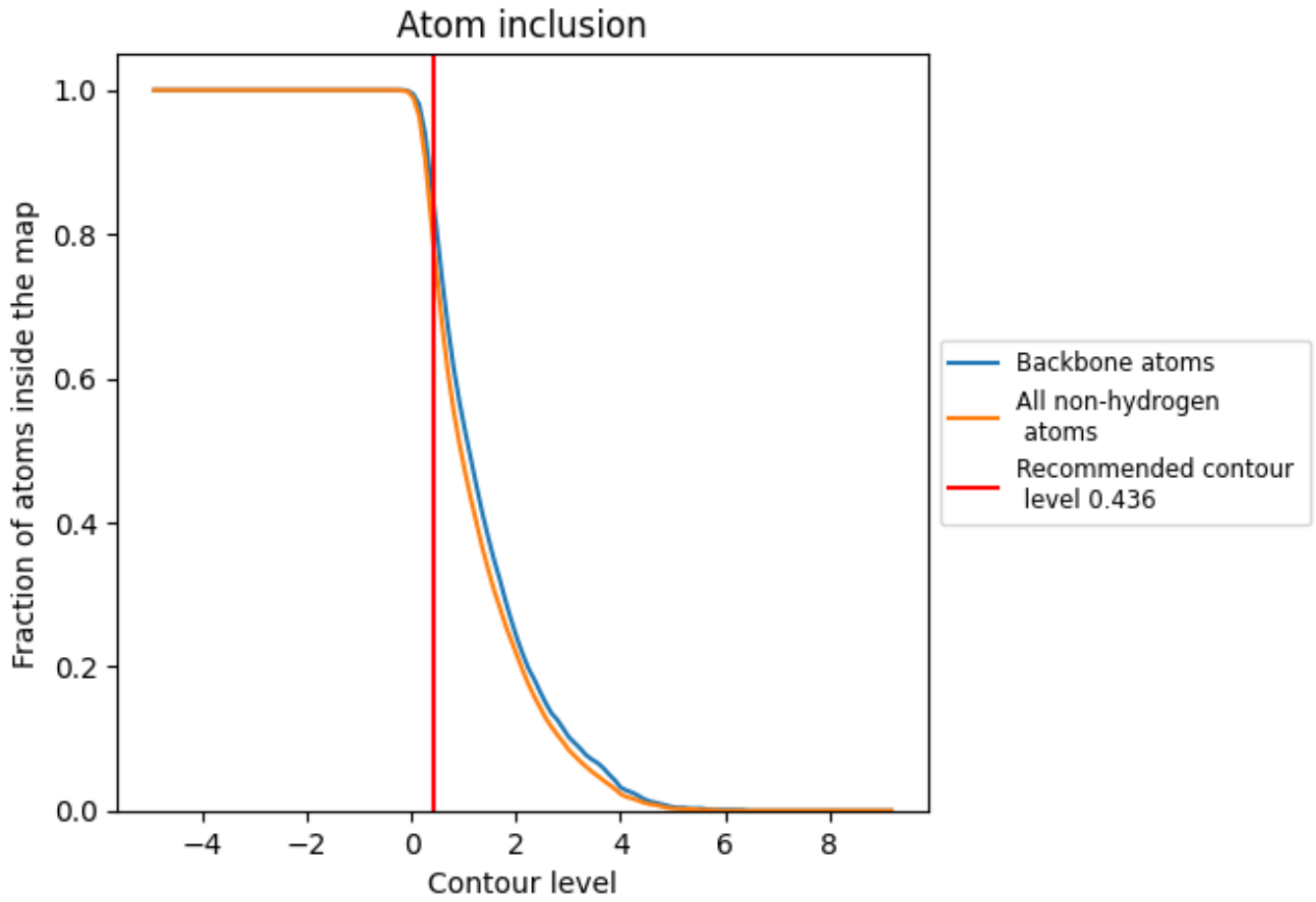
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.436).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.436) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7790	0.5180
A	0.7830	0.5140
B	0.7750	0.5210
C	0.7850	0.5170
D	0.7740	0.5180