



Full wwPDB EM Validation Report ⓘ

Jun 9, 2025 – 04:27 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

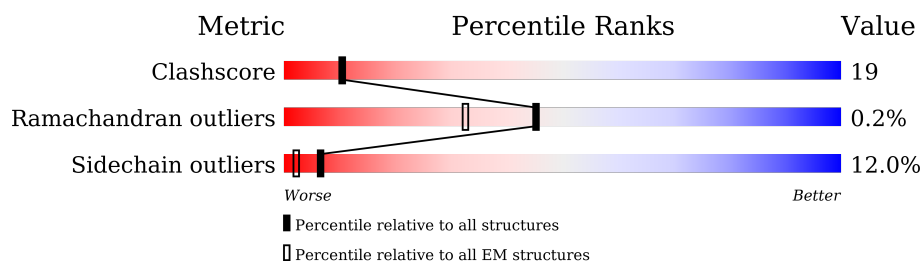
1 Overall quality at a glance

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 $\leq 5\%$. 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	895	<div> <div>5%</div> <div>32%</div> <div>16%</div> <div>•</div> <div>47%</div> </div>
1	B	895	<div> <div>7%</div> <div>32%</div> <div>16%</div> <div>• •</div> <div>48%</div> </div>
1	C	895	<div> <div>6%</div> <div>32%</div> <div>17%</div> <div>•</div> <div>47%</div> </div>
1	D	895	<div> <div>7%</div> <div>34%</div> <div>16%</div> <div>•</div> <div>48%</div> </div>

2 Entry composition

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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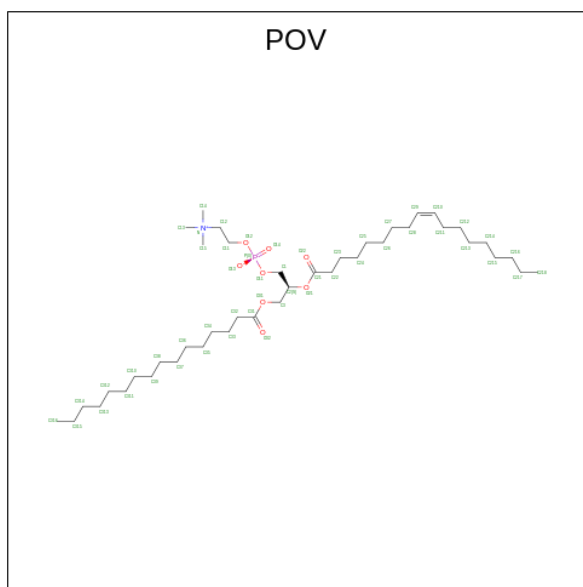
Chain	Residue	Modelled	Actual	Comment	Reference
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C	889	HIS	-	expression tag	UNP Q38998
C	890	HIS	-	expression tag	UNP Q38998
C	891	HIS	-	expression tag	UNP Q38998
C	892	HIS	-	expression tag	UNP Q38998
C	893	HIS	-	expression tag	UNP Q38998
C	894	HIS	-	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: C₄₂H₈₂NO₈P) (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	

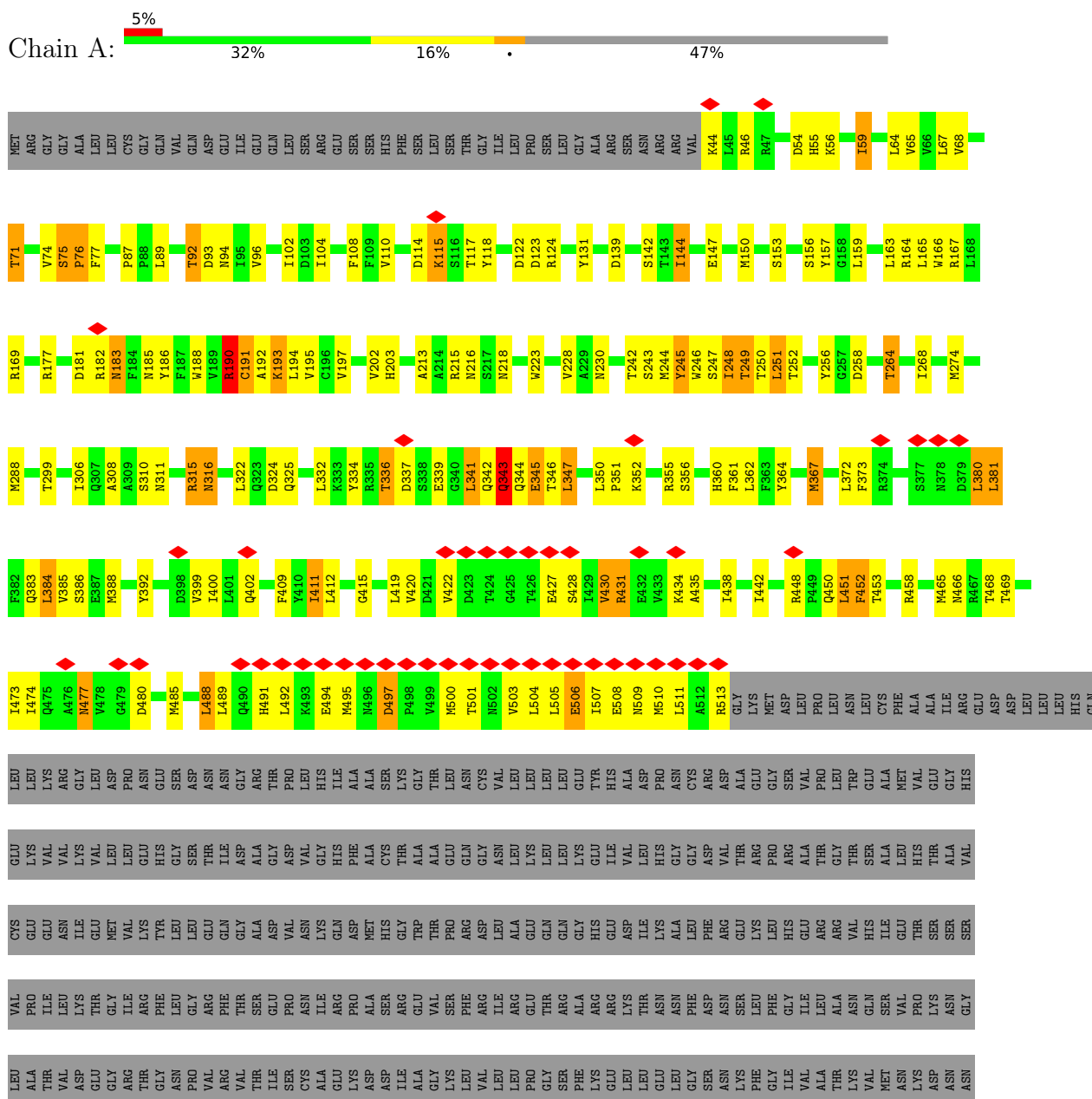
- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

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

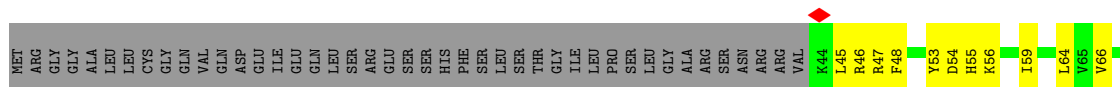
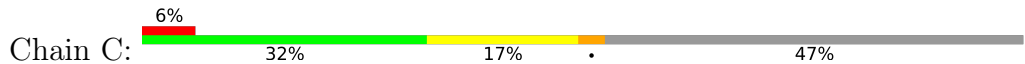
3 Residue-property plots

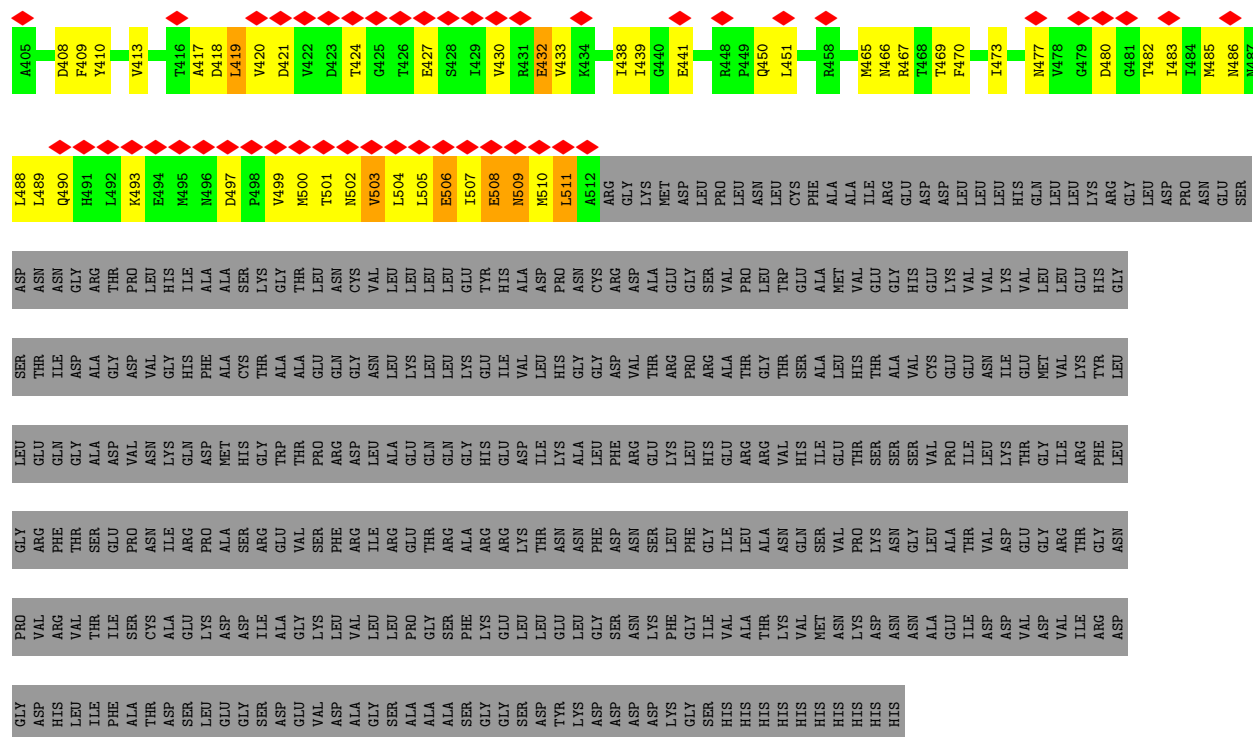
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 B: 7% 32% 16% 2% 48%





4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 (\AA)	258.552, 258.552, 258.552	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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: 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	0.63	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%)

All (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
1	D	246	TRP	C-O	-7.73	1.15	1.24
1	B	246	TRP	C-O	-7.69	1.15	1.24
1	B	247	SER	C-O	-7.45	1.15	1.24
1	A	247	SER	C-O	-7.39	1.15	1.24
1	D	247	SER	C-O	-7.39	1.15	1.24
1	A	249	THR	C-O	-7.32	1.15	1.24
1	B	250	THR	C-O	-7.30	1.15	1.24
1	A	246	TRP	C-O	-7.18	1.15	1.24
1	B	245	TYR	C-O	-6.93	1.15	1.24
1	A	75	SER	C-O	-6.42	1.18	1.24
1	A	75	SER	CA-CB	-6.30	1.45	1.53
1	C	75	SER	C-O	-6.29	1.18	1.24
1	D	245	TYR	C-O	-6.28	1.16	1.24
1	B	249	THR	C-O	-6.23	1.16	1.24
1	C	75	SER	CA-CB	-6.22	1.45	1.53
1	D	250	THR	C-O	-6.22	1.16	1.24
1	D	75	SER	CA-CB	-6.20	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	75	SER	CA-CB	-6.12	1.45	1.53
1	B	247	SER	CA-CB	-5.94	1.44	1.53
1	C	182	ARG	C-O	-5.88	1.16	1.24
1	D	247	SER	CA-CB	-5.78	1.44	1.53
1	A	247	SER	CA-CB	-5.72	1.44	1.53
1	C	77	PHE	C-O	-5.63	1.17	1.24
1	B	337	ASP	C-O	-5.52	1.17	1.24
1	A	77	PHE	C-O	-5.50	1.17	1.24
1	A	245	TYR	C-O	-5.48	1.17	1.24
1	D	249	THR	C-O	-5.42	1.16	1.24
1	A	344	GLN	C-O	-5.38	1.17	1.24
1	A	252	THR	C-O	-5.32	1.17	1.24
1	D	75	SER	C-O	-5.27	1.19	1.24
1	D	77	PHE	C-O	-5.27	1.18	1.24
1	B	75	SER	C-O	-5.25	1.19	1.24
1	B	77	PHE	C-O	-5.21	1.18	1.24
1	A	251	LEU	C-O	-5.19	1.18	1.24
1	B	251	LEU	C-O	-5.03	1.18	1.24

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	D	250	THR	CA-CB-OG1	-6.10	100.45	109.60
1	D	252	THR	CB-CA-C	-6.02	99.22	110.36
1	B	348	ASP	CA-CB-CG	5.77	118.37	112.60
1	C	314	HIS	CA-CB-CG	-5.68	108.12	113.80
1	A	252	THR	CA-CB-OG1	-5.67	101.10	109.60
1	C	187	PHE	CB-CA-C	5.61	120.39	110.85
1	D	252	THR	CA-C-N	5.57	131.79	123.05
1	D	252	THR	C-N-CA	5.57	131.79	123.05
1	B	347	LEU	N-CA-C	-5.37	106.73	113.72
1	B	298	ARG	CA-C-N	5.30	128.78	120.82
1	B	298	ARG	C-N-CA	5.30	128.78	120.82
1	A	252	THR	CA-C-N	5.30	131.37	123.05
1	A	252	THR	C-N-CA	5.30	131.37	123.05
1	B	303	ARG	CG-CD-NE	5.21	123.45	112.00
1	A	250	THR	CA-CB-OG1	-5.16	101.86	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	190	ARG	CG-CD-NE	-5.14	100.69	112.00
1	C	346	THR	CA-CB-OG1	-5.10	101.95	109.60
1	B	303	ARG	NE-CZ-NH1	-5.05	116.45	121.50
1	A	190	ARG	N-CA-C	-5.03	106.40	112.54
1	D	337	ASP	N-CA-C	-5.03	106.31	112.90
1	B	253	THR	CA-CB-OG1	-5.02	102.07	109.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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.

All (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:PHE:HB2	1:C:343:GLN:HG3	1.32	1.06
1:C:315:ARG:HD3	1:D:339:GLU:OE2	1.59	1.03
1:D:297:SER:O	1:D:300:ARG:HD2	1.62	0.98
1:B:312:PHE:CB	1:C:343:GLN:HG3	1.93	0.98
1:C:75:SER:OG	1:C:76:PRO:HD3	1.67	0.93
1:B:202:VAL:HG23	1:B:251:LEU:CD1	2.01	0.89
1:A:402:GLN:H	1:A:453:THR:HG22	1.38	0.88
1:C:335:ARG:HB2	1:C:335:ARG:NH1	1.90	0.87
1:D:75:SER:OG	1:D:76:PRO:HD3	1.76	0.86
1:B:341:LEU:O	1:B:341:LEU:HD12	1.76	0.85
1:B:75:SER:OG	1:B:76:PRO:HD3	1.77	0.84
1:B:202:VAL:CG2	1:B:251:LEU:CD1	2.55	0.84
1:A:341:LEU:CD1	1:A:392:TYR:OH	2.26	0.84
1:D:202:VAL:HG23	1:D:251:LEU:CD1	2.06	0.84
1:B:304:ASP:OD1	1:B:304:ASP:N	2.11	0.81
1:C:347:LEU:HD11	1:C:358:ILE:HD11	1.61	0.81
1:C:335:ARG:HD2	1:D:115:LYS:NZ	1.96	0.80
1:C:352:LYS:HD3	1:C:355:ARG:HE	1.44	0.80
1:C:185:ASN:HB2	1:C:188:TRP:HB2	1.60	0.80
1:D:202:VAL:CG2	1:D:251:LEU:CD1	2.58	0.80
1:A:75:SER:OG	1:A:76:PRO:HD3	1.82	0.79
1:C:497:ASP:HB2	1:C:500:MET:HB2	1.65	0.79
1:D:297:SER:HA	1:D:300:ARG:NE	1.97	0.79
1:A:343:GLN:CG	1:D:312:PHE:HB2	2.11	0.79
1:B:312:PHE:CG	1:C:343:GLN:HG3	2.18	0.79
1:C:185:ASN:HD22	1:C:185:ASN:H	1.30	0.79
1:D:400:ILE:HD11	1:D:450:GLN:HG3	1.64	0.79
1:B:301:ASN:O	1:B:301:ASN:ND2	2.17	0.78
1:B:312:PHE:HB2	1:C:343:GLN:HG2	1.65	0.77
1:A:402:GLN:HE21	1:A:452:PHE:HA	1.49	0.77
1:A:343:GLN:HG3	1:D:312:PHE:HB2	1.65	0.77
1:A:367:MET:HE3	1:A:385:VAL:HG22	1.65	0.76
1:C:190:ARG:CB	1:C:190:ARG:HH11	1.99	0.76
1:C:337:ASP:HA	1:C:342:GLN:HB3	1.68	0.75
1:D:150:MET:HE1	1:D:157:TYR:HB2	1.67	0.75
1:C:492:LEU:HD21	1:C:503:VAL:HB	1.69	0.75
1:B:150:MET:HE1	1:B:157:TYR:HB2	1.67	0.74
1:C:315:ARG:CD	1:D:339:GLU:OE2	2.34	0.73
1:B:388:MET:HB3	1:B:463:LEU:HD22	1.70	0.72
1:C:351:PRO:HD2	1:C:354:ILE:CG2	2.18	0.72
1:A:419:LEU:HD12	1:A:452:PHE:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:ARG:NH1	1:D:181:ASP:O	2.22	0.72
1:A:54:ASP:OD1	1:A:55:HIS:N	2.23	0.72
1:A:332:LEU:O	1:A:336:THR:HG23	1.90	0.72
1:C:480:ASP:HA	1:C:483:ILE:HD13	1.72	0.71
1:A:139:ASP:OD1	1:A:166:TRP:NE1	2.21	0.71
1:A:190:ARG:CZ	1:A:190:ARG:HB3	2.19	0.71
1:B:312:PHE:CD1	1:C:343:GLN:CB	2.74	0.71
1:A:202:VAL:CG2	1:A:251:LEU:HD22	2.21	0.71
1:B:218:ASN:HD21	1:B:221:LYS:HG3	1.55	0.70
1:A:46:ARG:NH1	1:A:122:ASP:O	2.24	0.70
1:A:477:ASN:HB3	1:D:424:THR:HB	1.74	0.70
1:B:251:LEU:HD23	1:B:251:LEU:O	1.91	0.69
1:B:489:LEU:HA	1:B:492:LEU:HD12	1.73	0.69
1:C:180:LYS:HB3	1:C:180:LYS:HZ2	1.57	0.69
1:A:185:ASN:HB3	1:A:188:TRP:HB2	1.75	0.69
1:A:181:ASP:OD1	1:A:182:ARG:N	2.24	0.69
1:B:202:VAL:HG22	1:B:251:LEU:HD12	1.73	0.69
1:B:341:LEU:HD12	1:B:341:LEU:C	2.14	0.69
2:C:901:POV:H3	2:C:901:POV:O13	1.92	0.69
1:B:312:PHE:CD1	1:C:343:GLN:HB3	2.27	0.68
1:A:341:LEU:O	1:A:341:LEU:HD13	1.92	0.68
1:A:186:TYR:CZ	1:A:190:ARG:HD2	2.29	0.68
1:C:46:ARG:HH22	1:C:124:ARG:H	1.41	0.68
1:C:332:LEU:O	1:C:336:THR:HG23	1.92	0.68
1:B:300:ARG:HB2	1:C:294:HIS:HE1	1.59	0.68
1:B:402:GLN:NE2	1:B:451:LEU:O	2.27	0.68
1:B:399:VAL:HG23	1:B:400:ILE:HG22	1.76	0.67
1:C:351:PRO:HD2	1:C:354:ILE:HG22	1.77	0.67
1:D:139:ASP:OD2	1:D:169:ARG:NH2	2.28	0.67
1:D:202:VAL:HG22	1:D:251:LEU:HD12	1.74	0.67
1:A:434:LYS:NZ	1:A:435:ALA:O	2.27	0.67
1:C:249:THR:HG22	1:D:274:MET:HE1	1.76	0.66
1:C:139:ASP:OD1	1:C:166:TRP:NE1	2.23	0.66
1:C:501:THR:O	1:C:504:LEU:HB2	1.96	0.66
1:A:400:ILE:HD11	1:A:450:GLN:HG3	1.78	0.65
1:B:318:LEU:HD12	1:B:322:LEU:HD21	1.78	0.65
1:A:402:GLN:NE2	1:A:451:LEU:O	2.30	0.65
1:A:501:THR:HA	1:A:504:LEU:HD13	1.78	0.65
1:A:341:LEU:HD11	1:A:392:TYR:OH	1.97	0.65
1:A:510:MET:HA	1:A:513:ARG:HB3	1.77	0.65
1:B:248:ILE:HD13	1:B:248:ILE:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:505:LEU:HA	1:C:508:GLU:HG2	1.79	0.64
1:D:71:THR:HG21	1:D:167:ARG:HH11	1.62	0.64
1:A:315:ARG:NE	1:B:339:GLU:OE2	2.29	0.64
1:B:71:THR:HG21	1:B:167:ARG:HH11	1.63	0.64
1:B:376:VAL:HA	1:B:483:ILE:HD11	1.79	0.64
1:C:345:GLU:CD	1:C:345:GLU:H	2.05	0.64
1:D:248:ILE:HD13	1:D:248:ILE:O	1.98	0.63
1:A:190:ARG:NH1	1:A:190:ARG:HA	2.13	0.63
1:C:258:ASP:N	1:C:258:ASP:OD1	2.31	0.63
1:B:76:PRO:HA	1:B:162:MET:HE2	1.80	0.63
1:D:482:THR:HG23	1:D:483:ILE:HD12	1.81	0.62
1:C:150:MET:HE1	1:C:157:TYR:HB2	1.81	0.62
1:C:352:LYS:N	1:C:352:LYS:HE2	2.14	0.62
1:C:190:ARG:HH11	1:C:190:ARG:CA	2.12	0.62
1:A:274:MET:HE1	1:D:249:THR:HG22	1.82	0.62
1:B:139:ASP:OD2	1:B:169:ARG:NH2	2.32	0.62
1:D:505:LEU:HA	1:D:508:GLU:OE1	2.00	0.62
1:C:185:ASN:HD22	1:C:185:ASN:N	1.98	0.62
1:D:506:GLU:O	1:D:509:ASN:ND2	2.32	0.62
1:C:419:LEU:HD22	1:C:452:PHE:HD2	1.65	0.62
1:C:71:THR:HG21	1:C:167:ARG:HH11	1.63	0.61
1:D:203:HIS:HA	1:D:244:MET:HE1	1.81	0.61
1:D:76:PRO:HA	1:D:162:MET:HE2	1.81	0.61
1:B:318:LEU:HD23	1:B:318:LEU:H	1.65	0.61
1:C:144:ILE:O	1:C:164:ARG:NH2	2.32	0.61
1:A:71:THR:HG21	1:A:167:ARG:HH11	1.64	0.61
1:A:144:ILE:O	1:A:164:ARG:NH2	2.31	0.61
1:C:376:VAL:HB	1:C:381:LEU:HD11	1.81	0.61
1:C:315:ARG:NE	1:D:339:GLU:CD	2.58	0.61
1:B:249:THR:HG22	1:C:274:MET:HE1	1.83	0.61
1:C:371:TYR:HA	1:C:374:ARG:HH21	1.66	0.61
1:B:501:THR:O	1:B:505:LEU:N	2.34	0.60
1:A:190:ARG:HH11	1:A:190:ARG:CG	2.14	0.60
1:A:420:VAL:HG21	1:A:427:GLU:HG2	1.81	0.60
1:B:203:HIS:HA	1:B:244:MET:HE1	1.82	0.60
1:A:248:ILE:HD13	1:A:248:ILE:O	2.01	0.60
1:C:400:ILE:HD11	1:C:450:GLN:HG3	1.82	0.60
1:A:190:ARG:HH12	1:A:193:LYS:HE2	1.66	0.60
1:D:251:LEU:HD23	1:D:251:LEU:O	2.01	0.60
1:C:509:ASN:O	1:C:513:ARG:N	2.34	0.60
1:B:258:ASP:OD1	1:B:258:ASP:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:PHE:CD1	1:C:343:GLN:CG	2.85	0.60
1:A:193:LYS:HB2	1:A:193:LYS:HZ3	1.67	0.59
1:D:298:ARG:NH2	1:D:298:ARG:HG3	2.17	0.59
1:B:441:GLU:OE2	1:B:441:GLU:N	2.34	0.59
1:D:258:ASP:OD1	1:D:258:ASP:N	2.32	0.59
1:C:434:LYS:NZ	1:C:435:ALA:O	2.36	0.59
1:B:477:ASN:OD1	1:B:477:ASN:N	2.34	0.59
1:C:376:VAL:HG12	1:C:380:LEU:HD21	1.83	0.59
1:C:410:TYR:HD1	1:C:439:ILE:HD11	1.66	0.59
1:B:398:ASP:OD1	1:B:398:ASP:N	2.36	0.59
1:B:466:ASN:OD1	1:B:467:ARG:N	2.36	0.58
1:A:448:ARG:HH22	1:A:503:VAL:HA	1.67	0.58
1:B:181:ASP:OD1	1:B:182:ARG:N	2.34	0.58
1:C:352:LYS:HE2	1:C:352:LYS:HA	1.84	0.58
1:B:321:ARG:O	1:B:321:ARG:NH1	2.33	0.58
1:C:352:LYS:HE2	1:C:352:LYS:CA	2.33	0.58
1:A:489:LEU:HD21	1:A:507:ILE:HG12	1.85	0.58
1:B:396:LYS:N	1:B:456:THR:O	2.26	0.58
1:C:352:LYS:HZ2	1:C:355:ARG:HD3	1.69	0.58
1:D:190:ARG:NH1	1:D:193:LYS:HD2	2.19	0.58
1:C:339:GLU:HB3	1:C:341:LEU:HD22	1.84	0.58
1:B:356:SER:O	1:B:356:SER:OG	2.21	0.57
1:A:190:ARG:HH11	1:A:190:ARG:HG2	1.69	0.57
1:A:324:ASP:OD1	1:A:325:GLN:N	2.37	0.57
1:C:335:ARG:HD2	1:D:115:LYS:HZ2	1.70	0.57
1:A:399:VAL:HG23	1:A:400:ILE:HG22	1.85	0.57
1:C:415:GLY:HA2	1:C:458:ARG:HD2	1.87	0.57
1:A:194:LEU:HA	1:A:197:VAL:HG12	1.87	0.57
1:C:380:LEU:O	1:C:384:LEU:N	2.30	0.57
1:D:500:MET:HA	1:D:503:VAL:HG23	1.87	0.57
1:A:308:ALA:HB1	1:B:342:GLN:HB2	1.87	0.57
1:B:312:PHE:CG	1:C:343:GLN:CG	2.87	0.57
1:C:92:THR:O	1:C:92:THR:OG1	2.23	0.56
1:A:190:ARG:CZ	1:A:190:ARG:CB	2.83	0.56
1:B:296:THR:HA	1:B:299:THR:CG2	2.34	0.56
2:B:901:POV:H3A	2:B:901:POV:O22	2.04	0.56
1:C:316:ASN:OD1	1:C:316:ASN:N	2.38	0.56
1:C:352:LYS:NZ	1:C:355:ARG:HD3	2.20	0.56
1:C:315:ARG:CD	1:D:339:GLU:CD	2.78	0.56
1:D:181:ASP:OD1	1:D:182:ARG:N	2.37	0.56
1:B:381:LEU:O	1:B:385:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:CYS:SG	1:C:332:LEU:N	2.78	0.56
1:C:366:LEU:HD11	1:C:413:VAL:HA	1.87	0.56
1:C:489:LEU:HD21	1:C:507:ILE:HG21	1.86	0.56
1:A:442:ILE:HD12	1:A:503:VAL:HG11	1.88	0.56
1:B:419:LEU:HD11	1:B:452:PHE:HB2	1.88	0.56
1:C:315:ARG:CZ	1:D:339:GLU:OE1	2.53	0.56
1:A:383:GLN:HE22	1:A:473:ILE:HG21	1.71	0.56
1:A:477:ASN:OD1	1:A:477:ASN:N	2.39	0.56
1:C:216:ASN:ND2	1:C:218:ASN:O	2.39	0.56
1:A:311:ASN:O	1:A:315:ARG:HD3	2.06	0.55
1:B:360:HIS:O	1:B:360:HIS:ND1	2.35	0.55
1:B:92:THR:O	1:B:92:THR:OG1	2.25	0.55
1:C:54:ASP:OD1	1:C:55:HIS:N	2.38	0.55
1:A:191:CYS:SG	1:A:192:ALA:N	2.79	0.55
1:A:216:ASN:ND2	1:A:218:ASN:O	2.39	0.55
1:C:335:ARG:HB2	1:C:335:ARG:HH11	1.68	0.55
1:C:75:SER:OG	1:C:76:PRO:CD	2.48	0.55
1:C:489:LEU:O	1:C:493:LYS:HE2	2.07	0.55
1:D:218:ASN:HD21	1:D:221:LYS:HG3	1.70	0.55
1:D:147:GLU:OE2	1:D:147:GLU:N	2.38	0.55
1:A:114:ASP:O	1:A:118:TYR:N	2.33	0.55
1:C:180:LYS:HZ2	1:C:180:LYS:CB	2.20	0.55
1:C:252:THR:O	1:C:253:THR:OG1	2.21	0.55
1:A:46:ARG:HH21	1:A:124:ARG:HG3	1.72	0.55
1:B:297:SER:CB	1:B:300:ARG:HH12	2.19	0.55
1:C:410:TYR:CD1	1:C:439:ILE:HD11	2.42	0.55
1:A:315:ARG:CZ	1:B:339:GLU:OE2	2.54	0.55
1:B:216:ASN:ND2	1:B:218:ASN:O	2.40	0.55
1:A:182:ARG:NH2	1:D:310:SER:HB3	2.22	0.54
1:D:54:ASP:OD1	1:D:56:LYS:N	2.39	0.54
1:D:114:ASP:OD1	1:D:115:LYS:N	2.40	0.54
1:A:341:LEU:HD12	1:A:392:TYR:OH	2.05	0.54
1:B:147:GLU:OE1	1:B:147:GLU:N	2.40	0.54
1:C:123:ASP:N	1:C:123:ASP:OD1	2.40	0.54
1:A:360:HIS:CD2	1:A:364:TYR:HB2	2.42	0.54
1:B:123:ASP:OD1	1:B:123:ASP:N	2.40	0.54
1:D:356:SER:O	1:D:356:SER:OG	2.24	0.54
1:D:298:ARG:HG3	1:D:298:ARG:HH21	1.72	0.54
1:C:108:PHE:HE1	1:C:131:TYR:HD2	1.55	0.54
1:D:190:ARG:HH12	1:D:193:LYS:HD2	1.73	0.54
1:D:216:ASN:ND2	1:D:218:ASN:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:LYS:CA	1:C:352:LYS:CE	2.85	0.54
1:D:304:ASP:OD1	1:D:304:ASP:N	2.40	0.53
1:D:360:HIS:ND1	1:D:360:HIS:O	2.42	0.53
1:A:67:LEU:HD13	1:A:96:VAL:HG13	1.90	0.53
1:D:504:LEU:O	1:D:507:ILE:HG22	2.08	0.53
1:C:186:TYR:CD1	1:C:186:TYR:C	2.86	0.53
1:C:190:ARG:CB	1:C:190:ARG:NH1	2.71	0.53
1:C:190:ARG:HH11	1:C:190:ARG:HB3	1.73	0.53
1:C:448:ARG:NH1	1:C:506:GLU:OE2	2.42	0.53
1:D:480:ASP:HA	1:D:483:ILE:HD13	1.90	0.53
1:A:337:ASP:HA	1:A:342:GLN:HB3	1.91	0.53
1:B:248:ILE:HG23	1:C:274:MET:HE3	1.91	0.53
1:C:315:ARG:NE	1:D:339:GLU:OE1	2.41	0.53
1:D:298:ARG:HH21	1:D:298:ARG:CG	2.22	0.53
1:A:190:ARG:NH1	1:A:190:ARG:CB	2.72	0.52
1:B:144:ILE:O	1:B:164:ARG:NH2	2.43	0.52
1:C:333:LYS:O	1:C:337:ASP:HB2	2.09	0.52
1:D:381:LEU:O	1:D:385:VAL:HG23	2.10	0.52
1:A:56:LYS:O	1:A:59:ILE:HG13	2.08	0.52
1:A:341:LEU:HD13	1:A:341:LEU:C	2.35	0.52
1:D:486:ASN:HA	1:D:489:LEU:HD12	1.90	0.52
1:B:73:TRP:HD1	1:B:74:VAL:HG23	1.73	0.52
1:D:183:ASN:OD1	1:D:183:ASN:N	2.42	0.52
1:D:73:TRP:HD1	1:D:74:VAL:HG23	1.75	0.52
1:A:192:ALA:HA	1:A:195:VAL:HG12	1.91	0.52
1:C:316:ASN:HD22	1:D:362:LEU:CD1	2.23	0.52
1:B:312:PHE:CB	1:C:343:GLN:CG	2.64	0.52
1:B:377:SER:HB3	1:B:480:ASP:OD2	2.10	0.52
1:A:430:VAL:HG12	1:A:431:ARG:H	1.75	0.51
1:B:251:LEU:HD23	1:B:251:LEU:C	2.35	0.51
1:C:335:ARG:HB2	1:C:335:ARG:CZ	2.40	0.51
1:A:388:MET:HG3	1:A:465:MET:HE3	1.92	0.51
1:A:505:LEU:O	1:A:509:ASN:N	2.43	0.51
1:C:400:ILE:HG21	1:C:439:ILE:HD13	1.93	0.51
1:D:311:ASN:O	1:D:315:ARG:HG2	2.11	0.51
1:D:418:ASP:HA	1:D:432:GLU:HA	1.91	0.51
1:A:190:ARG:NH1	1:A:190:ARG:CG	2.72	0.51
1:C:342:GLN:O	1:C:342:GLN:HG2	2.09	0.51
1:A:492:LEU:O	1:A:495:MET:HG2	2.11	0.51
1:C:203:HIS:HA	1:C:244:MET:HE1	1.93	0.51
1:A:508:GLU:HA	1:A:511:LEU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:LEU:HD12	1:B:477:ASN:ND2	2.25	0.51
1:C:316:ASN:HD22	1:D:362:LEU:HD13	1.75	0.51
1:C:191:CYS:SG	1:C:192:ALA:N	2.82	0.51
2:C:901:POV:O22	2:C:901:POV:H24	2.11	0.51
1:B:297:SER:OG	1:B:300:ARG:NH1	2.44	0.51
1:D:139:ASP:OD1	1:D:166:TRP:NE1	2.26	0.51
1:D:194:LEU:O	1:D:198:THR:HG22	2.11	0.51
1:A:193:LYS:NZ	1:A:193:LYS:CB	2.73	0.50
1:A:347:LEU:HD13	1:A:347:LEU:N	2.25	0.50
1:C:187:PHE:CE2	1:C:294:HIS:ND1	2.79	0.50
1:A:193:LYS:HB2	1:A:193:LYS:NZ	2.26	0.50
1:A:415:GLY:HA2	1:A:458:ARG:HD2	1.91	0.50
1:C:315:ARG:CZ	1:D:339:GLU:CD	2.84	0.50
1:C:369:LYS:O	1:C:374:ARG:NH2	2.42	0.50
1:A:108:PHE:HE1	1:A:131:TYR:HD2	1.58	0.50
1:B:387:GLU:OE2	1:B:473:ILE:HD11	2.11	0.50
1:C:53:TYR:HE1	1:C:113:LEU:HD11	1.77	0.50
1:B:400:ILE:HD11	1:B:450:GLN:HG3	1.93	0.50
1:C:147:GLU:OE2	1:C:147:GLU:N	2.41	0.50
1:A:258:ASP:OD1	1:A:258:ASP:N	2.34	0.50
1:B:103:ASP:O	1:B:107:THR:HG23	2.10	0.50
1:D:404:GLU:HB2	1:D:450:GLN:HB2	1.92	0.50
1:A:75:SER:HG	1:A:76:PRO:HD3	1.76	0.50
1:B:108:PHE:CE1	1:B:131:TYR:HD2	2.30	0.50
1:A:256:TYR:HH	1:B:250:THR:HG1	1.59	0.50
1:B:290:ASN:O	1:B:294:HIS:HB2	2.11	0.50
1:B:482:THR:HG23	1:B:483:ILE:HG23	1.94	0.50
1:B:298:ARG:O	1:B:301:ASN:N	2.45	0.50
1:C:352:LYS:CD	1:C:355:ARG:HE	2.20	0.50
1:C:360:HIS:CD2	1:C:364:TYR:HB2	2.47	0.50
1:C:335:ARG:HD2	1:D:115:LYS:CE	2.41	0.50
1:C:342:GLN:O	1:C:344:GLN:N	2.45	0.50
1:C:347:LEU:CD1	1:C:358:ILE:HD11	2.36	0.50
1:D:251:LEU:C	1:D:251:LEU:CD2	2.85	0.50
1:A:213:ALA:HB2	1:A:223:TRP:NE1	2.27	0.49
1:B:194:LEU:O	1:B:198:THR:HG23	2.12	0.49
1:B:388:MET:HE2	1:B:465:MET:HE2	1.94	0.49
1:B:251:LEU:C	1:B:251:LEU:CD2	2.85	0.49
1:C:245:TYR:O	1:C:249:THR:HG23	2.12	0.49
1:C:337:ASP:OD1	1:C:342:GLN:NE2	2.44	0.49
1:D:54:ASP:OD1	1:D:55:HIS:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ASN:OD1	1:A:183:ASN:N	2.46	0.49
1:D:377:SER:HB3	1:D:480:ASP:OD2	2.12	0.49
1:A:74:VAL:HG12	1:A:74:VAL:O	2.10	0.49
1:A:316:ASN:N	1:A:316:ASN:OD1	2.46	0.49
1:A:347:LEU:N	1:A:347:LEU:CD1	2.74	0.49
1:D:320:PRO:HA	1:D:323:GLN:HG3	1.93	0.49
1:A:67:LEU:O	1:A:71:THR:HG23	2.12	0.49
1:A:341:LEU:CD1	1:A:341:LEU:C	2.85	0.49
1:C:180:LYS:CB	1:C:180:LYS:NZ	2.72	0.49
1:D:108:PHE:CE1	1:D:131:TYR:HD2	2.29	0.49
1:D:240:TYR:OH	1:D:244:MET:HE3	2.13	0.49
1:C:309:ALA:HA	1:D:346:THR:HG21	1.95	0.49
1:D:311:ASN:O	1:D:315:ARG:NH1	2.46	0.49
1:A:451:LEU:HD22	1:A:451:LEU:H	1.78	0.49
1:B:318:LEU:HB2	1:B:319:PRO:HD2	1.94	0.49
1:B:490:GLN:OE1	1:B:490:GLN:N	2.45	0.49
1:C:45:LEU:HD21	1:C:120:ILE:HB	1.94	0.49
1:D:400:ILE:HG13	1:D:404:GLU:HG3	1.94	0.49
1:C:345:GLU:CD	1:C:345:GLU:N	2.70	0.49
1:C:497:ASP:O	1:C:501:THR:HG23	2.13	0.49
1:D:326:MET:HG3	1:D:327:LEU:HD12	1.94	0.49
1:A:202:VAL:HG23	1:A:251:LEU:HD22	1.93	0.49
1:B:292:VAL:O	1:B:296:THR:HG23	2.13	0.49
1:C:352:LYS:HA	1:C:352:LYS:CE	2.39	0.49
1:A:44:LYS:HZ2	1:A:44:LYS:N	2.11	0.48
1:A:352:LYS:HD3	1:A:355:ARG:HE	1.77	0.48
1:C:337:ASP:CG	1:C:342:GLN:NE2	2.71	0.48
1:C:483:ILE:HD12	1:C:483:ILE:H	1.76	0.48
2:D:901:POV:H1	2:D:901:POV:O22	2.12	0.48
1:D:123:ASP:OD2	1:D:126:GLN:HB2	2.14	0.48
1:B:337:ASP:OD1	1:B:337:ASP:N	2.41	0.48
1:C:115:LYS:H	1:C:115:LYS:HD3	1.79	0.48
1:C:350:LEU:H	1:C:350:LEU:HG	1.48	0.48
1:D:92:THR:O	1:D:92:THR:OG1	2.28	0.48
1:A:115:LYS:H	1:A:115:LYS:HD3	1.78	0.48
1:B:412:LEU:HD12	1:B:462:LEU:HG	1.95	0.48
1:A:497:ASP:O	1:A:501:THR:N	2.40	0.48
1:B:297:SER:CB	1:B:300:ARG:NH1	2.77	0.47
1:D:211:LEU:O	1:D:215:ARG:HG2	2.14	0.47
1:A:492:LEU:HA	1:A:495:MET:HE3	1.95	0.47
1:C:185:ASN:N	1:C:185:ASN:ND2	2.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:ASN:O	1:B:505:LEU:HB2	2.14	0.47
1:C:122:ASP:OD1	1:C:122:ASP:N	2.48	0.47
1:D:402:GLN:NE2	1:D:451:LEU:O	2.39	0.47
1:D:420:VAL:HA	1:D:430:VAL:HG23	1.96	0.47
1:A:448:ARG:HH21	1:A:506:GLU:HB2	1.80	0.47
1:B:240:TYR:OH	1:B:244:MET:HE3	2.13	0.47
1:B:301:ASN:HD22	1:B:301:ASN:C	2.22	0.47
1:A:93:ASP:OD1	1:A:94:ASN:N	2.47	0.47
1:A:147:GLU:OE2	1:A:147:GLU:N	2.43	0.47
1:A:215:ARG:HA	1:A:215:ARG:HD3	1.70	0.47
1:A:346:THR:O	1:A:350:LEU:HG	2.14	0.47
1:C:75:SER:HG	1:C:76:PRO:HD3	1.76	0.47
1:C:175:PHE:O	1:C:179:GLU:HG2	2.14	0.47
1:C:352:LYS:N	1:C:352:LYS:CE	2.78	0.47
2:C:901:POV:O22	2:C:901:POV:H1A	2.14	0.47
1:C:194:LEU:O	1:C:198:THR:HG22	2.15	0.47
1:C:215:ARG:HA	1:C:215:ARG:HD3	1.71	0.47
1:C:388:MET:HG3	1:C:465:MET:HE3	1.97	0.47
1:B:44:LYS:NZ	1:B:45:LEU:O	2.38	0.47
1:B:430:VAL:HG23	1:B:431:ARG:H	1.78	0.47
1:C:153:SER:HG	1:C:156:SER:HG	1.62	0.47
1:C:335:ARG:CZ	1:C:335:ARG:CB	2.92	0.47
1:B:484:ILE:HA	1:B:487:ASN:ND2	2.30	0.47
1:C:411:ILE:HD13	1:C:411:ILE:HA	1.71	0.47
1:D:505:LEU:HD23	1:D:505:LEU:H	1.80	0.47
1:A:190:ARG:NH1	1:A:190:ARG:CA	2.77	0.46
1:A:352:LYS:NZ	1:A:386:SER:O	2.43	0.46
1:A:491:HIS:HA	1:A:494:GLU:HG2	1.97	0.46
1:B:395:PRO:HB3	1:B:458:ARG:HA	1.96	0.46
1:A:367:MET:HE2	1:A:367:MET:HB2	1.76	0.46
1:B:114:ASP:O	1:B:118:TYR:N	2.49	0.46
1:C:399:VAL:HG13	1:C:400:ILE:HG22	1.97	0.46
1:A:153:SER:OG	1:A:156:SER:OG	2.28	0.46
1:B:415:GLY:HA2	1:B:458:ARG:HD2	1.97	0.46
1:A:343:GLN:CB	1:D:312:PHE:HB2	2.46	0.46
1:A:495:MET:HG3	1:A:500:MET:HB3	1.98	0.46
1:C:179:GLU:HB2	1:C:180:LYS:HZ3	1.80	0.46
1:C:468:THR:OG1	1:C:469:THR:N	2.48	0.46
1:A:186:TYR:CZ	1:A:190:ARG:CD	2.97	0.46
1:D:409:PHE:CD2	1:D:438:ILE:HD11	2.50	0.46
1:C:163:LEU:C	1:C:165:LEU:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:PHE:HD2	1:A:362:LEU:HD12	1.80	0.46
1:B:63:PHE:O	1:B:66:VAL:HG22	2.16	0.46
1:C:431:ARG:HH12	1:C:433:VAL:HG12	1.80	0.46
1:D:63:PHE:O	1:D:66:VAL:HG22	2.16	0.46
1:C:139:ASP:OD2	1:C:169:ARG:NH2	2.41	0.46
1:C:442:ILE:HD13	1:C:503:VAL:HG21	1.97	0.46
1:D:67:LEU:O	1:D:71:THR:HG23	2.16	0.46
1:A:108:PHE:CE1	1:A:131:TYR:HD2	2.34	0.45
1:D:344:GLN:C	1:D:344:GLN:CD	2.84	0.45
1:B:230:ASN:OD1	1:B:230:ASN:N	2.47	0.45
1:B:67:LEU:O	1:B:71:THR:HG23	2.15	0.45
1:C:190:ARG:NH1	1:C:190:ARG:CG	2.73	0.45
1:D:366:LEU:HD11	1:D:413:VAL:HG12	1.98	0.45
1:D:380:LEU:HD12	1:D:477:ASN:HB3	1.98	0.45
1:A:381:LEU:HA	1:A:384:LEU:HB2	1.98	0.45
1:B:297:SER:HA	1:B:300:ARG:NH1	2.31	0.45
1:C:75:SER:HB2	1:C:161:ASN:O	2.17	0.45
1:B:324:ASP:O	1:B:328:ALA:N	2.45	0.45
1:C:360:HIS:HD2	1:C:364:TYR:HB2	1.82	0.45
1:D:297:SER:C	1:D:300:ARG:HD2	2.39	0.45
1:A:182:ARG:NH1	1:D:306:ILE:HG22	2.32	0.45
1:A:411:ILE:HD13	1:A:411:ILE:HA	1.71	0.45
1:B:139:ASP:OD1	1:B:166:TRP:NE1	2.27	0.45
1:B:344:GLN:CD	1:B:344:GLN:C	2.85	0.45
1:C:489:LEU:O	1:C:492:LEU:N	2.50	0.45
1:C:495:MET:SD	1:C:500:MET:HB3	2.56	0.45
1:D:326:MET:HG3	1:D:327:LEU:N	2.31	0.45
1:C:190:ARG:HB3	1:C:190:ARG:NH1	2.31	0.45
1:C:333:LYS:O	1:C:337:ASP:CB	2.65	0.45
1:C:409:PHE:CD2	1:C:438:ILE:HD11	2.52	0.45
1:C:422:VAL:O	1:C:422:VAL:HG23	2.16	0.45
1:C:423:ASP:O	1:C:426:THR:N	2.43	0.45
1:A:468:THR:OG1	1:A:469:THR:N	2.50	0.44
1:D:332:LEU:O	1:D:336:THR:HG22	2.17	0.44
1:D:441:GLU:OE2	1:D:441:GLU:N	2.49	0.44
1:A:186:TYR:CE2	1:A:190:ARG:HD3	2.52	0.44
1:B:313:ALA:HA	1:B:318:LEU:HD21	1.99	0.44
1:B:500:MET:O	1:B:503:VAL:HG12	2.17	0.44
1:D:493:LYS:HD2	1:D:504:LEU:HD21	1.99	0.44
1:A:87:PRO:O	1:A:89:LEU:N	2.51	0.44
1:A:115:LYS:HD3	1:A:115:LYS:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ARG:HB2	1:B:117:THR:HB	1.99	0.44
1:B:296:THR:O	1:B:296:THR:OG1	2.24	0.44
1:B:352:LYS:O	1:B:356:SER:HB3	2.17	0.44
1:C:335:ARG:HH21	1:D:118:TYR:HE2	1.65	0.44
1:D:419:LEU:HD23	1:D:419:LEU:HA	1.65	0.44
1:B:321:ARG:HH11	1:B:321:ARG:C	2.24	0.44
1:C:138:LEU:HD23	1:C:138:LEU:HA	1.83	0.44
1:C:344:GLN:C	1:C:344:GLN:CD	2.85	0.44
1:C:509:ASN:O	1:C:512:ALA:N	2.50	0.44
1:D:137:LEU:HD12	1:D:137:LEU:HA	1.77	0.44
1:A:115:LYS:HA	1:A:118:TYR:CE1	2.53	0.44
1:C:48:PHE:HB2	1:C:124:ARG:HH12	1.82	0.44
1:D:251:LEU:HD23	1:D:251:LEU:C	2.43	0.44
1:A:341:LEU:HD12	1:A:392:TYR:CZ	2.53	0.44
1:C:418:ASP:OD1	1:C:419:LEU:N	2.50	0.44
1:C:115:LYS:HD3	1:C:115:LYS:N	2.33	0.44
1:C:183:ASN:OD1	1:C:183:ASN:N	2.49	0.44
1:D:485:MET:O	1:D:488:LEU:HB3	2.18	0.44
1:A:420:VAL:HG23	1:A:428:SER:C	2.43	0.43
1:C:46:ARG:NH1	1:C:123:ASP:HA	2.34	0.43
1:C:335:ARG:NH1	1:C:335:ARG:CB	2.73	0.43
1:C:402:GLN:H	1:C:453:THR:HG22	1.83	0.43
1:C:256:TYR:OH	1:D:250:THR:OG1	2.32	0.43
1:A:351:PRO:HD3	1:D:329:HIS:NE2	2.33	0.43
1:B:193:LYS:O	1:B:193:LYS:HG2	2.16	0.43
1:B:199:LEU:HD23	1:B:199:LEU:HA	1.84	0.43
1:C:380:LEU:HD23	1:C:380:LEU:H	1.82	0.43
1:B:500:MET:HE3	1:B:500:MET:HB3	1.78	0.43
1:C:352:LYS:HD3	1:C:352:LYS:HA	1.87	0.43
1:A:186:TYR:O	1:A:190:ARG:HG3	2.17	0.43
1:A:193:LYS:HZ3	1:A:193:LYS:CB	2.27	0.43
1:B:104:ILE:HD11	1:B:139:ASP:O	2.18	0.43
1:C:114:ASP:HB3	1:C:117:THR:OG1	2.18	0.43
1:D:73:TRP:CD1	1:D:73:TRP:C	2.96	0.43
1:D:288:MET:HB3	1:D:288:MET:HE2	1.75	0.43
1:D:300:ARG:H	1:D:300:ARG:HG3	1.63	0.43
1:D:508:GLU:O	1:D:511:LEU:HB3	2.18	0.43
1:B:115:LYS:HE3	1:B:115:LYS:HB3	1.67	0.43
1:B:137:LEU:HD12	1:B:137:LEU:HA	1.78	0.43
1:B:379:ASP:HA	1:B:382:PHE:CD2	2.54	0.43
1:B:421:ASP:OD1	1:B:421:ASP:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:TRP:CD1	1:B:73:TRP:C	2.96	0.43
1:C:342:GLN:HB3	1:C:342:GLN:HE21	1.59	0.43
1:B:108:PHE:HE1	1:B:131:TYR:HD2	1.66	0.43
1:B:508:GLU:CD	1:B:508:GLU:H	2.27	0.43
1:C:466:ASN:OD1	1:C:466:ASN:N	2.49	0.43
1:D:132:LEU:HA	1:D:136:PHE:HB3	2.01	0.43
1:A:114:ASP:HB3	1:A:117:THR:HG22	2.00	0.43
1:B:324:ASP:OD1	1:B:325:GLN:N	2.52	0.43
1:C:335:ARG:HD2	1:D:115:LYS:HZ1	1.79	0.43
1:A:163:LEU:C	1:A:165:LEU:H	2.27	0.42
1:B:59:ILE:HD12	1:B:59:ILE:HA	1.87	0.42
1:B:311:ASN:OD1	1:B:312:PHE:N	2.52	0.42
1:B:313:ALA:O	1:B:317:HIS:N	2.52	0.42
1:B:404:GLU:OE2	1:B:405:ALA:N	2.51	0.42
1:C:493:LYS:HZ2	1:C:504:LEU:HD13	1.83	0.42
1:C:509:ASN:OD1	1:C:510:MET:N	2.52	0.42
1:D:103:ASP:O	1:D:107:THR:HG23	2.19	0.42
1:D:420:VAL:HG22	1:D:427:GLU:HB2	2.01	0.42
1:A:203:HIS:HA	1:A:244:MET:HE1	2.00	0.42
1:B:233:GLU:OE1	1:B:233:GLU:N	2.52	0.42
1:B:236:LEU:HD12	1:B:236:LEU:HA	1.81	0.42
1:B:288:MET:HB3	1:B:288:MET:HE2	1.75	0.42
1:B:410:TYR:HB2	1:B:439:ILE:HD11	2.01	0.42
1:B:495:MET:HB3	1:B:500:MET:HE2	1.99	0.42
1:C:186:TYR:O	1:C:186:TYR:CG	2.69	0.42
1:D:341:LEU:HA	1:D:341:LEU:HD23	1.79	0.42
1:D:379:ASP:O	1:D:382:PHE:HB2	2.19	0.42
1:D:410:TYR:HB2	1:D:439:ILE:HD11	1.99	0.42
1:D:417:ALA:O	1:D:433:VAL:N	2.52	0.42
2:D:901:POV:C1	2:D:901:POV:C31	2.97	0.42
1:C:409:PHE:HE1	1:C:465:MET:HG2	1.84	0.42
1:A:139:ASP:OD2	1:A:169:ARG:NH2	2.43	0.42
1:A:150:MET:SD	1:A:157:TYR:HB2	2.59	0.42
1:A:466:ASN:ND2	1:A:469:THR:HG22	2.35	0.42
1:A:186:TYR:CE2	1:A:190:ARG:CD	3.02	0.42
1:A:501:THR:O	1:A:504:LEU:HB2	2.20	0.42
1:B:227:ASN:OD1	1:B:227:ASN:N	2.53	0.42
1:C:337:ASP:HA	1:C:342:GLN:HE21	1.85	0.42
1:C:354:ILE:HD12	1:C:357:SER:HB3	2.02	0.42
1:C:492:LEU:HD12	1:C:495:MET:SD	2.59	0.42
1:D:499:VAL:O	1:D:502:ASN:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:GLU:HG3	1:C:82:LEU:HD12	2.02	0.42
1:C:193:LYS:HE3	2:C:901:POV:H3A	2.01	0.42
1:D:318:LEU:HB2	1:D:319:PRO:HD2	2.01	0.42
1:D:387:GLU:OE2	1:D:473:ILE:HD11	2.20	0.42
1:D:507:ILE:O	1:D:510:MET:HB2	2.20	0.42
1:A:190:ARG:HH12	1:A:193:LYS:CE	2.33	0.42
1:A:488:LEU:O	1:A:492:LEU:N	2.52	0.42
1:D:469:THR:OG1	1:D:470:PHE:N	2.52	0.42
1:D:501:THR:O	1:D:504:LEU:HB3	2.20	0.42
1:A:352:LYS:HZ1	1:A:356:SER:HB2	1.83	0.42
1:D:465:MET:SD	1:D:470:PHE:HB2	2.60	0.42
1:A:306:ILE:HG22	1:B:182:ARG:HD3	2.02	0.41
1:B:370:VAL:HG21	1:B:411:ILE:HD13	2.02	0.41
1:C:351:PRO:HD2	1:C:354:ILE:HG21	1.98	0.41
1:D:56:LYS:O	1:D:59:ILE:HG22	2.20	0.41
1:D:319:PRO:HA	1:D:320:PRO:HD3	1.96	0.41
1:A:274:MET:HE1	1:D:249:THR:CG2	2.48	0.41
1:A:485:MET:O	1:A:489:LEU:HG	2.19	0.41
1:B:301:ASN:ND2	1:B:301:ASN:C	2.77	0.41
1:D:218:ASN:ND2	1:D:221:LYS:HG3	2.36	0.41
1:A:465:MET:HE3	1:A:465:MET:HB2	1.91	0.41
1:D:333:LYS:HE2	1:D:333:LYS:HB3	1.89	0.41
1:A:497:ASP:HB2	1:A:500:MET:HB2	2.02	0.41
1:B:376:VAL:HG21	1:B:380:LEU:HD22	2.01	0.41
1:C:190:ARG:HA	1:C:190:ARG:HD2	1.30	0.41
1:C:193:LYS:NZ	2:C:901:POV:H3A	2.35	0.41
1:D:297:SER:O	1:D:300:ARG:CD	2.51	0.41
1:D:330:LEU:HD13	1:D:330:LEU:HA	1.81	0.41
1:B:396:LYS:HZ2	1:C:354:ILE:HD13	1.86	0.41
1:C:193:LYS:O	1:C:193:LYS:HG2	2.20	0.41
1:C:502:ASN:O	1:C:505:LEU:HG	2.21	0.41
1:D:421:ASP:OD1	1:D:421:ASP:N	2.45	0.41
1:A:332:LEU:HD12	1:A:336:THR:CG2	2.50	0.41
1:A:409:PHE:HE1	1:A:465:MET:HG2	1.84	0.41
1:B:308:ALA:O	1:C:346:THR:HG21	2.20	0.41
1:B:312:PHE:CE1	1:C:343:GLN:HB3	2.56	0.41
1:B:345:GLU:OE2	1:B:345:GLU:CA	2.69	0.41
1:C:347:LEU:O	1:C:355:ARG:HG3	2.20	0.41
1:C:379:ASP:N	1:C:379:ASP:OD1	2.53	0.41
1:B:418:ASP:HA	1:B:432:GLU:HA	2.02	0.41
1:C:402:GLN:N	1:C:453:THR:HG22	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:TYR:OH	1:A:190:ARG:HD2	2.21	0.41
1:A:380:LEU:O	1:A:383:GLN:HG3	2.20	0.41
1:D:326:MET:HG3	1:D:327:LEU:H	1.86	0.41
1:D:331:CYS:SG	1:D:332:LEU:N	2.93	0.41
1:A:182:ARG:HH22	1:D:307:GLN:HA	1.85	0.41
1:A:256:TYR:OH	1:B:250:THR:OG1	2.30	0.41
1:A:334:TYR:HA	1:A:337:ASP:HB3	2.03	0.41
1:A:345:GLU:CA	1:A:345:GLU:OE2	2.69	0.41
1:B:186:TYR:OH	1:B:190:ARG:HD2	2.21	0.41
1:C:64:LEU:HD23	1:C:64:LEU:HA	1.84	0.41
1:D:79:PHE:CD2	1:D:162:MET:HE3	2.56	0.41
1:A:372:LEU:HD23	1:A:373:PHE:CE1	2.56	0.41
1:C:163:LEU:HD23	1:C:163:LEU:HA	1.88	0.41
1:C:492:LEU:HD21	1:C:503:VAL:CB	2.47	0.41
1:D:410:TYR:O	1:D:438:ILE:HG13	2.21	0.41
1:B:232:LEU:HD23	1:B:232:LEU:HA	1.94	0.40
1:B:296:THR:CA	1:B:299:THR:HG23	2.51	0.40
1:C:54:ASP:OD1	1:C:56:LYS:N	2.53	0.40
1:C:149:ALA:O	1:C:152:ILE:HG13	2.21	0.40
1:D:486:ASN:O	1:D:490:GLN:HG3	2.21	0.40
1:A:448:ARG:NH2	1:A:503:VAL:HA	2.32	0.40
1:B:54:ASP:OD1	1:B:55:HIS:N	2.53	0.40
1:B:296:THR:C	1:B:299:THR:HG23	2.46	0.40
1:B:316:ASN:C	1:B:317:HIS:CG	2.99	0.40
1:C:378:ASN:OD1	1:C:378:ASN:N	2.54	0.40
1:D:320:PRO:HA	1:D:323:GLN:CG	2.52	0.40
1:D:333:LYS:HA	1:D:336:THR:HG22	2.04	0.40
1:D:408:ASP:N	1:D:408:ASP:OD1	2.55	0.40
1:A:242:THR:O	1:A:245:TYR:HB3	2.21	0.40
1:C:231:PHE:O	1:C:239:ARG:HD3	2.21	0.40
1:A:409:PHE:CD2	1:A:438:ILE:HD11	2.56	0.40
1:B:275:LEU:HD23	1:B:275:LEU:HA	1.87	0.40
1:C:46:ARG:HH12	1:C:123:ASP:HA	1.87	0.40
1:D:466:ASN:OD1	1:D:467:ARG:N	2.54	0.40
1:A:46:ARG:HH12	1:A:123:ASP:HA	1.87	0.40
1:A:89:LEU:HA	1:A:92:THR:HG23	2.03	0.40
1:A:264:THR:O	1:A:268:ILE:HG13	2.22	0.40
1:A:274:MET:CE	1:D:249:THR:HG22	2.50	0.40
1:B:400:ILE:HD11	1:B:450:GLN:CD	2.46	0.40
1:B:432:GLU:OE1	1:B:432:GLU:N	2.52	0.40
1:C:46:ARG:HG2	1:C:47:ARG:H	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1678/3104 (54%)	1476 (88%)	202 (12%)	6 10

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ILE
1	A	64	LEU
1	A	65	VAL
1	A	68	VAL
1	A	71	THR
1	A	92	THR
1	A	102	ILE
1	A	104	ILE
1	A	110	VAL
1	A	115	LYS
1	A	142	SER
1	A	144	ILE
1	A	159	LEU
1	A	177	ARG
1	A	183	ASN
1	A	190	ARG
1	A	191	CYS
1	A	193	LYS
1	A	228	VAL
1	A	230	ASN
1	A	243	SER
1	A	248	ILE
1	A	249	THR
1	A	264	THR
1	A	288	MET
1	A	299	THR
1	A	310	SER
1	A	315	ARG
1	A	316	ASN
1	A	322	LEU
1	A	336	THR
1	A	339	GLU
1	A	341	LEU
1	A	343	GLN
1	A	345	GLU
1	A	347	LEU
1	A	367	MET

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Mol	Chain	Res	Type
1	A	380	LEU
1	A	381	LEU
1	A	384	LEU
1	A	411	ILE
1	A	412	LEU
1	A	422	VAL
1	A	430	VAL
1	A	431	ARG
1	A	451	LEU
1	A	452	PHE
1	A	474	ILE
1	A	477	ASN
1	A	480	ASP
1	A	488	LEU
1	A	497	ASP
1	A	506	GLU
1	B	59	ILE
1	B	60	TRP
1	B	66	VAL
1	B	78	GLU
1	B	92	THR
1	B	104	ILE
1	B	117	THR
1	B	134	SER
1	B	141	VAL
1	B	218	ASN
1	B	228	VAL
1	B	235	SER
1	B	243	SER
1	B	248	ILE
1	B	249	THR
1	B	251	LEU
1	B	288	MET
1	B	293	VAL
1	B	296	THR
1	B	298	ARG
1	B	299	THR
1	B	300	ARG
1	B	301	ASN
1	B	304	ASP
1	B	311	ASN
1	B	327	LEU

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Mol	Chain	Res	Type
1	B	337	ASP
1	B	338	SER
1	B	339	GLU
1	B	341	LEU
1	B	342	GLN
1	B	344	GLN
1	B	345	GLU
1	B	346	THR
1	B	348	ASP
1	B	352	LYS
1	B	354	ILE
1	B	356	SER
1	B	377	SER
1	B	389	LYS
1	B	401	LEU
1	B	420	VAL
1	B	422	VAL
1	B	437	ASP
1	B	471	LEU
1	B	477	ASN
1	B	487	ASN
1	B	495	MET
1	B	497	ASP
1	B	501	THR
1	B	507	ILE
1	B	508	GLU
1	C	59	ILE
1	C	66	VAL
1	C	71	THR
1	C	78	GLU
1	C	84	LYS
1	C	90	SER
1	C	92	THR
1	C	104	ILE
1	C	106	MET
1	C	110	VAL
1	C	115	LYS
1	C	116	SER
1	C	120	ILE
1	C	142	SER
1	C	143	THR
1	C	159	LEU

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Mol	Chain	Res	Type
1	C	180	LYS
1	C	182	ARG
1	C	183	ASN
1	C	185	ASN
1	C	190	ARG
1	C	191	CYS
1	C	221	LYS
1	C	228	VAL
1	C	249	THR
1	C	258	ASP
1	C	259	LEU
1	C	264	THR
1	C	314	HIS
1	C	316	ASN
1	C	324	ASP
1	C	335	ARG
1	C	336	THR
1	C	339	GLU
1	C	341	LEU
1	C	342	GLN
1	C	343	GLN
1	C	345	GLU
1	C	350	LEU
1	C	352	LYS
1	C	367	MET
1	C	383	GLN
1	C	401	LEU
1	C	411	ILE
1	C	421	ASP
1	C	424	THR
1	C	430	VAL
1	C	444	VAL
1	C	459	LEU
1	C	474	ILE
1	C	497	ASP
1	C	504	LEU
1	D	60	TRP
1	D	66	VAL
1	D	78	GLU
1	D	102	ILE
1	D	105	ILE
1	D	106	MET

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Mol	Chain	Res	Type
1	D	115	LYS
1	D	117	THR
1	D	134	SER
1	D	141	VAL
1	D	146	SER
1	D	183	ASN
1	D	202	VAL
1	D	218	ASN
1	D	235	SER
1	D	243	SER
1	D	248	ILE
1	D	249	THR
1	D	251	LEU
1	D	288	MET
1	D	293	VAL
1	D	298	ARG
1	D	300	ARG
1	D	311	ASN
1	D	317	HIS
1	D	330	LEU
1	D	333	LYS
1	D	337	ASP
1	D	339	GLU
1	D	341	LEU
1	D	346	THR
1	D	347	LEU
1	D	354	ILE
1	D	365	SER
1	D	366	LEU
1	D	377	SER
1	D	398	ASP
1	D	419	LEU
1	D	432	GLU
1	D	497	ASP
1	D	503	VAL
1	D	506	GLU
1	D	508	GLU
1	D	509	ASN
1	D	511	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	ASN
1	A	227	ASN
1	A	260	HIS
1	A	277	ASN
1	A	294	HIS
1	A	323	GLN
1	A	325	GLN
1	A	383	GLN
1	A	402	GLN
1	A	403	ASN
1	A	414	ASN
1	A	450	GLN
1	A	472	ASN
1	A	502	ASN
1	B	203	HIS
1	B	216	ASN
1	B	218	ASN
1	B	260	HIS
1	B	301	ASN
1	B	342	GLN
1	B	343	GLN
1	B	472	ASN
1	B	475	GLN
1	B	491	HIS
1	C	126	GLN
1	C	185	ASN
1	C	203	HIS
1	C	216	ASN
1	C	260	HIS
1	C	294	HIS
1	C	307	GLN
1	C	317	HIS
1	C	323	GLN
1	C	342	GLN
1	C	414	ASN
1	C	450	GLN
1	C	472	ASN
1	C	496	ASN
1	D	126	GLN
1	D	203	HIS
1	D	216	ASN
1	D	218	ASN
1	D	260	HIS

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Mol	Chain	Res	Type
1	D	277	ASN
1	D	311	ASN
1	D	323	GLN
1	D	343	GLN
1	D	383	GLN
1	D	477	ASN
1	D	509	ASN

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	A	901	-	38,38,51	0.55	0	42,43,59	0.69	2 (4%)
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%)

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	A	901	-	-	19/40/40/55	-
2	POV	D	901	-	-	25/40/40/55	-
2	POV	C	901	-	-	20/40/40/55	-
2	POV	B	901	-	-	18/40/40/55	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
2	C	901	POV	O21-C21-C22	2.36	116.60	111.50
2	D	901	POV	O13-P-O11	2.25	112.71	106.73
2	A	901	POV	O21-C21-C22	2.17	116.17	111.50

There are no chirality outliers.

All (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
2	D	901	POV	C1-O11-P-O12
2	D	901	POV	C1-O11-P-O13
2	D	901	POV	C1-O11-P-O14
2	D	901	POV	O32-C31-O31-C3
2	D	901	POV	C2-C3-O31-C31
2	D	901	POV	C32-C31-O31-C3
2	C	901	POV	O22-C21-O21-C2
2	A	901	POV	C22-C21-O21-C2
2	A	901	POV	O22-C21-O21-C2
2	D	901	POV	C22-C21-O21-C2
2	D	901	POV	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
2	C	901	POV	C31-C32-C33-C34
2	D	901	POV	O22-C21-O21-C2
2	B	901	POV	C311-C310-C39-C38
2	C	901	POV	C32-C31-O31-C3
2	D	901	POV	C311-C310-C39-C38
2	D	901	POV	C32-C33-C34-C35
2	D	901	POV	C23-C24-C25-C26
2	D	901	POV	C24-C25-C26-C27
2	B	901	POV	C22-C23-C24-C25
2	D	901	POV	C34-C35-C36-C37
2	C	901	POV	O32-C31-O31-C3
2	D	901	POV	C35-C36-C37-C38
2	C	901	POV	C35-C36-C37-C38
2	D	901	POV	C26-C27-C28-C29
2	B	901	POV	C32-C31-O31-C3
2	C	901	POV	C24-C25-C26-C27
2	A	901	POV	C24-C25-C26-C27
2	D	901	POV	C311-C312-C313-C314
2	D	901	POV	C310-C311-C312-C313
2	D	901	POV	O11-C1-C2-C3
2	B	901	POV	C31-C32-C33-C34
2	C	901	POV	C34-C35-C36-C37
2	A	901	POV	C311-C312-C313-C314
2	B	901	POV	C1-O11-P-O14
2	B	901	POV	O32-C31-O31-C3
2	A	901	POV	C39-C310-C311-C312
2	B	901	POV	C37-C38-C39-C310
2	D	901	POV	C37-C38-C39-C310
2	B	901	POV	C35-C36-C37-C38
2	C	901	POV	C311-C312-C313-C314
2	A	901	POV	C313-C314-C315-C316
2	B	901	POV	O11-C1-C2-O21
2	D	901	POV	O11-C1-C2-O21
2	A	901	POV	C33-C34-C35-C36
2	D	901	POV	C25-C26-C27-C28
2	A	901	POV	C311-C310-C39-C38
2	A	901	POV	C310-C311-C312-C313
2	A	901	POV	C37-C38-C39-C310
2	A	901	POV	C211-C210-C29-C28
2	C	901	POV	C211-C210-C29-C28
2	D	901	POV	C211-C210-C29-C28
2	A	901	POV	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	C	901	POV	C1-C2-O21-C21
2	C	901	POV	O11-C1-C2-O21
2	B	901	POV	O11-C1-C2-C3
2	C	901	POV	O11-C1-C2-C3
2	A	901	POV	O11-C1-C2-O21
2	C	901	POV	C2-C1-O11-P
2	B	901	POV	C32-C33-C34-C35
2	A	901	POV	C22-C23-C24-C25
2	C	901	POV	C1-O11-P-O14
2	D	901	POV	C27-C28-C29-C210
2	C	901	POV	C39-C310-C311-C312
2	A	901	POV	C2-C1-O11-P
2	A	901	POV	C27-C28-C29-C210
2	C	901	POV	C27-C28-C29-C210
2	B	901	POV	C313-C314-C315-C316
2	C	901	POV	C311-C310-C39-C38
2	B	901	POV	C1-C2-O21-C21
2	D	901	POV	C1-C2-O21-C21
2	C	901	POV	C1-C2-C3-O31
2	B	901	POV	C27-C28-C29-C210
2	C	901	POV	C1-O11-P-O12
2	A	901	POV	C312-C313-C314-C315
2	A	901	POV	C34-C35-C36-C37
2	B	901	POV	O31-C31-C32-C33

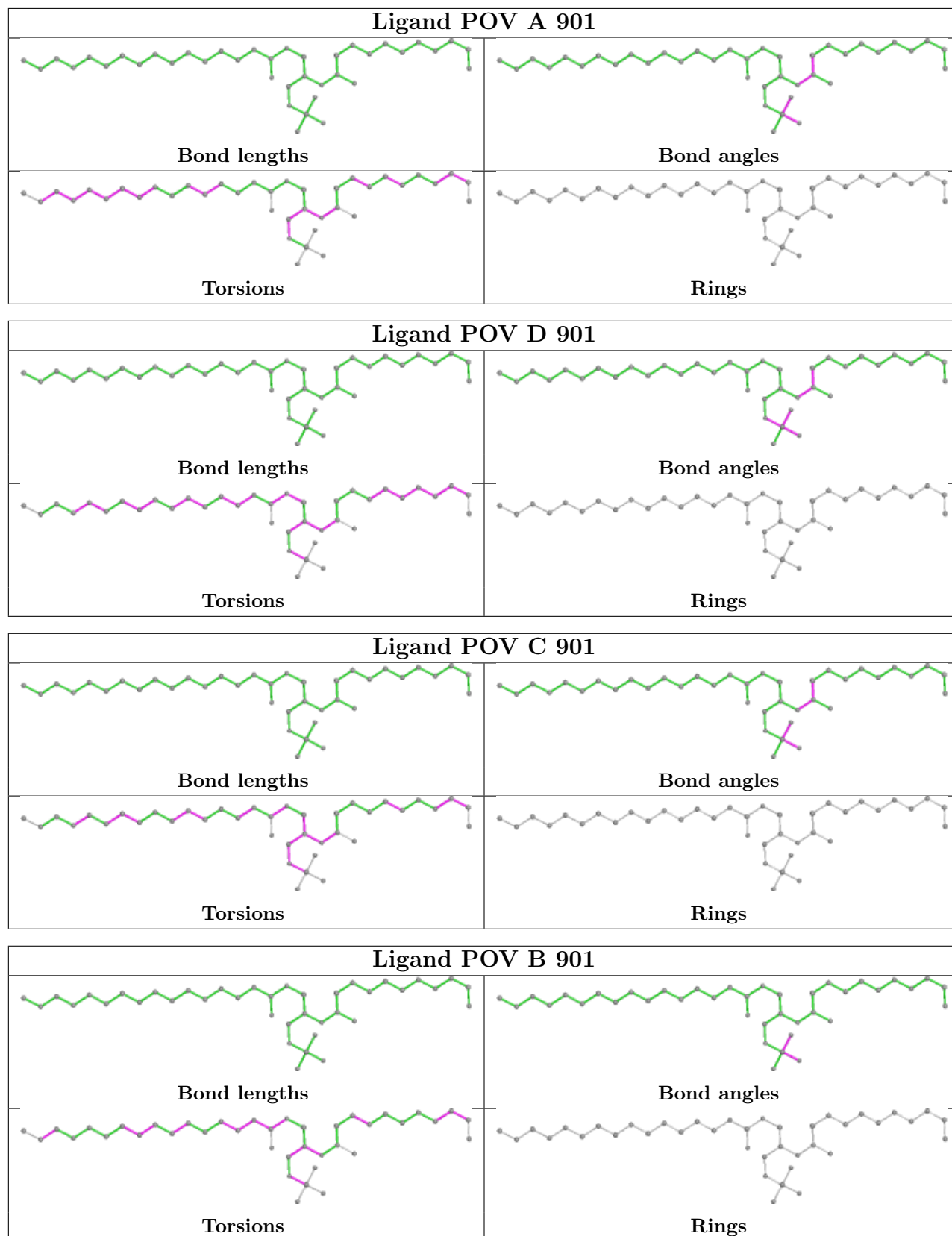
There are no ring outliers.

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 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.

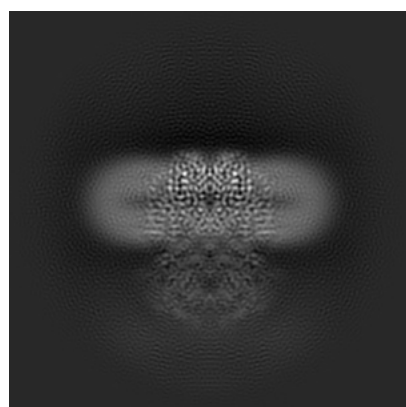
6 Map visualisation [i](#)

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

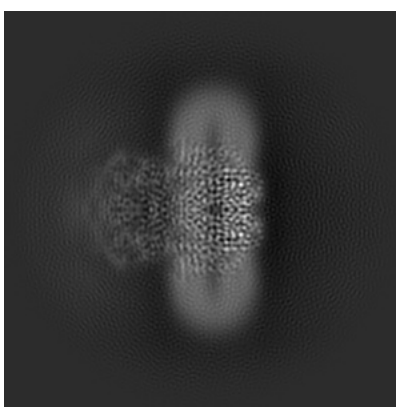
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

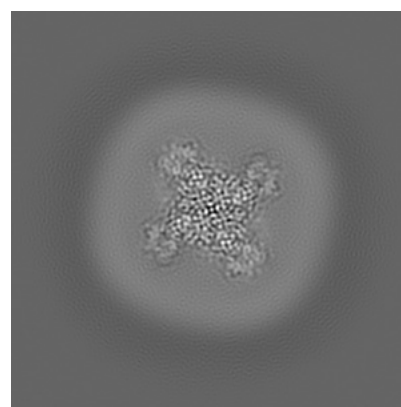
6.1.1 Primary map



X



Y

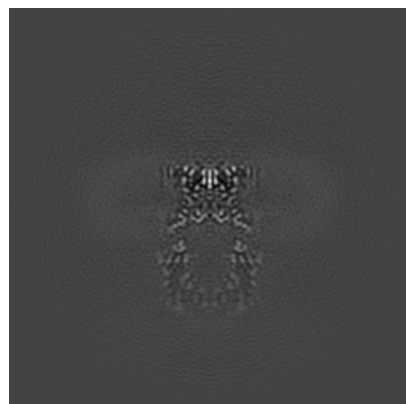


Z

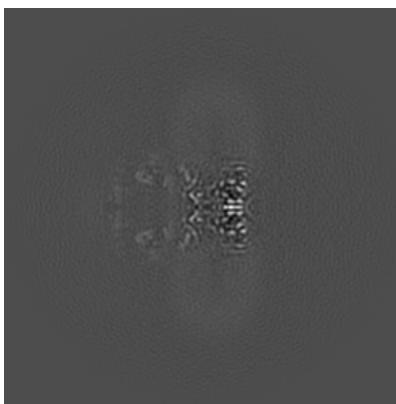
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

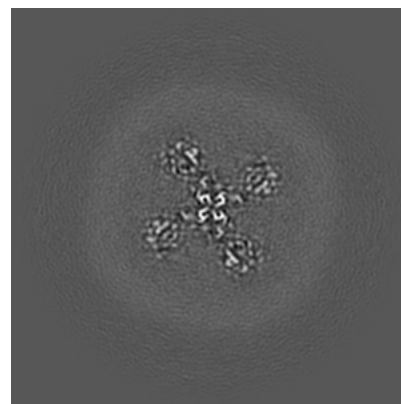
6.2.1 Primary map



X Index: 120



Y Index: 120

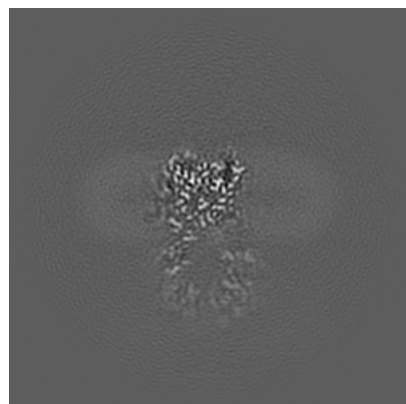


Z Index: 120

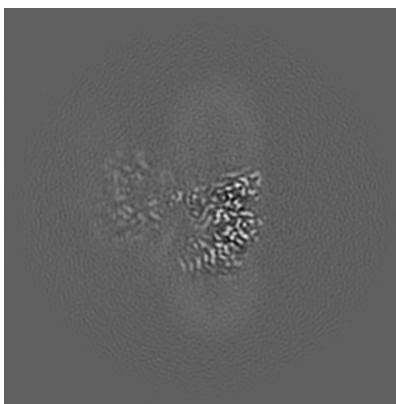
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

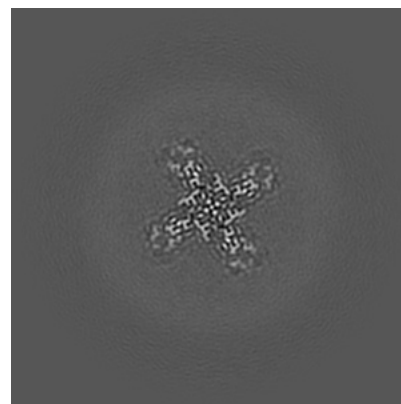
6.3.1 Primary map



X Index: 126



Y Index: 108

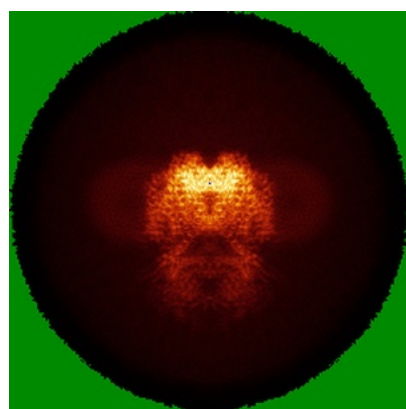


Z Index: 133

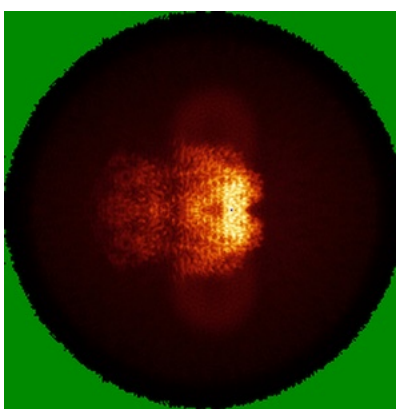
The images above show the largest variance slices of the map in three orthogonal directions.

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

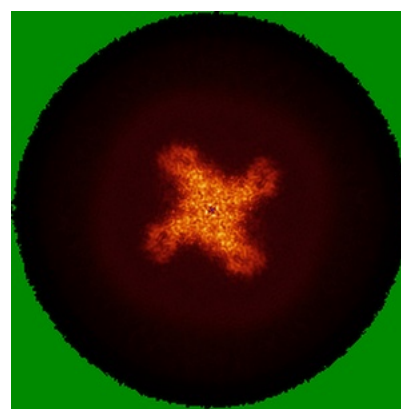
6.4.1 Primary map



X



Y

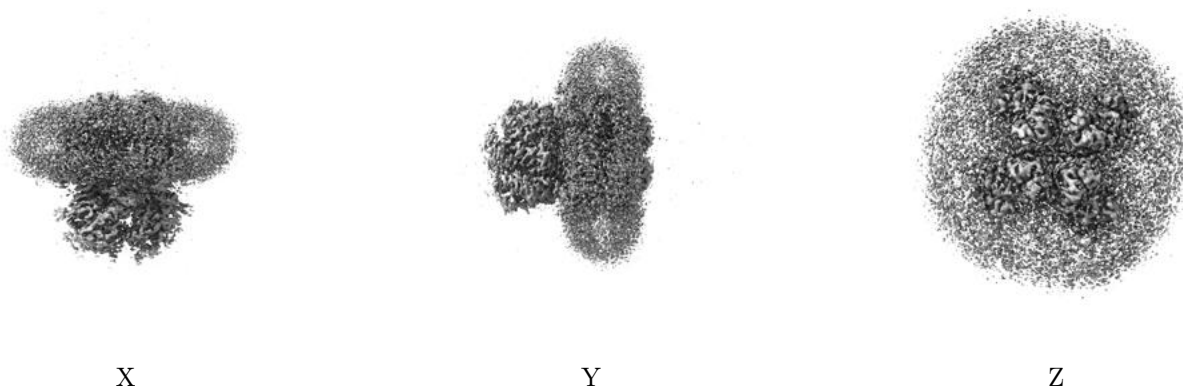


Z

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



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.

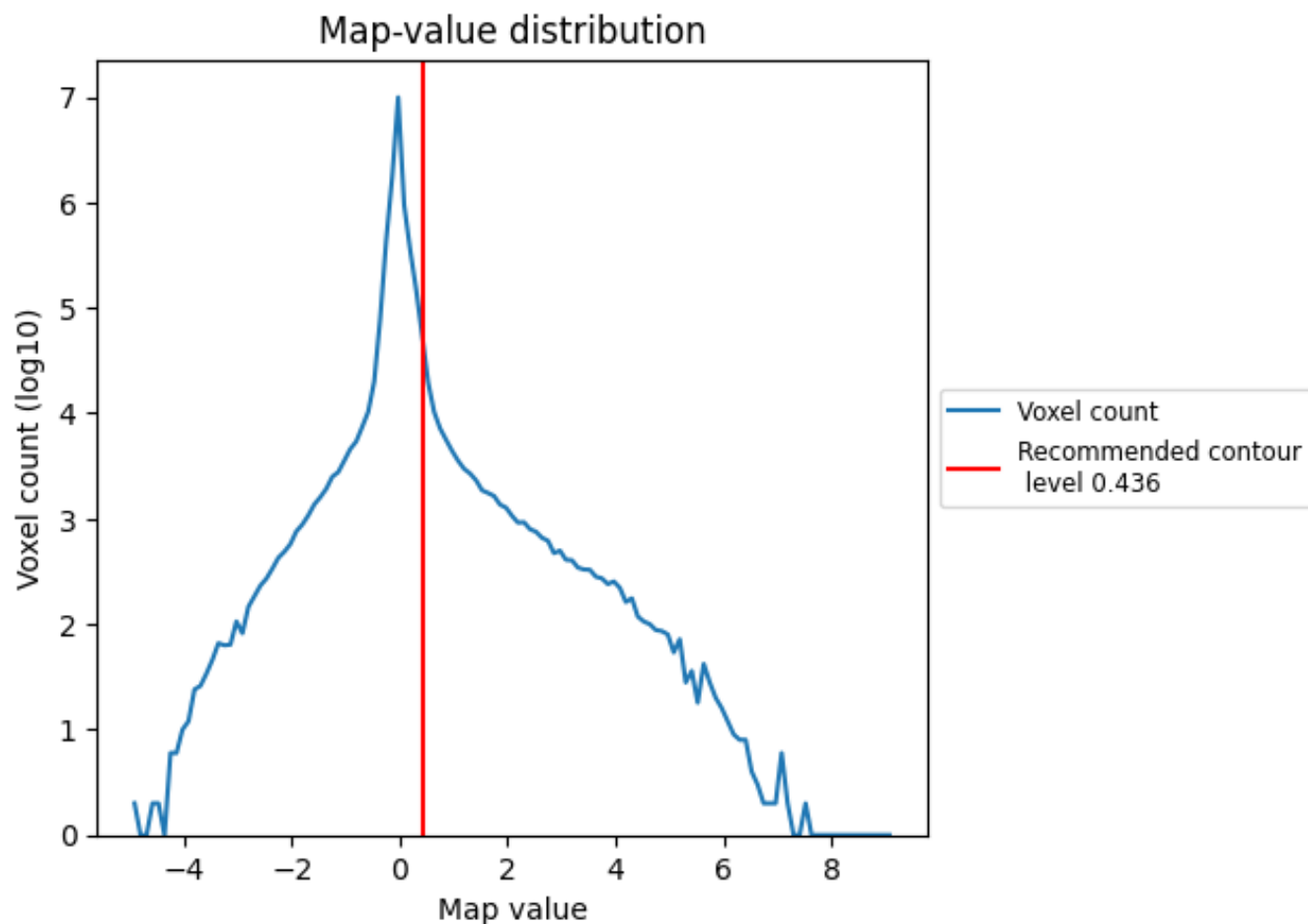
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

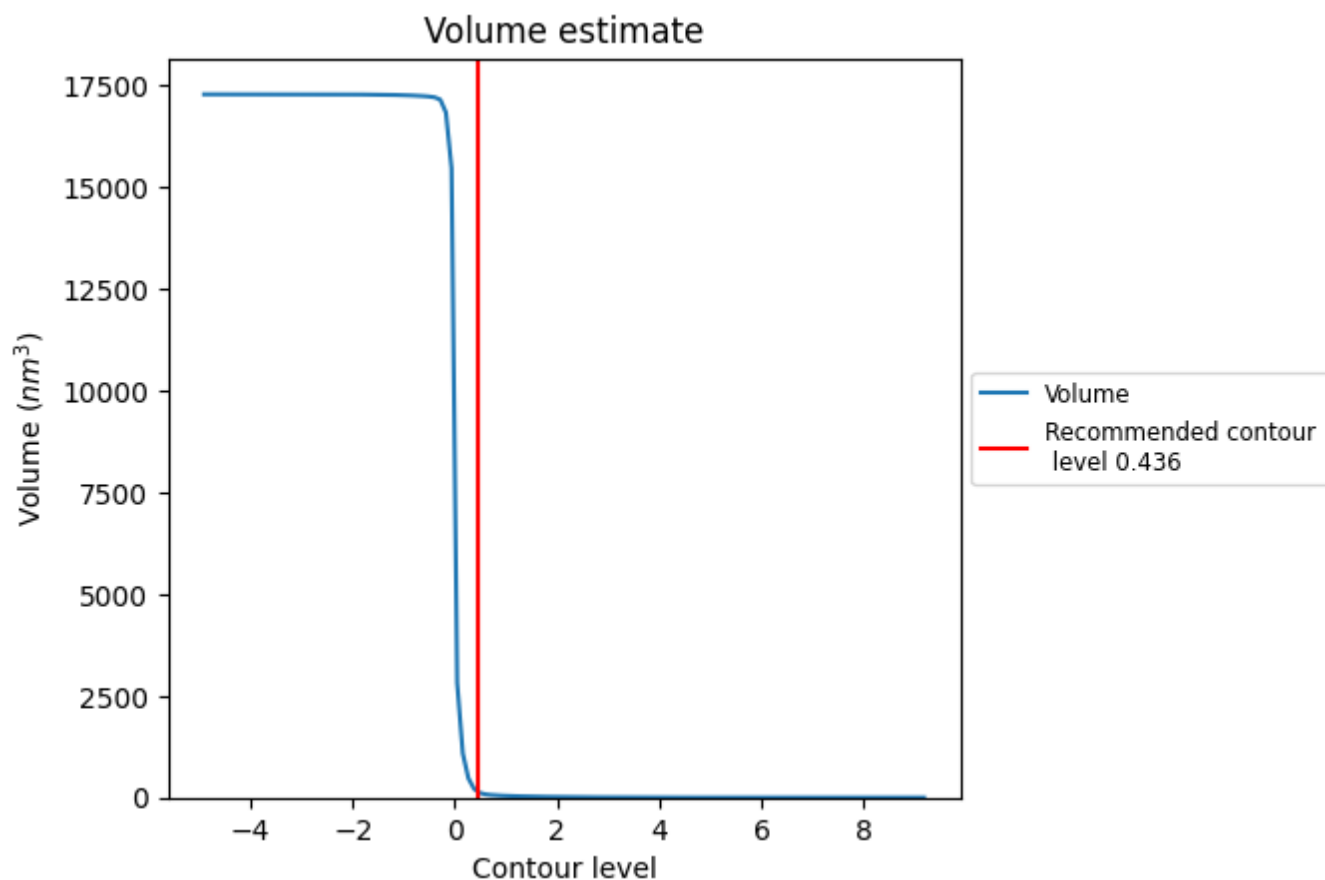
This section contains the results of statistical analysis of the map.

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.

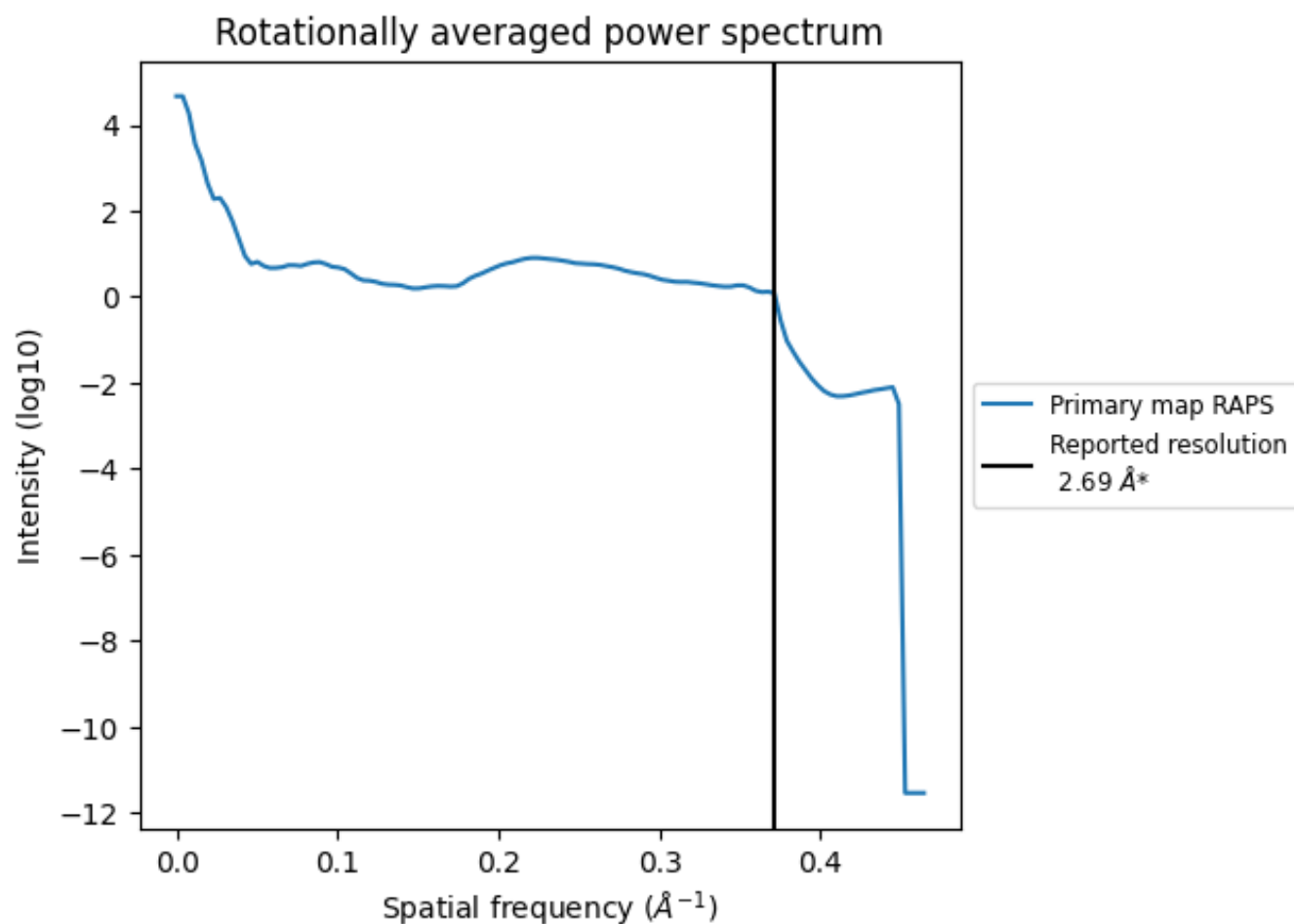
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 159 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.372 Å⁻¹

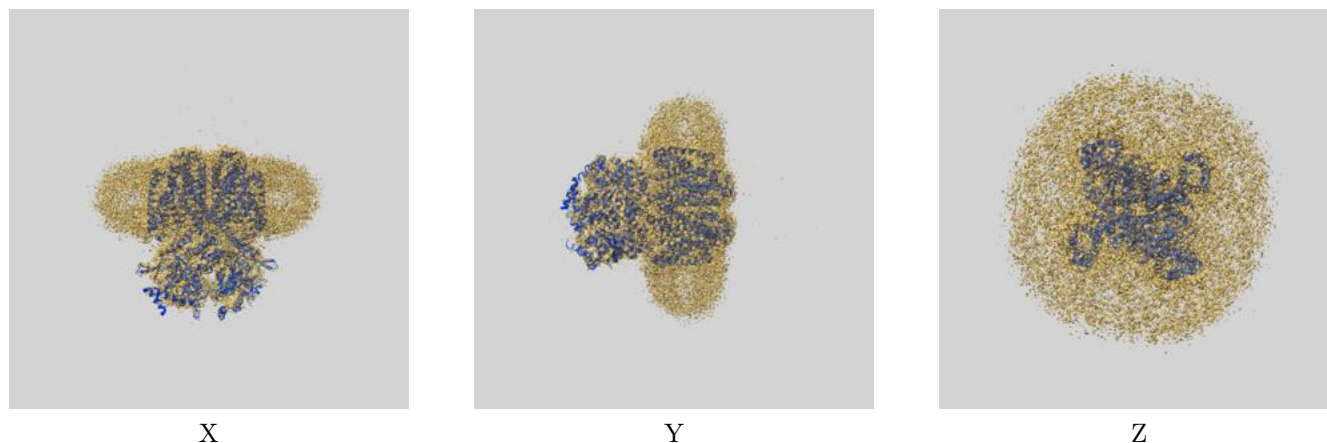
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

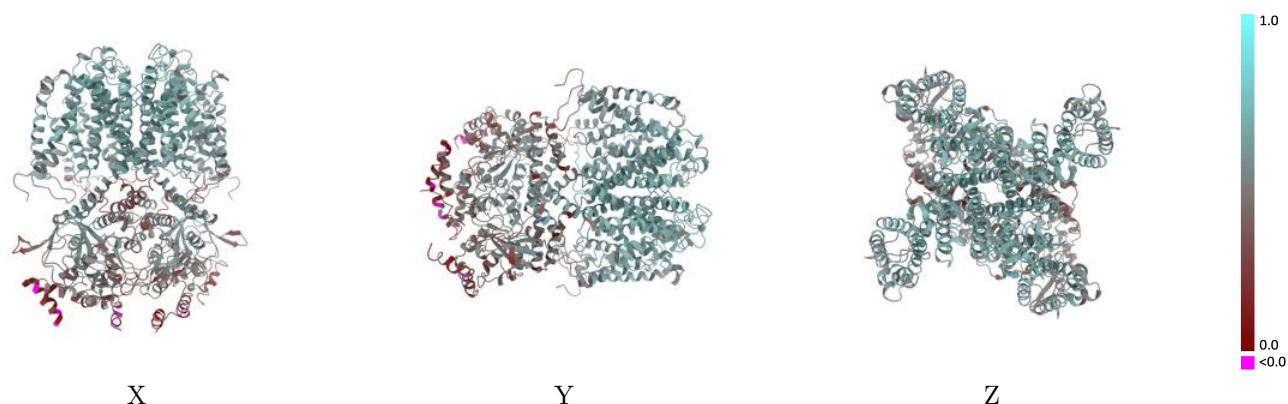
This section contains information regarding the fit between EMDB map EMD-32598 and PDB model 7WM2. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



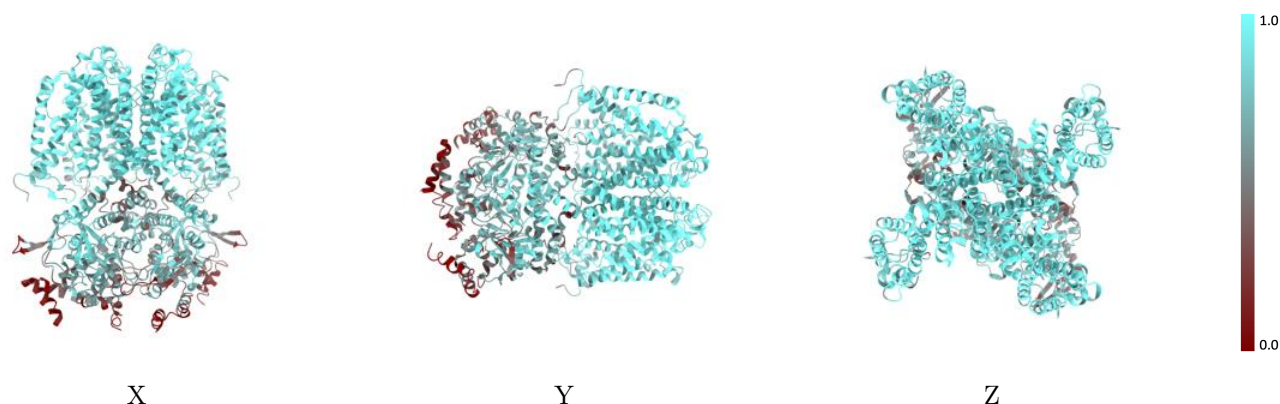
The images above show the 3D surface view of the map at the recommended contour level 0.436 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



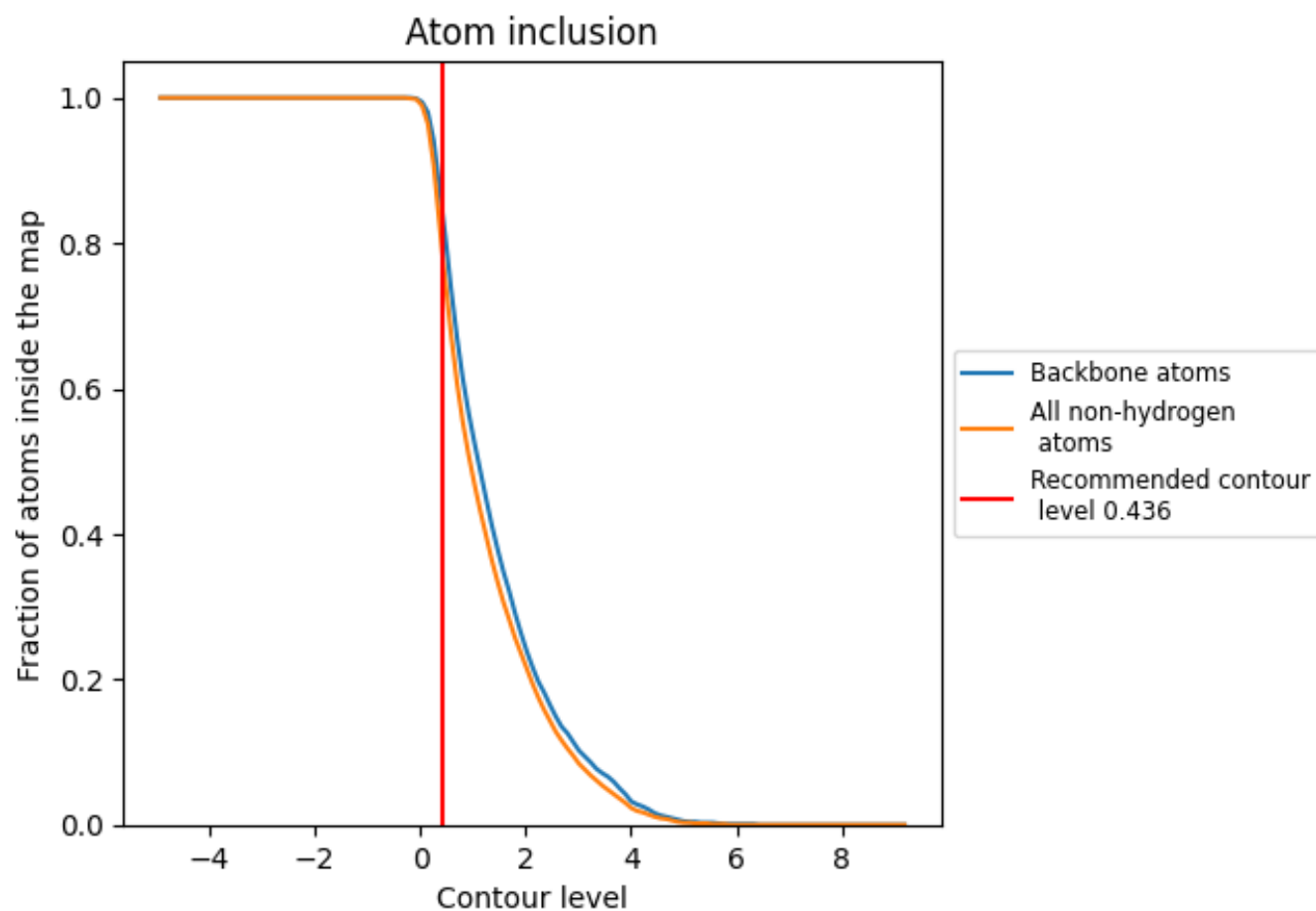
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.436).

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	<div></div> 0.7790	<div></div> 0.5180
A	<div></div> 0.7830	<div></div> 0.5140
B	<div></div> 0.7750	<div></div> 0.5210
C	<div></div> 0.7850	<div></div> 0.5170
D	<div></div> 0.7740	<div></div> 0.5180

