



Full wwPDB EM Validation Report ⓘ

Jun 20, 2024 – 12:21 AM JST

PDB ID : 7WM1
EMDB ID : EMD-32597
Title : Cryo-EM structure of AKT1-AtKC1
Authors : Dongliang, L.; Zijie, Z.; Yannan, Q.; Yuyue, T.; Huaizong, S.
Deposited on : 2022-01-14
Resolution : 2.80 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.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

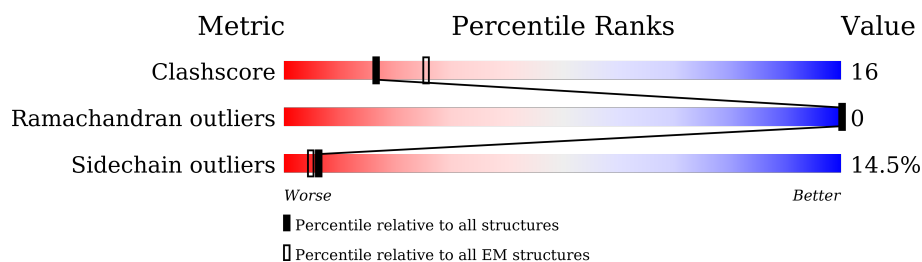
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	885	<div> <div>9%</div> <div>32%</div> <div>13%</div> <div>5%</div> <div>•</div> <div>49%</div> </div>
1	C	885	<div> <div>9%</div> <div>32%</div> <div>13%</div> <div>5%</div> <div>•</div> <div>49%</div> </div>
2	B	690	<div> <div>7%</div> <div>48%</div> <div>18%</div> <div>•</div> <div>31%</div> </div>
2	D	690	<div> <div>7%</div> <div>47%</div> <div>19%</div> <div>•</div> <div>31%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15197 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	449	Total	C	N	O	S	0	0
			3669	2387	623	639	20		
1	C	449	Total	C	N	O	S	0	0
			3669	2387	623	639	20		

There are 56 discrepancies between the modelled and reference sequences:

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

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

- Molecule 2 is a protein called Potassium channel KAT3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	473	Total	C	N	O	S	0	0
			3850	2527	635	672	16		
2	D	473	Total	C	N	O	S	0	0
			3850	2527	635	672	16		

There are 56 discrepancies between the modelled and reference sequences:

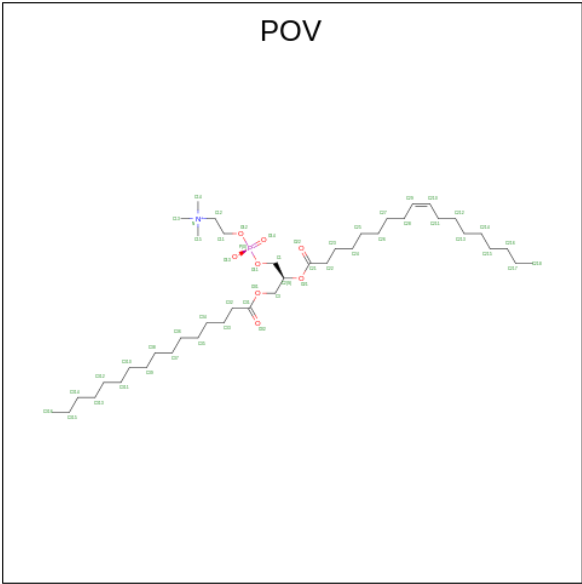
Chain	Residue	Modelled	Actual	Comment	Reference
B	663	LEU	-	expression tag	UNP P92960
B	664	GLU	-	expression tag	UNP P92960
B	665	GLY	-	expression tag	UNP P92960
B	666	SER	-	expression tag	UNP P92960
B	667	ASP	-	expression tag	UNP P92960
B	668	GLU	-	expression tag	UNP P92960
B	669	VAL	-	expression tag	UNP P92960
B	670	ASP	-	expression tag	UNP P92960
B	671	ALA	-	expression tag	UNP P92960
B	672	GLY	-	expression tag	UNP P92960
B	673	SER	-	expression tag	UNP P92960
B	674	ALA	-	expression tag	UNP P92960
B	675	ALA	-	expression tag	UNP P92960
B	676	ALA	-	expression tag	UNP P92960
B	677	SER	-	expression tag	UNP P92960
B	678	GLY	-	expression tag	UNP P92960
B	679	GLY	-	expression tag	UNP P92960
B	680	SER	-	expression tag	UNP P92960
B	681	GLY	-	expression tag	UNP P92960
B	682	SER	-	expression tag	UNP P92960
B	683	TRP	-	expression tag	UNP P92960
B	684	SER	-	expression tag	UNP P92960
B	685	HIS	-	expression tag	UNP P92960
B	686	PRO	-	expression tag	UNP P92960
B	687	GLN	-	expression tag	UNP P92960
B	688	PHE	-	expression tag	UNP P92960
B	689	GLU	-	expression tag	UNP P92960
B	690	LYS	-	expression tag	UNP P92960
D	663	LEU	-	expression tag	UNP P92960
D	664	GLU	-	expression tag	UNP P92960
D	665	GLY	-	expression tag	UNP P92960
D	666	SER	-	expression tag	UNP P92960
D	667	ASP	-	expression tag	UNP P92960
D	668	GLU	-	expression tag	UNP P92960
D	669	VAL	-	expression tag	UNP P92960
D	670	ASP	-	expression tag	UNP P92960
D	671	ALA	-	expression tag	UNP P92960
D	672	GLY	-	expression tag	UNP P92960
D	673	SER	-	expression tag	UNP P92960
D	674	ALA	-	expression tag	UNP P92960
D	675	ALA	-	expression tag	UNP P92960
D	676	ALA	-	expression tag	UNP P92960
D	677	SER	-	expression tag	UNP P92960

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Chain	Residue	Modelled	Actual	Comment	Reference
D	678	GLY	-	expression tag	UNP P92960
D	679	GLY	-	expression tag	UNP P92960
D	680	SER	-	expression tag	UNP P92960
D	681	GLY	-	expression tag	UNP P92960
D	682	SER	-	expression tag	UNP P92960
D	683	TRP	-	expression tag	UNP P92960
D	684	SER	-	expression tag	UNP P92960
D	685	HIS	-	expression tag	UNP P92960
D	686	PRO	-	expression tag	UNP P92960
D	687	GLN	-	expression tag	UNP P92960
D	688	PHE	-	expression tag	UNP P92960
D	689	GLU	-	expression tag	UNP P92960
D	690	LYS	-	expression tag	UNP P92960

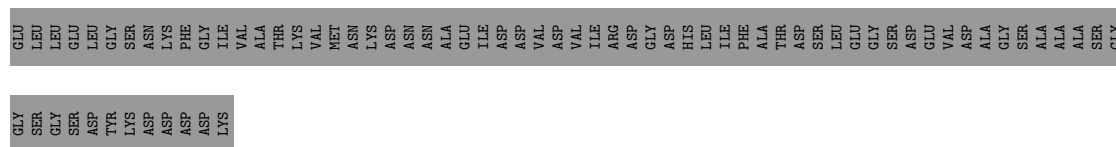
- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (three-letter code: POV) (formula: C₄₂H₈₂NO₈P).



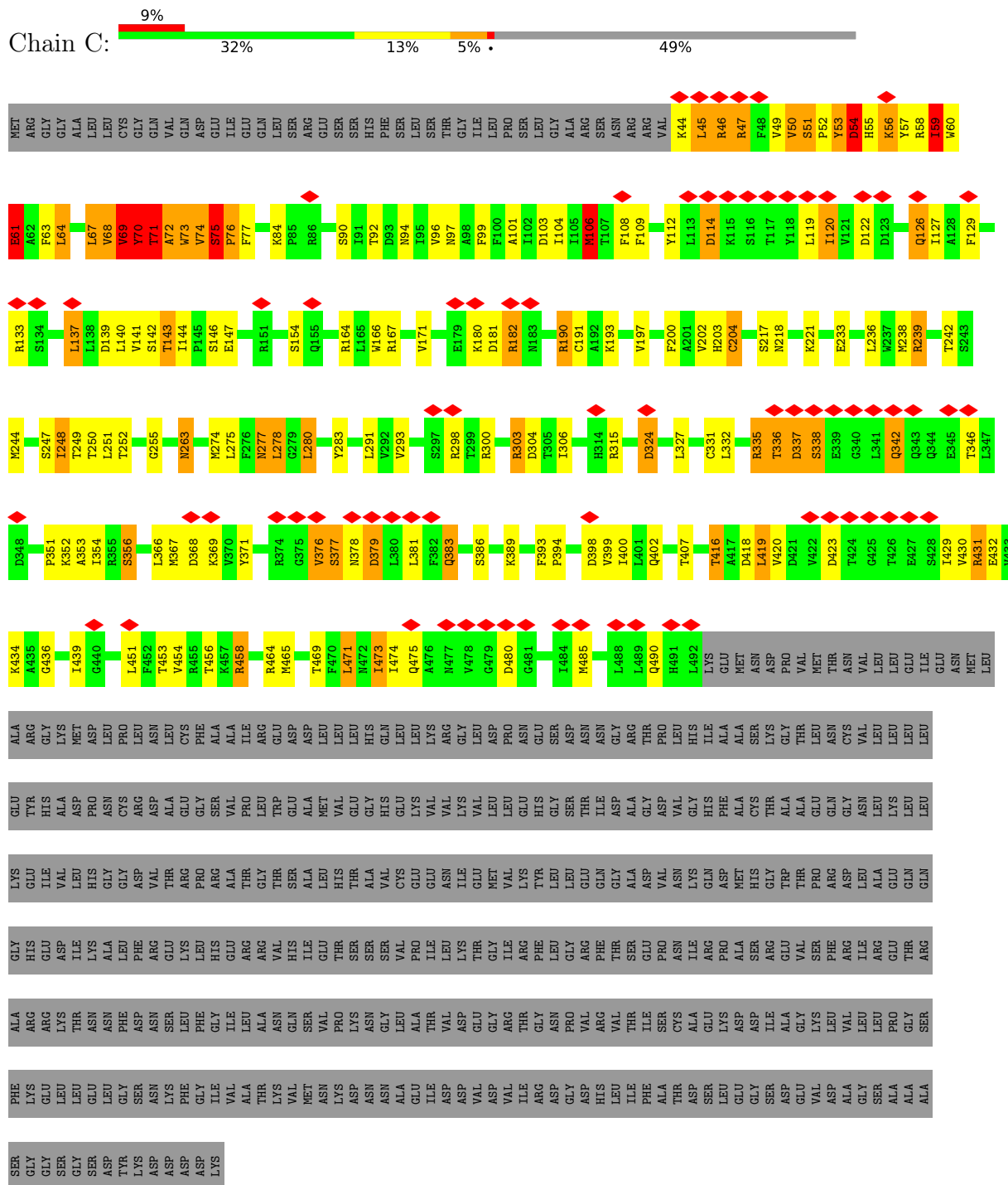
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			39	30	8	1	
3	B	1	Total	C	O	P	0
			39	30	8	1	
3	C	1	Total	C	O	P	0
			39	30	8	1	
3	D	1	Total	C	O	P	0
			39	30	8	1	

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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



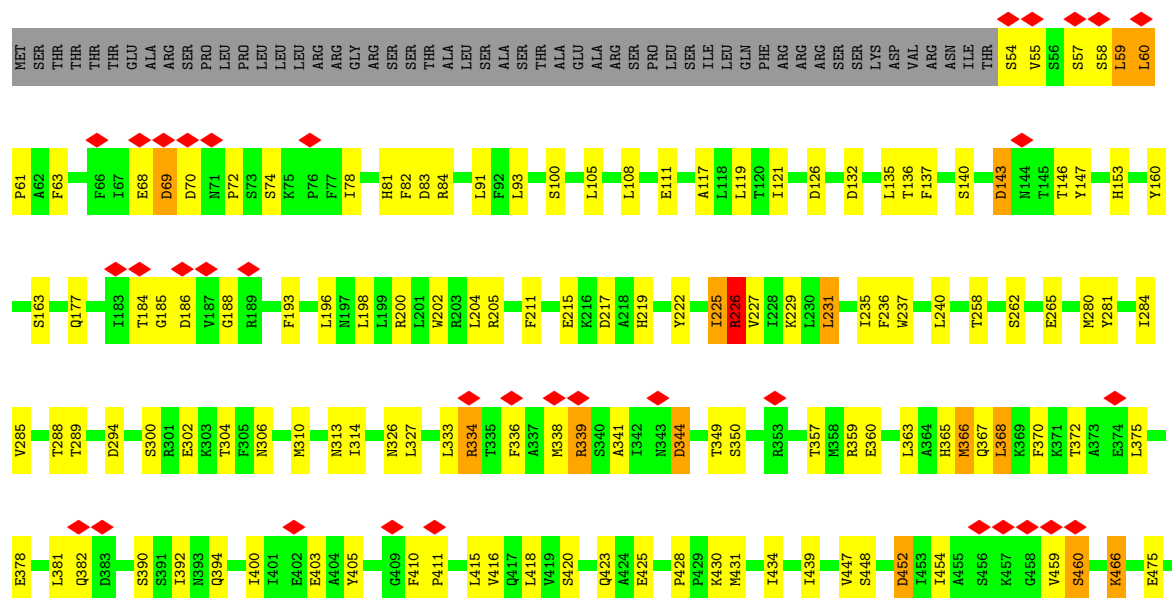
• Molecule 1: Potassium channel AKT1



• Molecule 2: Potassium channel KAT3



- Molecule 2: Potassium channel KAT3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	289326	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	8.034	Depositor
Minimum map value	-5.128	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.144	Depositor
Recommended contour level	0.633	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 [i](#)

5.1 Standard geometry [i](#)

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	0.62	6/3760 (0.2%)	0.76	15/5105 (0.3%)
1	C	0.83	19/3760 (0.5%)	0.80	15/5105 (0.3%)
2	B	0.45	0/3947	0.53	1/5352 (0.0%)
2	D	0.48	1/3947 (0.0%)	0.55	1/5352 (0.0%)
All	All	0.61	26/15414 (0.2%)	0.67	32/20914 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	3
2	B	0	1
All	All	0	6

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	72	ALA	C-O	-13.02	0.98	1.23
1	C	73	TRP	C-O	-12.99	0.98	1.23
1	C	71	THR	C-O	-11.52	1.01	1.23
1	C	77	PHE	C-O	-9.73	1.04	1.23
1	A	61	GLU	CD-OE2	-9.72	1.15	1.25
1	C	75	SER	CA-CB	-9.45	1.38	1.52
1	C	76	PRO	C-O	-9.33	1.04	1.23
2	D	60	LEU	C-N	8.66	1.50	1.34
1	C	74	VAL	C-O	-7.97	1.08	1.23
1	C	68	VAL	C-O	-7.30	1.09	1.23
1	C	61	GLU	CD-OE2	-7.29	1.17	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	ALA	C-O	-7.03	1.09	1.23
1	C	69	VAL	C-O	-6.87	1.10	1.23
1	C	70	TYR	C-O	-6.62	1.10	1.23
1	C	64	LEU	C-O	-6.49	1.11	1.23
1	C	75	SER	CB-OG	-6.28	1.34	1.42
1	C	61	GLU	C-O	-5.89	1.12	1.23
1	C	60	TRP	C-O	-5.67	1.12	1.23
1	C	76	PRO	N-CA	-5.62	1.37	1.47
1	A	247	SER	CA-CB	-5.39	1.44	1.52
1	C	57	TYR	C-O	-5.35	1.13	1.23
1	A	57	TYR	C-O	-5.32	1.13	1.23
1	A	59	ILE	C-O	-5.12	1.13	1.23
1	C	59	ILE	C-O	-5.10	1.13	1.23
1	C	75	SER	C-O	-5.06	1.13	1.23
1	A	332	LEU	C-O	-5.04	1.13	1.23

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	MET	O-C-N	-13.23	101.53	122.70
1	A	57	TYR	CB-CA-C	-11.33	87.75	110.40
1	C	57	TYR	CB-CA-C	-11.32	87.77	110.40
1	C	106	MET	O-C-N	-10.96	105.17	122.70
1	A	106	MET	CA-C-N	8.29	135.44	117.20
1	C	76	PRO	CA-N-CD	-7.78	100.61	111.50
1	C	458	ARG	CG-CD-NE	-7.29	96.49	111.80
1	C	57	TYR	CB-CG-CD1	-7.04	116.77	121.00
1	A	57	TYR	CB-CG-CD1	-7.01	116.79	121.00
1	A	277	ASN	CB-CA-C	-6.92	96.55	110.40
1	C	458	ARG	CB-CA-C	-6.91	96.58	110.40
1	C	106	MET	CA-C-N	6.86	132.29	117.20
1	C	277	ASN	CB-CA-C	-6.86	96.68	110.40
1	A	458	ARG	CB-CA-C	-6.74	96.92	110.40
1	C	126	GLN	O-C-N	-6.45	112.38	122.70
1	C	76	PRO	N-CA-CB	6.40	110.98	103.30
1	A	106	MET	C-N-CA	6.20	137.20	121.70
2	B	65	THR	CA-CB-OG1	-6.11	96.18	109.00
1	C	54	ASP	CB-CA-C	6.11	122.61	110.40
1	A	54	ASP	CB-CA-C	6.10	122.60	110.40
1	A	126	GLN	O-C-N	-5.82	113.38	122.70
2	D	226	ARG	CG-CD-NE	-5.58	100.08	111.80
1	A	198	THR	CB-CA-C	-5.54	96.63	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	THR	CA-CB-OG1	-5.45	97.56	109.00
1	A	283	TYR	CB-CA-C	5.41	121.22	110.40
1	C	58	ARG	CG-CD-NE	-5.26	100.75	111.80
1	C	250	THR	CA-CB-OG1	-5.25	97.98	109.00
1	A	58	ARG	CG-CD-NE	-5.24	100.79	111.80
1	A	122	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	122	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	334	TYR	CB-CA-C	5.18	120.76	110.40
1	C	106	MET	C-N-CA	5.05	134.32	121.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	MET	Mainchain
1	A	61	GLU	Mainchain
2	B	59	LEU	Mainchain
1	C	106	MET	Mainchain
1	C	126	GLN	Mainchain
1	C	72	ALA	Mainchain

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	3669	0	3694	148	0
1	C	3669	0	3695	158	0
2	B	3850	0	3899	95	0
2	D	3850	0	3899	102	0
3	A	39	0	52	1	0
3	B	39	0	52	5	0
3	C	39	0	52	4	0
3	D	39	0	52	5	0
4	A	3	0	0	0	0
All	All	15197	0	15395	479	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 16.

All (479) 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:C:335:ARG:HG2	2:D:147:TYR:OH	1.49	1.13
1:A:458:ARG:HH11	1:A:458:ARG:HB3	1.16	1.09
1:C:112:TYR:CD1	1:C:127:ILE:HG22	1.95	1.02
1:C:56:LYS:H	1:C:56:LYS:HD2	1.31	0.96
1:A:331:CYS:SG	2:B:60:LEU:HD22	2.06	0.96
1:A:56:LYS:H	1:A:56:LYS:HD2	1.32	0.95
1:A:112:TYR:CD1	1:A:127:ILE:HG22	2.04	0.93
1:C:112:TYR:HD1	1:C:127:ILE:HG22	1.29	0.92
1:A:112:TYR:HD1	1:A:127:ILE:HG22	1.35	0.89
1:A:47:ARG:HG3	1:A:47:ARG:HH11	1.38	0.88
1:C:47:ARG:HH11	1:C:47:ARG:HG3	1.37	0.88
1:C:68:VAL:HG22	1:C:167:ARG:O	1.76	0.86
1:C:280:LEU:HD12	1:C:280:LEU:O	1.76	0.85
2:D:68:GLU:HG3	2:D:69:ASP:H	1.41	0.85
1:A:108:PHE:O	1:A:127:ILE:HD11	1.76	0.84
1:A:278:LEU:HD12	1:A:278:LEU:O	1.77	0.83
2:D:344:ASP:OD1	2:D:344:ASP:N	2.08	0.83
2:B:68:GLU:HG3	2:B:69:ASP:H	1.41	0.83
2:D:334:ARG:HG3	2:D:334:ARG:HH11	1.44	0.82
1:A:280:LEU:HD12	1:A:280:LEU:O	1.79	0.81
1:C:335:ARG:HD3	1:C:335:ARG:N	1.92	0.81
1:C:47:ARG:HH11	1:C:47:ARG:H	1.29	0.80
1:A:47:ARG:HH11	1:A:47:ARG:H	1.29	0.80
2:B:60:LEU:HD12	2:B:60:LEU:O	1.83	0.78
2:D:334:ARG:HG3	2:D:334:ARG:NH1	1.98	0.78
1:C:251:LEU:HA	1:C:277:ASN:ND2	1.98	0.78
1:A:47:ARG:HG3	1:A:47:ARG:NH1	1.98	0.77
1:A:336:THR:HG23	1:A:342:GLN:HB2	1.66	0.76
2:B:60:LEU:N	2:B:61:PRO:HD2	2.00	0.76
1:A:458:ARG:HH11	1:A:458:ARG:CB	1.95	0.76
1:C:47:ARG:HG3	1:C:47:ARG:NH1	1.98	0.75
2:D:215:GLU:HG2	2:D:225:ILE:HD11	1.69	0.75
1:A:56:LYS:H	1:A:56:LYS:CD	1.97	0.75
1:A:45:LEU:O	1:A:45:LEU:HD12	1.86	0.74
1:A:336:THR:CG2	1:A:342:GLN:HB2	2.17	0.74
1:C:45:LEU:HD12	1:C:45:LEU:O	1.86	0.74
2:D:466:LYS:HB3	2:D:491:ARG:HH12	1.53	0.74
2:B:452:ASP:OD1	2:B:452:ASP:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:PHE:O	1:C:127:ILE:HD11	1.89	0.73
2:B:466:LYS:HB3	2:B:491:ARG:HH12	1.53	0.73
2:B:226:ARG:HG3	2:B:226:ARG:HH11	1.53	0.73
1:C:197:VAL:HG12	3:C:901:POV:H35A	1.70	0.72
1:A:458:ARG:HB3	1:A:458:ARG:NH1	2.00	0.72
1:C:331:CYS:SG	2:D:60:LEU:HD22	2.30	0.72
1:C:46:ARG:CG	1:C:46:ARG:HH11	2.03	0.71
1:C:56:LYS:H	1:C:56:LYS:CD	1.98	0.71
1:C:431:ARG:HB2	1:C:431:ARG:HH21	1.55	0.71
1:C:336:THR:HG23	1:C:342:GLN:HB2	1.72	0.71
1:A:46:ARG:HH11	1:A:46:ARG:CG	2.03	0.71
2:B:229:LYS:CE	3:B:701:POV:O32	2.39	0.71
2:D:452:ASP:OD1	2:D:452:ASP:N	2.21	0.71
3:B:701:POV:H1A	3:B:701:POV:O22	1.91	0.70
1:A:46:ARG:HH11	1:A:46:ARG:HG3	1.56	0.70
2:B:59:LEU:C	2:B:59:LEU:HD23	2.12	0.70
1:C:46:ARG:HH11	1:C:46:ARG:HG3	1.56	0.70
1:C:335:ARG:CG	2:D:147:TYR:OH	2.36	0.70
1:C:429:ILE:HD12	1:C:429:ILE:N	2.06	0.70
1:A:280:LEU:HD12	1:A:280:LEU:C	2.12	0.69
2:D:59:LEU:C	2:D:59:LEU:HD23	2.12	0.69
2:B:68:GLU:HG3	2:B:69:ASP:N	2.08	0.69
1:C:249:THR:CG2	1:C:255:GLY:H	2.06	0.69
1:A:51:SER:HB3	1:A:52:PRO:HD2	1.75	0.69
1:A:331:CYS:SG	2:B:60:LEU:CD2	2.79	0.69
1:C:139:ASP:OD1	1:C:166:TRP:NE1	2.26	0.69
1:C:278:LEU:C	1:C:278:LEU:HD12	2.13	0.69
1:C:280:LEU:HD12	1:C:280:LEU:C	2.12	0.69
1:A:331:CYS:HG	2:B:60:LEU:HD22	1.56	0.69
1:A:139:ASP:OD1	1:A:166:TRP:NE1	2.26	0.68
1:A:418:ASP:HA	1:A:432:GLU:HA	1.76	0.68
1:C:278:LEU:HD12	1:C:278:LEU:O	1.94	0.68
1:A:429:ILE:HD12	1:A:429:ILE:N	2.07	0.68
1:C:335:ARG:HG2	2:D:147:TYR:HH	1.59	0.68
1:C:336:THR:CG2	1:C:342:GLN:HB2	2.23	0.68
1:C:112:TYR:CE1	1:C:127:ILE:HG22	2.29	0.67
2:D:68:GLU:HG3	2:D:69:ASP:N	2.08	0.67
2:B:229:LYS:HE2	3:B:701:POV:O32	1.95	0.67
2:B:60:LEU:N	2:B:61:PRO:CD	2.59	0.66
1:C:67:LEU:HD21	1:C:99:PHE:HD2	1.59	0.66
2:D:63:PHE:HE2	2:D:91:LEU:HD22	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:VAL:CG2	1:C:167:ARG:O	2.44	0.66
1:C:67:LEU:HG	1:C:96:VAL:HG13	1.76	0.66
1:A:251:LEU:HD23	1:A:251:LEU:C	2.16	0.66
2:D:222:TYR:O	2:D:226:ARG:HB2	1.95	0.66
1:A:251:LEU:HA	1:A:277:ASN:ND2	2.11	0.66
1:C:61:GLU:N	1:C:61:GLU:OE2	2.29	0.66
1:C:251:LEU:C	1:C:251:LEU:HD23	2.16	0.66
2:B:288:THR:O	2:B:289:THR:OG1	2.14	0.65
2:D:288:THR:O	2:D:289:THR:OG1	2.14	0.65
1:A:108:PHE:O	1:A:127:ILE:CD1	2.45	0.65
1:A:251:LEU:HD23	1:A:251:LEU:O	1.97	0.65
1:C:335:ARG:HD3	1:C:335:ARG:H	1.62	0.65
2:D:60:LEU:HD12	2:D:60:LEU:O	1.97	0.65
1:C:332:LEU:HD13	1:C:394:PRO:HD3	1.78	0.65
2:D:60:LEU:N	2:D:61:PRO:CD	2.61	0.64
1:A:278:LEU:HD12	1:A:278:LEU:C	2.14	0.64
1:A:332:LEU:HD13	1:A:394:PRO:HD3	1.78	0.64
2:B:434:ILE:HG21	2:B:484:GLN:HG2	1.79	0.64
1:A:469:THR:O	1:A:473:ILE:HG22	1.98	0.64
1:C:429:ILE:HD12	1:C:429:ILE:H	1.62	0.64
2:B:226:ARG:HG3	2:B:226:ARG:NH1	2.08	0.64
1:C:332:LEU:HD12	1:C:394:PRO:HB3	1.80	0.63
2:D:434:ILE:HG21	2:D:484:GLN:HG2	1.79	0.63
1:C:469:THR:O	1:C:473:ILE:HG22	1.98	0.63
1:A:94:ASN:ND2	1:A:147:GLU:OE1	2.31	0.63
1:A:190:ARG:NH1	1:A:190:ARG:HG2	2.12	0.63
1:C:251:LEU:HD23	1:C:251:LEU:O	1.98	0.62
1:A:429:ILE:HD12	1:A:429:ILE:H	1.65	0.62
1:A:244:MET:O	1:A:248:ILE:HG12	2.00	0.62
1:C:431:ARG:HB2	1:C:431:ARG:NH2	2.14	0.62
1:C:249:THR:HG23	1:C:255:GLY:H	1.66	0.61
1:C:244:MET:O	1:C:248:ILE:HG12	2.00	0.61
2:D:338:MET:SD	2:D:370:PHE:HD2	2.23	0.61
1:C:252:THR:HG22	2:D:314:ILE:HD11	1.82	0.60
2:B:229:LYS:HE3	3:B:701:POV:O32	2.00	0.60
2:D:184:THR:HG22	2:D:185:GLY:H	1.67	0.60
2:D:225:ILE:HD12	2:D:225:ILE:C	2.21	0.60
2:D:59:LEU:HD23	2:D:59:LEU:O	2.02	0.60
2:B:184:THR:HG22	2:B:185:GLY:H	1.67	0.60
1:C:51:SER:OG	1:C:52:PRO:HD2	2.02	0.60
1:C:429:ILE:H	1:C:429:ILE:CD1	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ASN:ND2	1:C:147:GLU:OE1	2.31	0.59
1:C:68:VAL:HG11	1:C:171:VAL:HG23	1.85	0.59
2:D:339:ARG:CG	2:D:339:ARG:HH21	2.14	0.59
1:A:190:ARG:HG2	1:A:190:ARG:HH11	1.67	0.59
2:B:59:LEU:HD23	2:B:59:LEU:O	2.02	0.59
1:C:200:PHE:O	1:C:204:CYS:HB2	2.03	0.59
1:C:337:ASP:HB2	1:C:342:GLN:O	2.03	0.58
1:A:416:THR:HG22	1:A:434:LYS:HA	1.84	0.58
1:C:416:THR:HG22	1:C:434:LYS:HA	1.84	0.58
1:A:429:ILE:H	1:A:429:ILE:CD1	2.16	0.58
1:C:190:ARG:HG2	1:C:291:LEU:HD11	1.86	0.58
1:A:190:ARG:HH11	1:A:190:ARG:CG	2.14	0.58
2:D:237:TRP:CD1	2:D:240:LEU:HD23	2.39	0.58
2:B:466:LYS:HG2	2:B:491:ARG:HH22	1.69	0.58
1:A:451:LEU:H	1:A:451:LEU:HD23	1.69	0.58
2:D:363:LEU:O	2:D:367:GLN:HG2	2.04	0.58
1:A:97:ASN:HD21	1:A:164:ARG:HH21	1.51	0.57
1:A:200:PHE:O	1:A:204:CYS:HB2	2.03	0.57
1:C:74:VAL:O	1:C:74:VAL:HG12	2.03	0.57
1:C:97:ASN:HD21	1:C:164:ARG:HH21	1.51	0.57
2:B:237:TRP:CD1	2:B:240:LEU:HD23	2.39	0.57
1:C:249:THR:CG2	1:C:255:GLY:N	2.68	0.57
1:A:252:THR:HG22	2:B:314:ILE:HD11	1.86	0.57
1:A:61:GLU:OE2	1:A:61:GLU:N	2.38	0.57
2:B:363:LEU:O	2:B:367:GLN:HG2	2.04	0.57
1:C:143:THR:O	1:C:143:THR:OG1	2.23	0.57
2:D:466:LYS:HG2	2:D:491:ARG:HH22	1.69	0.57
2:B:502:HIS:HD2	2:D:439:ILE:HG12	1.70	0.56
1:C:451:LEU:HD23	1:C:451:LEU:H	1.69	0.56
2:B:365:HIS:CE1	1:C:351:PRO:HD3	2.41	0.56
2:B:439:ILE:HG12	2:D:502:HIS:HD2	1.70	0.56
2:D:60:LEU:N	2:D:61:PRO:HD3	2.19	0.56
2:D:63:PHE:CE2	2:D:91:LEU:HD22	2.39	0.56
2:D:334:ARG:HH11	2:D:334:ARG:CG	2.14	0.56
2:B:219:HIS:O	2:B:219:HIS:ND1	2.39	0.56
1:C:249:THR:CG2	1:C:255:GLY:HA2	2.36	0.56
1:C:471:LEU:O	1:C:475:GLN:HB2	2.06	0.56
3:C:901:POV:O22	3:C:901:POV:H24	2.06	0.56
1:C:389:LYS:HD3	1:C:464:ARG:NH1	2.21	0.55
1:A:471:LEU:O	1:A:475:GLN:HB2	2.06	0.55
2:B:258:THR:O	2:B:262:SER:OG	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:TRP:HD1	3:C:901:POV:H315	1.71	0.55
1:A:389:LYS:HD3	1:A:464:ARG:NH1	2.21	0.55
1:C:64:LEU:HD21	1:C:103:ASP:HB2	1.87	0.55
1:C:120:ILE:HG12	1:C:120:ILE:O	2.06	0.55
1:A:120:ILE:HG12	1:A:120:ILE:O	2.06	0.55
2:B:62:ALA:HB2	2:B:213:ARG:O	2.07	0.55
2:D:219:HIS:O	2:D:219:HIS:ND1	2.39	0.55
1:C:50:VAL:HG23	1:C:109:PHE:O	2.06	0.54
1:C:351:PRO:HD2	1:C:354:ILE:HD12	1.88	0.54
2:D:215:GLU:HG2	2:D:225:ILE:CD1	2.34	0.54
1:A:67:LEU:HD21	1:A:99:PHE:HD2	1.72	0.54
2:B:237:TRP:HD1	2:B:240:LEU:HD23	1.73	0.54
2:B:236:PHE:HB2	3:B:701:POV:H310	1.90	0.54
2:B:381:LEU:HD11	2:B:392:ILE:HD12	1.90	0.54
1:A:402:GLN:N	1:A:453:THR:OG1	2.41	0.54
1:C:402:GLN:N	1:C:453:THR:OG1	2.41	0.54
1:A:332:LEU:HD12	1:A:394:PRO:HB3	1.89	0.54
1:A:175:PHE:CD1	1:A:193:LYS:HB2	2.42	0.54
1:A:351:PRO:HD2	1:A:354:ILE:HD12	1.88	0.54
2:B:400:ILE:HG21	2:B:447:VAL:HG12	1.90	0.54
2:D:411:PRO:HD3	2:D:515:ASP:HB3	1.90	0.54
1:A:75:SER:CB	1:A:76:PRO:HD3	2.37	0.54
1:A:112:TYR:CE1	1:A:127:ILE:HG22	2.40	0.54
1:C:53:TYR:CD1	1:C:53:TYR:N	2.76	0.54
2:B:349:THR:HG21	2:B:359:ARG:HB2	1.90	0.53
1:A:278:LEU:HD22	2:D:288:THR:HG22	1.91	0.53
1:C:429:ILE:N	1:C:429:ILE:CD1	2.72	0.53
2:D:237:TRP:HD1	2:D:240:LEU:HD23	1.73	0.53
2:D:381:LEU:HD11	2:D:392:ILE:HD12	1.90	0.53
2:B:285:VAL:HA	1:C:274:MET:HE1	1.89	0.53
1:C:51:SER:CB	1:C:52:PRO:HD2	2.38	0.53
2:D:334:ARG:HD3	2:D:334:ARG:N	2.23	0.53
1:A:429:ILE:N	1:A:429:ILE:CD1	2.72	0.53
2:D:349:THR:HG21	2:D:359:ARG:HB2	1.90	0.53
2:B:411:PRO:HD3	2:B:515:ASP:HB3	1.90	0.53
1:C:46:ARG:CG	1:C:46:ARG:NH1	2.70	0.52
1:A:249:THR:HG23	1:A:255:GLY:H	1.75	0.52
1:A:379:ASP:O	1:A:383:GLN:HG3	2.10	0.52
1:C:164:ARG:O	1:C:167:ARG:HG2	2.09	0.52
2:D:117:ALA:O	2:D:121:ILE:HG12	2.09	0.52
2:B:117:ALA:O	2:B:121:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:344:ASP:OD1	2:B:344:ASP:N	2.42	0.52
2:D:126:ASP:OD2	2:D:200:ARG:NH2	2.40	0.52
1:A:459:LEU:O	1:A:459:LEU:HG	2.03	0.52
2:D:258:THR:O	2:D:262:SER:OG	2.25	0.52
1:A:71:THR:O	1:A:75:SER:HB2	2.09	0.52
1:A:164:ARG:O	1:A:167:ARG:HG2	2.09	0.52
1:C:249:THR:HG23	1:C:255:GLY:N	2.24	0.52
1:A:46:ARG:NH1	1:A:46:ARG:CB	2.73	0.52
1:A:398:ASP:N	1:A:398:ASP:OD1	2.43	0.52
2:B:126:ASP:OD2	2:B:200:ARG:NH2	2.40	0.52
1:C:431:ARG:NH2	1:C:431:ARG:CB	2.73	0.52
1:C:46:ARG:NH1	1:C:46:ARG:CB	2.73	0.52
1:C:137:LEU:HA	1:C:140:LEU:HB3	1.92	0.52
1:C:379:ASP:O	1:C:383:GLN:HG3	2.10	0.52
1:A:190:ARG:NH1	1:A:190:ARG:CG	2.73	0.51
1:C:108:PHE:O	1:C:127:ILE:CD1	2.57	0.51
1:A:46:ARG:NH1	1:A:46:ARG:CA	2.73	0.51
2:B:60:LEU:H	2:B:61:PRO:HD2	1.75	0.51
1:C:46:ARG:NH1	1:C:46:ARG:CA	2.73	0.51
1:C:293:VAL:HG12	2:D:326:ASN:HB2	1.91	0.51
2:B:302:GLU:O	2:B:306:ASN:HB2	2.10	0.51
2:D:400:ILE:HG21	2:D:447:VAL:HG12	1.90	0.51
1:A:53:TYR:N	1:A:53:TYR:CD1	2.76	0.51
1:C:249:THR:HG22	1:C:255:GLY:H	1.75	0.51
1:A:51:SER:CB	1:A:52:PRO:HD2	2.38	0.51
2:B:416:VAL:O	2:B:420:SER:OG	2.27	0.51
1:C:70:TYR:CD1	1:C:70:TYR:C	2.83	0.51
1:A:351:PRO:HD3	2:D:365:HIS:CE1	2.46	0.51
1:C:70:TYR:O	1:C:70:TYR:CG	2.63	0.51
1:C:393:PHE:CE2	1:C:399:VAL:HG12	2.46	0.51
3:A:901:POV:O22	3:A:901:POV:H1A	2.11	0.51
1:C:46:ARG:NH1	1:C:46:ARG:N	2.59	0.51
1:C:439:ILE:HD12	1:C:454:VAL:HG21	1.93	0.51
2:D:70:ASP:OD1	2:D:72:PRO:HD3	2.11	0.51
2:D:339:ARG:CG	2:D:339:ARG:NH2	2.72	0.51
1:A:114:ASP:OD1	1:A:114:ASP:N	2.44	0.51
1:A:218:ASN:HD22	1:A:221:LYS:HE2	1.76	0.50
1:A:191:CYS:SG	1:A:192:ALA:N	2.84	0.50
1:A:393:PHE:CE2	1:A:399:VAL:HG12	2.46	0.50
2:D:302:GLU:O	2:D:306:ASN:HB2	2.10	0.50
1:A:439:ILE:HD12	1:A:454:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:143:ASP:OD1	2:D:143:ASP:N	2.45	0.50
2:D:300:SER:O	2:D:304:THR:OG1	2.22	0.50
1:A:64:LEU:HD21	1:A:103:ASP:HB2	1.93	0.50
1:A:137:LEU:HA	1:A:140:LEU:HB3	1.93	0.50
1:A:143:THR:O	1:A:143:THR:OG1	2.23	0.50
1:A:249:THR:CG2	1:A:255:GLY:HA2	2.42	0.50
1:A:303:ARG:NH2	2:B:217:ASP:O	2.45	0.50
1:A:335:ARG:HB3	2:B:147:TYR:OH	2.12	0.50
2:B:70:ASP:OD1	2:B:72:PRO:HD3	2.11	0.50
2:B:105:LEU:HD13	2:B:240:LEU:HA	1.93	0.50
1:C:202:VAL:HG23	1:C:251:LEU:HD13	1.94	0.50
1:A:190:ARG:O	1:A:190:ARG:HD3	2.11	0.50
1:A:293:VAL:HG12	2:B:326:ASN:HB2	1.93	0.50
1:A:191:CYS:HA	1:A:194:LEU:HD12	1.93	0.50
1:C:56:LYS:CD	1:C:56:LYS:N	2.72	0.50
1:C:398:ASP:N	1:C:398:ASP:OD1	2.43	0.49
2:B:300:SER:O	2:B:304:THR:OG1	2.22	0.49
1:C:193:LYS:HE2	3:C:901:POV:H3	1.94	0.49
1:C:249:THR:CG2	1:C:255:GLY:CA	2.90	0.49
1:A:46:ARG:NH1	1:A:46:ARG:N	2.59	0.49
2:D:339:ARG:HH21	2:D:339:ARG:HG3	1.77	0.49
2:D:105:LEU:HD13	2:D:240:LEU:HA	1.93	0.49
2:D:416:VAL:O	2:D:420:SER:OG	2.27	0.49
1:C:59:ILE:N	1:C:59:ILE:HD13	2.28	0.49
2:B:281:TYR:O	2:B:285:VAL:HG13	2.13	0.49
2:D:281:TYR:O	2:D:285:VAL:HG13	2.13	0.49
1:C:137:LEU:O	1:C:141:VAL:HG22	2.13	0.49
2:D:294:ASP:OD1	2:D:294:ASP:N	2.46	0.49
1:A:180:LYS:HB3	1:A:180:LYS:HE2	1.53	0.48
2:B:62:ALA:CB	2:B:213:ARG:O	2.61	0.48
1:A:59:ILE:N	1:A:59:ILE:HD13	2.28	0.48
1:C:202:VAL:CG2	1:C:251:LEU:HD13	2.42	0.48
1:C:218:ASN:HD22	1:C:221:LYS:HE2	1.76	0.48
2:B:60:LEU:H	2:B:61:PRO:CD	2.25	0.48
3:D:701:POV:C1	3:D:701:POV:C31	2.89	0.48
1:A:458:ARG:CB	1:A:458:ARG:NH1	2.69	0.48
2:D:334:ARG:N	2:D:334:ARG:CD	2.72	0.48
1:A:50:VAL:HG12	1:A:54:ASP:OD2	2.13	0.48
2:B:143:ASP:N	2:B:143:ASP:OD1	2.45	0.48
1:C:114:ASP:OD1	1:C:114:ASP:N	2.45	0.48
1:C:249:THR:HG22	1:C:255:GLY:HA2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:MET:O	1:A:242:THR:HG22	2.14	0.48
1:A:129:PHE:O	1:A:133:ARG:HG2	2.14	0.48
1:A:202:VAL:HG11	1:A:248:ILE:HD13	1.96	0.48
1:C:59:ILE:N	1:C:59:ILE:CD1	2.77	0.48
1:C:70:TYR:CE1	1:C:96:VAL:HG21	2.49	0.48
1:C:303:ARG:NH2	2:D:217:ASP:O	2.47	0.48
2:D:202:TRP:O	2:D:205:ARG:HG2	2.13	0.48
1:A:274:MET:HE1	2:D:285:VAL:HA	1.96	0.48
1:C:418:ASP:HA	1:C:432:GLU:HA	1.95	0.48
2:D:111:GLU:O	2:D:111:GLU:HG2	2.14	0.48
2:B:202:TRP:O	2:B:205:ARG:HG2	2.13	0.48
1:C:50:VAL:HG12	1:C:54:ASP:OD2	2.13	0.48
1:C:238:MET:O	1:C:242:THR:HG22	2.14	0.48
1:C:74:VAL:O	1:C:74:VAL:CG1	2.61	0.47
3:D:701:POV:C31	3:D:701:POV:H1A	2.43	0.47
1:A:137:LEU:O	1:A:141:VAL:HG22	2.13	0.47
1:C:244:MET:O	1:C:248:ILE:CG1	2.62	0.47
1:C:379:ASP:OD1	1:C:379:ASP:N	2.40	0.47
2:B:294:ASP:N	2:B:294:ASP:OD1	2.46	0.47
2:B:226:ARG:NH1	2:B:226:ARG:CG	2.72	0.47
1:C:129:PHE:O	1:C:133:ARG:HG2	2.14	0.47
1:C:101:ALA:HA	1:C:104:ILE:HG12	1.97	0.47
1:A:202:VAL:HG11	1:A:248:ILE:CD1	2.45	0.47
1:C:47:ARG:HG3	1:C:47:ARG:H	1.53	0.47
2:D:341:ALA:CB	2:D:366:MET:HE1	2.45	0.47
2:D:81:HIS:HD2	2:D:140:SER:HB2	1.80	0.47
1:C:366:LEU:HD11	1:C:436:GLY:HA2	1.96	0.47
2:B:111:GLU:HG2	2:B:111:GLU:O	2.14	0.47
1:C:45:LEU:HD12	1:C:45:LEU:C	2.36	0.46
1:C:393:PHE:CD2	1:C:399:VAL:HG12	2.50	0.46
1:A:236:LEU:HD13	1:A:239:ARG:HH11	1.80	0.46
1:C:46:ARG:HH11	1:C:46:ARG:CB	2.29	0.46
1:C:480:ASP:OD1	1:C:480:ASP:N	2.48	0.46
1:A:59:ILE:HD12	1:A:59:ILE:HA	1.68	0.46
1:A:181:ASP:OD1	1:A:182:ARG:N	2.49	0.46
1:A:202:VAL:CG2	1:A:251:LEU:HD13	2.46	0.46
1:A:366:LEU:HD11	1:A:436:GLY:HA2	1.96	0.46
1:C:324:ASP:HB2	2:D:57:SER:OG	2.15	0.46
1:A:324:ASP:HB2	2:B:57:SER:OG	2.15	0.46
1:A:393:PHE:CD2	1:A:399:VAL:HG12	2.50	0.46
2:B:81:HIS:HD2	2:B:140:SER:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:LEU:HD13	1:C:239:ARG:HH11	1.80	0.46
1:C:352:LYS:O	1:C:356:SER:HB3	2.16	0.46
1:A:46:ARG:CG	1:A:46:ARG:NH1	2.70	0.46
1:A:59:ILE:N	1:A:59:ILE:CD1	2.77	0.46
2:B:160:TYR:O	2:B:163:SER:OG	2.30	0.46
2:B:215:GLU:HG2	2:B:225:ILE:HD13	1.96	0.46
2:B:430:LYS:NZ	1:C:353:ALA:HB3	2.30	0.46
2:B:310:MET:HA	2:B:313:ASN:HB2	1.98	0.46
1:C:181:ASP:OD1	1:C:182:ARG:N	2.49	0.46
1:A:101:ALA:HA	1:A:104:ILE:HG12	1.97	0.45
2:B:186:ASP:OD1	2:B:186:ASP:N	2.42	0.45
1:A:419:LEU:HD13	1:A:431:ARG:HH11	1.82	0.45
1:A:419:LEU:HD13	1:A:431:ARG:NH1	2.31	0.45
1:A:44:LYS:HB2	1:A:44:LYS:NZ	2.32	0.45
2:B:61:PRO:O	2:B:61:PRO:HG2	2.16	0.45
1:C:218:ASN:ND2	1:C:221:LYS:HE2	2.31	0.45
2:D:284:ILE:O	2:D:288:THR:OG1	2.27	0.45
2:B:475:GLU:O	2:B:479:VAL:HG23	2.17	0.45
1:C:44:LYS:HB2	1:C:44:LYS:NZ	2.32	0.45
2:D:186:ASP:OD1	2:D:186:ASP:N	2.42	0.45
1:A:218:ASN:ND2	1:A:221:LYS:HE2	2.31	0.45
2:B:188:GLY:HA3	2:B:193:PHE:CE1	2.52	0.45
1:A:190:ARG:C	1:A:190:ARG:CD	2.85	0.45
1:C:144:ILE:O	1:C:164:ARG:NH2	2.35	0.45
2:D:475:GLU:O	2:D:479:VAL:HG23	2.16	0.45
1:A:202:VAL:HG23	1:A:251:LEU:HD13	1.98	0.45
1:A:352:LYS:O	1:A:356:SER:HB3	2.16	0.45
2:D:502:HIS:O	2:D:506:GLU:HG3	2.17	0.45
2:D:236:PHE:HB2	3:D:701:POV:H31C	1.98	0.45
1:A:249:THR:CG2	1:A:255:GLY:H	2.30	0.44
2:B:502:HIS:O	2:B:506:GLU:HG3	2.17	0.44
1:A:46:ARG:HH11	1:A:46:ARG:CB	2.29	0.44
1:C:71:THR:O	1:C:71:THR:CG2	2.65	0.44
2:D:188:GLY:HA3	2:D:193:PHE:CE1	2.52	0.44
1:C:68:VAL:O	1:C:68:VAL:CG1	2.66	0.44
2:D:83:ASP:OD1	2:D:84:ARG:N	2.50	0.44
2:D:310:MET:HA	2:D:313:ASN:HB2	1.98	0.44
2:B:368:LEU:HD12	2:B:368:LEU:HA	1.81	0.44
1:C:376:VAL:HG23	1:C:377:SER:H	1.82	0.44
2:D:60:LEU:H	2:D:61:PRO:HD3	1.83	0.44
1:A:45:LEU:HD12	1:A:45:LEU:C	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:PRO:HG2	1:A:53:TYR:HD1	1.83	0.44
1:A:334:TYR:CD1	1:A:334:TYR:N	2.84	0.44
1:C:52:PRO:HG2	1:C:53:TYR:HD1	1.83	0.44
2:D:231:LEU:O	2:D:235:ILE:HG23	2.17	0.44
2:B:231:LEU:O	2:B:235:ILE:HG23	2.18	0.44
1:A:92:THR:O	1:A:96:VAL:HG23	2.17	0.44
1:A:249:THR:HG23	1:A:255:GLY:N	2.33	0.44
1:A:376:VAL:HG23	1:A:377:SER:H	1.82	0.44
1:C:399:VAL:HG23	1:C:400:ILE:HG13	2.00	0.44
1:C:53:TYR:N	1:C:53:TYR:HD1	2.16	0.43
1:A:72:ALA:HB2	1:A:168:LEU:HD11	2.00	0.43
2:B:430:LYS:HZ3	1:C:353:ALA:HB3	1.83	0.43
1:C:68:VAL:CG1	1:C:171:VAL:HG23	2.46	0.43
1:A:353:ALA:HB3	2:D:430:LYS:NZ	2.33	0.43
2:B:74:SER:O	2:B:74:SER:OG	2.37	0.43
1:C:92:THR:O	1:C:96:VAL:HG23	2.17	0.43
1:A:263:ASN:OD1	1:A:263:ASN:N	2.50	0.43
2:B:64:GLY:HA3	2:B:87:ARG:HG3	2.00	0.43
2:B:148:LEU:HD23	2:B:148:LEU:HA	1.81	0.43
2:D:211:PHE:HB3	2:D:229:LYS:HE2	2.01	0.43
2:D:237:TRP:HZ3	2:D:313:ASN:OD1	2.02	0.43
1:A:84:LYS:HB2	1:A:84:LYS:HE3	1.87	0.43
2:B:333:LEU:HD12	2:B:333:LEU:HA	1.87	0.43
1:A:144:ILE:O	1:A:164:ARG:NH2	2.35	0.43
2:B:425:GLU:OE2	2:B:498:ARG:NH1	2.52	0.43
1:C:275:LEU:HD23	1:C:275:LEU:HA	1.66	0.43
2:B:339:ARG:O	2:B:343:ASN:HB2	2.19	0.43
1:C:251:LEU:HA	1:C:277:ASN:HD21	1.80	0.43
2:D:368:LEU:O	2:D:372:THR:HG23	2.19	0.43
1:A:315:ARG:NH1	2:B:378:GLU:OE2	2.43	0.42
2:B:507:MET:HA	2:B:511:ASP:OD2	2.19	0.42
1:C:97:ASN:HD21	1:C:164:ARG:NH2	2.16	0.42
1:A:312:PHE:O	1:A:316:ASN:ND2	2.46	0.42
1:A:335:ARG:HD2	1:A:335:ARG:N	2.35	0.42
1:A:399:VAL:HG23	1:A:400:ILE:HG13	2.00	0.42
2:D:341:ALA:HB1	2:D:366:MET:HE1	2.00	0.42
1:A:336:THR:CG2	1:A:342:GLN:CB	2.94	0.42
2:B:89:TRP:NE1	2:B:132:ASP:OD1	2.37	0.42
2:B:237:TRP:HZ3	2:B:313:ASN:OD1	2.02	0.42
1:C:75:SER:HB3	1:C:76:PRO:CD	2.50	0.42
1:C:298:ARG:HH21	1:C:338:SER:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PHE:CE1	1:A:131:TYR:HD2	2.37	0.42
2:B:63:PHE:CE2	2:B:214:LEU:HD21	2.55	0.42
1:C:64:LEU:CD2	1:C:103:ASP:HB2	2.50	0.42
1:C:389:LYS:HD3	1:C:464:ARG:HH12	1.85	0.42
2:D:160:TYR:O	2:D:163:SER:OG	2.30	0.42
2:D:196:LEU:HD12	2:D:196:LEU:HA	1.78	0.42
1:C:263:ASN:OD1	1:C:263:ASN:N	2.50	0.42
1:C:419:LEU:HD13	1:C:431:ARG:NH1	2.35	0.42
1:A:248:ILE:HG12	1:A:248:ILE:H	1.48	0.42
1:C:142:SER:O	1:C:167:ARG:NH1	2.53	0.42
2:D:509:GLN:HE21	2:D:509:GLN:HB3	1.53	0.42
1:C:233:GLU:O	1:C:233:GLU:HG2	2.20	0.42
1:A:61:GLU:OE2	1:A:61:GLU:CA	2.67	0.42
2:B:509:GLN:HE21	2:B:509:GLN:HB3	1.53	0.42
1:A:53:TYR:N	1:A:53:TYR:HD1	2.16	0.41
1:A:108:PHE:CE1	1:A:131:TYR:CD2	3.08	0.41
2:B:366:MET:HE2	2:B:366:MET:HB2	1.89	0.41
1:C:76:PRO:HG2	1:C:203:HIS:HE2	1.84	0.41
1:C:383:GLN:HG3	1:C:383:GLN:H	1.61	0.41
1:A:233:GLU:O	1:A:233:GLU:HG2	2.20	0.41
2:B:368:LEU:O	2:B:372:THR:HG23	2.19	0.41
1:C:371:TYR:CE1	1:C:490:GLN:HB2	2.55	0.41
2:D:425:GLU:OE2	2:D:498:ARG:NH1	2.52	0.41
1:A:97:ASN:HD21	1:A:164:ARG:NH2	2.16	0.41
1:C:119:LEU:HD23	1:C:119:LEU:HA	1.81	0.41
1:A:142:SER:O	1:A:167:ARG:NH1	2.53	0.41
1:A:175:PHE:CE1	1:A:193:LYS:HB2	2.54	0.41
1:A:389:LYS:HD3	1:A:464:ARG:HH12	1.85	0.41
1:C:180:LYS:HB3	1:C:180:LYS:HE2	1.53	0.41
2:B:78:ILE:HG12	2:B:153:HIS:HE2	1.86	0.41
1:C:251:LEU:C	1:C:251:LEU:CD2	2.85	0.41
2:D:507:MET:HA	2:D:511:ASP:OD2	2.19	0.41
1:A:190:ARG:HD3	1:A:190:ARG:HA	1.59	0.41
1:C:44:LYS:NZ	1:C:44:LYS:CB	2.84	0.41
1:A:47:ARG:NH1	1:A:47:ARG:CG	2.73	0.41
1:A:353:ALA:HB3	2:D:430:LYS:HZ3	1.86	0.41
1:C:315:ARG:NH1	2:D:378:GLU:OE2	2.45	0.41
2:B:400:ILE:HD12	2:B:447:VAL:HA	2.02	0.41
2:D:306:ASN:O	2:D:310:MET:HG2	2.21	0.41
3:D:701:POV:H312	3:D:701:POV:H315	1.88	0.41
1:A:44:LYS:NZ	1:A:44:LYS:CB	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:SER:HB3	1:A:52:PRO:CD	2.49	0.41
1:A:275:LEU:HD23	1:A:275:LEU:HA	1.93	0.41
2:B:137:PHE:CE1	2:B:160:TYR:HD2	2.38	0.41
1:C:46:ARG:HH11	1:C:46:ARG:CA	2.33	0.41
1:C:69:VAL:O	1:C:69:VAL:CG1	2.66	0.41
2:D:204:LEU:HD22	3:D:701:POV:H38A	2.03	0.41
2:B:306:ASN:O	2:B:310:MET:HG2	2.21	0.41
2:B:332:ALA:HB1	2:B:336:PHE:CD1	2.56	0.41
1:C:84:LYS:HB2	1:C:84:LYS:HE3	1.87	0.41
2:D:132:ASP:O	2:D:136:THR:OG1	2.39	0.41
2:D:137:PHE:CE1	2:D:160:TYR:HD2	2.39	0.41
2:D:363:LEU:O	2:D:366:MET:HG3	2.21	0.41
1:A:306:ILE:HG23	1:A:327:LEU:HD22	2.03	0.40
2:B:59:LEU:O	2:B:59:LEU:CG	2.69	0.40
2:B:363:LEU:O	2:B:366:MET:HG3	2.21	0.40
2:D:459:VAL:O	2:D:460:SER:HB2	2.22	0.40
1:C:306:ILE:HG23	1:C:327:LEU:HD22	2.03	0.40
2:D:59:LEU:O	2:D:59:LEU:CG	2.69	0.40
2:D:501:HIS:CD2	2:D:502:HIS:H	2.40	0.40
2:B:405:TYR:OH	2:B:475:GLU:HG3	2.21	0.40
2:B:459:VAL:O	2:B:460:SER:HB2	2.22	0.40
2:D:215:GLU:OE2	2:D:226:ARG:HD3	2.21	0.40
2:D:454:ILE:HB	2:D:487:THR:HB	2.03	0.40
1:A:371:TYR:CE1	1:A:490:GLN:HB2	2.56	0.40
2:B:418:LEU:HD22	2:B:507:MET:SD	2.62	0.40
1:C:458:ARG:HG2	2:D:146:THR:HG23	2.02	0.40
1:C:67:LEU:HD12	1:C:67:LEU:HA	1.75	0.40
2:D:78:ILE:HG12	2:D:153:HIS:HE2	1.86	0.40
2:D:226:ARG:HB3	2:D:327:LEU:HD11	2.04	0.40
2:D:400:ILE:HD12	2:D:447:VAL:HA	2.02	0.40
2:D:428:PRO:HG2	2:D:431:MET:HE3	2.04	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	447/885 (50%)	418 (94%)	29 (6%)	0	100	100
1	C	447/885 (50%)	414 (93%)	33 (7%)	0	100	100
2	B	471/690 (68%)	442 (94%)	29 (6%)	0	100	100
2	D	471/690 (68%)	441 (94%)	30 (6%)	0	100	100
All	All	1836/3150 (58%)	1715 (93%)	121 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	400/766 (52%)	332 (83%)	68 (17%)	2	6
1	C	400/766 (52%)	328 (82%)	72 (18%)	1	5
2	B	418/603 (69%)	371 (89%)	47 (11%)	6	18
2	D	418/603 (69%)	367 (88%)	51 (12%)	5	15
All	All	1636/2738 (60%)	1398 (86%)	238 (14%)	6	9

All (238) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	46	ARG
1	A	47	ARG
1	A	49	VAL
1	A	50	VAL
1	A	53	TYR
1	A	54	ASP
1	A	55	HIS
1	A	56	LYS
1	A	59	ILE

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Mol	Chain	Res	Type
1	A	61	GLU
1	A	71	THR
1	A	75	SER
1	A	90	SER
1	A	106	MET
1	A	114	ASP
1	A	120	ILE
1	A	137	LEU
1	A	143	THR
1	A	146	SER
1	A	154	SER
1	A	182	ARG
1	A	190	ARG
1	A	191	CYS
1	A	197	VAL
1	A	204	CYS
1	A	217	SER
1	A	239	ARG
1	A	247	SER
1	A	248	ILE
1	A	263	ASN
1	A	278	LEU
1	A	280	LEU
1	A	283	TYR
1	A	303	ARG
1	A	304	ASP
1	A	324	ASP
1	A	332	LEU
1	A	336	THR
1	A	342	GLN
1	A	346	THR
1	A	356	SER
1	A	367	MET
1	A	368	ASP
1	A	369	LYS
1	A	376	VAL
1	A	377	SER
1	A	378	ASN
1	A	379	ASP
1	A	381	LEU
1	A	383	GLN
1	A	386	SER

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Mol	Chain	Res	Type
1	A	407	THR
1	A	416	THR
1	A	419	LEU
1	A	420	VAL
1	A	423	ASP
1	A	430	VAL
1	A	431	ARG
1	A	456	THR
1	A	457	LYS
1	A	458	ARG
1	A	459	LEU
1	A	465	MET
1	A	471	LEU
1	A	473	ILE
1	A	474	ILE
1	A	485	MET
2	B	54	SER
2	B	55	VAL
2	B	58	SER
2	B	59	LEU
2	B	60	LEU
2	B	69	ASP
2	B	74	SER
2	B	82	PHE
2	B	84	ARG
2	B	93	LEU
2	B	100	SER
2	B	108	LEU
2	B	119	LEU
2	B	135	LEU
2	B	143	ASP
2	B	177	GLN
2	B	198	LEU
2	B	226	ARG
2	B	231	LEU
2	B	265	GLU
2	B	280	MET
2	B	334	ARG
2	B	350	SER
2	B	357	THR
2	B	360	GLU
2	B	366	MET

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Mol	Chain	Res	Type
2	B	368	LEU
2	B	375	LEU
2	B	382	GLN
2	B	390	SER
2	B	394	GLN
2	B	403	GLU
2	B	405	TYR
2	B	410	PHE
2	B	415	LEU
2	B	418	LEU
2	B	423	GLN
2	B	448	SER
2	B	452	ASP
2	B	460	SER
2	B	466	LYS
2	B	484	GLN
2	B	489	ARG
2	B	506	GLU
2	B	509	GLN
2	B	513	ASP
2	B	524	MET
1	C	45	LEU
1	C	46	ARG
1	C	47	ARG
1	C	49	VAL
1	C	50	VAL
1	C	51	SER
1	C	53	TYR
1	C	54	ASP
1	C	55	HIS
1	C	56	LYS
1	C	59	ILE
1	C	61	GLU
1	C	63	PHE
1	C	67	LEU
1	C	69	VAL
1	C	70	TYR
1	C	71	THR
1	C	75	SER
1	C	90	SER
1	C	106	MET
1	C	114	ASP

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Mol	Chain	Res	Type
1	C	120	ILE
1	C	137	LEU
1	C	143	THR
1	C	146	SER
1	C	154	SER
1	C	182	ARG
1	C	190	ARG
1	C	191	CYS
1	C	204	CYS
1	C	217	SER
1	C	239	ARG
1	C	247	SER
1	C	248	ILE
1	C	263	ASN
1	C	278	LEU
1	C	280	LEU
1	C	283	TYR
1	C	300	ARG
1	C	303	ARG
1	C	304	ASP
1	C	324	ASP
1	C	335	ARG
1	C	336	THR
1	C	337	ASP
1	C	338	SER
1	C	342	GLN
1	C	346	THR
1	C	356	SER
1	C	367	MET
1	C	368	ASP
1	C	369	LYS
1	C	376	VAL
1	C	377	SER
1	C	378	ASN
1	C	379	ASP
1	C	381	LEU
1	C	383	GLN
1	C	386	SER
1	C	407	THR
1	C	416	THR
1	C	419	LEU
1	C	420	VAL

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Mol	Chain	Res	Type
1	C	423	ASP
1	C	430	VAL
1	C	431	ARG
1	C	456	THR
1	C	465	MET
1	C	471	LEU
1	C	473	ILE
1	C	474	ILE
1	C	485	MET
2	D	54	SER
2	D	55	VAL
2	D	58	SER
2	D	59	LEU
2	D	69	ASP
2	D	74	SER
2	D	82	PHE
2	D	93	LEU
2	D	100	SER
2	D	108	LEU
2	D	119	LEU
2	D	135	LEU
2	D	143	ASP
2	D	177	GLN
2	D	198	LEU
2	D	225	ILE
2	D	226	ARG
2	D	227	VAL
2	D	231	LEU
2	D	265	GLU
2	D	280	MET
2	D	333	LEU
2	D	334	ARG
2	D	336	PHE
2	D	339	ARG
2	D	344	ASP
2	D	350	SER
2	D	357	THR
2	D	360	GLU
2	D	366	MET
2	D	368	LEU
2	D	375	LEU
2	D	382	GLN

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Mol	Chain	Res	Type
2	D	390	SER
2	D	394	GLN
2	D	403	GLU
2	D	405	TYR
2	D	410	PHE
2	D	415	LEU
2	D	418	LEU
2	D	423	GLN
2	D	448	SER
2	D	452	ASP
2	D	460	SER
2	D	466	LYS
2	D	484	GLN
2	D	489	ARG
2	D	506	GLU
2	D	509	GLN
2	D	513	ASP
2	D	524	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	218	ASN
1	A	317	HIS
1	A	323	GLN
1	A	342	GLN
1	A	378	ASN
1	A	461	GLN
1	A	486	ASN
1	A	491	HIS
2	B	81	HIS
2	B	299	ASN
2	B	306	ASN
2	B	436	GLN
2	B	501	HIS
2	B	502	HIS
2	B	509	GLN
1	C	97	ASN
1	C	218	ASN
1	C	290	ASN
1	C	317	HIS

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Mol	Chain	Res	Type
1	C	323	GLN
1	C	342	GLN
1	C	378	ASN
1	C	461	GLN
1	C	486	ASN
1	C	491	HIS
2	D	81	HIS
2	D	299	ASN
2	D	306	ASN
2	D	436	GLN
2	D	501	HIS
2	D	502	HIS
2	D	509	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	POV	A	901	-	38,38,51	0.46	0	42,43,59	0.65	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	POV	C	901	-	38,38,51	0.44	0	42,43,59	0.65	1 (2%)
3	POV	B	701	-	38,38,51	0.49	0	42,43,59	0.67	1 (2%)
3	POV	D	701	-	38,38,51	0.49	0	42,43,59	0.63	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
3	POV	A	901	-	-	18/40/40/55	-
3	POV	C	901	-	-	19/40/40/55	-
3	POV	B	701	-	-	23/40/40/55	-
3	POV	D	701	-	-	23/40/40/55	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	POV	O13-P-O14	2.56	120.69	110.68
3	C	901	POV	O13-P-O14	2.54	120.61	110.68
3	D	701	POV	O13-P-O14	2.46	120.31	110.68
3	B	701	POV	O13-P-O14	2.39	120.03	110.68

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	701	POV	C1-O11-P-O12
3	B	701	POV	C1-O11-P-O13
3	B	701	POV	C1-O11-P-O14
3	B	701	POV	C211-C210-C29-C28
3	C	901	POV	O22-C21-O21-C2
3	D	701	POV	C1-O11-P-O12
3	D	701	POV	C1-O11-P-O13
3	D	701	POV	C1-O11-P-O14
3	D	701	POV	C22-C21-O21-C2
3	D	701	POV	O32-C31-O31-C3
3	A	901	POV	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
3	D	701	POV	O22-C21-O21-C2
3	D	701	POV	C32-C31-O31-C3
3	A	901	POV	C22-C21-O21-C2
3	C	901	POV	C22-C21-O21-C2
3	C	901	POV	C32-C31-O31-C3
3	C	901	POV	O32-C31-O31-C3
3	D	701	POV	C2-C3-O31-C31
3	B	701	POV	O22-C21-O21-C2
3	B	701	POV	C22-C21-O21-C2
3	A	901	POV	C312-C313-C314-C315
3	C	901	POV	C312-C313-C314-C315
3	A	901	POV	C1-C2-O21-C21
3	B	701	POV	C1-C2-O21-C21
3	A	901	POV	C310-C311-C312-C313
3	D	701	POV	C311-C312-C313-C314
3	B	701	POV	C22-C23-C24-C25
3	A	901	POV	C39-C310-C311-C312
3	B	701	POV	C35-C36-C37-C38
3	C	901	POV	C31-C32-C33-C34
3	D	701	POV	C310-C311-C312-C313
3	A	901	POV	C37-C38-C39-C310
3	C	901	POV	C311-C310-C39-C38
3	C	901	POV	C310-C311-C312-C313
3	A	901	POV	C35-C36-C37-C38
3	D	701	POV	C24-C25-C26-C27
3	D	701	POV	C39-C310-C311-C312
3	D	701	POV	C35-C36-C37-C38
3	B	701	POV	C312-C313-C314-C315
3	B	701	POV	O21-C2-C3-O31
3	D	701	POV	C26-C27-C28-C29
3	C	901	POV	C22-C23-C24-C25
3	D	701	POV	O11-C1-C2-C3
3	A	901	POV	C24-C25-C26-C27
3	B	701	POV	C39-C310-C311-C312
3	B	701	POV	C1-C2-C3-O31
3	D	701	POV	C311-C310-C39-C38
3	C	901	POV	C37-C38-C39-C310
3	C	901	POV	O21-C2-C3-O31
3	A	901	POV	C25-C26-C27-C28
3	B	701	POV	C37-C38-C39-C310
3	B	701	POV	C25-C26-C27-C28
3	C	901	POV	C211-C210-C29-C28

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Mol	Chain	Res	Type	Atoms
3	D	701	POV	C211-C210-C29-C28
3	B	701	POV	O11-C1-C2-C3
3	D	701	POV	C23-C24-C25-C26
3	D	701	POV	C1-C2-C3-O31
3	A	901	POV	O11-C1-C2-O21
3	B	701	POV	O11-C1-C2-O21
3	D	701	POV	O11-C1-C2-O21
3	B	701	POV	C31-C32-C33-C34
3	C	901	POV	C26-C27-C28-C29
3	C	901	POV	C1-C2-C3-O31
3	D	701	POV	O21-C2-C3-O31
3	A	901	POV	C1-O11-P-O14
3	B	701	POV	C21-C22-C23-C24
3	C	901	POV	C32-C33-C34-C35
3	A	901	POV	C2-C1-O11-P
3	D	701	POV	C25-C26-C27-C28
3	C	901	POV	C24-C25-C26-C27
3	B	701	POV	C311-C310-C39-C38
3	A	901	POV	C27-C28-C29-C210
3	C	901	POV	C311-C312-C313-C314
3	A	901	POV	O21-C2-C3-O31
3	B	701	POV	C311-C312-C313-C314
3	A	901	POV	C211-C210-C29-C28
3	C	901	POV	O31-C31-C32-C33
3	B	701	POV	C34-C35-C36-C37
3	A	901	POV	C1-O11-P-O12
3	D	701	POV	C312-C313-C314-C315
3	A	901	POV	C22-C23-C24-C25
3	C	901	POV	C27-C28-C29-C210
3	B	701	POV	C313-C314-C315-C316

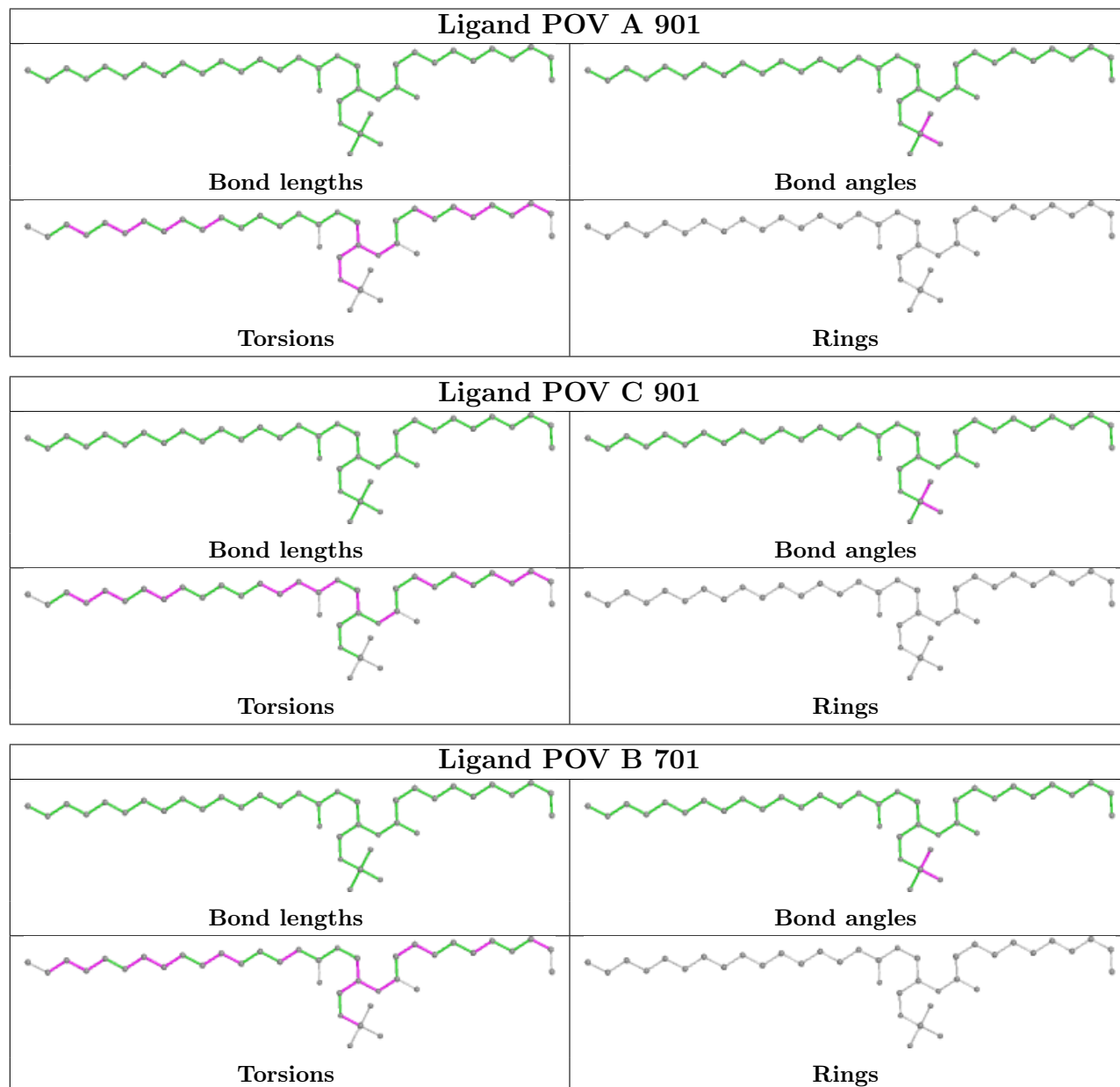
There are no ring outliers.

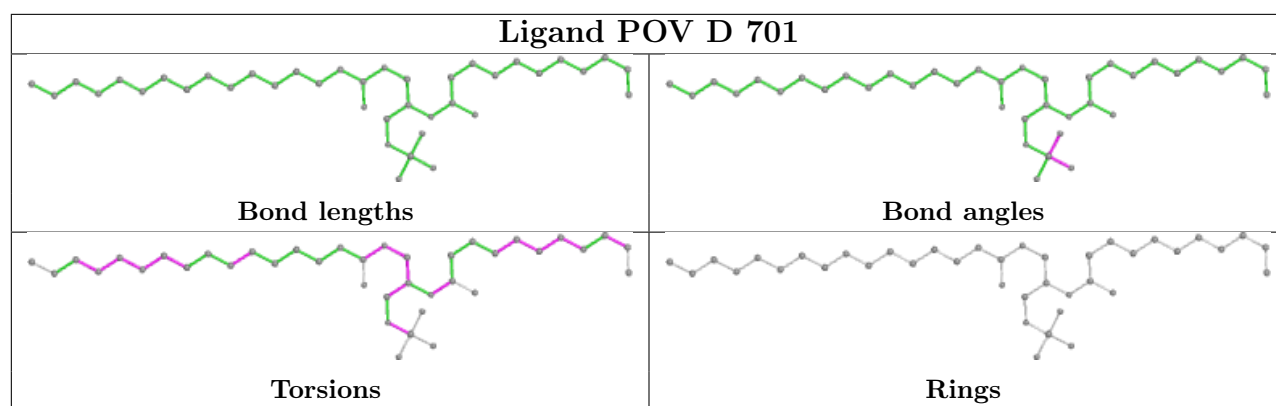
4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	POV	1	0
3	C	901	POV	4	0
3	B	701	POV	5	0
3	D	701	POV	5	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.

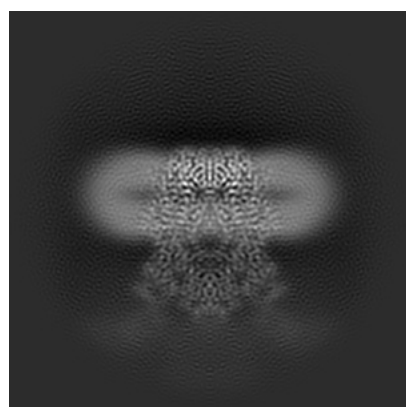
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32597. These allow visual inspection of the internal detail of the map and identification of artifacts.

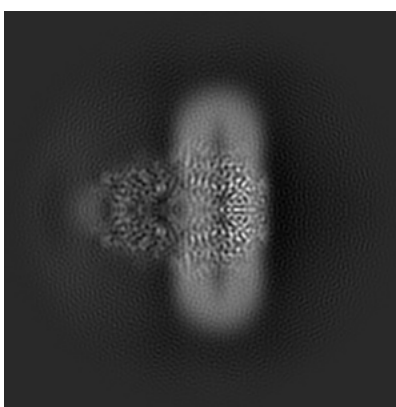
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

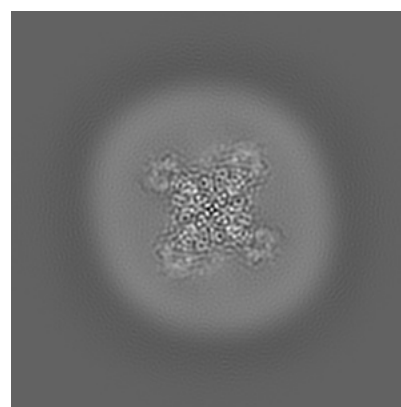
6.1.1 Primary map



X



Y

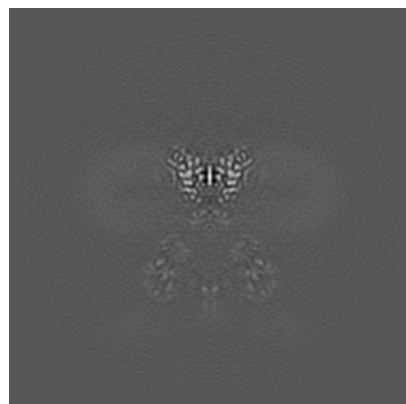


Z

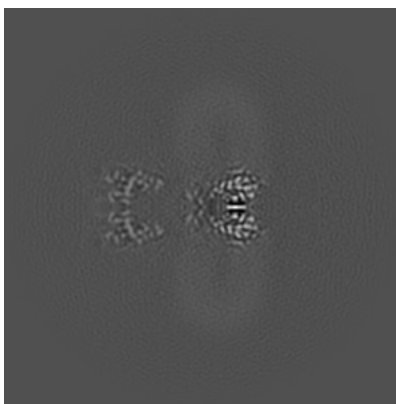
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

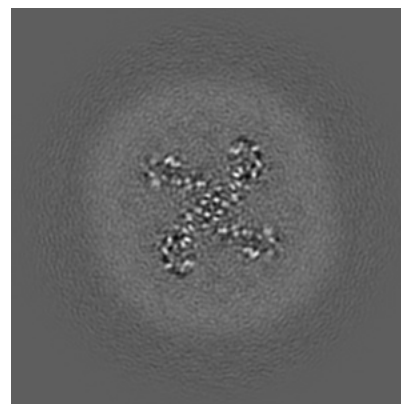
6.2.1 Primary map



X Index: 120



Y Index: 120

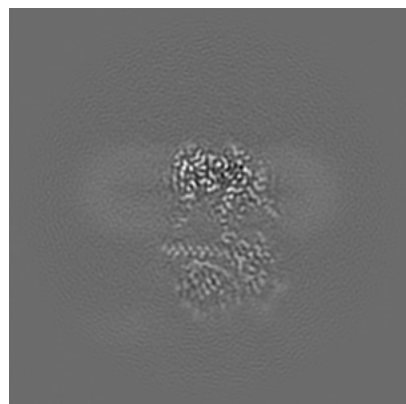


Z Index: 120

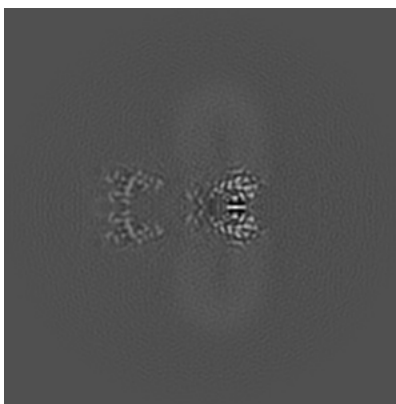
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

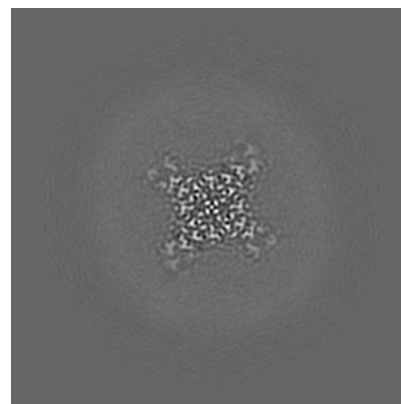
6.3.1 Primary map



X Index: 133



Y Index: 120

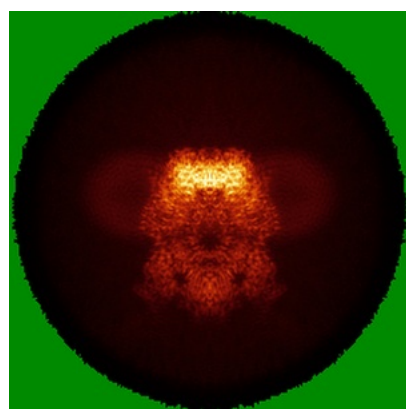


Z Index: 140

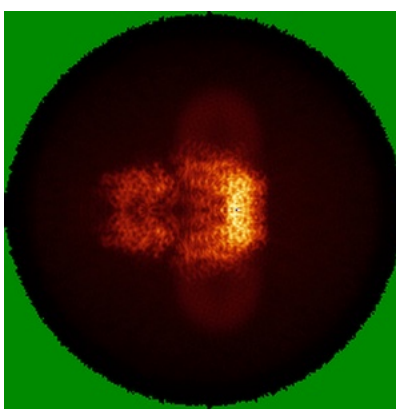
The images above show the largest variance slices of the map in three orthogonal directions.

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

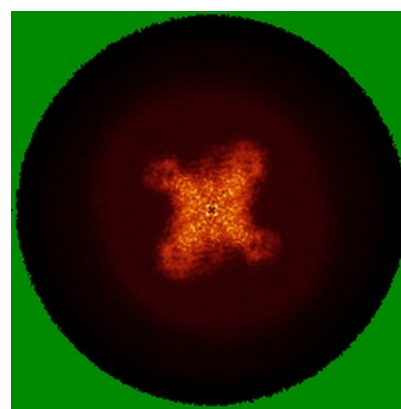
6.4.1 Primary map



X



Y

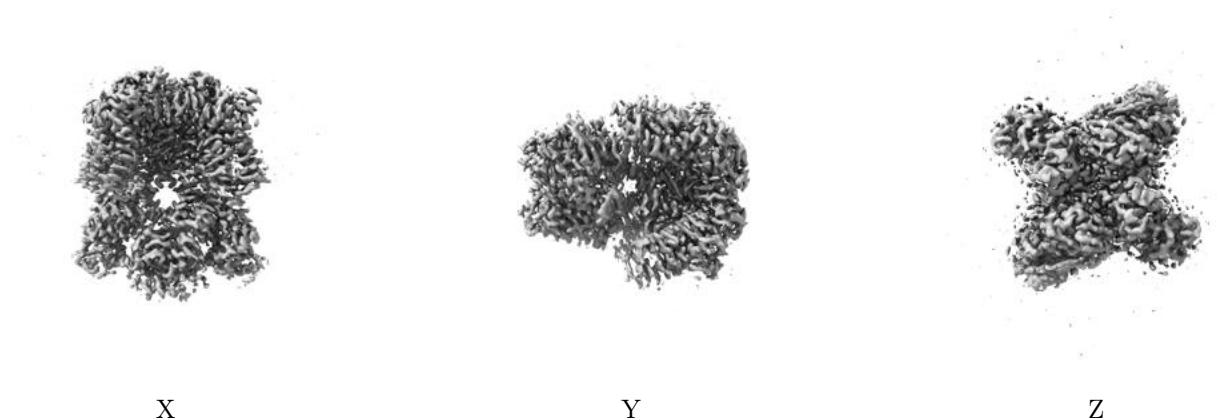


Z

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 0.633. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

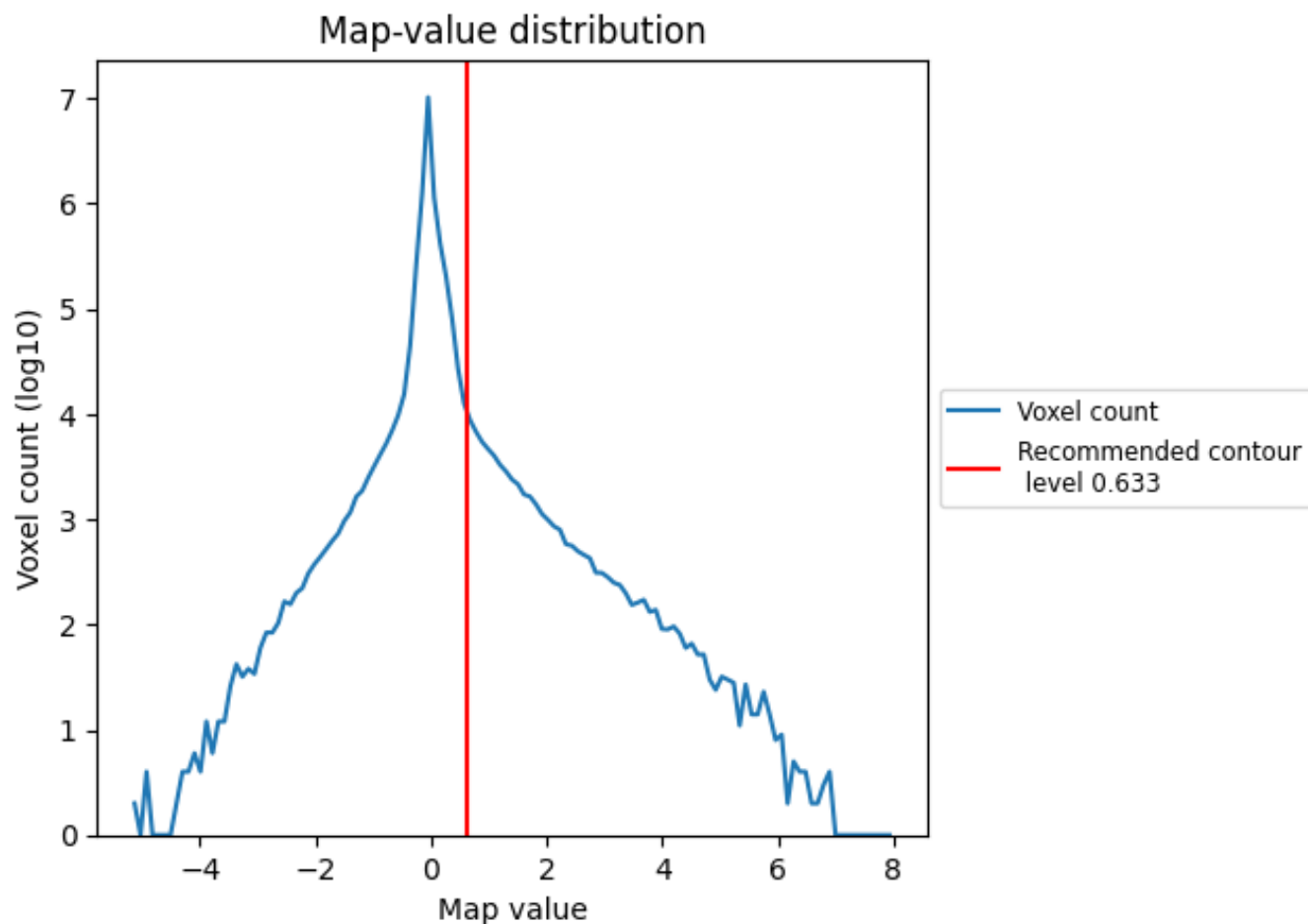
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

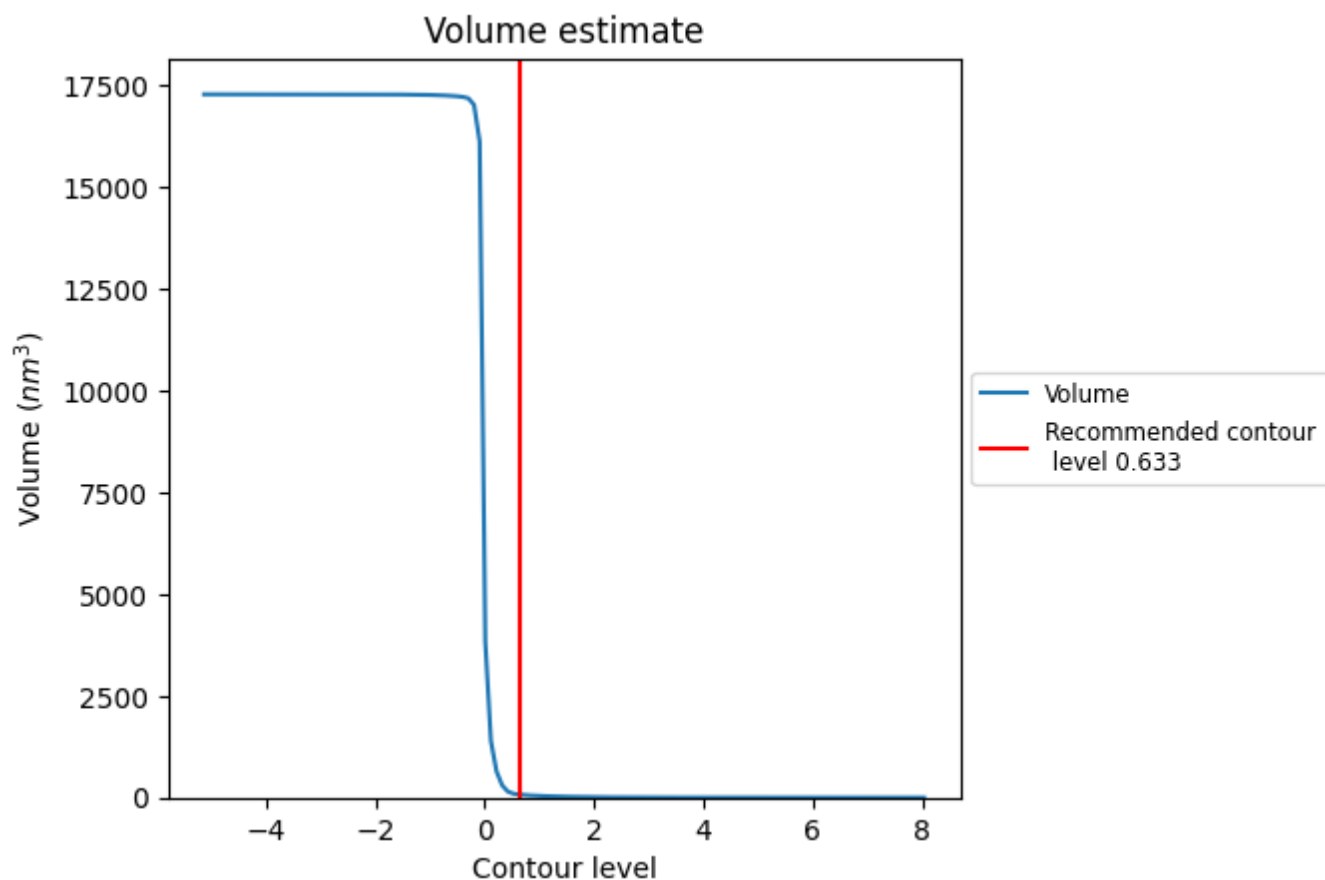
This section contains the results of statistical analysis of the map.

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.

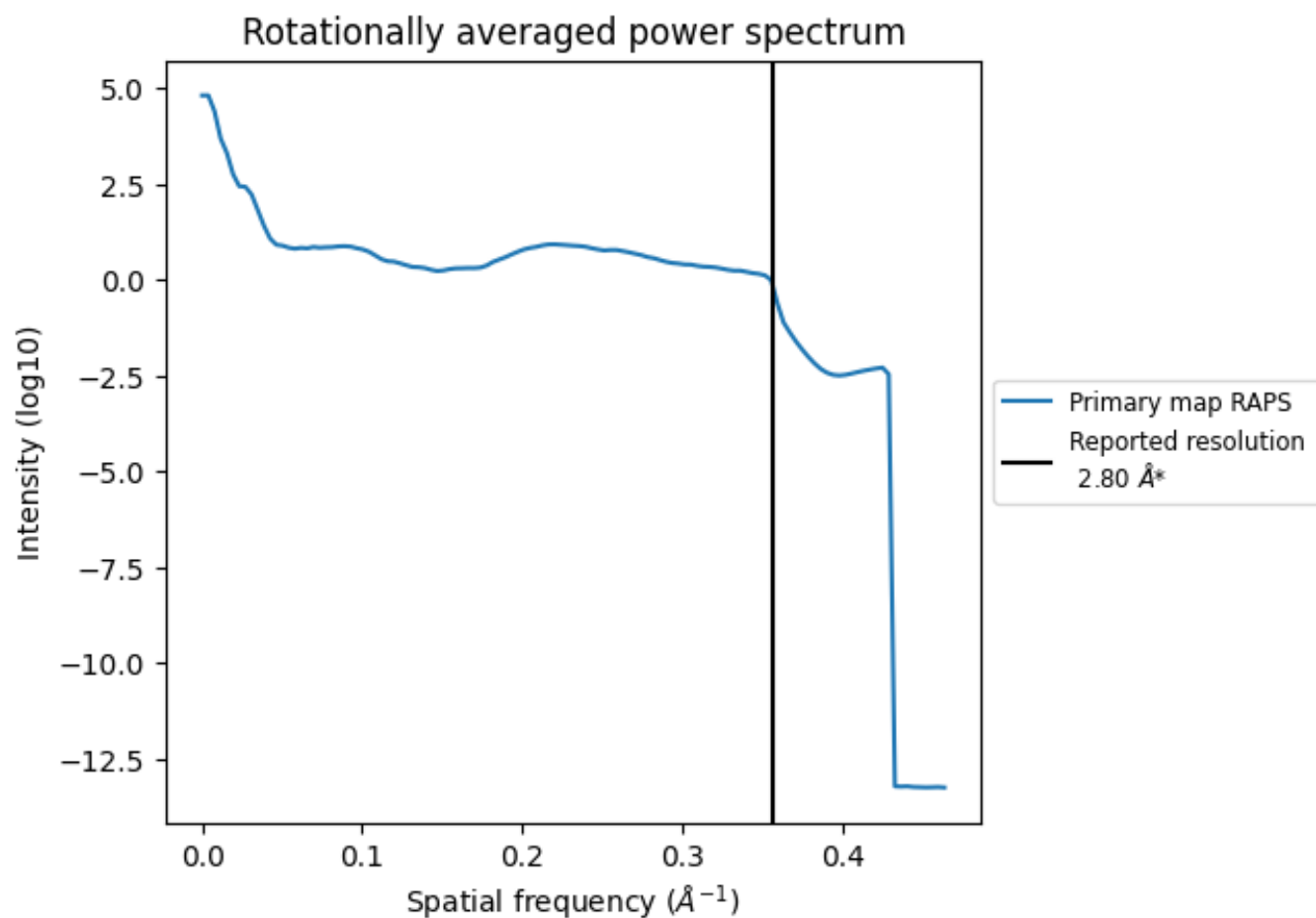
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 74 nm³; this corresponds to an approximate mass of 67 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

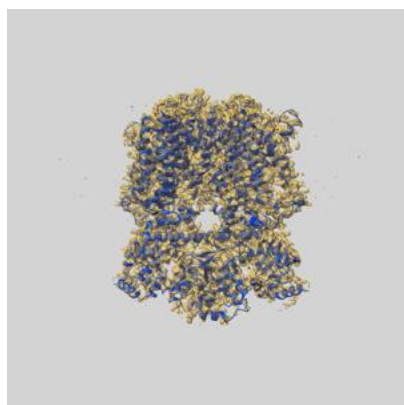
8 Fourier-Shell correlation ⓘ

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

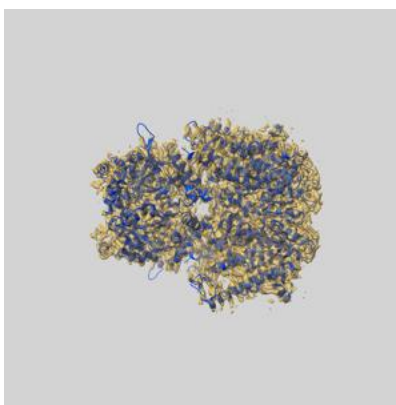
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32597 and PDB model 7WM1. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

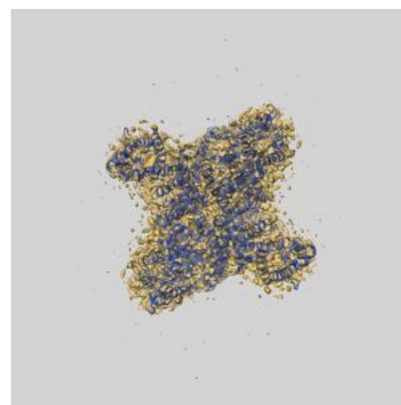
9.1 Map-model overlay [i](#)



X



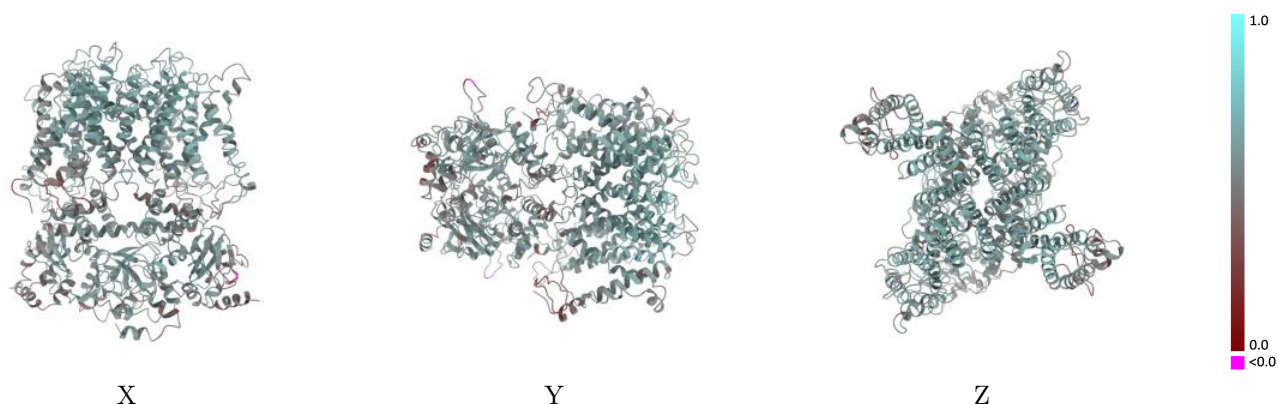
Y



Z

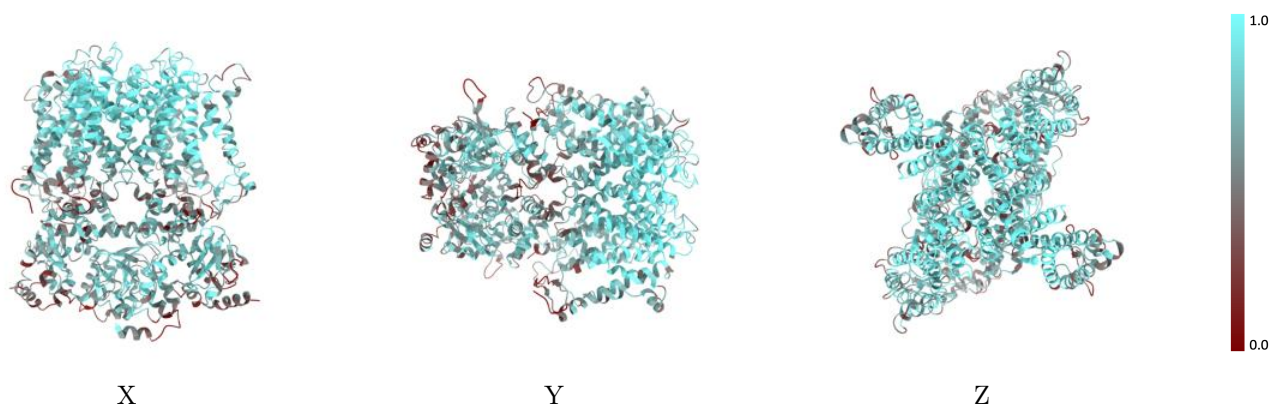
The images above show the 3D surface view of the map at the recommended contour level 0.633 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



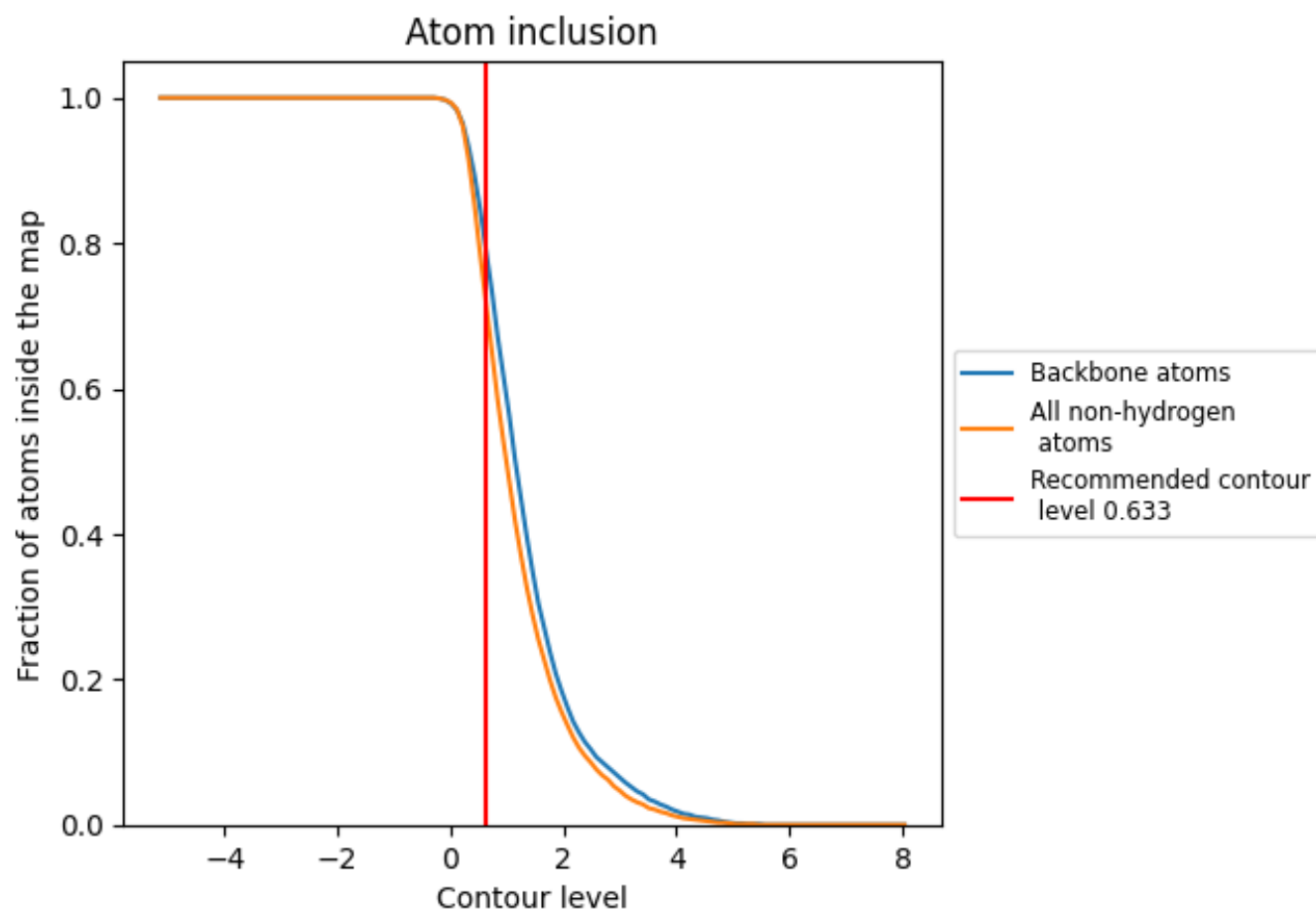
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.633).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 72% 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 (0.633) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7170	<div></div> 0.5480
A	<div></div> 0.6930	<div></div> 0.5340
B	<div></div> 0.7380	<div></div> 0.5620
C	<div></div> 0.6960	<div></div> 0.5350
D	<div></div> 0.7380	<div></div> 0.5600

