



Full wwPDB EM Validation Report ⓘ

Aug 24, 2026 – 06:29 PM JST

PDB ID : 25LE / pdb_000025le
EMDB ID : EMD-80182
Title : Cryo-EM structure of the Arabidopsis thaliana potassium transporter 5 mutant
- H527A
Authors : Wang, C.; Wang, X.H.; Qu, Y.N.; Shen, H.Z.
Deposited on : 2026-04-08
Resolution : 3.22 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

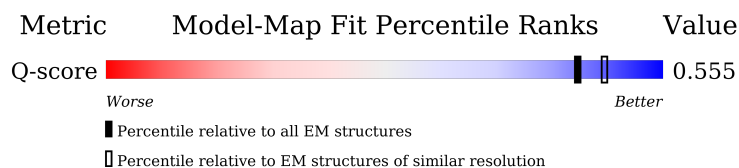
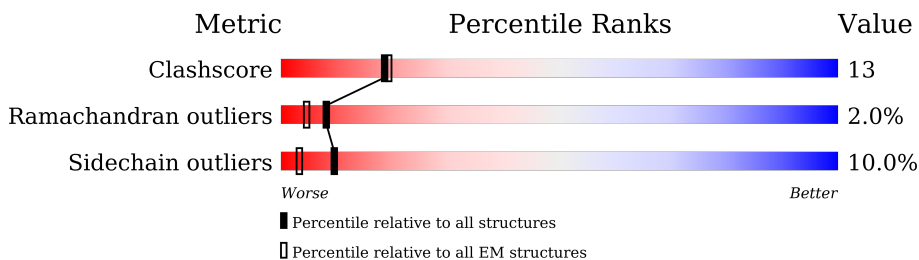
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.22 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14612 (2.72 - 3.72)

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	798	
1	B	798	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10586 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 transporter 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	664	Total	C	N	O	S	0	0
			5259	3460	840	929	30		
1	B	664	Total	C	N	O	S	0	0
			5259	3460	840	929	30		

There are 28 discrepancies between the modelled and reference sequences:

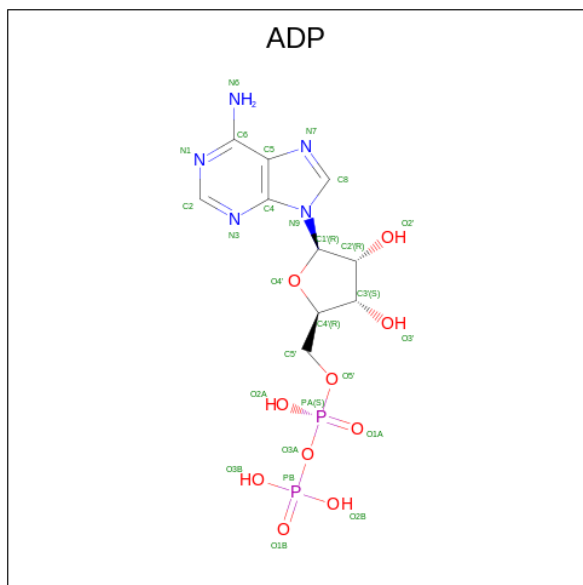
Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP Q9M7K4
A	-11	ASP	-	expression tag	UNP Q9M7K4
A	-10	TYR	-	expression tag	UNP Q9M7K4
A	-9	LYS	-	expression tag	UNP Q9M7K4
A	-8	ASP	-	expression tag	UNP Q9M7K4
A	-7	ASP	-	expression tag	UNP Q9M7K4
A	-6	ASP	-	expression tag	UNP Q9M7K4
A	-5	ASP	-	expression tag	UNP Q9M7K4
A	-4	LYS	-	expression tag	UNP Q9M7K4
A	-3	GLY	-	expression tag	UNP Q9M7K4
A	-2	CYS	-	expression tag	UNP Q9M7K4
A	-1	GLY	-	expression tag	UNP Q9M7K4
A	0	ARG	-	expression tag	UNP Q9M7K4
A	527	ALA	HIS	engineered mutation	UNP Q9M7K4
B	-12	MET	-	initiating methionine	UNP Q9M7K4
B	-11	ASP	-	expression tag	UNP Q9M7K4
B	-10	TYR	-	expression tag	UNP Q9M7K4
B	-9	LYS	-	expression tag	UNP Q9M7K4
B	-8	ASP	-	expression tag	UNP Q9M7K4
B	-7	ASP	-	expression tag	UNP Q9M7K4
B	-6	ASP	-	expression tag	UNP Q9M7K4
B	-5	ASP	-	expression tag	UNP Q9M7K4
B	-4	LYS	-	expression tag	UNP Q9M7K4
B	-3	GLY	-	expression tag	UNP Q9M7K4
B	-2	CYS	-	expression tag	UNP Q9M7K4
B	-1	GLY	-	expression tag	UNP Q9M7K4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ARG	-	expression tag	UNP Q9M7K4
B	527	ALA	HIS	engineered mutation	UNP Q9M7K4

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	K	0
			1	1	
3	B	1	Total	K	0
			1	1	

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	6	Total	O	0
			6	6	

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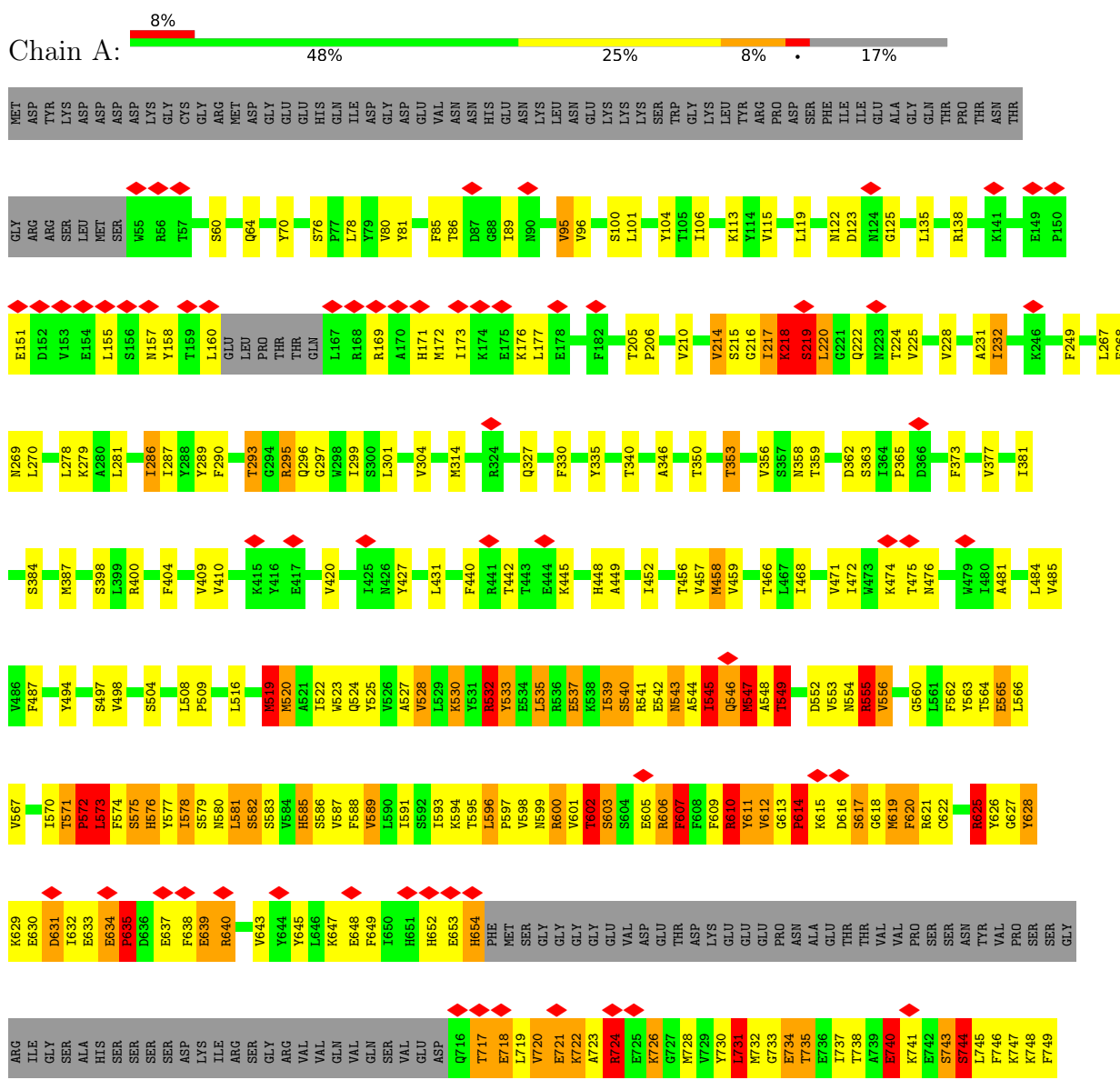
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Mol	Chain	Residues	Atoms		AltConf
4	B	6	Total	O	0
			6	6	

3 Residue-property plots

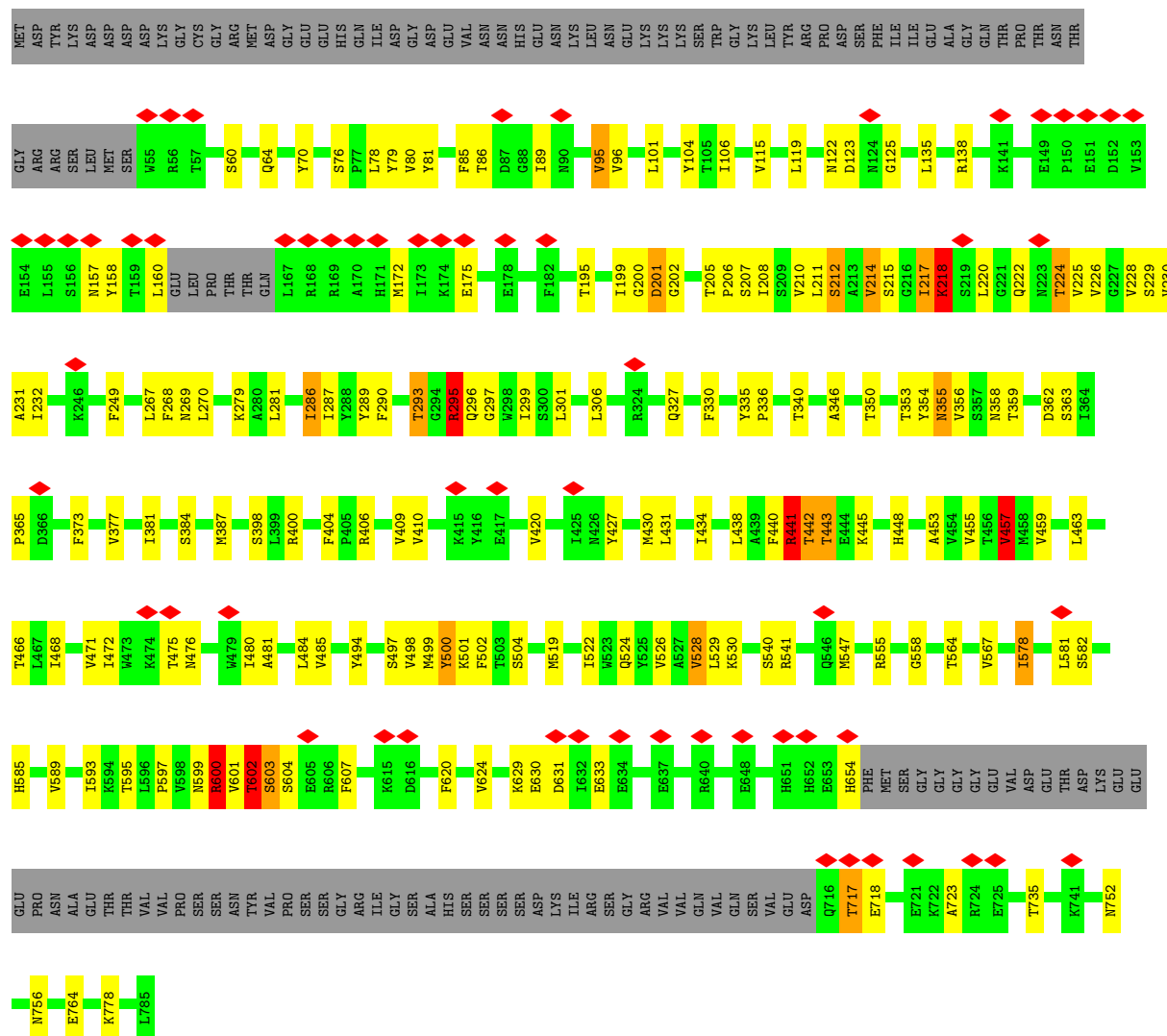
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 transporter 5





• Molecule 1: Potassium transporter 5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	271609	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	7.831	Depositor
Minimum map value	-5.732	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.144	Depositor
Recommended contour level	1	Depositor
Map size (Å)	278.272, 278.272, 278.272	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, 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	0.67	2/5381 (0.0%)	1.09	49/7301 (0.7%)
1	B	0.36	0/5381	0.65	12/7301 (0.2%)
All	All	0.54	2/10762 (0.0%)	0.90	61/14602 (0.4%)

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	11
1	B	0	3
All	All	0	14

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	560	GLY	CA-C	-7.32	1.47	1.52
1	A	744	SER	CA-CB	-5.21	1.44	1.53

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	772	PRO	N-CA-CB	-11.45	93.71	103.32
1	A	635	PRO	N-CA-CB	-9.93	92.83	103.25
1	A	218	LYS	N-CA-C	-9.65	95.59	110.17
1	A	220	LEU	N-CA-C	-9.59	98.72	113.02
1	A	537	GLU	N-CA-CB	-9.03	100.24	110.35
1	B	354	TYR	N-CA-CB	-7.92	98.77	110.49
1	B	231	ALA	N-CA-C	-7.85	104.86	114.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	ALA	N-CA-C	-7.81	104.91	114.75
1	B	295	ARG	CB-CA-C	-7.77	96.32	109.38
1	A	572	PRO	N-CA-CB	-7.64	95.41	101.83
1	A	772	PRO	CA-C-O	-7.62	112.89	121.43
1	B	201	ASP	CA-CB-CG	7.61	120.21	112.60
1	A	528	VAL	N-CA-C	-7.45	104.06	113.22
1	B	218	LYS	N-CA-C	-7.30	104.62	113.97
1	B	528	VAL	N-CA-C	-7.23	104.33	113.22
1	A	614	PRO	N-CA-CB	-6.79	96.12	103.25
1	A	622	CYS	CB-CA-C	-6.62	99.54	110.14
1	A	458	MET	N-CA-C	-6.61	105.84	114.04
1	B	601	VAL	N-CA-CB	6.56	119.62	110.56
1	B	296	GLN	N-CA-C	-6.48	105.19	113.23
1	A	296	GLN	N-CA-C	-6.45	105.23	113.23
1	A	773	ARG	N-CA-CB	6.38	120.47	110.46
1	A	293	THR	CA-CB-OG1	-6.34	100.10	109.60
1	A	731	LEU	N-CA-CB	-6.25	99.69	109.87
1	A	219	SER	N-CA-C	-6.21	100.64	113.31
1	A	543	ASN	N-CA-C	-6.11	103.95	111.40
1	A	611	TYR	N-CA-CB	-6.05	101.54	110.49
1	A	555	ARG	N-CA-CB	-6.04	101.54	110.49
1	A	585	HIS	CB-CA-C	6.01	119.51	109.89
1	A	607	PHE	N-CA-CB	6.01	120.64	110.49
1	A	630	GLU	CB-CG-CD	-6.00	102.41	112.60
1	A	724	ARG	N-CA-C	-5.79	105.71	112.89
1	A	625	ARG	N-CA-CB	-5.76	101.36	110.06
1	A	764	GLU	N-CA-CB	-5.63	102.64	110.29
1	A	766	ASP	CB-CA-C	-5.62	101.29	110.85
1	A	520	MET	N-CA-C	-5.58	106.52	113.38
1	A	749	PHE	CB-CA-C	-5.55	102.12	110.90
1	A	532	ARG	N-CA-C	-5.55	106.35	113.23
1	A	549	THR	N-CA-C	-5.55	105.45	113.21
1	A	573	LEU	N-CA-C	-5.53	106.31	113.16
1	A	620	PHE	CA-CB-CG	5.52	119.32	113.80
1	A	745	LEU	N-CA-C	-5.50	106.62	113.38
1	A	735	THR	CA-CB-OG1	-5.45	101.42	109.60
1	A	779	VAL	CA-C-O	-5.43	116.14	121.58
1	B	541	ARG	N-CA-C	-5.41	105.36	112.72
1	A	628	TYR	N-CA-C	-5.34	106.81	113.38
1	A	552	ASP	N-CA-C	-5.33	106.54	114.64
1	A	576	HIS	N-CA-C	-5.31	105.57	111.36
1	A	218	LYS	CA-C-O	-5.28	115.01	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	767	LYS	N-CA-CB	-5.25	102.37	110.20
1	A	519	MET	N-CA-C	-5.25	99.61	110.80
1	B	295	ARG	N-CA-CB	5.23	118.10	110.88
1	A	766	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	547	MET	N-CA-C	-5.20	107.31	113.97
1	A	734	GLU	CB-CA-C	-5.18	102.31	111.22
1	B	630	GLU	CB-CG-CD	-5.15	103.85	112.60
1	A	775	LYS	N-CA-C	-5.12	108.05	114.56
1	A	757	PHE	CB-CA-C	-5.10	101.37	110.70
1	A	556	VAL	CA-C-O	-5.09	115.28	119.76
1	B	529	LEU	N-CA-C	-5.07	106.79	113.12
1	A	628	TYR	CB-CA-C	5.05	118.44	109.65

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	216	GLY	Mainchain
1	A	295	ARG	Sidechain
1	A	532	ARG	Sidechain
1	A	555	ARG	Sidechain
1	A	606	ARG	Sidechain
1	A	610	ARG	Sidechain
1	A	625	ARG	Sidechain
1	A	640	ARG	Sidechain
1	A	724	ARG	Sidechain
1	A	763	ARG	Sidechain
1	A	773	ARG	Sidechain
1	B	295	ARG	Sidechain
1	B	441	ARG	Sidechain
1	B	600	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5259	0	5389	177	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5259	0	5389	104	0
2	A	27	0	12	2	0
2	B	27	0	12	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
All	All	10586	0	10802	278	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 13.

All (278) 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:A:545:ILE:HD13	1:A:613:GLY:HA2	1.48	0.93
1:A:544:ALA:O	1:A:546:GLN:N	2.23	0.72
1:B:499:MET:O	1:B:500:TYR:C	2.35	0.70
1:B:735:THR:OG1	2:B:901:ADP:O1A	2.11	0.69
1:B:158:TYR:HD1	1:B:160:LEU:HD23	1.58	0.68
1:A:158:TYR:HD1	1:A:160:LEU:HD23	1.58	0.68
1:A:721:GLU:C	1:A:723:ALA:H	2.01	0.68
1:B:200:GLY:C	1:B:202:GLY:H	2.02	0.68
1:B:81:TYR:HB2	1:B:359:THR:HG21	1.76	0.67
1:A:471:VAL:HG23	1:A:472:ILE:HG13	1.77	0.67
1:B:471:VAL:HG23	1:B:472:ILE:HG13	1.76	0.67
1:B:589:VAL:HG22	1:B:620:PHE:HB2	1.77	0.67
1:B:499:MET:O	1:B:501:LYS:N	2.29	0.66
1:A:96:VAL:HG11	1:A:279:LYS:HZ3	1.59	0.66
1:A:81:TYR:HB2	1:A:359:THR:HG21	1.76	0.66
1:A:528:VAL:O	1:A:532:ARG:HG3	1.96	0.65
1:A:544:ALA:C	1:A:546:GLN:H	2.05	0.65
1:B:499:MET:O	1:B:502:PHE:N	2.30	0.64
1:B:138:ARG:NH1	1:B:597:PRO:O	2.30	0.64
1:B:226:VAL:HG11	1:B:441:ARG:HD3	1.79	0.64
1:A:445:LYS:NZ	1:A:504:SER:O	2.32	0.63
1:B:96:VAL:HG11	1:B:279:LYS:HZ3	1.63	0.63
1:A:535:LEU:HG	1:A:566:LEU:HD11	1.82	0.62
1:A:599:ASN:O	1:A:629:LYS:HB2	2.00	0.62
1:A:115:VAL:CG2	1:A:314:MET:HE1	2.30	0.61
1:A:735:THR:OG1	2:A:901:ADP:O2A	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:THR:HB	1:A:572:PRO:HD2	1.83	0.61
1:A:764:GLU:CD	1:A:764:GLU:H	2.06	0.61
1:B:208:ILE:O	1:B:212:SER:OG	2.19	0.60
1:A:563:TYR:O	2:A:901:ADP:O2'	2.20	0.60
1:A:205:THR:HG21	1:A:387:MET:HG3	1.83	0.60
1:B:123:ASP:OD1	1:B:138:ARG:NH2	2.30	0.59
1:A:214:VAL:O	1:A:217:ILE:HG13	2.02	0.59
1:B:499:MET:C	1:B:501:LYS:N	2.60	0.59
1:A:494:TYR:O	1:A:498:VAL:HG23	2.03	0.59
1:A:746:PHE:O	1:A:747:LYS:C	2.46	0.59
1:B:157:ASN:ND2	1:B:600:ARG:O	2.36	0.58
1:A:638:PHE:O	1:A:640:ARG:N	2.37	0.58
1:B:205:THR:HG21	1:B:387:MET:HG3	1.85	0.58
1:B:406:ARG:NH1	2:B:901:ADP:O2B	2.36	0.58
1:B:230:VAL:HG13	1:B:434:ILE:HD12	1.86	0.58
1:B:295:ARG:O	1:B:299:ILE:HG13	2.05	0.57
1:A:524:GLN:HG3	1:A:524:GLN:O	2.05	0.56
1:A:652:HIS:C	1:A:654:HIS:H	2.12	0.56
1:A:532:ARG:HH11	1:A:532:ARG:HB3	1.69	0.56
1:A:717:THR:O	1:A:718:GLU:HB3	2.06	0.56
1:A:595:THR:HG23	1:A:627:GLY:O	2.04	0.56
1:B:224:THR:O	1:B:228:VAL:HG23	2.06	0.56
1:A:115:VAL:HG23	1:A:314:MET:HE1	1.88	0.55
1:B:555:ARG:NH1	1:B:585:HIS:O	2.39	0.55
1:A:730:TYR:CD2	1:A:771:ILE:HG23	2.41	0.55
1:B:602:THR:OG1	1:B:603:SER:N	2.36	0.55
1:A:762:CYS:O	1:A:763:ARG:C	2.49	0.55
1:B:85:PHE:HB2	1:B:356:VAL:HG11	1.88	0.54
1:A:544:ALA:HB2	1:A:570:ILE:HD13	1.88	0.54
1:A:589:VAL:HG22	1:A:620:PHE:HB2	1.87	0.54
1:B:218:LYS:HE2	1:B:225:VAL:HG21	1.89	0.54
1:A:95:VAL:HG21	1:A:350:THR:HG22	1.90	0.54
1:A:224:THR:O	1:A:228:VAL:HG23	2.07	0.54
1:B:211:LEU:HD23	1:B:443:THR:OG1	2.07	0.54
1:A:400:ARG:O	1:A:595:THR:HG21	2.08	0.54
1:A:85:PHE:HB2	1:A:356:VAL:HG11	1.90	0.54
1:B:95:VAL:HG21	1:B:350:THR:HG22	1.90	0.54
1:A:603:SER:O	1:A:605:GLU:N	2.38	0.54
1:A:171:HIS:HB2	1:A:172:MET:HE2	1.90	0.54
1:A:577:TYR:C	1:A:579:SER:H	2.16	0.54
1:A:731:LEU:HD23	1:A:777:LEU:HD23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ARG:O	1:A:299:ILE:HG13	2.08	0.54
1:B:226:VAL:HG21	1:B:441:ARG:HB2	1.90	0.54
1:B:524:GLN:O	1:B:528:VAL:HG23	2.08	0.53
1:A:577:TYR:O	1:A:579:SER:N	2.42	0.53
1:A:594:LYS:O	1:A:626:TYR:N	2.41	0.53
1:B:104:TYR:OH	1:B:281:LEU:O	2.22	0.53
1:B:442:THR:HG21	1:B:445:LYS:HB2	1.91	0.53
1:A:602:THR:OG1	1:A:603:SER:N	2.39	0.53
1:A:777:LEU:HD21	1:B:581:LEU:HD11	1.90	0.53
1:A:155:LEU:HD22	1:A:596:LEU:HD22	1.91	0.53
1:A:157:ASN:ND2	1:A:600:ARG:O	2.41	0.53
1:B:599:ASN:O	1:B:629:LYS:HB2	2.09	0.53
1:A:616:ASP:OD1	1:A:617:SER:N	2.42	0.53
1:A:643:VAL:O	1:A:647:LYS:NZ	2.41	0.53
1:A:206:PRO:O	1:A:210:VAL:HG22	2.10	0.52
1:B:214:VAL:O	1:B:217:ILE:HG13	2.09	0.52
1:B:717:THR:HG22	1:B:718:GLU:H	1.75	0.52
1:A:123:ASP:OD1	1:A:138:ARG:NH2	2.30	0.51
1:A:290:PHE:HZ	1:A:301:LEU:HD21	1.76	0.51
1:A:554:ASN:HB2	1:A:583:SER:OG	2.09	0.51
1:B:81:TYR:OH	1:B:346:ALA:HB2	2.10	0.51
1:B:226:VAL:CG2	1:B:441:ARG:HB2	2.40	0.51
1:A:732:MET:HG3	1:A:733:GLY:N	2.25	0.51
1:B:206:PRO:O	1:B:210:VAL:HG22	2.09	0.51
1:A:466:THR:HG21	1:A:484:LEU:HD22	1.93	0.51
1:A:427:TYR:O	1:A:431:LEU:HG	2.10	0.51
1:A:758:LEU:O	1:A:762:CYS:HB3	2.11	0.51
1:B:89:ILE:HG13	1:B:356:VAL:HG21	1.92	0.51
1:B:200:GLY:C	1:B:202:GLY:N	2.67	0.51
1:A:721:GLU:C	1:A:723:ALA:N	2.68	0.51
1:B:215:SER:O	1:B:215:SER:OG	2.25	0.51
1:A:220:LEU:O	1:A:224:THR:HG21	2.10	0.50
1:B:290:PHE:HZ	1:B:301:LEU:HD21	1.75	0.50
1:A:562:PHE:CE1	1:A:573:LEU:HD23	2.47	0.50
1:B:442:THR:CG2	1:B:445:LYS:HB2	2.42	0.50
1:B:453:ALA:O	1:B:457:VAL:HG23	2.11	0.50
1:A:747:LYS:O	1:A:751:VAL:HG23	2.12	0.50
1:A:750:ILE:HA	1:A:754:ALA:HB3	1.94	0.50
1:B:358:ASN:HB3	1:B:362:ASP:OD2	2.12	0.50
1:A:81:TYR:OH	1:A:346:ALA:HB2	2.11	0.50
1:A:89:ILE:HG13	1:A:356:VAL:HG21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:VAL:HG13	1:A:583:SER:HB3	1.92	0.50
1:B:466:THR:HG21	1:B:484:LEU:HD22	1.93	0.50
1:A:104:TYR:OH	1:A:281:LEU:O	2.22	0.50
1:A:522:ILE:O	1:A:523:TRP:C	2.54	0.50
1:A:541:ARG:HH22	1:A:610:ARG:HD2	1.76	0.50
1:A:268:PHE:CD2	1:A:365:PRO:HG3	2.47	0.50
1:B:355:ASN:OD1	1:B:355:ASN:N	2.45	0.50
1:A:547:MET:SD	1:A:575:SER:OG	2.69	0.50
1:A:549:THR:O	1:A:549:THR:OG1	2.29	0.50
1:A:218:LYS:O	1:A:219:SER:HB3	2.12	0.49
1:A:562:PHE:CD2	1:A:588:PHE:HZ	2.30	0.49
1:A:652:HIS:O	1:A:654:HIS:N	2.45	0.49
1:B:268:PHE:CD2	1:B:365:PRO:HG3	2.47	0.49
1:A:138:ARG:NH1	1:A:597:PRO:O	2.45	0.49
1:A:562:PHE:HE1	1:A:573:LEU:HD23	1.78	0.49
1:A:607:PHE:HD2	1:A:645:TYR:CD2	2.30	0.49
1:B:206:PRO:HB3	1:B:384:SER:HB3	1.94	0.49
1:A:442:THR:HG23	1:A:445:LYS:H	1.78	0.48
1:A:737:ILE:HD13	1:A:783:TYR:HB2	1.95	0.48
1:A:358:ASN:HB3	1:A:362:ASP:OD1	2.13	0.48
1:A:737:ILE:HG23	1:A:785:LEU:CD1	2.43	0.48
1:A:60:SER:O	1:A:64:GLN:HG2	2.13	0.48
1:A:732:MET:HG3	1:A:733:GLY:H	1.79	0.48
1:A:645:TYR:O	1:A:648:GLU:HB3	2.14	0.48
1:B:442:THR:HG23	1:B:445:LYS:H	1.78	0.48
1:A:215:SER:O	1:A:215:SER:OG	2.24	0.48
1:B:269:ASN:ND2	1:B:363:SER:HB2	2.29	0.48
1:A:743:SER:OG	1:A:748:LYS:HG3	2.14	0.47
1:B:60:SER:O	1:B:64:GLN:HG2	2.13	0.47
1:A:596:LEU:HD13	1:A:625:ARG:HB3	1.96	0.47
1:A:269:ASN:ND2	1:A:363:SER:HB2	2.29	0.47
1:B:547:MET:HG3	1:B:578:ILE:HD12	1.96	0.47
1:A:548:ALA:O	1:A:549:THR:HG22	2.15	0.47
1:A:773:ARG:HG3	1:A:773:ARG:O	2.14	0.47
1:A:600:ARG:O	1:A:600:ARG:HG3	2.14	0.47
1:A:540:SER:C	1:A:542:GLU:H	2.21	0.47
1:A:546:GLN:HG2	1:A:546:GLN:O	2.16	0.46
1:B:445:LYS:HA	1:B:448:HIS:CD2	2.50	0.46
1:A:115:VAL:HG22	1:A:314:MET:HE1	1.96	0.46
1:A:777:LEU:HD13	1:B:581:LEU:HD21	1.96	0.46
1:B:200:GLY:O	1:B:202:GLY:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ARG:HD2	1:A:612:VAL:HG13	1.96	0.46
1:A:740:GLU:HB2	1:A:741:LYS:H	1.60	0.46
1:B:409:VAL:HG13	1:B:420:VAL:HB	1.97	0.46
1:B:430:MET:O	1:B:434:ILE:HG12	2.15	0.46
1:B:400:ARG:O	1:B:595:THR:HG21	2.15	0.46
1:A:638:PHE:O	1:A:639:GLU:C	2.58	0.46
1:A:721:GLU:O	1:A:723:ALA:N	2.45	0.46
1:A:409:VAL:HG13	1:A:420:VAL:HB	1.97	0.46
1:B:195:THR:O	1:B:199:ILE:HG13	2.16	0.46
1:B:232:ILE:HG21	1:B:381:ILE:HD11	1.98	0.46
1:B:764:GLU:H	1:B:764:GLU:CD	2.24	0.46
1:A:574:PHE:O	1:A:578:ILE:HG12	2.16	0.46
1:A:581:LEU:HD22	1:A:581:LEU:H	1.80	0.46
1:B:603:SER:OG	1:B:604:SER:N	2.49	0.46
1:A:96:VAL:HG11	1:A:279:LYS:NZ	2.31	0.46
1:A:373:PHE:O	1:A:377:VAL:HG23	2.16	0.46
1:A:481:ALA:O	1:A:485:VAL:HG13	2.16	0.45
1:A:643:VAL:HG12	1:A:647:LYS:HZ2	1.81	0.45
1:A:778:LYS:HE3	1:A:778:LYS:HB3	1.24	0.45
1:B:373:PHE:O	1:B:377:VAL:HG23	2.16	0.45
1:B:481:ALA:O	1:B:485:VAL:HG13	2.16	0.45
1:A:232:ILE:HG21	1:A:381:ILE:HD11	1.98	0.45
1:B:70:TYR:OH	1:B:330:PHE:HB2	2.17	0.45
1:A:70:TYR:OH	1:A:330:PHE:HB2	2.17	0.45
1:A:122:ASN:HD22	1:A:125:GLY:HA2	1.81	0.45
1:A:535:LEU:HG	1:A:566:LEU:CD1	2.46	0.45
1:A:440:PHE:HD2	1:A:445:LYS:HB3	1.82	0.45
1:B:199:ILE:HG22	1:B:199:ILE:O	2.16	0.45
1:A:220:LEU:O	1:A:224:THR:CG2	2.65	0.45
1:A:539:ILE:HG22	1:A:543:ASN:HB2	1.98	0.45
1:B:122:ASN:HD22	1:B:125:GLY:HA2	1.82	0.45
1:A:89:ILE:HB	1:A:353:THR:HG22	1.98	0.44
1:A:609:PHE:HB3	1:A:649:PHE:CD2	2.52	0.44
1:B:218:LYS:C	1:B:220:LEU:N	2.74	0.44
1:A:562:PHE:HD2	1:A:588:PHE:HZ	1.64	0.44
1:A:582:SER:O	1:A:582:SER:OG	2.29	0.44
1:A:249:PHE:H	1:A:249:PHE:HD1	1.66	0.44
1:A:456:THR:O	1:A:459:VAL:HG22	2.17	0.44
1:B:96:VAL:HG11	1:B:279:LYS:NZ	2.31	0.44
1:A:637:GLU:O	1:A:638:PHE:C	2.61	0.44
1:A:289:TYR:O	1:A:293:THR:OG1	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:LEU:HD12	1:A:508:LEU:HA	1.85	0.44
1:A:530:LYS:HE2	1:A:530:LYS:HB2	1.58	0.44
1:A:647:LYS:HG2	1:A:720:VAL:HB	1.98	0.44
1:A:571:THR:HB	1:A:572:PRO:CD	2.47	0.43
1:A:581:LEU:O	1:A:582:SER:HB2	2.18	0.43
1:B:522:ILE:O	1:B:526:VAL:HG23	2.18	0.43
1:A:600:ARG:NH2	1:A:602:THR:HA	2.34	0.43
1:A:445:LYS:HA	1:A:448:HIS:CD2	2.53	0.43
1:A:544:ALA:CB	1:A:570:ILE:HD13	2.48	0.43
1:A:547:MET:HE3	1:A:547:MET:HB3	1.88	0.43
1:A:565:GLU:H	1:A:565:GLU:HG3	1.59	0.43
1:B:494:TYR:O	1:B:498:VAL:HG23	2.18	0.43
1:B:249:PHE:HD1	1:B:249:PHE:H	1.66	0.43
1:B:442:THR:CG2	1:B:445:LYS:H	2.31	0.43
1:A:176:LYS:HE2	1:A:176:LYS:HB2	1.81	0.43
1:A:545:ILE:HG21	1:A:614:PRO:HD3	1.99	0.43
1:A:611:TYR:O	1:A:613:GLY:N	2.47	0.43
1:A:440:PHE:CD2	1:A:445:LYS:HE3	2.54	0.43
1:A:556:VAL:HG23	1:A:585:HIS:CD2	2.53	0.43
1:B:267:LEU:HG	1:B:340:THR:HG21	2.01	0.43
1:A:169:ARG:HA	1:A:172:MET:HG2	2.01	0.42
1:A:516:LEU:O	1:A:520:MET:HG3	2.19	0.42
1:B:582:SER:O	1:B:582:SER:OG	2.32	0.42
1:A:218:LYS:O	1:A:219:SER:CB	2.67	0.42
1:A:135:LEU:HD23	1:A:468:ILE:HD13	2.00	0.42
1:B:752:ASN:O	1:B:756:ASN:ND2	2.52	0.42
1:A:173:ILE:O	1:A:177:LEU:HB2	2.20	0.42
1:A:206:PRO:HB3	1:A:384:SER:HB3	2.01	0.42
1:A:222:GLN:O	1:A:225:VAL:HG22	2.19	0.42
1:A:652:HIS:C	1:A:654:HIS:N	2.77	0.42
1:A:734:GLU:OE2	1:B:778:LYS:HD2	2.19	0.42
1:B:135:LEU:HD23	1:B:468:ILE:HD13	2.02	0.42
1:A:155:LEU:HD23	1:A:601:VAL:HG22	2.02	0.42
1:A:267:LEU:HG	1:A:340:THR:HG21	2.01	0.42
1:A:533:TYR:CE2	1:A:537:GLU:HG3	2.53	0.42
1:A:562:PHE:HB2	1:A:588:PHE:CZ	2.54	0.42
1:A:726:LYS:H	1:A:726:LYS:HG2	1.55	0.42
1:A:400:ARG:HD3	1:A:628:TYR:O	2.20	0.42
1:B:172:MET:HA	1:B:175:GLU:HG2	2.02	0.42
1:A:588:PHE:N	1:A:618:GLY:O	2.33	0.42
1:B:440:PHE:CD2	1:B:445:LYS:HE3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ILE:HG22	1:A:335:TYR:HE1	1.85	0.42
1:A:606:ARG:CZ	1:A:626:TYR:CE1	3.03	0.42
1:B:398:SER:OG	1:B:404:PHE:HB2	2.20	0.42
1:B:455:VAL:O	1:B:459:VAL:HG22	2.20	0.42
1:A:278:LEU:HD23	1:A:278:LEU:HA	1.85	0.41
1:A:771:ILE:HG21	1:A:776:LEU:HD13	2.00	0.41
1:B:211:LEU:O	1:B:215:SER:HB3	2.19	0.41
1:B:289:TYR:O	1:B:293:THR:OG1	2.15	0.41
1:A:456:THR:C	1:A:458:MET:H	2.28	0.41
1:A:525:TYR:C	1:A:527:ALA:H	2.27	0.41
1:A:540:SER:C	1:A:542:GLU:N	2.77	0.41
1:A:619:MET:HB3	1:A:619:MET:HE2	1.55	0.41
1:B:76:SER:O	1:B:80:VAL:HG23	2.20	0.41
1:B:76:SER:C	1:B:78:LEU:H	2.28	0.41
1:B:207:SER:O	1:B:211:LEU:HB2	2.20	0.41
1:A:290:PHE:HE1	1:A:297:GLY:C	2.29	0.41
1:B:101:LEU:HG	1:B:286:ILE:HG23	2.02	0.41
1:B:106:ILE:HG22	1:B:335:TYR:HE1	1.85	0.41
1:A:101:LEU:HB3	1:A:304:VAL:HG11	2.01	0.41
1:B:115:VAL:HG13	1:B:327:GLN:HG2	2.03	0.41
1:B:427:TYR:O	1:B:431:LEU:HG	2.20	0.41
1:B:443:THR:HG22	1:B:443:THR:O	2.20	0.41
1:B:480:ILE:H	1:B:480:ILE:HG13	1.69	0.41
1:B:290:PHE:HE1	1:B:297:GLY:C	2.29	0.41
1:A:452:ILE:HG13	1:A:498:VAL:HG12	2.03	0.41
1:A:634:GLU:O	1:A:635:PRO:C	2.63	0.41
1:B:211:LEU:HD12	1:B:229:SER:OG	2.20	0.41
1:A:449:ALA:HB1	1:A:509:PRO:HD3	2.03	0.41
1:A:456:THR:O	1:A:458:MET:N	2.54	0.41
1:B:222:GLN:O	1:B:225:VAL:HG22	2.21	0.41
1:B:459:VAL:O	1:B:463:LEU:HG	2.21	0.41
1:A:113:LYS:HB2	1:A:487:PHE:CE1	2.56	0.40
1:A:524:GLN:O	1:A:528:VAL:HG23	2.21	0.40
1:A:631:ASP:HB2	1:A:632:ILE:H	1.70	0.40
1:B:336:PRO:O	1:B:340:THR:OG1	2.27	0.40
1:B:607:PHE:CD1	1:B:624:VAL:HG22	2.56	0.40
1:A:76:SER:O	1:A:80:VAL:HG23	2.20	0.40
1:A:581:LEU:O	1:A:582:SER:CB	2.68	0.40
1:B:440:PHE:HD2	1:B:445:LYS:HB3	1.85	0.40
1:B:558:GLY:O	1:B:723:ALA:HB1	2.21	0.40
1:A:101:LEU:HG	1:A:286:ILE:HG23	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:VAL:HG13	1:A:327:GLN:HG2	2.02	0.40
1:A:771:ILE:O	1:A:772:PRO:C	2.65	0.40
1:B:79:TYR:HD1	1:B:306:LEU:HD13	1.87	0.40
1:A:76:SER:C	1:A:78:LEU:H	2.29	0.40
1:A:398:SER:OG	1:A:404:PHE:HB2	2.20	0.40
1:B:445:LYS:NZ	1:B:504:SER:O	2.36	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	658/798 (82%)	549 (83%)	90 (14%)	19 (3%)	3	23
1	B	658/798 (82%)	582 (88%)	69 (10%)	7 (1%)	11	42
All	All	1316/1596 (82%)	1131 (86%)	159 (12%)	26 (2%)	8	30

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	545	ILE
1	A	581	LEU
1	A	582	SER
1	A	607	PHE
1	A	744	SER
1	A	457	VAL
1	A	602	THR
1	A	612	VAL
1	A	639	GLU
1	A	653	GLU
1	A	722	LYS
1	B	443	THR

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Mol	Chain	Res	Type
1	B	500	TYR
1	B	602	THR
1	A	476	ASN
1	A	519	MET
1	A	580	ASN
1	B	201	ASP
1	B	441	ARG
1	B	476	ASN
1	A	578	ILE
1	A	614	PRO
1	A	635	PRO
1	A	740	GLU
1	B	457	VAL
1	A	571	THR

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	577/694 (83%)	497 (86%)	80 (14%)	3	16
1	B	577/694 (83%)	542 (94%)	35 (6%)	17	47
All	All	1154/1388 (83%)	1039 (90%)	115 (10%)	9	29

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	THR
1	A	95	VAL
1	A	100	SER
1	A	119	LEU
1	A	151	GLU
1	A	214	VAL
1	A	217	ILE
1	A	218	LYS
1	A	219	SER

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Mol	Chain	Res	Type
1	A	232	ILE
1	A	270	LEU
1	A	286	ILE
1	A	287	ILE
1	A	353	THR
1	A	410	VAL
1	A	474	LYS
1	A	475	THR
1	A	497	SER
1	A	519	MET
1	A	530	LYS
1	A	532	ARG
1	A	533	TYR
1	A	535	LEU
1	A	539	ILE
1	A	540	SER
1	A	545	ILE
1	A	546	GLN
1	A	547	MET
1	A	549	THR
1	A	553	VAL
1	A	555	ARG
1	A	564	THR
1	A	565	GLU
1	A	567	VAL
1	A	572	PRO
1	A	573	LEU
1	A	575	SER
1	A	576	HIS
1	A	586	SER
1	A	587	VAL
1	A	589	VAL
1	A	591	ILE
1	A	593	ILE
1	A	596	LEU
1	A	598	VAL
1	A	600	ARG
1	A	602	THR
1	A	603	SER
1	A	610	ARG
1	A	615	LYS
1	A	617	SER

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Mol	Chain	Res	Type
1	A	619	MET
1	A	621	ARG
1	A	631	ASP
1	A	633	GLU
1	A	634	GLU
1	A	635	PRO
1	A	654	HIS
1	A	717	THR
1	A	718	GLU
1	A	719	LEU
1	A	720	VAL
1	A	721	GLU
1	A	722	LYS
1	A	724	ARG
1	A	726	LYS
1	A	728	MET
1	A	731	LEU
1	A	738	THR
1	A	740	GLU
1	A	743	SER
1	A	744	SER
1	A	759	LYS
1	A	760	LYS
1	A	762	CYS
1	A	766	ASP
1	A	767	LYS
1	A	772	PRO
1	A	778	LYS
1	A	781	MET
1	B	86	THR
1	B	95	VAL
1	B	119	LEU
1	B	212	SER
1	B	214	VAL
1	B	217	ILE
1	B	218	LYS
1	B	224	THR
1	B	270	LEU
1	B	286	ILE
1	B	287	ILE
1	B	293	THR
1	B	353	THR

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Mol	Chain	Res	Type
1	B	355	ASN
1	B	410	VAL
1	B	438	LEU
1	B	441	ARG
1	B	442	THR
1	B	457	VAL
1	B	475	THR
1	B	497	SER
1	B	519	MET
1	B	530	LYS
1	B	540	SER
1	B	564	THR
1	B	567	VAL
1	B	578	ILE
1	B	593	ILE
1	B	600	ARG
1	B	602	THR
1	B	603	SER
1	B	631	ASP
1	B	633	GLU
1	B	654	HIS
1	B	717	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	223	ASN
1	A	240	GLN
1	A	273	HIS
1	A	419	GLN
1	A	524	GLN
1	A	543	ASN
1	A	568	ASN
1	A	585	HIS
1	A	641	HIS
1	B	171	HIS
1	B	179	ASN
1	B	223	ASN
1	B	240	GLN
1	B	273	HIS
1	B	448	HIS

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Mol	Chain	Res	Type
1	B	543	ASN
1	B	761	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	ADP	A	901	-	27,29,29	1.34	4 (14%)	42,45,45	2.04	10 (23%)
2	ADP	B	901	-	27,29,29	1.34	4 (14%)	42,45,45	1.97	10 (23%)

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	ADP	A	901	-	-	2/16/32/32	0/3/3/3

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	901	-	-	5/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	ADP	C5-C4	4.39	1.47	1.39
2	B	901	ADP	C5-C4	4.38	1.47	1.39
2	A	901	ADP	C5-C6	2.63	1.48	1.41
2	B	901	ADP	C5-C6	2.60	1.48	1.41
2	A	901	ADP	C8-N7	2.32	1.36	1.31
2	B	901	ADP	C8-N7	2.29	1.35	1.31
2	B	901	ADP	C5-N7	-2.28	1.34	1.39
2	A	901	ADP	C5-N7	-2.21	1.34	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	ADP	C5-C4-N3	-6.58	118.17	126.75
2	B	901	ADP	C5-C4-N3	-6.45	118.33	126.75
2	A	901	ADP	N3-C4-N9	5.09	135.47	127.08
2	B	901	ADP	N3-C4-N9	4.99	135.30	127.08
2	A	901	ADP	C2-N3-C4	4.03	121.27	111.75
2	B	901	ADP	C2-N3-C4	3.92	121.02	111.75
2	A	901	ADP	PA-O3A-PB	-3.59	120.52	132.83
2	A	901	ADP	C4-C5-N7	-3.28	106.62	110.62
2	B	901	ADP	C4-C5-N7	-3.24	106.68	110.62
2	A	901	ADP	N3-C2-N1	-3.17	123.64	128.60
2	B	901	ADP	N3-C2-N1	-3.06	123.82	128.60
2	B	901	ADP	PA-O3A-PB	-2.99	122.56	132.83
2	A	901	ADP	C3'-C2'-C1'	2.81	106.76	101.43
2	A	901	ADP	C5-N7-C8	2.77	107.44	103.51
2	B	901	ADP	C5-N7-C8	2.70	107.35	103.51
2	B	901	ADP	C3'-C2'-C1'	2.54	106.25	101.43
2	A	901	ADP	C4-N9-C8	2.37	108.30	105.73
2	B	901	ADP	C4-N9-C8	2.35	108.28	105.73
2	A	901	ADP	C6-C5-N7	2.08	135.89	132.02
2	B	901	ADP	C6-C5-N7	2.02	135.78	132.02

There are no chirality outliers.

All (7) torsion outliers are listed below:

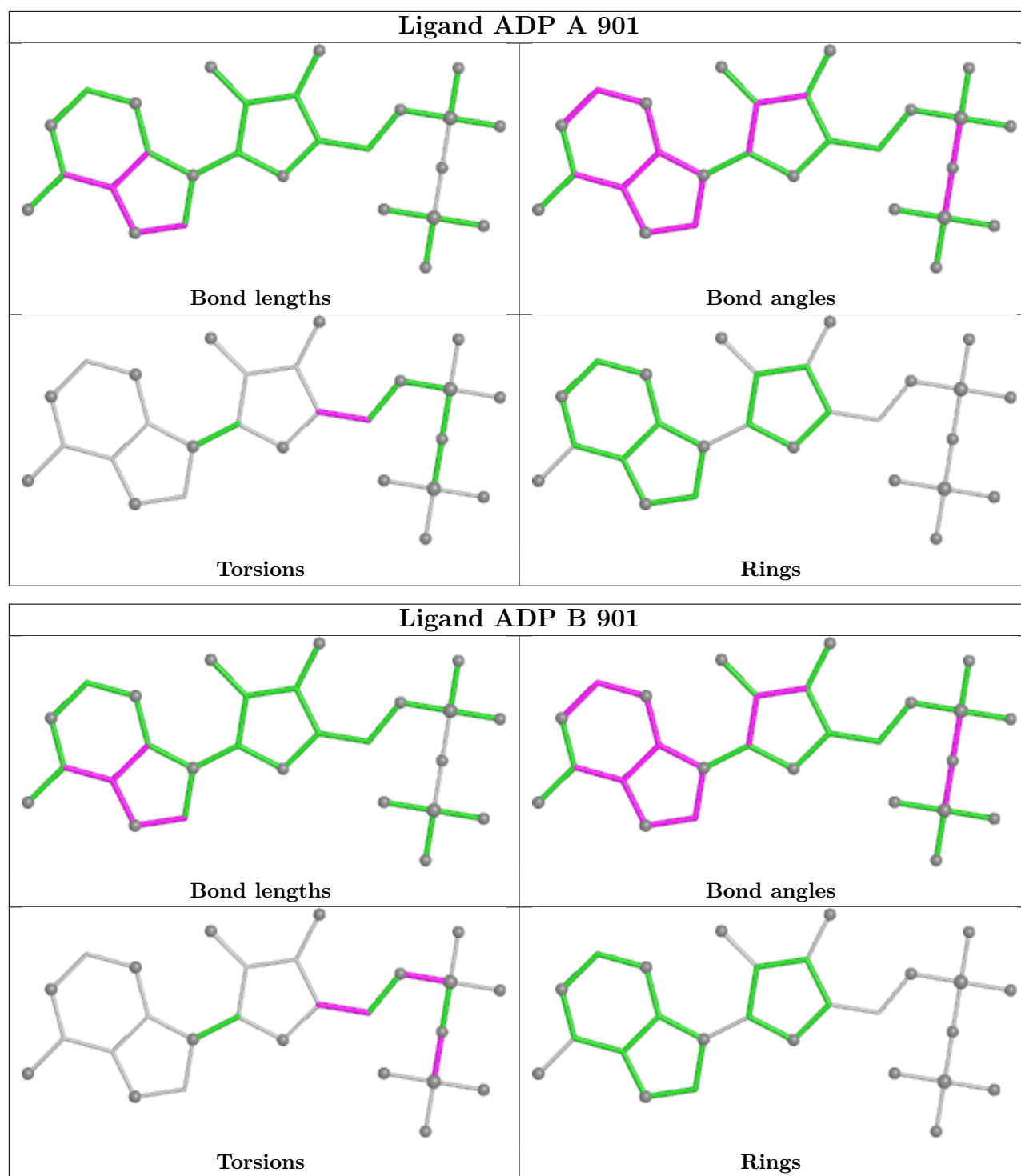
Mol	Chain	Res	Type	Atoms
2	B	901	ADP	PA-O3A-PB-O3B
2	B	901	ADP	C5'-O5'-PA-O3A
2	A	901	ADP	O4'-C4'-C5'-O5'
2	A	901	ADP	C3'-C4'-C5'-O5'
2	B	901	ADP	O4'-C4'-C5'-O5'
2	B	901	ADP	C5'-O5'-PA-O1A
2	B	901	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	ADP	2	0
2	B	901	ADP	2	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

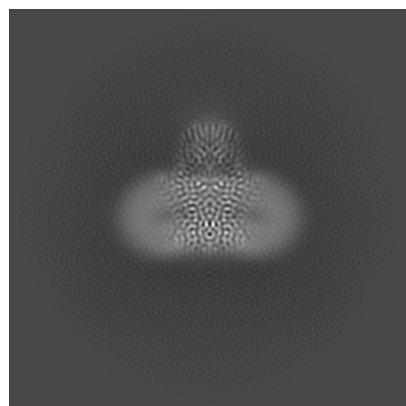
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-80182. These allow visual inspection of the internal detail of the map and identification of artifacts.

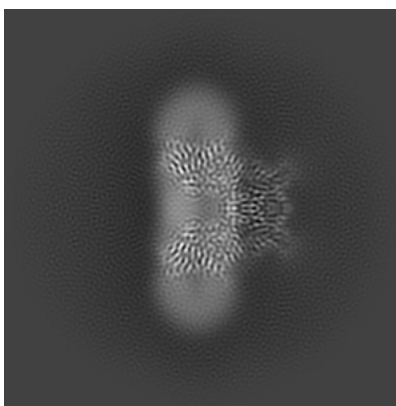
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

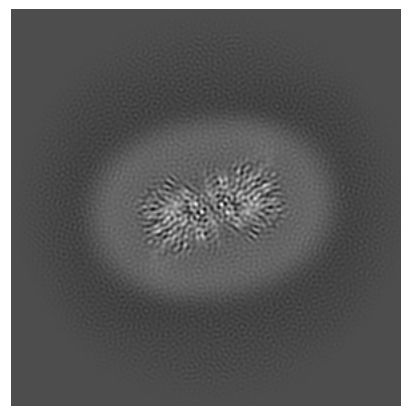
6.1.1 Primary map



X

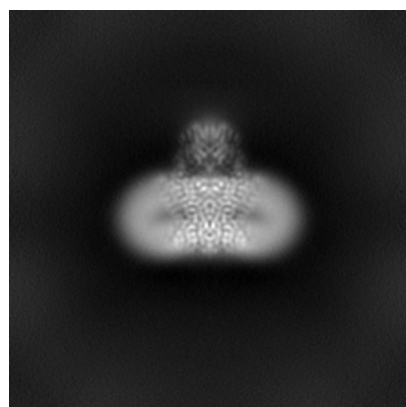


Y

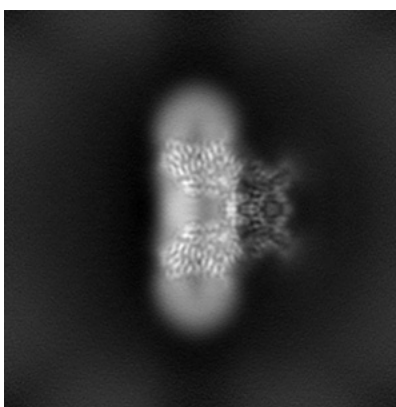


Z

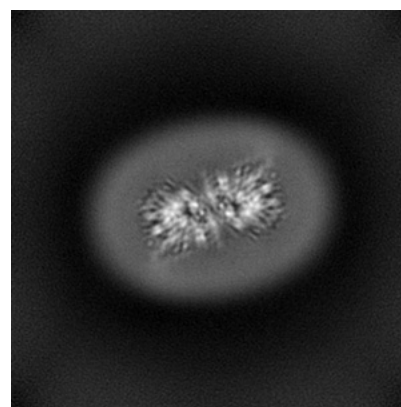
6.1.2 Raw map



X



Y

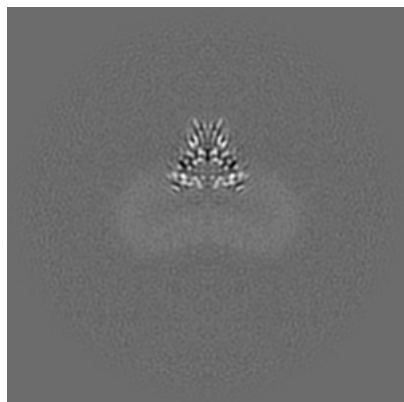


Z

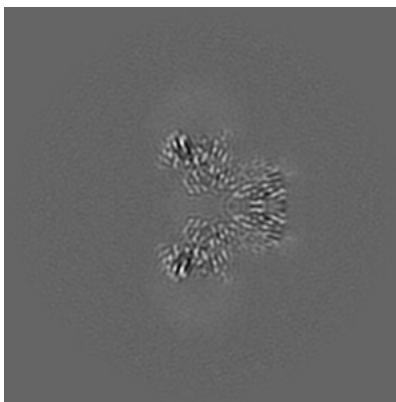
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

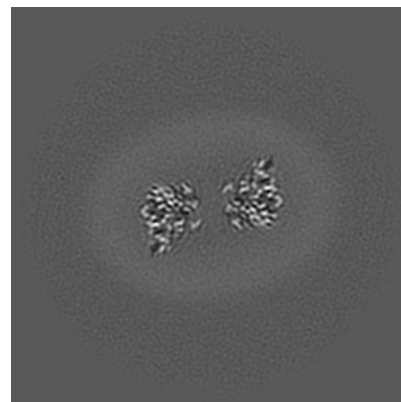
6.2.1 Primary map



X Index: 128

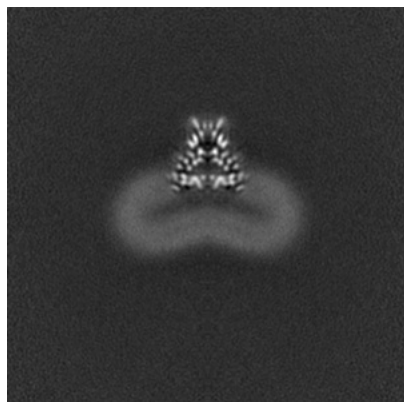


Y Index: 128

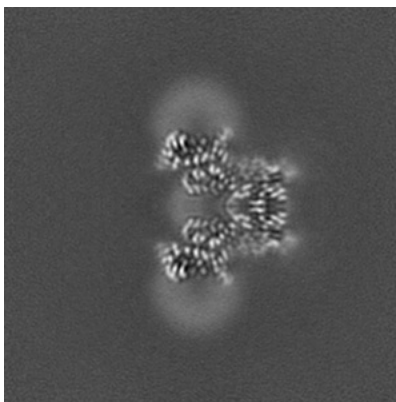


Z Index: 128

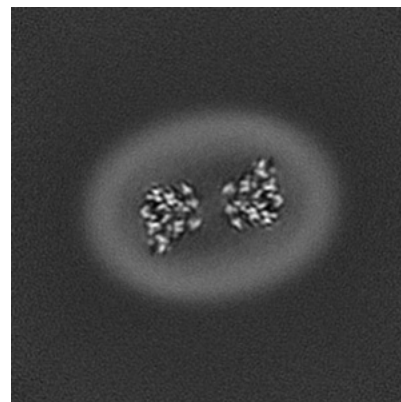
6.2.2 Raw map



X Index: 128



Y Index: 128

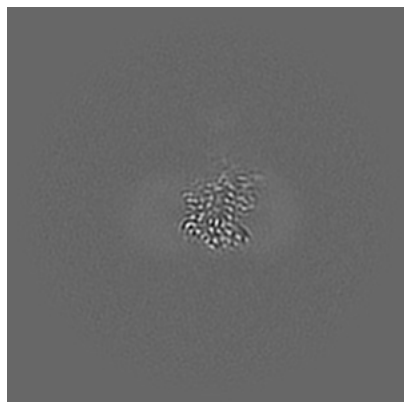


Z Index: 128

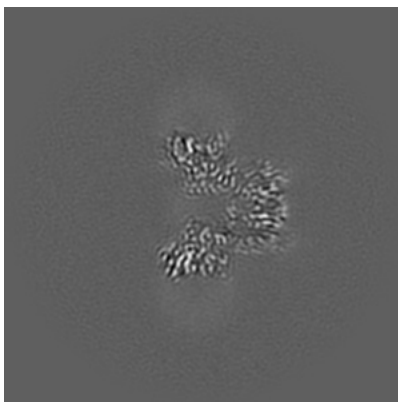
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

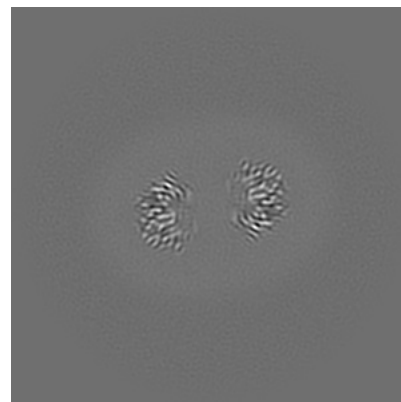
6.3.1 Primary map



X Index: 161

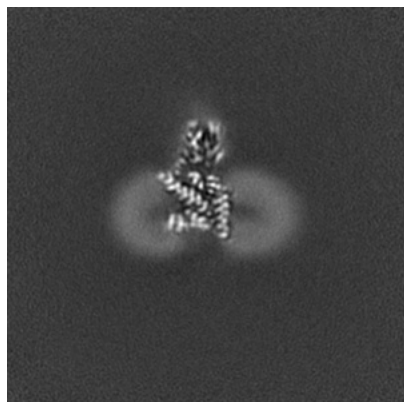


Y Index: 126

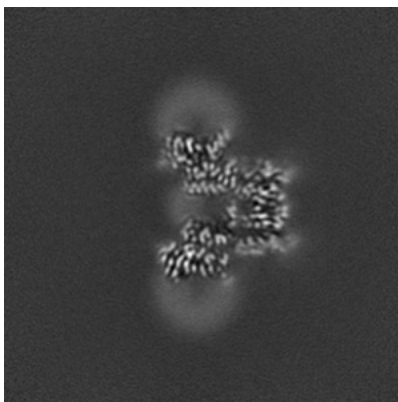


Z Index: 112

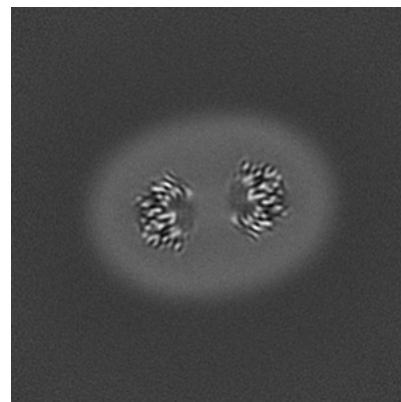
6.3.2 Raw map



X Index: 111



Y Index: 126

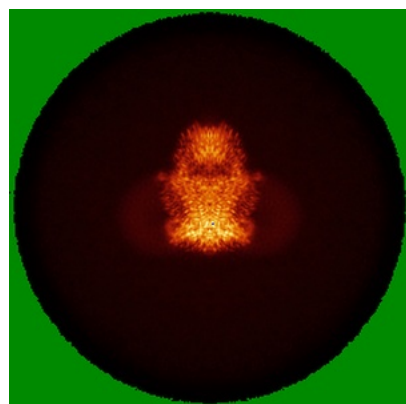


Z Index: 112

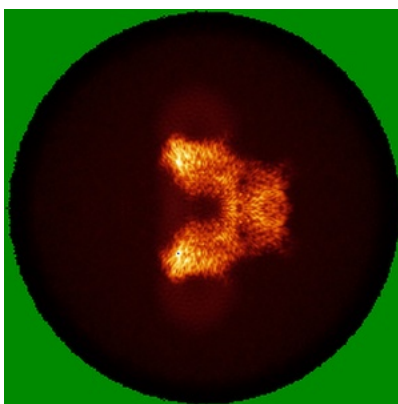
The images above show the largest variance slices of the map in three orthogonal directions.

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

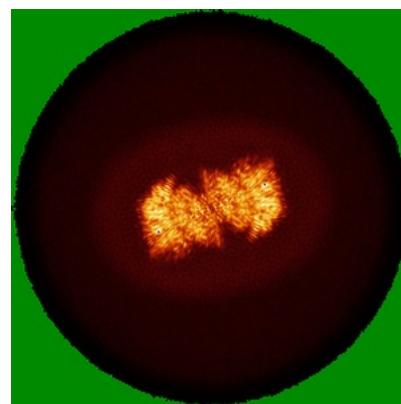
6.4.1 Primary map



X

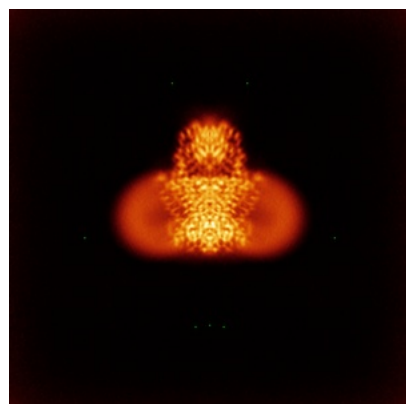


Y

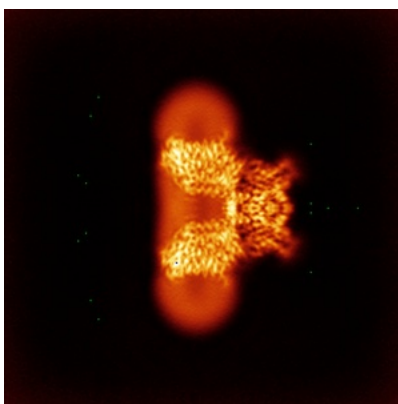


Z

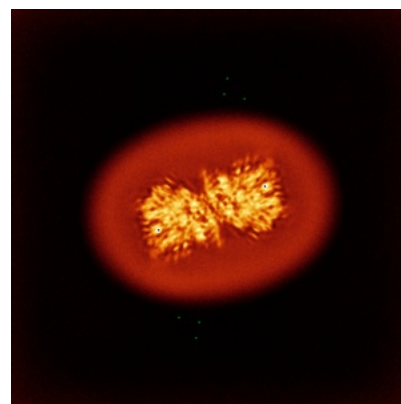
6.4.2 Raw map



X



Y

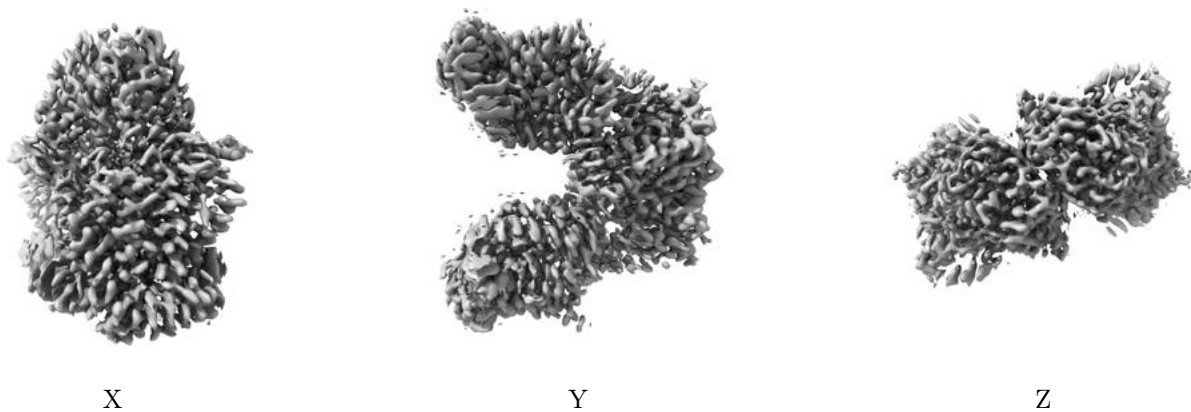


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

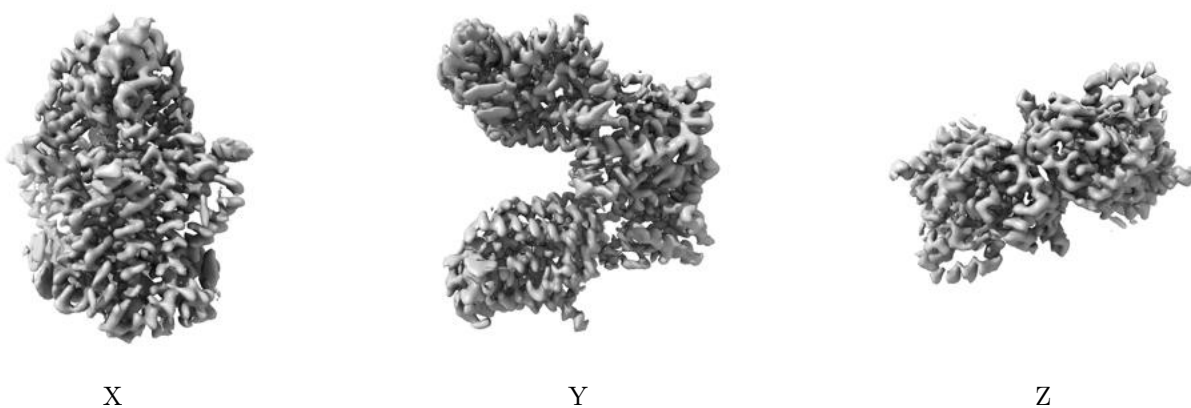
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

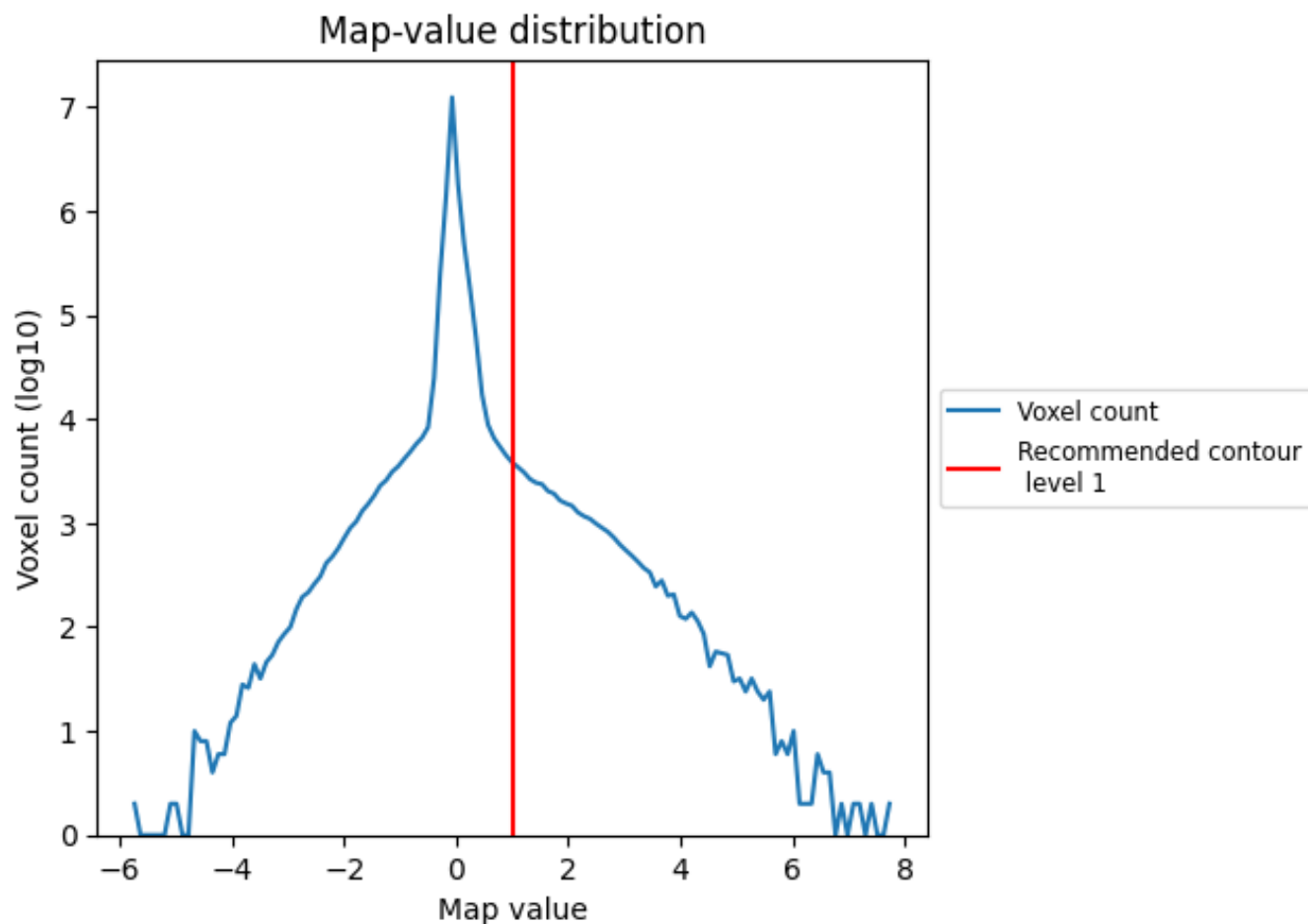
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

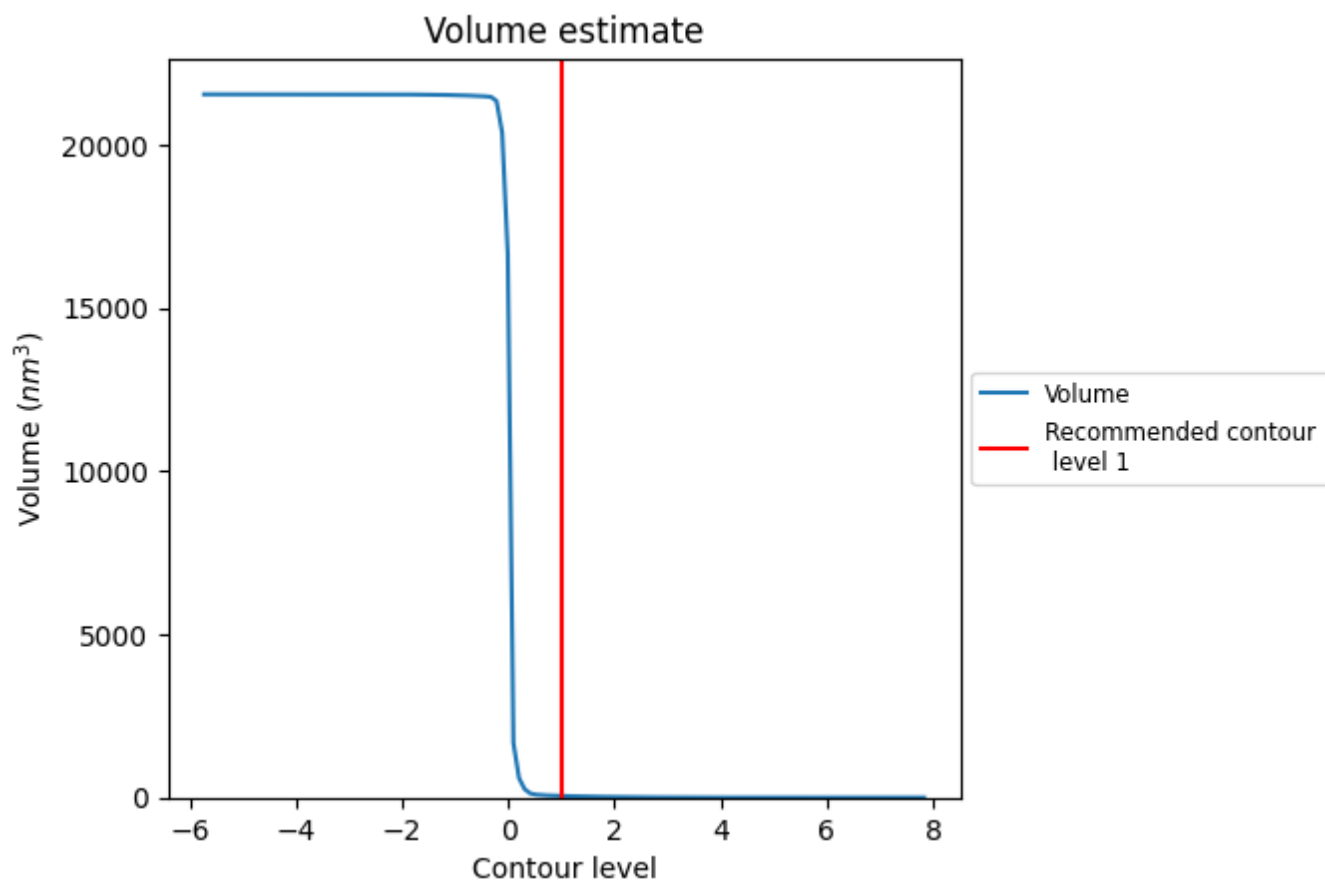
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

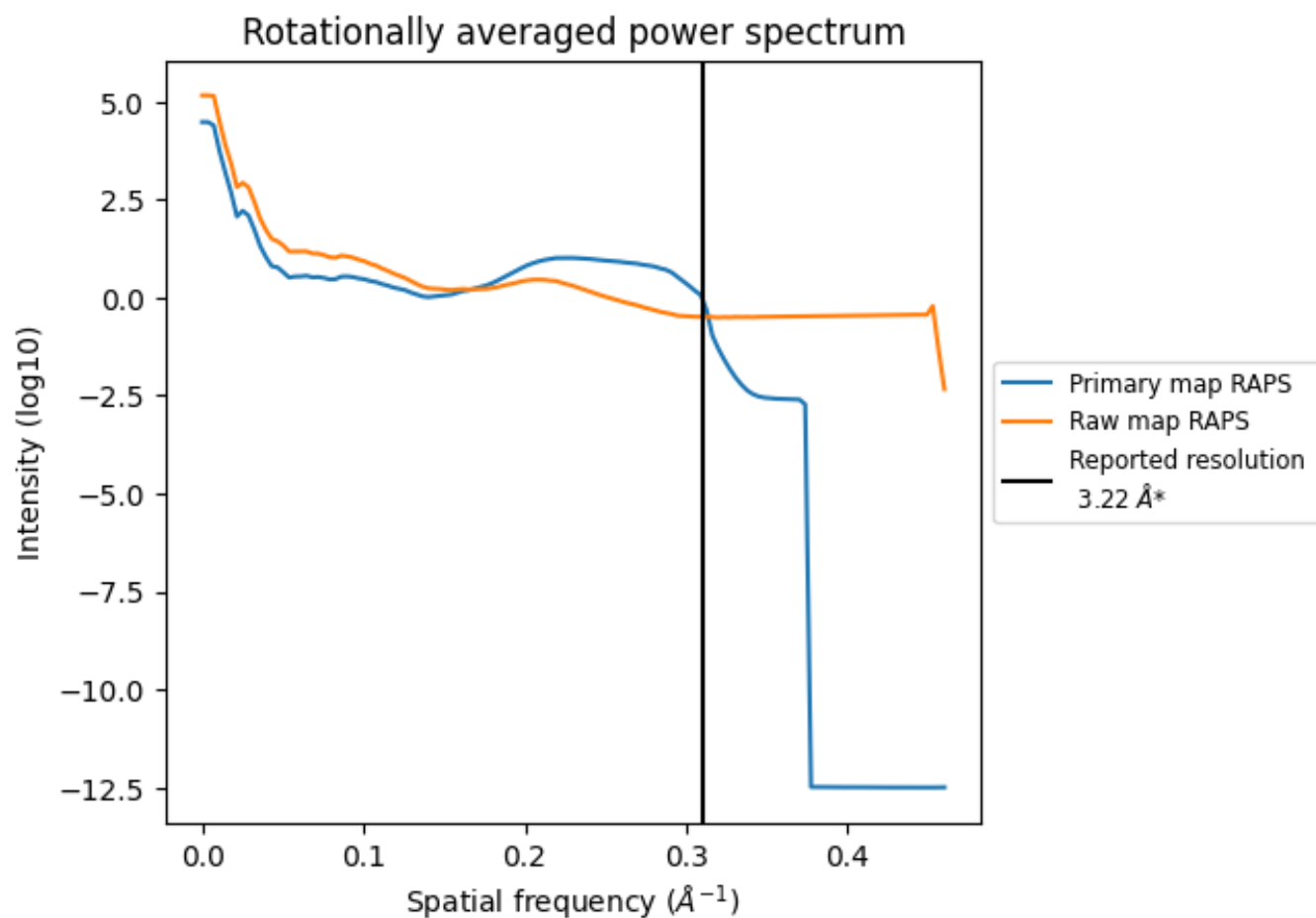
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 49 nm³; this corresponds to an approximate mass of 44 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 ⓘ

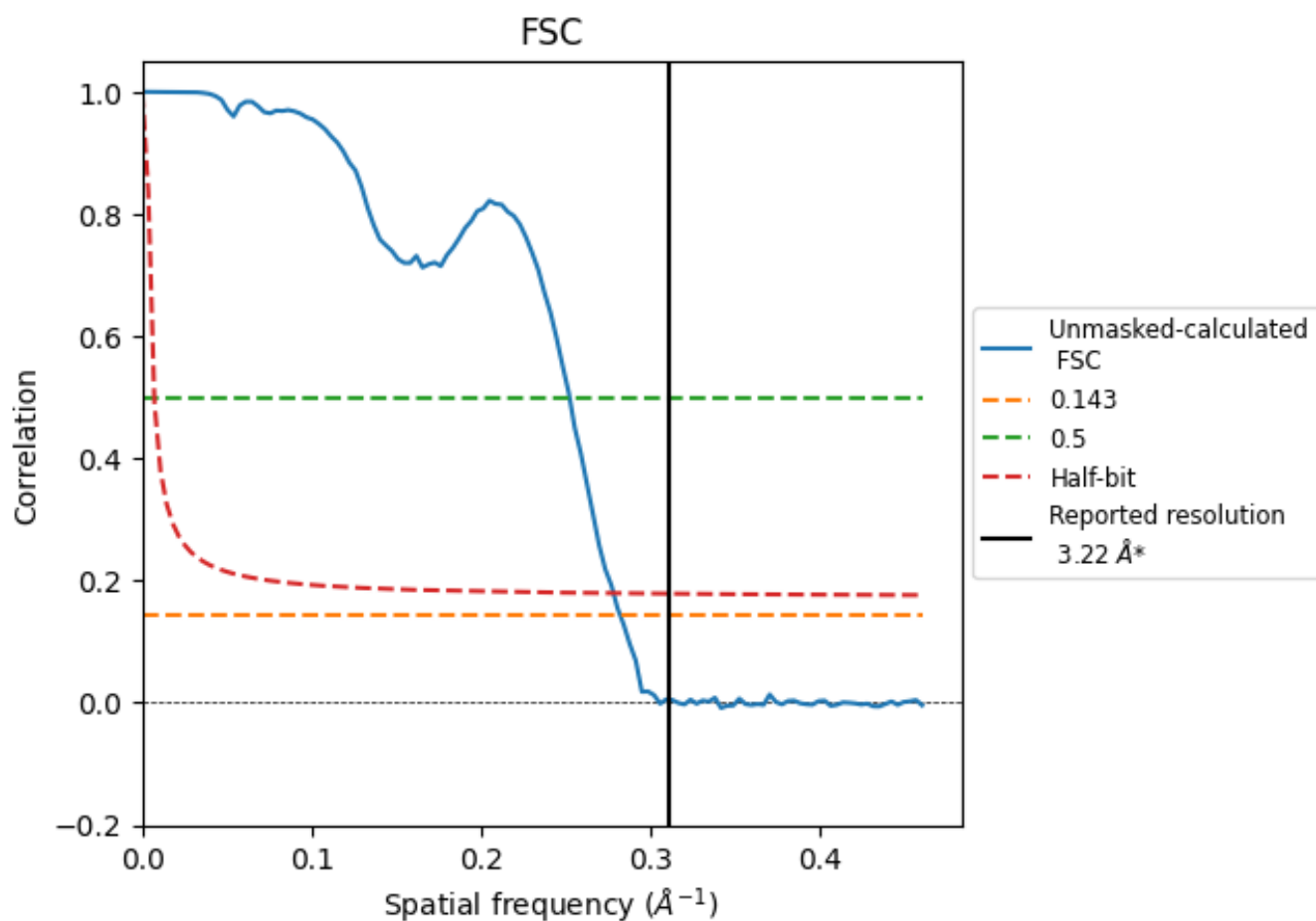


*Reported resolution corresponds to spatial frequency of 0.311 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.311 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

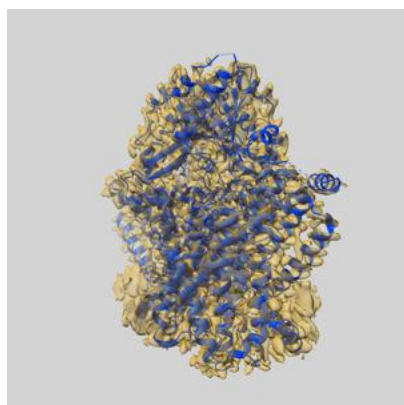
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.22	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.55	3.97	3.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.55 differs from the reported value 3.22 by more than 10 %

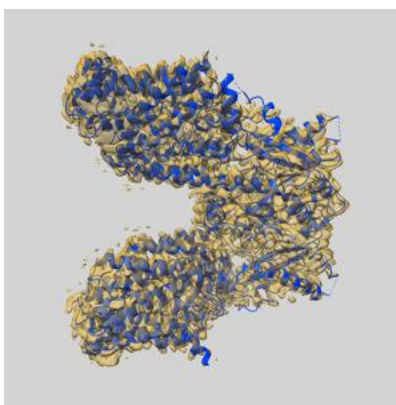
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-80182 and PDB model 25LE. Per-residue inclusion information can be found in section [3](#) on page [6](#).

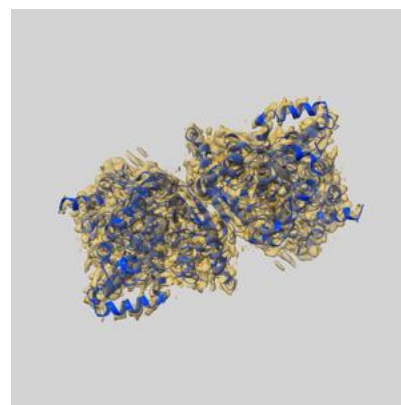
9.1 Map-model overlay [i](#)



X



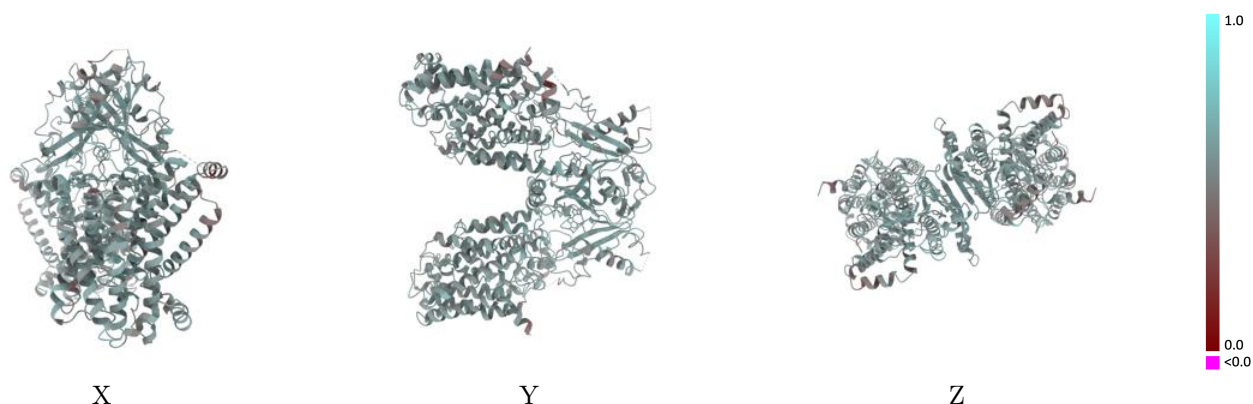
Y



Z

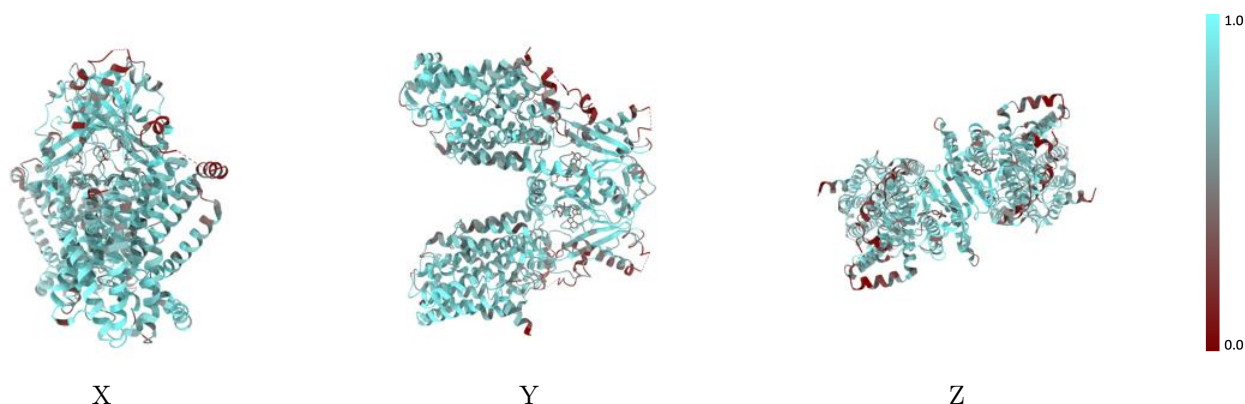
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



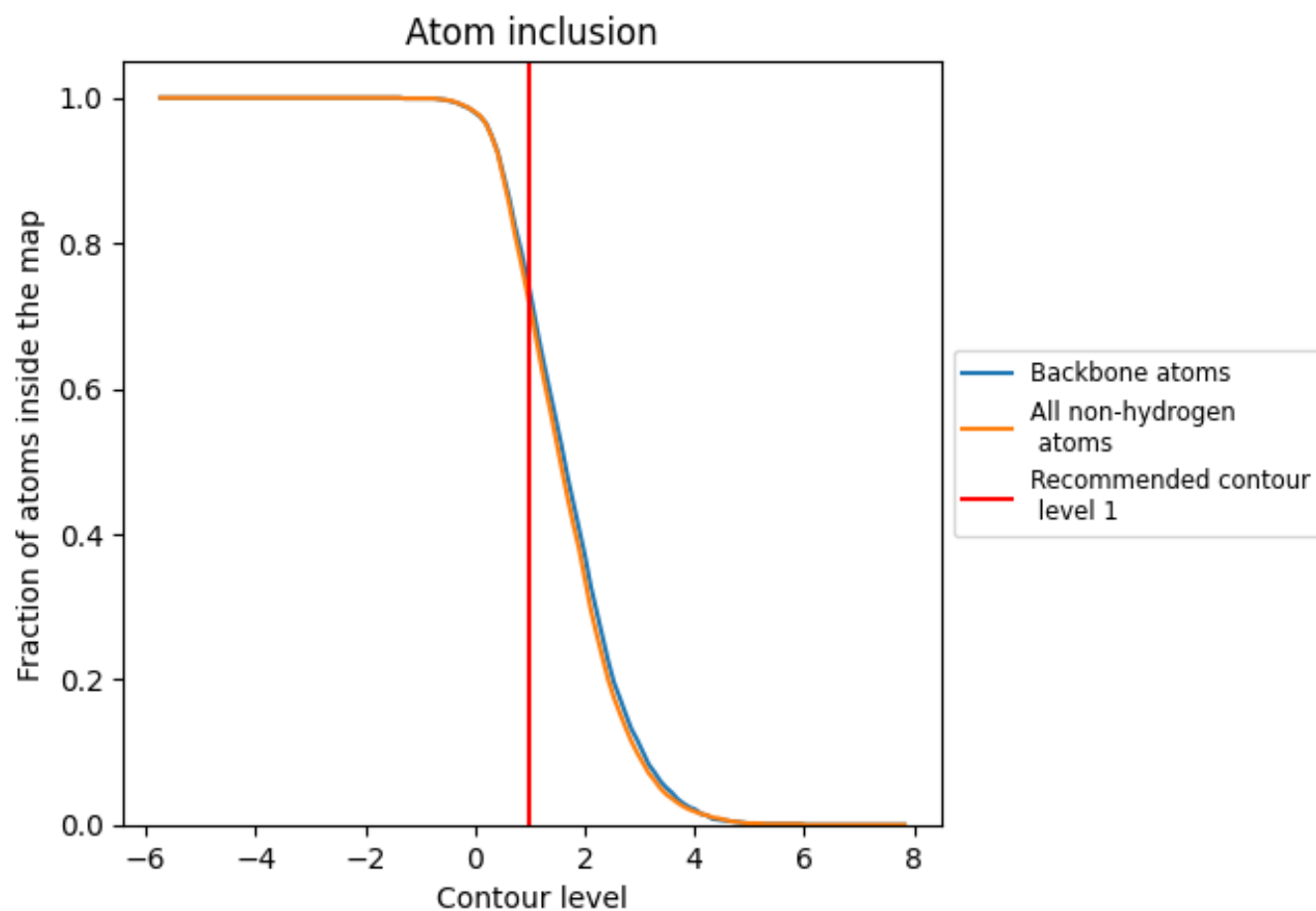
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 71% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7140	0.5550
A	0.7170	0.5580
B	0.7170	0.5510

