



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:17 AM UTC

PDB ID : 8A5P / pdb_00008a5p
EMDB ID : EMD-15180
Title : Structure of Arp4-Ies4-N-actin-Arp8-Ino80HSA subcomplex (A-module) of Chaetomium thermophilum INO80 on curved DNA
Authors : Kunert, F.; Metzner, F.J.; Eustermann, S.; Jung, J.; Woike, S.; Schall, K.; Kostrewa, D.; Hopfner, K.P.
Deposited on : 2022-06-15
Resolution : 3.40 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:

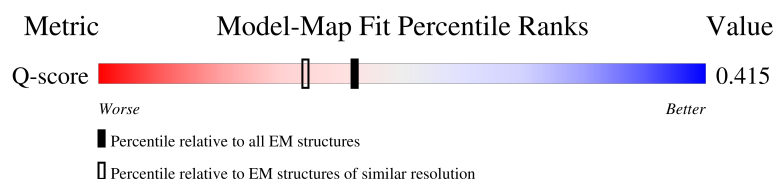
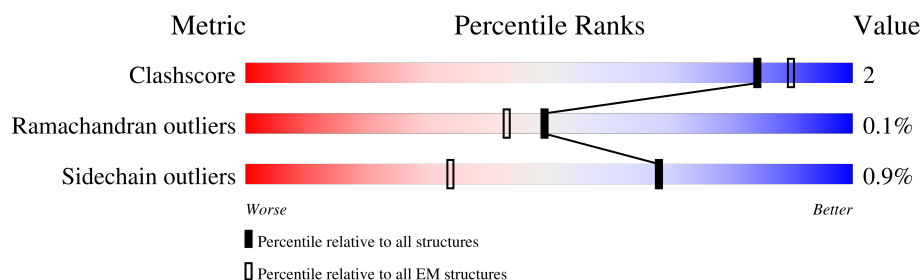
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

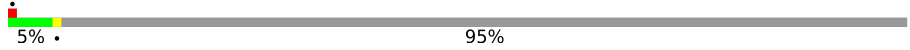
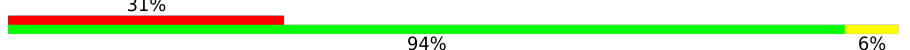
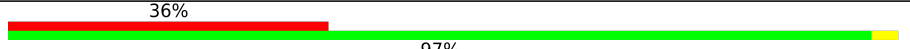
The reported resolution of this entry is 3.40 Å.

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	14717 (2.90 - 3.90)

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	G	1856	
2	K	36	
3	L	36	
4	U	747	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	V	375	87% 9%
6	W	468	85% 7% 8%
7	X	284	16% 82%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13937 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 Ino80 ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	99	Total	C	N	O	S	0	0
			831	519	164	145	3		

- Molecule 2 is a DNA chain called DNA (36-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	36	Total	C	N	O	P	0	0
			739	350	136	217	36		

- Molecule 3 is a DNA chain called DNA (36-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	36	Total	C	N	O	P	0	0
			737	349	137	215	36		

- Molecule 4 is a protein called Actin-related protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	605	Total	C	N	O	S	0	0
			4913	3115	856	915	27		

- Molecule 5 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	V	362	Total	C	N	O	S	0	0
			2831	1796	481	539	15		

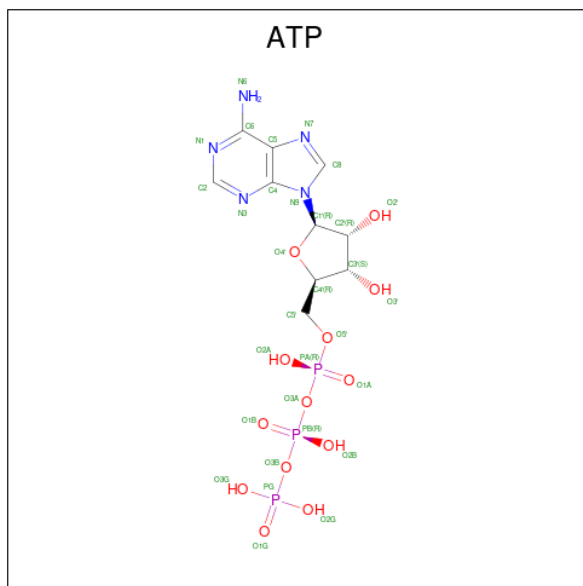
- Molecule 6 is a protein called Actin related protein 4 (Arp4).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	W	432	Total	C	N	O	S	0	0
			3377	2143	593	627	14		

- Molecule 7 is a protein called Ies4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	52	Total	C	N	O	S	0	0
			413	263	82	66	2		

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

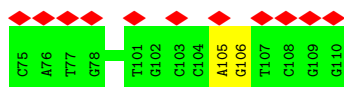


Mol	Chain	Residues	Atoms					AltConf
8	U	1	Total	C	N	O	P	0
			31	10	5	13	3	
8	V	1	Total	C	N	O	P	0
			31	10	5	13	3	
8	W	1	Total	C	N	O	P	0
			31	10	5	13	3	

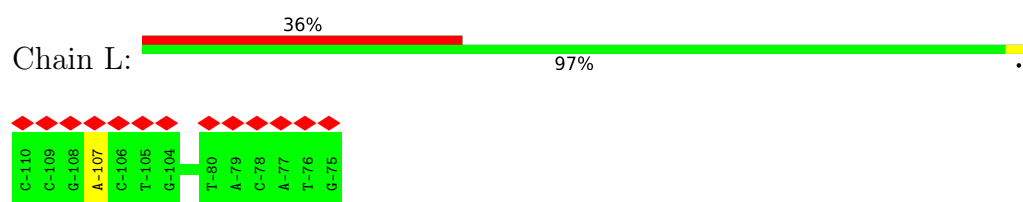
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	U	1	Total	Mg	0
			1	1	
9	V	1	Total	Mg	0
			1	1	
9	W	1	Total	Mg	0
			1	1	

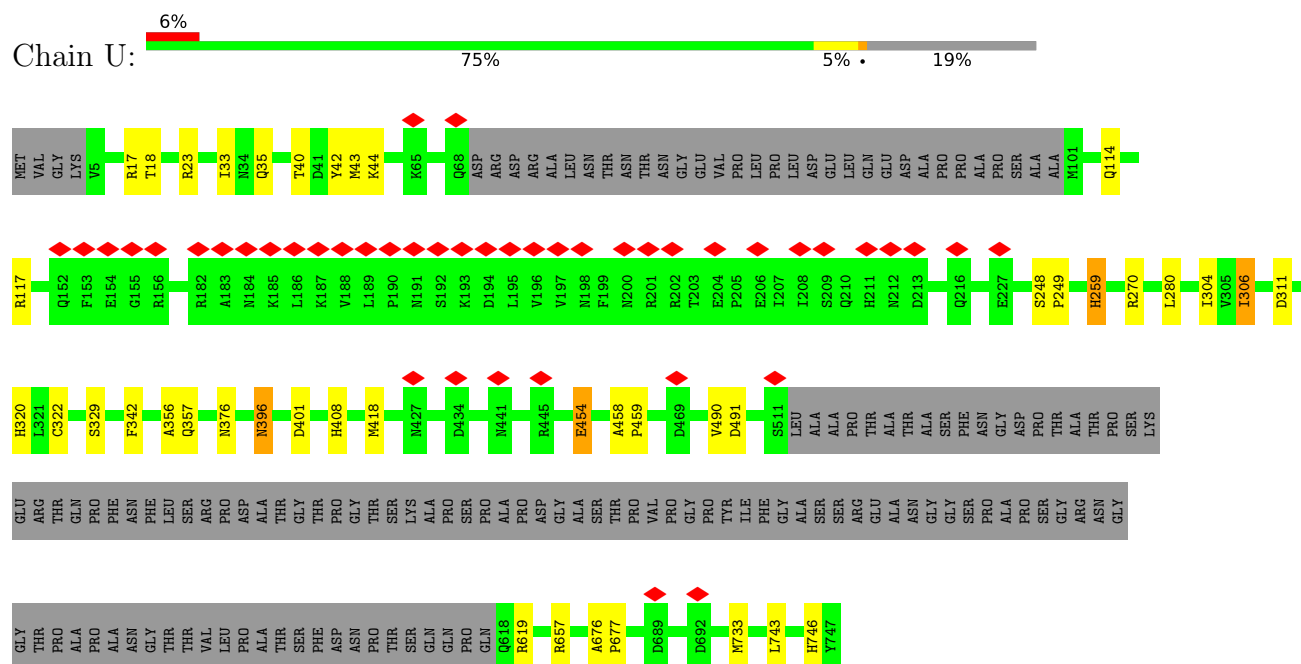
- Molecule 2: DNA (36-MER)



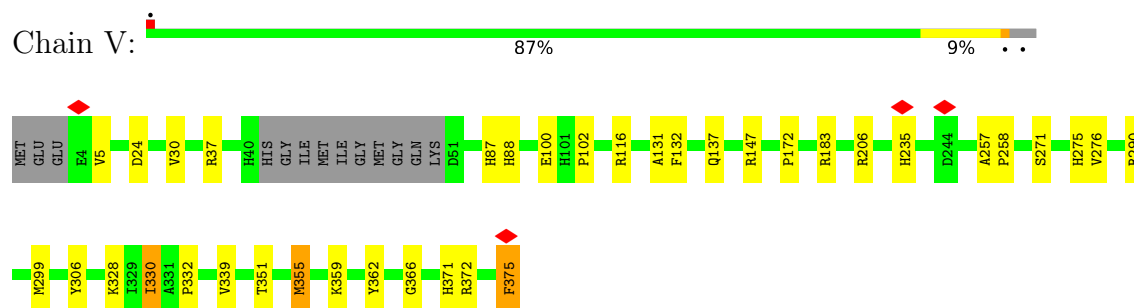
- Molecule 3: DNA (36-MER)



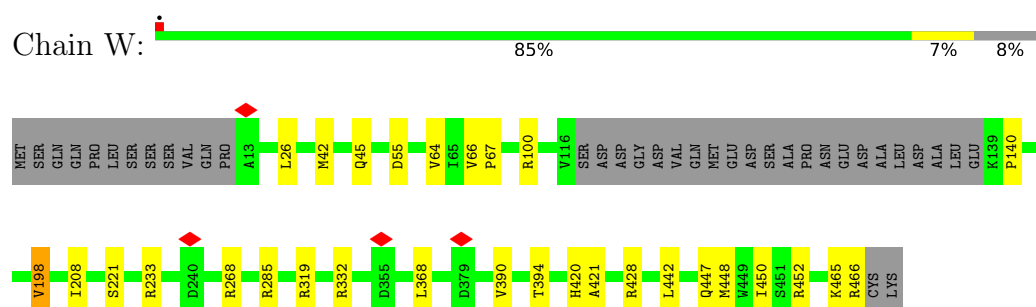
• Molecule 4: Actin-related protein 8



• Molecule 5: Actin



• Molecule 6: Actin related protein 4 (Arp4)



• Molecule 7: Ies4



ALA	PRO	VAL	PRO	ILE	ALA	VAL	VAL	ALA																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
-----	-----	-----	-----	-----	-----	-----	-----	-----	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	325000	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 ($e^-/\text{\AA}^2$)	50.5	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.088	Depositor
Minimum map value	-0.024	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	257.28, 257.28, 257.28	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

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

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	G	0.64	0/842	1.14	0/1119
2	K	0.56	0/828	0.83	0/1276
3	L	0.57	0/826	0.81	0/1272
4	U	0.69	4/5016 (0.1%)	1.07	3/6779 (0.0%)
5	V	0.81	4/2894 (0.1%)	1.15	6/3921 (0.2%)
6	W	0.72	0/3464	1.08	2/4711 (0.0%)
7	X	0.70	0/426	1.19	0/576
All	All	0.71	8/14296 (0.1%)	1.07	11/19654 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	3
4	U	0	5
5	V	0	7
6	W	0	7
7	X	0	1
All	All	0	23

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	V	371	HIS	CE1-NE2	7.38	1.40	1.32
4	U	320	HIS	CE1-NE2	7.02	1.39	1.32
4	U	746	HIS	CE1-NE2	5.83	1.38	1.32
4	U	408	HIS	CE1-NE2	5.47	1.38	1.32
5	V	355	MET	CG-SD	5.25	1.93	1.80
5	V	88	HIS	CE1-NE2	5.24	1.37	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	U	259	HIS	CE1-NE2	5.19	1.37	1.32
5	V	87	HIS	CE1-NE2	5.04	1.37	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	V	271	SER	CA-C-N	5.99	125.79	120.10
5	V	271	SER	C-N-CA	5.99	125.79	120.10
5	V	24	ASP	CA-CB-CG	5.97	118.57	112.60
4	U	401	ASP	CA-CB-CG	5.89	118.49	112.60
5	V	306	TYR	CB-CA-C	-5.85	100.43	109.62
4	U	311	ASP	CA-CB-CG	5.70	118.30	112.60
4	U	306	ILE	N-CA-CB	-5.52	108.02	111.83
5	V	375	PHE	CA-CB-CG	5.49	119.29	113.80
5	V	299	MET	CG-SD-CE	-5.19	89.48	100.90
6	W	140	PRO	N-CA-C	5.17	121.36	114.18
6	W	55	ASP	CA-CB-CG	5.11	117.71	112.60

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	748	ARG	Sidechain
1	G	778	ARG	Sidechain
1	G	803	ARG	Sidechain
4	U	17	ARG	Sidechain
4	U	23	ARG	Sidechain
4	U	270	ARG	Sidechain
4	U	619	ARG	Sidechain
4	U	657	ARG	Sidechain
5	V	116	ARG	Sidechain
5	V	147	ARG	Sidechain
5	V	183	ARG	Sidechain
5	V	206	ARG	Sidechain
5	V	290	ARG	Sidechain
5	V	37	ARG	Sidechain
5	V	372	ARG	Peptide
6	W	100	ARG	Sidechain
6	W	233	ARG	Sidechain
6	W	268	ARG	Sidechain
6	W	285	ARG	Sidechain
6	W	319	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
6	W	332	ARG	Sidechain
6	W	452	ARG	Sidechain
7	X	190	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	G	831	0	866	14	0
2	K	739	0	405	2	0
3	L	737	0	404	1	0
4	U	4913	0	4896	27	0
5	V	2831	0	2795	22	0
6	W	3377	0	3308	20	0
7	X	413	0	424	7	0
8	U	31	0	12	4	0
8	V	31	0	12	0	0
8	W	31	0	12	0	0
9	U	1	0	0	0	0
9	V	1	0	0	0	0
9	W	1	0	0	0	0
All	All	13937	0	13134	63	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 2.

All (63) 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)
4:U:33:ILE:HD11	5:V:355:MET:HE3	1.59	0.84
1:G:738:LEU:HD11	6:W:442:LEU:HD12	1.66	0.76
5:V:172:PRO:HD2	6:W:42:MET:HE3	1.67	0.75
1:G:771:GLU:OE1	4:U:40:THR:HG21	1.90	0.71
1:G:735:TRP:NE1	6:W:448:MET:HE2	2.11	0.66
1:G:763:LYS:HB3	4:U:35:GLN:OE1	1.98	0.64
4:U:490:VAL:HG22	4:U:490:VAL:O	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:100:GLU:O	7:X:163:ARG:NH1	2.31	0.64
5:V:366:GLY:HA2	7:X:171:TRP:CE2	2.36	0.61
1:G:746:VAL:HG21	6:W:442:LEU:CD2	2.31	0.60
4:U:33:ILE:HD11	5:V:355:MET:CE	2.31	0.60
1:G:738:LEU:CD1	6:W:442:LEU:HD12	2.32	0.60
1:G:727:TYR:OH	6:W:465:LYS:HG3	2.02	0.59
1:G:746:VAL:HG21	6:W:442:LEU:HD22	1.85	0.57
4:U:676:ALA:HB3	4:U:677:PRO:HD3	1.86	0.56
5:V:330:ILE:HG22	5:V:330:ILE:O	2.03	0.56
5:V:257:ALA:HB3	5:V:258:PRO:HD3	1.88	0.56
1:G:748:ARG:NH2	2:K:105:DA:OP1	2.40	0.54
6:W:190:LYS:HE3	6:W:420:HIS:CE1	2.42	0.54
5:V:5:VAL:CG2	7:X:163:ARG:HH12	2.21	0.53
1:G:727:TYR:OH	6:W:465:LYS:HA	2.08	0.53
4:U:117:ARG:NH2	8:U:900:ATP:O1A	2.43	0.51
6:W:26:LEU:HD23	6:W:148:MET:HE2	1.93	0.51
4:U:418:MET:HE2	8:U:900:ATP:C8	2.47	0.49
1:G:738:LEU:CD1	6:W:442:LEU:CD1	2.91	0.48
4:U:490:VAL:O	4:U:490:VAL:CG2	2.62	0.48
4:U:33:ILE:HD13	5:V:351:THR:CG2	2.44	0.47
4:U:248:SER:HB2	4:U:249:PRO:CD	2.44	0.47
5:V:366:GLY:HA2	7:X:171:TRP:NE1	2.29	0.47
1:G:757:LYS:HE2	5:V:375:PHE:HB3	1.97	0.47
4:U:491:ASP:OD1	5:V:328:LYS:HE2	2.15	0.46
5:V:275:HIS:CE1	5:V:276:VAL:HG23	2.51	0.46
5:V:359:LYS:NZ	7:X:166:LYS:O	2.47	0.46
4:U:40:THR:HG23	4:U:44:LYS:HE2	1.97	0.46
1:G:797:MET:HG3	4:U:342:PHE:CG	2.51	0.45
4:U:454:GLU:H	4:U:454:GLU:CD	2.24	0.45
6:W:66:VAL:HG22	6:W:67:PRO:HD2	1.99	0.45
1:G:731:TYR:CE2	6:W:448:MET:HE1	2.53	0.44
4:U:733:MET:HE1	5:V:30:VAL:HG21	1.99	0.44
4:U:42:TYR:CE2	4:U:43:MET:SD	3.10	0.44
4:U:248:SER:HB2	4:U:249:PRO:HD3	2.00	0.44
6:W:195:VAL:HG23	6:W:208:ILE:HD13	1.99	0.43
5:V:330:ILE:O	5:V:332:PRO:HD3	2.18	0.43
4:U:458:ALA:HB3	4:U:459:PRO:HD3	2.01	0.43
4:U:33:ILE:CD1	5:V:355:MET:HE3	2.41	0.43
4:U:114:GLN:OE1	8:U:900:ATP:O3'	2.35	0.43
5:V:102:PRO:HA	5:V:131:ALA:O	2.19	0.42
4:U:280:LEU:C	4:U:280:LEU:HD23	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:W:198:VAL:HG12	6:W:394:THR:HB	2.00	0.42
2:K:106:DG:O6	3:L:-107:DA:N6	2.53	0.42
6:W:450:ILE:HD13	6:W:465:LYS:HE2	2.02	0.41
6:W:421:ALA:HB1	6:W:428:ARG:HG2	2.01	0.41
5:V:137:GLN:HG2	5:V:339:VAL:HG11	2.02	0.41
6:W:45:GLN:NE2	6:W:45:GLN:HA	2.34	0.41
4:U:356:ALA:HB2	8:U:900:ATP:O3'	2.21	0.41
5:V:235:HIS:CD2	5:V:235:HIS:H	2.39	0.41
4:U:18:THR:N	6:W:447:GLN:OE1	2.30	0.41
4:U:306:ILE:HG21	4:U:306:ILE:HD13	1.77	0.40
5:V:362:TYR:CZ	7:X:171:TRP:HD1	2.40	0.40
6:W:221:SER:HB2	6:W:368:LEU:HD11	2.03	0.40
4:U:259:HIS:HA	4:U:357:GLN:HB3	2.02	0.40
4:U:304:ILE:HD11	4:U:322:CYS:SG	2.61	0.40
5:V:5:VAL:CG2	7:X:163:ARG:NH1	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	G	97/1856 (5%)	94 (97%)	3 (3%)	0	100	100
4	U	599/747 (80%)	580 (97%)	18 (3%)	1 (0%)	43	71
5	V	358/375 (96%)	348 (97%)	10 (3%)	0	100	100
6	W	428/468 (92%)	413 (96%)	15 (4%)	0	100	100
7	X	50/284 (18%)	45 (90%)	4 (8%)	1 (2%)	6	25
All	All	1532/3730 (41%)	1480 (97%)	50 (3%)	2 (0%)	49	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	X	154	ILE
4	U	396	ASN

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	G	85/1604 (5%)	85 (100%)	0	100	100
4	U	537/645 (83%)	532 (99%)	5 (1%)	70	76
5	V	308/318 (97%)	306 (99%)	2 (1%)	78	80
6	W	355/387 (92%)	351 (99%)	4 (1%)	65	74
7	X	42/214 (20%)	41 (98%)	1 (2%)	43	62
All	All	1327/3168 (42%)	1315 (99%)	12 (1%)	68	76

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	U	329	SER
4	U	376	ASN
4	U	396	ASN
4	U	454	GLU
4	U	743	LEU
5	V	132	PHE
5	V	330	ILE
6	W	64	VAL
6	W	198	VAL
6	W	390	VAL
6	W	466	ARG
7	X	161	LEU

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

Mol	Chain	Res	Type
4	U	24	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	U	152	GLN
4	U	160	GLN
4	U	161	GLN
4	U	221	ASN
4	U	223	ASN
4	U	238	GLN
4	U	376	ASN
4	U	396	ASN
4	U	408	HIS
4	U	431	GLN
4	U	436	HIS
4	U	746	HIS
5	V	92	ASN
6	W	154	ASN
6	W	405	ASN
6	W	458	ASN
7	X	177	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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
8	ATP	W	500	9	32,33,33	1.17	1 (3%)	48,52,52	1.13	5 (10%)
8	ATP	V	500	9	32,33,33	1.59	2 (6%)	48,52,52	0.82	2 (4%)
8	ATP	U	900	9	32,33,33	0.84	2 (6%)	48,52,52	0.82	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
8	ATP	W	500	9	-	10/22/38/38	0/3/3/3
8	ATP	V	500	9	-	0/22/38/38	0/3/3/3
8	ATP	U	900	9	-	4/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	V	500	ATP	PA-O3A	-7.02	1.51	1.59
8	W	500	ATP	PA-O3A	-4.85	1.54	1.59
8	V	500	ATP	PB-O3A	-4.64	1.54	1.59
8	U	900	ATP	PB-O3A	-2.59	1.56	1.59
8	U	900	ATP	C1'-N9	-2.04	1.40	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	W	500	ATP	O2A-PA-O3A	3.69	117.26	107.27
8	W	500	ATP	O4'-C4'-C3'	-2.25	100.68	105.15
8	U	900	ATP	O2B-PB-O1B	2.21	122.75	112.44
8	V	500	ATP	O3G-PG-O2G	2.21	116.08	107.80
8	W	500	ATP	O2G-PG-O3B	2.18	111.95	104.64
8	W	500	ATP	O2B-PB-O1B	2.09	122.15	112.44
8	V	500	ATP	O2B-PB-O3A	2.05	112.82	107.27
8	W	500	ATP	O2B-PB-O3A	2.03	112.76	107.27

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	W	500	ATP	PB-O3B-PG-O2G

Continued on next page...

Continued from previous page...

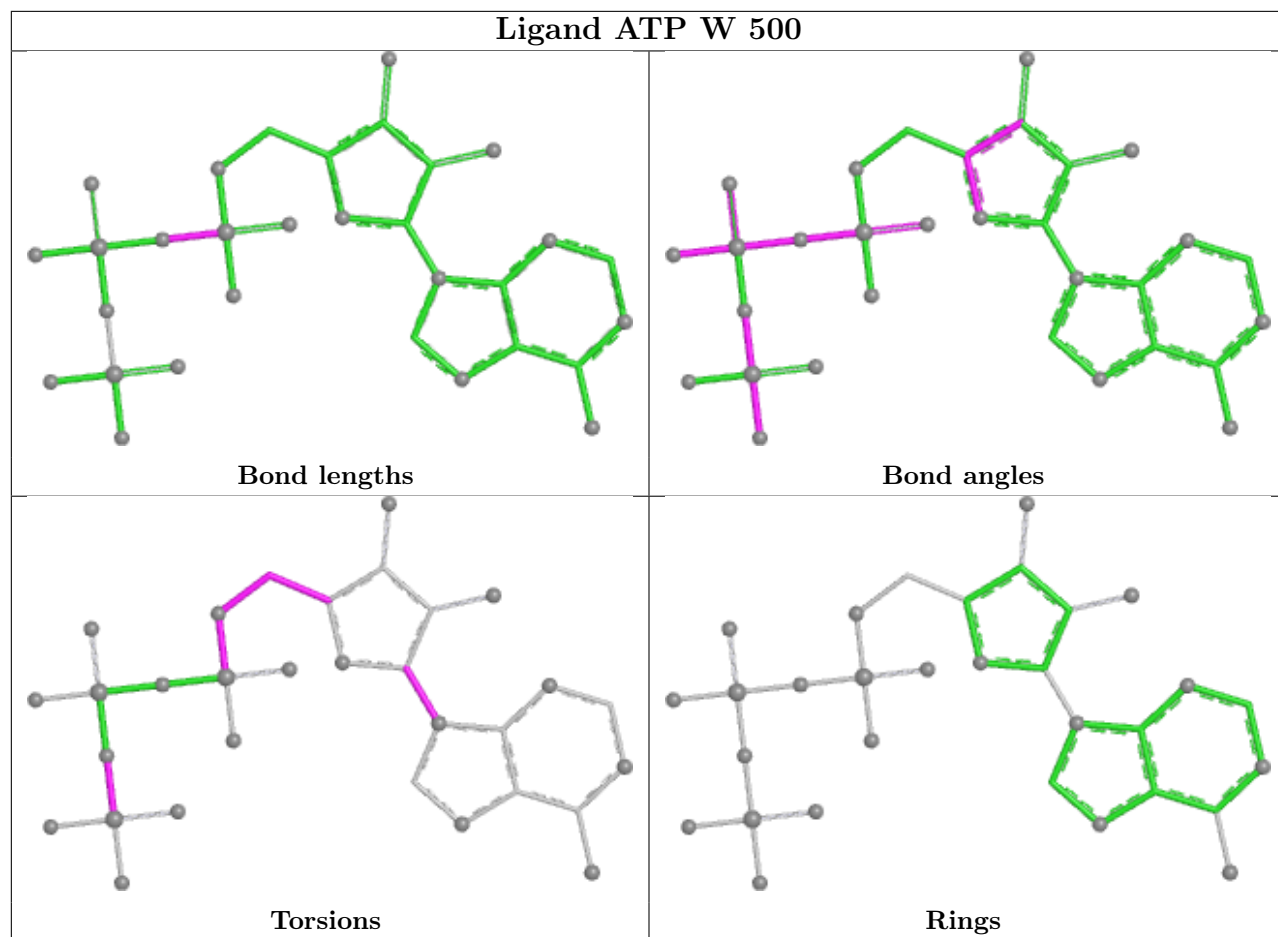
Mol	Chain	Res	Type	Atoms
8	W	500	ATP	C5'-O5'-PA-O1A
8	W	500	ATP	C5'-O5'-PA-O2A
8	W	500	ATP	C5'-O5'-PA-O3A
8	W	500	ATP	O4'-C4'-C5'-O5'
8	W	500	ATP	C3'-C4'-C5'-O5'
8	W	500	ATP	C4'-C5'-O5'-PA
8	U	900	ATP	C3'-C4'-C5'-O5'
8	W	500	ATP	PB-O3B-PG-O1G
8	W	500	ATP	PB-O3B-PG-O3G
8	U	900	ATP	O4'-C4'-C5'-O5'
8	U	900	ATP	C2'-C1'-N9-C8
8	W	500	ATP	C2'-C1'-N9-C8
8	U	900	ATP	PA-O3A-PB-O2B

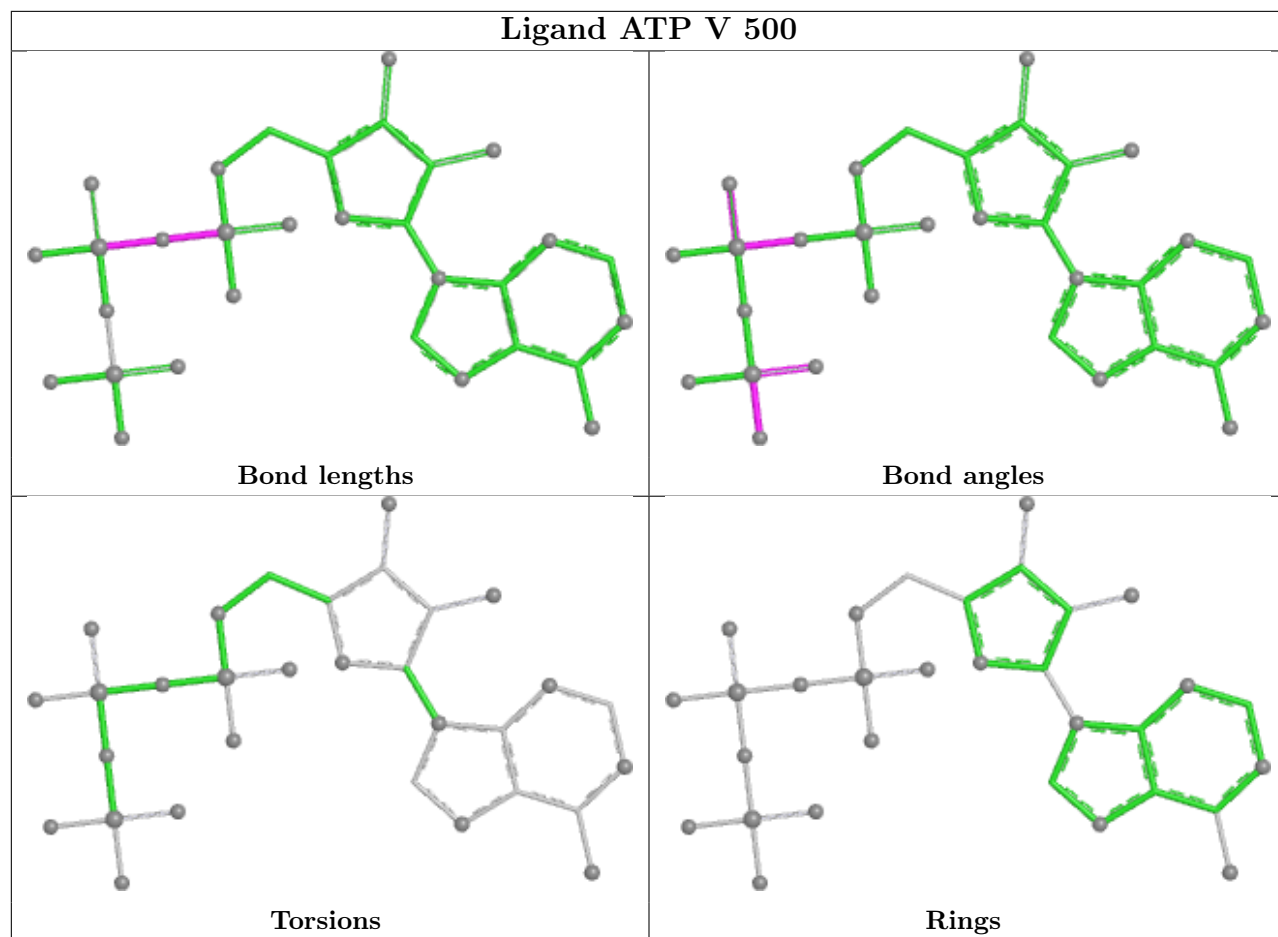
There are no ring outliers.

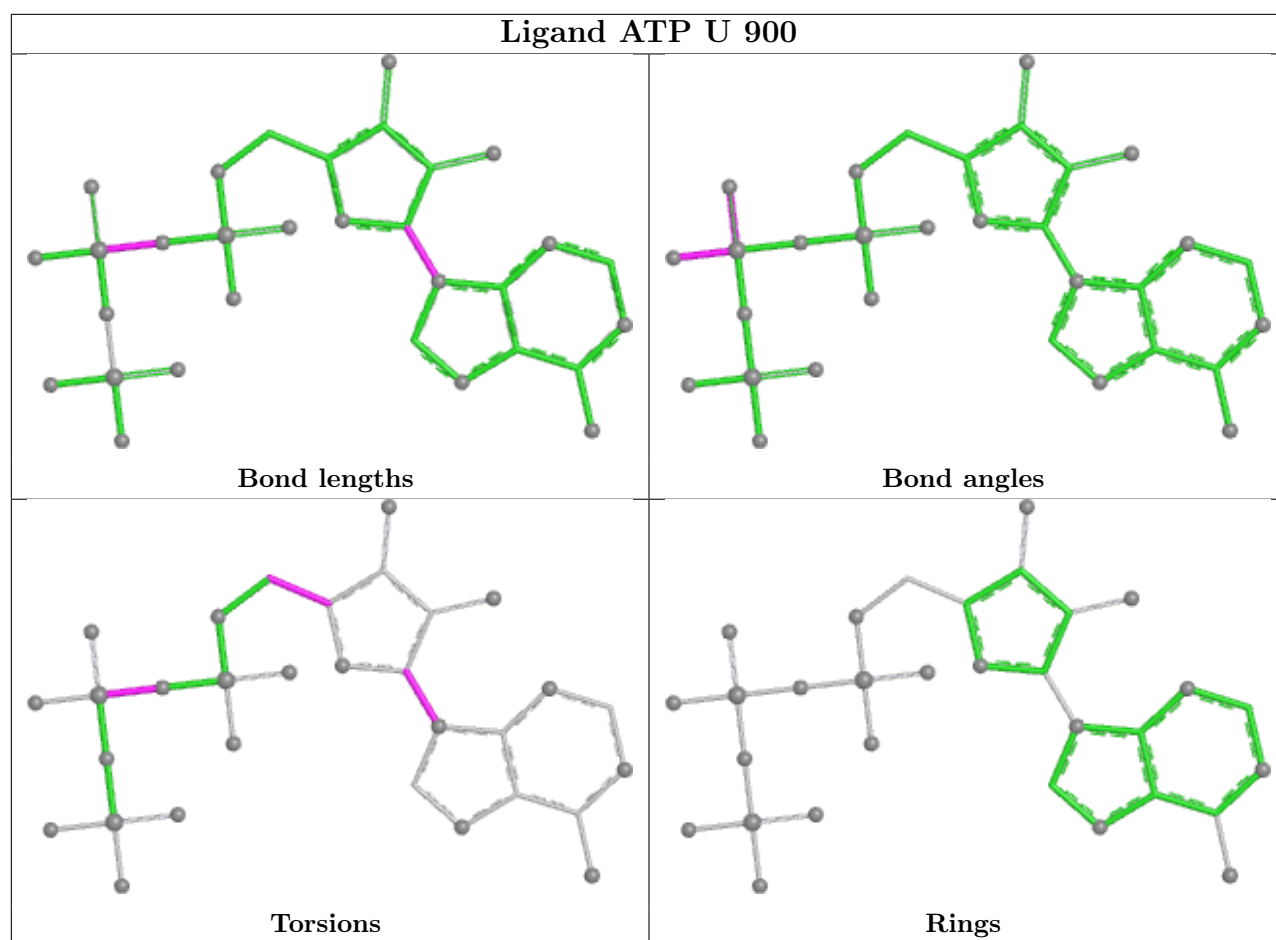
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	U	900	ATP	4	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.

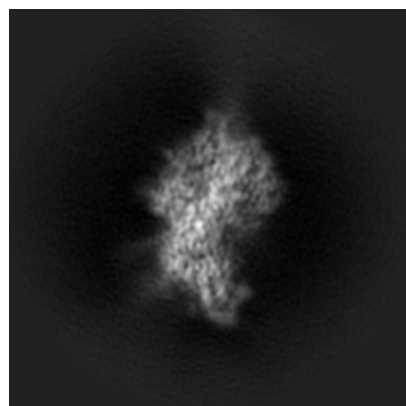
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15180. These allow visual inspection of the internal detail of the map and identification of artifacts.

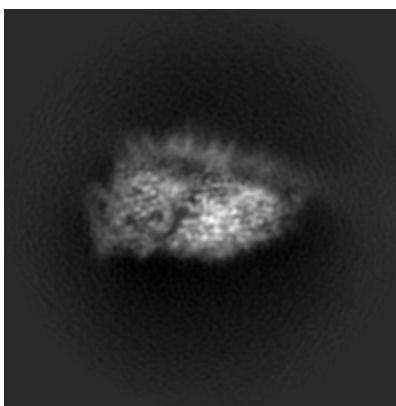
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

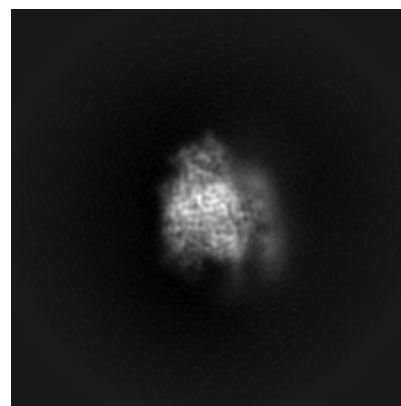
6.1.1 Primary map



X

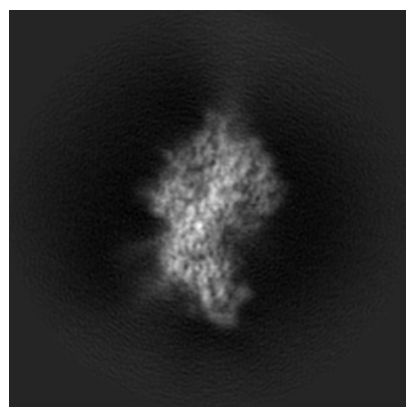


Y

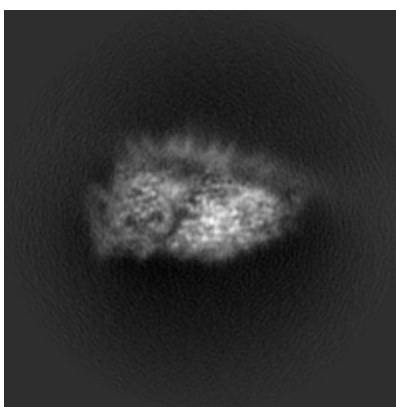


Z

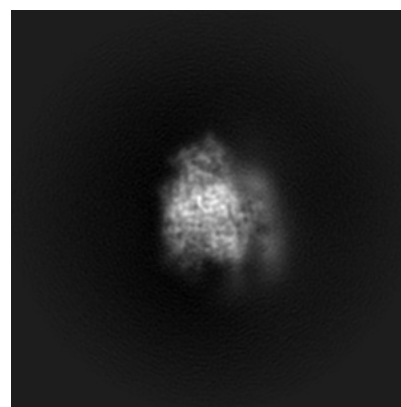
6.1.2 Raw map



X



Y

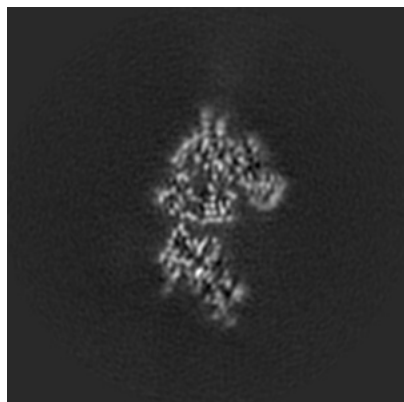


Z

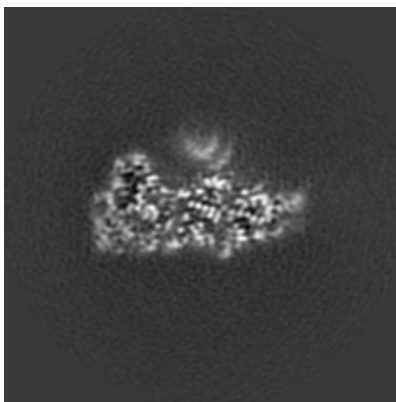
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

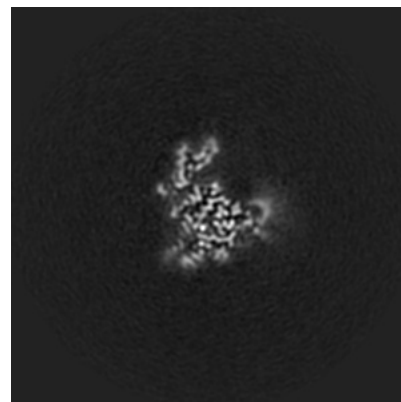
6.2.1 Primary map



X Index: 96

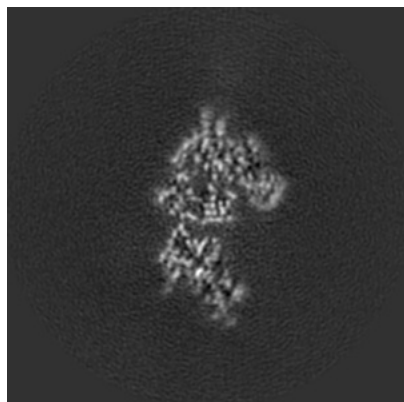


Y Index: 96

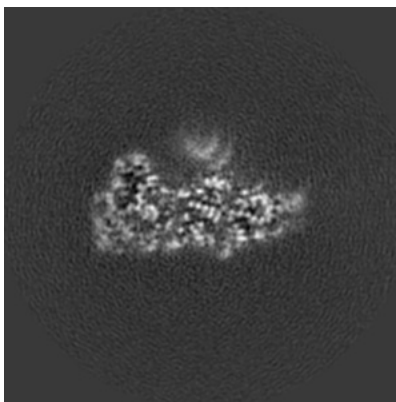


Z Index: 96

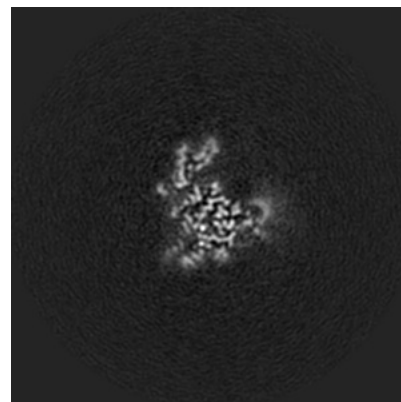
6.2.2 Raw map



X Index: 96



Y Index: 96

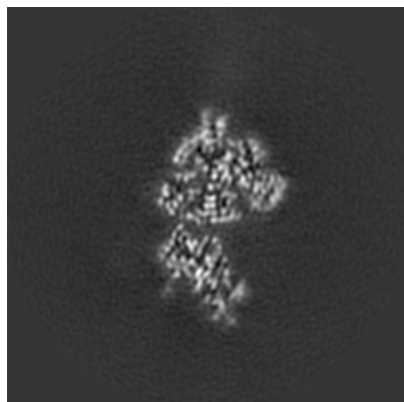


Z Index: 96

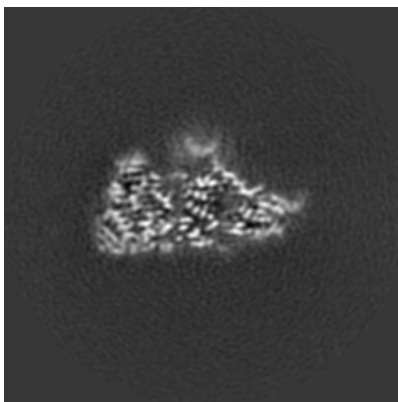
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

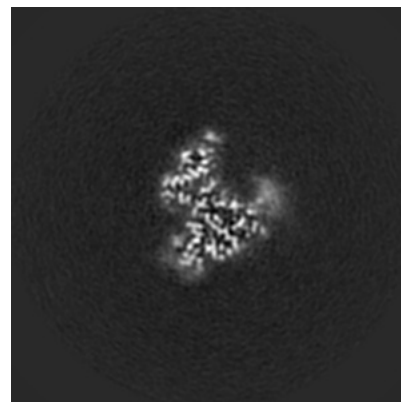
6.3.1 Primary map



X Index: 95

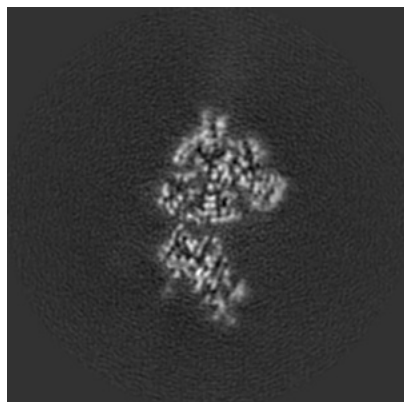


Y Index: 94

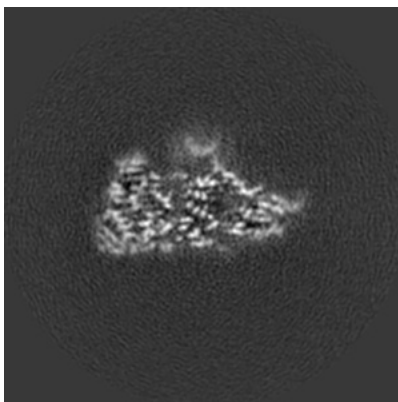


Z Index: 102

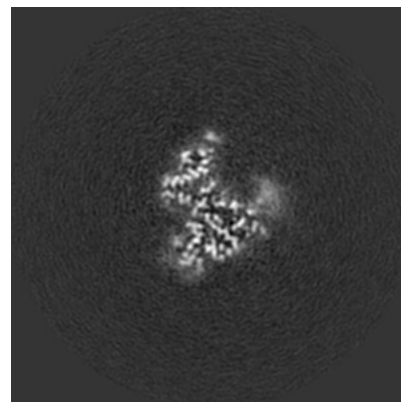
6.3.2 Raw map



X Index: 95



Y Index: 94

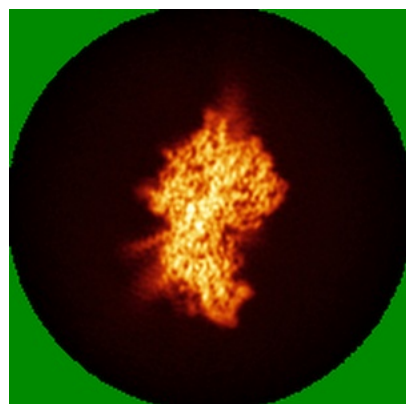


Z Index: 102

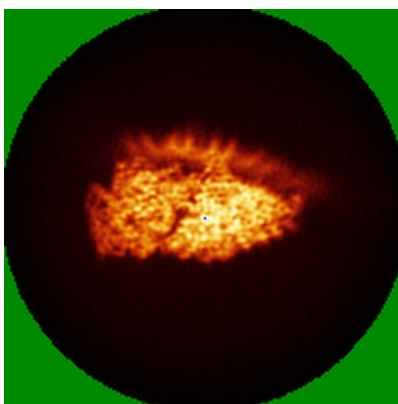
The images above show the largest variance slices of the map in three orthogonal directions.

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

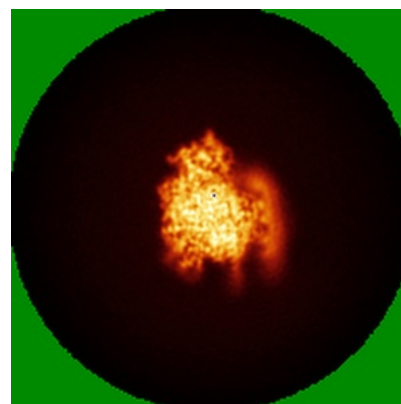
6.4.1 Primary map



X

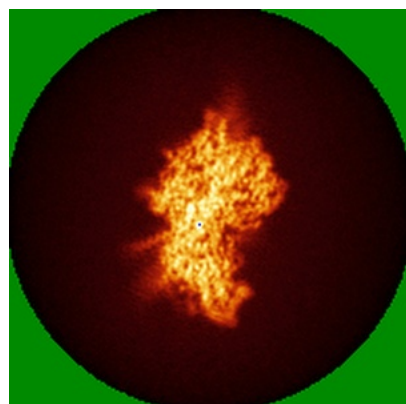


Y

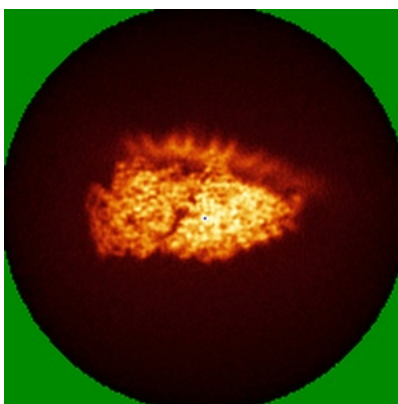


Z

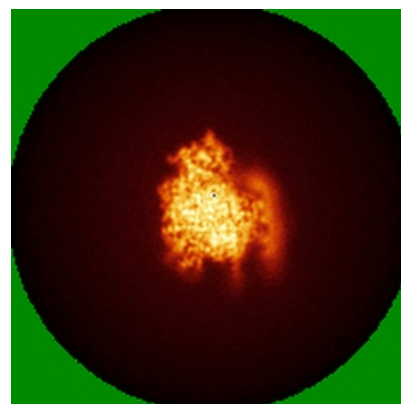
6.4.2 Raw map



X



Y

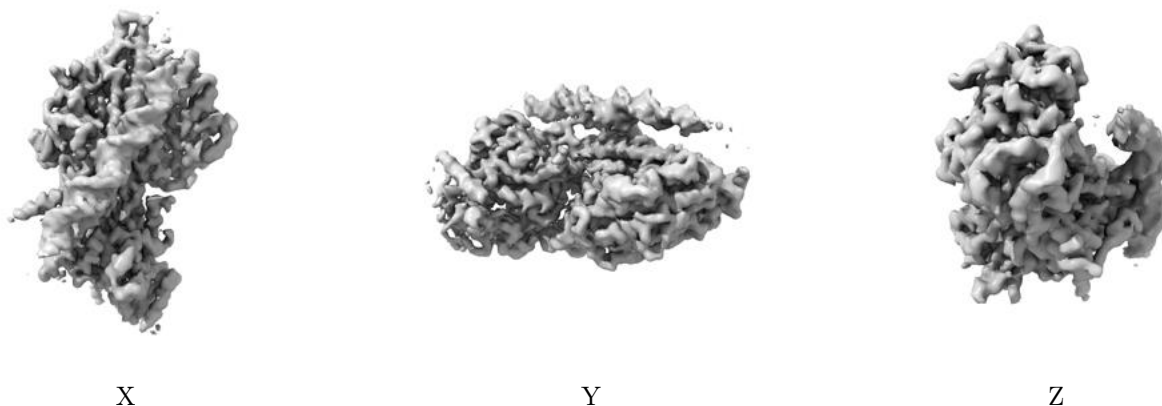


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

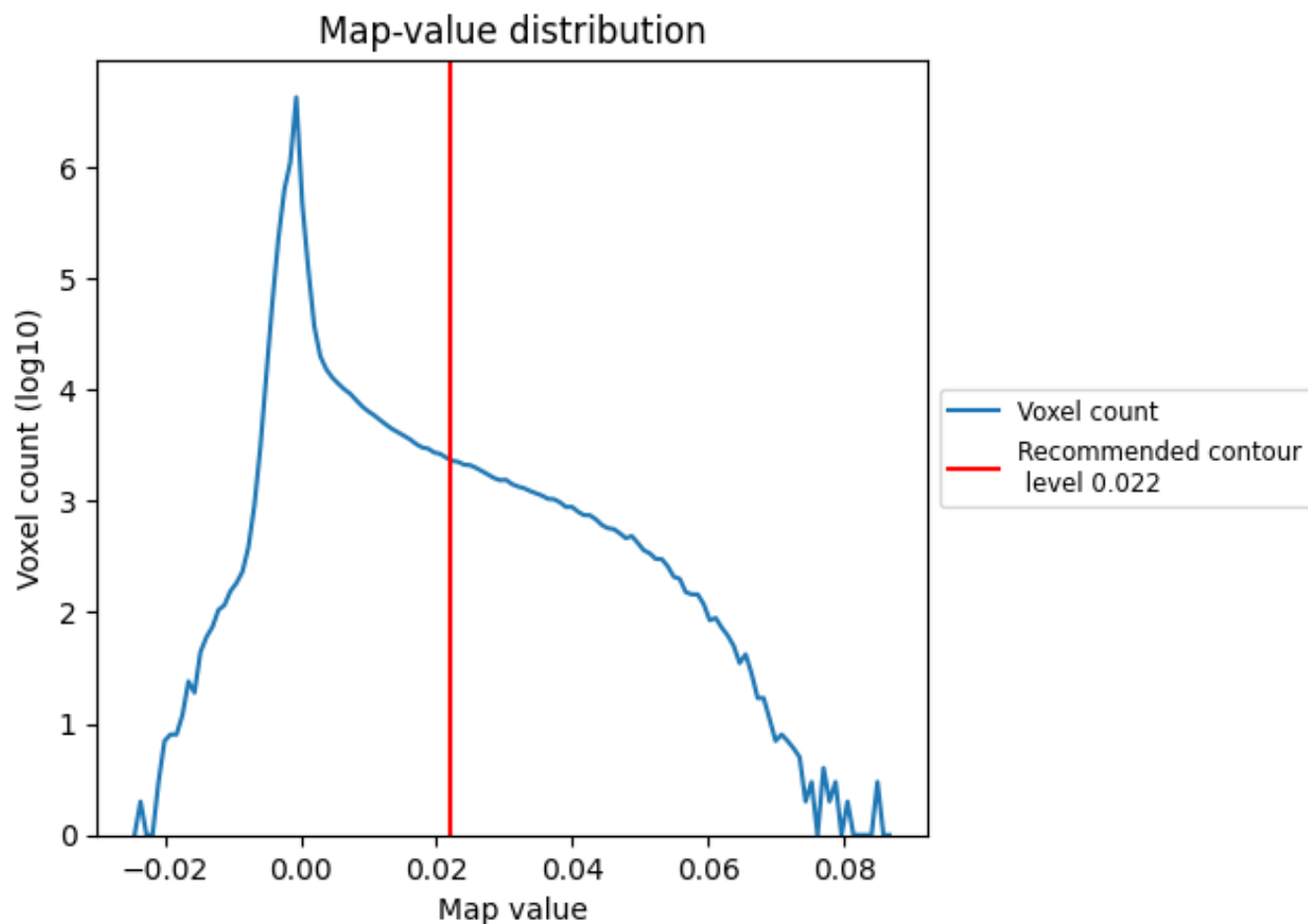
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

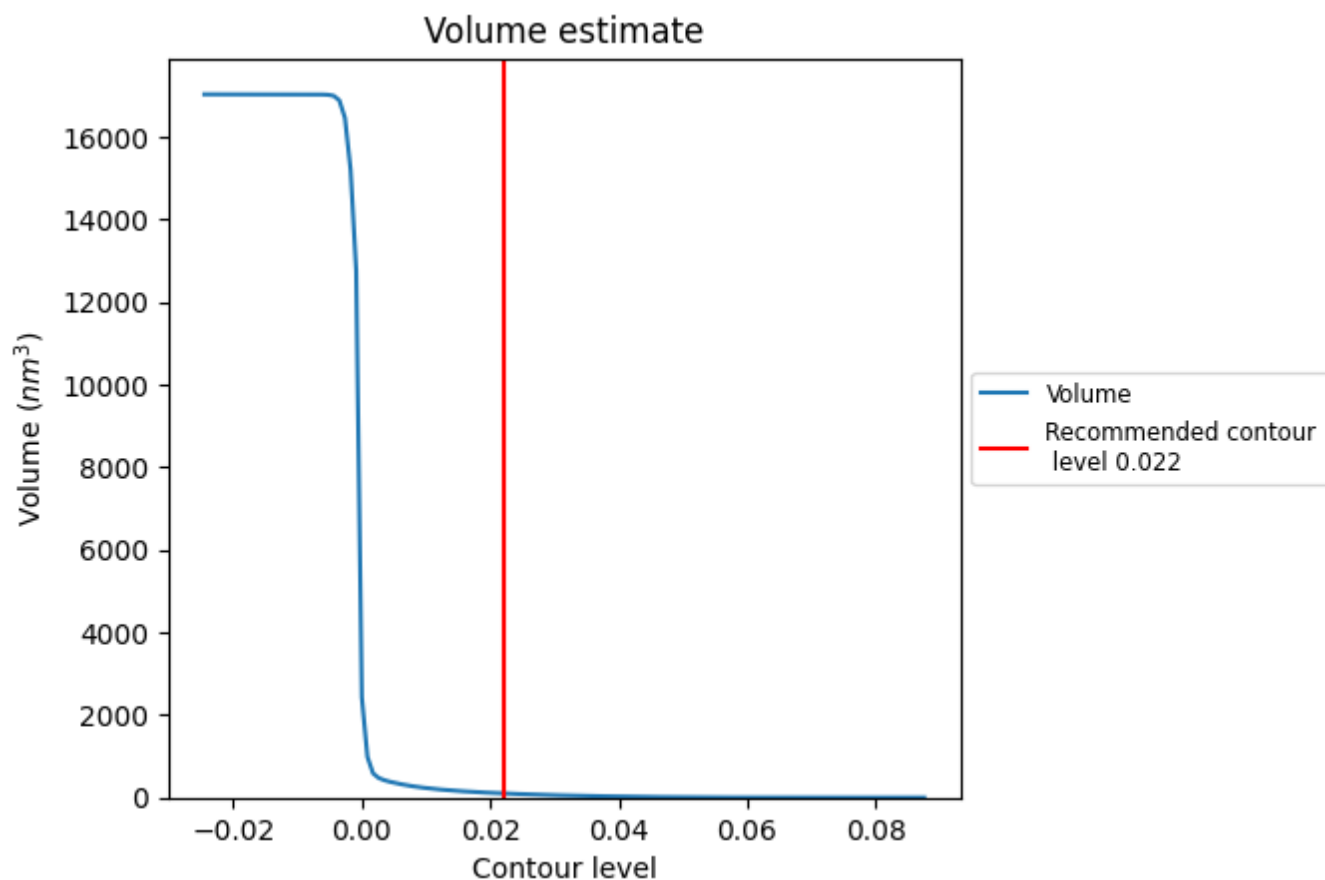
This section contains the results of statistical analysis of the map.

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.

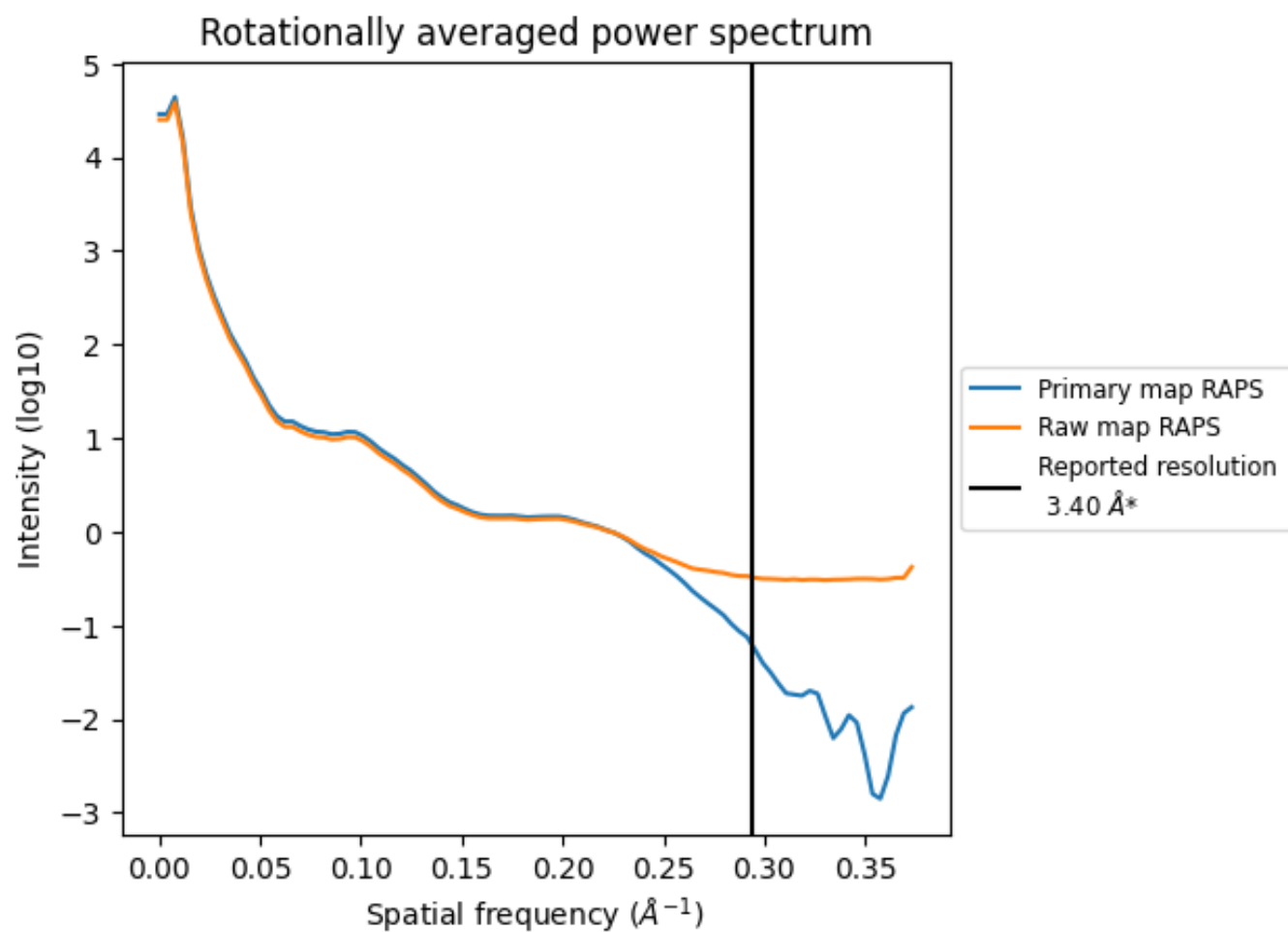
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 101 nm³; this corresponds to an approximate mass of 91 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 ⓘ

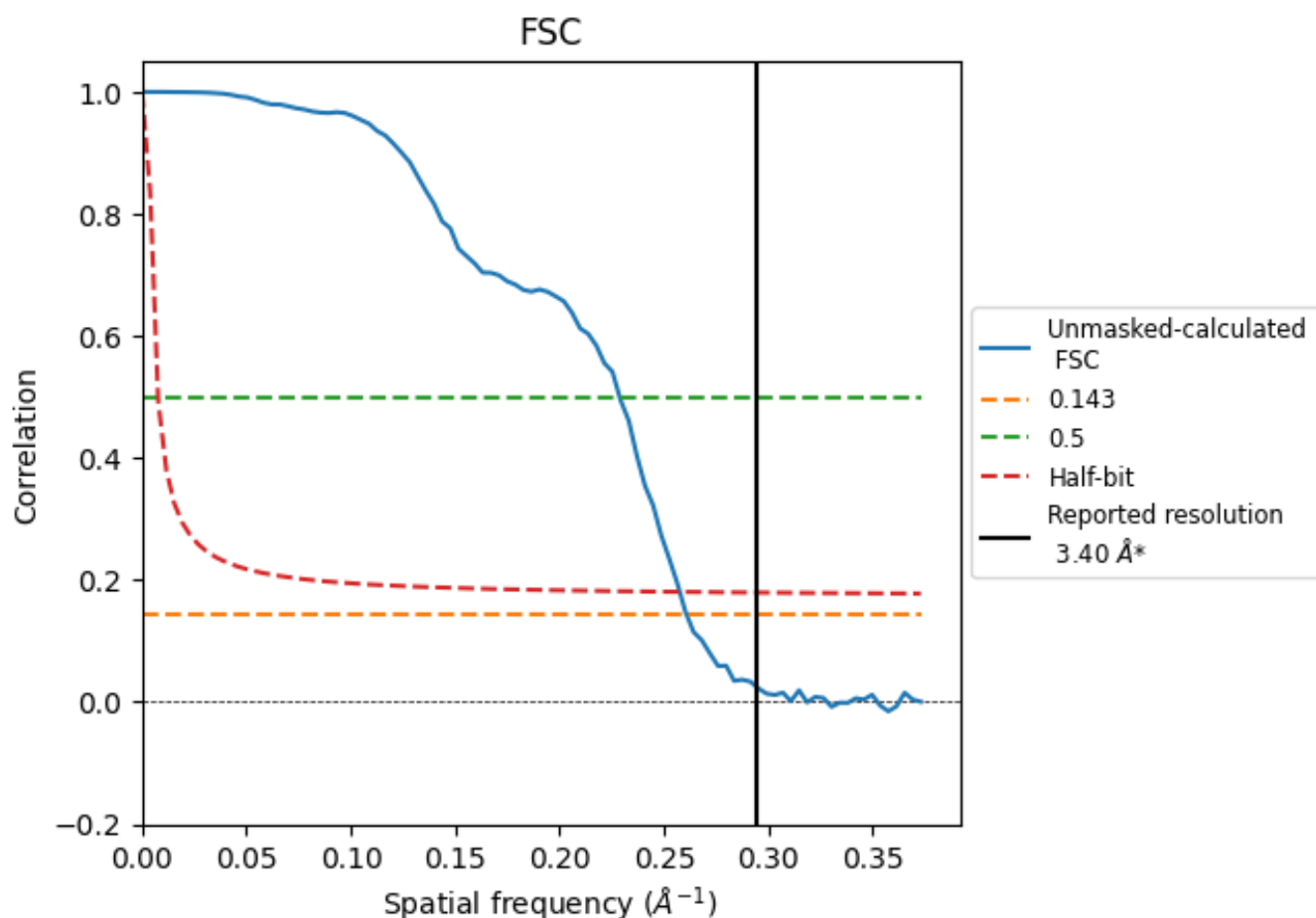


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

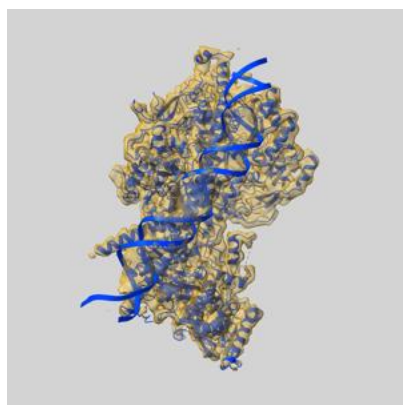
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.83	4.37	3.88

*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 3.83 differs from the reported value 3.4 by more than 10 %

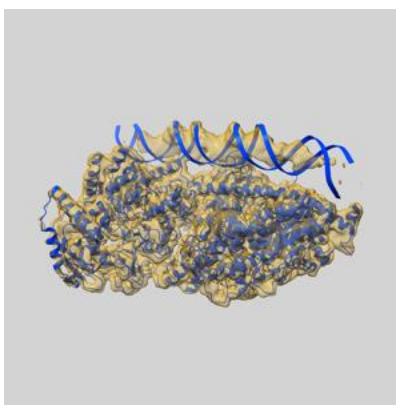
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15180 and PDB model 8A5P. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

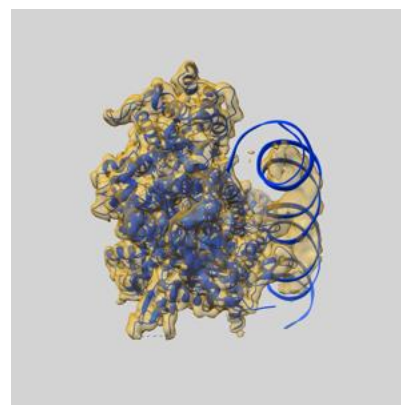
9.1 Map-model overlay [i](#)



X



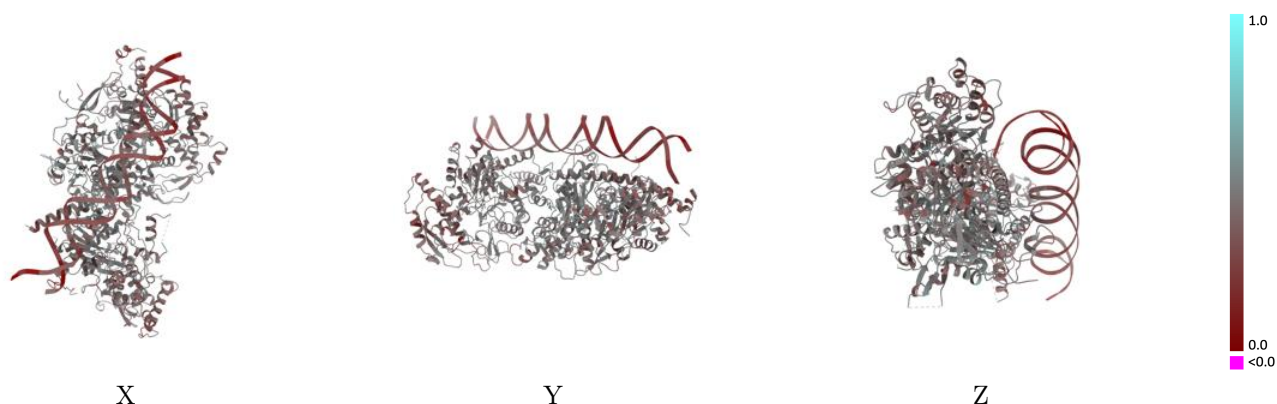
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

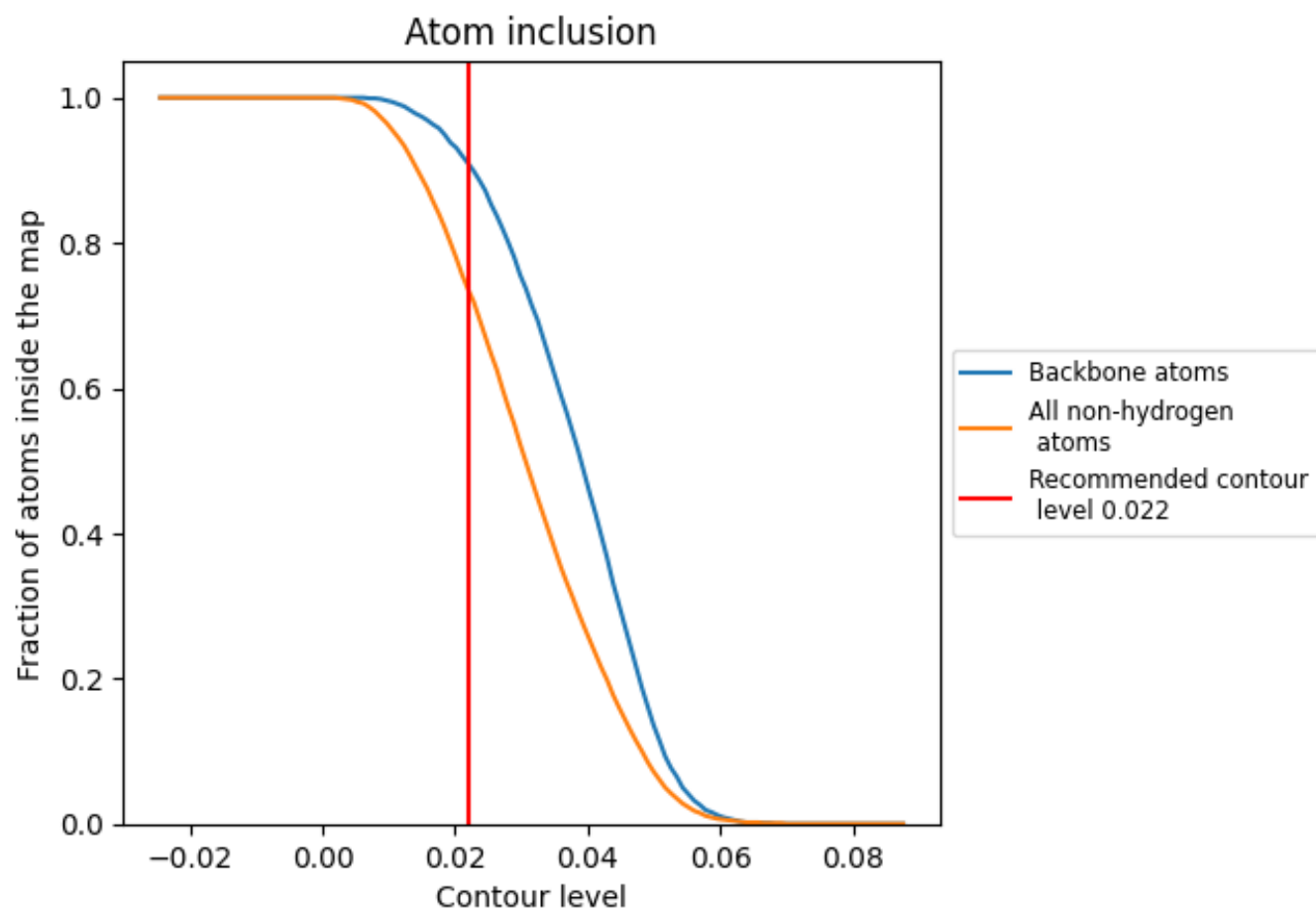


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 74% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7350	0.4150
G	0.6970	0.4020
K	0.4800	0.2510
L	0.4690	0.2500
U	0.7160	0.4260
V	0.8170	0.4550
W	0.8120	0.4370
X	0.7940	0.4550

1.0

0.0

<0.0