



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 11:57 AM UTC

PDB ID : 8A5A / pdb_00008a5a
EMDB ID : EMD-15163
Title : Structure of Arp4-Ies4-N-actin-Arp8-Ino80HSA subcomplex (A-module) of INO80
Authors : Kunert, F.; Metzner, F.J.; Eustermann, S.; Jung, J.; Woike, S.; Schall, K.; Kostrewa, D.; Hopfner, K.P.
Deposited on : 2022-06-14
Resolution : 3.30 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

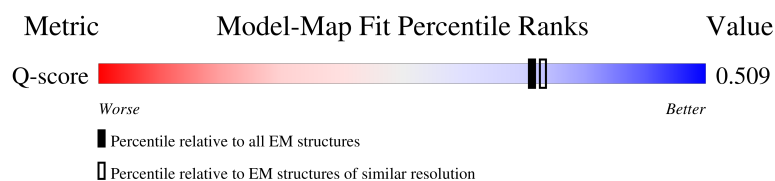
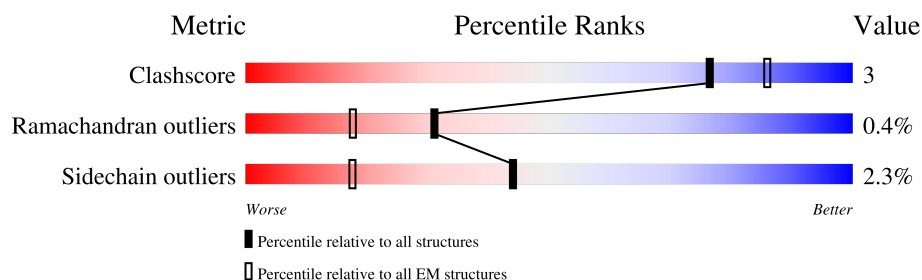
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	616	
2	U	881	
3	V	375	
4	W	489	

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Mol	Chain	Length	Quality of chain
5	X	116	 A horizontal bar chart showing the quality of chain 5. The bar is divided into three segments: a green segment on the left labeled '24%', a yellow segment in the middle labeled '9%', and a grey segment on the right labeled '66%'. A small black dot is located at the end of the yellow segment.

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13191 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 Chromatin-remodeling ATPase INO80.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	110	Total	C	N	O	S	0	0
			938	580	184	168	6		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	599	ASP	-	expression tag	UNP P53115
G	600	TYR	-	expression tag	UNP P53115
G	601	LYS	-	expression tag	UNP P53115
G	602	ASP	-	expression tag	UNP P53115
G	603	ASP	-	expression tag	UNP P53115
G	604	ASP	-	expression tag	UNP P53115
G	605	ASP	-	expression tag	UNP P53115
G	606	LYS	-	expression tag	UNP P53115
G	607	GLY	-	expression tag	UNP P53115
G	608	THR	-	expression tag	UNP P53115
G	609	ASP	-	expression tag	UNP P53115
G	610	TYR	-	expression tag	UNP P53115
G	611	LYS	-	expression tag	UNP P53115
G	612	ASP	-	expression tag	UNP P53115
G	613	ASP	-	expression tag	UNP P53115
G	614	ASP	-	expression tag	UNP P53115
G	615	ASP	-	expression tag	UNP P53115
G	616	LYS	-	expression tag	UNP P53115

- Molecule 2 is a protein called Actin-like protein ARP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	690	Total	C	N	O	S	0	0
			5582	3567	934	1066	15		

- Molecule 3 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	V	362	Total	C	N	O	S	0	0
			2830	1795	476	542	17		

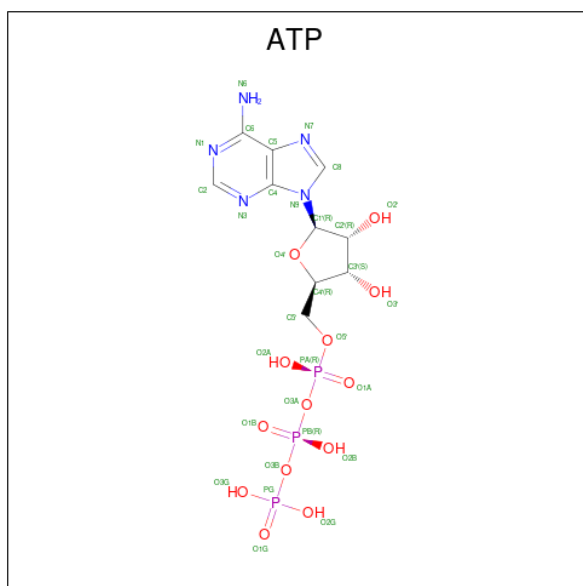
- Molecule 4 is a protein called Actin-related protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	W	427	Total	C	N	O	S	0	0
			3398	2166	564	657	11		

- Molecule 5 is a protein called Ino eighty subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	X	40	Total	C	N	O	0	0
			347	223	65	59		

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

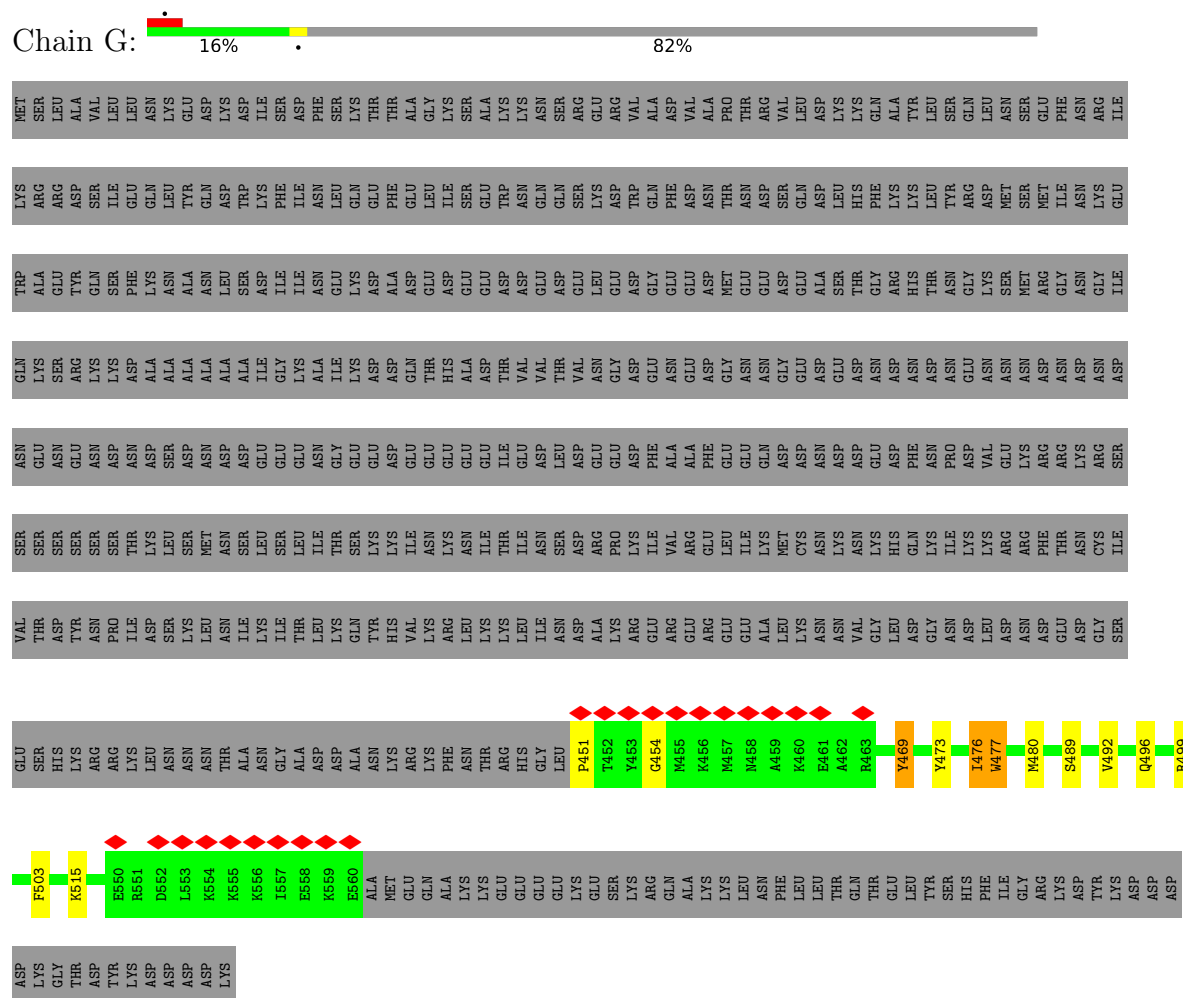


Mol	Chain	Residues	Atoms		AltConf
7	U	1	Total 1	Mg 1	0
7	V	1	Total 1	Mg 1	0
7	W	1	Total 1	Mg 1	0

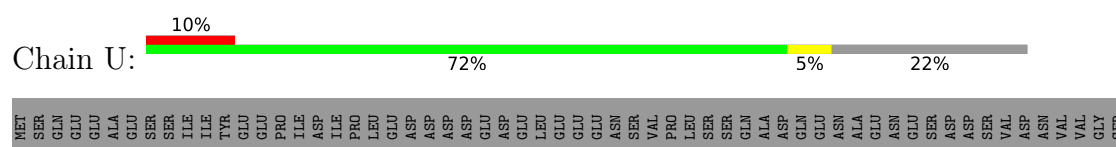
3 Residue-property plots

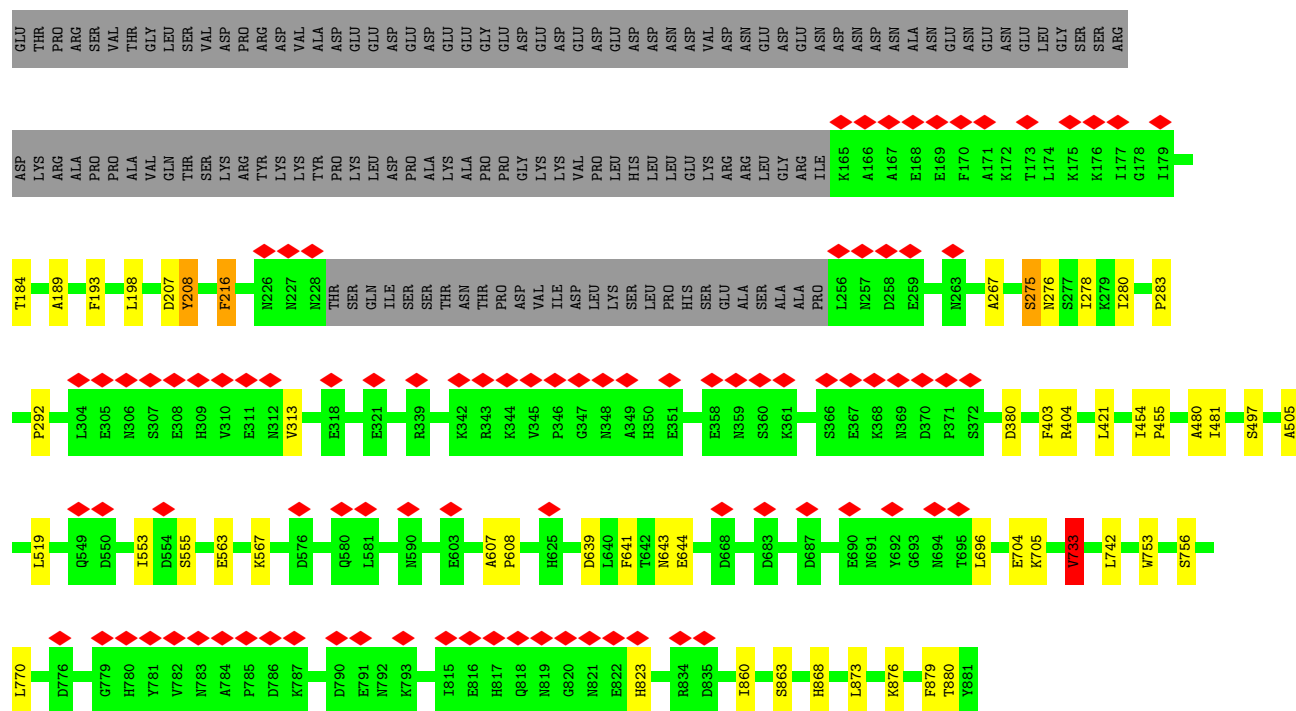
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Chromatin-remodeling ATPase INO80

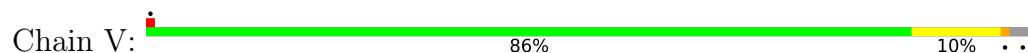


• Molecule 2: Actin-like protein ARP8

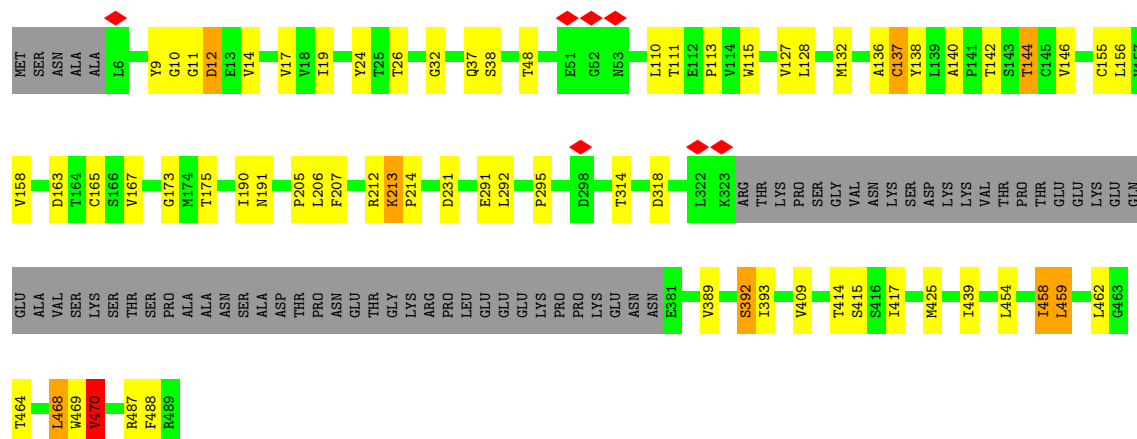
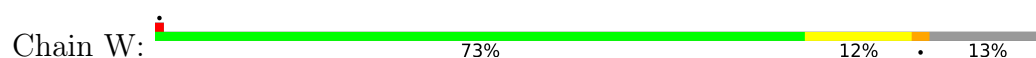




• Molecule 3: Actin

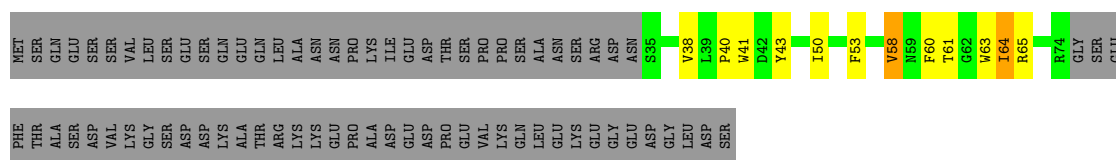


• Molecule 4: Actin-related protein 4



• Molecule 5: Ino eighty subunit 4

Service	Percentage
Used	24%
Not used	9%
Don't know	66%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	327293	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 ($e^-/\text{\AA}^2$)	44.68	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	7.521	Depositor
Minimum map value	-4.734	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.157	Depositor
Recommended contour level	0.735	Depositor
Map size (Å)	271.104, 271.104, 271.104	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.11	1/952 (0.1%)	1.68	8/1261 (0.6%)
2	U	1.09	1/5702 (0.0%)	1.43	13/7723 (0.2%)
3	V	1.15	1/2892 (0.0%)	1.46	7/3916 (0.2%)
4	W	1.24	11/3474 (0.3%)	1.55	14/4712 (0.3%)
5	X	1.16	2/356 (0.6%)	1.51	3/477 (0.6%)
All	All	1.15	16/13376 (0.1%)	1.49	45/18089 (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
2	U	0	4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	W	136	ALA	C-O	13.86	1.39	1.23
4	W	11	GLY	C-O	9.95	1.35	1.24
4	W	26	THR	C-O	9.20	1.35	1.23
4	W	175	THR	C-O	6.82	1.32	1.23
1	G	477	TRP	C-O	6.65	1.32	1.24
4	W	137	CYS	C-O	-6.51	1.15	1.23
2	U	292	PRO	C-O	-6.29	1.16	1.23
4	W	38	SER	CA-CB	-6.12	1.44	1.53
4	W	470	VAL	C-O	5.61	1.30	1.24
5	X	63	TRP	C-O	5.55	1.30	1.23
3	V	164	PRO	C-O	-5.53	1.18	1.23
4	W	415	SER	CA-CB	-5.32	1.45	1.53
4	W	392	SER	CA-CB	-5.17	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	W	205	PRO	C-O	-5.10	1.17	1.23
4	W	459	LEU	C-O	-5.06	1.17	1.24
5	X	40	PRO	C-O	-5.01	1.18	1.23

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	454	ILE	N-CA-CB	-9.89	105.01	111.83
4	W	458	ILE	N-CA-C	-9.73	101.39	110.53
3	V	372	HIS	CA-CB-CG	7.64	121.44	113.80
4	W	113	PRO	CB-CA-C	-7.59	99.76	111.22
4	W	24	TYR	N-CA-C	-6.72	105.08	113.55
2	U	380	ASP	CA-CB-CG	6.66	119.26	112.60
3	V	301	GLY	CA-C-O	-6.23	117.24	122.29
2	U	455	PRO	CA-C-O	-6.12	114.54	122.12
1	G	476	ILE	N-CA-C	-6.11	104.39	110.62
3	V	275	ASP	CA-CB-CG	6.05	118.65	112.60
4	W	191	ASN	N-CA-C	-6.00	104.65	111.07
3	V	208	ILE	N-CA-C	-5.86	105.02	110.53
1	G	503	PHE	CA-C-O	-5.69	114.39	120.42
3	V	293	LEU	CA-C-O	-5.67	114.86	120.70
1	G	469	TYR	O-C-N	5.64	128.12	122.08
2	U	480	ALA	CA-C-O	-5.60	114.22	120.66
2	U	863	SER	CA-C-O	-5.60	113.78	120.10
1	G	492	VAL	CA-C-O	-5.56	114.96	120.85
2	U	280	ILE	CA-C-O	-5.55	115.48	121.19
4	W	462	LEU	CB-CA-C	5.47	117.67	110.06
1	G	489	SER	O-C-N	5.47	127.71	122.07
2	U	208	TYR	N-CA-CB	5.44	118.21	110.16
2	U	639	ASP	CA-CB-CG	5.40	118.00	112.60
1	G	489	SER	CA-C-O	-5.39	115.16	120.82
4	W	389	VAL	CA-C-O	-5.34	114.86	120.57
1	G	499	ARG	N-CA-C	-5.33	105.36	111.07
5	X	63	TRP	O-C-N	5.33	128.99	122.96
4	W	144	THR	CA-CB-OG1	-5.29	101.67	109.60
4	W	231	ASP	N-CA-C	-5.28	105.52	111.28
4	W	212	ARG	CG-CD-NE	-5.23	100.49	112.00
2	U	189	ALA	CA-C-O	-5.20	114.23	120.10
2	U	276	ASN	N-CA-C	-5.14	106.17	112.90
4	W	14	VAL	CA-C-O	-5.13	115.75	121.23
1	G	496	GLN	CA-C-O	-5.12	115.44	120.82
3	V	345	ILE	CA-C-O	-5.12	115.75	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	63	TRP	CA-C-O	-5.10	115.60	121.47
2	U	275	SER	N-CA-C	-5.09	105.81	111.36
2	U	733	VAL	O-C-N	5.08	128.92	122.57
4	W	146	VAL	CA-C-O	-5.08	115.67	120.95
4	W	318	ASP	CA-CB-CG	5.07	117.67	112.60
2	U	267	ALA	CA-C-O	-5.06	114.84	122.38
4	W	163	ASP	N-CA-C	-5.05	105.97	111.82
5	X	58	VAL	CA-C-O	-5.03	116.73	120.96
4	W	37	GLN	N-CA-CB	5.02	118.27	110.44
3	V	174	ALA	CA-C-O	-5.01	113.56	119.48

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	U	184	THR	Peptide
2	U	207	ASP	Peptide
2	U	696	LEU	Peptide
2	U	876	LYS	Peptide

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	G	938	0	963	7	0
2	U	5582	0	5549	26	0
3	V	2830	0	2795	15	0
4	W	3398	0	3361	35	0
5	X	347	0	349	11	0
6	U	31	0	12	4	0
6	V	31	0	12	0	0
6	W	31	0	12	1	0
7	U	1	0	0	0	0
7	V	1	0	0	0	0
7	W	1	0	0	0	0
All	All	13191	0	13053	79	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 3.

All (79) 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)
2:U:567:LYS:HE2	6:U:900:ATP:O2'	1.74	0.86
1:G:477:TRP:HH2	4:W:459:LEU:HD21	1.43	0.82
4:W:414:THR:HG22	4:W:414:THR:O	1.78	0.82
2:U:505:ALA:HB2	6:U:900:ATP:H5'2	1.75	0.67
5:X:50:ILE:HD12	5:X:60:PHE:CD2	2.33	0.65
3:V:257:ALA:HB3	3:V:258:PRO:HD3	1.79	0.64
4:W:19:ILE:HG22	4:W:110:LEU:HD12	1.80	0.63
4:W:19:ILE:HG22	4:W:110:LEU:CD1	2.29	0.62
5:X:50:ILE:HD12	5:X:60:PHE:CE2	2.35	0.62
4:W:414:THR:O	4:W:414:THR:CG2	2.46	0.61
1:G:473:TYR:OH	4:W:138:TYR:OH	2.18	0.61
2:U:733:VAL:HG12	2:U:733:VAL:O	2.00	0.61
1:G:477:TRP:CH2	4:W:459:LEU:HD21	2.32	0.60
1:G:477:TRP:CZ3	4:W:459:LEU:HD11	2.38	0.58
4:W:190:ILE:HD11	4:W:292:LEU:HD12	1.85	0.58
3:V:121:GLN:NE2	5:X:41:TRP:O	2.36	0.58
1:G:469:TYR:CZ	5:X:53:PHE:CZ	2.94	0.56
4:W:127:VAL:HG12	4:W:132:MET:HE2	1.87	0.56
3:V:82:MET:SD	3:V:85:ILE:HD11	2.46	0.56
4:W:115:TRP:HA	4:W:314:THR:HG22	1.87	0.56
3:V:96:VAL:O	3:V:96:VAL:HG23	2.07	0.54
2:U:567:LYS:CE	6:U:900:ATP:O2'	2.51	0.54
4:W:470:VAL:O	4:W:470:VAL:HG12	2.09	0.53
2:U:705:LYS:HE2	2:U:753:TRP:CE3	2.45	0.52
4:W:9:TYR:HE2	5:X:41:TRP:CH2	2.27	0.52
2:U:193:PHE:CE1	4:W:32:GLY:O	2.63	0.52
4:W:468:LEU:HD12	5:X:53:PHE:CD1	2.46	0.50
2:U:278:ILE:HD11	2:U:403:PHE:CE2	2.47	0.50
3:V:250:ILE:HG23	3:V:253:GLU:HB2	1.93	0.50
4:W:213:LYS:HB2	4:W:214:PRO:HD3	1.93	0.49
2:U:742:LEU:C	2:U:742:LEU:HD13	2.37	0.49
4:W:213:LYS:CB	4:W:214:PRO:HD3	2.42	0.49
4:W:128:LEU:HD13	4:W:137:CYS:SG	2.53	0.49
4:W:144:THR:OG1	4:W:173:GLY:O	2.29	0.48
4:W:12:ASP:OD1	5:X:64:ILE:HG23	2.13	0.48
2:U:193:PHE:CE2	4:W:32:GLY:HA2	2.49	0.48
3:V:178:ILE:HG22	3:V:180:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:155:CYS:HB2	4:W:409:VAL:HG23	1.96	0.47
4:W:156:LEU:HD22	4:W:393:ILE:HD11	1.97	0.47
1:G:476:ILE:O	1:G:480:MET:HG3	2.15	0.46
3:V:124:PHE:HB3	5:X:38:VAL:HG11	1.97	0.46
4:W:291:GLU:HG3	4:W:295:PRO:HA	1.97	0.46
2:U:193:PHE:CZ	4:W:32:GLY:O	2.69	0.46
4:W:19:ILE:CG2	4:W:110:LEU:CD1	2.93	0.46
4:W:207:PHE:C	4:W:207:PHE:CD1	2.94	0.46
4:W:167:VAL:HG11	4:W:392:SER:OG	2.16	0.45
3:V:162:VAL:HG11	3:V:281:SER:OG	2.17	0.45
2:U:607:ALA:HB3	2:U:608:PRO:HD3	1.99	0.44
1:G:515:LYS:HG2	2:U:641:PHE:CD1	2.52	0.44
4:W:9:TYR:CE2	5:X:41:TRP:CH2	3.05	0.44
3:V:346:LEU:HD11	3:V:355:MET:HE1	2.00	0.43
4:W:138:TYR:HA	4:W:488:PHE:HE1	1.83	0.43
5:X:43:TYR:CZ	5:X:61:THR:CG2	3.00	0.43
2:U:860:ILE:HD11	2:U:873:LEU:HD21	2.00	0.43
2:U:880:THR:HG22	2:U:880:THR:O	2.18	0.43
3:V:151:ILE:CG2	3:V:297:ILE:HG12	2.47	0.43
2:U:563:GLU:OE1	6:U:900:ATP:O2'	2.33	0.43
2:U:733:VAL:O	2:U:733:VAL:CG1	2.67	0.42
4:W:137:CYS:N	4:W:469:TRP:O	2.43	0.42
4:W:111:THR:HA	4:W:140:ALA:O	2.19	0.42
2:U:481:ILE:HD13	2:U:481:ILE:HG21	1.79	0.42
3:V:142:LEU:HD22	3:V:165:ILE:HD12	2.01	0.42
2:U:278:ILE:HD11	2:U:403:PHE:CD2	2.55	0.41
2:U:770:LEU:HD23	2:U:770:LEU:O	2.20	0.41
4:W:156:LEU:CD2	4:W:393:ILE:HD11	2.49	0.41
2:U:216:PHE:CE2	2:U:868:HIS:CD2	3.09	0.41
2:U:208:TYR:CD1	2:U:208:TYR:O	2.74	0.41
2:U:519:LEU:HD23	2:U:519:LEU:HA	1.91	0.41
2:U:275:SER:HB3	2:U:404:ARG:HA	2.03	0.41
4:W:158:VAL:HG22	4:W:167:VAL:HG22	2.02	0.41
4:W:487:ARG:O	4:W:488:PHE:CD1	2.74	0.41
3:V:10:ILE:HD11	3:V:90:PHE:CE1	2.56	0.41
3:V:370:VAL:HG22	3:V:370:VAL:O	2.20	0.41
6:W:500:ATP:O1A	6:W:500:ATP:O1B	2.34	0.41
3:V:363:ASP:O	5:X:65:ARG:NH1	2.52	0.40
2:U:860:ILE:HD11	2:U:873:LEU:CD2	2.51	0.40
2:U:879:PHE:CD1	2:U:879:PHE:C	2.99	0.40
2:U:313:VAL:O	2:U:313:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:27:PRO:HD3	3:V:340:TRP:CE3	2.57	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	G	108/616 (18%)	106 (98%)	1 (1%)	1 (1%)	14	43
2	U	686/881 (78%)	648 (94%)	36 (5%)	2 (0%)	36	65
3	V	358/375 (96%)	345 (96%)	13 (4%)	0	100	100
4	W	423/489 (86%)	393 (93%)	27 (6%)	3 (1%)	18	49
5	X	38/116 (33%)	36 (95%)	2 (5%)	0	100	100
All	All	1613/2477 (65%)	1528 (95%)	79 (5%)	6 (0%)	31	60

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	U	643	ASN
4	W	213	LYS
2	U	823	HIS
4	W	10	GLY
4	W	470	VAL
1	G	454	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	101/561 (18%)	100 (99%)	1 (1%)	68	76
2	U	629/802 (78%)	618 (98%)	11 (2%)	53	71
3	V	310/320 (97%)	303 (98%)	7 (2%)	44	66
4	W	380/434 (88%)	367 (97%)	13 (3%)	32	59
5	X	37/104 (36%)	35 (95%)	2 (5%)	20	49
All	All	1457/2221 (66%)	1423 (98%)	34 (2%)	44	66

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	451	PRO
2	U	198	LEU
2	U	216	PHE
2	U	283	PRO
2	U	421	LEU
2	U	497	SER
2	U	553	ILE
2	U	555	SER
2	U	644	GLU
2	U	704	GLU
2	U	733	VAL
2	U	756	SER
3	V	32	PRO
3	V	113	LYS
3	V	132	PHE
3	V	222	ASP
3	V	281	SER
3	V	293	LEU
3	V	375	PHE
4	W	12	ASP
4	W	17	VAL
4	W	48	THR
4	W	142	THR
4	W	165	CYS
4	W	206	LEU
4	W	417	ILE
4	W	425	MET
4	W	439	ILE

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Mol	Chain	Res	Type
4	W	454	LEU
4	W	458	ILE
4	W	464	THR
4	W	468	LEU
5	X	58	VAL
5	X	64	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	471	ASN
1	G	494	GLN
1	G	541	ASN
2	U	203	ASN
2	U	312	ASN
2	U	319	GLN
2	U	325	ASN
2	U	615	GLN
2	U	709	GLN
2	U	821	ASN
2	U	823	HIS
2	U	862	ASN
3	V	87	HIS
3	V	92	ASN
3	V	115	ASN
3	V	252	ASN
4	W	60	GLN
4	W	77	ASN
4	W	449	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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$
6	ATP	W	500	7	32,33,33	1.33	6 (18%)	48,52,52	1.32	7 (14%)
6	ATP	V	500	7	32,33,33	1.12	2 (6%)	48,52,52	1.21	5 (10%)
6	ATP	U	900	7	32,33,33	0.52	0	48,52,52	0.69	0

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
6	ATP	W	500	7	-	8/22/38/38	0/3/3/3
6	ATP	V	500	7	-	1/22/38/38	0/3/3/3
6	ATP	U	900	7	-	1/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	500	ATP	PA-O3A	-5.14	1.54	1.59
6	W	500	ATP	PB-O3A	-3.51	1.55	1.59
6	W	500	ATP	PB-O2B	-3.27	1.40	1.55
6	W	500	ATP	C8-N9	-2.53	1.33	1.37
6	W	500	ATP	PG-O1G	-2.49	1.42	1.50
6	W	500	ATP	PA-O3A	-2.42	1.56	1.59
6	W	500	ATP	PB-O1B	2.20	1.58	1.50
6	V	500	ATP	PB-O3A	-2.14	1.57	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	V	500	ATP	O3A-PA-O1A	-3.86	99.11	110.70
6	W	500	ATP	O3B-PB-O1B	3.08	119.96	110.70
6	W	500	ATP	O3B-PG-O1G	-2.99	95.29	111.04
6	W	500	ATP	O4'-C4'-C3'	-2.98	99.23	105.15
6	V	500	ATP	O2A-PA-O1A	2.68	124.90	112.44
6	W	500	ATP	O2G-PG-O3B	2.47	112.93	104.64
6	W	500	ATP	O2B-PB-O1B	2.44	123.82	112.44
6	W	500	ATP	O2A-PA-O1A	2.39	123.57	112.44
6	V	500	ATP	O2B-PB-O1B	2.35	123.40	112.44
6	V	500	ATP	O2G-PG-O3B	2.28	112.29	104.64
6	W	500	ATP	C3'-C2'-C1'	-2.26	97.18	101.46
6	V	500	ATP	O3B-PG-O1G	-2.04	100.32	111.04

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	W	500	ATP	C5'-O5'-PA-O1A
6	W	500	ATP	C5'-O5'-PA-O2A
6	W	500	ATP	C5'-O5'-PA-O3A
6	W	500	ATP	C4'-C5'-O5'-PA
6	W	500	ATP	C3'-C4'-C5'-O5'
6	W	500	ATP	O4'-C4'-C5'-O5'
6	W	500	ATP	C2'-C1'-N9-C8
6	U	900	ATP	C2'-C1'-N9-C8
6	V	500	ATP	PA-O3A-PB-O1B
6	W	500	ATP	O4'-C1'-N9-C8

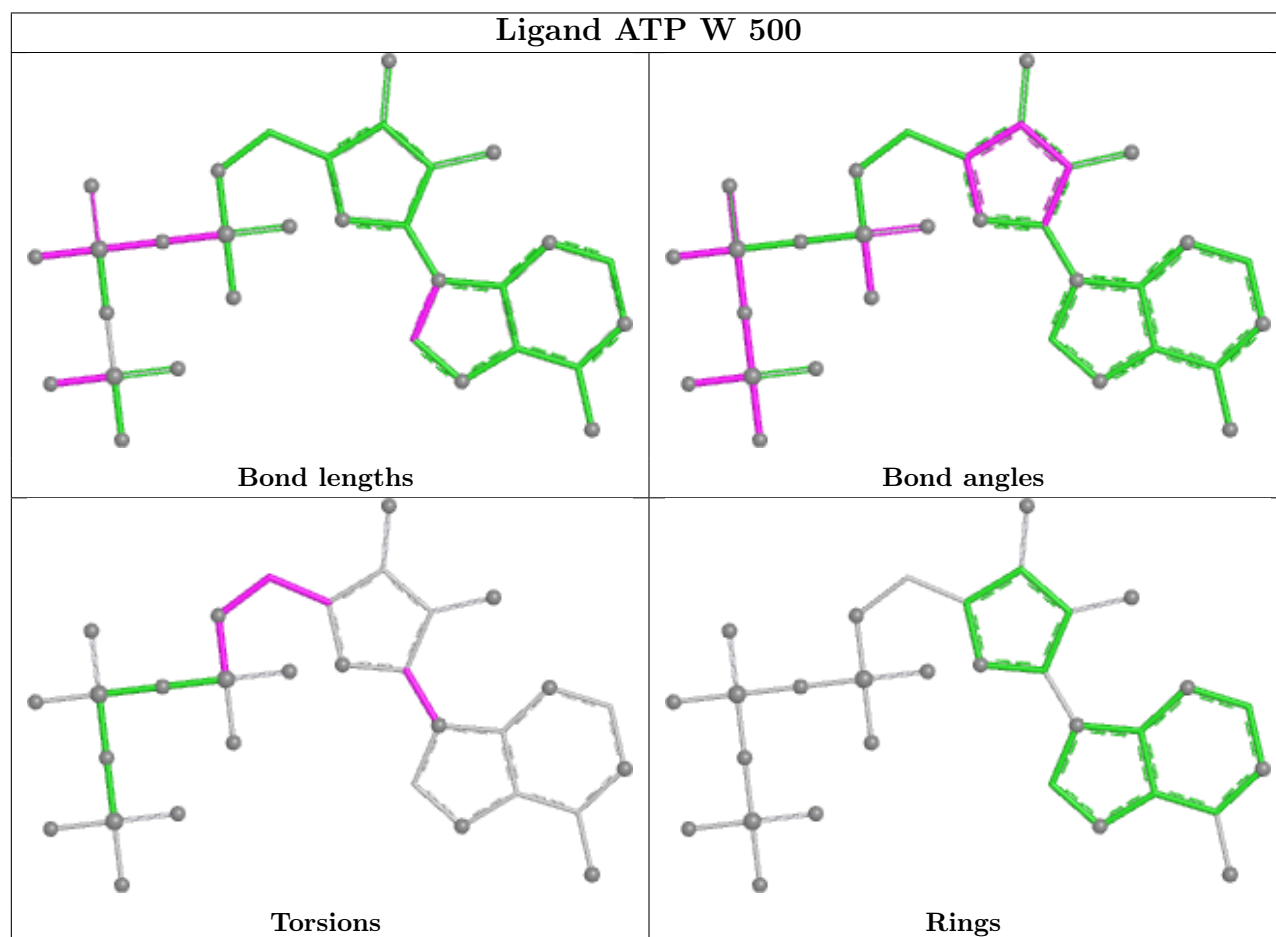
There are no ring outliers.

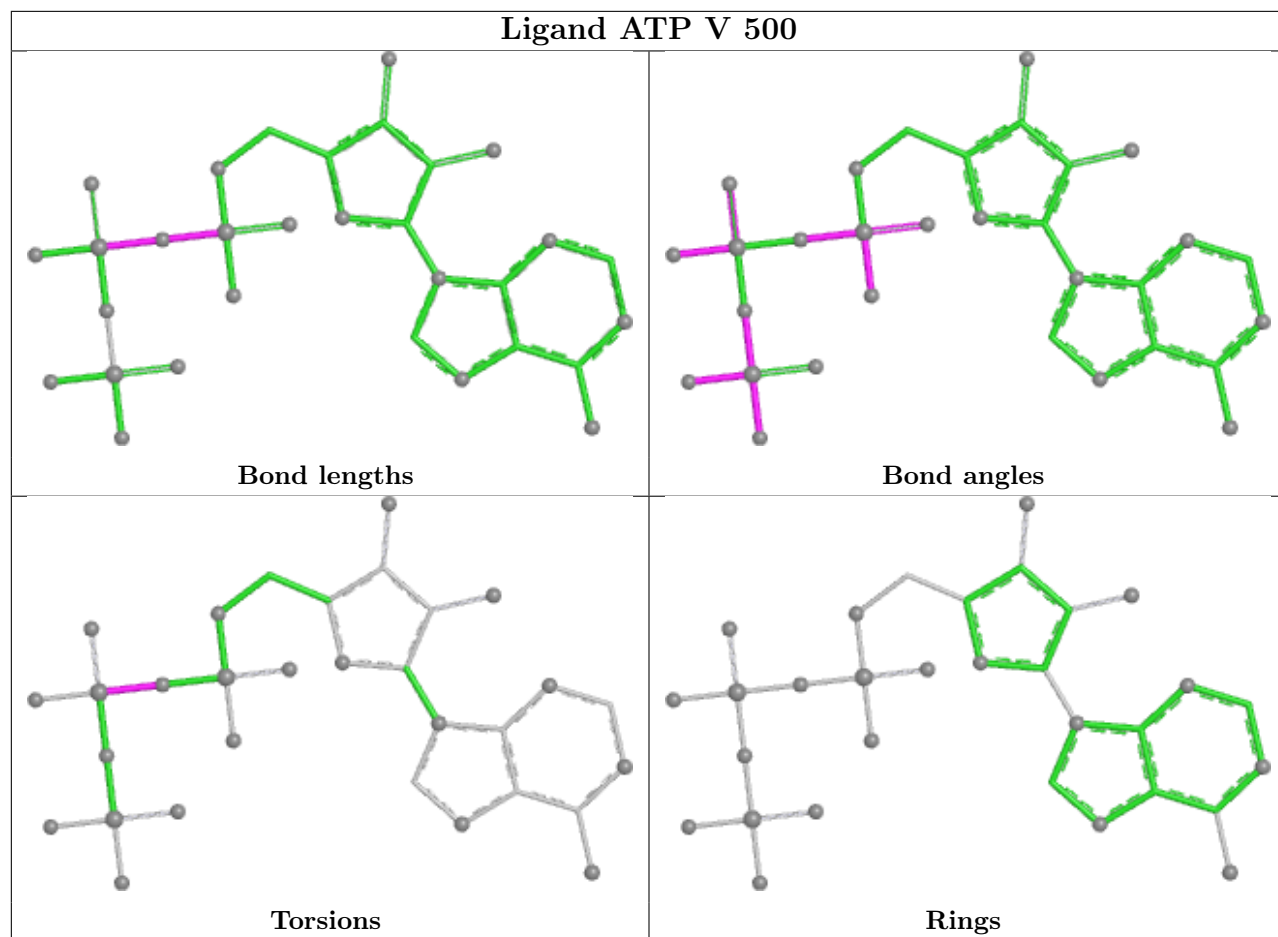
2 monomers are involved in 5 short contacts:

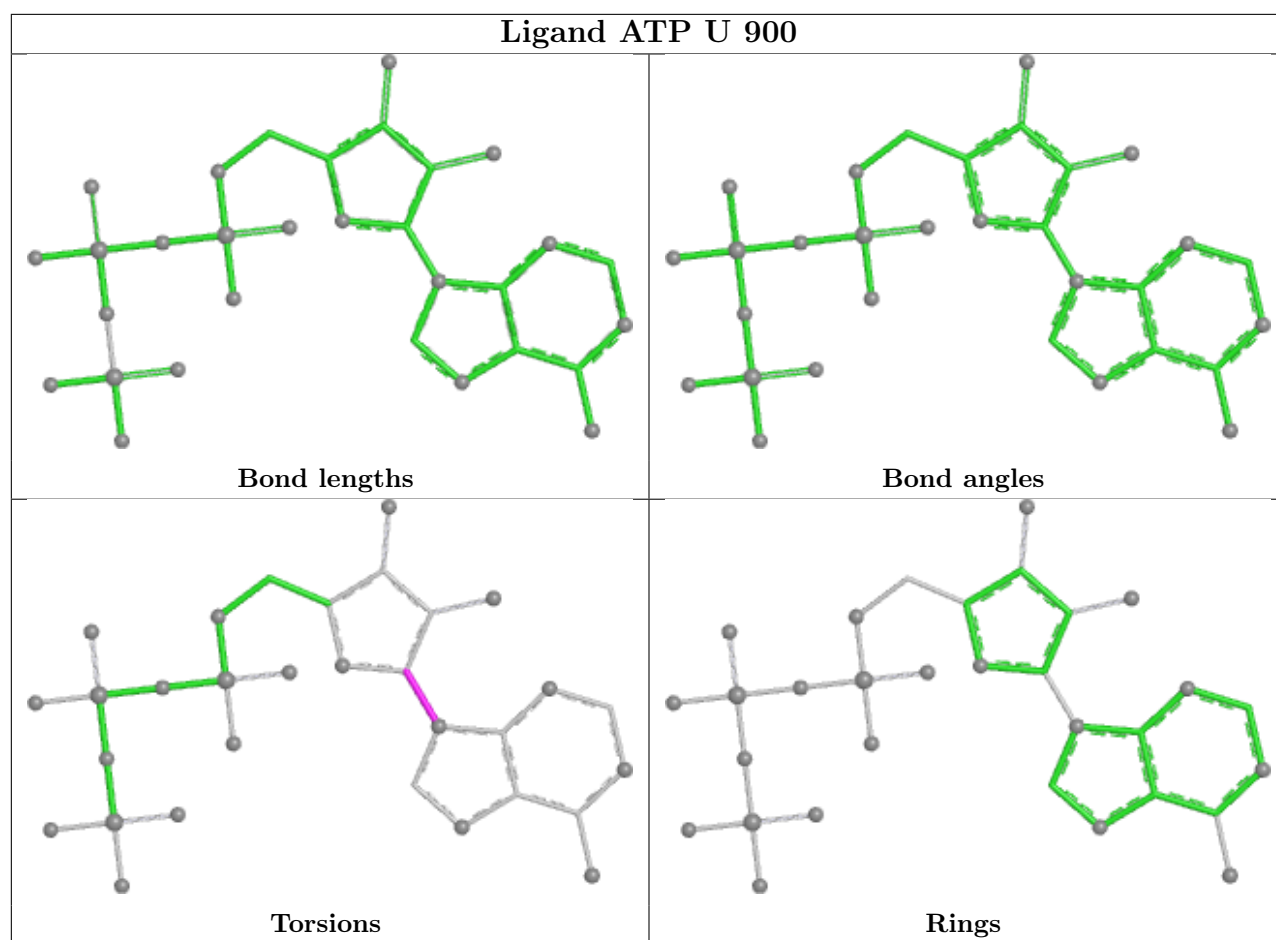
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	W	500	ATP	1	0
6	U	900	ATP	4	0

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.

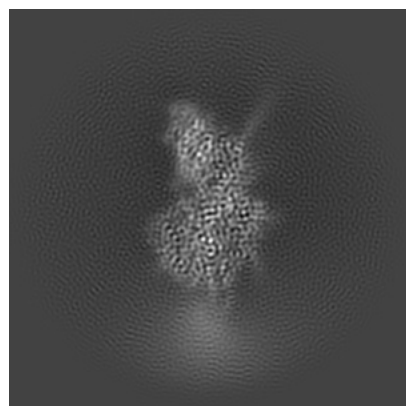
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15163. These allow visual inspection of the internal detail of the map and identification of artifacts.

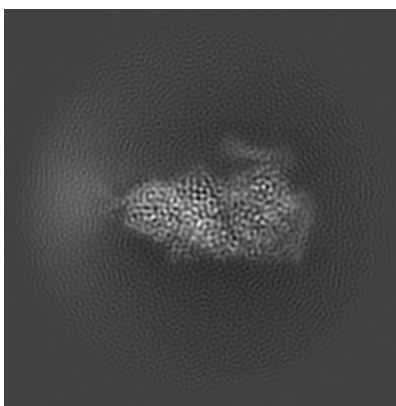
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

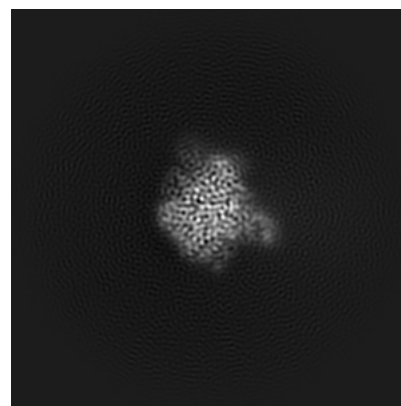
6.1.1 Primary map



X

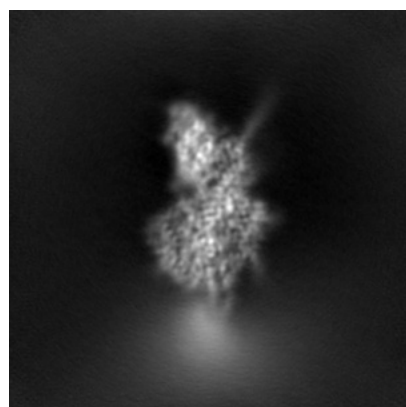


Y

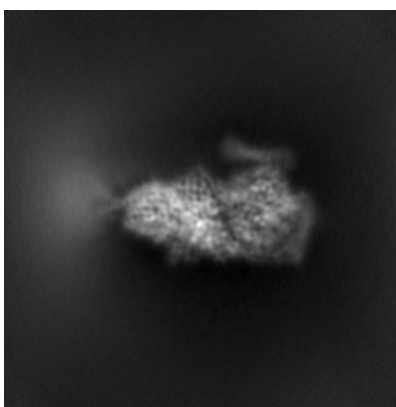


Z

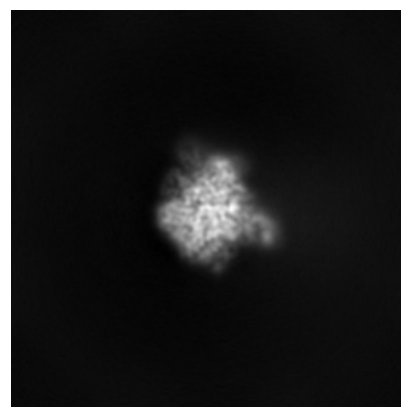
6.1.2 Raw map



X



Y

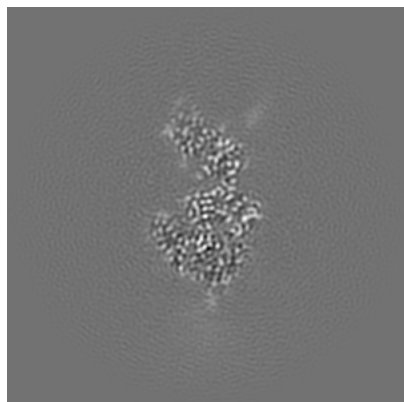


Z

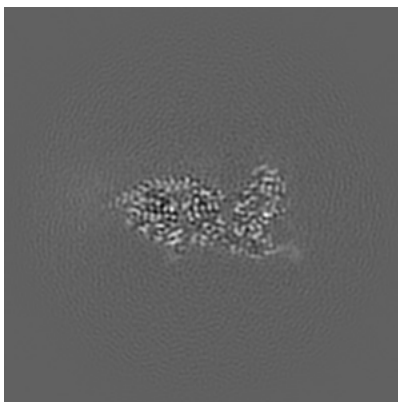
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

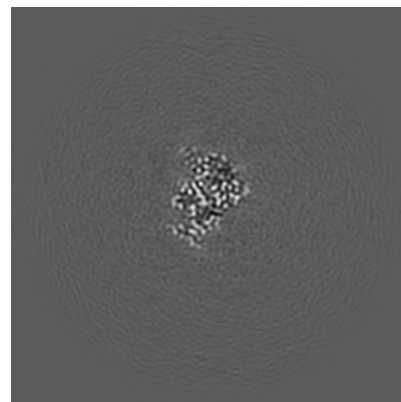
6.2.1 Primary map



X Index: 128

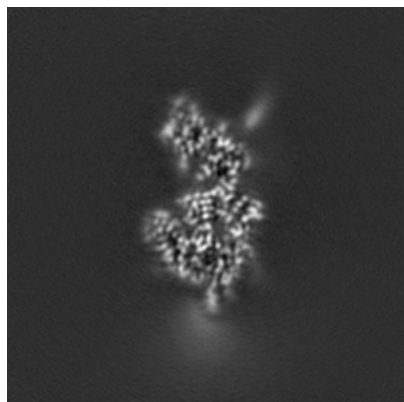


Y Index: 128

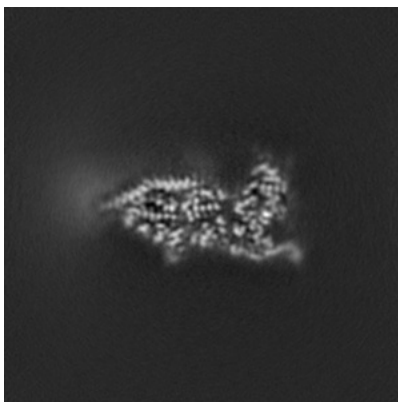


Z Index: 128

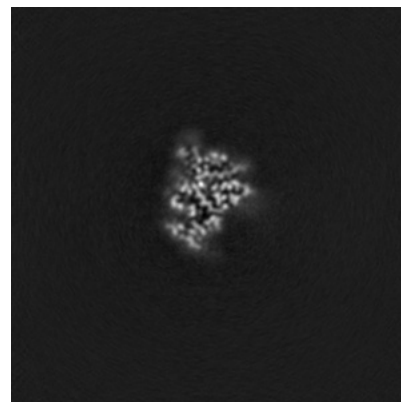
6.2.2 Raw map



X Index: 128



Y Index: 128

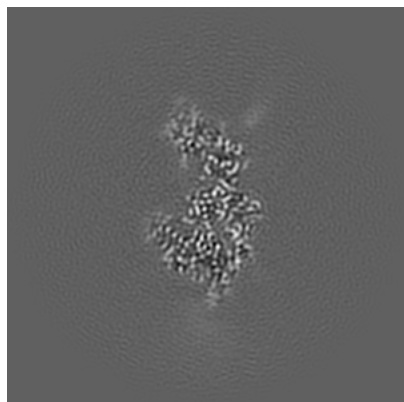


Z Index: 128

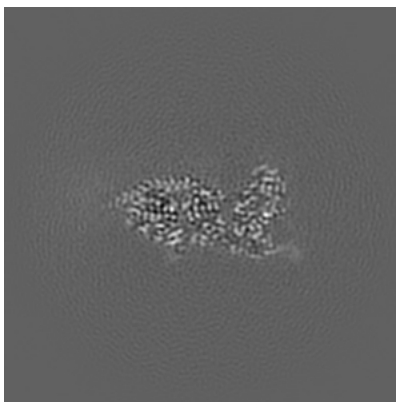
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

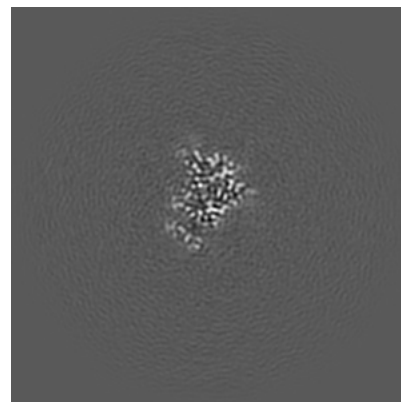
6.3.1 Primary map



X Index: 129

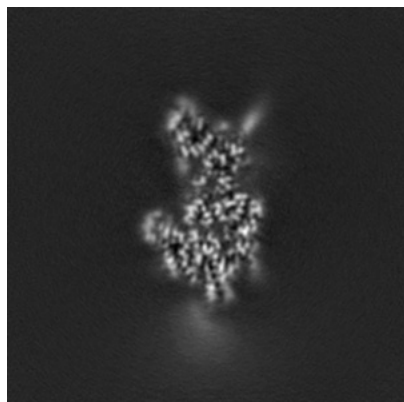


Y Index: 128

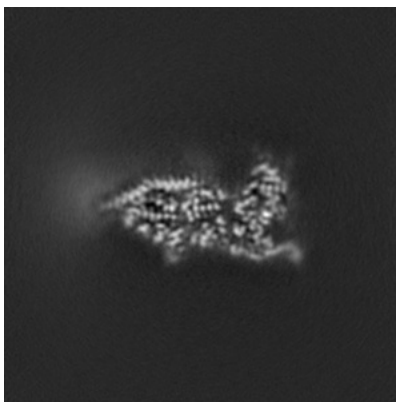


Z Index: 126

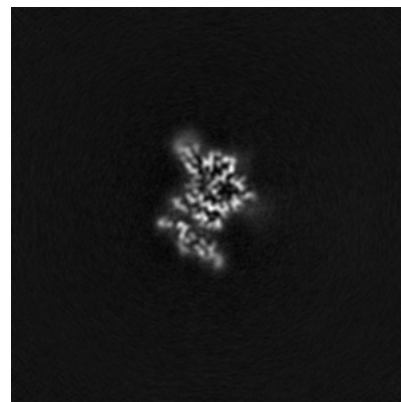
6.3.2 Raw map



X Index: 131



Y Index: 128

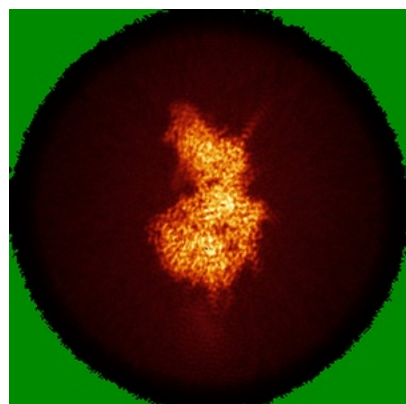


Z Index: 122

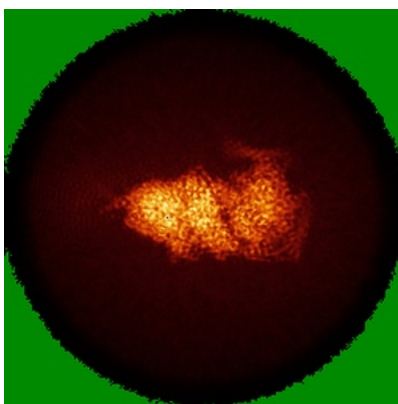
The images above show the largest variance slices of the map in three orthogonal directions.

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

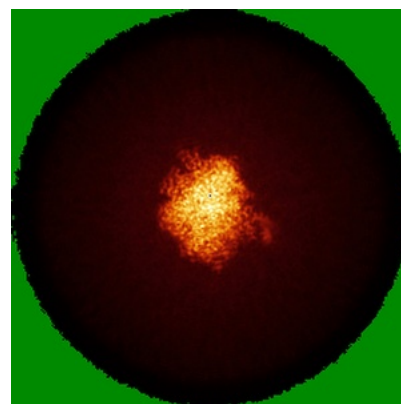
6.4.1 Primary map



X

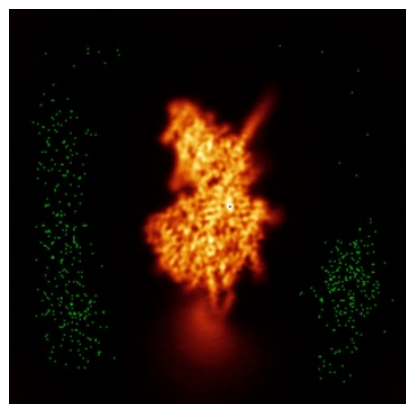


Y

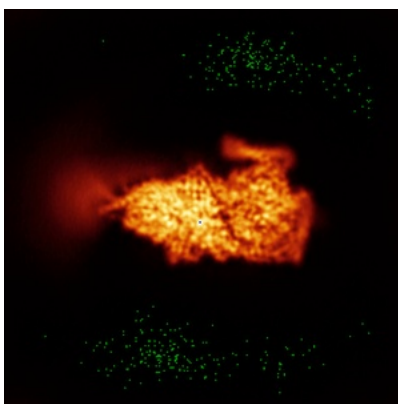


Z

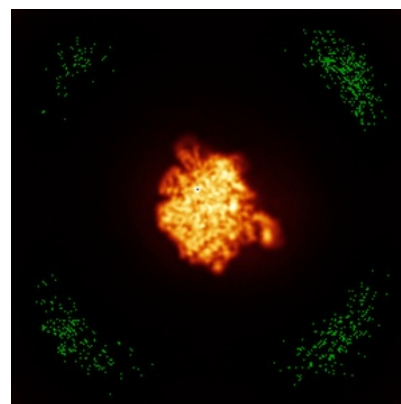
6.4.2 Raw map



X



Y

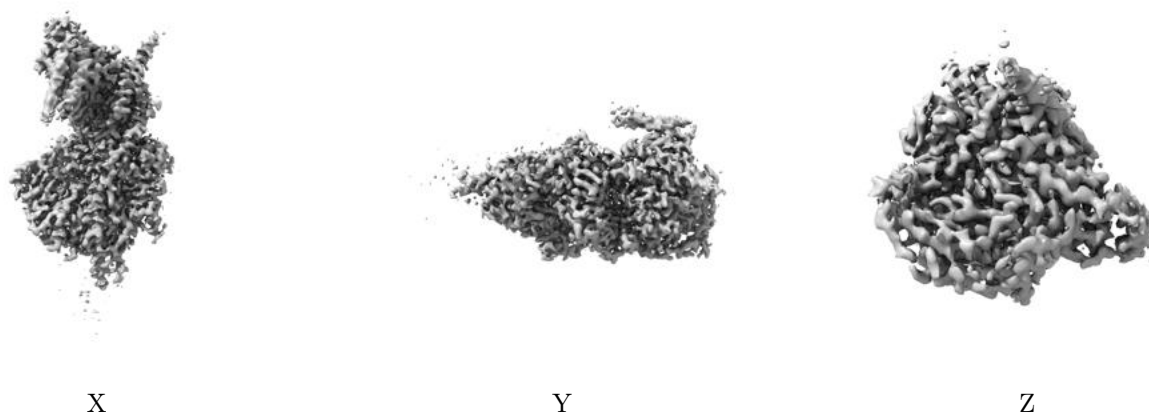


Z

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 0.735. 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.

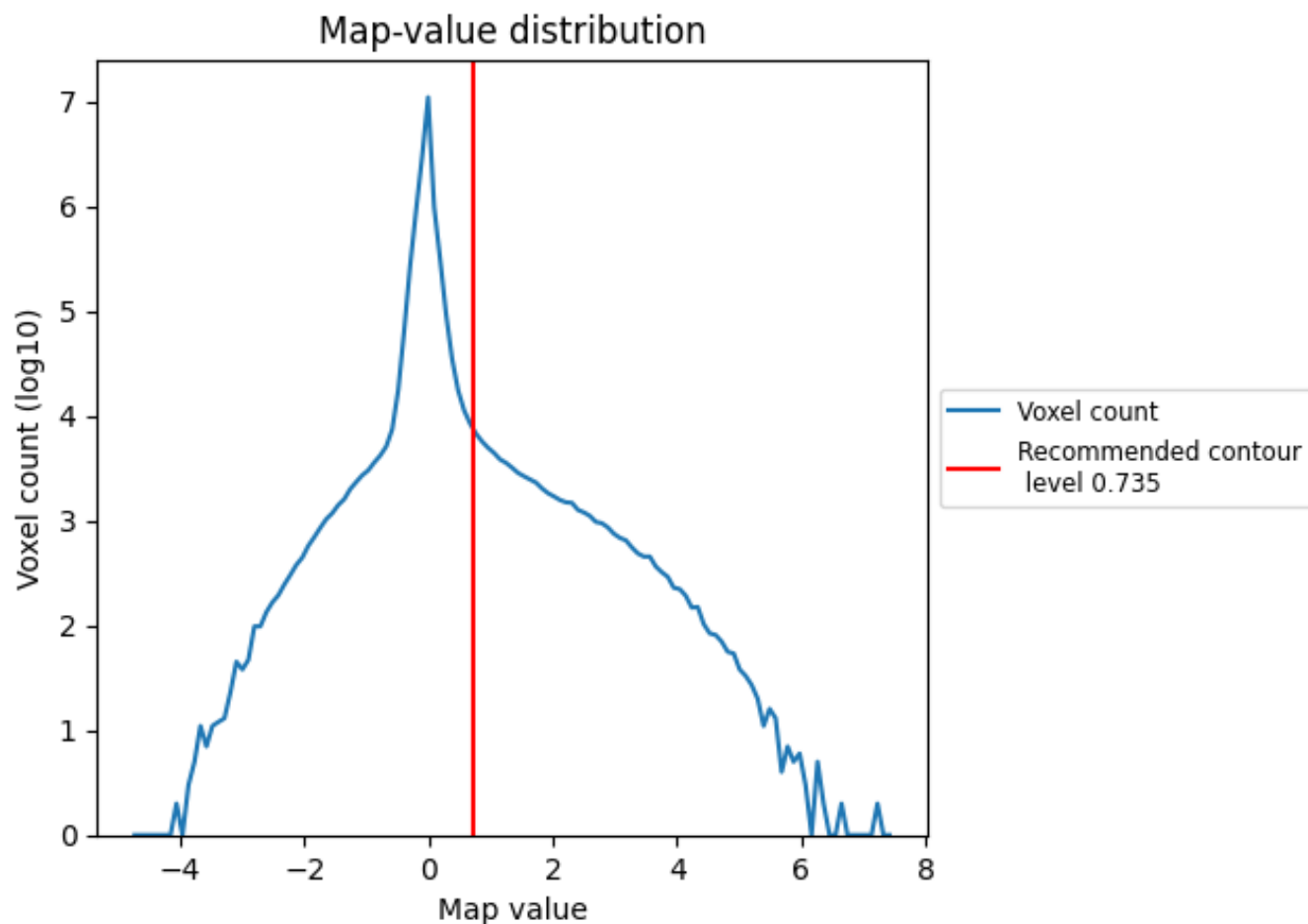
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

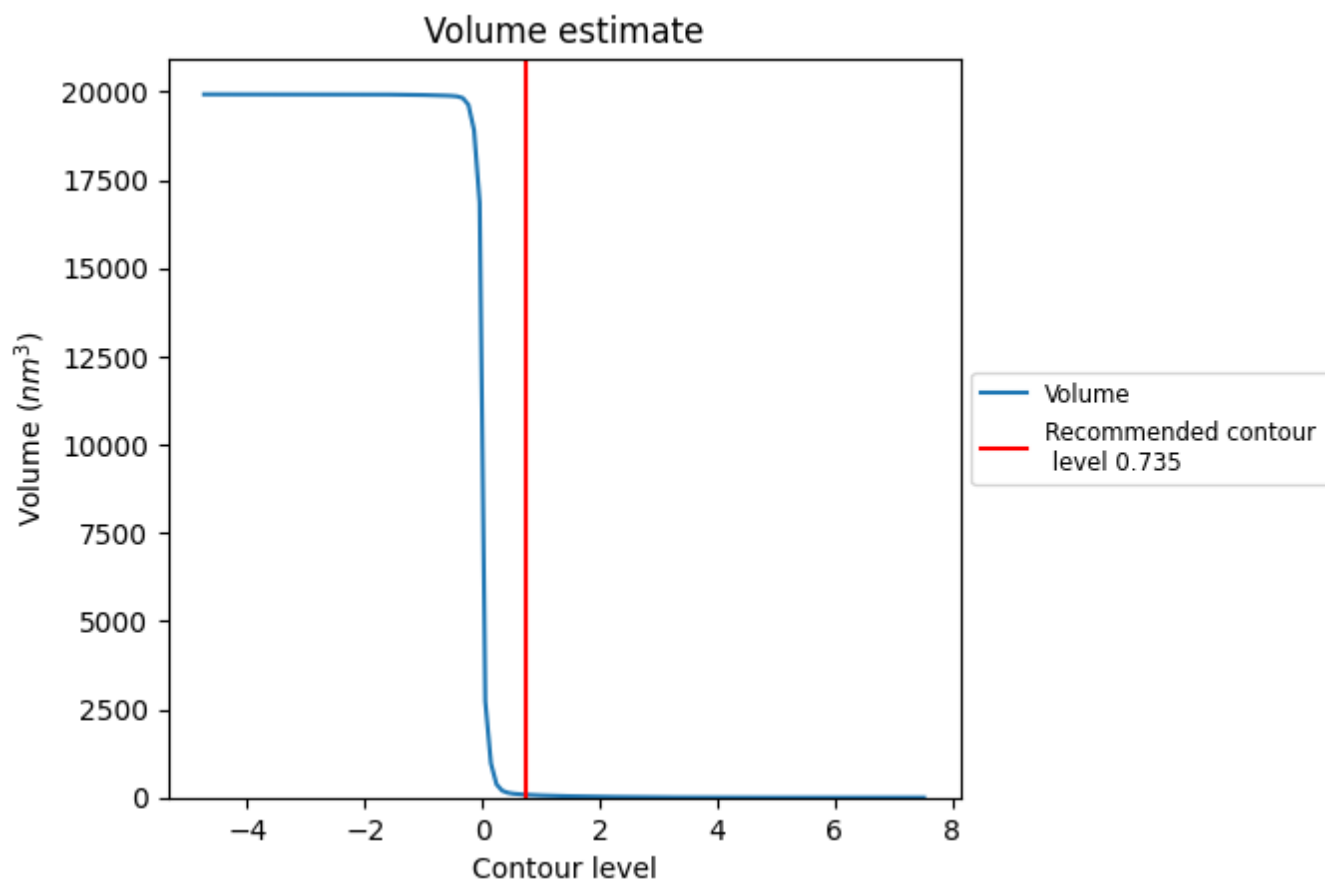
This section contains the results of statistical analysis of the map.

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.

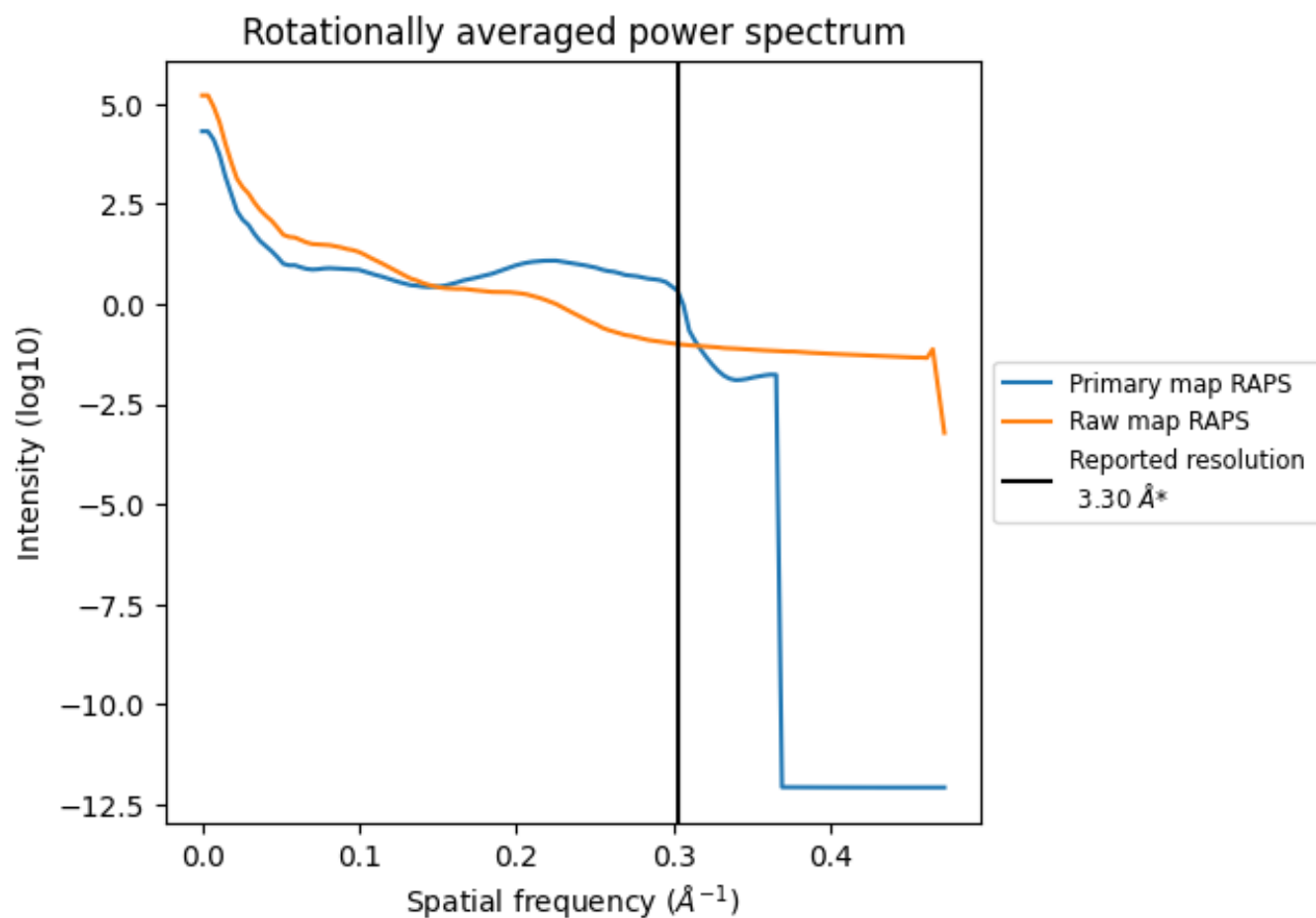
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 81 nm³; this corresponds to an approximate mass of 73 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 ⓘ

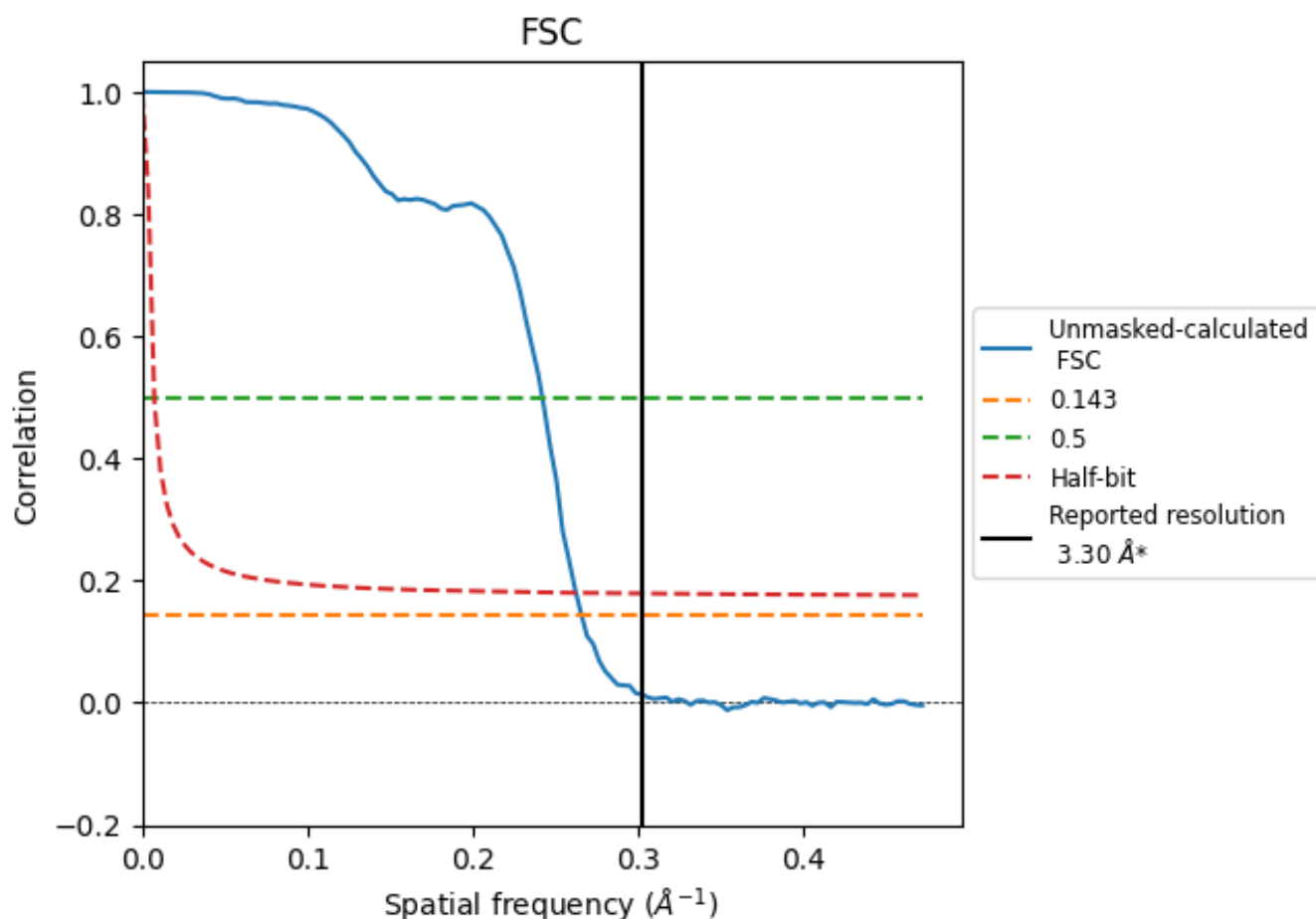


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

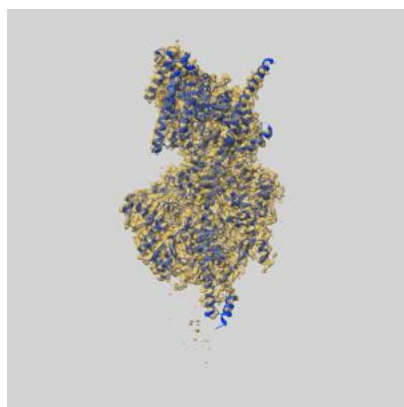
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.76	4.13	3.81

*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 3.76 differs from the reported value 3.3 by more than 10 %

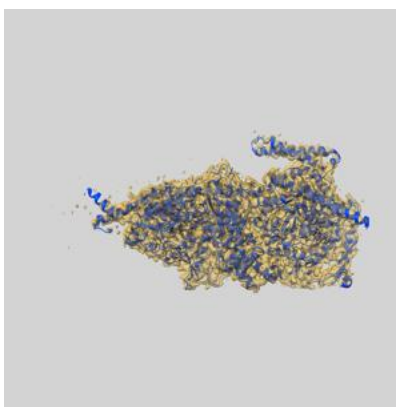
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15163 and PDB model 8A5A. Per-residue inclusion information can be found in section [3](#) on page [7](#).

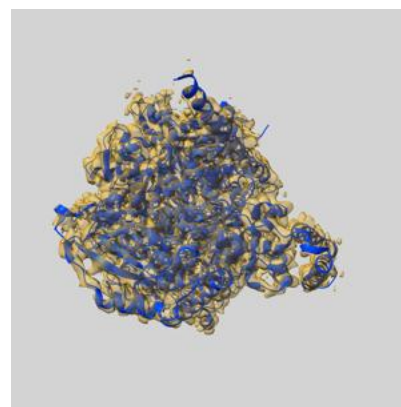
9.1 Map-model overlay [i](#)



X



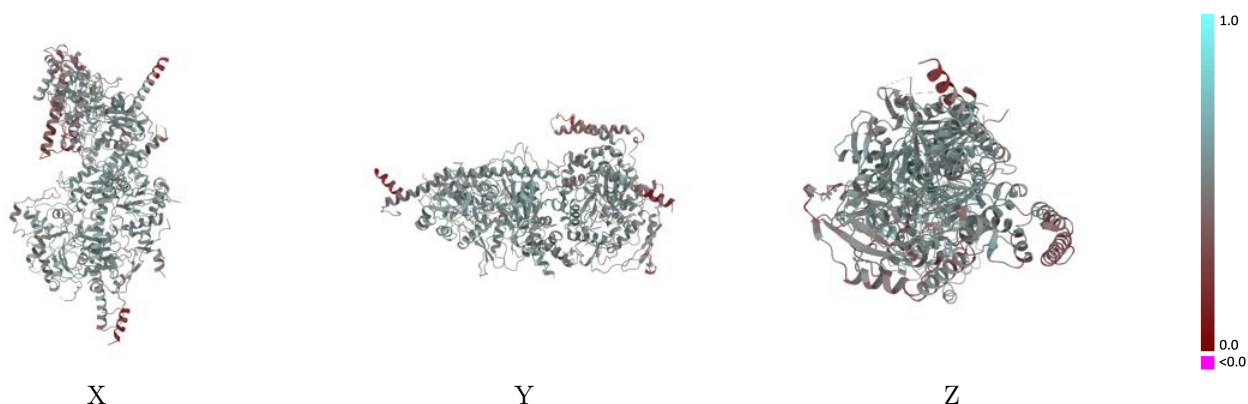
Y



Z

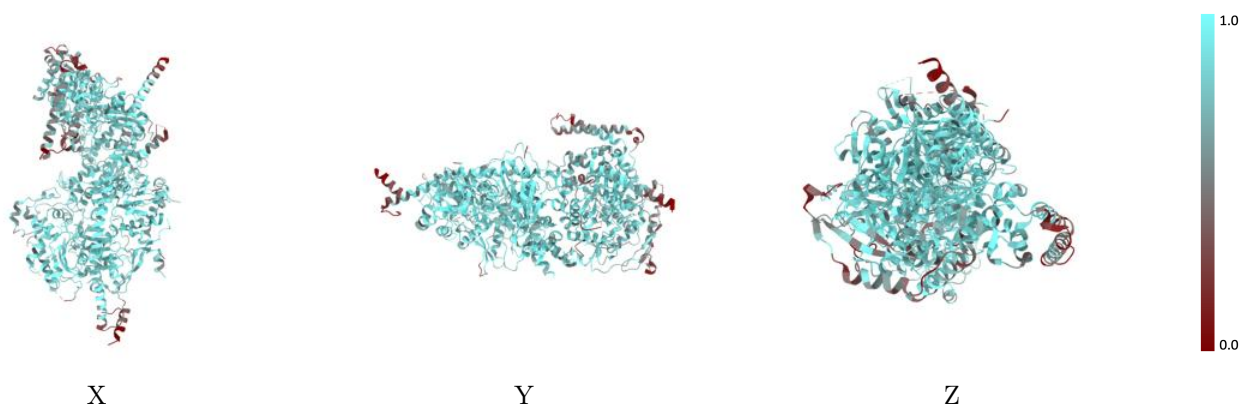
The images above show the 3D surface view of the map at the recommended contour level 0.735 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



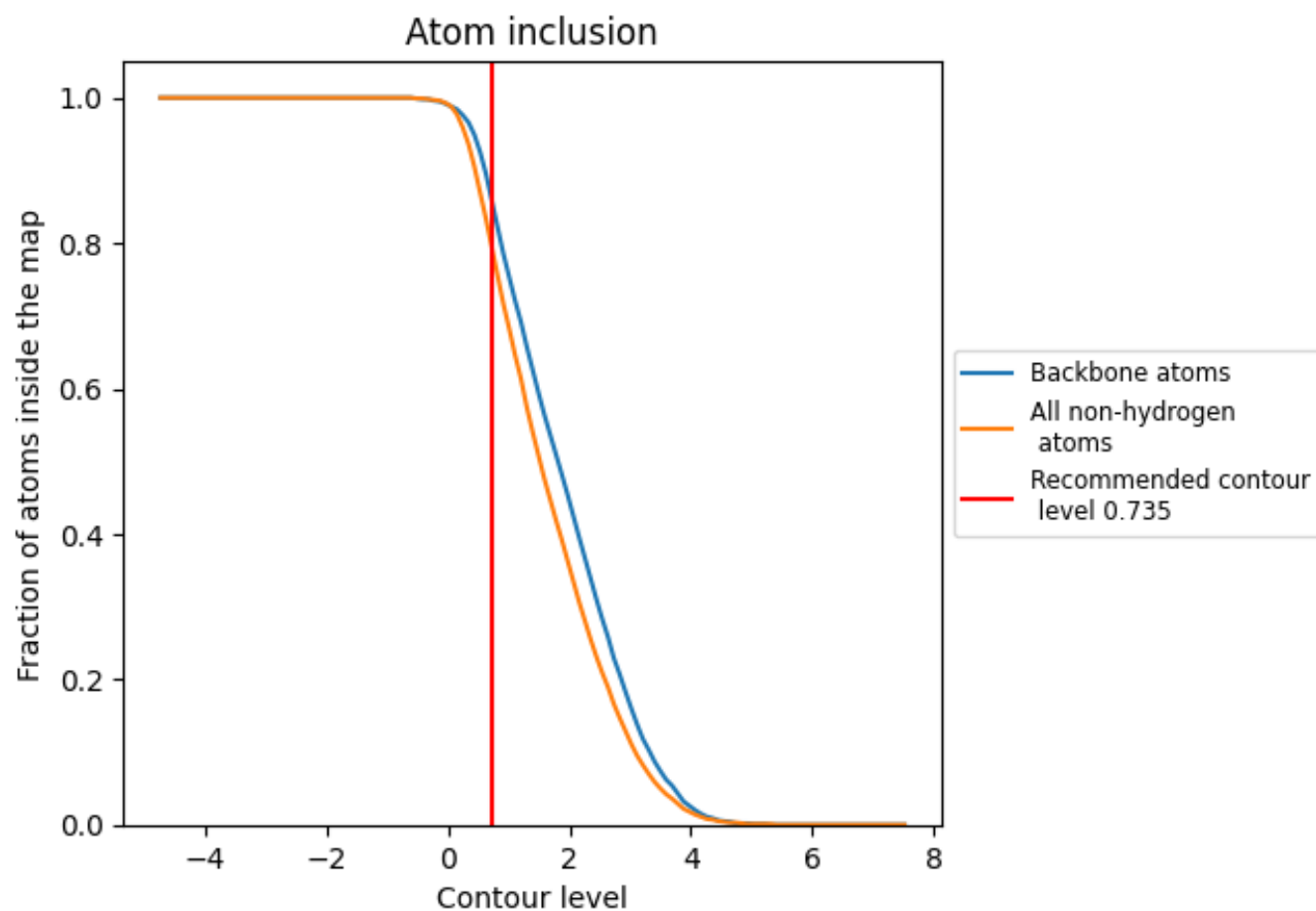
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.735).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 79% 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 (0.735) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7890	0.5090
G	0.7080	0.4770
U	0.7250	0.4820
V	0.8690	0.5460
W	0.8460	0.5290
X	0.8410	0.5250

