



Full wwPDB EM Validation Report ⓘ

Aug 3, 2026 – 12:14 PM JST

PDB ID : 9W5I / pdb_00009w5i
EMDB ID : EMD-65663
Title : AGO maturation complex (AMC): AGO2-miRNA duplex in complex with Hsp90 beta and co-chaperone p23
Authors : Lee, H.; Jeong, M.-S.; Lee, Y.-Y.; Lee, J.-H.; Lee, D.; Kim, V.N.; Roh, S.-H.
Deposited on : 2025-08-01
Resolution : 2.63 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

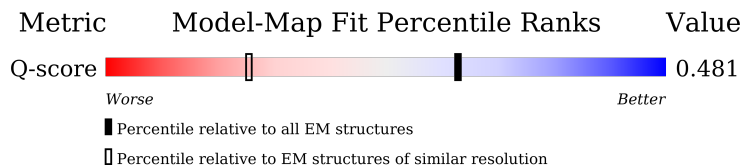
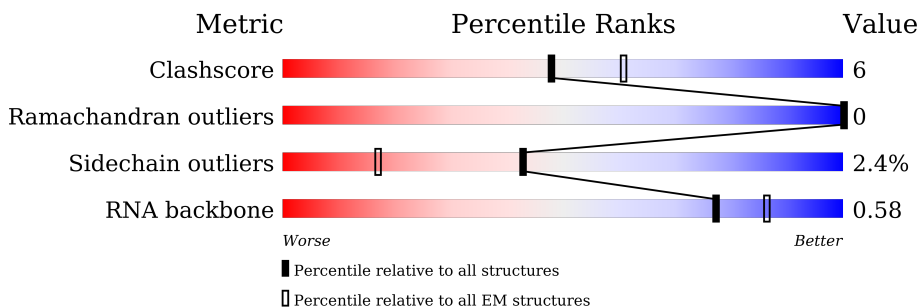
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.63 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	8888 (2.13 - 3.13)

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	724	
1	B	724	
2	C	160	

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Mol	Chain	Length	Quality of chain
3	D	859	7% 68% 18% • 13%
4	E	22	5% 45% 45% 9%
5	F	22	5% 41% 45% 14%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18185 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 Heat shock protein HSP 90-beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	628	Total	C	N	O	S	0	0
			5088	3226	856	983	23		
1	B	624	Total	C	N	O	S	0	0
			5050	3204	848	975	23		

- Molecule 2 is a protein called Prostaglandin E synthase 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	129	Total	C	N	O	S	0	0
			1077	670	188	210	9		

- Molecule 3 is a protein called Protein argonaute-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	747	Total	C	N	O	S	0	0
			5977	3792	1085	1063	37		

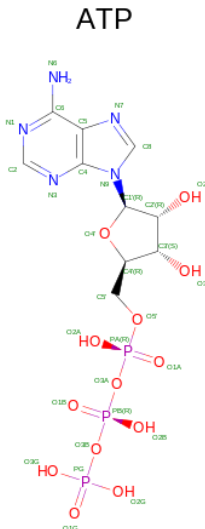
- Molecule 4 is a RNA chain called RNA (5'-R(P*UP*GP*AP*GP*GP*UP*AP*GP*UP*AP*GP*GP*UP*UP*GP*UP*AP*UP*AP*GP*UP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	22	Total	C	N	O	P	0	0
			475	211	83	159	22		

- Molecule 5 is a RNA chain called RNA (5'-R(P*CP*UP*AP*UP*AP*CP*AP*AP*UP*CP*UP*AP*CP*UP*GP*UP*CP*UP*UP*UP*CP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	22	Total	C	N	O	P	0	0
			453	204	68	159	22		

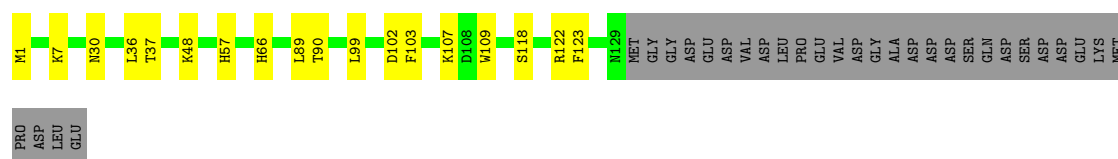
- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



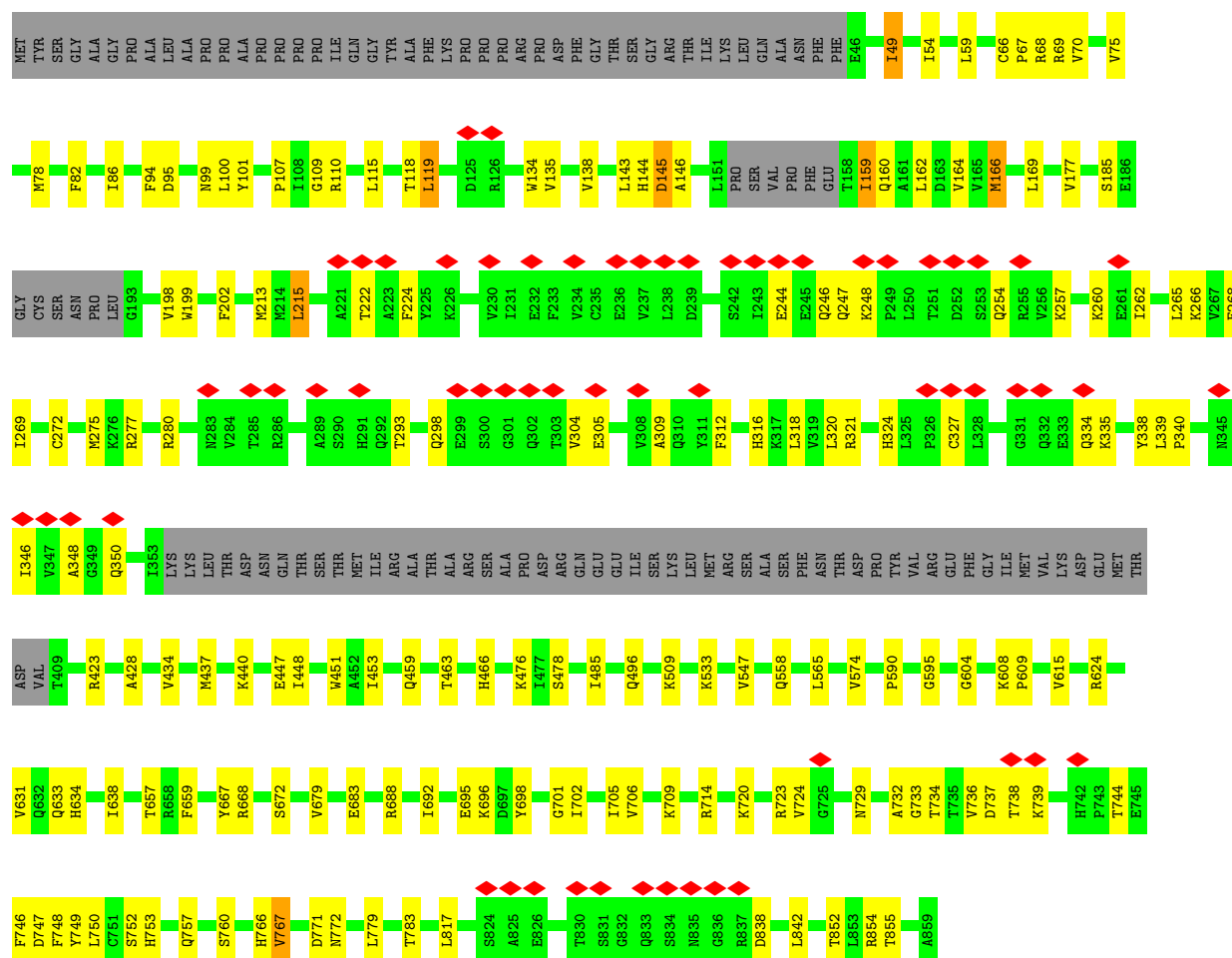
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total 31	C 10	N 5	O 13	P 3	0
6	B	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

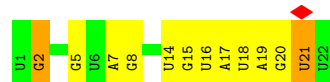
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total 1	Mg 1	0
7	B	1	Total 1	Mg 1	0
7	D	1	Total 1	Mg 1	0



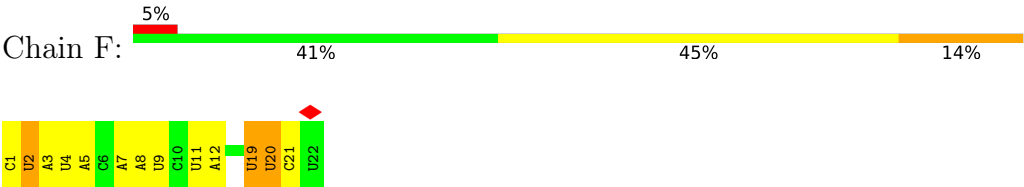
• Molecule 3: Protein argonaute-2



• Molecule 4: RNA (5'-R(P*UP*GP*AP*GP*GP*UP*AP*GP*UP*AP*GP*GP*UP*UP*GP*U P*AP*UP*AP*GP*UP*U)-3')



• Molecule 5: RNA (5'-R(P*CP*UP*AP*UP*AP*CP*AP*AP*UP*CP*UP*AP*CP*UP*GP*U P*CP*UP*UP*UP*CP*U)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1225410	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 ($e^-/\text{\AA}^2$)	69.9	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.499	Depositor
Minimum map value	-0.948	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.0834	Depositor
Map size (Å)	318.71997, 318.71997, 318.71997	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1382856, 1.1382856, 1.1382856	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	A	0.11	0/5172	0.26	0/6952
1	B	0.13	0/5134	0.27	0/6903
2	C	0.11	0/1103	0.32	0/1483
3	D	0.14	0/6116	0.32	0/8273
4	E	0.12	0/531	0.20	0/825
5	F	0.13	0/502	0.28	0/776
All	All	0.13	0/18558	0.28	0/25212

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5088	0	5127	46	0
1	B	5050	0	5089	45	0
2	C	1077	0	1002	8	0
3	D	5977	0	6015	101	0
4	E	475	0	234	11	0
5	F	453	0	233	15	0
6	A	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	31	0	12	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
All	All	18185	0	17724	211	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 6.

All (211) 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)
3:D:49:ILE:HD11	3:D:144:HIS:HB2	1.70	0.74
1:A:65:LEU:HD23	1:A:177:ARG:HH12	1.52	0.73
1:A:567:MET:HA	1:A:567:MET:HE3	1.71	0.72
3:D:272:CYS:HB2	3:D:275:MET:HB3	1.71	0.71
3:D:213:MET:HA	3:D:213:MET:HE2	1.70	0.71
1:A:620:MET:HE3	1:A:620:MET:HA	1.72	0.70
3:D:720:LYS:HA	3:D:723:ARG:HB3	1.73	0.69
1:B:567:MET:HA	1:B:567:MET:HE2	1.75	0.69
3:D:748:PHE:HB2	3:D:767:VAL:HG21	1.77	0.67
1:A:93:MET:HG3	1:A:147:THR:HG21	1.76	0.67
3:D:339:LEU:HD22	3:D:340:PRO:HD2	1.76	0.67
3:D:224:PHE:HZ	3:D:348:ALA:HA	1.61	0.66
3:D:318:LEU:HD12	3:D:321:ARG:HH12	1.62	0.65
1:B:621:MET:HE2	1:B:621:MET:H	1.62	0.64
1:A:576:GLU:HG3	1:A:623:LYS:HD2	1.78	0.64
3:D:185:SER:HA	3:D:198:VAL:HG21	1.81	0.62
1:B:154:GLN:HE21	1:B:175:ILE:HG12	1.64	0.62
1:A:219:LYS:HB2	1:A:276:TYR:HB2	1.80	0.62
3:D:714:ARG:HG2	3:D:760:SER:HB3	1.82	0.61
3:D:729:ASN:HA	3:D:760:SER:HB2	1.83	0.60
3:D:744:THR:HG23	3:D:746:PHE:H	1.67	0.59
2:C:118:SER:C	2:C:122:ARG:HH21	2.11	0.59
3:D:736:VAL:HG12	3:D:738:THR:H	1.69	0.58
3:D:737:ASP:HA	3:D:739:LYS:HZ2	1.68	0.58
3:D:246:GLN:HA	3:D:248:LYS:HE3	1.85	0.58
4:E:16:U:H2'	4:E:17:A:C8	2.38	0.58
4:E:2:G:H1	5:F:19:U:H3	1.53	0.57
1:A:53:LYS:HE3	1:A:125:MET:HE1	1.85	0.57
3:D:739:LYS:HE2	3:D:747:ASP:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:SER:HB3	1:B:510:VAL:HG12	1.86	0.57
1:A:567:MET:HE1	1:A:655:VAL:HG22	1.87	0.56
1:B:567:MET:HE1	1:B:655:VAL:HG21	1.87	0.56
3:D:706:VAL:HG23	3:D:766:HIS:HB2	1.88	0.56
4:E:19:A:H2'	4:E:20:G:C8	2.41	0.56
3:D:702:ILE:H	3:D:771:ASP:HB2	1.70	0.55
3:D:262:ILE:HG23	3:D:265:LEU:HD12	1.88	0.55
1:B:154:GLN:NE2	1:B:175:ILE:HG12	2.22	0.55
3:D:609:PRO:HG3	3:D:842:LEU:HD13	1.89	0.55
3:D:312:PHE:HA	3:D:316:HIS:HB2	1.90	0.54
1:A:450:ARG:HG2	1:A:450:ARG:HH11	1.71	0.54
2:C:89:LEU:HD23	2:C:99:LEU:HD21	1.89	0.54
4:E:2:G:N2	5:F:19:U:O2	2.39	0.54
3:D:59:LEU:HD11	3:D:100:LEU:HB2	1.89	0.54
5:F:2:U:H2'	5:F:3:A:H8	1.73	0.53
3:D:69:ARG:N	3:D:69:ARG:HD3	2.24	0.53
1:B:196:ARG:HH22	1:B:197:ARG:HD3	1.74	0.53
1:B:619:TYR:HB2	1:B:620:MET:SD	2.48	0.53
3:D:733:GLY:HA2	3:D:752:SER:HB2	1.91	0.52
2:C:7:LYS:HB3	2:C:102:ASP:HB2	1.92	0.52
3:D:346:ILE:HD11	3:D:350:GLN:HA	1.91	0.52
1:A:312:TRP:H	1:A:312:TRP:CD1	2.26	0.52
1:A:327:LEU:HD21	1:A:400:ILE:HG23	1.92	0.52
1:B:612:ARG:HH22	1:B:617:MET:HG3	1.74	0.52
1:B:526:LYS:HB3	3:D:146:ALA:HB2	1.92	0.51
3:D:68:ARG:HB3	3:D:69:ARG:HH11	1.74	0.51
4:E:14:U:H2'	4:E:15:G:H8	1.74	0.51
5:F:1:C:HO2'	5:F:2:U:H6	1.58	0.51
4:E:18:U:H2'	4:E:19:A:C4	2.45	0.51
1:A:663:LEU:HD23	1:A:670:LEU:HD23	1.93	0.51
1:A:365:SER:HB2	1:A:369:LEU:HD12	1.93	0.51
5:F:19:U:H5'	5:F:20:U:H5''	1.92	0.51
2:C:30:ASN:HB2	2:C:37:THR:HB	1.92	0.50
3:D:558:GLN:HG2	5:F:19:U:H2'	1.93	0.50
3:D:668:ARG:HB3	3:D:706:VAL:HG12	1.94	0.50
1:A:563:LEU:HD22	1:A:639:ARG:HB2	1.93	0.50
1:A:98:LEU:HD21	1:A:157:TRP:HB2	1.94	0.50
1:B:485:TYR:CZ	1:B:535:SER:HB2	2.47	0.50
3:D:723:ARG:HA	3:D:729:ASN:HB2	1.93	0.50
3:D:86:ILE:HD12	3:D:107:PRO:HG2	1.93	0.50
3:D:734:THR:H	3:D:752:SER:HA	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:638:ILE:HG22	3:D:679:VAL:HG22	1.93	0.50
1:A:18:GLN:HB2	1:B:104:THR:HG22	1.92	0.49
1:A:602:MET:HE2	1:A:602:MET:HA	1.93	0.49
5:F:11:U:H2'	5:F:12:A:C8	2.47	0.49
5:F:11:U:H2'	5:F:12:A:H8	1.77	0.49
1:A:573:LYS:C	1:A:573:LYS:HD2	2.37	0.49
3:D:75:VAL:HG11	3:D:94:PHE:CD2	2.48	0.49
3:D:95:ASP:HB2	3:D:99:ASN:HB2	1.94	0.49
3:D:254:GLN:HA	3:D:257:LYS:HE3	1.93	0.49
4:E:14:U:H2'	4:E:15:G:C8	2.46	0.49
3:D:437:MET:HE1	3:D:565:LEU:HD11	1.94	0.49
5:F:7:A:H2'	5:F:8:A:C8	2.47	0.49
3:D:134:TRP:HD1	3:D:135:VAL:N	2.11	0.49
5:F:2:U:H2'	5:F:3:A:C8	2.48	0.48
5:F:7:A:H2'	5:F:8:A:H8	1.78	0.48
3:D:779:LEU:O	3:D:783:THR:HG22	2.13	0.48
3:D:82:PHE:HB3	3:D:86:ILE:HG22	1.94	0.48
1:B:618:GLY:C	1:B:621:MET:HE1	2.39	0.48
3:D:724:VAL:HG21	3:D:757:GLN:HA	1.95	0.48
1:A:638:LEU:HD13	1:A:654:LEU:HD22	1.94	0.48
3:D:118:THR:HB	3:D:119:LEU:HD22	1.95	0.48
3:D:293:THR:HG22	3:D:305:GLU:HB3	1.95	0.48
4:E:18:U:H2'	4:E:19:A:C5	2.48	0.47
3:D:78:MET:SD	3:D:115:LEU:HD11	2.54	0.47
1:B:657:LEU:HD13	1:B:679:ARG:HD2	1.97	0.47
1:A:649:LYS:HA	1:A:652:LYS:HD2	1.97	0.47
3:D:166:MET:HE2	3:D:166:MET:HB3	1.72	0.47
3:D:110:ARG:HD2	3:D:134:TRP:HE1	1.79	0.47
3:D:169:LEU:HD12	3:D:169:LEU:O	2.14	0.47
3:D:247:GLN:HE21	3:D:324:HIS:HB2	1.80	0.47
3:D:309:ALA:HA	3:D:320:LEU:HD13	1.96	0.47
1:A:573:LYS:H	3:D:423:ARG:NH1	2.12	0.47
1:B:591:ILE:HG22	1:B:626:LEU:HD12	1.97	0.46
3:D:753:HIS:CE1	3:D:783:THR:HG23	2.50	0.46
5:F:4:U:H2'	5:F:5:A:C8	2.50	0.46
1:B:471:GLU:HB3	1:B:475:ARG:HH21	1.80	0.46
3:D:496:GLN:N	3:D:496:GLN:OE1	2.49	0.46
3:D:244:GLU:HA	3:D:247:GLN:HB2	1.98	0.46
3:D:705:ILE:HG12	3:D:767:VAL:HG12	1.96	0.46
1:B:584:LEU:HD22	1:B:587:SER:HB2	1.97	0.46
1:B:461:GLN:HE22	1:B:475:ARG:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:448:ILE:HD11	3:D:451:TRP:HB3	1.96	0.46
3:D:67:PRO:HB2	3:D:70:VAL:HG23	1.98	0.46
1:B:196:ARG:O	1:B:200:GLU:HG2	2.16	0.45
3:D:269:ILE:HG22	3:D:277:ARG:H	1.79	0.45
2:C:109:TRP:CD1	2:C:109:TRP:H	2.34	0.45
3:D:160:GLN:CD	3:D:160:GLN:H	2.25	0.45
3:D:199:TRP:HZ3	3:D:657:THR:HG21	1.80	0.45
3:D:696:LYS:HA	3:D:696:LYS:HD2	1.78	0.45
3:D:854:ARG:NH1	3:D:854:ARG:HB2	2.32	0.45
4:E:20:G:H2'	4:E:21:U:C5	2.51	0.45
1:A:338:ARG:HE	3:D:109:GLY:N	2.14	0.45
1:B:527:GLU:HB3	3:D:145:ASP:OD1	2.17	0.45
3:D:509:LYS:HE2	3:D:509:LYS:HB3	1.85	0.45
3:D:82:PHE:HB3	3:D:86:ILE:CG2	2.46	0.45
4:E:7:A:H2'	4:E:8:G:C8	2.51	0.45
1:B:547:GLU:O	1:B:550:LYS:HG2	2.16	0.45
1:B:663:LEU:HD22	1:B:670:LEU:HD23	1.99	0.44
1:A:40:LEU:HD23	1:A:40:LEU:HA	1.79	0.44
3:D:134:TRP:CD1	3:D:135:VAL:N	2.86	0.44
3:D:266:LYS:HD2	3:D:280:ARG:HH11	1.81	0.44
1:A:539:GLU:HG3	1:A:594:SER:HA	1.98	0.44
1:A:369:LEU:HD21	1:A:401:LEU:HD22	2.00	0.44
1:A:551:LYS:O	1:A:554:GLU:HG2	2.18	0.44
1:A:621:MET:HE2	1:A:621:MET:HA	2.00	0.44
2:C:122:ARG:HD2	2:C:123:PHE:N	2.33	0.44
3:D:66:CYS:SG	3:D:70:VAL:HB	2.58	0.43
3:D:268:GLU:OE1	3:D:346:ILE:HA	2.19	0.43
3:D:428:ALA:HB2	3:D:440:LYS:HE2	2.00	0.43
3:D:817:LEU:HD12	3:D:842:LEU:HD22	2.01	0.43
1:B:629:ASN:O	1:B:635:VAL:HG21	2.19	0.43
1:B:652:LYS:HB3	1:B:652:LYS:HE3	1.82	0.43
1:A:427:LYS:HD3	1:A:427:LYS:HA	1.80	0.43
1:A:51:LEU:HD22	1:A:71:LEU:HB3	2.01	0.43
1:A:196:ARG:HG3	1:A:196:ARG:HH11	1.83	0.43
1:B:94:THR:HG23	1:B:97:ASP:H	1.84	0.43
1:A:442:HIS:HE2	3:D:177:VAL:H	1.65	0.43
3:D:733:GLY:CA	3:D:752:SER:HB2	2.49	0.43
1:B:557:LYS:HB3	1:B:557:LYS:HE3	1.78	0.43
3:D:298:GLN:HB2	3:D:304:VAL:HG12	2.01	0.43
3:D:54:ILE:HD12	3:D:101:TYR:HB3	2.01	0.42
3:D:327:CYS:SG	3:D:338:TYR:HB3	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:688:ARG:O	3:D:692:ILE:HG12	2.18	0.42
1:A:79:PRO:HA	1:A:193:LEU:HD13	2.01	0.42
1:B:394:MET:HE2	1:B:394:MET:HB3	1.85	0.42
3:D:476:LYS:HE3	3:D:476:LYS:HB3	1.90	0.42
1:B:400:ILE:H	1:B:400:ILE:HG12	1.65	0.42
1:B:466:MET:HE2	1:B:466:MET:HB3	1.95	0.42
3:D:447:GLU:O	3:D:447:GLU:HG3	2.19	0.42
1:A:399:LYS:HE3	1:A:399:LYS:HB3	1.90	0.42
1:A:430:TYR:O	1:A:434:SER:HB3	2.19	0.42
1:B:477:LYS:HD2	1:B:508:PHE:HE1	1.83	0.42
1:B:619:TYR:N	1:B:621:MET:HE1	2.34	0.42
3:D:215:LEU:HD23	3:D:215:LEU:H	1.85	0.42
3:D:590:PRO:HG3	3:D:659:PHE:HD2	1.85	0.42
1:B:621:MET:H	1:B:621:MET:CE	2.29	0.42
3:D:118:THR:O	3:D:119:LEU:HD13	2.20	0.42
5:F:8:A:H2'	5:F:9:U:C6	2.54	0.42
1:A:485:TYR:CZ	1:A:535:SER:HB2	2.55	0.42
1:A:634:ILE:HD11	1:B:685:LYS:HG3	2.01	0.42
1:B:374:LEU:HD12	1:B:374:LEU:HA	1.84	0.42
3:D:260:LYS:HA	3:D:260:LYS:HD3	1.71	0.42
3:D:604:GLY:HA3	3:D:608:LYS:HD2	2.01	0.42
4:E:7:A:H2'	4:E:8:G:H8	1.85	0.42
3:D:248:LYS:H	3:D:248:LYS:HG3	1.57	0.42
1:A:168:ARG:HE	1:A:168:ARG:HB3	1.70	0.41
3:D:679:VAL:HG13	3:D:683:GLU:HG3	2.02	0.41
1:B:36:LYS:HE2	1:B:36:LYS:HB3	1.77	0.41
1:A:82:ARG:HA	1:A:193:LEU:HD11	2.01	0.41
2:C:1:MET:HE1	2:C:48:LYS:HD2	2.03	0.41
3:D:732:ALA:HA	3:D:752:SER:O	2.19	0.41
1:A:28:ILE:O	1:A:32:PHE:HB2	2.21	0.41
1:B:387:PRO:HD3	2:C:103:PHE:CD2	2.56	0.41
1:A:341:PHE:CE1	3:D:135:VAL:HG11	2.56	0.41
3:D:478:SER:OG	3:D:485:ILE:HG13	2.20	0.41
5:F:4:U:H2'	5:F:5:A:H8	1.86	0.41
1:A:53:LYS:HD2	1:A:91:ILE:HG21	2.02	0.41
1:A:657:LEU:HD23	1:B:684:ILE:HD11	2.02	0.41
1:B:87:VAL:HG22	1:B:180:LYS:HG3	2.02	0.41
1:B:461:GLN:OE1	1:B:461:GLN:O	2.39	0.41
3:D:159:ILE:HD13	3:D:159:ILE:HA	1.87	0.41
1:B:350:LYS:O	1:B:365:SER:HB3	2.21	0.41
1:B:501:GLU:HB3	1:B:585:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:68:ARG:HB3	3:D:69:ARG:NH1	2.35	0.41
3:D:138:VAL:HG11	3:D:164:VAL:O	2.21	0.41
3:D:533:LYS:HD2	3:D:533:LYS:HA	1.84	0.41
3:D:701:GLY:HA3	3:D:772:ASN:OD1	2.21	0.41
1:A:347:LYS:HE2	1:A:349:LYS:HE2	2.02	0.41
1:A:466:MET:H	1:A:466:MET:HG2	1.53	0.41
3:D:334:GLN:HG2	3:D:335:LYS:H	1.86	0.41
3:D:595:GLY:HA2	3:D:667:TYR:O	2.21	0.41
3:D:695:GLU:HB3	3:D:698:TYR:HB2	2.02	0.41
3:D:709:LYS:H	3:D:709:LYS:HG2	1.62	0.41
1:B:277:ILE:HD12	1:B:277:ILE:HA	1.93	0.40
3:D:633:GLN:HG2	3:D:634:HIS:N	2.36	0.40
1:A:568:LYS:HZ2	1:A:568:LYS:HG3	1.74	0.40
1:A:24:LEU:HD11	1:B:24:LEU:HD21	2.03	0.40
3:D:463:THR:HG22	3:D:466:HIS:ND1	2.36	0.40
1:B:606:MET:HE2	3:D:169:LEU:HD22	2.04	0.40
1:B:683:MET:HE3	1:B:683:MET:HB2	1.84	0.40
5:F:2:U:C2	5:F:3:A:C8	3.10	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	624/724 (86%)	612 (98%)	12 (2%)	0	100	100
1	B	620/724 (86%)	602 (97%)	18 (3%)	0	100	100
2	C	127/160 (79%)	124 (98%)	3 (2%)	0	100	100
3	D	739/859 (86%)	699 (95%)	40 (5%)	0	100	100
All	All	2110/2467 (86%)	2037 (96%)	73 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	567/652 (87%)	561 (99%)	6 (1%)	65	79
1	B	563/652 (86%)	554 (98%)	9 (2%)	55	73
2	C	122/149 (82%)	117 (96%)	5 (4%)	27	44
3	D	657/752 (87%)	632 (96%)	25 (4%)	29	48
All	All	1909/2205 (87%)	1864 (98%)	45 (2%)	43	64

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	48	SER
1	A	179	THR
1	A	381	VAL
1	A	596	TYR
1	A	619	TYR
1	B	36	LYS
1	B	38	ILE
1	B	67	SER
1	B	125	MET
1	B	147	THR
1	B	282	LEU
1	B	467	THR
1	B	532	SER
1	B	617	MET
2	C	36	LEU
2	C	57	HIS
2	C	66	HIS
2	C	90	THR
2	C	107	LYS
3	D	49	ILE
3	D	119	LEU
3	D	143	LEU
3	D	145	ASP

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Mol	Chain	Res	Type
3	D	159	ILE
3	D	162	LEU
3	D	166	MET
3	D	202	PHE
3	D	215	LEU
3	D	222	THR
3	D	434	VAL
3	D	453	ILE
3	D	459	GLN
3	D	547	VAL
3	D	574	VAL
3	D	615	VAL
3	D	624	ARG
3	D	631	VAL
3	D	672	SER
3	D	749	TYR
3	D	750	LEU
3	D	767	VAL
3	D	838	ASP
3	D	852	THR
3	D	855	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	ASN
1	B	30	ASN
1	B	326	GLN
2	C	128	ASN
3	D	204	GLN
3	D	228	GLN
3	D	568	ASN
3	D	677	GLN
3	D	788	HIS
3	D	816	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	E	21/22 (95%)	3 (14%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	F	21/22 (95%)	4 (19%)	0
All	All	42/44 (95%)	7 (16%)	0

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	E	2	G
4	E	5	G
4	E	21	U
5	F	2	U
5	F	19	U
5	F	20	U
5	F	21	C

There are no RNA pucker outliers to report.

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 5 ligands modelled in this entry, 3 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	$\# Z > 2$
6	ATP	A	801	7	29,33,33	0.35	0	44,52,52	0.52	1 (2%)
6	ATP	B	801	7	29,33,33	0.34	0	44,52,52	0.50	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
6	ATP	A	801	7	-	2/22/38/38	0/3/3/3
6	ATP	B	801	7	-	4/22/38/38	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	ATP	PB-O3B-PG	2.07	139.91	132.83
6	B	801	ATP	PB-O3B-PG	2.06	139.91	132.83

There are no chirality outliers.

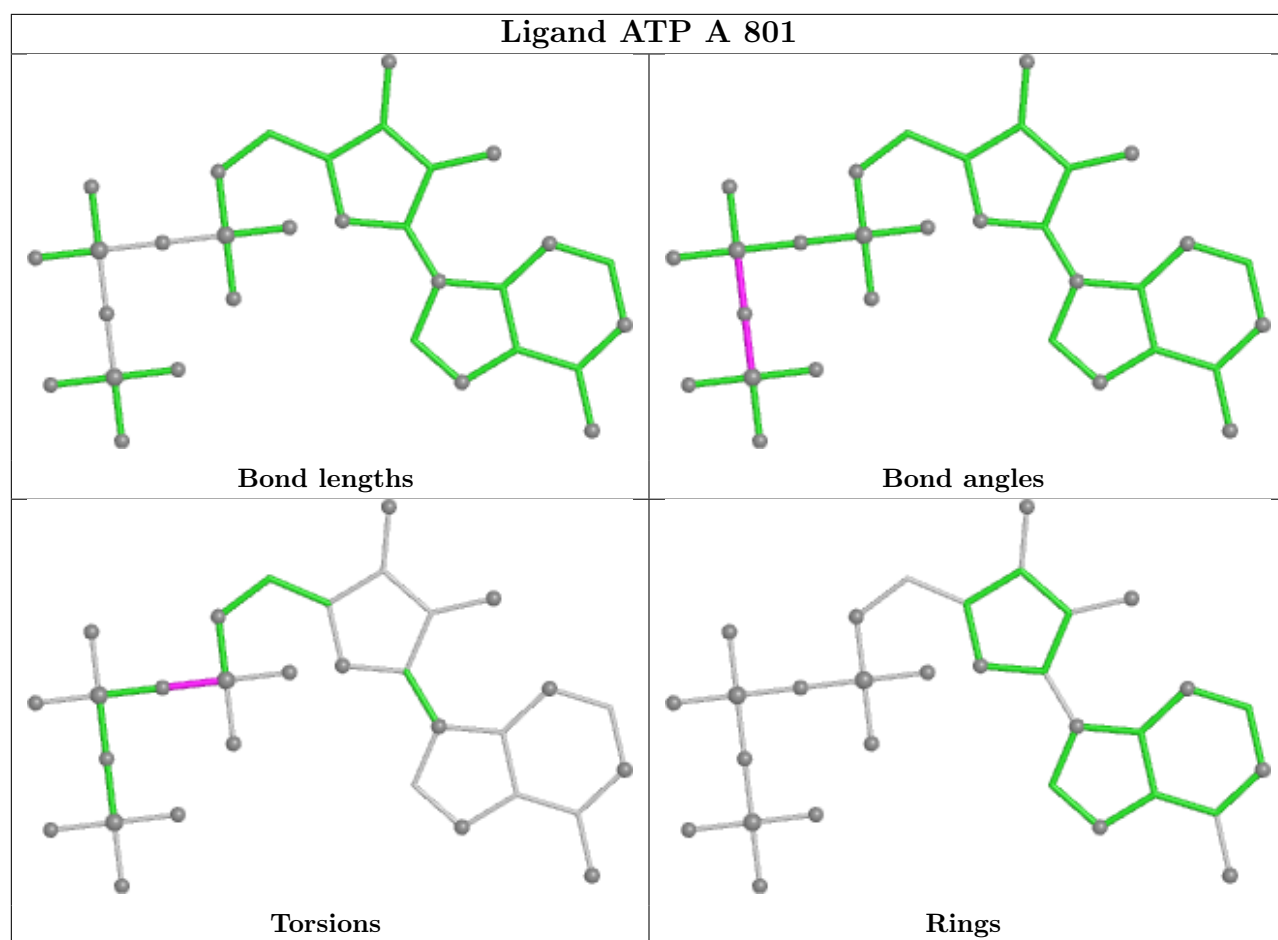
All (6) torsion outliers are listed below:

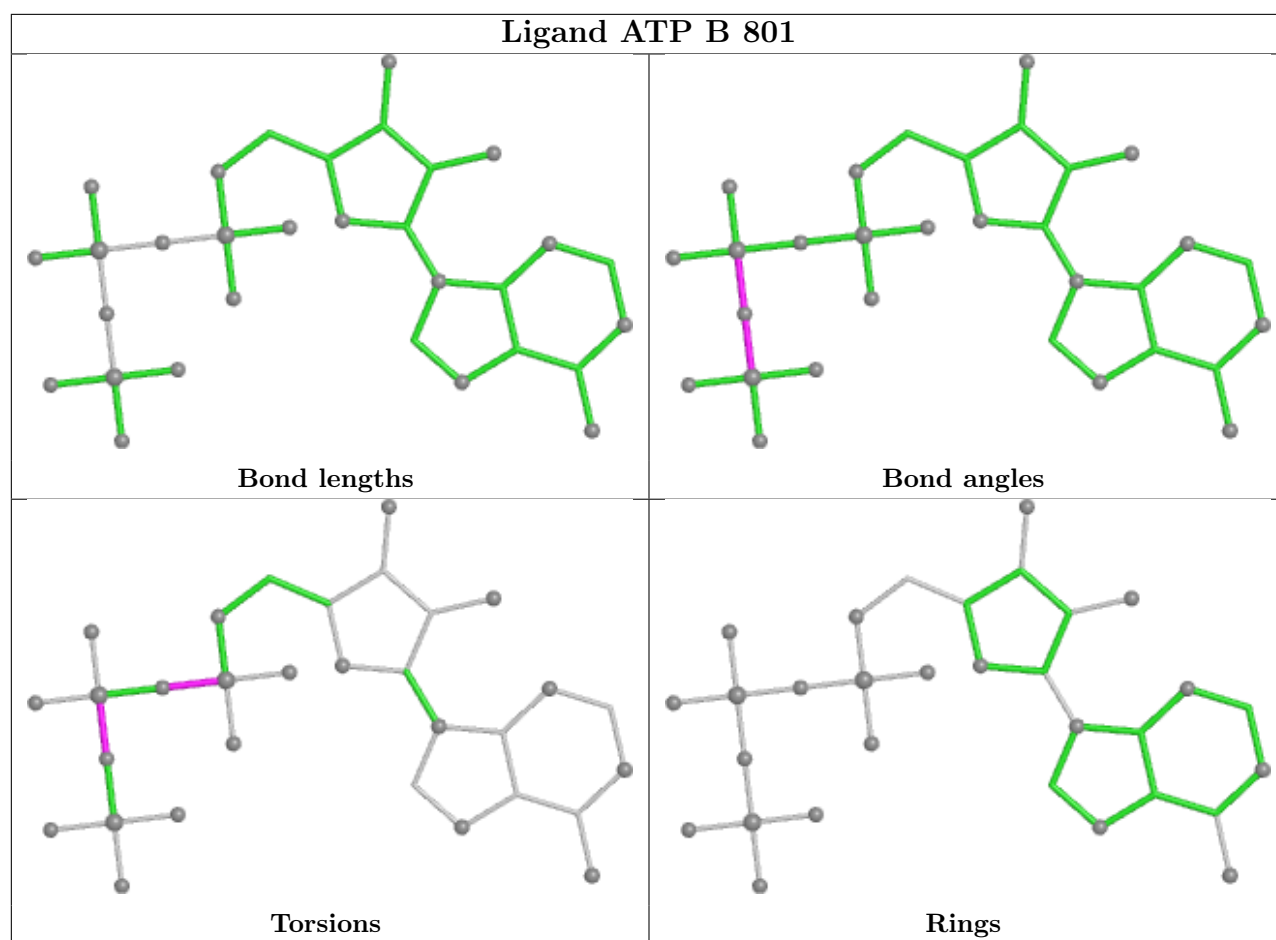
Mol	Chain	Res	Type	Atoms
6	A	801	ATP	PB-O3A-PA-O1A
6	B	801	ATP	PG-O3B-PB-O2B
6	B	801	ATP	PB-O3A-PA-O2A
6	A	801	ATP	PB-O3A-PA-O2A
6	B	801	ATP	PG-O3B-PB-O1B
6	B	801	ATP	PB-O3A-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

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.

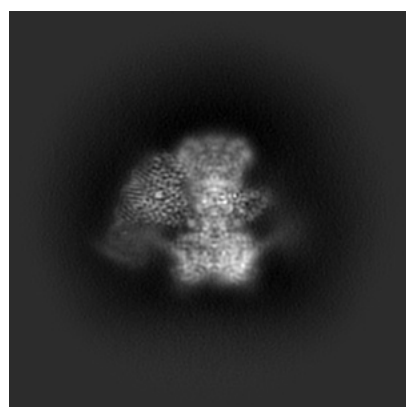
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65663. These allow visual inspection of the internal detail of the map and identification of artifacts.

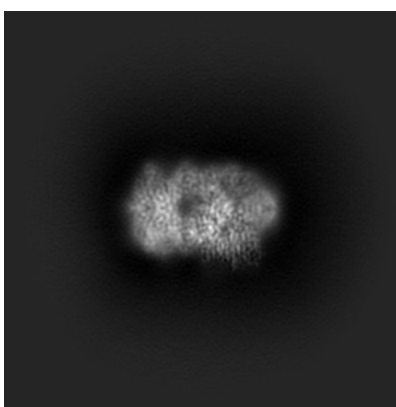
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

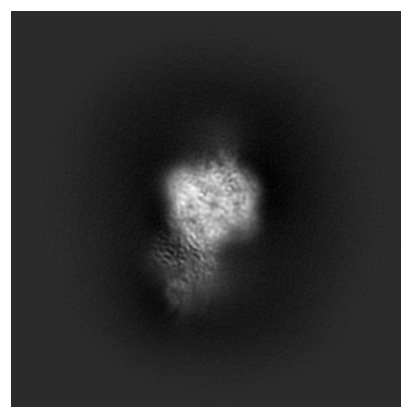
6.1.1 Primary map



X



Y

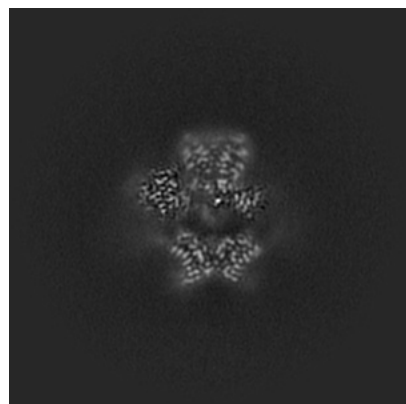


Z

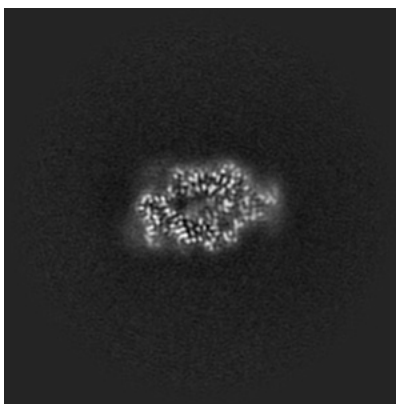
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

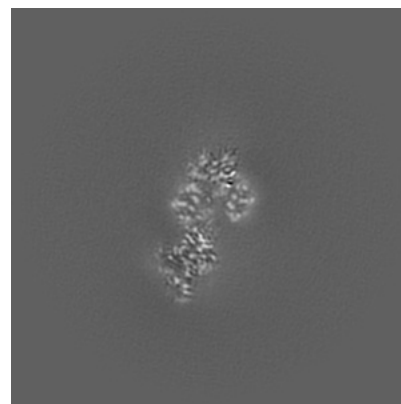
6.2.1 Primary map



X Index: 140



Y Index: 140

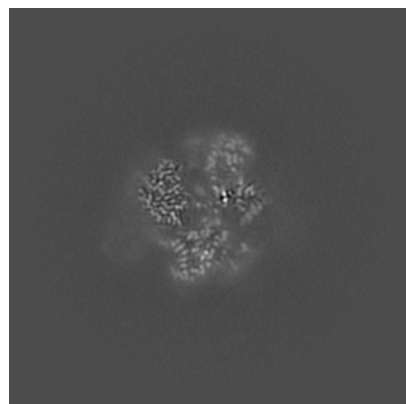


Z Index: 140

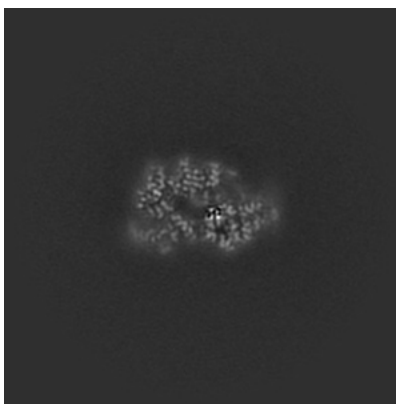
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

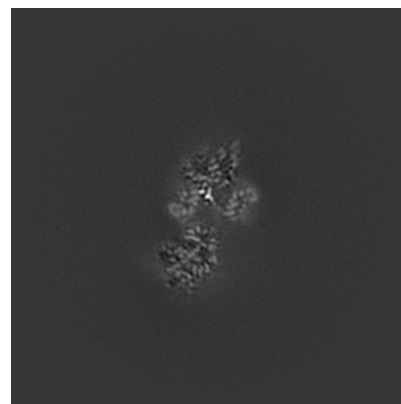
6.3.1 Primary map



X Index: 133



Y Index: 150

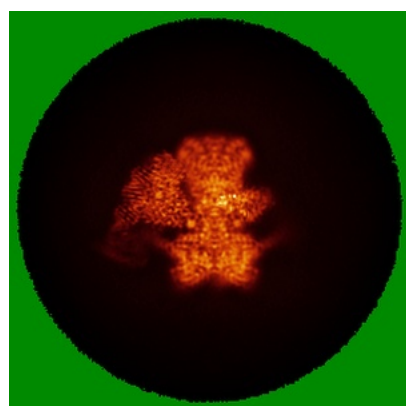


Z Index: 145

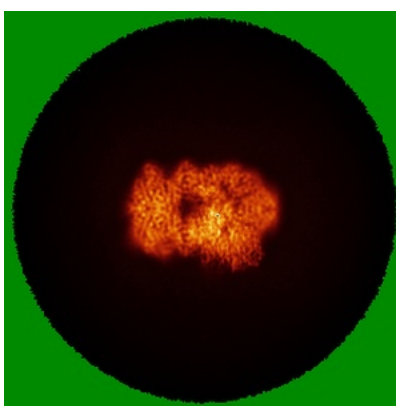
The images above show the largest variance slices of the map in three orthogonal directions.

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

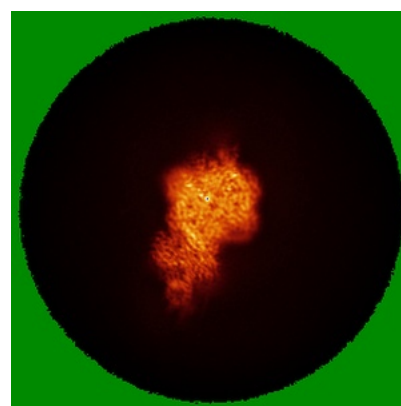
6.4.1 Primary map



X



Y



Z

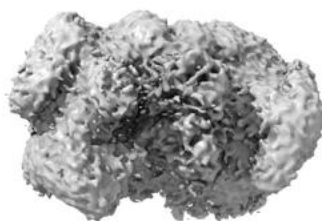
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0834. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

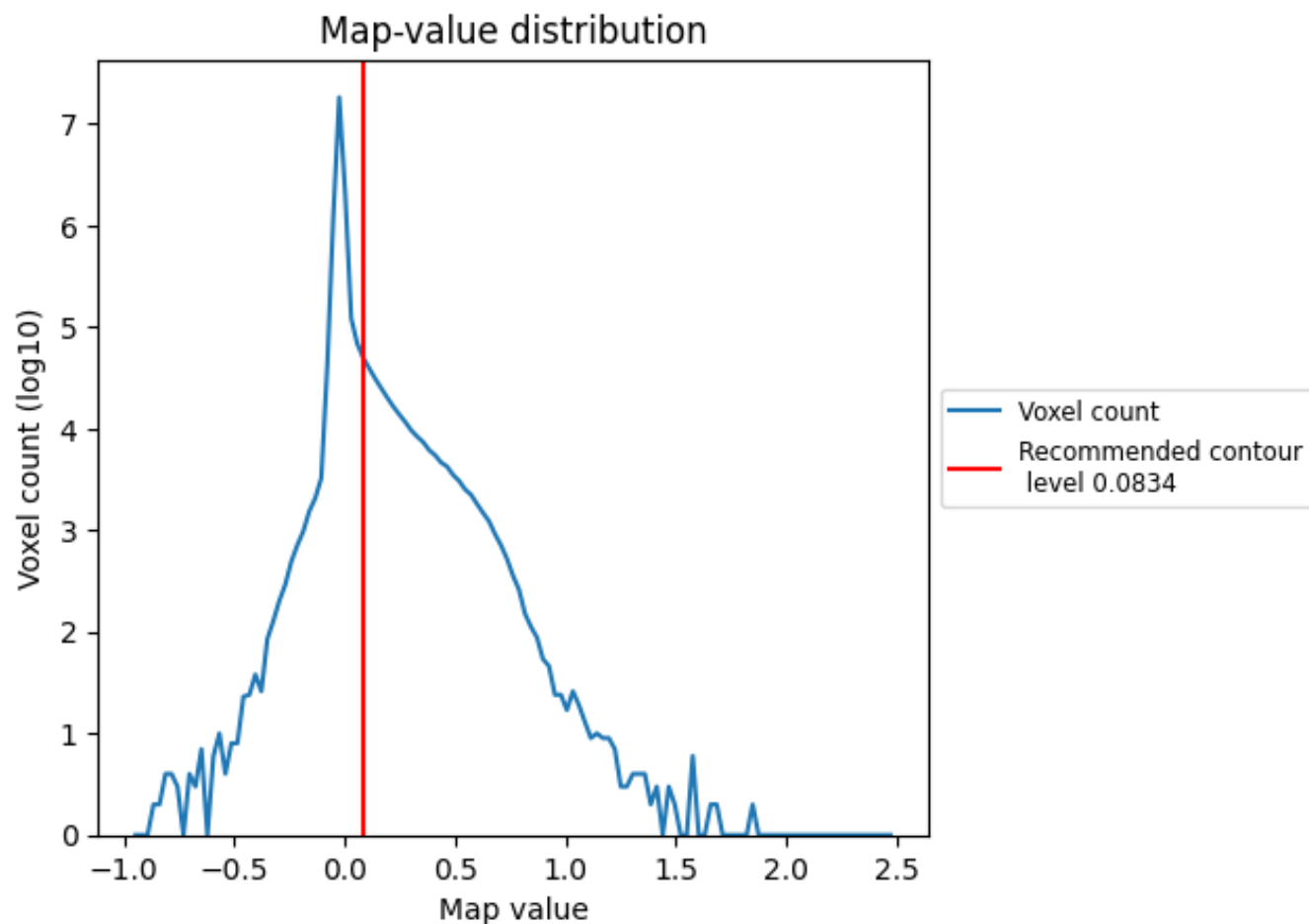
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

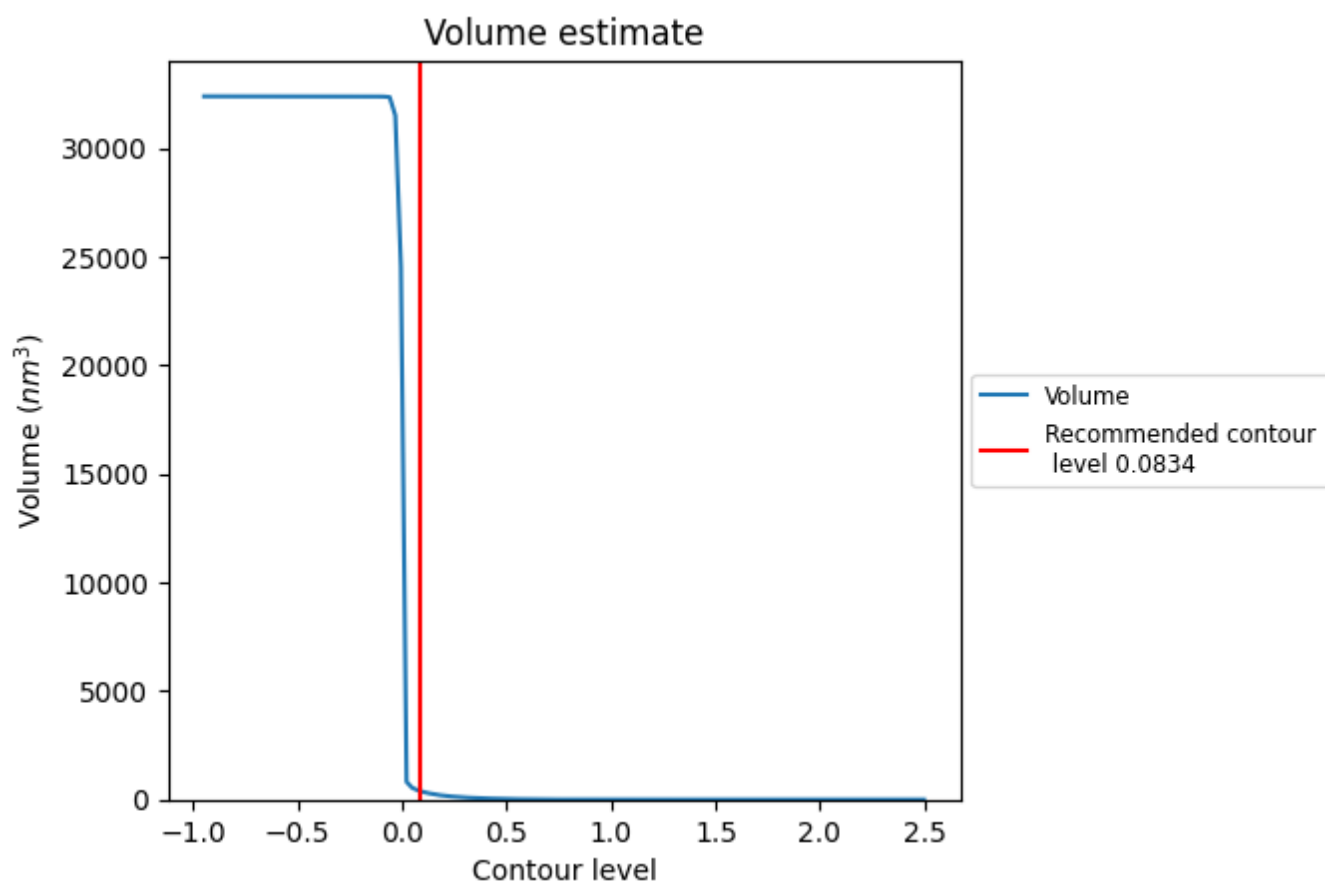
This section contains the results of statistical analysis of the map.

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.

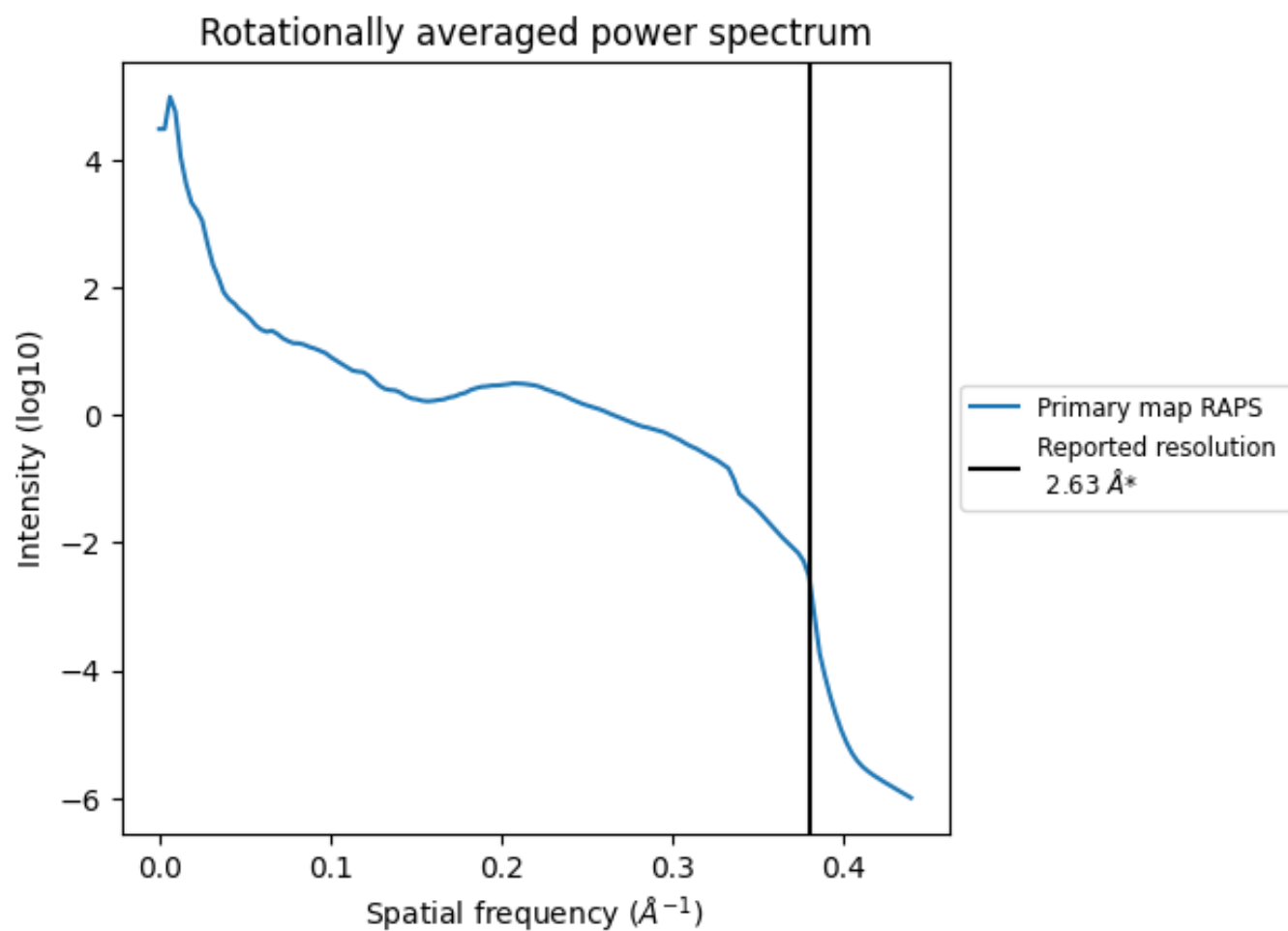
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 405 nm^3 ; this corresponds to an approximate mass of 366 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 0.380 Å⁻¹

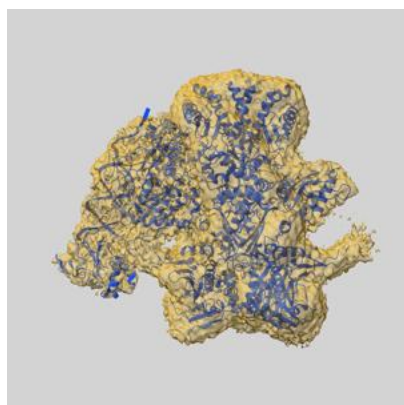
8 Fourier-Shell correlation ⓘ

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

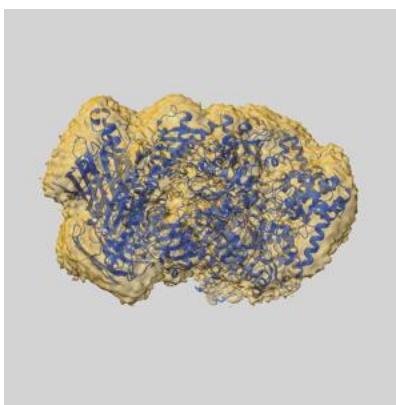
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65663 and PDB model 9W5I. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

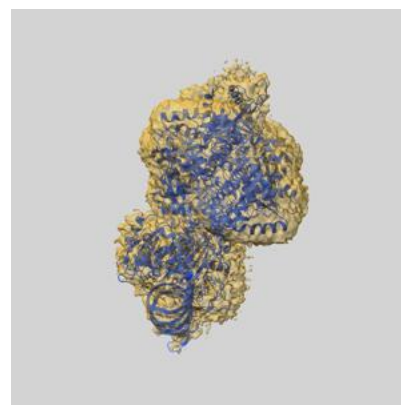
9.1 Map-model overlay [i](#)



X



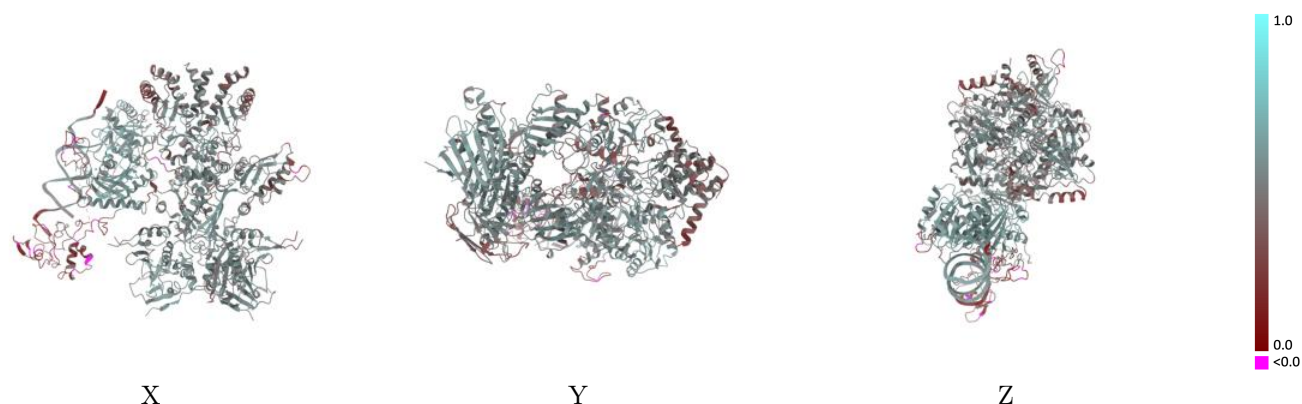
Y



Z

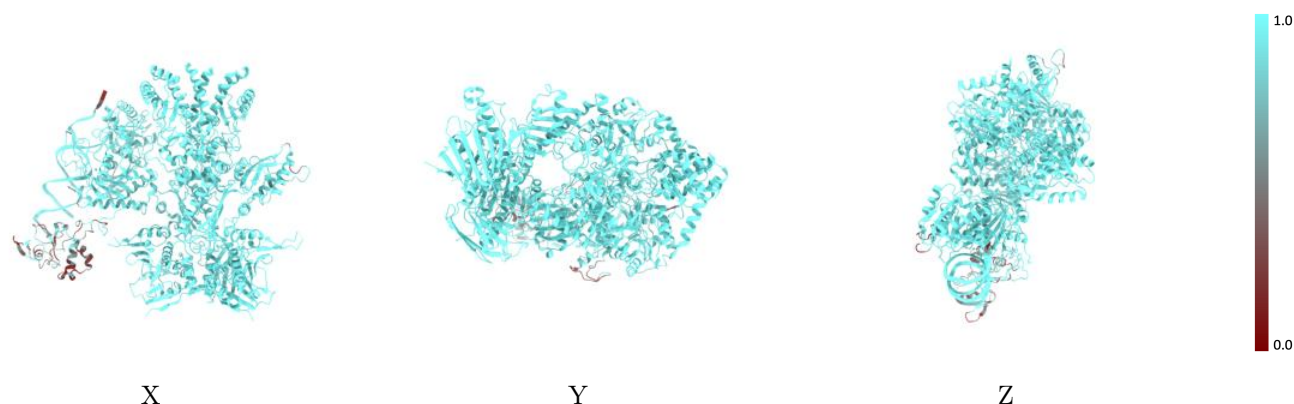
The images above show the 3D surface view of the map at the recommended contour level 0.0834 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



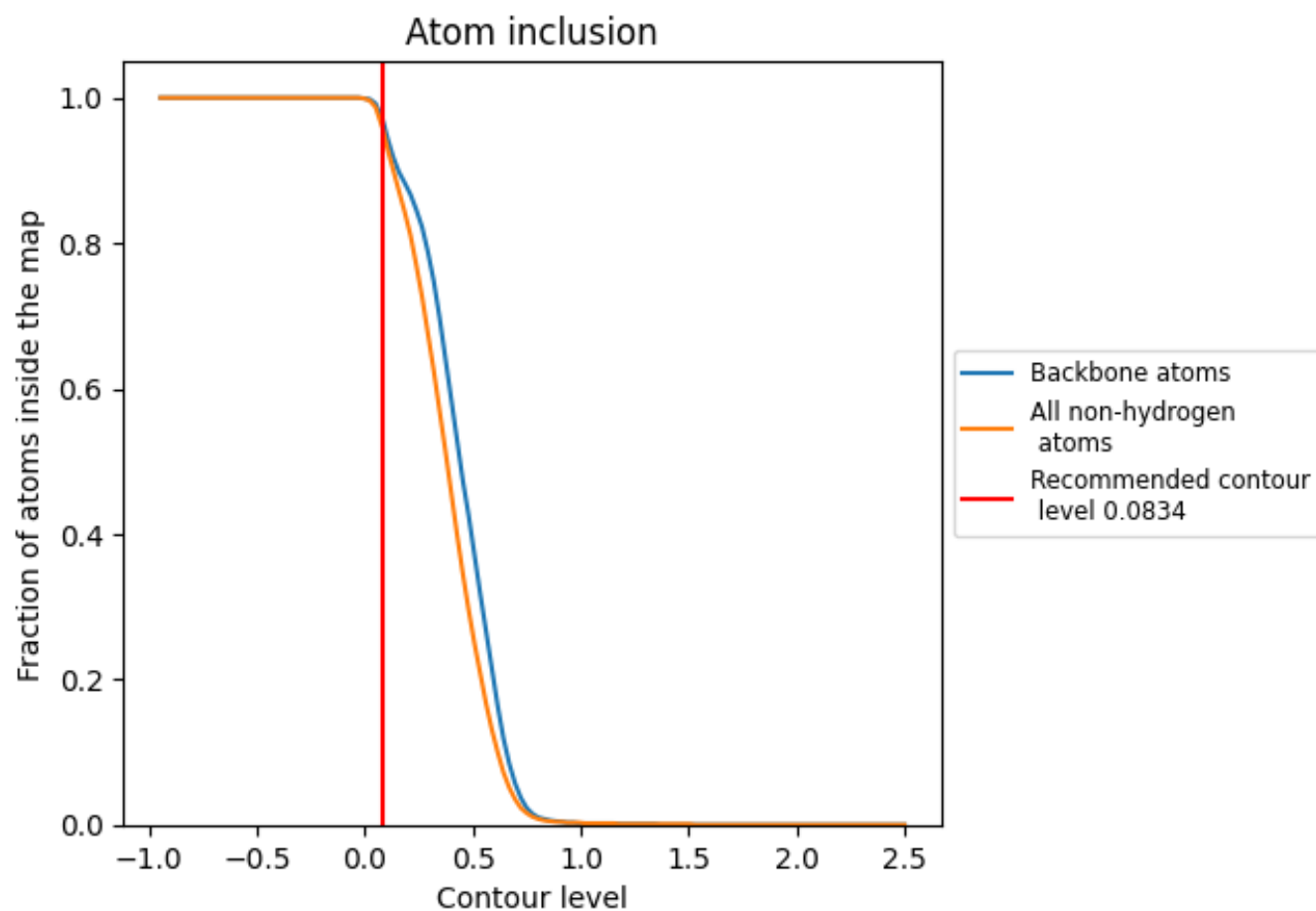
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0834).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 96% 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 (0.0834) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9560	0.4810
A	0.9990	0.5040
B	1.0000	0.5040
C	0.9940	0.4300
D	0.8800	0.4500
E	0.9370	0.4850
F	0.9090	0.4890

1.0

0.0

<0.0