



Full wwPDB EM Validation Report ⓘ

Jul 6, 2026 – 12:36 PM EDT

PDB ID : 10ML / pdb_000010ml
EMDB ID : EMD-75289
Title : AAP-SO2 bound Open Mtb-EC: Cryo-EM structure of Mtb RNAP elongation complex (substrate loading mimic) with an open active site (open TL and RH-FL)
Authors : Dhingra, Y.; Darst, S.A.
Deposited on : 2026-01-27
Resolution : 3.00 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:

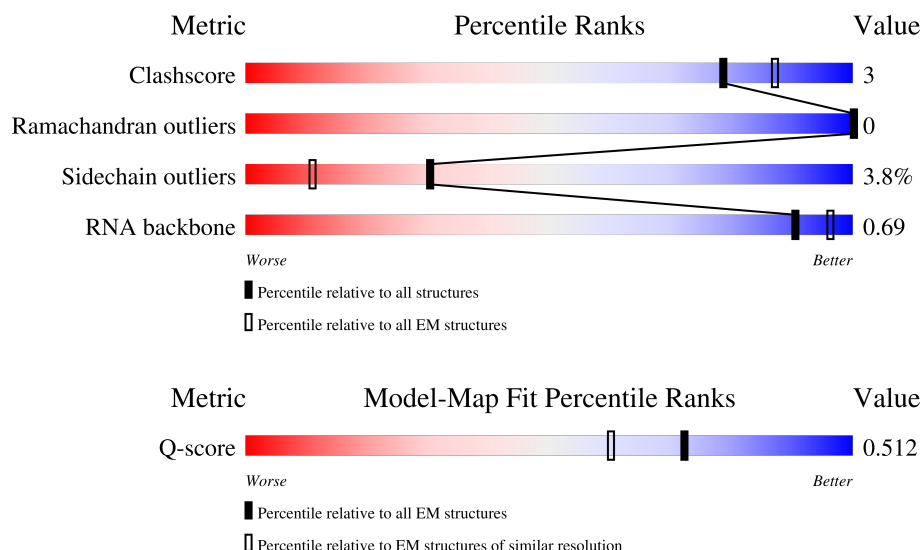
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	347	
1	B	347	
2	E	110	

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Mol	Chain	Length	Quality of chain
3	Q	54	24% 17% 59%
4	P	54	41% 13% 46%
5	R	20	50% 50%
6	C	1178	84% 9% 7%
7	D	1318	87% 9% • •

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 24620 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	226	Total	C	N	O	S	0	0
			1724	1085	297	339	3		
1	B	237	Total	C	N	O	S	0	0
			1775	1120	304	348	3		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	82	Total	C	N	O	0	0
			645	412	107	126		

- Molecule 3 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	22	Total	C	N	O	P	0	0
			451	213	84	132	22		

- Molecule 4 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	29	Total	C	N	O	P	0	0
			586	278	103	176	29		

- Molecule 5 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	10	Total	C	N	O	P	0	0
			221	98	45	68	10		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	1095	Total	C	N	O	S	0	0
			8489	5313	1491	1646	39		

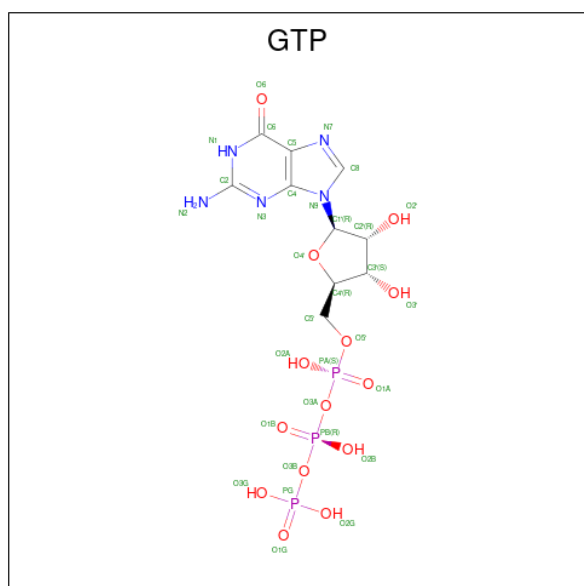
- Molecule 7 is a protein called DNA-directed RNA polymerase subunit beta'.

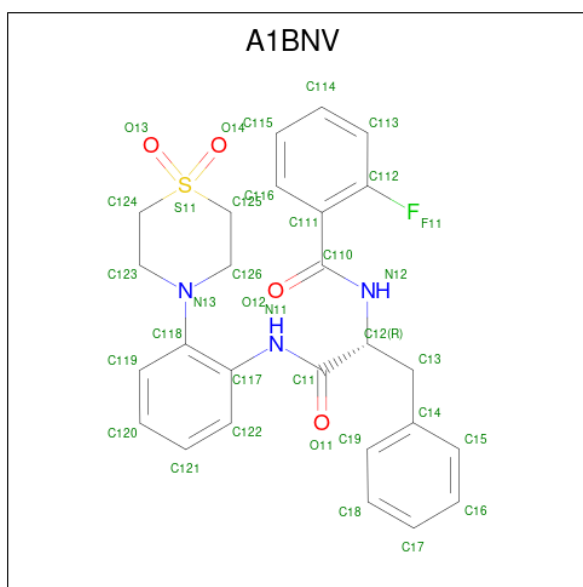
Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	1269	Total	C	N	O	S	0	0
			9916	6212	1802	1860	42		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP P9WGY7
D	0	ALA	-	expression tag	UNP P9WGY7

- Molecule 8 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).





Mol	Chain	Residues	Atoms						AltConf
9	C	1	Total	C	F	N	O	S	0
			35	26	1	3	4	1	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total	Mg	0
			2	2	

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
11	D	2	Total	Zn	0
			2	2	

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
12	A	58	Total	O	0
			58	58	
12	B	43	Total	O	0
			43	43	
12	E	20	Total	O	0
			20	20	
12	Q	13	Total	O	0
			13	13	

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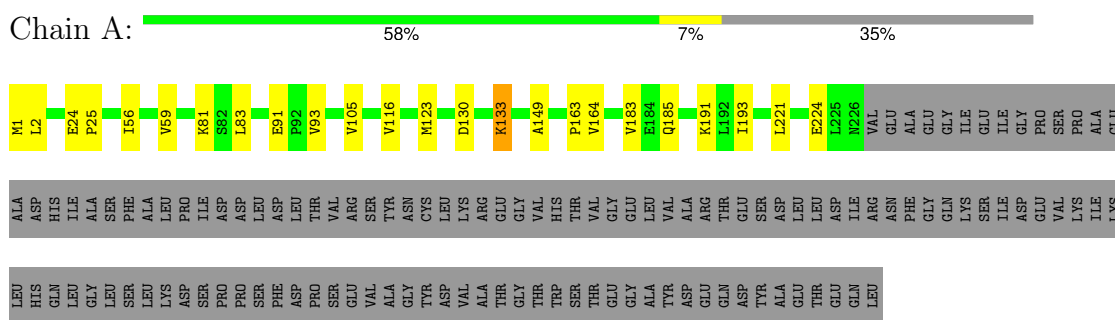
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Mol	Chain	Residues	Atoms		AltConf
12	P	25	Total 25	O 25	0
12	R	15	Total 15	O 15	0
12	C	260	Total 260	O 260	0
12	D	308	Total 308	O 308	0

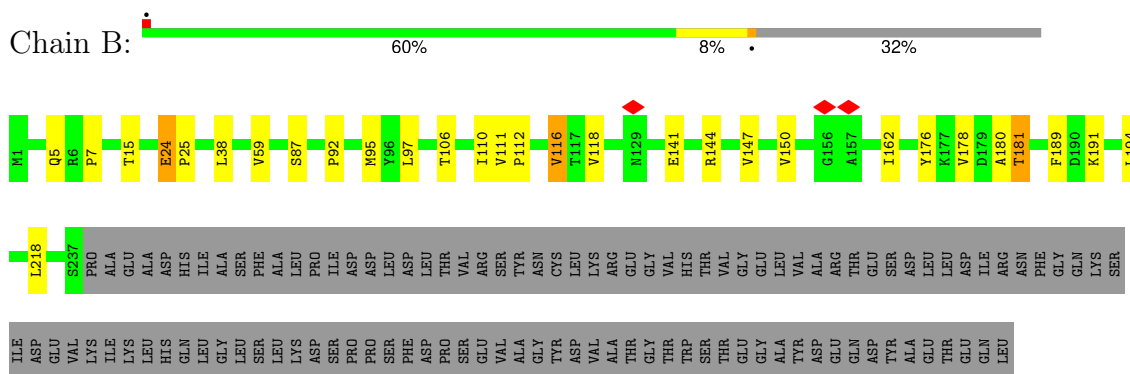
3 Residue-property plots

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.

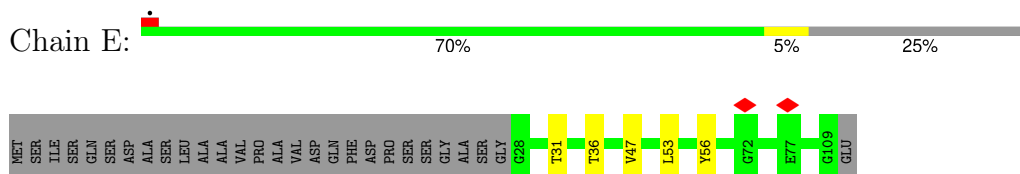
- Molecule 1: DNA-directed RNA polymerase subunit alpha



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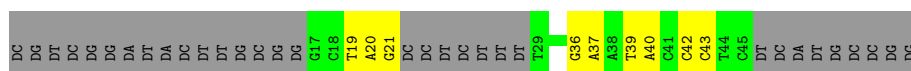


- Molecule 2: DNA-directed RNA polymerase subunit omega

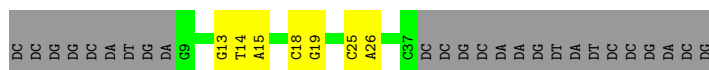


- Molecule 3: Non-template DNA

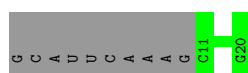




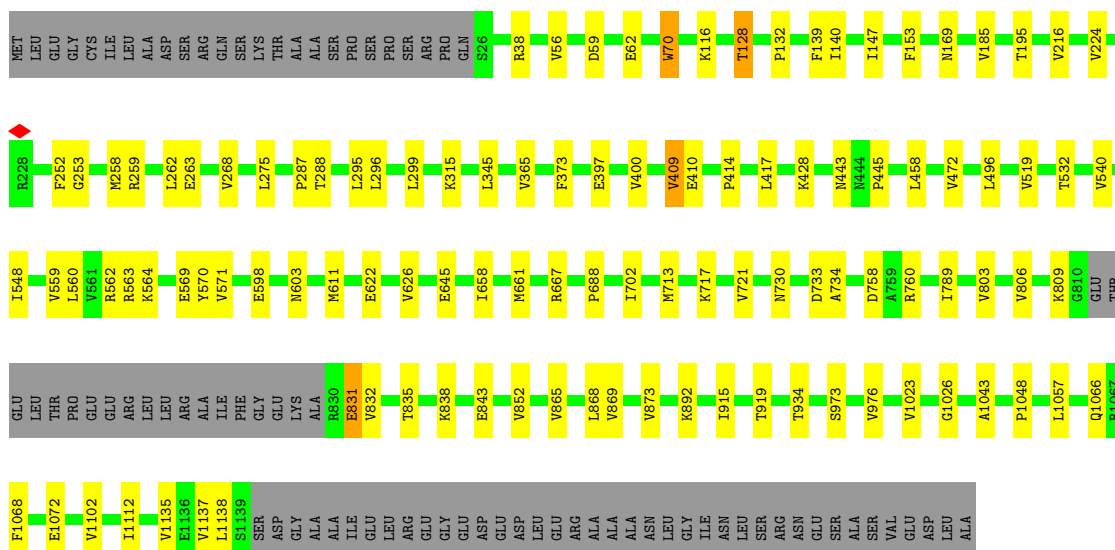
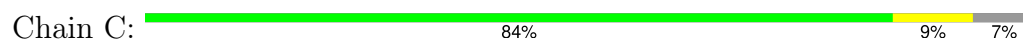
• Molecule 4: Template DNA



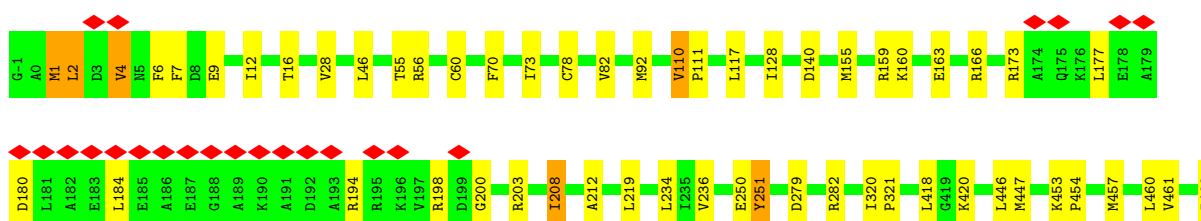
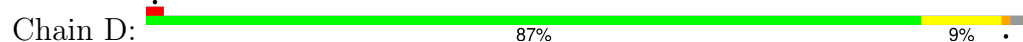
• Molecule 5: RNA

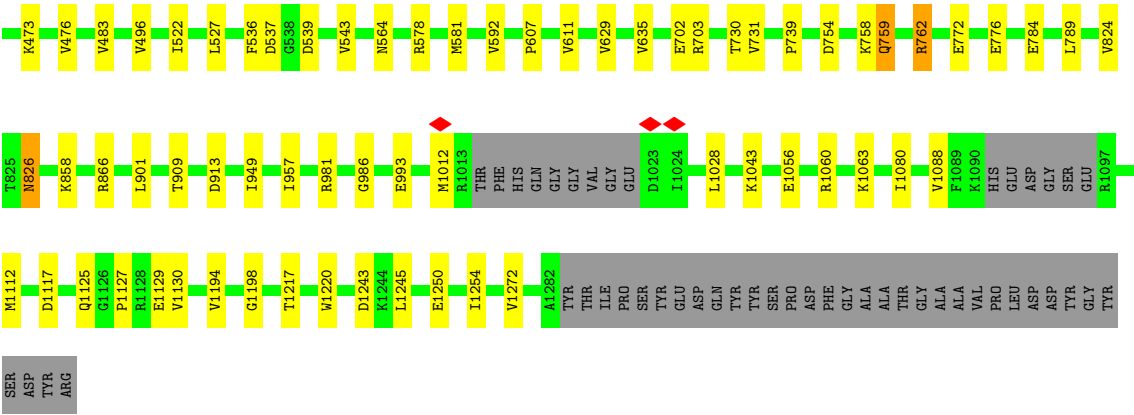


• Molecule 6: DNA-directed RNA polymerase subunit beta



• Molecule 7: DNA-directed RNA polymerase subunit beta'





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	274167	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.7	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.205	Depositor
Minimum map value	-0.087	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	325.248, 325.248, 325.248	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.84699994, 0.84699994, 0.84699994	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, A1BNV, MG, GTP

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	0/1750	0.34	0/2380
1	B	0.10	0/1802	0.28	0/2454
2	E	0.11	0/658	0.33	0/896
3	Q	0.15	0/504	0.31	0/773
4	P	0.18	0/654	0.37	0/1005
5	R	0.37	0/248	0.40	0/386
6	C	0.16	0/8645	0.35	3/11720 (0.0%)
7	D	0.15	0/10080	0.32	2/13625 (0.0%)
All	All	0.15	0/24341	0.34	5/33239 (0.0%)

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
6	C	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	564	LYS	N-CA-C	7.77	119.75	111.28
7	D	536	PHE	CB-CA-C	5.85	120.89	112.12
7	D	536	PHE	N-CA-CB	-5.66	103.63	110.53
6	C	564	LYS	CA-C-N	-5.65	115.45	123.03
6	C	564	LYS	C-N-CA	-5.65	115.45	123.03

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	C	562	ARG	Sidechain

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	1724	0	1768	13	0
1	B	1775	0	1809	17	0
2	E	645	0	642	2	0
3	Q	451	0	248	6	0
4	P	586	0	326	7	0
5	R	221	0	108	0	0
6	C	8489	0	8426	44	0
7	D	9916	0	10007	57	0
8	C	32	0	12	0	0
9	C	35	0	0	0	0
10	D	2	0	0	0	0
11	D	2	0	0	0	0
12	A	58	0	0	0	0
12	B	43	0	0	0	0
12	C	260	0	0	0	0
12	D	308	0	0	0	0
12	E	20	0	0	0	0
12	P	25	0	0	0	0
12	Q	13	0	0	0	0
12	R	15	0	0	0	0
All	All	24620	0	23346	134	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 (134) 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)
7:D:166:ARG:HG3	7:D:212:ALA:HB2	1.66	0.77
6:C:1138:LEU:HB2	7:D:9:GLU:HB2	1.73	0.68
1:A:24:GLU:HA	1:A:191:LYS:HG3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:14:DT:H2'	4:P:15:DA:C8	2.29	0.66
6:C:611:MET:HE1	6:C:892:LYS:HB3	1.77	0.64
7:D:1056:GLU:HB3	7:D:1063:LYS:HB3	1.80	0.63
7:D:177:LEU:HD22	7:D:198:ARG:HH21	1.65	0.61
1:A:56:ILE:HB	1:A:59:VAL:HB	1.81	0.61
6:C:1043:ALA:HB2	7:D:447:MET:HG3	1.82	0.60
6:C:540:VAL:HG12	6:C:563:ARG:HG2	1.83	0.60
7:D:1080:ILE:HG21	7:D:1112:MET:HE3	1.84	0.59
6:C:445:PRO:HB2	6:C:713:MET:HE1	1.85	0.58
7:D:1245:LEU:HD13	7:D:1254:ILE:HD13	1.84	0.58
6:C:733:ASP:HB3	7:D:537:ASP:OD2	2.04	0.58
3:Q:39:DT:H2''	3:Q:40:DA:C8	2.38	0.58
1:A:183:VAL:HG13	1:A:185:GLN:H	1.68	0.57
3:Q:36:DG:H2''	3:Q:37:DA:C8	2.39	0.57
7:D:454:PRO:HA	7:D:457:MET:HE2	1.86	0.57
7:D:180:ASP:HB2	7:D:198:ARG:HH22	1.70	0.57
6:C:760:ARG:HG2	6:C:865:VAL:HG12	1.86	0.56
2:E:47:VAL:HG21	2:E:53:LEU:HB2	1.88	0.56
3:Q:42:DC:H2''	3:Q:43:DC:H5'	1.87	0.56
7:D:578:ARG:H	7:D:581:MET:HE3	1.72	0.55
7:D:981:ARG:HD3	7:D:986:GLY:HA2	1.89	0.54
6:C:721:VAL:HG23	6:C:915:ILE:HG23	1.90	0.54
1:A:191:LYS:HE3	1:A:193:ILE:HD11	1.90	0.53
1:A:83:LEU:HG	1:A:123:MET:HE1	1.91	0.53
7:D:1194:VAL:HA	7:D:1198:GLY:HA2	1.90	0.53
1:A:24:GLU:HB3	1:A:25:PRO:HD3	1.91	0.53
1:B:181:THR:OG1	1:B:191:LYS:HB2	2.08	0.53
1:A:1:MET:HG2	1:B:147:VAL:HG21	1.90	0.53
7:D:70:PHE:HB3	7:D:73:ILE:HD11	1.90	0.52
7:D:60:CYS:HB3	7:D:78:CYS:SG	2.49	0.52
6:C:1102:VAL:HG22	6:C:1112:ILE:HG23	1.91	0.52
6:C:400:VAL:HG23	6:C:417:LEU:HB3	1.92	0.52
7:D:155:MET:HE1	7:D:219:LEU:HB3	1.91	0.52
6:C:140:ILE:HG12	6:C:147:ILE:HG13	1.91	0.51
7:D:155:MET:HE3	7:D:159:ARG:HD2	1.91	0.51
7:D:739:PRO:HD3	7:D:789:LEU:HD13	1.93	0.51
6:C:658:ILE:HD11	6:C:688:PRO:HB3	1.91	0.51
6:C:569:GLU:HG2	6:C:570:TYR:N	2.26	0.50
1:B:95:MET:HE2	1:B:112:PRO:HB3	1.94	0.50
6:C:275:LEU:HG	6:C:287:PRO:HB2	1.93	0.50
7:D:1:MET:SD	7:D:4:VAL:HG13	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:453:LYS:HZ1	7:D:473:LYS:HE3	1.78	0.49
1:B:110:ILE:HD11	1:B:118:VAL:HG21	1.95	0.48
6:C:733:ASP:CB	7:D:537:ASP:OD2	2.62	0.48
7:D:320:ILE:HG12	7:D:321:PRO:HD2	1.96	0.47
6:C:128:THR:HG22	6:C:169:ASN:H	1.79	0.47
7:D:2:LEU:H	7:D:2:LEU:HD13	1.79	0.47
7:D:160:LYS:HA	7:D:163:GLU:HG2	1.95	0.47
7:D:1012:MET:HG3	7:D:1028:LEU:HB3	1.96	0.47
7:D:28:VAL:HG11	7:D:46:LEU:HD23	1.96	0.47
1:B:38:LEU:HD23	1:B:194:LEU:HD11	1.96	0.47
6:C:62:GLU:HG3	6:C:70:TRP:HB2	1.97	0.47
7:D:702:GLU:HG3	7:D:703:ARG:HG3	1.97	0.47
1:B:162:ILE:HG23	7:D:607:PRO:HG2	1.98	0.46
6:C:758:ASP:HB3	6:C:868:LEU:HD13	1.97	0.46
7:D:250:GLU:HG3	7:D:251:TYR:H	1.80	0.46
6:C:622:GLU:HG2	6:C:717:LYS:HD3	1.98	0.46
1:B:7:PRO:HB3	1:B:25:PRO:O	2.15	0.46
6:C:919:THR:HG23	7:D:731:VAL:HG23	1.97	0.46
1:B:87:SER:HB2	1:B:116:VAL:HG13	1.97	0.46
6:C:1048:PRO:HB2	6:C:1057:LEU:HD12	1.98	0.46
6:C:789:ILE:HG23	6:C:803:VAL:HG22	1.98	0.46
6:C:809:LYS:H	6:C:831:GLU:HB3	1.81	0.46
7:D:460:LEU:HD11	7:D:483:VAL:HG12	1.98	0.46
6:C:1135:VAL:HG22	7:D:12:ILE:HG13	1.97	0.45
1:B:92:PRO:HB3	1:B:141:GLU:HG2	1.97	0.45
7:D:461:VAL:HG21	7:D:469:ILE:HD13	1.98	0.45
6:C:59:ASP:HA	6:C:62:GLU:HG2	1.97	0.45
6:C:560:LEU:HD13	6:C:570:TYR:CE2	2.52	0.45
4:P:25:DC:H2'	4:P:26:DA:H8	1.82	0.45
7:D:1125:GLN:HB3	7:D:1129:GLU:HG3	1.99	0.45
1:A:93:VAL:HG21	1:A:116:VAL:HG21	1.99	0.45
4:P:18:DC:H2''	4:P:19:DG:H8	1.81	0.45
6:C:38:ARG:HD3	6:C:973:SER:HB3	1.98	0.45
7:D:200:GLY:O	7:D:203:ARG:HG2	2.16	0.45
7:D:759:GLN:HA	7:D:762:ARG:HD2	2.00	0.44
1:A:2:LEU:HD11	1:B:144:ARG:HH21	1.83	0.44
1:B:97:LEU:HB2	1:B:110:ILE:HG22	1.99	0.44
3:Q:20:DA:H2''	3:Q:21:DG:C8	2.52	0.44
6:C:661:MET:HE1	6:C:667:ARG:HH11	1.83	0.44
6:C:934:THR:HG23	6:C:1026:GLY:HA3	1.98	0.44
7:D:826:ASN:HD22	7:D:826:ASN:HA	1.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:184:LEU:HB3	7:D:194:ARG:HG2	1.99	0.44
6:C:409:VAL:O	6:C:410:GLU:HG3	2.18	0.44
7:D:55:THR:HG23	7:D:56:ARG:HG3	2.00	0.44
4:P:13:DG:H2'	4:P:14:DT:O4'	2.17	0.44
6:C:253:GLY:HA2	6:C:259:ARG:HH12	1.83	0.44
4:P:14:DT:H2''	4:P:15:DA:H5'	2.00	0.44
6:C:132:PRO:HB3	6:C:153:PHE:HE1	1.83	0.44
1:A:149:ALA:HB1	1:A:163:PRO:HB2	1.99	0.43
7:D:173:ARG:HE	7:D:208:ILE:HG13	1.81	0.43
1:B:176:TYR:HB3	1:B:194:LEU:HD23	1.99	0.43
6:C:252:PHE:HB3	6:C:258:MET:HG3	2.00	0.43
6:C:397:GLU:HA	6:C:400:VAL:HG12	2.00	0.43
7:D:901:LEU:O	7:D:913:ASP:HB2	2.19	0.43
1:B:178:VAL:HA	1:B:191:LYS:O	2.19	0.43
6:C:730:ASN:HA	6:C:734:ALA:HB3	2.01	0.43
7:D:60:CYS:SG	7:D:82:VAL:HG22	2.58	0.43
6:C:458:LEU:HD21	6:C:496:LEU:HD13	2.00	0.43
6:C:139:PHE:HB2	6:C:414:PRO:HG3	2.00	0.43
7:D:772:GLU:O	7:D:776:GLU:HG2	2.19	0.43
4:P:18:DC:H2''	4:P:19:DG:C8	2.54	0.42
7:D:1127:PRO:O	7:D:1130:VAL:HG12	2.19	0.42
7:D:128:ILE:HD11	7:D:234:LEU:HD11	2.00	0.42
7:D:92:MET:HG2	7:D:321:PRO:HD3	2.02	0.42
3:Q:19:DT:H2''	3:Q:20:DA:C8	2.55	0.42
6:C:299:LEU:HD23	6:C:299:LEU:HA	1.83	0.42
7:D:1220:TRP:NE1	7:D:1243:ASP:HB2	2.35	0.42
1:A:81:LYS:NZ	1:A:164:VAL:HG13	2.35	0.42
6:C:1023:VAL:HA	7:D:730:THR:HG21	2.02	0.42
7:D:110:VAL:HG22	7:D:111:PRO:HD3	2.01	0.42
7:D:140:ASP:HB3	7:D:251:TYR:HB3	2.01	0.41
6:C:806:VAL:HB	6:C:832:VAL:HB	2.02	0.41
6:C:1068:PHE:CZ	6:C:1072:GLU:HB3	2.55	0.41
7:D:866:ARG:HD3	7:D:1012:MET:HB2	2.01	0.41
3:Q:39:DT:H2''	3:Q:40:DA:N7	2.36	0.41
7:D:453:LYS:HG3	7:D:476:VAL:HG11	2.01	0.41
1:B:38:LEU:HD12	1:B:38:LEU:HA	1.91	0.41
4:P:25:DC:H2'	4:P:26:DA:C8	2.55	0.41
6:C:1137:VAL:HG12	7:D:1:MET:HE1	2.03	0.41
7:D:1043:LYS:HE2	7:D:1117:ASP:HB2	2.02	0.41
6:C:315:LYS:HE2	6:C:315:LYS:HB3	1.93	0.41
7:D:447:MET:HE1	7:D:522:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LYS:HD3	1:A:133:LYS:H	1.86	0.40
1:B:5:GLN:HG3	1:B:7:PRO:HD3	2.02	0.40
1:B:24:GLU:HA	1:B:191:LYS:HG3	2.04	0.40
7:D:279:ASP:HA	7:D:282:ARG:HG2	2.03	0.40
1:A:221:LEU:O	1:A:224:GLU:HG2	2.21	0.40
1:B:180:ALA:HA	1:B:189:PHE:O	2.22	0.40
2:E:56:TYR:HE1	7:D:1272:VAL:HG13	1.85	0.40
6:C:259:ARG:O	6:C:263:GLU:HG2	2.21	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	224/347 (65%)	216 (96%)	8 (4%)	0	100	100
1	B	235/347 (68%)	229 (97%)	6 (3%)	0	100	100
2	E	80/110 (73%)	76 (95%)	4 (5%)	0	100	100
6	C	1091/1178 (93%)	1059 (97%)	32 (3%)	0	100	100
7	D	1263/1318 (96%)	1235 (98%)	28 (2%)	0	100	100
All	All	2893/3300 (88%)	2815 (97%)	78 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A	195/297 (66%)	191 (98%)	4 (2%)	47	75
1	B	197/297 (66%)	188 (95%)	9 (5%)	24	58
2	E	69/90 (77%)	67 (97%)	2 (3%)	37	70
6	C	929/998 (93%)	890 (96%)	39 (4%)	26	61
7	D	1050/1095 (96%)	1011 (96%)	39 (4%)	30	64
All	All	2440/2777 (88%)	2347 (96%)	93 (4%)	30	63

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	GLU
1	A	105	VAL
1	A	130	ASP
1	A	133	LYS
1	B	15	THR
1	B	24	GLU
1	B	59	VAL
1	B	106	THR
1	B	111	VAL
1	B	116	VAL
1	B	150	VAL
1	B	181	THR
1	B	218	LEU
2	E	31	THR
2	E	36	THR
6	C	56	VAL
6	C	70	TRP
6	C	116	LYS
6	C	128	THR
6	C	185	VAL
6	C	195	THR
6	C	216	VAL
6	C	224	VAL
6	C	262	LEU
6	C	268	VAL
6	C	288	THR
6	C	295	LEU
6	C	296	LEU
6	C	345	LEU

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Mol	Chain	Res	Type
6	C	365	VAL
6	C	373	PHE
6	C	409	VAL
6	C	428	LYS
6	C	443	ASN
6	C	472	VAL
6	C	519	VAL
6	C	532	THR
6	C	548	ILE
6	C	559	VAL
6	C	571	VAL
6	C	598	GLU
6	C	603	ASN
6	C	626	VAL
6	C	645	GLU
6	C	702	ILE
6	C	831	GLU
6	C	835	THR
6	C	838	LYS
6	C	843	GLU
6	C	852	VAL
6	C	869	VAL
6	C	873	VAL
6	C	976	VAL
6	C	1066	GLN
7	D	1	MET
7	D	2	LEU
7	D	4	VAL
7	D	6	PHE
7	D	7	PHE
7	D	16	THR
7	D	110	VAL
7	D	117	LEU
7	D	208	ILE
7	D	236	VAL
7	D	251	TYR
7	D	418	LEU
7	D	420	LYS
7	D	446	LEU
7	D	496	VAL
7	D	527	LEU
7	D	539	ASP

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Mol	Chain	Res	Type
7	D	543	VAL
7	D	564	ASN
7	D	592	VAL
7	D	611	VAL
7	D	629	VAL
7	D	635	VAL
7	D	754	ASP
7	D	758	LYS
7	D	759	GLN
7	D	762	ARG
7	D	784	GLU
7	D	824	VAL
7	D	826	ASN
7	D	858	LYS
7	D	909	THR
7	D	949	ILE
7	D	957	ILE
7	D	993	GLU
7	D	1060	ARG
7	D	1088	VAL
7	D	1217	THR
7	D	1250	GLU

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

Mol	Chain	Res	Type
2	E	69	ASN
6	C	142	ASN
6	C	150	GLN
6	C	419	ASN
6	C	686	GLN
6	C	941	HIS
6	C	1042	HIS
6	C	1062	GLN
6	C	1066	GLN
7	D	35	ASN
7	D	439	HIS
7	D	540	GLN
7	D	748	HIS
7	D	787	GLN
7	D	797	ASN
7	D	826	ASN

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Mol	Chain	Res	Type
7	D	1001	GLN
7	D	1246	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	R	8/20 (40%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 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	$\# Z > 2$
9	A1BNV	C	1202	-	38,38,38	2.83	20 (52%)	48,53,53	3.73	21 (43%)
8	GTP	C	1201	10	33,34,34	1.14	1 (3%)	50,54,54	1.45	6 (12%)

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
9	A1BNV	C	1202	-	-	1/24/36/36	0/4/4/4
8	GTP	C	1201	10	-	3/22/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1202	A1BNV	O11-C11	-7.13	1.09	1.23
9	C	1202	A1BNV	O12-C110	-5.40	1.10	1.23
9	C	1202	A1BNV	C110-N12	4.72	1.45	1.34
9	C	1202	A1BNV	C116-C111	-4.64	1.32	1.39
9	C	1202	A1BNV	O13-S11	-4.35	1.36	1.44
9	C	1202	A1BNV	C11-N11	4.14	1.45	1.35
9	C	1202	A1BNV	C119-C118	-3.89	1.33	1.39
9	C	1202	A1BNV	C18-C19	-3.80	1.32	1.38
8	C	1201	GTP	PA-O3A	-3.67	1.55	1.59
9	C	1202	A1BNV	C115-C116	-3.58	1.32	1.38
9	C	1202	A1BNV	C18-C17	-3.29	1.31	1.38
9	C	1202	A1BNV	C114-C113	-3.23	1.33	1.38
9	C	1202	A1BNV	O14-S11	-3.00	1.38	1.44
9	C	1202	A1BNV	C17-C16	-2.84	1.32	1.38
9	C	1202	A1BNV	C122-C117	-2.56	1.35	1.39
9	C	1202	A1BNV	C125-S11	-2.26	1.74	1.76
9	C	1202	A1BNV	C120-C119	-2.19	1.35	1.38
9	C	1202	A1BNV	C123-N13	-2.03	1.43	1.46
9	C	1202	A1BNV	C124-S11	-2.02	1.74	1.76
9	C	1202	A1BNV	C12-N12	-2.01	1.41	1.45
9	C	1202	A1BNV	C117-N11	2.00	1.45	1.41

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1202	A1BNV	O14-S11-O13	-14.46	105.86	117.89
9	C	1202	A1BNV	C125-S11-C124	12.64	120.68	101.11
9	C	1202	A1BNV	O13-S11-C124	-7.71	101.64	109.19
9	C	1202	A1BNV	C111-C110-N12	6.00	129.69	116.67
8	C	1201	GTP	O2A-PA-O3A	-5.44	92.56	107.27
9	C	1202	A1BNV	O11-C11-N11	-5.18	112.97	123.92
9	C	1202	A1BNV	O12-C110-C111	-3.90	113.88	121.03
9	C	1202	A1BNV	C12-C11-N11	3.87	126.46	115.28
9	C	1202	A1BNV	F11-C112-C111	3.56	125.63	119.62
9	C	1202	A1BNV	O12-C110-N12	-3.38	116.05	122.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1202	A1BNV	O14-S11-C124	3.30	112.42	109.19
9	C	1202	A1BNV	O13-S11-C125	-3.26	106.00	109.19
8	C	1201	GTP	O2'-C2'-C3'	-3.25	101.40	111.82
9	C	1202	A1BNV	C116-C111-C110	-3.02	110.46	118.53
9	C	1202	A1BNV	C126-N13-C123	2.97	118.25	111.57
9	C	1202	A1BNV	C18-C17-C16	2.95	123.91	119.87
8	C	1201	GTP	O2B-PB-O3A	2.86	115.00	107.27
9	C	1202	A1BNV	F11-C112-C113	-2.77	112.22	118.65
9	C	1202	A1BNV	C115-C114-C113	2.71	123.58	120.24
8	C	1201	GTP	O3A-PA-O1A	2.66	118.70	110.70
9	C	1202	A1BNV	C13-C12-C11	2.60	116.96	110.30
9	C	1202	A1BNV	C112-C111-C110	2.53	131.20	124.32
9	C	1202	A1BNV	C17-C18-C19	-2.52	117.13	120.24
8	C	1201	GTP	O3G-PG-O2G	2.46	117.04	107.80
9	C	1202	A1BNV	C119-C118-N13	-2.25	118.90	122.42
9	C	1202	A1BNV	C118-C117-N11	2.15	122.57	118.61
8	C	1201	GTP	O3G-PG-O1G	2.05	118.81	110.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

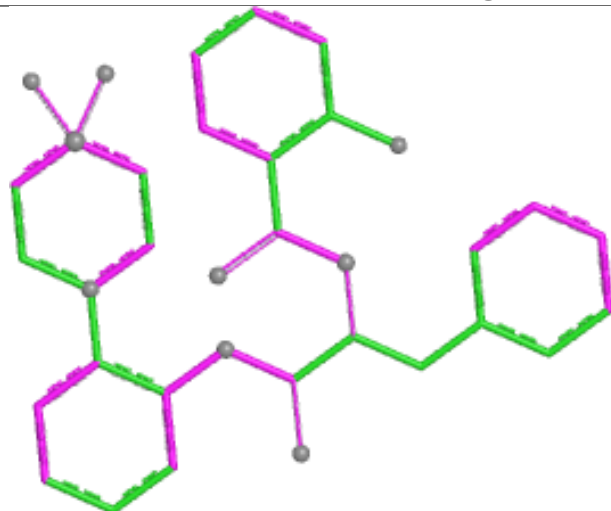
Mol	Chain	Res	Type	Atoms
8	C	1201	GTP	C3'-C4'-C5'-O5'
8	C	1201	GTP	O4'-C4'-C5'-O5'
8	C	1201	GTP	PA-O3A-PB-O1B
9	C	1202	A1BNV	C119-C118-N13-C123

There are no ring outliers.

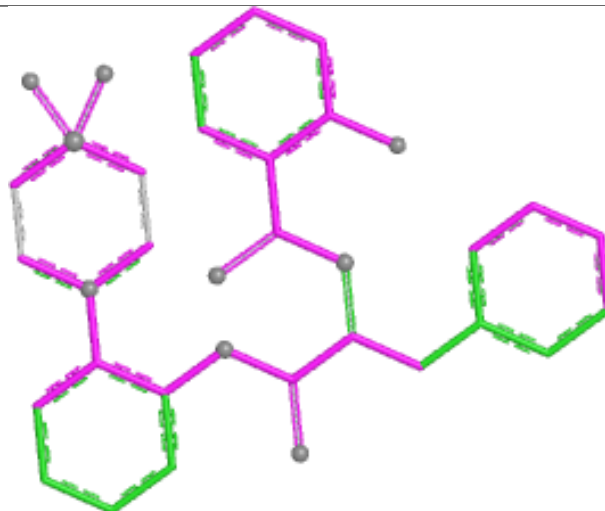
No monomer is involved in short contacts.

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.

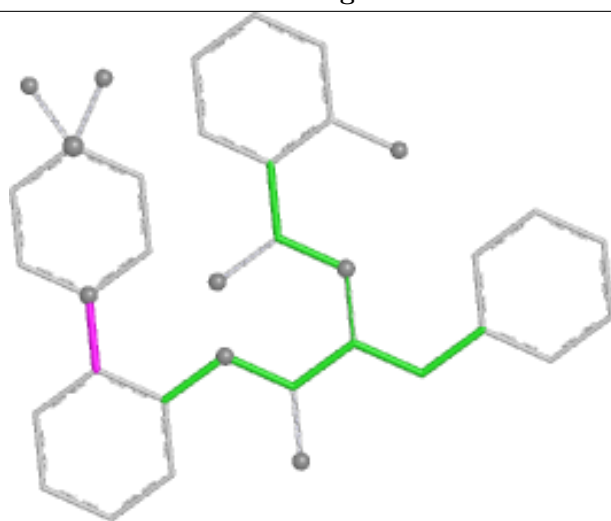
Ligand A1BNV C 1202



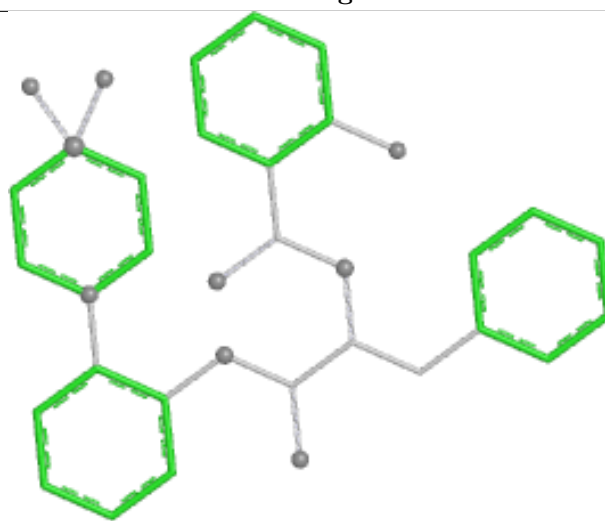
Bond lengths



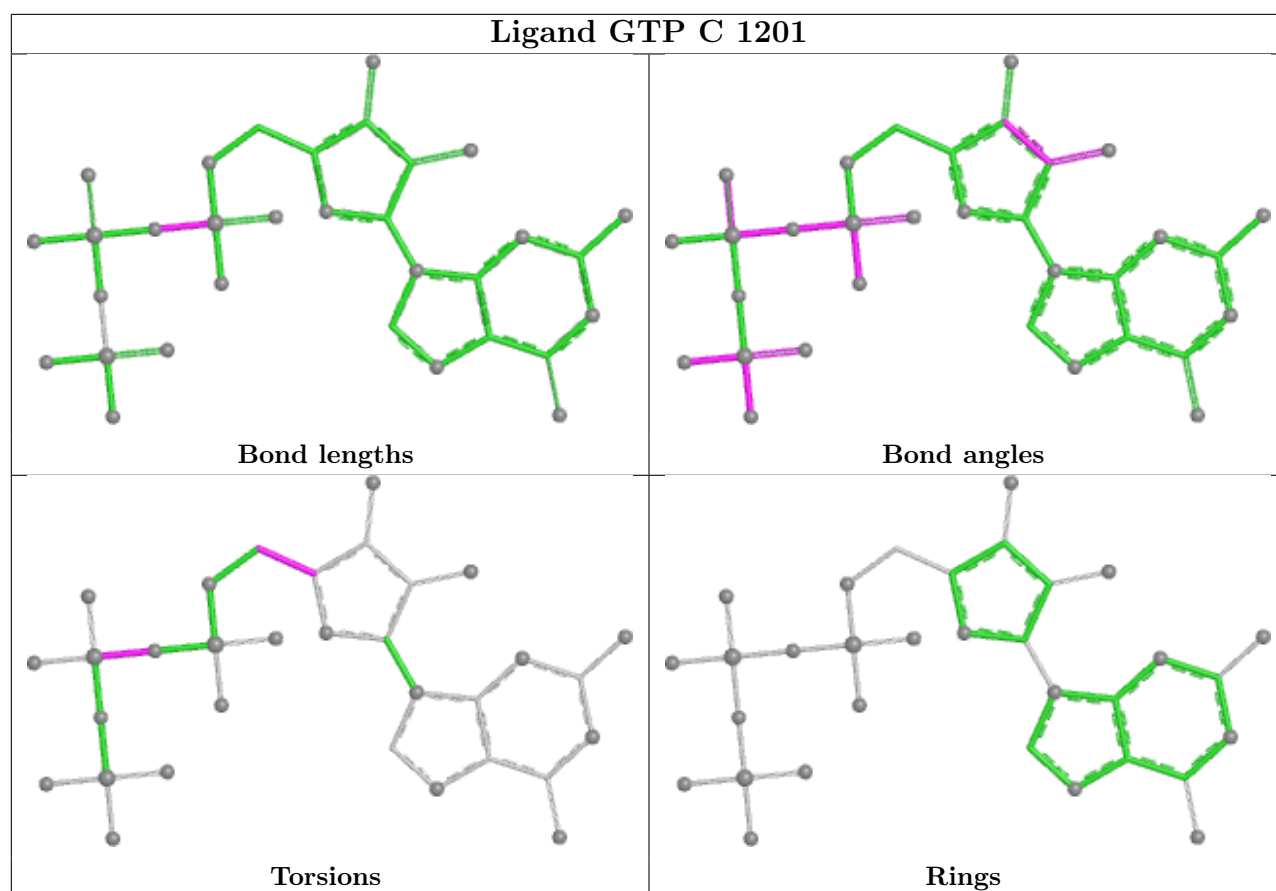
Bond angles



Torsions



Rings



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.

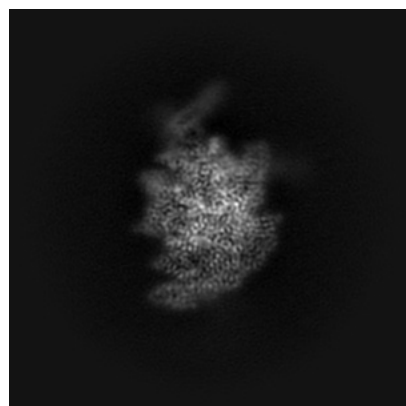
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75289. These allow visual inspection of the internal detail of the map and identification of artifacts.

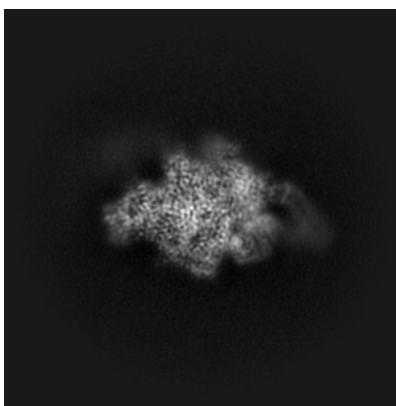
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

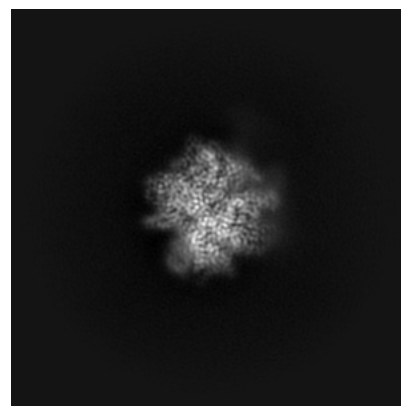
6.1.1 Primary map



X

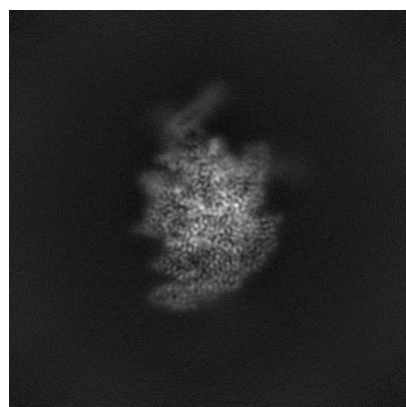


Y

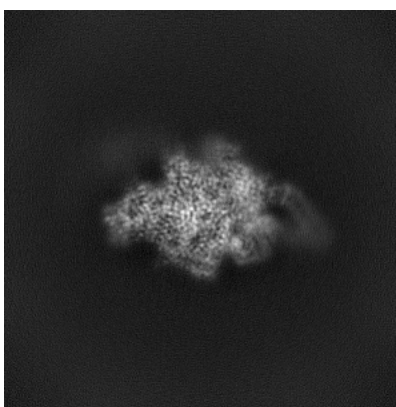


Z

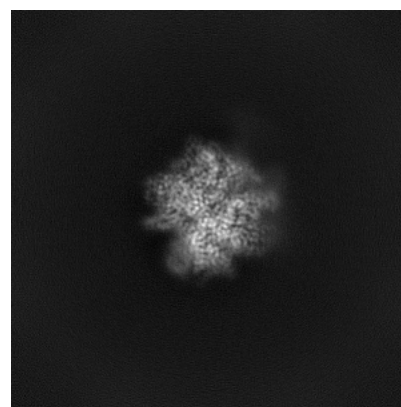
6.1.2 Raw map



X



Y

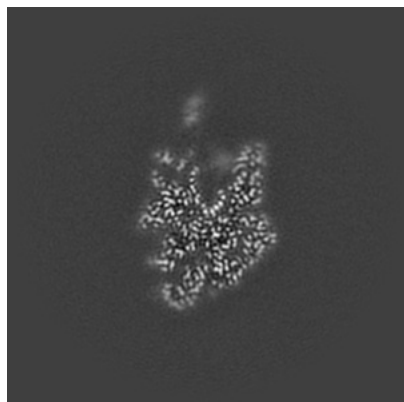


Z

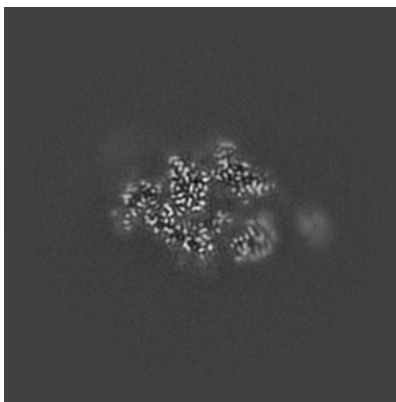
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

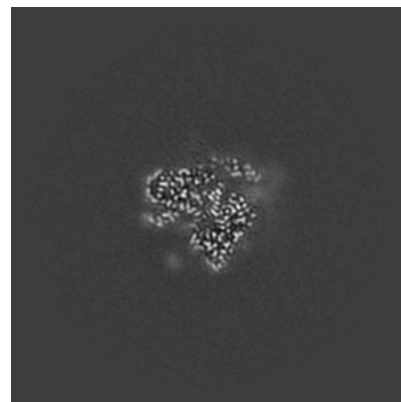
6.2.1 Primary map



X Index: 192

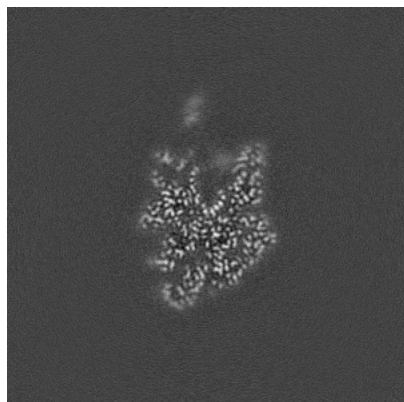


Y Index: 192

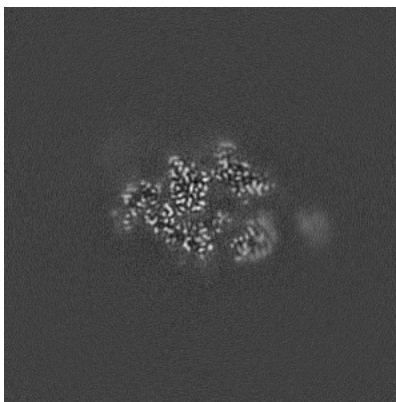


Z Index: 192

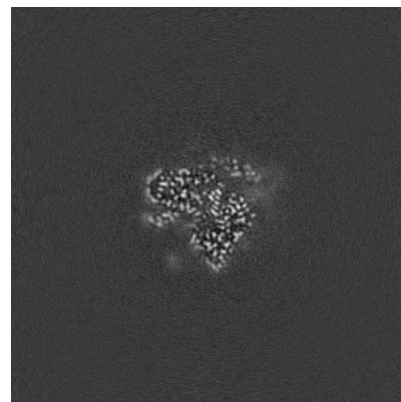
6.2.2 Raw map



X Index: 192



Y Index: 192

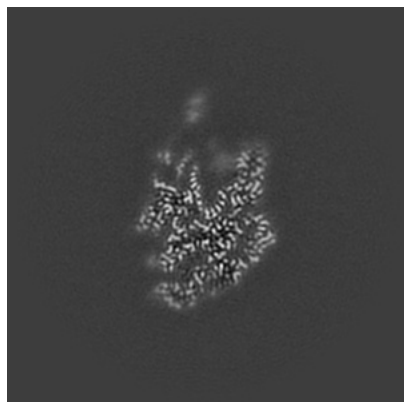


Z Index: 192

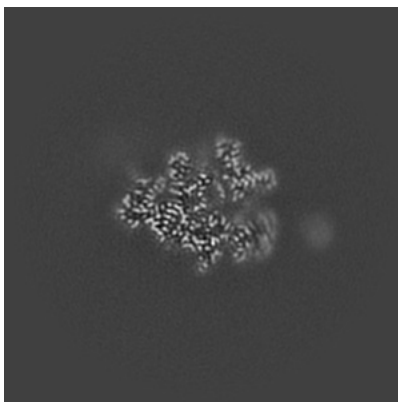
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

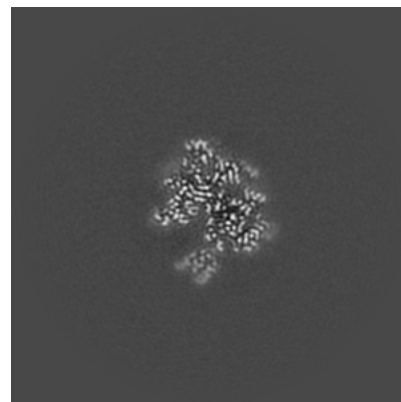
6.3.1 Primary map



X Index: 190

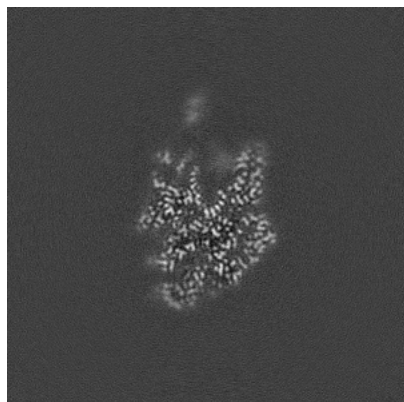


Y Index: 199

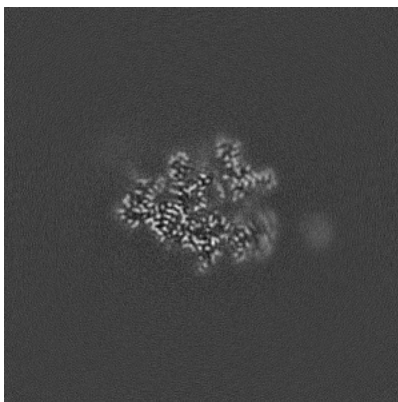


Z Index: 172

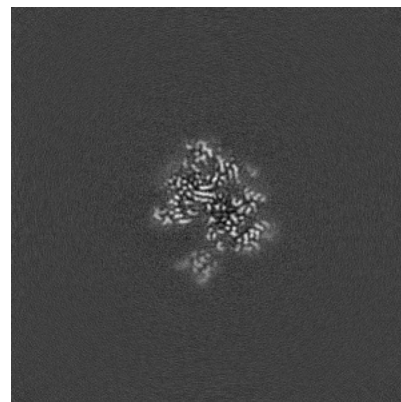
6.3.2 Raw map



X Index: 191



Y Index: 199

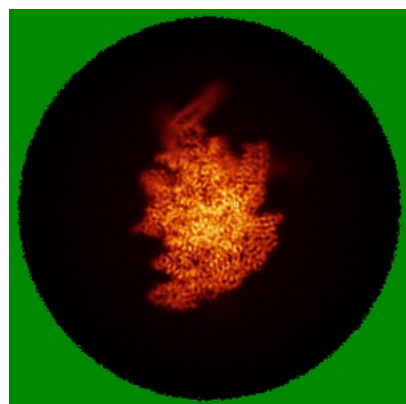


Z Index: 171

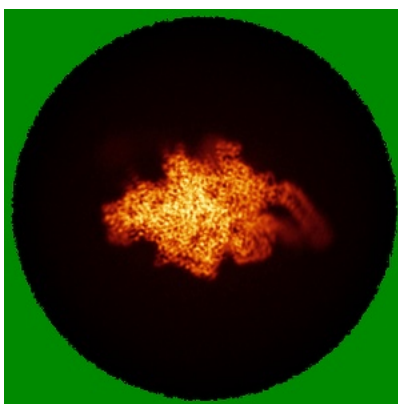
The images above show the largest variance slices of the map in three orthogonal directions.

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

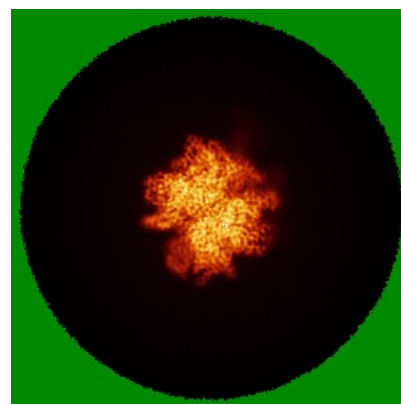
6.4.1 Primary map



X

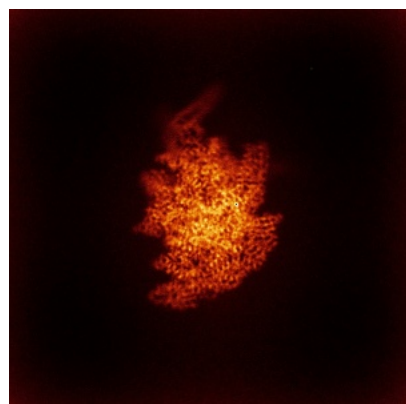


Y

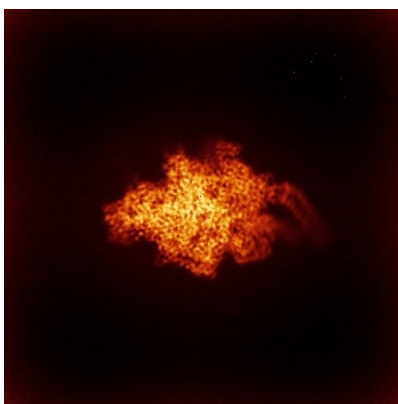


Z

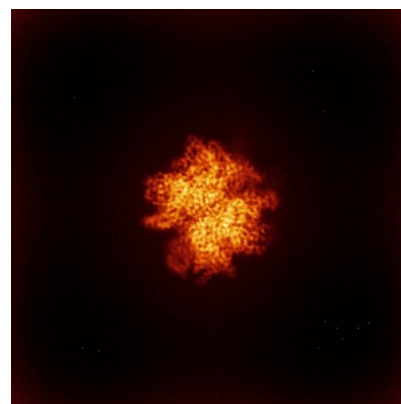
6.4.2 Raw map



X



Y

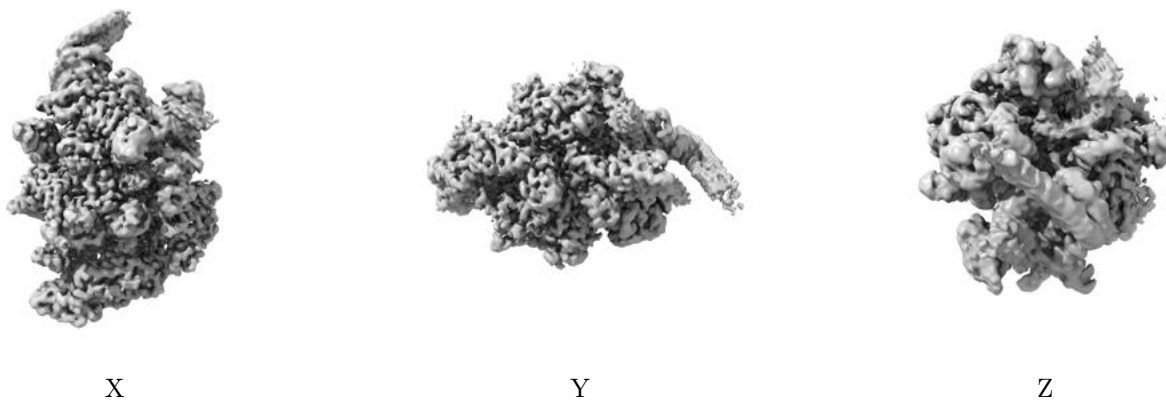


Z

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.

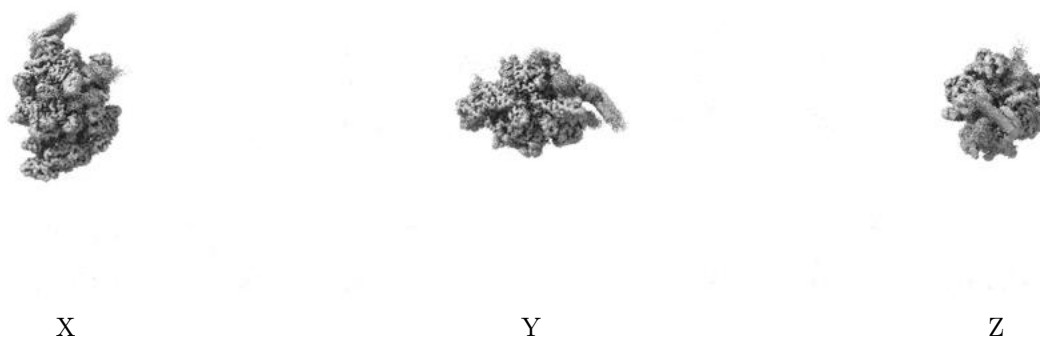
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

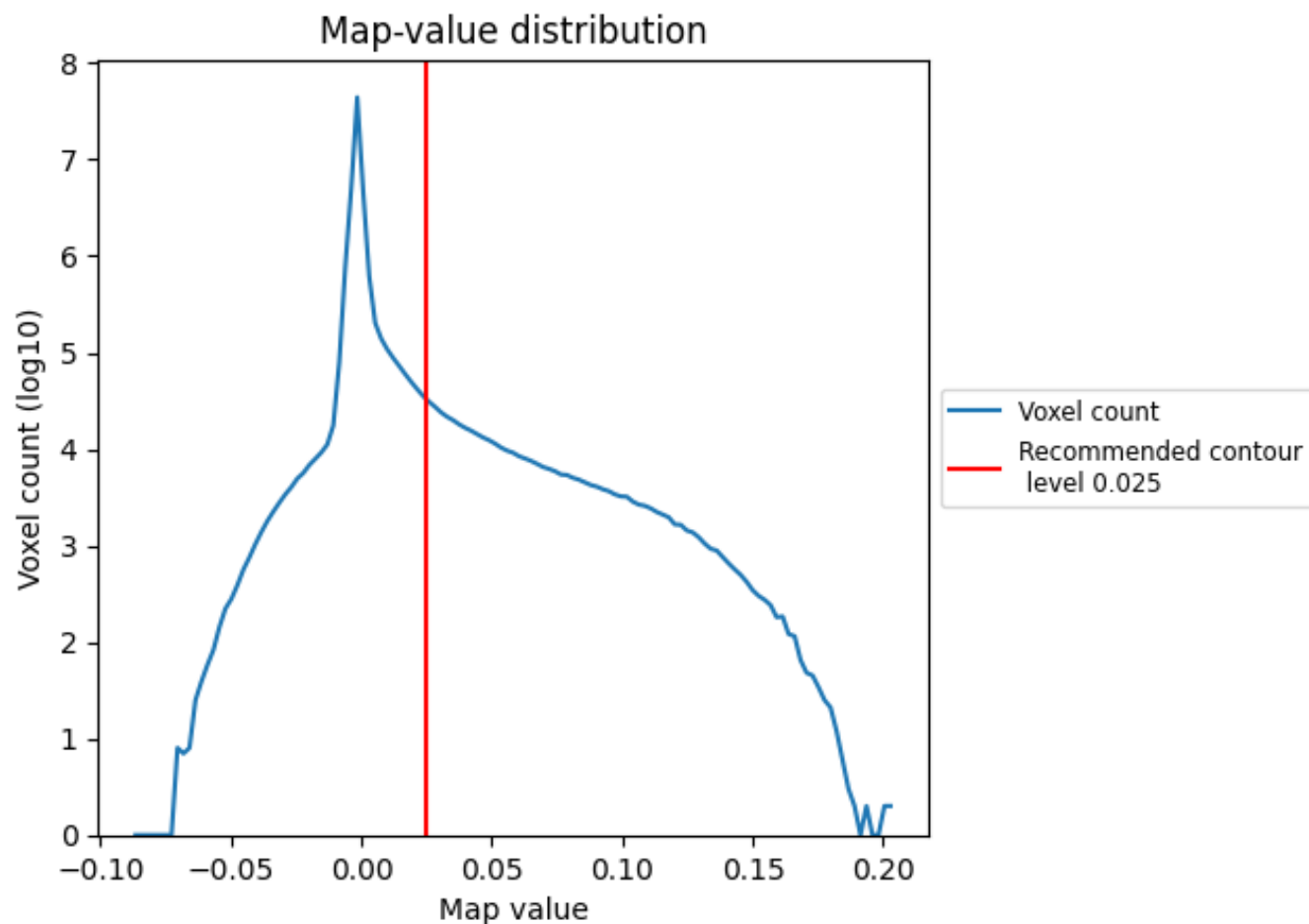
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

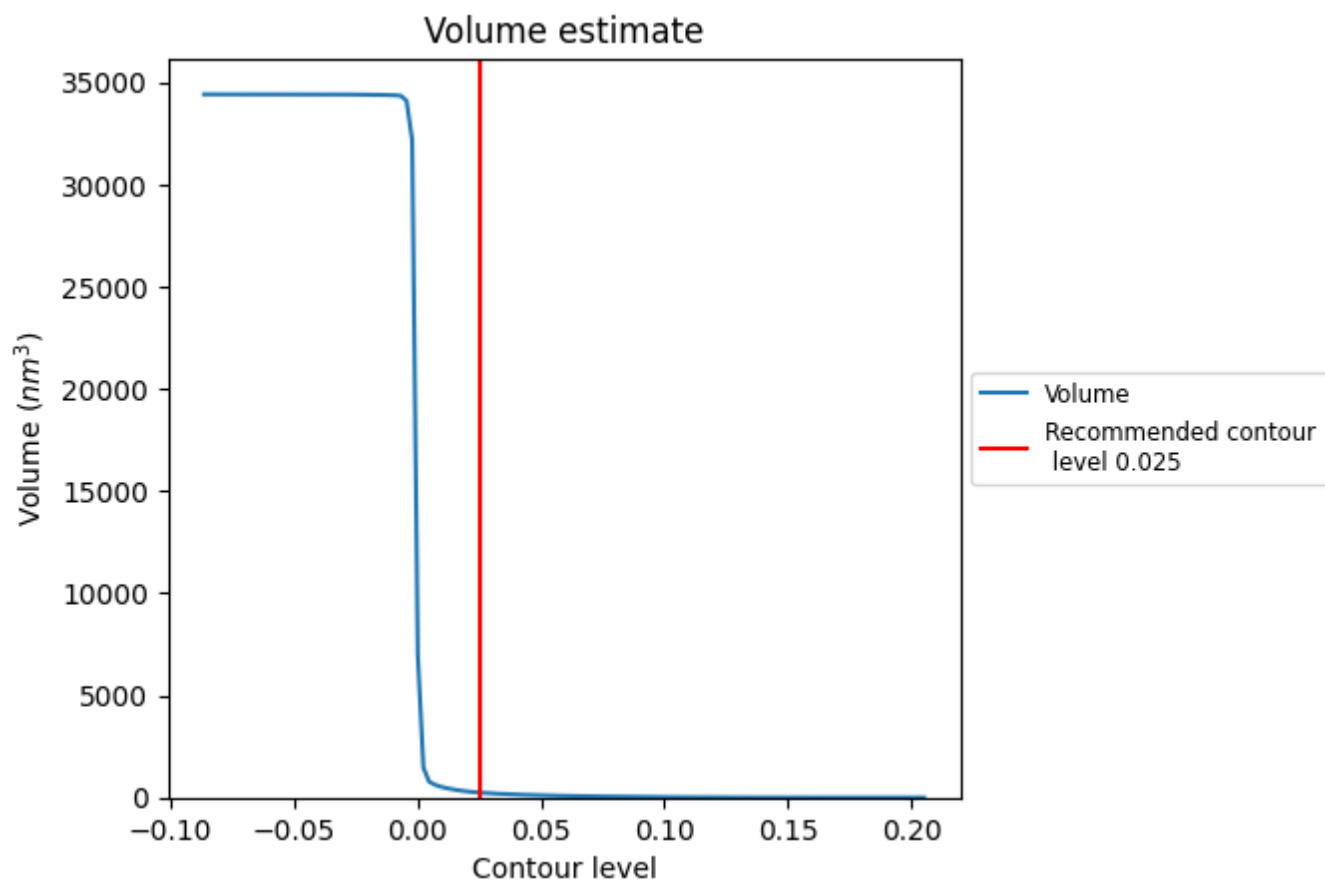
This section contains the results of statistical analysis of the map.

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.

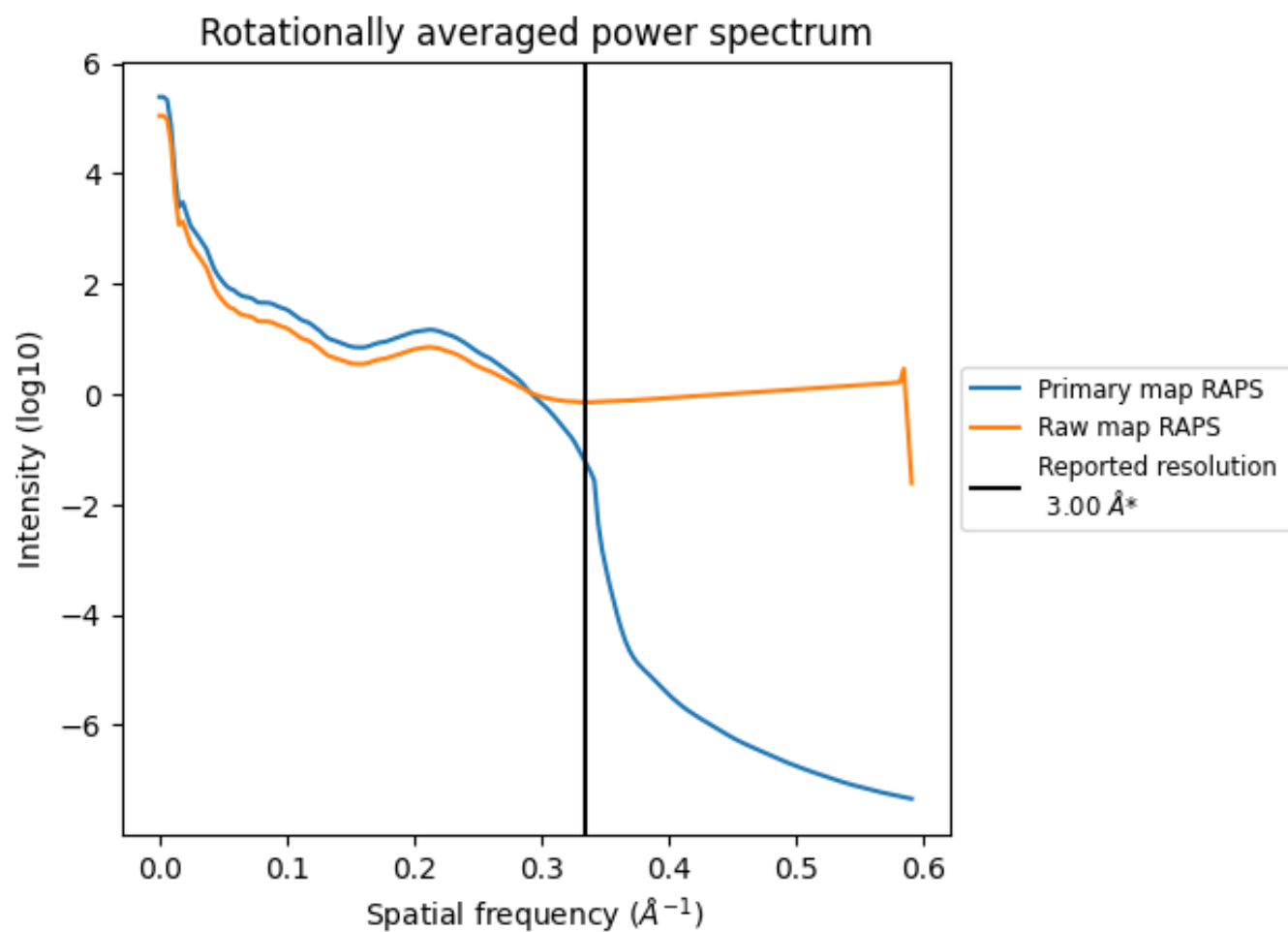
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 244 nm³; this corresponds to an approximate mass of 220 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 ⓘ

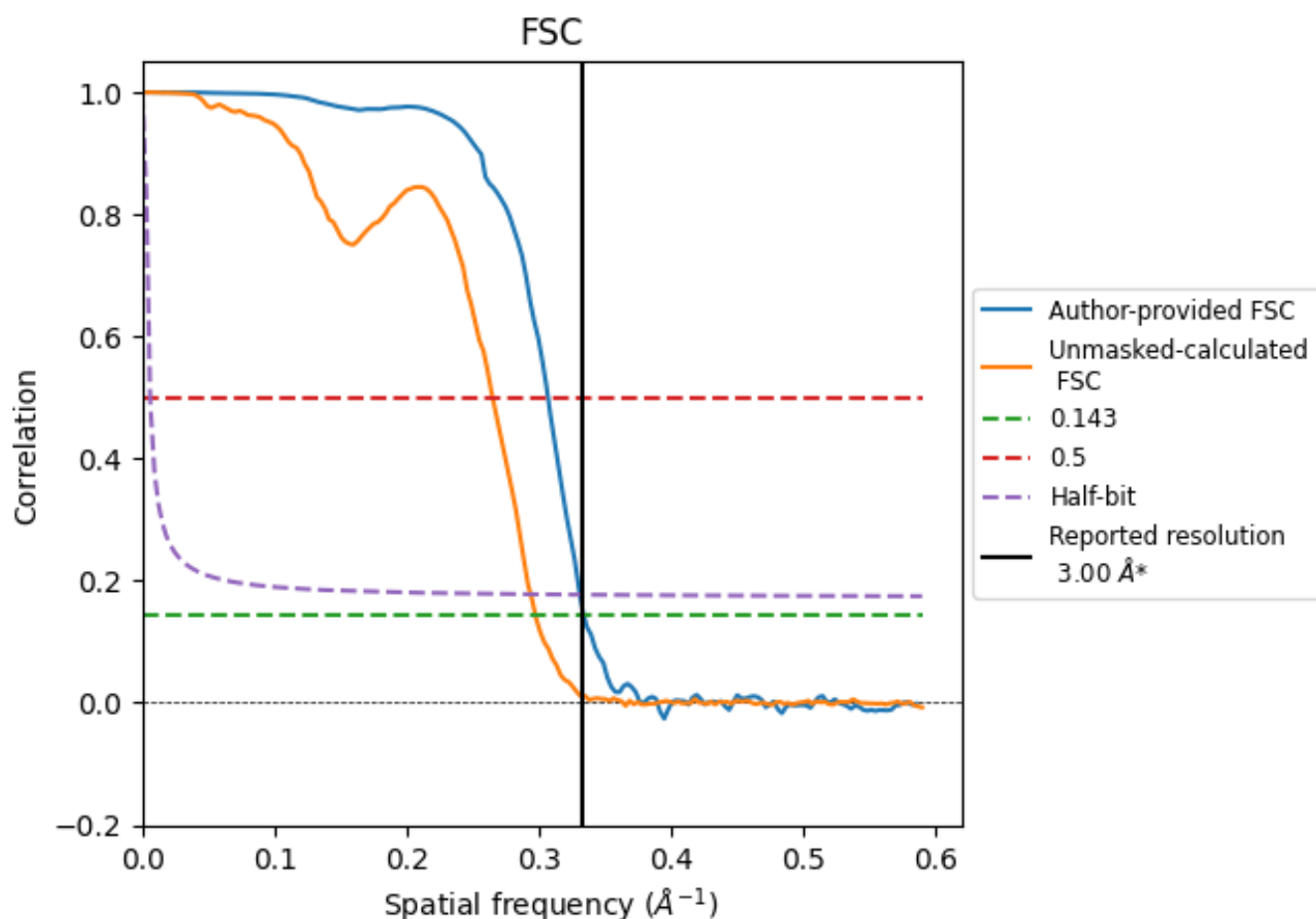


*Reported resolution corresponds to spatial frequency of $0.333 \text{ \AA}^{-1}$

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

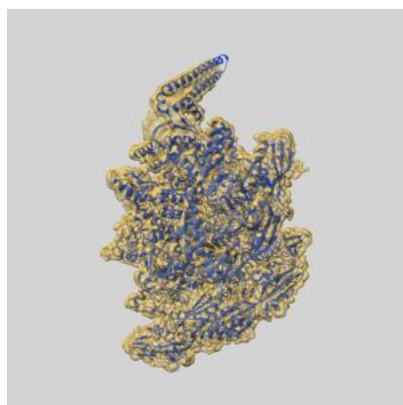
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.99	3.26	3.02
Unmasked-calculated*	3.36	3.77	3.40

*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 3.36 differs from the reported value 3.0 by more than 10 %

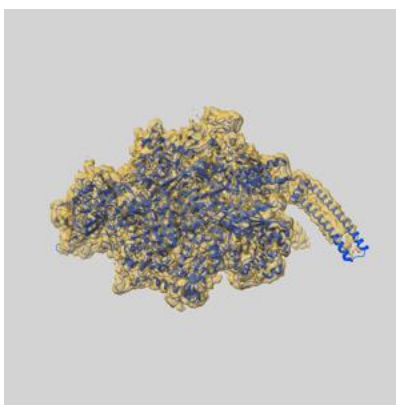
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-75289 and PDB model 10ML. Per-residue inclusion information can be found in section 3 on page 8.

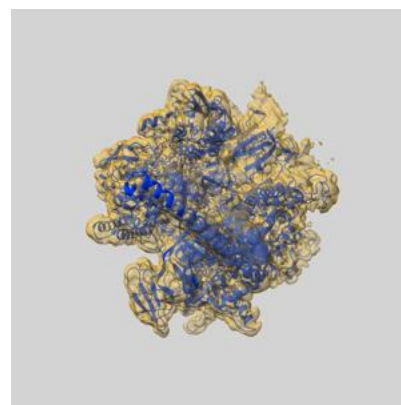
9.1 Map-model overlay [i](#)



X



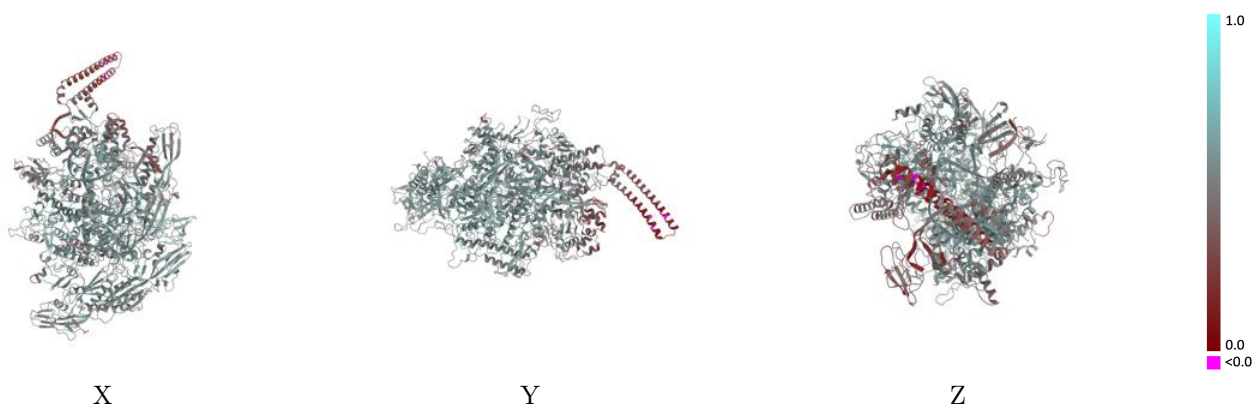
Y



Z

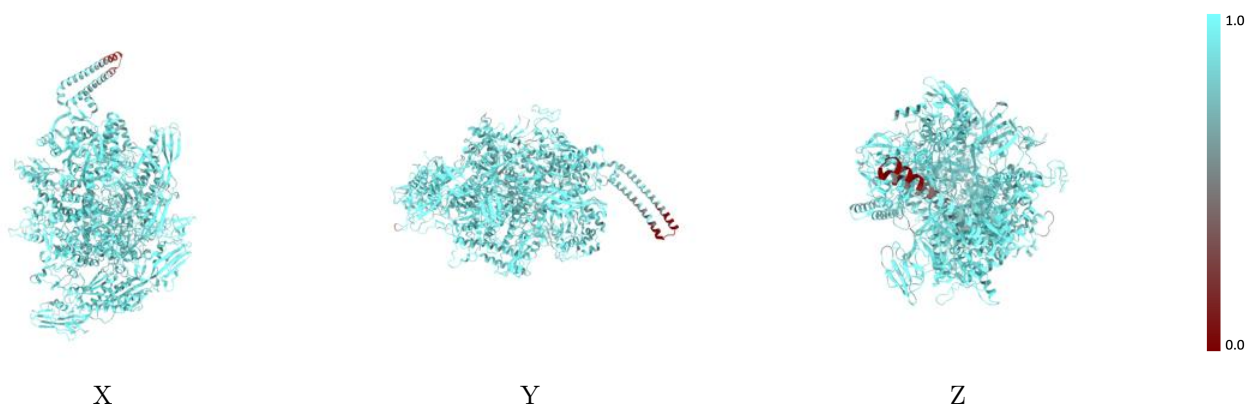
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



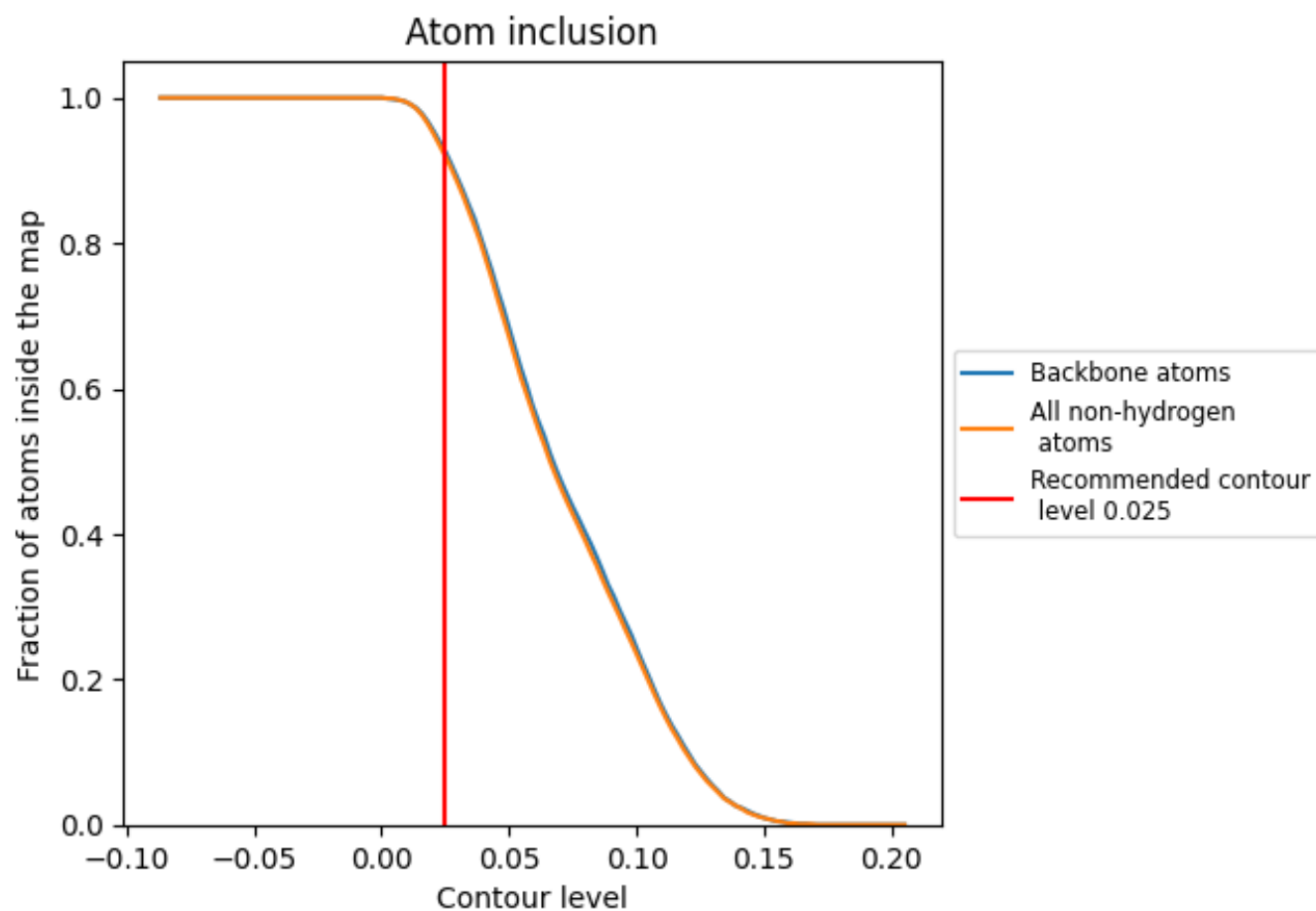
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 92% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9200	0.5120
A	0.9340	0.5360
B	0.9090	0.5030
C	0.9330	0.5290
D	0.9140	0.5000
E	0.9030	0.5120
P	0.9880	0.4840
Q	0.9420	0.4090
R	0.9820	0.5730

