



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 05:34 AM UTC

PDB ID : 6OF3 / pdb_00006of3
EMDB ID : EMD-20041
Title : Precursor ribosomal RNA processing complex, State 1.
Authors : Pillon, M.C.; Hsu, A.L.; Krahn, J.M.; Williams, J.G.; Goslen, K.H.; Sobhany, M.; Borgnia, M.J.; Stanley, R.E.
Deposited on : 2019-03-28
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:

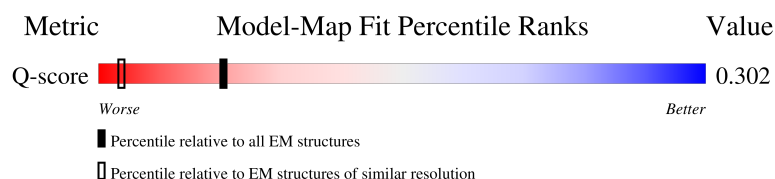
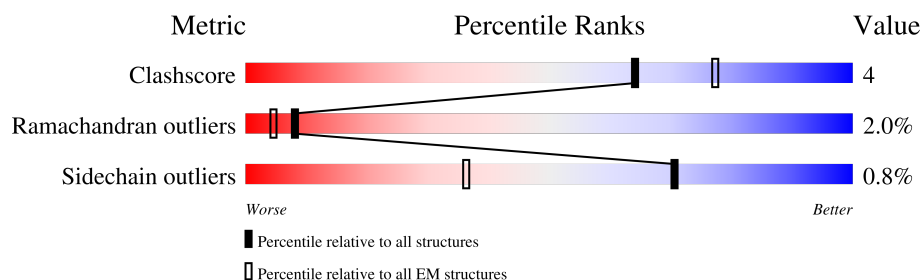
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

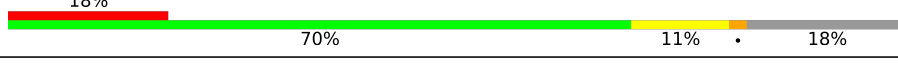
The reported resolution of this entry is 3.00 Å.

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	-
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	391	
1	D	391	
2	B	640	
2	E	640	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11096 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 Ribonuclease.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	187	Total	C	N	O	S	0	0
			1471	940	262	263	6		
1	D	187	Total	C	N	O	S	0	0
			1471	940	262	263	6		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP G0SGE9
A	-26	SER	-	expression tag	UNP G0SGE9
A	-25	TYR	-	expression tag	UNP G0SGE9
A	-24	TYR	-	expression tag	UNP G0SGE9
A	-23	HIS	-	expression tag	UNP G0SGE9
A	-22	HIS	-	expression tag	UNP G0SGE9
A	-21	HIS	-	expression tag	UNP G0SGE9
A	-20	HIS	-	expression tag	UNP G0SGE9
A	-19	HIS	-	expression tag	UNP G0SGE9
A	-18	HIS	-	expression tag	UNP G0SGE9
A	-17	ASP	-	expression tag	UNP G0SGE9
A	-16	TYR	-	expression tag	UNP G0SGE9
A	-15	ASP	-	expression tag	UNP G0SGE9
A	-14	ILE	-	expression tag	UNP G0SGE9
A	-13	PRO	-	expression tag	UNP G0SGE9
A	-12	THR	-	expression tag	UNP G0SGE9
A	-11	THR	-	expression tag	UNP G0SGE9
A	-10	GLU	-	expression tag	UNP G0SGE9
A	-9	ASN	-	expression tag	UNP G0SGE9
A	-8	LEU	-	expression tag	UNP G0SGE9
A	-7	TYR	-	expression tag	UNP G0SGE9
A	-6	PHE	-	expression tag	UNP G0SGE9
A	-5	GLN	-	expression tag	UNP G0SGE9
A	-4	GLY	-	expression tag	UNP G0SGE9
A	-3	ALA	-	expression tag	UNP G0SGE9
A	-2	MET	-	expression tag	UNP G0SGE9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP G0SGE9
A	0	SER	-	expression tag	UNP G0SGE9
D	-27	MET	-	initiating methionine	UNP G0SGE9
D	-26	SER	-	expression tag	UNP G0SGE9
D	-25	TYR	-	expression tag	UNP G0SGE9
D	-24	TYR	-	expression tag	UNP G0SGE9
D	-23	HIS	-	expression tag	UNP G0SGE9
D	-22	HIS	-	expression tag	UNP G0SGE9
D	-21	HIS	-	expression tag	UNP G0SGE9
D	-20	HIS	-	expression tag	UNP G0SGE9
D	-19	HIS	-	expression tag	UNP G0SGE9
D	-18	HIS	-	expression tag	UNP G0SGE9
D	-17	ASP	-	expression tag	UNP G0SGE9
D	-16	TYR	-	expression tag	UNP G0SGE9
D	-15	ASP	-	expression tag	UNP G0SGE9
D	-14	ILE	-	expression tag	UNP G0SGE9
D	-13	PRO	-	expression tag	UNP G0SGE9
D	-12	THR	-	expression tag	UNP G0SGE9
D	-11	THR	-	expression tag	UNP G0SGE9
D	-10	GLU	-	expression tag	UNP G0SGE9
D	-9	ASN	-	expression tag	UNP G0SGE9
D	-8	LEU	-	expression tag	UNP G0SGE9
D	-7	TYR	-	expression tag	UNP G0SGE9
D	-6	PHE	-	expression tag	UNP G0SGE9
D	-5	GLN	-	expression tag	UNP G0SGE9
D	-4	GLY	-	expression tag	UNP G0SGE9
D	-3	ALA	-	expression tag	UNP G0SGE9
D	-2	MET	-	expression tag	UNP G0SGE9
D	-1	GLY	-	expression tag	UNP G0SGE9
D	0	SER	-	expression tag	UNP G0SGE9

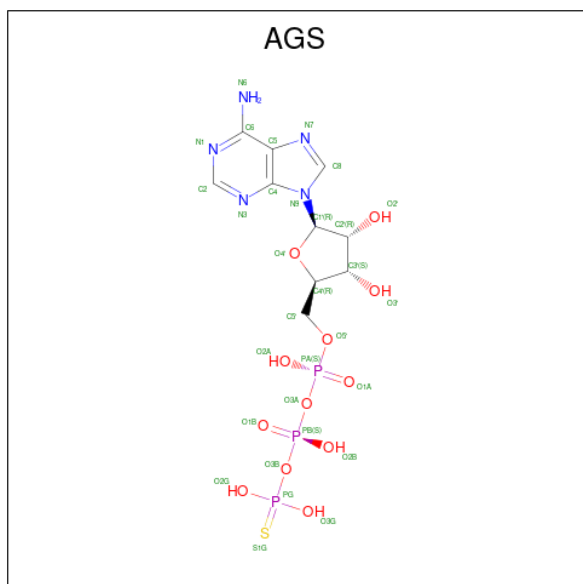
- Molecule 2 is a protein called CLP1_P domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	528	Total	C	N	O	S	0	0
			4045	2585	702	737	21		
2	E	528	Total	C	N	O	S	0	0
			4045	2585	702	737	21		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	109	MET	-	initiating methionine	UNP G0S263
E	109	MET	-	initiating methionine	UNP G0S263

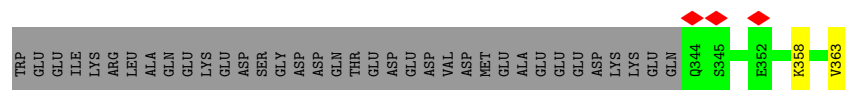
- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



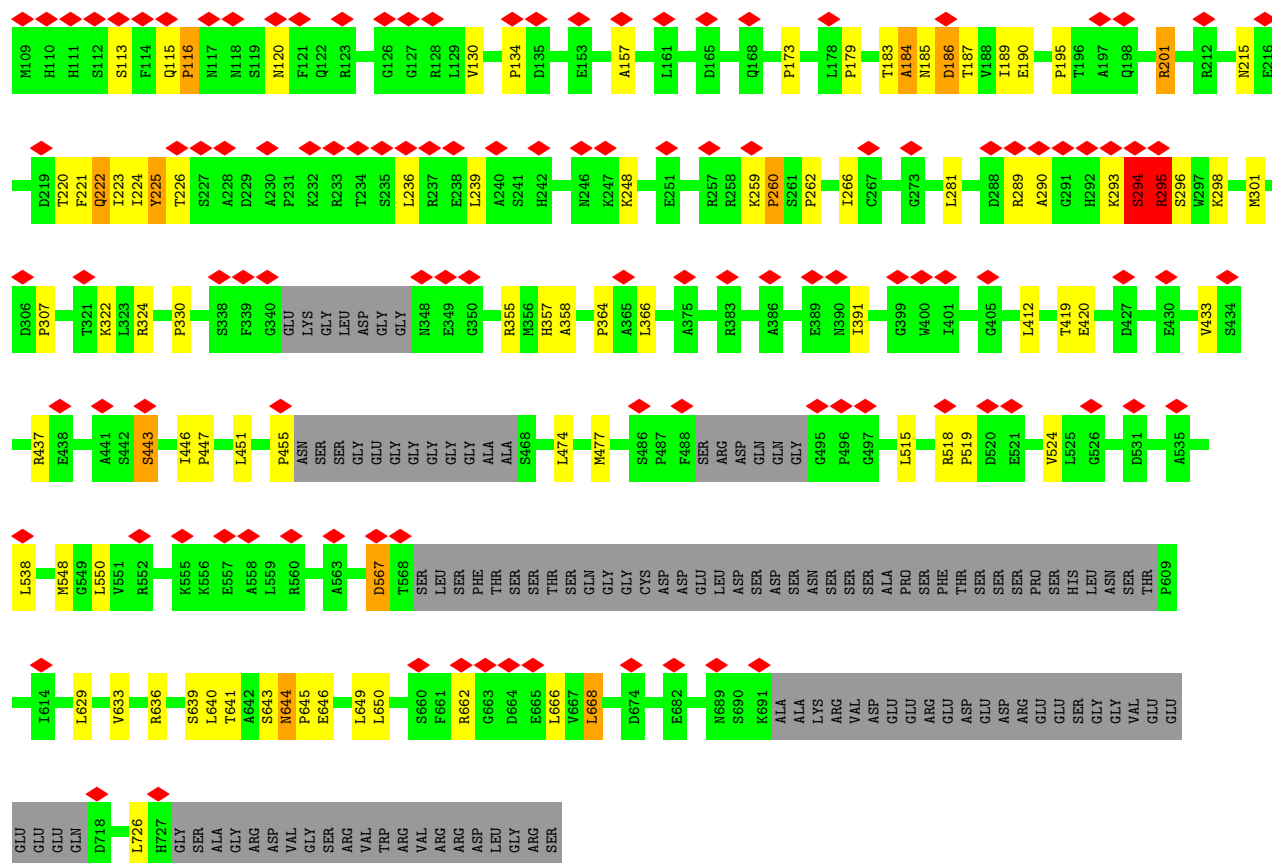
Mol	Chain	Residues	Atoms						AltConf
3	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

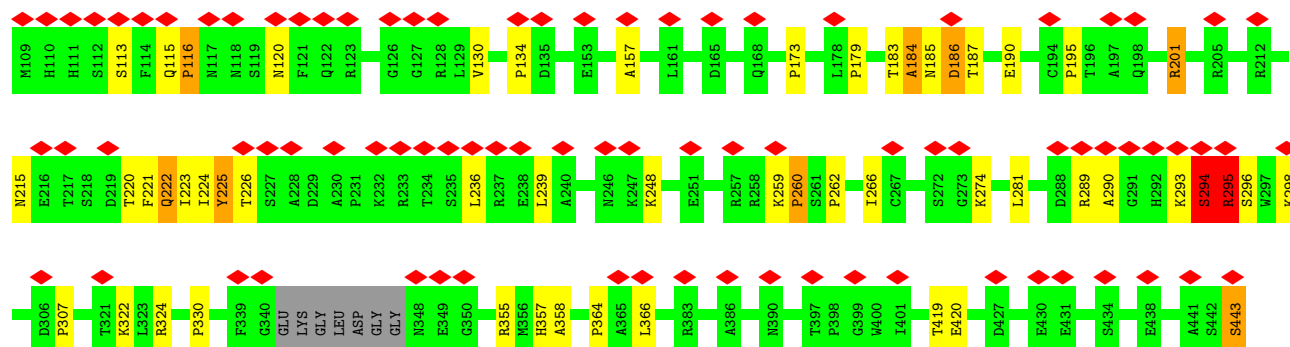
Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	



• Molecule 2: CLP1_P domain-containing protein



• Molecule 2: CLP1_P domain-containing protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74582	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	27.610	Depositor
Minimum map value	-0.709	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.657	Depositor
Recommended contour level	4.5	Depositor
Map size ($\text{\AA}$)	241.92001, 241.92001, 241.92001	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.35	0/1511	0.85	1/2052 (0.0%)
1	D	0.35	0/1511	0.85	1/2052 (0.0%)
2	B	0.38	0/4155	1.03	17/5679 (0.3%)
2	E	0.38	0/4155	1.03	17/5679 (0.3%)
All	All	0.37	0/11332	0.99	36/15462 (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	B	0	2
2	E	0	2
All	All	0	4

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	641	THR	CA-C-N	8.65	138.06	121.54
2	B	641	THR	C-N-CA	8.65	138.06	121.54
2	E	641	THR	CA-C-N	8.62	138.00	121.54
2	E	641	THR	C-N-CA	8.62	138.00	121.54
2	E	184	ALA	CA-C-N	8.61	137.98	121.54
2	E	184	ALA	C-N-CA	8.61	137.98	121.54
2	B	184	ALA	CA-C-N	8.60	137.97	121.54
2	B	184	ALA	C-N-CA	8.60	137.97	121.54
2	B	293	LYS	CA-C-N	8.28	137.35	121.54
2	B	293	LYS	C-N-CA	8.28	137.35	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	293	LYS	CA-C-N	8.25	137.30	121.54
2	E	293	LYS	C-N-CA	8.25	137.30	121.54
2	B	294	SER	CA-C-N	6.83	134.59	121.54
2	B	294	SER	C-N-CA	6.83	134.59	121.54
2	E	294	SER	CA-C-N	6.79	134.52	121.54
2	E	294	SER	C-N-CA	6.79	134.52	121.54
2	B	455	PRO	N-CA-CB	6.75	110.43	103.00
2	E	455	PRO	N-CA-CB	6.75	110.43	103.00
2	B	113	SER	CA-C-N	6.70	134.34	121.54
2	B	113	SER	C-N-CA	6.70	134.34	121.54
2	E	113	SER	CA-C-N	6.68	134.30	121.54
2	E	113	SER	C-N-CA	6.68	134.30	121.54
2	B	295	ARG	N-CA-CB	6.23	121.02	110.49
2	E	295	ARG	N-CA-CB	6.21	120.98	110.49
2	E	443	SER	CA-C-N	6.16	133.30	121.54
2	E	443	SER	C-N-CA	6.16	133.30	121.54
1	D	147	GLU	N-CA-C	6.14	119.15	109.39
2	B	443	SER	CA-C-N	6.13	133.25	121.54
2	B	443	SER	C-N-CA	6.13	133.25	121.54
1	A	147	GLU	N-CA-C	6.13	119.14	109.39
2	B	296	SER	N-CA-C	-5.93	100.76	109.18
2	E	296	SER	N-CA-C	-5.90	100.80	109.18
2	E	293	LYS	N-CA-C	-5.04	100.07	110.80
2	E	366	LEU	N-CA-C	-5.03	106.99	114.64
2	B	293	LYS	N-CA-C	-5.03	100.08	110.80
2	B	366	LEU	N-CA-C	-5.03	107.00	114.64

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	184	ALA	Peptide
2	B	225	TYR	Peptide
2	E	184	ALA	Peptide
2	E	225	TYR	Peptide

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1471	0	1411	8	0
1	D	1471	0	1411	7	0
2	B	4045	0	4019	43	0
2	E	4045	0	4019	40	0
3	B	31	0	12	1	0
3	E	31	0	12	1	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
All	All	11096	0	10884	89	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 4.

All (89) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ALA:HB2	1:D:102:ALA:HB2	1.74	0.69
2:E:116:PRO:HG3	2:E:225:TYR:HA	1.82	0.61
2:B:644:ASN:ND2	2:B:646:GLU:OE1	2.34	0.60
2:E:644:ASN:ND2	2:E:646:GLU:OE1	2.34	0.60
2:B:116:PRO:HG3	2:B:225:TYR:HA	1.82	0.60
2:B:201:ARG:NH2	2:B:215:ASN:OD1	2.37	0.58
2:B:239:LEU:HA	3:B:801:AGS:H2	1.86	0.57
2:E:201:ARG:NH2	2:E:215:ASN:OD1	2.36	0.57
2:E:239:LEU:HA	3:E:801:AGS:H2	1.86	0.57
2:E:289:ARG:HD2	2:E:294:SER:HB3	1.88	0.56
2:B:289:ARG:HD2	2:B:294:SER:HB3	1.88	0.56
2:B:322:LYS:HE2	2:B:324:ARG:HE	1.70	0.56
1:A:146:HIS:O	1:D:106:ARG:NH1	2.39	0.56
2:E:322:LYS:HE2	2:E:324:ARG:HE	1.70	0.55
1:A:47:ARG:NH2	1:A:84:GLU:O	2.39	0.55
1:D:47:ARG:NH2	1:D:84:GLU:O	2.39	0.54
1:D:55:ALA:HB1	2:E:538:LEU:HD11	1.90	0.53
1:A:3:GLN:HB2	2:B:726:LEU:HB2	1.91	0.53
1:D:363:VAL:HG11	2:E:639:SER:HB3	1.89	0.53
2:E:518:ARG:HA	2:E:567:ASP:HB3	1.92	0.52
2:B:518:ARG:HA	2:B:567:ASP:HB3	1.92	0.51
2:B:130:VAL:HG22	2:B:190:GLU:HG2	1.93	0.51
1:D:358:LYS:O	2:E:636:ARG:NH2	2.44	0.51
2:E:130:VAL:HG22	2:E:190:GLU:HG2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:636:ARG:HD2	2:E:650:LEU:HD23	1.94	0.50
1:A:363:VAL:HG11	2:B:639:SER:HB3	1.93	0.50
2:B:295:ARG:HH11	2:B:298:LYS:HE2	1.77	0.50
2:B:134:PRO:HA	2:B:186:ASP:HA	1.94	0.50
2:B:636:ARG:HD2	2:B:650:LEU:HD23	1.93	0.49
2:E:295:ARG:HH11	2:E:298:LYS:HE2	1.77	0.49
2:E:419:THR:HG22	2:E:420:GLU:HG3	1.95	0.48
1:A:55:ALA:HB1	2:B:538:LEU:HD11	1.95	0.48
2:E:134:PRO:HA	2:E:186:ASP:HA	1.94	0.48
2:E:515:LEU:HB2	2:E:645:PRO:HB2	1.96	0.48
2:B:419:THR:HG22	2:B:420:GLU:HG3	1.95	0.48
2:E:157:ALA:HB2	2:E:179:PRO:HB3	1.95	0.48
2:B:157:ALA:HB2	2:B:179:PRO:HB3	1.95	0.48
2:B:515:LEU:HB2	2:B:645:PRO:HB2	1.96	0.48
2:E:224:ILE:HD13	2:E:236:LEU:HD11	1.97	0.47
2:B:518:ARG:HG2	2:B:519:PRO:HD2	1.97	0.47
2:B:224:ILE:HD13	2:B:236:LEU:HD11	1.96	0.47
2:B:220:THR:HG23	2:B:221:PHE:HD1	1.80	0.46
2:E:220:THR:HG23	2:E:221:PHE:HD1	1.80	0.46
2:E:355:ARG:HE	2:E:357:HIS:HE1	1.63	0.46
2:E:518:ARG:HG2	2:E:519:PRO:HD2	1.97	0.46
2:E:259:LYS:HG2	2:E:260:PRO:HD2	1.98	0.46
2:E:474:LEU:HA	2:E:477:MET:HE3	1.98	0.46
2:B:474:LEU:HA	2:B:477:MET:HE3	1.98	0.45
2:B:548:MET:HE3	2:B:548:MET:HB2	1.60	0.45
2:B:355:ARG:HE	2:B:357:HIS:HE1	1.63	0.45
2:B:524:VAL:HG21	2:B:668:LEU:HD22	1.99	0.45
1:A:358:LYS:O	2:B:636:ARG:NH2	2.50	0.44
2:E:524:VAL:HG21	2:E:668:LEU:HD22	1.99	0.44
2:B:550:LEU:HD22	2:B:666:LEU:HD11	2.00	0.44
2:B:259:LYS:HG2	2:B:260:PRO:HD2	1.98	0.44
2:E:358:ALA:HB2	2:E:629:LEU:HD22	2.00	0.44
2:E:266:ILE:HD11	2:E:281:LEU:HD12	2.00	0.44
2:B:222:GLN:NE2	2:B:223:ILE:O	2.51	0.43
2:B:173:PRO:HG2	2:B:330:PRO:HG2	2.00	0.43
2:B:266:ILE:HD11	2:B:281:LEU:HD12	2.00	0.43
2:B:358:ALA:HB2	2:B:629:LEU:HD22	2.00	0.43
2:B:633:VAL:HG11	2:B:649:LEU:HD22	2.01	0.43
2:E:222:GLN:NE2	2:E:223:ILE:O	2.51	0.43
2:E:420:GLU:HG2	2:E:447:PRO:HB2	2.00	0.43
2:E:443:SER:HB2	2:E:446:ILE:HD11	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:550:LEU:HD22	2:E:666:LEU:HD11	2.00	0.42
2:B:260:PRO:O	2:B:262:PRO:HD3	2.19	0.42
2:E:633:VAL:HG11	2:E:649:LEU:HD22	2.00	0.42
2:E:248:LYS:HG2	2:E:451:LEU:HD11	2.01	0.42
2:E:173:PRO:HG2	2:E:330:PRO:HG2	2.00	0.42
2:B:289:ARG:HB3	2:B:294:SER:HA	2.02	0.42
2:B:420:GLU:HG2	2:B:447:PRO:HB2	2.00	0.42
2:B:183:THR:HB	2:B:187:THR:HG21	2.02	0.41
2:E:183:THR:HB	2:E:187:THR:HG21	2.02	0.41
2:E:289:ARG:HB3	2:E:294:SER:HA	2.02	0.41
2:E:548:MET:HE3	2:E:548:MET:HB2	1.60	0.41
2:B:412:LEU:HD23	2:B:412:LEU:HA	1.95	0.41
2:B:248:LYS:HG2	2:B:451:LEU:HD11	2.01	0.41
2:B:301:MET:HG3	2:B:391:ILE:HD12	2.03	0.41
2:B:307:PRO:HG2	2:B:364:PRO:HG3	2.03	0.41
2:E:274:LYS:HE3	2:E:274:LYS:HB2	1.84	0.41
2:B:443:SER:HB2	2:B:446:ILE:HD11	2.01	0.41
1:D:172:LYS:HE3	1:D:172:LYS:HB3	1.92	0.41
2:E:260:PRO:O	2:E:262:PRO:HD3	2.19	0.40
2:E:668:LEU:HA	2:E:668:LEU:HD12	1.87	0.40
1:A:57:VAL:HG11	1:A:74:ALA:HB2	2.03	0.40
2:B:189:ILE:HG21	2:B:189:ILE:HD13	1.86	0.40
2:B:433:VAL:HG12	2:B:437:ARG:HH12	1.87	0.40
2:E:307:PRO:HG2	2:E:364:PRO:HG3	2.03	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	181/391 (46%)	163 (90%)	18 (10%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	181/391 (46%)	163 (90%)	18 (10%)	0	100	100
2	B	516/640 (81%)	408 (79%)	94 (18%)	14 (3%)	4	22
2	E	516/640 (81%)	408 (79%)	94 (18%)	14 (3%)	4	22
All	All	1394/2062 (68%)	1142 (82%)	224 (16%)	28 (2%)	8	28

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	120	ASN
2	B	185	ASN
2	B	290	ALA
2	B	295	ARG
2	E	120	ASN
2	E	185	ASN
2	E	290	ALA
2	E	295	ARG
2	B	186	ASP
2	B	260	PRO
2	B	643	SER
2	B	644	ASN
2	E	186	ASP
2	E	260	PRO
2	E	643	SER
2	E	644	ASN
2	B	116	PRO
2	B	195	PRO
2	B	662	ARG
2	E	116	PRO
2	E	195	PRO
2	E	662	ARG
2	B	294	SER
2	B	567	ASP
2	E	294	SER
2	E	567	ASP
2	B	115	GLN
2	E	115	GLN

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	144/316 (46%)	144 (100%)	0	100	100
1	D	144/316 (46%)	144 (100%)	0	100	100
2	B	445/542 (82%)	440 (99%)	5 (1%)	65	83
2	E	445/542 (82%)	440 (99%)	5 (1%)	65	83
All	All	1178/1716 (69%)	1168 (99%)	10 (1%)	70	86

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	201	ARG
2	B	222	GLN
2	B	226	THR
2	B	640	LEU
2	B	668	LEU
2	E	201	ARG
2	E	222	GLN
2	E	226	THR
2	E	640	LEU
2	E	668	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	45	HIS
1	A	51	GLN
1	A	143	GLN
2	B	115	GLN
2	B	144	ASN
2	B	168	GLN
2	B	222	GLN
2	B	242	HIS
2	B	309	GLN
2	B	370	HIS
2	B	544	ASN
1	D	21	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	45	HIS
1	D	51	GLN
1	D	143	GLN
2	E	115	GLN
2	E	144	ASN
2	E	222	GLN
2	E	242	HIS
2	E	370	HIS
2	E	544	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	AGS	E	801	4	32,33,33	0.64	0	45,52,52	0.96	1 (2%)
3	AGS	B	801	4	32,33,33	0.65	0	45,52,52	0.96	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
3	AGS	E	801	4	-	3/21/38/38	0/3/3/3
3	AGS	B	801	4	-	3/21/38/38	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(°)
3	E	801	AGS	PB-O3B-PG	-4.39	117.12	133.17
3	B	801	AGS	PB-O3B-PG	-4.38	117.13	133.17

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	801	AGS	PB-O3B-PG-O3G
3	E	801	AGS	PB-O3B-PG-O3G
3	B	801	AGS	C5'-O5'-PA-O3A
3	E	801	AGS	C5'-O5'-PA-O3A
3	B	801	AGS	PB-O3B-PG-O2G
3	E	801	AGS	PB-O3B-PG-O2G

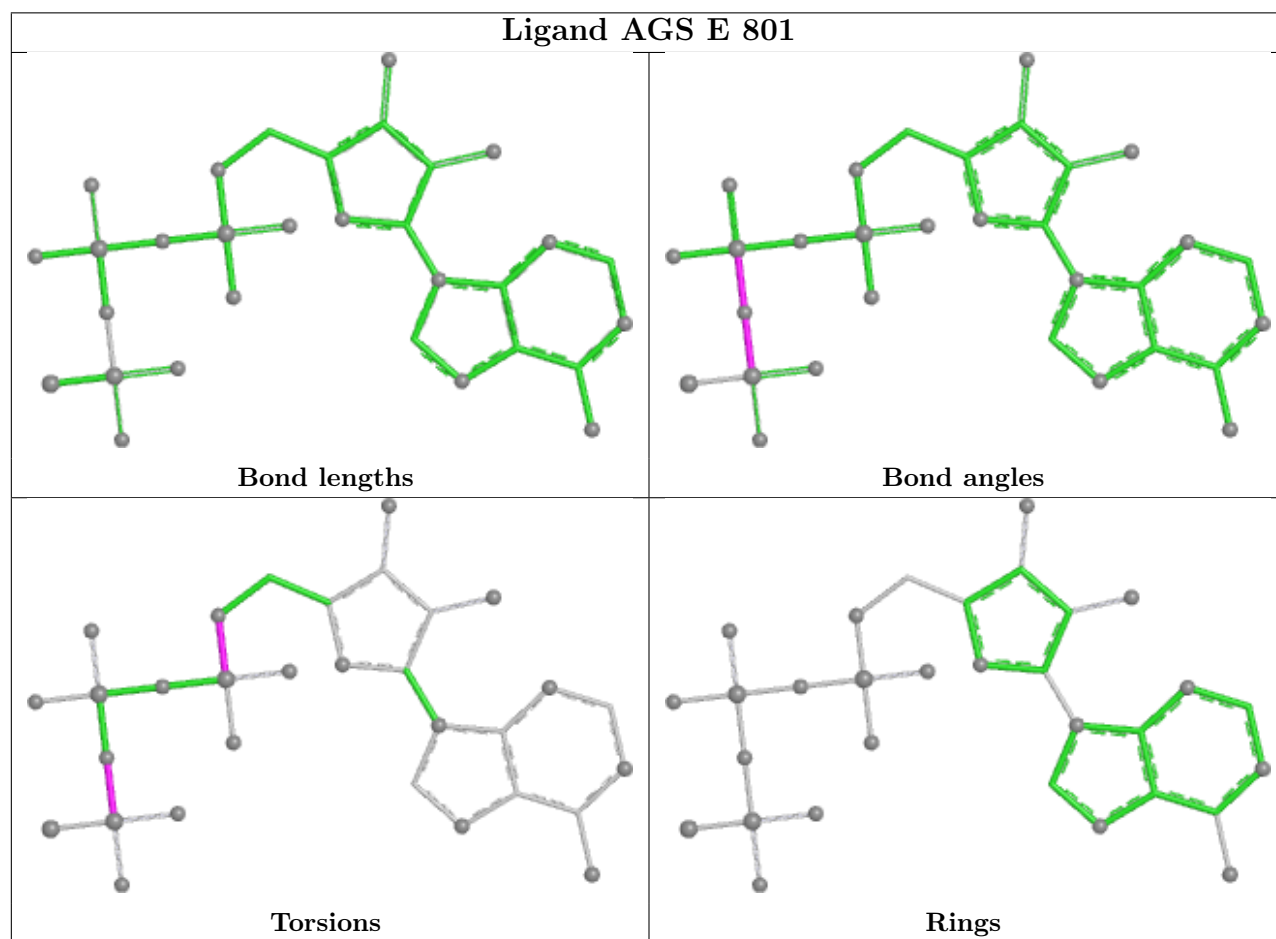
There are no ring outliers.

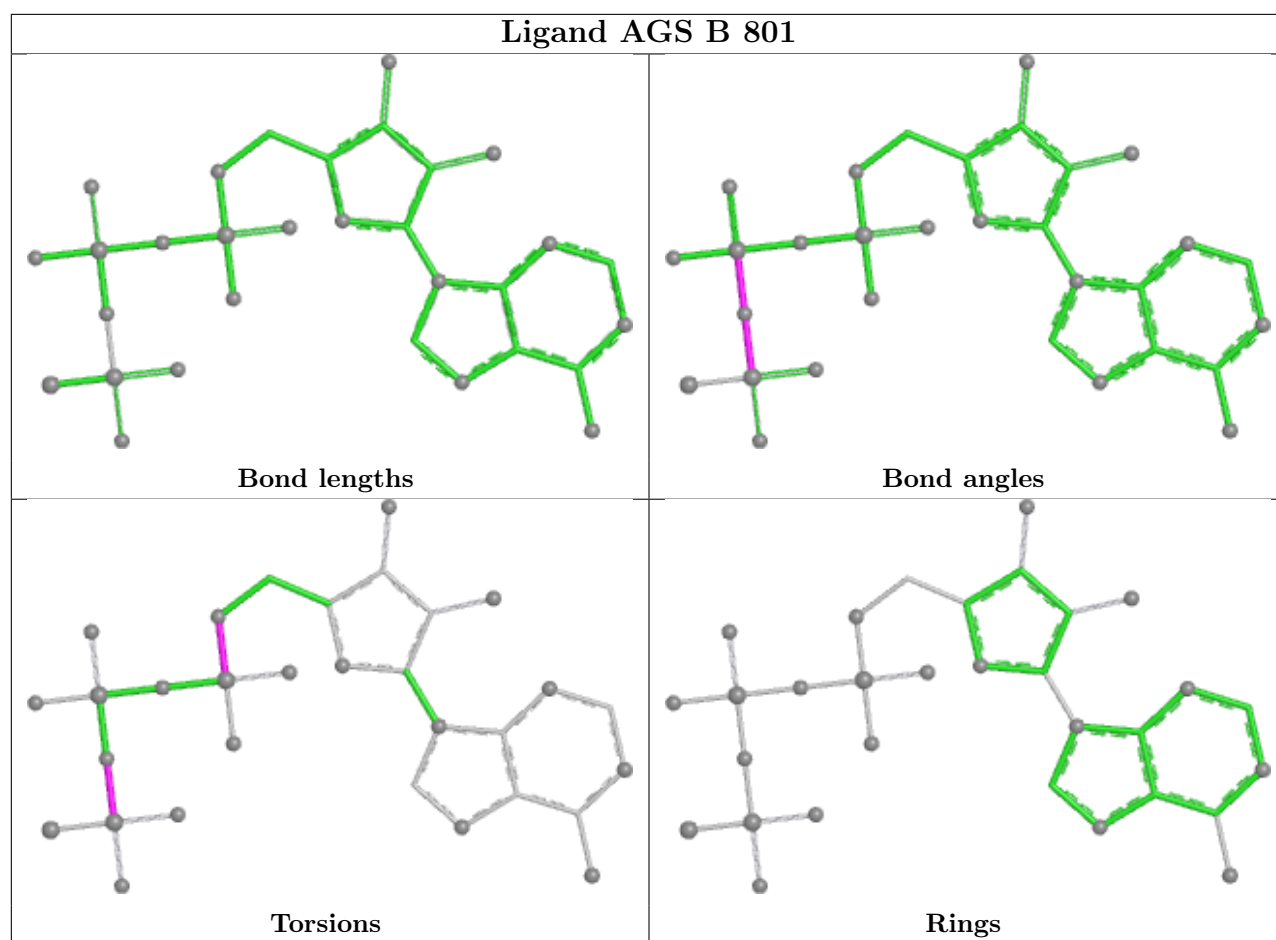
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	801	AGS	1	0
3	B	801	AGS	1	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.

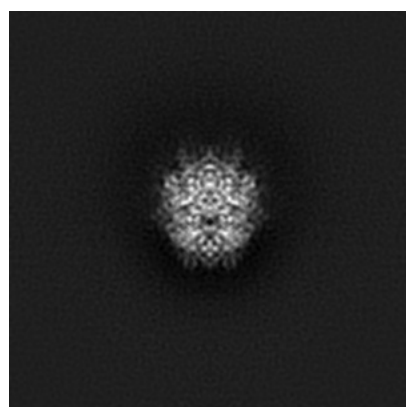
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20041. These allow visual inspection of the internal detail of the map and identification of artifacts.

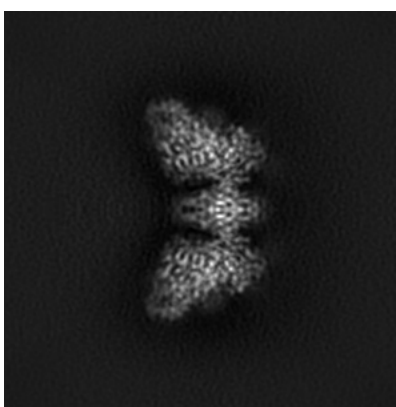
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

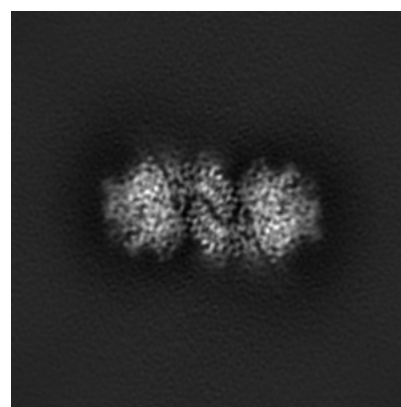
6.1.1 Primary map



X



Y

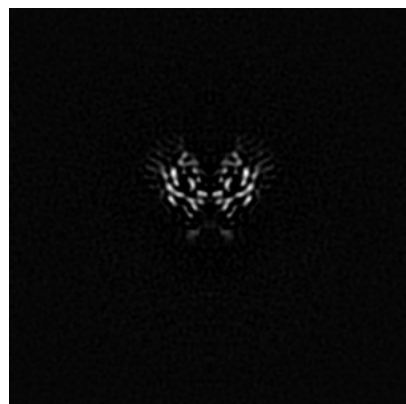


Z

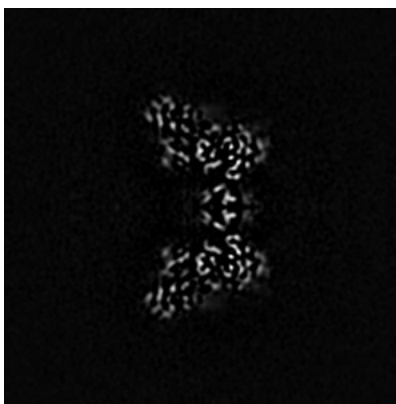
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

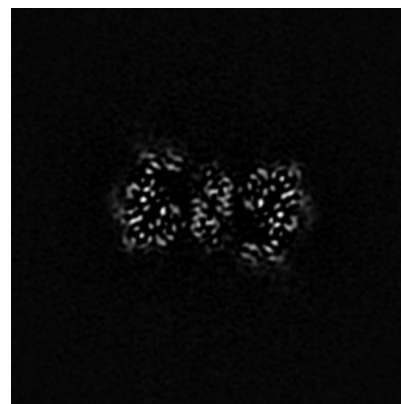
6.2.1 Primary map



X Index: 112



Y Index: 112

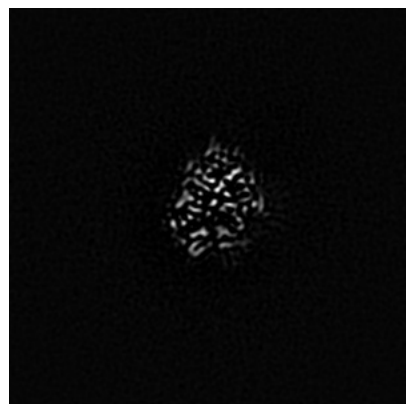


Z Index: 112

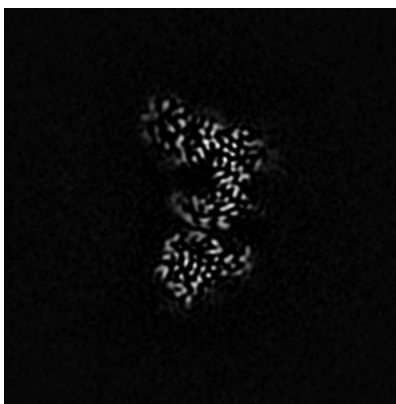
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

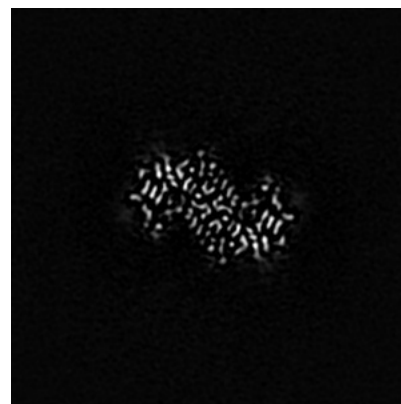
6.3.1 Primary map



X Index: 78



Y Index: 102

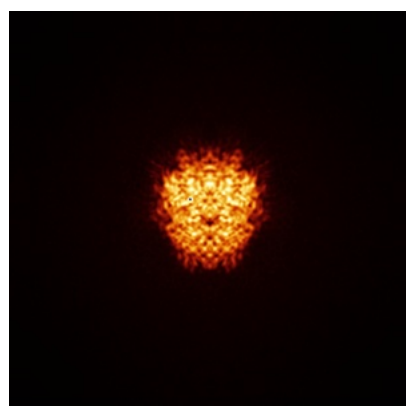


Z Index: 124

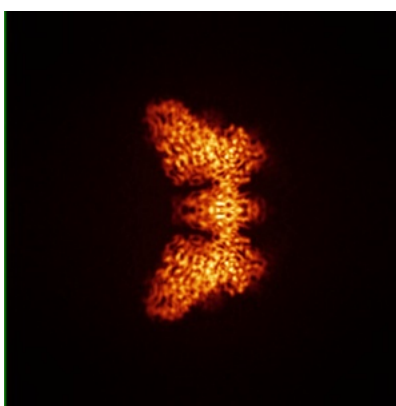
The images above show the largest variance slices of the map in three orthogonal directions.

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

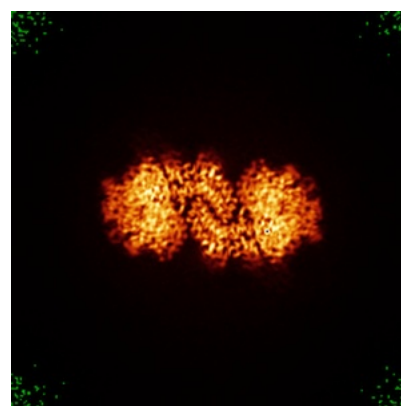
6.4.1 Primary map



X



Y

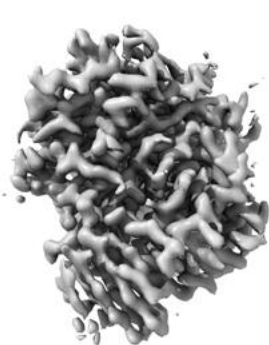


Z

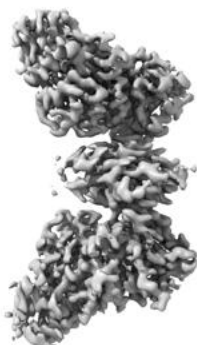
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

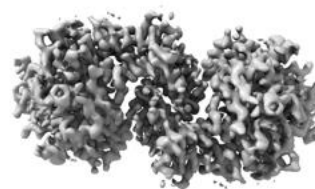
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

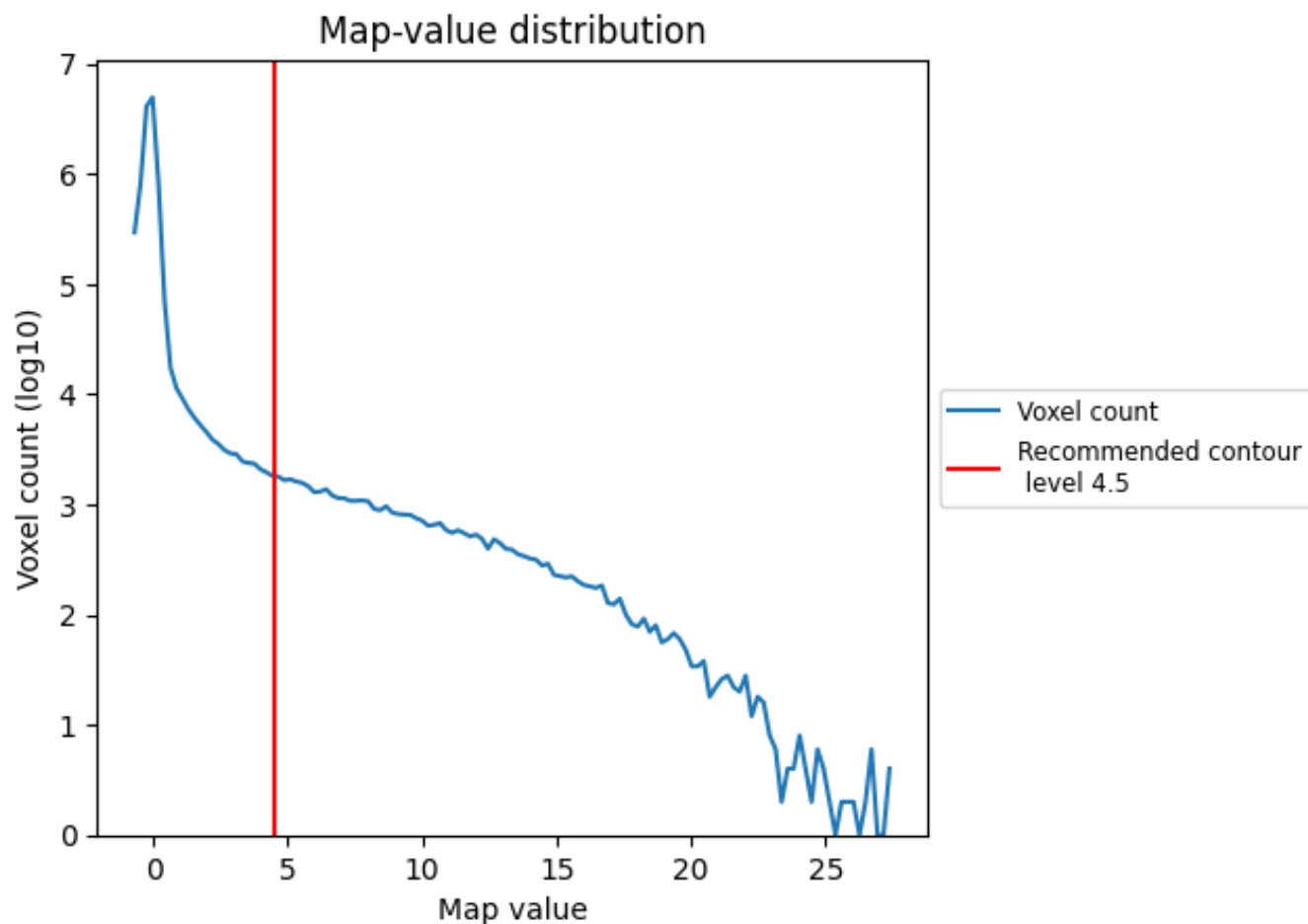
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

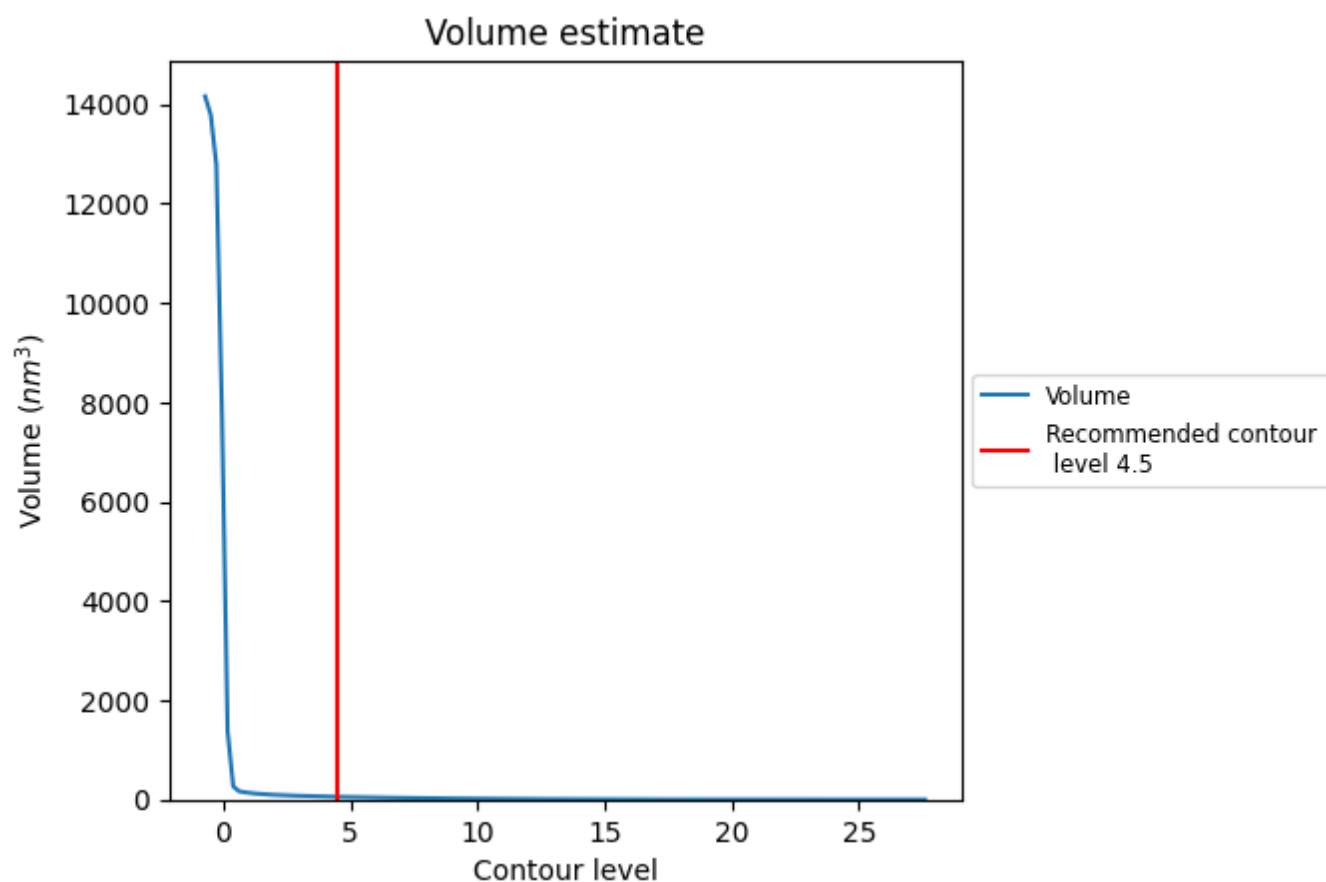
This section contains the results of statistical analysis of the map.

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.

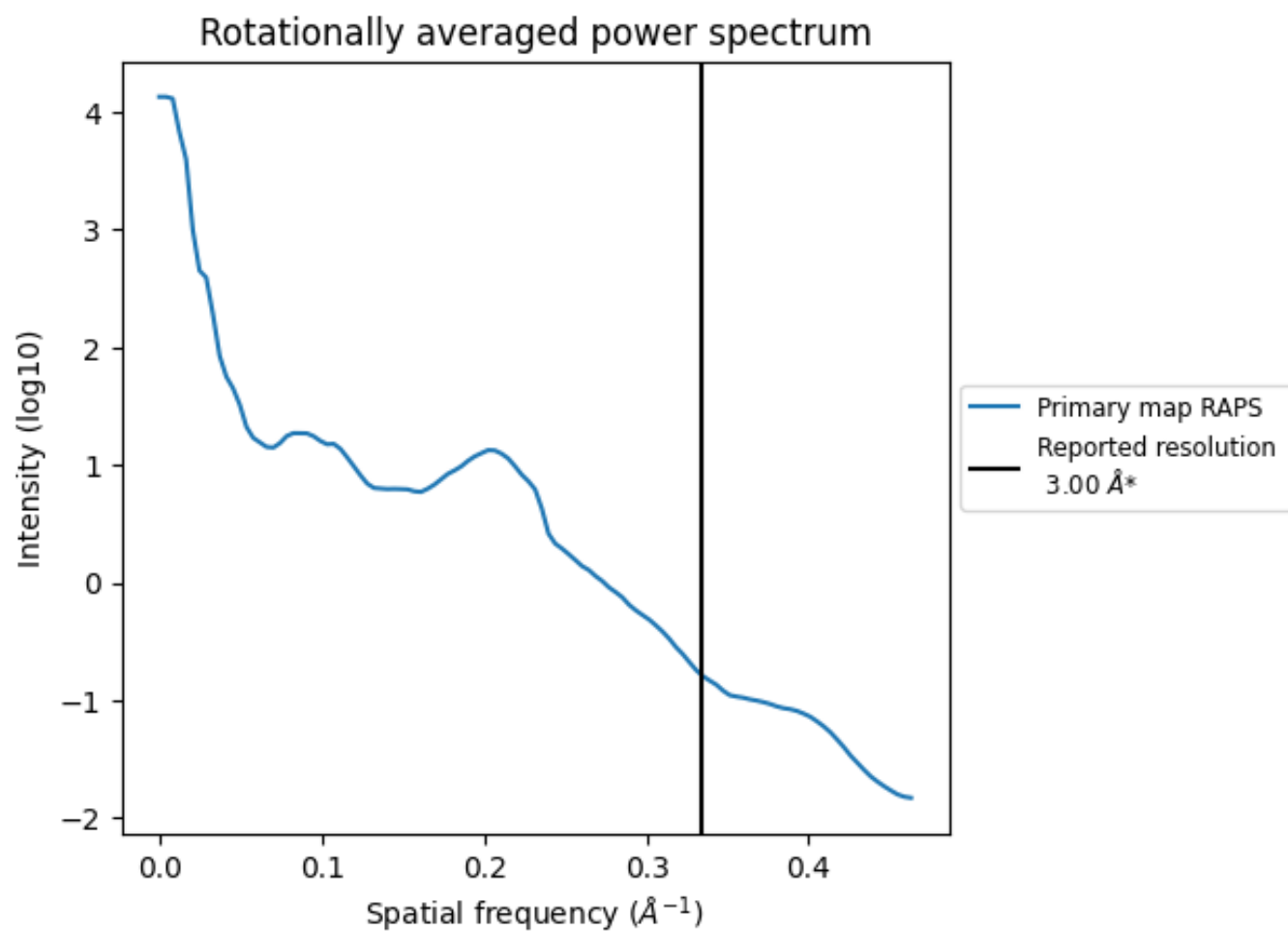
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 55 nm^3 ; this corresponds to an approximate mass of 49 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 Å⁻¹

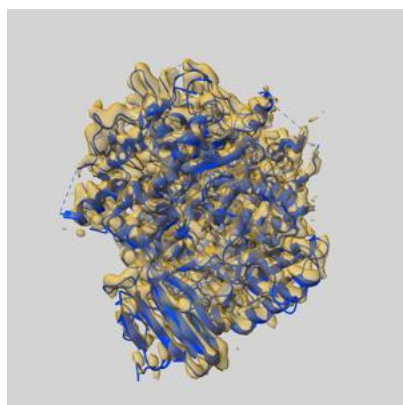
8 Fourier-Shell correlation ⓘ

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

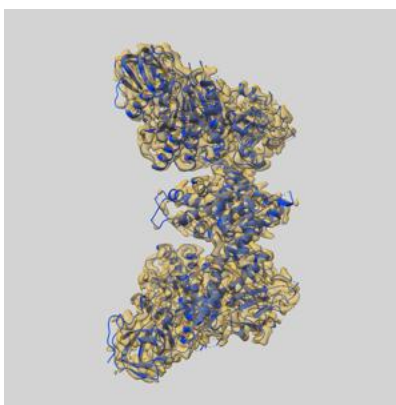
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20041 and PDB model 6OF3. Per-residue inclusion information can be found in section [3](#) on page [6](#).

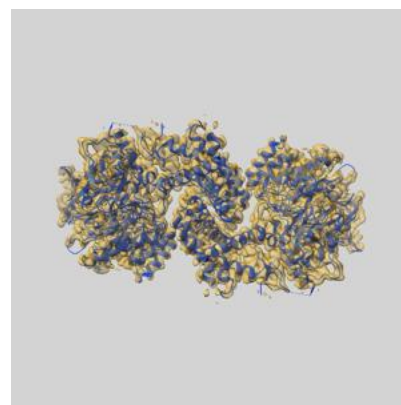
9.1 Map-model overlay [i](#)



X



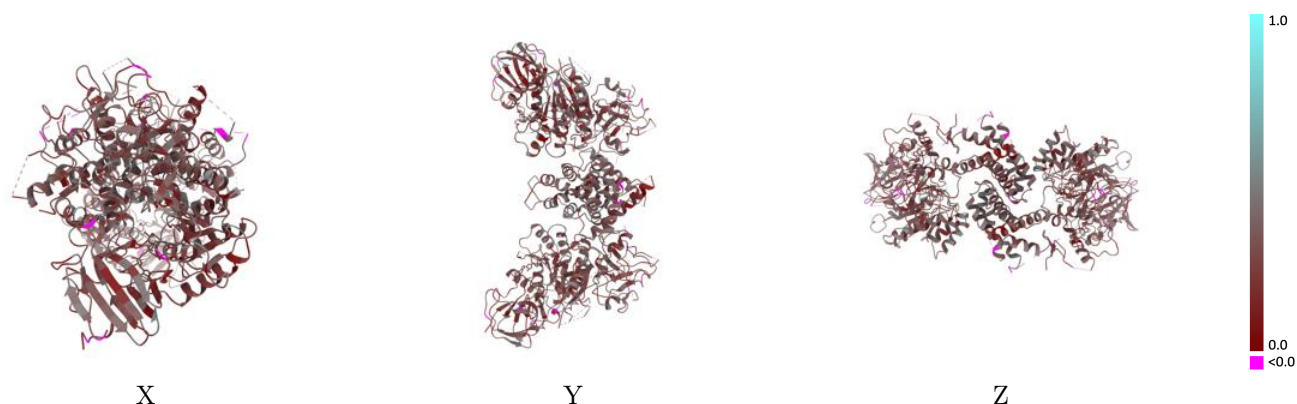
Y



Z

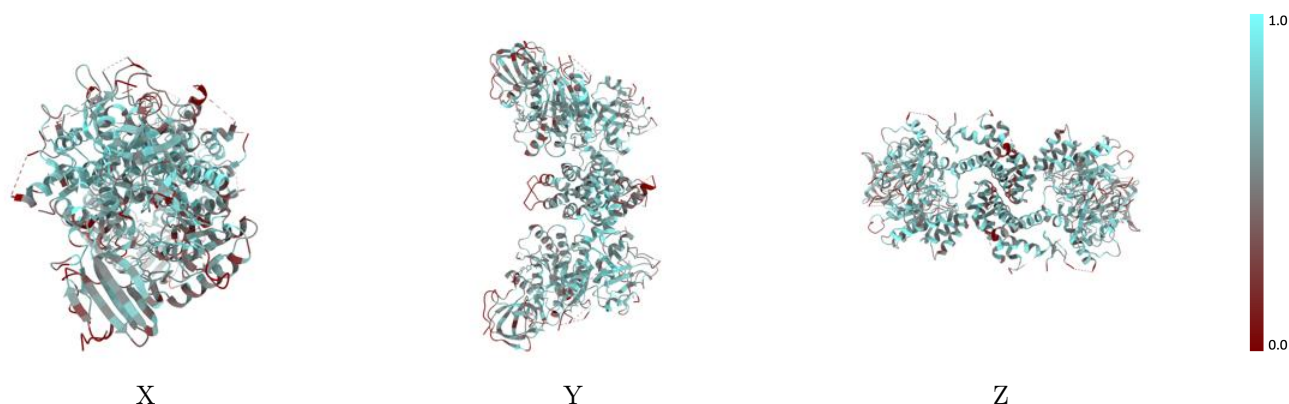
The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



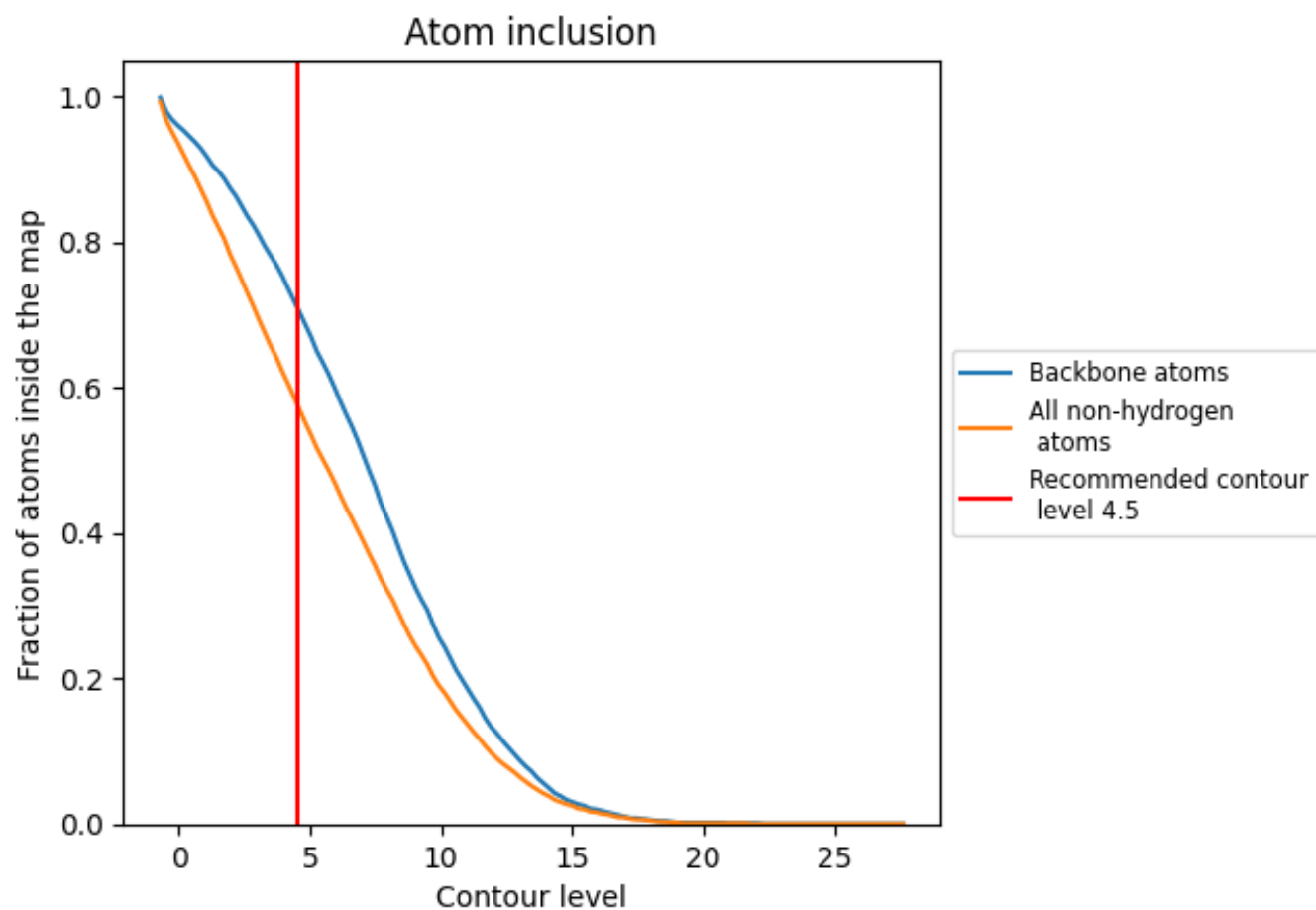
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 58% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5770	0.3020
A	0.6100	0.3430
B	0.5720	0.2940
D	0.5820	0.3110
E	0.5680	0.2930

