



## Full wwPDB EM Validation Report ⓘ

Jun 16, 2026 – 06:27 PM EDT

PDB ID : 10MG / pdb\_000010mg  
EMDB ID : EMD-75285  
Title : CBR9379 bound Open2 Eco-ePEC: Cryo-EM structure of Eco RNAP his-  
elemental paused elongation complex with an open active site (open TL, SI3  
and RH-FL)  
Authors : Dhingra, Y.; Darst, S.A.  
Deposited on : 2026-01-27  
Resolution : 2.90 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](mailto: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>.

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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

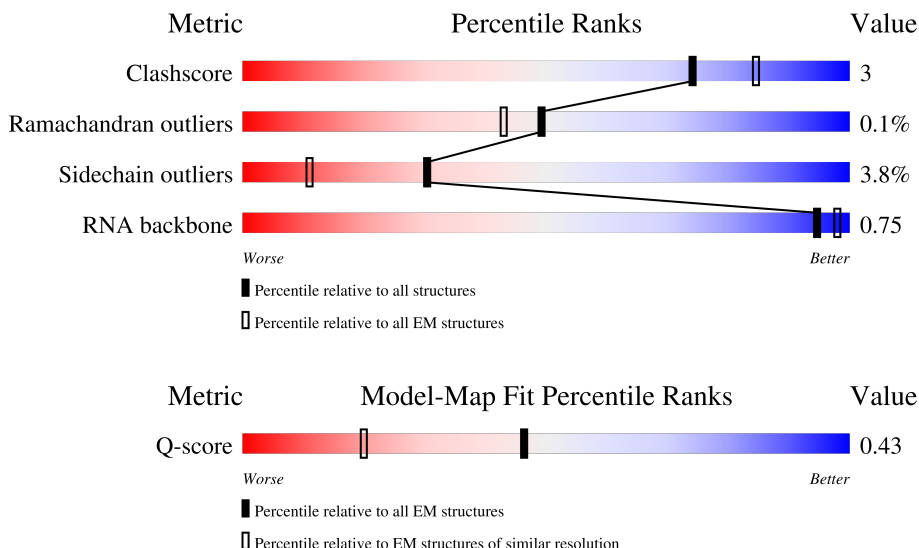
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 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	13054 ( 2.40 - 3.40 )

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  $\geq 3$ , 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	B	32	
2	K	91	
3	R	19	

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Mol	Chain	Length	Quality of chain
4	A	32	<div><div><div></div><div></div><div></div></div><div>50%22%28%</div></div>
5	G	329	<div><div><div></div><div></div><div></div></div><div>61%5%34%</div></div>
5	H	329	<div><div><div></div><div></div><div></div></div><div>54%11%33%</div></div>
6	I	1342	<div><div><div></div><div></div><div></div></div><div>89%8%..</div></div>
7	J	1407	<div><div><div></div><div></div><div></div></div><div>83%11%5%</div></div>

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 26909 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 DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	30	Total	C	N	O	P	0	0
			608	290	109	179	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	79	Total	C	N	O	S	0	0
			627	382	118	126	1		

- Molecule 3 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	10	Total	C	N	O	P	0	0
			214	95	36	73	10		

- Molecule 4 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	23	Total	C	N	O	P	0	0
			470	225	87	136	22		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	218	Total	C	N	O	S	0	0
			1679	1051	297	325	6		
5	H	219	Total	C	N	O	S	0	0
			1689	1056	298	329	6		

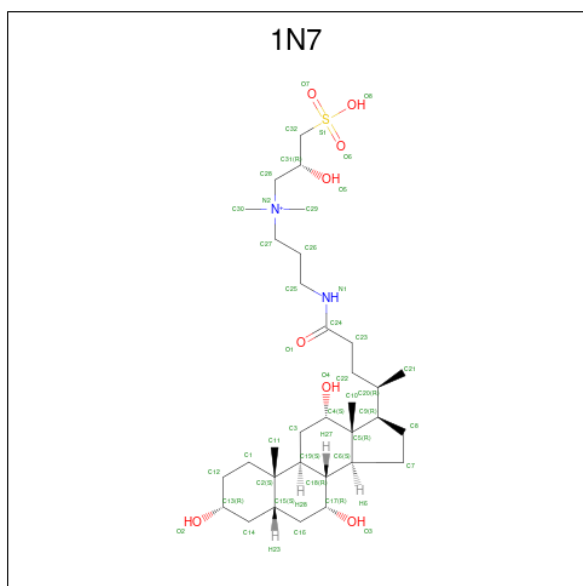
- Molecule 6 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	1316	Total	C	N	O	S	0	0
			10381	6514	1810	2014	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	1337	Total	C	N	O	S	0	0
			10403	6536	1856	1961	50		

- Molecule 8 is CHAPSO (CCD ID: 1N7) (formula: C<sub>32</sub>H<sub>59</sub>N<sub>2</sub>O<sub>8</sub>S).



Mol	Chain	Residues	Atoms			AltConf
8	I	1	Total	C	O	0
			27	24	3	

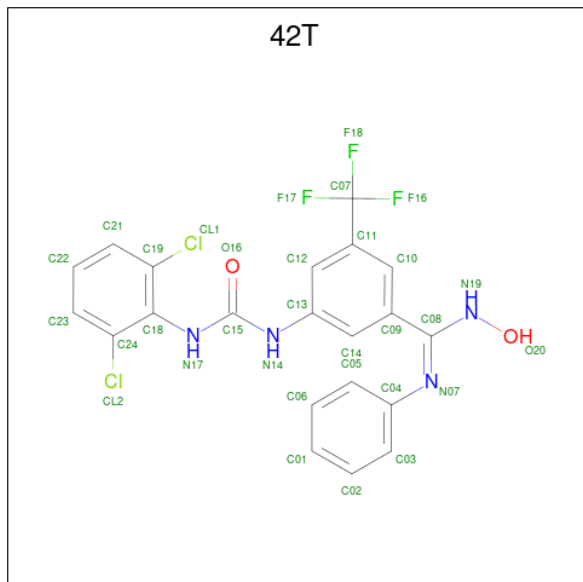
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	J	1	Total	Mg	0
			1	1	

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
10	J	2	Total	Zn	0
			2	2	

- Molecule 11 is 3-[[[(2,6-dichlorophenyl)carbamoyl]amino}-N-hydroxy-N'-phenyl-5-(trifluoromethyl)benzenecarboximidamide (CCD ID: 42T) (formula:  $C_{21}H_{15}Cl_2F_3N_4O_2$ ).



Mol	Chain	Residues	Atoms						AltConf
11	J	1	Total	C	Cl	F	N	O	0
			32	21	2	3	4	2	

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
12	B	20	Total	O	0
			20	20	
12	K	10	Total	O	0
			10	10	
12	R	19	Total	O	0
			19	19	
12	A	10	Total	O	0
			10	10	
12	G	50	Total	O	0
			50	50	
12	H	36	Total	O	0
			36	36	
12	I	369	Total	O	0
			369	369	
12	J	262	Total	O	0
			262	262	

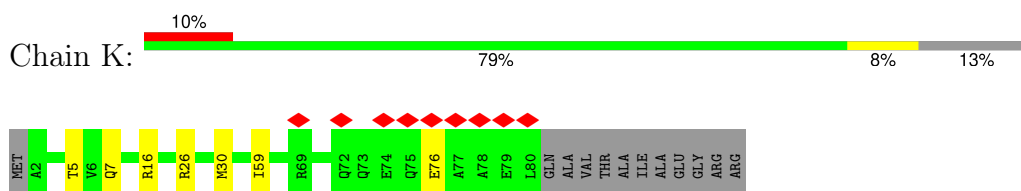
### 3 Residue-property plots

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.

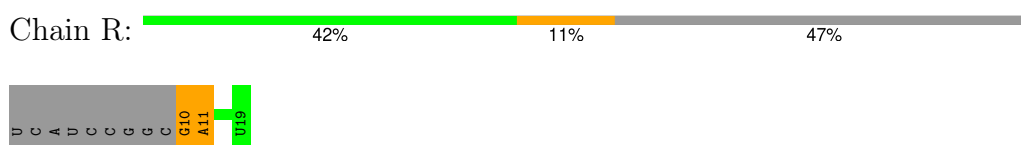
- Molecule 1: template DNA



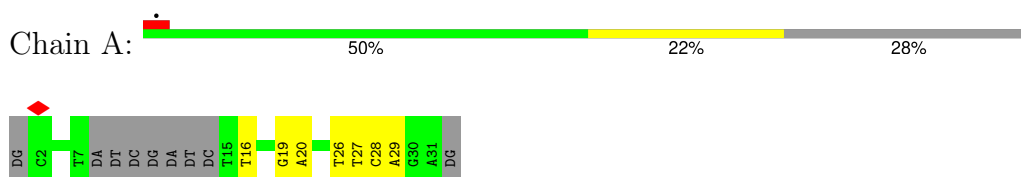
- Molecule 2: DNA-directed RNA polymerase subunit omega



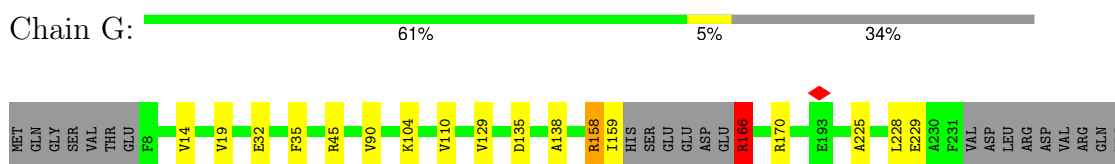
- Molecule 3: RNA

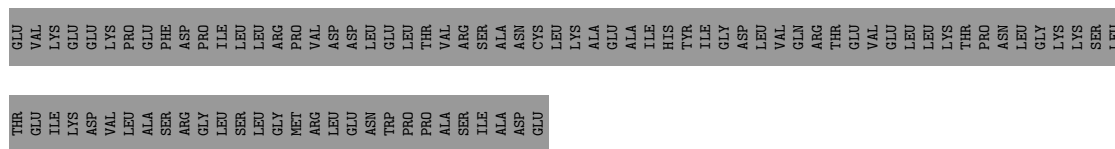


- Molecule 4: non-template DNA

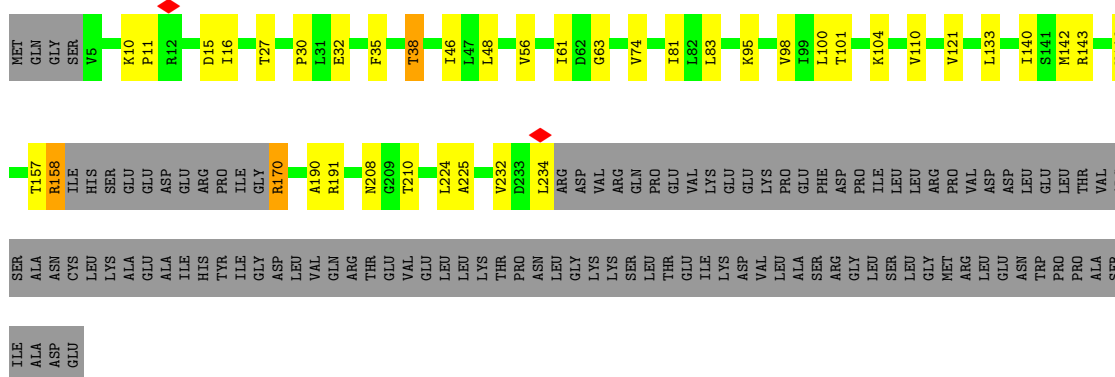


- Molecule 5: DNA-directed RNA polymerase subunit alpha

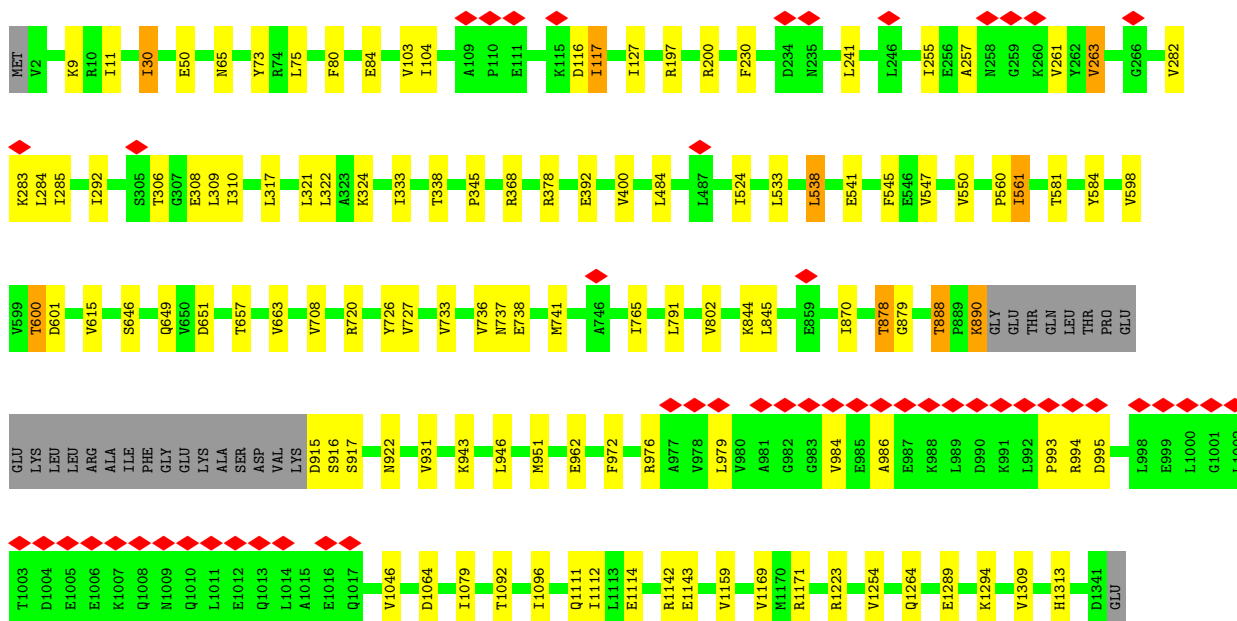
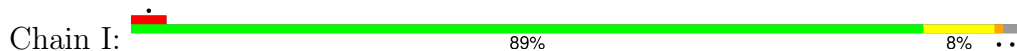




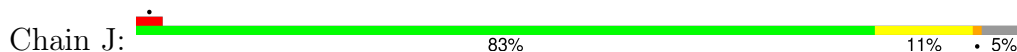
• Molecule 5: DNA-directed RNA polymerase subunit alpha



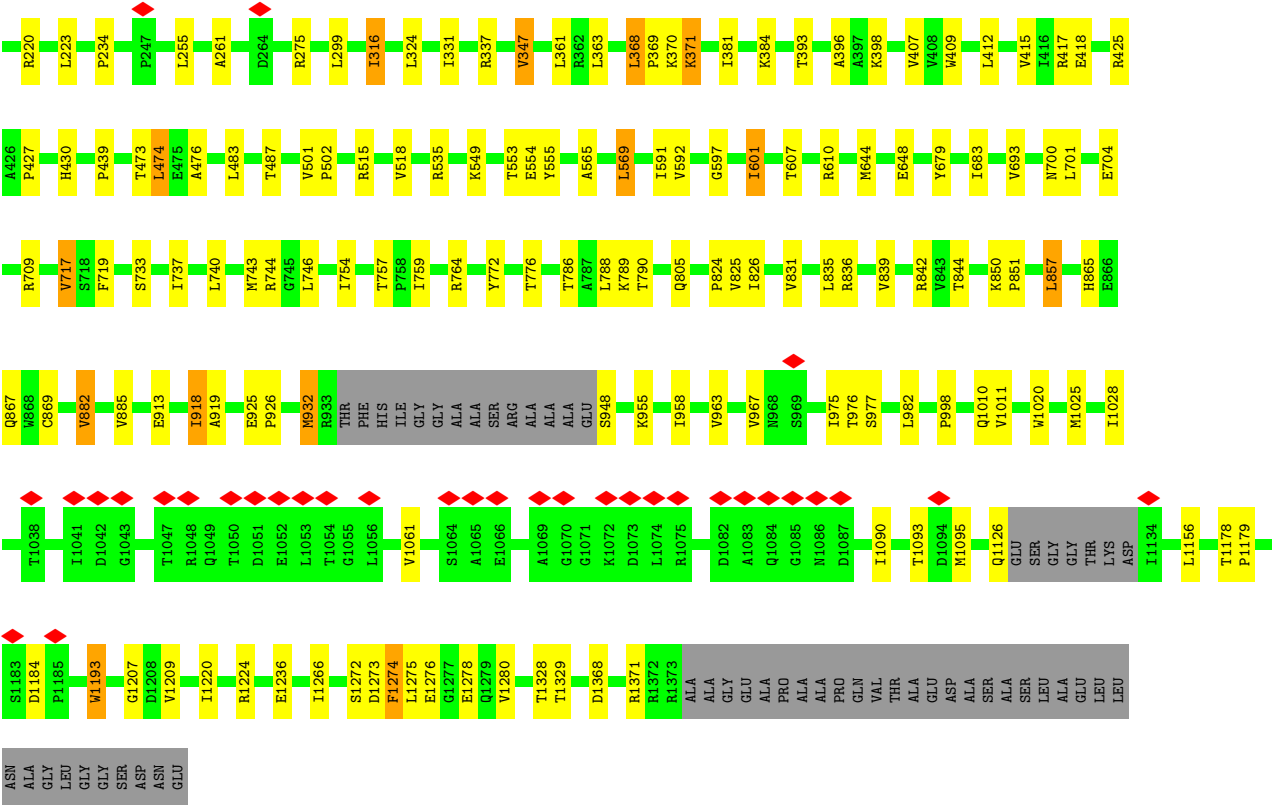
• Molecule 6: DNA-directed RNA polymerase subunit beta



• 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	146977	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	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	0.454	Depositor
Minimum map value	-0.326	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	259.58398, 259.58398, 259.58398	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.67599994, 0.67599994, 0.67599994	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1N7, 42T, MG, ZN

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	B	0.35	0/680	0.55	0/1045
2	K	0.10	0/629	0.24	0/847
3	R	0.12	0/238	0.31	0/369
4	A	0.31	0/526	0.49	0/808
5	G	0.16	0/1699	0.32	0/2302
5	H	0.14	0/1708	0.30	0/2315
6	I	0.12	0/10547	0.28	0/14232
7	J	0.15	0/10560	0.30	0/14257
All	All	0.15	0/26587	0.31	0/36175

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
5	G	0	2
5	H	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	G	158	ARG	Sidechain
5	G	166	ARG	Sidechain
5	H	158	ARG	Sidechain

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Mol	Chain	Res	Type	Group
5	H	170	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	B	608	0	338	10	0
2	K	627	0	634	3	0
3	R	214	0	106	2	0
4	A	470	0	262	7	0
5	G	1679	0	1717	7	0
5	H	1689	0	1725	20	0
6	I	10381	0	10392	49	0
7	J	10403	0	10628	84	0
8	I	27	0	39	0	0
9	J	1	0	0	0	0
10	J	2	0	0	0	0
11	J	32	0	15	0	0
12	A	10	0	0	0	0
12	B	20	0	0	0	0
12	G	50	0	0	0	0
12	H	36	0	0	0	0
12	I	369	0	0	0	0
12	J	262	0	0	0	0
12	K	10	0	0	0	0
12	R	19	0	0	0	0
All	All	26909	0	25856	168	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 (168) 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:B:13:DT:H3	4:A:19:DG:H1	0.84	0.82
7:J:201:LEU:HD11	7:J:220:ARG:HH11	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:976:ARG:HH21	6:I:986:ALA:HB1	1.61	0.66
7:J:85:CYS:HB3	7:J:88:CYS:SG	2.37	0.64
6:I:888:THR:HG23	6:I:890:LYS:HE3	1.79	0.63
3:R:10:G:H2'	3:R:11:A:C8	2.34	0.63
6:I:738:GLU:HA	6:I:741:MET:HE2	1.81	0.62
7:J:417:ARG:HG2	7:J:418:GLU:HG3	1.82	0.62
7:J:1178:THR:HG22	7:J:1184:ASP:HB3	1.82	0.61
7:J:826:ILE:HG22	7:J:831:VAL:HG12	1.81	0.61
7:J:549:LYS:HB3	7:J:569:LEU:HD11	1.83	0.61
1:B:11:DC:H2''	1:B:12:DT:H71	1.84	0.60
6:I:915:ASP:C	6:I:917:SER:H	2.10	0.59
7:J:1093:THR:HG22	7:J:1095:MET:H	1.68	0.59
1:B:13:DT:O4	4:A:19:DG:O6	2.21	0.58
1:B:20:DC:H2'	1:B:21:DA:C8	2.38	0.58
6:I:104:ILE:HG21	6:I:484:LEU:HB3	1.86	0.57
1:B:30:DC:H2''	1:B:31:DG:H5'	1.85	0.57
7:J:255:LEU:HD21	7:J:261:ALA:HB2	1.87	0.57
7:J:1273:ASP:O	7:J:1274:PHE:C	2.47	0.57
6:I:241:LEU:HD13	6:I:285:ILE:HG13	1.87	0.56
4:A:28:DC:H2''	4:A:29:DA:C8	2.40	0.56
5:H:56:VAL:HA	5:H:146:VAL:HG12	1.86	0.56
6:I:75:LEU:HD21	6:I:127:ILE:HD11	1.87	0.56
6:I:306:THR:HG23	6:I:308:GLU:H	1.70	0.56
5:G:45:ARG:HE	5:H:38:THR:HG22	1.71	0.56
6:I:9:LYS:HG2	6:I:1171:ARG:HE	1.72	0.56
6:I:50:GLU:HG2	6:I:73:TYR:HE1	1.71	0.56
7:J:607:THR:HA	7:J:610:ARG:HG2	1.87	0.55
5:H:101:THR:HG22	5:H:143:ARG:HG2	1.88	0.55
5:H:95:LYS:HE2	5:H:98:VAL:HG22	1.89	0.55
6:I:560:PRO:HB2	7:J:776:THR:HG21	1.88	0.55
6:I:255:ILE:HB	6:I:263:VAL:HG21	1.88	0.54
7:J:1275:LEU:HB3	7:J:1278:GLU:HB2	1.89	0.54
5:H:140:ILE:HD11	5:H:142:MET:HE3	1.89	0.54
7:J:693:VAL:HG21	7:J:743:MET:HE3	1.90	0.54
6:I:197:ARG:HD3	6:I:200:ARG:HA	1.89	0.54
7:J:85:CYS:CB	7:J:88:CYS:SG	2.95	0.54
7:J:368:LEU:HD12	7:J:439:PRO:HB3	1.90	0.54
1:B:20:DC:H2'	1:B:21:DA:H8	1.74	0.53
6:I:400:VAL:HG22	6:I:584:TYR:HD1	1.73	0.53
7:J:644:MET:HE3	7:J:740:LEU:HB3	1.91	0.53
7:J:865:HIS:CE1	7:J:867:GLN:HB2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:850:LYS:HG2	7:J:851:PRO:HD2	1.91	0.52
6:I:309:LEU:H	6:I:309:LEU:HD23	1.75	0.52
6:I:230:PHE:HB2	6:I:333:ILE:HB	1.92	0.52
5:H:30:PRO:HG3	5:H:190:ALA:HB1	1.92	0.51
7:J:744:ARG:HB3	7:J:759:ILE:HB	1.92	0.51
6:I:283:LYS:HG3	6:I:284:LEU:HD12	1.92	0.51
5:H:10:LYS:HG3	5:H:11:PRO:HD2	1.91	0.50
7:J:502:PRO:HD2	7:J:601:ILE:HD11	1.92	0.50
7:J:918:ILE:HG13	7:J:919:ALA:N	2.25	0.50
7:J:1025:MET:HG3	7:J:1126:GLN:HG2	1.93	0.50
7:J:381:ILE:HD11	7:J:412:LEU:HD13	1.93	0.50
6:I:317:LEU:HA	6:I:321:LEU:HD12	1.94	0.50
6:I:1294:LYS:HG3	7:J:347:VAL:HG22	1.94	0.50
7:J:597:GLY:O	7:J:601:ILE:HG23	2.12	0.50
6:I:726:TYR:HB3	6:I:733:VAL:HB	1.94	0.49
7:J:121:PRO:HG2	7:J:123:ARG:HH12	1.77	0.49
2:K:5:THR:HG22	2:K:7:GLN:H	1.77	0.49
5:H:98:VAL:HG11	5:H:121:VAL:HG21	1.94	0.49
7:J:1266:ILE:HG13	7:J:1274:PHE:HB3	1.94	0.49
7:J:368:LEU:HD23	7:J:369:PRO:HD2	1.93	0.49
6:I:870:ILE:HG21	6:I:931:VAL:HG11	1.95	0.49
7:J:824:PRO:HD3	7:J:835:LEU:HB2	1.94	0.49
6:I:1313:HIS:HB2	7:J:474:LEU:HD13	1.94	0.48
7:J:842:ARG:HD3	7:J:882:VAL:HG11	1.95	0.48
2:K:16:ARG:HD3	7:J:483:LEU:HD23	1.95	0.48
1:B:13:DT:O2	4:A:19:DG:N2	2.41	0.48
6:I:720:ARG:HE	6:I:736:VAL:HG11	1.79	0.48
5:H:46:ILE:HD12	5:H:224:LEU:HB2	1.96	0.47
7:J:1220:ILE:HG23	7:J:1224:ARG:HD2	1.96	0.47
4:A:19:DG:H2"	4:A:20:DA:C8	2.49	0.47
6:I:600:THR:HG22	6:I:601:ASP:H	1.79	0.47
7:J:371:LYS:H	7:J:371:LYS:HG2	1.44	0.47
7:J:975:ILE:HG13	7:J:977:SER:H	1.80	0.47
6:I:310:ILE:HG23	6:I:324:LYS:HE2	1.96	0.47
6:I:878:THR:HG22	6:I:879:GLY:H	1.80	0.47
5:H:32:GLU:HB3	5:H:35:PHE:CD1	2.49	0.47
5:G:166:ARG:HB2	5:G:170:ARG:HH21	1.79	0.47
7:J:473:THR:HG23	7:J:476:ALA:H	1.79	0.46
7:J:836:ARG:HG3	7:J:869:CYS:HB3	1.98	0.46
5:G:104:LYS:HG2	5:G:110:VAL:HG22	1.96	0.46
7:J:1193:TRP:CD1	7:J:1193:TRP:H	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:155:GLU:HG2	7:J:158:GLN:HB2	1.97	0.46
5:H:74:VAL:HG11	5:H:81:ILE:HD11	1.97	0.46
6:I:844:LYS:HD2	6:I:845:LEU:N	2.31	0.45
5:H:61:ILE:HG22	5:H:63:GLY:H	1.82	0.45
2:K:26:ARG:HG3	2:K:30:MET:HE2	1.97	0.45
6:I:80:PHE:HB3	6:I:84:GLU:HB2	1.98	0.45
6:I:972:PHE:CG	6:I:994:ARG:HB3	2.51	0.45
3:R:10:G:H2'	3:R:11:A:H8	1.80	0.45
7:J:1090:ILE:HB	7:J:1093:THR:HB	1.98	0.45
7:J:84:ILE:HG12	7:J:91:GLU:HB3	1.98	0.45
6:I:1289:GLU:O	6:I:1294:LYS:HG2	2.17	0.44
7:J:393:THR:HG23	7:J:396:ALA:H	1.82	0.44
7:J:932:MET:HE2	7:J:932:MET:HB3	1.64	0.44
1:B:21:DA:H2'	1:B:22:DC:C6	2.52	0.44
6:I:561:ILE:HD13	7:J:772:TYR:HE2	1.82	0.44
6:I:943:LYS:HA	6:I:946:LEU:HG	1.99	0.44
7:J:963:VAL:HG23	7:J:975:ILE:HD13	2.00	0.44
7:J:591:ILE:HG23	7:J:592:VAL:HG13	2.00	0.44
7:J:958:ILE:HG23	7:J:982:LEU:HD11	2.00	0.44
7:J:786:THR:O	7:J:790:THR:HG23	2.19	0.43
7:J:1156:LEU:HD23	7:J:1207:GLY:HA2	2.00	0.43
1:B:26:DA:C2'	1:B:27:DG:OP2	2.66	0.43
6:I:524:ILE:HD12	6:I:708:VAL:HG13	2.00	0.43
7:J:733:SER:O	7:J:737:ILE:HG12	2.19	0.43
7:J:955:LYS:HE3	7:J:955:LYS:HB3	1.89	0.43
7:J:275:ARG:HA	7:J:275:ARG:HD3	1.78	0.43
4:A:26:DT:H2'	4:A:27:DT:H71	2.01	0.43
6:I:257:ALA:HB1	6:I:282:VAL:HG21	2.01	0.43
6:I:104:ILE:HD11	6:I:116:ASP:HB3	1.99	0.43
7:J:127:LEU:HD21	7:J:234:PRO:HB3	2.01	0.43
7:J:168:ALA:HA	7:J:171:GLU:HG2	1.99	0.43
5:H:232:VAL:HG22	5:H:234:LEU:H	1.84	0.43
7:J:555:TYR:CE2	7:J:565:ALA:HB2	2.54	0.43
7:J:398:LYS:HE3	7:J:398:LYS:HB2	1.82	0.42
7:J:789:LYS:HG3	7:J:932:MET:HB2	2.00	0.42
6:I:103:VAL:HG12	6:I:117:ILE:HB	2.00	0.42
7:J:47:ARG:HG3	7:J:48:THR:HG23	2.01	0.42
5:H:48:LEU:HD11	7:J:535:ARG:HG3	2.02	0.42
5:H:15:ASP:HB2	5:H:27:THR:OG1	2.20	0.42
7:J:746:LEU:HD13	7:J:754:ILE:HG21	2.01	0.42
5:G:228:LEU:HD23	5:H:225:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:1111:GLN:HG3	6:I:1112:ILE:HD12	2.01	0.42
7:J:955:LYS:HD3	7:J:1010:GLN:HE21	1.84	0.42
6:I:545:PHE:CZ	7:J:788:LEU:HD22	2.54	0.42
5:G:32:GLU:HB2	5:G:35:PHE:HD2	1.85	0.42
5:H:104:LYS:HD3	5:H:110:VAL:HG22	2.00	0.42
7:J:201:LEU:HD22	7:J:217:LEU:HD22	2.01	0.42
7:J:384:LYS:HG3	7:J:415:VAL:HG12	2.02	0.42
7:J:1272:SER:HB3	7:J:1274:PHE:HD2	1.85	0.42
6:I:993:PRO:HB2	6:I:995:ASP:OD1	2.20	0.42
7:J:316:ILE:HD11	7:J:324:LEU:HD12	2.00	0.42
5:H:133:LEU:HD11	5:H:140:ILE:HG22	2.02	0.41
7:J:425:ARG:HG2	7:J:427:PRO:HD2	2.01	0.41
5:H:100:LEU:HD21	5:H:121:VAL:HG11	2.00	0.41
6:I:30:ILE:H	6:I:30:ILE:HG13	1.25	0.41
7:J:679:TYR:O	7:J:683:ILE:HG12	2.19	0.41
6:I:338:THR:HG21	6:I:345:PRO:HB3	2.02	0.41
7:J:126:LEU:HD23	7:J:223:LEU:HD22	2.02	0.41
1:B:8:DT:H2''	1:B:9:DC:H5'	2.01	0.41
7:J:1179:PRO:HD2	7:J:1184:ASP:HA	2.02	0.41
6:I:646:SER:HB3	6:I:649:GLN:HG3	2.02	0.41
7:J:700:ASN:O	7:J:704:GLU:HB2	2.20	0.41
6:I:737:ASN:O	6:I:741:MET:HG3	2.20	0.41
6:I:802:VAL:HG12	6:I:1096:ILE:HB	2.03	0.41
7:J:337:ARG:HA	7:J:337:ARG:HD3	1.95	0.41
7:J:925:GLU:HB3	7:J:926:PRO:HD3	2.02	0.41
6:I:292:ILE:HG21	6:I:322:LEU:HD11	2.02	0.41
7:J:370:LYS:HG2	7:J:409:TRP:CZ3	2.56	0.41
7:J:998:PRO:HG2	7:J:1020:TRP:CE2	2.56	0.41
7:J:865:HIS:HE1	7:J:867:GLN:HB2	1.86	0.41
6:I:1223:ARG:NH2	7:J:719:PHE:HB3	2.36	0.40
7:J:850:LYS:HG3	7:J:857:LEU:HG	2.03	0.40
7:J:976:THR:HG22	7:J:1028:ILE:HD11	2.03	0.40
4:A:16:DT:O2	6:I:200:ARG:HG2	2.21	0.40
7:J:371:LYS:HB3	7:J:371:LYS:HE2	1.88	0.40
5:G:135:ASP:HB3	5:G:138:ALA:HB2	2.01	0.40
6:I:1142:ARG:HG2	6:I:1169:VAL:HG11	2.03	0.40
5:G:225:ALA:O	5:G:229:GLU:HG2	2.22	0.40
5:H:208:ASN:OD1	5:H:210:THR:HG22	2.21	0.40
6:I:533:LEU:HD23	6:I:538:LEU:HD12	2.03	0.40
7:J:24:LEU:HD21	7:J:116:PHE:CZ	2.57	0.40
7:J:331:ILE:HG22	7:J:1328:THR:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:1368:ASP:O	7:J:1371:ARG:HG2	2.22	0.40
7:J:515:ARG:NH2	7:J:717:VAL:HG13	2.36	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	
2	K	77/91 (85%)	75 (97%)	2 (3%)	0	100	100
5	G	214/329 (65%)	207 (97%)	7 (3%)	0	100	100
5	H	215/329 (65%)	211 (98%)	4 (2%)	0	100	100
6	I	1312/1342 (98%)	1271 (97%)	40 (3%)	1 (0%)	48	77
7	J	1331/1407 (95%)	1299 (98%)	30 (2%)	2 (0%)	43	72
All	All	3149/3498 (90%)	3063 (97%)	83 (3%)	3 (0%)	49	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	J	1274	PHE
7	J	1276	GLU
6	I	916	SER

### 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	
2	K	67/75 (89%)	65 (97%)	2 (3%)	36	70
5	G	185/286 (65%)	178 (96%)	7 (4%)	29	64
5	H	187/286 (65%)	180 (96%)	7 (4%)	30	64
6	I	1135/1157 (98%)	1093 (96%)	42 (4%)	30	64
7	J	1122/1168 (96%)	1077 (96%)	45 (4%)	28	62
All	All	2696/2972 (91%)	2593 (96%)	103 (4%)	30	64

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	59	ILE
2	K	76	GLU
5	G	14	VAL
5	G	19	VAL
5	G	90	VAL
5	G	129	VAL
5	G	158	ARG
5	G	159	ILE
5	G	166	ARG
5	H	16	ILE
5	H	38	THR
5	H	83	LEU
5	H	157	THR
5	H	158	ARG
5	H	170	ARG
5	H	191	ARG
6	I	11	ILE
6	I	30	ILE
6	I	65	ASN
6	I	117	ILE
6	I	261	VAL
6	I	263	VAL
6	I	368	ARG
6	I	378	ARG
6	I	392	GLU
6	I	538	LEU
6	I	541	GLU
6	I	547	VAL
6	I	550	VAL
6	I	561	ILE
6	I	581	THR

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Mol	Chain	Res	Type
6	I	598	VAL
6	I	600	THR
6	I	615	VAL
6	I	651	ASP
6	I	657	THR
6	I	663	VAL
6	I	727	VAL
6	I	765	ILE
6	I	791	LEU
6	I	878	THR
6	I	888	THR
6	I	890	LYS
6	I	922	ASN
6	I	951	MET
6	I	962	GLU
6	I	979	LEU
6	I	984	VAL
6	I	1046	VAL
6	I	1064	ASP
6	I	1079	ILE
6	I	1092	THR
6	I	1114	GLU
6	I	1143	GLU
6	I	1159	VAL
6	I	1254	VAL
6	I	1264	GLN
6	I	1309	VAL
7	J	53	ARG
7	J	86	GLU
7	J	92	VAL
7	J	299	LEU
7	J	316	ILE
7	J	347	VAL
7	J	361	LEU
7	J	363	LEU
7	J	368	LEU
7	J	371	LYS
7	J	407	VAL
7	J	430	HIS
7	J	474	LEU
7	J	487	THR
7	J	501	VAL

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Mol	Chain	Res	Type
7	J	518	VAL
7	J	553	THR
7	J	554	GLU
7	J	569	LEU
7	J	601	ILE
7	J	648	GLU
7	J	701	LEU
7	J	709	ARG
7	J	717	VAL
7	J	757	THR
7	J	764	ARG
7	J	805	GLN
7	J	825	VAL
7	J	839	VAL
7	J	844	THR
7	J	857	LEU
7	J	882	VAL
7	J	885	VAL
7	J	913	GLU
7	J	918	ILE
7	J	932	MET
7	J	948	SER
7	J	967	VAL
7	J	1011	VAL
7	J	1061	VAL
7	J	1193	TRP
7	J	1209	VAL
7	J	1236	GLU
7	J	1280	VAL
7	J	1329	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	K	31	GLN
5	H	66	HIS
6	I	173	ASN
6	I	808	ASN
6	I	1220	GLN
6	I	1244	HIS
6	I	1336	ASN
7	J	158	GLN

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Mol	Chain	Res	Type
7	J	720	ASN
7	J	792	ASN
7	J	979	ASN
7	J	1086	ASN
7	J	1249	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	R	10/19 (52%)	1 (10%)	1 (10%)

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	R	11	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	R	10	G

## 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	$\# Z  > 2$
8	1N7	I	1401	-	30,30,46	0.40	0	47,48,72	0.78	0
11	42T	J	1504	-	34,34,34	0.61	0	47,48,48	0.91	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	1N7	I	1401	-	-	0/7/72/92	0/4/4/4
11	42T	J	1504	-	-	0/23/24/24	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(°)
11	J	1504	42T	C09-C08-N19	-2.46	110.65	114.61
11	J	1504	42T	C04-N07-C08	2.28	125.45	120.49

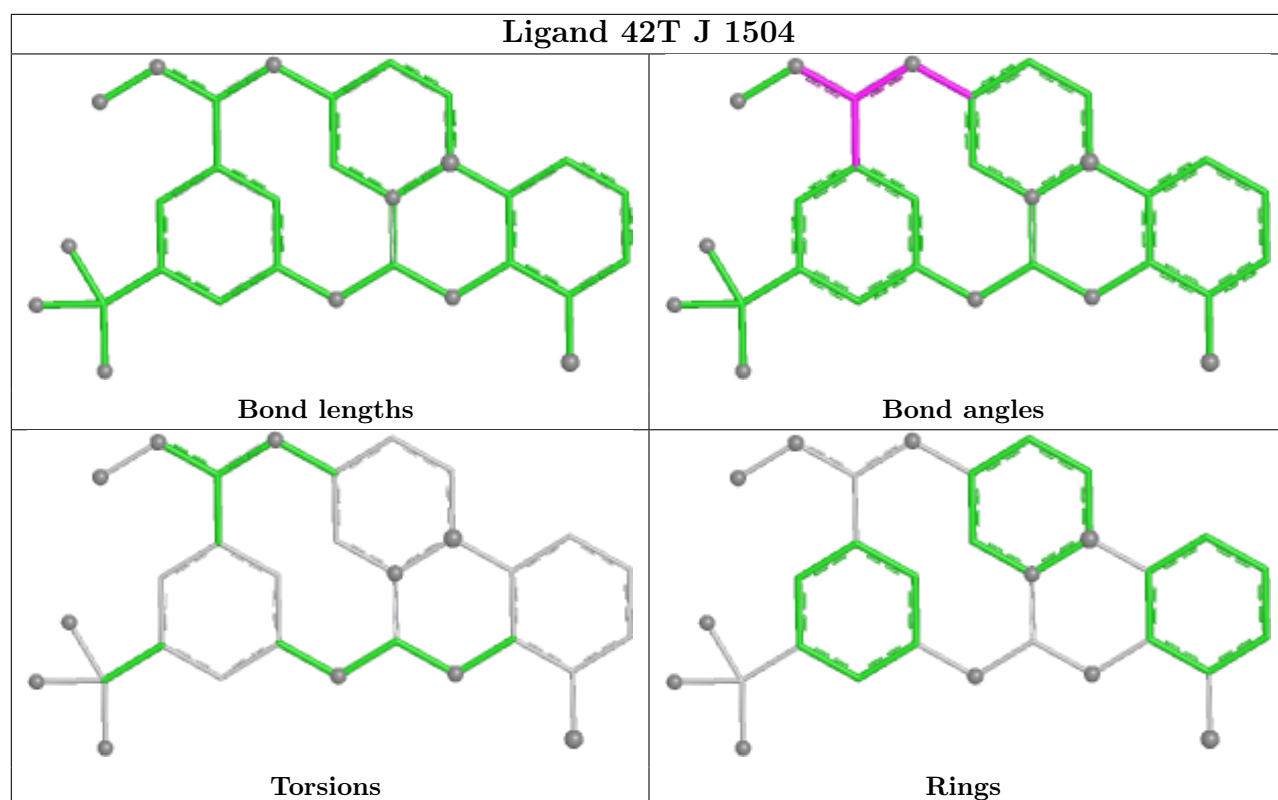
There are no chirality outliers.

There are no torsion outliers.

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.

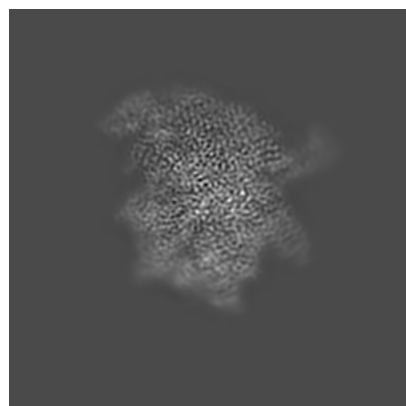
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75285. These allow visual inspection of the internal detail of the map and identification of artifacts.

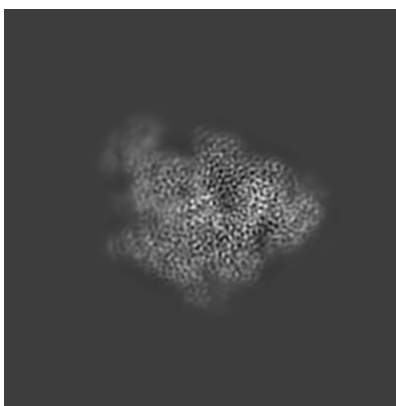
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

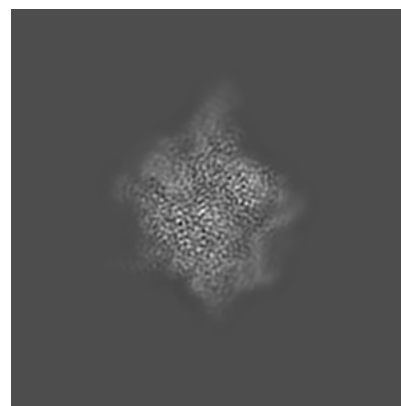
#### 6.1.1 Primary map



X

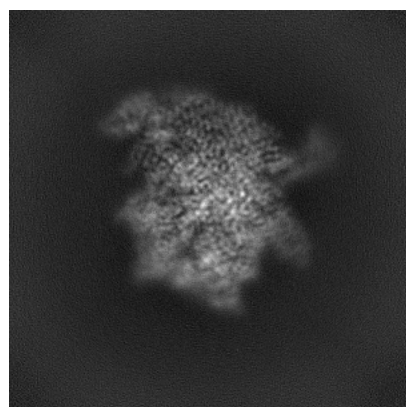


Y

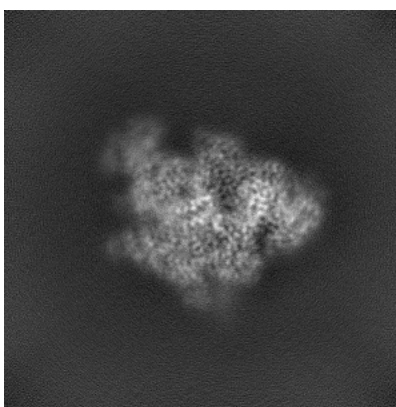


Z

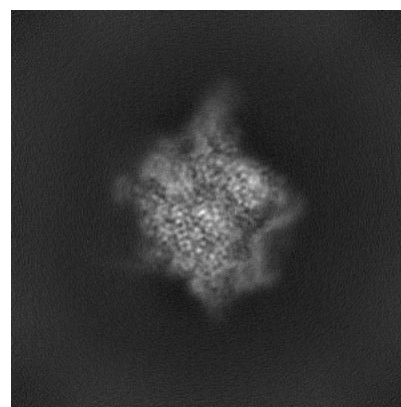
#### 6.1.2 Raw map



X



Y



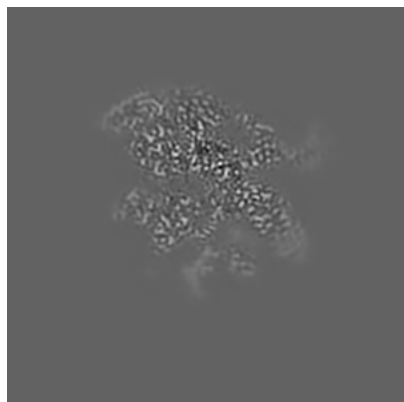
Z

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

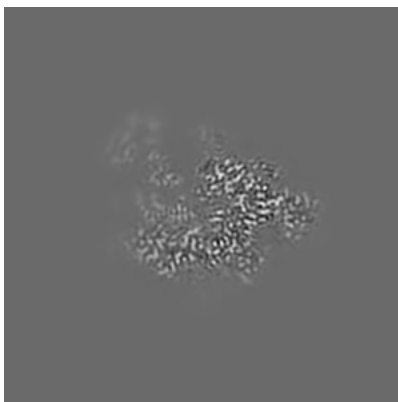


## 6.2 Central slices [i](#)

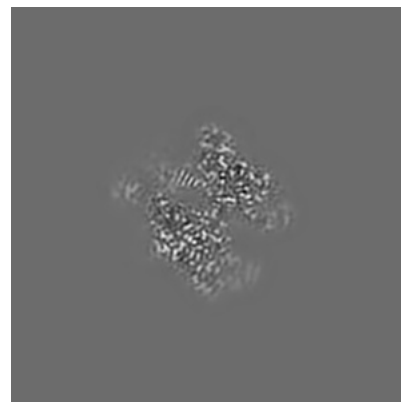
### 6.2.1 Primary map



X Index: 192

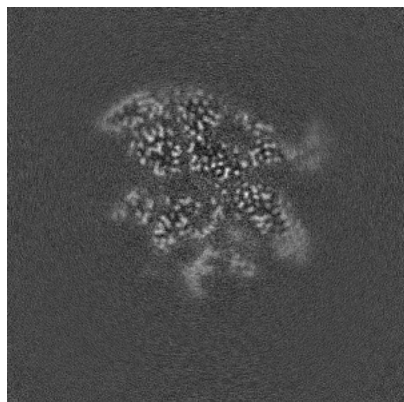


Y Index: 192

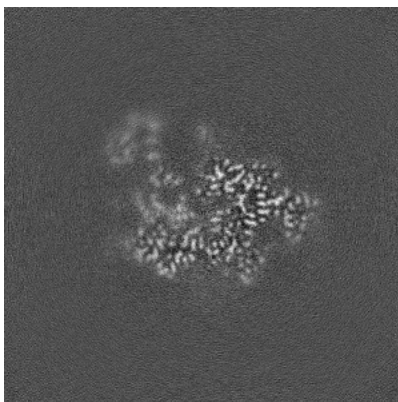


Z Index: 192

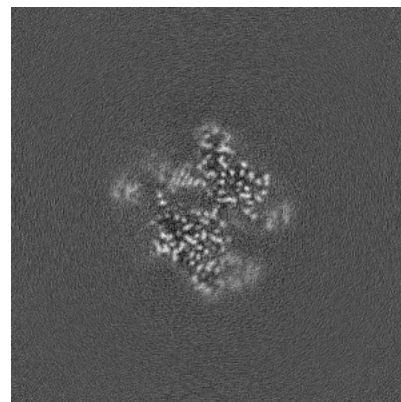
### 6.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

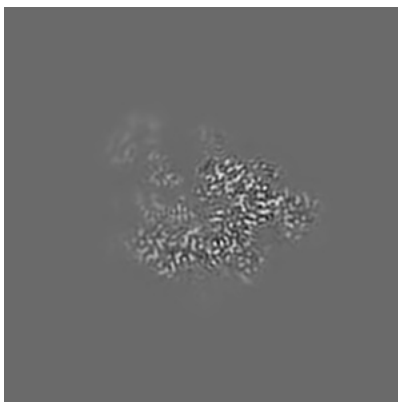
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

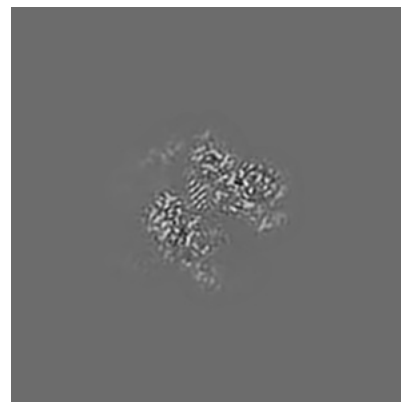
### 6.3.1 Primary map



X Index: 199

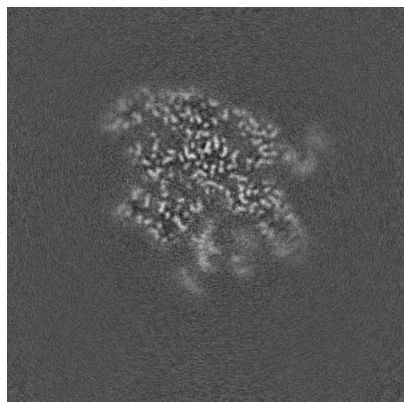


Y Index: 192

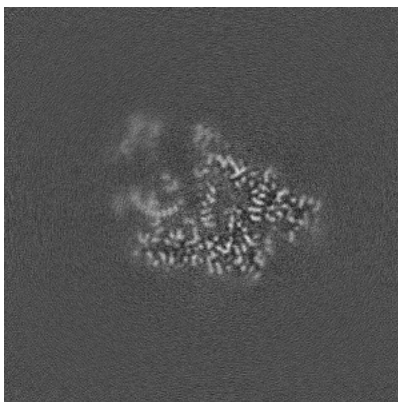


Z Index: 204

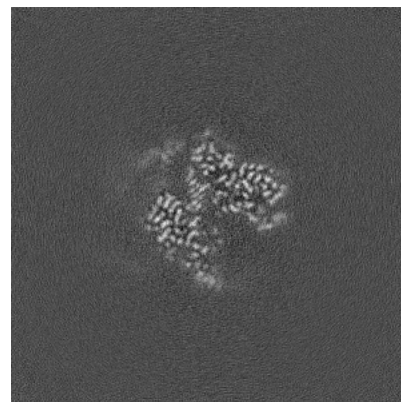
### 6.3.2 Raw map



X Index: 187



Y Index: 186

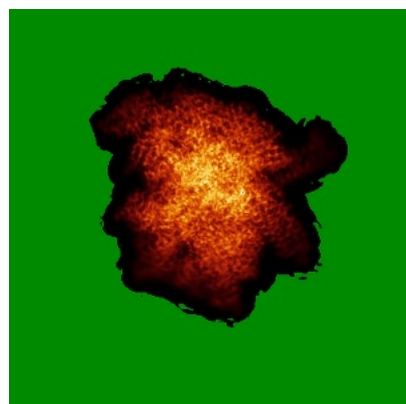


Z Index: 203

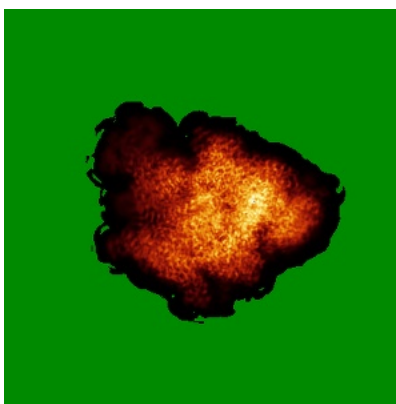
The images above show the largest variance slices of the map in three orthogonal directions.

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

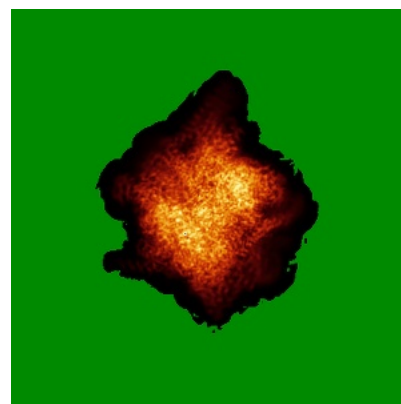
### 6.4.1 Primary map



X

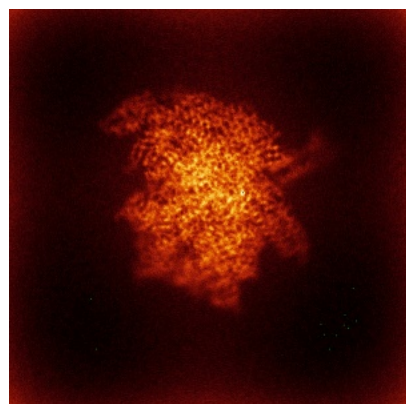


Y

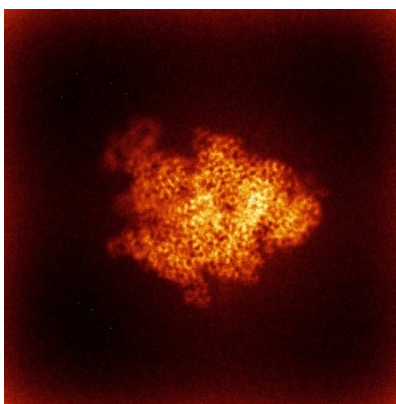


Z

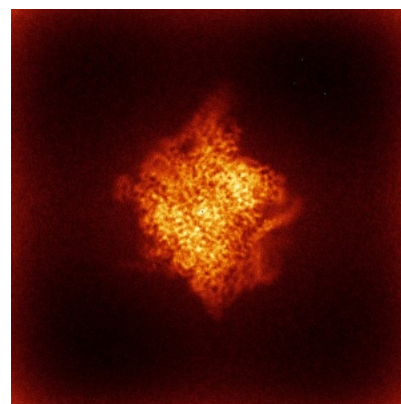
### 6.4.2 Raw map



X



Y

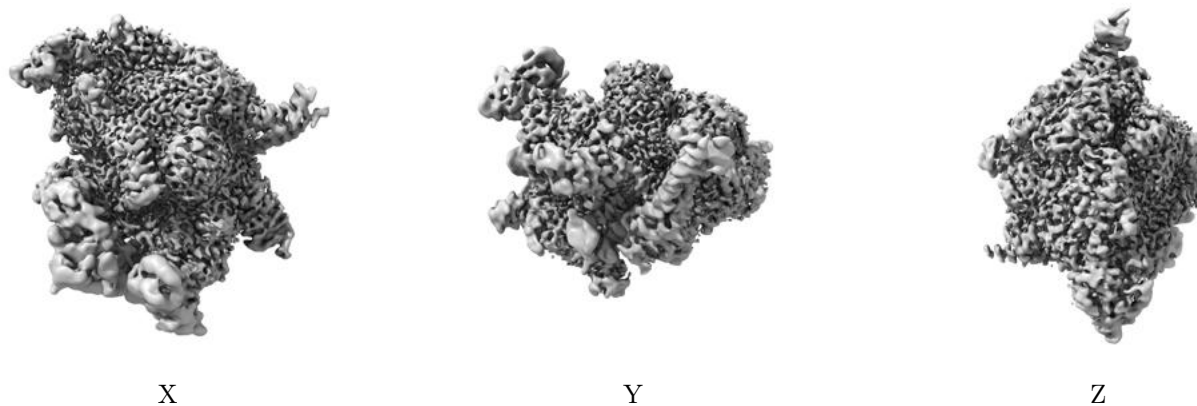


Z

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.

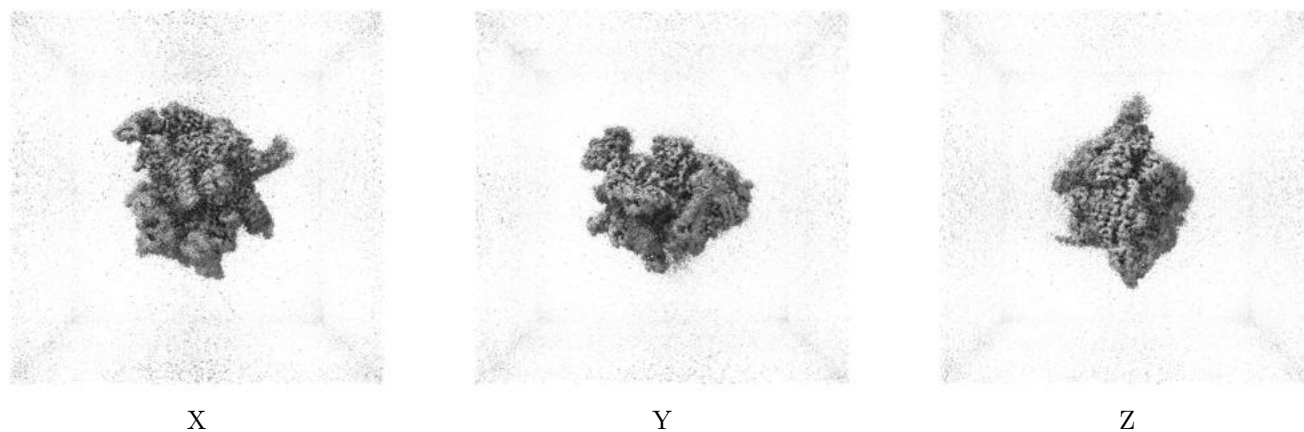
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

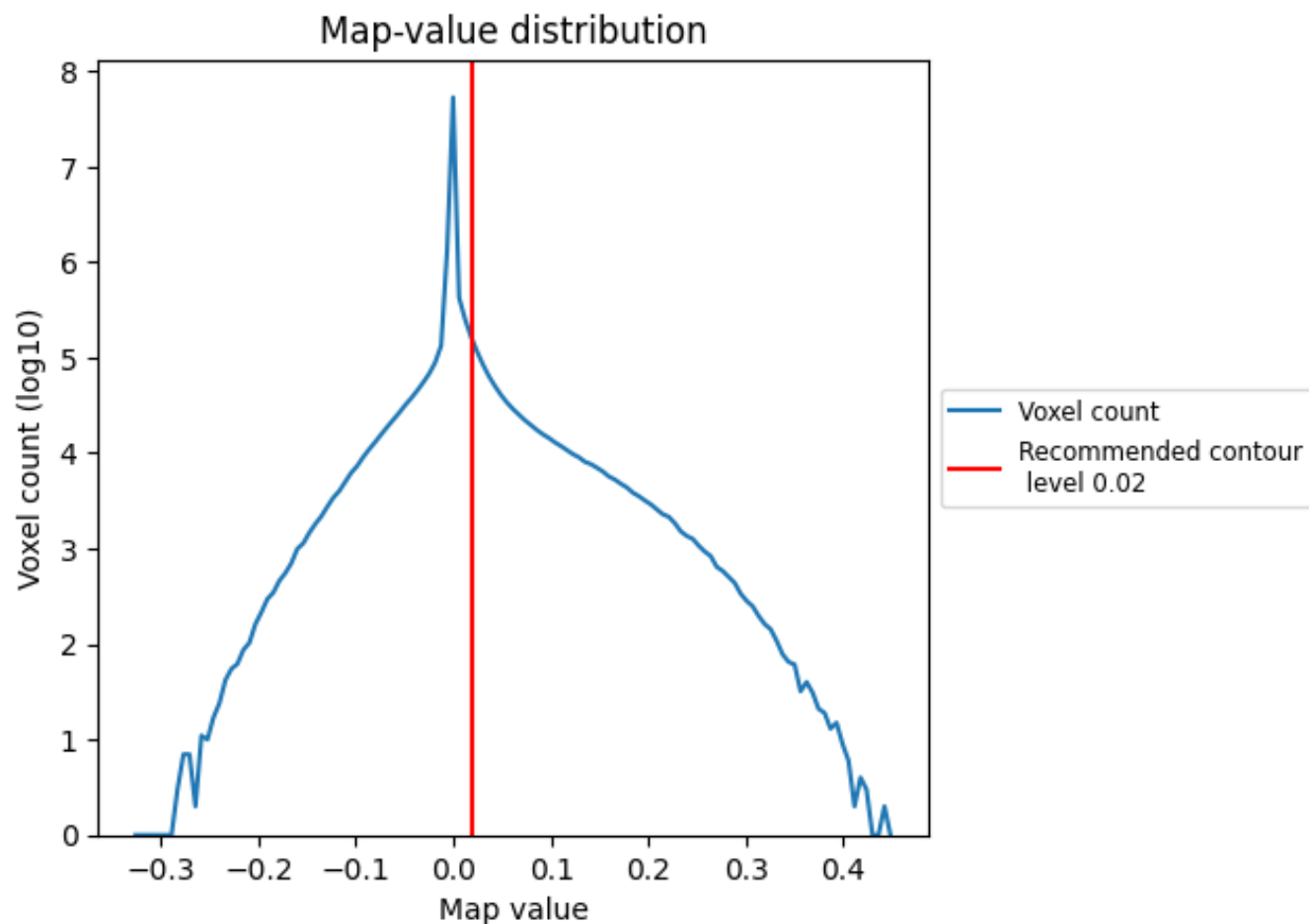
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

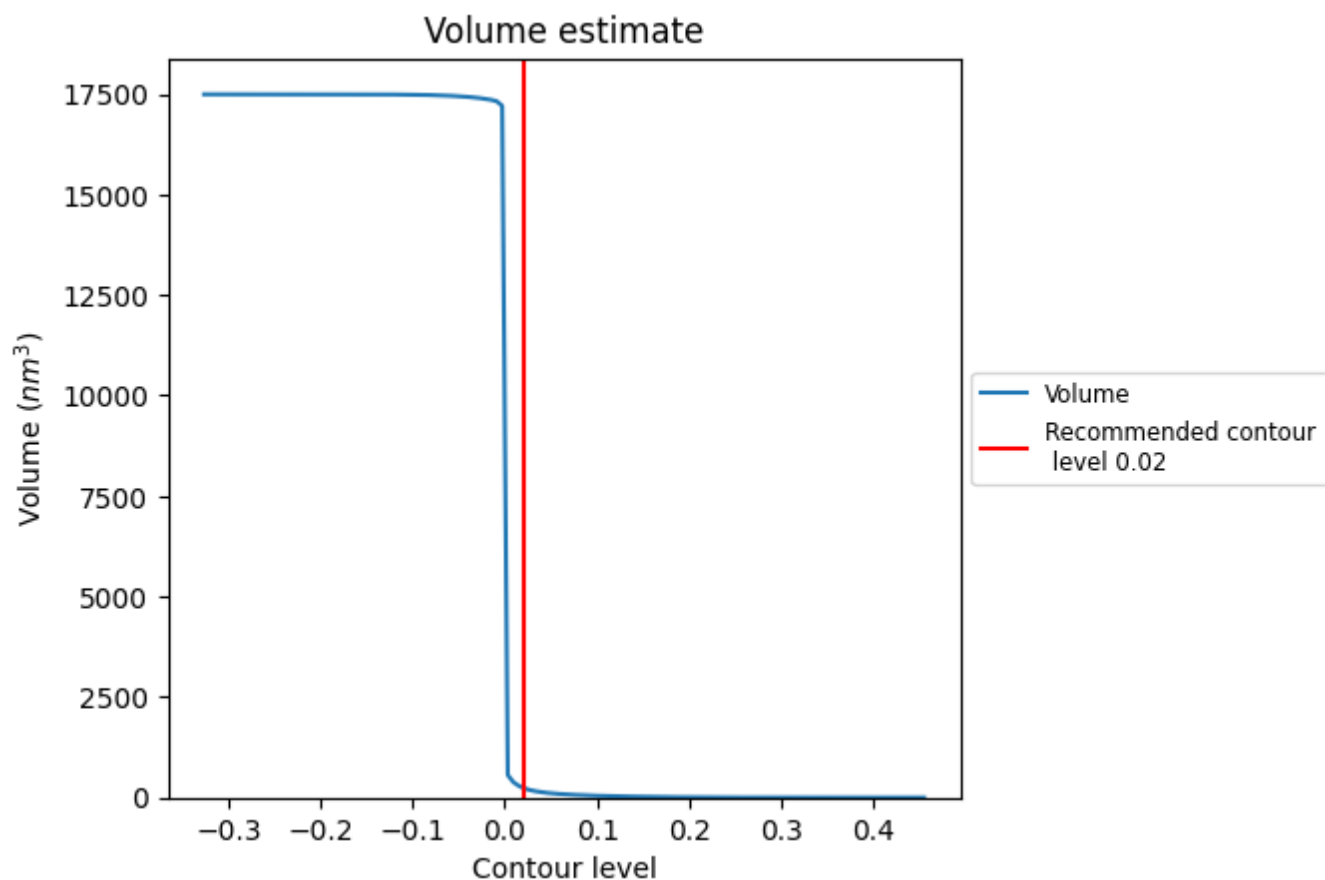
This section contains the results of statistical analysis of the map.

### 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.

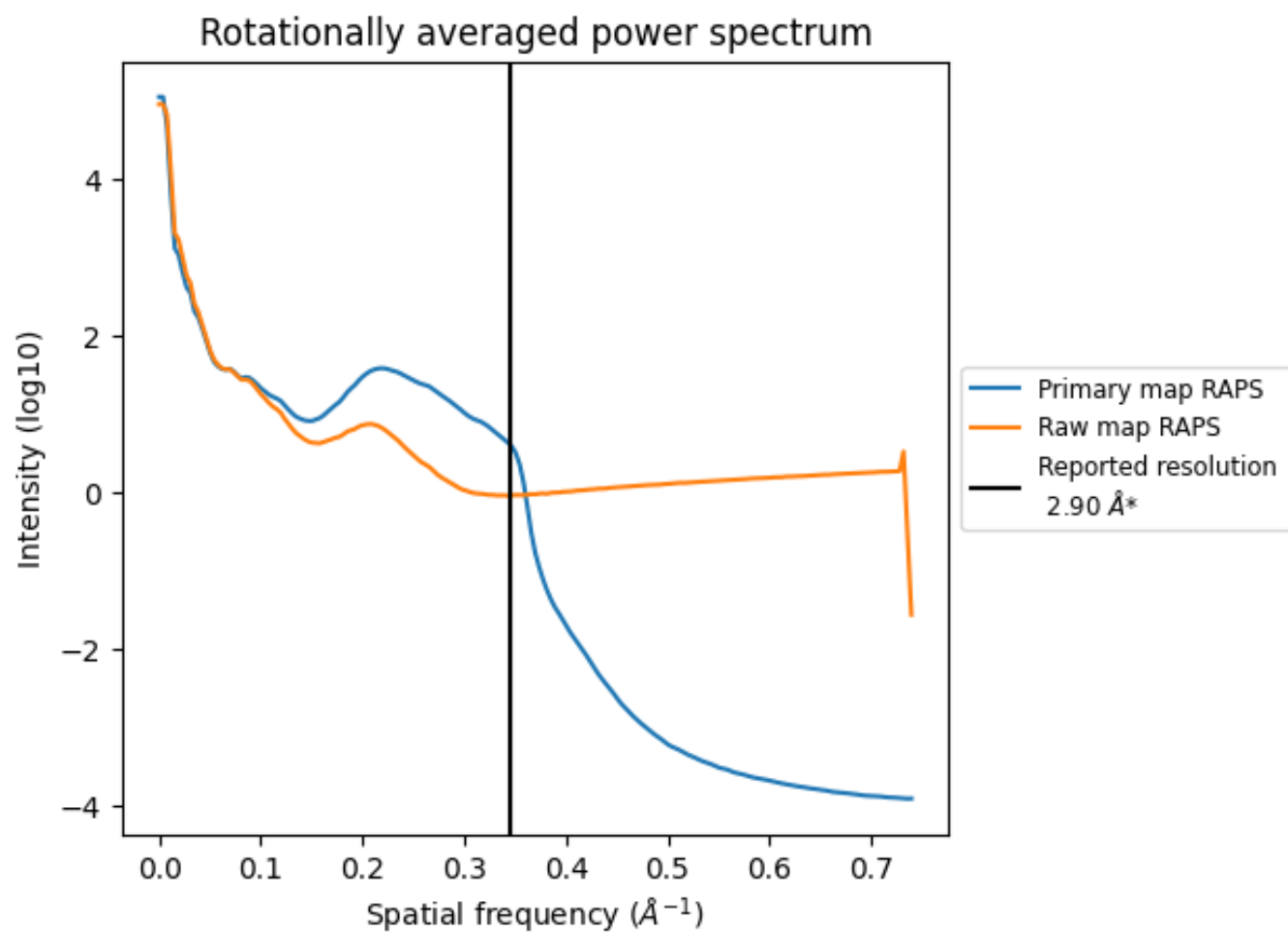
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 242 nm<sup>3</sup>; this corresponds to an approximate mass of 219 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 ⓘ



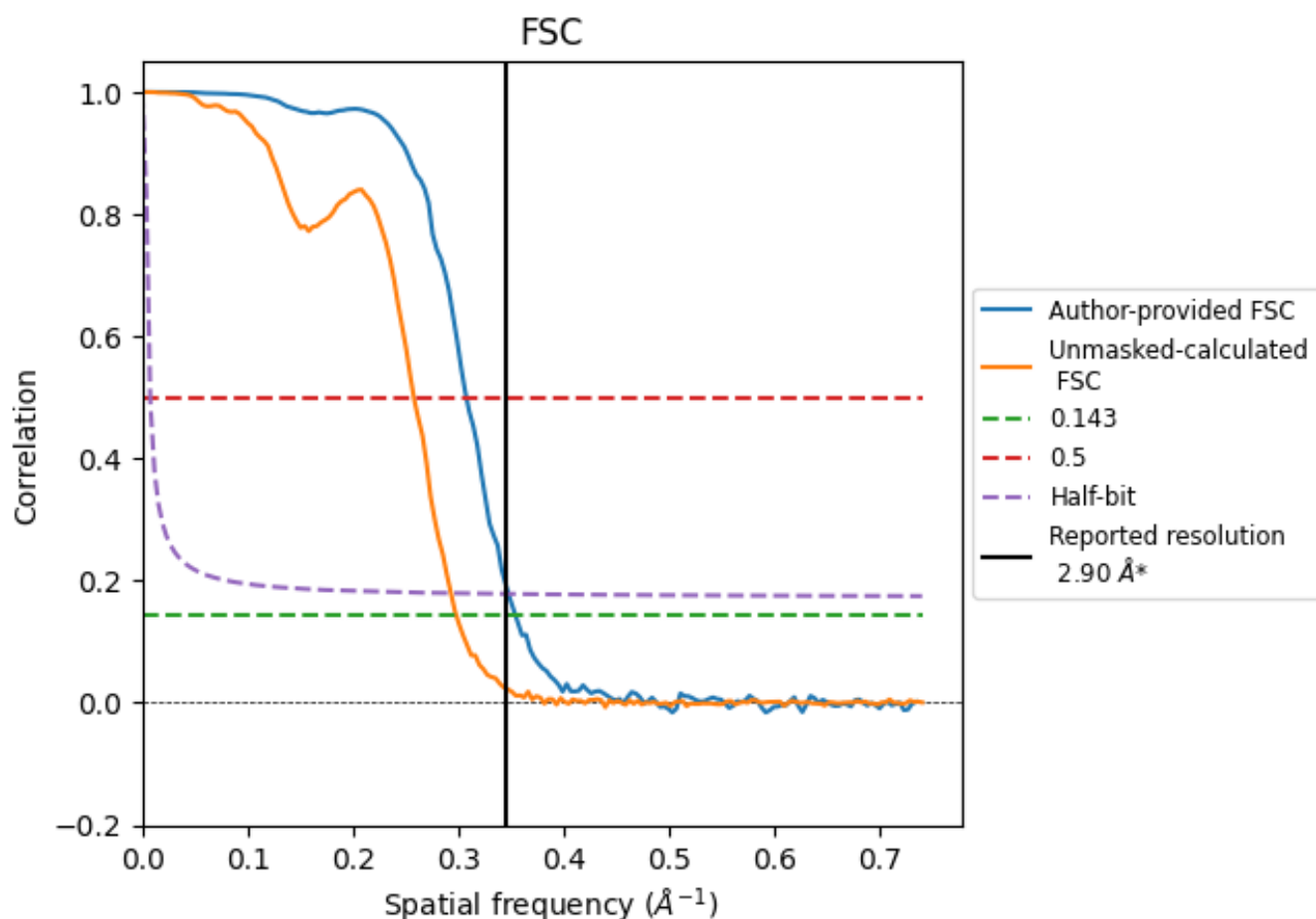
\*Reported resolution corresponds to spatial frequency of  $0.345 \text{ \AA}^{-1}$



## 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 0.345  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

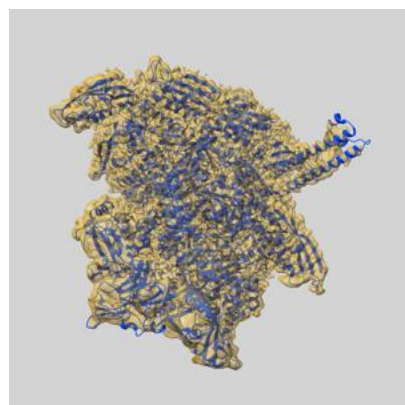
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.83	3.25	2.88
Unmasked-calculated*	3.36	3.88	3.41

\*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 2.9 by more than 10 %

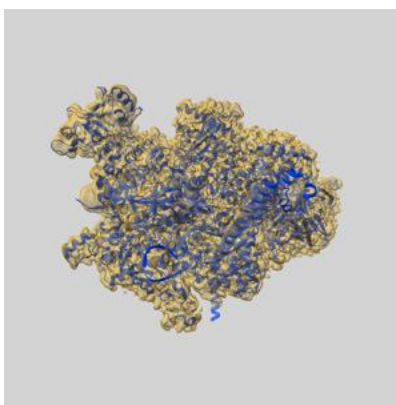
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-75285 and PDB model 10MG. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

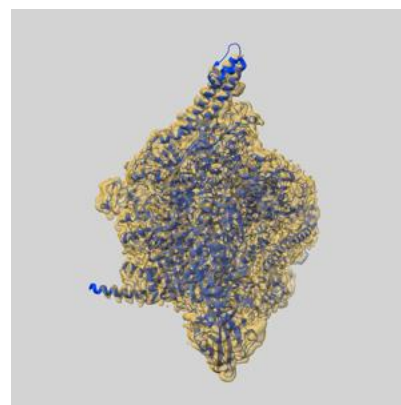
### 9.1 Map-model overlay [i](#)



X



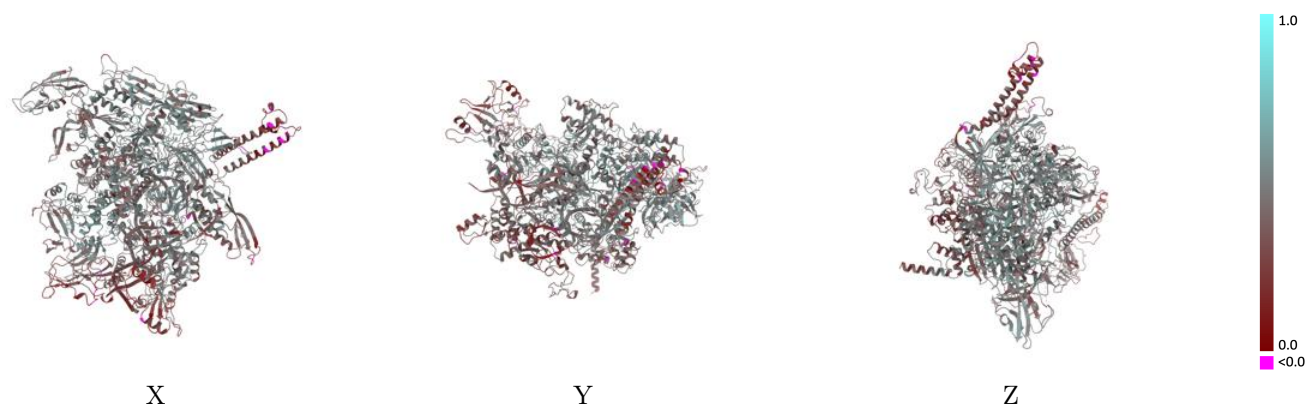
Y



Z

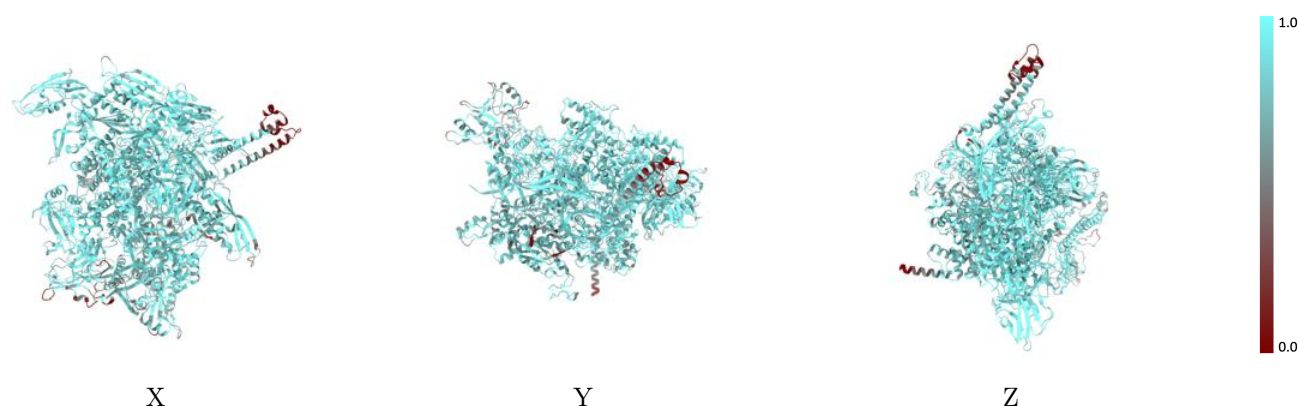
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



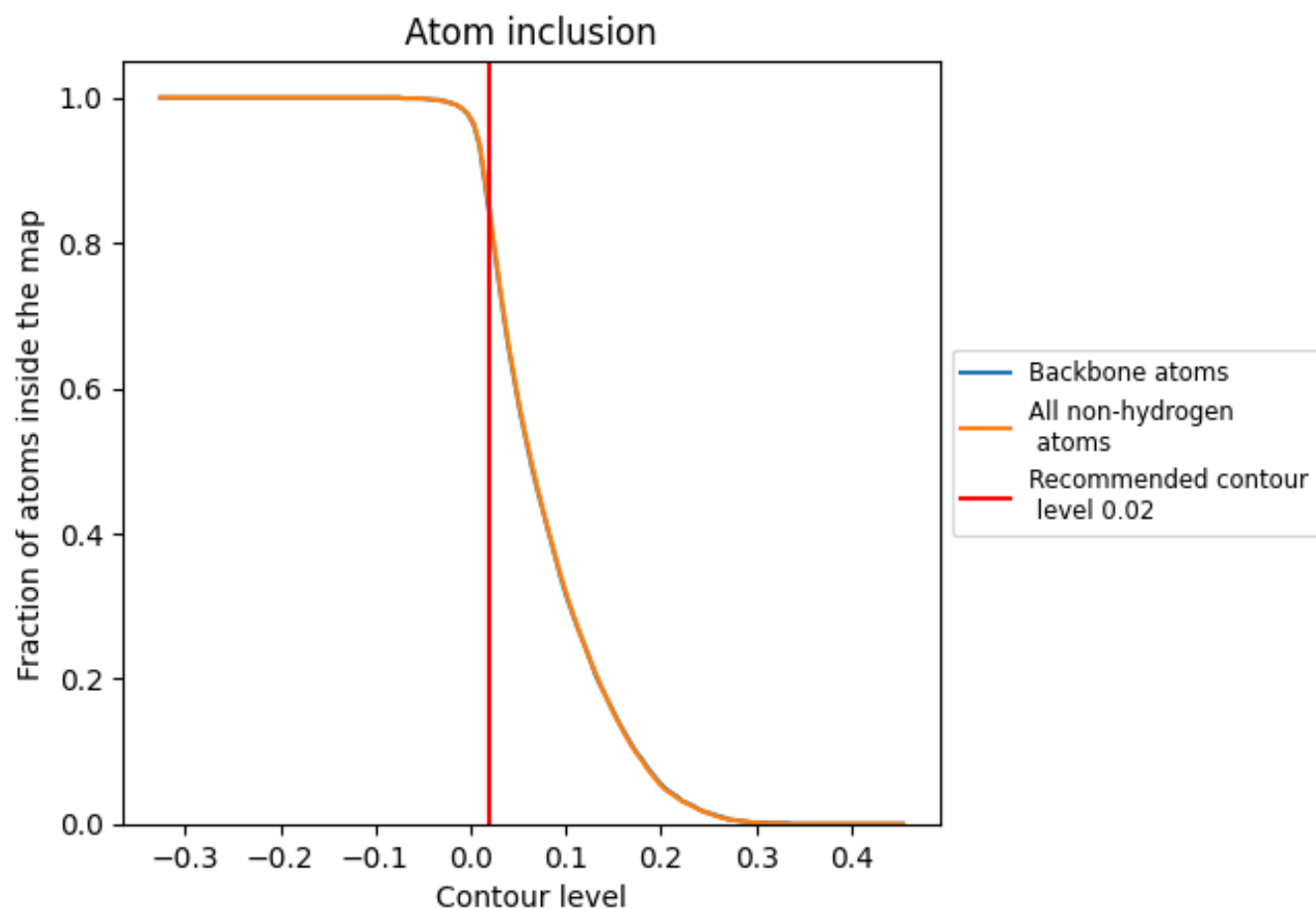
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8450	<div></div> 0.4300
A	<div></div> 0.8110	<div></div> 0.3130
B	<div></div> 0.7980	<div></div> 0.3290
G	<div></div> 0.8960	<div></div> 0.4900
H	<div></div> 0.8530	<div></div> 0.4470
I	<div></div> 0.8520	<div></div> 0.4370
J	<div></div> 0.8500	<div></div> 0.4240
K	<div></div> 0.6840	<div></div> 0.3750
R	<div></div> 0.9630	<div></div> 0.4970

1.0

0.0

<0.0