



## Full wwPDB EM Validation Report ⓘ

Dec 18, 2023 – 01:17 PM EST

PDB ID : 8SY6  
EMDB ID : EMD-40863  
Title : E. coli DNA-directed RNA polymerase transcription elongation complex bound the unnatural dB-UTP base pair in the active site  
Authors : Shan, Z.; Lyumkis, D.; Oh, J.; Wang, D.  
Deposited on : 2023-05-24  
Resolution : 3.28 Å(reported)  
Based on initial model : .

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.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

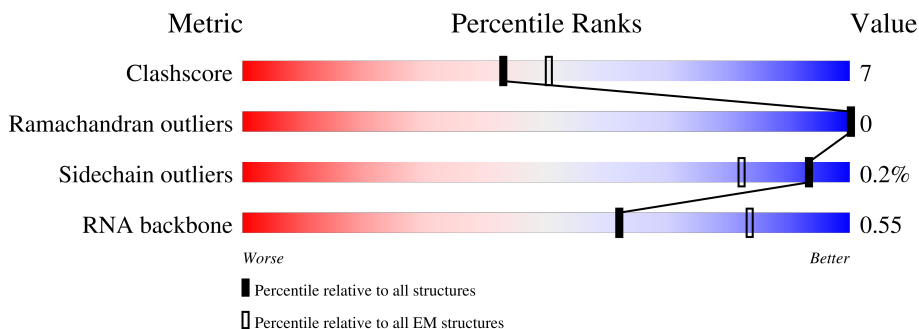
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.28 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.



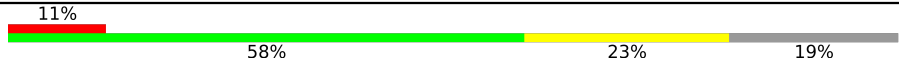
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	N	18	44% (green), 17% (yellow), 39% (grey)
2	T	29	31% (green), 38% (yellow), 28% (grey), 1% (orange)
3	A	329	15% (red), 51% (green), 16% (yellow), 32% (grey)
3	G	329	56% (green), 12% (yellow), 33% (grey), 1% (orange)
4	I	1342	74% (green), 11% (yellow), 15% (grey), 1% (orange)
5	J	1430	11% (red), 72% (green), 16% (yellow), 11% (grey)
6	R	9	44% (green), 56% (yellow)

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Mol	Chain	Length	Quality of chain
7	K	91	 <p>A horizontal bar chart showing the quality distribution of chain K. The bar is divided into four segments: 11% red, 58% green, 23% yellow, and 19% grey. The percentages are labeled below the corresponding segments.</p>

## 2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 23373 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 Non-template single stranded DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	N	11	227	108	48	61	10	0	0

- Molecule 2 is a DNA chain called Template single stranded DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	T	21	422	202	68	131	21	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	221	1681	1053	293	329	6	0	0
3	A	223	1705	1066	301	332	6	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	I	1135	8780	5509	1541	1691	39	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	J	1269	9730	6108	1740	1836	46	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1408	LEU	-	expression tag	UNP P0A8T7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1409	GLU	-	expression tag	UNP P0A8T7
J	1410	LEU	-	expression tag	UNP P0A8T7
J	1411	GLU	-	expression tag	UNP P0A8T7
J	1412	VAL	-	expression tag	UNP P0A8T7
J	1413	LEU	-	expression tag	UNP P0A8T7
J	1414	PHE	-	expression tag	UNP P0A8T7
J	1415	GLN	-	expression tag	UNP P0A8T7
J	1416	GLY	-	expression tag	UNP P0A8T7
J	1417	PRO	-	expression tag	UNP P0A8T7
J	1418	SER	-	expression tag	UNP P0A8T7
J	1419	SER	-	expression tag	UNP P0A8T7
J	1420	GLY	-	expression tag	UNP P0A8T7
J	1421	HIS	-	expression tag	UNP P0A8T7
J	1422	HIS	-	expression tag	UNP P0A8T7
J	1423	HIS	-	expression tag	UNP P0A8T7
J	1424	HIS	-	expression tag	UNP P0A8T7
J	1425	HIS	-	expression tag	UNP P0A8T7
J	1426	HIS	-	expression tag	UNP P0A8T7
J	1427	HIS	-	expression tag	UNP P0A8T7
J	1428	HIS	-	expression tag	UNP P0A8T7
J	1429	HIS	-	expression tag	UNP P0A8T7
J	1430	HIS	-	expression tag	UNP P0A8T7

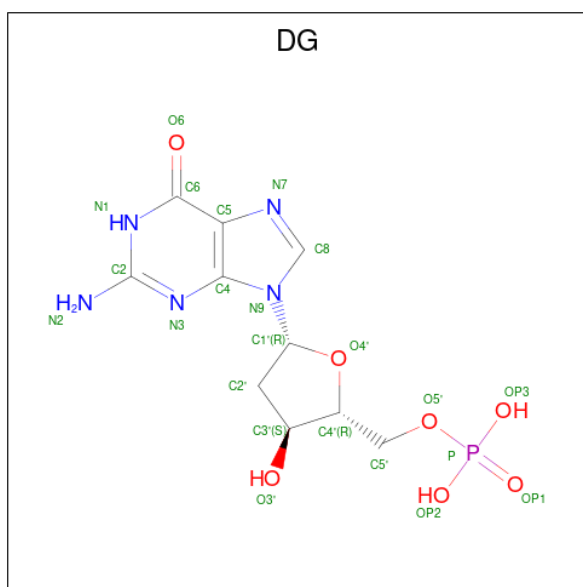
- Molecule 6 is a RNA chain called RNA oligomer.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O	P		
6	R	9	194	88	40	58	8	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O	S		
7	K	74	580	353	111	114	2	0	0

- Molecule 8 is 2'-DEOXYGUANOSINE-5'-MONOPHOSPHATE (three-letter code: DG) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	T	1	Total	C	N	O	P	0
			22	10	5	6	1	

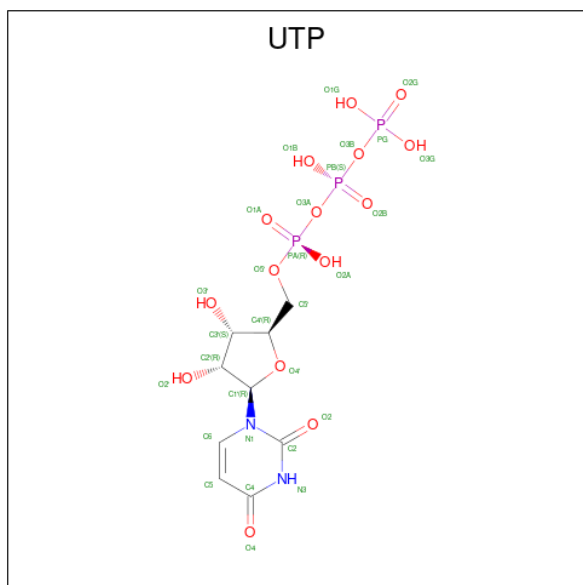
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 11 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: C<sub>9</sub>H<sub>15</sub>N<sub>2</sub>O<sub>15</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
11	J	1	29	9	2	15	3	0

### 3 Residue-property plots

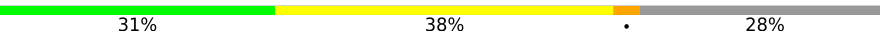
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain N: 



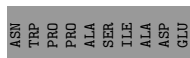
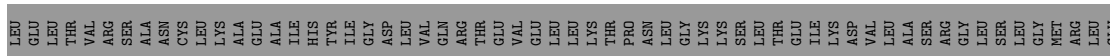
- Molecule 2: Template single stranded DNA

Chain T: 



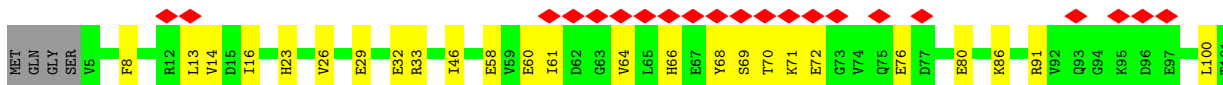
- Molecule 3: DNA-directed RNA polymerase subunit alpha

Chain G: 

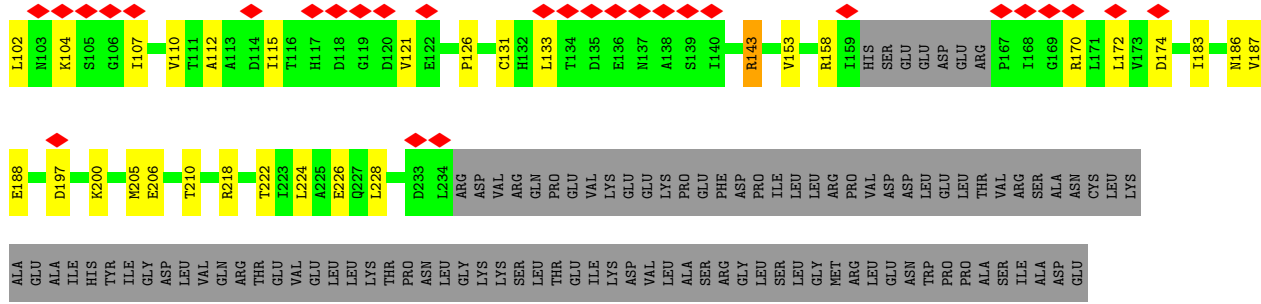


- Molecule 3: DNA-directed RNA polymerase subunit alpha

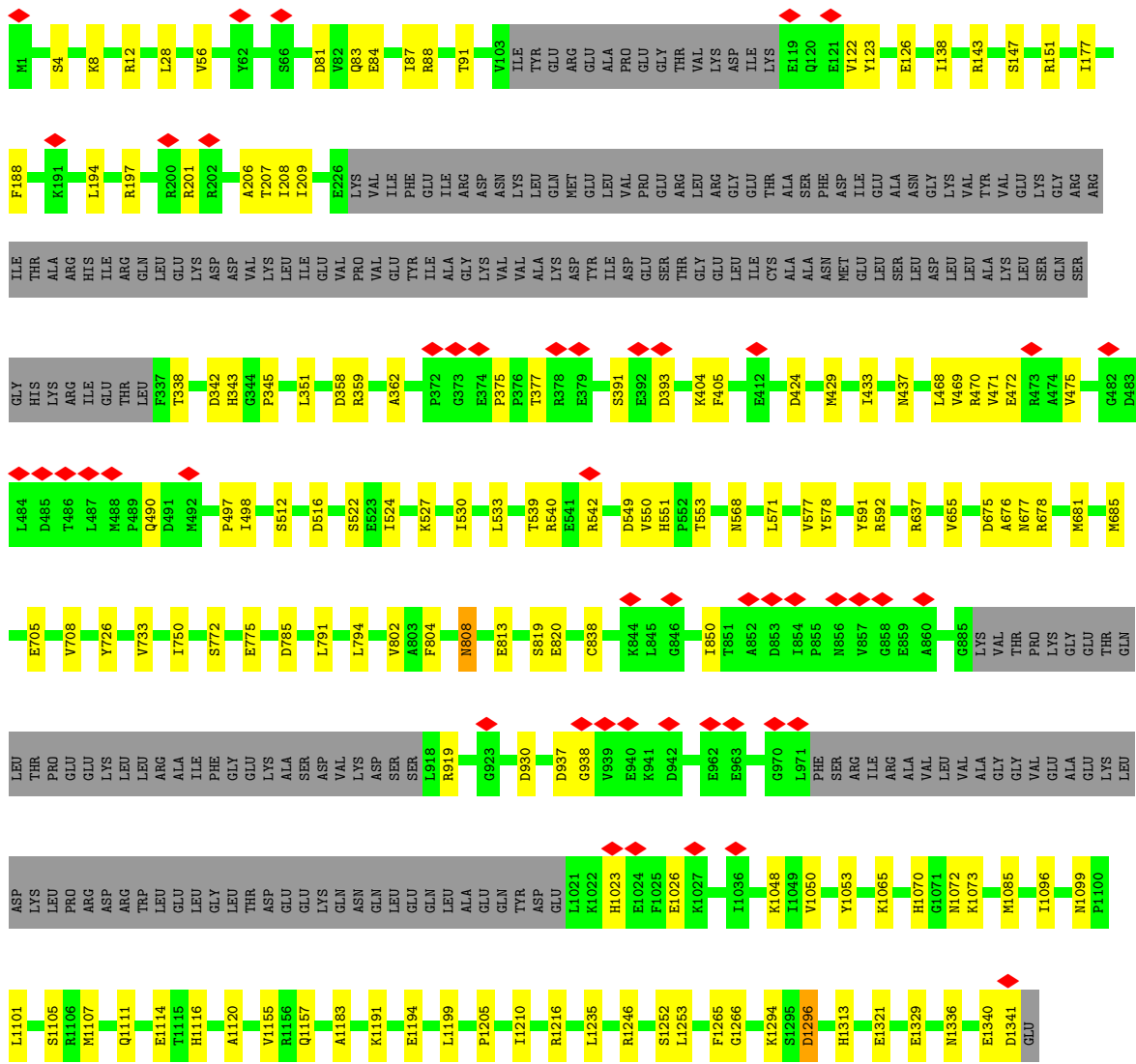
Chain A: 





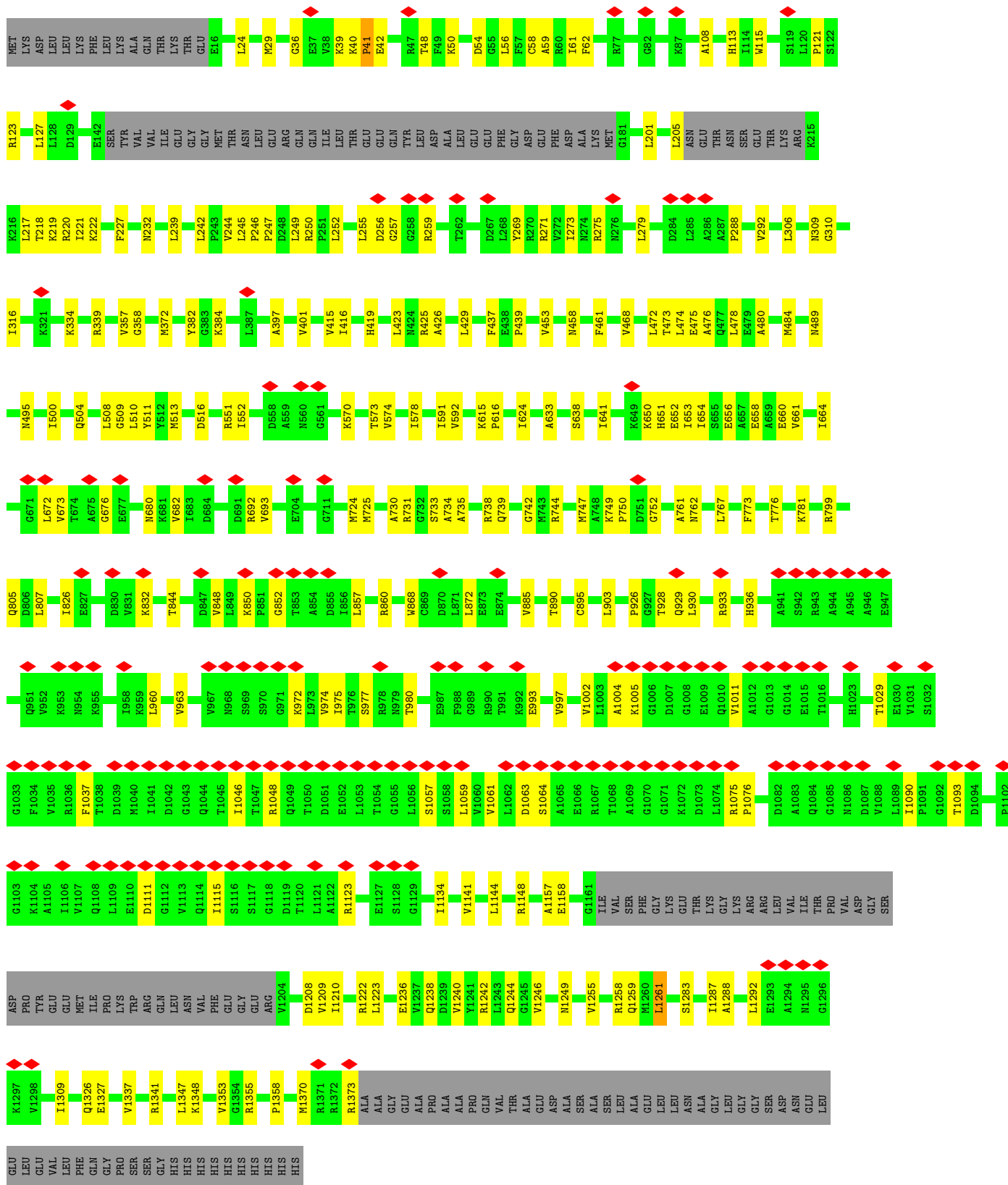


● Molecule 4: DNA-directed RNA polymerase subunit beta



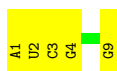
● Molecule 5: DNA-directed RNA polymerase subunit beta'



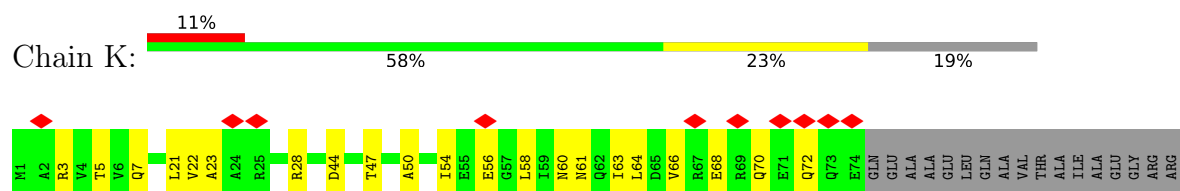


• Molecule 6: RNA oligomer





- Molecule 7: DNA-directed RNA polymerase subunit omega



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	268973	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	33.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	60240	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.513	Depositor
Minimum map value	-0.109	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	265.6, 265.6, 265.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	N	0.46	0/256	0.74	0/394
2	T	0.49	0/443	0.96	0/677
3	A	0.24	0/1724	0.51	0/2336
3	G	0.24	0/1701	0.50	0/2307
4	I	0.25	0/8923	0.50	1/12058 (0.0%)
5	J	0.25	0/9874	0.52	2/13347 (0.0%)
6	R	0.29	0/218	0.90	0/339
7	K	0.26	0/582	0.56	0/784
All	All	0.26	0/23721	0.53	3/32242 (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
5	J	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	1261	LEU	CA-CB-CG	5.76	128.56	115.30
4	I	1296	ASP	CB-CG-OD1	5.69	123.42	118.30
5	J	41	PRO	CA-N-CD	-5.03	104.45	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	J	40	LYS	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	N	227	0	124	2	0
2	T	422	0	239	15	0
3	A	1705	0	1737	33	0
3	G	1681	0	1698	25	0
4	I	8780	0	8609	97	0
5	J	9730	0	9872	159	0
6	R	194	0	98	7	0
7	K	580	0	583	14	0
8	T	22	0	12	3	0
9	J	2	0	0	0	0
10	J	1	0	0	0	0
11	J	29	0	10	2	0
All	All	23373	0	22982	330	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 7.

All (330) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:19:IGU:C1'	2:T:19:IGU:O4'	1.66	1.26
11:J:1504:UTP:O4'	11:J:1504:UTP:C1'	1.67	1.16
3:A:14:VAL:HG21	3:A:29:GLU:HG2	1.68	0.74
3:G:61:ILE:HG12	3:G:142:MET:HG2	1.68	0.74
8:T:101:DG:N2	6:R:1:A:N1	2.39	0.71
3:G:224:LEU:HD23	3:A:228:LEU:HD11	1.72	0.71
4:I:850:ILE:HD12	4:I:1048:LYS:HD2	1.74	0.69
5:J:334:LYS:HG2	5:J:339:ARG:HH12	1.58	0.69
3:A:100:LEU:HD21	3:A:121:VAL:HG21	1.74	0.69
2:T:25:DC:H2'	2:T:26:DG:C8	2.27	0.69
5:J:850:LYS:HB3	5:J:857:LEU:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:903:LEU:HD11	5:J:1249:ASN:HD22	1.58	0.69
7:K:60:ASN:OD1	7:K:61:ASN:N	2.26	0.68
8:T:101:DG:N7	5:J:259:ARG:NH1	2.42	0.68
5:J:1326:GLN:HG3	5:J:1327:GLU:HG3	1.76	0.68
4:I:549:ASP:OD1	4:I:550:VAL:N	2.27	0.67
4:I:122:VAL:HG23	4:I:490:GLN:HG2	1.78	0.66
5:J:1063:ASP:OD2	5:J:1064:SER:N	2.28	0.65
3:A:29:GLU:HB3	3:A:200:LYS:HG3	1.77	0.65
3:G:233:ASP:HB2	3:A:218:ARG:HE	1.62	0.64
4:I:188:PHE:HE1	4:I:194:LEU:HD23	1.63	0.64
5:J:56:LEU:HD22	5:J:250:ARG:HH21	1.62	0.63
5:J:653:ILE:HA	5:J:656:GLU:HG2	1.81	0.63
5:J:58:CYS:SG	5:J:59:ALA:N	2.71	0.63
4:I:1246:ARG:NH1	4:I:1265:PHE:O	2.32	0.62
5:J:591:ILE:HG13	5:J:592:VAL:HG13	1.80	0.62
5:J:977:SER:OG	5:J:980:THR:OG1	2.17	0.62
5:J:742:GLY:O	5:J:762:ASN:ND2	2.32	0.61
3:G:60:GLU:OE2	3:G:143:ARG:NH2	2.33	0.61
4:I:808:ASN:H	5:J:633:ALA:HB2	1.65	0.61
4:I:338:THR:HG21	4:I:345:PRO:HB3	1.83	0.60
5:J:62:PHE:CD1	5:J:247:PRO:HD3	2.36	0.60
7:K:22:VAL:HG22	7:K:54:ILE:HD13	1.83	0.60
2:T:25:DC:H2'	2:T:26:DG:H8	1.66	0.60
4:I:1073:LYS:NZ	6:R:9:G:OP1	2.32	0.60
5:J:1370:MET:SD	5:J:1373:ARG:NH2	2.74	0.60
5:J:246:PRO:HB2	5:J:249:LEU:HD23	1.83	0.60
5:J:24:LEU:HD12	5:J:232:ASN:HB3	1.83	0.60
4:I:342:ASP:O	4:I:437:ASN:ND2	2.24	0.60
5:J:1158:GLU:HA	5:J:1223:LEU:HD11	1.83	0.60
5:J:653:ILE:HD11	5:J:693:VAL:HB	1.84	0.59
5:J:271:ARG:HH12	5:J:316:ILE:HG13	1.68	0.59
3:A:71:LYS:NZ	3:A:72:GLU:O	2.36	0.59
4:I:471:VAL:O	4:I:475:VAL:HG23	2.04	0.58
5:J:653:ILE:HB	5:J:692:ARG:HH11	1.67	0.58
5:J:201:LEU:HD11	5:J:220:ARG:HH11	1.69	0.57
5:J:552:ILE:HD11	5:J:570:LYS:HD2	1.87	0.57
5:J:1157:ALA:HB2	5:J:1210:ILE:HD11	1.86	0.57
3:A:61:ILE:HB	3:A:64:VAL:HG12	1.87	0.57
4:I:802:VAL:HG12	4:I:1096:ILE:HB	1.87	0.57
7:K:21:LEU:HD21	7:K:60:ASN:HA	1.87	0.57
5:J:807:LEU:HD21	5:J:1255:VAL:HG13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:66:VAL:O	7:K:70:GLN:HG2	2.05	0.57
5:J:205:LEU:HG	5:J:217:LEU:HD23	1.87	0.56
3:G:14:VAL:HG13	3:G:15:ASP:OD1	2.05	0.56
4:I:83:GLN:O	4:I:87:ILE:HD12	2.06	0.56
3:G:111:THR:HG22	3:G:129:VAL:HG12	1.87	0.56
4:I:675:ASP:OD1	4:I:676:ALA:N	2.38	0.56
5:J:127:LEU:O	5:J:220:ARG:NH2	2.38	0.56
5:J:227:PHE:HE1	5:J:1337:VAL:HG13	1.71	0.55
4:I:524:ILE:HD12	4:I:708:VAL:HG13	1.87	0.55
5:J:509:GLY:O	5:J:513:MET:HG3	2.05	0.55
5:J:382:TYR:HE1	5:J:401:VAL:HG21	1.71	0.55
5:J:744:ARG:NH1	5:J:747:MET:SD	2.80	0.55
5:J:1208:ASP:OD1	5:J:1209:VAL:N	2.38	0.55
3:G:91:ARG:HG2	3:G:210:THR:HG23	1.88	0.55
4:I:813:GLU:OE1	5:J:504:GLN:NE2	2.40	0.55
3:A:107:ILE:HA	3:A:133:LEU:O	2.08	0.54
4:I:391:SER:OG	4:I:393:ASP:OD1	2.24	0.54
3:A:46:ILE:HD11	3:A:224:LEU:HD13	1.90	0.54
5:J:36:GLY:HA3	5:J:61:ILE:HG23	1.88	0.54
5:J:574:VAL:O	5:J:578:ILE:HD12	2.08	0.54
4:I:207:THR:HG21	4:I:351:LEU:HD13	1.88	0.54
3:A:66:HIS:CE1	3:A:68:TYR:HB2	2.43	0.54
5:J:108:ALA:HB3	5:J:279:LEU:HD23	1.91	0.53
4:I:539:THR:HB	4:I:542:ARG:HG2	1.90	0.53
5:J:1283:SER:O	5:J:1287:ILE:HD12	2.09	0.53
5:J:510:LEU:HD11	5:J:624:ILE:HG23	1.91	0.53
4:I:1065:LYS:HE3	4:I:1235:LEU:HD12	1.91	0.53
5:J:478:LEU:HG	7:K:23:ALA:HB2	1.90	0.53
5:J:495:ASN:HA	5:J:903:LEU:HD13	1.91	0.52
5:J:41:PRO:HD2	5:J:42:GLU:H	1.75	0.52
5:J:1148:ARG:HH11	5:J:1148:ARG:HG2	1.75	0.52
4:I:358:ASP:OD1	4:I:359:ARG:N	2.42	0.52
3:A:222:THR:O	3:A:226:GLU:HG3	2.10	0.52
4:I:1340:GLU:OE2	5:J:1341:ARG:NE	2.39	0.52
5:J:500:ILE:HG13	5:J:500:ILE:O	2.10	0.52
5:J:41:PRO:HG3	5:J:54:ASP:HB3	1.90	0.52
5:J:357:VAL:HG13	5:J:358:GLY:H	1.75	0.52
5:J:926:PRO:HB3	5:J:1246:VAL:HG21	1.92	0.52
5:J:848:VAL:H	5:J:860:ARG:NH2	2.08	0.52
5:J:936:HIS:NE2	11:J:1504:UTP:O1B	2.38	0.52
5:J:661:VAL:HG23	5:J:682:VAL:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:5:THR:HG22	7:K:7:GLN:H	1.75	0.52
5:J:885:VAL:HG12	5:J:1258:ARG:HD2	1.90	0.52
5:J:244:VAL:HG12	5:J:269:TYR:HE2	1.75	0.51
5:J:1075:ARG:HD3	5:J:1076:PRO:HD2	1.93	0.51
4:I:592:ARG:HG3	4:I:655:VAL:HG12	1.93	0.51
4:I:4:SER:O	4:I:8:LYS:N	2.43	0.51
6:R:2:U:H2'	6:R:3:C:C6	2.45	0.51
3:A:33:ARG:HD3	3:A:197:ASP:HB2	1.92	0.51
2:T:20:DC:H2'	2:T:21:DC:C6	2.46	0.51
5:J:437:PHE:HZ	5:J:453:VAL:HG11	1.75	0.51
4:I:813:GLU:HB2	5:J:461:PHE:HD2	1.76	0.51
5:J:733:SER:OG	5:J:734:ALA:N	2.44	0.51
3:G:104:LYS:HG2	3:G:110:VAL:HG22	1.93	0.50
5:J:218:THR:HA	5:J:221:ILE:HG12	1.94	0.50
4:I:143:ARG:NH1	4:I:512:SER:O	2.44	0.50
4:I:1296:ASP:OD1	4:I:1321:GLU:N	2.45	0.50
5:J:242:LEU:HD21	5:J:306:LEU:HD23	1.94	0.50
5:J:676:GLY:O	5:J:680:ASN:ND2	2.44	0.50
4:I:540:ARG:NH1	4:I:568:ASN:OD1	2.42	0.50
5:J:890:THR:HG21	5:J:895:CYS:HB3	1.93	0.50
6:R:3:C:H2'	6:R:4:G:C8	2.47	0.50
3:G:61:ILE:HB	3:G:64:VAL:HG22	1.93	0.50
4:I:1294:LYS:HE2	5:J:472:LEU:HD13	1.92	0.50
3:A:112:ALA:HB3	3:A:126:PRO:HA	1.92	0.50
2:T:26:DG:H2'	2:T:27:DA:H5'	1.93	0.50
5:J:868:TRP:O	5:J:872:LEU:HG	2.12	0.50
3:G:28:LEU:HD12	3:G:201:LEU:HD23	1.94	0.50
4:I:147:SER:HB2	4:I:530:ILE:HG22	1.94	0.49
4:I:1101:LEU:HD22	5:J:725:MET:HE3	1.95	0.49
5:J:1222:ARG:HG3	5:J:1223:LEU:HD22	1.93	0.49
4:I:151:ARG:HH21	4:I:177:ILE:HD11	1.77	0.49
2:T:20:DC:H2'	2:T:21:DC:H6	1.77	0.49
5:J:739:GLN:HG2	5:J:744:ARG:HA	1.95	0.49
5:J:1029:THR:HG21	5:J:1115:ILE:HD12	1.94	0.49
3:A:16:ILE:HG12	3:A:26:VAL:HG22	1.95	0.49
4:I:551:HIS:HD2	4:I:553:THR:HG23	1.78	0.49
5:J:113:HIS:CE1	5:J:115:TRP:HB2	2.48	0.49
4:I:469:VAL:O	4:I:472:GLU:HG3	2.13	0.48
5:J:334:LYS:HG2	5:J:339:ARG:NH1	2.26	0.48
5:J:475:GLU:OE2	7:K:28:ARG:NH2	2.46	0.48
5:J:121:PRO:O	5:J:123:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:504:GLN:HE22	5:J:731:ARG:NH2	2.11	0.48
5:J:1261:LEU:HD12	5:J:1261:LEU:O	2.12	0.48
3:G:62:ASP:OD1	3:G:62:ASP:N	2.46	0.48
5:J:425:ARG:HG2	5:J:426:ALA:H	1.79	0.48
2:T:24:DT:H2'	2:T:25:DC:H6	1.79	0.48
2:T:24:DT:H2'	2:T:25:DC:C6	2.49	0.48
4:I:405:PHE:HE2	4:I:424:ASP:HB3	1.77	0.48
3:A:188:GLU:OE1	3:A:200:LYS:NZ	2.40	0.48
4:I:81:ASP:OD1	4:I:84:GLU:HG3	2.13	0.48
7:K:50:ALA:O	7:K:54:ILE:HD12	2.13	0.48
3:A:76:GLU:HG3	3:A:131:CYS:HA	1.94	0.48
5:J:672:LEU:HD12	5:J:673:VAL:HB	1.94	0.47
4:I:1120:ALA:HB2	4:I:1199:LEU:HG	1.96	0.47
5:J:423:LEU:HG	5:J:468:VAL:HG12	1.96	0.47
5:J:489:ASN:HD22	5:J:489:ASN:N	2.11	0.47
5:J:773:PHE:O	5:J:776:THR:OG1	2.32	0.47
4:I:375:PRO:HB2	4:I:377:THR:HG23	1.96	0.47
4:I:1252:SER:OG	4:I:1253:LEU:N	2.48	0.47
5:J:974:VAL:HG22	5:J:1002:VAL:HG12	1.97	0.47
7:K:56:GLU:OE1	7:K:58:LEU:HG	2.14	0.47
4:I:208:ILE:HG23	4:I:362:ALA:HB1	1.96	0.47
4:I:1246:ARG:HH11	4:I:1266:GLY:HA2	1.80	0.47
5:J:826:ILE:HD13	5:J:993:GLU:HA	1.95	0.47
5:J:1005:LYS:HD3	5:J:1011:VAL:HG12	1.96	0.47
5:J:1090:ILE:HB	5:J:1093:THR:HB	1.97	0.47
7:K:60:ASN:HB3	7:K:63:ILE:HD13	1.97	0.47
4:I:1341:ASP:OD1	4:I:1341:ASP:N	2.48	0.47
5:J:504:GLN:HA	5:J:730:ALA:HB1	1.97	0.47
5:J:844:THR:HB	5:J:848:VAL:HG21	1.97	0.47
3:G:180:VAL:HA	3:G:207:THR:HG22	1.97	0.46
5:J:256:ASP:OD1	5:J:257:GLY:N	2.49	0.46
4:I:677:ASN:O	4:I:681:MET:HG3	2.15	0.46
4:I:705:GLU:HB3	4:I:794:LEU:H	1.80	0.46
4:I:516:ASP:HB3	4:I:522:SER:OG	2.16	0.46
5:J:738:ARG:O	5:J:742:GLY:N	2.47	0.46
4:I:819:SER:HB2	4:I:1085:MET:HG3	1.98	0.46
5:J:1141:VAL:HG23	5:J:1240:VAL:HG11	1.96	0.46
4:I:342:ASP:OD1	4:I:343:HIS:ND1	2.45	0.46
4:I:919:ARG:NH1	4:I:919:ARG:HB3	2.30	0.46
5:J:807:LEU:HD23	5:J:1259:GLN:NE2	2.31	0.46
4:I:1070:HIS:NE2	4:I:1114:GLU:OE1	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:1353:VAL:HG13	5:J:1355:ARG:HG3	1.98	0.46
8:T:101:DG:C6	5:J:255:LEU:HD21	2.50	0.46
5:J:516:ASP:HB3	5:J:573:THR:HG21	1.96	0.46
5:J:799:ARG:HB3	5:J:1309:ILE:HD12	1.98	0.46
3:G:107:ILE:H	3:G:107:ILE:HD12	1.81	0.45
2:T:9:DC:H2''	2:T:10:DT:C5	2.51	0.45
5:J:850:LYS:O	5:J:852:GLY:N	2.44	0.45
2:T:23:DC:H2'	2:T:24:DT:H6	1.81	0.45
5:J:458:ASN:ND2	5:J:929:GLN:OE1	2.49	0.45
4:I:84:GLU:O	4:I:88:ARG:HG2	2.17	0.45
5:J:651:HIS:CE1	5:J:652:GLU:HG2	2.52	0.45
3:G:199:ASP:OD1	3:G:199:ASP:N	2.50	0.45
7:K:68:GLU:O	7:K:72:GLN:HG2	2.17	0.45
3:G:67:GLU:HG2	3:G:171:LEU:HD23	1.99	0.45
4:I:804:PHE:O	5:J:638:SER:OG	2.17	0.45
5:J:416:ILE:HG12	5:J:439:PRO:HG2	1.98	0.45
3:A:153:VAL:HG12	3:A:158:ARG:HH11	1.81	0.45
4:I:56:VAL:HG11	4:I:468:LEU:HG	1.98	0.45
5:J:658:GLU:HA	5:J:661:VAL:HG12	1.98	0.45
3:A:102:LEU:HD13	3:A:115:ILE:HG12	1.97	0.45
4:I:28:LEU:HD22	4:I:527:LYS:HD2	1.98	0.45
5:J:848:VAL:HG12	5:J:848:VAL:O	2.17	0.45
2:T:22:DT:H2'	2:T:23:DC:H6	1.82	0.44
5:J:271:ARG:O	5:J:275:ARG:HG2	2.17	0.44
4:I:188:PHE:CE1	4:I:194:LEU:HD23	2.48	0.44
4:I:498:ILE:HD12	4:I:498:ILE:H	1.82	0.44
4:I:591:TYR:OH	4:I:637:ARG:NH2	2.49	0.44
4:I:1116:HIS:CE1	5:J:641:ILE:HG22	2.52	0.44
5:J:48:THR:HG23	5:J:50:LYS:H	1.83	0.44
5:J:761:ALA:HB3	5:J:767:LEU:HD23	2.00	0.44
5:J:219:LYS:HE2	5:J:219:LYS:HB2	1.83	0.44
5:J:244:VAL:HG12	5:J:269:TYR:CE2	2.52	0.44
5:J:384:LYS:HD3	5:J:415:VAL:HG22	1.99	0.44
5:J:615:LYS:HB3	5:J:616:PRO:HD3	1.98	0.44
1:N:2:DC:H2''	1:N:3:DA:H5'	2.00	0.44
5:J:750:PRO:HG3	5:J:781:LYS:HA	2.00	0.44
6:R:3:C:H2'	6:R:4:G:H8	1.82	0.44
5:J:39:LYS:HZ3	5:J:56:LEU:HA	1.81	0.44
3:G:182:ARG:HB3	3:G:206:GLU:HB3	1.99	0.44
3:G:197:ASP:OD1	3:G:197:ASP:N	2.51	0.44
6:R:1:A:H2'	6:R:2:U:H6	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:1072:ASN:ND2	4:I:1111:GLN:OE1	2.46	0.44
5:J:489:ASN:N	5:J:489:ASN:ND2	2.66	0.44
5:J:508:LEU:HA	5:J:511:TYR:CE1	2.53	0.44
3:A:60:GLU:HG2	3:A:170:ARG:HA	2.00	0.44
4:I:1023:HIS:HA	4:I:1026:GLU:HG2	1.99	0.43
5:J:551:ARG:NH2	3:A:80:GLU:OE1	2.51	0.43
5:J:397:ALA:O	5:J:401:VAL:HG23	2.17	0.43
3:A:60:GLU:OE1	3:A:143:ARG:NH2	2.51	0.43
5:J:309:ASN:OD1	5:J:310:GLY:N	2.50	0.43
5:J:429:LEU:HD22	5:J:928:THR:HG21	2.00	0.43
5:J:511:TYR:HE2	5:J:724:MET:HG2	1.83	0.43
4:I:577:VAL:HG23	4:I:578:TYR:CD2	2.53	0.43
5:J:269:TYR:CE1	5:J:306:LEU:HD11	2.54	0.43
5:J:975:ILE:HG13	5:J:997:VAL:HG11	2.01	0.43
5:J:227:PHE:CE1	5:J:1337:VAL:HG13	2.50	0.43
5:J:735:ALA:O	5:J:738:ARG:HG2	2.19	0.43
5:J:749:LYS:N	5:J:752:GLY:O	2.52	0.43
6:R:1:A:H2'	6:R:2:U:C6	2.53	0.43
5:J:903:LEU:HD11	5:J:1249:ASN:ND2	2.31	0.43
5:J:1288:ALA:O	5:J:1292:LEU:HG	2.19	0.43
5:J:357:VAL:HG13	5:J:358:GLY:N	2.34	0.43
4:I:681:MET:O	4:I:685:MET:HG3	2.19	0.43
5:J:201:LEU:HD22	5:J:217:LEU:HD11	2.01	0.43
5:J:930:LEU:HB3	5:J:1134:ILE:HG21	1.99	0.43
4:I:785:ASP:OD2	4:I:791:LEU:N	2.43	0.43
3:A:58:GLU:HG2	3:A:172:LEU:HA	2.01	0.43
4:I:91:THR:HG23	4:I:138:ILE:HA	2.00	0.43
4:I:123:TYR:OH	4:I:126:GLU:OE1	2.36	0.42
4:I:429:MET:O	4:I:433:ILE:HG12	2.19	0.42
4:I:1191:LYS:N	4:I:1194:GLU:OE1	2.38	0.42
4:I:1205:PRO:HG3	4:I:1210:ILE:HG22	2.01	0.42
4:I:1313:HIS:HB2	5:J:474:LEU:HG	2.01	0.42
5:J:1148:ARG:HG2	5:J:1148:ARG:NH1	2.33	0.42
3:G:107:ILE:HA	3:G:133:LEU:O	2.19	0.42
4:I:197:ARG:NE	4:I:201:ARG:O	2.46	0.42
4:I:937:ASP:OD1	4:I:938:GLY:N	2.52	0.42
4:I:1155:VAL:HG12	4:I:1157:GLN:H	1.83	0.42
5:J:832:LYS:HE3	5:J:832:LYS:HB3	1.82	0.42
5:J:660:GLU:O	5:J:664:ILE:HG12	2.19	0.42
7:K:3:ARG:NH1	7:K:44:ASP:OD2	2.51	0.42
3:A:8:PHE:HD2	3:A:32:GLU:HG3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:233:ASP:HA	3:A:13:LEU:HD22	2.02	0.42
4:I:1101:LEU:HD13	5:J:725:MET:HE1	2.02	0.42
5:J:1046:ILE:HD11	5:J:1059:LEU:HB3	2.01	0.42
5:J:1238:GLN:HB3	5:J:1242:ARG:NH2	2.35	0.42
4:I:551:HIS:CD2	4:I:553:THR:HG23	2.54	0.42
4:I:838:CYS:HB3	4:I:1050:VAL:HG23	2.00	0.42
4:I:1105:SER:O	4:I:1107:MET:HG3	2.20	0.42
4:I:802:VAL:HA	4:I:1096:ILE:O	2.20	0.42
5:J:480:ALA:HA	5:J:484:MET:HB2	2.01	0.42
3:A:104:LYS:HG2	3:A:110:VAL:HG22	2.02	0.42
4:I:470:ARG:HD2	4:I:497:PRO:HB3	2.01	0.42
4:I:471:VAL:HB	4:I:498:ILE:HD11	2.02	0.42
2:T:19:IGU:H2''	2:T:20:DC:H6	1.84	0.42
4:I:468:LEU:HA	4:I:471:VAL:HG12	2.00	0.42
4:I:819:SER:OG	4:I:820:GLU:N	2.53	0.42
4:I:1116:HIS:HE1	5:J:641:ILE:HG22	1.85	0.42
5:J:288:PRO:O	5:J:292:VAL:HG13	2.20	0.42
3:G:31:LEU:HD13	3:G:36:GLY:HA2	2.01	0.41
3:G:228:LEU:HD11	3:A:224:LEU:HD23	2.01	0.41
5:J:805:GLN:OE1	5:J:1348:LYS:HG3	2.19	0.41
5:J:1048:ARG:NH2	5:J:1057:SER:OG	2.52	0.41
3:A:23:HIS:ND1	3:A:206:GLU:HB2	2.35	0.41
4:I:206:ALA:O	4:I:209:ILE:HG22	2.20	0.41
4:I:533:LEU:HD21	4:I:571:LEU:HD13	2.01	0.41
5:J:478:LEU:HD21	7:K:47:THR:HB	2.02	0.41
5:J:1347:LEU:HD23	5:J:1358:PRO:HD2	2.01	0.41
2:T:23:DC:H2'	2:T:24:DT:C6	2.55	0.41
4:I:733:VAL:HG22	4:I:750:ILE:HG12	2.03	0.41
5:J:219:LYS:HA	5:J:222:LYS:HE3	2.01	0.41
5:J:960:LEU:HD23	5:J:963:VAL:HG21	2.02	0.41
1:N:10:DG:N2	2:T:10:DT:O2	2.53	0.41
3:G:30:PRO:HB2	3:G:198:LEU:HD13	2.02	0.41
3:G:120:ASP:OD1	3:G:121:VAL:N	2.52	0.41
5:J:217:LEU:HD12	5:J:217:LEU:HA	1.93	0.41
5:J:372:MET:HB2	5:J:372:MET:HE3	1.89	0.41
4:I:56:VAL:HG21	4:I:468:LEU:HB3	2.03	0.41
4:I:468:LEU:HA	4:I:468:LEU:HD12	1.91	0.41
4:I:930:ASP:HB3	4:I:1053:TYR:CD1	2.56	0.41
4:I:1296:ASP:OD1	4:I:1296:ASP:O	2.38	0.41
5:J:1134:ILE:HB	5:J:1244:GLN:HG3	2.03	0.41
5:J:1144:LEU:HD11	5:J:1236:GLU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:113:HIS:HD2	5:J:239:LEU:HD11	1.86	0.41
5:J:252:LEU:HD12	5:J:252:LEU:HA	1.89	0.41
5:J:929:GLN:OE1	5:J:933:ARG:NE	2.54	0.41
3:A:86:LYS:HD2	3:A:174:ASP:HB2	2.02	0.41
2:T:14:DG:H5'	2:T:14:DG:C8	2.56	0.41
3:G:39:LEU:HD23	3:G:39:LEU:HA	1.89	0.41
3:G:186:ASN:OD1	3:G:187:VAL:N	2.54	0.41
4:I:726:TYR:HB3	4:I:733:VAL:HB	2.02	0.41
4:I:772:SER:N	4:I:775:GLU:OE2	2.45	0.41
5:J:269:TYR:O	5:J:273:ILE:HG13	2.21	0.41
5:J:972:LYS:HG3	5:J:1004:ALA:HA	2.02	0.41
5:J:1046:ILE:HG13	5:J:1061:VAL:HA	2.02	0.41
7:K:21:LEU:HD11	7:K:64:LEU:HD12	2.02	0.41
4:I:12:ARG:HD3	4:I:1183:ALA:HB2	2.03	0.41
4:I:678:ARG:HA	4:I:678:ARG:HD3	1.88	0.41
5:J:1037:PHE:HD2	5:J:1111:ASP:HB2	1.85	0.41
4:I:405:PHE:CE2	4:I:424:ASP:HB3	2.55	0.40
4:I:1099:ASN:OD1	4:I:1101:LEU:HD23	2.21	0.40
4:I:1329:GLU:HA	5:J:245:LEU:HD21	2.04	0.40
5:J:650:LYS:O	5:J:654:ILE:HG13	2.21	0.40
3:A:69:SER:OG	3:A:70:THR:N	2.54	0.40
3:A:91:ARG:HG2	3:A:210:THR:HG23	2.02	0.40
5:J:113:HIS:ND1	5:J:115:TRP:HB2	2.37	0.40
5:J:735:ALA:HA	5:J:738:ARG:HG2	2.04	0.40
3:A:183:ILE:HD13	3:A:205:MET:HG3	2.03	0.40
4:I:404:LYS:HD2	4:I:404:LYS:HA	1.92	0.40
5:J:473:THR:HG23	5:J:476:ALA:H	1.86	0.40
3:A:66:HIS:HB3	3:A:69:SER:HB2	2.02	0.40
4:I:1216:ARG:HE	4:I:1216:ARG:HB2	1.63	0.40
4:I:1336:ASN:ND2	5:J:29:MET:SD	2.94	0.40
5:J:39:LYS:HE3	5:J:39:LYS:HB3	1.81	0.40
3:A:186:ASN:OD1	3:A:187:VAL:N	2.55	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	
3	A	219/329 (67%)	214 (98%)	5 (2%)	0	100	100
3	G	217/329 (66%)	214 (99%)	3 (1%)	0	100	100
4	I	1125/1342 (84%)	1099 (98%)	26 (2%)	0	100	100
5	J	1261/1430 (88%)	1214 (96%)	47 (4%)	0	100	100
7	K	72/91 (79%)	71 (99%)	1 (1%)	0	100	100
All	All	2894/3521 (82%)	2812 (97%)	82 (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	
3	A	187/286 (65%)	186 (100%)	1 (0%)	88	93
3	G	183/286 (64%)	183 (100%)	0	100	100
4	I	929/1157 (80%)	928 (100%)	1 (0%)	93	97
5	J	1032/1189 (87%)	1030 (100%)	2 (0%)	93	97
7	K	61/75 (81%)	61 (100%)	0	100	100
All	All	2392/2993 (80%)	2388 (100%)	4 (0%)	93	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	I	808	ASN
5	J	419	HIS
5	J	1123	ARG
3	A	143	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such

sidechains are listed below:

Mol	Chain	Res	Type
4	I	551	HIS
4	I	1116	HIS
5	J	762	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	R	7/9 (77%)	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 [i](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z  > 2$
2	IGU	T	19	2	21,24,25	4.82	14 (66%)	30,35,38	1.41	3 (10%)

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
2	IGU	T	19	2	-	0/7/21/22	0/3/3/3

All (14) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	19	IGU	O4'-C1'	10.90	1.66	1.42
2	T	19	IGU	C4-N3	9.06	1.51	1.33
2	T	19	IGU	C5-C6	7.78	1.58	1.40
2	T	19	IGU	O4'-C4'	-7.61	1.28	1.45
2	T	19	IGU	C2'-C1'	-6.35	1.34	1.52
2	T	19	IGU	C6-N6	5.11	1.44	1.33
2	T	19	IGU	C2-N1	4.76	1.50	1.39
2	T	19	IGU	C2-N3	4.42	1.47	1.36
2	T	19	IGU	O3'-C3'	-4.38	1.34	1.43
2	T	19	IGU	C3'-C4'	3.58	1.62	1.53
2	T	19	IGU	C5-N7	-2.45	1.34	1.39
2	T	19	IGU	C8-N7	2.36	1.39	1.32
2	T	19	IGU	C6-N1	2.22	1.41	1.37
2	T	19	IGU	O2-C2	-2.05	1.20	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	19	IGU	C5-C6-N6	-3.29	120.23	124.60
2	T	19	IGU	C5-C4-N3	-3.19	120.28	127.52
2	T	19	IGU	N9-C8-N7	-2.66	108.38	113.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	19	IGU	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	DG	T	101	-	18,24,25	1.10	2 (11%)	19,35,38	0.63	1 (5%)
11	UTP	J	1504	10	22,30,30	6.45	9 (40%)	27,47,47	1.05	2 (7%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	DG	T	101	-	-	0/3/21/22	0/3/3/3
11	UTP	J	1504	10	-	8/20/38/38	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	J	1504	UTP	O4'-C1'	18.86	1.67	1.41
11	J	1504	UTP	C2'-C1'	-16.54	1.28	1.53
11	J	1504	UTP	C6-N1	8.60	1.46	1.35
11	J	1504	UTP	C4-N3	7.39	1.45	1.33
11	J	1504	UTP	O4'-C4'	-6.61	1.30	1.45
11	J	1504	UTP	C2-N3	5.97	1.50	1.38
11	J	1504	UTP	C6-C5	5.69	1.50	1.38
11	J	1504	UTP	O3'-C3'	-4.41	1.32	1.43
11	J	1504	UTP	O2'-C2'	3.22	1.50	1.43
8	T	101	DG	C5-C6	-2.72	1.41	1.47
8	T	101	DG	C8-N7	-2.55	1.30	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	J	1504	UTP	PB-O3B-PG	-2.74	123.41	132.83
11	J	1504	UTP	C3'-C2'-C1'	2.20	104.29	100.98
8	T	101	DG	O6-C6-C5	2.02	128.33	124.37

There are no chirality outliers.

All (8) torsion outliers are listed below:

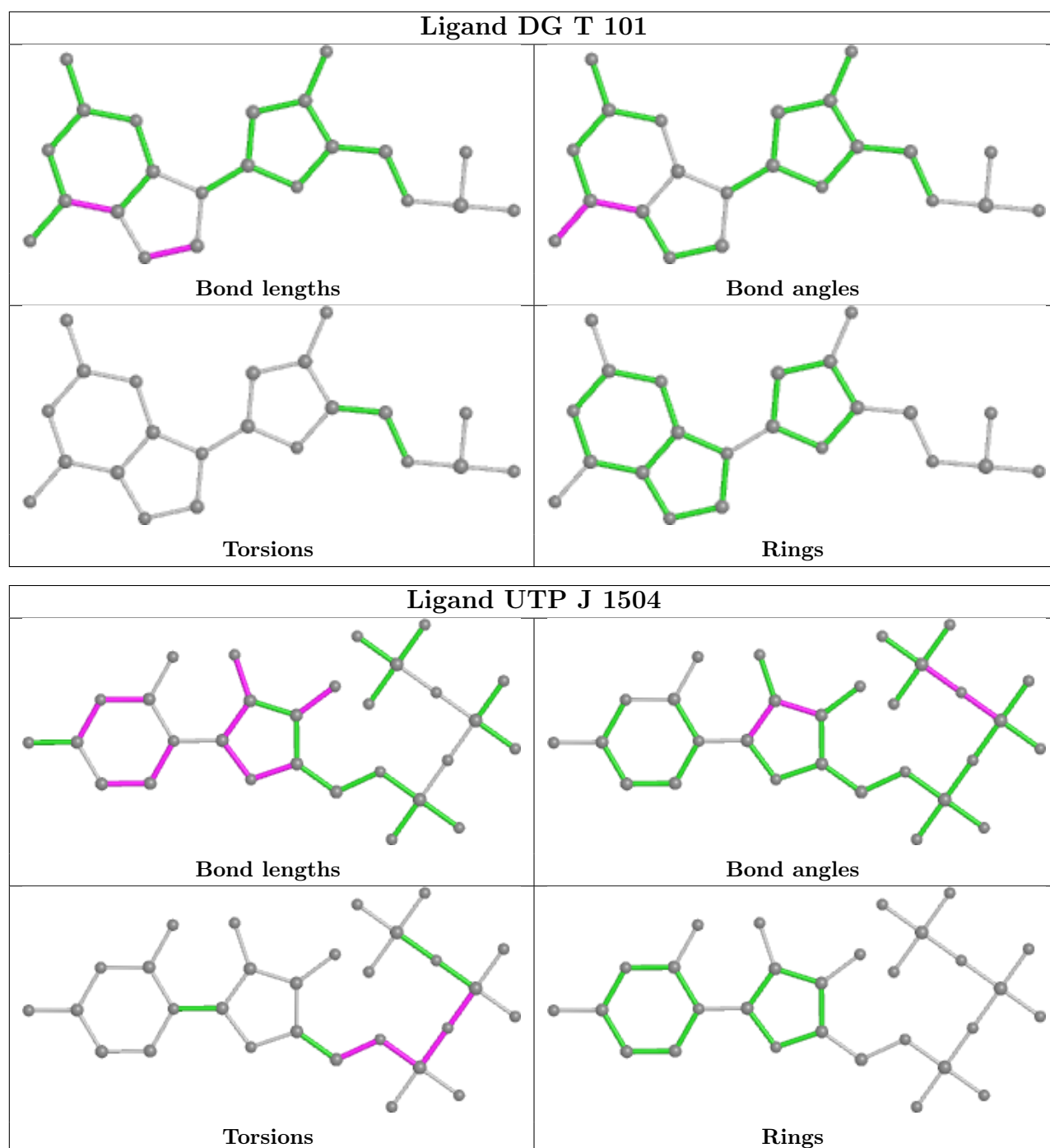
Mol	Chain	Res	Type	Atoms
11	J	1504	UTP	C5'-O5'-PA-O3A
11	J	1504	UTP	C4'-C5'-O5'-PA
11	J	1504	UTP	C5'-O5'-PA-O1A
11	J	1504	UTP	C5'-O5'-PA-O2A
11	J	1504	UTP	PA-O3A-PB-O3B
11	J	1504	UTP	PB-O3A-PA-O2A
11	J	1504	UTP	PB-O3A-PA-O1A
11	J	1504	UTP	PA-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	T	101	DG	3	0
11	J	1504	UTP	2	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.

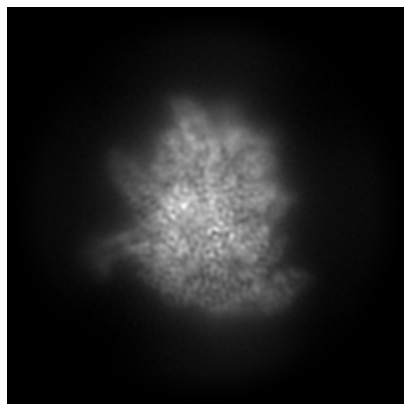
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40863. These allow visual inspection of the internal detail of the map and identification of artifacts.

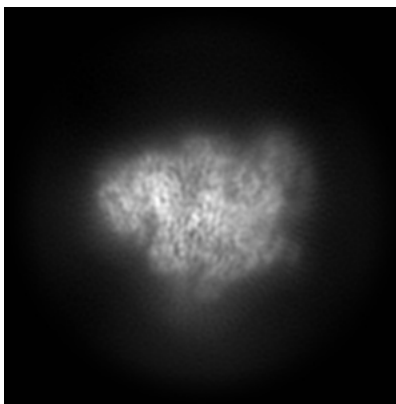
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

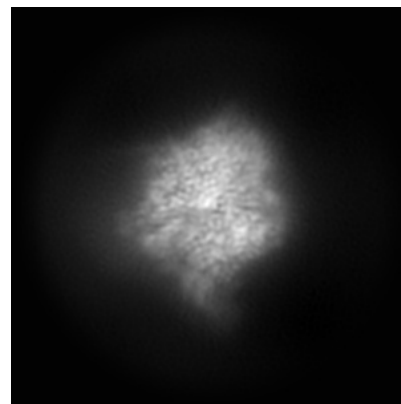
#### 6.1.1 Primary map



X

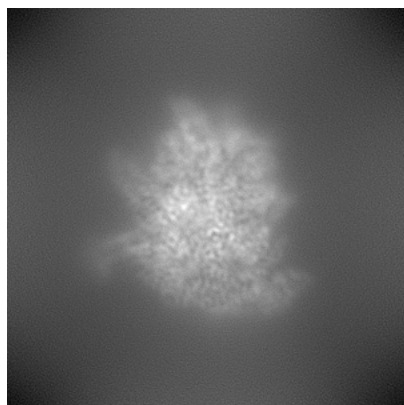


Y

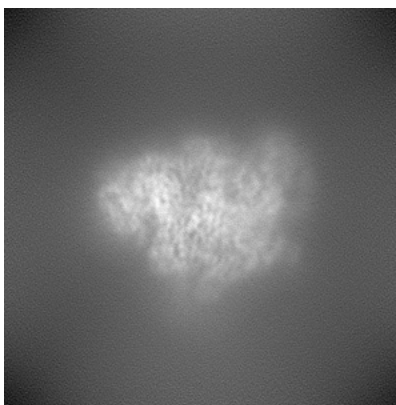


Z

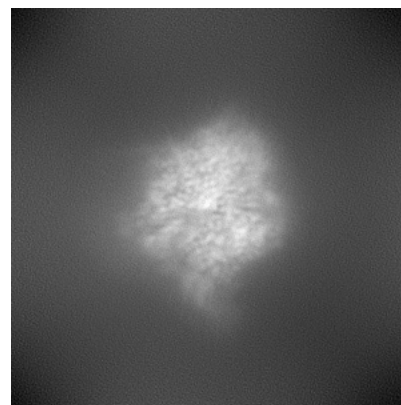
#### 6.1.2 Raw map



X



Y

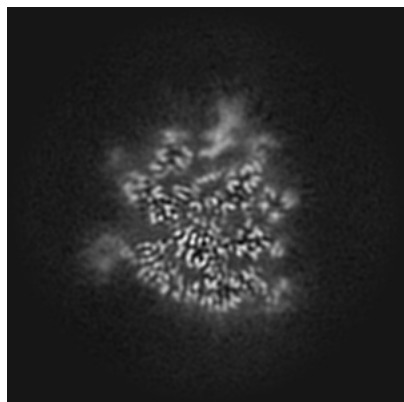


Z

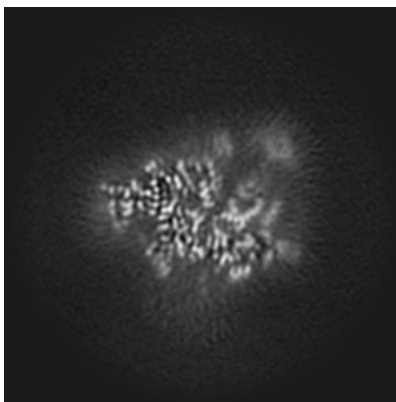
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

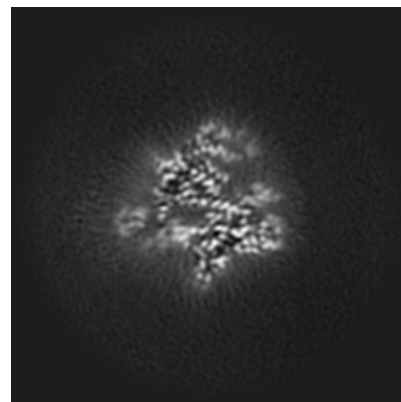
### 6.2.1 Primary map



X Index: 160

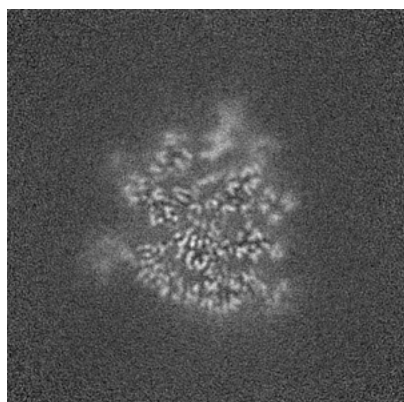


Y Index: 160

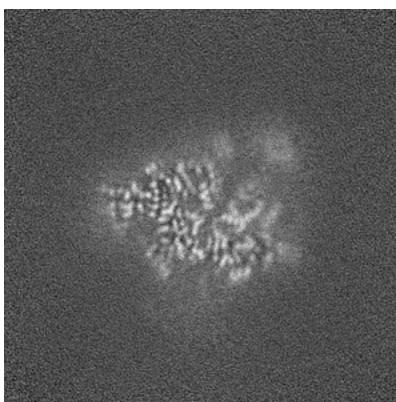


Z Index: 160

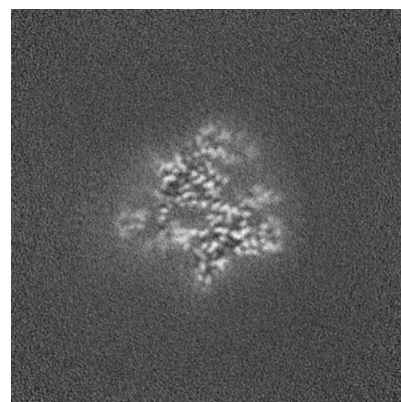
### 6.2.2 Raw map



X Index: 160



Y Index: 160

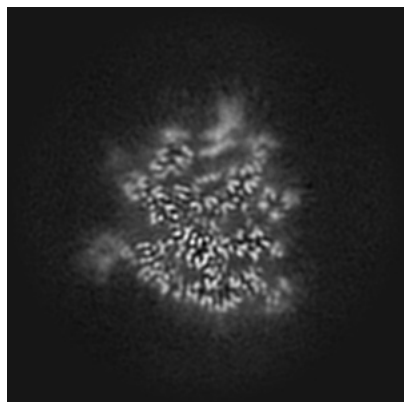


Z Index: 160

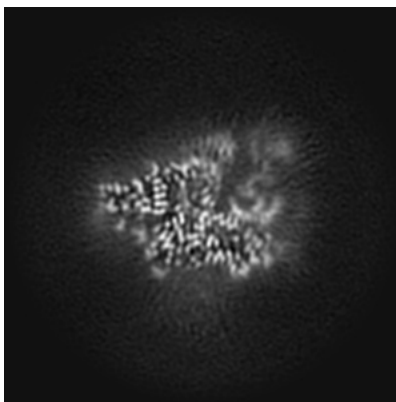
The images above show central slices of the map in three orthogonal directions.

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

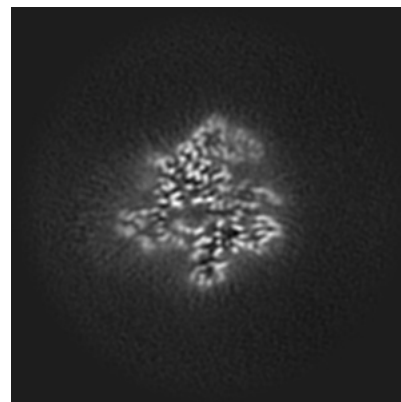
### 6.3.1 Primary map



X Index: 161

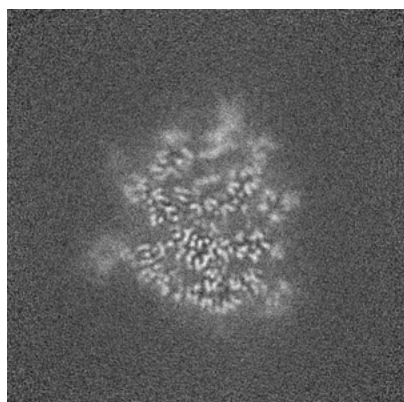


Y Index: 163

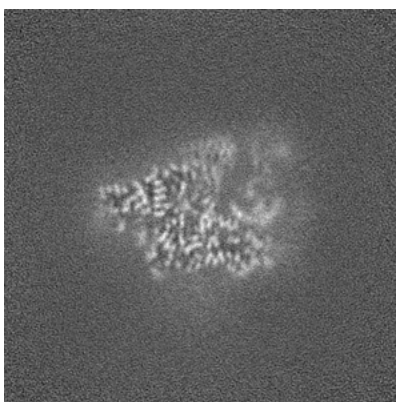


Z Index: 164

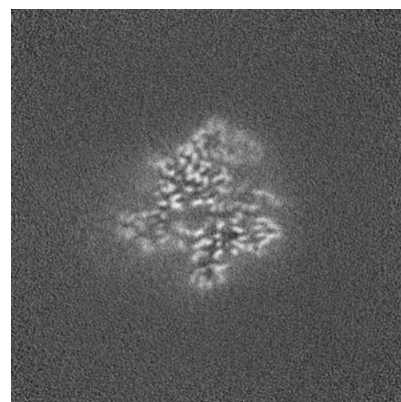
### 6.3.2 Raw map



X Index: 161



Y Index: 164

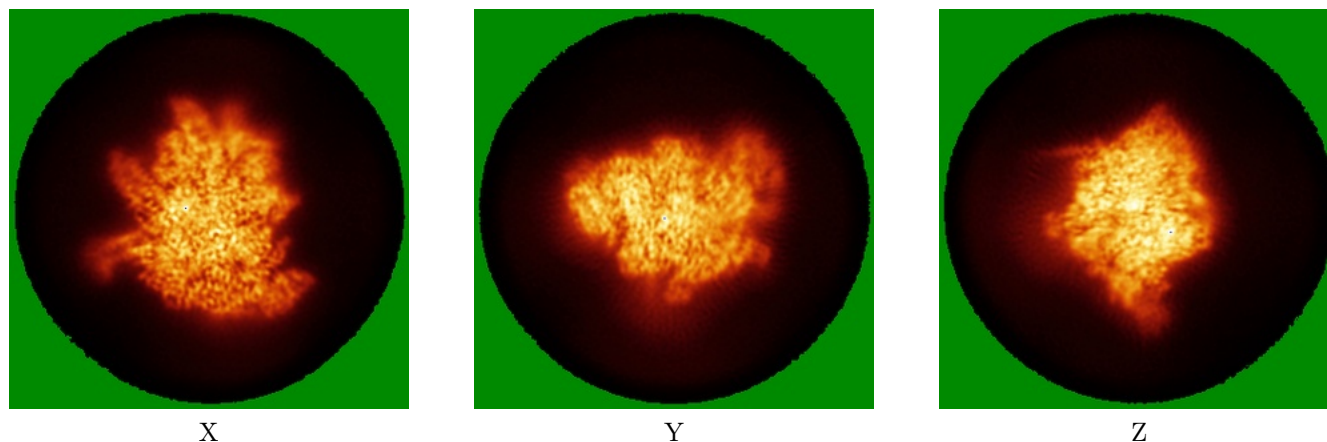


Z Index: 164

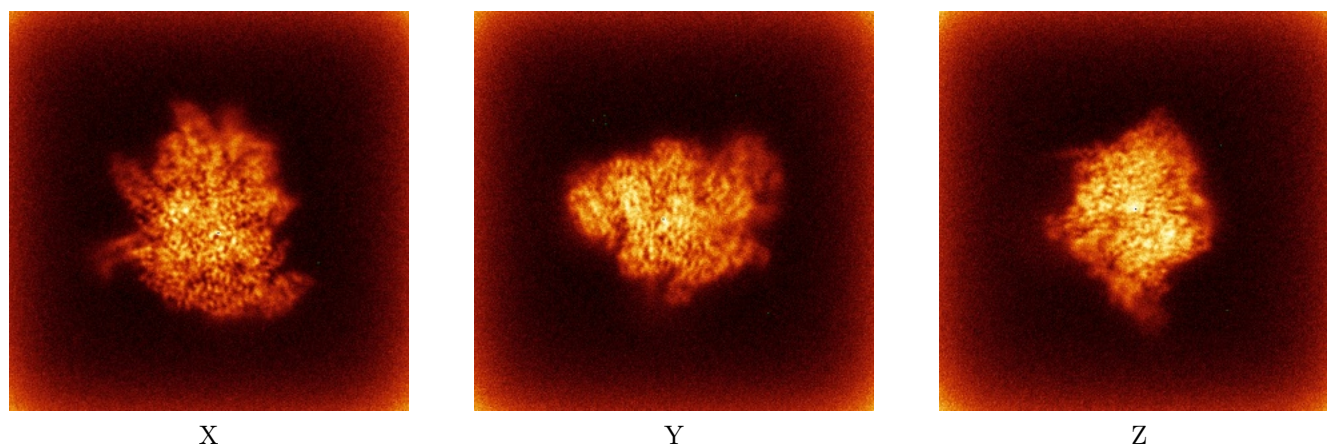
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map

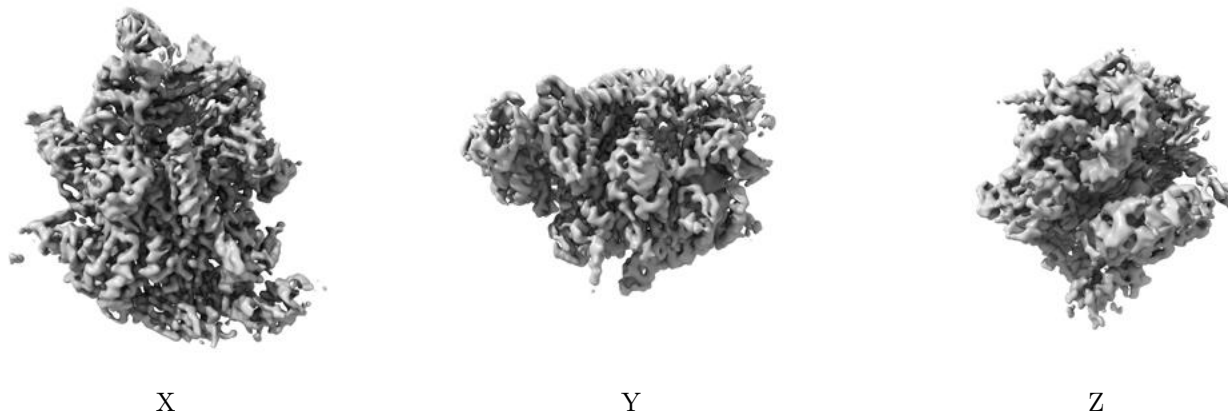


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



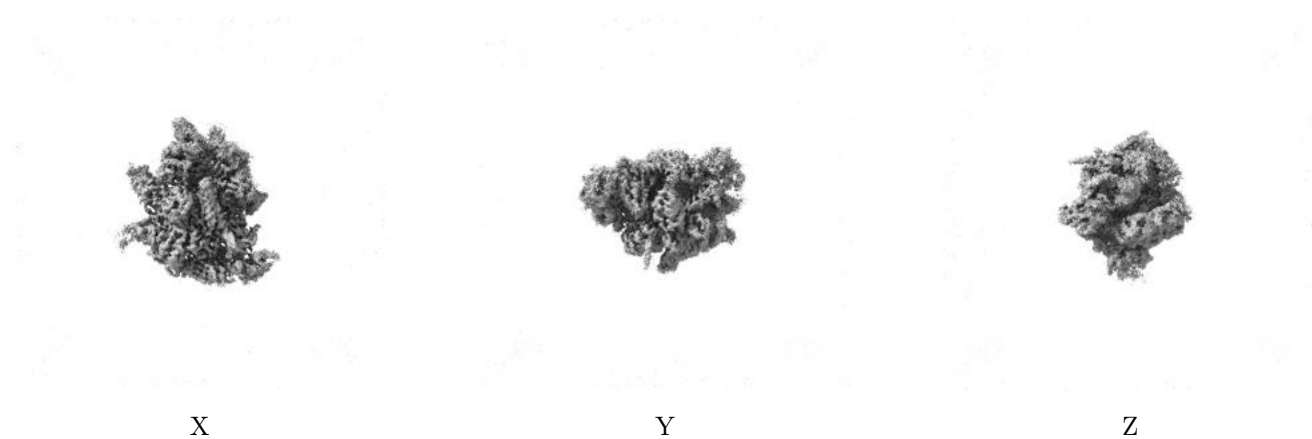
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. 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.

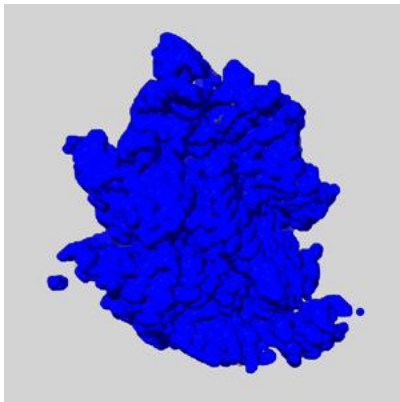
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

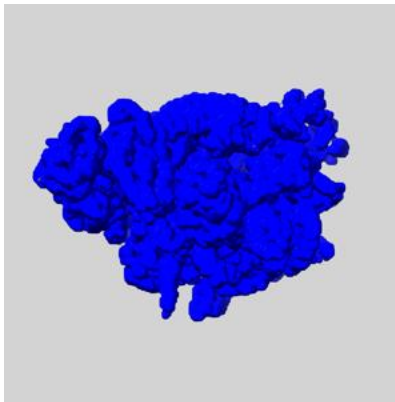
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

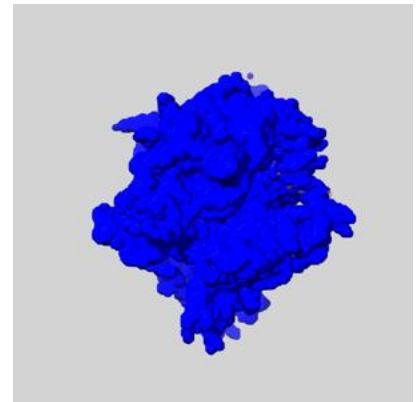
### 6.6.1 emd\_40863\_msk\_1.map [i](#)



X



Y

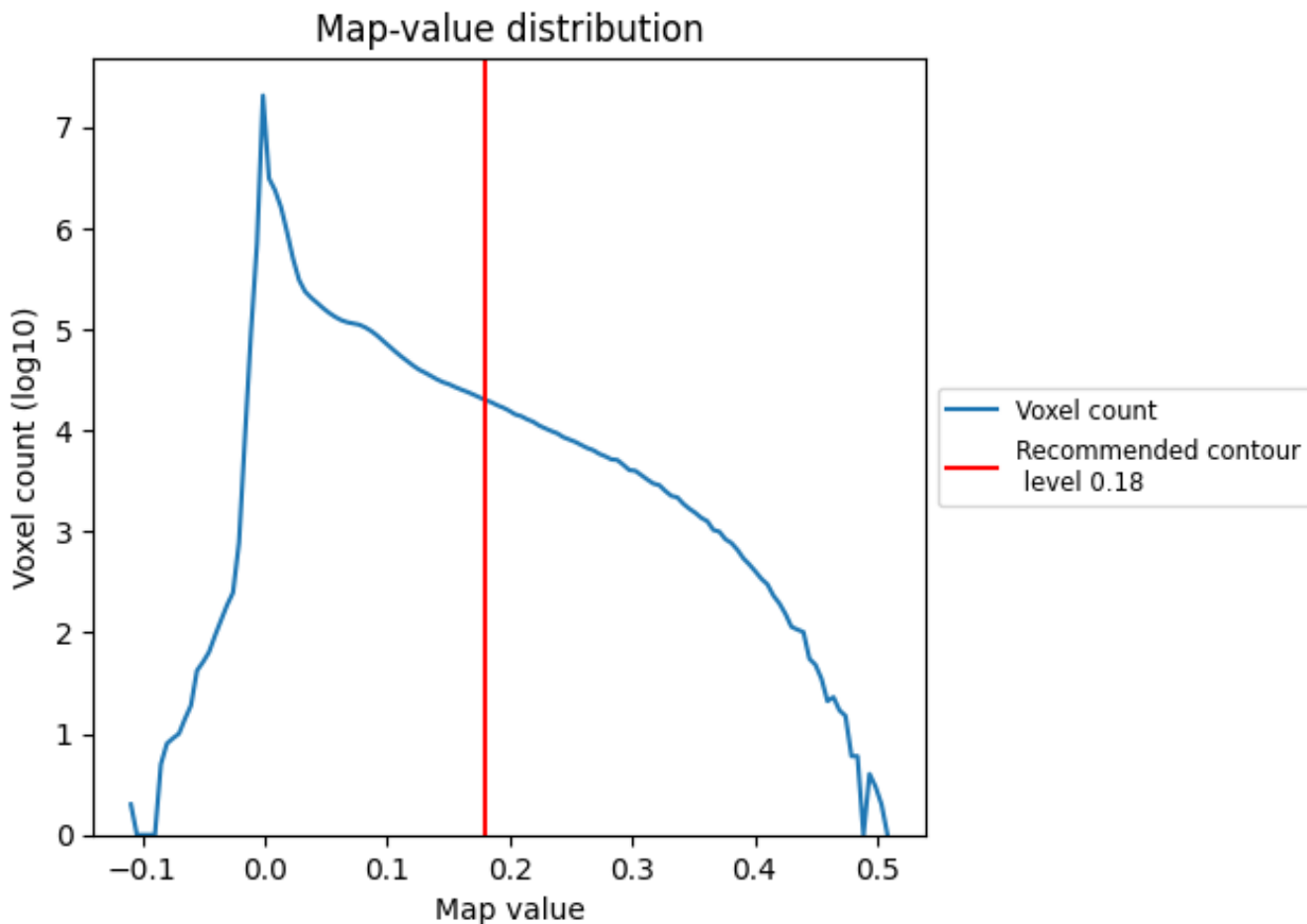


Z

## 7 Map analysis [i](#)

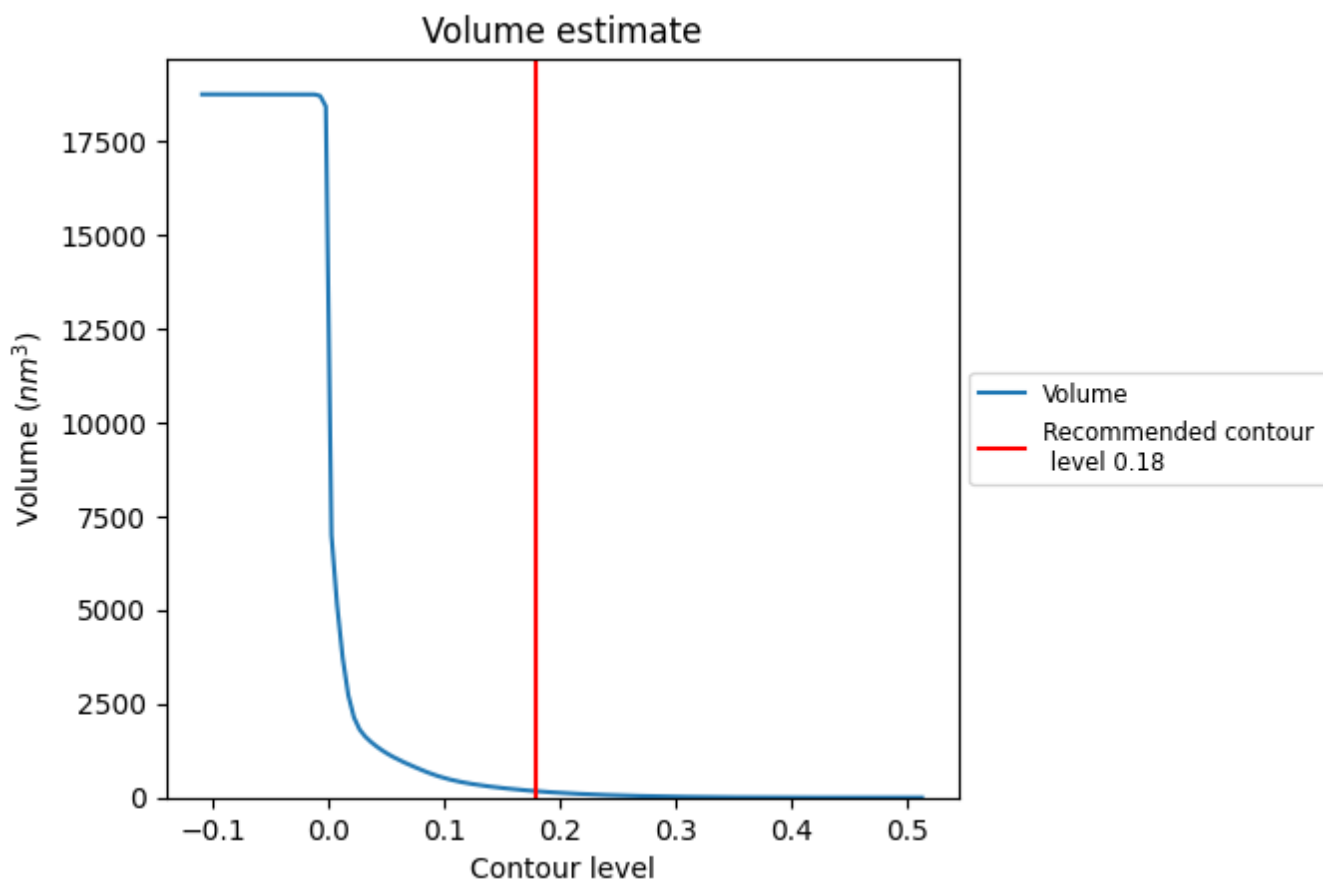
This section contains the results of statistical analysis of the map.

### 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.

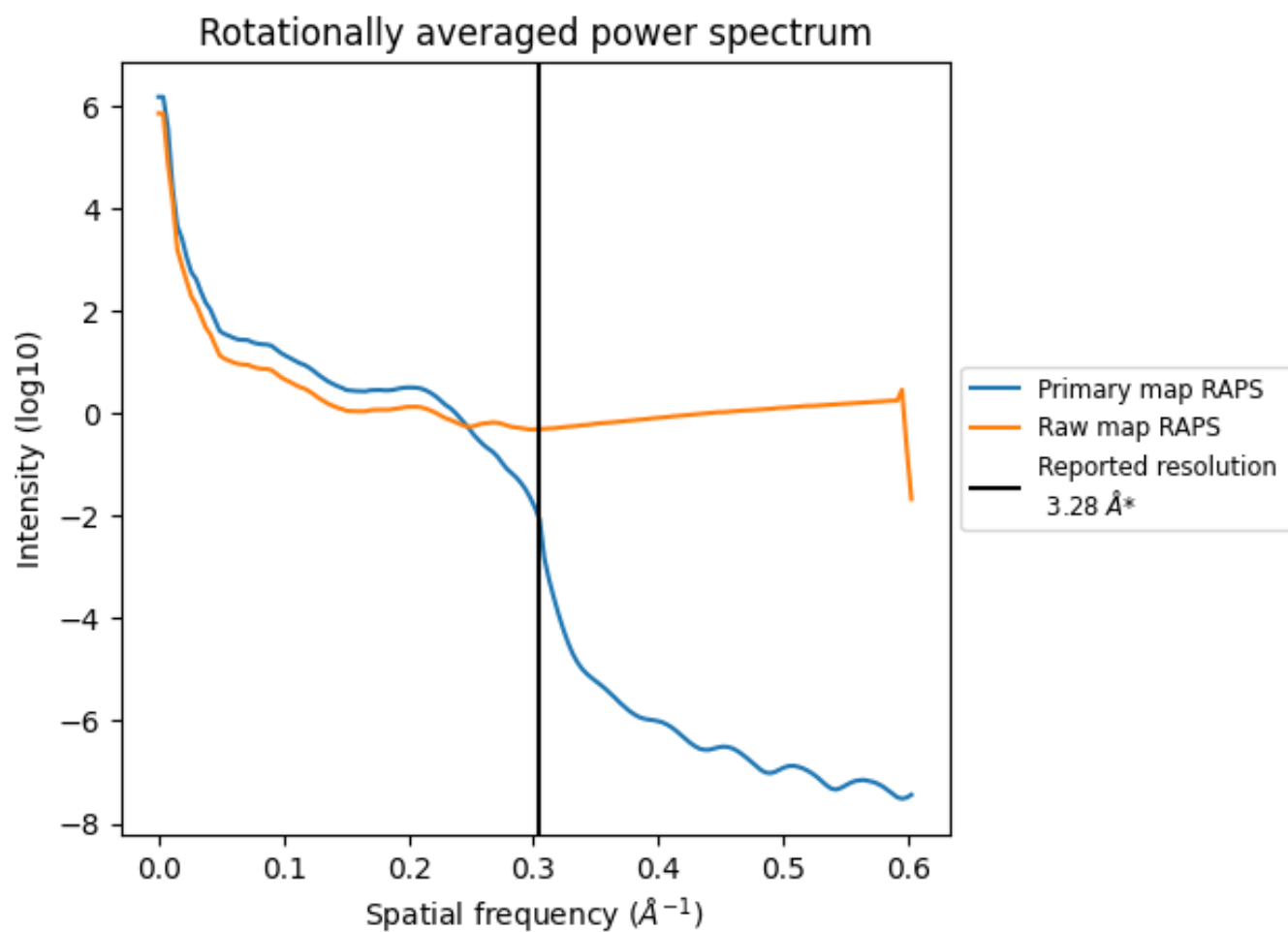
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 170 nm<sup>3</sup>; this corresponds to an approximate mass of 153 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 i

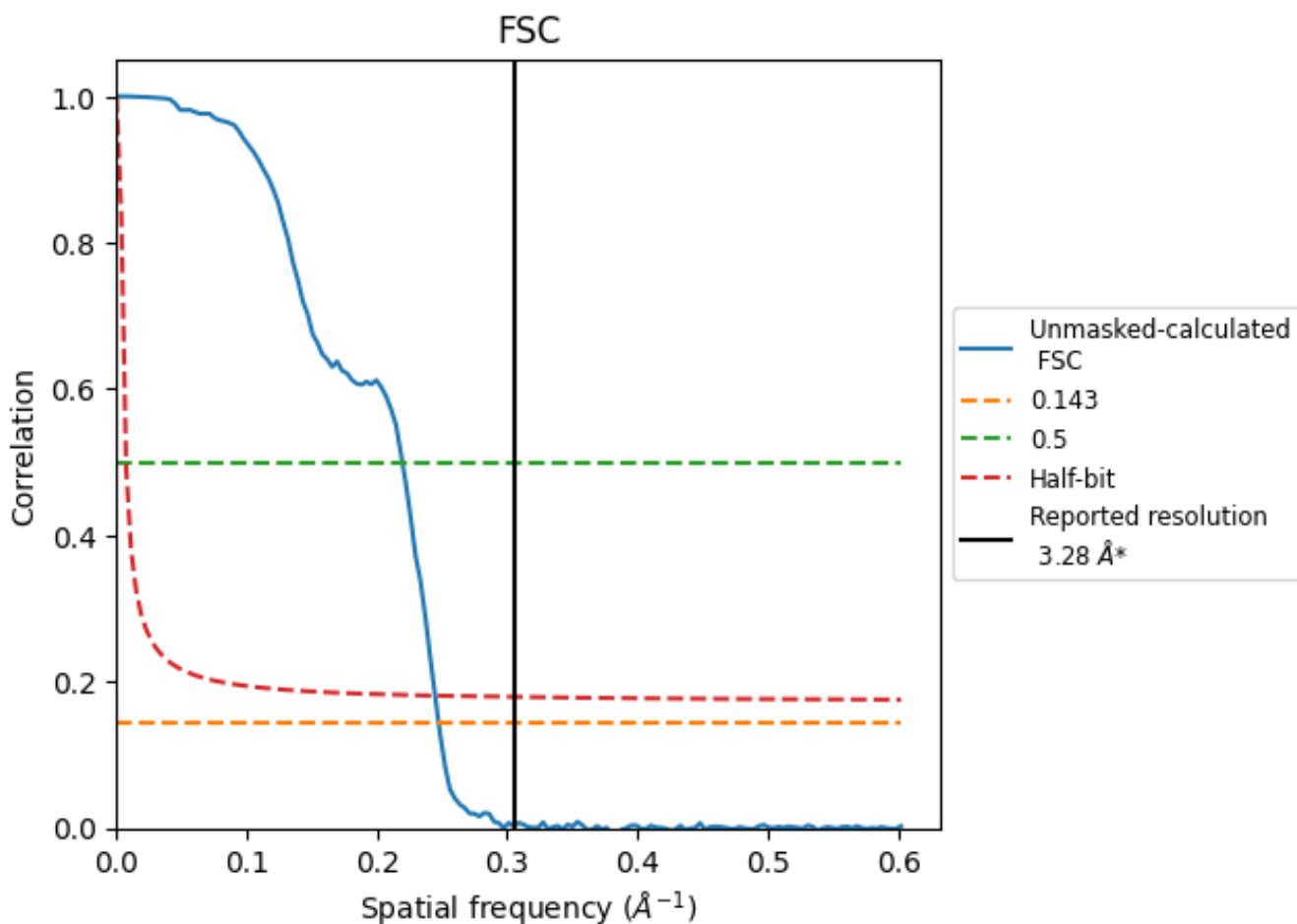


\*Reported resolution corresponds to spatial frequency of 0.305 Å<sup>-1</sup>

## 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  $0.305 \text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

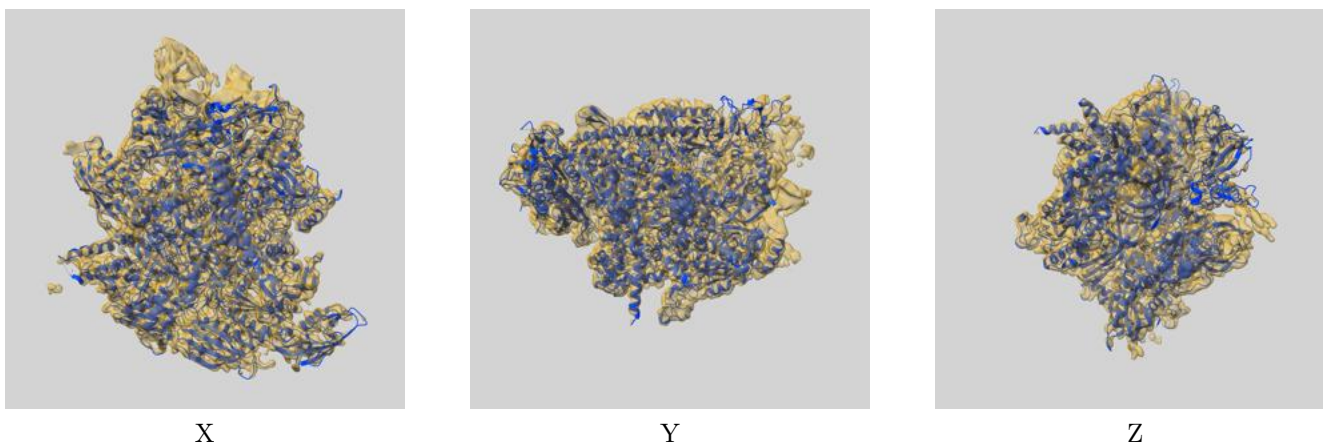
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.04	4.56	4.09

\*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 4.04 differs from the reported value 3.28 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-40863 and PDB model 8SY6. Per-residue inclusion information can be found in section 3 on page 8.

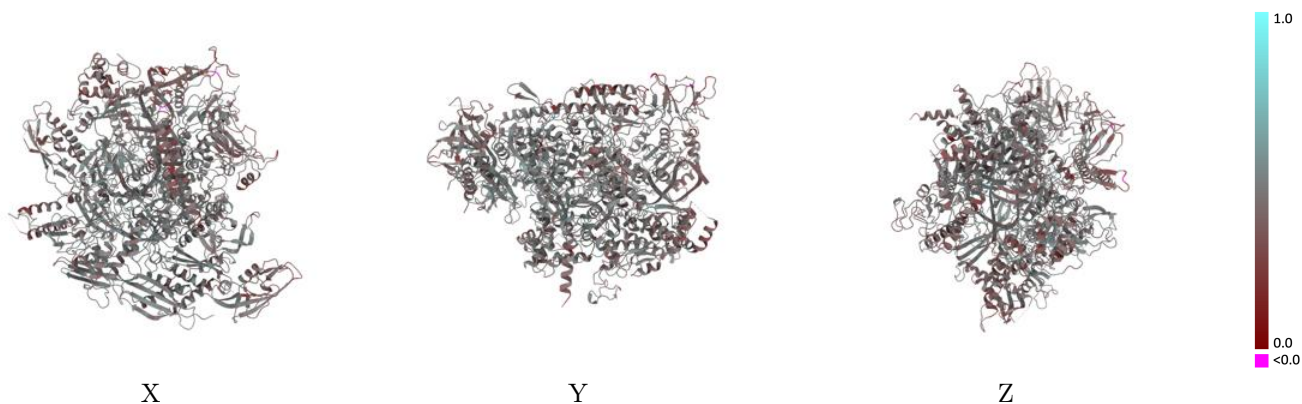
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.18 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.

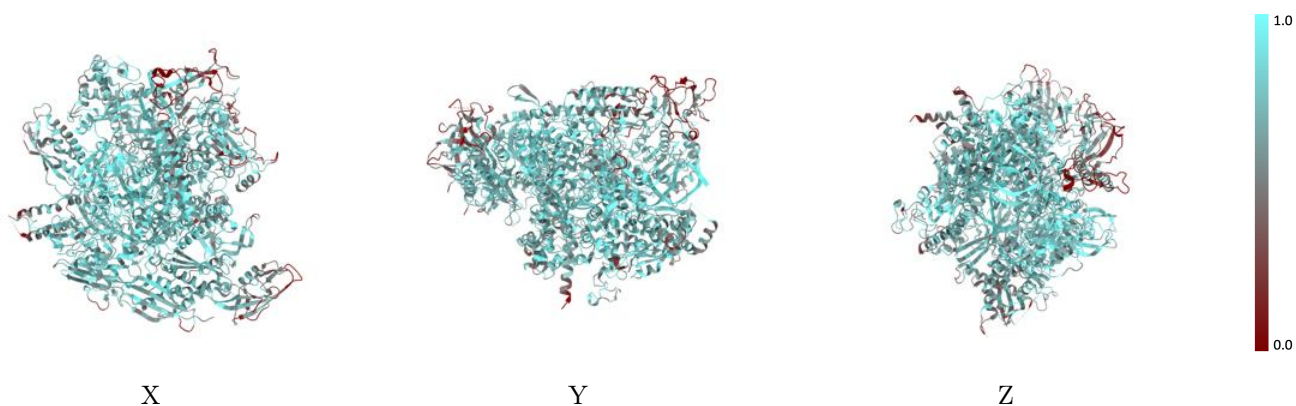


## 9.2 Q-score mapped to coordinate model [i](#)



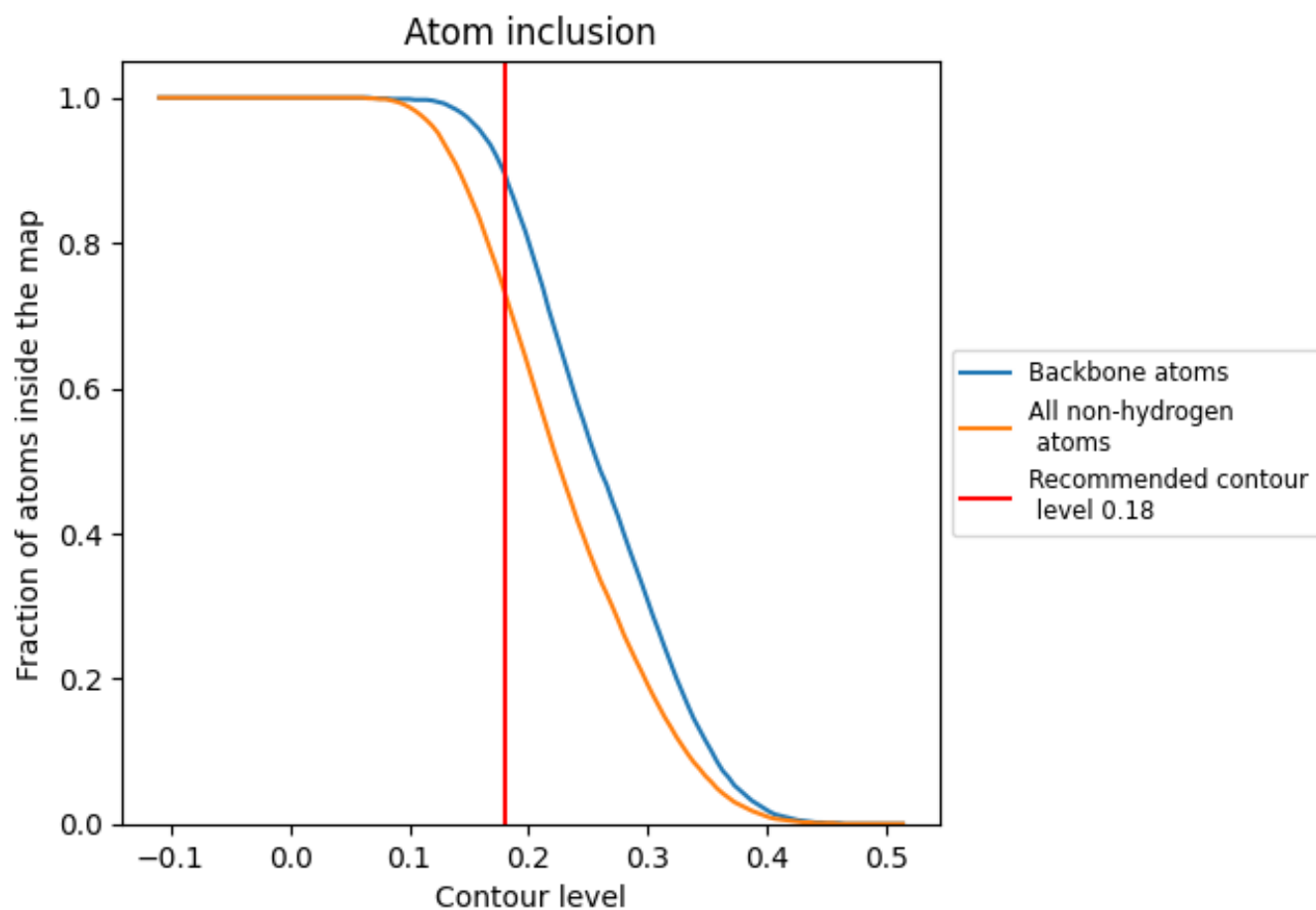
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).



















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 73% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7320	 0.4490
A	 0.5970	 0.4320
G	 0.7230	 0.4730
I	 0.7740	 0.4610
J	 0.7090	 0.4390
K	 0.6050	 0.4350
N	 0.9290	 0.4160
R	 0.9490	 0.4270
T	 0.9530	 0.4430

