



## Full wwPDB EM Validation Report ⓘ

Jul 18, 2024 – 06:30 PM JST

PDB ID : 8XMB  
EMDB ID : EMD-38470  
Title : NTP-bound Pol IV transcription elongation complex  
Authors : Huang, K.; Fang, C.L.; Zhang, Y.  
Deposited on : 2023-12-27  
Resolution : 3.40 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:

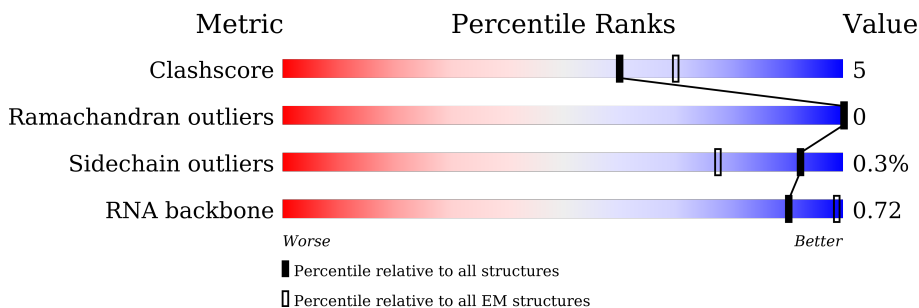
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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.









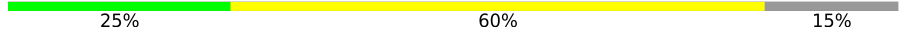
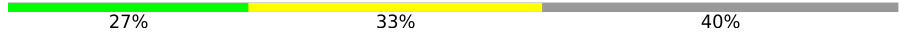

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	A	1498	
2	B	1172	
3	C	319	
4	D	205	
5	E	205	
6	F	144	
7	G	174	

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Mol	Chain	Length	Quality of chain
8	H	146	 73% 12% 14%
9	I	114	 11% 81% 18%
10	J	71	 70% 15% 13%
11	K	116	 72% 9% 19%
12	L	51	 67% 16% 18%
13	M	1133	 11% 80% 13% 7%
14	N	20	 25% 60% 15%
15	O	15	 27% 33% 40%
16	Q	33	 55% 27% 18%

## 2 Entry composition i

There are 19 unique types of molecules in this entry. The entry contains 35299 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase IV subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1159	8582	5452	1487	1589	54	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1454	GLY	-	expression tag	UNP Q9LQ02
A	1455	SER	-	expression tag	UNP Q9LQ02
A	1456	GLY	-	expression tag	UNP Q9LQ02
A	1457	SER	-	expression tag	UNP Q9LQ02
A	1458	GLY	-	expression tag	UNP Q9LQ02
A	1459	SER	-	expression tag	UNP Q9LQ02
A	1460	ASP	-	expression tag	UNP Q9LQ02
A	1461	TYR	-	expression tag	UNP Q9LQ02
A	1462	LYS	-	expression tag	UNP Q9LQ02
A	1463	ASP	-	expression tag	UNP Q9LQ02
A	1464	HIS	-	expression tag	UNP Q9LQ02
A	1465	ASP	-	expression tag	UNP Q9LQ02
A	1466	GLY	-	expression tag	UNP Q9LQ02
A	1467	ASP	-	expression tag	UNP Q9LQ02
A	1468	TYR	-	expression tag	UNP Q9LQ02
A	1469	LYS	-	expression tag	UNP Q9LQ02
A	1470	ASP	-	expression tag	UNP Q9LQ02
A	1471	HIS	-	expression tag	UNP Q9LQ02
A	1472	ASP	-	expression tag	UNP Q9LQ02
A	1473	ILE	-	expression tag	UNP Q9LQ02
A	1474	ASP	-	expression tag	UNP Q9LQ02
A	1475	TYR	-	expression tag	UNP Q9LQ02
A	1476	LYS	-	expression tag	UNP Q9LQ02
A	1477	ASP	-	expression tag	UNP Q9LQ02
A	1478	ASP	-	expression tag	UNP Q9LQ02
A	1479	ASP	-	expression tag	UNP Q9LQ02
A	1480	ASP	-	expression tag	UNP Q9LQ02
A	1481	LYS	-	expression tag	UNP Q9LQ02

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1482	GLU	-	expression tag	UNP Q9LQ02
A	1483	ASN	-	expression tag	UNP Q9LQ02
A	1484	LEU	-	expression tag	UNP Q9LQ02
A	1485	TYR	-	expression tag	UNP Q9LQ02
A	1486	PHE	-	expression tag	UNP Q9LQ02
A	1487	GLN	-	expression tag	UNP Q9LQ02
A	1488	GLY	-	expression tag	UNP Q9LQ02
A	1489	HIS	-	expression tag	UNP Q9LQ02
A	1490	HIS	-	expression tag	UNP Q9LQ02
A	1491	HIS	-	expression tag	UNP Q9LQ02
A	1492	HIS	-	expression tag	UNP Q9LQ02
A	1493	HIS	-	expression tag	UNP Q9LQ02
A	1494	HIS	-	expression tag	UNP Q9LQ02
A	1495	HIS	-	expression tag	UNP Q9LQ02
A	1496	HIS	-	expression tag	UNP Q9LQ02
A	1497	HIS	-	expression tag	UNP Q9LQ02
A	1498	HIS	-	expression tag	UNP Q9LQ02

- Molecule 2 is a protein called DNA-directed RNA polymerases IV and V subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1064	8080	5148	1459	1425	48	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases II, IV and V subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	291	2148	1367	372	395	14	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerases IV and V subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	113	869	550	139	173	7	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases II and IV subunit 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	198	1505	973	269	254	9	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases II, IV and V subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	76	568	363	101	101	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	174	1096	707	185	200	4	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases II, IV and V subunit 8B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	126	949	624	155	163	7	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerases II, IV and V subunit 9A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	113	823	505	156	150	12	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases II, IV and V subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	62	476	310	84	76	6	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerases II, IV and V subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	94	715	458	131	125	1	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerases II, IV and V subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	42	312	192	59	57	4	0	0

- Molecule 13 is a protein called RNA-dependent RNA polymerase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	1052	8044	5139	1378	1476	51	0	0

- Molecule 14 is a DNA chain called Nontemplate\_DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	N	17	351	168	60	106	17	0	0

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
15	O	9	197	88	40	60	9	0	0

- Molecule 16 is a DNA chain called Template\_DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	Q	27	541	259	95	160	27	0	0

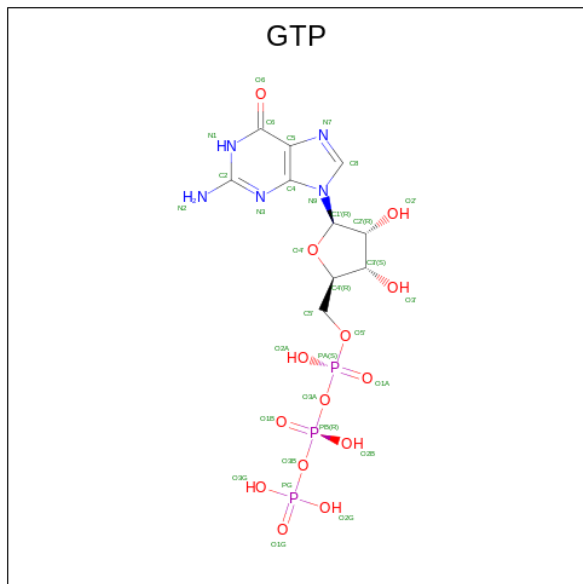
- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	A	3	Total	Zn	0
			3	3	
17	B	1	Total	Zn	0
			1	1	
17	C	1	Total	Zn	0
			1	1	
17	I	2	Total	Zn	0
			2	2	
17	J	1	Total	Zn	0
			1	1	
17	L	1	Total	Zn	0
			1	1	

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
18	A	2	Total	Mg	0
			2	2	

- Molecule 19 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ) (labeled as "Ligand of Interest" by depositor).



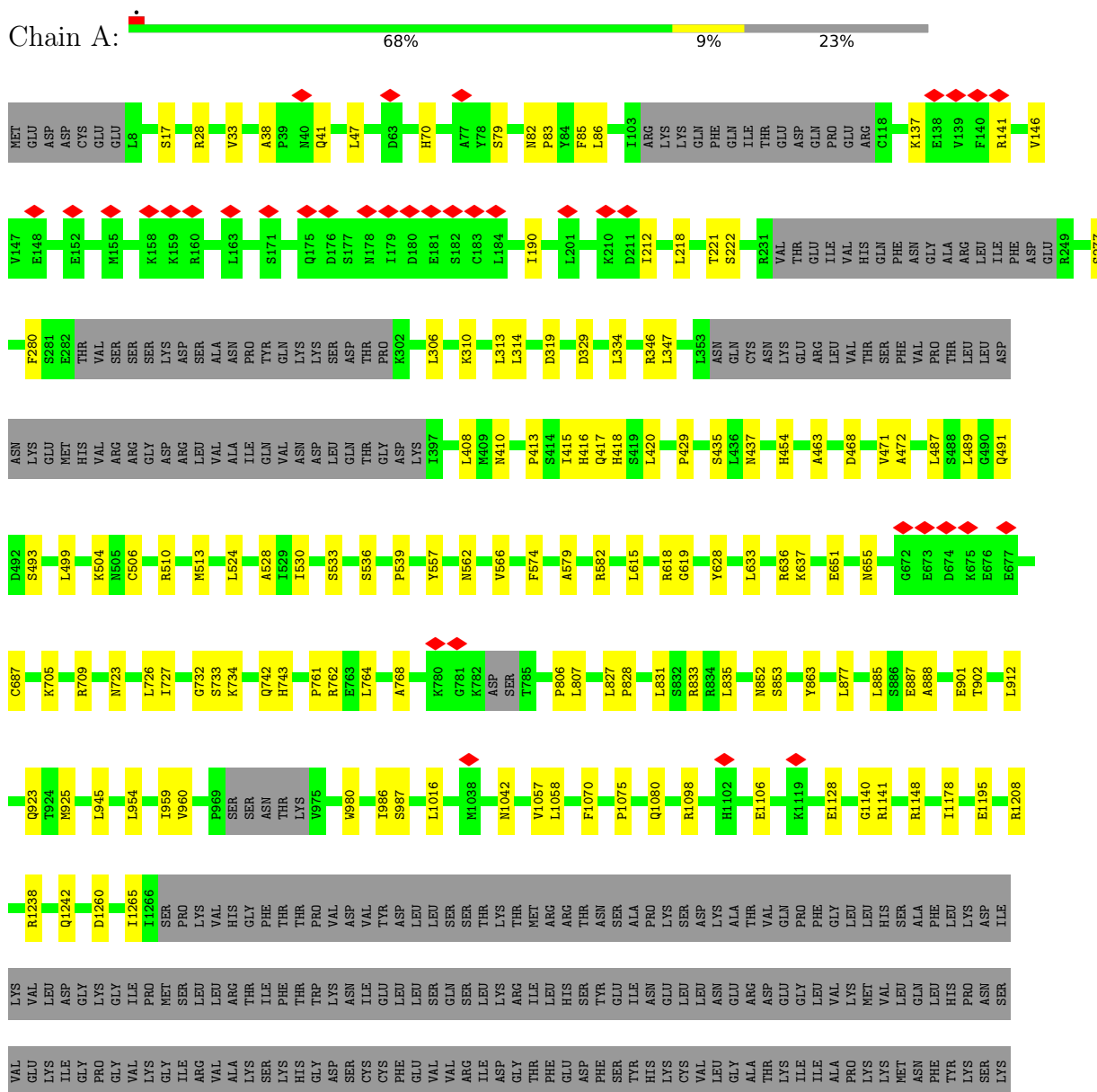
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
19	Q	1	32	10	5	14	3	0



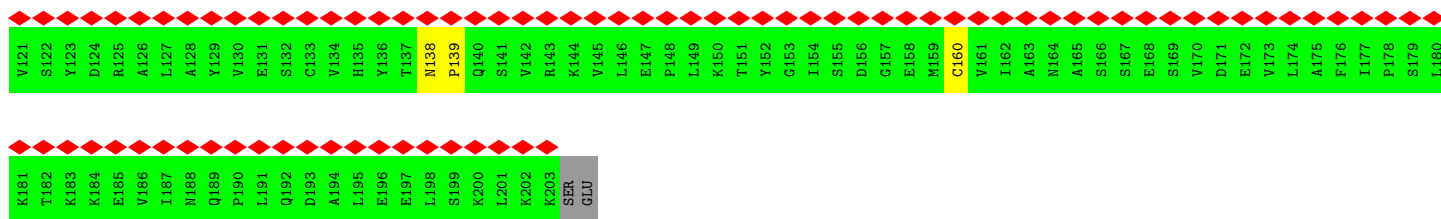
### 3 Residue-property plots

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: DNA-directed RNA polymerase IV subunit 1







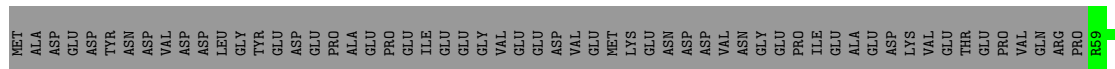
- Molecule 5: DNA-directed RNA polymerases II and IV subunit 5A

Chain E: 87% 9%



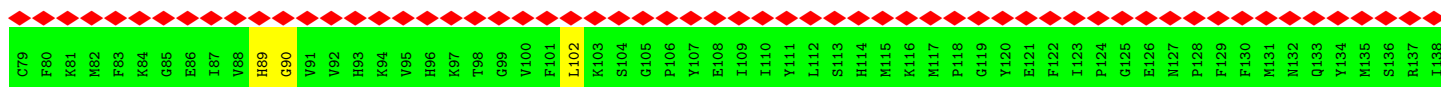
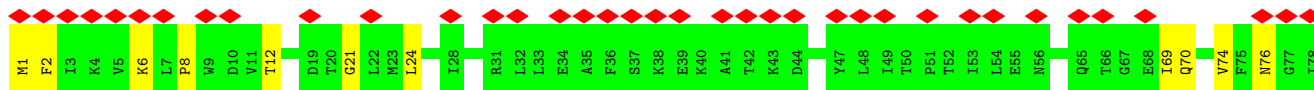
- Molecule 6: DNA-directed RNA polymerases II, IV and V subunit 6A

Chain F: 50% 47%



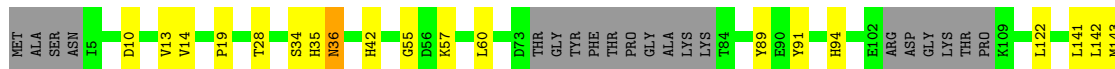
- Molecule 7: DNA-directed RNA polymerase IV subunit 7

Chain G: 75% 90% 10%

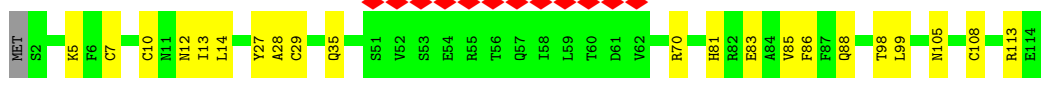
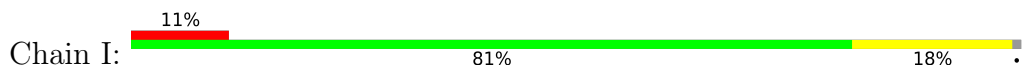


- Molecule 8: DNA-directed RNA polymerases II, IV and V subunit 8B

Chain H: 73% 12% 14%



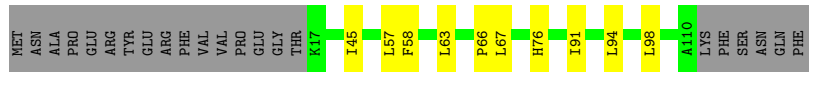
- Molecule 9: DNA-directed RNA polymerases II, IV and V subunit 9A



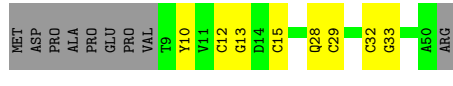
• Molecule 10: DNA-directed RNA polymerases II, IV and V subunit 10



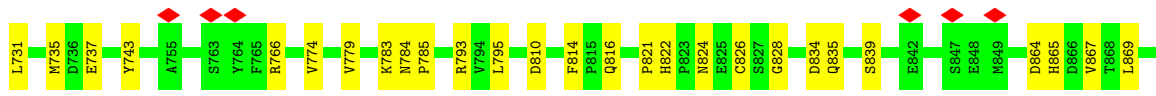
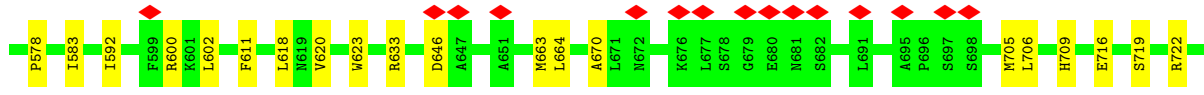
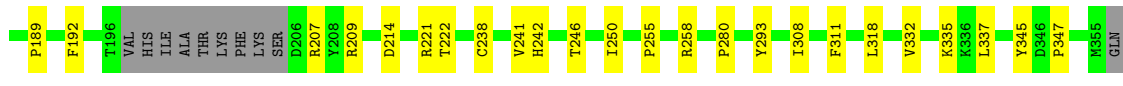
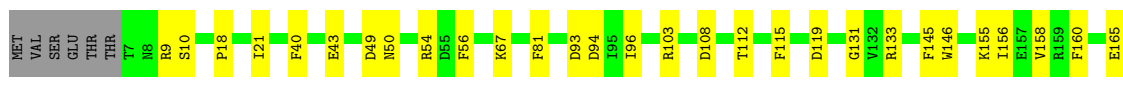
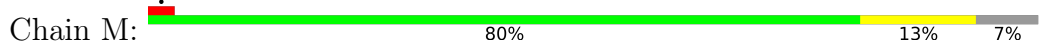
• Molecule 11: DNA-directed RNA polymerases II, IV and V subunit 11

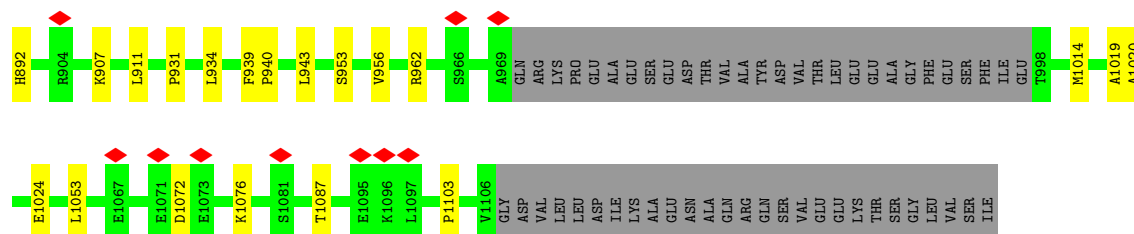


• Molecule 12: DNA-directed RNA polymerases II, IV and V subunit 12

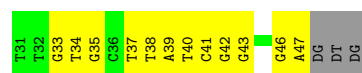


• Molecule 13: RNA-dependent RNA polymerase 2

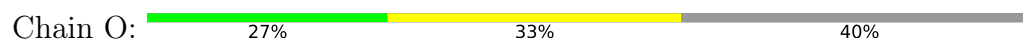




- Molecule 14: Nontemplate\_DNA



- Molecule 15: RNA



- Molecule 16: Template\_DNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	89938	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.064	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.008	Depositor
Map size ( $\text{\AA}$ )	281.6, 281.6, 281.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.1, 1.1, 1.1	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, 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	A	0.24	0/8747	0.45	0/11890
2	B	0.24	0/8250	0.46	0/11161
3	C	0.24	0/2178	0.48	0/2954
4	D	0.23	0/881	0.40	0/1190
5	E	0.24	0/1529	0.47	0/2073
6	F	0.24	0/578	0.48	0/783
7	G	0.25	0/1112	0.44	0/1528
8	H	0.25	0/964	0.46	0/1297
9	I	0.24	0/839	0.50	0/1139
10	J	0.23	0/483	0.49	0/654
11	K	0.23	0/729	0.43	0/992
12	L	0.23	0/315	0.50	0/423
13	M	0.24	0/8213	0.46	0/11127
14	N	0.47	0/392	1.03	0/604
15	O	0.19	0/221	0.75	0/343
16	Q	0.53	0/604	0.88	0/926
All	All	0.25	0/36035	0.48	0/49084

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8582	0	8230	86	0
2	B	8080	0	7823	77	0
3	C	2148	0	2129	18	0
4	D	869	0	887	4	0
5	E	1505	0	1474	11	0
6	F	568	0	542	2	0
7	G	1096	0	896	10	0
8	H	949	0	922	10	0
9	I	823	0	720	13	0
10	J	476	0	484	10	0
11	K	715	0	681	8	0
12	L	312	0	278	5	0
13	M	8044	0	7734	82	0
14	N	351	0	195	11	0
15	O	197	0	97	5	0
16	Q	541	0	303	5	0
17	A	3	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	2	0	0	0	0
19	Q	32	0	12	2	0
All	All	35299	0	33407	321	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 5.

All (321) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:PRO:HG3	19:Q:101:GTP:HN22	1.46	0.80
2:B:1049:LYS:HE2	2:B:1072:GLY:H	1.45	0.79
1:A:489:LEU:HB3	1:A:493:SER:HB2	1.73	0.71
1:A:528:ALA:HA	8:H:94:HIS:HB3	1.73	0.71
14:N:41:DC:H2'	14:N:42:DG:C8	2.26	0.70
1:A:137:LYS:HA	1:A:141:ARG:HA	1.75	0.68
1:A:417:GLN:O	2:B:1086:HIS:NE2	2.26	0.68
14:N:42:DG:H2''	14:N:43:DG:H5'	1.78	0.65
8:H:35:HIS:O	8:H:36:ASN:ND2	2.29	0.64
16:Q:19:DC:N3	19:Q:101:GTP:N1	2.38	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:774:VAL:HG22	2:B:944:ILE:HB	1.79	0.64
9:I:10:CYS:SG	9:I:12:ASN:ND2	2.70	0.64
1:A:429:PRO:HD2	11:K:67:LEU:HD13	1.79	0.64
3:C:297:ARG:HB2	11:K:91:ILE:HG21	1.78	0.63
14:N:41:DC:H2'	14:N:42:DG:H8	1.61	0.62
13:M:1087:THR:HG21	13:M:1103:PRO:HG2	1.81	0.61
2:B:226:LYS:HD3	2:B:577:ASN:HB3	1.81	0.61
1:A:17:SER:HB2	1:A:1238:ARG:HE	1.65	0.61
1:A:1128:GLU:OE1	5:E:9:ARG:NH1	2.33	0.61
5:E:77:VAL:HB	5:E:81:THR:HG21	1.82	0.60
14:N:33:DG:H2''	14:N:34:DT:H5''	1.83	0.60
5:E:113:ILE:HG13	5:E:122:LEU:HD12	1.82	0.60
2:B:963:ALA:HB1	2:B:1033:GLY:HA3	1.82	0.60
14:N:38:DT:H2''	14:N:39:DA:H2'	1.83	0.60
13:M:735:MET:HG2	13:M:814:PHE:HB2	1.84	0.60
1:A:742:GLN:HE21	2:B:955:GLN:HE22	1.48	0.59
13:M:119:ASP:HA	13:M:345:TYR:HB3	1.83	0.59
8:H:13:VAL:HG22	8:H:57:LYS:HG2	1.84	0.59
10:J:3:ILE:HD12	10:J:18:TRP:HB2	1.83	0.59
13:M:633:ARG:NH2	13:M:719:SER:O	2.36	0.59
2:B:771:ASN:HD21	10:J:51:THR:HG21	1.66	0.59
2:B:354:LEU:O	2:B:368:LYS:NZ	2.37	0.58
8:H:19:PRO:HG2	8:H:28:THR:HG22	1.84	0.58
7:G:21:GLY:HA2	7:G:24:LEU:HD23	1.85	0.58
13:M:318:LEU:HD11	13:M:347:PRO:HG2	1.85	0.58
13:M:108:ASP:HA	13:M:131:GLY:HA2	1.85	0.58
2:B:516:ARG:NH1	2:B:667:GLU:OE1	2.37	0.58
1:A:212:ILE:HG21	1:A:218:LEU:HD21	1.85	0.57
8:H:10:ASP:OD2	8:H:34:SER:OG	2.22	0.57
1:A:1098:ARG:HH22	1:A:1140:GLY:HA3	1.69	0.57
12:L:28:GLN:HE21	12:L:33:GLY:HA2	1.70	0.57
1:A:1148:ARG:NH2	1:A:1195:GLU:OE2	2.37	0.57
2:B:790:MET:HG2	2:B:944:ILE:HG12	1.87	0.57
2:B:629:ARG:NH2	2:B:667:GLU:OE2	2.38	0.57
6:F:108:ARG:NH2	6:F:129:ASP:O	2.33	0.57
13:M:133:ARG:HB3	13:M:146:TRP:HB2	1.87	0.57
1:A:506:CYS:SG	2:B:1027:ARG:NH2	2.77	0.57
4:D:92:MET:SD	4:D:92:MET:N	2.76	0.57
9:I:98:THR:HG21	9:I:113:ARG:HH21	1.70	0.56
9:I:5:LYS:HG3	9:I:14:LEU:HD12	1.88	0.56
2:B:749:GLN:NE2	2:B:771:ASN:OD1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:783:LYS:NZ	13:M:835:GLN:O	2.35	0.56
16:Q:8:DG:H2''	16:Q:9:DA:C8	2.40	0.56
13:M:558:GLY:HA3	13:M:592:ILE:HG22	1.87	0.56
13:M:821:PRO:HG2	13:M:824:ASN:HB2	1.88	0.56
13:M:892:HIS:HA	13:M:911:LEU:HD13	1.87	0.56
12:L:12:CYS:SG	12:L:13:GLY:N	2.78	0.55
1:A:346:ARG:O	2:B:1052:ASN:ND2	2.39	0.55
3:C:158:ARG:HE	10:J:60:LEU:HB3	1.70	0.55
2:B:414:HIS:HB3	2:B:448:ILE:HG12	1.88	0.55
13:M:705:MET:O	13:M:709:HIS:ND1	2.39	0.55
1:A:562:ASN:HD21	1:A:579:ALA:HB3	1.71	0.55
3:C:62:LEU:HD12	3:C:155:VAL:HG12	1.88	0.55
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.89	0.55
14:N:37:DT:H2''	14:N:38:DT:H5''	1.88	0.55
12:L:29:CYS:SG	12:L:32:CYS:HB3	2.46	0.55
1:A:582:ARG:HD3	1:A:732:GLY:HA3	1.90	0.54
3:C:99:CYS:HB3	3:C:103:SER:H	1.72	0.54
13:M:221:ARG:NH1	13:M:422:GLU:OE2	2.40	0.54
2:B:718:GLN:NE2	2:B:916:SER:O	2.40	0.54
3:C:186:VAL:HG12	3:C:270:VAL:HA	1.89	0.54
7:G:154:ARG:H	7:G:158:LYS:HA	1.73	0.54
4:D:91:CYS:N	7:G:2:PHE:O	2.41	0.53
1:A:510:ARG:NH2	11:K:57:LEU:O	2.41	0.53
13:M:9:ARG:O	13:M:67:LYS:NZ	2.34	0.53
1:A:960:VAL:HA	1:A:986:ILE:HG12	1.91	0.53
3:C:190:TYR:HB2	3:C:240:TYR:OH	2.09	0.53
2:B:859:ILE:HG13	2:B:874:LYS:HG2	1.90	0.53
1:A:306:LEU:HD21	1:A:833:ARG:HH22	1.74	0.53
13:M:531:VAL:HG11	13:M:602:LEU:HD22	1.90	0.53
14:N:34:DT:H2''	14:N:35:DG:H5''	1.90	0.53
2:B:674:TRP:HB3	2:B:693:LEU:HD21	1.91	0.52
13:M:663:MET:HG3	13:M:670:ALA:HA	1.91	0.52
13:M:388:PRO:HB3	13:M:450:ILE:HD12	1.90	0.52
1:A:734:LYS:HG3	2:B:953:SER:HB2	1.92	0.52
9:I:14:LEU:HD23	9:I:29:CYS:HB3	1.92	0.52
3:C:286:ILE:HG23	11:K:98:LEU:HD22	1.92	0.51
13:M:373:LEU:O	13:M:377:ASN:ND2	2.43	0.51
13:M:377:ASN:HB3	13:M:401:ALA:HB3	1.93	0.51
1:A:1075:PRO:HD3	1:A:1080:GLN:HE21	1.75	0.51
2:B:220:GLN:HE22	2:B:496:GLN:HE21	1.58	0.51
1:A:47:LEU:HA	1:A:70:HIS:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:104:VAL:HG11	3:C:132:VAL:HG11	1.93	0.51
13:M:373:LEU:HA	13:M:377:ASN:HA	1.92	0.51
13:M:332:VAL:HA	13:M:335:LYS:HE3	1.93	0.51
11:K:45:ILE:HD12	11:K:94:LEU:HD21	1.93	0.50
2:B:577:ASN:HD21	2:B:622:THR:H	1.59	0.50
2:B:916:SER:HB3	2:B:920:GLN:HB2	1.93	0.50
13:M:50:ASN:O	13:M:207:ARG:NH2	2.45	0.50
14:N:38:DT:H1'	14:N:39:DA:H5'	1.92	0.50
2:B:606:GLU:O	2:B:626:ARG:NH2	2.45	0.50
1:A:1265:ILE:HD12	7:G:69:ILE:HD12	1.94	0.50
2:B:617:GLU:OE2	2:B:619:ARG:NH2	2.45	0.50
1:A:306:LEU:HG	1:A:310:LYS:HE3	1.93	0.50
1:A:513:MET:HG3	1:A:524:LEU:HD11	1.94	0.50
2:B:795:LEU:HD22	2:B:908:PRO:HG2	1.93	0.50
13:M:18:PRO:HB2	13:M:21:ILE:HG23	1.93	0.50
13:M:583:ILE:HD11	13:M:618:LEU:HD11	1.94	0.50
2:B:918:HIS:NE2	2:B:962:GLU:OE1	2.45	0.50
3:C:99:CYS:SG	3:C:100:GLU:N	2.85	0.50
13:M:165:GLU:OE2	13:M:258:ARG:NH2	2.44	0.50
15:O:4:A:H2'	15:O:5:G:C8	2.46	0.50
2:B:1101:ASP:N	2:B:1101:ASP:OD1	2.45	0.49
1:A:499:LEU:HD21	1:A:727:ILE:HD13	1.94	0.49
1:A:764:LEU:HA	1:A:807:LEU:HD23	1.94	0.49
3:C:108:LEU:HD12	3:C:125:LEU:HD13	1.93	0.49
3:C:46:PRO:HB3	3:C:173:ILE:HD13	1.93	0.49
13:M:280:PRO:HG3	13:M:390:LYS:HB2	1.95	0.49
1:A:723:ASN:HB3	1:A:726:LEU:HB2	1.94	0.49
1:A:806:PRO:HG3	2:B:693:LEU:HD23	1.94	0.49
3:C:191:GLU:OE1	3:C:265:SER:OG	2.29	0.49
7:G:6:LYS:HA	7:G:76:ASN:HA	1.95	0.49
15:O:4:A:H2'	15:O:5:G:H8	1.77	0.49
2:B:913:LYS:HD2	2:B:1040:LEU:HD12	1.95	0.49
2:B:634:VAL:HA	2:B:637:LEU:HB2	1.95	0.49
7:G:90:GLY:HA3	7:G:102:LEU:HD21	1.95	0.49
13:M:308:ILE:HD11	13:M:337:LEU:HD21	1.95	0.49
1:A:38:ALA:HB3	1:A:41:GLN:HB3	1.93	0.49
1:A:619:GLY:O	2:B:1028:SER:OG	2.27	0.48
1:A:742:GLN:NE2	2:B:955:GLN:HE22	2.11	0.48
13:M:145:PHE:HB2	13:M:156:ILE:HB	1.95	0.48
5:E:95:PHE:HA	5:E:120:PHE:HD1	1.78	0.48
2:B:917:MET:SD	2:B:1038:GLN:NE2	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:824:ASN:HA	13:M:828:GLY:HA2	1.95	0.48
13:M:378:ILE:HD12	13:M:1053:LEU:HD21	1.96	0.48
13:M:940:PRO:HD2	13:M:943:LEU:HD13	1.96	0.48
8:H:42:HIS:HB2	8:H:122:LEU:HB3	1.95	0.48
8:H:14:VAL:HG23	8:H:55:GLY:H	1.78	0.48
13:M:93:ASP:OD1	13:M:94:ASP:N	2.47	0.48
1:A:1106:GLU:OE2	1:A:1141:ARG:NH1	2.40	0.47
2:B:707:ALA:HB3	2:B:991:PRO:HB3	1.96	0.47
1:A:853:SER:OG	1:A:1242:GLN:O	2.32	0.47
1:A:83:PRO:HA	1:A:86:LEU:HG	1.96	0.47
3:C:71:LEU:HD21	3:C:154:ILE:HD13	1.95	0.47
13:M:241:VAL:HG22	13:M:242:HIS:H	1.78	0.47
13:M:373:LEU:HD21	13:M:379:MET:HB3	1.97	0.47
13:M:469:PHE:HB3	13:M:486:MET:HB3	1.96	0.47
2:B:516:ARG:NH2	2:B:662:ILE:O	2.47	0.47
1:A:980:TRP:NE1	1:A:1058:LEU:O	2.35	0.47
9:I:28:ALA:HB2	9:I:35:GLN:HG2	1.95	0.47
1:A:945:LEU:HD13	9:I:88:GLN:HG3	1.96	0.47
2:B:67:VAL:HG13	2:B:412:ARG:HG2	1.97	0.47
2:B:1097:PHE:HZ	2:B:1146:TYR:HB3	1.79	0.47
8:H:60:LEU:HD11	8:H:141:LEU:HD11	1.97	0.47
13:M:795:LEU:HD21	13:M:822:HIS:HD2	1.79	0.47
13:M:158:VAL:HG22	13:M:189:PRO:HB3	1.95	0.47
13:M:222:THR:HB	13:M:449:ASN:HD22	1.79	0.47
2:B:800:PHE:O	2:B:1039:ARG:NH1	2.48	0.47
16:Q:11:DA:H2''	16:Q:12:DA:H5'	1.97	0.47
13:M:907:LYS:HG3	13:M:934:LEU:HD11	1.96	0.47
13:M:10:SER:HA	13:M:67:LYS:HD2	1.97	0.46
8:H:91:TYR:HB3	8:H:143:MET:HB3	1.96	0.46
1:A:416:HIS:CD2	1:A:418:HIS:HB2	2.50	0.46
1:A:618:ARG:HG3	2:B:1027:ARG:HH11	1.80	0.46
13:M:155:LYS:HB3	13:M:192:PHE:HB2	1.96	0.46
13:M:578:PRO:HG2	13:M:623:TRP:HB2	1.98	0.46
13:M:783:LYS:HG2	13:M:826:CYS:HB3	1.97	0.46
1:A:831:LEU:HD11	1:A:912:LEU:HD12	1.98	0.46
1:A:1075:PRO:HD3	1:A:1080:GLN:NE2	2.31	0.46
13:M:115:PHE:HE2	13:M:311:PHE:HB2	1.79	0.46
13:M:280:PRO:HG2	13:M:391:ILE:HG22	1.98	0.46
1:A:651:GLU:OE2	1:A:655:ASN:ND2	2.47	0.46
2:B:537:LEU:HB3	2:B:630:PRO:HD2	1.97	0.46
5:E:17:LEU:HD11	5:E:100:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:35:LEU:HD13	10:J:46:ARG:HB3	1.98	0.46
13:M:103:ARG:HB3	13:M:250:ILE:HD11	1.97	0.46
13:M:1020:ALA:N	13:M:1024:GLU:OE2	2.37	0.46
2:B:278:PRO:HD2	2:B:281:LEU:HD12	1.97	0.46
1:A:277:SER:HB3	1:A:280:PHE:HD1	1.81	0.46
5:E:50:ARG:NH1	5:E:127:GLU:OE2	2.48	0.46
13:M:520:GLN:HE21	13:M:611:PHE:HE1	1.63	0.46
1:A:79:SER:HA	1:A:221:THR:HG22	1.98	0.45
1:A:633:LEU:HG	1:A:637:LYS:HE3	1.98	0.45
13:M:384:ALA:HB3	13:M:418:VAL:HG22	1.97	0.45
1:A:491:GLN:HB2	1:A:733:SER:HB3	1.98	0.45
1:A:347:LEU:HD21	2:B:1050:PHE:HB2	1.99	0.45
13:M:214:ASP:OD1	13:M:214:ASP:N	2.49	0.45
1:A:408:LEU:HD11	1:A:420:LEU:HB3	1.98	0.45
7:G:8:PRO:HA	7:G:74:VAL:HA	1.99	0.45
9:I:81:HIS:CE1	9:I:83:GLU:HB3	2.51	0.45
1:A:415:ILE:HG13	1:A:416:HIS:ND1	2.30	0.45
13:M:49:ASP:OD1	13:M:49:ASP:N	2.50	0.45
1:A:410:ASN:HD22	1:A:454:HIS:CE1	2.35	0.45
1:A:954:LEU:HD21	1:A:959:ILE:HD11	1.98	0.45
2:B:365:LEU:HD12	2:B:368:LYS:HD2	1.98	0.45
2:B:491:ARG:NH2	2:B:535:SER:O	2.36	0.45
1:A:33:VAL:HA	2:B:1134:ARG:HH11	1.82	0.45
1:A:533:SER:HB2	1:A:536:SER:HB3	1.98	0.45
2:B:1158:LEU:HA	2:B:1161:MET:HG2	1.99	0.45
3:C:52:LEU:HD23	3:C:168:ILE:HD11	1.98	0.45
8:H:89:TYR:CG	8:H:142:LEU:HB3	2.52	0.44
13:M:537:GLU:HB3	13:M:600:ARG:NH2	2.32	0.44
1:A:82:ASN:HB3	1:A:85:PHE:HD2	1.82	0.44
2:B:510:HIS:CG	2:B:511:PRO:HD2	2.52	0.44
4:D:160:CYS:SG	7:G:1:MET:N	2.71	0.44
13:M:931:PRO:HG2	13:M:934:LEU:HB2	1.99	0.44
14:N:39:DA:C8	14:N:40:DT:H72	2.52	0.44
2:B:586:ASP:OD1	2:B:586:ASP:N	2.43	0.44
2:B:722:HIS:CE1	2:B:915:SER:HG	2.34	0.44
3:C:158:ARG:HG2	10:J:60:LEU:HD22	1.99	0.44
13:M:716:GLU:OE2	13:M:722:ARG:NH1	2.43	0.44
13:M:864:ASP:OD1	13:M:865:HIS:ND1	2.45	0.44
2:B:722:HIS:CG	2:B:915:SER:HG	2.34	0.44
13:M:18:PRO:HD2	13:M:21:ILE:HD13	1.98	0.44
13:M:160:PHE:HB3	13:M:255:PRO:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:3:G:H2'	15:O:4:A:H8	1.82	0.44
1:A:319:ASP:OD1	2:B:1051:ARG:NE	2.43	0.44
1:A:835:LEU:HD21	1:A:885:LEU:HD12	1.99	0.44
2:B:721:LYS:HD3	15:O:9:U:OP1	2.17	0.44
7:G:12:THR:HA	7:G:70:GLN:HA	2.00	0.44
10:J:30:THR:HG23	10:J:33:ASP:H	1.82	0.44
5:E:21:LEU:HD11	5:E:69:ILE:HD11	2.00	0.43
15:O:3:G:H2'	15:O:4:A:C8	2.53	0.43
1:A:923:GLN:HG3	1:A:925:MET:HE2	1.99	0.43
2:B:315:ILE:HG21	9:I:13:ILE:HG21	1.99	0.43
13:M:867:VAL:HG12	13:M:869:LEU:H	1.83	0.43
6:F:77:ARG:NE	6:F:104:GLU:OE1	2.50	0.43
13:M:737:GLU:OE1	13:M:816:GLN:NE2	2.51	0.43
1:A:557:TYR:HB3	1:A:566:VAL:HB	2.00	0.43
1:A:761:PRO:HB2	1:A:768:ALA:HB1	2.01	0.43
9:I:86:PHE:HB2	9:I:99:LEU:HD11	1.99	0.43
12:L:15:CYS:HB2	12:L:32:CYS:SG	2.57	0.43
1:A:310:LYS:HG2	1:A:314:LEU:HD12	2.01	0.43
13:M:422:GLU:HG2	13:M:423:GLU:H	1.84	0.43
2:B:903:ARG:NH1	3:C:65:GLU:OE1	2.52	0.43
2:B:610:LYS:HB3	2:B:619:ARG:HB3	2.01	0.43
2:B:714:ARG:NH2	2:B:954:ARG:HG2	2.33	0.43
1:A:329:ASP:HB2	1:A:435:SER:HB3	2.01	0.43
2:B:598:ARG:HA	2:B:603:LEU:HB2	2.01	0.43
1:A:146:VAL:HG22	1:A:190:ILE:HG12	2.01	0.43
2:B:1097:PHE:CZ	2:B:1146:TYR:HB3	2.54	0.43
13:M:21:ILE:HG21	13:M:81:PHE:HE2	1.84	0.43
13:M:103:ARG:NH2	13:M:246:THR:O	2.52	0.43
13:M:664:LEU:HA	13:M:706:LEU:HD21	2.00	0.43
1:A:888:ALA:HB2	1:A:1178:ILE:HD11	2.00	0.42
1:A:1260:ASP:OD1	1:A:1260:ASP:N	2.50	0.42
1:A:987:SER:HA	1:A:1042:ASN:HA	2.01	0.42
13:M:646:ASP:HB3	13:M:956:VAL:HG12	2.00	0.42
2:B:236:THR:HB	2:B:251:ARG:HG3	2.02	0.42
13:M:40:PHE:HE2	13:M:96:ILE:HD12	1.84	0.42
16:Q:4:DT:H2'	16:Q:5:DA:C8	2.54	0.42
2:B:634:VAL:HG22	2:B:687:THR:HA	2.01	0.42
3:C:75:PRO:HG3	10:J:13:VAL:HG21	2.01	0.42
13:M:953:SER:O	13:M:962:ARG:NH2	2.52	0.42
1:A:334:LEU:HG	1:A:437:ASN:HD22	1.84	0.42
1:A:743:HIS:NE2	2:B:955:GLN:HG3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:632:LEU:O	2:B:689:CYS:N	2.51	0.42
1:A:334:LEU:HD23	1:A:487:LEU:HD13	2.02	0.42
1:A:615:LEU:O	1:A:619:GLY:N	2.47	0.42
1:A:628:TYR:O	1:A:636:ARG:NH1	2.53	0.42
1:A:687:CYS:HB2	1:A:762:ARG:HD3	2.01	0.42
1:A:705:LYS:O	1:A:709:ARG:HG3	2.18	0.42
2:B:797:ARG:HD2	10:J:8:PHE:HA	2.02	0.42
2:B:990:THR:HB	2:B:993:SER:HB3	2.01	0.42
14:N:46:DG:H2''	14:N:47:DA:C8	2.53	0.42
1:A:852:ASN:OD1	1:A:853:SER:N	2.53	0.42
1:A:901:GLU:HG2	1:A:902:THR:HG22	2.02	0.42
5:E:113:ILE:HD11	5:E:122:LEU:HB2	2.01	0.42
10:J:7:CYS:O	10:J:10:CYS:N	2.52	0.42
1:A:530:ILE:HA	1:A:539:PRO:HB3	2.02	0.42
2:B:237:VAL:HG12	2:B:379:LEU:HD22	2.02	0.42
3:C:289:LEU:HD23	11:K:98:LEU:HD21	2.02	0.42
13:M:766:ARG:O	13:M:774:VAL:N	2.52	0.42
13:M:731:LEU:HD22	13:M:810:ASP:HB3	2.02	0.41
1:A:28:ARG:HD2	1:A:222:SER:HB2	2.01	0.41
2:B:1158:LEU:HD12	2:B:1165:LEU:HD11	2.01	0.41
7:G:89:HIS:HA	7:G:145:ARG:HA	2.00	0.41
9:I:14:LEU:HB3	9:I:27:TYR:HB3	2.02	0.41
1:A:310:LYS:HA	1:A:314:LEU:HB2	2.02	0.41
1:A:468:ASP:HA	1:A:472:ALA:HB2	2.02	0.41
2:B:788:ILE:O	2:B:925:GLY:N	2.42	0.41
1:A:863:TYR:CD1	1:A:877:LEU:HD13	2.55	0.41
1:A:1016:LEU:HD11	1:A:1070:PHE:CG	2.55	0.41
9:I:70:ARG:HG2	9:I:85:VAL:HG12	2.03	0.41
13:M:112:THR:HG23	13:M:238:CYS:HB3	2.02	0.41
13:M:1072:ASP:O	13:M:1076:LYS:N	2.45	0.41
1:A:313:LEU:HD11	2:B:1154:LEU:HD22	2.03	0.41
1:A:463:ALA:HB1	2:B:1091:ASN:ND2	2.36	0.41
13:M:779:VAL:HG13	13:M:839:SER:H	1.85	0.41
2:B:633:VAL:HG12	2:B:688:HIS:CD2	2.55	0.41
2:B:797:ARG:NH1	10:J:8:PHE:O	2.50	0.41
5:E:24:ARG:NH2	5:E:177:TYR:O	2.51	0.41
11:K:63:LEU:HD21	11:K:66:PRO:HA	2.03	0.41
2:B:845:ASP:OD2	12:L:10:TYR:OH	2.26	0.41
14:N:42:DG:C2'	14:N:43:DG:H5'	2.48	0.41
1:A:1208:ARG:HD3	1:A:1208:ARG:HA	1.93	0.41
2:B:359:PHE:HD2	2:B:368:LYS:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:747:TYR:O	2:B:770:GLN:NE2	2.53	0.41
2:B:1080:ARG:HG3	2:B:1092:LEU:HD11	2.03	0.41
13:M:783:LYS:HZ1	13:M:834:ASP:HB2	1.86	0.41
13:M:939:PHE:HD2	13:M:943:LEU:HD22	1.85	0.41
4:D:138:ASN:HB3	4:D:139:PRO:HD3	2.03	0.40
5:E:166:PRO:HB2	5:E:202:ARG:HD2	2.02	0.40
9:I:105:ASN:HD22	9:I:108:CYS:HB2	1.85	0.40
13:M:499:ARG:HH12	13:M:869:LEU:HD22	1.86	0.40
1:A:504:LYS:NZ	1:A:574:PHE:O	2.32	0.40
2:B:362:LEU:HD23	2:B:367:LYS:HB3	2.04	0.40
13:M:474:PHE:HB3	13:M:484:VAL:HG23	2.02	0.40
1:A:454:HIS:O	1:A:454:HIS:ND1	2.54	0.40
1:A:827:LEU:HB2	1:A:828:PRO:HD3	2.03	0.40
2:B:523:PRO:HG2	2:B:531:VAL:HB	2.01	0.40
11:K:58:PHE:HB3	11:K:76:HIS:HB2	2.04	0.40
13:M:54:ARG:HE	13:M:56:PHE:HE1	1.69	0.40
13:M:743:TYR:OH	13:M:793:ARG:NH1	2.54	0.40
5:E:58:ALA:HA	5:E:66:GLN:HA	2.03	0.40
13:M:43:GLU:HG3	13:M:209:ARG:HG2	2.02	0.40
13:M:293:TYR:CZ	13:M:467:LYS:HD2	2.57	0.40
13:M:583:ILE:HG13	13:M:620:VAL:HG12	2.04	0.40
13:M:784:ASN:HB3	13:M:785:PRO:HD3	2.03	0.40
13:M:1014:MET:O	13:M:1019:ALA:N	2.55	0.40
16:Q:15:DA:H2'	16:Q:16:DC:C6	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
1	A	1145/1498 (76%)	1110 (97%)	35 (3%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1046/1172 (89%)	1017 (97%)	29 (3%)	0	100	100
3	C	287/319 (90%)	279 (97%)	8 (3%)	0	100	100
4	D	111/205 (54%)	105 (95%)	6 (5%)	0	100	100
5	E	194/205 (95%)	191 (98%)	3 (2%)	0	100	100
6	F	74/144 (51%)	72 (97%)	2 (3%)	0	100	100
7	G	172/174 (99%)	164 (95%)	8 (5%)	0	100	100
8	H	120/146 (82%)	117 (98%)	3 (2%)	0	100	100
9	I	111/114 (97%)	109 (98%)	2 (2%)	0	100	100
10	J	60/71 (84%)	57 (95%)	3 (5%)	0	100	100
11	K	92/116 (79%)	91 (99%)	1 (1%)	0	100	100
12	L	40/51 (78%)	38 (95%)	2 (5%)	0	100	100
13	M	1044/1133 (92%)	1005 (96%)	39 (4%)	0	100	100
All	All	4496/5348 (84%)	4355 (97%)	141 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	882/1332 (66%)	879 (100%)	3 (0%)	92	97
2	B	821/1029 (80%)	819 (100%)	2 (0%)	93	98
3	C	220/280 (79%)	220 (100%)	0	100	100
4	D	101/181 (56%)	100 (99%)	1 (1%)	76	88
5	E	145/191 (76%)	145 (100%)	0	100	100
6	F	53/128 (41%)	53 (100%)	0	100	100
7	G	74/151 (49%)	74 (100%)	0	100	100
8	H	90/127 (71%)	89 (99%)	1 (1%)	73	86
9	I	80/104 (77%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	48/66 (73%)	47 (98%)	1 (2%)	53	76
11	K	68/105 (65%)	68 (100%)	0	100	100
12	L	28/45 (62%)	28 (100%)	0	100	100
13	M	820/1005 (82%)	819 (100%)	1 (0%)	93	98
All	All	3430/4744 (72%)	3421 (100%)	9 (0%)	92	97

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	471	VAL
1	A	887	GLU
1	A	1057	VAL
2	B	184	LEU
2	B	921	LYS
4	D	92	MET
8	H	36	ASN
10	J	3	ILE
13	M	491	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	70	HIS
1	A	410	ASN
1	A	462	GLN
1	A	476	GLN
1	A	562	ASN
1	A	634	GLN
1	A	652	GLN
1	A	736	ASN
1	A	742	GLN
1	A	857	GLN
1	A	1008	GLN
1	A	1080	GLN
1	A	1149	GLN
1	A	1182	HIS
1	A	1227	GLN
2	B	66	ASN
2	B	220	GLN

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Mol	Chain	Res	Type
2	B	222	GLN
2	B	417	HIS
2	B	450	ASN
2	B	477	ASN
2	B	495	GLN
2	B	543	GLN
2	B	577	ASN
2	B	600	GLN
2	B	711	HIS
2	B	718	GLN
2	B	749	GLN
2	B	768	ASN
2	B	771	ASN
2	B	779	HIS
2	B	949	HIS
2	B	1042	HIS
2	B	1106	HIS
3	C	280	GLN
4	D	140	GLN
5	E	126	GLN
8	H	124	GLN
9	I	12	ASN
9	I	80	GLN
9	I	81	HIS
11	K	89	GLN
11	K	104	GLN
12	L	17	GLN
12	L	28	GLN
12	L	47	GLN
13	M	84	HIS
13	M	298	GLN
13	M	306	GLN
13	M	376	GLN
13	M	377	ASN
13	M	449	ASN
13	M	482	ASN
13	M	567	GLN
13	M	822	HIS
13	M	1002	HIS
13	M	1059	HIS

### 5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	O	7/15 (46%)	1 (14%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	O	6	A

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 11 are monoatomic - leaving 1 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
19	GTP	Q	101	16,18	26,34,34	1.14	2 (7%)	32,54,54	1.71	6 (18%)

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
19	GTP	Q	101	16,18	-	4/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Q	101	GTP	C5-C6	-4.20	1.38	1.47
19	Q	101	GTP	C2-N3	2.21	1.38	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Q	101	GTP	PB-O3B-PG	-3.69	120.17	132.83
19	Q	101	GTP	C5-C6-N1	3.65	120.40	113.95
19	Q	101	GTP	PA-O3A-PB	-3.64	120.35	132.83
19	Q	101	GTP	C3'-C2'-C1'	3.32	105.97	100.98
19	Q	101	GTP	C2-N1-C6	-3.22	119.17	125.10
19	Q	101	GTP	C8-N7-C5	2.88	108.47	102.99

There are no chirality outliers.

All (4) torsion outliers are listed below:

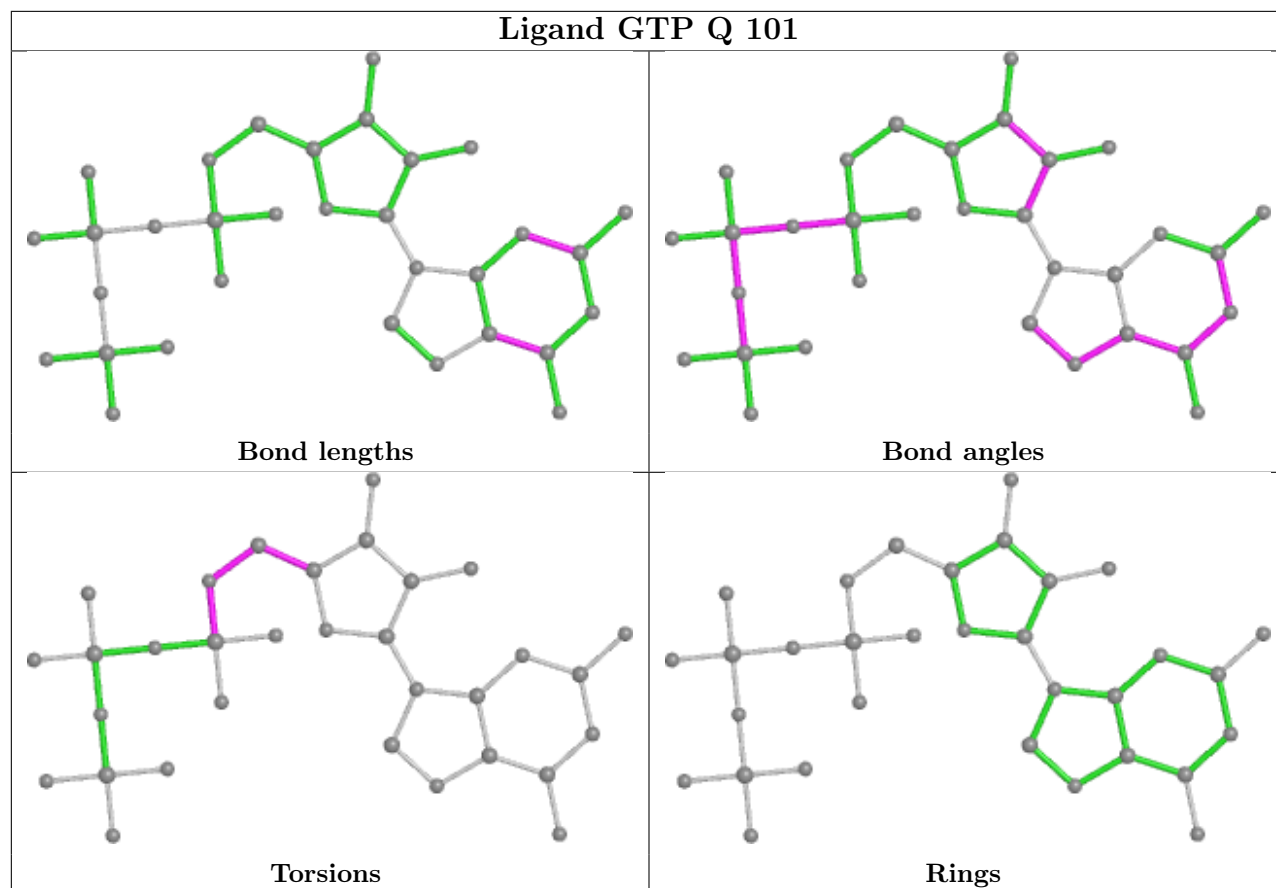
Mol	Chain	Res	Type	Atoms
19	Q	101	GTP	C5'-O5'-PA-O1A
19	Q	101	GTP	O4'-C4'-C5'-O5'
19	Q	101	GTP	C3'-C4'-C5'-O5'
19	Q	101	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	Q	101	GTP	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.

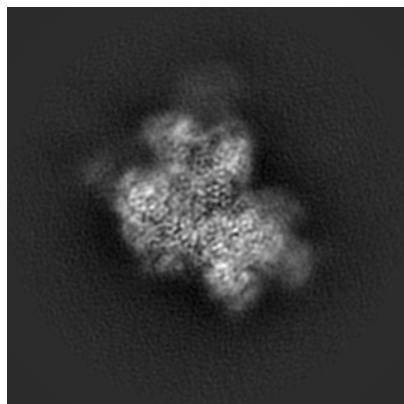
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38470. These allow visual inspection of the internal detail of the map and identification of artifacts.

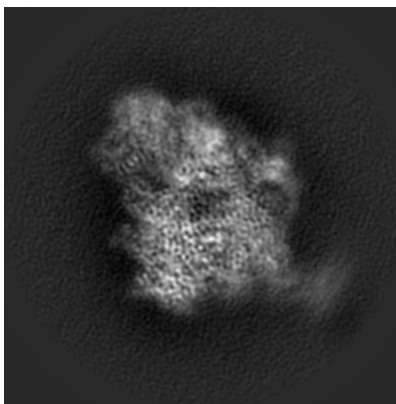
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

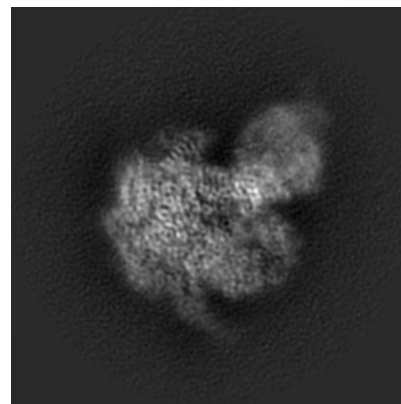
#### 6.1.1 Primary map



X

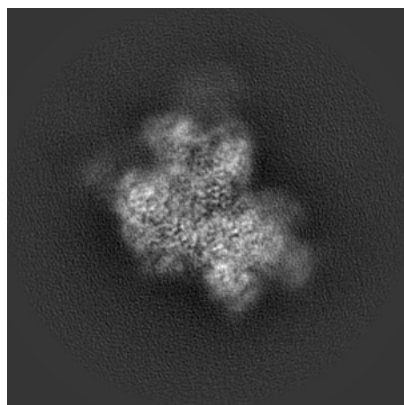


Y

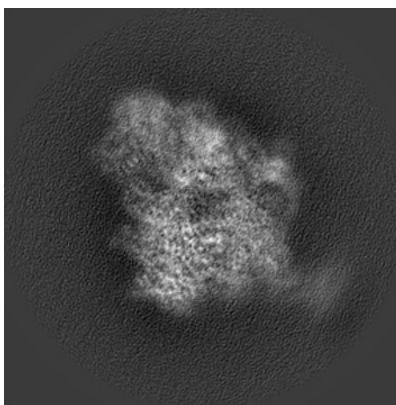


Z

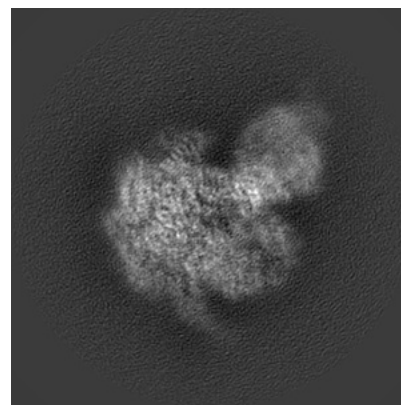
#### 6.1.2 Raw map



X



Y

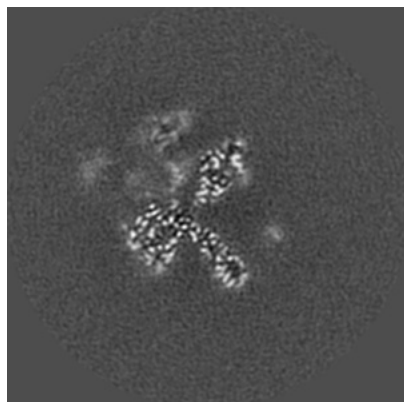


Z

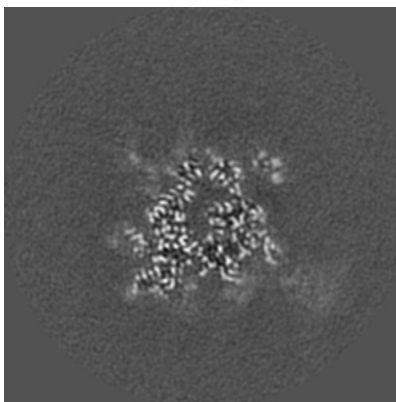
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

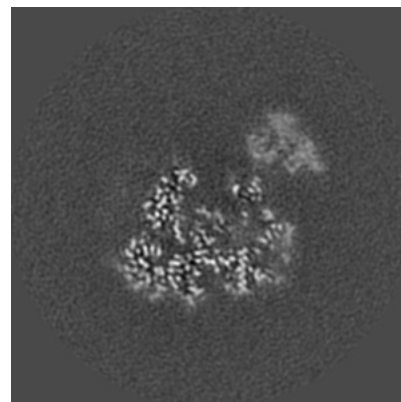
### 6.2.1 Primary map



X Index: 128

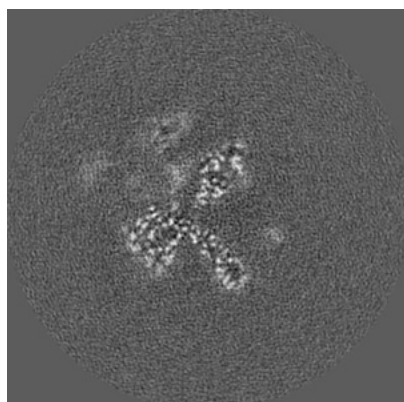


Y Index: 128

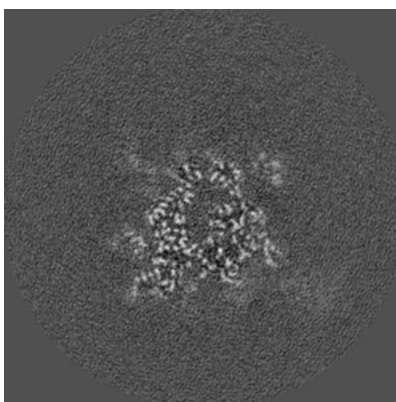


Z Index: 128

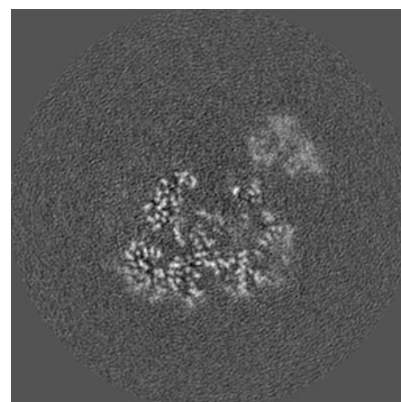
### 6.2.2 Raw map



X Index: 128



Y Index: 128



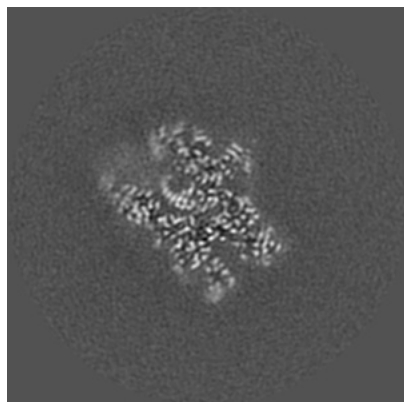
Z Index: 128

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

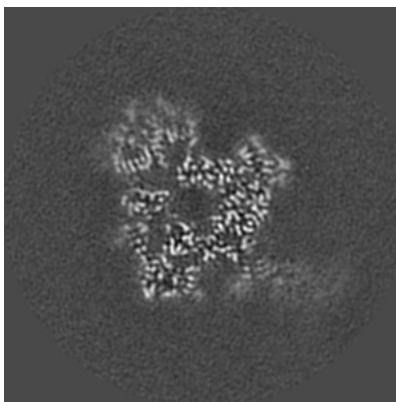


## 6.3 Largest variance slices [i](#)

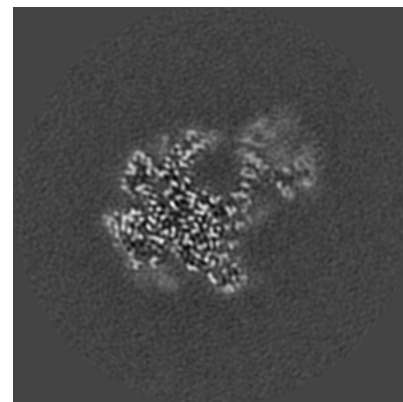
### 6.3.1 Primary map



X Index: 106

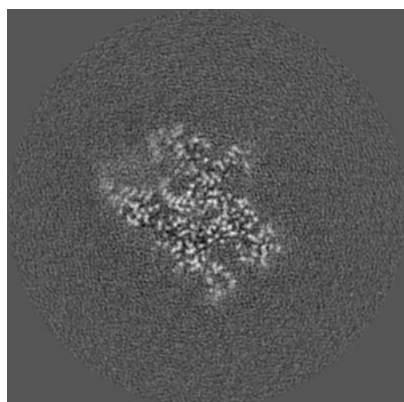


Y Index: 138

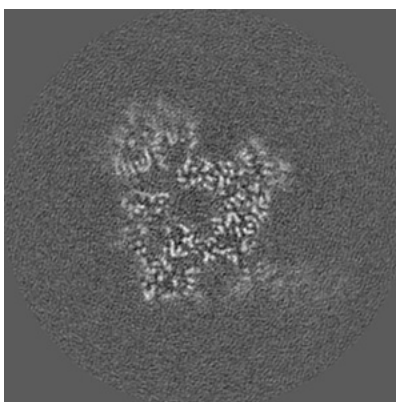


Z Index: 110

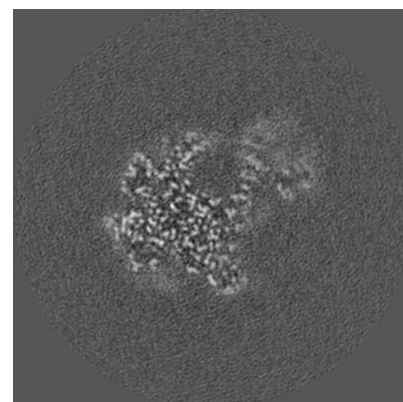
### 6.3.2 Raw map



X Index: 107



Y Index: 138

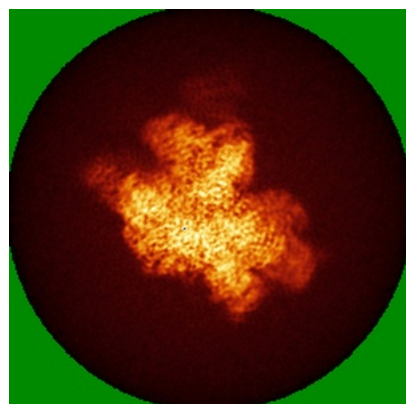


Z Index: 110

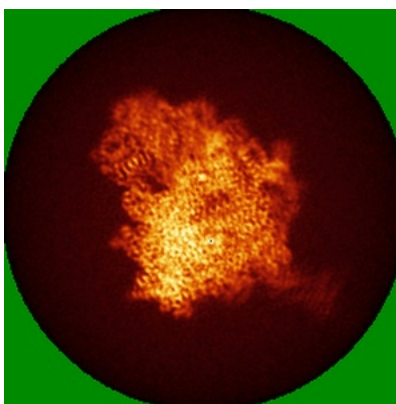
The images above show the largest variance slices of the map in three orthogonal directions.

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

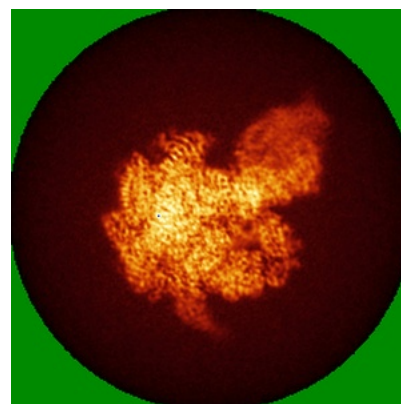
### 6.4.1 Primary map



X

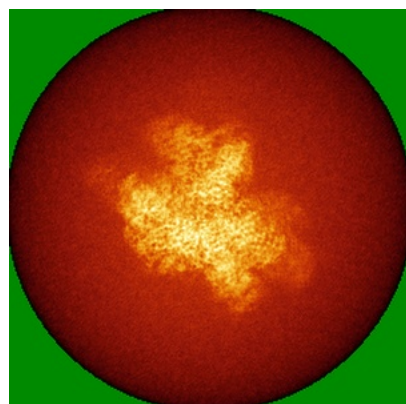


Y

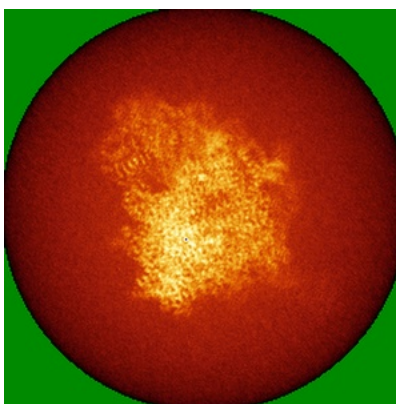


Z

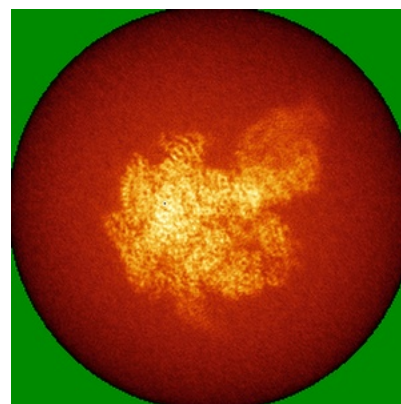
### 6.4.2 Raw map



X



Y

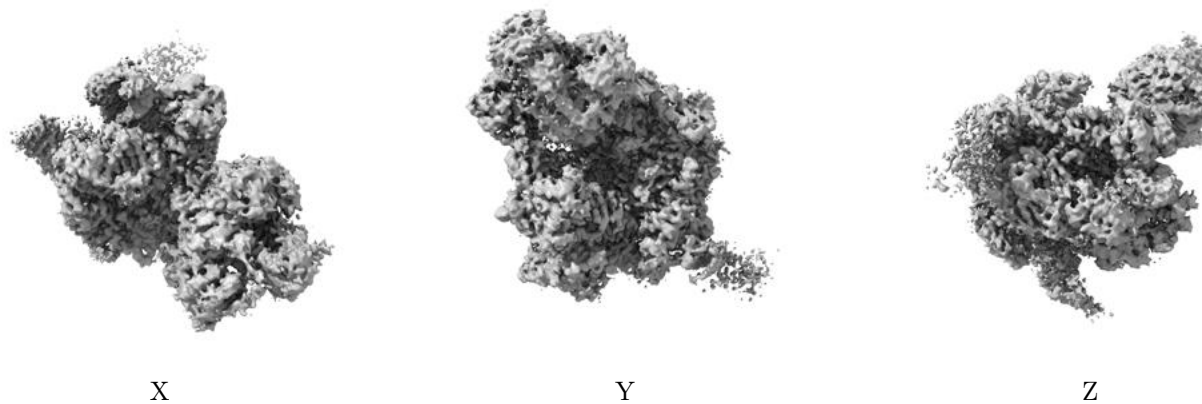


Z

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.

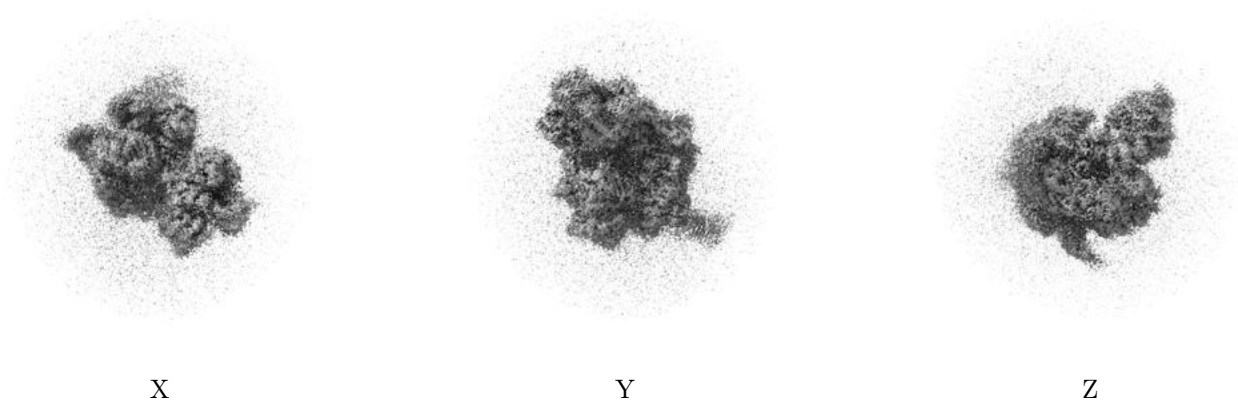
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. 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.

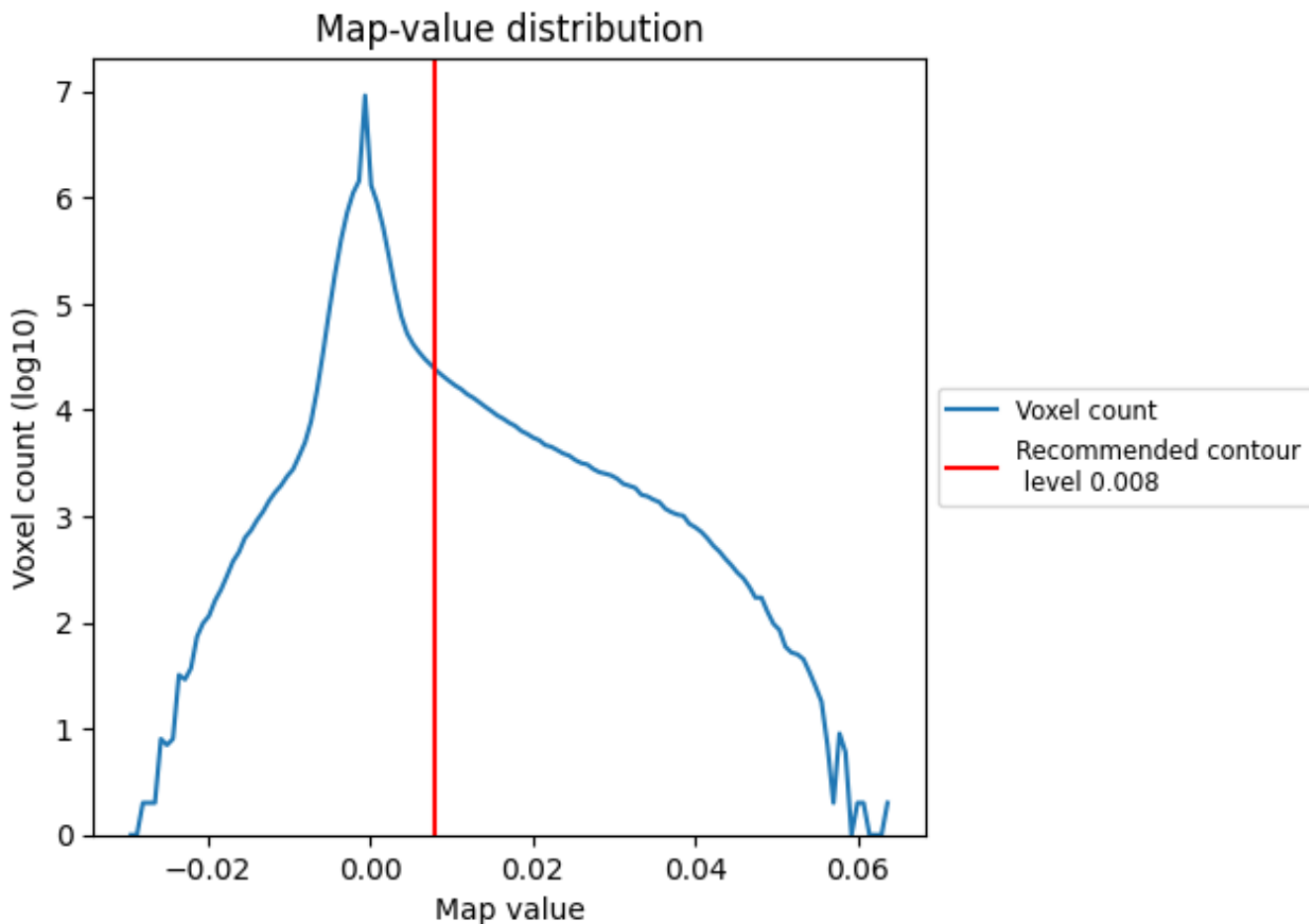
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

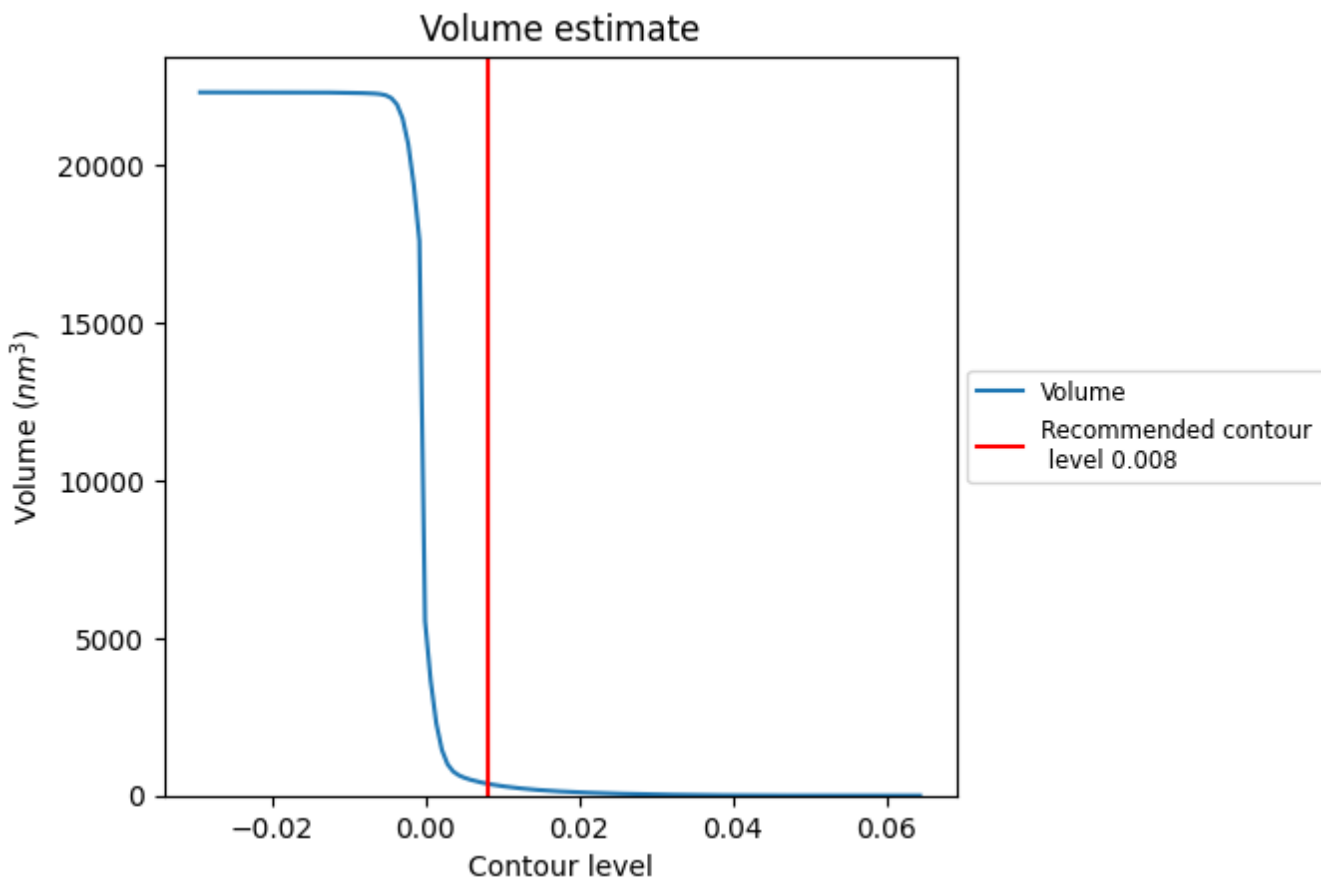
This section contains the results of statistical analysis of the map.

### 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.

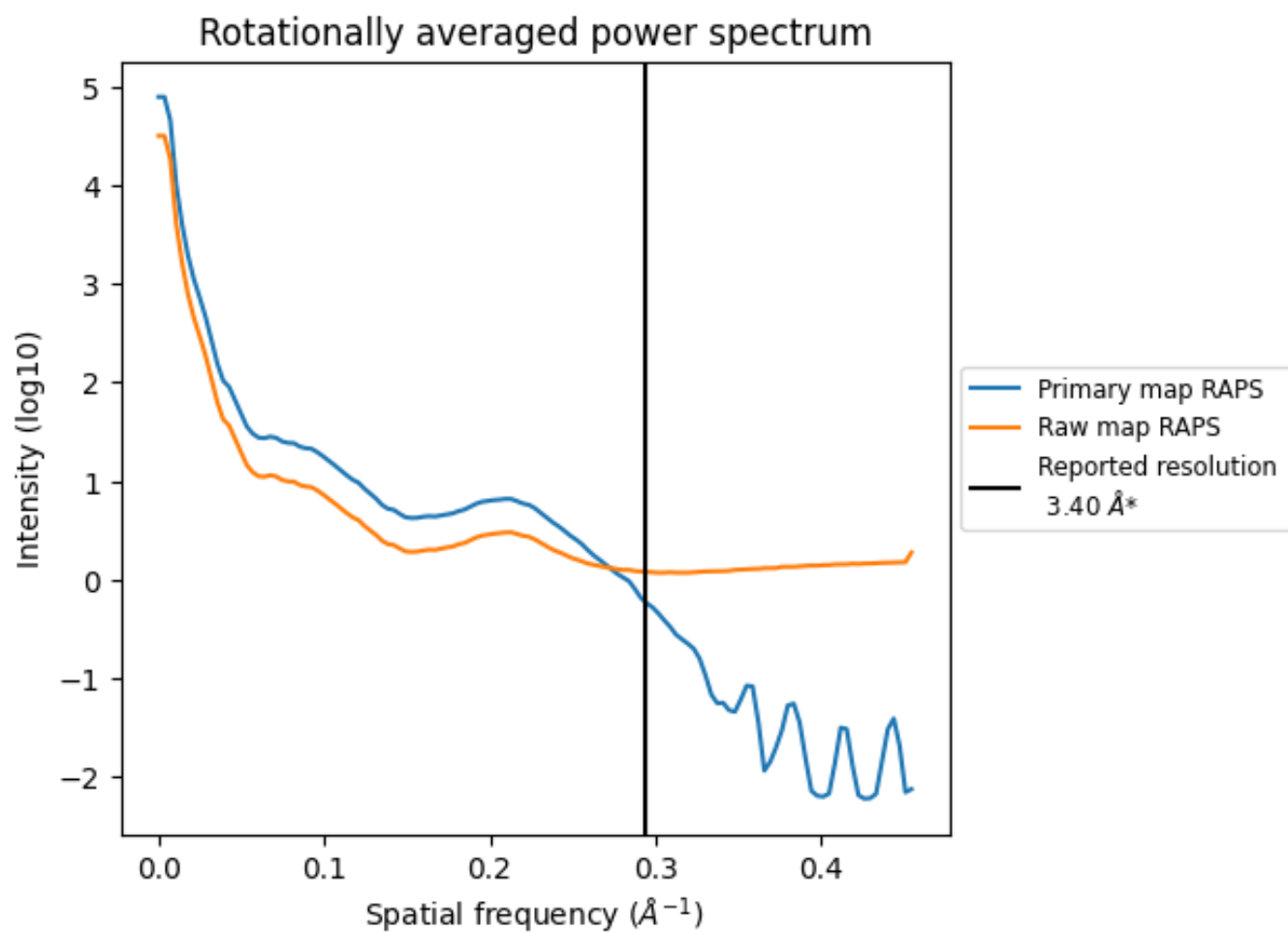
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 378 nm<sup>3</sup>; this corresponds to an approximate mass of 342 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

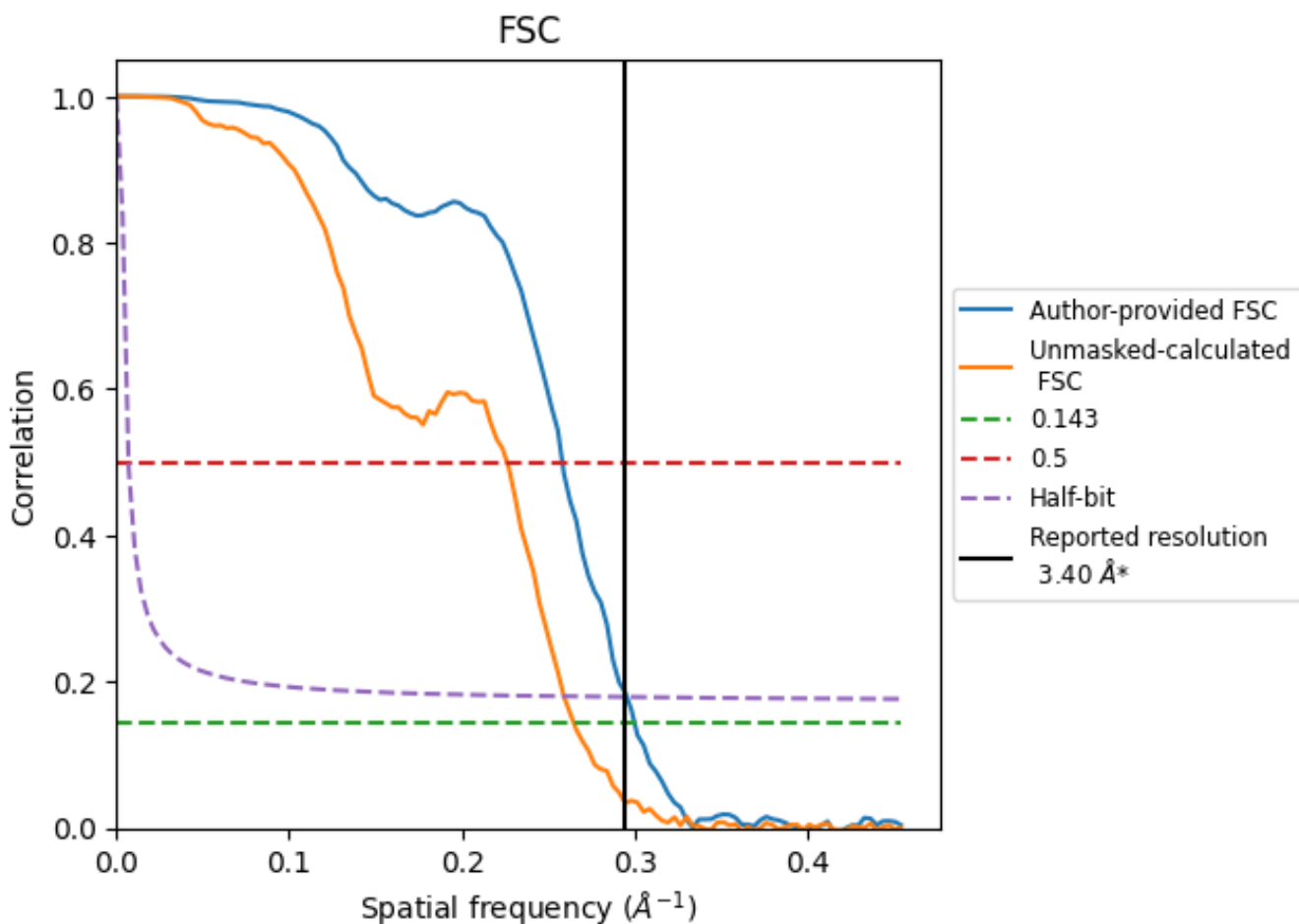


\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 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 0.294 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.33	3.87	3.38
Unmasked-calculated*	3.78	4.42	3.86

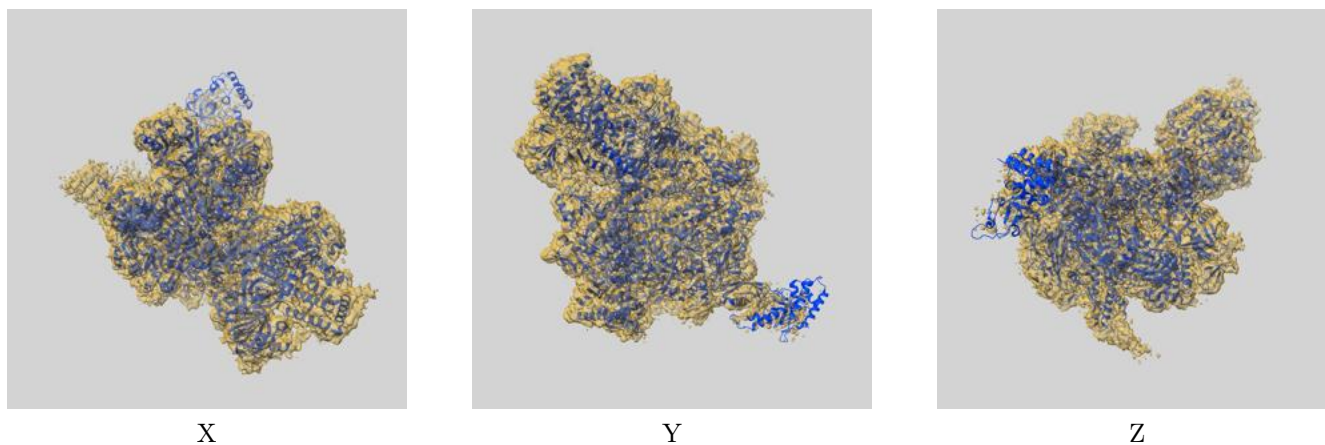
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.78 differs from the reported value 3.4 by more than 10 %



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

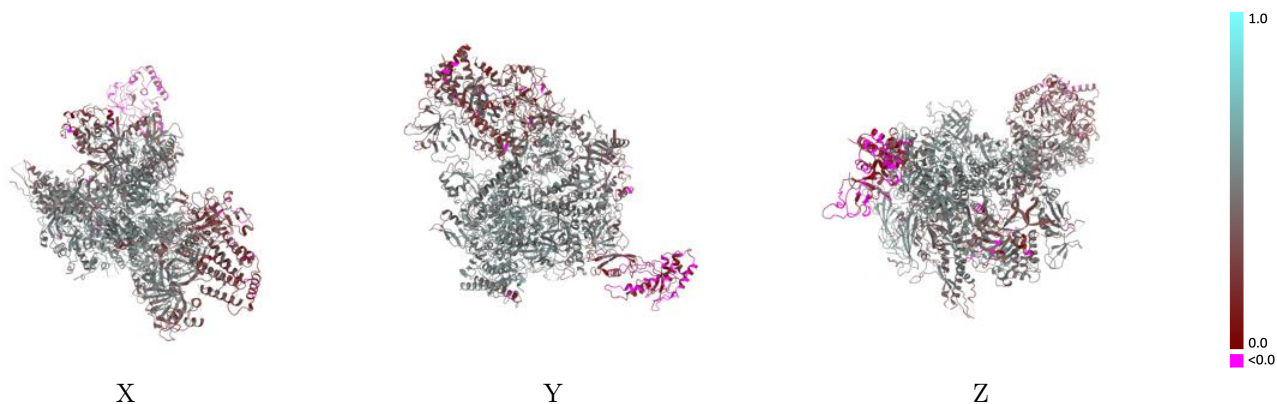
This section contains information regarding the fit between EMDB map EMD-38470 and PDB model 8XMB. Per-residue inclusion information can be found in section [3](#) on page [9](#).

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



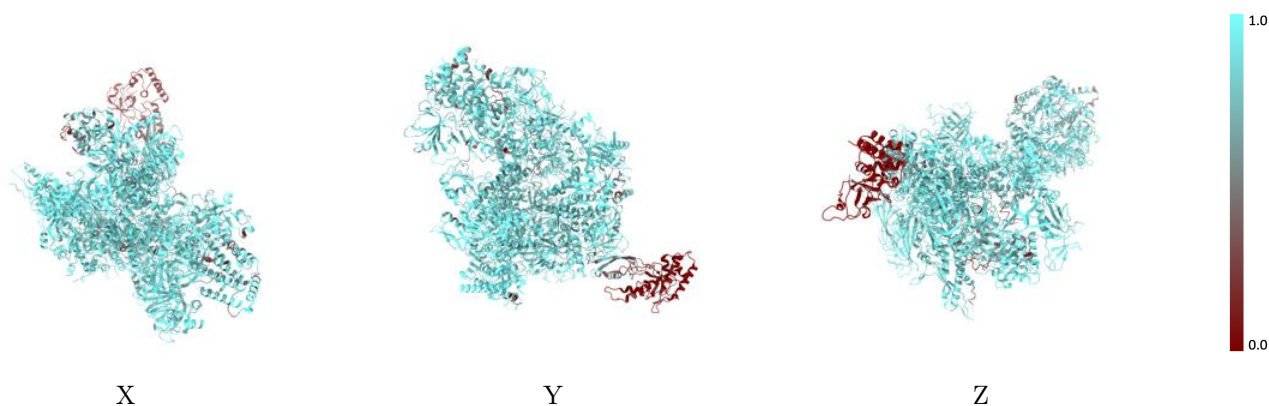
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



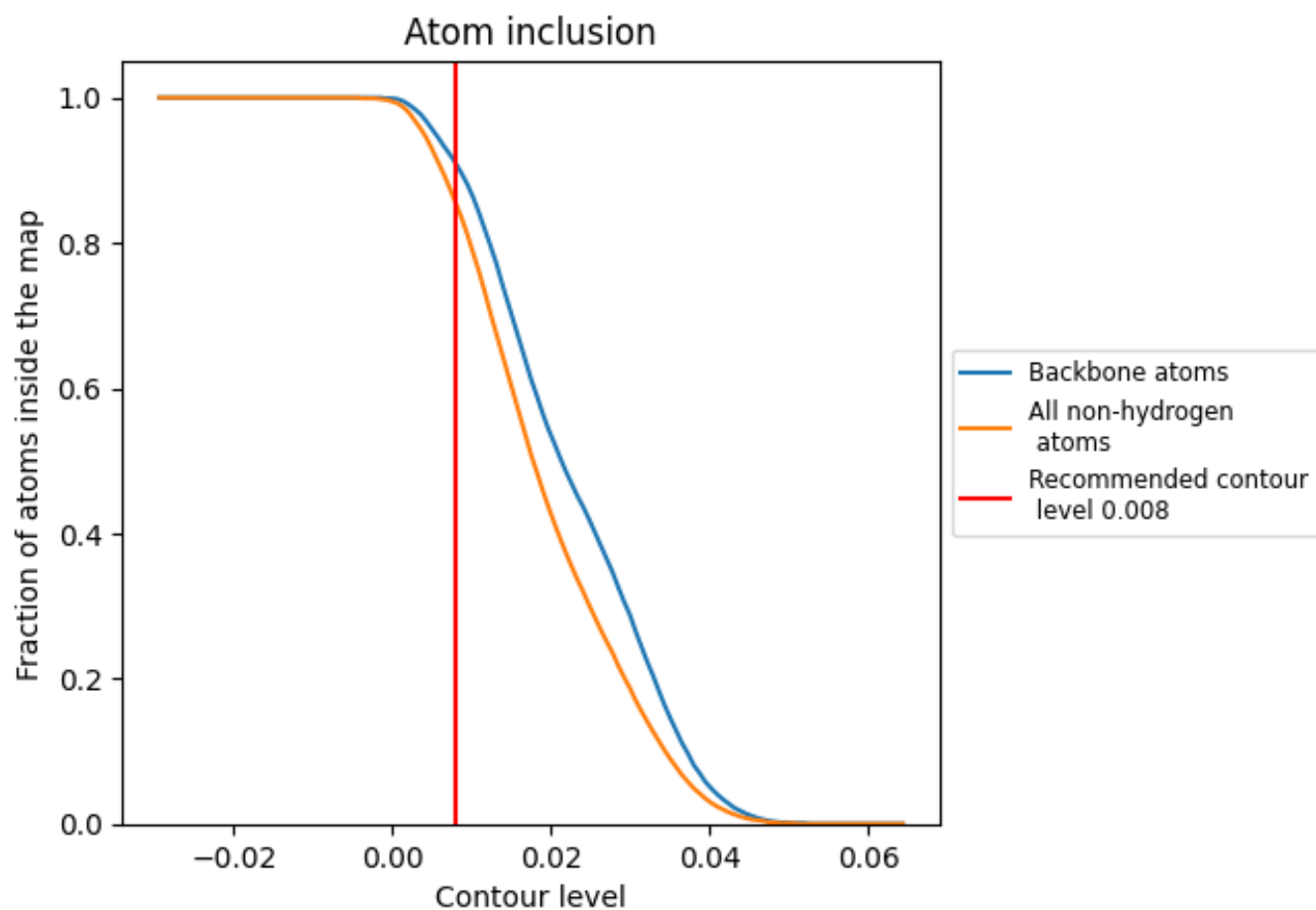
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).



































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 85% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8540	 0.4300
A	 0.8770	 0.4580
B	 0.9250	 0.4970
C	 0.9340	 0.4900
D	 0.0240	 0.0390
E	 0.9260	 0.4620
F	 0.9190	 0.4650
G	 0.2500	 0.1280
H	 0.9330	 0.4950
I	 0.8580	 0.4550
J	 0.9380	 0.5050
K	 0.9670	 0.5220
L	 0.9600	 0.4910
M	 0.8550	 0.3700
N	 0.9320	 0.3700
O	 0.9340	 0.4730
Q	 0.9420	 0.4170

