



## Full wwPDB EM Validation Report ⓘ

Apr 16, 2026 – 04:34 PM EDT

PDB ID : 9YNP / pdb\_00009ynp  
EMDB ID : EMD-73220  
Title : Cryo-EM structure of Escherichia coli transcription initiation complex with GpA and pseudouridimycin (PUM)  
Authors : You, L.L.; Ebright, R.H.  
Deposited on : 2025-10-11  
Resolution : 3.06 Å(reported)  
Based on initial model : 4MEY

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>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

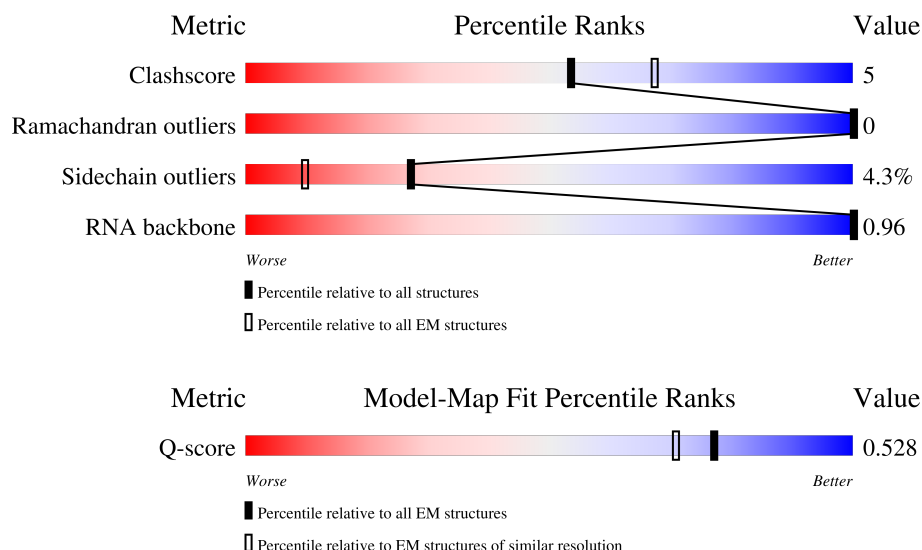
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.06 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13976 ( 2.56 - 3.56 )

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	329	
1	B	329	
2	C	1342	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	1407	<div><div></div><div>8%</div><div>80%</div><div>16%</div><div></div><div></div></div>
4	E	91	<div><div></div><div>5%</div><div>75%</div><div>11%</div><div>14%</div><div></div></div>
5	F	613	<div><div></div><div>8%</div><div>46%</div><div>8%</div><div>46%</div><div></div></div>
6	G	27	<div><div></div><div>52%</div><div>48%</div><div></div></div>
7	H	21	<div><div></div><div>5%</div><div>33%</div><div>67%</div><div></div></div>
8	I	2	<div><div></div><div>100%</div><div></div></div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 29059 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	230	Total	C	N	O	S	0	0
			1780	1109	314	351	6		
1	B	229	Total	C	N	O	S	0	0
			1774	1105	313	350	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0
			10567	6631	1841	2052	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1362	Total	C	N	O	S	0	0
			10562	6630	1884	1998	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	78	Total	C	N	O	S	0	0
			619	376	117	125	1		

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	331	Total	C	N	O	S	0	0
			2689	1672	493	506	18		

- Molecule 6 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	27	Total	C	N	O	P	0	0
			560	266	109	159	26		

- Molecule 7 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	21	Total	C	N	O	P	0	0
			429	204	81	124	20		

- Molecule 8 is a RNA chain called RNA (5'-R(\*GP\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	2	Total	C	N	O	P	0	0
			42	20	10	11	1		

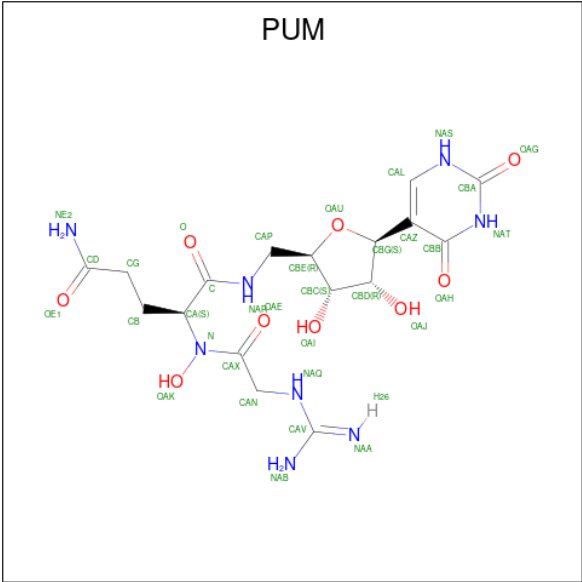
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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

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

- Molecule 11 is (1S)-1,4-anhydro-5-[(N-carbamimidoylglycyl-N 2 -hydroxy-L-glutaminy)amino]-5-deoxy-1-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-5-yl)-D-ribitol (CCD ID: PUM) (formula: C<sub>17</sub>H<sub>26</sub>N<sub>8</sub>O<sub>9</sub>).

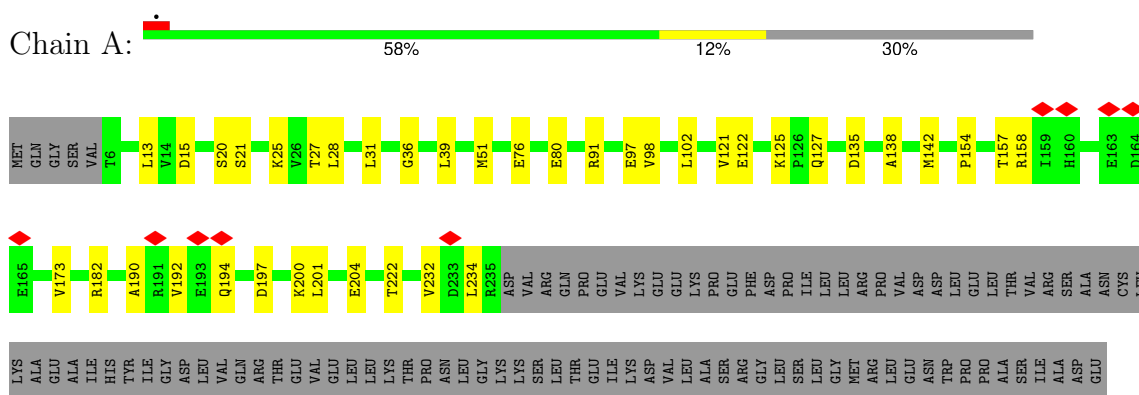


Mol	Chain	Residues	Atoms				AltConf
11	I	1	Total	C	N	O	0
			34	17	8	9	

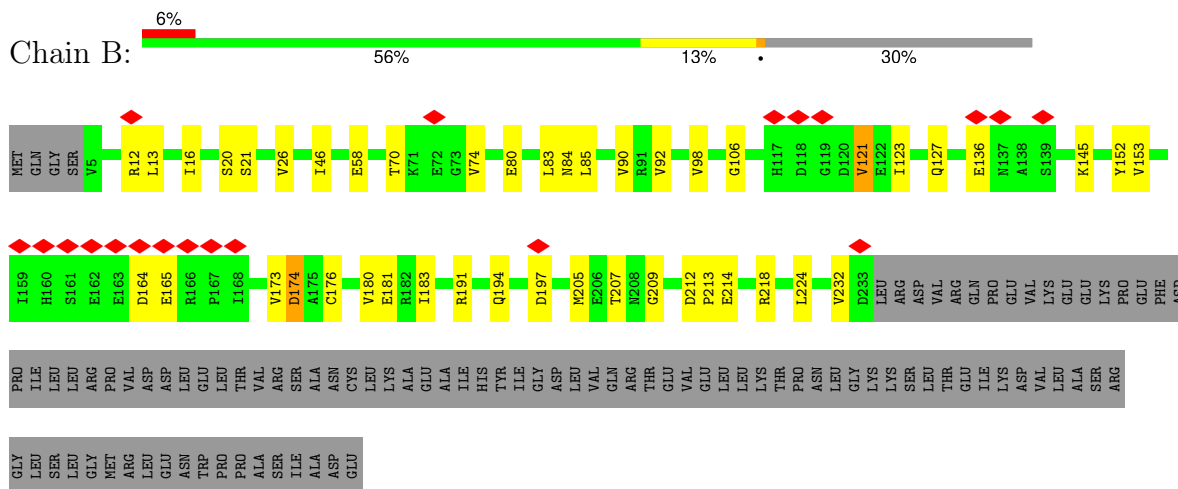
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

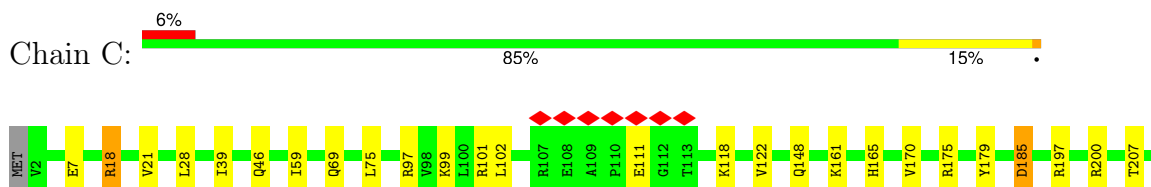
- Molecule 1: DNA-directed RNA polymerase subunit alpha

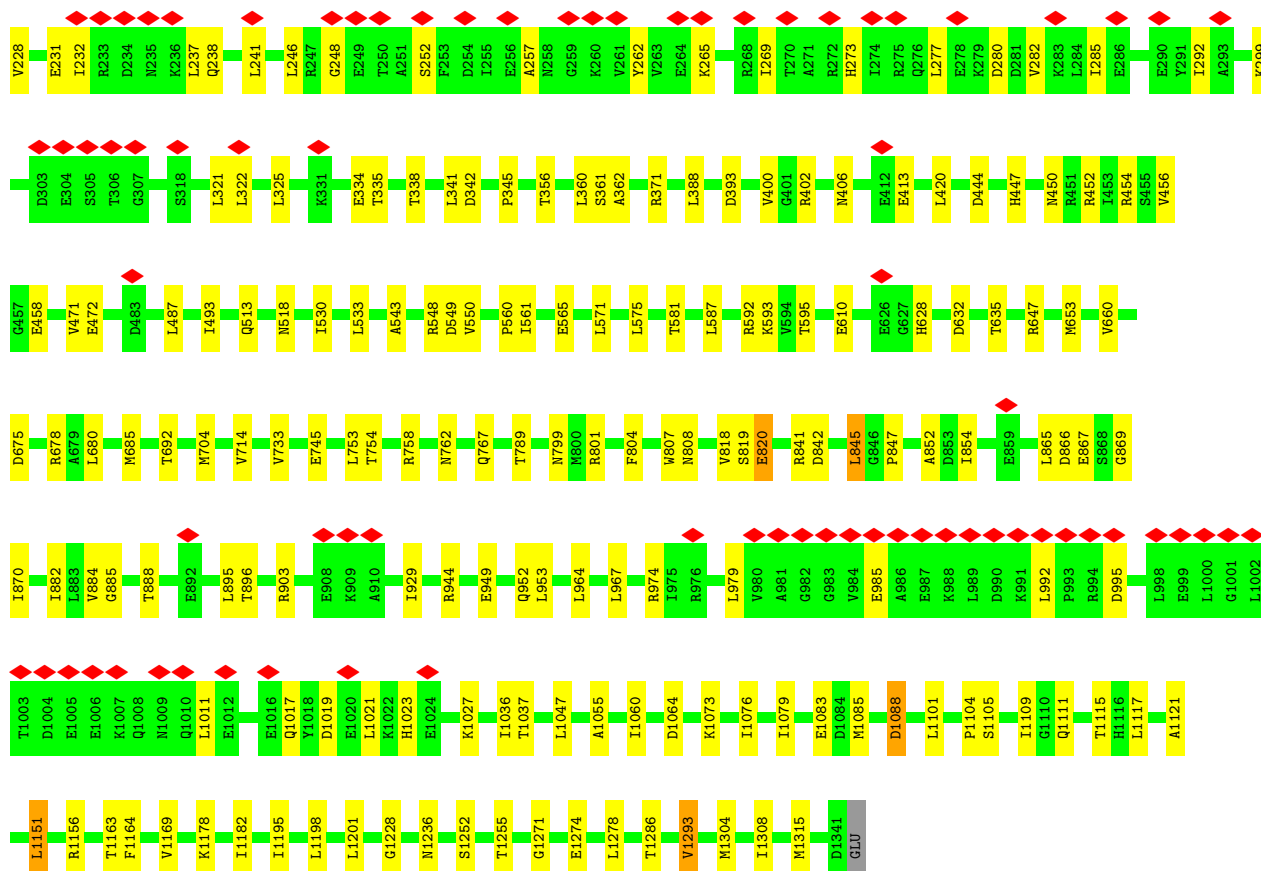


- Molecule 1: DNA-directed RNA polymerase subunit alpha

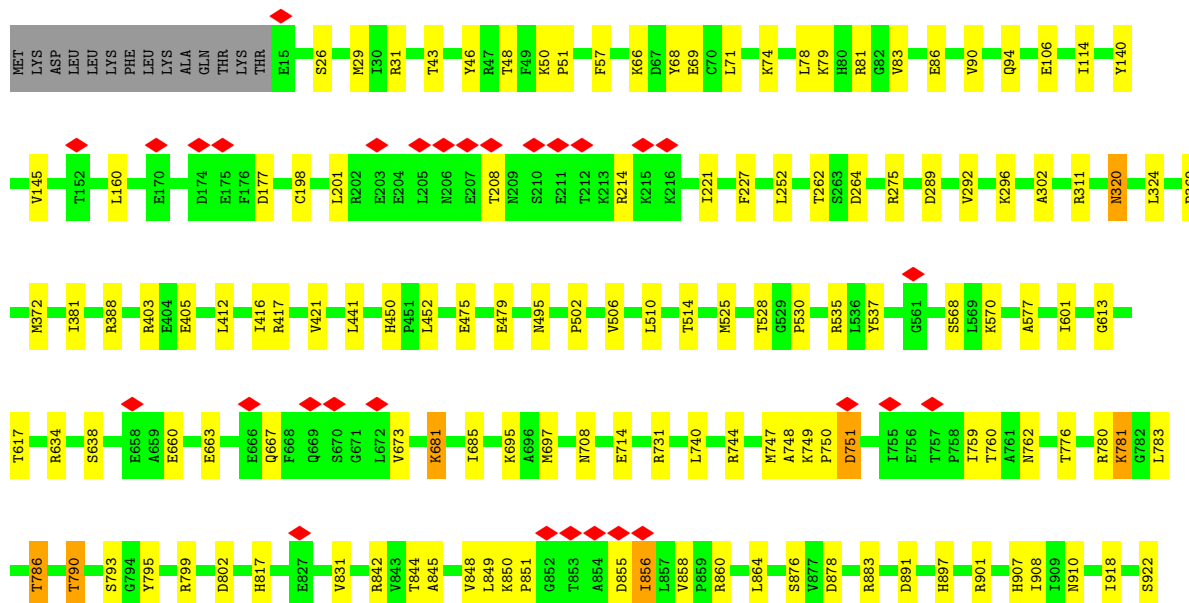
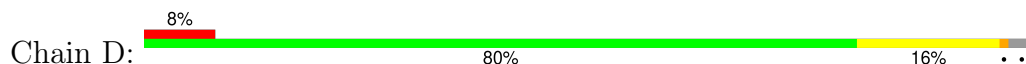


- Molecule 2: DNA-directed RNA polymerase subunit beta

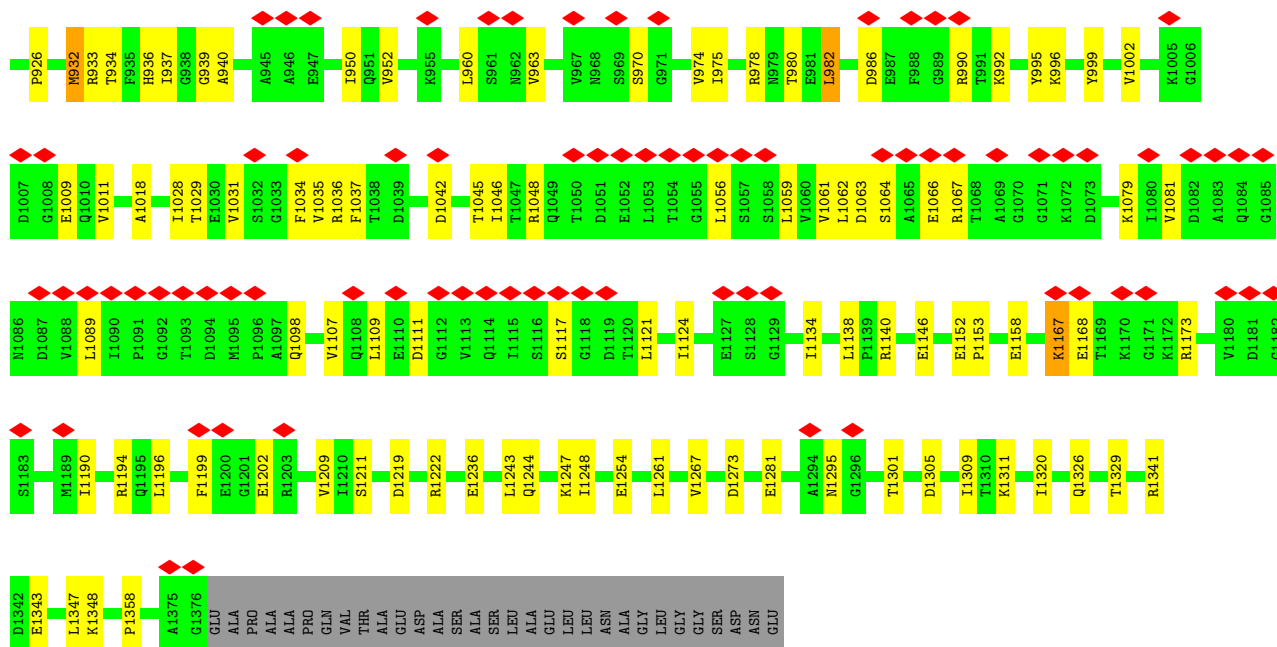




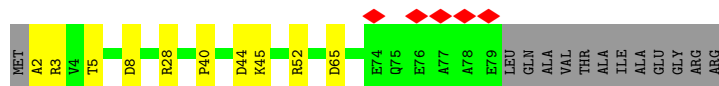
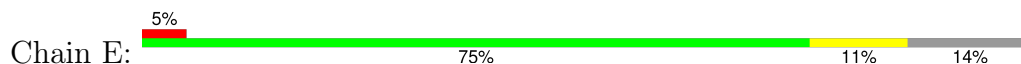
• Molecule 3: DNA-directed RNA polymerase subunit beta'



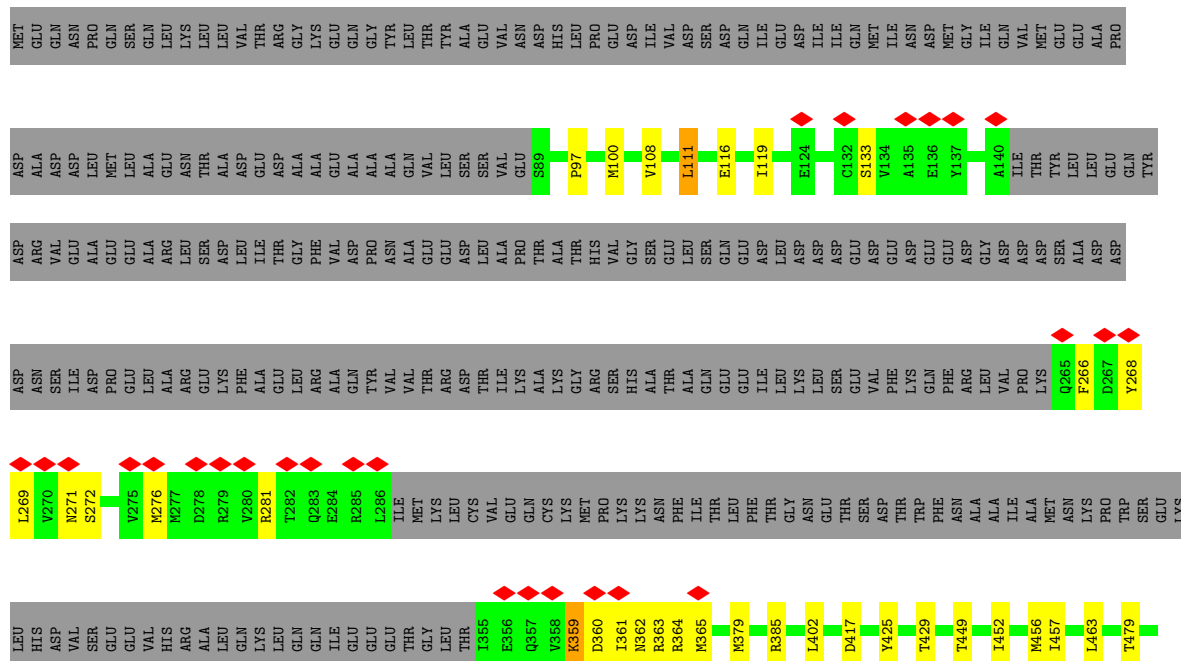


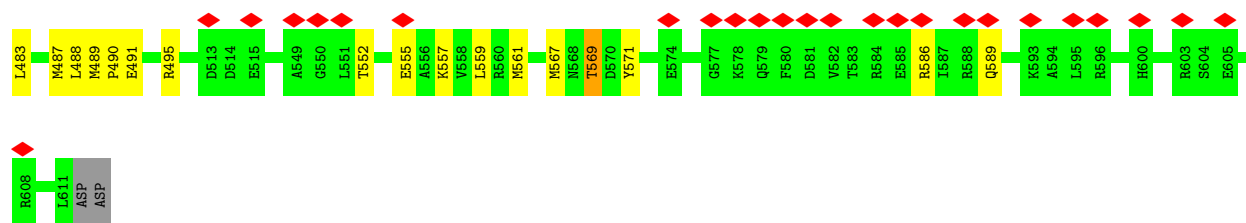


- Molecule 4: DNA-directed RNA polymerase subunit omega



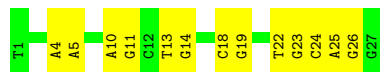
- Molecule 5: RNA polymerase sigma factor RpoD





- Molecule 6: DNA (27-MER)

Chain G: 52% 48%



- Molecule 7: DNA

Chain H: 5% 33% 67%



- Molecule 8: RNA (5'-R(\*GP\*A)-3')

Chain I: 100%

There are no outlier residues recorded for this chain.

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46892	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	32.1	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.684	Depositor
Minimum map value	-0.380	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.085	Depositor
Map size ( $\text{\AA}$ )	311.4, 311.4, 311.4	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.038, 1.038, 1.038	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: MG, ZN, PUM

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	0.08	0/1802	0.20	0/2443
1	B	0.08	0/1796	0.21	0/2435
2	C	0.10	0/10736	0.23	0/14487
3	D	0.13	0/10723	0.25	0/14480
4	E	0.08	0/621	0.17	0/836
5	F	0.10	0/2719	0.20	0/3645
6	G	0.16	0/630	0.30	0/973
7	H	0.18	0/481	0.33	0/741
8	I	0.13	0/47	0.28	0/72
All	All	0.11	0/29555	0.23	0/40112

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1780	0	1802	18	0
1	B	1774	0	1798	24	0
2	C	10567	0	10585	102	0
3	D	10562	0	10768	124	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	619	0	623	5	0
5	F	2689	0	2752	28	0
6	G	560	0	305	11	0
7	H	429	0	237	10	0
8	I	42	0	23	0	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
11	I	34	0	0	0	0
All	All	29059	0	28893	301	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 (301) 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)
5:F:425:TYR:CG	5:F:425:TYR:CE1	2.41	0.96
1:B:80:GLU:O	1:B:84:ASN:ND2	2.10	0.85
2:C:801:ARG:NH2	2:C:1088:ASP:OD2	2.22	0.73
3:D:502:PRO:HB3	3:D:506:VAL:HB	1.71	0.71
1:A:192:VAL:HG13	1:A:194:GLN:H	1.56	0.70
3:D:802:ASP:OD2	3:D:1348:LYS:NZ	2.27	0.68
1:A:102:LEU:HD23	1:A:142:MET:HE3	1.76	0.67
2:C:560:PRO:HB2	3:D:776:THR:HG21	1.75	0.66
2:C:400:VAL:HG21	2:C:452:ARG:HD2	1.78	0.65
6:G:4:DA:H2''	6:G:5:DA:H5''	1.79	0.64
2:C:804:PHE:O	3:D:638:SER:OG	2.15	0.63
2:C:185:ASP:OD1	2:C:185:ASP:N	2.32	0.62
2:C:444:ASP:O	2:C:450:ASN:ND2	2.32	0.62
3:D:795:TYR:OH	3:D:1326:GLN:NE2	2.33	0.62
3:D:926:PRO:HG2	3:D:1248:ILE:HD11	1.80	0.62
1:B:180:VAL:HG13	1:B:205:MET:HE3	1.82	0.61
5:F:281:ARG:NH1	5:F:362:ASN:OD1	2.33	0.60
3:D:1219:ASP:OD1	3:D:1222:ARG:NH2	2.35	0.60
3:D:252:LEU:HD13	3:D:262:THR:HB	1.84	0.60
5:F:561:MET:HA	5:F:567:MET:HE1	1.83	0.60
3:D:876:SER:HB2	3:D:990:ARG:HH21	1.66	0.59
3:D:1158:GLU:OE2	3:D:1222:ARG:NH1	2.34	0.59
2:C:341:LEU:HG	2:C:342:ASP:H	1.68	0.59
2:C:895:LEU:HD12	2:C:903:ARG:HH11	1.67	0.59
1:B:98:VAL:HG11	1:B:121:VAL:HG11	1.85	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:963:VAL:HG11	3:D:980:THR:HG23	1.83	0.59
3:D:974:VAL:HG12	3:D:1002:VAL:HG12	1.84	0.58
3:D:1140:ARG:NH2	3:D:1236:GLU:OE1	2.35	0.58
2:C:1151:LEU:HD13	2:C:1201:LEU:HD22	1.86	0.58
3:D:749:LYS:HG3	3:D:751:ASP:H	1.69	0.58
3:D:748:ALA:H	3:D:940:ALA:HB3	1.69	0.58
3:D:403:ARG:NH1	3:D:405:GLU:OE2	2.37	0.57
3:D:781:LYS:O	3:D:781:LYS:HG2	2.04	0.57
3:D:1134:ILE:HD13	3:D:1244:GLN:HG3	1.86	0.57
3:D:978:ARG:HA	3:D:999:TYR:HB2	1.85	0.57
1:A:182:ARG:NH2	1:A:204:GLU:OE2	2.37	0.57
1:B:20:SER:OG	1:B:21:SER:N	2.38	0.57
1:B:92:VAL:HG13	1:B:121:VAL:HG12	1.86	0.57
3:D:66:LYS:HB3	3:D:69:GLU:HB3	1.85	0.57
2:C:1151:LEU:HD22	2:C:1198:LEU:HD13	1.86	0.57
4:E:3:ARG:NH1	4:E:44:ASP:OD2	2.37	0.57
3:D:475:GLU:OE2	4:E:28:ARG:NH1	2.35	0.57
3:D:878:ASP:OD1	3:D:878:ASP:N	2.37	0.57
2:C:745:GLU:O	2:C:974:ARG:NH1	2.37	0.56
2:C:59:ILE:HG21	2:C:472:GLU:HG3	1.86	0.56
6:G:22:DT:H2"	6:G:23:DG:C8	2.40	0.56
2:C:18:ARG:O	2:C:1156:ARG:NH1	2.39	0.56
1:B:106:GLY:HA2	1:B:136:GLU:HA	1.86	0.56
2:C:292:ILE:HG13	2:C:322:LEU:HD22	1.87	0.55
5:F:569:THR:HG23	5:F:571:TYR:HE1	1.70	0.55
7:H:3:DT:H2"	7:H:4:DG:C8	2.41	0.55
3:D:568:SER:OG	3:D:570:LYS:NZ	2.36	0.55
3:D:74:LYS:NZ	3:D:86:GLU:OE2	2.38	0.55
1:B:46:ILE:HD11	1:B:224:LEU:HD13	1.89	0.55
3:D:844:THR:HG23	3:D:864:LEU:HD11	1.89	0.55
3:D:292:VAL:HG12	3:D:296:LYS:HE2	1.89	0.54
5:F:133:SER:OG	5:F:364:ARG:NH1	2.39	0.54
3:D:416:ILE:HD13	3:D:441:LEU:HD21	1.89	0.54
3:D:986:ASP:HB3	3:D:992:LYS:HD3	1.90	0.54
4:E:40:PRO:O	4:E:52:ARG:NH2	2.39	0.54
3:D:799:ARG:HB3	3:D:1309:ILE:HG21	1.89	0.54
4:E:2:ALA:N	4:E:5:THR:O	2.41	0.54
1:A:125:LYS:NZ	1:A:127:GLN:OE1	2.41	0.54
2:C:1088:ASP:N	2:C:1088:ASP:OD1	2.39	0.54
2:C:852:ALA:HB2	2:C:869:GLY:HA2	1.89	0.53
2:C:929:ILE:HD11	2:C:1055:ALA:HB2	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:241:LEU:HB3	2:C:285:ILE:HD13	1.90	0.53
2:C:444:ASP:HB3	2:C:447:HIS:HB2	1.89	0.53
2:C:1117:LEU:HD13	2:C:1195:ILE:HG12	1.90	0.53
2:C:842:ASP:HA	2:C:847:PRO:HA	1.90	0.53
1:A:28:LEU:HD12	1:A:201:LEU:HD23	1.91	0.53
1:B:181:GLU:O	3:D:535:ARG:NH1	2.42	0.53
2:C:179:TYR:OH	2:C:458:GLU:OE2	2.26	0.53
2:C:257:ALA:HB3	2:C:262:TYR:HE2	1.73	0.52
3:D:952:VAL:HG21	3:D:1011:VAL:HG21	1.89	0.52
1:B:12:ARG:HG3	1:B:13:LEU:HG	1.92	0.52
2:C:1109:ILE:HD11	3:D:740:LEU:HD22	1.90	0.52
3:D:1295:ASN:OD1	3:D:1295:ASN:N	2.43	0.52
3:D:762:ASN:OD1	3:D:762:ASN:N	2.42	0.52
6:G:25:DA:H2''	6:G:26:DG:N7	2.25	0.51
2:C:356:THR:HG23	2:C:361:SER:HB2	1.90	0.51
1:B:83:LEU:HG	3:D:528:THR:HG22	1.92	0.51
3:D:208:THR:O	3:D:214:ARG:NH1	2.41	0.51
3:D:510:LEU:O	3:D:514:THR:OG1	2.23	0.51
2:C:530:ILE:HD11	2:C:575:LEU:HD13	1.93	0.51
7:H:1:DC:H2''	7:H:2:DC:H5'	1.92	0.51
1:B:205:MET:HG2	1:B:213:PRO:HB3	1.92	0.51
3:D:1034:PHE:HB2	3:D:1081:VAL:HG23	1.92	0.51
1:B:207:THR:HG23	1:B:209:GLY:H	1.76	0.51
3:D:1347:LEU:HD23	3:D:1358:PRO:HD2	1.93	0.51
3:D:845:ALA:HB2	3:D:883:ARG:HG3	1.93	0.51
3:D:1194:ARG:HD3	3:D:1211:SER:HB3	1.92	0.51
2:C:543:ALA:HB3	2:C:548:ARG:HH21	1.75	0.50
1:A:20:SER:OG	1:A:21:SER:N	2.42	0.50
1:B:214:GLU:OE1	1:B:214:GLU:N	2.26	0.50
3:D:901:ARG:HA	3:D:908:ILE:HA	1.92	0.50
3:D:750:PRO:HG3	3:D:781:LYS:HB2	1.91	0.50
7:H:18:DA:H2''	7:H:19:DG:C8	2.47	0.50
5:F:97:PRO:HB2	5:F:402:LEU:HD11	1.94	0.50
3:D:933:ARG:HB2	3:D:936:HIS:NE2	2.26	0.50
3:D:1029:THR:HG22	3:D:1121:LEU:HG	1.93	0.50
5:F:268:TYR:HA	5:F:271:ASN:HD21	1.77	0.50
3:D:970:SER:OG	3:D:1117:SER:OG	2.27	0.50
3:D:1063:ASP:OD1	3:D:1063:ASP:N	2.37	0.50
3:D:934:THR:O	3:D:937:ILE:HG22	2.12	0.49
3:D:1267:VAL:O	3:D:1301:THR:OG1	2.23	0.49
2:C:870:ILE:HD12	2:C:944:ARG:HG2	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:489:MET:HG3	5:F:490:PRO:HD2	1.94	0.49
6:G:25:DA:H2''	6:G:26:DG:C8	2.47	0.49
2:C:533:LEU:HD21	2:C:571:LEU:HD13	1.94	0.49
2:C:632:ASP:HA	2:C:647:ARG:HH21	1.78	0.49
6:G:23:DG:H1	7:H:5:DC:H42	1.59	0.49
2:C:560:PRO:O	3:D:780:ARG:NH2	2.45	0.49
2:C:979:LEU:HD21	2:C:1011:LEU:HD11	1.94	0.49
3:D:1167:LYS:H	3:D:1167:LYS:HD3	1.77	0.49
5:F:429:THR:HG23	6:G:4:DA:H2'	1.94	0.49
1:A:234:LEU:O	1:B:218:ARG:NH1	2.42	0.49
2:C:995:ASP:OD1	2:C:995:ASP:N	2.41	0.49
3:D:708:ASN:HB3	3:D:714:GLU:HG3	1.94	0.49
2:C:753:LEU:HB3	2:C:767:GLN:HB2	1.93	0.49
3:D:747:MET:HE1	3:D:939:GLY:HA3	1.95	0.49
3:D:790:THR:HG21	3:D:932:MET:SD	2.53	0.49
3:D:975:ILE:HD13	3:D:980:THR:HG21	1.95	0.49
2:C:820:GLU:HG2	2:C:1079:ILE:HG22	1.93	0.49
1:A:76:GLU:HG2	1:A:80:GLU:HG2	1.95	0.48
3:D:786:THR:HB	3:D:932:MET:HA	1.94	0.48
3:D:918:ILE:O	3:D:922:SER:OG	2.27	0.48
1:A:135:ASP:HB3	1:A:138:ALA:HB2	1.94	0.48
2:C:406:ASN:ND2	2:C:413:GLU:O	2.34	0.48
3:D:848:VAL:HB	3:D:858:VAL:HB	1.96	0.48
5:F:491:GLU:OE2	5:F:495:ARG:NH2	2.47	0.48
3:D:750:PRO:CD	3:D:781:LYS:HB2	2.43	0.48
6:G:18:DC:H2''	6:G:19:DG:C8	2.49	0.48
2:C:581:THR:HG22	2:C:587:LEU:HD23	1.95	0.48
3:D:381:ILE:HD11	3:D:412:LEU:HD13	1.96	0.48
2:C:277:LEU:HD13	2:C:282:VAL:HG21	1.96	0.47
3:D:68:TYR:OH	3:D:81:ARG:NH2	2.47	0.47
3:D:1109:LEU:HD21	3:D:1121:LEU:HA	1.96	0.47
2:C:321:LEU:O	2:C:325:LEU:HD23	2.14	0.47
2:C:1121:ALA:HB2	2:C:1182:ILE:HD12	1.95	0.47
3:D:851:PRO:HA	3:D:855:ASP:HA	1.95	0.47
3:D:1037:PHE:HE2	3:D:1111:ASP:HB2	1.78	0.47
5:F:119:ILE:HG21	5:F:379:MET:HB2	1.96	0.47
7:H:20:DG:H2''	7:H:21:DG:C8	2.49	0.47
5:F:487:MET:O	5:F:487:MET:HG2	2.14	0.47
2:C:252:SER:O	2:C:265:LYS:NZ	2.42	0.47
3:D:320:ASN:OD1	3:D:320:ASN:N	2.40	0.47
3:D:530:PRO:HB3	3:D:577:ALA:O	2.15	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:786:THR:O	3:D:786:THR:OG1	2.31	0.47
5:F:359:LYS:HB2	5:F:359:LYS:HE3	1.71	0.47
5:F:361:ILE:O	5:F:365:MET:HG2	2.14	0.47
2:C:338:THR:HG21	2:C:345:PRO:HB3	1.95	0.47
1:A:222:THR:HA	1:B:232:VAL:HG23	1.96	0.47
3:D:799:ARG:NH1	3:D:1146:GLU:OE2	2.44	0.47
2:C:99:LYS:HE3	2:C:99:LYS:HB2	1.75	0.47
2:C:161:LYS:HA	2:C:170:VAL:HG22	1.97	0.47
7:H:19:DG:H2''	7:H:20:DG:C8	2.50	0.47
1:B:191:ARG:HH21	1:B:194:GLN:H	1.63	0.46
5:F:586:ARG:NH1	5:F:589:GLN:OE1	2.48	0.46
2:C:413:GLU:OE2	2:C:413:GLU:N	2.34	0.46
2:C:518:ASN:OD1	2:C:1236:ASN:ND2	2.45	0.46
1:B:16:ILE:HG23	1:B:26:VAL:HG12	1.97	0.46
2:C:231:GLU:O	2:C:238:GLN:N	2.37	0.46
3:D:31:ARG:NH1	3:D:106:GLU:OE2	2.49	0.46
3:D:495:ASN:OD1	3:D:495:ASN:N	2.48	0.46
5:F:557:LYS:HD3	5:F:557:LYS:HA	1.60	0.46
5:F:463:LEU:HD11	5:F:483:LEU:HD13	1.98	0.46
1:A:158:ARG:NH2	1:A:173:VAL:O	2.49	0.45
2:C:1023:HIS:O	2:C:1027:LYS:HG3	2.17	0.45
1:B:85:LEU:HD23	1:B:85:LEU:HA	1.81	0.45
2:C:685:MET:SD	2:C:1073:LYS:HB3	2.55	0.45
2:C:39:ILE:HD11	2:C:75:LEU:HD11	1.98	0.45
2:C:388:LEU:HD23	2:C:388:LEU:HA	1.85	0.45
3:D:275:ARG:HH11	3:D:302:ALA:HB2	1.81	0.45
6:G:10:DA:H2''	6:G:11:DG:C8	2.51	0.45
2:C:549:ASP:HA	3:D:780:ARG:HD2	1.99	0.45
2:C:952:GLN:HB3	2:C:1036:ILE:HD13	1.99	0.45
2:C:1111:GLN:O	2:C:1115:THR:OG1	2.31	0.45
2:C:593:LYS:HZ3	2:C:595:THR:HG22	1.82	0.45
2:C:248:GLY:HA2	2:C:269:ILE:HB	1.99	0.45
3:D:750:PRO:CG	3:D:781:LYS:HB2	2.47	0.44
5:F:108:VAL:O	5:F:385:ARG:NH1	2.48	0.44
3:D:79:LYS:HB2	3:D:79:LYS:HE3	1.68	0.44
3:D:94:GLN:H	3:D:94:GLN:HG2	1.56	0.44
3:D:1341:ARG:NH1	3:D:1343:GLU:OE2	2.50	0.44
1:A:31:LEU:HD13	1:A:36:GLY:HA2	1.99	0.44
2:C:356:THR:HG21	2:C:362:ALA:HB2	1.99	0.44
3:D:214:ARG:H	3:D:214:ARG:HG2	1.64	0.44
3:D:1046:ILE:HG22	3:D:1061:VAL:HG22	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1273:ASP:OD1	3:D:1273:ASP:N	2.49	0.44
3:D:369:PRO:HG2	3:D:372:MET:HB2	1.99	0.44
3:D:613:GLY:O	3:D:617:THR:OG1	2.22	0.44
7:H:9:DC:H2"	7:H:10:DG:C8	2.53	0.44
2:C:592:ARG:HG3	2:C:653:MET:HB3	2.00	0.44
5:F:452:ILE:HG22	5:F:457:ILE:HG12	1.98	0.44
3:D:264:ASP:HB3	3:D:324:LEU:HD22	2.00	0.44
3:D:1064:SER:HA	3:D:1067:ARG:HB2	1.97	0.44
1:B:127:GLN:O	1:B:127:GLN:NE2	2.50	0.44
3:D:177:ASP:N	3:D:177:ASP:OD1	2.51	0.44
3:D:1311:LYS:HB3	3:D:1311:LYS:HE3	1.61	0.44
5:F:111:LEU:HD13	5:F:116:GLU:HG3	1.99	0.44
1:A:91:ARG:HG3	1:A:122:GLU:HG3	2.00	0.44
1:B:164:ASP:OD1	1:B:165:GLU:N	2.49	0.44
3:D:681:LYS:O	3:D:685:ILE:HG13	2.18	0.44
3:D:1042:ASP:HA	3:D:1046:ILE:HG13	2.00	0.44
3:D:1190:ILE:HG21	3:D:1196:LEU:HD11	2.00	0.44
3:D:817:HIS:HD2	3:D:860:ARG:HH12	1.66	0.43
2:C:102:LEU:HB3	2:C:118:LYS:HB2	2.00	0.43
2:C:197:ARG:HD3	2:C:200:ARG:HA	1.99	0.43
2:C:228:VAL:HG12	2:C:335:THR:HB	2.00	0.43
2:C:1064:ASP:HB2	2:C:1076:ILE:HD12	1.99	0.43
3:D:537:TYR:OH	3:D:634:ARG:NH1	2.51	0.43
2:C:854:ILE:HD11	2:C:885:GLY:HA3	2.00	0.43
3:D:201:LEU:HD23	3:D:221:ILE:HB	2.00	0.43
2:C:1286:THR:HG22	3:D:479:GLU:OE2	2.18	0.43
3:D:26:SER:H	3:D:29:MET:HE3	1.83	0.43
1:B:152:TYR:OH	1:B:174:ASP:OD2	2.34	0.43
2:C:704:MET:HE3	2:C:704:MET:HB3	1.80	0.43
3:D:450:HIS:HD2	3:D:452:LEU:HB2	1.84	0.43
2:C:262:TYR:OH	2:C:280:ASP:OD2	2.31	0.43
2:C:949:GLU:O	2:C:953:LEU:HG	2.19	0.43
3:D:842:ARG:NH2	3:D:1254:GLU:OE1	2.50	0.43
3:D:1062:LEU:HD12	3:D:1062:LEU:H	1.82	0.43
2:C:341:LEU:HG	2:C:342:ASP:N	2.34	0.43
2:C:865:LEU:HD21	2:C:882:ILE:HG22	2.01	0.43
2:C:1011:LEU:HD23	2:C:1011:LEU:HA	1.84	0.43
3:D:502:PRO:HG2	3:D:601:ILE:HG21	2.01	0.43
2:C:148:GLN:OE1	2:C:454:ARG:NH1	2.51	0.43
2:C:866:ASP:OD1	2:C:867:GLU:N	2.48	0.43
3:D:907:HIS:ND1	3:D:908:ILE:O	2.48	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1017:GLN:HE21	2:C:1021:LEU:HG	1.84	0.43
1:A:98:VAL:HG11	1:A:121:VAL:HG21	2.01	0.42
2:C:1293:VAL:HG21	2:C:1315:MET:HG2	2.00	0.42
3:D:43:THR:HG21	5:F:449:THR:HG22	2.00	0.42
6:G:24:DC:H2''	6:G:25:DA:C8	2.54	0.42
7:H:15:DT:H2'	7:H:16:DC:C6	2.53	0.42
1:A:25:LYS:HB3	1:A:25:LYS:HE3	1.82	0.42
2:C:122:VAL:HG11	2:C:493:ILE:HG13	2.01	0.42
3:D:1079:LYS:HG2	3:D:1098:GLN:HG2	1.99	0.42
2:C:420:LEU:HD23	2:C:420:LEU:HA	1.88	0.42
3:D:417:ARG:O	4:E:45:LYS:HE2	2.19	0.42
3:D:667:GLN:HB3	3:D:673:VAL:HG21	2.02	0.42
1:B:90:VAL:HG13	1:B:123:ILE:HD13	2.02	0.42
2:C:402:ARG:HA	2:C:402:ARG:HD3	1.91	0.42
3:D:982:LEU:HB3	3:D:995:TYR:HB2	2.02	0.42
7:H:4:DG:H4'	7:H:5:DC:OP1	2.17	0.42
2:C:28:LEU:HD12	2:C:28:LEU:O	2.19	0.42
2:C:200:ARG:HG3	6:G:13:DT:H2''	2.00	0.42
2:C:819:SER:HB2	2:C:1085:MET:HG3	2.02	0.42
3:D:71:LEU:HB2	3:D:90:VAL:HG21	2.00	0.42
3:D:114:ILE:HD11	3:D:311:ARG:HB3	2.01	0.42
3:D:1028:ILE:HD12	3:D:1028:ILE:HA	1.90	0.42
1:A:190:ALA:HB2	1:A:200:LYS:HE2	2.02	0.42
2:C:675:ASP:HB3	2:C:678:ARG:HG2	2.01	0.42
5:F:552:THR:OG1	5:F:555:GLU:OE1	2.36	0.42
2:C:175:ARG:NH1	6:G:14:DG:OP1	2.44	0.42
2:C:299:LYS:NZ	2:C:334:GLU:OE1	2.41	0.42
3:D:51:PRO:HB3	3:D:57:PHE:O	2.20	0.42
3:D:140:TYR:CD2	5:F:100:MET:HE1	2.55	0.42
3:D:1326:GLN:HG2	7:H:12:DG:H5''	2.02	0.42
2:C:241:LEU:HD11	2:C:246:LEU:HD21	2.02	0.41
2:C:1304:MET:HE3	2:C:1308:ILE:HG13	2.02	0.41
3:D:48:THR:O	3:D:50:LYS:N	2.52	0.41
1:A:154:PRO:HG2	1:A:157:THR:HG23	2.01	0.41
2:C:758:ARG:NH2	2:C:762:ASN:OD1	2.30	0.41
2:C:842:ASP:HB3	2:C:1047:LEU:HD11	2.02	0.41
3:D:744:ARG:HB2	3:D:759:ILE:HB	2.02	0.41
3:D:950:ILE:HG12	3:D:1018:ALA:HB3	2.01	0.41
3:D:996:LYS:HA	3:D:996:LYS:HD3	1.77	0.41
3:D:1134:ILE:HD12	3:D:1134:ILE:HA	1.88	0.41
3:D:660:GLU:HB3	3:D:685:ILE:HD13	2.01	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ARG:NH2	1:B:194:GLN:H	2.19	0.41
2:C:69:GLN:OE1	2:C:101:ARG:NE	2.49	0.41
2:C:1115:THR:HG22	2:C:1228:GLY:HA3	2.01	0.41
3:D:1152:GLU:OE2	3:D:1194:ARG:NH2	2.53	0.41
3:D:1153:PRO:O	3:D:1194:ARG:NH2	2.54	0.41
5:F:452:ILE:HG23	5:F:456:MET:HB3	2.02	0.41
3:D:697:MET:HE3	3:D:697:MET:HB3	1.83	0.41
2:C:232:ILE:HA	2:C:237:LEU:HA	2.03	0.41
2:C:967:LEU:HD23	2:C:967:LEU:HA	1.92	0.41
2:C:1164:PHE:HB3	2:C:1169:VAL:HG23	2.03	0.41
3:D:856:ILE:H	3:D:856:ILE:HG12	1.66	0.41
5:F:272:SER:O	5:F:276:MET:HG2	2.21	0.41
5:F:360:ASP:HA	5:F:363:ARG:HG2	2.03	0.41
2:C:845:LEU:HD13	2:C:845:LEU:HA	1.94	0.40
5:F:266:PHE:HD1	5:F:269:LEU:HD12	1.84	0.40
2:C:487:LEU:HD12	2:C:487:LEU:HA	1.90	0.40
2:C:1104:PRO:HA	3:D:740:LEU:HD11	2.04	0.40
2:C:1105:SER:HB2	3:D:731:ARG:HG3	2.02	0.40
2:C:1271:GLY:N	2:C:1274:GLU:OE1	2.52	0.40
3:D:1247:LYS:HB3	3:D:1247:LYS:HE2	1.88	0.40
2:C:807:TRP:CG	2:C:808:ASN:H	2.39	0.40
2:C:870:ILE:HG23	2:C:884:VAL:HG22	2.03	0.40
1:B:58:GLU:HB3	1:B:145:LYS:HD2	2.02	0.40
2:C:1278:LEU:HD23	2:C:1278:LEU:HA	1.91	0.40
2:C:1293:VAL:HG11	2:C:1304:MET:HG2	2.03	0.40
3:D:388:ARG:H	3:D:388:ARG:HG2	1.68	0.40
1:A:39:LEU:HD23	1:A:39:LEU:HA	1.92	0.40
2:C:273:HIS:O	2:C:277:LEU:HD23	2.22	0.40
3:D:850:LYS:HD3	3:D:850:LYS:HA	1.82	0.40
5:F:487:MET:O	5:F:488:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	228/329 (69%)	225 (99%)	3 (1%)	0	100	100
1	B	227/329 (69%)	220 (97%)	7 (3%)	0	100	100
2	C	1338/1342 (100%)	1295 (97%)	43 (3%)	0	100	100
3	D	1360/1407 (97%)	1315 (97%)	45 (3%)	0	100	100
4	E	76/91 (84%)	76 (100%)	0	0	100	100
5	F	325/613 (53%)	323 (99%)	2 (1%)	0	100	100
All	All	3554/4111 (86%)	3454 (97%)	100 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/286 (69%)	190 (96%)	7 (4%)	31	58
1	B	197/286 (69%)	187 (95%)	10 (5%)	21	48
2	C	1155/1157 (100%)	1105 (96%)	50 (4%)	26	53
3	D	1134/1168 (97%)	1079 (95%)	55 (5%)	22	50
4	E	66/75 (88%)	64 (97%)	2 (3%)	36	62
5	F	292/540 (54%)	286 (98%)	6 (2%)	47	68
All	All	3041/3512 (87%)	2911 (96%)	130 (4%)	27	53

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	15	ASP
1	A	27	THR
1	A	51	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	97	GLU
1	A	197	ASP
1	A	232	VAL
1	B	70	THR
1	B	74	VAL
1	B	121	VAL
1	B	153	VAL
1	B	173	VAL
1	B	174	ASP
1	B	176	CYS
1	B	183	ILE
1	B	197	ASP
1	B	212	ASP
2	C	7	GLU
2	C	18	ARG
2	C	21	VAL
2	C	46	GLN
2	C	97	ARG
2	C	111	GLU
2	C	165	HIS
2	C	185	ASP
2	C	207	THR
2	C	360	LEU
2	C	371	ARG
2	C	393	ASP
2	C	456	VAL
2	C	471	VAL
2	C	513	GLN
2	C	550	VAL
2	C	561	ILE
2	C	565	GLU
2	C	610	GLU
2	C	628	HIS
2	C	635	THR
2	C	660	VAL
2	C	680	LEU
2	C	692	THR
2	C	714	VAL
2	C	733	VAL
2	C	754	THR
2	C	789	THR
2	C	799	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	818	VAL
2	C	820	GLU
2	C	841	ARG
2	C	845	LEU
2	C	888	THR
2	C	896	THR
2	C	964	LEU
2	C	985	GLU
2	C	992	LEU
2	C	1019	ASP
2	C	1037	THR
2	C	1060	ILE
2	C	1083	GLU
2	C	1088	ASP
2	C	1101	LEU
2	C	1151	LEU
2	C	1163	THR
2	C	1178	LYS
2	C	1252	SER
2	C	1255	THR
2	C	1293	VAL
3	D	46	TYR
3	D	78	LEU
3	D	83	VAL
3	D	145	VAL
3	D	160	LEU
3	D	198	CYS
3	D	227	PHE
3	D	289	ASP
3	D	320	ASN
3	D	421	VAL
3	D	525	MET
3	D	663	GLU
3	D	681	LYS
3	D	695	LYS
3	D	751	ASP
3	D	760	THR
3	D	781	LYS
3	D	783	LEU
3	D	786	THR
3	D	790	THR
3	D	793	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	D	831	VAL
3	D	849	LEU
3	D	856	ILE
3	D	891	ASP
3	D	897	HIS
3	D	910	ASN
3	D	932	MET
3	D	960	LEU
3	D	982	LEU
3	D	1009	GLU
3	D	1031	VAL
3	D	1035	VAL
3	D	1036	ARG
3	D	1045	THR
3	D	1048	ARG
3	D	1056	LEU
3	D	1059	LEU
3	D	1066	GLU
3	D	1089	LEU
3	D	1107	VAL
3	D	1124	ILE
3	D	1138	LEU
3	D	1167	LYS
3	D	1168	GLU
3	D	1173	ARG
3	D	1199	PHE
3	D	1202	GLU
3	D	1209	VAL
3	D	1243	LEU
3	D	1261	LEU
3	D	1281	GLU
3	D	1305	ASP
3	D	1320	ILE
3	D	1329	THR
4	E	8	ASP
4	E	65	ASP
5	F	111	LEU
5	F	359	LYS
5	F	417	ASP
5	F	479	THR
5	F	559	LEU
5	F	569	THR



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	132	HIS
1	A	147	GLN
1	B	103	ASN
2	C	327	GLN
2	C	447	HIS
2	C	517	GLN
2	C	526	HIS
2	C	618	GLN
2	C	688	GLN
2	C	767	GLN
2	C	1009	ASN
2	C	1017	GLN
2	C	1116	HIS
2	C	1136	GLN
3	D	335	GLN
3	D	341	ASN
3	D	364	HIS
3	D	448	GLN
3	D	450	HIS
3	D	488	ASN
3	D	545	HIS
3	D	739	GLN
3	D	817	HIS
3	D	897	HIS
3	D	921	GLN
3	D	1086	ASN
3	D	1098	GLN
3	D	1108	GLN
3	D	1227	HIS
3	D	1249	ASN
3	D	1259	GLN
3	D	1326	GLN
3	D	1367	GLN
4	E	31	GLN
4	E	73	GLN
5	F	271	ASN
5	F	469	GLN

### 5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	1/2 (50%)	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](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 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	$\# Z  > 2$
11	PUM	I	1601	-	35,35,35	0.81	1 (2%)	39,49,49	0.59	0

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
11	PUM	I	1601	-	-	11/31/47/47	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	1601	PUM	CAL-CAZ	3.67	1.39	1.35

There are no bond angle outliers.

There are no chirality outliers.

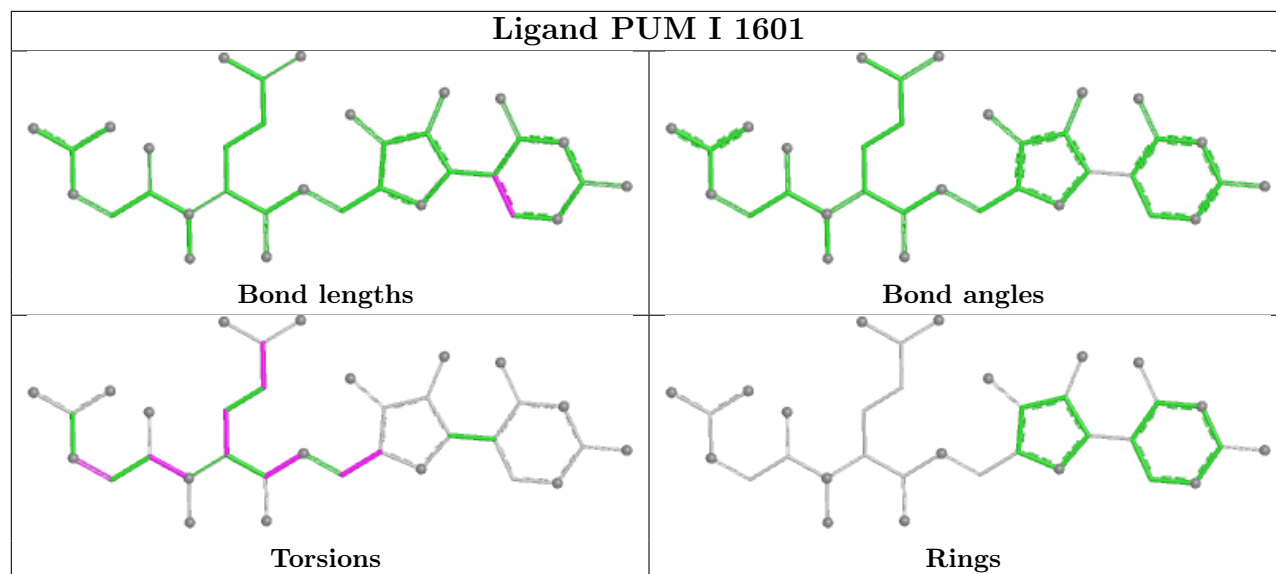
All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	I	1601	PUM	NAR-CAP-CBE-OAU
11	I	1601	PUM	C-CA-CB-CG
11	I	1601	PUM	N-CA-CB-CG
11	I	1601	PUM	O-C-NAR-CAP
11	I	1601	PUM	CA-C-NAR-CAP
11	I	1601	PUM	OE1-CD-CG-CB
11	I	1601	PUM	NE2-CD-CG-CB
11	I	1601	PUM	OAE-CAX-N-CA
11	I	1601	PUM	CAX-CAN-NAQ-CAV
11	I	1601	PUM	NAR-CAP-CBE-CBC
11	I	1601	PUM	OAE-CAX-N-OAK

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

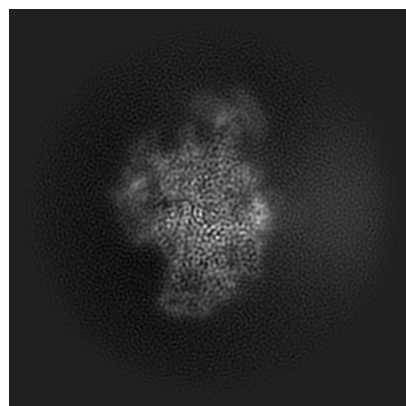
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73220. These allow visual inspection of the internal detail of the map and identification of artifacts.

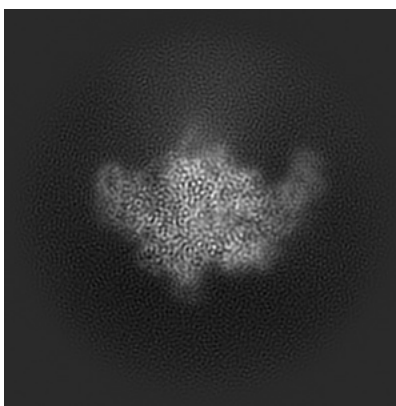
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

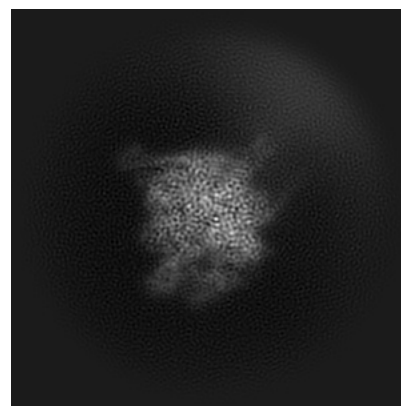
#### 6.1.1 Primary map



X

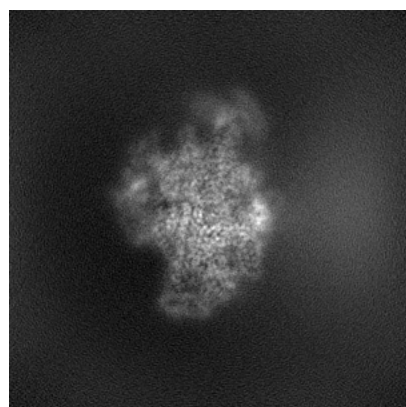


Y

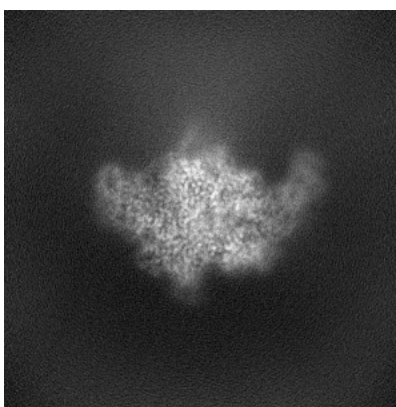


Z

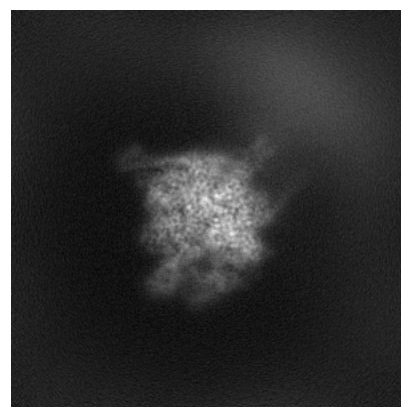
#### 6.1.2 Raw map



X



Y

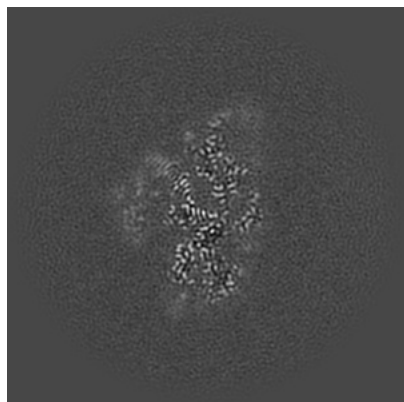


Z

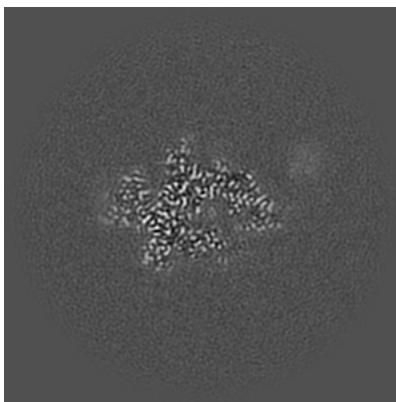
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

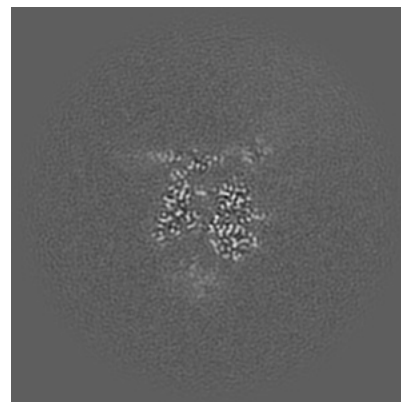
### 6.2.1 Primary map



X Index: 150

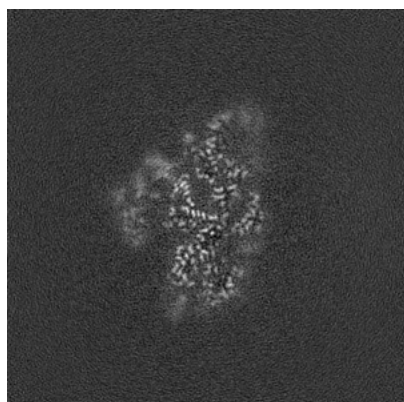


Y Index: 150

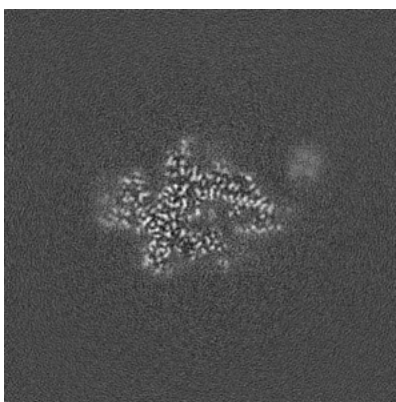


Z Index: 150

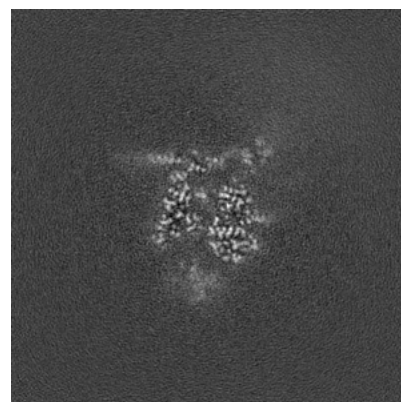
### 6.2.2 Raw map



X Index: 150



Y Index: 150



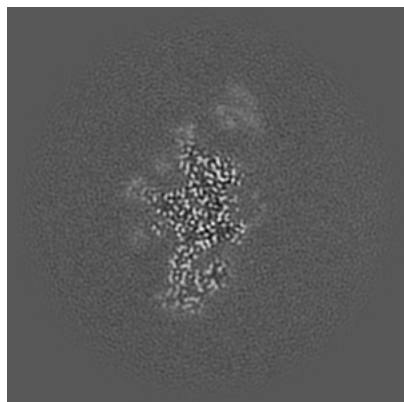
Z Index: 150

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

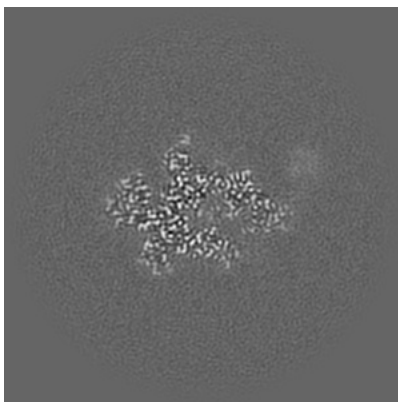


## 6.3 Largest variance slices [i](#)

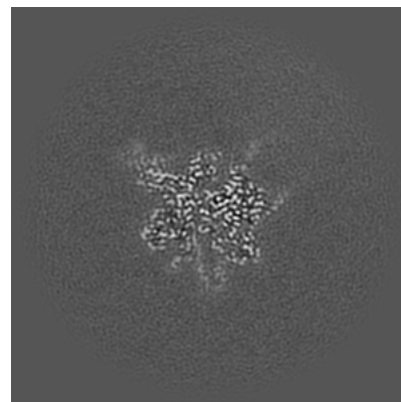
### 6.3.1 Primary map



X Index: 165

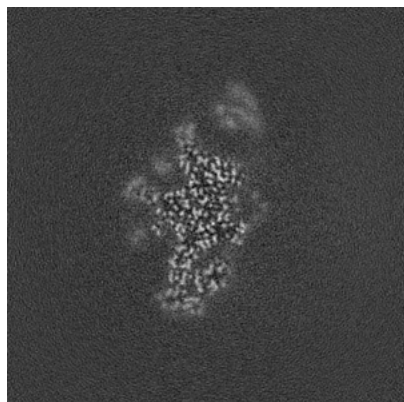


Y Index: 153

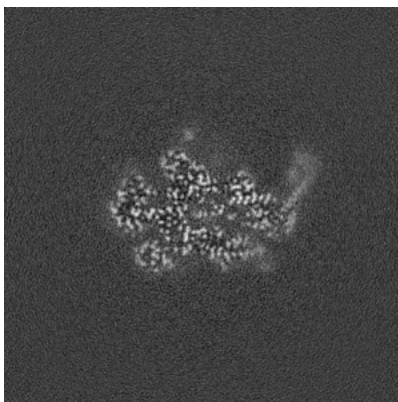


Z Index: 136

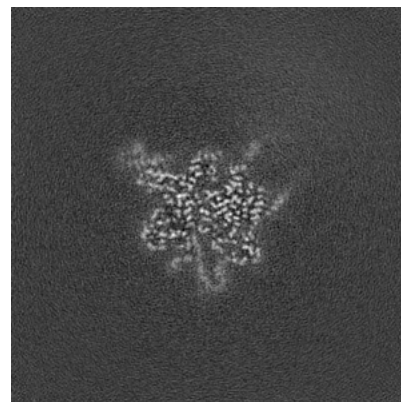
### 6.3.2 Raw map



X Index: 165



Y Index: 158

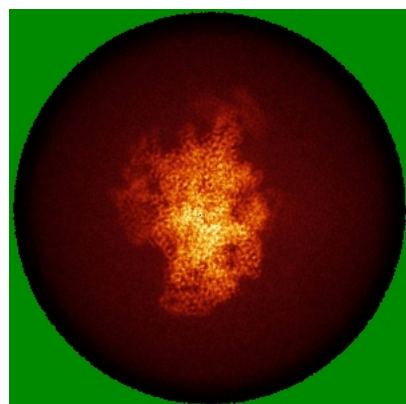


Z Index: 136

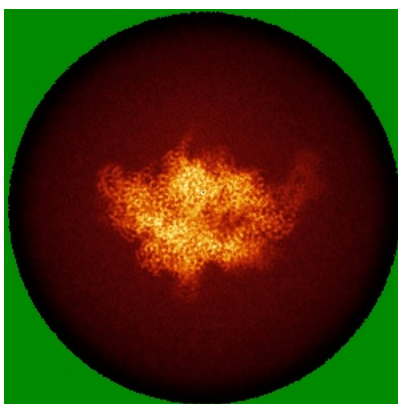
The images above show the largest variance slices of the map in three orthogonal directions.

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

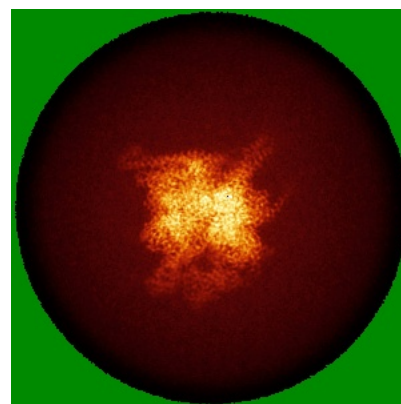
### 6.4.1 Primary map



X

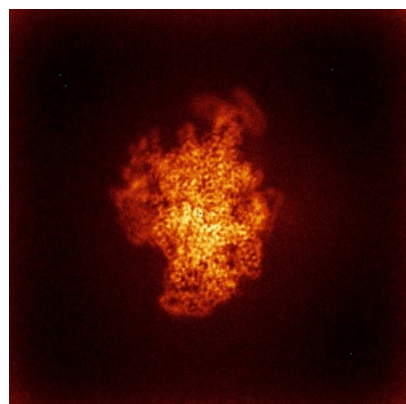


Y

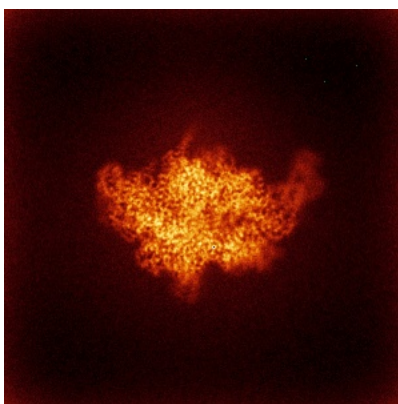


Z

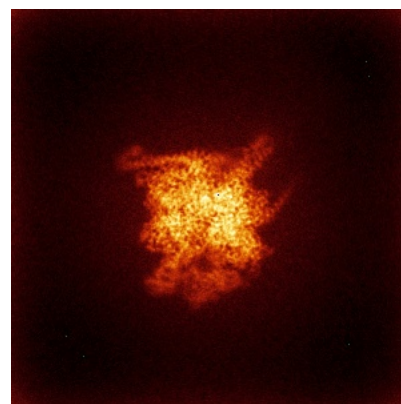
### 6.4.2 Raw map



X



Y



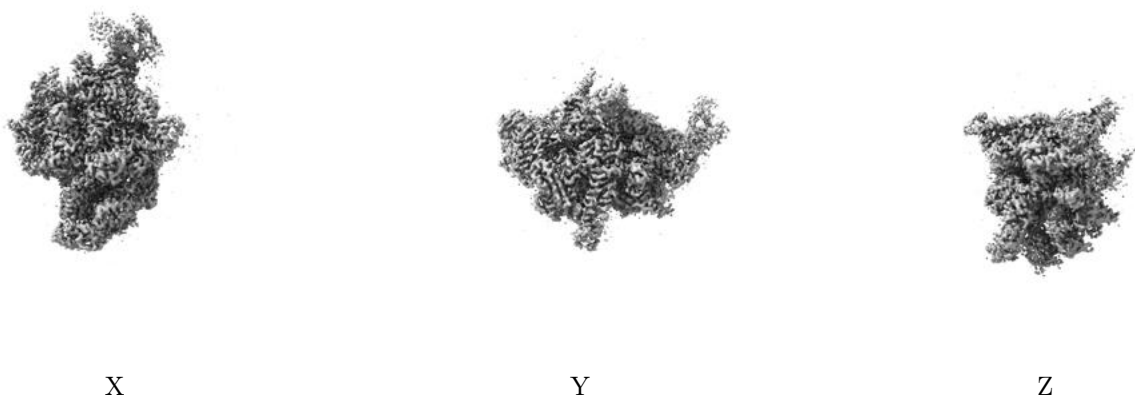
Z

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.



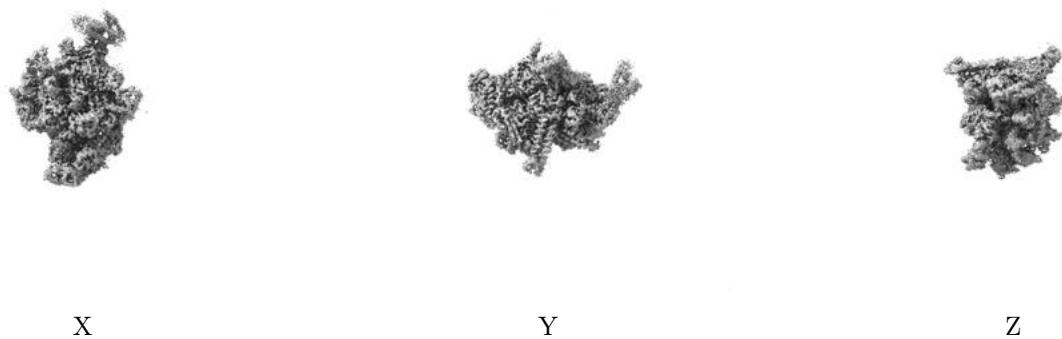
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.085. 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.

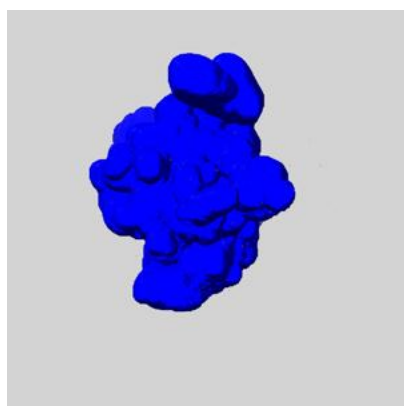
## 6.6 Mask visualisation [i](#)

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

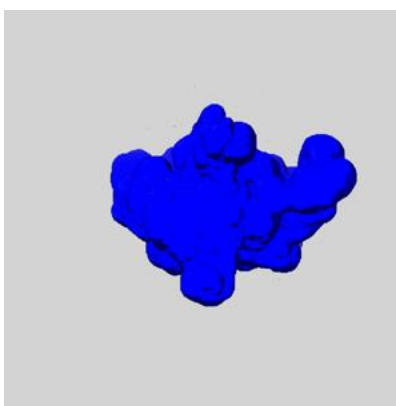
A mask typically either:

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

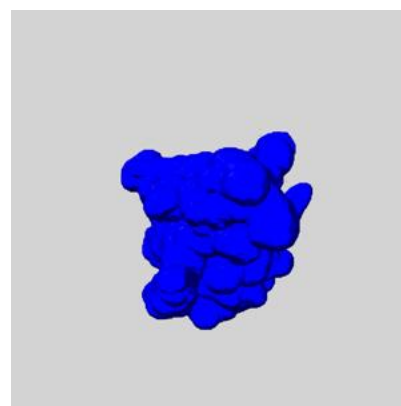
### 6.6.1 emd\_73220\_msk\_1.map [i](#)



X



Y

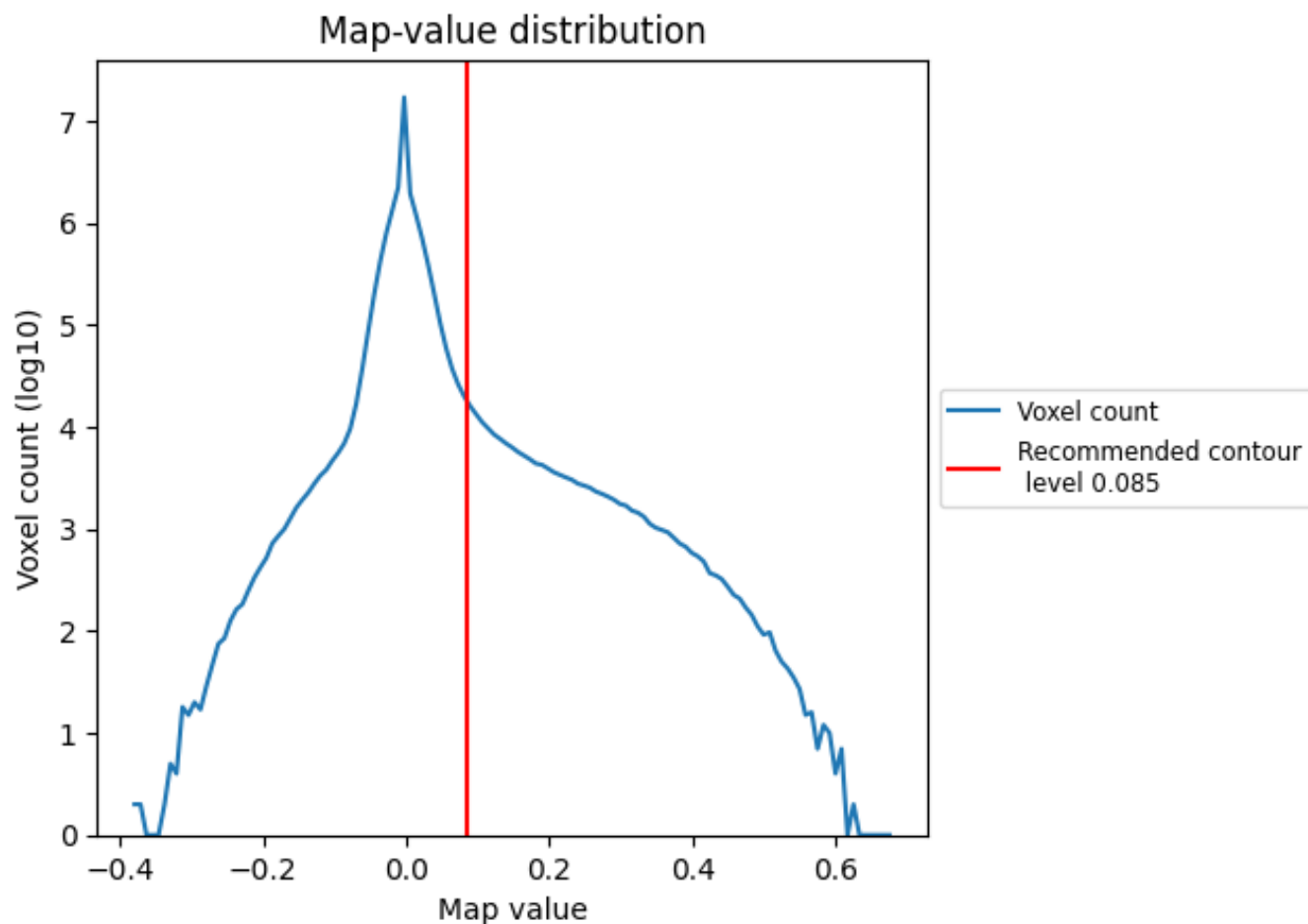


Z

## 7 Map analysis [i](#)

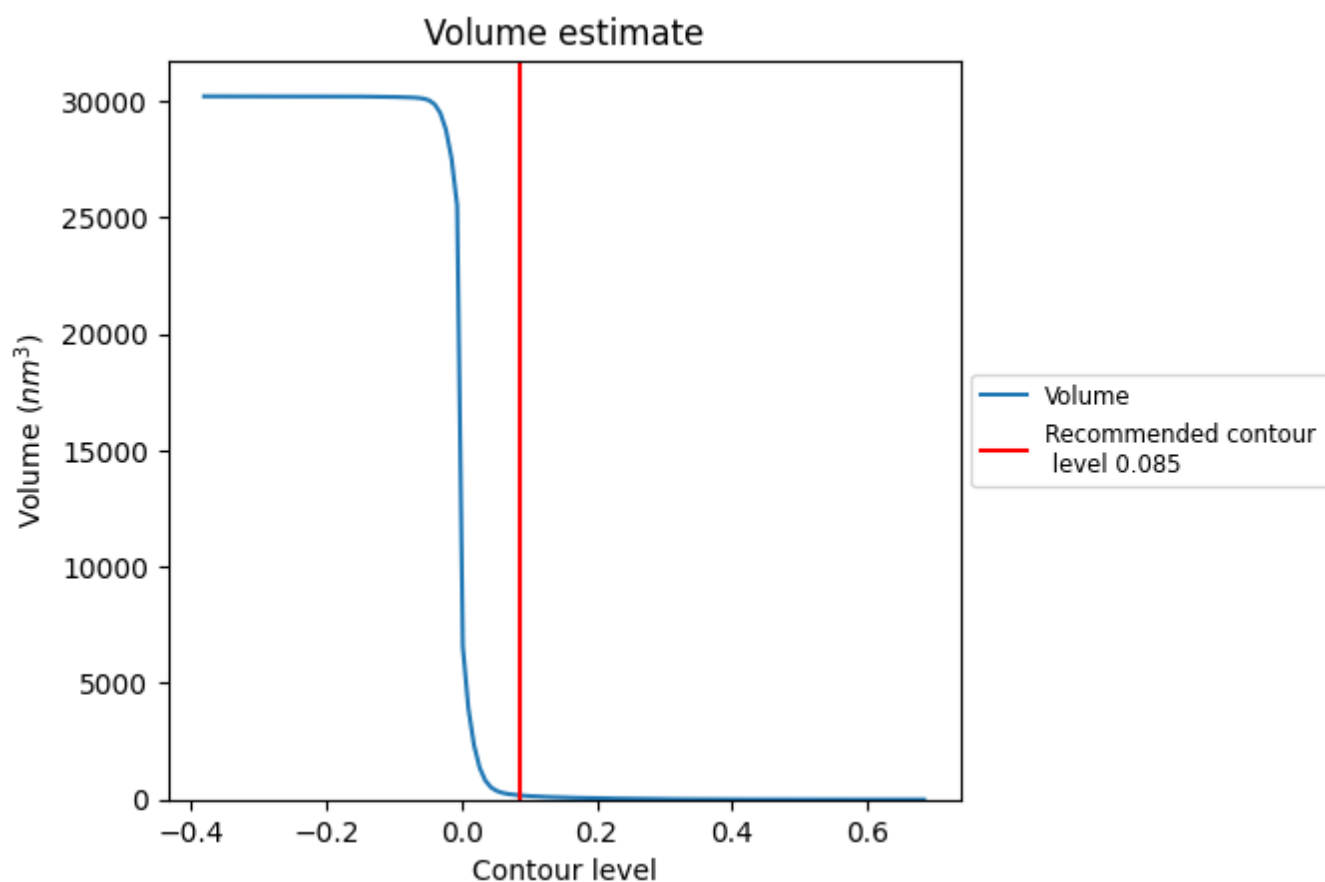
This section contains the results of statistical analysis of the map.

### 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.

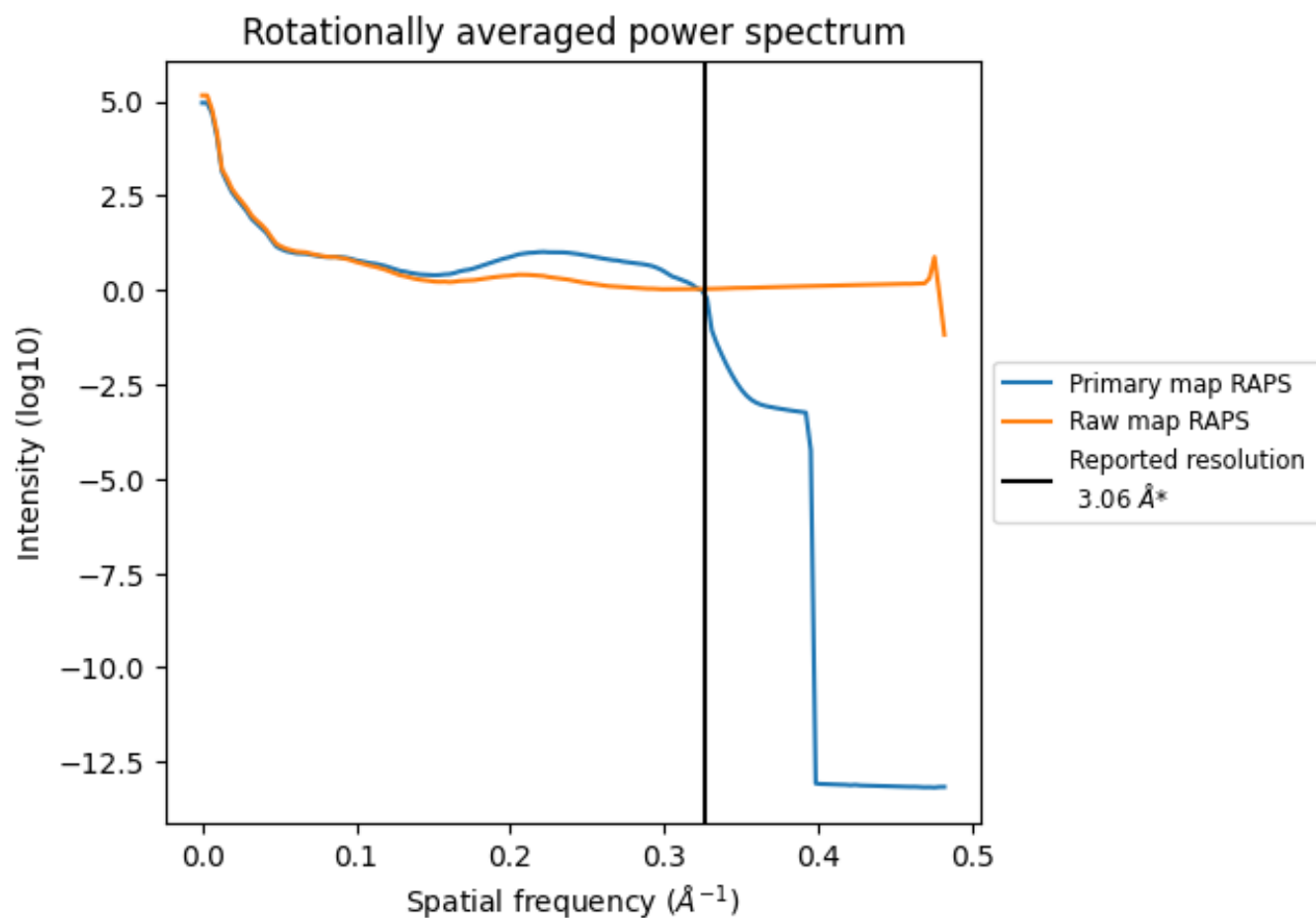
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 184 nm<sup>3</sup>; this corresponds to an approximate mass of 166 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

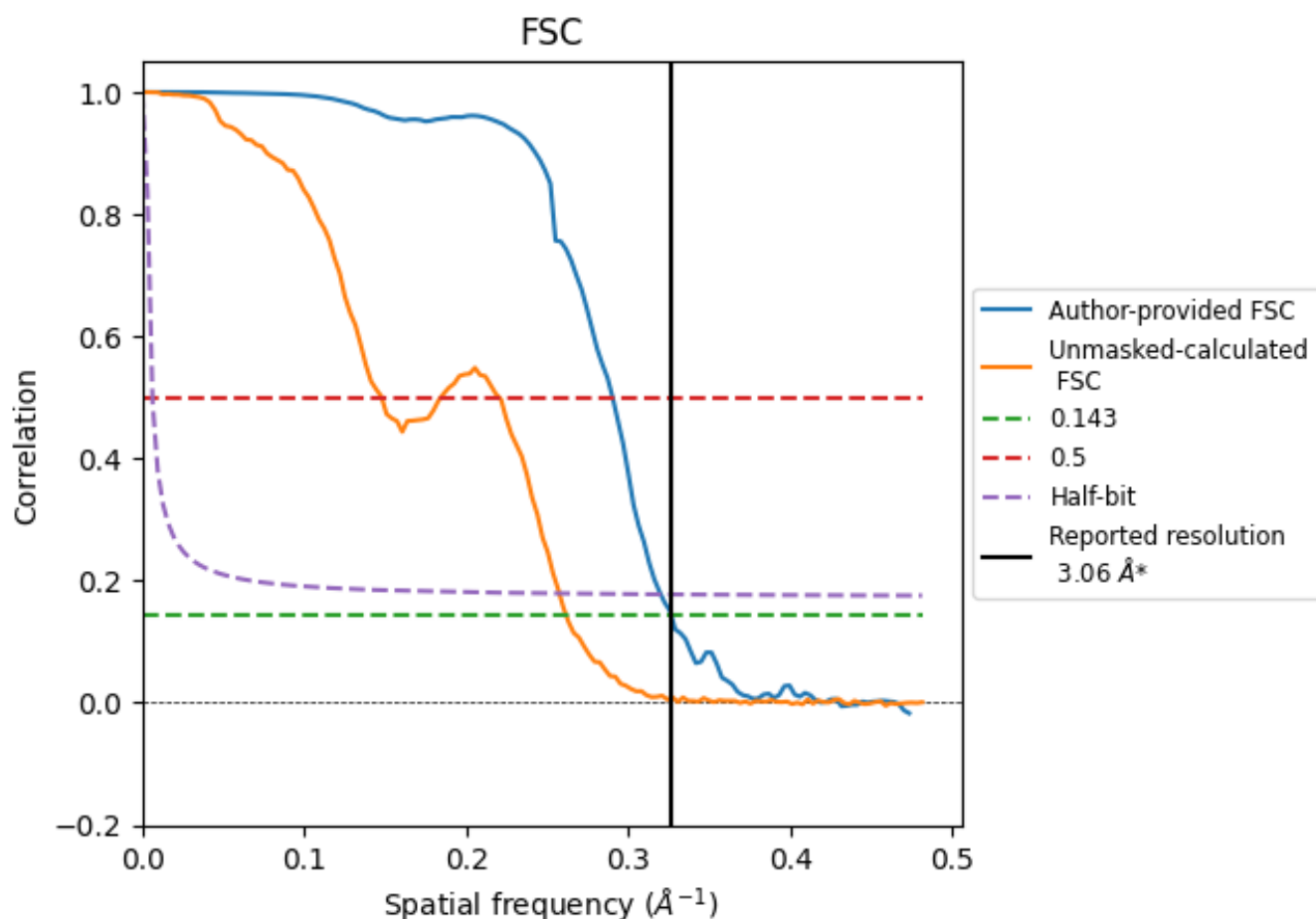


\*Reported resolution corresponds to spatial frequency of 0.327  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.327 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

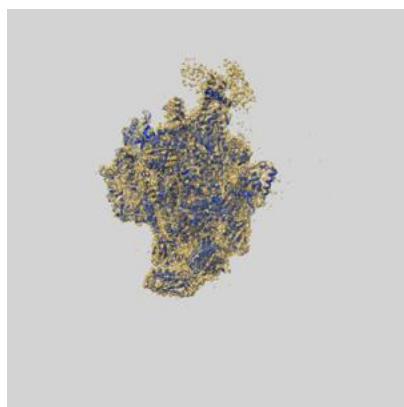
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	3.06	3.44	3.12
Unmasked-calculated*	3.82	6.76	3.88

\*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 3.82 differs from the reported value 3.06 by more than 10 %

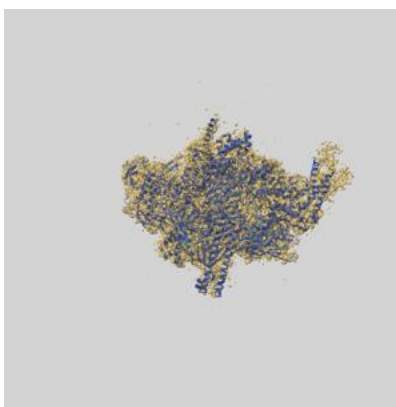
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73220 and PDB model 9YNP. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

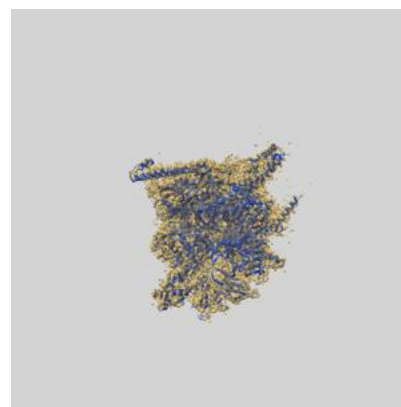
### 9.1 Map-model overlay [i](#)



X



Y

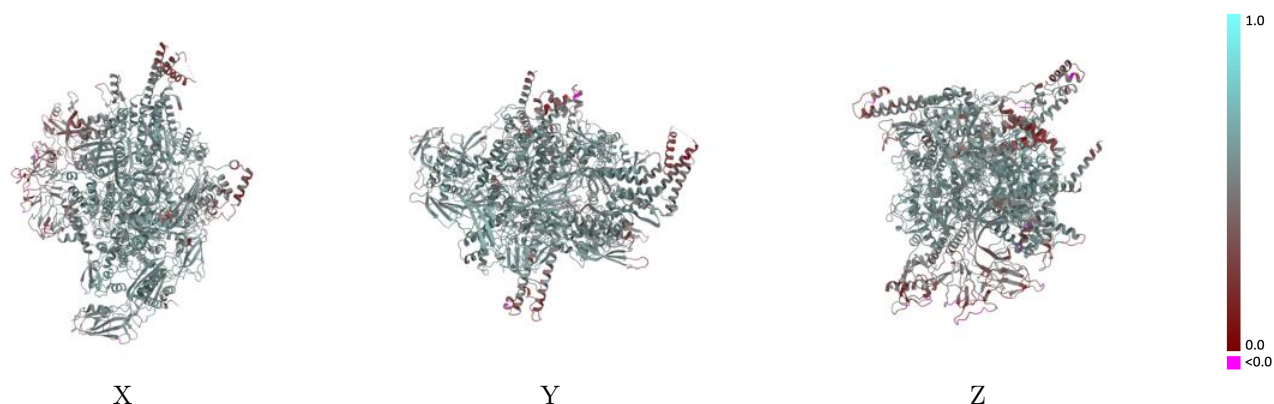


Z

The images above show the 3D surface view of the map at the recommended contour level 0.085 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.

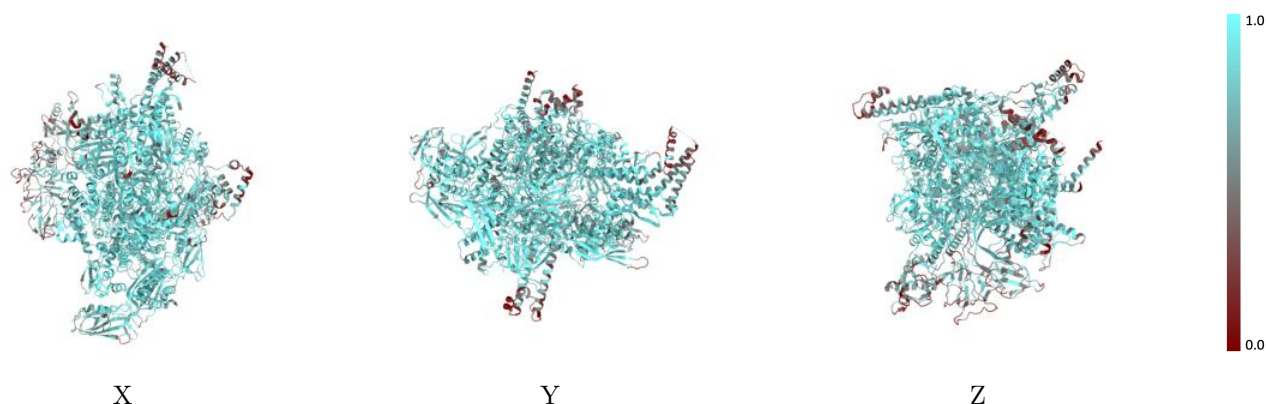


## 9.2 Q-score mapped to coordinate model [i](#)



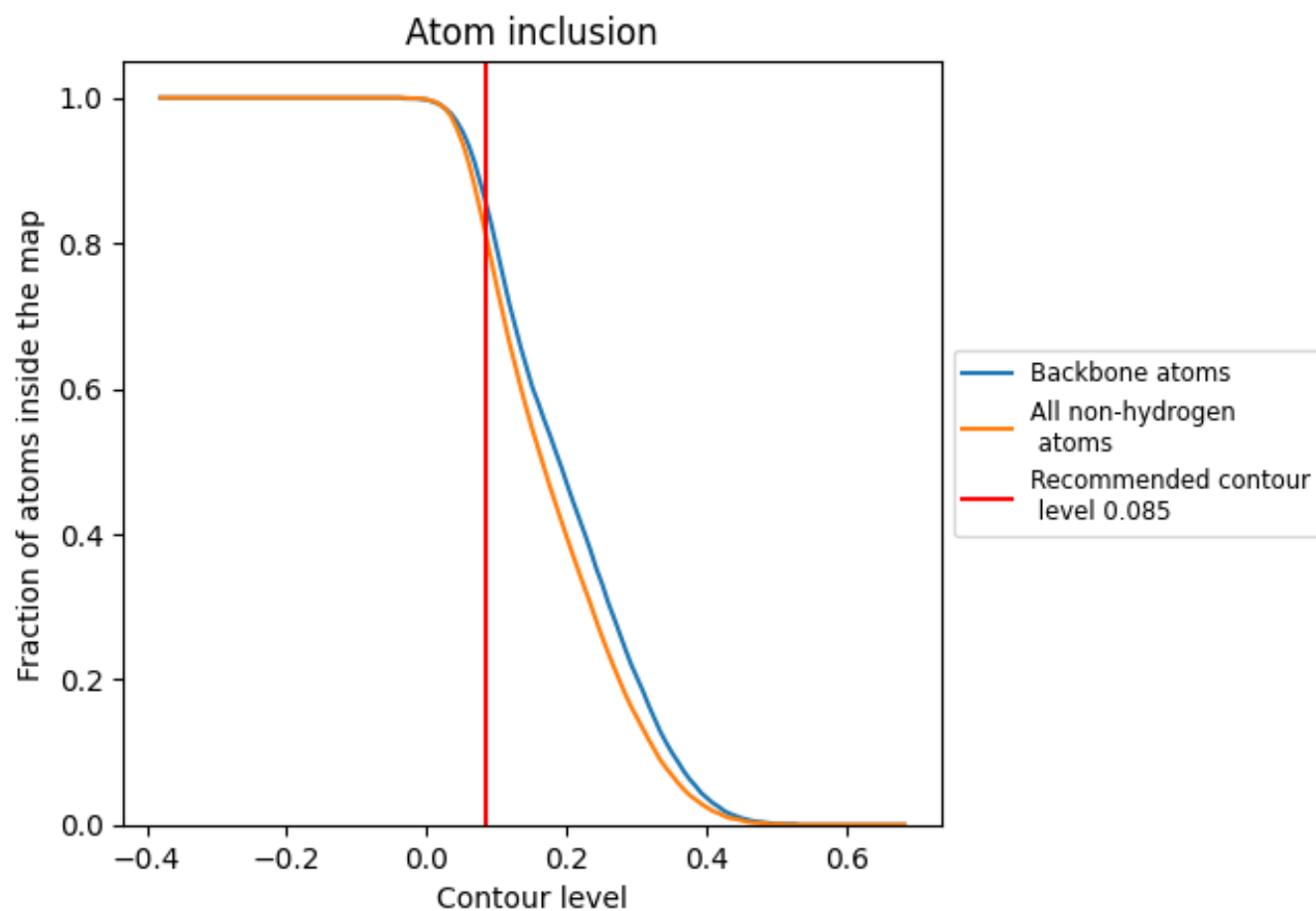
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.085).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 81% 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 (0.085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8110	<div></div> 0.5280
A	<div></div> 0.8640	<div></div> 0.5580
B	<div></div> 0.7520	<div></div> 0.5150
C	<div></div> 0.8290	<div></div> 0.5400
D	<div></div> 0.8120	<div></div> 0.5260
E	<div></div> 0.7960	<div></div> 0.5350
F	<div></div> 0.7110	<div></div> 0.4730
G	<div></div> 0.8640	<div></div> 0.5190
H	<div></div> 0.8830	<div></div> 0.5300
I	<div></div> 0.9730	<div></div> 0.6010

1.0

0.0

<0.0