



## wwPDB EM Validation Summary Report ⓘ

Jun 10, 2024 – 08:34 AM EDT

PDB ID : 8G4W  
EMDB ID : EMD-29732  
Title : Cryo-EM consensus structure of Escherichia coli que-PEC (paused elongation complex) RNA Polymerase plus preQ1 ligand  
Authors : Porta, J.C.; Chauvier, A.; Deb, I.; Ellinger, E.; Frank, A.T.; Meze, K.; Ohi, M.D.; Walter, N.G.  
Deposited on : 2023-02-10  
Resolution : 3.80 Å (reported)  
Based on initial model : 6ASX

This is a wwPDB EM Validation Summary 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) : 2.36.2

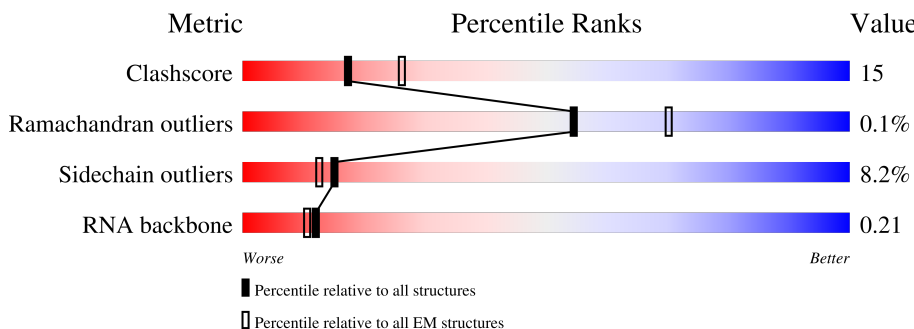
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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	39	<div> <div>21%</div> <div>13% 36% 51%</div> </div>
2	B	31	<div> <div>35%</div> <div>52% 48%</div> </div>
3	G	235	<div> <div>23%</div> <div>61% 33% 6%</div> </div>
3	H	235	<div> <div>42%</div> <div>40% 38% 15% 7%</div> </div>
4	K	79	<div> <div>52%</div> <div>61% 34% 5%</div> </div>
5	R	47	<div> <div>83%</div> <div>34% 51% 13%</div> </div>
6	I	1340	<div> <div>41%</div> <div>65% 32%</div> </div>

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Mol	Chain	Length	Quality of chain
7	J	1358	<div><div></div><div>45%</div><div>63%</div><div>34%</div><div>..</div></div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 26842 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a DNA chain called DNA (39-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	19	Total	C	N	O	P	0	0
			388	186	78	107	17		

- Molecule 2 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	31	Total	C	N	O	P	0	0
			631	301	107	192	31		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	221	Total	C	N	O	S	0	0
			1708	1069	303	330	6		
3	H	219	Total	C	N	O	S	0	0
			1693	1058	298	331	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	235	GLU	-	expression tag	UNP A0A5B9AW69
H	235	GLU	-	expression tag	UNP A0A5B9AW69

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

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

- Molecule 5 is a RNA chain called RNA (47-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	47	Total	C	N	O	P	0	0
			997	449	185	317	46		

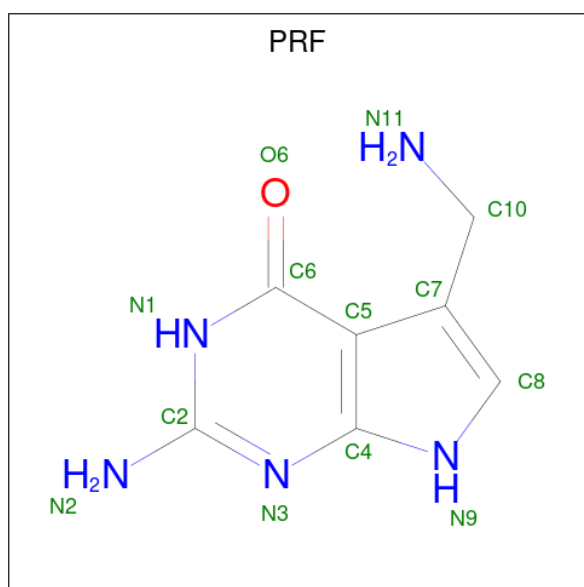
- Molecule 6 is a protein called DNA-directed RNA polymerase subunit beta.

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

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

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

- Molecule 8 is 7-DEAZA-7-AMINOMETHYL-GUANINE (three-letter code: PRF) (formula:  $C_7H_9N_5O$ ) (labeled as "Ligand of Interest" by depositor).

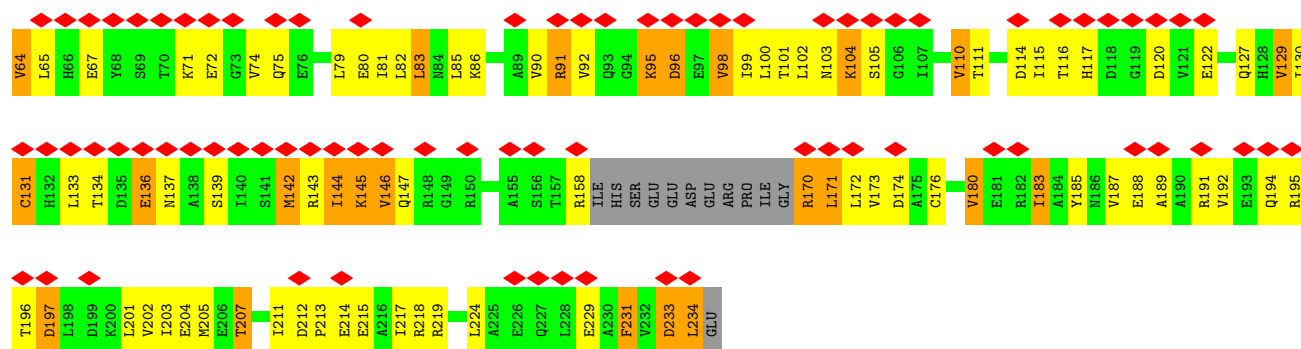


Mol	Chain	Residues	Atoms				AltConf
8	R	1	Total	C	N	O	0
			13	7	5	1	

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

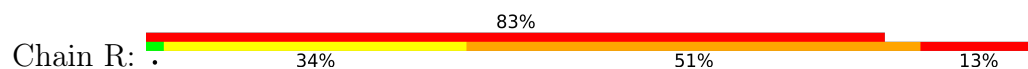




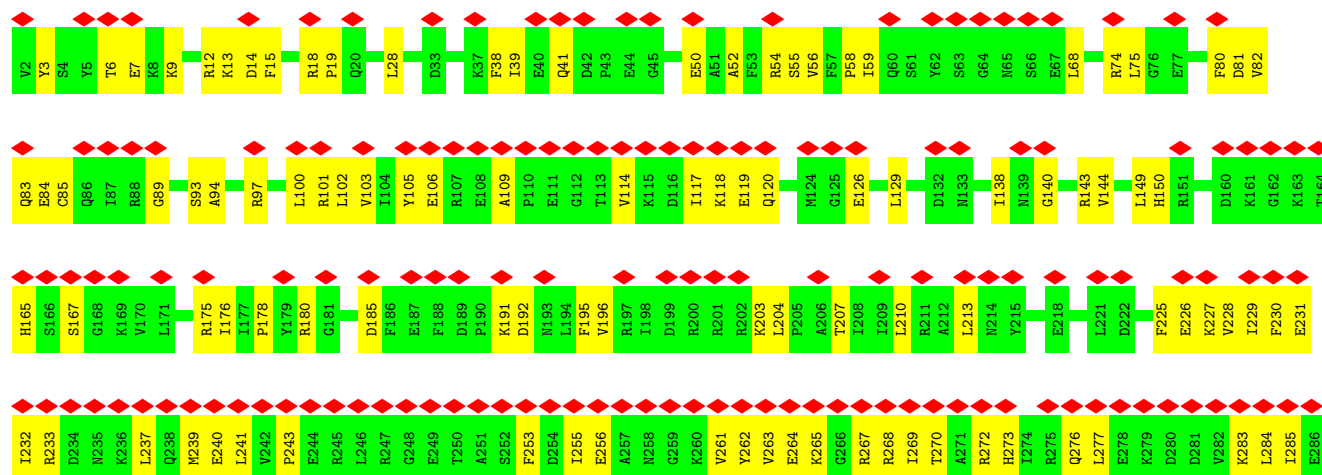
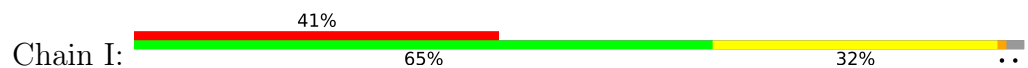
• Molecule 4: DNA-directed RNA polymerase subunit omega



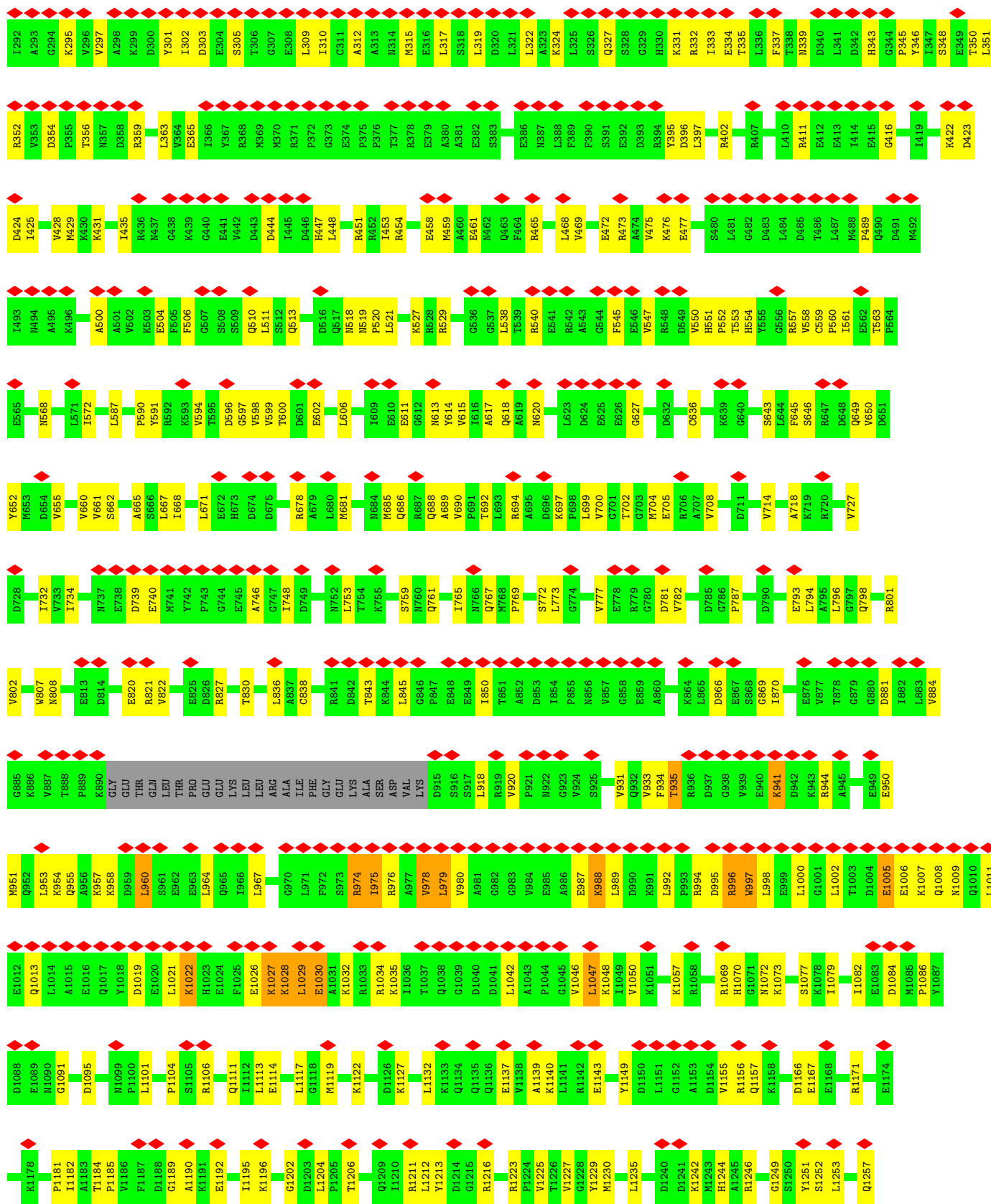
• Molecule 5: RNA (47-MER)

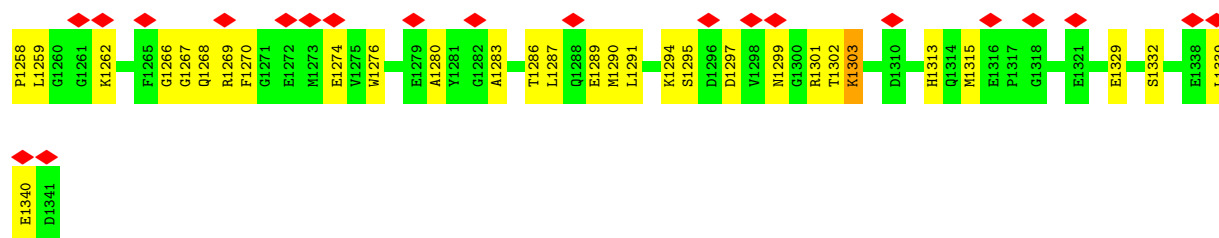


• Molecule 6: DNA-directed RNA polymerase subunit beta

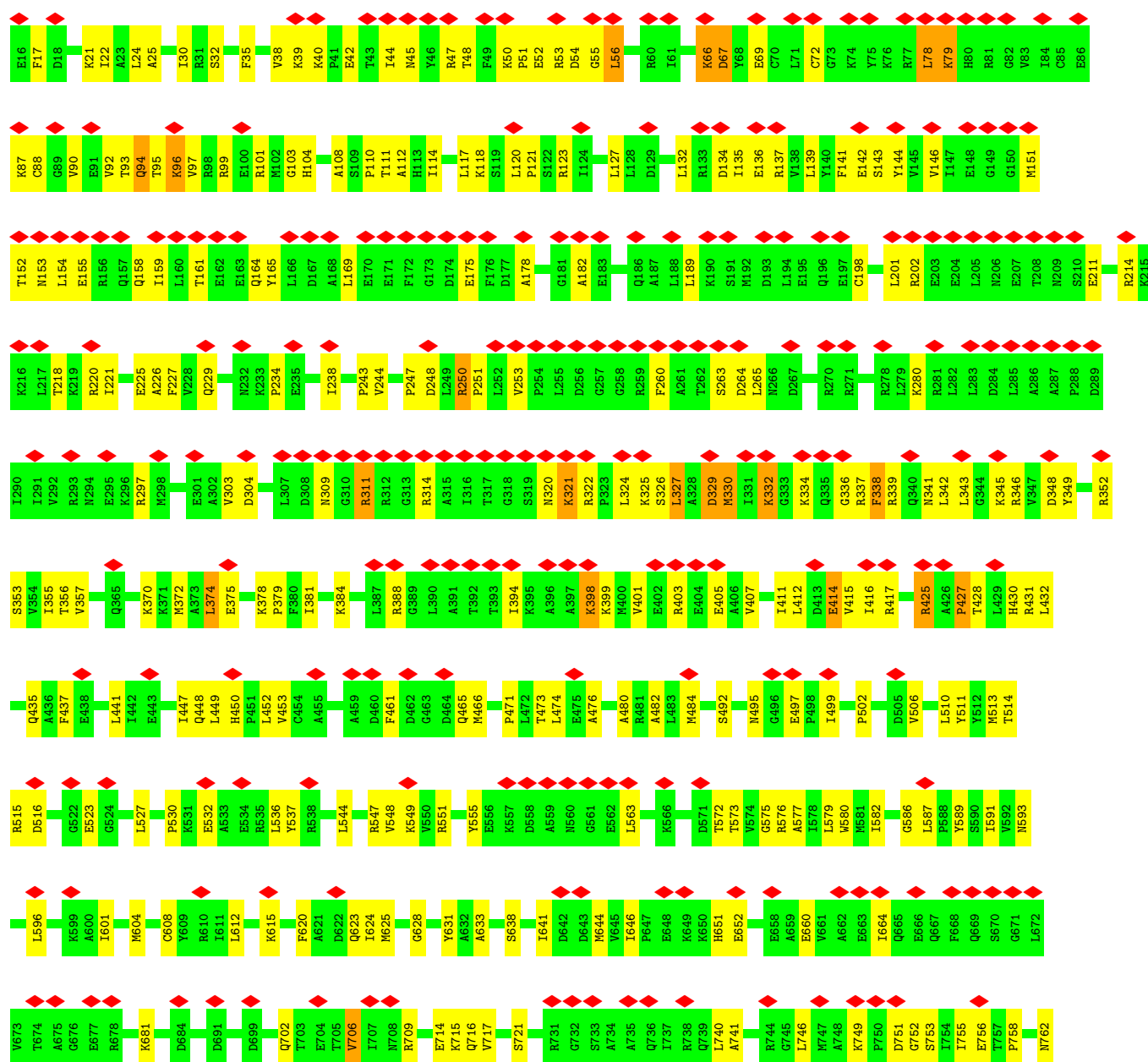
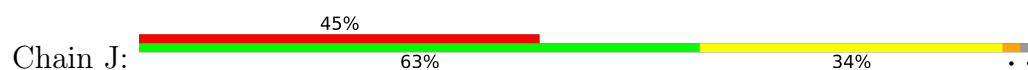








• Molecule 7: DNA-directed RNA polymerase subunit beta'



Y1302	V1229	E1168	A1105	T1045	I985	I923	F763
D1305	T1230	T1169	I1106	I1046	D986	G924	R764
L1306	R1231	K1170	V1107	T1047	E987	E765	G766
K1311	E1236	G1171	Q1108	R1048	F988	L767	L768
L1314	V1237	K1172	L1109	Q1049	R989	W769	W770
A1315	Q1238	R1173	E1110	T1050	T991	L770	F773
T1316	V1239	R1174	D1111	D1051	M932	T791	T776
E1317	T1241	L1175	G1112	E1052	R933	H777	H777
A1322	R1242	L1178	V1113	T1053	THR	R780	K781
F1325	L1243	P1179	Q1114	G1055	HIS	G852	K781
Q1326	Q1244	V1180	I1115	L1056	ILE	I856	A784
E1327	G1245	D1181	S1117	S1057	GLY	L857	D785
R1330	D1250	G1182	G1118	S1058	ALA	V858	T786
E1334	T1253	S1183	D1119	L1059	Y999	H865	A787
V1337	I1256	D1184	T1120	V1060	G1000	E866	L788
A1338	V1257	P1185	L1121	V1061	A1001	Q867	K789
G1339	R1258	E1187	R1123	D1063	V1002	N792	S793
K1340	Q1259	E1188	I1124	S1064	L1003	G794	G794
R1341	R1263	M1189	P1125	A1065	A1004	R799	R799
D1342	K1266	T1190	Q1126	E1066	K1005	L800	V801
E1343	I1267	K1192	GLU	R1067	G1006	D802	V803
L1344	V1268	W1193	SER	T1068	D1007	A804	Q805
R1345	N1268	G1194	GLY	A1069	E1009	D806	D812
R1346	A1269	Q1195	THR	G1070	Q1010	C814	D813
G1346	G1270	L1196	LYS	G1071	V1011	T816	T816
L1347	S1271	R1197	ASP	K1072	A1012	H817	H817
K1348	S1272	V1198	I1134	D1074	G1013	E818	E818
E1349	D1273	F1199	T1135	L1074	G1014	M821	M821
N1350	F1274	E1200	G1136	R1075	E1015	M822	M822
V1351	L1275	G1201	G1137	P1076	T1016	T823	T823
I1352	E1276	E1202	L1138	A1077	V1017	P824	P824
G1354	G1277	R1203	P1139	L1078	N962	V825	V825
R1355	E1278	V1204	D1143	K1079	V963	I826	I826
L1356	Q1279	E1205	E1146	T1080	W1020	E827	E827
I1357	V1280	R1206	A1147	V1081	D1021	G828	G828
Y1363	E1281	G1207	R1148	D1082	P1022	G906	G906
A1364	Y1282	D1208	R1149	A1083	H1023	H907	H907
Y1365	S1283	V1209	P1150	Q1084	T1024	N910	N910
H1366	R1284	L1210	K1151	G1085	M1025	K911	K911
Q1367	V1285	S1211	E1152	N1086	P1026	G912	G912
D1368	K1286	D1212	P1153	D1087	V1027	E913	E913
R1369	N1289	G1213	A1154	V1088	I1028	I918	I918
M1370	E1293	P1214	I1155	L1089	T1029		
R1371	A1294	E1215	L1156	T1090	E1030		
R1372	N1295	A1216	A1157	P1091	V1031		
R1373	G1296	G1217	E1158	G1092	S1032		
	K1297	H1218	I1159	T1093	F1034		
	V1298	D1219	S1160	D1094	T1035		
	G1299	L1220	G1161	M1095	V1035		
	A1300	L1221	V1163	P1096	R1036		
	T1301	R1222	S1164	A1097	F1037		
		L1223	F1165	Q1098	T1038		
		R1224	G1166	Y1099	D1039		
		G1225	K1167	F1100	M1040		
		V1226		L1101	I1041		
		A1227		P1102	D1042		
				G1103	G1043		
				K1104	Q1044		

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51824	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	62.00	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.135	Depositor
Minimum map value	-0.541	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.4	Depositor
Map size ( $\text{\AA}$ )	300.0, 300.0, 300.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.0, 1.0, 1.0	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, PRF

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	0.57	0/436	0.85	0/670
2	B	0.49	0/704	0.95	0/1084
3	G	0.27	0/1728	0.50	0/2341
3	H	0.62	0/1712	0.73	0/2320
4	K	0.59	0/629	0.68	0/847
5	R	2.95	109/1116 (9.8%)	3.01	179/1736 (10.3%)
6	I	0.34	0/10547	0.53	0/14232
7	J	0.35	0/10560	0.54	0/14257
All	All	0.70	109/27432 (0.4%)	0.86	179/37487 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	R	0	13

The worst 5 of 109 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	13	G	C6-N1	12.38	1.48	1.39
5	R	18	A	N7-C5	-11.81	1.32	1.39
5	R	4	G	N7-C5	-11.62	1.32	1.39
5	R	28	A	C6-N6	11.09	1.42	1.33
5	R	4	G	N1-C2	10.81	1.46	1.37

The worst 5 of 179 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	18	A	N1-C6-N6	16.24	128.34	118.60
5	R	27	A	N1-C6-N6	16.08	128.25	118.60
5	R	3	A	N1-C6-N6	14.99	127.59	118.60
5	R	29	A	N1-C6-N6	14.57	127.34	118.60
5	R	14	C	N3-C4-N4	13.81	127.67	118.00

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	R	1	G	Sidechain
5	R	10	C	Sidechain
5	R	4	G	Sidechain
5	R	7	G	Sidechain
5	R	9	U	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	388	0	216	11	0
2	B	631	0	352	13	0
3	G	1708	0	1752	53	0
3	H	1693	0	1727	66	0
4	K	627	0	634	10	0
5	R	997	0	511	10	0
6	I	10381	0	10391	321	0
7	J	10403	0	10636	374	0
8	R	13	0	9	0	0
9	J	1	0	0	0	0
All	All	26842	0	26228	792	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 15.

The worst 5 of 792 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)
3:H:16:ILE:CG2	3:H:26:VAL:HG13	1.63	1.25
7:J:1048:ARG:HG2	7:J:1059:LEU:CD2	1.68	1.21
7:J:1048:ARG:CG	7:J:1059:LEU:CD2	2.19	1.19
7:J:118:LYS:CE	7:J:136:GLU:OE2	1.90	1.19
6:I:1294:LYS:HG2	7:J:348:ASP:OD1	1.44	1.15

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	217/235 (92%)	212 (98%)	5 (2%)	0	100	100
3	H	215/235 (92%)	204 (95%)	9 (4%)	2 (1%)	17	54
4	K	77/79 (98%)	75 (97%)	2 (3%)	0	100	100
6	I	1312/1340 (98%)	1271 (97%)	40 (3%)	1 (0%)	51	83
7	J	1331/1358 (98%)	1293 (97%)	37 (3%)	1 (0%)	51	83
All	All	3152/3247 (97%)	3055 (97%)	93 (3%)	4 (0%)	54	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	30	PRO
3	H	90	VAL
6	I	58	PRO
7	J	427	PRO

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	189/202 (94%)	188 (100%)	1 (0%)	88	94
3	H	188/202 (93%)	102 (54%)	86 (46%)	0	0
4	K	67/67 (100%)	43 (64%)	24 (36%)	0	1
6	I	1135/1155 (98%)	1084 (96%)	51 (4%)	27	57
7	J	1122/1134 (99%)	1062 (95%)	60 (5%)	22	54
All	All	2701/2760 (98%)	2479 (92%)	222 (8%)	15	40

5 of 222 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	I	734	ILE
7	J	1046	ILE
6	I	1006	GLU
7	J	716	GLN
7	J	372	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
6	I	1268	GLN
7	J	229	GLN
7	J	1114	GLN
7	J	424	ASN
4	K	61	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	R	47/47 (100%)	27 (57%)	2 (4%)

5 of 27 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	R	2	C
5	R	3	A
5	R	8	U

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Mol	Chain	Res	Type
5	R	9	U
5	R	10	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	R	1	G
5	R	15	U

## 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 2 ligands modelled in this entry, 1 is 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	$\# Z  > 2$
8	PRF	R	101	-	13,14,14	0.87	1 (7%)	9,20,20	1.43	2 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PRF	R	101	-	-	0/0/2/2	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	R	101	PRF	C5-C6	-2.18	1.42	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	101	PRF	C5-C6-N1	-2.66	113.10	115.36
8	R	101	PRF	C10-C7-C8	2.62	132.25	126.96

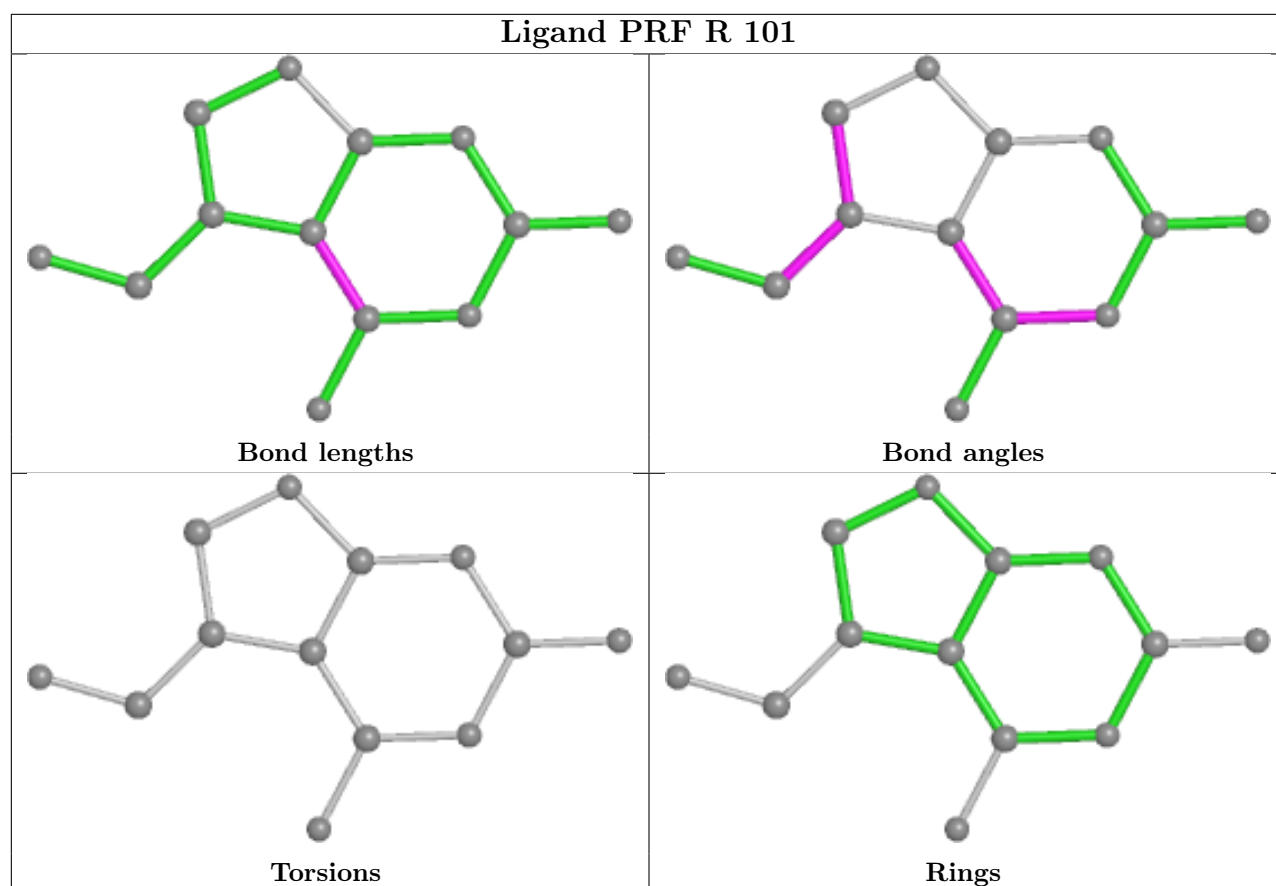
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

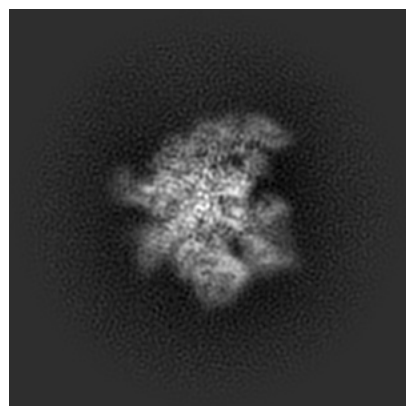
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29732. These allow visual inspection of the internal detail of the map and identification of artifacts.

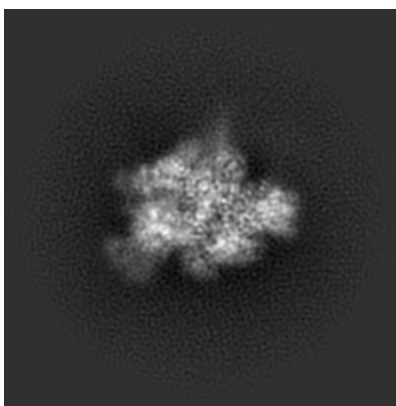
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

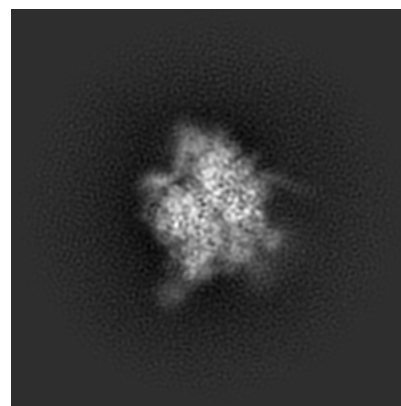
#### 6.1.1 Primary map



X

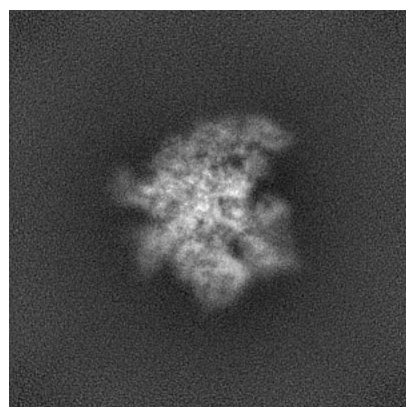


Y

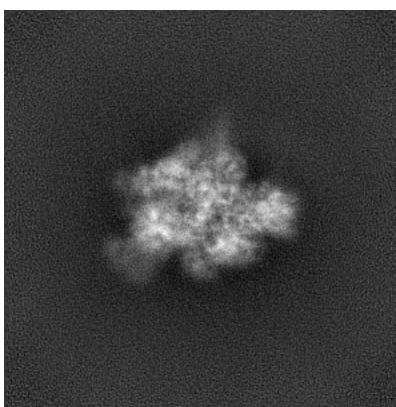


Z

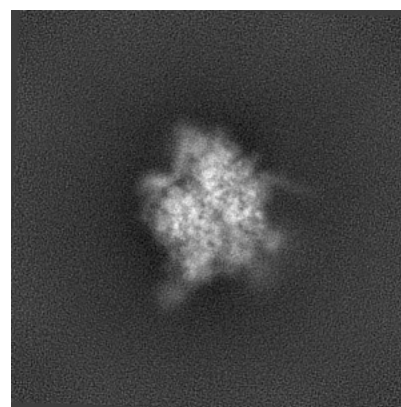
#### 6.1.2 Raw map



X



Y

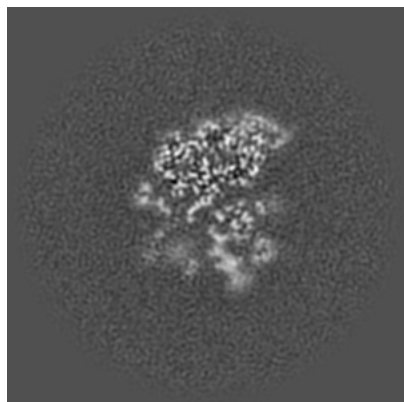


Z

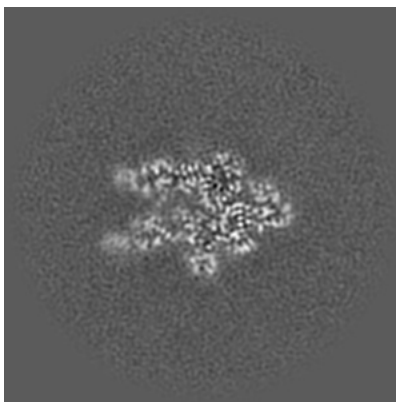
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

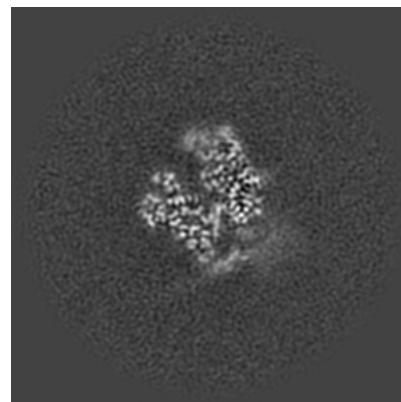
### 6.2.1 Primary map



X Index: 150

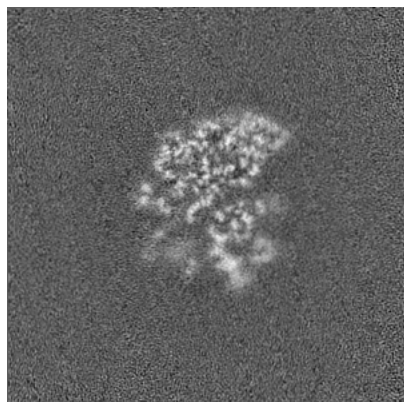


Y Index: 150

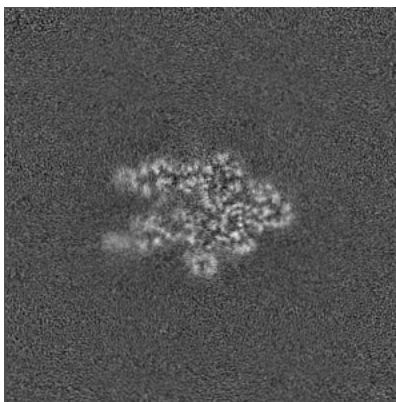


Z Index: 150

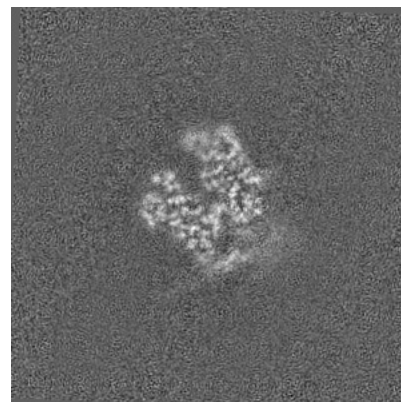
### 6.2.2 Raw map



X Index: 150



Y Index: 150

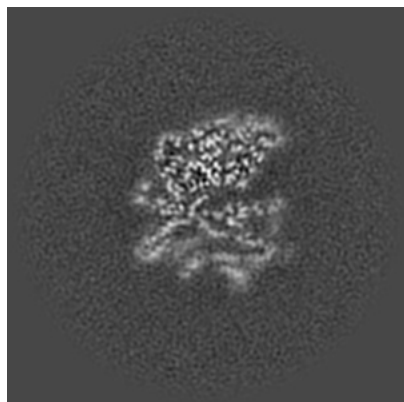


Z Index: 150

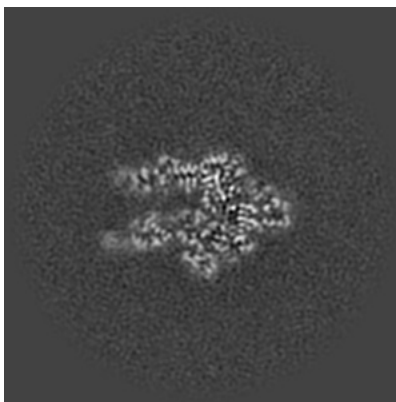
The images above show central slices of the map in three orthogonal directions.

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

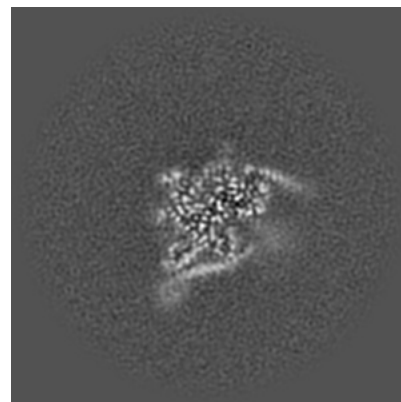
### 6.3.1 Primary map



X Index: 146

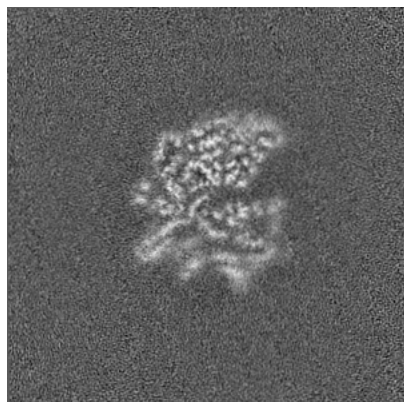


Y Index: 148

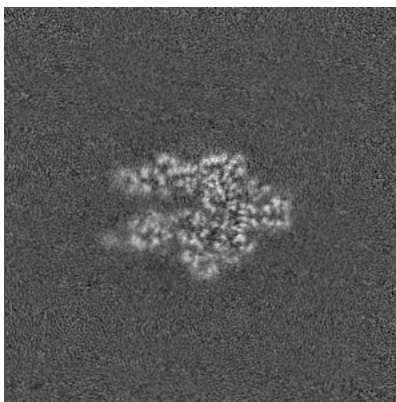


Z Index: 165

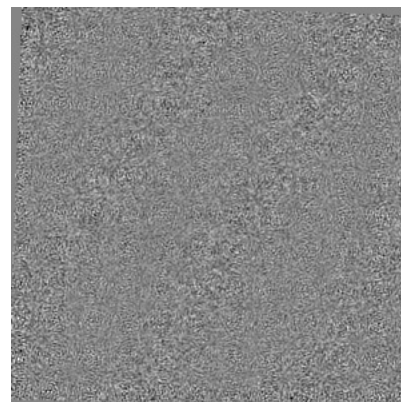
### 6.3.2 Raw map



X Index: 146



Y Index: 147



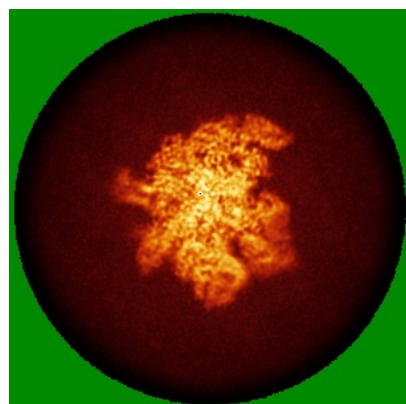
Z Index: 297

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

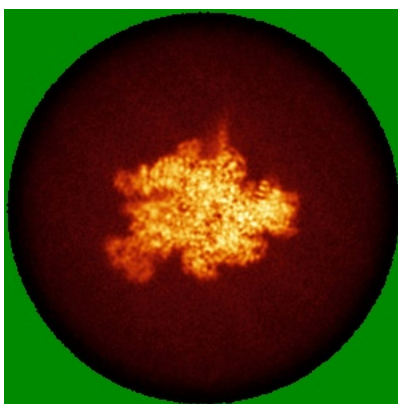


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

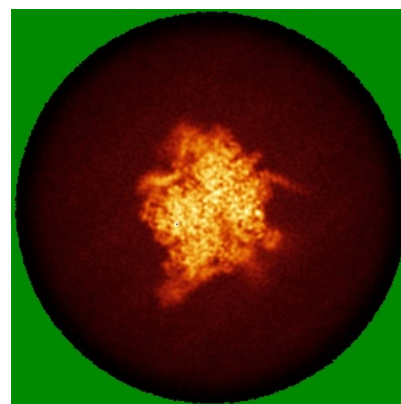
### 6.4.1 Primary map



X

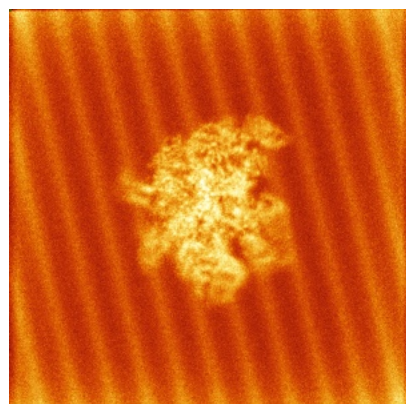


Y

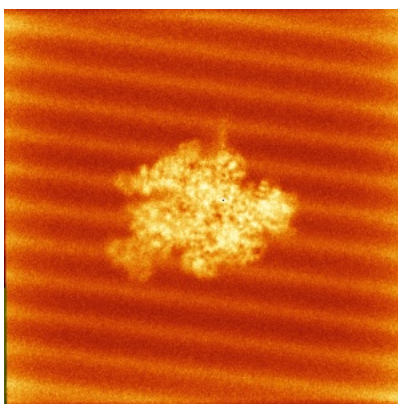


Z

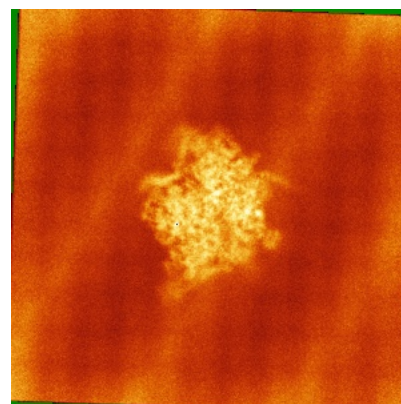
### 6.4.2 Raw map



X



Y

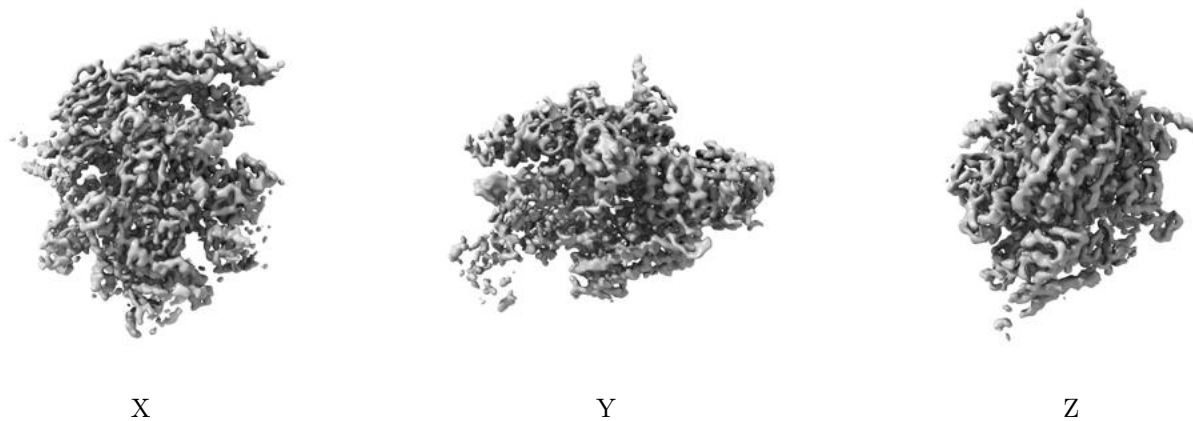


Z

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.

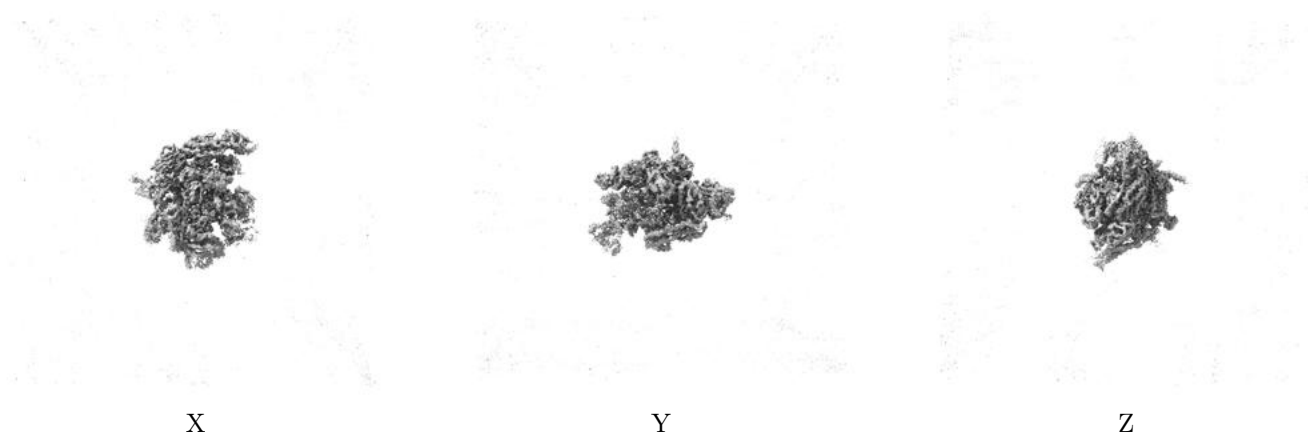
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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](#)

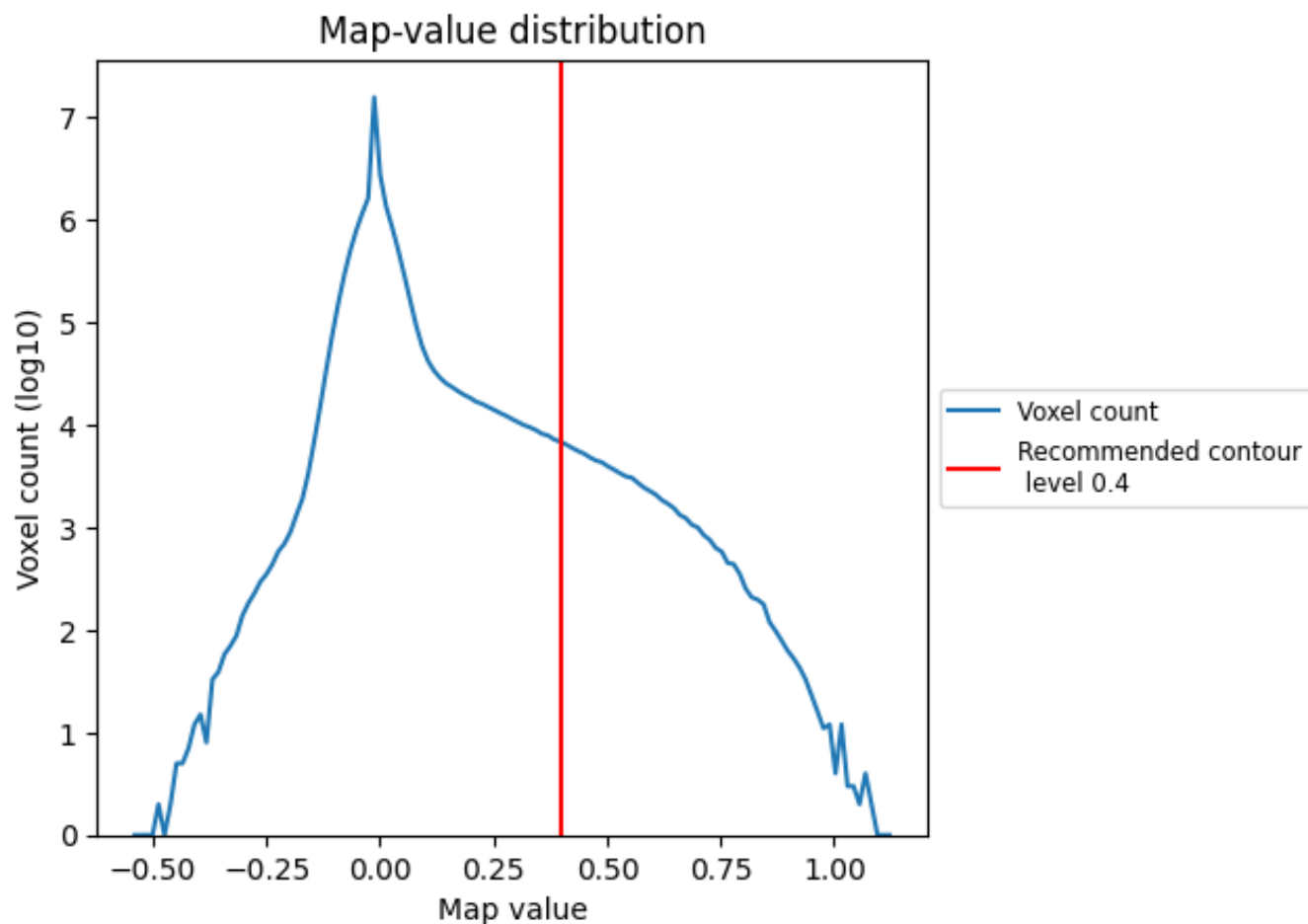
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

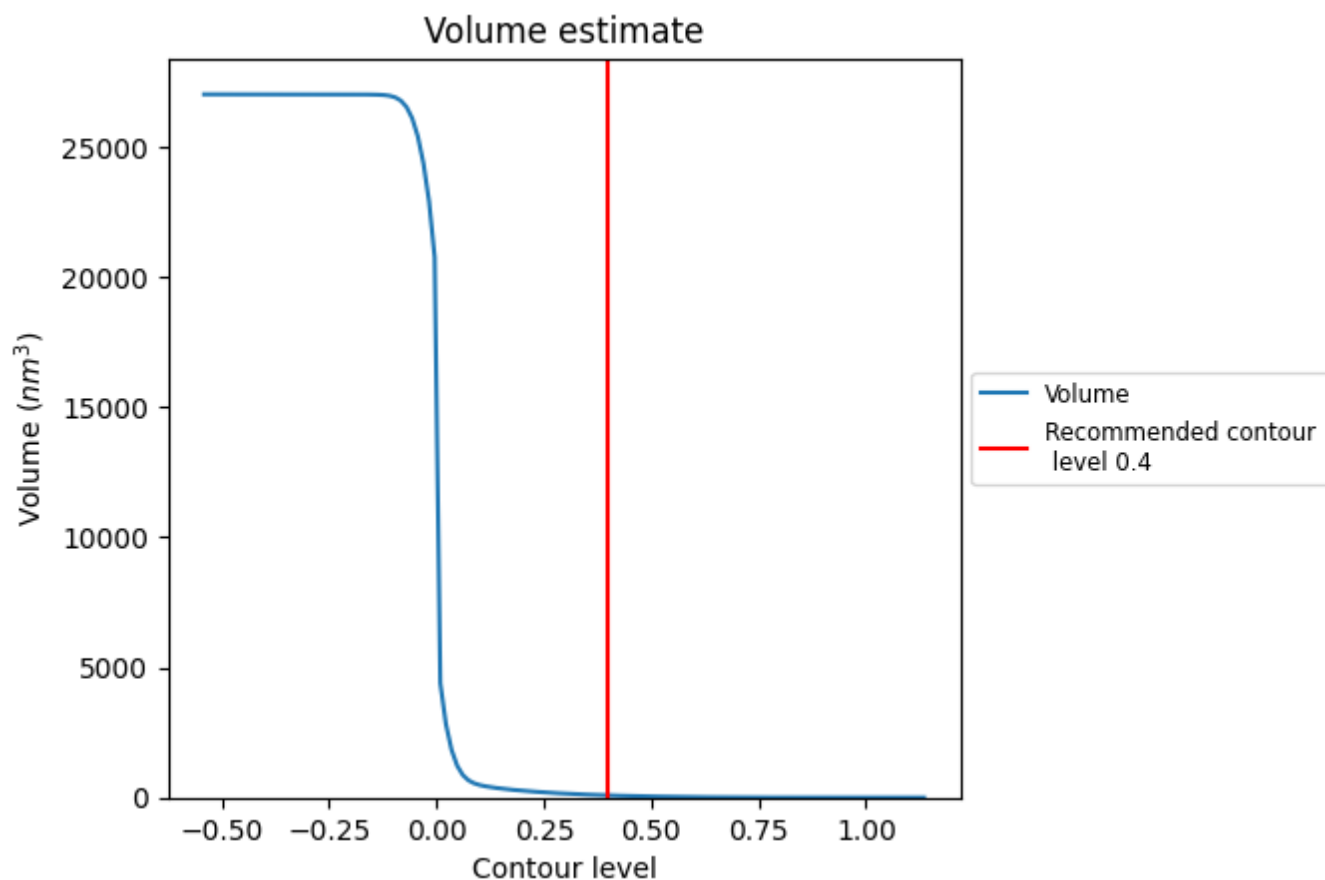
This section contains the results of statistical analysis of the map.

### 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.

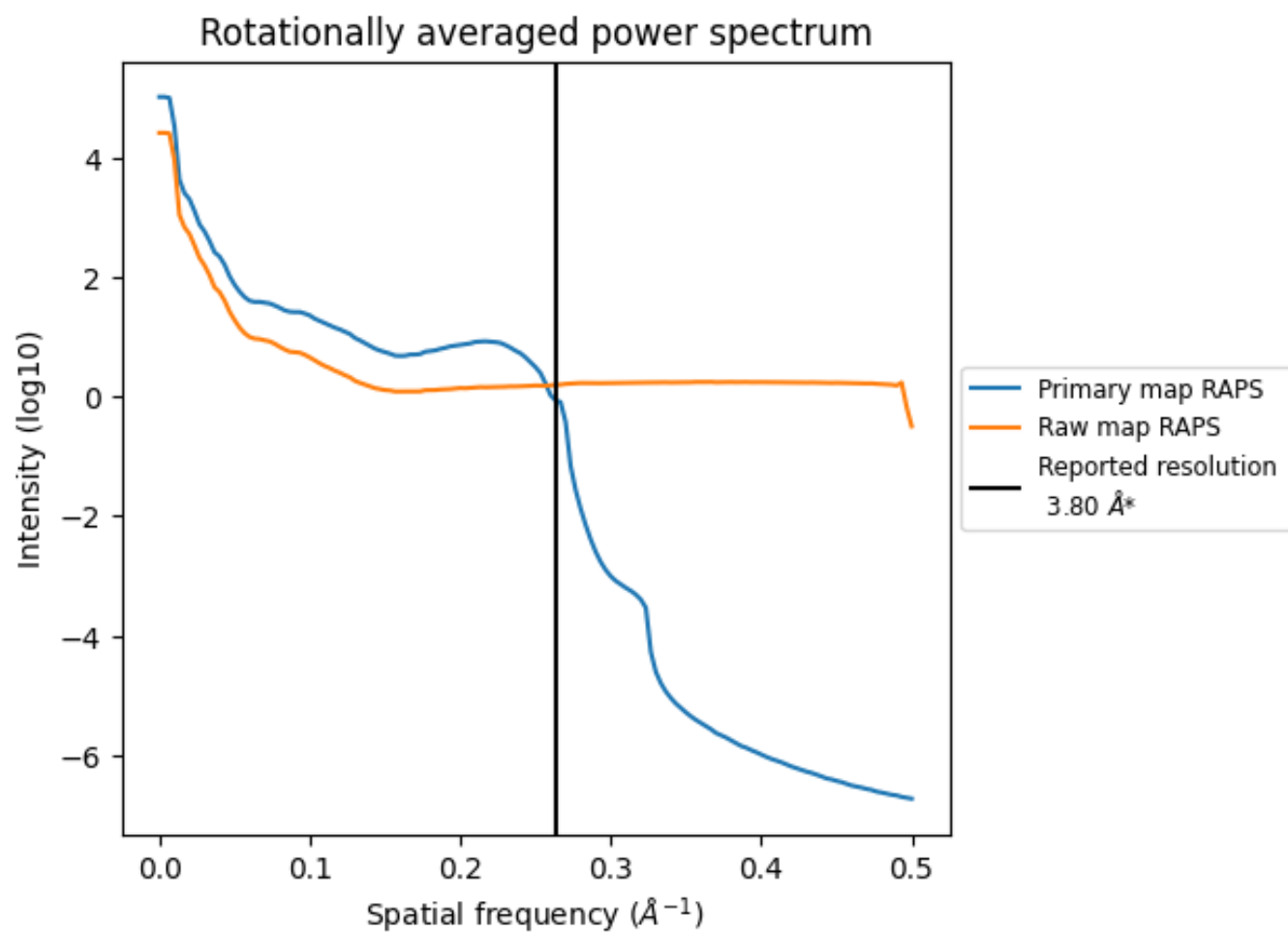
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 84 nm<sup>3</sup>; this corresponds to an approximate mass of 76 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 ⓘ

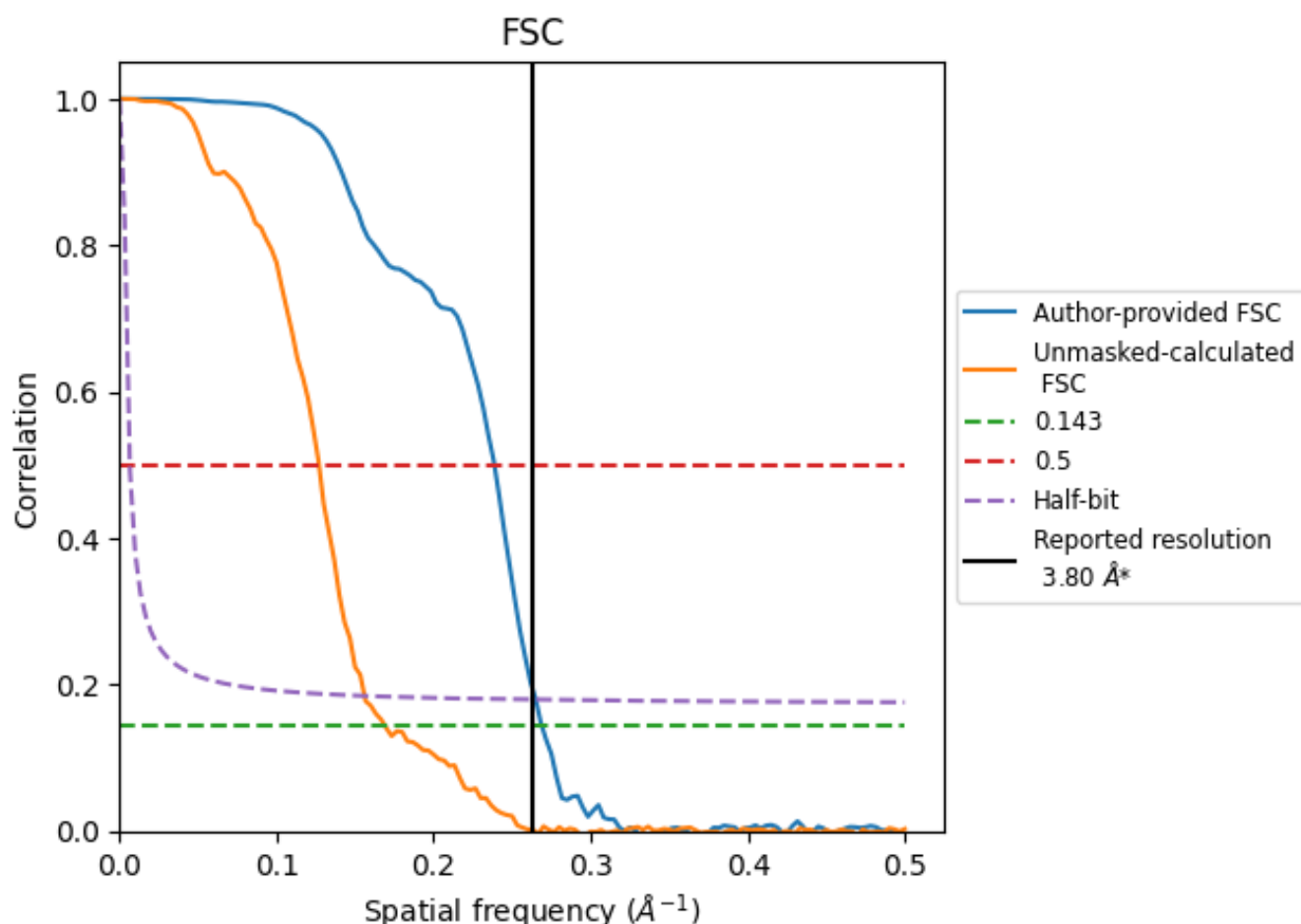


\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

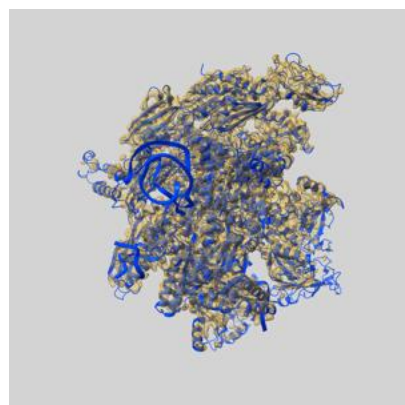
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.72	4.19	3.77
Unmasked-calculated*	5.91	7.87	6.41

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.91 differs from the reported value 3.8 by more than 10 %

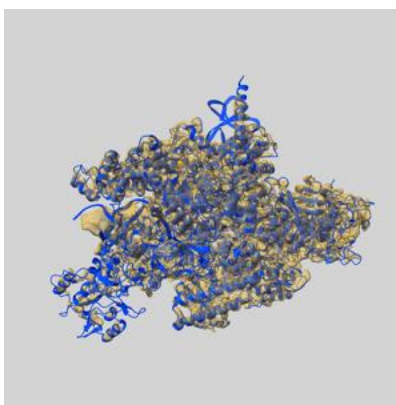
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29732 and PDB model 8G4W. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

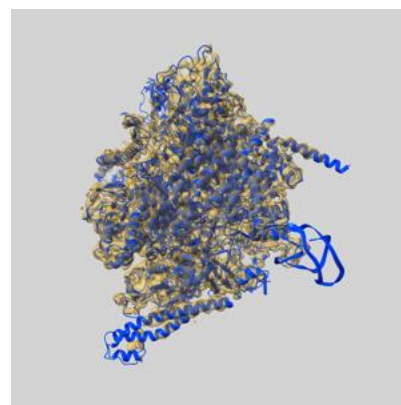
### 9.1 Map-model overlay [i](#)



X



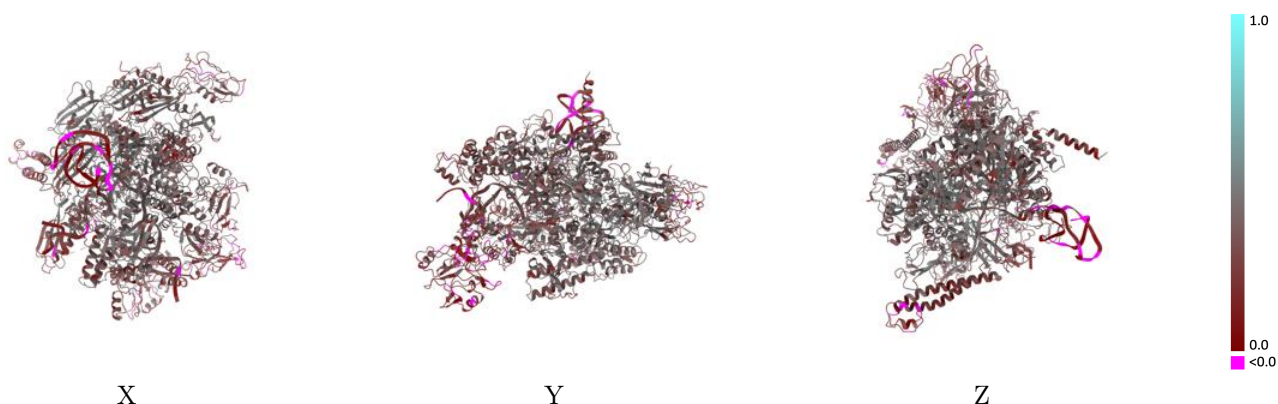
Y



Z

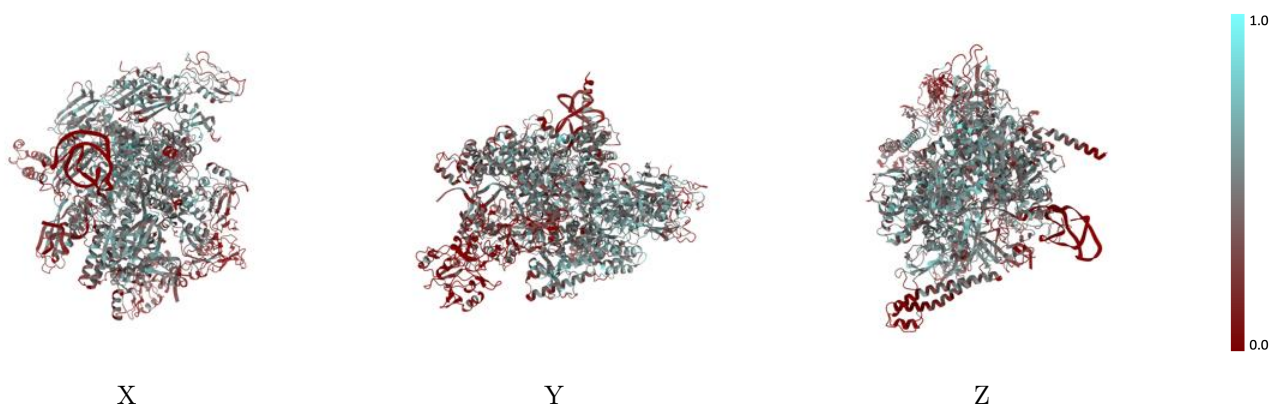
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



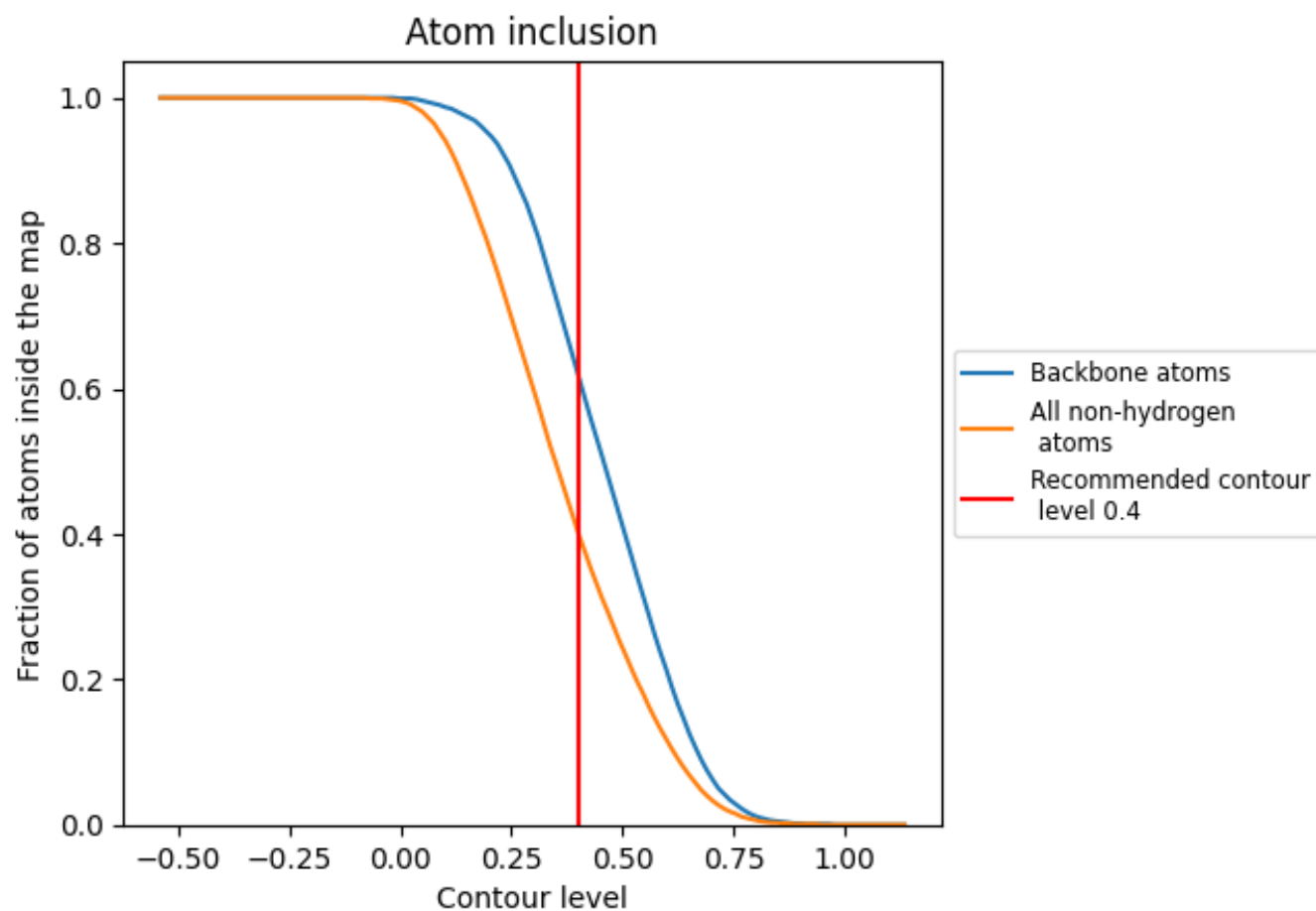
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 40% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4020	<div></div> 0.3380
A	<div></div> 0.4200	<div></div> 0.2700
B	<div></div> 0.4470	<div></div> 0.2870
G	<div></div> 0.5080	<div></div> 0.4040
H	<div></div> 0.3990	<div></div> 0.3080
I	<div></div> 0.4160	<div></div> 0.3580
J	<div></div> 0.3970	<div></div> 0.3410
K	<div></div> 0.3630	<div></div> 0.3290
R	<div></div> 0.1210	<div></div> 0.1030

1.0

0.0

<0.0