



## wwPDB EM Validation Summary Report ⓘ

Nov 13, 2022 – 10:40 PM EST

PDB ID : 6WMT  
EMDB ID : EMD-21852  
Title : F. tularensis RNAPs70-(MglA-SspA)-ppGpp-PigR-iglA DNA complex  
Authors : Travis, B.A.; Brennan, R.G.; Schumacher, M.A.  
Deposited on : 2020-04-21  
Resolution : 4.43 Å(reported)

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.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

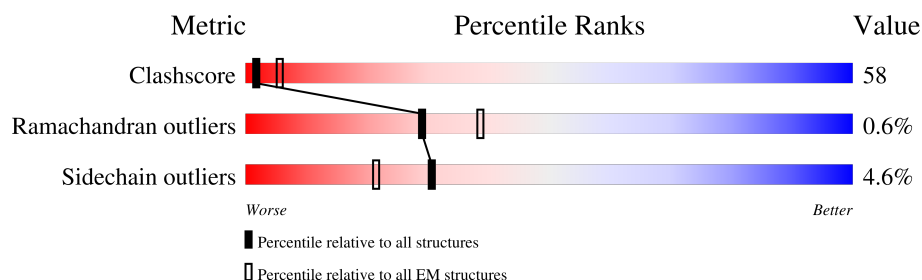
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

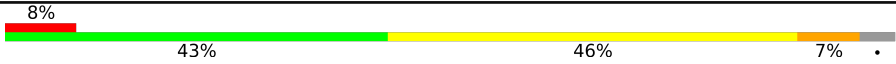
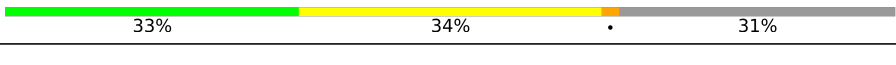
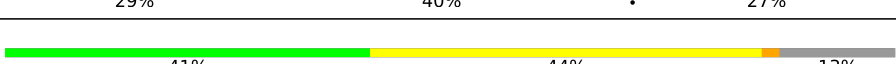
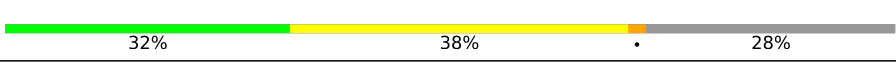
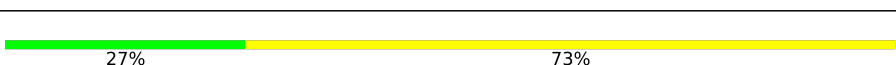


The reported resolution of this entry is 4.43 Å.

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

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	E	72	
2	A	323	
3	B	317	
4	C	1358	
5	D	1604	
6	G	52	
7	H	42	
8	J	11	

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Mol	Chain	Length	Quality of chain
9	K	73	<div><div></div><div>74%</div><div></div><div>88%</div><div></div><div>12%</div></div>
9	L	73	<div><div></div><div>90%</div><div></div><div>88%</div><div></div><div>12%</div></div>
10	M	205	<div><div></div><div>19%</div><div></div><div>32%</div><div></div><div>61%</div><div></div><div>5%</div><div></div></div>
11	S	210	<div><div></div><div>20%</div><div></div><div>37%</div><div></div><div>53%</div><div></div><div>6%</div><div></div></div>
12	X	11	<div><div></div><div>100%</div><div></div></div>
13	Z	577	<div><div></div><div></div><div>25%</div><div></div><div>51%</div><div></div><div>6%</div><div></div><div>19%</div></div>

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 31942 atoms, of which 11 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 omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	69	Total	C	N	O	S	0	0
			543	335	92	113	3		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit alpha 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	223	Total	C	N	O	S	0	0
			1688	1075	280	331	2		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit alpha 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	230	Total	C	N	O	S	0	0
			1769	1116	289	358	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	1187	Total	C	N	O	S	0	0
			8926	5618	1561	1710	37		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	1159	Total	C	N	O	S	0	0
			8874	5586	1565	1681	42		

- Molecule 6 is a DNA chain called DNA NT-strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	52	Total	C	N	O	P	0	0
			1069	515	181	321	52		

- Molecule 7 is a DNA chain called DNA T-strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	42	Total	C	N	O	P	0	0
			852	411	156	244	41		

- Molecule 8 is a DNA chain called DNA T-strand downstream.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	11	Total	C	N	O	P	0	0
			226	106	44	65	11		

- Molecule 9 is a protein called aCTDs.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	K	73	Total	C	N	O	0	0
			365	219	73	73		
9	L	73	Total	C	N	O	0	0
			365	219	73	73		

- Molecule 10 is a protein called Macrophage growth locus, subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	201	Total	C	N	O	S	0	0
			1598	1042	258	293	5		

- Molecule 11 is a protein called Glutathione S-transferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	202	Total	C	N	O	S	0	0
			1583	1024	265	287	7		

- Molecule 12 is a DNA chain called DNA NT-strand downstream.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	11	Total	C	N	O	P	0	0
			225	106	41	67	11		

- Molecule 13 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Z	470	Total	C	N	O	S	0	0
			3772	2392	666	698	16		

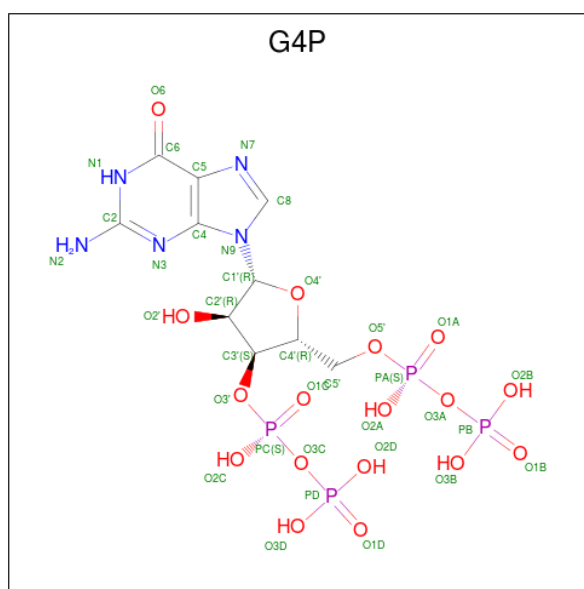
- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
14	D	1	Total	Mg	0
			1	1	
14	S	1	Total	Mg	0
			1	1	

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 16 is GUANOSINE-5',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>5</sub>O<sub>17</sub>P<sub>4</sub>).

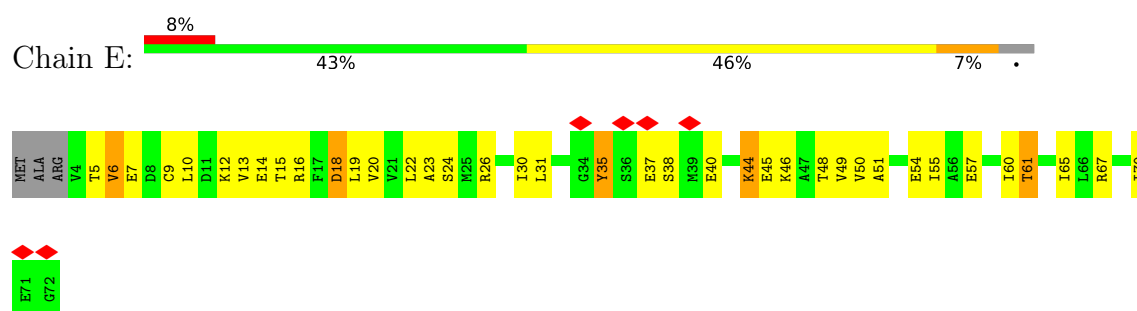


Mol	Chain	Residues	Atoms					AltConf	
16	D	1	Total 36	C 10	N 5	O 17	P 4	0	
16	M	1	Total 47	C 10	H 11	N 5	O 17	P 4	0

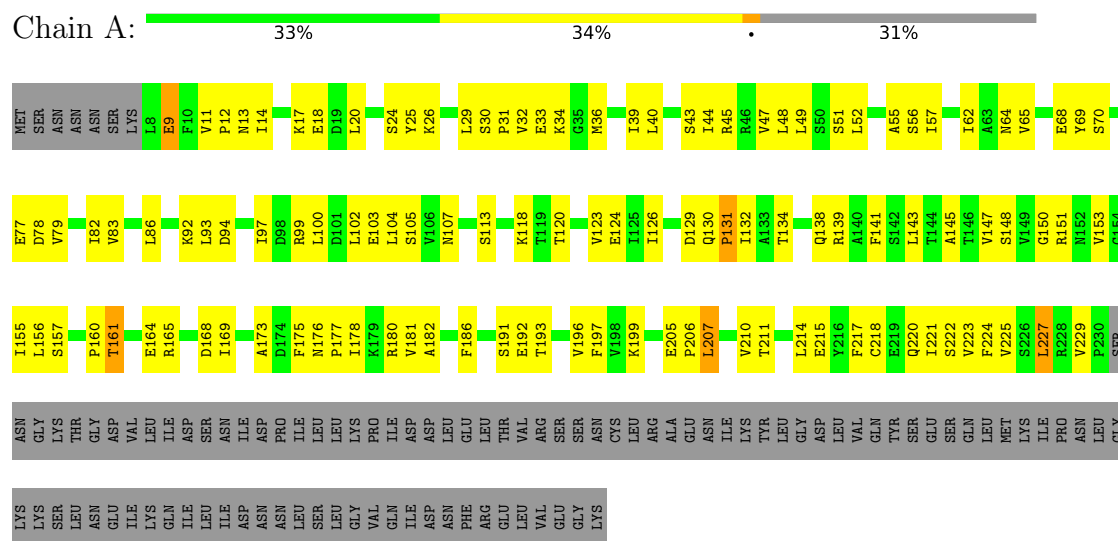
### 3 Residue-property plots [i](#)

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.

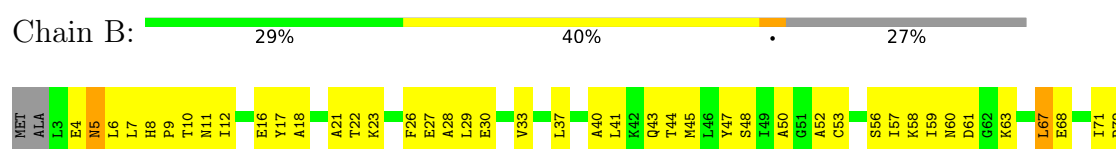
- Molecule 1: DNA-directed RNA polymerase subunit omega



- Molecule 2: DNA-directed RNA polymerase subunit alpha 1

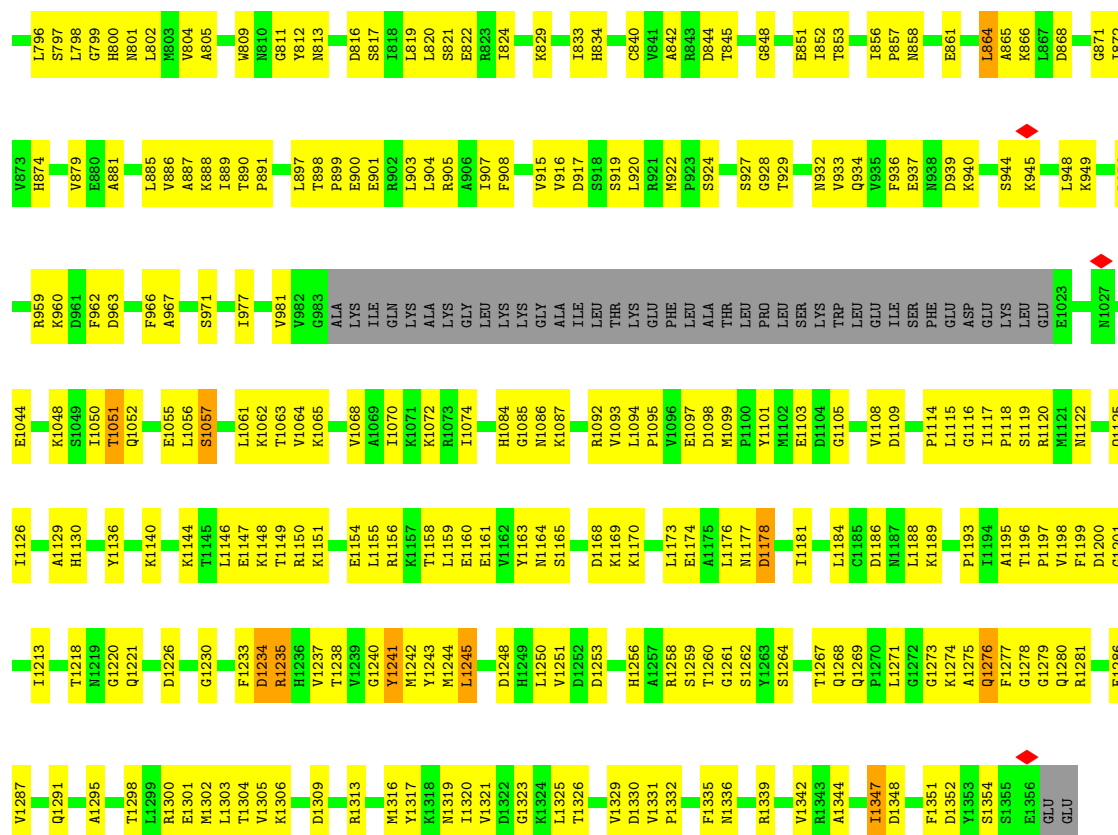


- Molecule 3: DNA-directed RNA polymerase subunit alpha 2

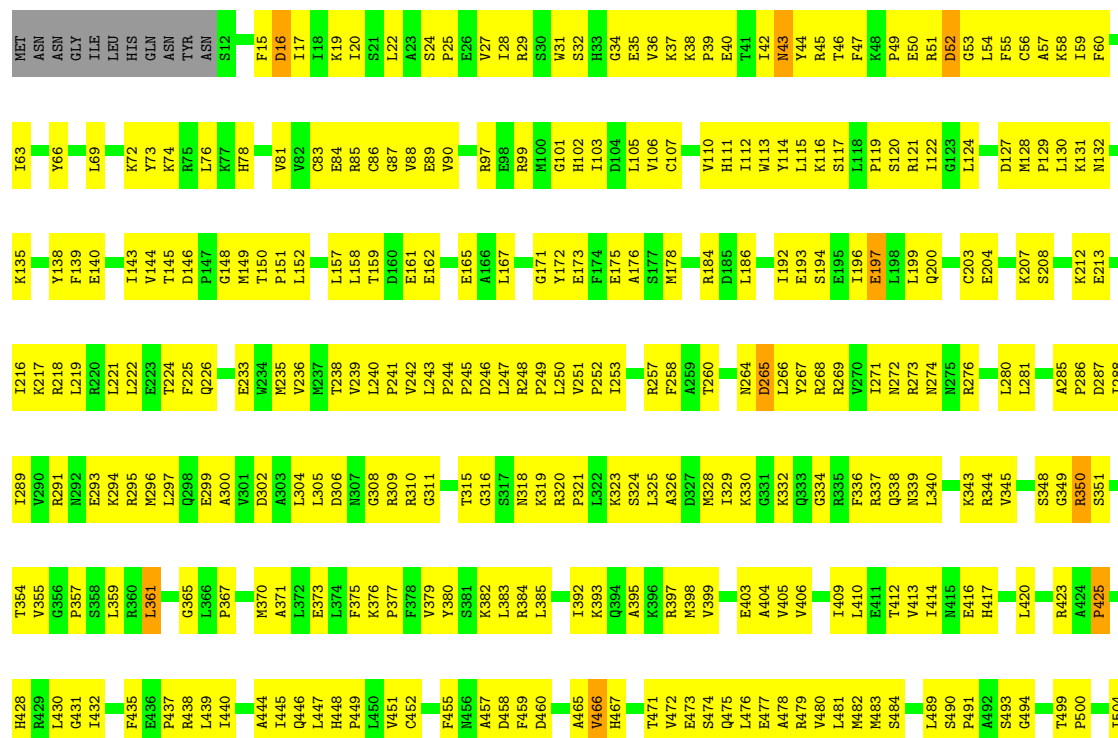




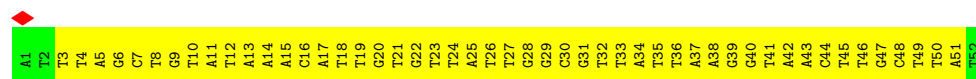




• Molecule 5: DNA-directed RNA polymerase subunit beta'

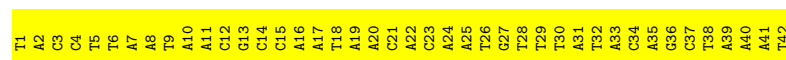






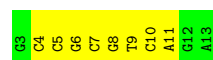
• Molecule 7: DNA T-strand

Chain H: 100%



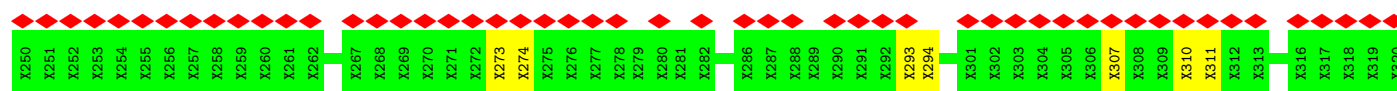
• Molecule 8: DNA T-strand downstream

Chain J: 27%



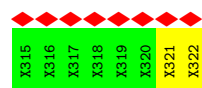
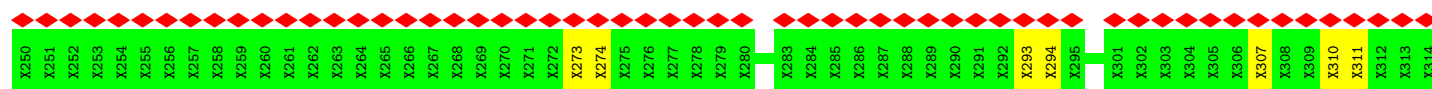
• Molecule 9: aCTDs

Chain K: 74%



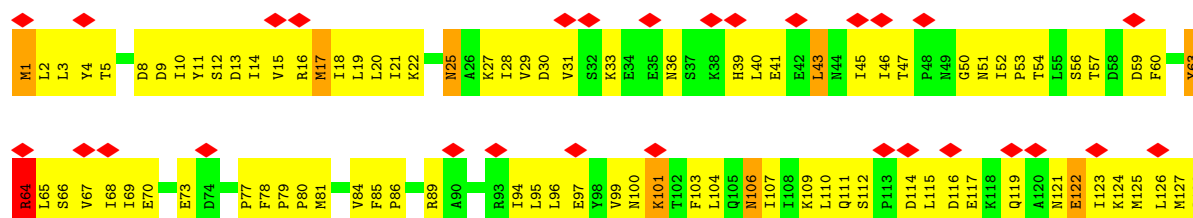
• Molecule 9: aCTDs

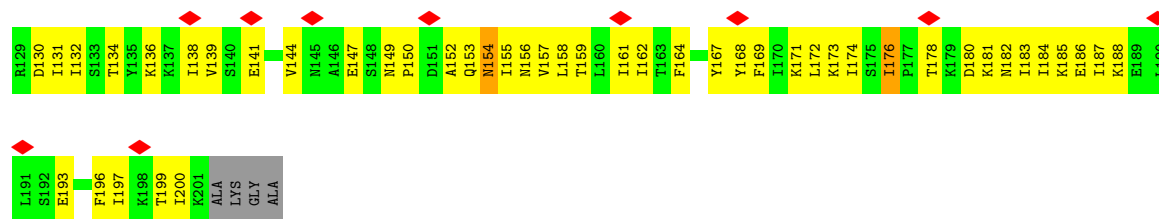
Chain L: 90%



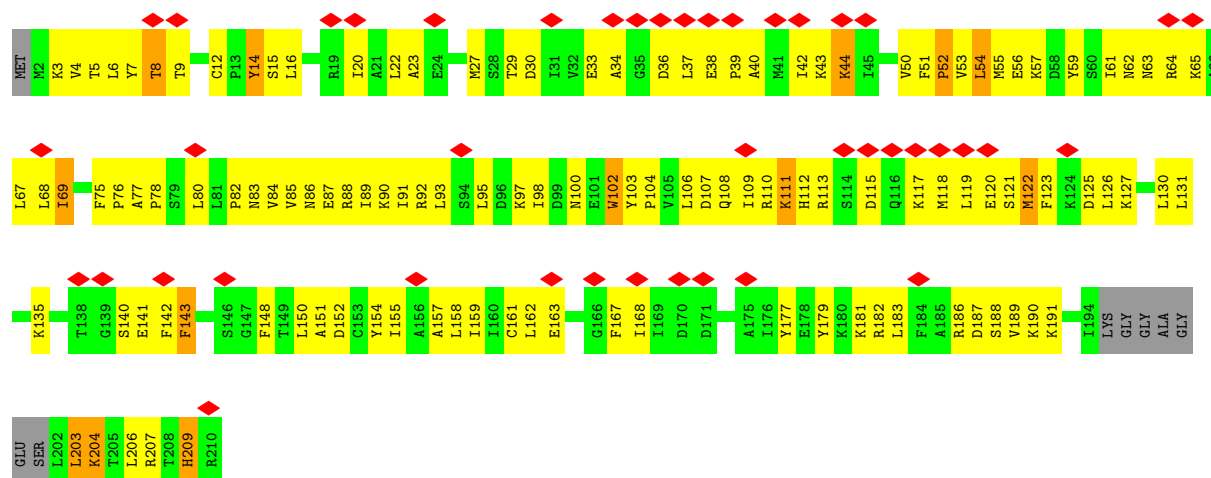
• Molecule 10: Macrophage growth locus, subunit A

Chain M: 19%

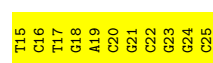




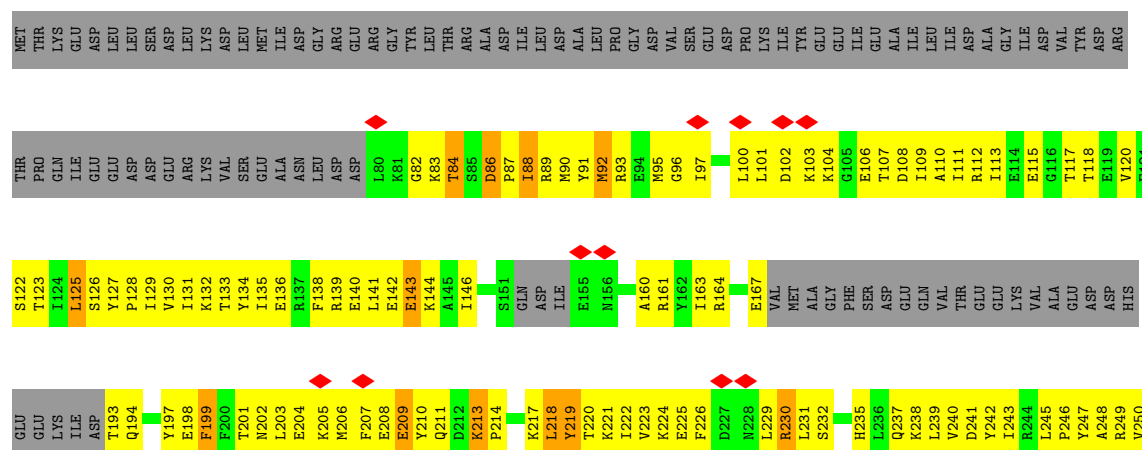
• Molecule 11: Glutathione S-transferase

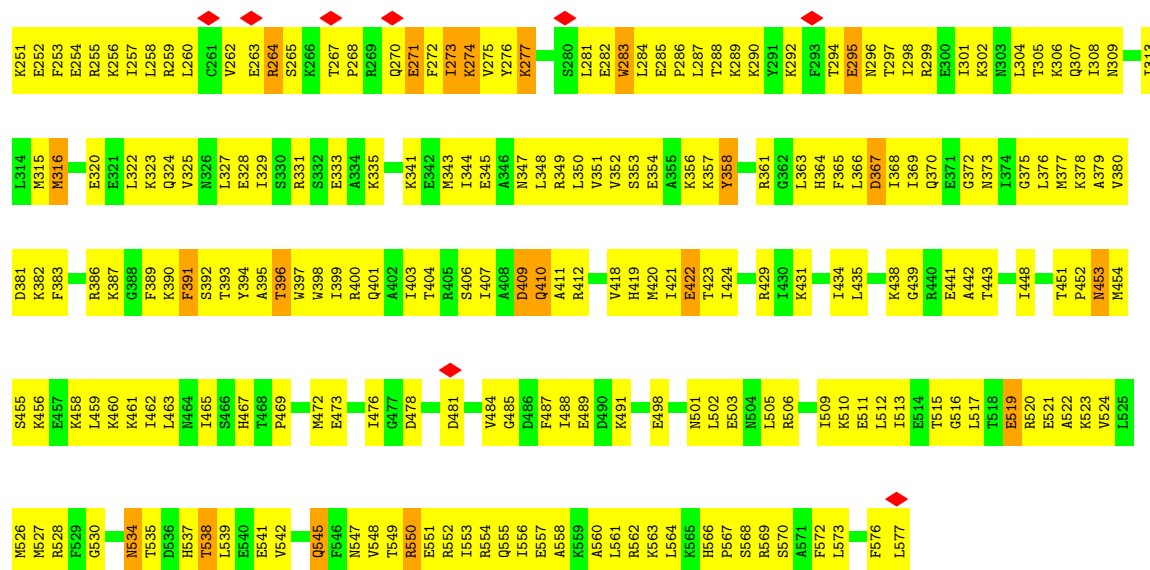


• Molecule 12: DNA NT-strand downstream



• Molecule 13: RNA polymerase sigma factor RpoD





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	116936	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.026	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	376.64, 376.64, 376.64	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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, G4P, 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	E	0.68	0/544	0.60	0/729
2	A	0.68	0/1708	0.61	0/2318
3	B	0.67	0/1789	0.59	0/2414
4	C	0.67	0/9068	0.61	0/12269
5	D	0.67	0/8994	0.61	0/12142
6	G	0.24	0/1196	1.08	0/1846
7	H	0.20	0/956	1.11	0/1471
8	J	0.20	0/253	1.07	0/388
10	M	0.65	0/1626	0.60	0/2208
11	S	0.66	0/1611	0.61	0/2173
12	X	0.20	0/251	1.11	0/385
13	Z	0.66	0/3825	0.61	0/5138
All	All	0.64	0/31821	0.67	0/43481

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	E	543	0	551	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1688	0	1726	186	0
3	B	1769	0	1767	211	0
4	C	8926	0	8670	781	0
5	D	8874	0	8944	856	0
6	G	1069	0	596	361	0
7	H	852	0	476	337	0
8	J	226	0	123	30	0
9	K	365	0	75	6	0
9	L	365	0	75	5	0
10	M	1598	0	1650	218	0
11	S	1583	0	1600	192	0
12	X	225	0	124	63	0
13	Z	3772	0	3813	579	0
14	D	1	0	0	0	0
14	S	1	0	0	0	0
15	D	2	0	0	0	0
16	D	36	0	11	1	0
16	M	36	11	11	3	0
All	All	31931	11	30212	3596	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 58.

The worst 5 of 3596 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)
6:G:49:DT:H2''	6:G:50:DT:C5'	0.98	1.46
6:G:49:DT:C2'	6:G:50:DT:H5'	0.99	1.44
7:H:9:DT:H2'	7:H:10:DA:C8	1.74	1.21
6:G:28:DG:H2''	6:G:29:DG:H5'	1.21	1.20
2:A:12:PRO:HA	2:A:31:PRO:HG2	1.23	1.19

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	E	67/72 (93%)	62 (92%)	3 (4%)	2 (3%)	4	31
2	A	221/323 (68%)	211 (96%)	8 (4%)	2 (1%)	17	56
3	B	228/317 (72%)	222 (97%)	4 (2%)	2 (1%)	17	56
4	C	1181/1358 (87%)	1135 (96%)	39 (3%)	7 (1%)	25	65
5	D	1155/1604 (72%)	1116 (97%)	36 (3%)	3 (0%)	41	76
10	M	199/205 (97%)	194 (98%)	4 (2%)	1 (0%)	29	68
11	S	198/210 (94%)	185 (93%)	10 (5%)	3 (2%)	10	46
13	Z	464/577 (80%)	444 (96%)	17 (4%)	3 (1%)	25	65
All	All	3713/4666 (80%)	3569 (96%)	121 (3%)	23 (1%)	29	65

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	6	VAL
4	C	64	SER
4	C	113	LEU
4	C	114	PRO
5	D	709	GLU

### 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	E	61/64 (95%)	58 (95%)	3 (5%)	25	51
2	A	189/287 (66%)	185 (98%)	4 (2%)	53	72
3	B	194/276 (70%)	186 (96%)	8 (4%)	30	56
4	C	911/1169 (78%)	876 (96%)	35 (4%)	33	58
5	D	936/1374 (68%)	902 (96%)	34 (4%)	35	60
10	M	179/191 (94%)	168 (94%)	11 (6%)	18	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	S	165/184 (90%)	155 (94%)	10 (6%)	18	46
13	Z	401/527 (76%)	365 (91%)	36 (9%)	9	32
All	All	3036/4072 (75%)	2895 (95%)	141 (5%)	31	53

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	Z	218	LEU
13	Z	271	GLU
13	Z	396	THR
4	C	1276	GLN
4	C	1245	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
5	D	475	GLN
13	Z	537	HIS
5	D	1154	ASN
13	Z	464	ASN
11	S	112	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
16	G4P	M	301	-	30,38,38	0.89	1 (3%)	42,61,61	1.33	5 (11%)
16	G4P	D	1704	-	30,38,38	0.89	1 (3%)	42,61,61	1.34	5 (11%)

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
16	G4P	M	301	-	-	3/23/43/43	0/3/3/3
16	G4P	D	1704	-	-	10/23/43/43	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	1704	G4P	C6-N1	-2.46	1.34	1.37
16	M	301	G4P	C6-N1	-2.35	1.34	1.37

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	1704	G4P	PA-O3A-PB	-3.62	120.39	132.83
16	M	301	G4P	PC-O3C-PD	-3.58	120.53	132.83
16	D	1704	G4P	PC-O3C-PD	-3.47	120.91	132.83
16	M	301	G4P	PA-O3A-PB	-3.41	121.12	132.83
16	M	301	G4P	C8-N7-C5	2.65	108.03	102.99

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	D	1704	G4P	C5'-O5'-PA-O3A
16	D	1704	G4P	C5'-O5'-PA-O1A

*Continued on next page...*

*Continued from previous page...*

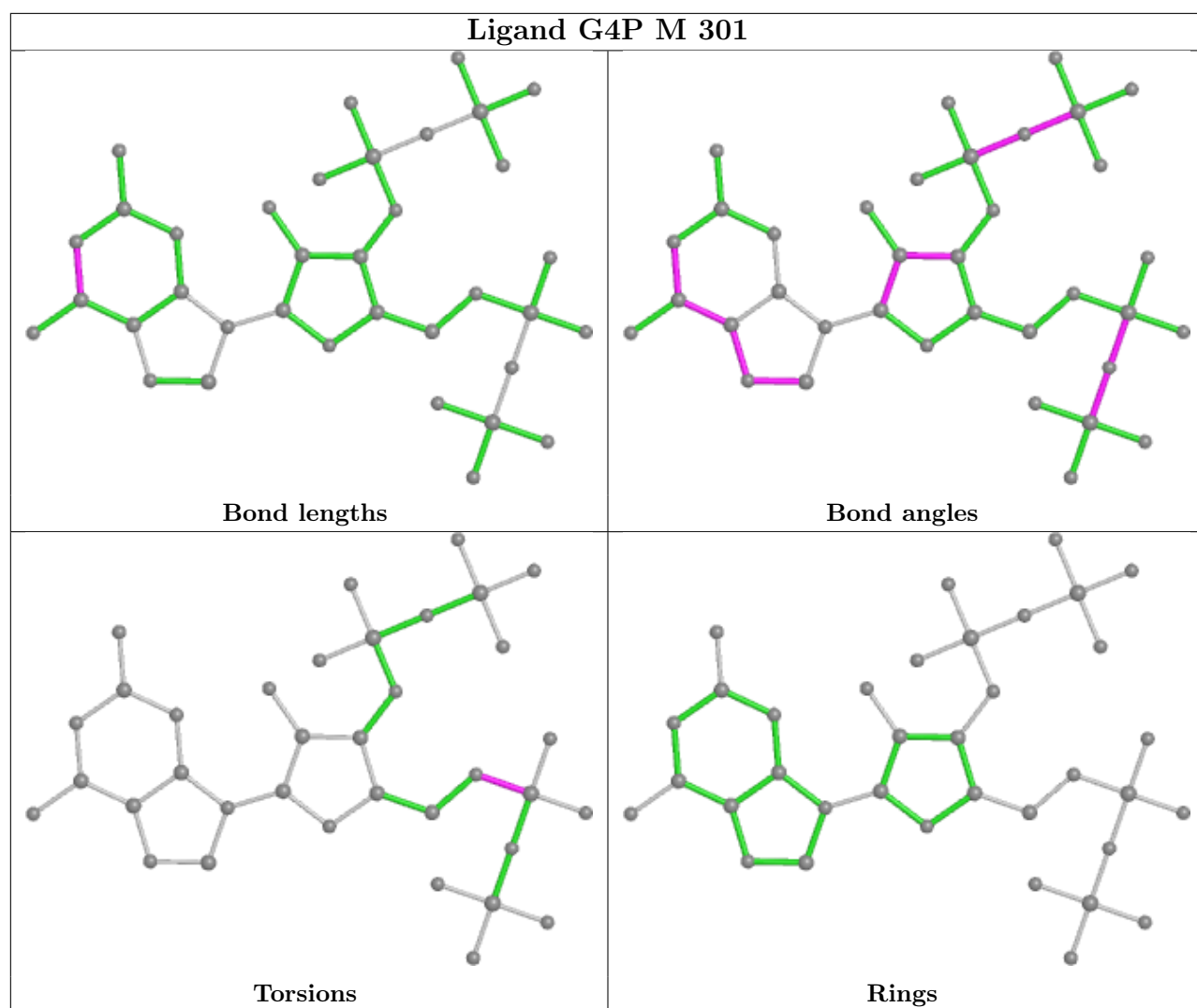
Mol	Chain	Res	Type	Atoms
16	D	1704	G4P	C5'-O5'-PA-O2A
16	D	1704	G4P	O4'-C4'-C5'-O5'
16	D	1704	G4P	C3'-O3'-PC-O2C

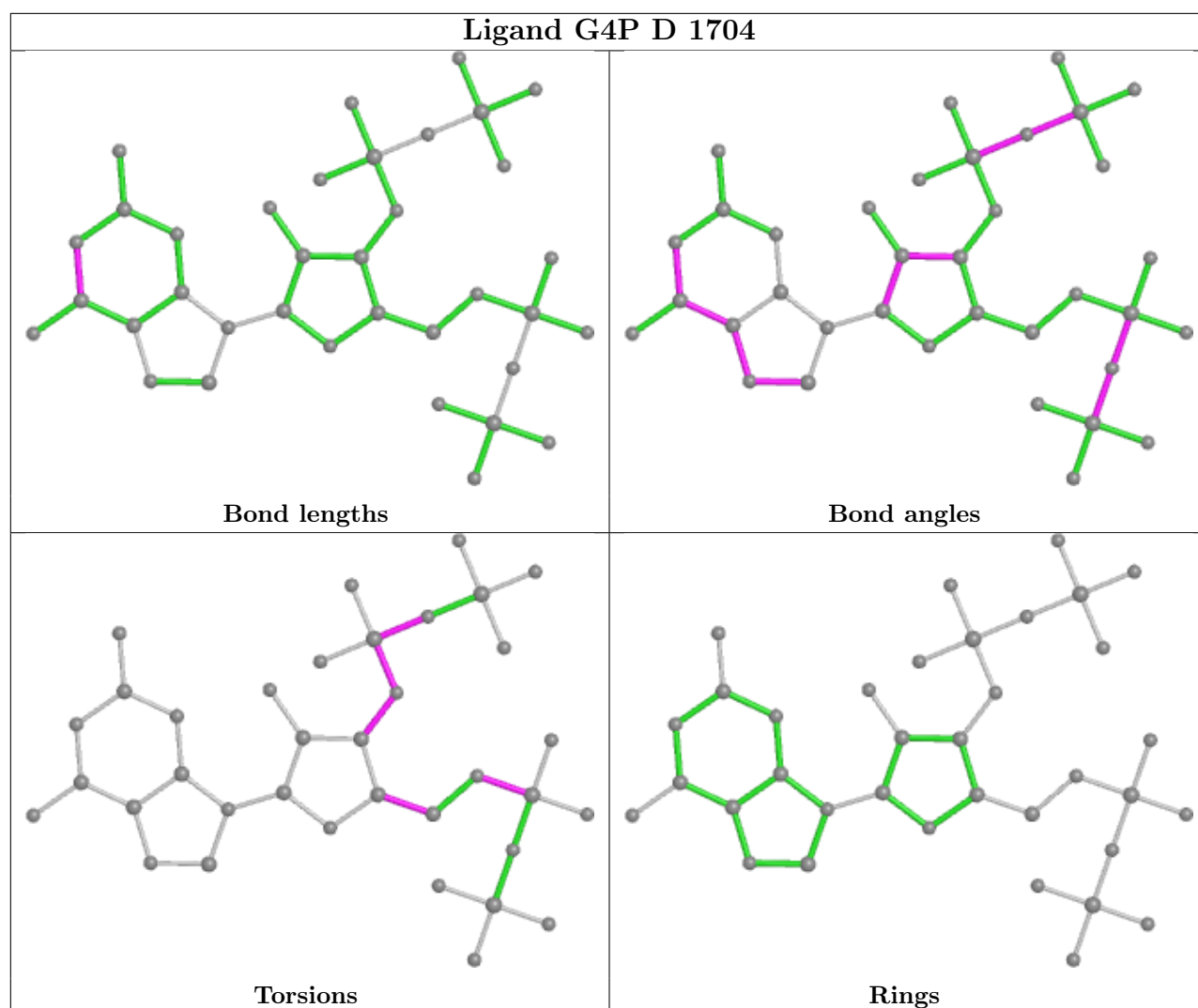
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	M	301	G4P	3	0
16	D	1704	G4P	1	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.

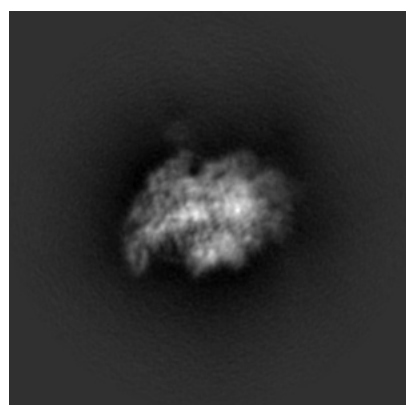
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21852. These allow visual inspection of the internal detail of the map and identification of artifacts.

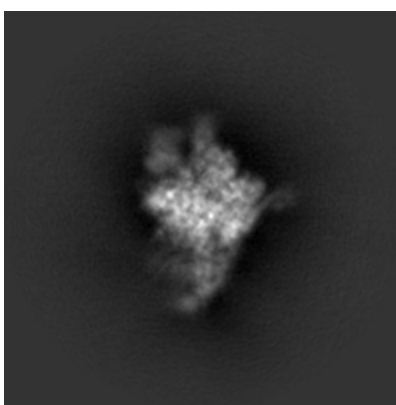
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

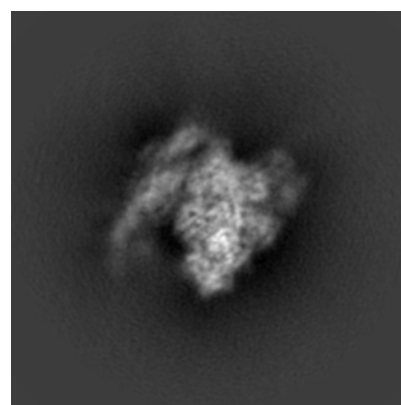
#### 6.1.1 Primary map



X



Y

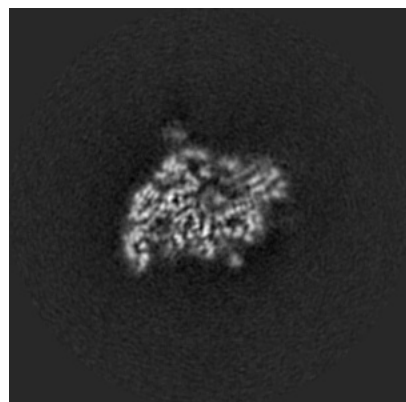


Z

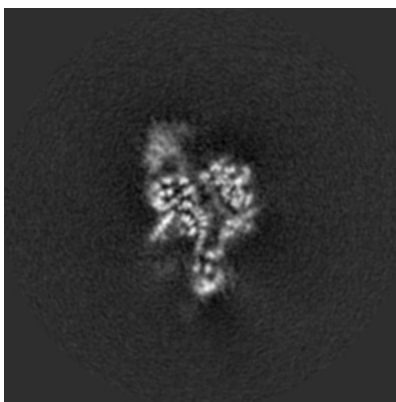
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

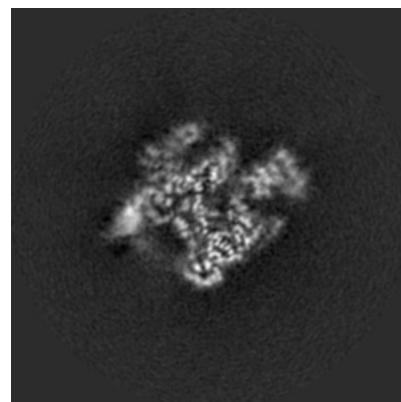
#### 6.2.1 Primary map



X Index: 176



Y Index: 176

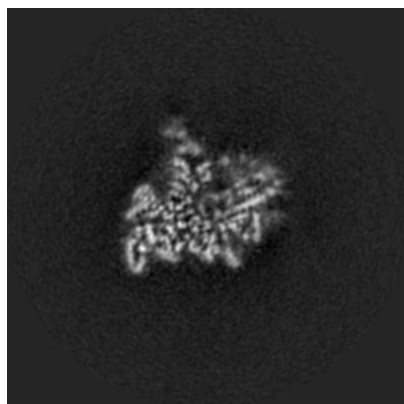


Z Index: 176

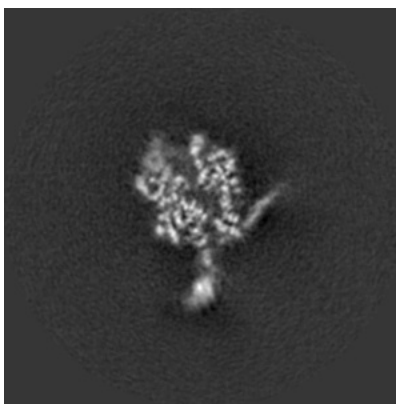
The images above show central slices of the map in three orthogonal directions.

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

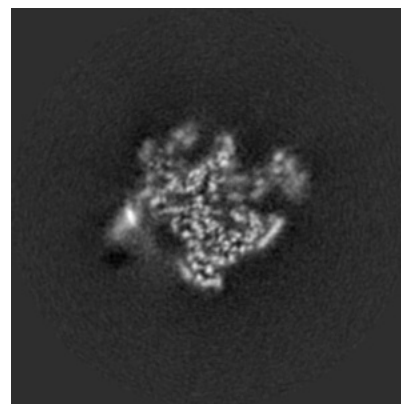
### 6.3.1 Primary map



X Index: 180



Y Index: 165



Z Index: 172

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

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



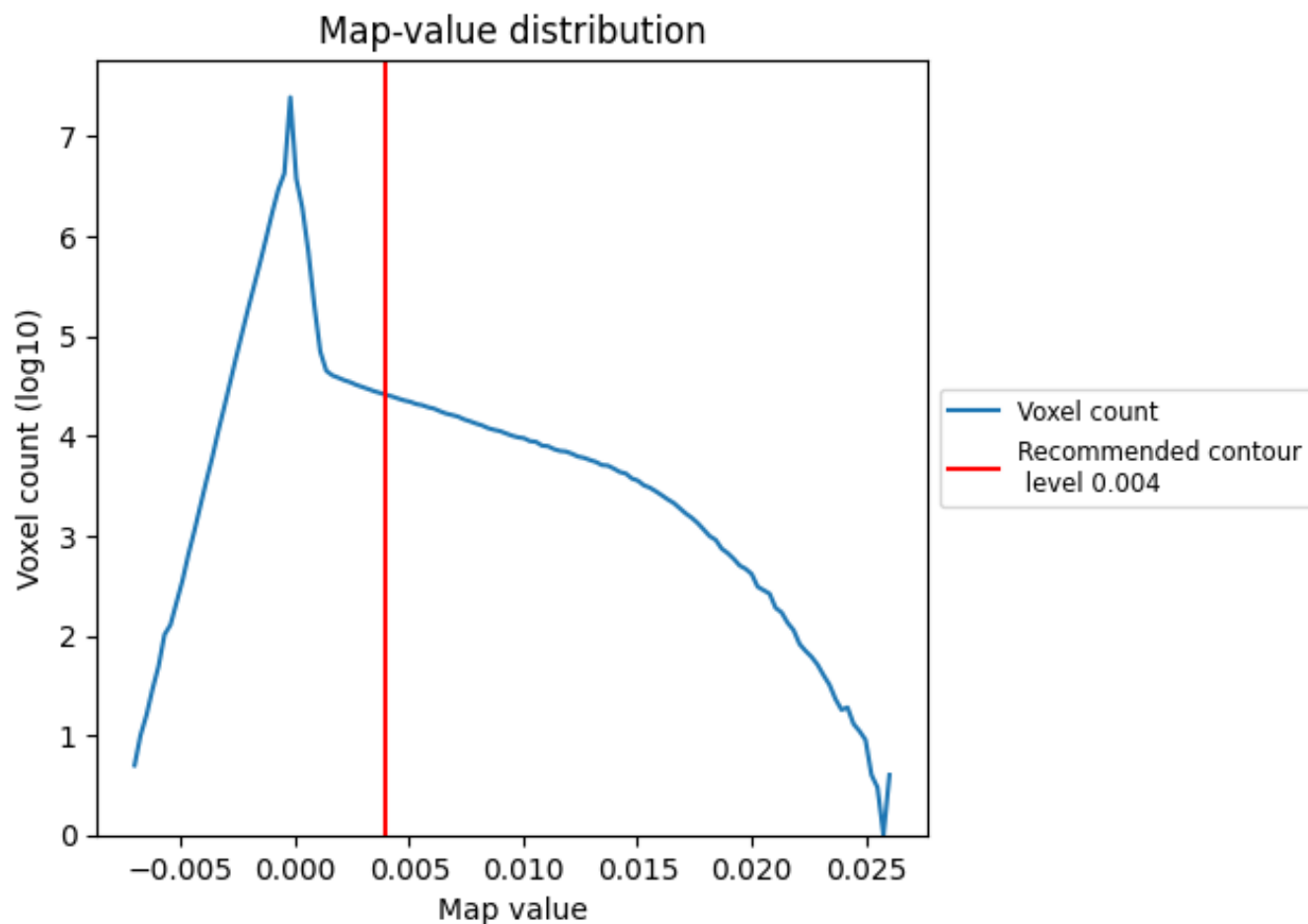
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

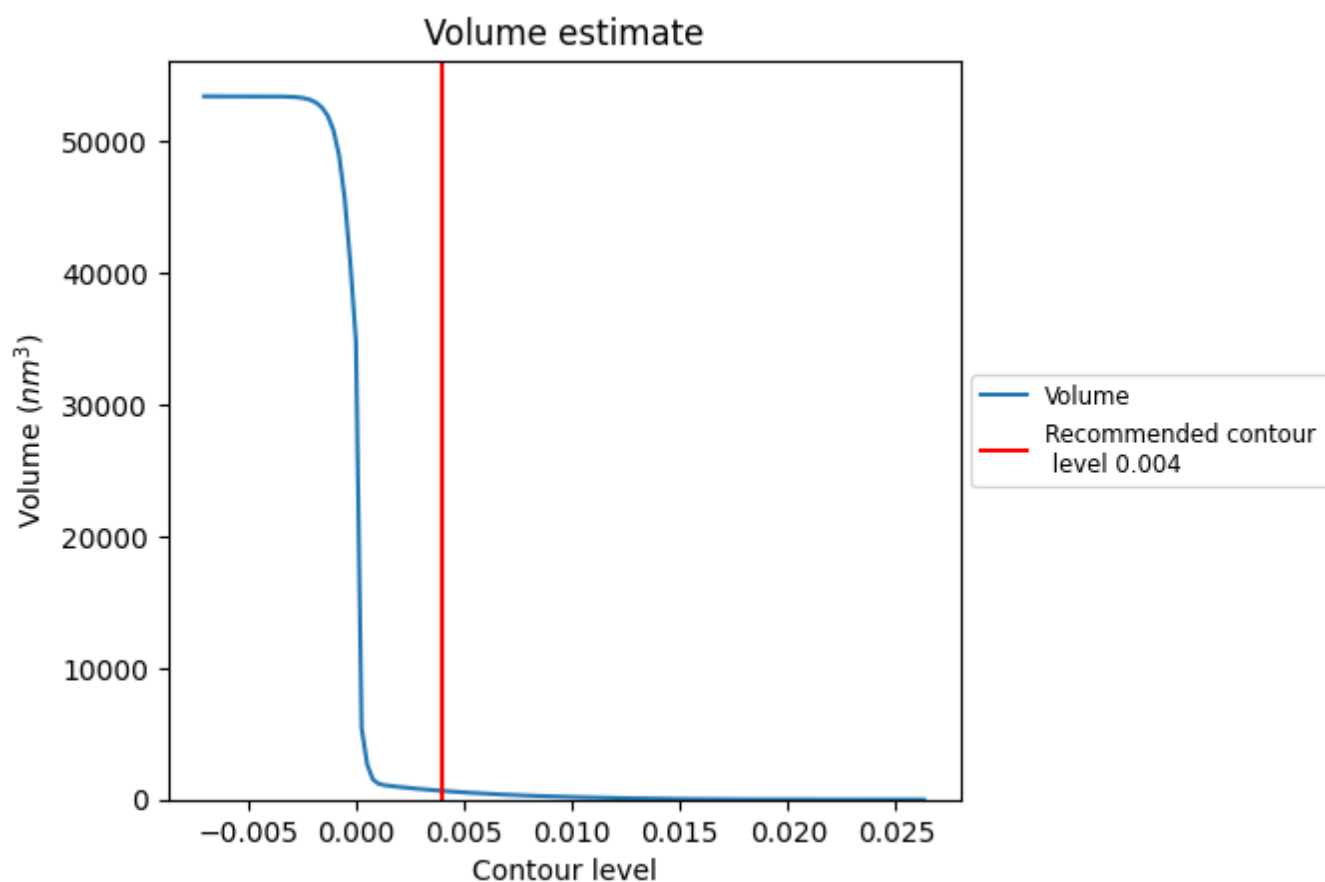
This section contains the results of statistical analysis of the map.

### 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.

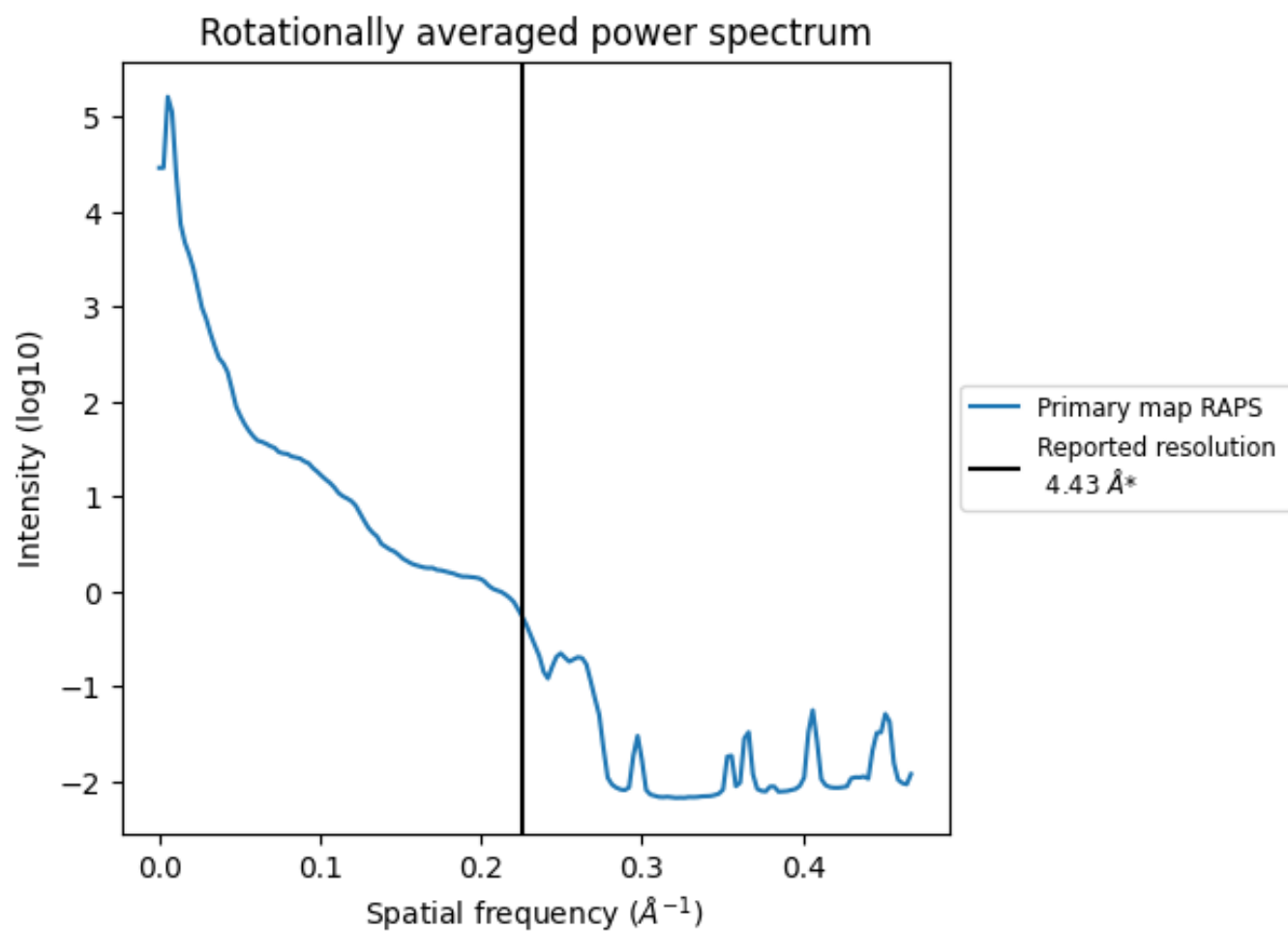
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 662 nm<sup>3</sup>; this corresponds to an approximate mass of 598 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 ⓘ

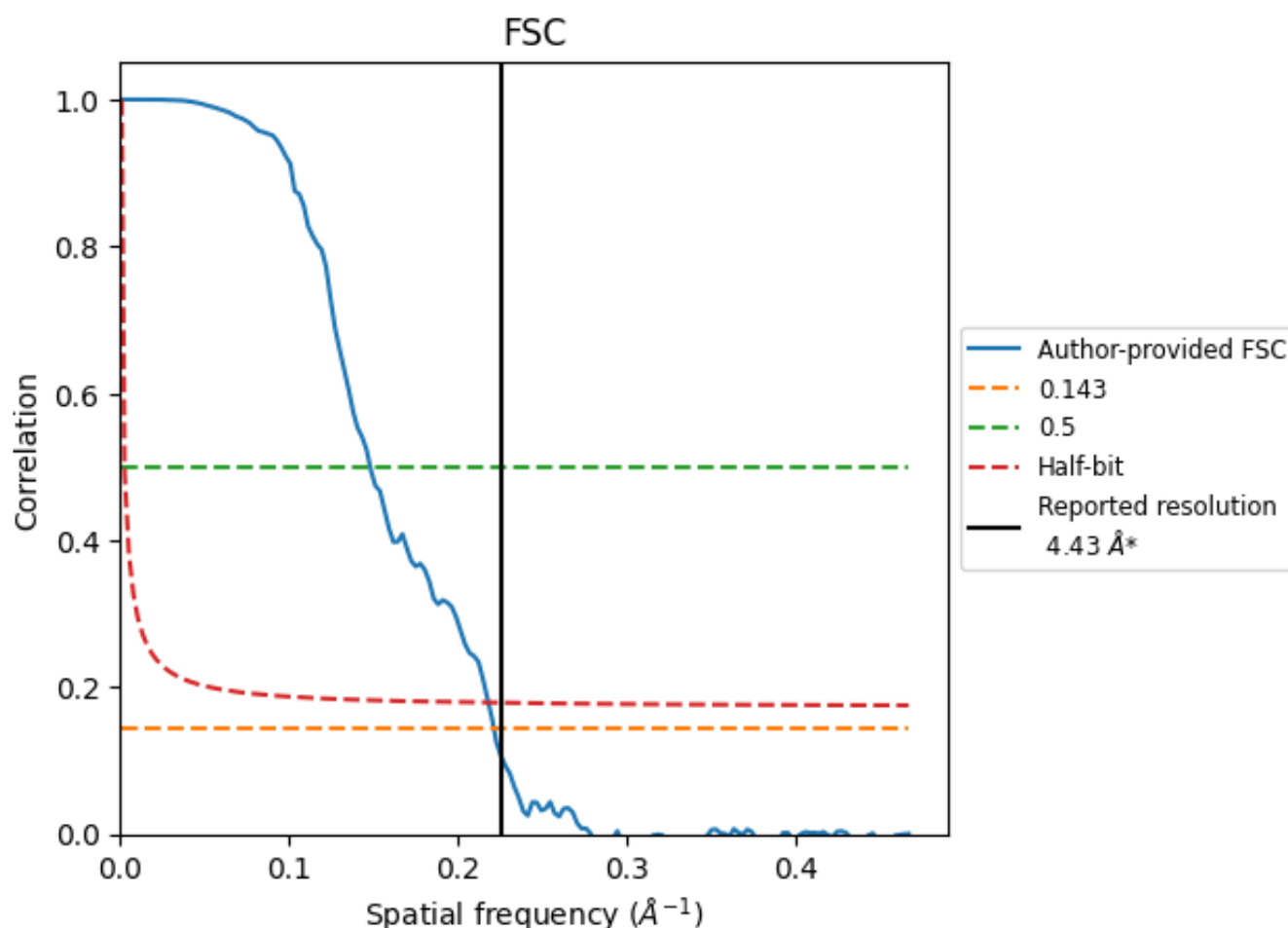


\*Reported resolution corresponds to spatial frequency of 0.226 Å<sup>-1</sup>

## 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 0.226 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

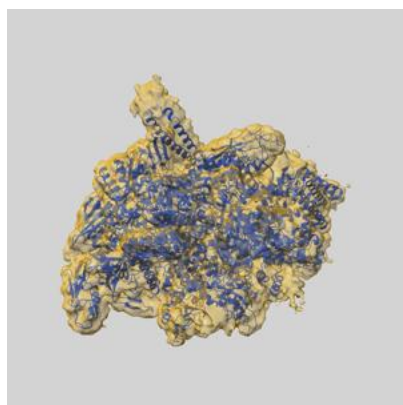
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.43	-	-
Author-provided FSC curve	4.51	6.75	4.58
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

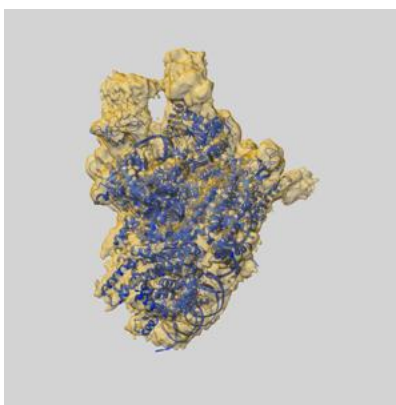
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21852 and PDB model 6WMT. Per-residue inclusion information can be found in section [3](#) on page [7](#).

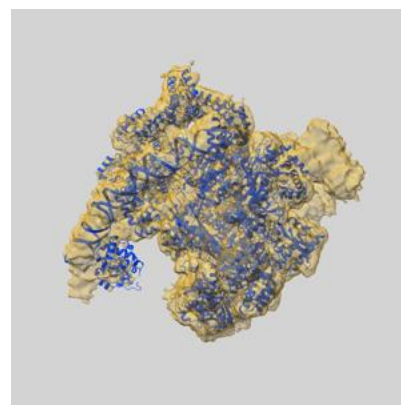
### 9.1 Map-model overlay [i](#)



X



Y



Z

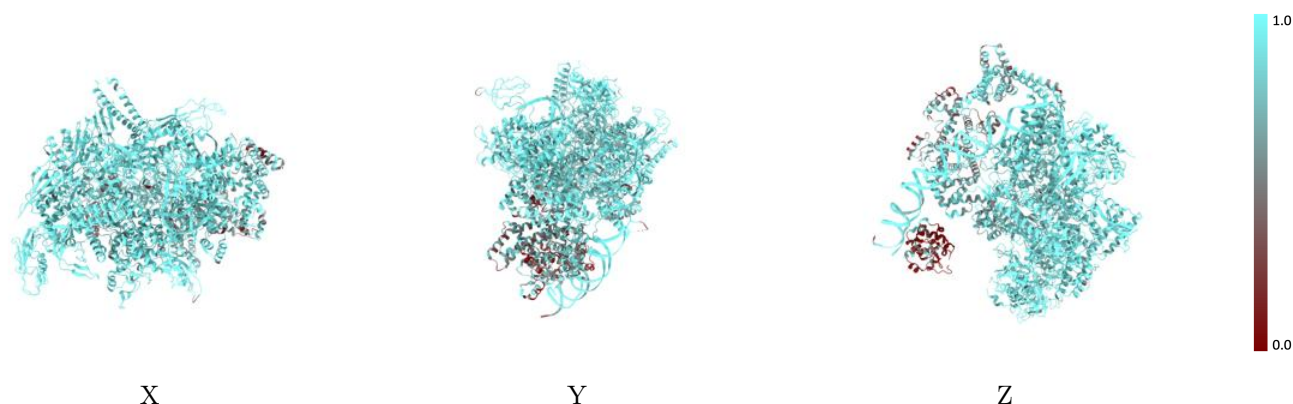
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

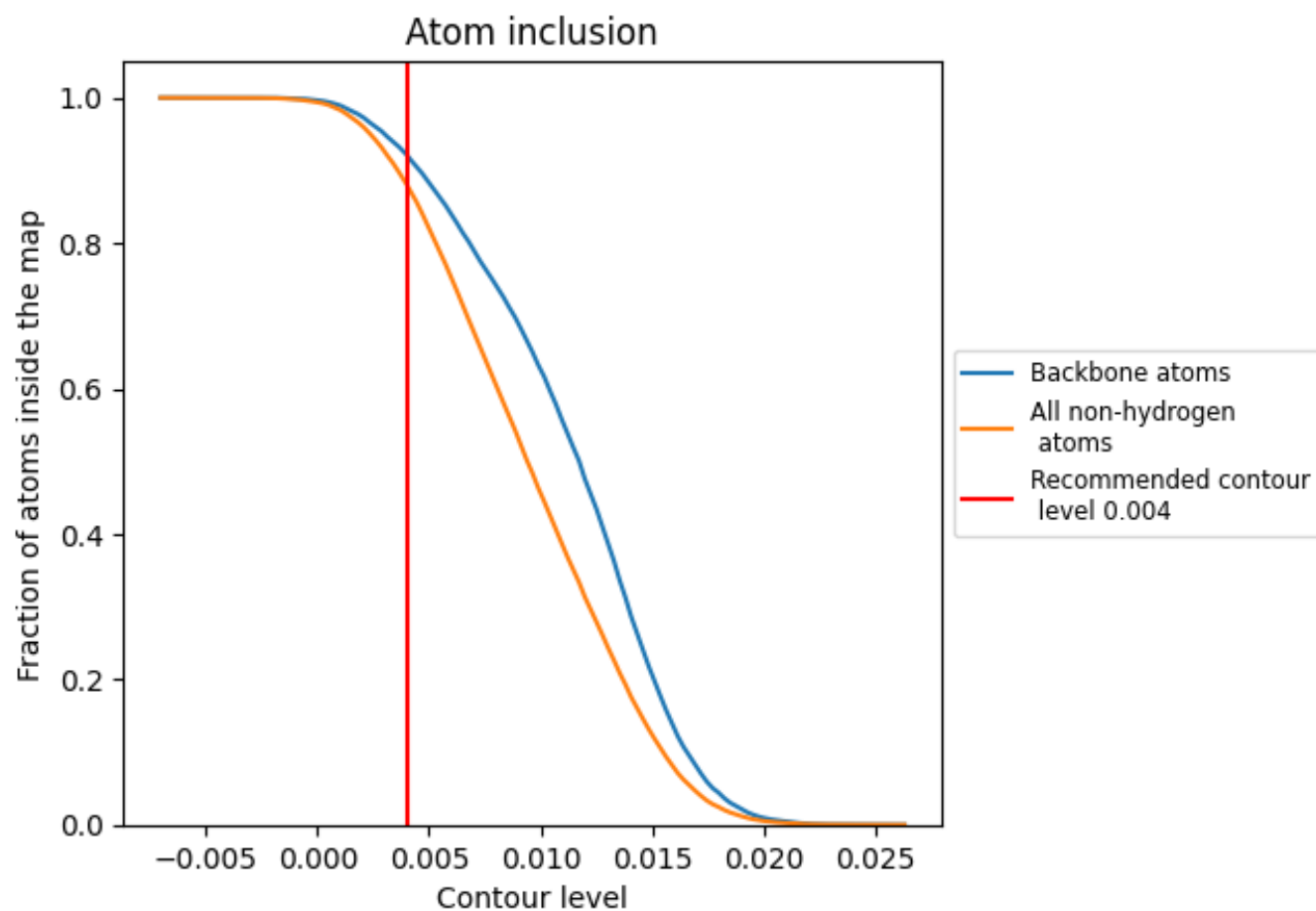
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.004).

































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8808	 0.2120
A	 0.9467	 0.1830
B	 0.9589	 0.2040
C	 0.9396	 0.2540
D	 0.9427	 0.2530
E	 0.8165	 0.1590
G	 0.9149	 0.0980
H	 0.9683	 0.1490
J	 0.9690	 0.2570
K	 0.2822	 0.0640
L	 0.1041	 0.0250
M	 0.6654	 0.1380
S	 0.6358	 0.1560
X	 0.9378	 0.2070
Z	 0.8417	 0.1760

