



# wwPDB EM Validation Summary Report ⓘ

Dec 26, 2023 – 10:48 AM JST

PDB ID : 8WAV  
EMDB ID : EMD-37406  
Title : De novo transcribing complex 12 (TC12), the early elongation complex with Pol II positioned 12nt downstream of TSS  
Authors : Chen, X.; Liu, W.; Wang, Q.; Wang, X.; Ren, Y.; Qu, X.; Li, W.; Xu, Y.  
Deposited on : 2023-09-08  
Resolution : 2.72 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.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

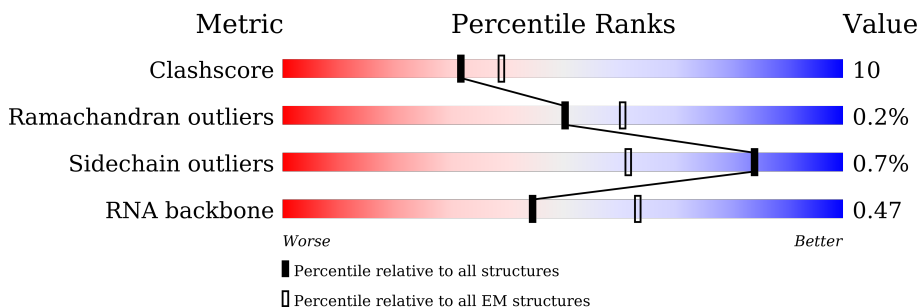
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.72 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	N	8	50% 50%
2	S	517	27% 23% 73%
3	T	249	41% 36% 5% 59%
4	X	99	25% 13% 30% 57%
5	Y	99	29% 34% 19% 45%
6	Z	12	17% 25% 42% 25% 8%
7	o	1970	73% 26%

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Mol	Chain	Length	Quality of chain
8	p	1174	
9	q	275	
10	r	142	
11	s	210	
12	t	127	
13	u	172	
14	v	150	
15	w	125	
16	x	67	
17	y	117	
18	z	58	

## 2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 35748 atoms, of which 30 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 Alpha-amanitin.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	N	8	94	39	30	10	14	1	0	0

- Molecule 2 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	S	138	1138	719	208	208	3	0	0

- Molecule 3 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	T	103	789	492	142	154	1	0	0

- Molecule 4 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	X	43	879	418	158	260	43	0	0

- Molecule 5 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	Y	54	1111	527	208	322	54	0	0

- Molecule 6 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	Z	12	261	114	42	91	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	o	1452	Total	C	N	O	S	0	0
			11510	7235	2056	2146	73		

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	p	1146	Total	C	N	O	S	0	0
			9149	5782	1610	1693	64		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	q	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	r	128	Total	C	N	O	S	0	0
			1050	656	178	212	4		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	s	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	t	82	Total	C	N	O	S	0	0
			657	418	113	121	5		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	u	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	v	148	1186	750	194	237	5	0	0

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	w	114	927	571	166	179	11	0	0

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	x	67	533	345	90	92	6	0	0

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	y	115	920	593	152	173	2	0	0

- Molecule 18 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	z	44	372	231	72	63	6	0	0

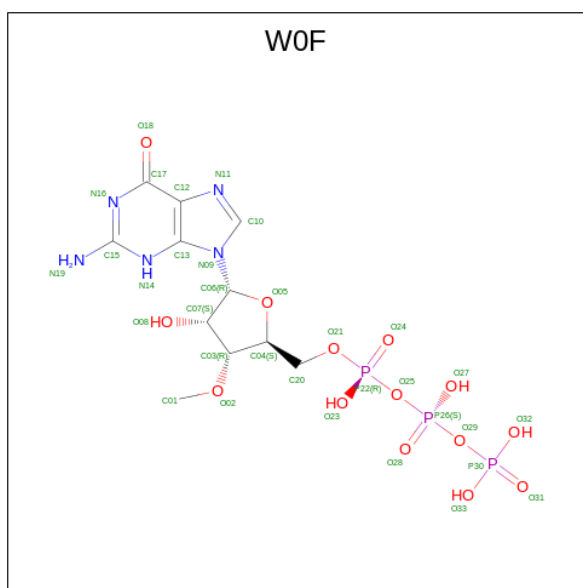
- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	o	2	Total	Zn	0
			2	2	
19	p	1	Total	Zn	0
			1	1	
19	q	1	Total	Zn	0
			1	1	
19	w	2	Total	Zn	0
			2	2	
19	x	1	Total	Zn	0
			1	1	
19	z	1	Total	Zn	0
			1	1	

- Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
20	o	1	1	1	0

- Molecule 21 is [[(2 {S},3 {R},4 {S},5 {R})-5-(2-azanyl-6-oxidanylidene-3 {H}-purin-9-yl)-3-methoxy-4-oxidanyl-oxolan-2-yl]methoxy-oxidanyl-phosphoryl] phosphono hydrogen phosphate (three-letter code: WOF) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



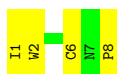
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
21	p	1	33	11	5	14	3	0

### 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.

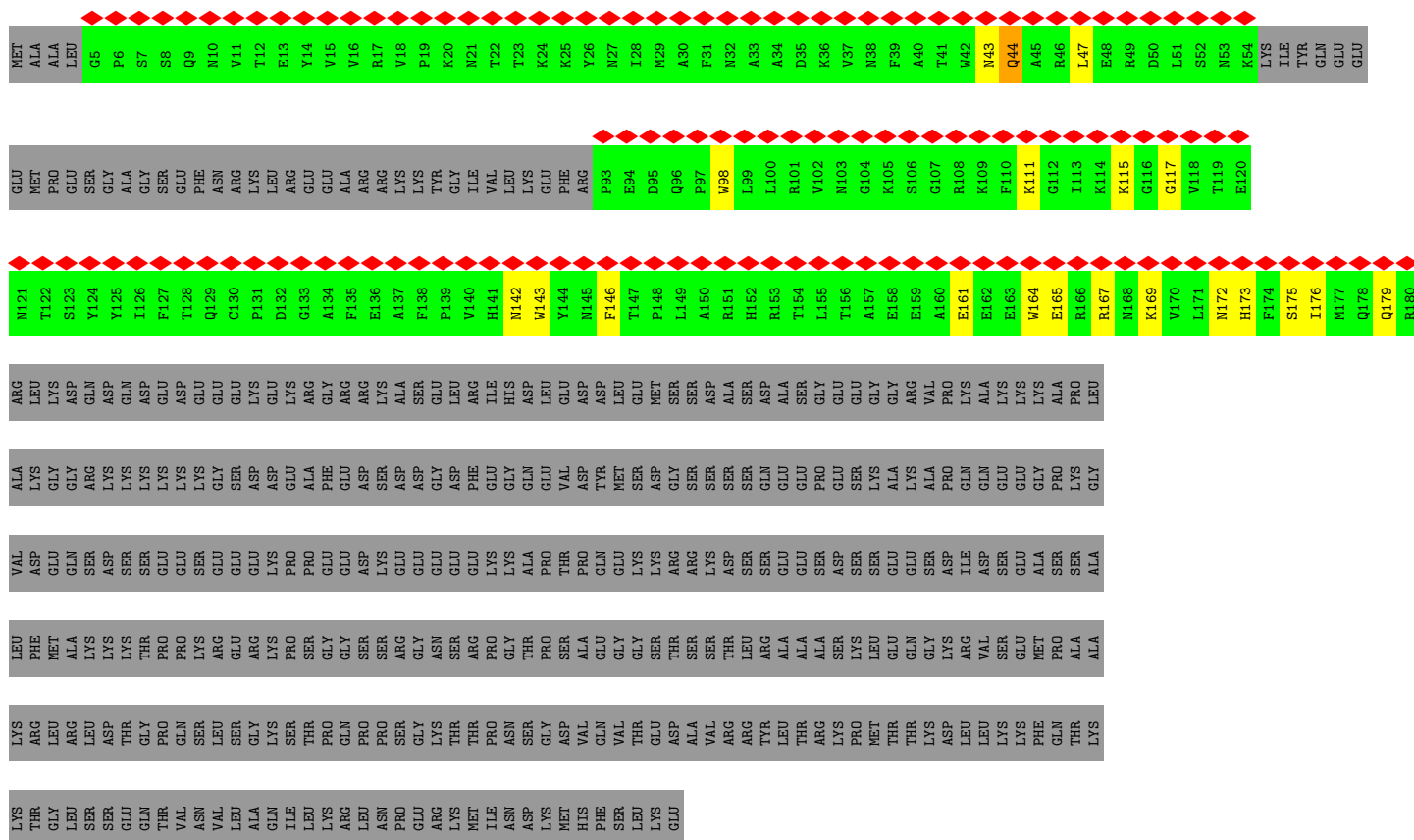
- Molecule 1: Alpha-amanitin

Chain N: 



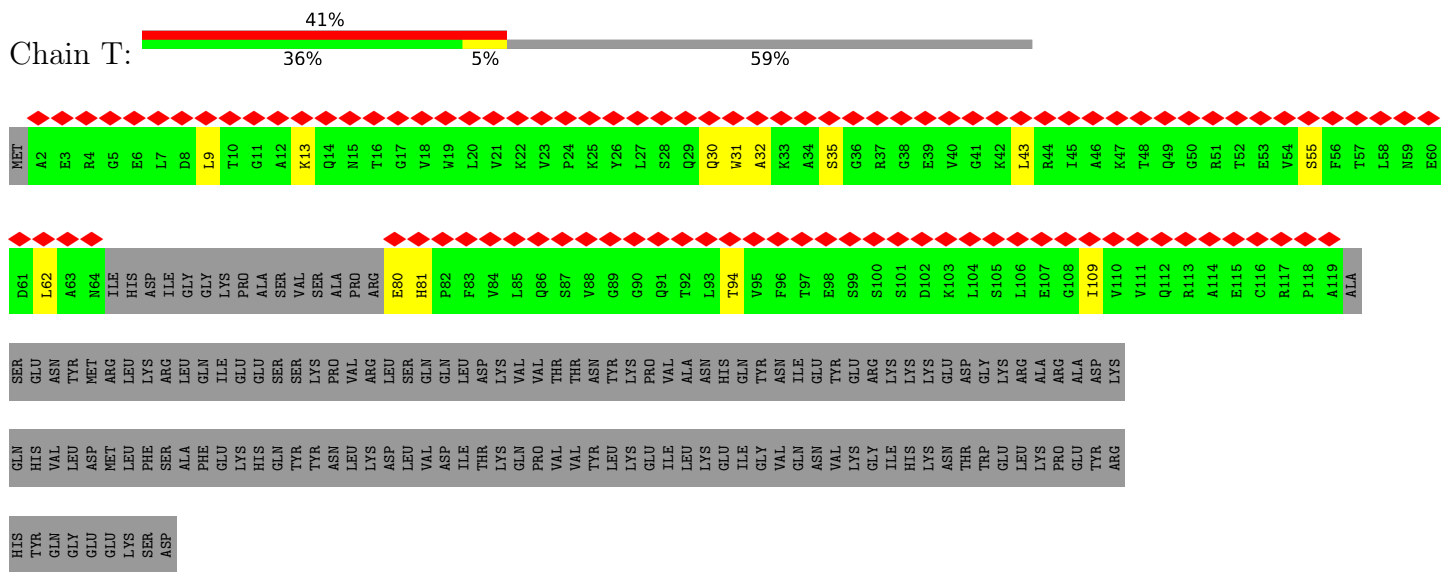
- Molecule 2: General transcription factor IIF subunit 1

Chain S: 

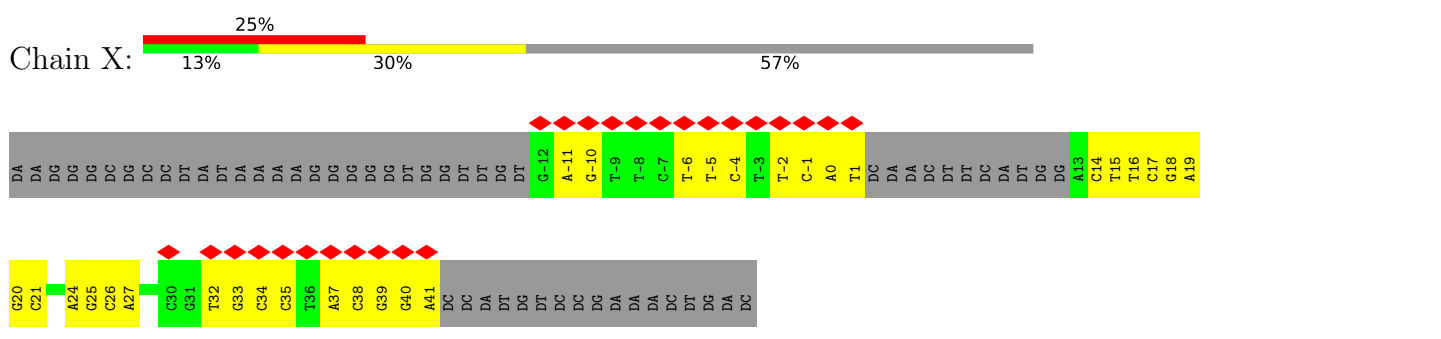


- Molecule 3: General transcription factor IIF subunit 2

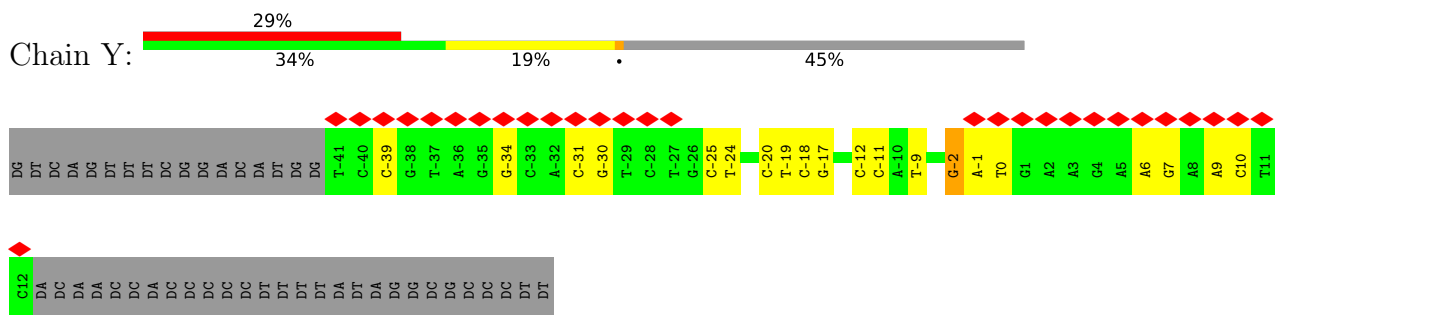




• Molecule 4: non-template DNA



• Molecule 5: template DNA

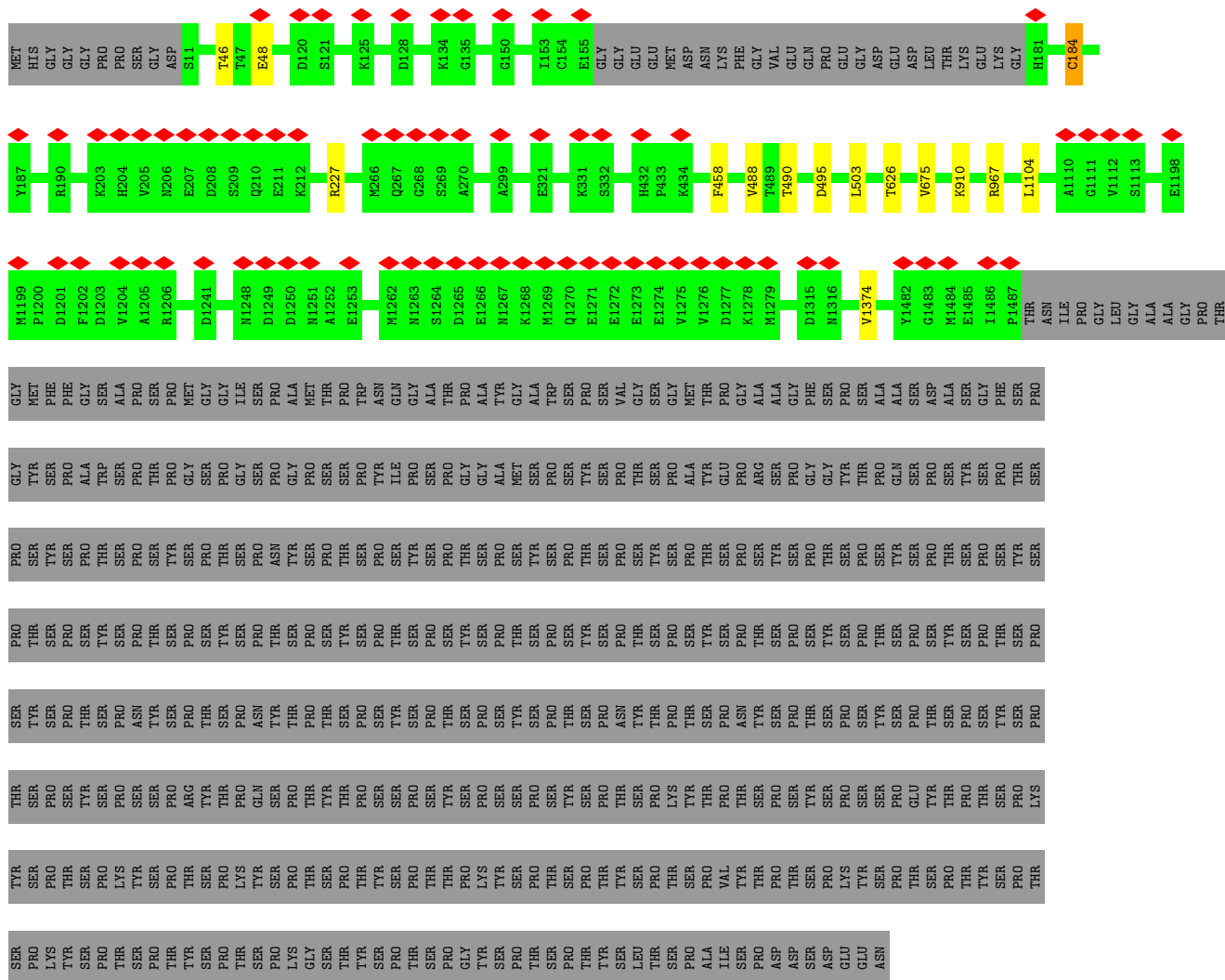


• Molecule 6: RNA

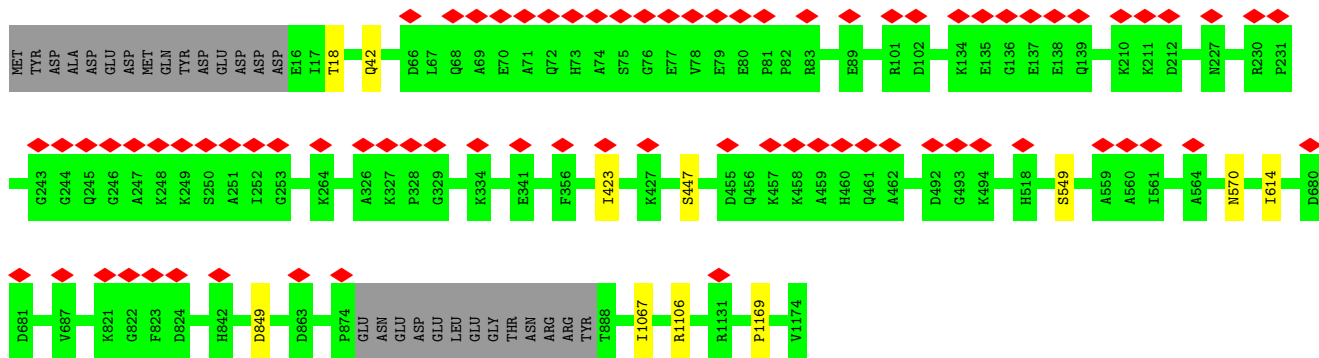


• Molecule 7: DNA-directed RNA polymerase subunit

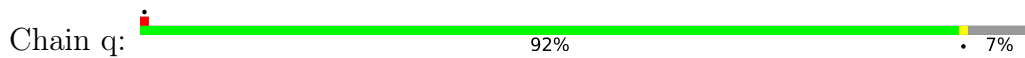


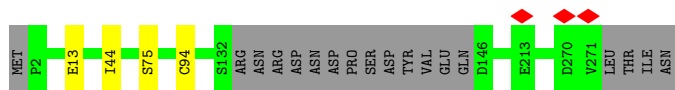


• Molecule 8: DNA-directed RNA polymerase subunit beta

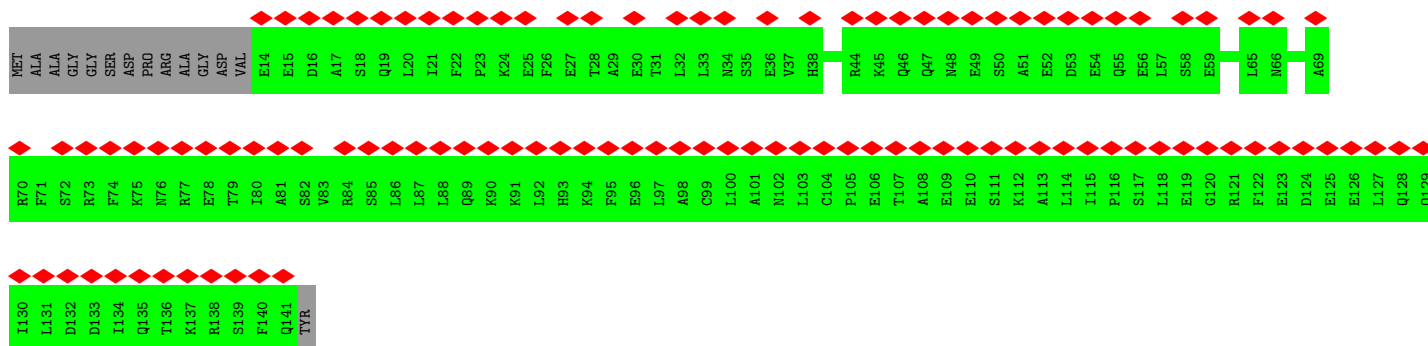
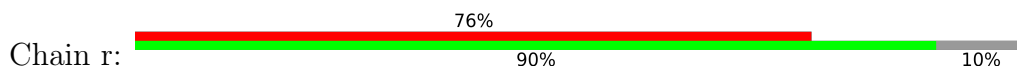


• Molecule 9: DNA-directed RNA polymerase II subunit RPB3

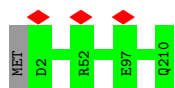




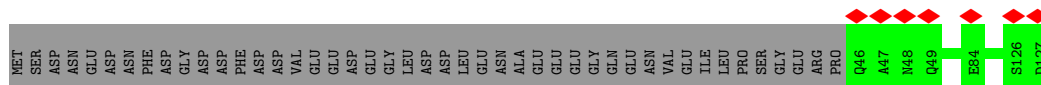
- Molecule 10: DNA-directed RNA polymerase II subunit RPB4



- Molecule 11: DNA-directed RNA polymerase II subunit E



- Molecule 12: DNA-directed RNA polymerase II subunit F

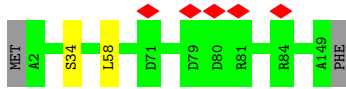


- Molecule 13: DNA-directed RNA polymerase II subunit RPB7

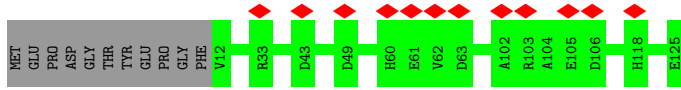
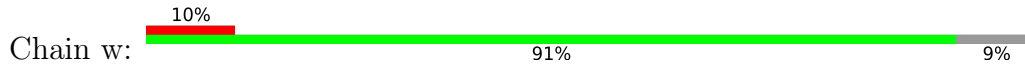


- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC3

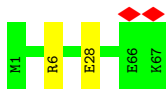




- Molecule 15: DNA-directed RNA polymerase II subunit RPB9



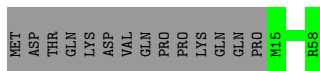
- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 17: DNA-directed RNA polymerase II subunit RPB11-a



- Molecule 18: RPB12



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	539000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	7.704	Depositor
Minimum map value	-5.165	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.115	Depositor
Recommended contour level	0.7	Depositor
Map size ( $\text{\AA}$ )	426.88, 426.88, 426.88	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.334, 1.334, 1.334	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: CSX, ZN, ILX, ATP, G2L, TRX, HYP, W0F, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	N	0.44	0/22	1.00	0/26
2	S	0.24	0/1167	0.48	0/1576
3	T	0.24	0/799	0.50	0/1077
4	X	0.78	0/983	1.11	1/1512 (0.1%)
5	Y	0.86	0/1247	1.06	2/1923 (0.1%)
6	Z	0.94	0/228	2.00	5/351 (1.4%)
7	o	0.49	1/11723 (0.0%)	0.59	1/15830 (0.0%)
8	p	0.53	0/9332	0.60	0/12598
9	q	0.57	0/2102	0.60	0/2857
10	r	0.26	0/1064	0.43	0/1428
11	s	0.47	0/1751	0.57	0/2366
12	t	0.50	0/667	0.55	0/901
13	u	0.34	0/1382	0.50	0/1874
14	v	0.56	0/1207	0.60	0/1628
15	w	0.46	0/948	0.54	0/1284
16	x	0.55	0/542	0.57	0/730
17	y	0.52	0/939	0.56	0/1271
18	z	0.48	0/377	0.64	0/500
All	All	0.52	1/36480 (0.0%)	0.65	9/49732 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	o	1374	VAL	CB-CG2	-5.32	1.41	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	2	U	P-O3'-C3'	23.59	148.00	119.70
5	Y	-2	DG	O5'-P-OP1	8.95	121.44	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	3	C	C5-C6-N1	-7.47	117.26	121.00
5	Y	-9	DT	O4'-C4'-C3'	-6.30	101.98	104.50
6	Z	3	C	C2-N3-C4	-5.42	117.19	119.90

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	N	64	30	51	0	0
2	S	1138	0	1103	12	0
3	T	789	0	795	8	0
4	X	879	0	486	18	0
5	Y	1111	0	607	20	0
6	Z	261	0	128	12	0
7	o	11510	0	11616	0	0
8	p	9149	0	9178	0	0
9	q	2059	0	2007	0	0
10	r	1050	0	1033	0	0
11	s	1720	0	1737	0	0
12	t	657	0	684	0	0
13	u	1351	0	1358	0	0
14	v	1186	0	1147	0	0
15	w	927	0	859	0	0
16	x	533	0	553	0	0
17	y	920	0	942	0	0
18	z	372	0	378	0	0
19	o	2	0	0	0	0
19	p	1	0	0	0	0
19	q	1	0	0	0	0
19	w	2	0	0	0	0
19	x	1	0	0	0	0
19	z	1	0	0	0	0
20	o	1	0	0	0	0
21	p	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	35718	30	34662	64	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 10.

The worst 5 of 64 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:Z:1:ATP:O3'	6:Z:1:ATP:C3'	1.64	1.42
5:Y:-11:DC:O2	6:Z:12:G2L:N2	1.89	1.04
5:Y:-2:DG:H1	6:Z:3:C:H42	1.21	0.86
4:X:15:DT:H4'	4:X:16:DT:H5'	1.57	0.84
5:Y:-2:DG:H8	5:Y:-2:DG:H5''	1.42	0.84

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	4/8 (50%)	3 (75%)	1 (25%)	0	100	100
2	S	134/517 (26%)	134 (100%)	0	0	100	100
3	T	99/249 (40%)	95 (96%)	4 (4%)	0	100	100
7	o	1448/1970 (74%)	1393 (96%)	53 (4%)	2 (0%)	51	77
8	p	1142/1174 (97%)	1077 (94%)	62 (5%)	3 (0%)	41	65
9	q	253/275 (92%)	246 (97%)	7 (3%)	0	100	100
10	r	126/142 (89%)	126 (100%)	0	0	100	100
11	s	207/210 (99%)	197 (95%)	10 (5%)	0	100	100
12	t	80/127 (63%)	79 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	u	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
14	v	146/150 (97%)	138 (94%)	7 (5%)	1 (1%)	22	45
15	w	112/125 (90%)	104 (93%)	8 (7%)	0	100	100
16	x	65/67 (97%)	63 (97%)	0	2 (3%)	4	9
17	y	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
18	z	42/58 (72%)	39 (93%)	3 (7%)	0	100	100
All	All	4140/5361 (77%)	3969 (96%)	163 (4%)	8 (0%)	50	72

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	o	910	LYS
16	x	28	GLU
8	p	549	SER
14	v	34	SER
7	o	184	CYS

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	2/2 (100%)	2 (100%)	0	100	100
2	S	121/448 (27%)	120 (99%)	1 (1%)	81	92
3	T	85/218 (39%)	85 (100%)	0	100	100
7	o	1280/1749 (73%)	1268 (99%)	12 (1%)	78	91
8	p	1001/1027 (98%)	993 (99%)	8 (1%)	81	92
9	q	234/252 (93%)	230 (98%)	4 (2%)	60	83
10	r	118/126 (94%)	118 (100%)	0	100	100
11	s	191/192 (100%)	191 (100%)	0	100	100
12	t	71/111 (64%)	71 (100%)	0	100	100
13	u	152/153 (99%)	152 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	v	129/131 (98%)	128 (99%)	1 (1%)	81	92
15	w	103/112 (92%)	103 (100%)	0	100	100
16	x	56/56 (100%)	56 (100%)	0	100	100
17	y	104/106 (98%)	104 (100%)	0	100	100
18	z	41/55 (74%)	41 (100%)	0	100	100
All	All	3688/4738 (78%)	3662 (99%)	26 (1%)	84	93

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	p	42	GLN
8	p	849	ASP
9	q	94	CYS
8	p	447	SER
8	p	1067	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
8	p	518	HIS
8	p	1094	GLN
8	p	639	HIS
8	p	838	GLN
9	q	217	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	Z	10/12 (83%)	2 (20%)	1 (10%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	Z	3	C
6	Z	5	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	Z	1	ATP

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CSX	N	6	1	3,6,7	1.01	0	1,6,8	2.20	1 (100%)
6	G2L	Z	12	6,5,20	19,26,30	1.00	1 (5%)	18,38,44	1.33	3 (16%)
1	TRX	N	2	1	14,16,17	1.01	0	15,22,24	1.98	4 (26%)
1	HYP	N	8	1	6,8,9	0.75	0	5,10,12	2.14	2 (40%)
1	ILX	N	1	1	8,9,10	0.61	0	9,11,13	1.32	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSX	N	6	1	-	1/1/5/7	-
6	G2L	Z	12	6,5,20	-	2/5/27/31	0/3/3/3
1	TRX	N	2	1	-	0/4/6/8	0/2/2/2
1	HYP	N	8	1	-	0/0/11/13	0/1/1/1
1	ILX	N	1	1	-	7/11/12/14	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Z	12	G2L	C6-N1	-2.37	1.34	1.37

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	2	TRX	CG-CB-CA	5.79	123.47	114.53
1	N	8	HYP	O-C-CA	-3.27	116.21	124.78
1	N	2	TRX	CB-CG-CD1	-2.96	124.31	127.97
1	N	8	HYP	CB-CG-CD	2.94	106.86	103.27
1	N	1	ILX	OD1-CD1-CG1	-2.93	104.69	111.07

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	N	1	ILX	C-CA-CB-CG2
1	N	1	ILX	OD1-CD1-CG1-CB
1	N	1	ILX	OD1-CD1-CG1-OG1
1	N	6	CSX	N-CA-CB-SG
6	Z	12	G2L	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Z	12	G2L	3	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 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
21	W0F	p	1201	-	25,35,35	3.21	7 (28%)	31,55,55	2.54	12 (38%)

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
21	W0F	p	1201	-	-	3/20/40/40	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	p	1201	W0F	C03-C04	-9.40	1.27	1.52
21	p	1201	W0F	O05-C06	-9.24	1.28	1.41
21	p	1201	W0F	O05-C04	6.86	1.60	1.45
21	p	1201	W0F	C07-C03	-2.90	1.46	1.52
21	p	1201	W0F	C20-C04	2.46	1.59	1.51

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	p	1201	W0F	O05-C06-C07	-6.30	97.72	106.93
21	p	1201	W0F	O05-C04-C03	-5.68	92.70	104.87
21	p	1201	W0F	O05-C04-C20	4.79	125.15	109.37
21	p	1201	W0F	O21-C20-C04	3.93	122.51	108.99
21	p	1201	W0F	O32-P30-O29	3.90	117.72	104.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

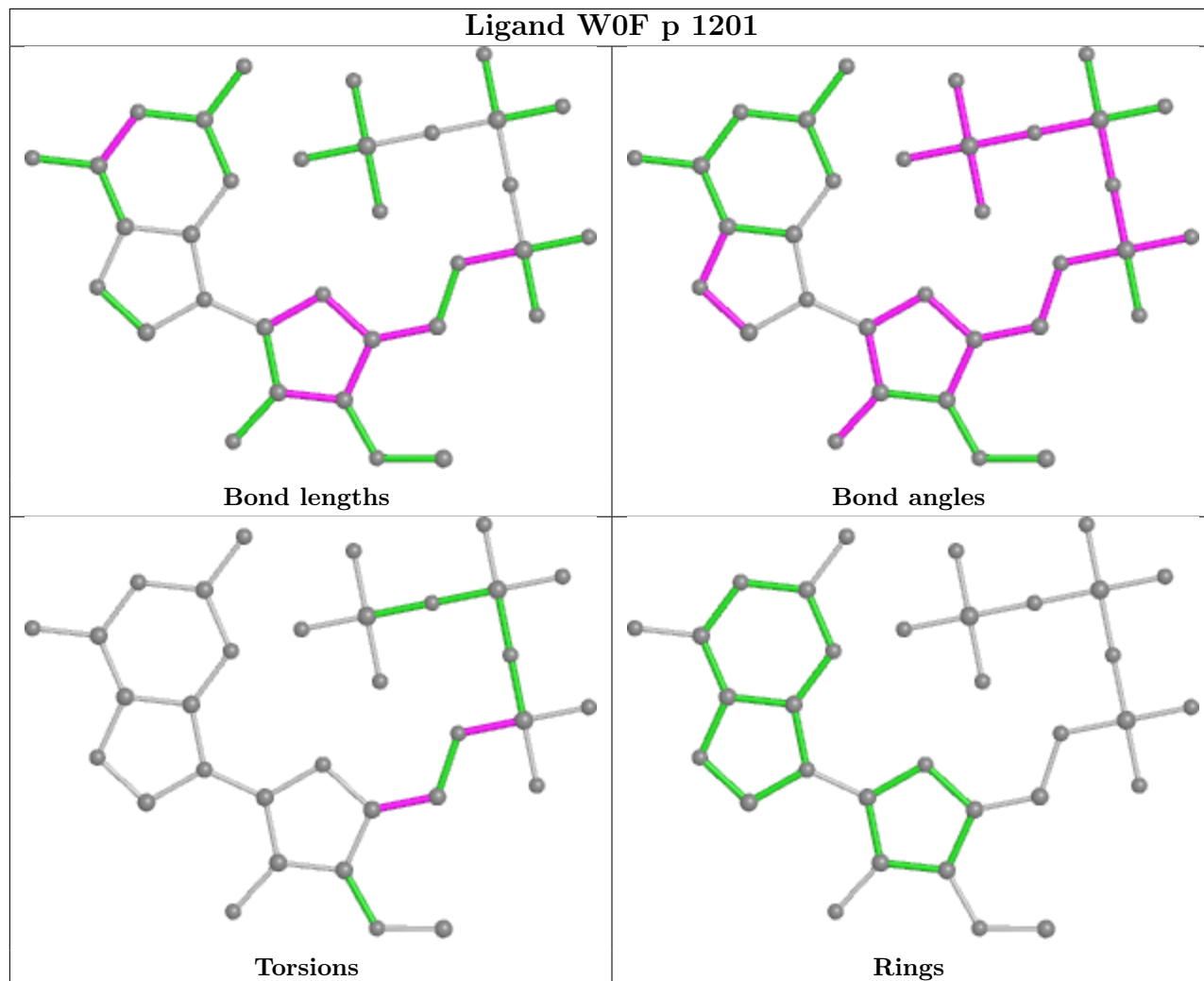
Mol	Chain	Res	Type	Atoms
21	p	1201	W0F	C20-O21-P22-O24
21	p	1201	W0F	C20-O21-P22-O25
21	p	1201	W0F	C03-C04-C20-O21

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.

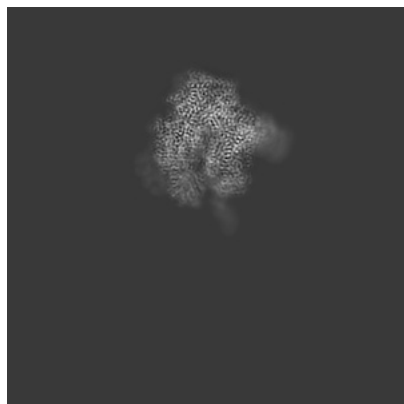
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37406. These allow visual inspection of the internal detail of the map and identification of artifacts.

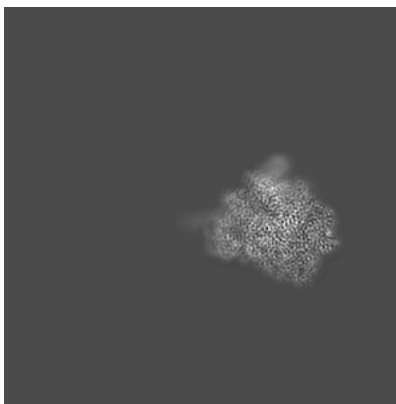
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

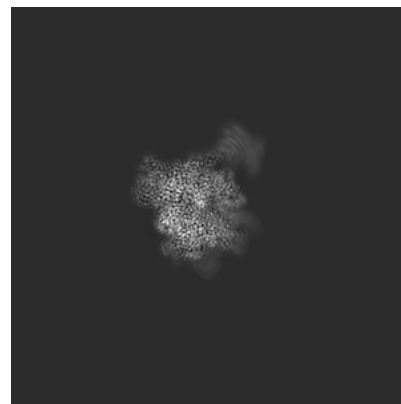
#### 6.1.1 Primary map



X

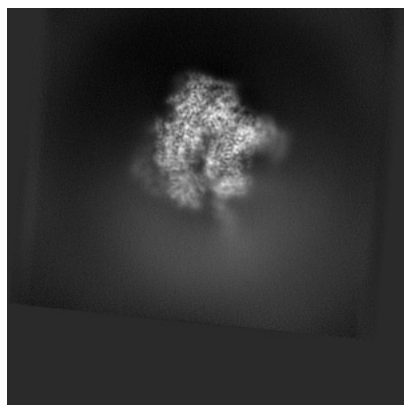


Y

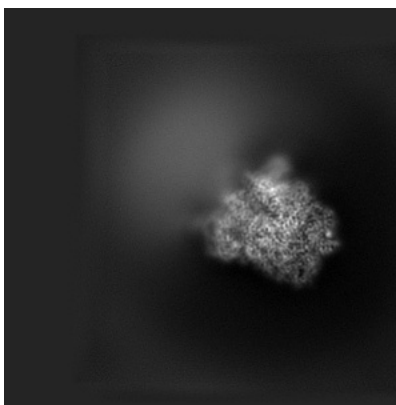


Z

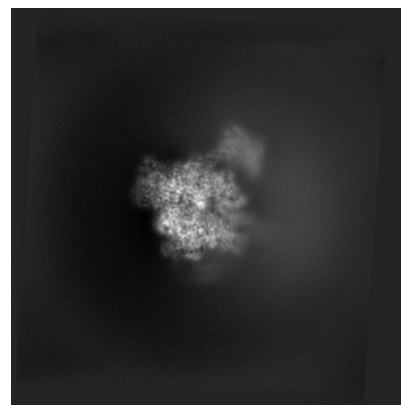
#### 6.1.2 Raw map



X



Y



Z

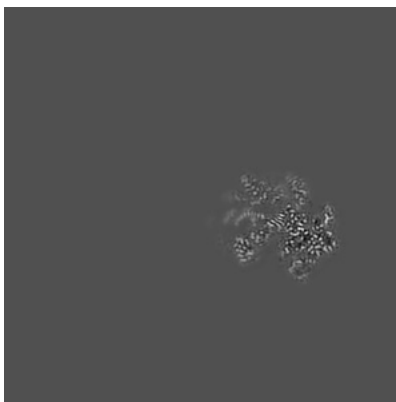
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

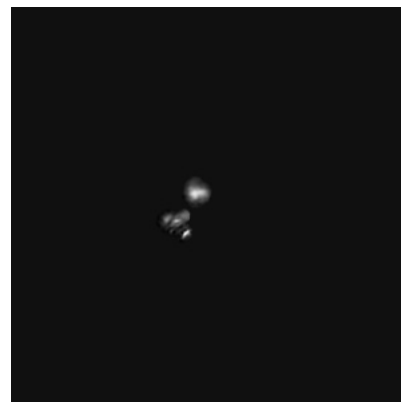
### 6.2.1 Primary map



X Index: 160

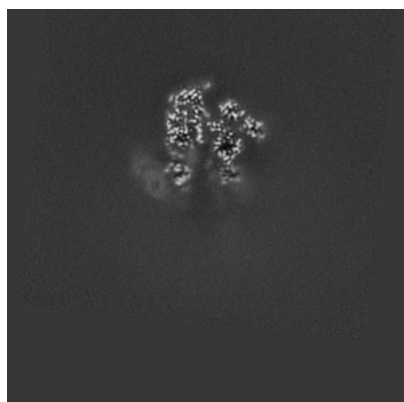


Y Index: 160

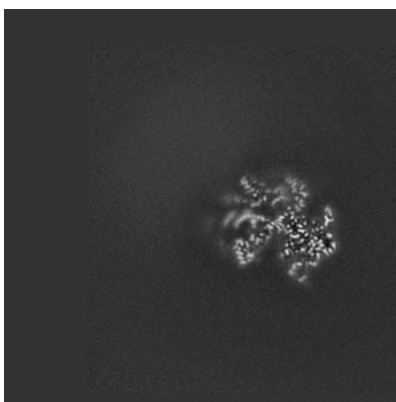


Z Index: 160

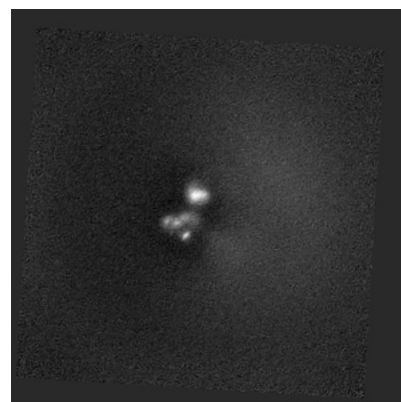
### 6.2.2 Raw map



X Index: 160



Y Index: 160



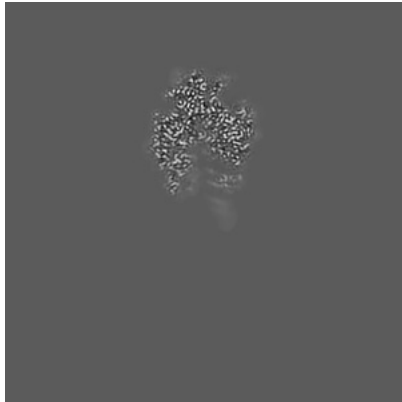
Z Index: 160

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

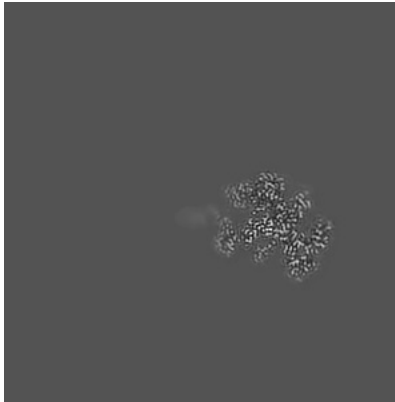


## 6.3 Largest variance slices [i](#)

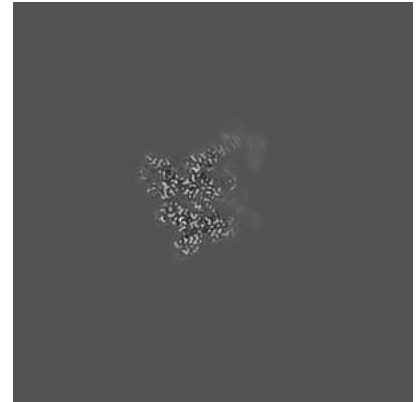
### 6.3.1 Primary map



X Index: 144

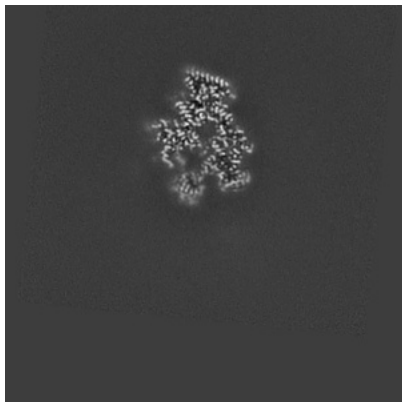


Y Index: 175

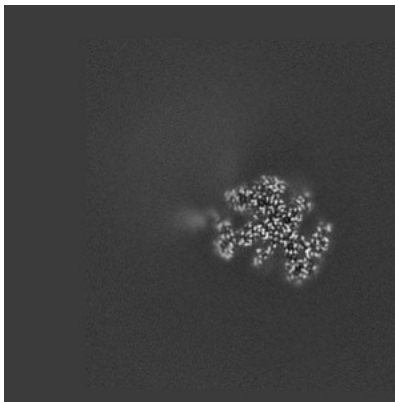


Z Index: 224

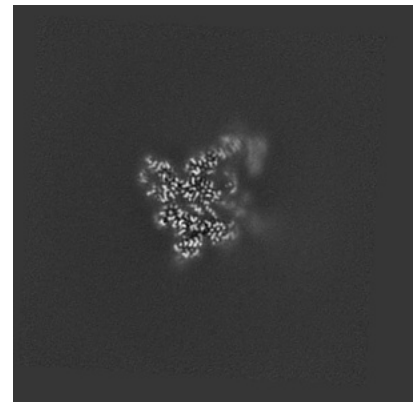
### 6.3.2 Raw map



X Index: 133



Y Index: 176

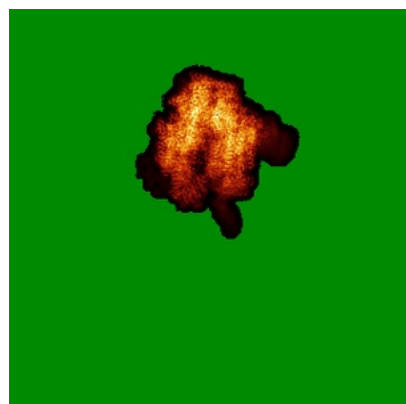


Z Index: 224

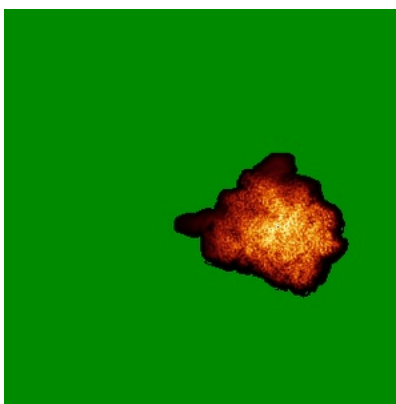
The images above show the largest variance slices of the map in three orthogonal directions.

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

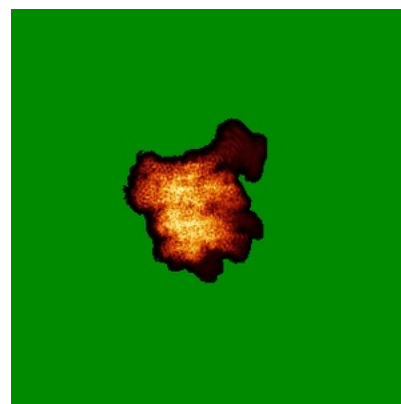
### 6.4.1 Primary map



X



Y



Z

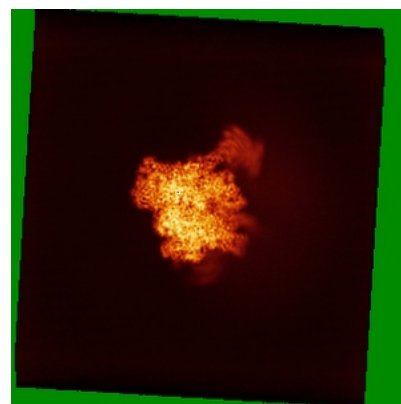
### 6.4.2 Raw map



X



Y

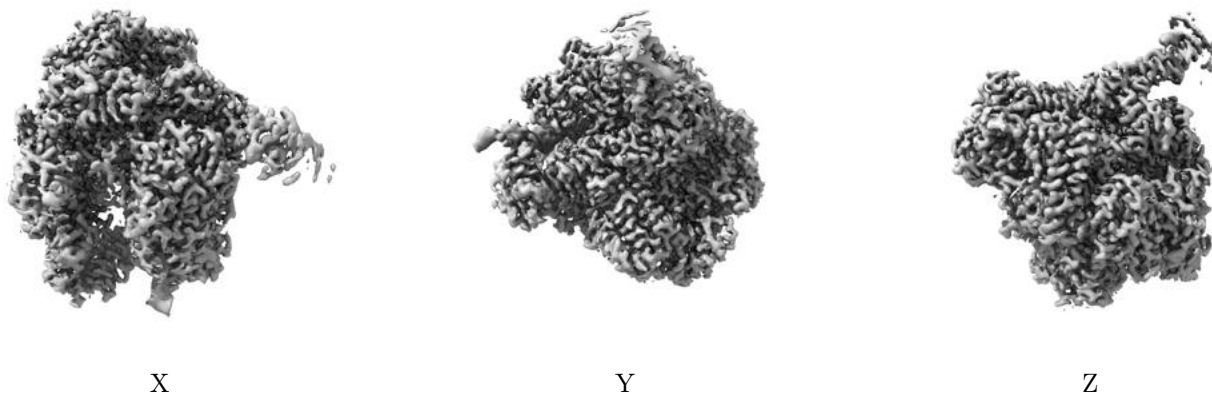


Z

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.

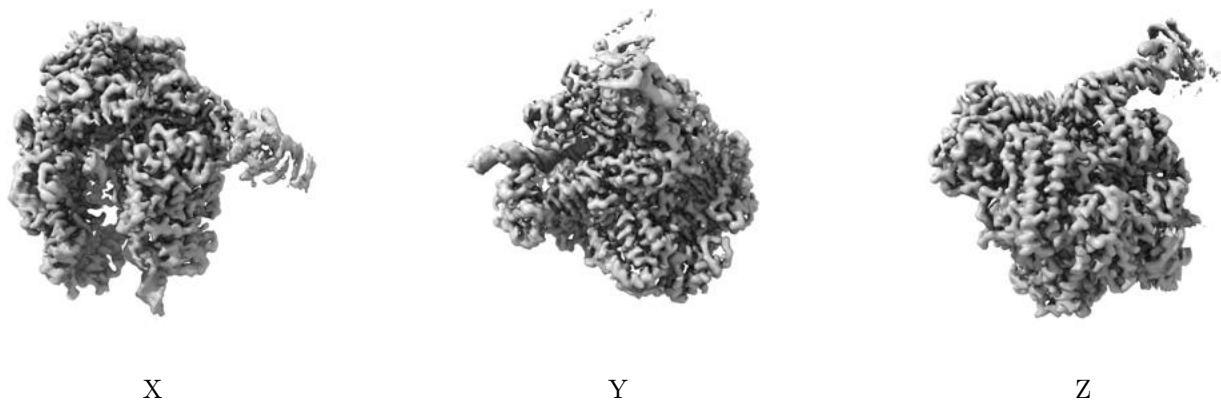
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. 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.

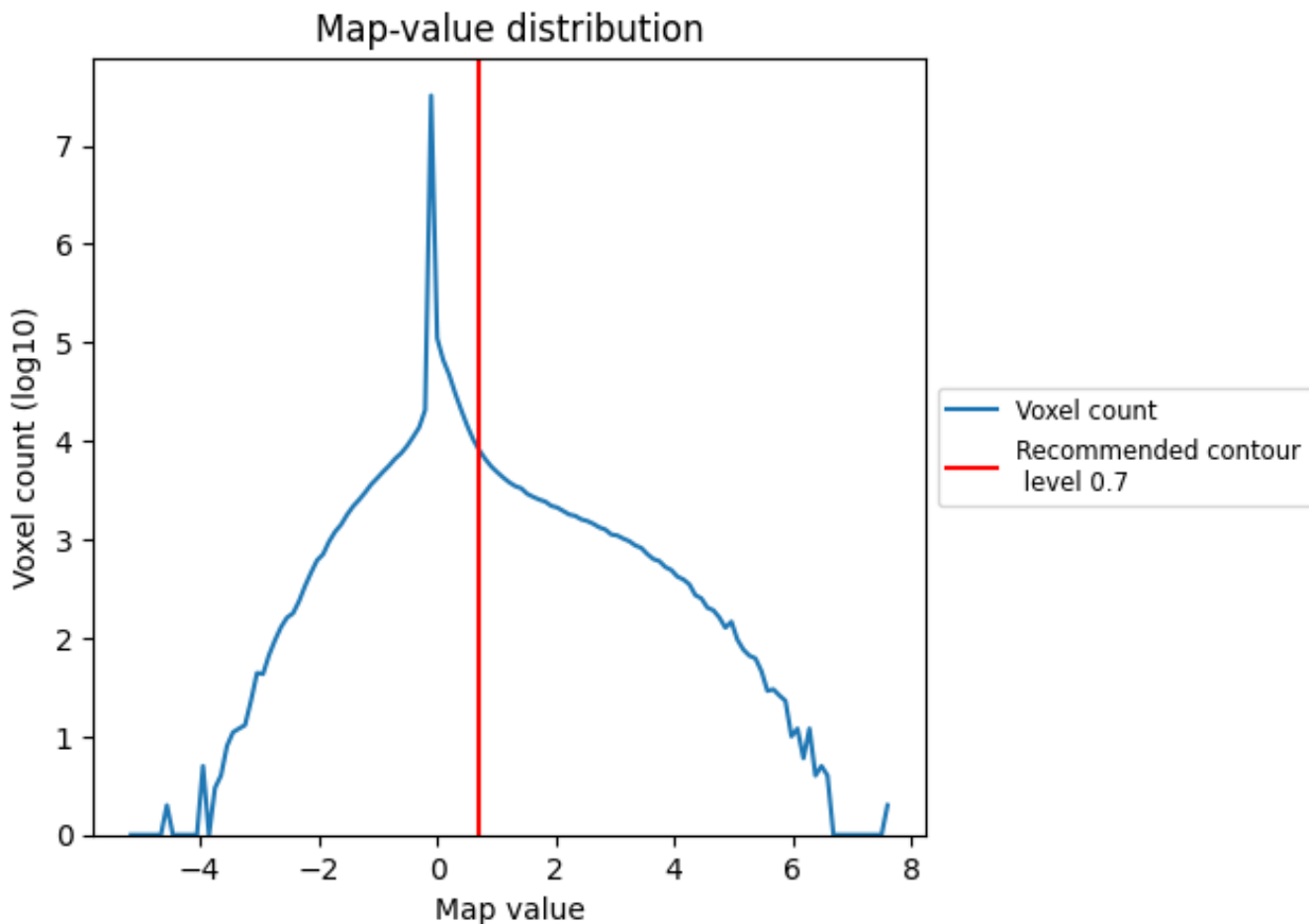
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

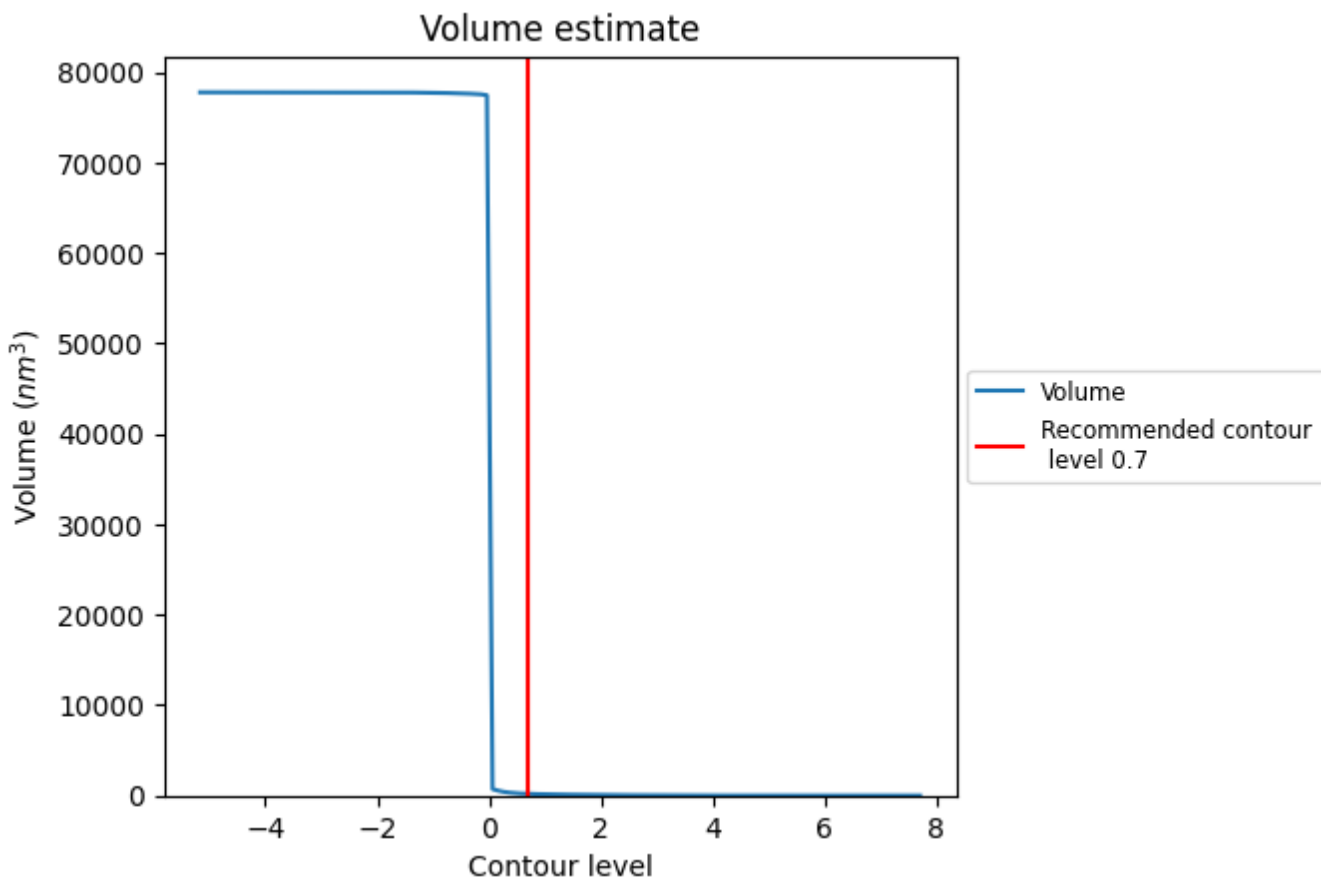
This section contains the results of statistical analysis of the map.

### 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.

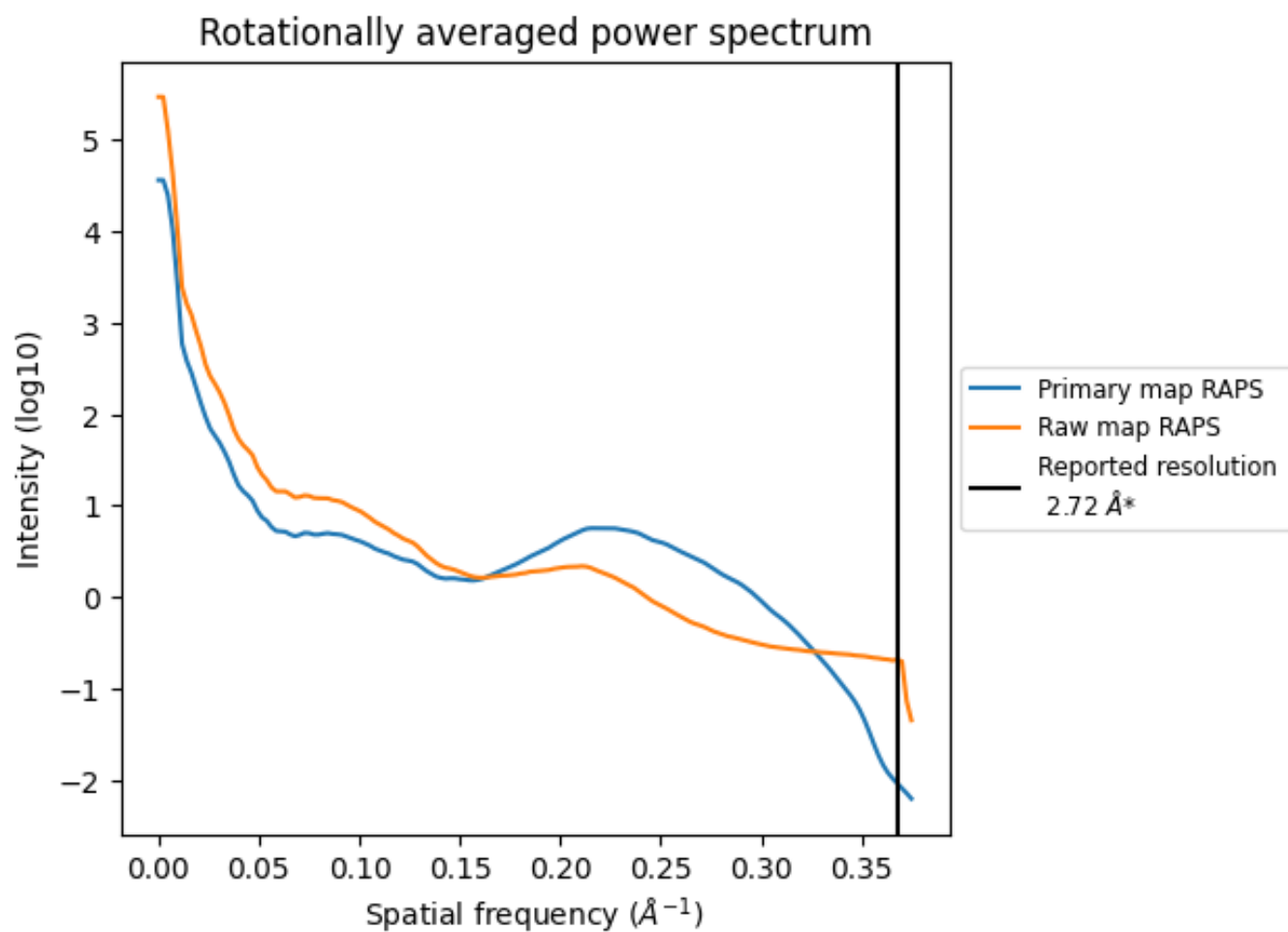
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 191 nm<sup>3</sup>; this corresponds to an approximate mass of 173 kDa.

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

### 7.3 Rotationally averaged power spectrum i

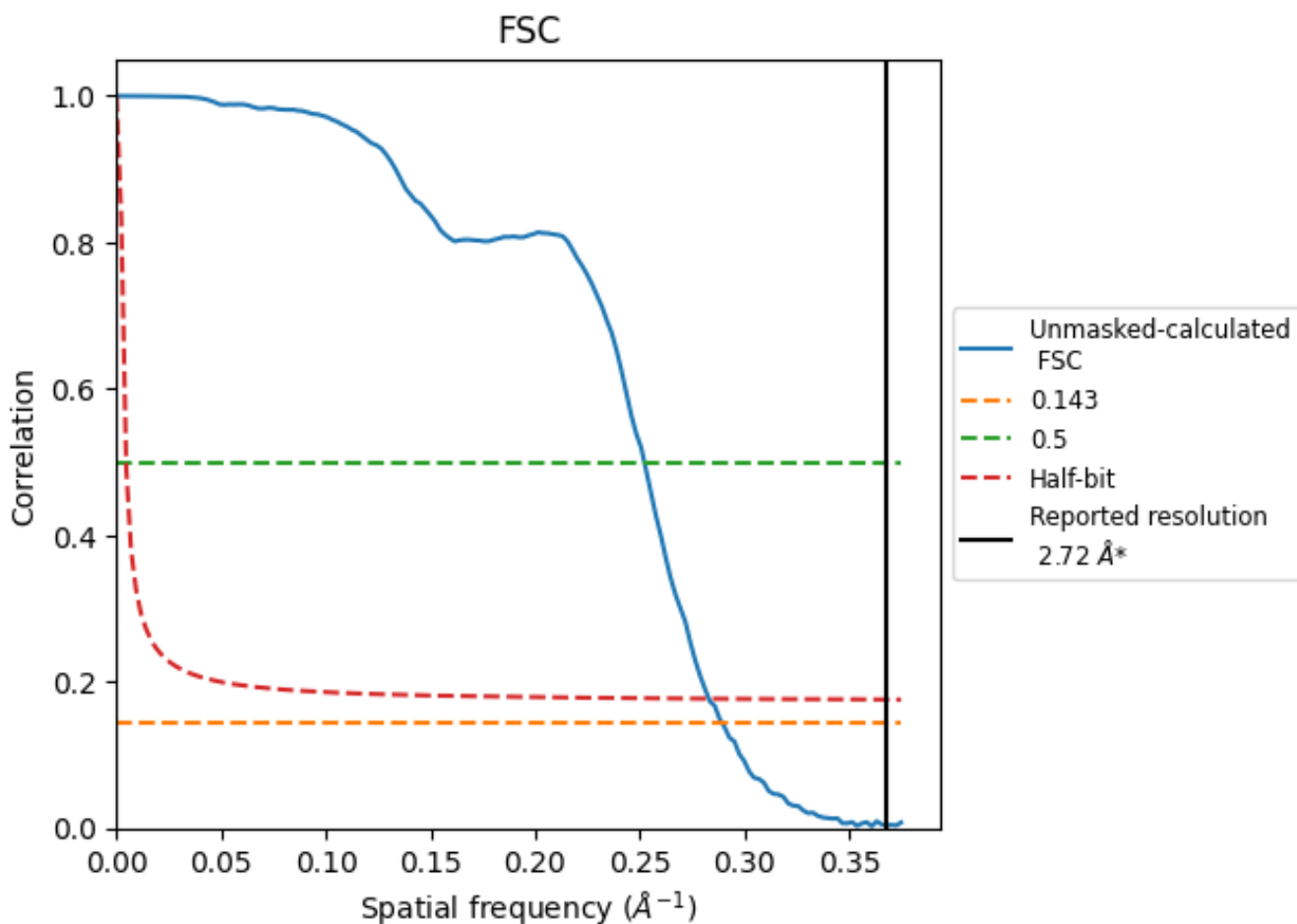


\*Reported resolution corresponds to spatial frequency of  $0.368 \text{ \AA}^{-1}$

## 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  $0.368 \text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.46	3.97	3.53

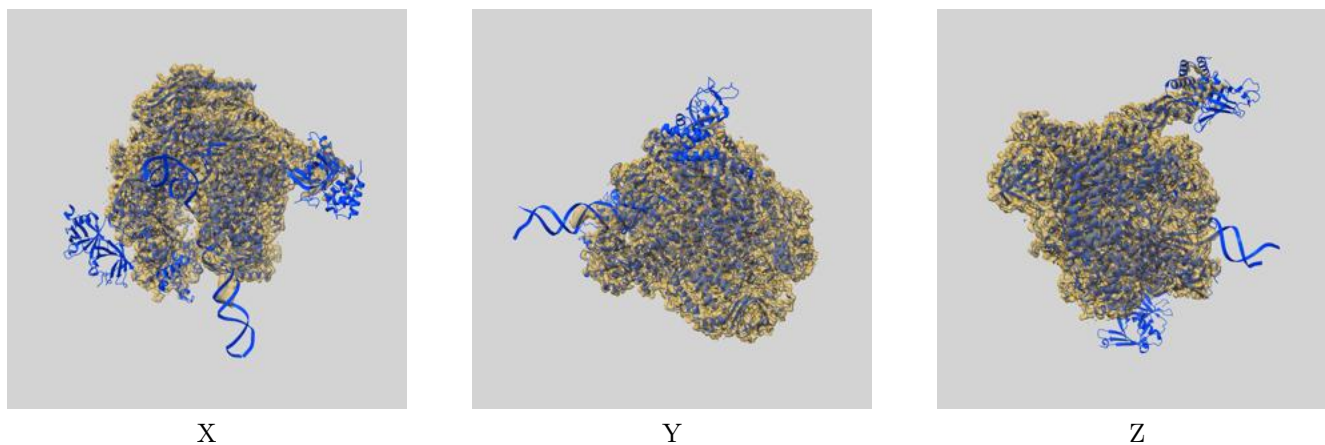
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.46 differs from the reported value 2.72 by more than 10 %



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

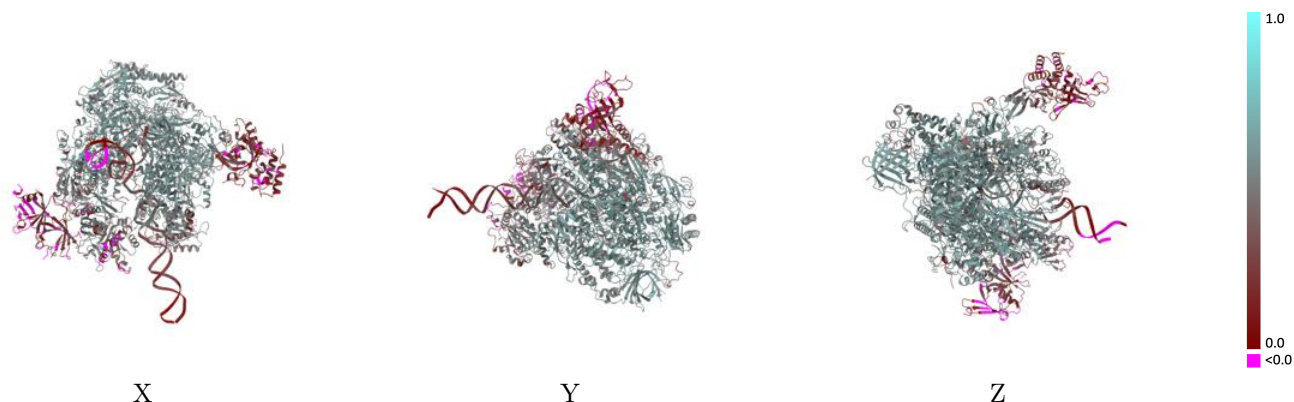
This section contains information regarding the fit between EMDB map EMD-37406 and PDB model 8WAV. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



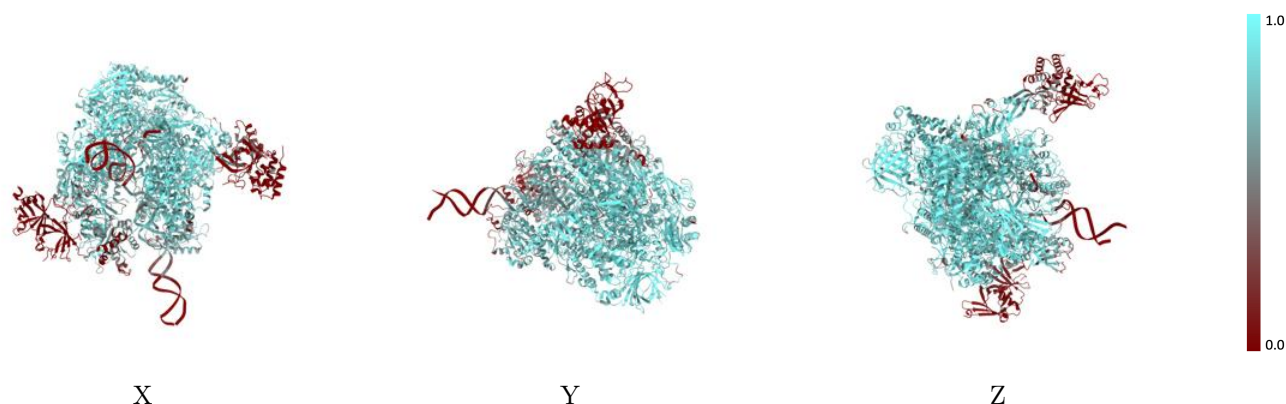
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



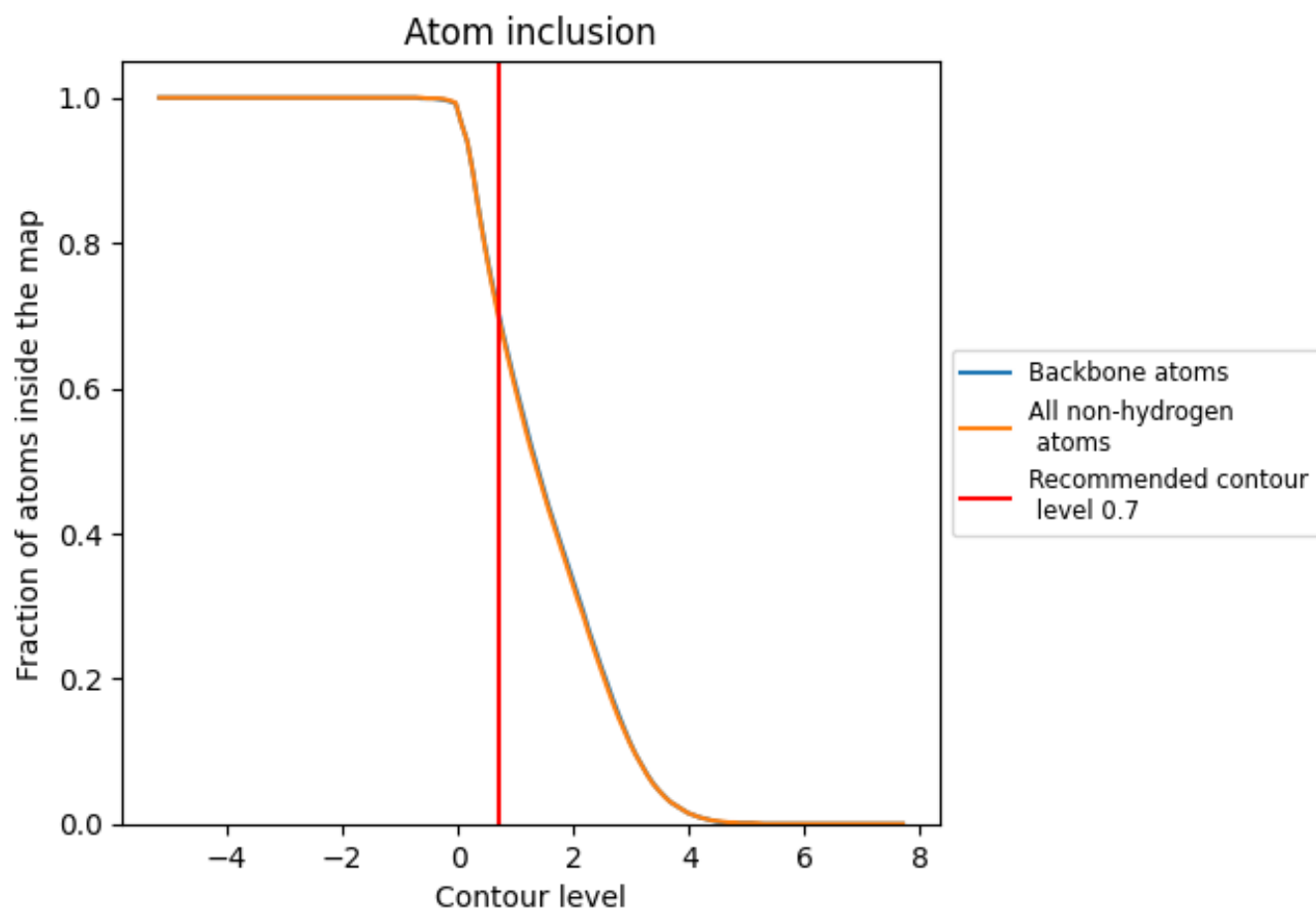
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).







































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 70% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6990	 0.4650
N	 0.9350	 0.5970
S	 0.0010	 0.1370
T	 0.0000	 0.0890
X	 0.2890	 0.2030
Y	 0.4360	 0.3030
Z	 0.7400	 0.4610
o	 0.8040	 0.5200
p	 0.8040	 0.5190
q	 0.8740	 0.5460
r	 0.1410	 0.1990
s	 0.8020	 0.5000
t	 0.8350	 0.5400
u	 0.3340	 0.2810
v	 0.8350	 0.5190
w	 0.7260	 0.4520
x	 0.8700	 0.5580
y	 0.8870	 0.5650
z	 0.7980	 0.4860

