



## wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 04:04 AM UTC

PDB ID : 8BWS / pdb\_00008bws  
EMDB ID : EMD-16299  
Title : Structure of yeast RNA Polymerase III elongation complex at 3.3 Å  
Authors : Nguyen, P.Q.; Fernandez-Tornero, C.  
Deposited on : 2022-12-07  
Resolution : 3.20 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:

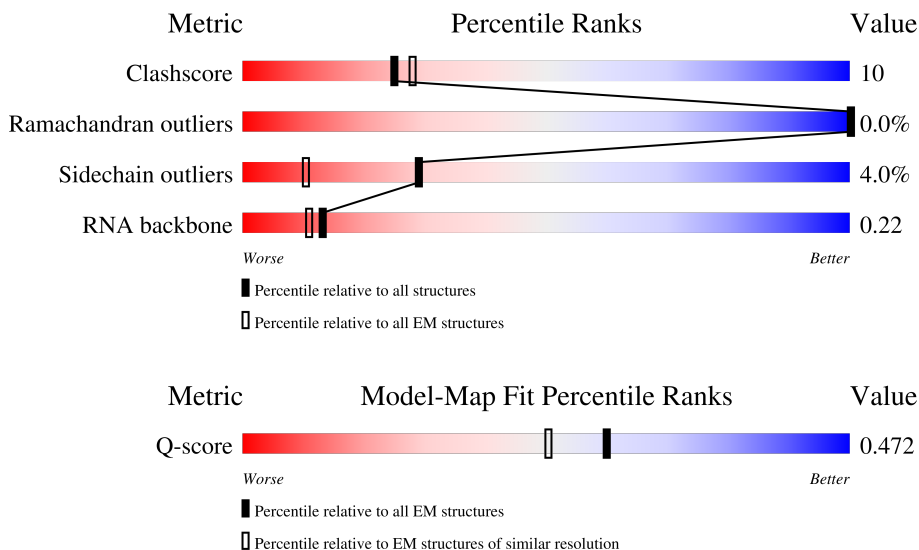
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 ( 2.70 - 3.70 )

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	1460	73% 24%
2	B	1149	67% 27%
3	C	335	73% 25%

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Mol	Chain	Length	Quality of chain
4	D	161	10% 54% 34% 11%
5	E	215	73% 27%
6	F	155	39% 14% 46%
7	G	212	9% 58% 31% 8%
8	H	146	5% 68% 27% 5%
9	I	110	7% 34% 15% 50%
10	J	70	67% 24%
11	K	142	64% 6% 29%
12	L	76	50% 14% 34%
13	M	282	9% 49% 16% 35%
14	N	422	16% 8% 75%
15	O	654	61% 24% 13%
16	P	317	31% 12% 57%
17	Q	251	5% 33% 12% 53%
18	S	52	15% 21% 63%
19	T	52	23% 25% 52%
20	R	10	50% 20% 30% 20% 30%

## 2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 41013 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1424	11145	7026	1968	2093	58	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1104	8715	5515	1502	1638	60	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	335	2655	1681	454	511	9	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	143	1169	745	197	221	6	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	215	1759	1116	310	321	12	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	83	671	429	114	125	3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	196	1569	1022	255	286	6	0	0

- Molecule 8 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		
8	H	138	1103	694	186	218	5	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	55	432	274	69	83	6	0	0

- Molecule 10 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		
10	J	67	549	350	95	98	6	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	101	792	496	130	161	5	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	50	381	235	76	66	4	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	183	1492	953	250	288	1	0	0

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	105	Total	C	N	O	S	0	0
			802	508	144	147	3		

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	568	Total	C	N	O	S	0	0
			4558	2897	784	858	19		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	137	Total	C	N	O	S	0	0
			1134	740	177	213	4		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	119	Total	C	N	O	S	0	0
			947	612	158	175	2		

- Molecule 18 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	19	Total	C	N	O	P	0	0
			402	187	89	107	19		

- Molecule 19 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	25	Total	C	N	O	P	0	0
			492	238	68	161	25		

- Molecule 20 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	7	Total	C	N	O	P	0	0
			158	70	35	46	7		

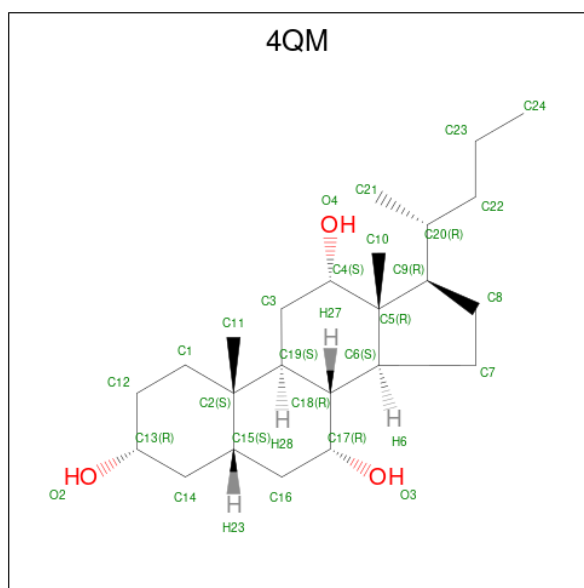
- Molecule 21 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
21	A	2	Total Zn 2 2	0
21	B	1	Total Zn 1 1	0
21	I	1	Total Zn 1 1	0
21	J	1	Total Zn 1 1	0
21	L	1	Total Zn 1 1	0

- Molecule 22 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total Mg 1 1	0

- Molecule 23 is (3R,5S,7R,8R,9S,10S,12S,13R,14S,17R)-10,13-dimethyl-17-[(2R)-pentan-2-yl]-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthrene-3,7,12-triol (CCD ID: 4QM) (formula: C<sub>24</sub>H<sub>42</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C O 27 24 3	0
23	C	1	Total C O 27 24 3	0

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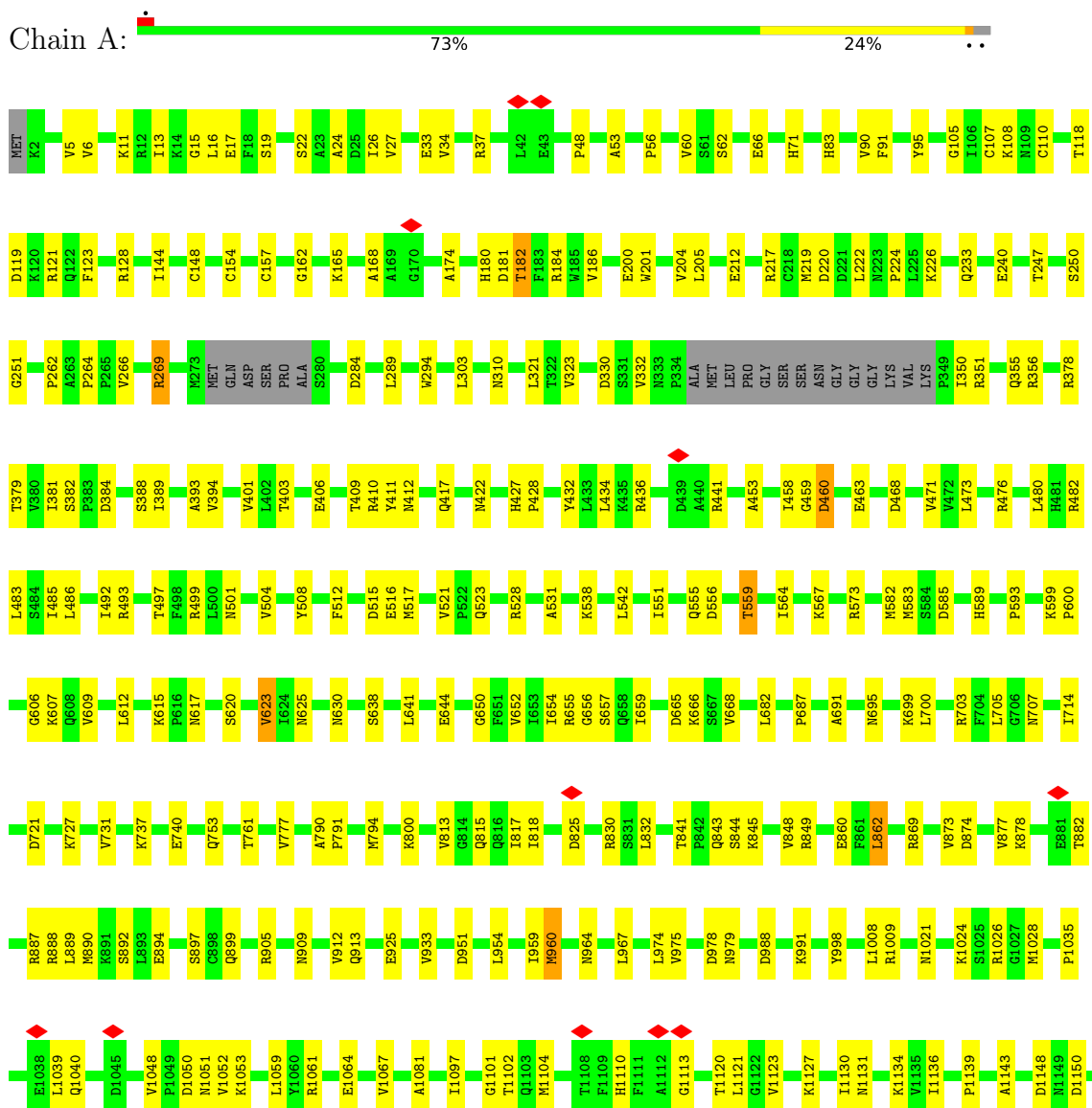
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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	I	1	27	24	3	0

### 3 Residue-property plots

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

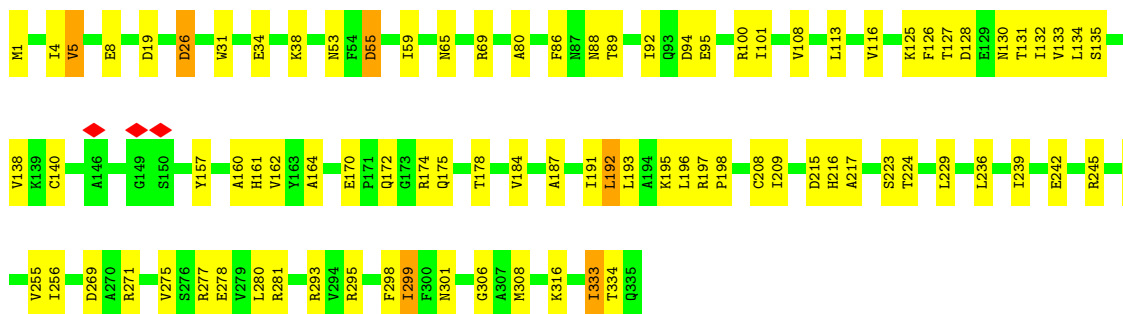
- Molecule 1: DNA-directed RNA polymerase III subunit RPC1



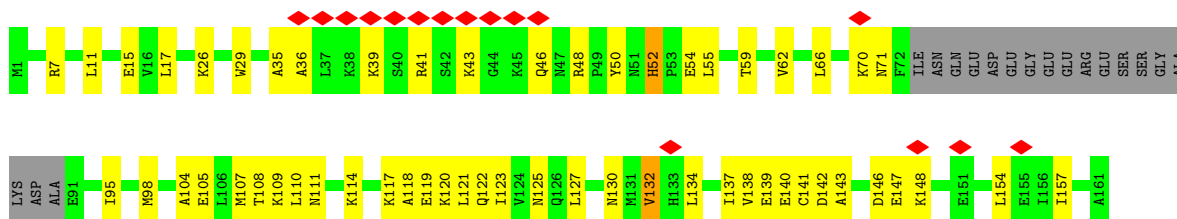




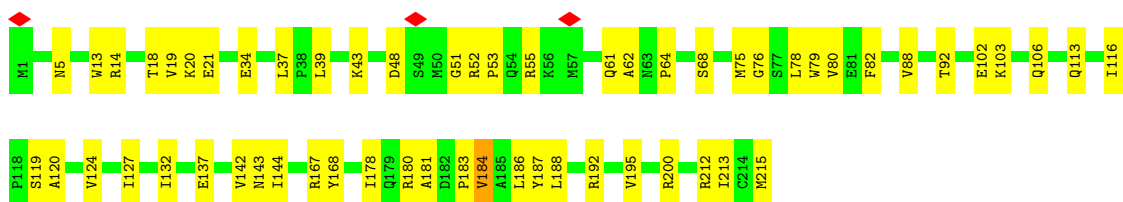
- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



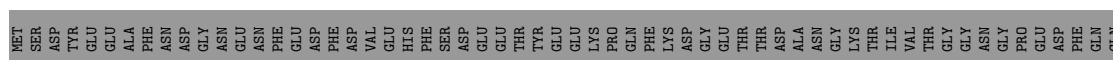
- Molecule 4: DNA-directed RNA polymerase III subunit RPC9



- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



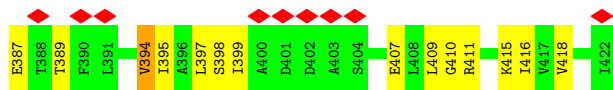
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



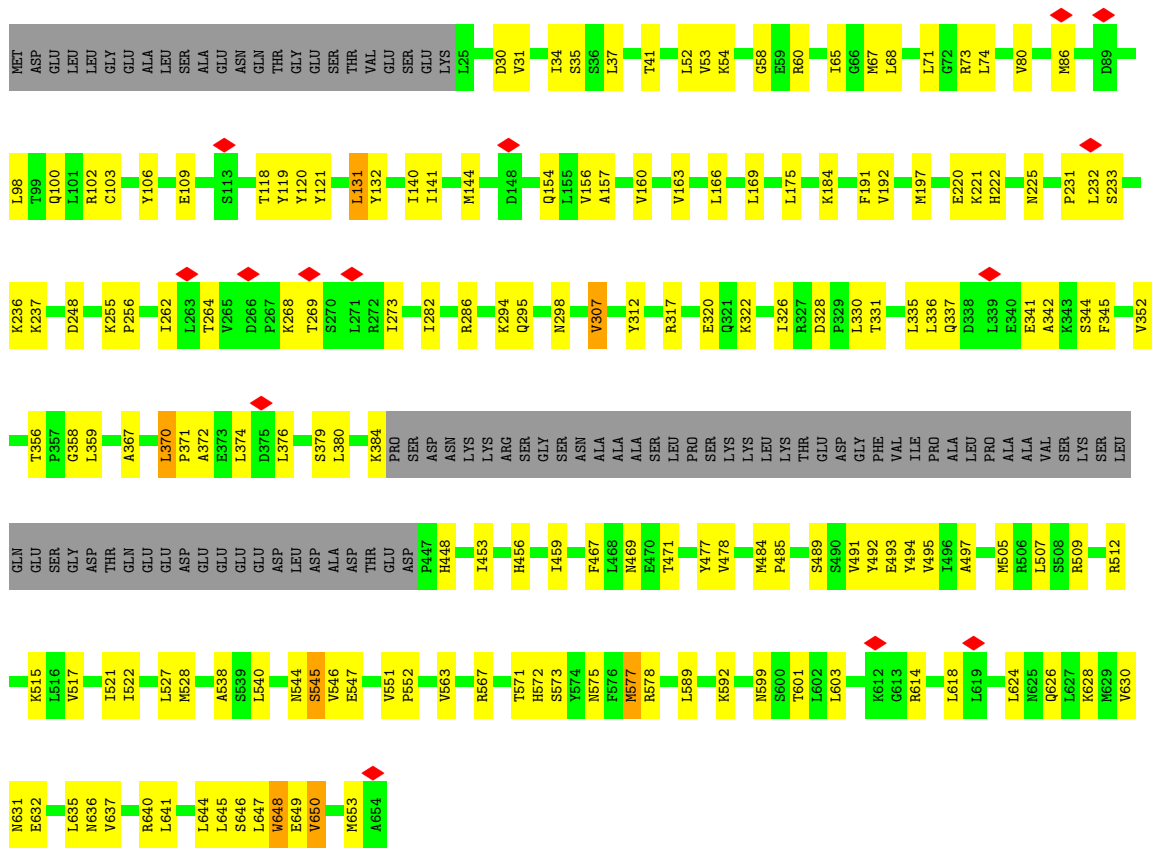
- Molecule 7: DNA-directed RNA polymerase III subunit RPC8



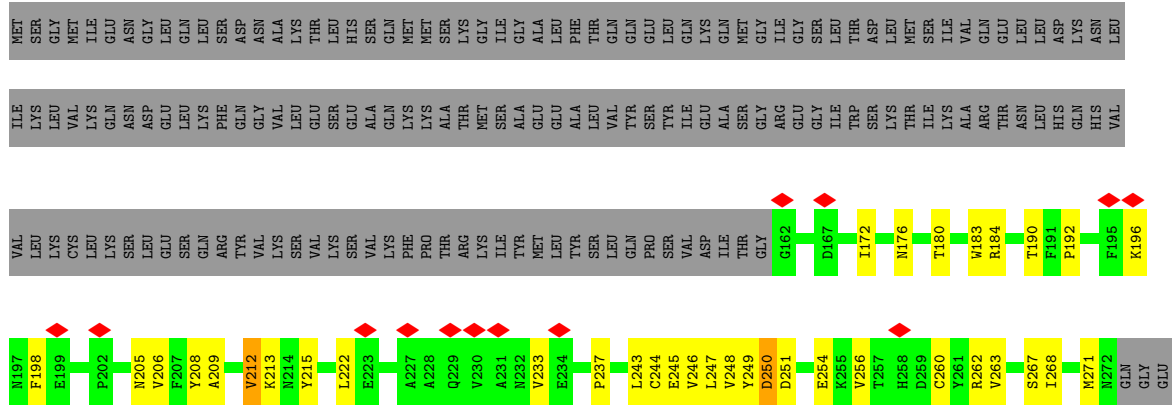




• Molecule 15: DNA-directed RNA polymerase III subunit RPC3



• Molecule 16: DNA-directed RNA polymerase III subunit RPC6





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101928	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS TALOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30.96	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.523	Depositor
Minimum map value	-1.351	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.252	Depositor
Map size (Å)	427.5, 427.5, 427.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.855, 0.855, 0.855	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: ZN, MG, 4QM

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	0.15	0/11344	0.30	0/15325
2	B	0.24	0/8867	0.38	0/11959
3	C	0.19	0/2711	0.34	0/3676
4	D	0.11	0/1187	0.28	0/1588
5	E	0.12	0/1795	0.28	0/2416
6	F	0.32	0/683	0.49	0/923
7	G	0.22	0/1609	0.39	0/2184
8	H	0.13	0/1121	0.30	0/1517
9	I	0.18	0/440	0.43	0/594
10	J	0.41	0/558	0.54	1/750 (0.1%)
11	K	0.24	0/803	0.35	0/1083
12	L	0.11	0/353	0.29	0/468
13	M	0.10	0/1524	0.31	0/2061
14	N	0.13	0/810	0.34	0/1088
15	O	0.13	0/4627	0.31	0/6243
16	P	0.10	0/1165	0.27	0/1582
17	Q	0.31	0/969	0.58	3/1307 (0.2%)
18	S	0.28	0/455	0.47	0/702
19	T	0.35	0/543	0.60	0/832
20	R	0.14	0/178	0.41	0/277
All	All	0.19	0/41742	0.35	4/56575 (0.0%)

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
2	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	61	PHE	N-CA-C	-6.67	101.28	110.35
17	Q	57	LYS	N-CA-C	-5.77	106.22	113.20
17	Q	58	TYR	N-CA-C	-5.65	106.93	113.88
10	J	8	PHE	CA-CB-CG	5.09	118.89	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	227	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11145	0	11269	232	0
2	B	8715	0	8835	199	0
3	C	2655	0	2628	63	0
4	D	1169	0	1189	49	0
5	E	1759	0	1788	39	0
6	F	671	0	692	19	0
7	G	1569	0	1551	57	0
8	H	1103	0	1079	26	0
9	I	432	0	430	20	0
10	J	549	0	560	13	0
11	K	792	0	790	11	0
12	L	381	0	383	11	0
13	M	1492	0	1456	38	0
14	N	802	0	851	31	0
15	O	4558	0	4735	105	0
16	P	1134	0	1085	27	0
17	Q	947	0	950	32	0
18	S	402	0	210	10	0
19	T	492	0	287	10	0
20	R	158	0	77	2	0
21	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	B	1	0	0	0	0
21	I	1	0	0	0	0
21	J	1	0	0	0	0
21	L	1	0	0	0	0
22	A	1	0	0	0	0
23	A	27	0	0	0	0
23	C	27	0	0	0	0
23	I	27	0	0	0	0
All	All	41013	0	40845	854	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 854 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)
10:J:10:CYS:SG	10:J:45:CYS:SG	2.66	0.93
9:I:32:GLU:HB2	13:M:132:ASN:HB2	1.54	0.90
9:I:26:CYS:O	9:I:29:CYS:SG	2.32	0.88
13:M:132:ASN:HD21	13:M:135:LYS:HB2	1.45	0.82
9:I:5:CYS:SG	9:I:8:CYS:HB3	2.21	0.80

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1416/1460 (97%)	1323 (93%)	93 (7%)	0	100   100
2	B	1100/1149 (96%)	1016 (92%)	83 (8%)	1 (0%)	48   79
3	C	333/335 (99%)	304 (91%)	29 (9%)	0	100   100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	139/161 (86%)	124 (89%)	15 (11%)	0	100	100
5	E	213/215 (99%)	201 (94%)	12 (6%)	0	100	100
6	F	81/155 (52%)	77 (95%)	4 (5%)	0	100	100
7	G	192/212 (91%)	167 (87%)	25 (13%)	0	100	100
8	H	134/146 (92%)	125 (93%)	9 (7%)	0	100	100
9	I	53/110 (48%)	45 (85%)	8 (15%)	0	100	100
10	J	65/70 (93%)	61 (94%)	4 (6%)	0	100	100
11	K	99/142 (70%)	91 (92%)	8 (8%)	0	100	100
12	L	42/76 (55%)	40 (95%)	2 (5%)	0	100	100
13	M	179/282 (64%)	161 (90%)	18 (10%)	0	100	100
14	N	101/422 (24%)	83 (82%)	18 (18%)	0	100	100
15	O	564/654 (86%)	533 (94%)	31 (6%)	0	100	100
16	P	133/317 (42%)	125 (94%)	8 (6%)	0	100	100
17	Q	115/251 (46%)	108 (94%)	7 (6%)	0	100	100
All	All	4959/6157 (80%)	4584 (92%)	374 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	503	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	
1	A	1230/1257 (98%)	1183 (96%)	47 (4%)	29	62
2	B	966/1006 (96%)	916 (95%)	50 (5%)	21	54
3	C	296/296 (100%)	286 (97%)	10 (3%)	32	64
4	D	131/145 (90%)	129 (98%)	2 (2%)	57	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	197/197 (100%)	194 (98%)	3 (2%)	57	76
6	F	73/137 (53%)	68 (93%)	5 (7%)	14	46
7	G	170/190 (90%)	161 (95%)	9 (5%)	20	53
8	H	121/128 (94%)	119 (98%)	2 (2%)	53	75
9	I	51/98 (52%)	50 (98%)	1 (2%)	48	72
10	J	62/65 (95%)	58 (94%)	4 (6%)	15	47
11	K	91/130 (70%)	89 (98%)	2 (2%)	45	71
12	L	39/57 (68%)	38 (97%)	1 (3%)	40	69
13	M	159/249 (64%)	157 (99%)	2 (1%)	61	78
14	N	88/360 (24%)	80 (91%)	8 (9%)	9	34
15	O	521/593 (88%)	501 (96%)	20 (4%)	29	62
16	P	127/285 (45%)	123 (97%)	4 (3%)	35	66
17	Q	105/212 (50%)	99 (94%)	6 (6%)	18	51
All	All	4427/5405 (82%)	4251 (96%)	176 (4%)	29	61

5 of 176 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	137	TYR
14	N	389	THR
7	G	42	VAL
10	J	7	CYS
15	O	307	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	69	ASN
14	N	288	GLN
8	H	33	GLN
10	J	23	ASN
15	O	544	ASN

### 5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	R	6/10 (60%)	4 (66%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	R	5	A
20	R	6	G
20	R	8	G
20	R	9	G

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 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	$\# Z  > 2$
23	4QM	I	2001	-	30,30,30	0.44	0	47,48,48	0.52	0
23	4QM	C	2001	-	30,30,30	0.41	0	47,48,48	0.58	0
23	4QM	A	1504	-	30,30,30	0.42	0	47,48,48	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	4QM	I	2001	-	-	7/7/72/72	0/4/4/4
23	4QM	C	2001	-	-	6/7/72/72	0/4/4/4
23	4QM	A	1504	-	-	6/7/72/72	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

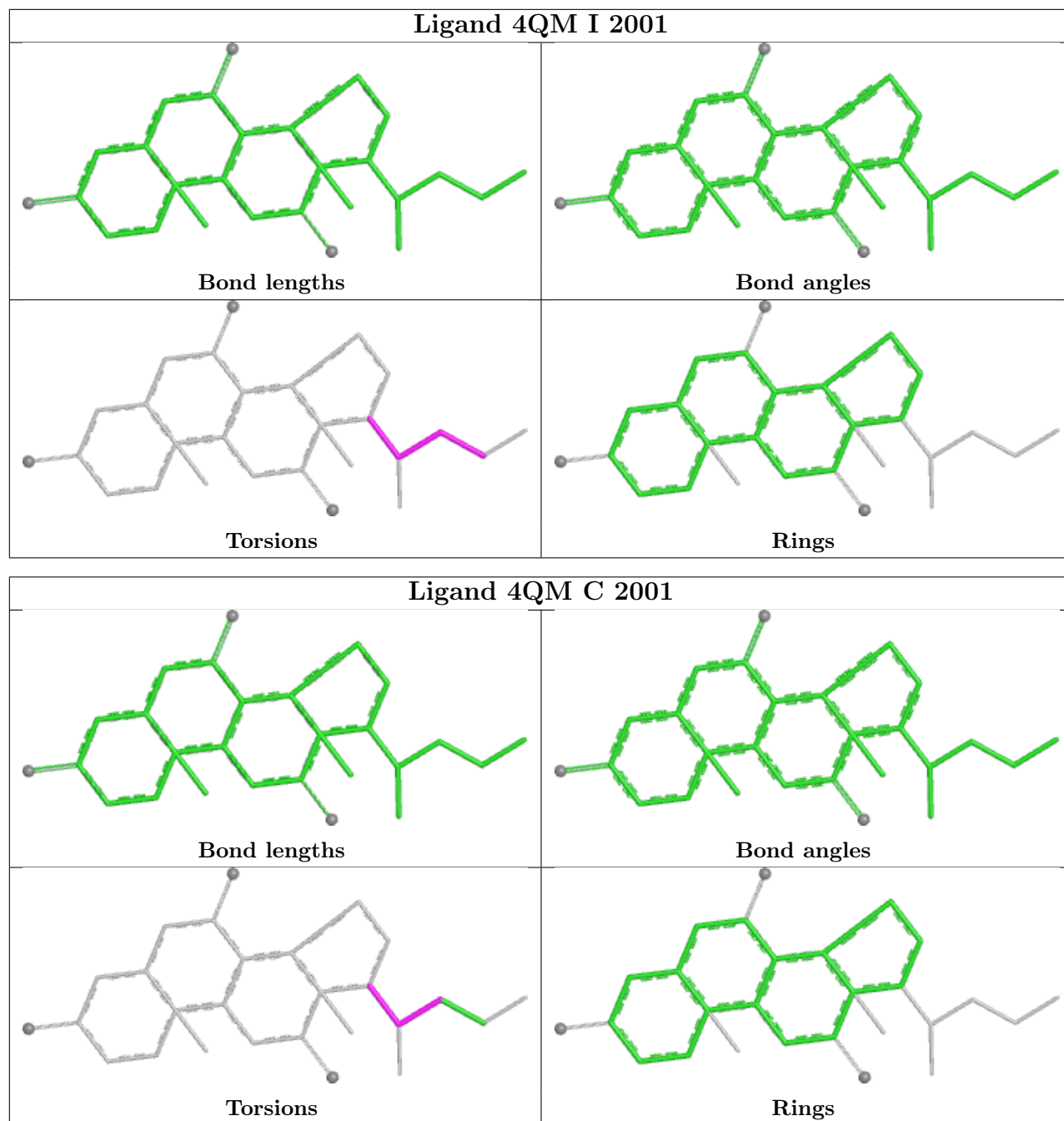
5 of 19 torsion outliers are listed below:

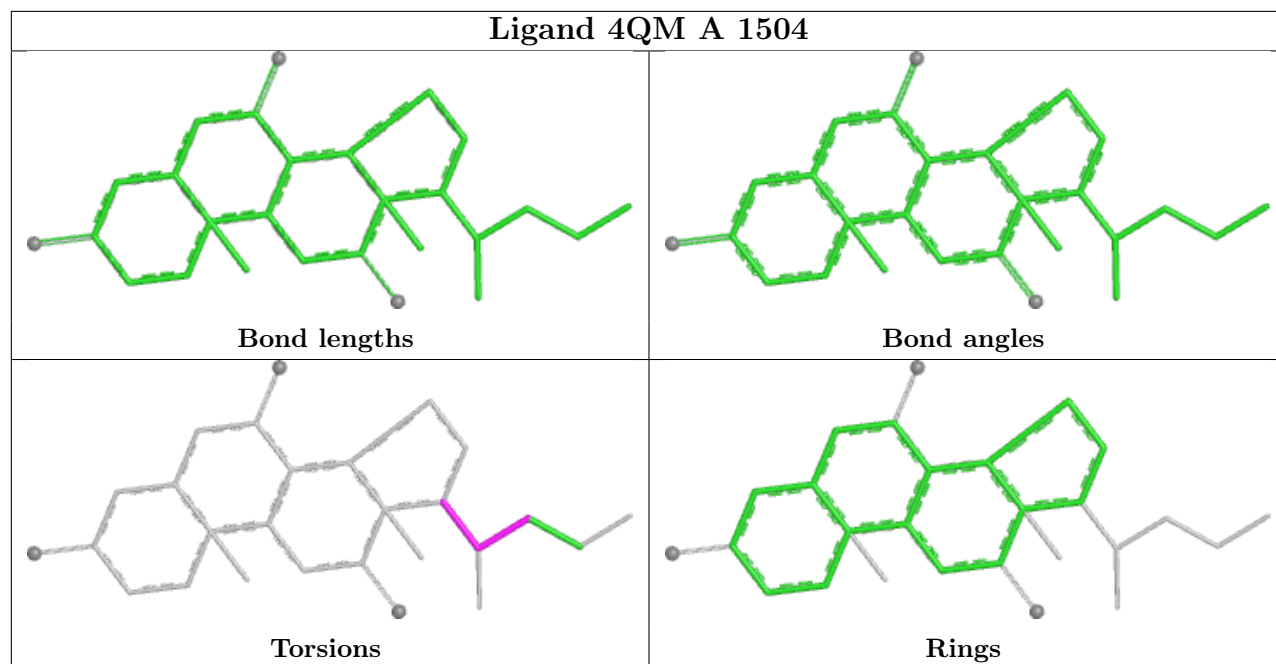
Mol	Chain	Res	Type	Atoms
23	A	1504	4QM	C21-C20-C9-C5
23	A	1504	4QM	C21-C20-C9-C8
23	C	2001	4QM	C21-C20-C9-C5
23	A	1504	4QM	C22-C20-C9-C8
23	A	1504	4QM	C22-C20-C9-C5

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.

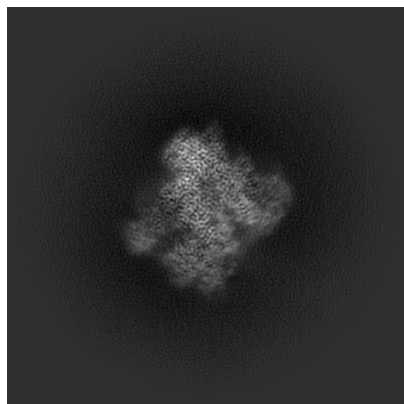
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16299. These allow visual inspection of the internal detail of the map and identification of artifacts.

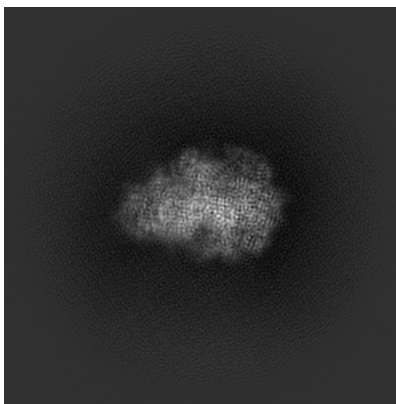
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

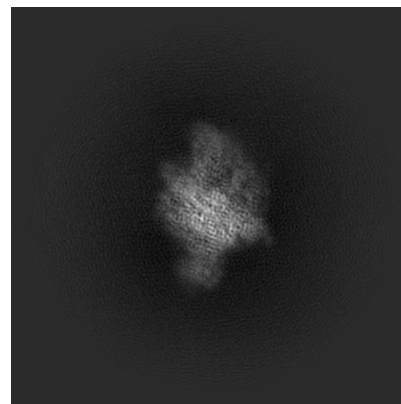
#### 6.1.1 Primary map



X

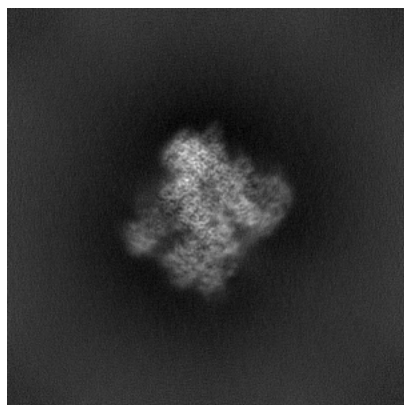


Y

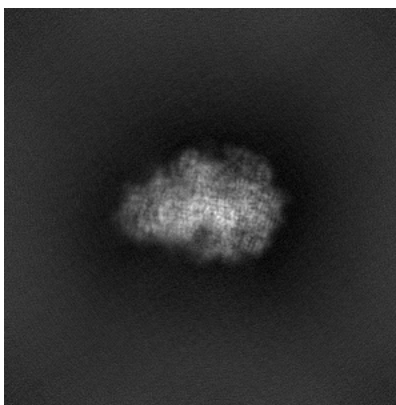


Z

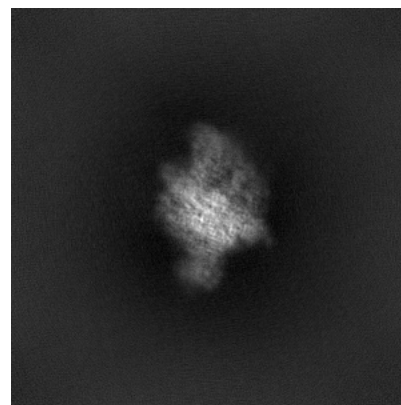
#### 6.1.2 Raw map



X



Y

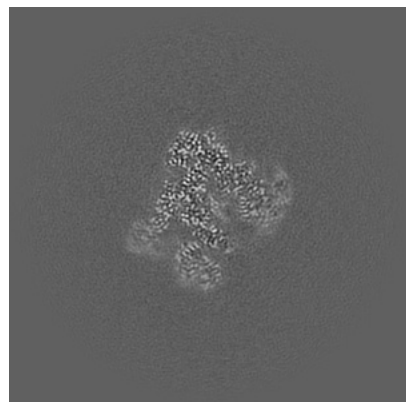


Z

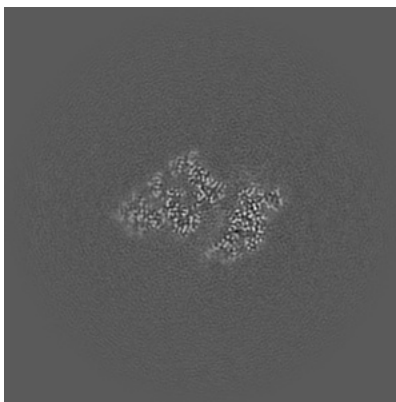
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

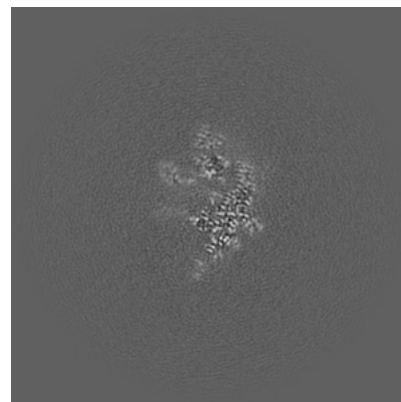
### 6.2.1 Primary map



X Index: 250

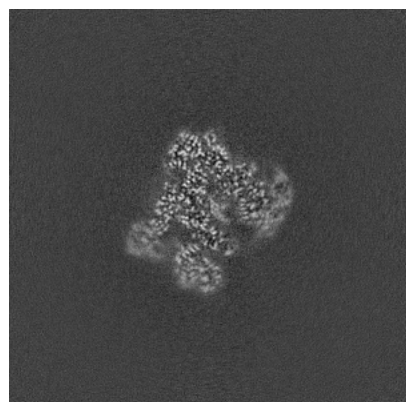


Y Index: 250

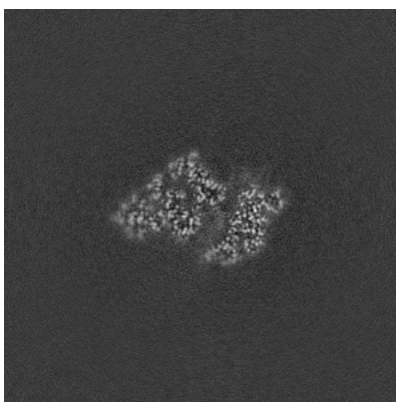


Z Index: 250

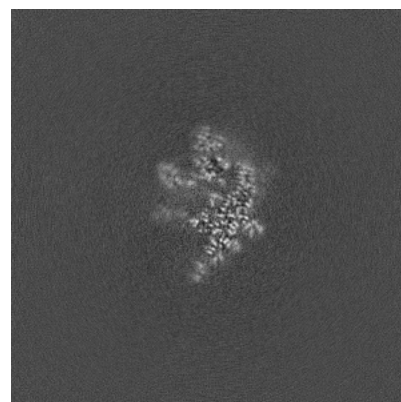
### 6.2.2 Raw map



X Index: 250



Y Index: 250

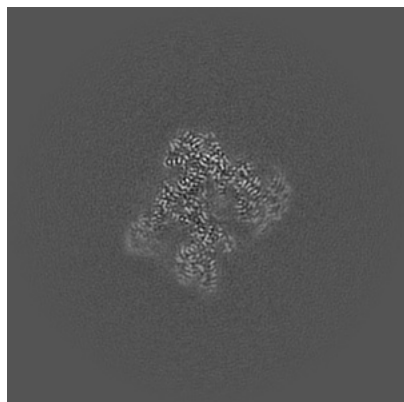


Z Index: 250

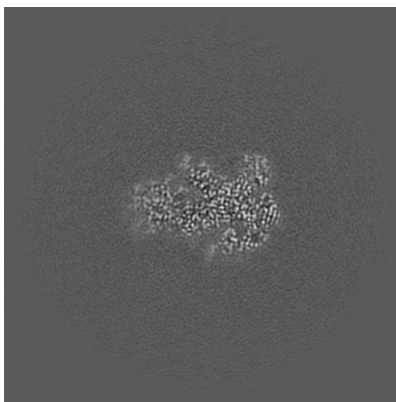
The images above show central slices of the map in three orthogonal directions.

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

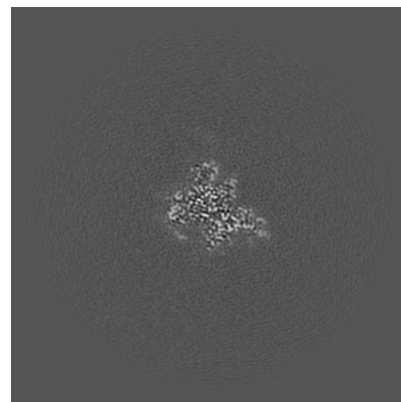
### 6.3.1 Primary map



X Index: 247

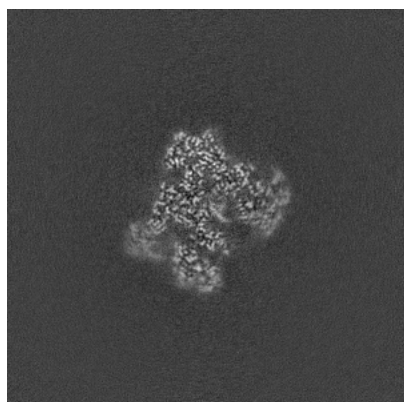


Y Index: 234

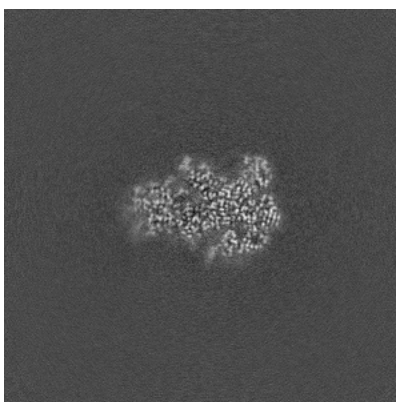


Z Index: 302

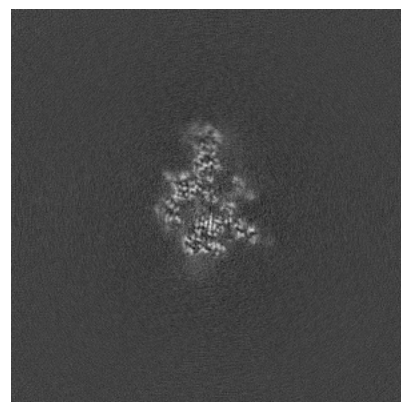
### 6.3.2 Raw map



X Index: 252



Y Index: 234

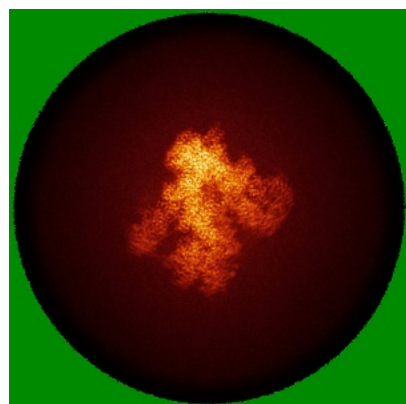


Z Index: 273

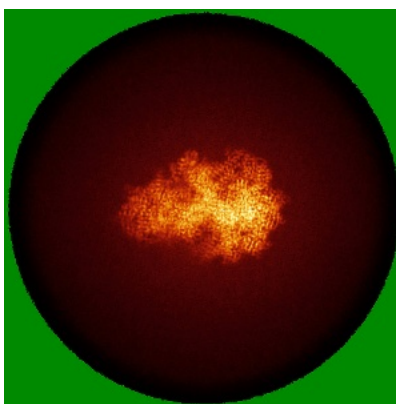
The images above show the largest variance slices of the map in three orthogonal directions.

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

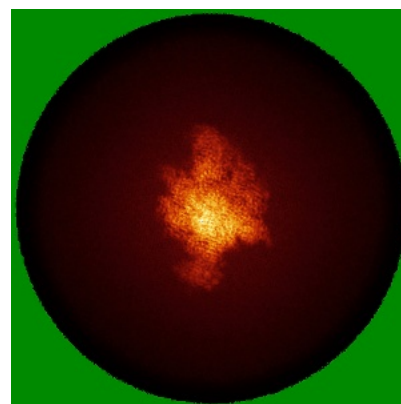
### 6.4.1 Primary map



X

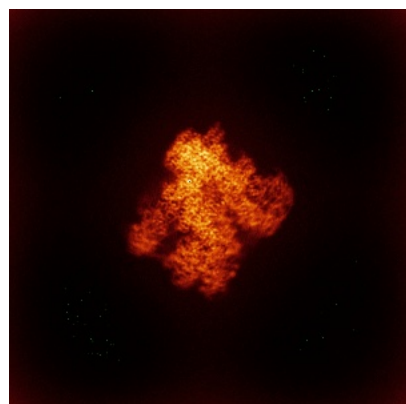


Y

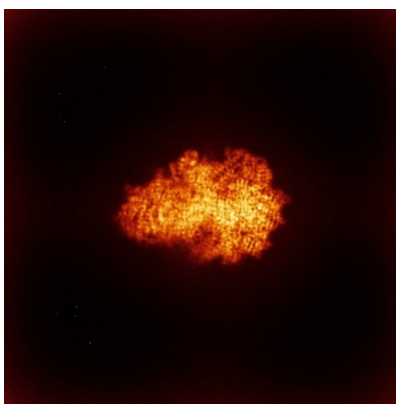


Z

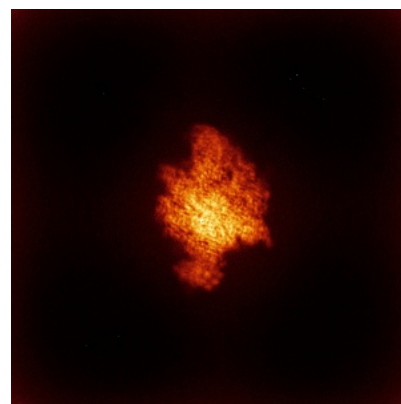
### 6.4.2 Raw map



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.

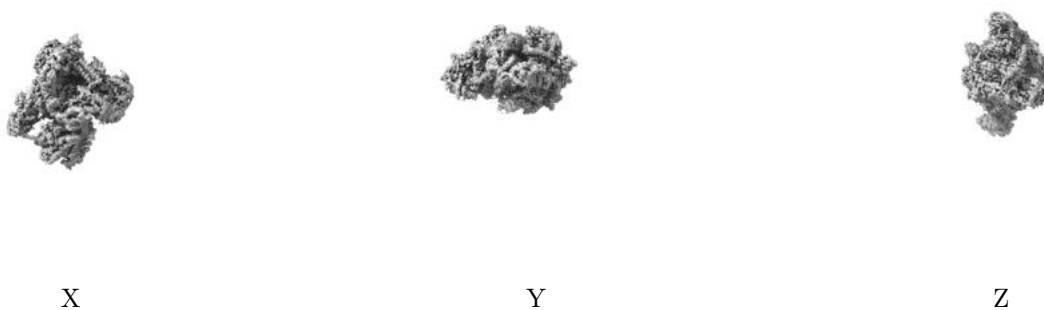
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.252. 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.

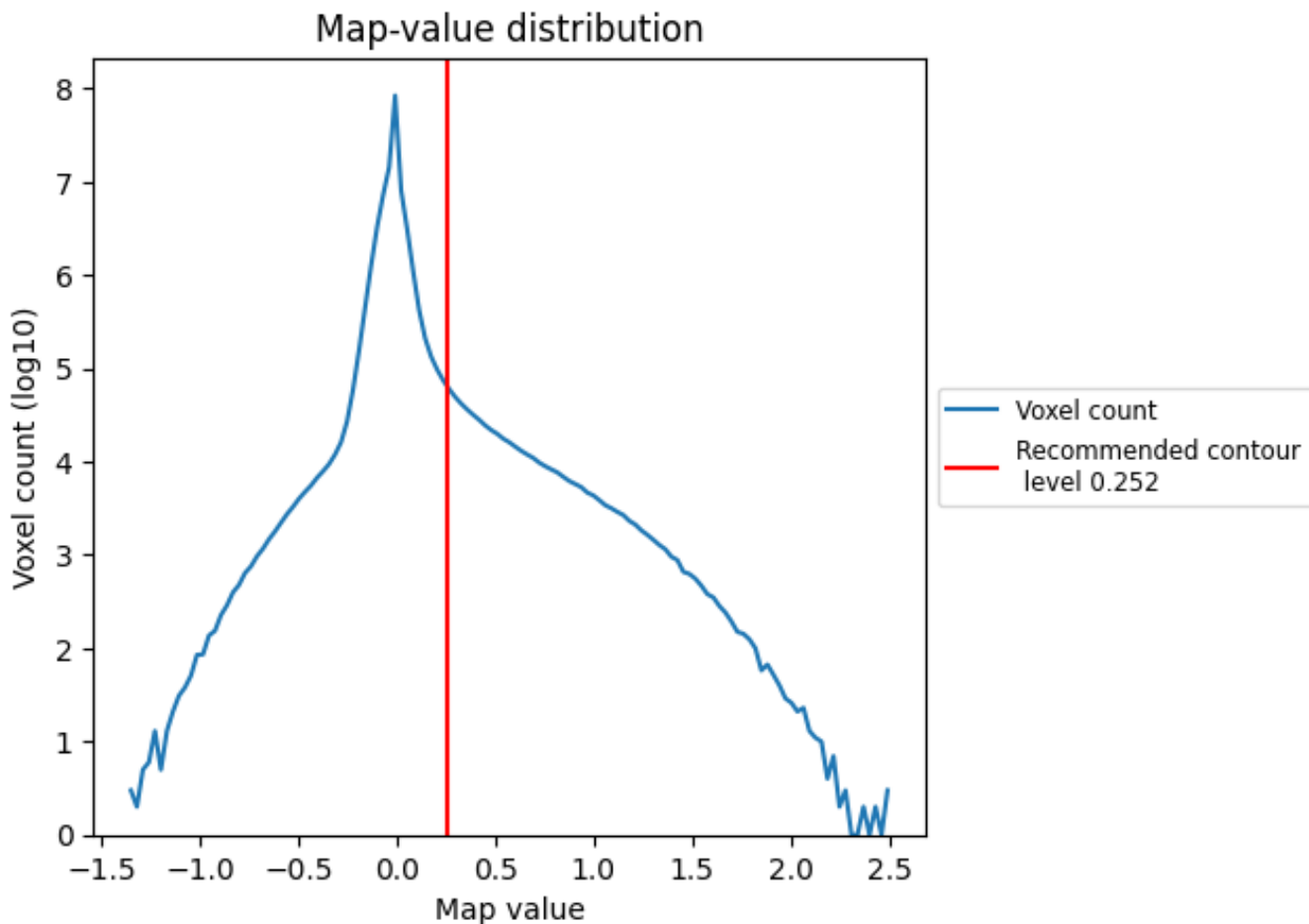
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

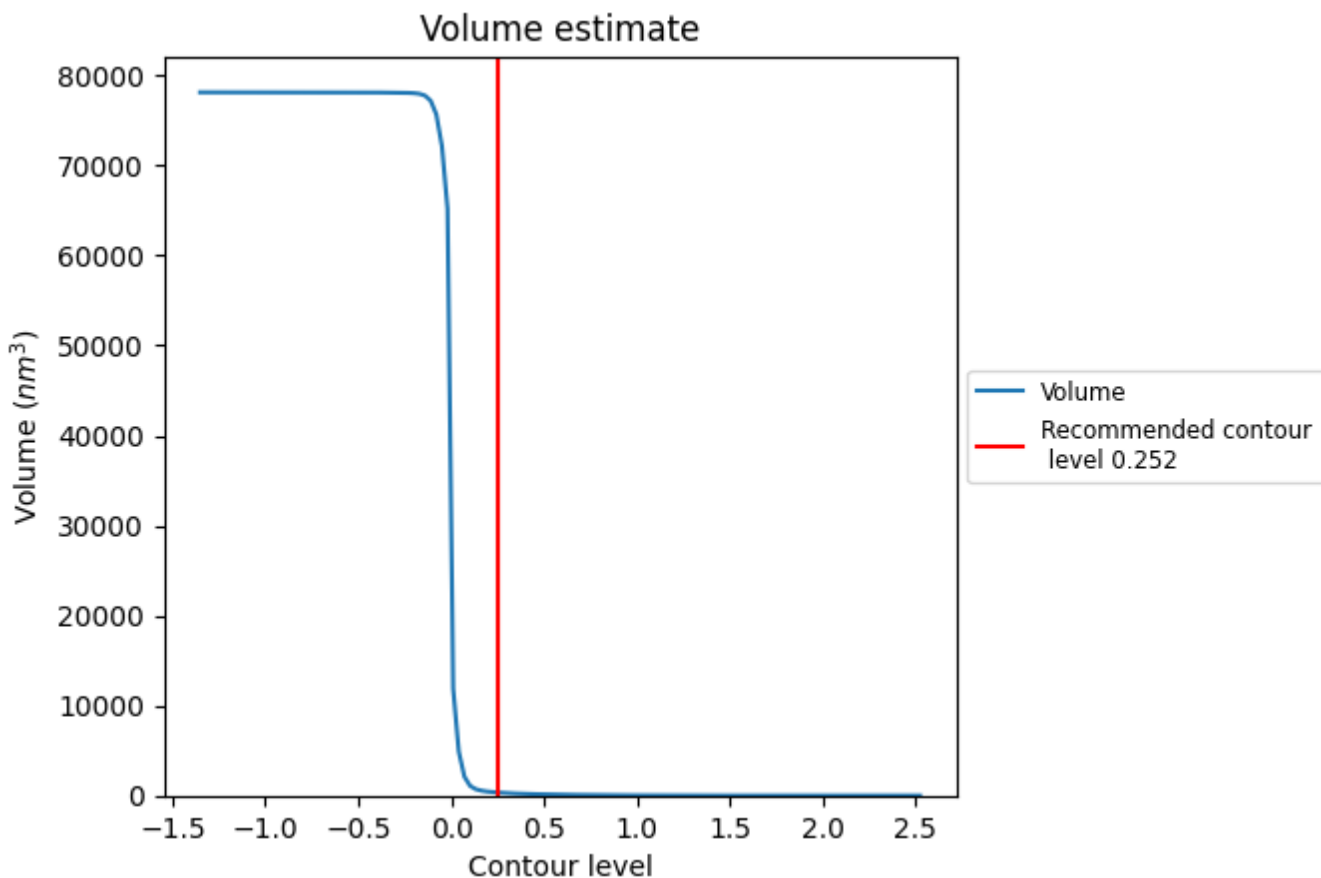
This section contains the results of statistical analysis of the map.

### 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.

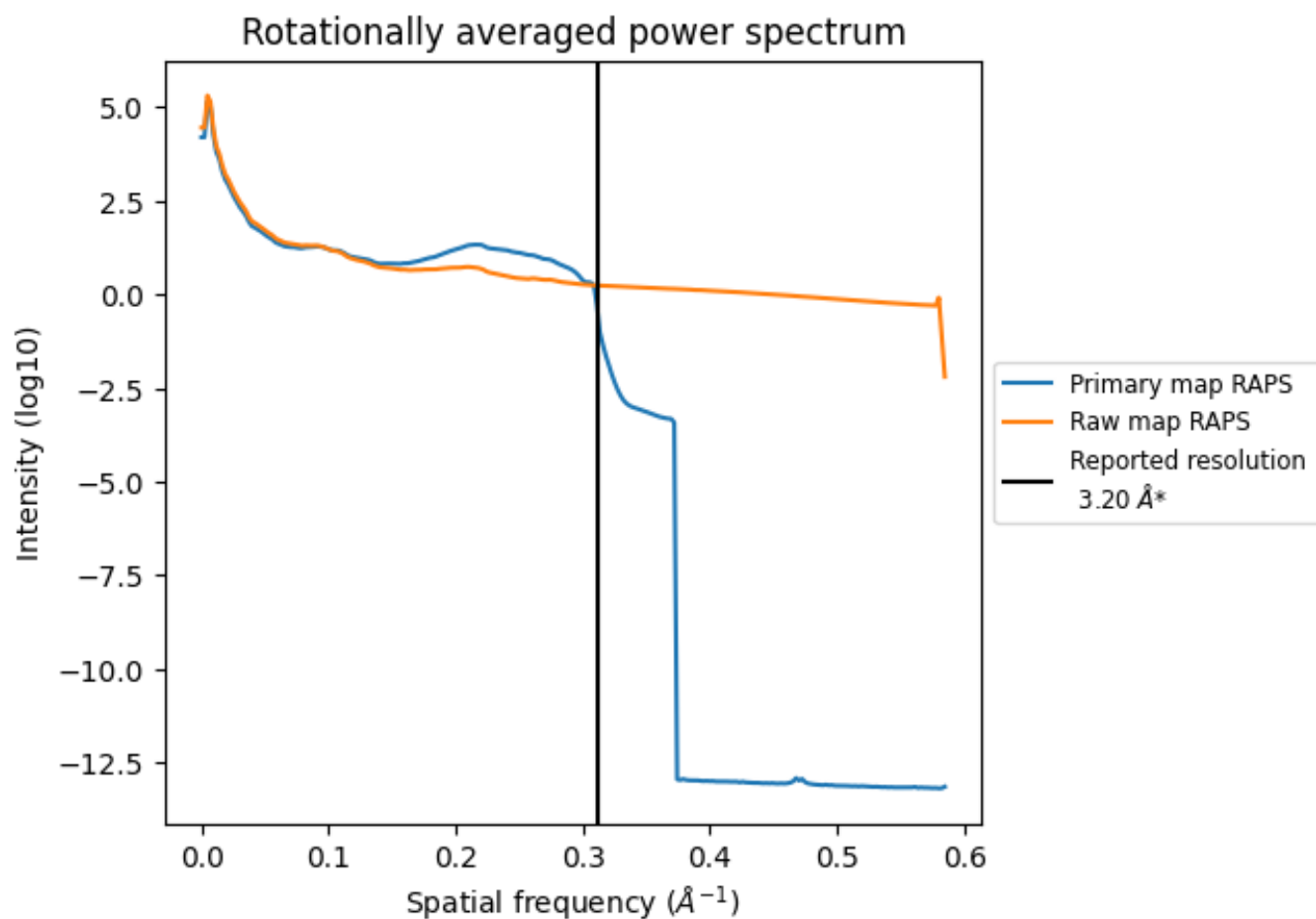
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 333 nm<sup>3</sup>; this corresponds to an approximate mass of 301 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](#)

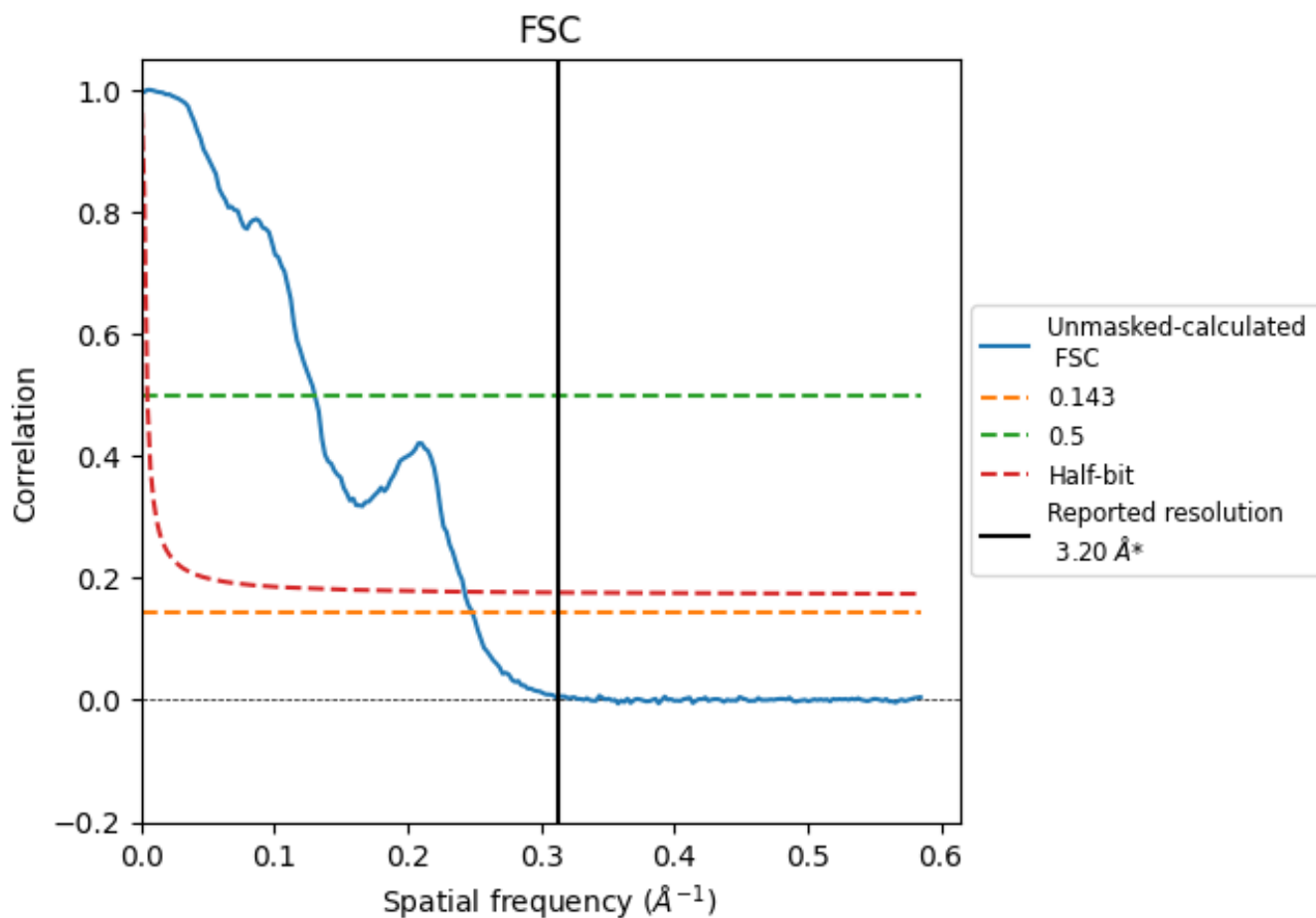


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

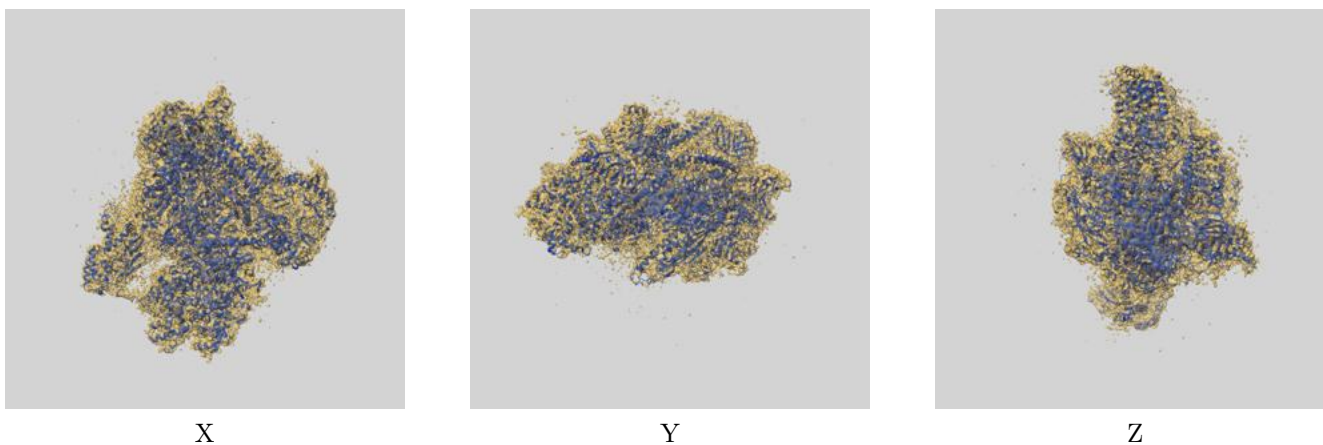
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	3.20	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.02	7.67	4.12

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.5 CUT-OFF 7.67 differs from the reported value 3.2 by more than 10 %

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

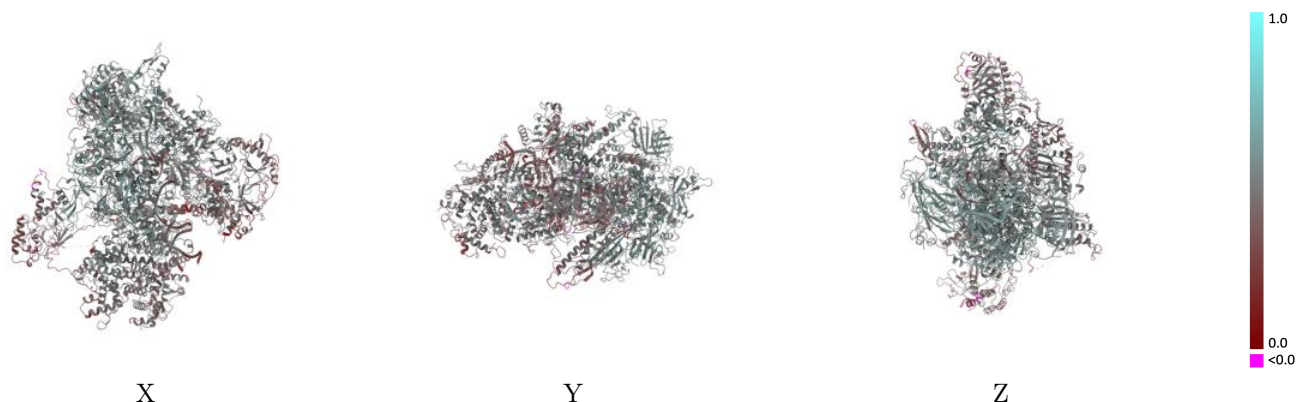
This section contains information regarding the fit between EMDB map EMD-16299 and PDB model 8BWS. Per-residue inclusion information can be found in section [3](#) on page [9](#).

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



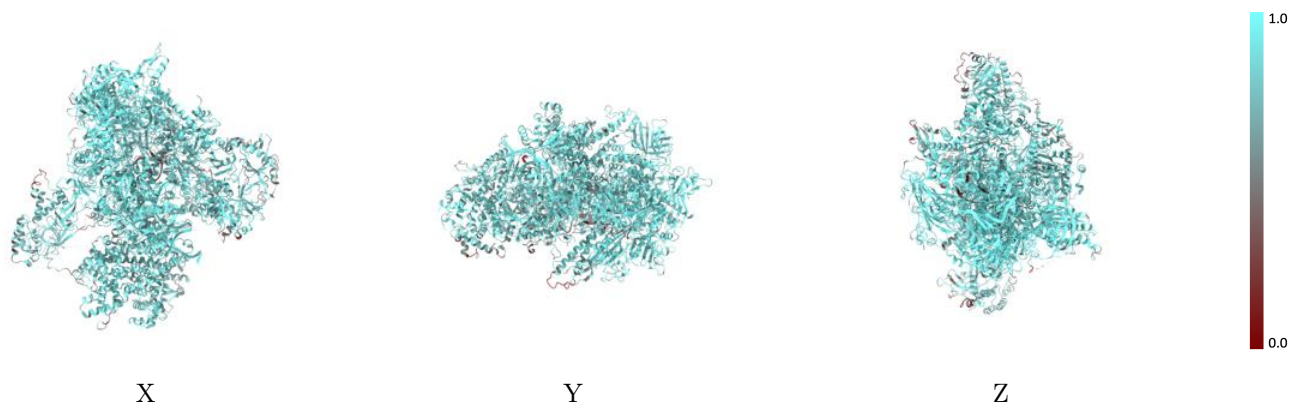
The images above show the 3D surface view of the map at the recommended contour level 0.252 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



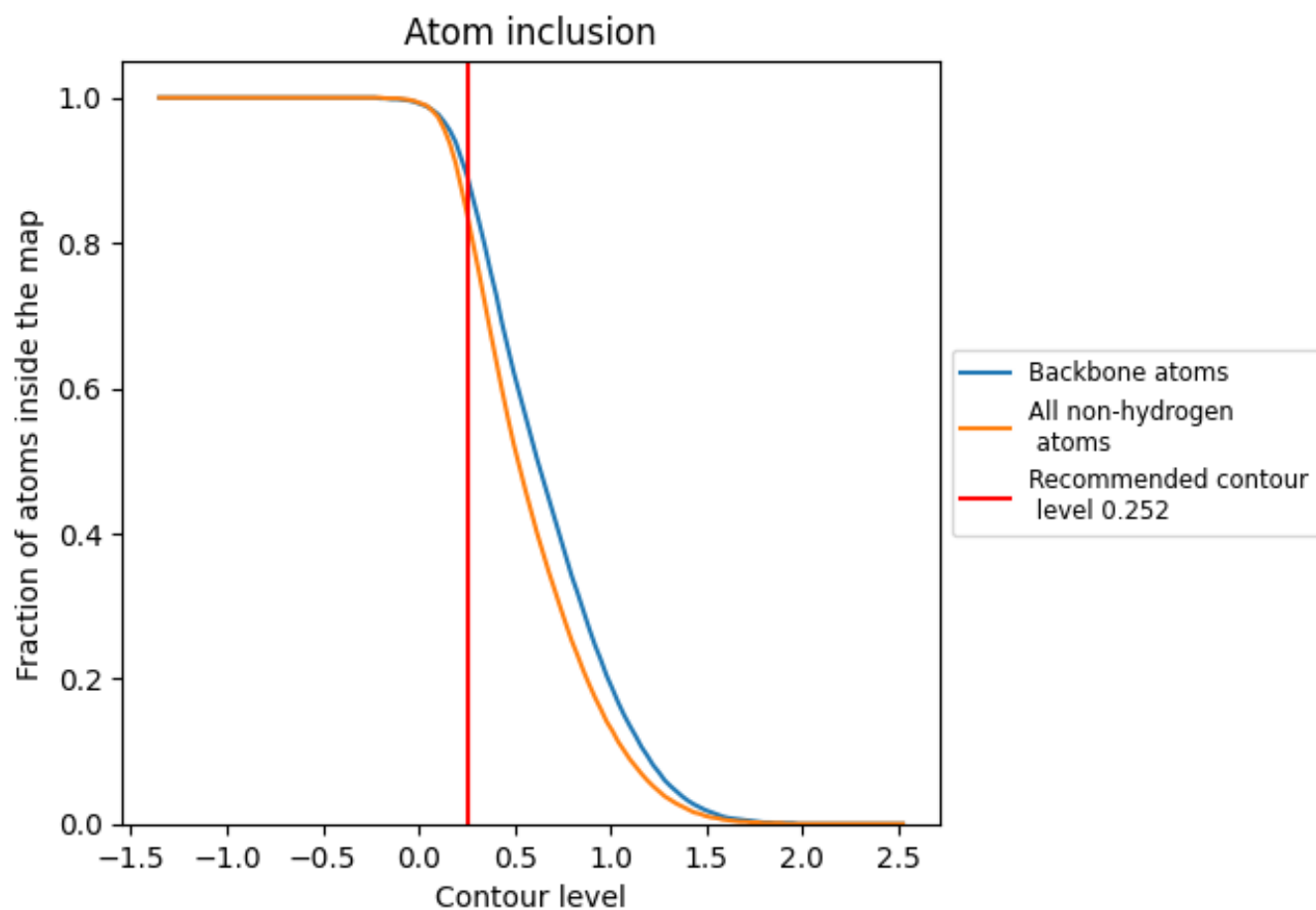
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.252).











































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% 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 (0.252) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8410	 0.4720
A	 0.8750	 0.5010
B	 0.8660	 0.4990
C	 0.9060	 0.5130
D	 0.7120	 0.3430
E	 0.8570	 0.4770
F	 0.9030	 0.5300
G	 0.7790	 0.4130
H	 0.8790	 0.4920
I	 0.7140	 0.3750
J	 0.9290	 0.5290
K	 0.9040	 0.5180
L	 0.8730	 0.5030
M	 0.7110	 0.3750
N	 0.7110	 0.3820
O	 0.8270	 0.4550
P	 0.7320	 0.4120
Q	 0.7480	 0.4240
R	 0.2720	 0.3110
S	 0.8580	 0.3800
T	 0.7540	 0.3500

