



# wwPDB EM Validation Summary Report ⓘ

May 18, 2026 – 05:05 pm BST

PDB ID : 9QEB / pdb\_00009qeb  
EMDB ID : EMD-53053  
Title : CryoEM structure of transcribing RNA polymerase II elongation complex  
Authors : Yi, G.; Li, Q.; Wang, D.; Zhang, P.  
Deposited on : 2025-03-08  
Resolution : 2.26 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:

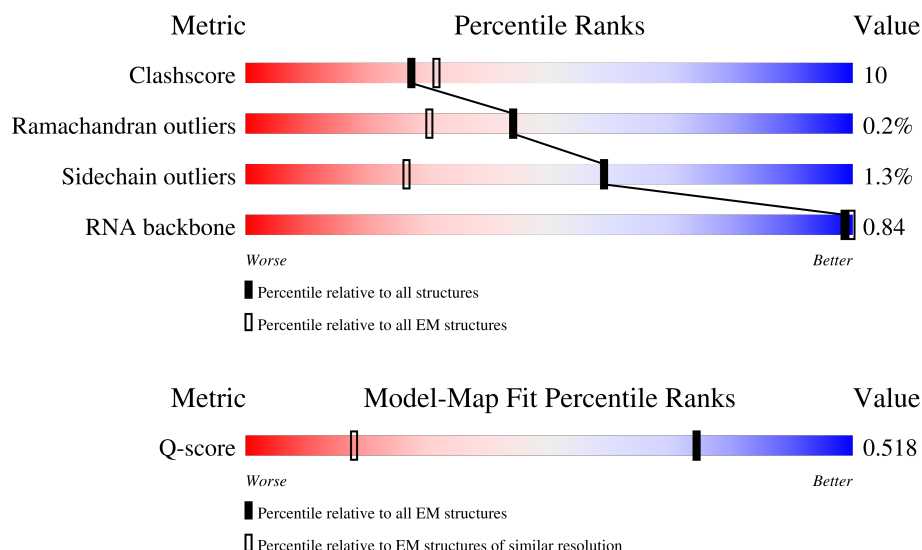
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using 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 2.26 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	3535 ( 1.76 - 2.76 )

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	1733	
2	B	1224	
3	C	318	

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Mol	Chain	Length	Quality of chain
4	D	221	<p>64% 56% 19% 24%</p>
5	E	215	<p>90% 9%</p>
6	F	155	<p>42% 11% 46%</p>
7	G	171	<p>62% 79% 21%</p>
8	H	146	<p>79% 12% 8%</p>
9	I	122	<p>82% 57% 34% 8%</p>
10	J	70	<p>69% 24% 7%</p>
11	K	120	<p>82% 11% 7%</p>
12	L	70	<p>11% 21% 31% 10% 36%</p>
13	N	44	<p>57% 36% 64%</p>
14	R	9	<p>33% 67%</p>
15	T	44	<p>36% 55% 45%</p>

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 33807 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1390	Total	C	N	O	S	0	0
			10942	6911	1913	2056	62		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1150	Total	C	N	O	S	0	0
			9155	5787	1602	1711	55		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	266	Total	C	N	O	S	0	0
			2095	1317	348	417	13		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	167	Total	C	N	O	S	0	0
			1327	821	230	273	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1744	1107	308	318	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			670	428	114	125	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	134	Total	C	N	O	S	0	0
			1077	679	182	212	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	112	Total	C	N	O	S	0	0
			909	561	164	173	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	112	Total	C	N	O	S	0	0
			904	580	154	168	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			359	221	71	63	4		

- Molecule 13 is a DNA chain called DNA (44-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	44	Total	C	N	O	P	0	0
			914	431	181	258	44		

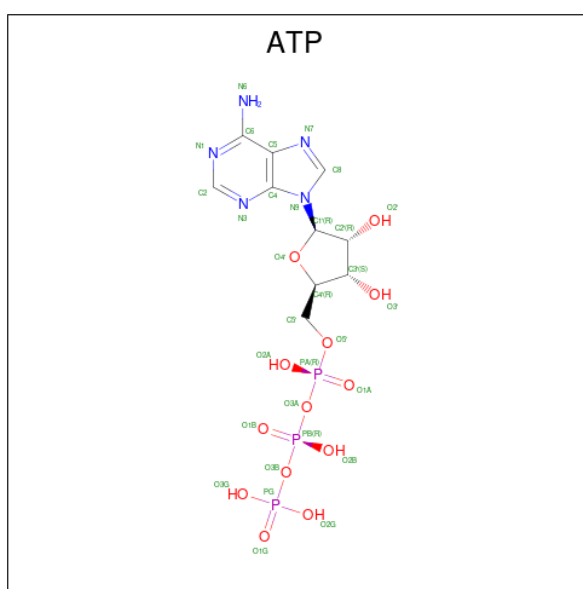
- Molecule 14 is a RNA chain called RNA (5'-R(P\*AP\*UP\*CP\*GP\*AP\*GP\*AP\*GP\*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	9	Total	C	N	O	P	0	0
			197	88	40	60	9		

- Molecule 15 is a DNA chain called DNA (44-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	44	Total	C	N	O	P	0	0
			879	421	140	274	44		

- Molecule 16 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
17	A	2	Total	Mg	0
			2	2	

- Molecule 18 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	K	0
			1	1	

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		AltConf
20	A	275	Total	O	0
			275	275	
20	B	229	Total	O	0
			229	229	
20	C	63	Total	O	0
			63	63	
20	E	27	Total	O	0
			27	27	
20	F	14	Total	O	0
			14	14	
20	H	11	Total	O	0
			11	11	
20	J	19	Total	O	0
			19	19	
20	K	32	Total	O	0
			32	32	
20	L	6	Total	O	0
			6	6	
20	R	20	Total	O	0
			20	20	

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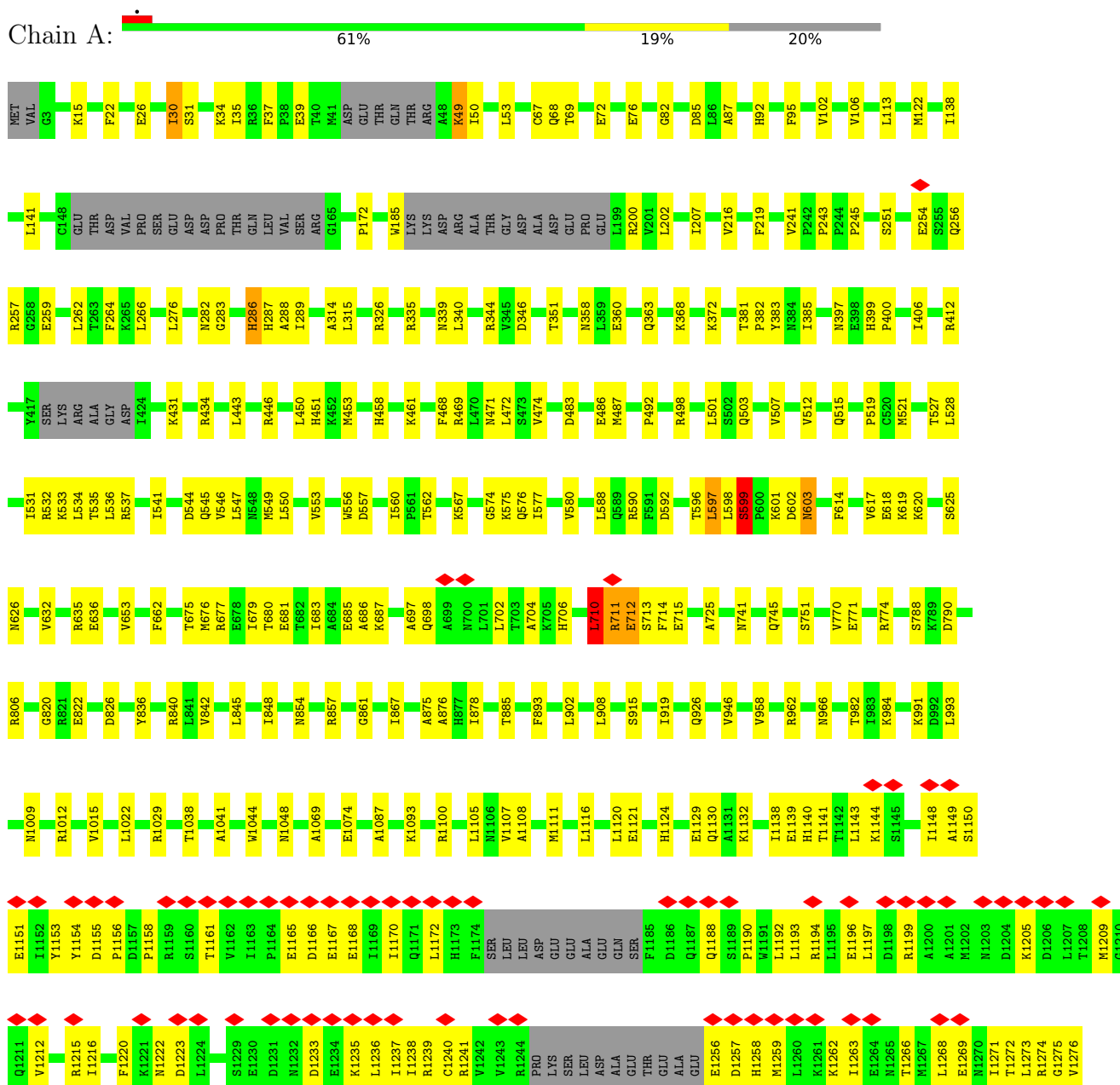
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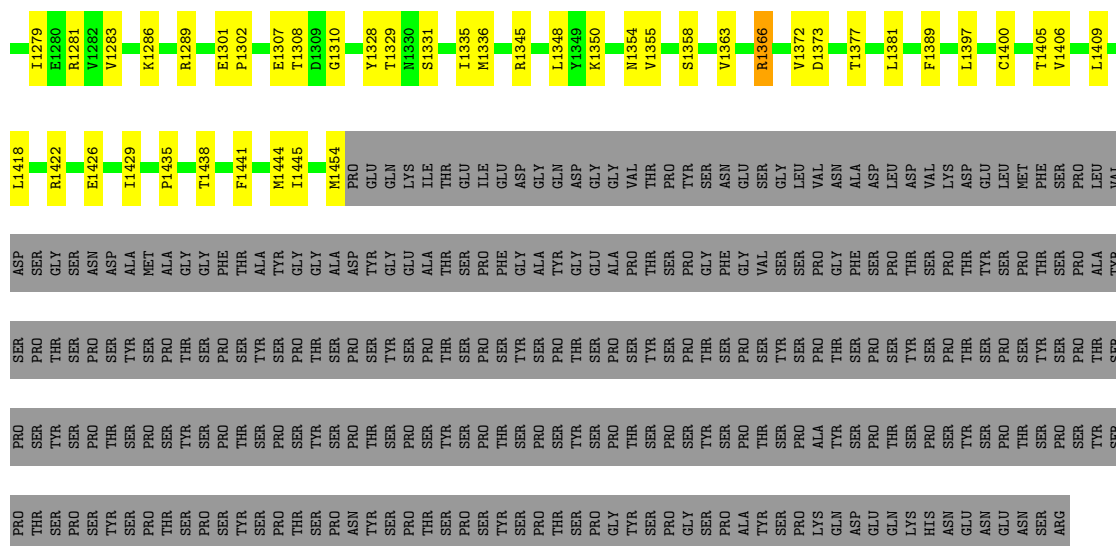
Mol	Chain	Residues	Atoms		AltConf
20	T	25	Total	O	0
			25	25	

### 3 Residue-property plots

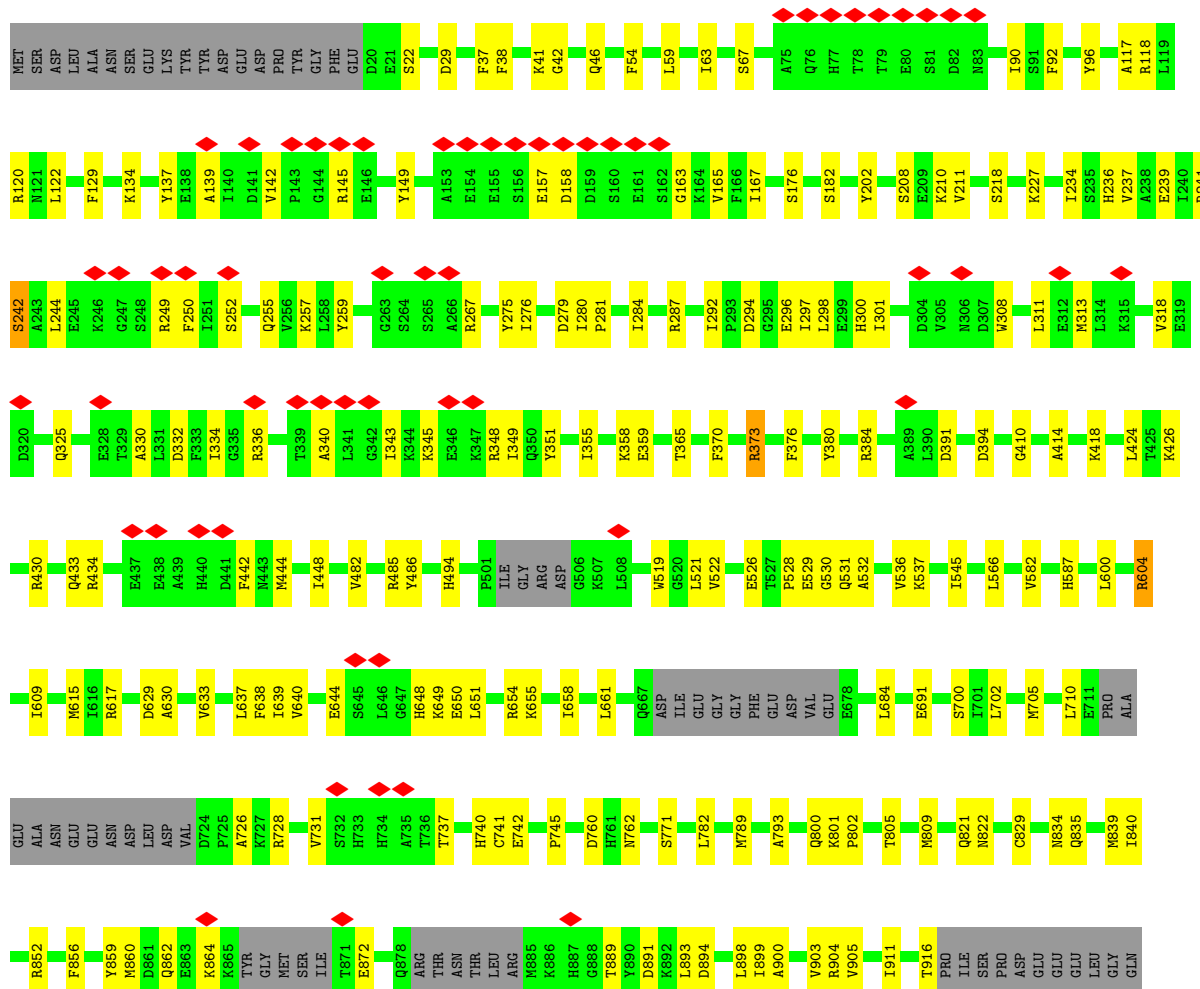
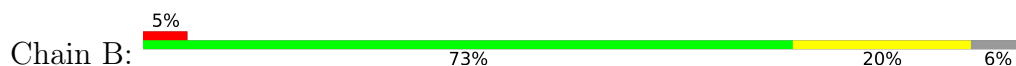
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 II subunit RPB1





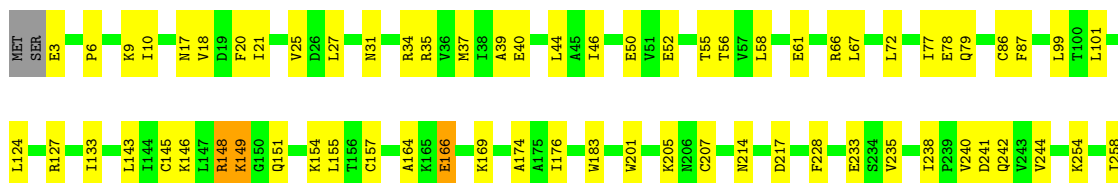
### ● Molecule 2: DNA-directed RNA polymerase II subunit RPB2





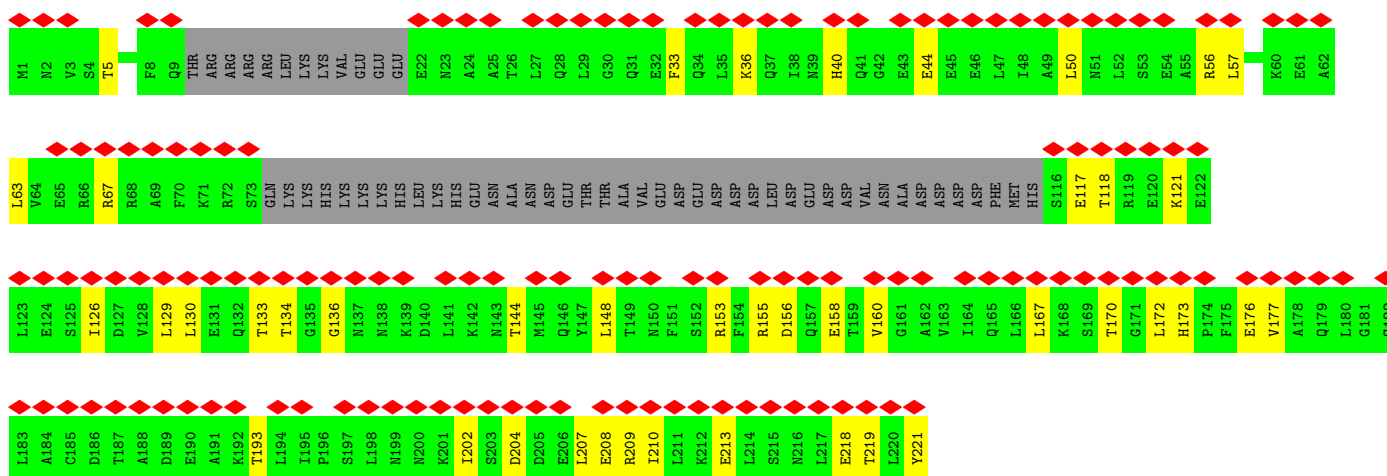
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 63% 20% 16%



• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D: 64% 56% 19% 24%



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

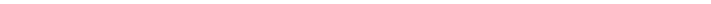
Chain E: 90% 9%

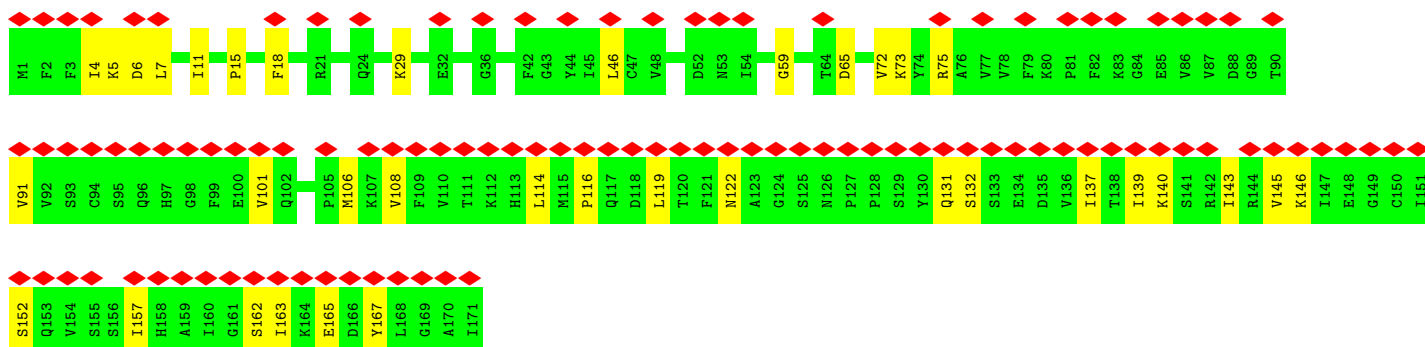


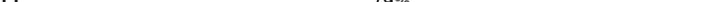
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

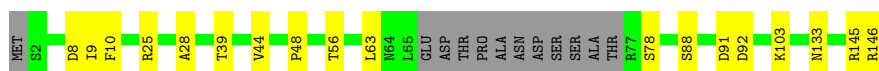
Chain F: 42% 11% 46%

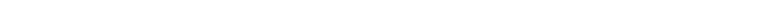


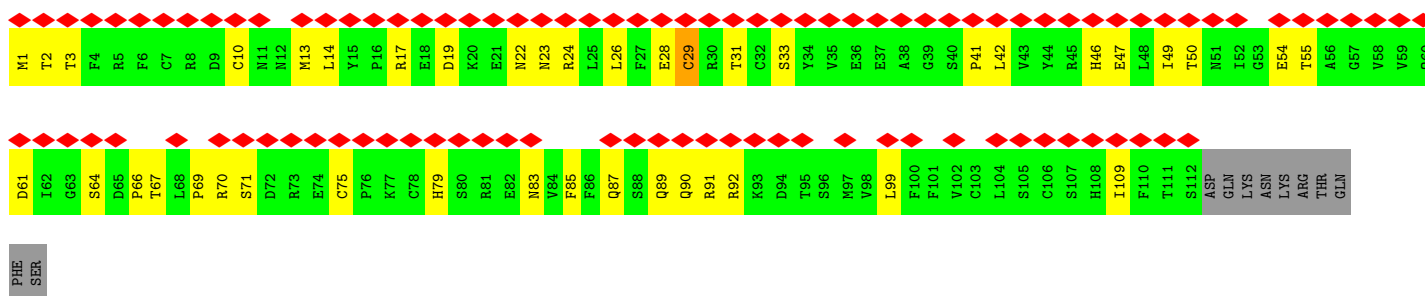
Chain G:  62% 79% 21%

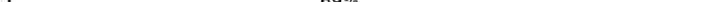


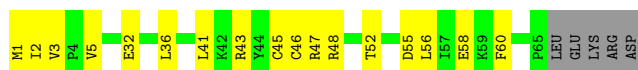
Chain H:  79% 12% 8%




Chain I: 



Chain J:  69% 24% 7%




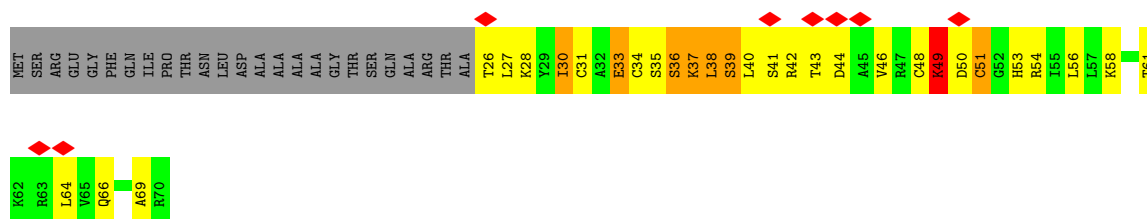
WORLD WIDE  
PDB  
PROTEIN DATA BANK

Chain K:  82% 11% 7%



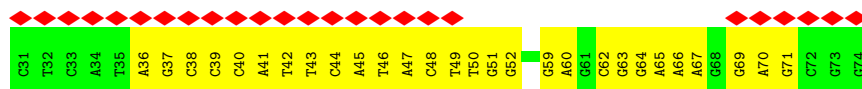
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:  11% 21% 31% 10% 36%




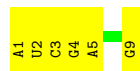
- Molecule 13: DNA (44-MER)

Chain N:  57% 36% 64%



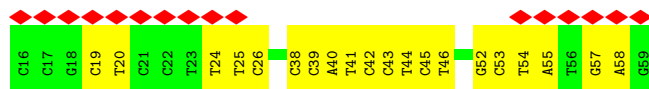
- Molecule 14: RNA (5'-R(P\*AP\*UP\*CP\*GP\*AP\*GP\*AP\*GP\*G)-3')

Chain R:  33% 67%



- Molecule 15: DNA (44-MER)

Chain T:  36% 55% 45%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	692163	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.986	Depositor
Minimum map value	-1.187	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.12	Depositor
Map size ( $\text{\AA}$ )	348.18, 348.18, 348.18	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.829, 0.829, 0.829	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: K, ZN, ATP, 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	A	0.58	18/11139 (0.2%)	0.62	24/15057 (0.2%)
2	B	0.41	4/9332 (0.0%)	0.47	4/12579 (0.0%)
3	C	0.47	0/2133	0.51	2/2891 (0.1%)
4	D	0.10	0/1336	0.30	0/1794
5	E	0.19	0/1780	0.34	0/2395
6	F	0.36	0/682	0.52	0/922
7	G	0.10	0/1368	0.25	0/1844
8	H	0.15	0/1095	0.32	0/1482
9	I	0.51	2/926 (0.2%)	0.66	1/1246 (0.1%)
10	J	0.35	0/541	0.39	0/727
11	K	0.19	0/922	0.35	0/1244
12	L	0.64	0/361	0.99	1/478 (0.2%)
13	N	0.20	0/1029	0.42	0/1588
14	R	0.23	0/221	0.31	0/343
15	T	0.20	0/977	0.47	0/1501
All	All	0.44	24/33842 (0.1%)	0.51	32/46091 (0.1%)

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
1	A	0	1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	710	LEU	C-N	-9.62	1.20	1.33
1	A	399	HIS	CE1-NE2	-8.76	1.23	1.32
1	A	1108	ALA	CA-C	8.55	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	286	HIS	CA-C	-7.58	1.42	1.52
1	A	95	PHE	N-CA	-7.19	1.38	1.46

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	THR	N-CA-C	-9.44	100.37	112.93
1	A	288	ALA	N-CA-C	-8.81	102.66	113.41
1	A	287	HIS	CE1-NE2-CD2	-8.73	100.27	109.00
1	A	287	HIS	ND1-CE1-NE2	7.63	116.03	108.40
2	B	992	ILE	CA-C-O	-7.51	114.93	121.09

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	286	HIS	Mainchain

## 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	10942	0	11025	238	0
2	B	9155	0	9161	195	0
3	C	2095	0	2051	48	0
4	D	1327	0	1331	28	0
5	E	1744	0	1772	11	0
6	F	670	0	690	18	0
7	G	1340	0	1357	36	0
8	H	1077	0	1050	12	0
9	I	909	0	867	55	0
10	J	532	0	542	13	0
11	K	904	0	911	12	0
12	L	359	0	381	32	0
13	N	914	0	492	32	0
14	R	197	0	97	5	0
15	T	879	0	499	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	A	31	0	12	1	0
17	A	2	0	0	0	0
18	A	1	0	0	0	0
19	A	2	0	0	0	0
19	B	1	0	0	0	0
19	C	1	0	0	0	0
19	I	2	0	0	0	0
19	J	1	0	0	0	0
19	L	1	0	0	0	0
20	A	275	0	0	13	0
20	B	229	0	0	7	0
20	C	63	0	0	1	0
20	E	27	0	0	0	0
20	F	14	0	0	0	0
20	H	11	0	0	0	0
20	J	19	0	0	0	0
20	K	32	0	0	4	0
20	L	6	0	0	0	0
20	R	20	0	0	0	0
20	T	25	0	0	0	0
All	All	33807	0	32238	640	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 640 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)
9:I:1:MET:H2	9:I:2:THR:N	1.12	1.40
9:I:1:MET:N	9:I:2:THR:N	1.96	1.13
6:F:103:MET:HE1	7:G:65:ASP:O	1.46	1.13
2:B:394:ASP:OD1	9:I:91:ARG:HG3	1.54	1.07
2:B:617:ARG:NH1	9:I:61:ASP:OD2	1.90	1.05

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1376/1733 (79%)	1333 (97%)	39 (3%)	4 (0%)	36	40
2	B	1136/1224 (93%)	1104 (97%)	32 (3%)	0	100	100
3	C	264/318 (83%)	258 (98%)	6 (2%)	0	100	100
4	D	161/221 (73%)	159 (99%)	2 (1%)	0	100	100
5	E	211/215 (98%)	204 (97%)	7 (3%)	0	100	100
6	F	81/155 (52%)	79 (98%)	2 (2%)	0	100	100
7	G	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
8	H	130/146 (89%)	129 (99%)	1 (1%)	0	100	100
9	I	109/122 (89%)	97 (89%)	12 (11%)	0	100	100
10	J	63/70 (90%)	62 (98%)	1 (2%)	0	100	100
11	K	110/120 (92%)	108 (98%)	2 (2%)	0	100	100
12	L	43/70 (61%)	28 (65%)	12 (28%)	3 (7%)	1	0
All	All	3853/4565 (84%)	3727 (97%)	119 (3%)	7 (0%)	44	50

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	710	LEU
1	A	711	ARG
12	L	51	CYS
12	L	33	GLU
12	L	36	SER

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1213/1520 (80%)	1200 (99%)	13 (1%)	65	75
2	B	997/1061 (94%)	987 (99%)	10 (1%)	68	77
3	C	234/274 (85%)	227 (97%)	7 (3%)	36	45
4	D	149/200 (74%)	149 (100%)	0	100	100
5	E	195/197 (99%)	194 (100%)	1 (0%)	81	87
6	F	73/137 (53%)	69 (94%)	4 (6%)	19	20
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	118/128 (92%)	118 (100%)	0	100	100
9	I	106/116 (91%)	105 (99%)	1 (1%)	70	79
10	J	60/65 (92%)	60 (100%)	0	100	100
11	K	97/102 (95%)	97 (100%)	0	100	100
12	L	40/57 (70%)	31 (78%)	9 (22%)	1	0
All	All	3434/4009 (86%)	3389 (99%)	45 (1%)	59	72

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	235	VAL
9	I	29	CYS
3	C	238	ILE
6	F	93	ILE
12	L	30	ILE

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

Mol	Chain	Res	Type
2	B	1025	HIS
4	D	34	GLN
2	B	1104	HIS
3	C	231	ASN
5	E	146	HIS

### 5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	R	7/9 (77%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 11 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	$\# Z  > 2$
16	ATP	A	1801	17	29,33,33	2.90	9 (31%)	44,52,52	2.73	12 (27%)

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	ATP	A	1801	17	-	6/22/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	1801	ATP	C8-N9	-9.12	1.21	1.37
16	A	1801	ATP	C4-N9	-8.57	1.18	1.37
16	A	1801	ATP	C6-N6	4.21	1.44	1.34
16	A	1801	ATP	C5-N7	3.50	1.45	1.39
16	A	1801	ATP	O4'-C1'	2.91	1.48	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	1801	ATP	C4-N9-C8	12.84	119.64	105.73
16	A	1801	ATP	N3-C2-N1	-6.07	119.11	128.60
16	A	1801	ATP	N3-C4-N9	3.88	133.47	127.08
16	A	1801	ATP	C5-C4-N3	-3.87	121.70	126.75
16	A	1801	ATP	N9-C8-N7	-3.45	109.20	113.91

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

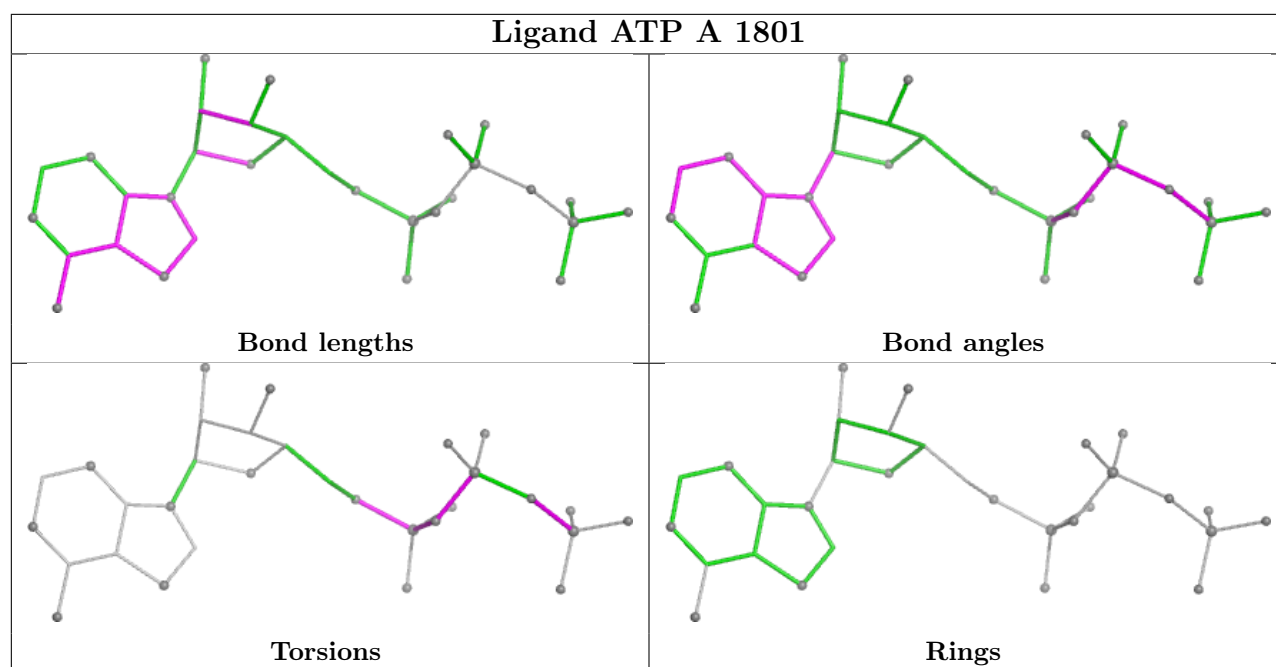
Mol	Chain	Res	Type	Atoms
16	A	1801	ATP	C5'-O5'-PA-O3A
16	A	1801	ATP	PA-O3A-PB-O2B
16	A	1801	ATP	C5'-O5'-PA-O1A
16	A	1801	ATP	C5'-O5'-PA-O2A
16	A	1801	ATP	PB-O3A-PA-O1A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	1801	ATP	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	I	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	1:MET	C	2:THR	N	2.38
1	A	710:LEU	C	711:ARG	N	1.20

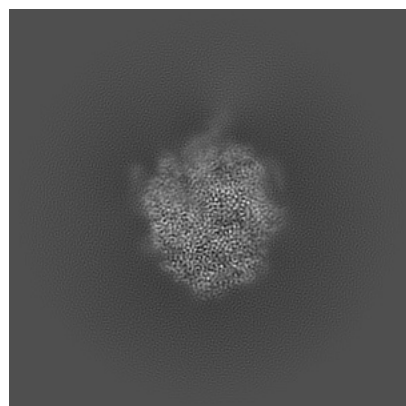
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53053. These allow visual inspection of the internal detail of the map and identification of artifacts.

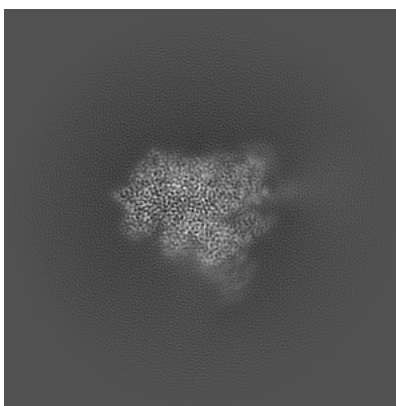
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

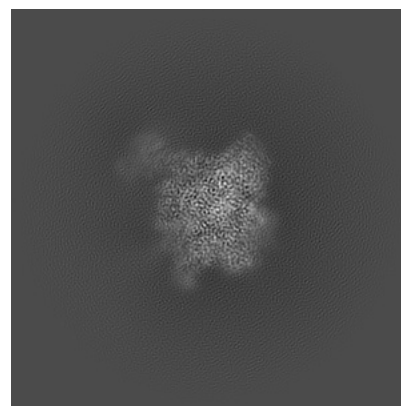
#### 6.1.1 Primary map



X

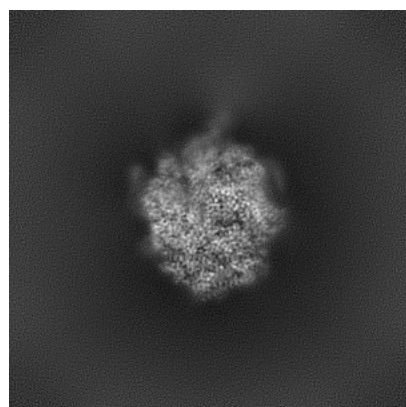


Y

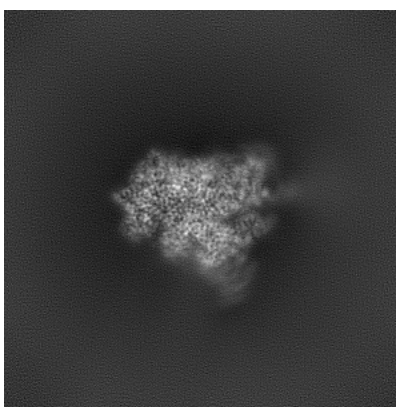


Z

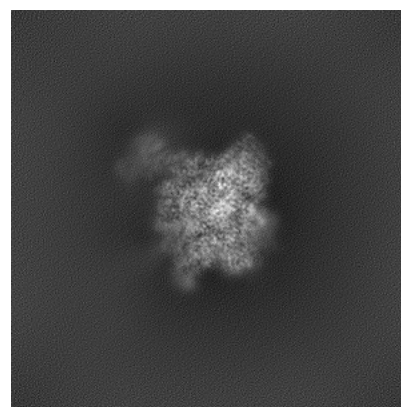
#### 6.1.2 Raw map



X



Y

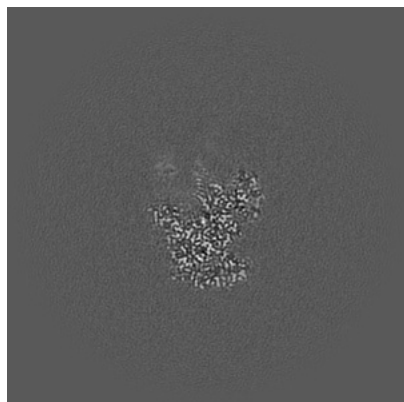


Z

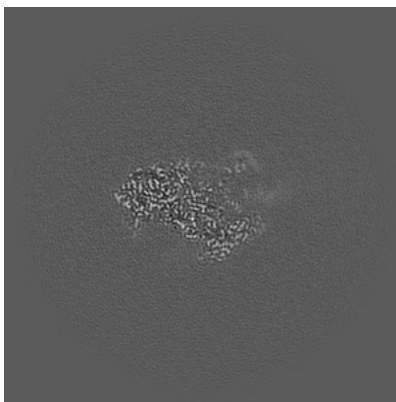
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

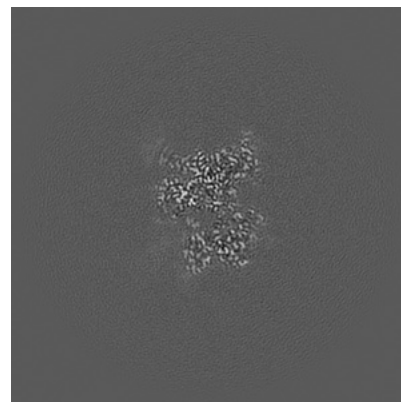
### 6.2.1 Primary map



X Index: 210

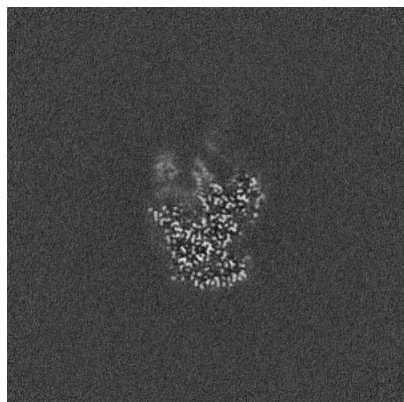


Y Index: 210

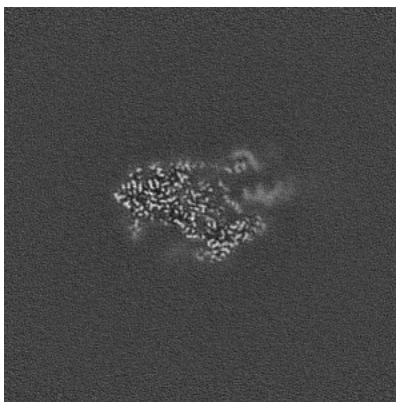


Z Index: 210

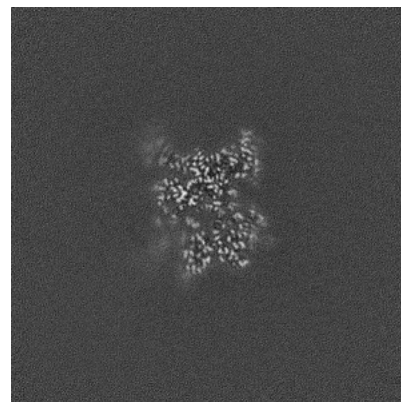
### 6.2.2 Raw map



X Index: 210



Y Index: 210

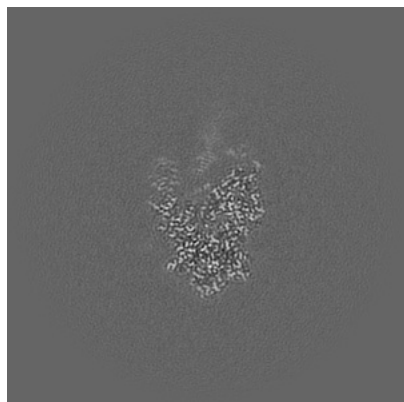


Z Index: 210

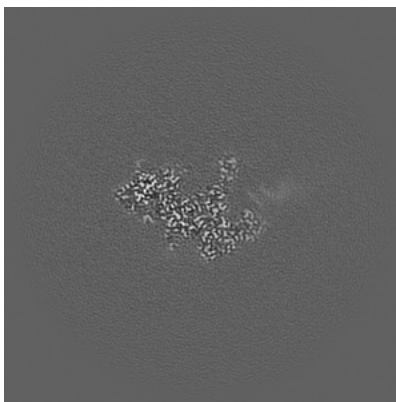
The images above show central slices of the map in three orthogonal directions.

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

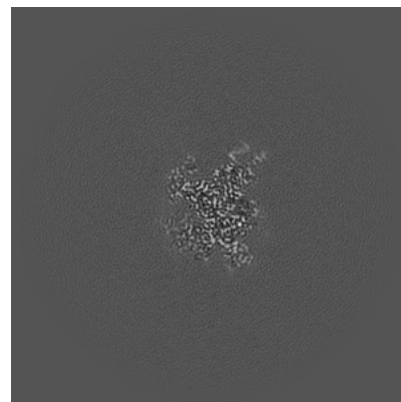
### 6.3.1 Primary map



X Index: 220

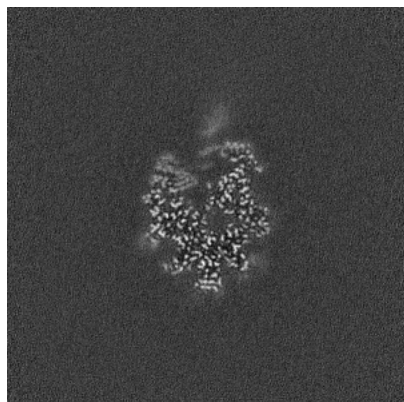


Y Index: 218

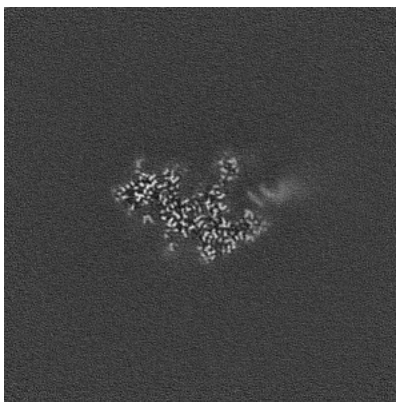


Z Index: 179

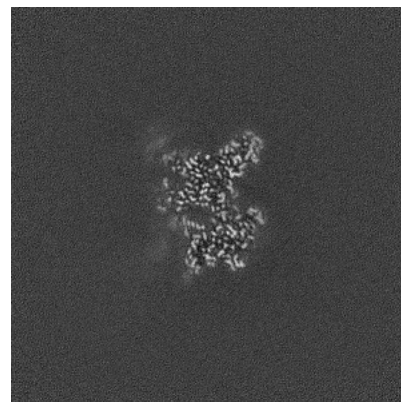
### 6.3.2 Raw map



X Index: 229



Y Index: 218

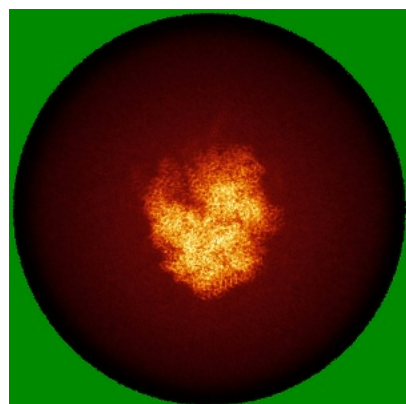


Z Index: 205

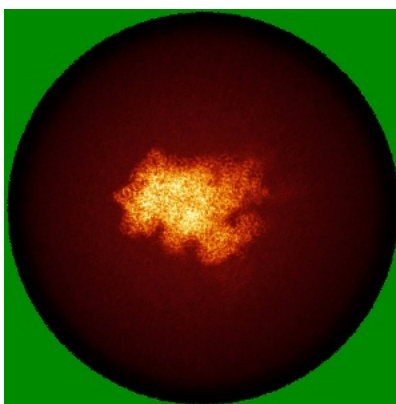
The images above show the largest variance slices of the map in three orthogonal directions.

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

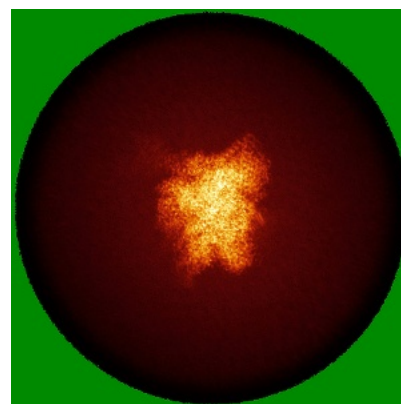
### 6.4.1 Primary map



X

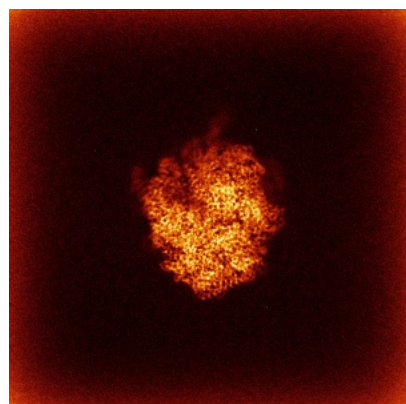


Y

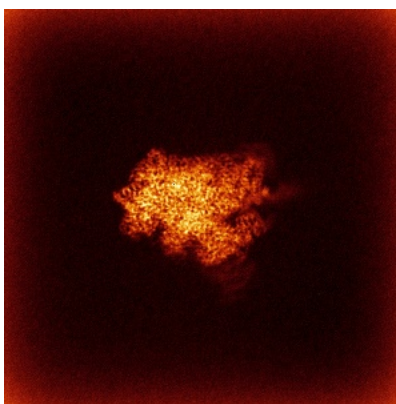


Z

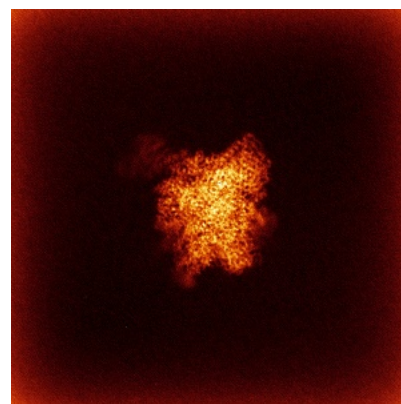
### 6.4.2 Raw map



X



Y

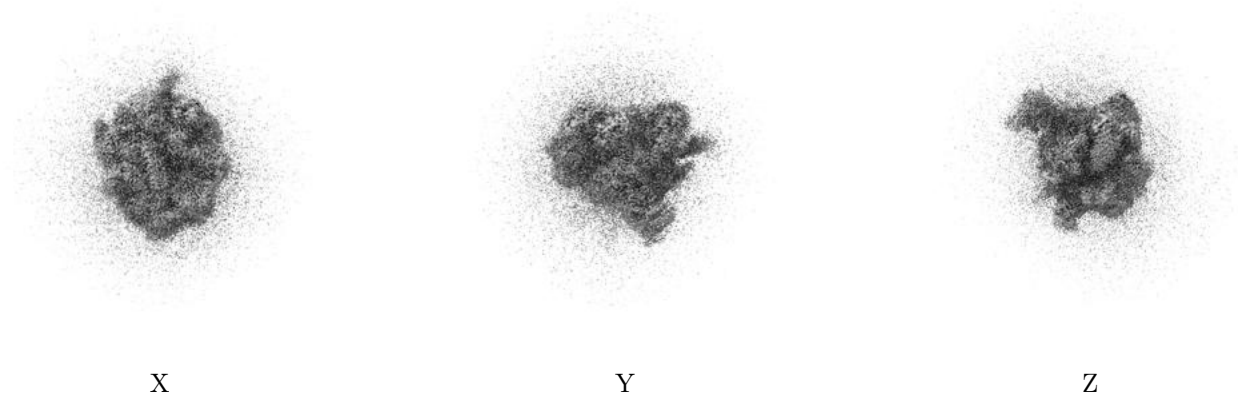


Z

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.

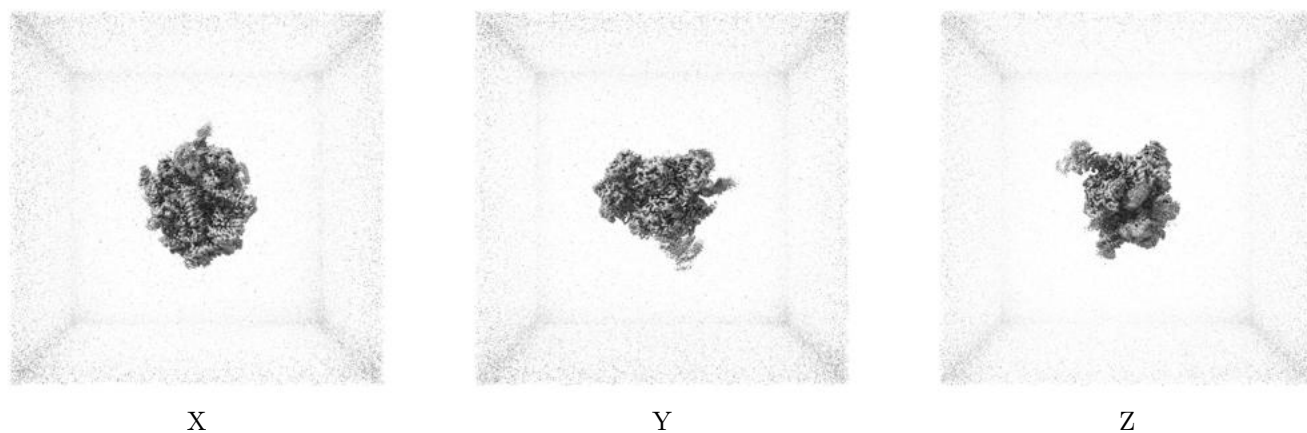
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

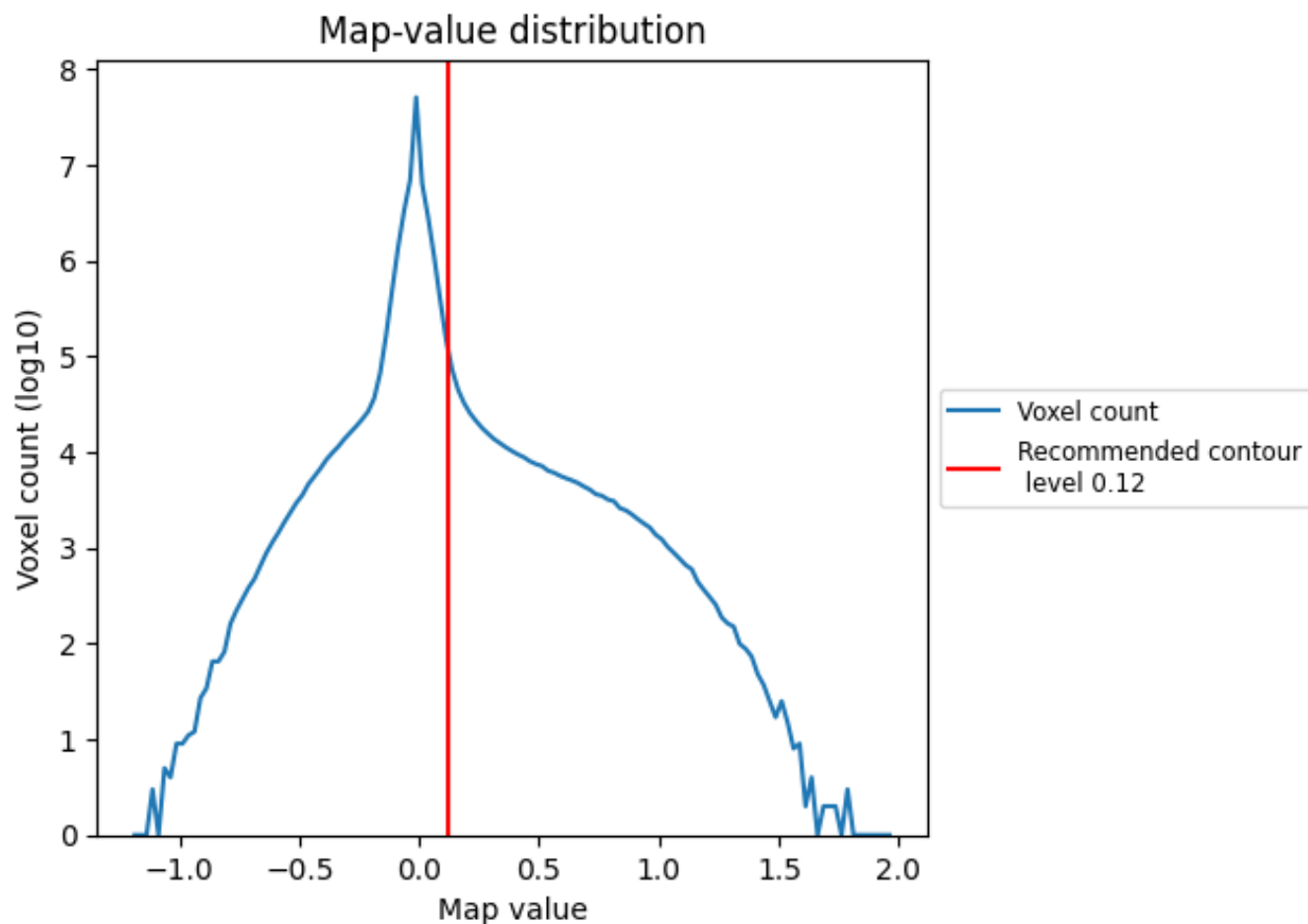
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

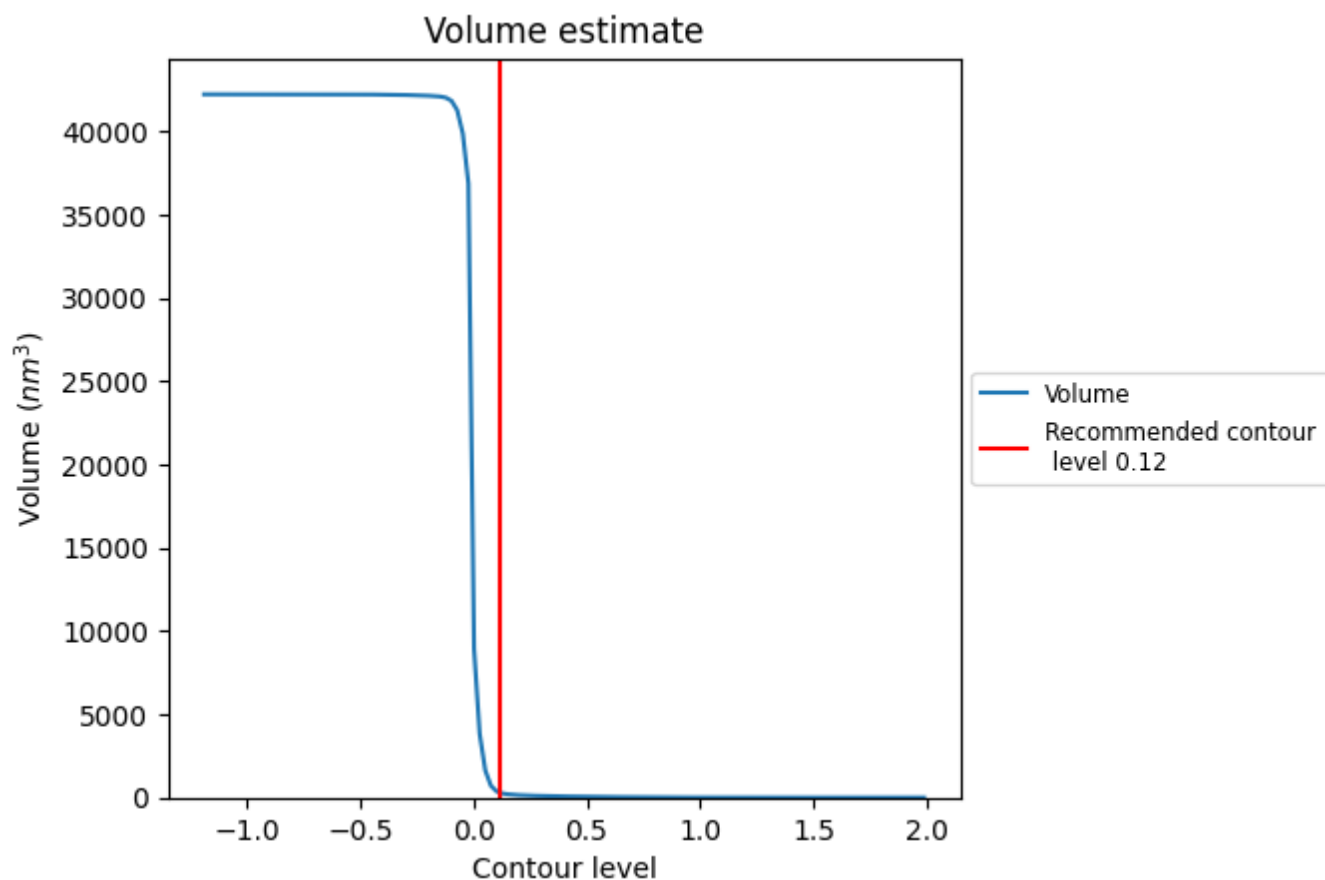
This section contains the results of statistical analysis of the map.

### 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.

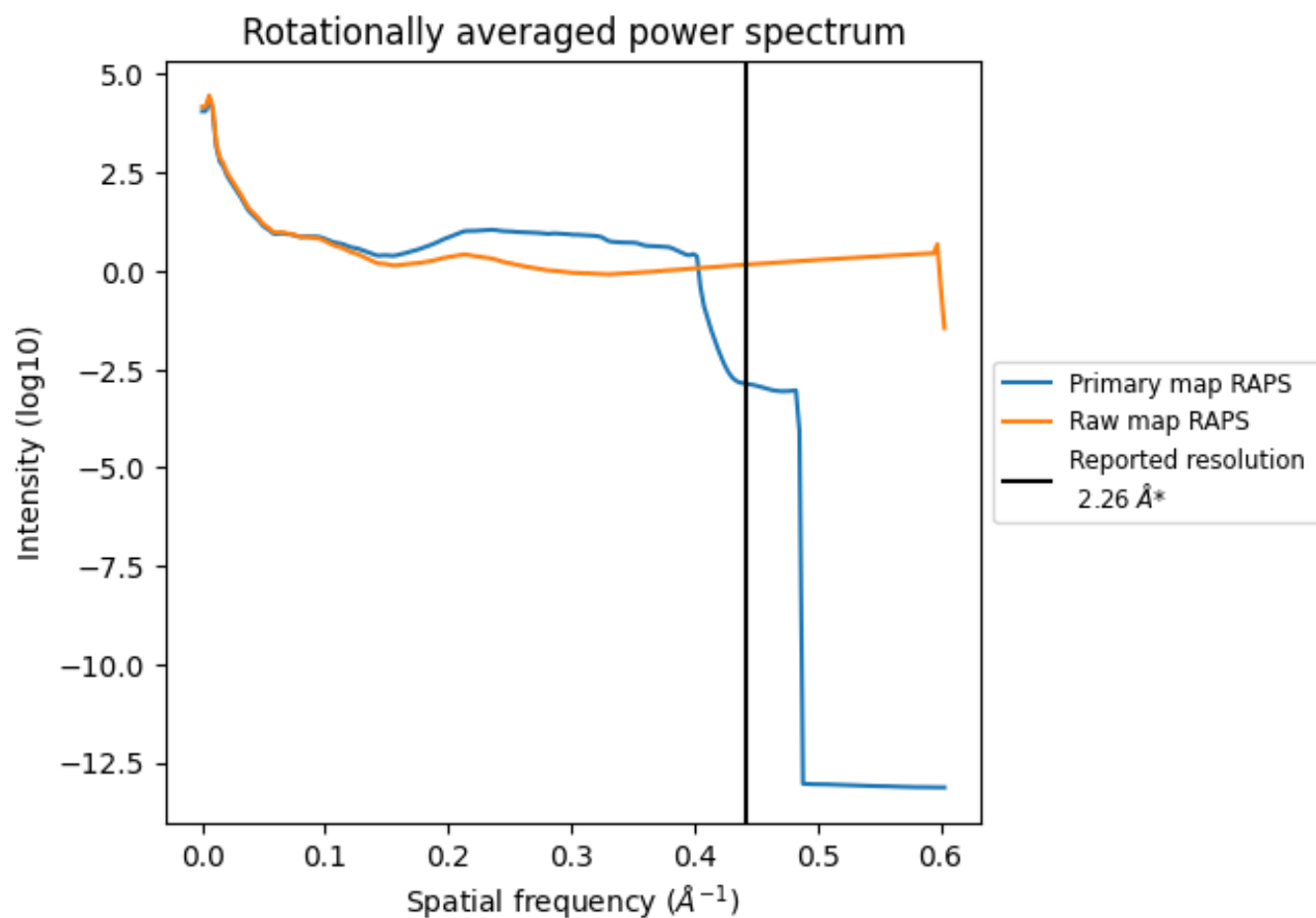
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 286 nm<sup>3</sup>; this corresponds to an approximate mass of 258 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 ⓘ

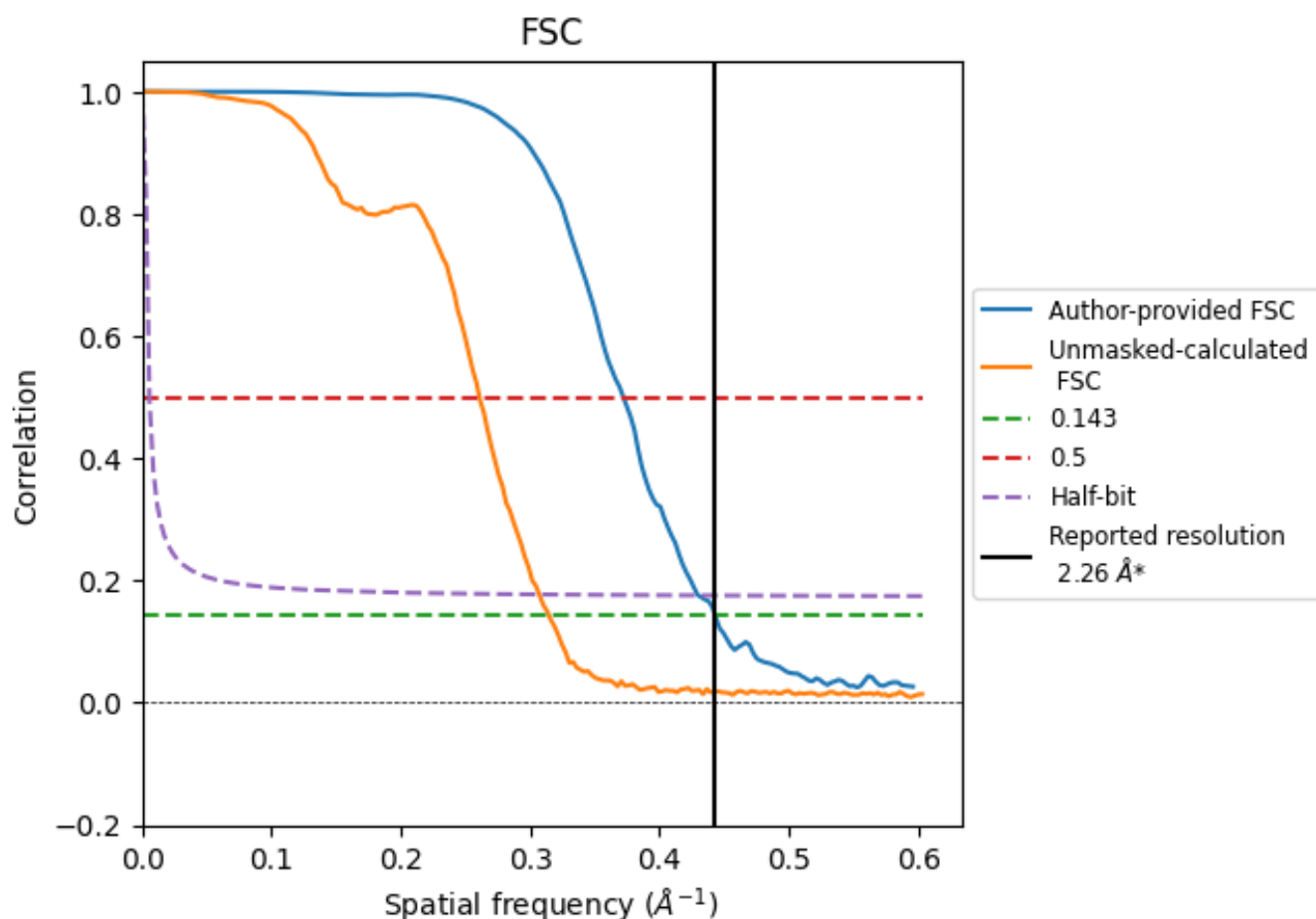


\*Reported resolution corresponds to spatial frequency of 0.442  $\text{\AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

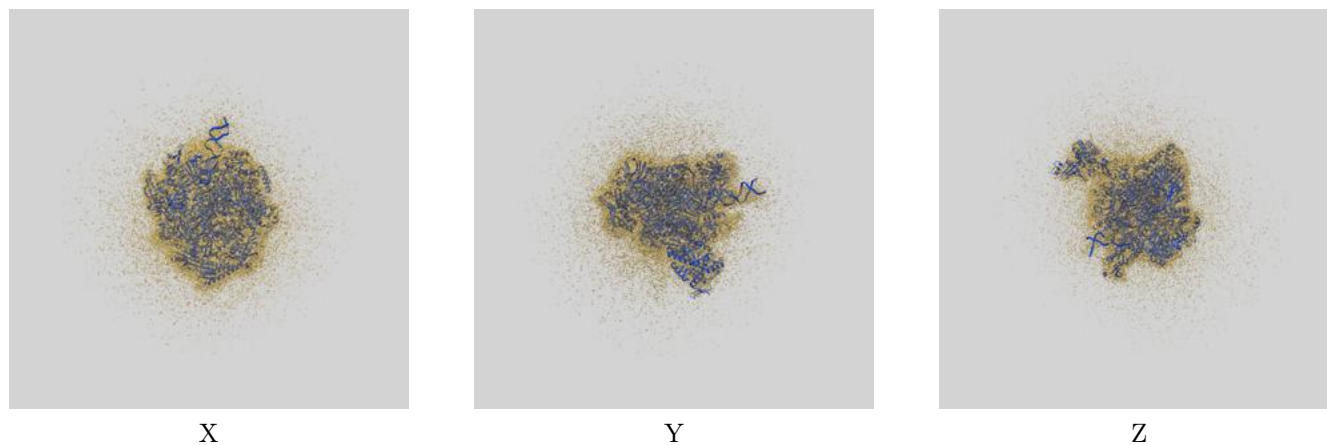
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.26	-	-
Author-provided FSC curve	2.26	2.69	2.33
Unmasked-calculated*	3.18	3.84	3.26

\*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 3.18 differs from the reported value 2.26 by more than 10 %

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

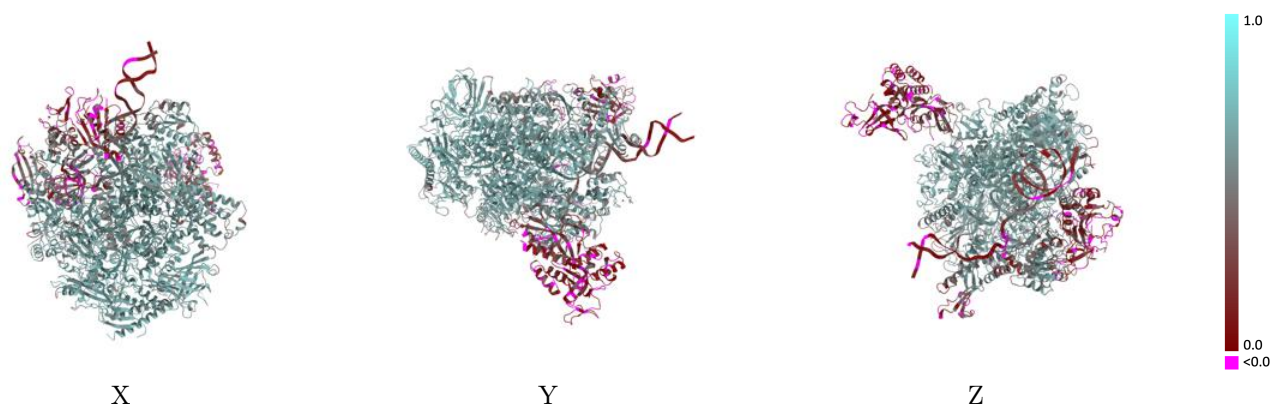
This section contains information regarding the fit between EMDB map EMD-53053 and PDB model 9QEB. Per-residue inclusion information can be found in section [3](#) on page [9](#).

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



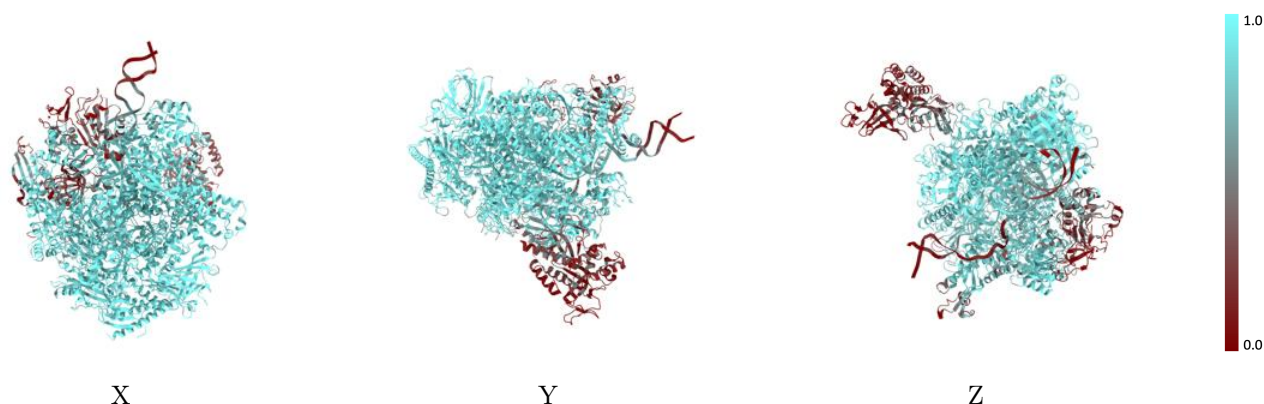
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



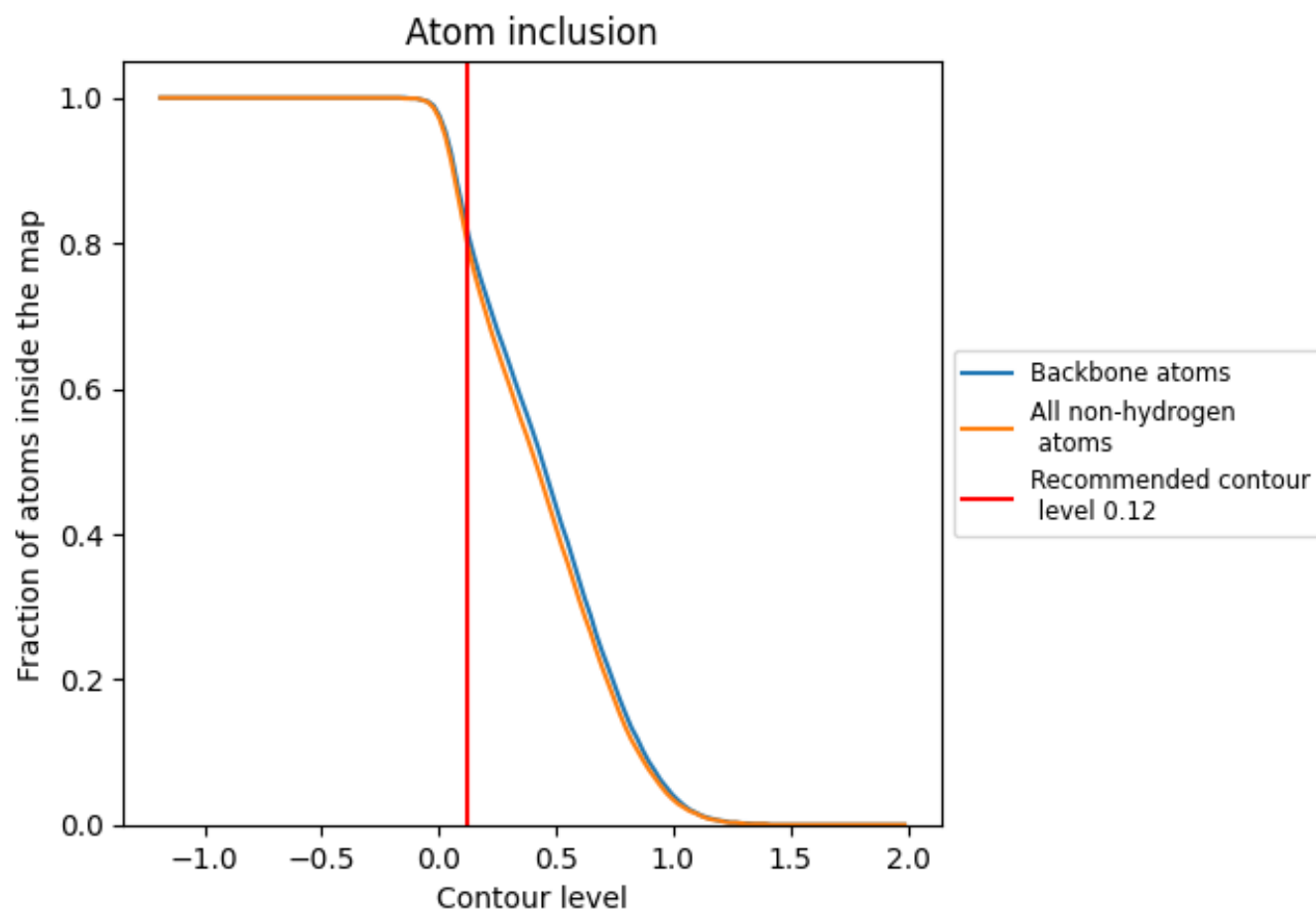
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 80% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8020	<div></div> 0.5180
A	<div></div> 0.8940	<div></div> 0.5820
B	<div></div> 0.8770	<div></div> 0.5650
C	<div></div> 0.9360	<div></div> 0.6210
D	<div></div> 0.2100	<div></div> 0.1140
E	<div></div> 0.9080	<div></div> 0.5840
F	<div></div> 0.9570	<div></div> 0.6280
G	<div></div> 0.3240	<div></div> 0.1510
H	<div></div> 0.9240	<div></div> 0.6060
I	<div></div> 0.1590	<div></div> 0.1360
J	<div></div> 0.9540	<div></div> 0.6360
K	<div></div> 0.9650	<div></div> 0.6380
L	<div></div> 0.6570	<div></div> 0.4820
N	<div></div> 0.3990	<div></div> 0.2110
R	<div></div> 0.9650	<div></div> 0.6340
T	<div></div> 0.5830	<div></div> 0.3460

