



## wwPDB EM Validation Summary Report ⓘ

Sep 17, 2025 – 10:21 AM EDT

PDB ID : 9EI4 / pdb\_00009ei4  
EMDB ID : EMD-48076  
Title : Cryo-EM structure of Human RNA polymerase II Elongation Complex bound to the RECQL5 helicase in the presence of ADP  
Authors : Florez Ariza, A.; Lue, N.; Nogales, E.  
Deposited on : 2024-11-25  
Resolution : 3.70 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:

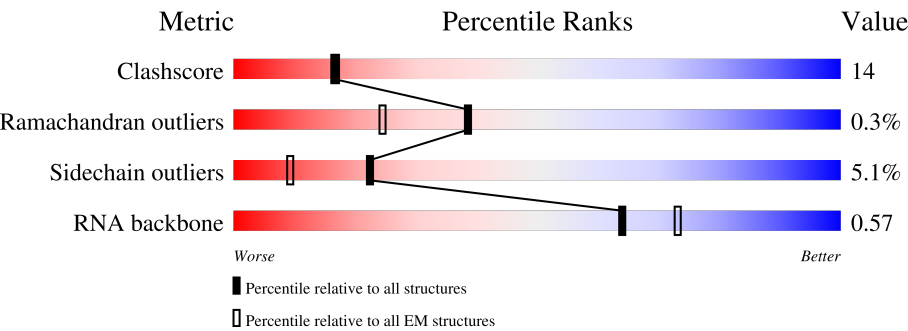
EMDB validation analysis : 0.0.1.dev126  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

# 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 3.70 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.





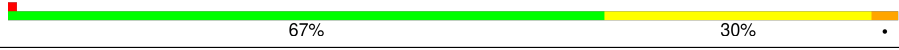



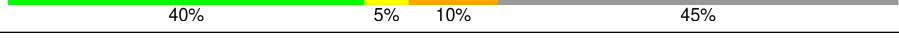
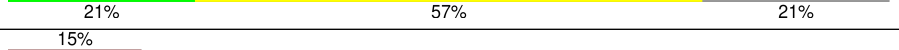
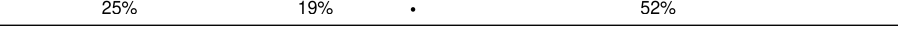
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1970	<div><div></div><div>48%23%28%</div></div>
2	B	1174	<div><div></div><div>68%27%</div></div>
3	C	275	<div><div></div><div>58%32%7%</div></div>
4	D	142	<div><div>39%</div><div>63%25%10%</div></div>
5	E	210	<div><div></div><div>70%27%</div></div>
6	F	127	<div><div></div><div>47%17%35%</div></div>
7	G	172	<div><div></div><div>45%74%25%</div></div>

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Mol	Chain	Length	Quality of chain
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	N	43	
14	P	20	
15	T	28	
16	U	991	

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 35854 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	1428	Total	C	N	O	S	0	0
			11317	7123	2025	2097	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1134	Total	C	N	O	S	0	0
			9062	5732	1595	1671	64		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	257	Total	C	N	O	S	0	0
			2060	1296	351	407	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	128	Total	C	N	O	S	0	0
			1005	632	172	197	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1711	1084	300	319	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	44	PHE	SER	conflict	UNP P19388

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	S	0	0
			658	419	113	121	5		

- 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
			1334	867	216	243	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	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	114	Total	C	N	O	S	0	0
			927	571	166	179	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	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	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	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 13 is a DNA chain called Non-template DNA, nucleic acid scaffold.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	17	Total	C	N	O	P	0	0
			355	169	68	101	17		

- Molecule 14 is a RNA chain called RNA, nucleic acid scaffold.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	11	Total	C	N	O	P	0	0
			239	107	49	72	11		

- Molecule 15 is a DNA chain called Template DNA, nucleic acid scaffold.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	22	Total	C	N	O	P	0	0
			447	214	77	134	22		

- Molecule 16 is a protein called ATP-dependent DNA helicase Q5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	472	Total	C	N	O	S	1	0
			3692	2330	665	672	25		

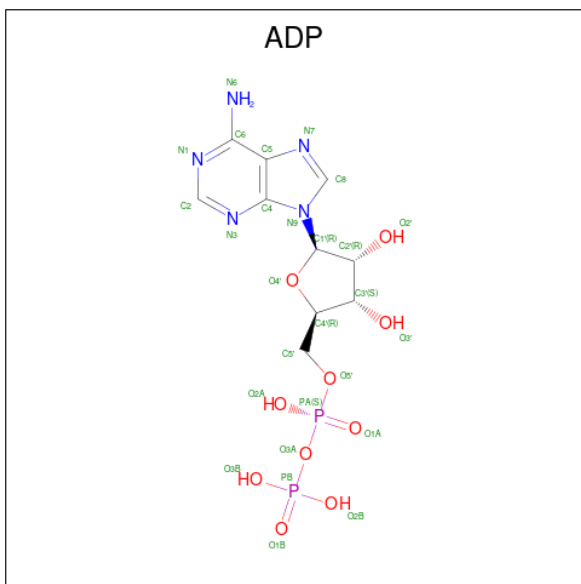
- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

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

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

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).

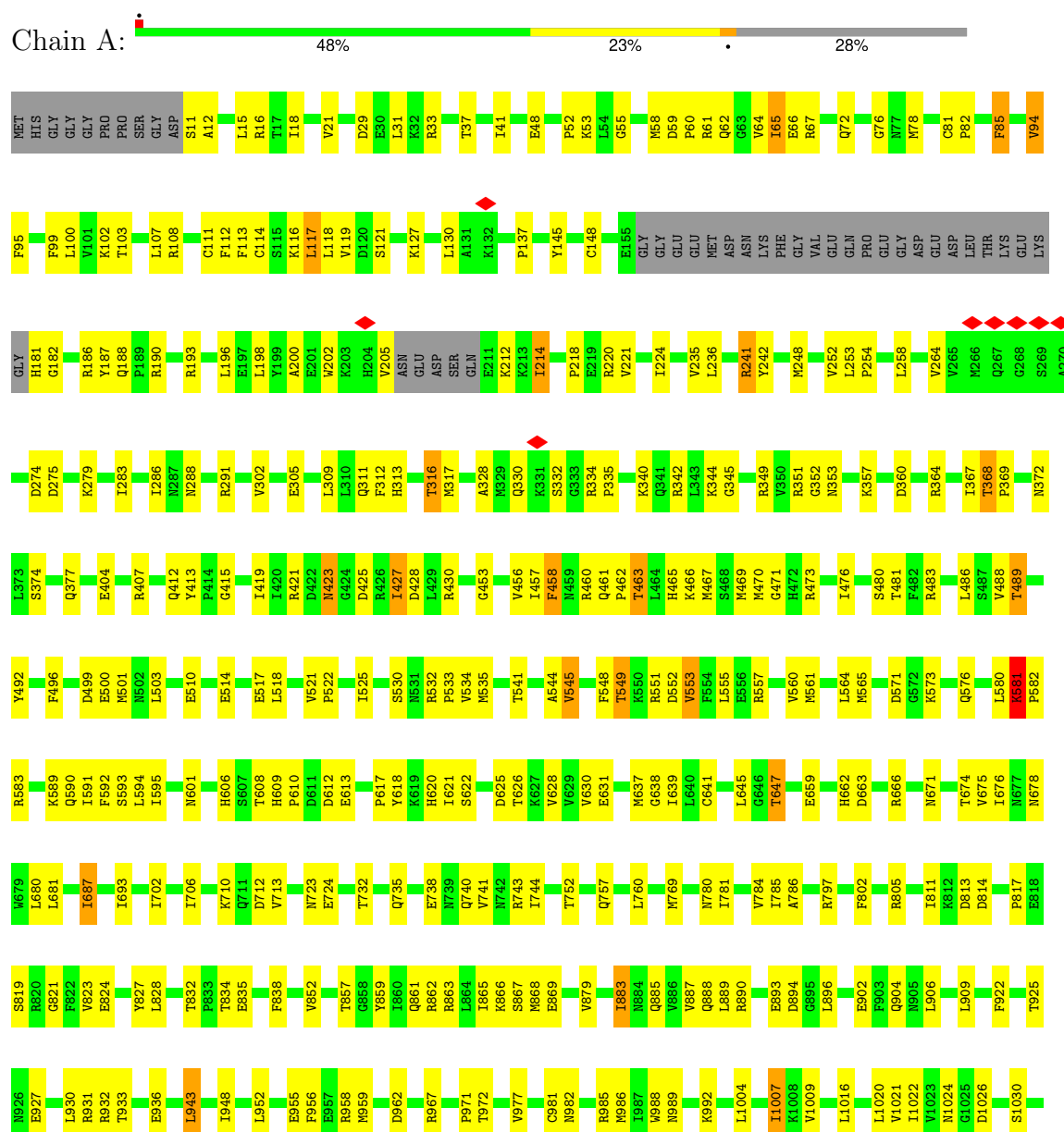


Mol	Chain	Residues	Atoms					AltConf
19	U	1	Total	C	N	O	P	0
			27	10	5	10	2	

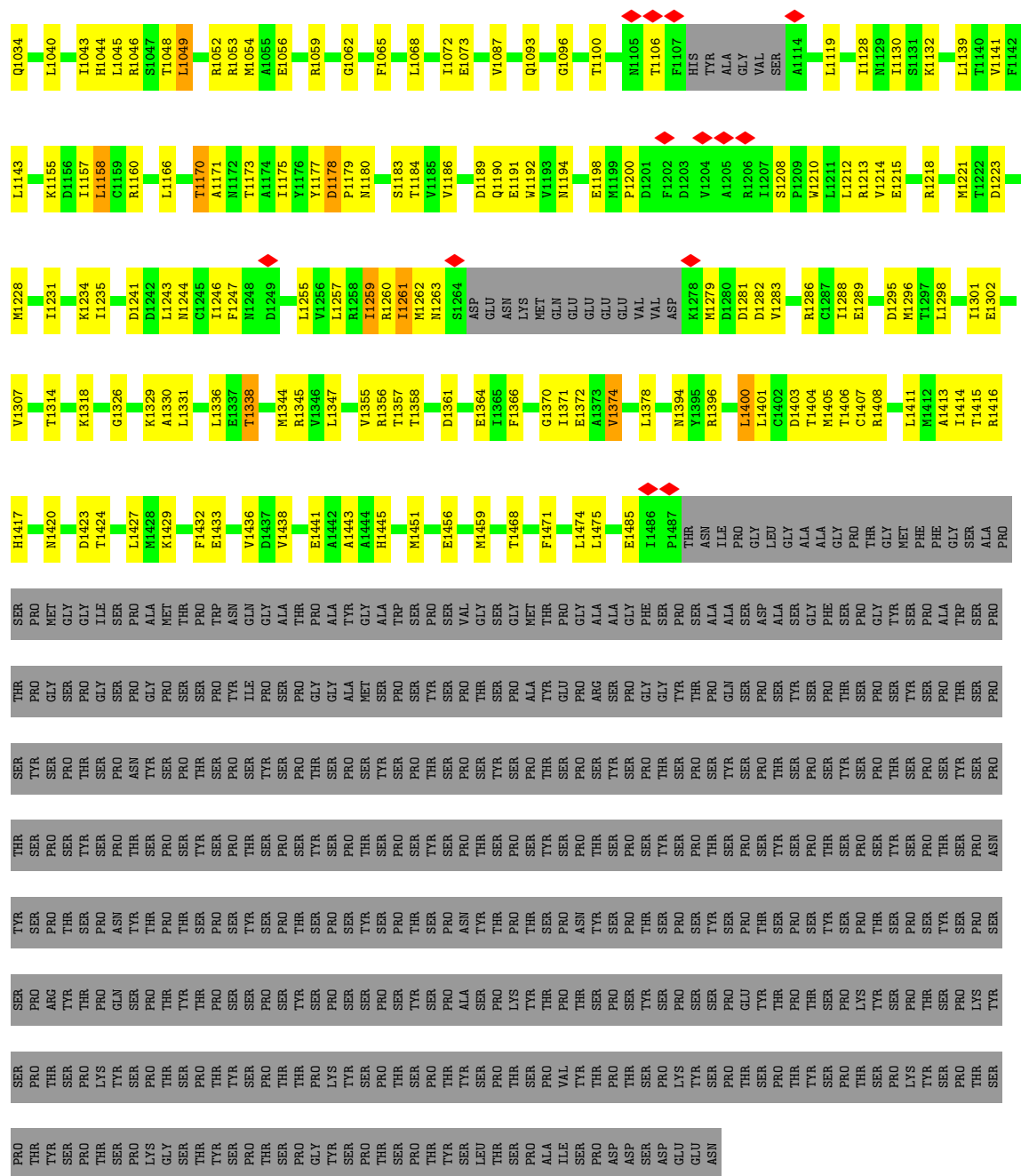
### 3 Residue-property plots

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

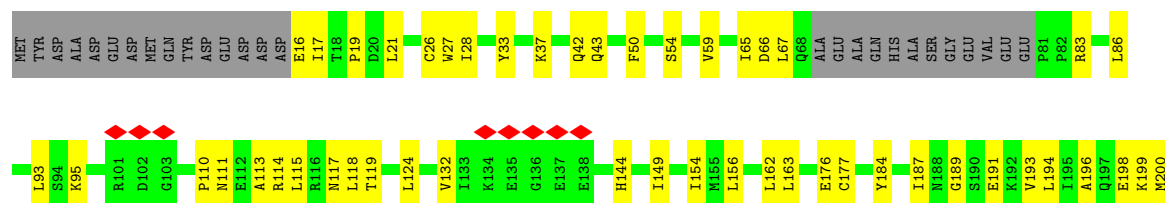


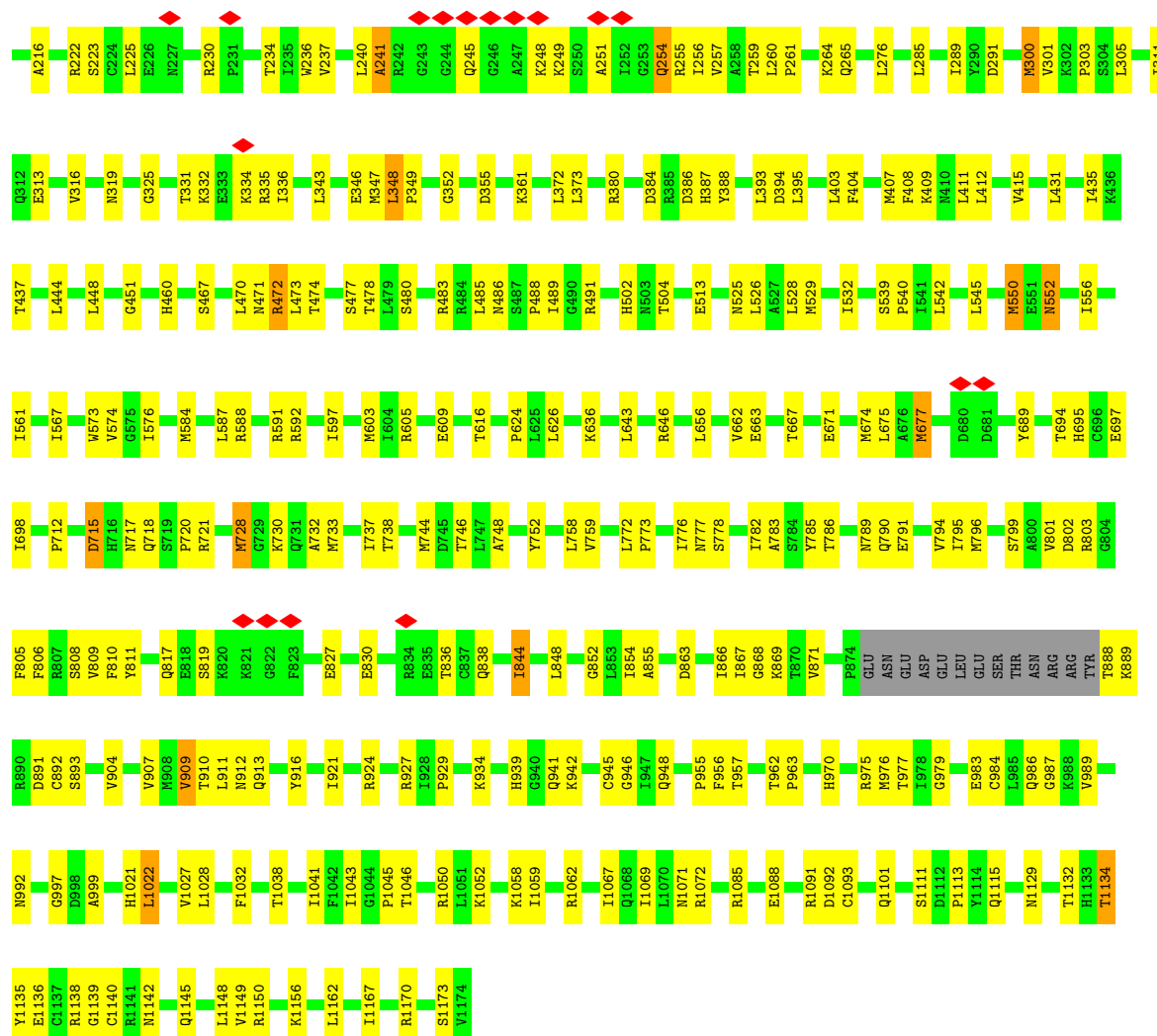




### • Molecule 2: DNA-directed RNA polymerase II subunit RPB2

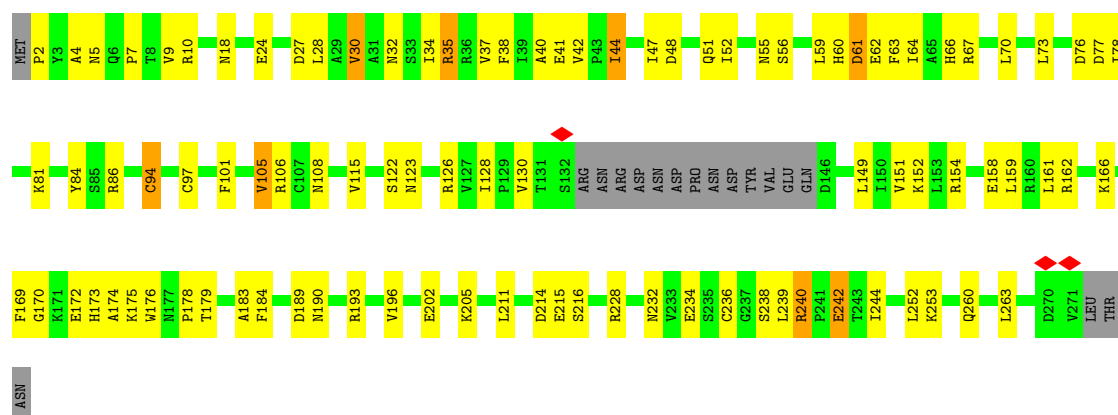
Chain B: 68% 27%



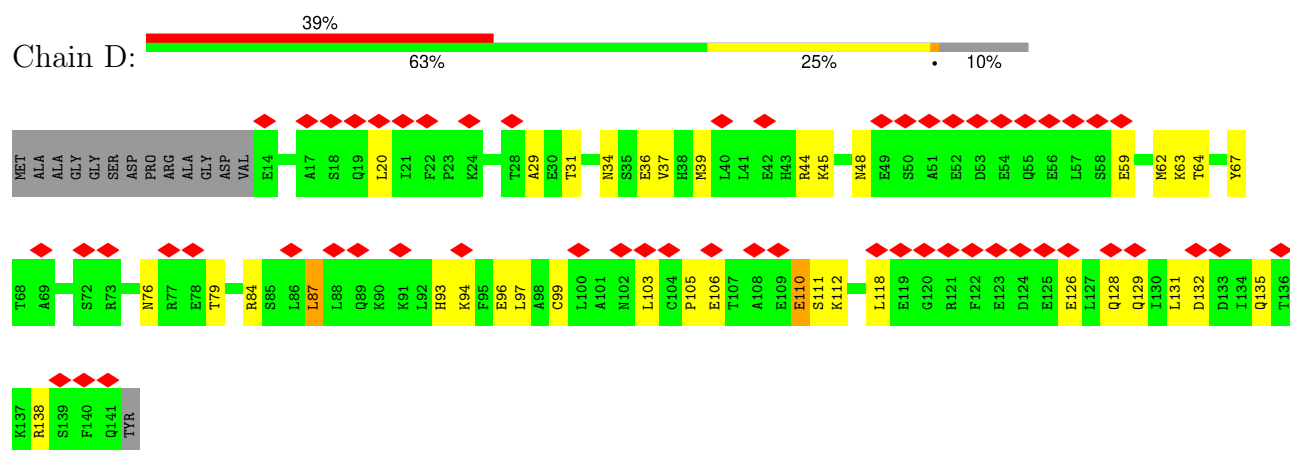


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

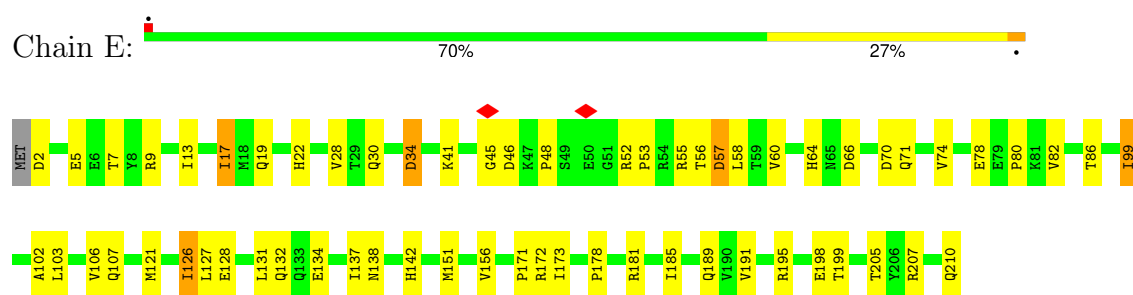
Chain C: 58% 32% 7%



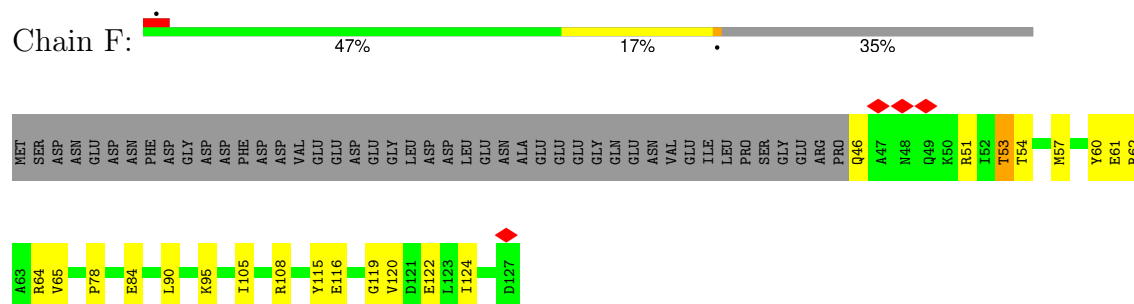
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



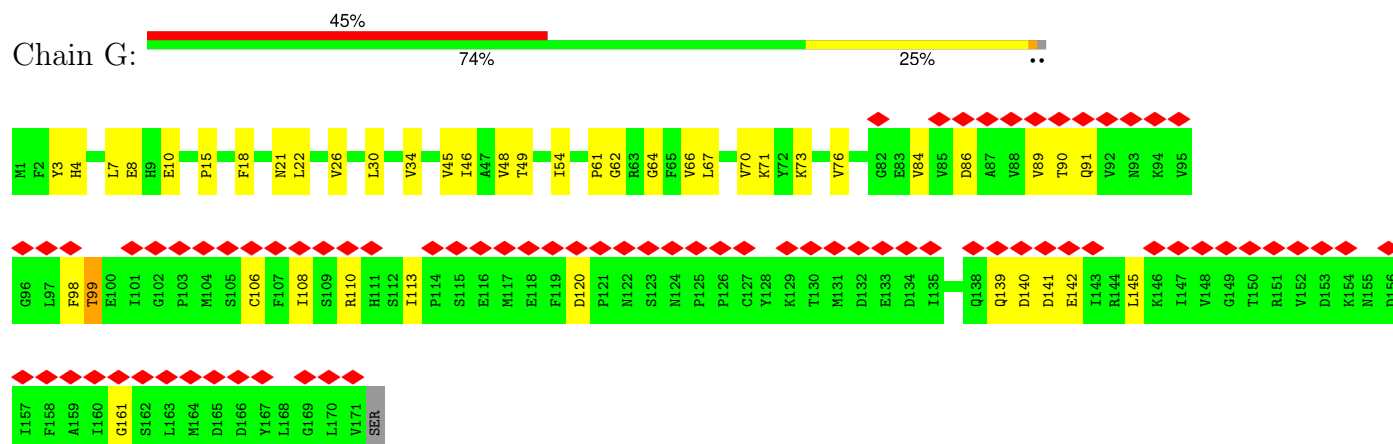
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



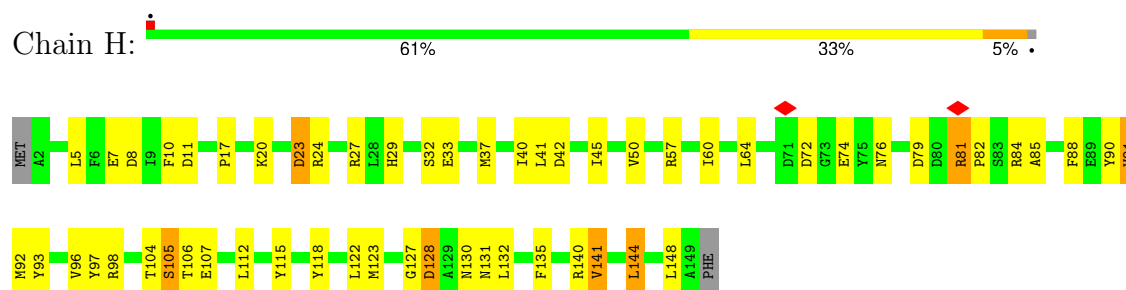
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



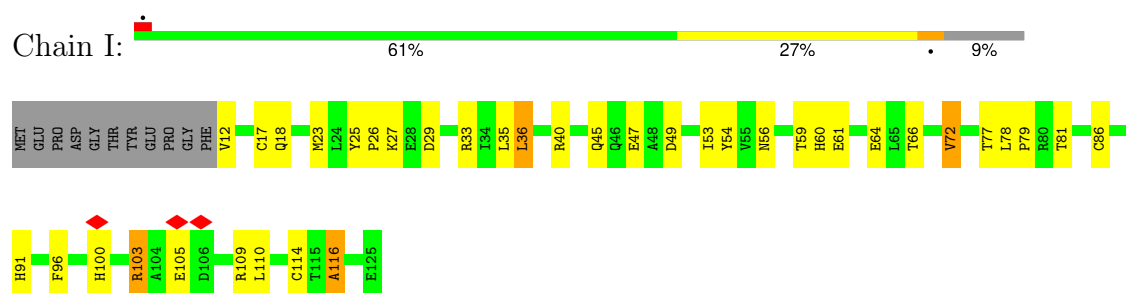
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



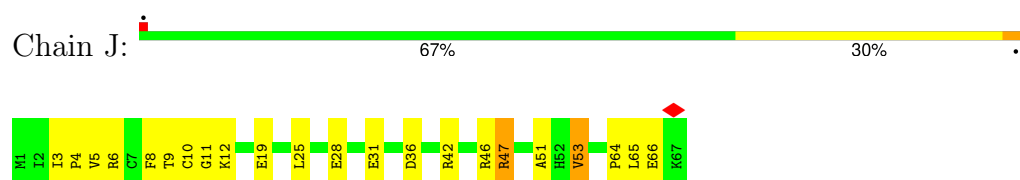
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



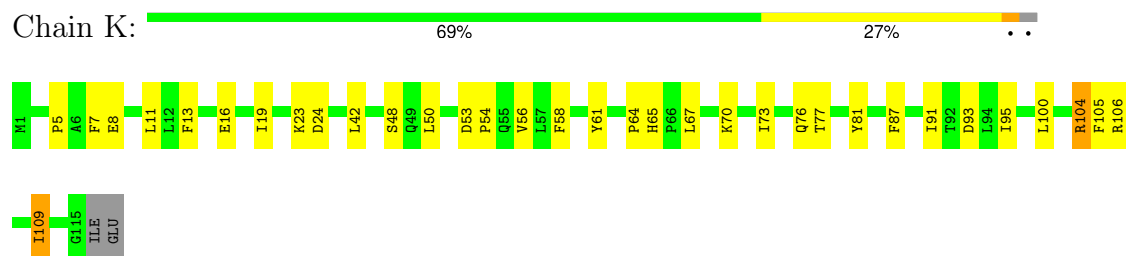
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



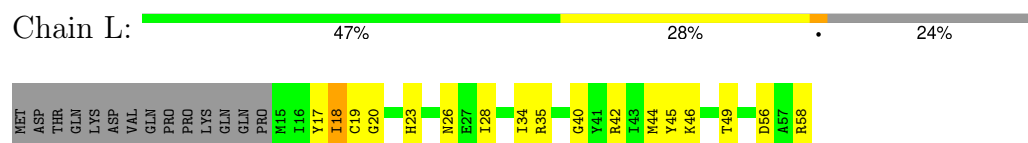
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a



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



- Molecule 13: Non-template DNA, nucleic acid scaffold







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17442	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.220	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	335.36, 335.36, 335.36	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.34	0/11525	0.37	0/15558
2	B	0.36	0/9243	0.37	1/12475 (0.0%)
3	C	0.38	0/2103	0.38	0/2858
4	D	0.10	0/1019	0.29	0/1374
5	E	0.29	0/1742	0.33	0/2353
6	F	0.32	0/668	0.33	0/903
7	G	0.20	0/1365	0.32	0/1853
8	H	0.32	0/1207	0.38	0/1628
9	I	0.29	0/948	0.34	0/1284
10	J	0.38	0/542	0.36	0/730
11	K	0.35	0/939	0.36	0/1271
12	L	0.31	0/377	0.47	0/500
13	N	0.30	0/398	0.50	0/611
14	P	0.41	0/268	0.36	0/416
15	T	0.45	0/499	0.56	0/767
16	U	0.21	0/3756	0.41	0/5066
All	All	0.33	0/36599	0.38	1/49647 (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
1	A	0	1
10	J	0	1
16	U	0	5
All	All	0	7

There are no bond length outliers.



All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	241	ALA	CB-CA-C	-5.46	109.29	115.79

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	583	ARG	Sidechain
10	J	28	GLU	Peptide
16	U	25	GLY	Peptide
16	U	76	VAL	Mainchain
16	U	77[A]	SER	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	11317	0	11453	337	0
2	B	9062	0	9107	243	0
3	C	2060	0	2011	76	0
4	D	1005	0	964	26	0
5	E	1711	0	1729	42	0
6	F	658	0	686	17	0
7	G	1334	0	1333	24	0
8	H	1186	0	1147	46	0
9	I	927	0	859	24	0
10	J	533	0	553	23	0
11	K	920	0	942	24	0
12	L	372	0	378	15	0
13	N	355	0	194	13	0
14	P	239	0	121	2	0
15	T	447	0	250	19	0
16	U	3692	0	3686	173	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
19	U	27	0	11	5	0
All	All	35854	0	35424	979	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 14.

The worst 5 of 979 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)
1:A:11:SER:N	2:B:1135:TYR:HH	1.54	1.05
1:A:1210:TRP:HD1	1:A:1281:ASP:HB2	1.35	0.88
16:U:31:THR:O	16:U:34:GLN:N	2.07	0.87
1:A:1128:ILE:HG23	1:A:1414:ILE:HB	1.57	0.86
1:A:1130:ILE:HG12	1:A:1413:ALA:HB2	1.64	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	1418/1970 (72%)	1323 (93%)	94 (7%)	1 (0%)	48 78
2	B	1128/1174 (96%)	1052 (93%)	73 (6%)	3 (0%)	37 67
3	C	253/275 (92%)	238 (94%)	15 (6%)	0	100 100
4	D	126/142 (89%)	118 (94%)	8 (6%)	0	100 100
5	E	207/210 (99%)	193 (93%)	13 (6%)	1 (0%)	25 57
6	F	80/127 (63%)	78 (98%)	2 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
8	H	146/150 (97%)	134 (92%)	11 (8%)	1 (1%)	19	51
9	I	112/125 (90%)	104 (93%)	7 (6%)	1 (1%)	14	47
10	J	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
11	K	113/117 (97%)	107 (95%)	6 (5%)	0	100	100
12	L	42/58 (72%)	36 (86%)	6 (14%)	0	100	100
16	U	453/991 (46%)	397 (88%)	50 (11%)	6 (1%)	10	40
All	All	4312/5578 (77%)	4002 (93%)	297 (7%)	13 (0%)	38	67

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	581	LYS
5	E	46	ASP
8	H	105	SER
16	U	78	PRO
16	U	328	VAL

### 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	1258/1748 (72%)	1198 (95%)	60 (5%)	21	48
2	B	993/1028 (97%)	962 (97%)	31 (3%)	35	57
3	C	234/252 (93%)	224 (96%)	10 (4%)	25	50
4	D	106/126 (84%)	103 (97%)	3 (3%)	38	60
5	E	189/192 (98%)	176 (93%)	13 (7%)	13	39
6	F	71/111 (64%)	67 (94%)	4 (6%)	17	45
7	G	147/153 (96%)	139 (95%)	8 (5%)	18	46
8	H	129/131 (98%)	119 (92%)	10 (8%)	10	36
9	I	103/112 (92%)	96 (93%)	7 (7%)	13	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	56/56 (100%)	54 (96%)	2 (4%)	30	55
11	K	104/106 (98%)	100 (96%)	4 (4%)	28	53
12	L	41/55 (74%)	40 (98%)	1 (2%)	44	63
16	U	391/820 (48%)	348 (89%)	43 (11%)	5	24
All	All	3822/4890 (78%)	3626 (95%)	196 (5%)	22	47

5 of 196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	198	GLU
9	I	103	ARG
6	F	90	LEU
8	H	23	ASP
11	K	104	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	157	GLN
5	E	71	GLN
16	U	433	HIS
3	C	173	HIS
4	D	66	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	10/20 (50%)	2 (20%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	11	A
14	P	13	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, 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
19	ADP	U	1000	-	24,29,29	3.29	8 (33%)	29,45,45	2.16	3 (10%)

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
19	ADP	U	1000	-	-	8/12/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	U	1000	ADP	C3'-C4'	-8.66	1.31	1.53
19	U	1000	ADP	O4'-C4'	7.64	1.62	1.45
19	U	1000	ADP	O4'-C1'	-7.50	1.31	1.40
19	U	1000	ADP	PA-O3A	5.25	1.65	1.59
19	U	1000	ADP	C6-N6	3.19	1.45	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	U	1000	ADP	C1'-N9-C4	8.42	141.43	126.64
19	U	1000	ADP	N3-C2-N1	-6.52	119.82	128.67
19	U	1000	ADP	C4'-O4'-C1'	-2.16	107.94	109.92

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

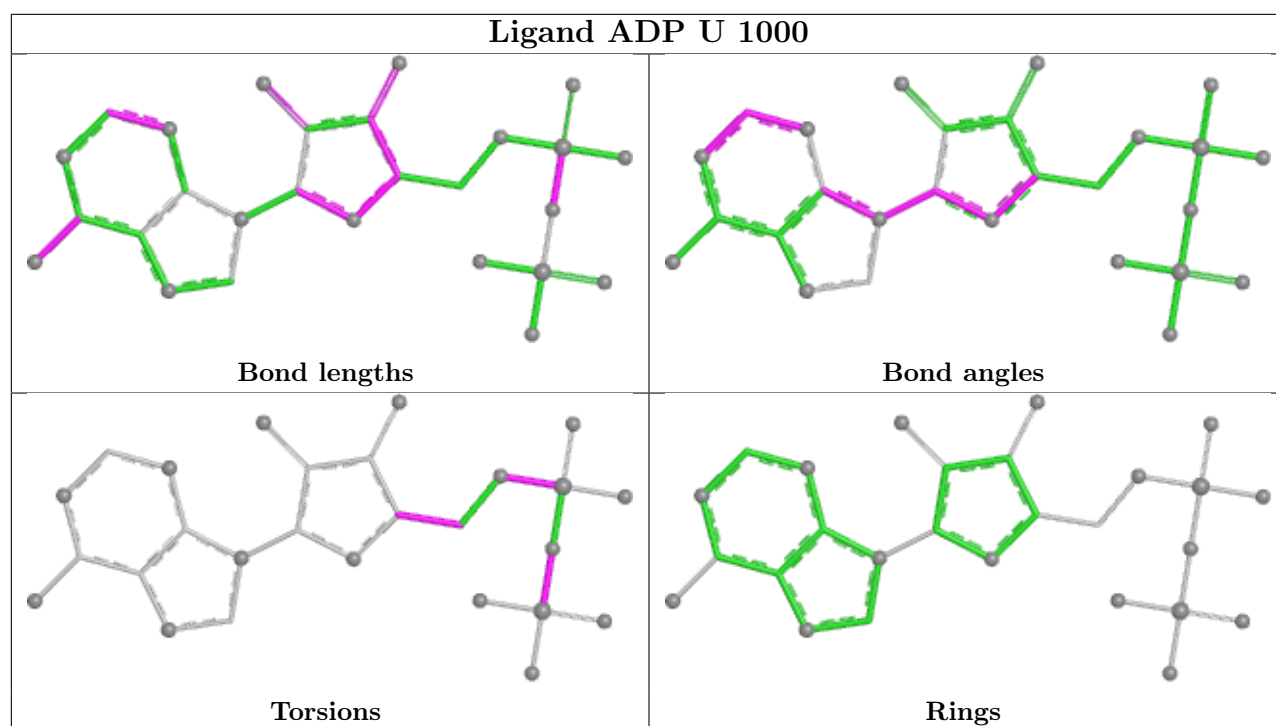
Mol	Chain	Res	Type	Atoms
19	U	1000	ADP	PA-O3A-PB-O2B
19	U	1000	ADP	PA-O3A-PB-O3B
19	U	1000	ADP	C5'-O5'-PA-O1A
19	U	1000	ADP	C5'-O5'-PA-O2A
19	U	1000	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	U	1000	ADP	5	0

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

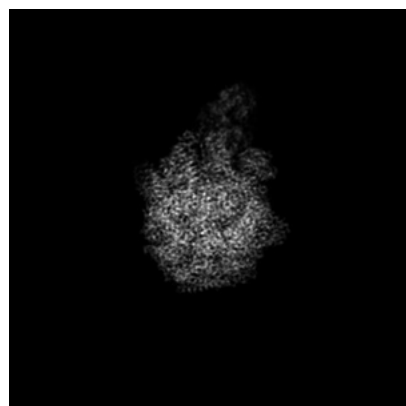
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48076. These allow visual inspection of the internal detail of the map and identification of artifacts.

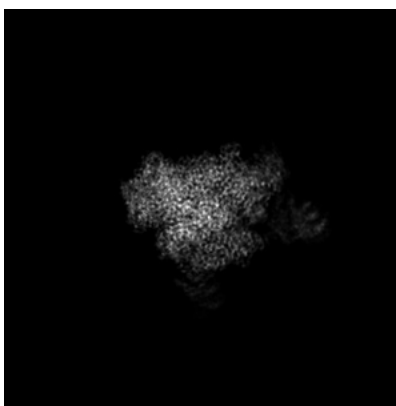
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

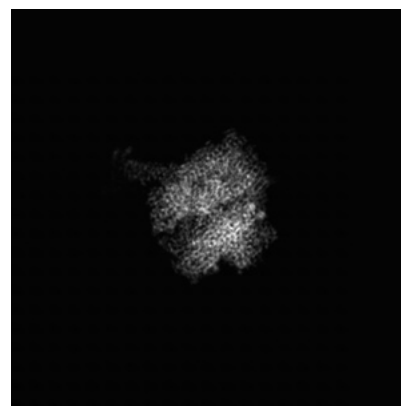
#### 6.1.1 Primary map



X

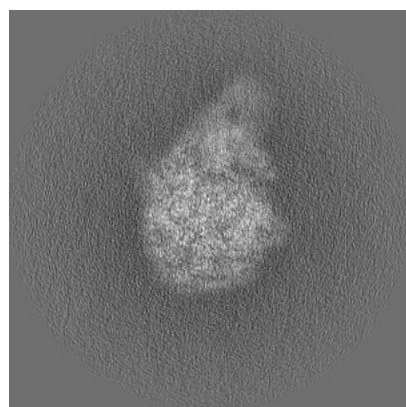


Y

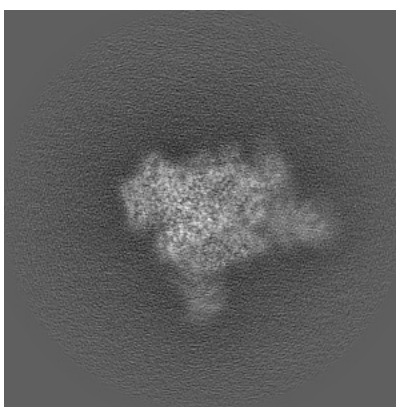


Z

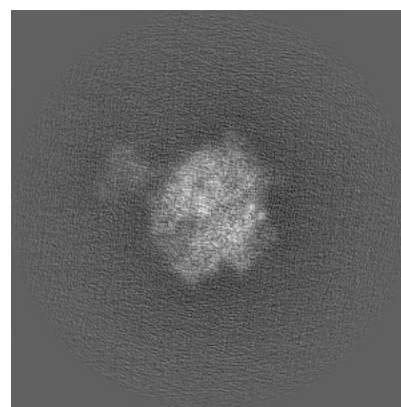
#### 6.1.2 Raw map



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

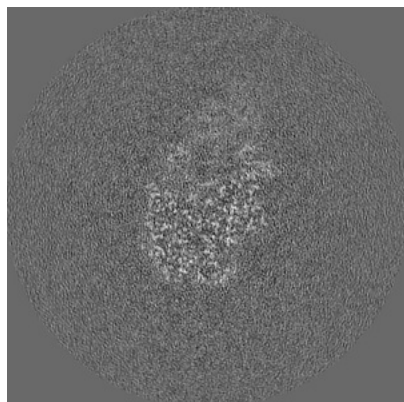


Y Index: 160

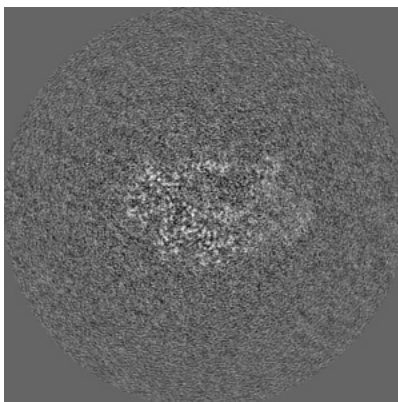


Z Index: 160

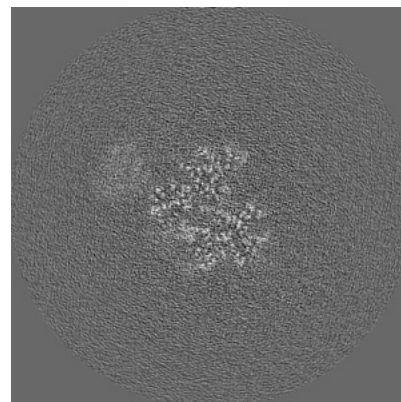
### 6.2.2 Raw map



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: 165

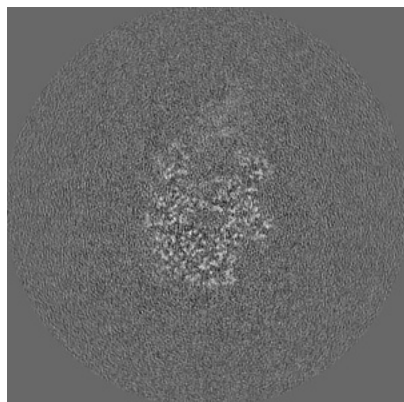


Y Index: 134

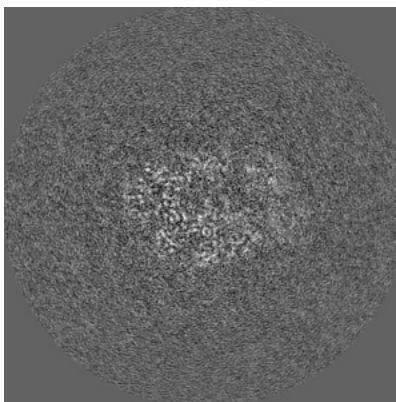


Z Index: 157

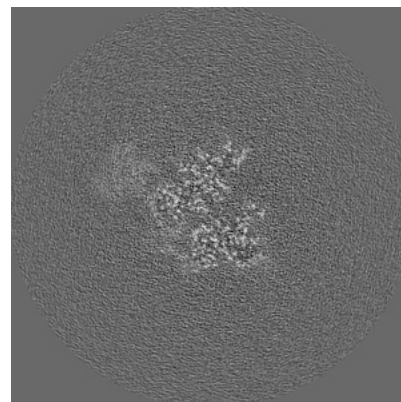
### 6.3.2 Raw map



X Index: 165



Y Index: 159

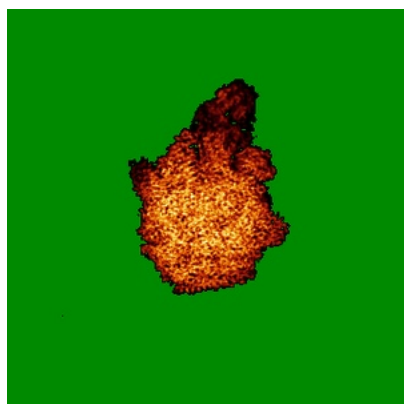


Z Index: 156

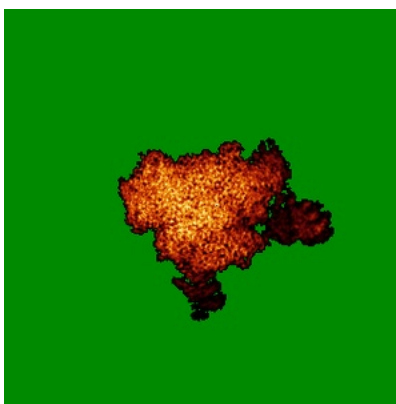
The images above show the largest variance slices of the map in three orthogonal directions.

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

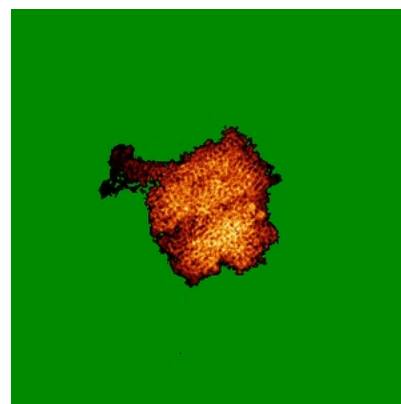
### 6.4.1 Primary map



X

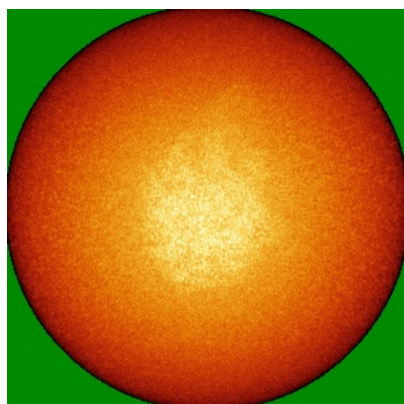


Y

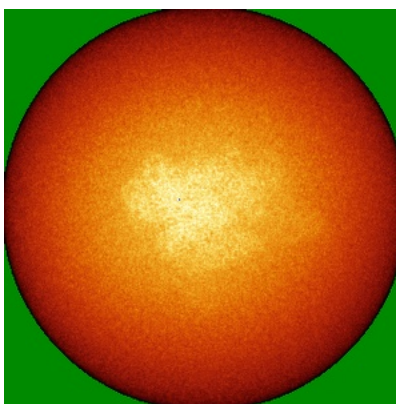


Z

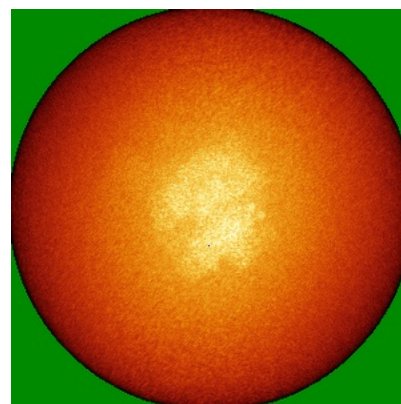
### 6.4.2 Raw map



X



Y

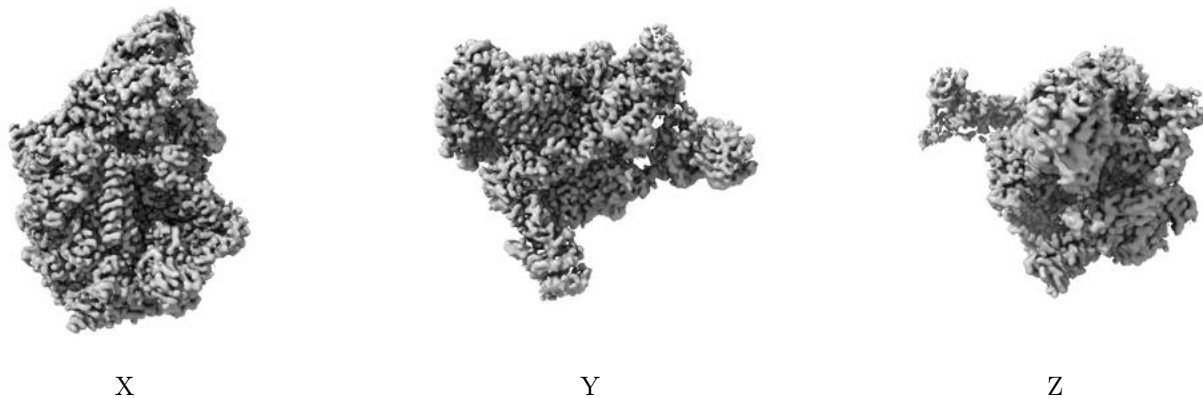


Z

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.

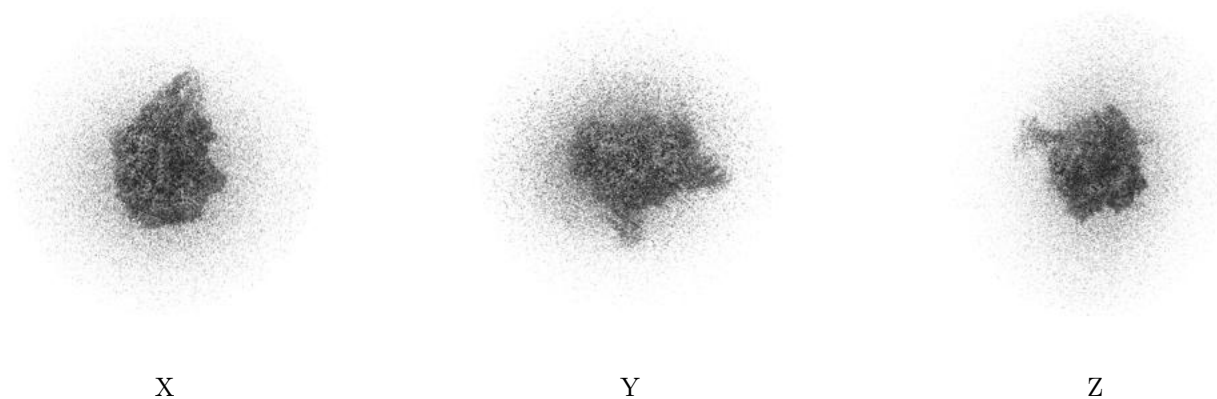
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

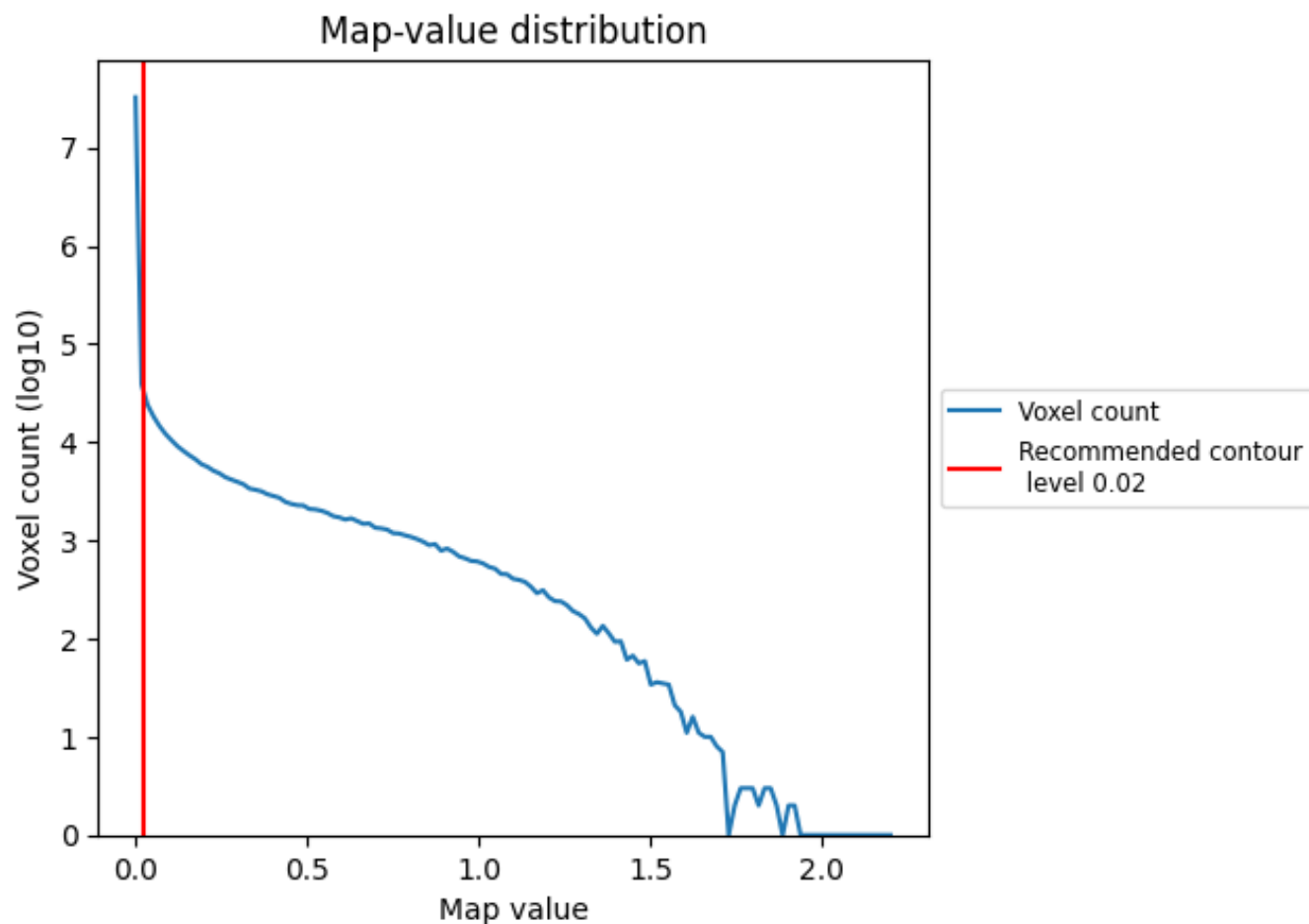
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

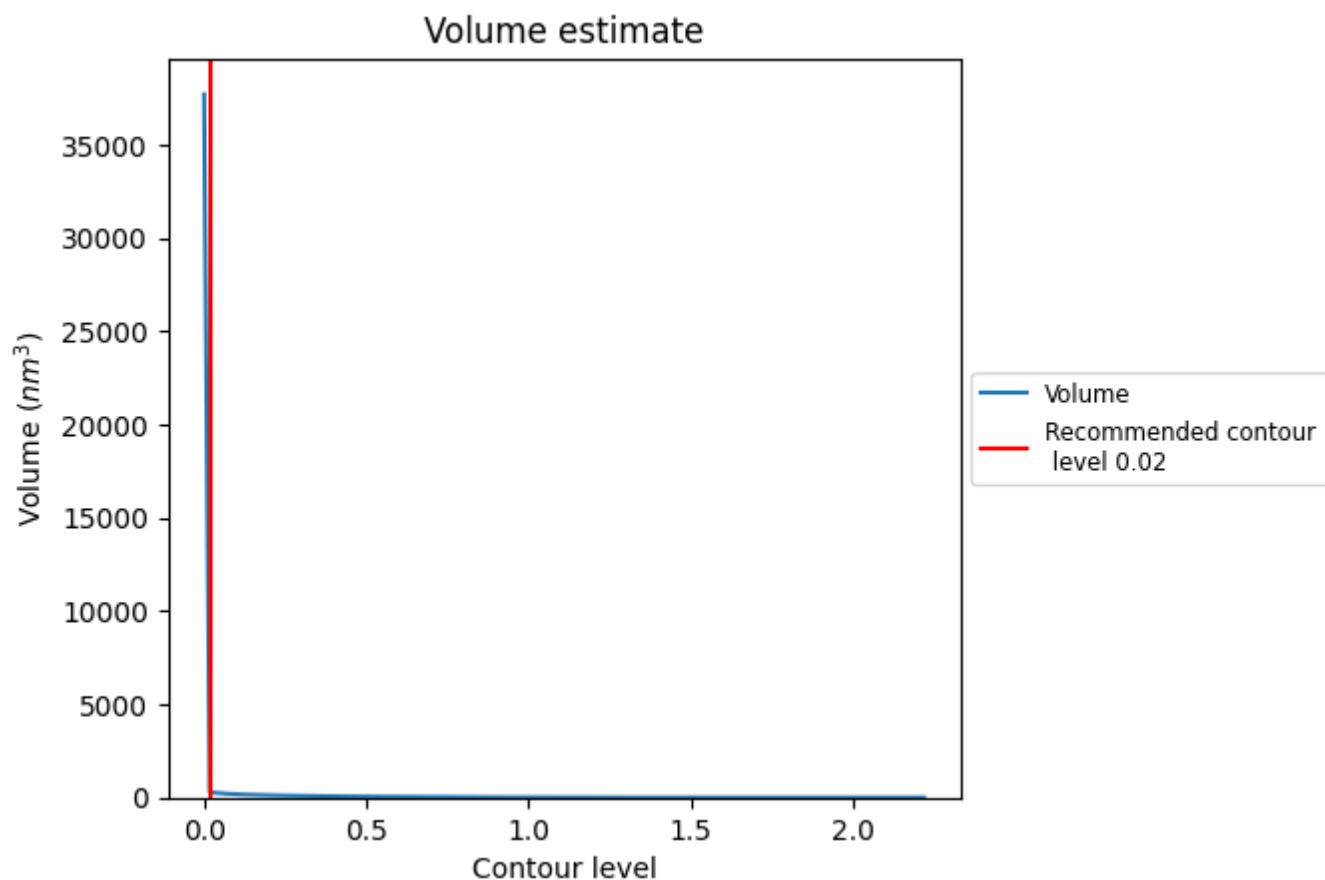
This section contains the results of statistical analysis of the map.

### 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.

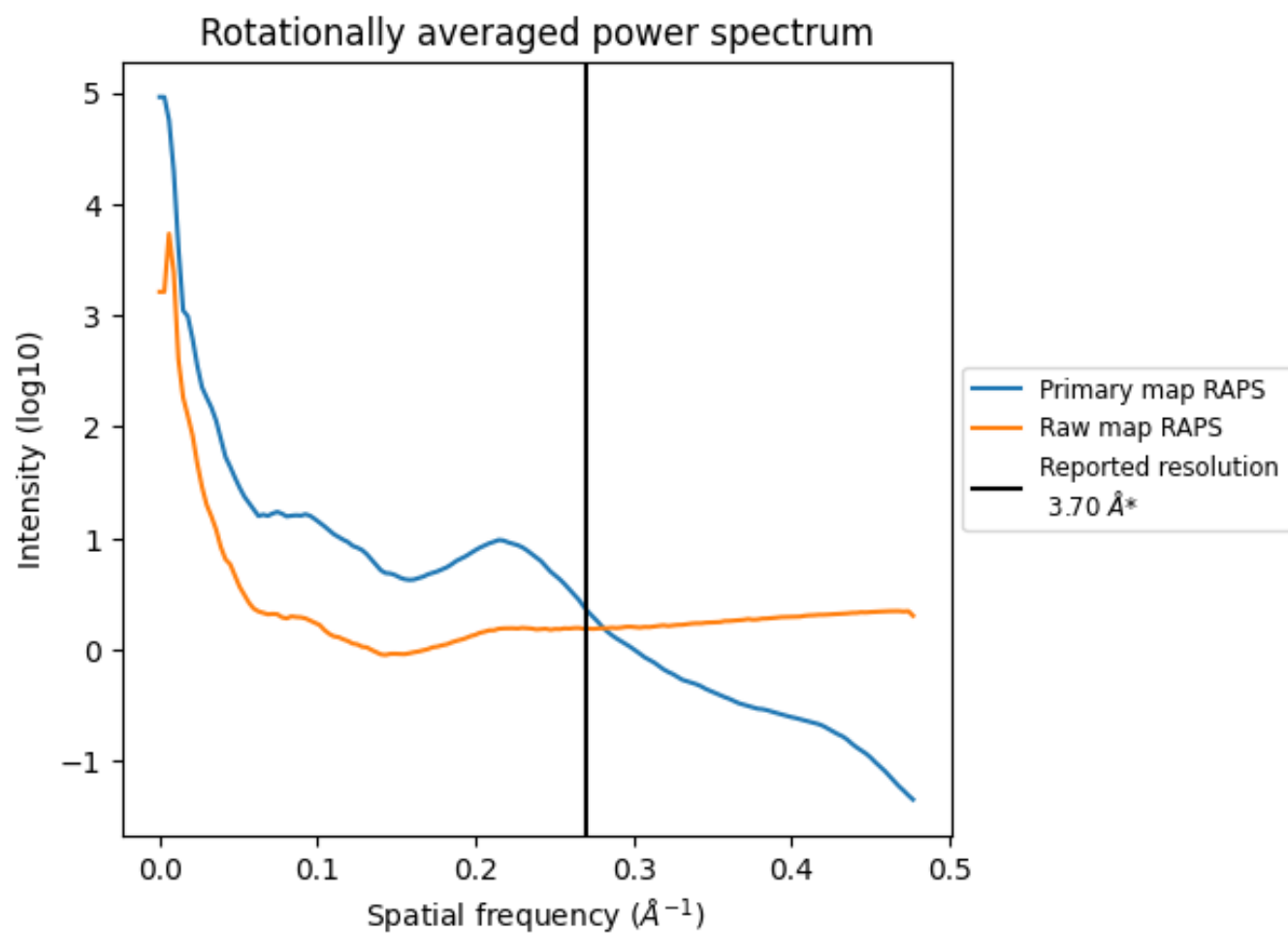
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 287  $\text{nm}^3$ ; this corresponds to an approximate mass of 260 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 ⓘ

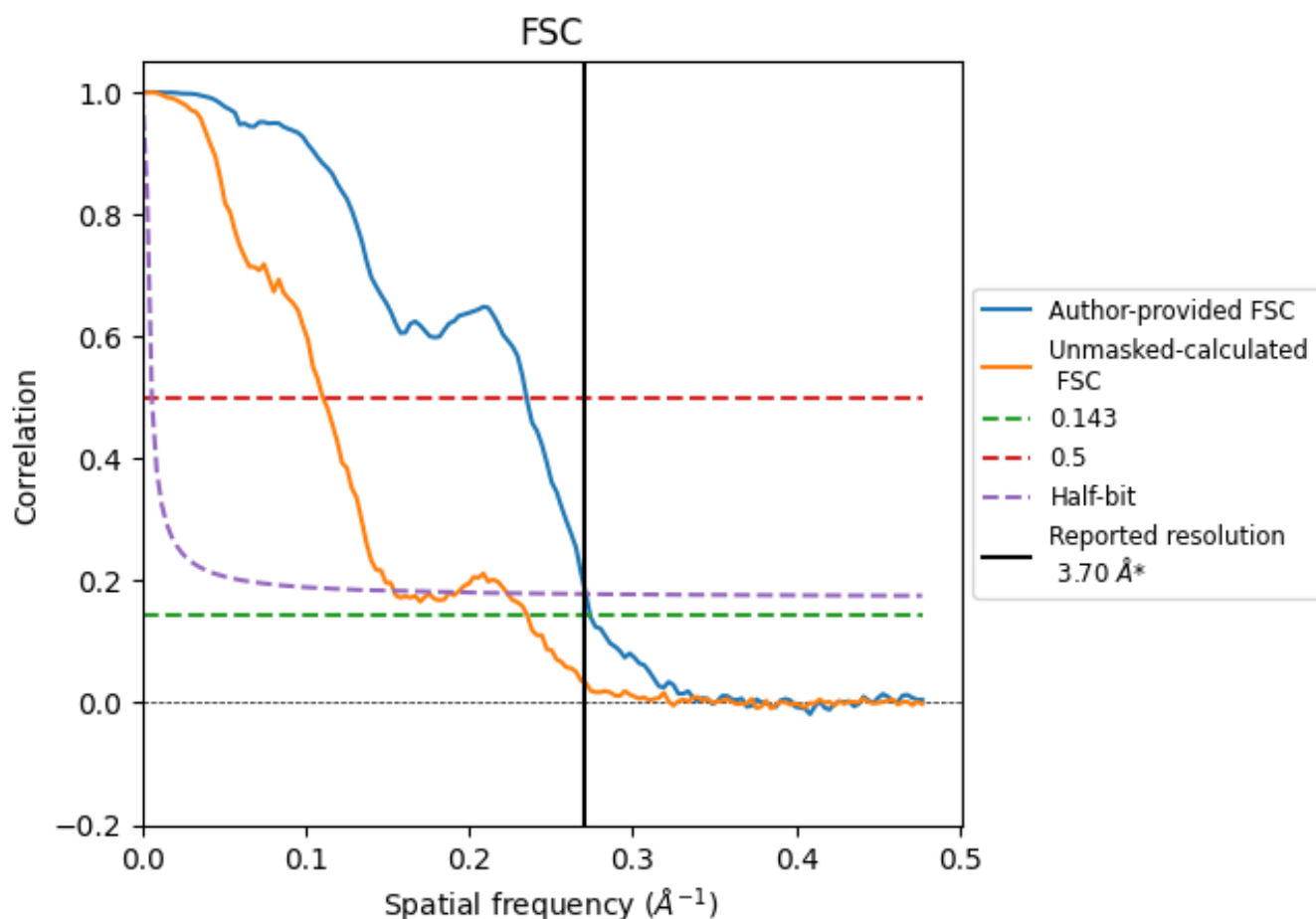


\*Reported resolution corresponds to spatial frequency of 0.270  $\text{\AA}^{-1}$

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



## 8.2 Resolution estimates [i](#)

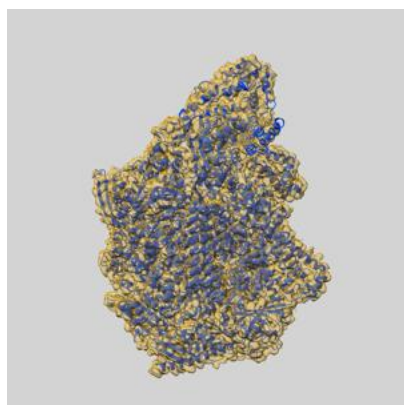
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.65	4.25	3.68
Unmasked-calculated*	4.24	9.04	6.49

\*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 4.24 differs from the reported value 3.7 by more than 10 %

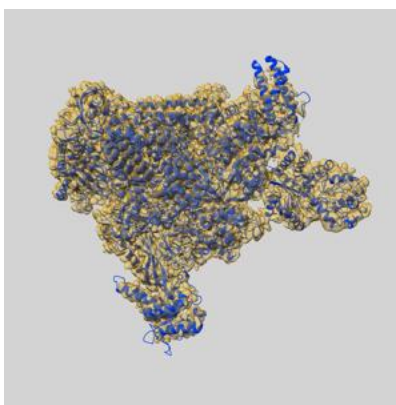
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48076 and PDB model 9EI4. Per-residue inclusion information can be found in section [3](#) on page [8](#).

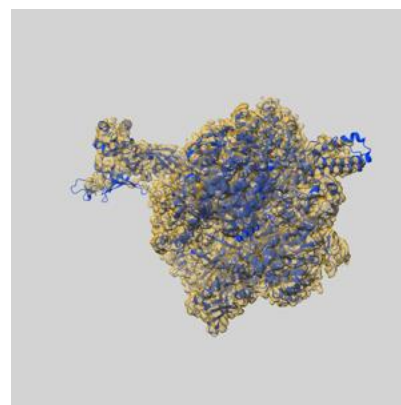
### 9.1 Map-model overlay [i](#)



X



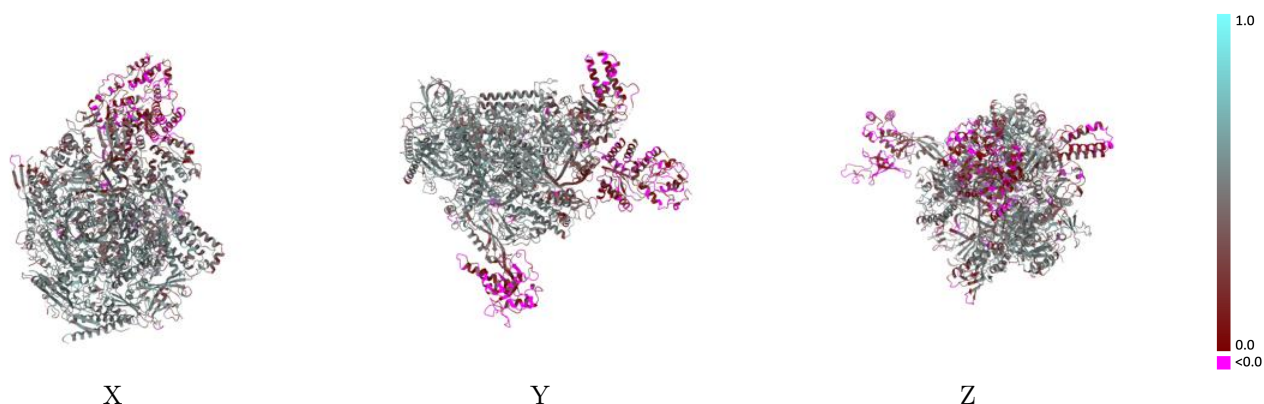
Y



Z

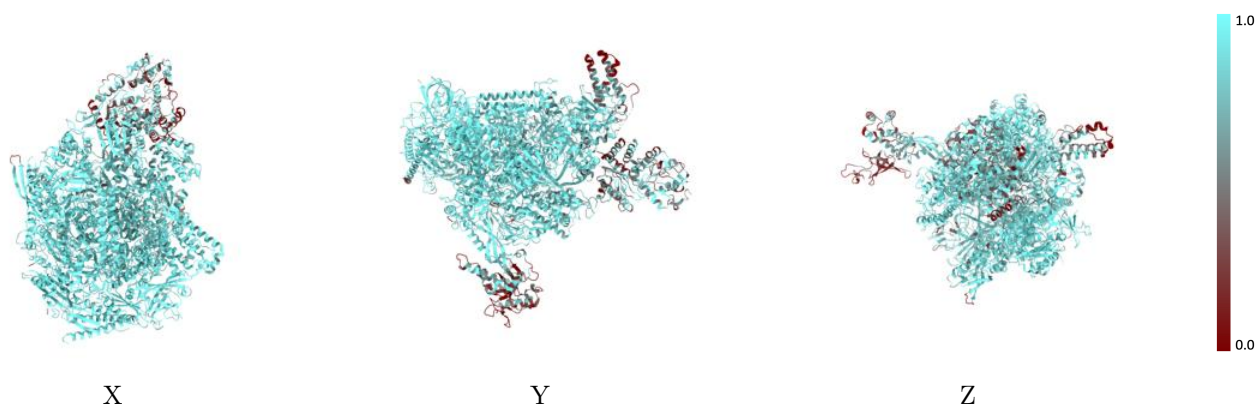
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



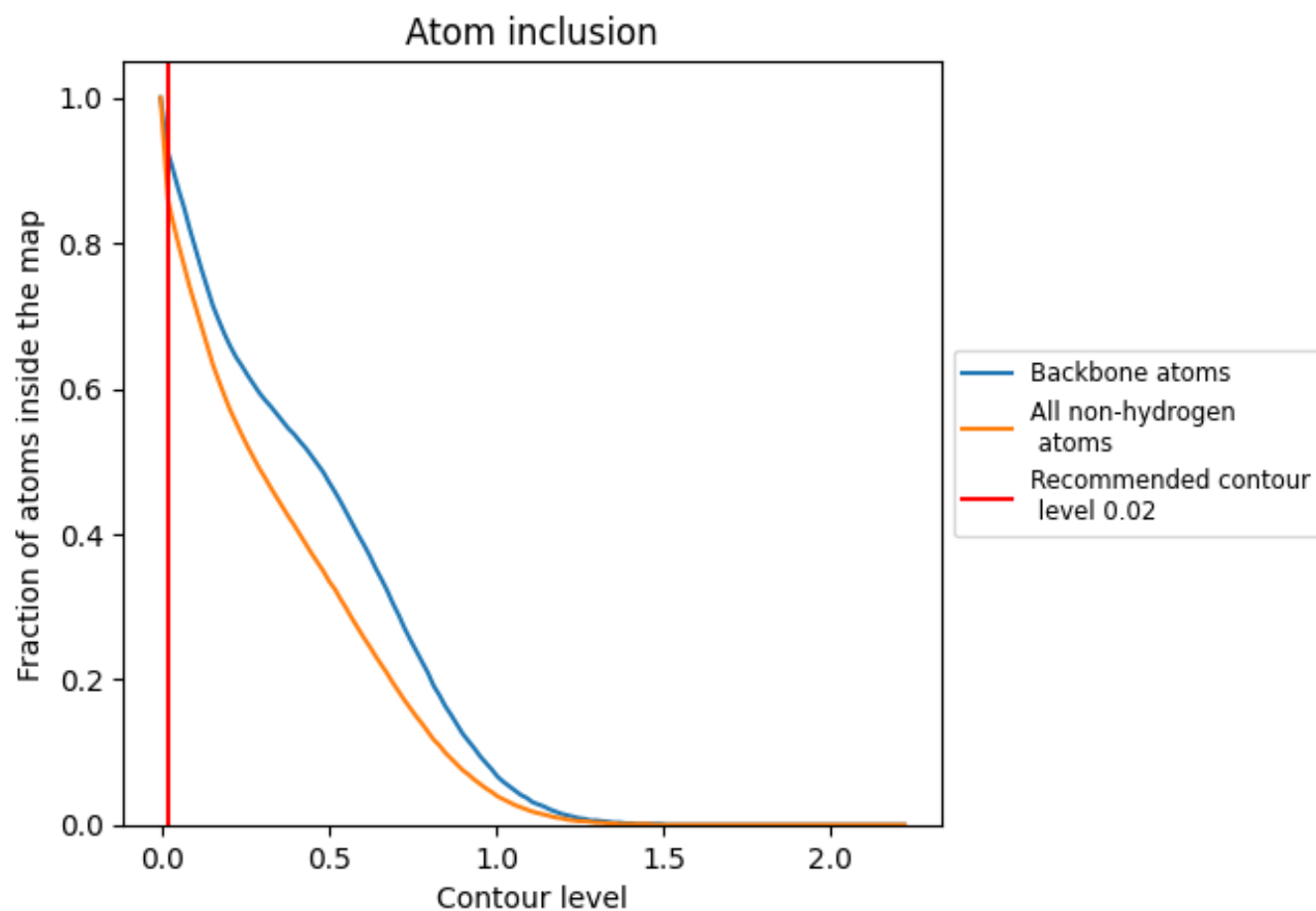
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).



































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8610	 0.4100
A	 0.9330	 0.4750
B	 0.9270	 0.4780
C	 0.9440	 0.4990
D	 0.5160	 0.0720
E	 0.9040	 0.4380
F	 0.9140	 0.4850
G	 0.5060	 0.1790
H	 0.9210	 0.4630
I	 0.8880	 0.4140
J	 0.9440	 0.5060
K	 0.9570	 0.4990
L	 0.8880	 0.4300
N	 0.8390	 0.2690
P	 0.8830	 0.3870
T	 0.9150	 0.3960
U	 0.5620	 0.1050

