

wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 11:02 am GMT

PDB ID : 5M3F EMDB ID : EMD-4147

Title: Yeast RNA polymerase I elongation complex at 3.8A

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Deposited on : 2016-10-14

Resolution : 3.80 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
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43

Mogul : 1.8.4, CSD as541be (2020)

MolProbity : 4.02b-467

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

MapQ: 1.9.9

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

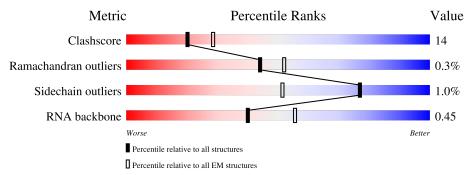
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 Å.

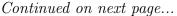
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive $(\# \mathrm{Entries})$	${ m EM\ structures} \ (\#{ m Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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	<u> </u>	
			38%		
1	A	1664	65%	22%	12%
			32%		
2	В	1203	71%	27%	•
			35%		
3	С	335	72%	19%	9%
			67%	_	
4	Е	215	81%		17% •
			30%		
5	F	155	49% 15%	35%	
			36%		
6	Н	146	71%	19%	10%
			50%		
7	I	125	30% 20%	50%	





Mol	Chain	Length			Qua	dity of c	hain	
8	J	70	17%		76%			23% •
9	K	142	22%	57%		•	14%	29%
10	L	70	23%	51%		11%	0	37%
11	Т	39	26%	51%	3	38%		36%
12	U	39	13%	23%	_		64%	
13	R	20	25% 15%	20%	5%		60%	
14	M	415	26% 17%	8% •			74%	
15	N	233		42%	·%	19%	-	38%
16	D	137	28%		10% •		61%	
17	G	326		45%	, o	13%		41%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	SO4	В	1301	_	_	X	-



2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 34032 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 I subunit RPA190.

Mol	Chain	Residues		A	AltConf	Trace			
1	A	1459	Total 11526	C 7281	N 2004	O 2180	S 61	0	0

• Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues		A	AltConf	Trace			
2	В	1177	Total 9350	C 5913	N 1639	O 1747	S 51	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	С	305	Total 2423	C 1539	N 416	O 460	S 8	0	0

• Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues		At	AltConf	Trace			
4	Е	212	Total 1735	C 1102	N 306	O 316	S 11	0	0

• Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues		At	oms	AltConf	Trace		
5	F	100	Total 823	C 522	N 144	O 154	S 3	0	0

• Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues		At	oms	AltConf	Trace		
6	Н	131	Total 1052	C 664	N 176	O 208	S 4	0	0



• Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues		Ato	ms	AltConf	Trace		
7	т	62	Total	С	N	О	S	0	0
1	1	63	466	292	77	93	4	0	0

• Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues		At	oms	AltConf	Trace		
8	J	69	Total 569	C 362	N 101	O 100	S 6	0	0

• Molecule 9 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms				AltConf	Trace	
9	К	101	Total 793	C 496	N 130	O 162	S 5	0	0

• Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms			AltConf	Trace		
10	Т	4.4	Total	С	N	О	S	0	0
10	П	44	352	217	70	61	4	0	U

• Molecule 11 is a DNA chain called template DNA.

Mol	Chain	Residues		At	oms			AltConf	Trace
11	Т	25	Total 509	C 244	N 95	O 146	P 24	0	0

• Molecule 12 is a DNA chain called non-template DNA.

Mol	Chain	Residues		Atoms				AltConf	Trace
12	U	14	Total 285	C 138	N 51	O 83	P 13	0	0

• Molecule 13 is a RNA chain called RNA.

Mol	Chain	Residues		\mathbf{At}	oms			AltConf	Trace
13	D	Q	Total	С	N	О	Р	0	0
10	16	8	173	77	34	54	8	0	0

• Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA49.



Mol	Chain	Residues		Ato	ms		AltConf	Trace
14	M	108	Total	C 5.40	N	0	0	0
			856	543	142	171		

• Molecule 15 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms			AltConf	Trace		
15	N	1.45	Total	С	N	О	S	0	0
10	IN .	145	1151	735	188	224	4	U	U

• Molecule 16 is a protein called DNA-directed RNA polymerase I subunit RPA14.

M	ol	Chain	Residues	Atoms			AltConf	Trace	
16	j	D	54	Total 431	C 270	N 73	O 88	0	0

• Molecule 17 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms			AltConf	Trace		
17	С	193	Total	С	N	О	S	0	0
11	G	195	1526	985	262	274	5	0	U

• Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

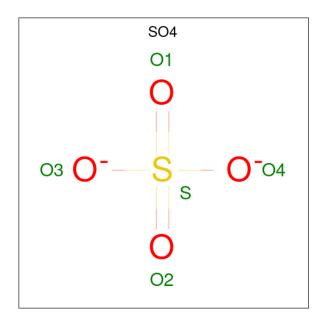
Mol	Chain	Residues	Atoms	AltConf
18	A	2	Total Zn 2 2	0
18	В	1	Total Zn 1 1	0
18	I	1	Total Zn 1 1	0
18	J	1	Total Zn 1 1	0
18	L	1	Total Zn 1 1	0

• Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

 \bullet Molecule 20 is SULFATE ION (three-letter code: SO4) (formula: $\mathrm{O_4S}).$





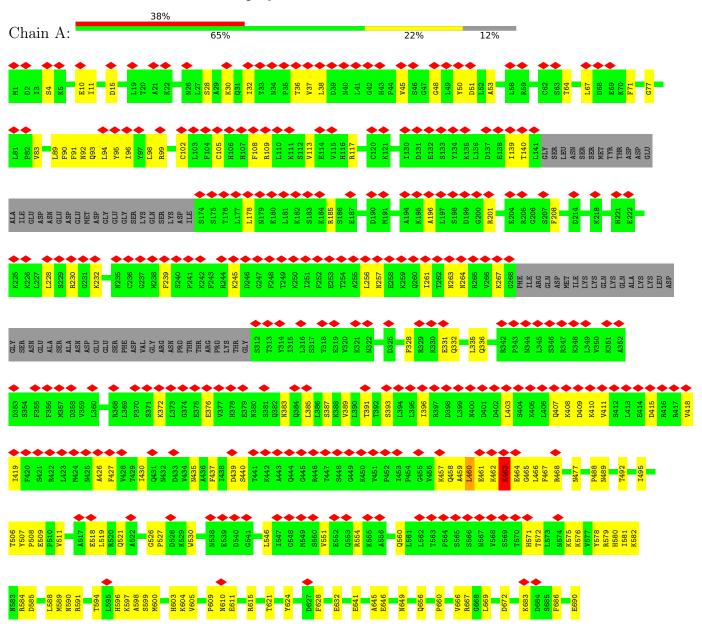
Mol	Chain	Residues	Atoms	AltConf
20	В	1	Total O S 5 4 1	0



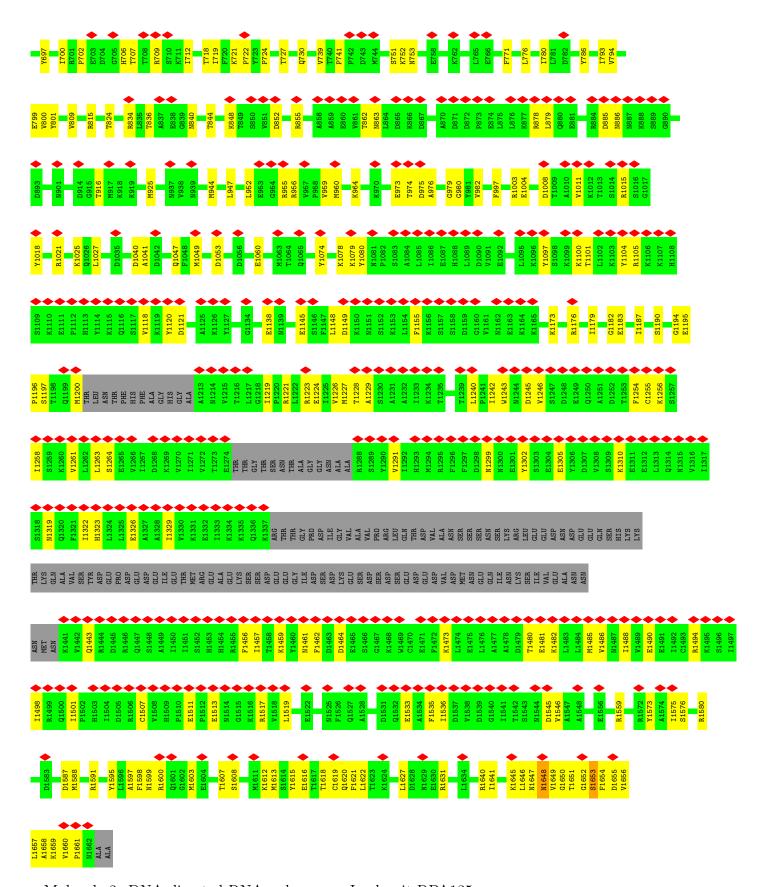
3 Residue-property plots (i)

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

• Molecule 1: DNA-directed RNA polymerase I subunit RPA190

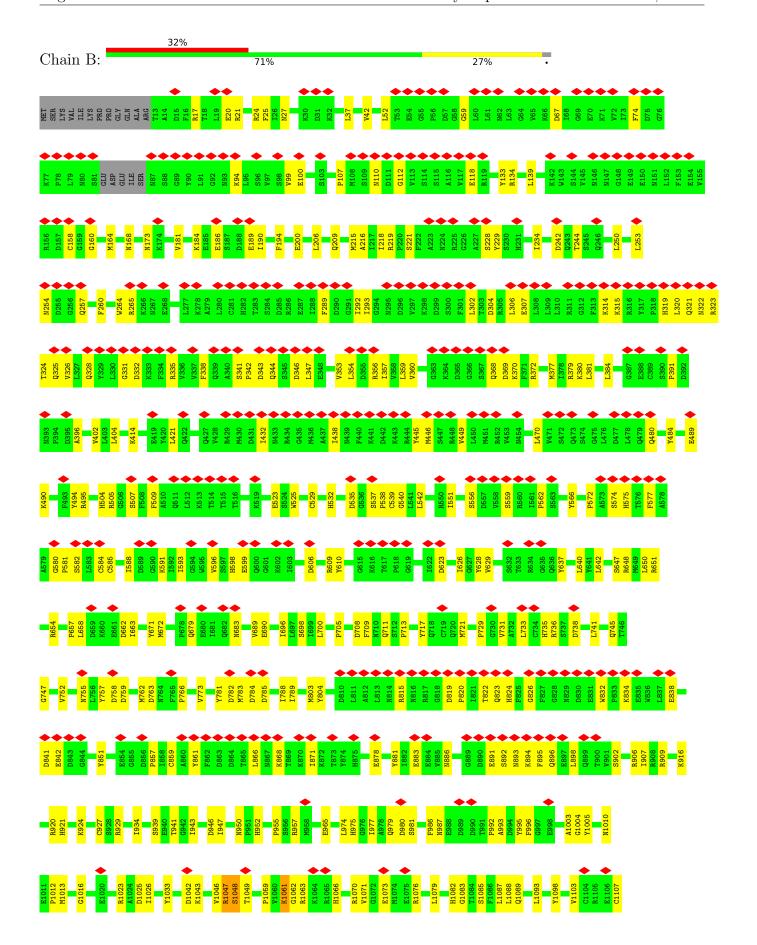




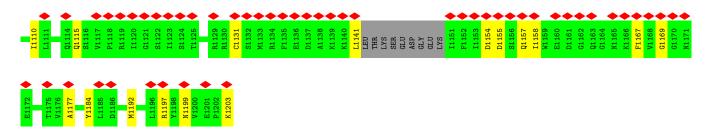


• Molecule 2: DNA-directed RNA polymerase I subunit RPA135

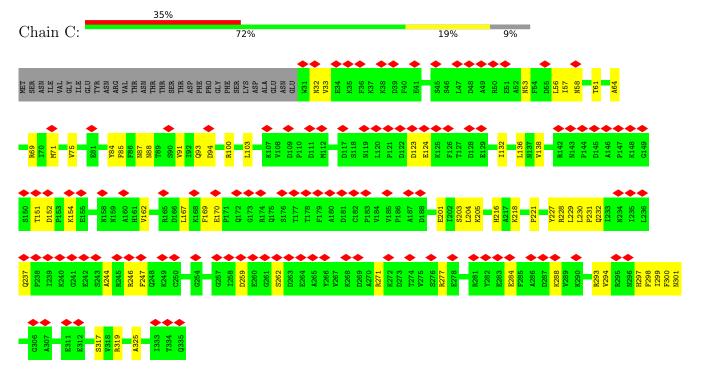




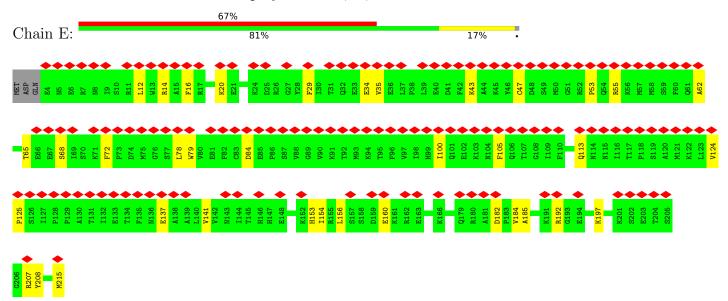




• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

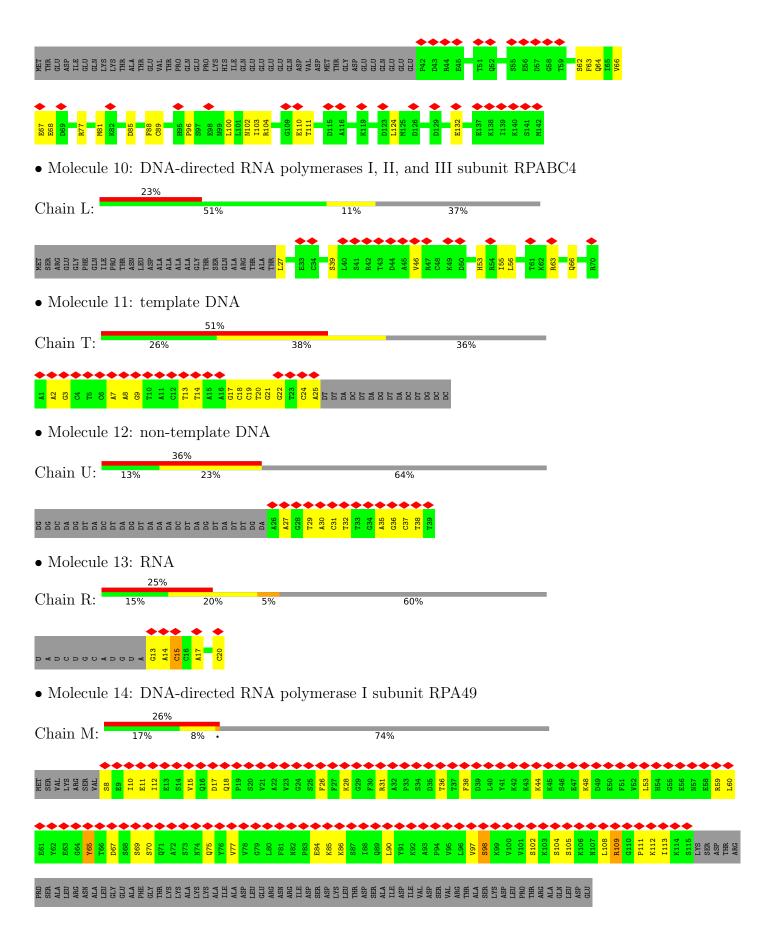


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

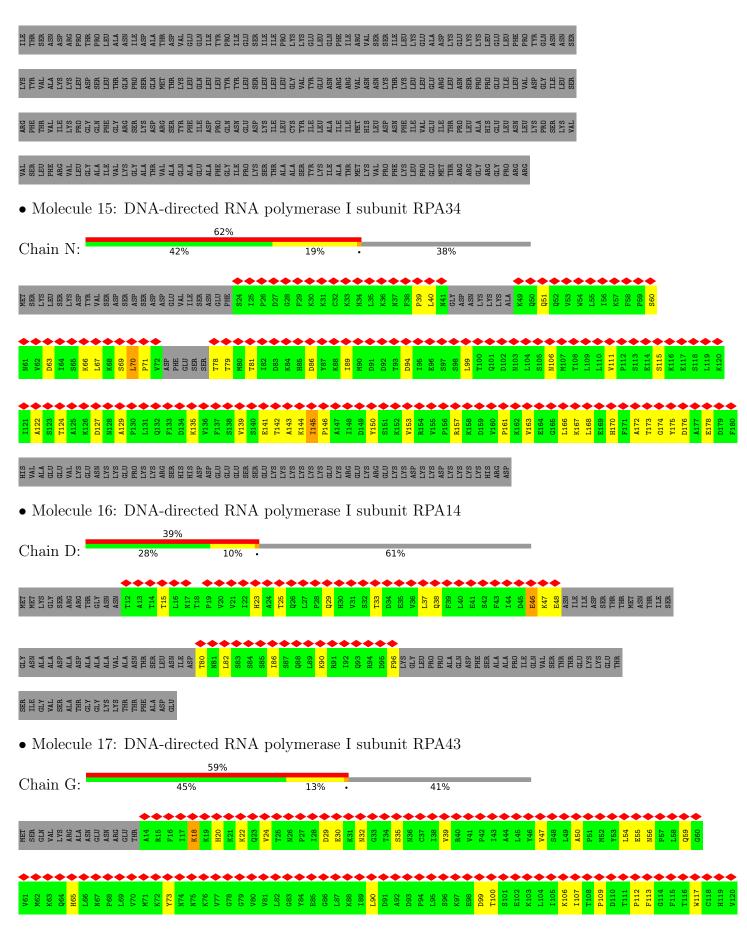




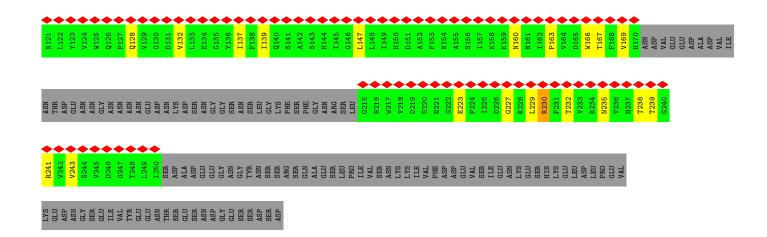














4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	94000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.218	Depositor
Minimum map value	-0.142	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	241.49998, 241.49998, 241.49998	wwPDB
Map dimensions	230, 230, 230	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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: SO4, ZN, 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	Во	ond angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.35	0/11738	0.50	0/15851
2	В	0.37	0/9557	0.52	0/12918
3	С	0.35	0/2475	0.49	0/3354
4	Е	0.31	0/1771	0.46	0/2383
5	F	0.32	0/838	0.46	0/1129
6	Н	0.34	0/1070	0.49	0/1449
7	I	0.26	0/472	0.48	0/639
8	J	0.37	0/578	0.47	0/775
9	K	0.35	0/804	0.51	0/1083
10	L	0.33	0/354	0.50	0/468
11	Т	0.60	0/571	0.87	0/879
12	U	0.58	0/319	0.97	0/491
13	R	0.48	0/193	1.08	0/299
14	M	0.41	0/872	0.55	0/1170
15	N	0.42	0/1172	0.57	1/1580 (0.1%)
16	D	0.38	0/436	0.51	0/591
17	G	0.37	0/1564	0.66	3/2127 (0.1%)
All	All	0.37	0/34784	0.54	4/47186 (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	В	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
17	G	241	ARG	NE-CZ-NH1	11.89	126.25	120.30
17	G	241	ARG	NE-CZ-NH2	-11.70	114.45	120.30
17	G	241	ARG	CD-NE-CZ	6.04	132.05	123.60
15	N	145	ILE	C-N-CD	5.04	138.99	128.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	В	1048	SER	Peptide
2	В	1061	LYS	Peptide
2	В	319	HIS	Peptide

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	11526	0	11614	326	0
2	В	9350	0	9240	362	0
3	С	2423	0	2412	68	0
4	Е	1735	0	1764	25	0
5	F	823	0	840	46	0
6	Н	1052	0	1021	20	0
7	I	466	0	466	29	0
8	J	569	0	585	21	0
9	K	793	0	790	17	0
10	L	352	0	376	7	0
11	Т	509	0	283	16	0
12	U	285	0	161	9	0
13	R	173	0	89	6	0
14	M	856	0	852	97	0
15	N	1151	0	1169	99	0
16	D	431	0	428	11	0
17	G	1526	0	1540	90	0
18	A	2	0	0	0	0
18	В	1	0	0	0	0
18	I	1	0	0	0	0
18	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	L	1	0	0	0	0
19	A	1	0	0	0	0
20	В	5	0	0	2	0
All	All	34032	0	33630	918	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 918 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
2:B:328:GLN:NE2	14:M:112:LYS:HA	1.22	1.49
1:A:1661:PRO:CD	17:G:55:GLU:CA	1.86	1.44
2:B:987:ASN:ND2	15:N:157:ARG:CD	1.85	1.39
2:B:328:GLN:CD	14:M:112:LYS:HA	1.39	1.39
3:C:301:ASN:ND2	15:N:173:THR:HB	1.37	1.37

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	1447/1664 (87%)	1325 (92%)	119 (8%)	3 (0%)	47	79
2	В	1171/1203 (97%)	1109 (95%)	60 (5%)	2 (0%)	47	79
3	С	303/335 (90%)	286 (94%)	17 (6%)	0	100	100
4	E	210/215 (98%)	200 (95%)	10 (5%)	0	100	100
5	F	98/155 (63%)	96 (98%)	2 (2%)	0	100	100
6	Н	127/146 (87%)	124 (98%)	3 (2%)	0	100	100
7	I	61/125 (49%)	53 (87%)	8 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
8	J	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
9	K	99/142 (70%)	93 (94%)	6 (6%)	0	100	100
10	L	42/70 (60%)	37 (88%)	5 (12%)	0	100	100
14	M	106/415~(26%)	96 (91%)	8 (8%)	2 (2%)	8	42
15	N	139/233 (60%)	122 (88%)	14 (10%)	3 (2%)	6	39
16	D	50/137 (36%)	48 (96%)	2 (4%)	0	100	100
17	G	189/326 (58%)	174 (92%)	13 (7%)	2 (1%)	14	51
All	All	4109/5236 (78%)	3826 (93%)	271 (7%)	12 (0%)	44	74

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	LYS
1	A	1653	SER
1	A	91	PHE
2	В	1047	ARG
14	M	85	LYS

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	Percer	ntiles
1	A	1289/1465 (88%)	1284 (100%)	5 (0%)	91	95
2	В	1030/1053 (98%)	1030 (100%)	0	100	100
3	С	269/296 (91%)	269 (100%)	0	100	100
4	E	194/197 (98%)	194 (100%)	0	100	100
5	F	90/137 (66%)	90 (100%)	0	100	100
6	Н	115/128 (90%)	115 (100%)	0	100	100
7	I	55/110 (50%)	55 (100%)	0	100	100
8	J	64/65 (98%)	64 (100%)	0	100	100
9	K	91/130 (70%)	91 (100%)	0	100	100

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Mol	Chain	hain Analysed Rotameric Outliers		Outliers	Percentiles		
10	L	39/57~(68%)	39 (100%)	0	100 100)	
14	M	98/371 (26%)	88 (90%)	10 (10%)	7 31		
15	N	135/220 (61%)	129 (96%)	6 (4%)	28 57		
16	D	52/116 (45%)	47 (90%)	5 (10%)	8 34		
17	G	171/291 (59%)	159 (93%)	12 (7%)	15 46		
All	All	3692/4636 (80%)	3654 (99%)	38 (1%)	77 86		

5 of 38 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
17	G	35	SER
17	G	230	ARG
17	G	39	VAL
17	G	167	THR
17	G	243	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	59	GLN
17	G	235	ASN
5	F	100	GLN
9	K	106	GLN
2	В	27	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	7/20 (35%)	2 (28%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	R	15	С
13	R	17	A

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 7 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	В	ond leng	$_{ m gths}$	В	ond ang	gles
WIOI	Moi Type Chain Res		nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	SO4	В	1301	-	4,4,4	0.16	0	6,6,6	0.09	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	В	1301	SO4	2	0

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.



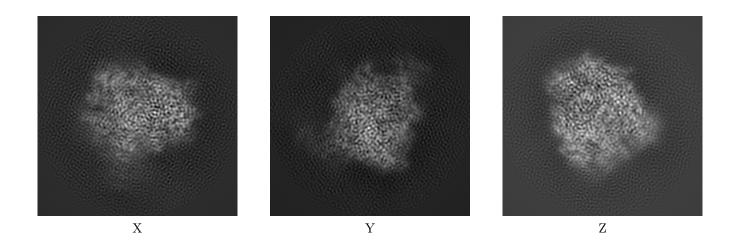
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4147. These allow visual inspection of the internal detail of the map and identification of artifacts.

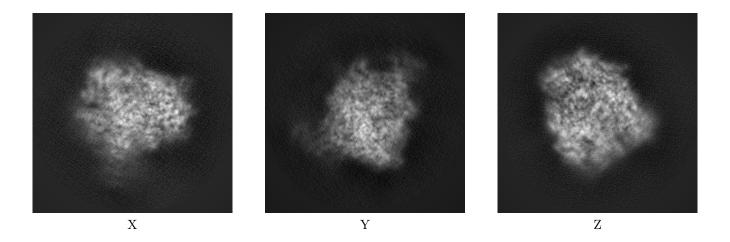
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map

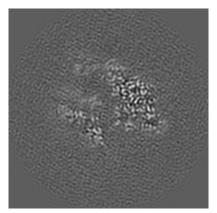


The images above show the map projected in three orthogonal directions.

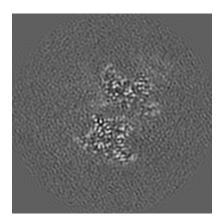


6.2 Central slices (i)

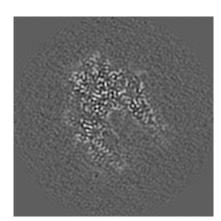
6.2.1 Primary map





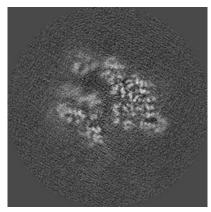


Y Index: 115

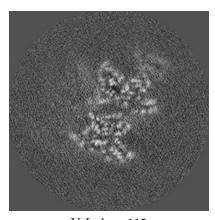


Z Index: 115

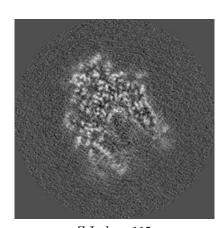
6.2.2 Raw map



X Index: 115



Y Index: 115



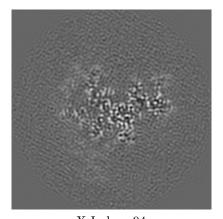
Z Index: 115

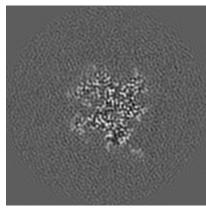
The images above show central slices of the map in three orthogonal directions.

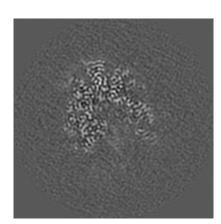


6.3 Largest variance slices (i)

6.3.1 Primary map





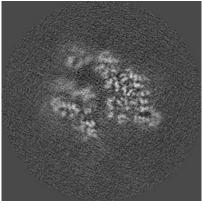


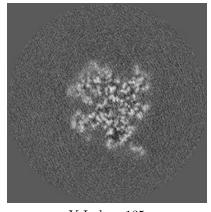
X Index: 94

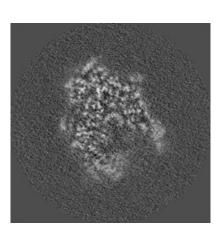
Y Index: 135

Z Index: 122

6.3.2 Raw map







X Index: 115

Y Index: 135

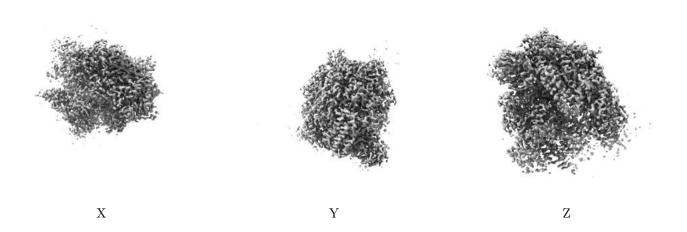
Z Index: 113

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



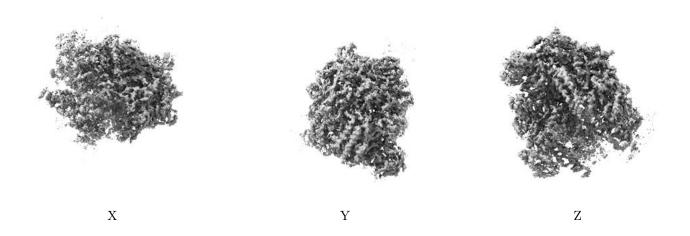
6.4 Orthogonal surface views (i)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

6.5 Mask visualisation (i)

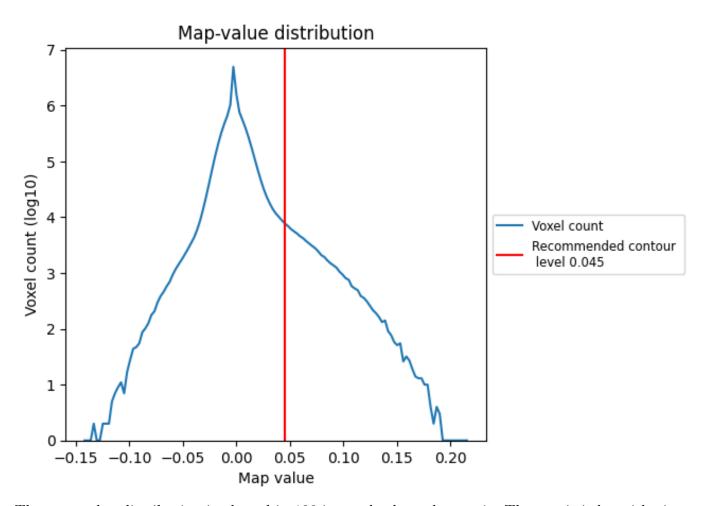
This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

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

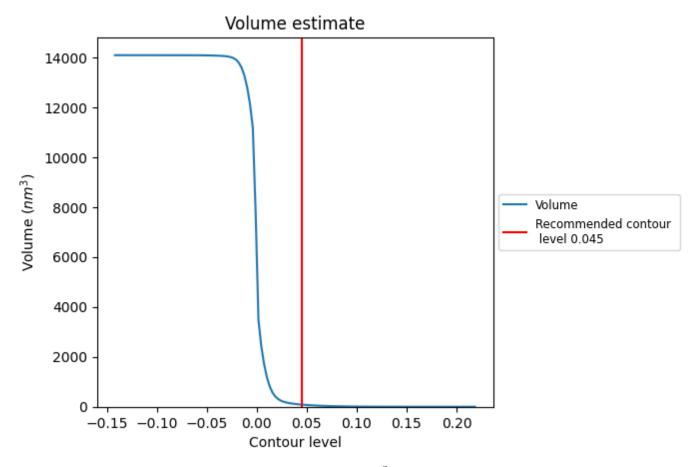
7.1 Map-value distribution (i)



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)

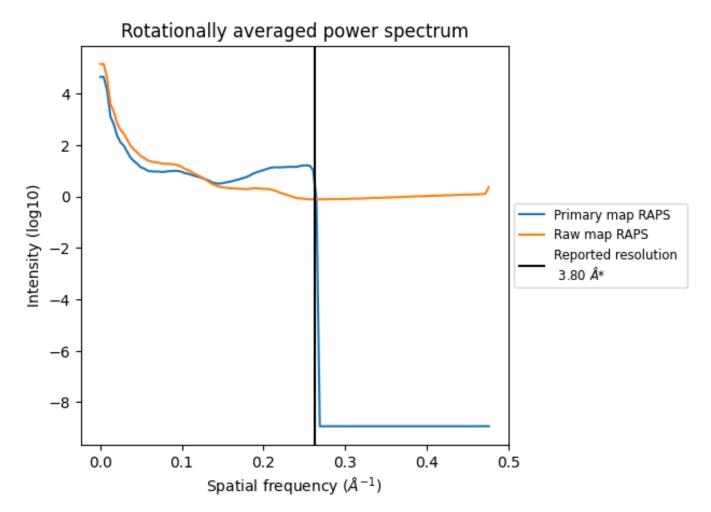


The volume at the recommended contour level is $87~\mathrm{nm}^3$; this corresponds to an approximate mass of $78~\mathrm{kDa}$.

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)



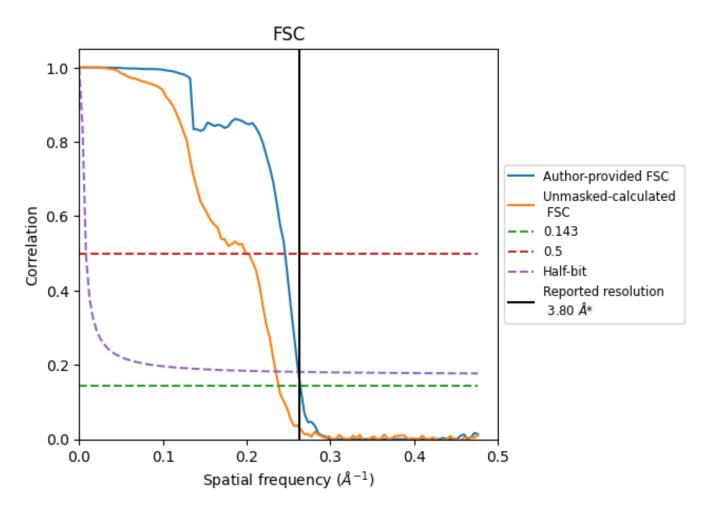
^{*}Reported resolution corresponds to spatial frequency of 0.263 $\rm \mathring{A}^{-1}$



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 0.263 $\rm \mathring{A}^{-1}$



8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
rtesolution estimate (A)	0.143	0.5	Half-bit	
Reported by author	3.80	-	-	
Author-provided FSC curve	3.79	4.07	3.82	
Unmasked-calculated*	4.20	5.01	4.26	

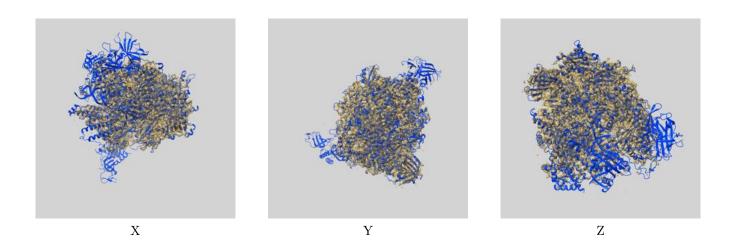
^{*}Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.20 differs from the reported value 3.8 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4147 and PDB model 5M3F. Per-residue inclusion information can be found in section 3 on page 8.

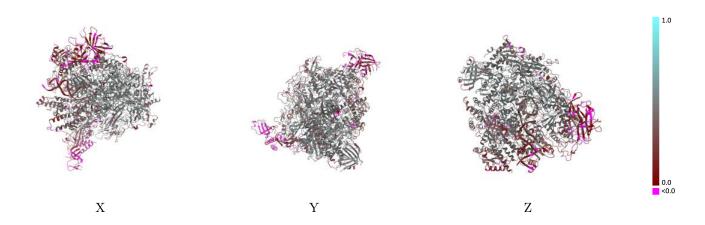
9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.045 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.

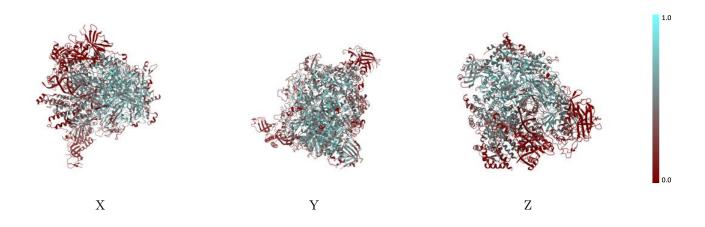


9.2 Q-score mapped to coordinate model (i)



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.

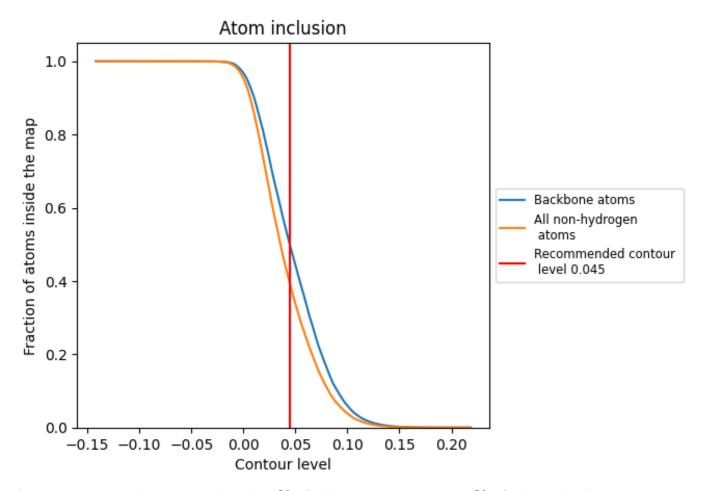
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.045).



9.4 Atom inclusion (i)



At the recommended contour level, 50% of all backbone atoms, 39% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3900	0.3830
A	0.4301	0.4240
В	0.5100	0.4500
С	0.4636	0.4480
D	0.0211	0.0430
Е	0.2908	0.3670
F	0.4207	0.4200
G	0.0332	0.0420
Н	0.4327	0.4430
I	0.0409	0.2560
J	0.6033	0.4880
K	0.4987	0.4600
L	0.4706	0.4510
M	0.0024	0.0870
N	0.0026	0.0760
R	0.2948	0.3370
Т	0.1709	0.2880
U	0.0246	0.1580



