



wwPDB EM Validation Summary Report ⓘ

Mar 30, 2026 – 12:35 AM UTC

PDB ID : 7Z2Z / pdb_00007z2z
EMDB ID : EMD-14468
Title : Structure of yeast RNA Polymerase III-DNA-Ty1 integrase complex (Pol III-DNA-IN1) at 3.1 Å
Authors : Nguyen, P.Q.; Fernandez-Tornero, C.
Deposited on : 2022-03-01
Resolution : 3.07 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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>.

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

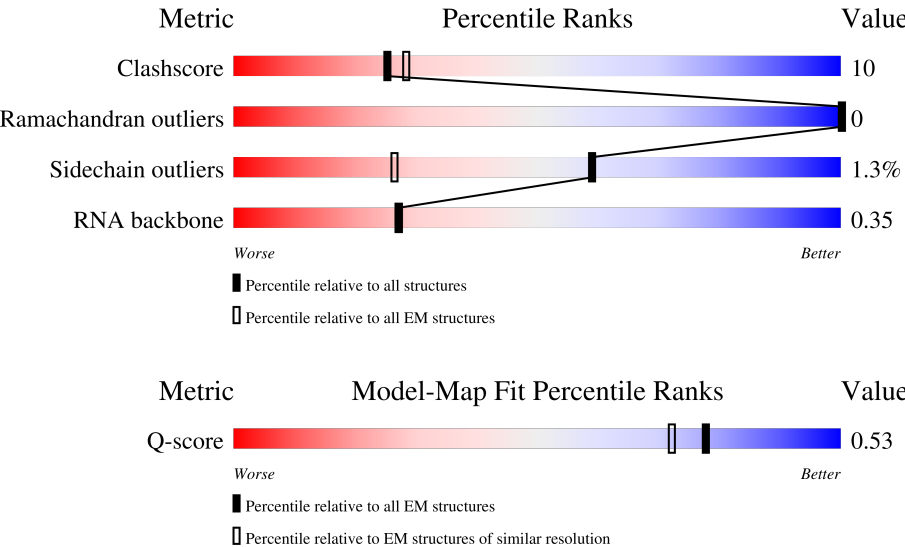
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.07 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	13977 (2.57 - 3.57)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1460	9% 76% 22% .
2	B	1149	10% 72% 24% .
3	C	335	5% 84% 16%

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Mol	Chain	Length	Quality of chain
4	D	161	
5	E	215	
6	F	155	
7	G	212	
8	H	146	
9	I	110	
10	J	70	
11	K	142	
12	L	70	
13	M	282	
14	N	422	
15	O	654	
16	P	317	
17	Q	251	
18	R	10	
19	S	52	
20	T	52	
21	W	635	
22	X	11	

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 41670 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1431	Total	C	N	O	S	0	0
			11192	7056	1976	2101	59		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	145	Total	C	N	O	S	0	0
			1140	723	191	220	6		

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

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

- 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
			671	429	114	125	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	191	Total	C	N	O	S	0	0
			1544	1007	250	281	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	138	Total	C	N	O	S	0	0
			1103	694	186	218	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	109	Total	C	N	O	S	0	0
			864	542	143	168	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
			549	350	95	98	6		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	151	Total	C	N	O	S	0	0
			1171	740	215	213	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	136	Total	C	N	O	S	0	0
			1126	736	175	211	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0
			829	535	137	154	3		

- Molecule 18 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	3	Total	C	N	O	P	0	0
			68	30	15	20	3		

- Molecule 19 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	18	Total	C	N	O	P	0	0
			383	178	86	101	18		

- Molecule 20 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	23	Total	C	N	O	P	0	0
			453	219	63	148	23		

- Molecule 21 is a protein called Integrase.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	W	16	Total	C	N	O	S	
			134	81	26	26	1	
								0
								0

- Molecule 22 is a protein called Unknown RNA polymerase III chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	11	Total	C	N	O		
			55	33	11	11		
							0	0

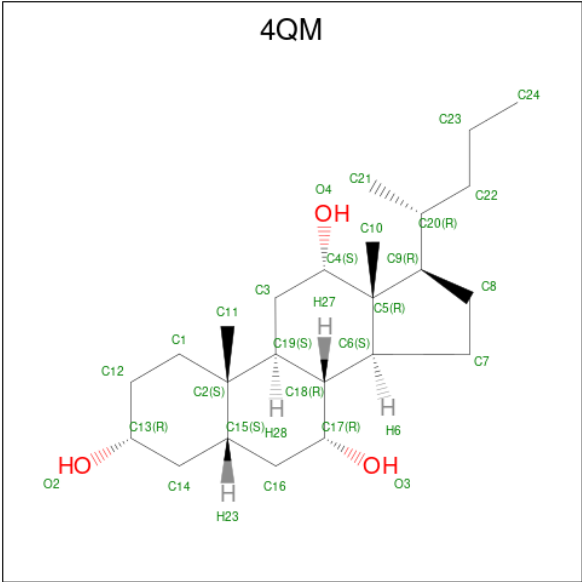
- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 24 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	Mg	
			1	1	
					0
24	I	1	Total	Mg	
			1	1	
					0

- Molecule 25 is (3R,5S,7R,8R,9S,10S,12S,13R,14S,17R)-10,13-dimethyl-17-[(2R)-pentan-2-yl]-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthrene-3,7,12-triol (CCD ID: 4QM) (formula: C₂₄H₄₂O₃).

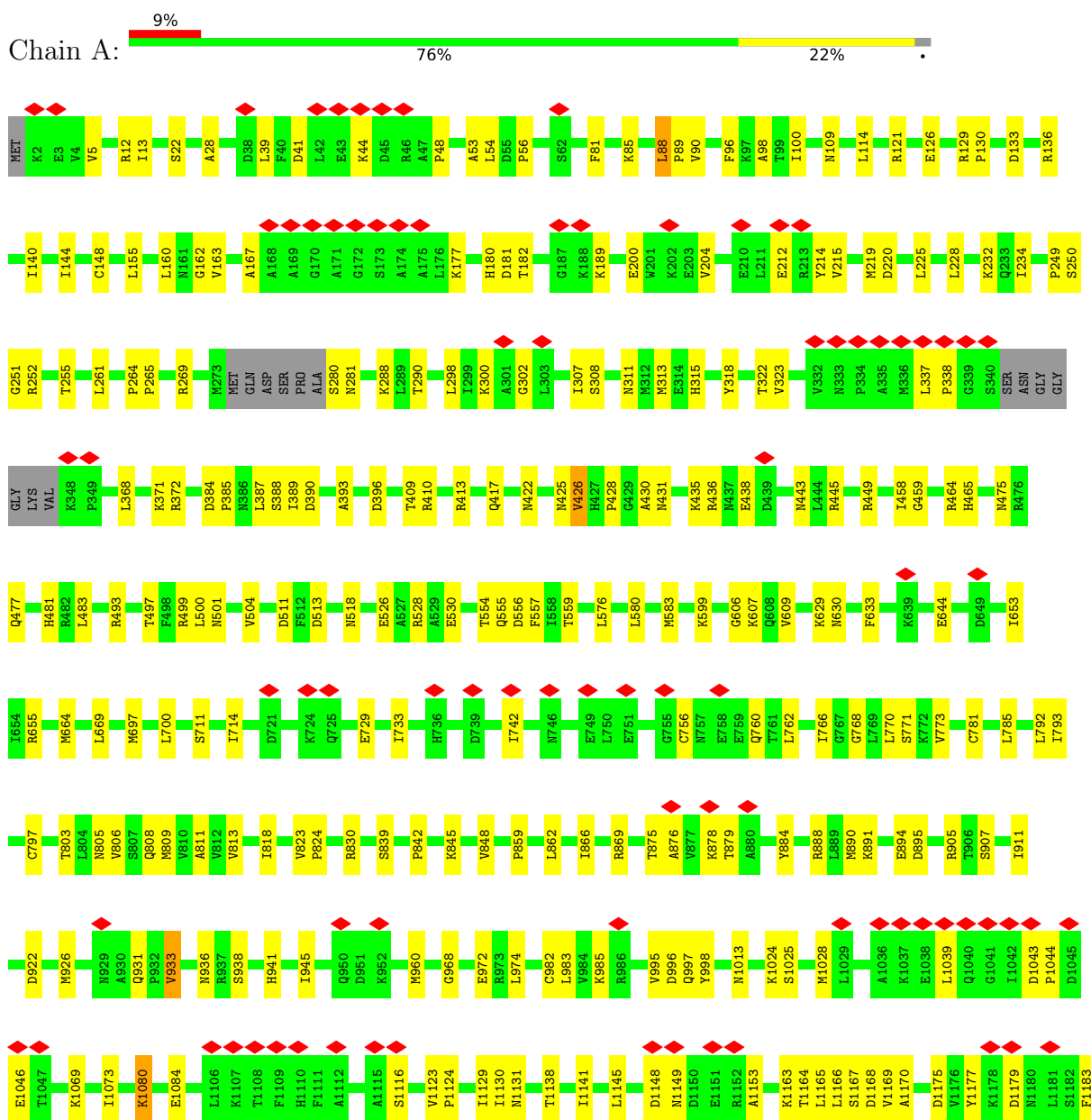


Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			27	24	3	

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.

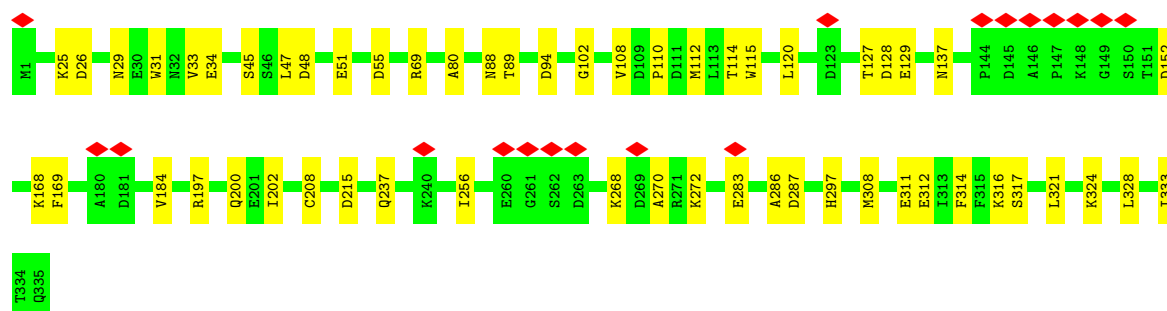
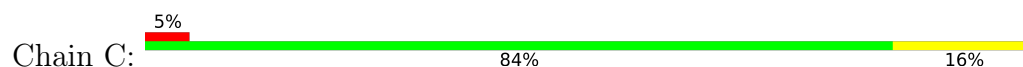
- Molecule 1: DNA-directed RNA polymerase III subunit RPC1



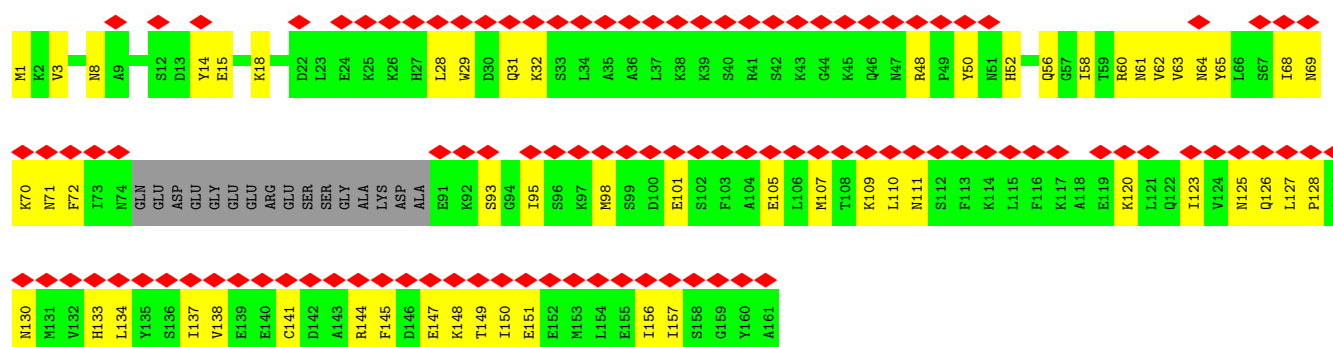




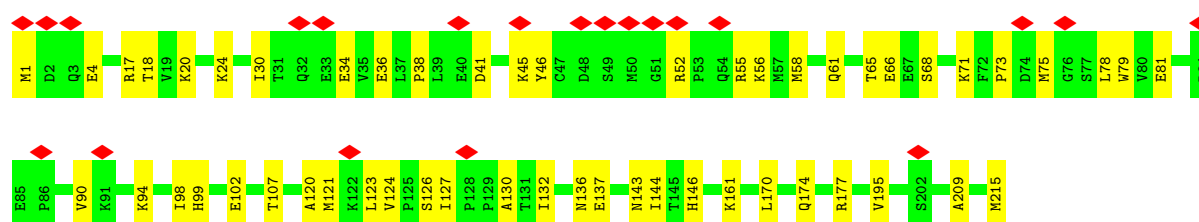
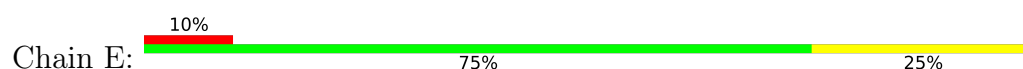
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



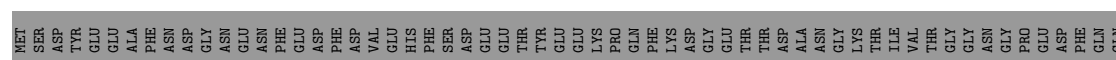
• Molecule 4: DNA-directed RNA polymerase III subunit RPC9



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

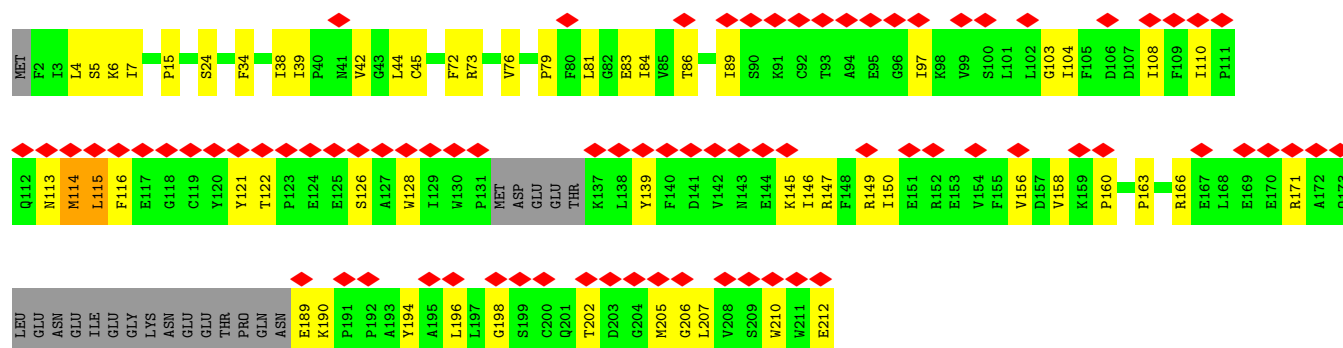
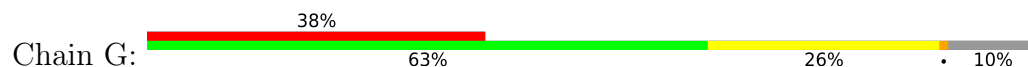


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

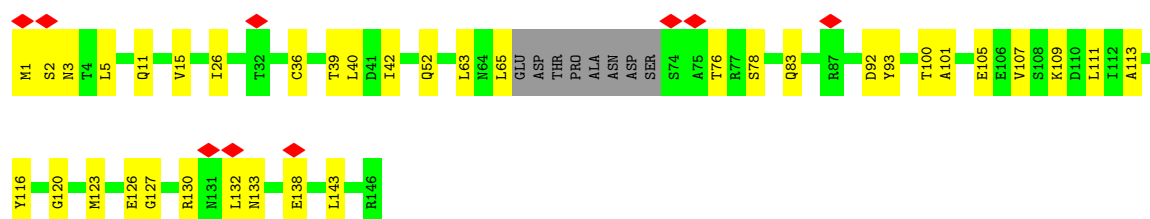




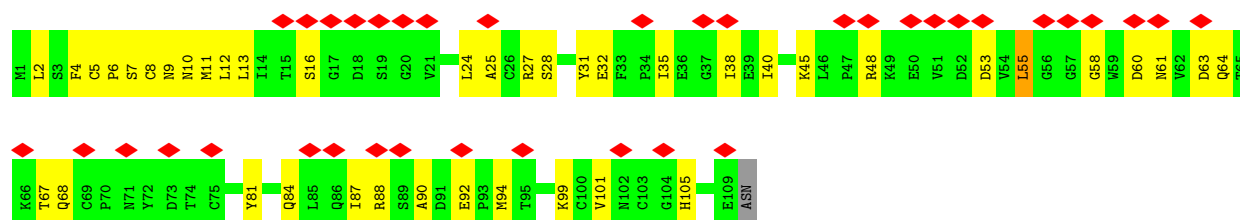
- Molecule 7: DNA-directed RNA polymerase III subunit RPC8



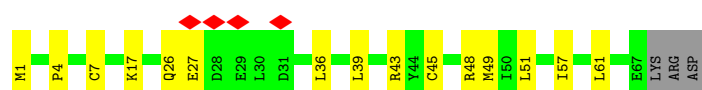
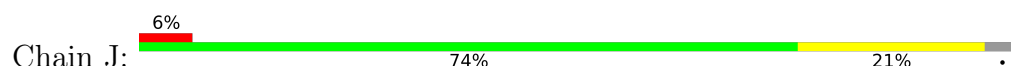
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



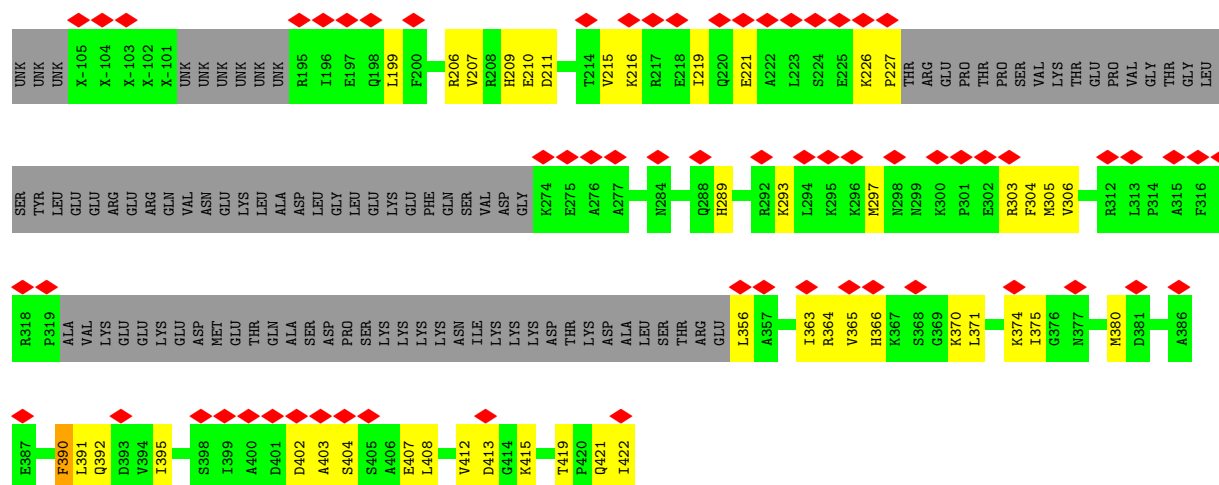
- Molecule 9: DNA-directed RNA polymerase III subunit RPC10



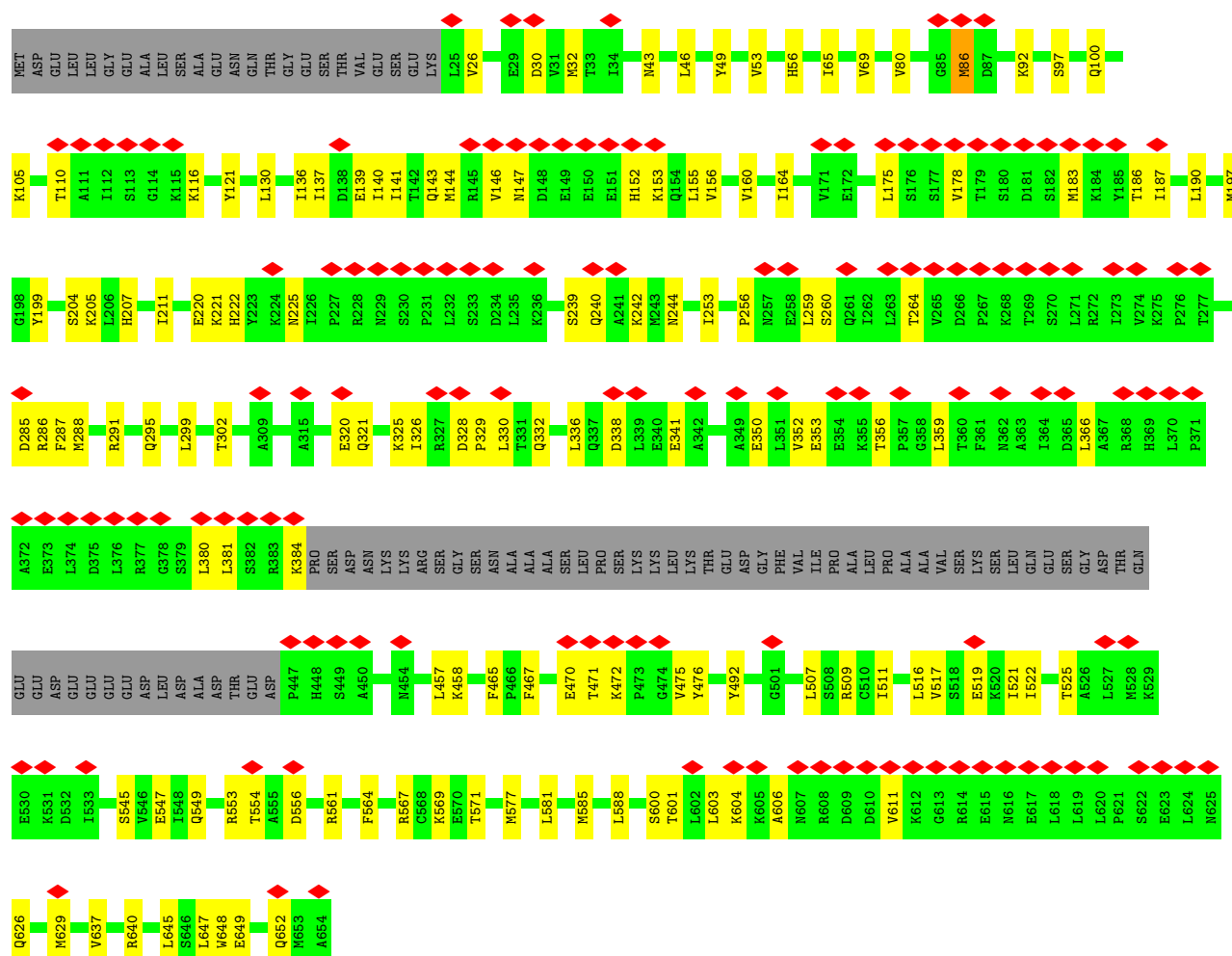
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



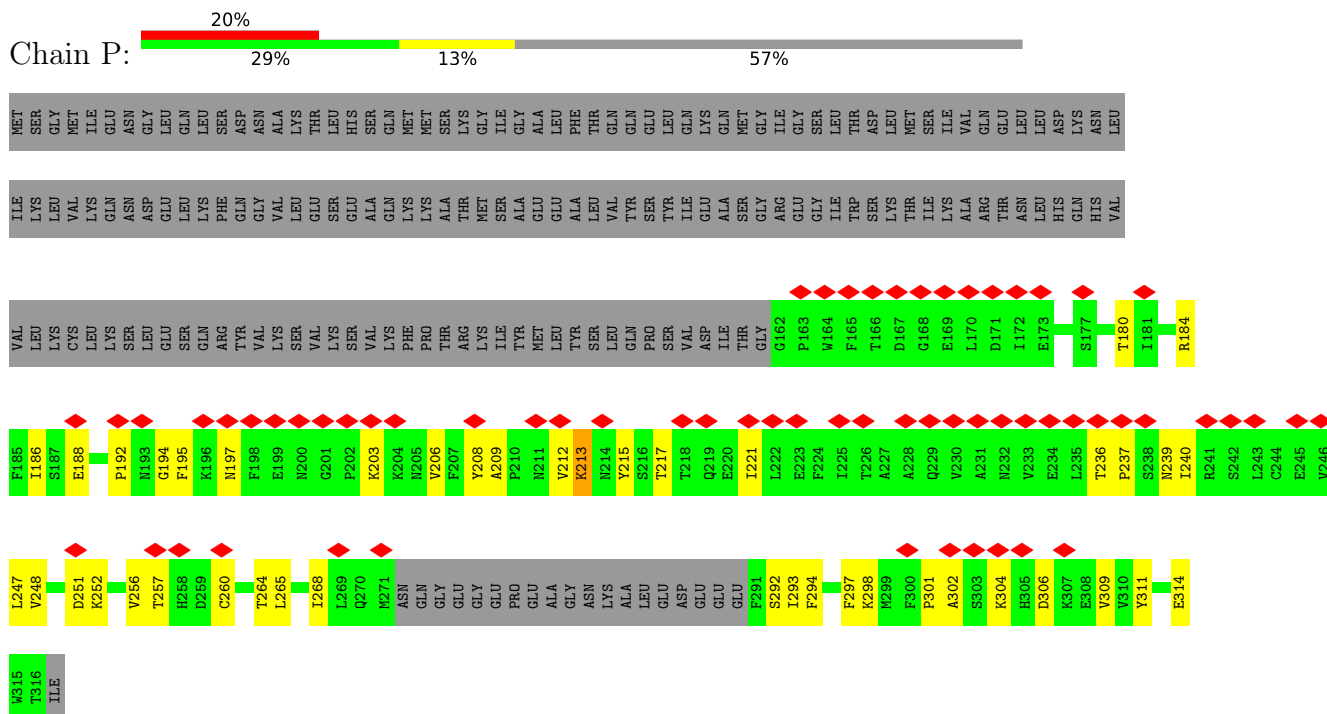
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2



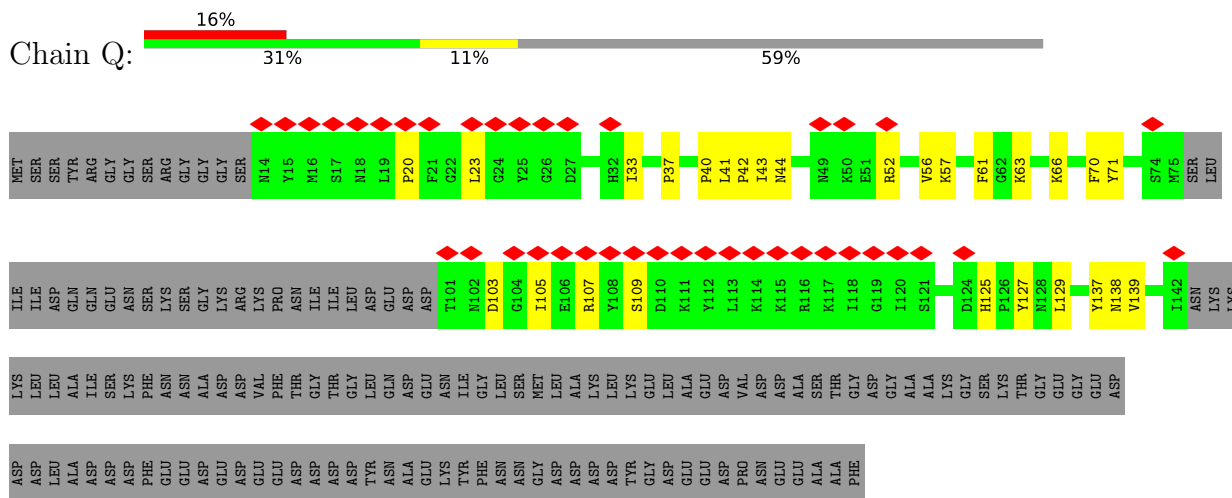
• Molecule 15: DNA-directed RNA polymerase III subunit RPC3



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



- Molecule 17: DNA-directed RNA polymerase III subunit RPC7

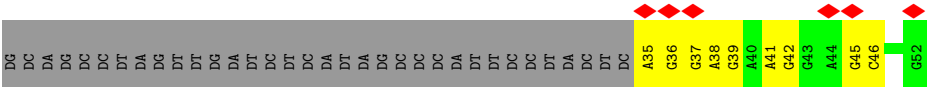


- Molecule 18: RNA

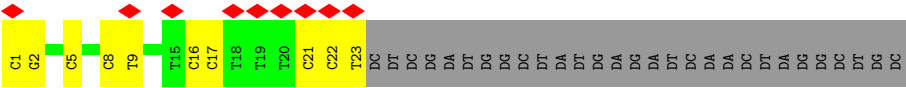


- Molecule 19: Non-template DNA

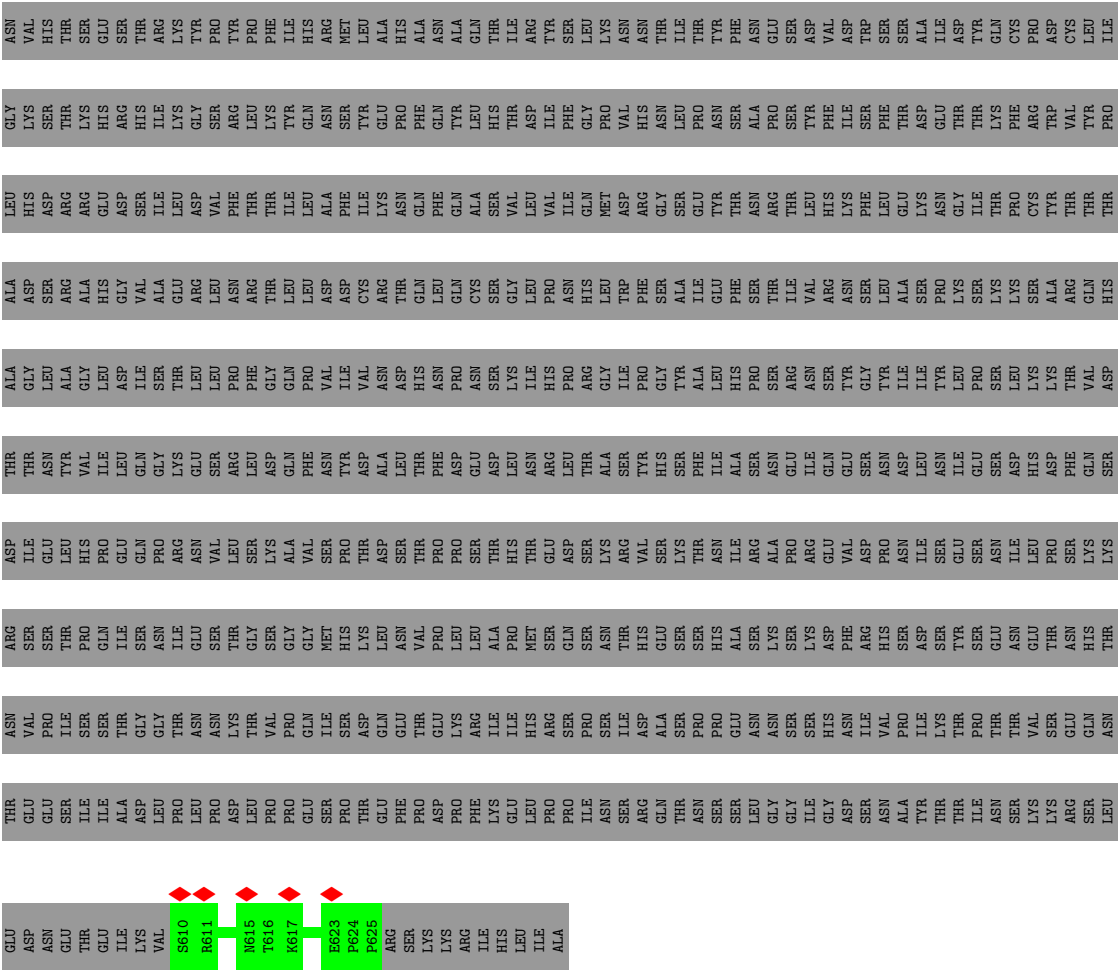




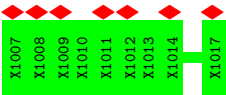
• Molecule 20: Template DNA



• Molecule 21: Integrase



• Molecule 22: Unknown RNA polymerase III chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	305253	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42.45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.148	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0235	Depositor
Map size ($\text{\AA}$)	325.5, 325.5, 325.5	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.085, 1.085, 1.085	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4QM, MG, 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	0.27	0/11392	0.40	0/15390
2	B	0.28	0/8867	0.41	0/11959
3	C	0.29	0/2711	0.41	0/3676
4	D	0.16	0/1158	0.39	0/1550
5	E	0.20	0/1795	0.35	0/2416
6	F	0.21	0/683	0.34	0/923
7	G	0.29	0/1583	0.45	0/2146
8	H	0.22	0/1121	0.40	0/1517
9	I	0.38	0/885	0.52	0/1197
10	J	0.24	0/558	0.32	0/750
11	K	0.24	0/803	0.34	0/1083
12	L	0.22	0/353	0.35	0/468
13	M	0.24	0/1524	0.42	0/2061
14	N	0.20	0/1160	0.39	0/1558
15	O	0.21	0/4627	0.38	0/6243
16	P	0.39	0/1157	0.58	1/1571 (0.1%)
17	Q	0.15	0/850	0.36	0/1148
18	R	0.13	0/76	0.29	0/117
19	S	0.20	0/434	0.31	0/670
20	T	0.24	0/500	0.45	0/766
21	W	0.15	0/137	0.26	0/185
All	All	0.26	0/42374	0.41	1/57394 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	301	PRO	CA-N-CD	-5.29	104.59	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	11192	0	11321	234	0
2	B	8715	0	8835	192	0
3	C	2655	0	2628	34	0
4	D	1140	0	1112	47	0
5	E	1759	0	1788	34	0
6	F	671	0	692	11	0
7	G	1544	0	1540	46	0
8	H	1103	0	1079	25	0
9	I	864	0	811	38	0
10	J	549	0	559	12	0
11	K	792	0	790	12	0
12	L	381	0	382	12	0
13	M	1492	0	1456	74	0
14	N	1171	0	1215	43	0
15	O	4558	0	4735	101	0
16	P	1126	0	1079	31	0
17	Q	829	0	819	28	0
18	R	68	0	34	0	0
19	S	383	0	199	5	0
20	T	453	0	264	7	0
21	W	134	0	128	0	0
22	X	55	0	13	0	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	I	2	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
24	A	1	0	0	0	0
24	I	1	0	0	0	0
25	A	27	0	0	0	0
All	All	41670	0	41479	858	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 858 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)
13:M:164:LYS:CE	13:M:256:LYS:HD2	1.34	1.53
13:M:164:LYS:HE3	13:M:256:LYS:CD	1.53	1.39
13:M:164:LYS:CE	13:M:256:LYS:CD	2.26	0.96
2:B:217:GLN:NE2	2:B:352:MET:SD	2.45	0.90
1:A:768:GLY:HA3	9:I:61:ASN:HB3	1.56	0.85

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	1423/1460 (98%)	1306 (92%)	117 (8%)	0	100	100
2	B	1100/1149 (96%)	1006 (92%)	94 (8%)	0	100	100
3	C	333/335 (99%)	303 (91%)	30 (9%)	0	100	100
4	D	141/161 (88%)	122 (86%)	19 (14%)	0	100	100
5	E	213/215 (99%)	201 (94%)	12 (6%)	0	100	100
6	F	81/155 (52%)	75 (93%)	6 (7%)	0	100	100
7	G	185/212 (87%)	160 (86%)	25 (14%)	0	100	100
8	H	134/146 (92%)	116 (87%)	18 (13%)	0	100	100
9	I	107/110 (97%)	86 (80%)	21 (20%)	0	100	100
10	J	65/70 (93%)	62 (95%)	3 (5%)	0	100	100
11	K	99/142 (70%)	93 (94%)	6 (6%)	0	100	100
12	L	42/70 (60%)	38 (90%)	4 (10%)	0	100	100
13	M	179/282 (64%)	156 (87%)	23 (13%)	0	100	100
14	N	140/422 (33%)	132 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	564/654 (86%)	531 (94%)	33 (6%)	0	100	100
16	P	132/317 (42%)	119 (90%)	13 (10%)	0	100	100
17	Q	100/251 (40%)	90 (90%)	10 (10%)	0	100	100
21	W	14/635 (2%)	14 (100%)	0	0	100	100
All	All	5052/6786 (74%)	4610 (91%)	442 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	1235/1257 (98%)	1220 (99%)	15 (1%)	63	75
2	B	966/1006 (96%)	950 (98%)	16 (2%)	53	71
3	C	296/296 (100%)	290 (98%)	6 (2%)	48	69
4	D	123/145 (85%)	123 (100%)	0	100	100
5	E	197/197 (100%)	197 (100%)	0	100	100
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	170/190 (90%)	165 (97%)	5 (3%)	37	63
8	H	121/128 (94%)	121 (100%)	0	100	100
9	I	97/98 (99%)	94 (97%)	3 (3%)	35	61
10	J	62/65 (95%)	62 (100%)	0	100	100
11	K	91/130 (70%)	91 (100%)	0	100	100
12	L	39/39 (100%)	39 (100%)	0	100	100
13	M	159/249 (64%)	156 (98%)	3 (2%)	50	70
14	N	126/200 (63%)	125 (99%)	1 (1%)	73	79
15	O	521/593 (88%)	519 (100%)	2 (0%)	84	84
16	P	126/285 (44%)	119 (94%)	7 (6%)	19	46
17	Q	92/212 (43%)	92 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	W	16/586 (3%)	16 (100%)	0	100	100
All	All	4510/5813 (78%)	4452 (99%)	58 (1%)	59	74

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	889	SER
16	P	292	SER
3	C	47	LEU
16	P	264	THR
15	O	86	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	115	ASN
15	O	523	ASN
9	I	10	ASN
15	O	454	ASN
15	O	152	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	R	2/10 (20%)	1 (50%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
18	R	10	A

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	$\# Z > 2$
25	4QM	A	1504	-	30,30,30	0.42	0	47,48,48	0.75	1 (2%)

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
25	4QM	A	1504	-	-	5/7/72/72	0/4/4/4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1504	4QM	C2-C19-C18	-2.56	108.98	111.84

There are no chirality outliers.

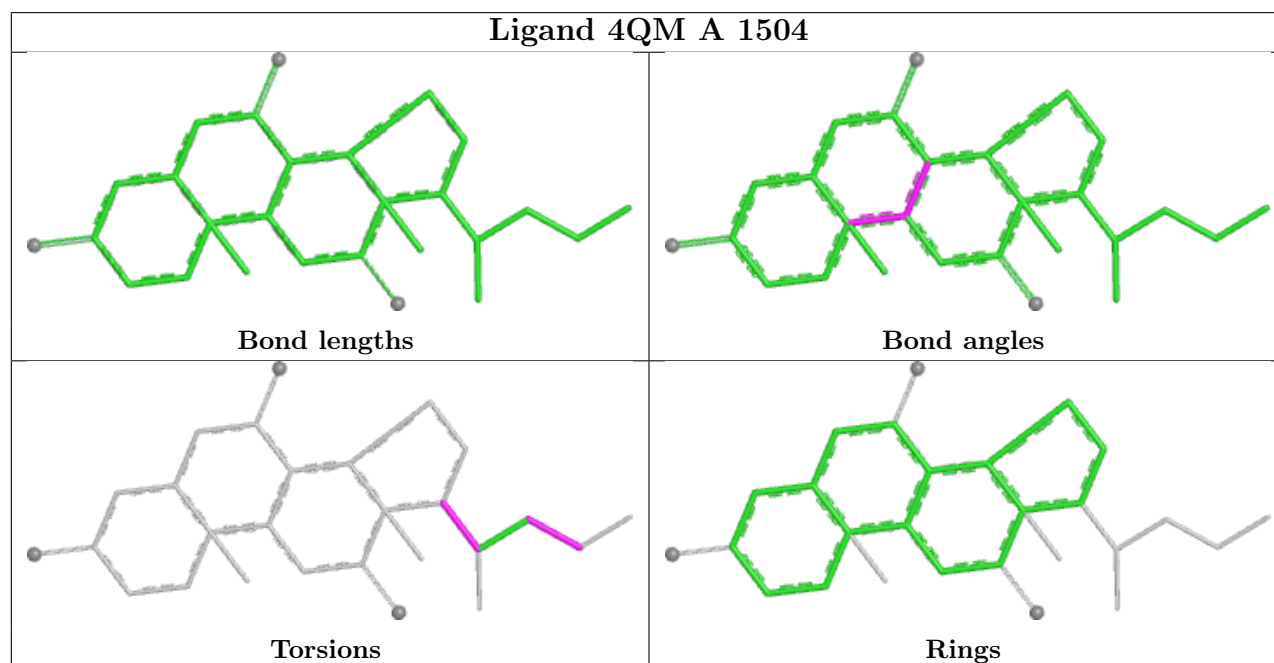
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	1504	4QM	C22-C20-C9-C5
25	A	1504	4QM	C21-C20-C9-C5
25	A	1504	4QM	C21-C20-C9-C8
25	A	1504	4QM	C22-C20-C9-C8
25	A	1504	4QM	C20-C22-C23-C24

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

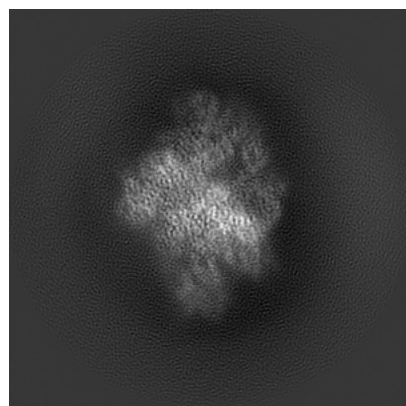
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14468. These allow visual inspection of the internal detail of the map and identification of artifacts.

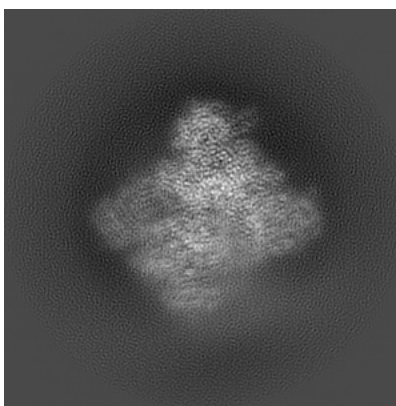
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

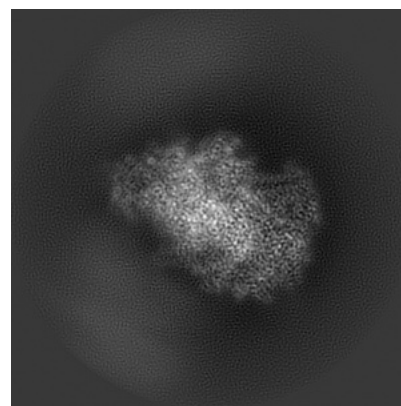
6.1.1 Primary map



X

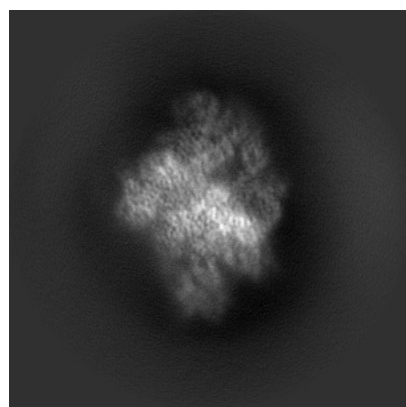


Y

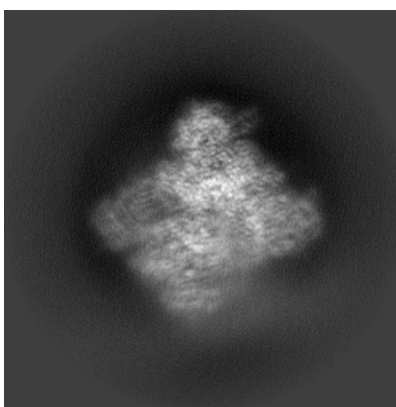


Z

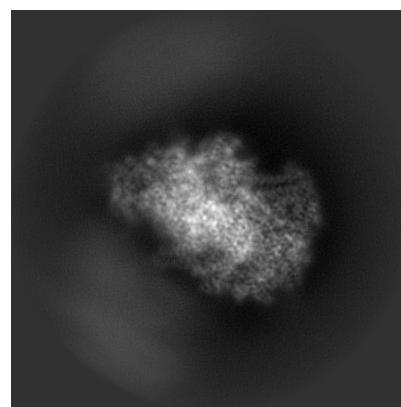
6.1.2 Raw map



X



Y

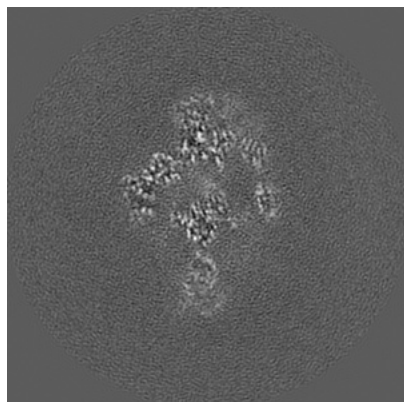


Z

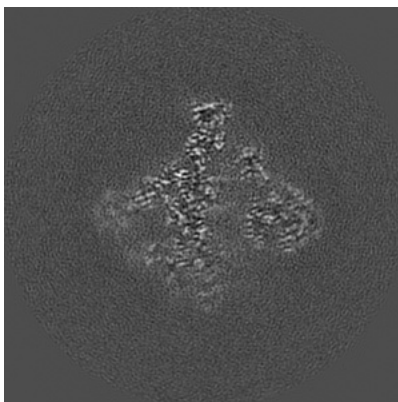
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

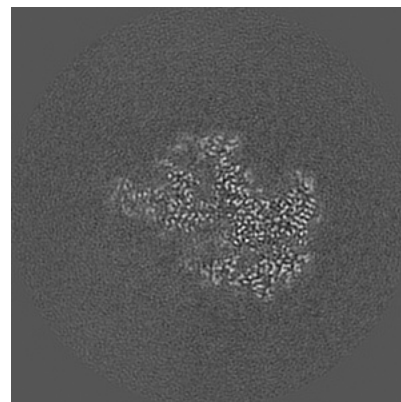
6.2.1 Primary map



X Index: 150

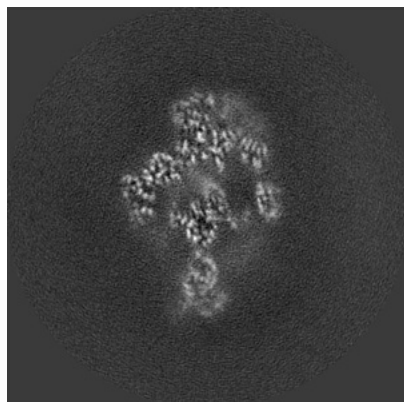


Y Index: 150

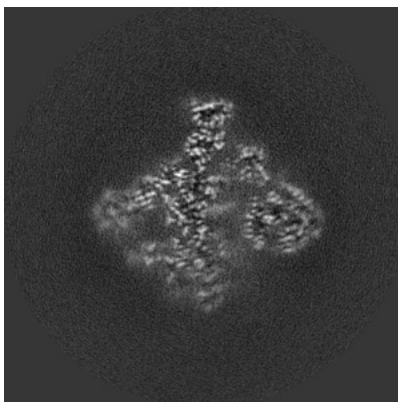


Z Index: 150

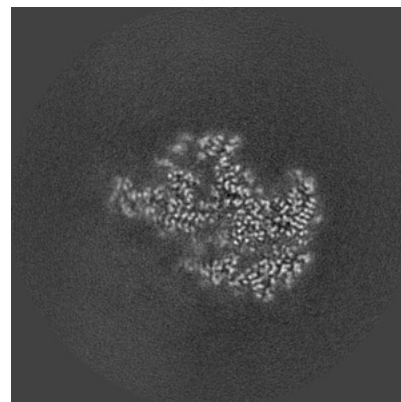
6.2.2 Raw map



X Index: 150



Y Index: 150

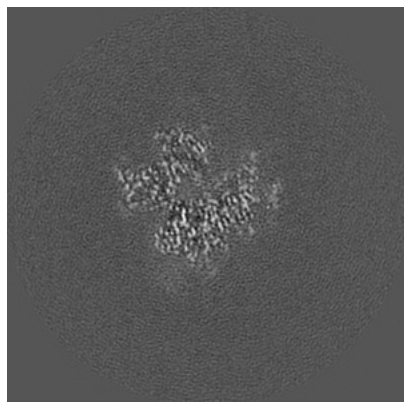


Z Index: 150

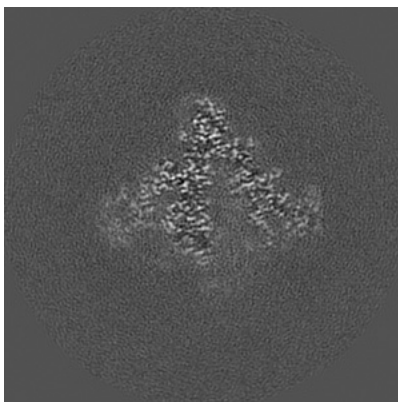
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

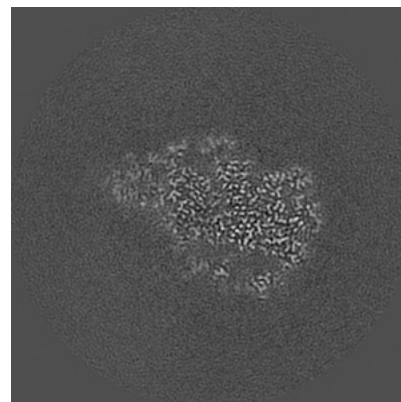
6.3.1 Primary map



X Index: 169

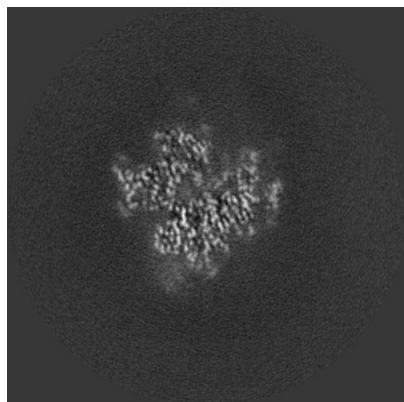


Y Index: 141

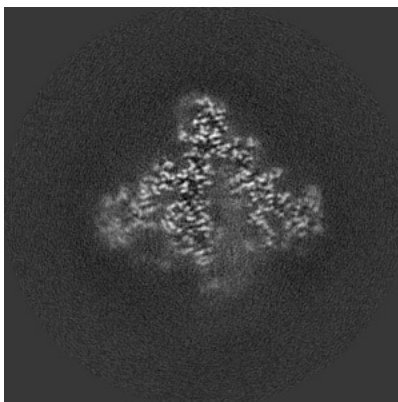


Z Index: 143

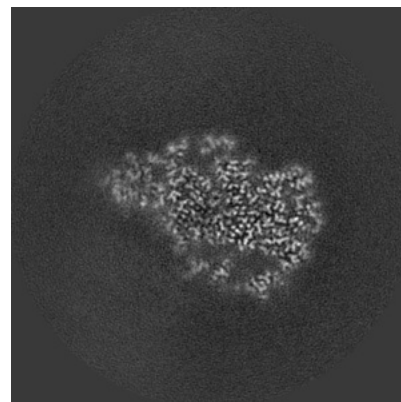
6.3.2 Raw map



X Index: 169



Y Index: 141

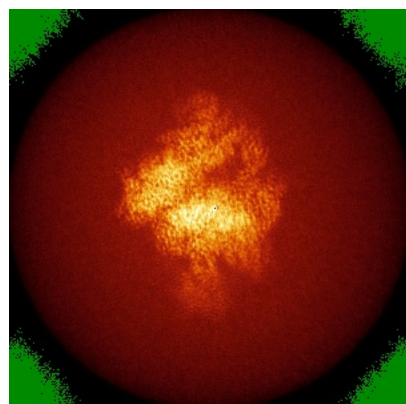


Z Index: 143

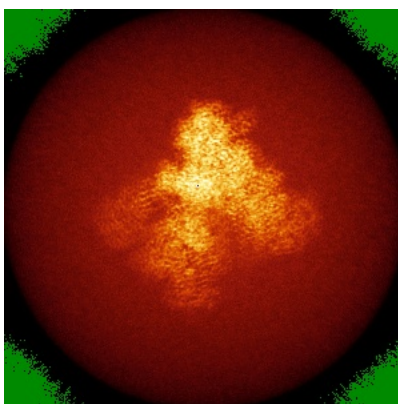
The images above show the largest variance slices of the map in three orthogonal directions.

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

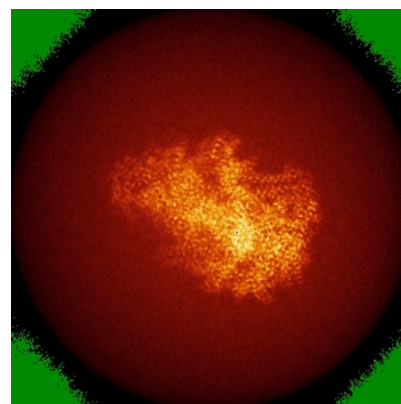
6.4.1 Primary map



X

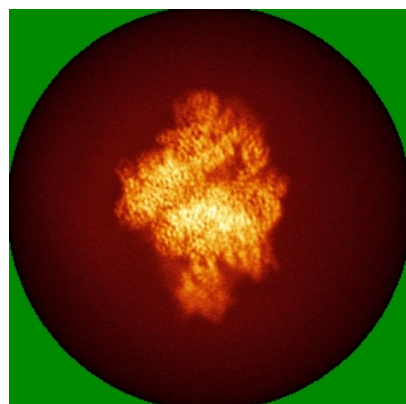


Y

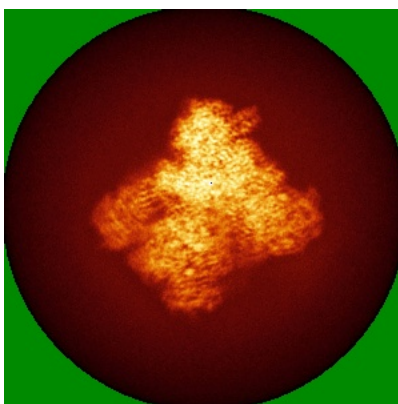


Z

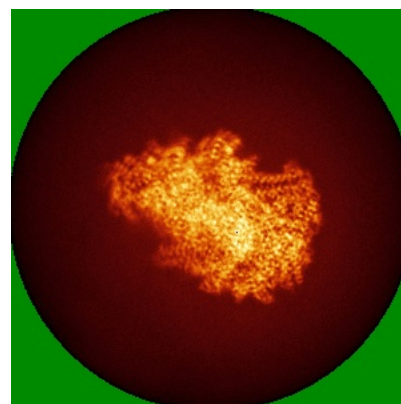
6.4.2 Raw map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0235. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

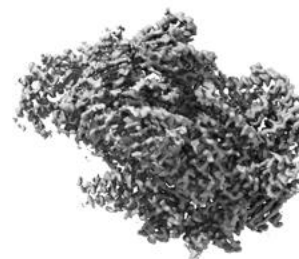
6.5.2 Raw map



X



Y



Z

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.

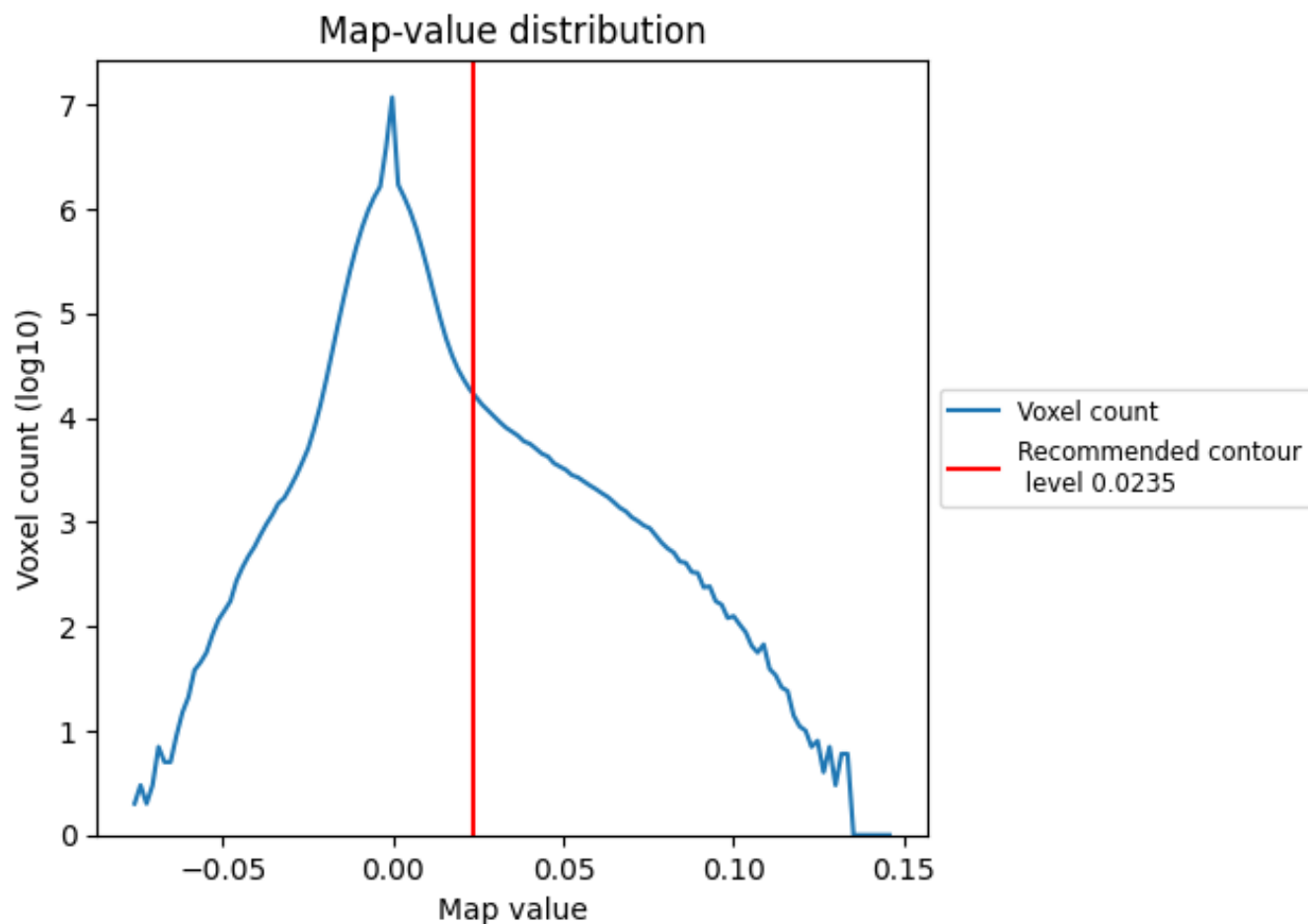
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

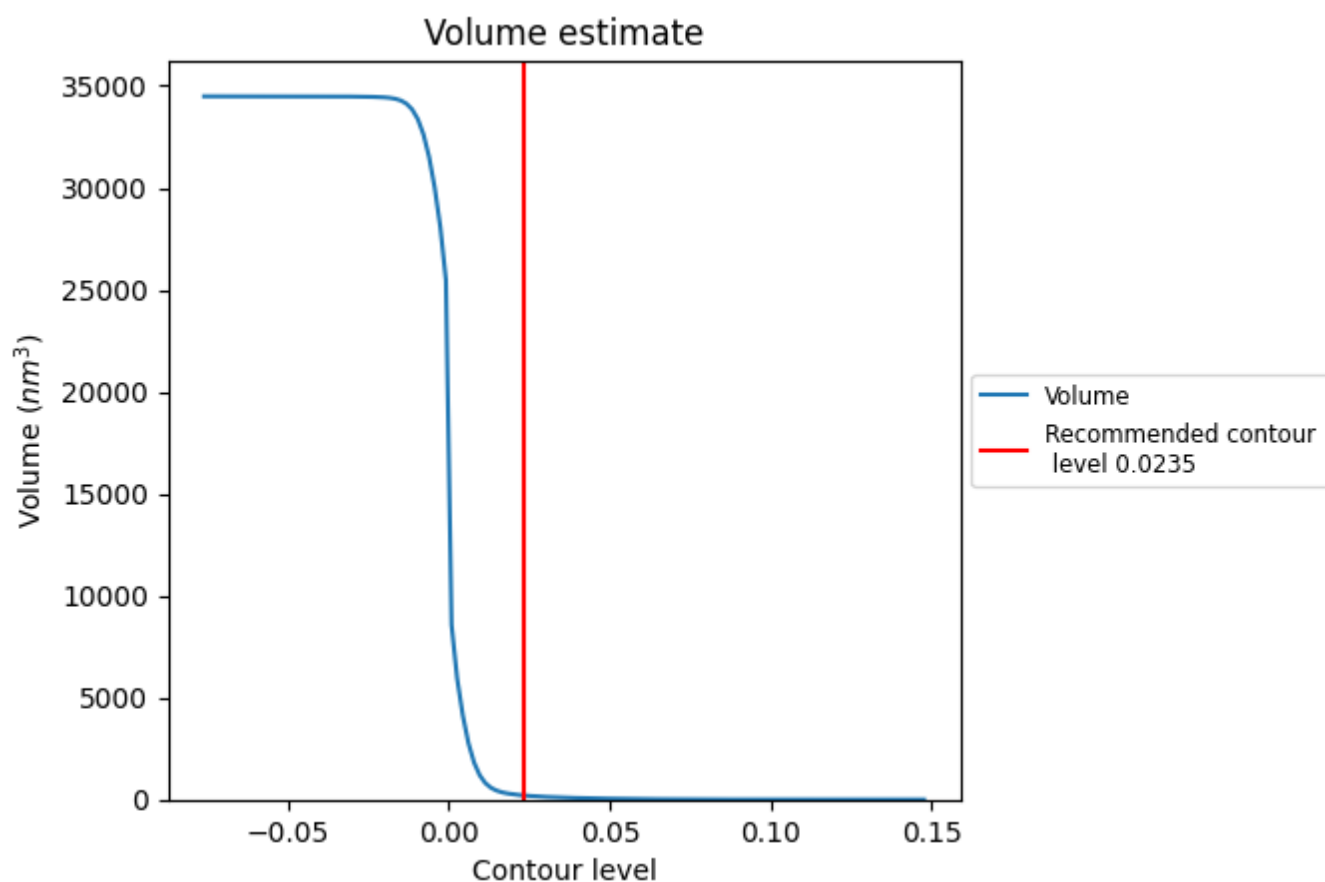
This section contains the results of statistical analysis of the map.

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.

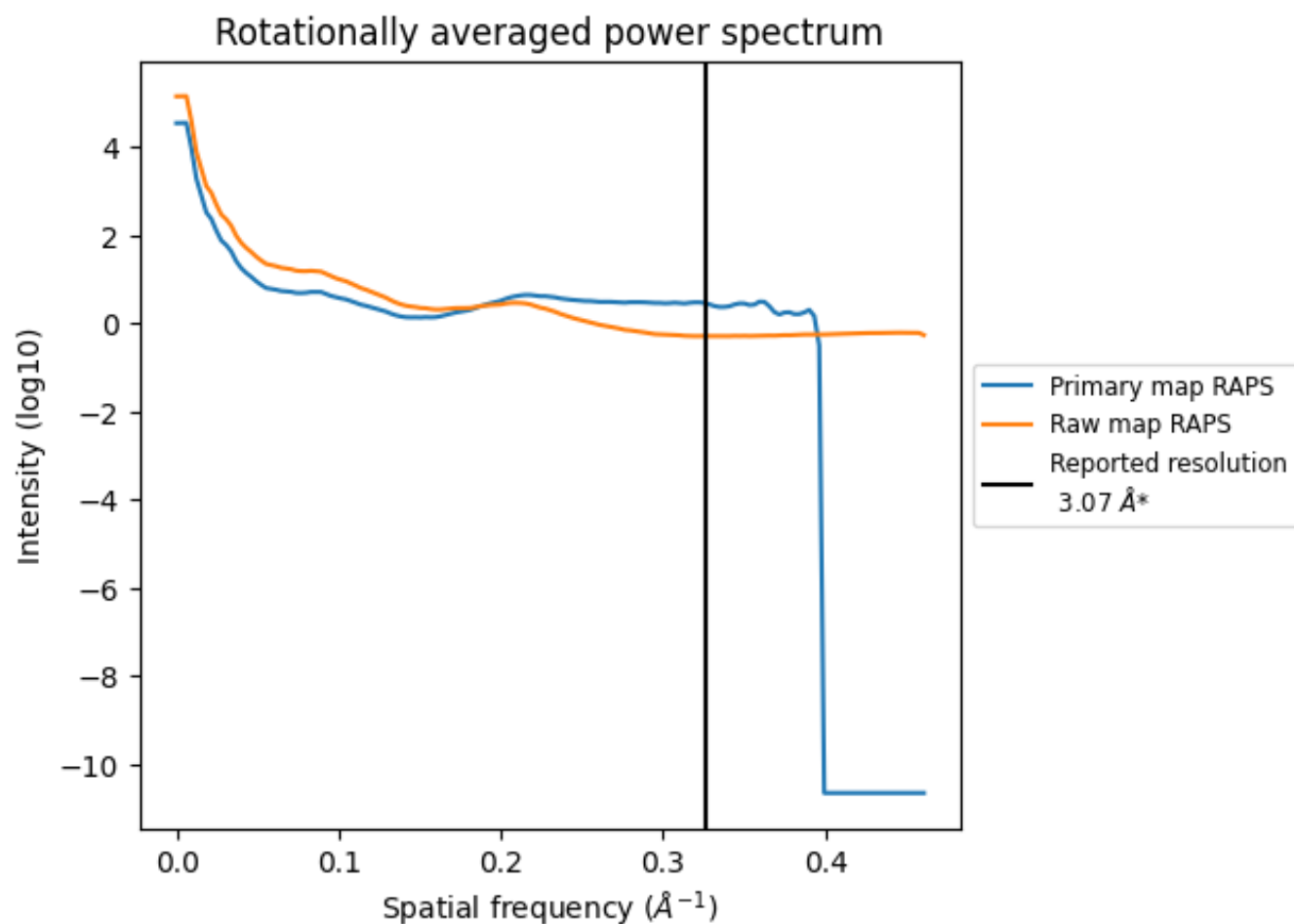
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 199 nm³; this corresponds to an approximate mass of 180 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 ⓘ

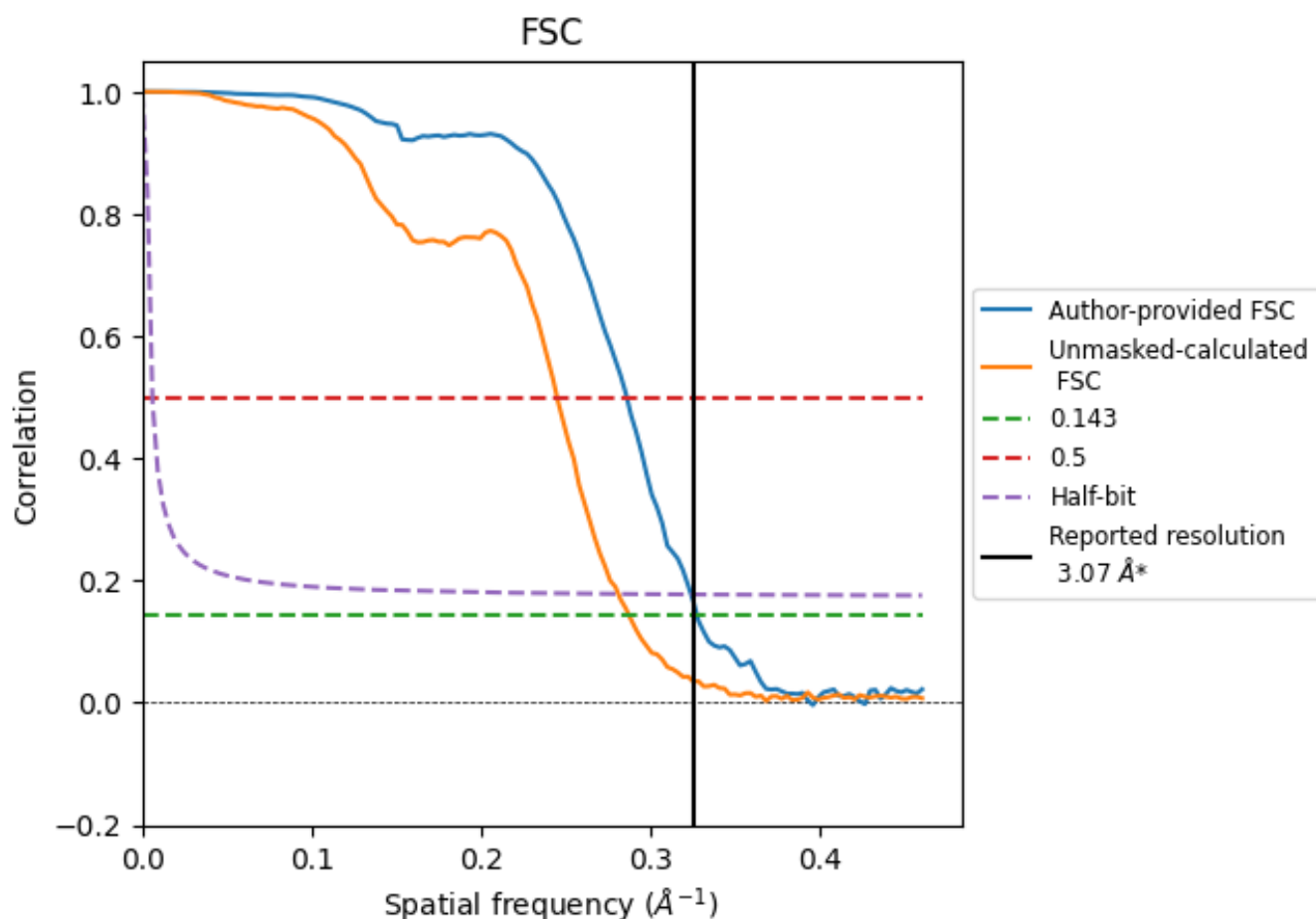


*Reported resolution corresponds to spatial frequency of 0.326 Å⁻¹

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 0.326 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	3.07	-
Author-provided FSC curve	3.05	3.49	3.08
Unmasked-calculated*	3.48	4.08	3.55

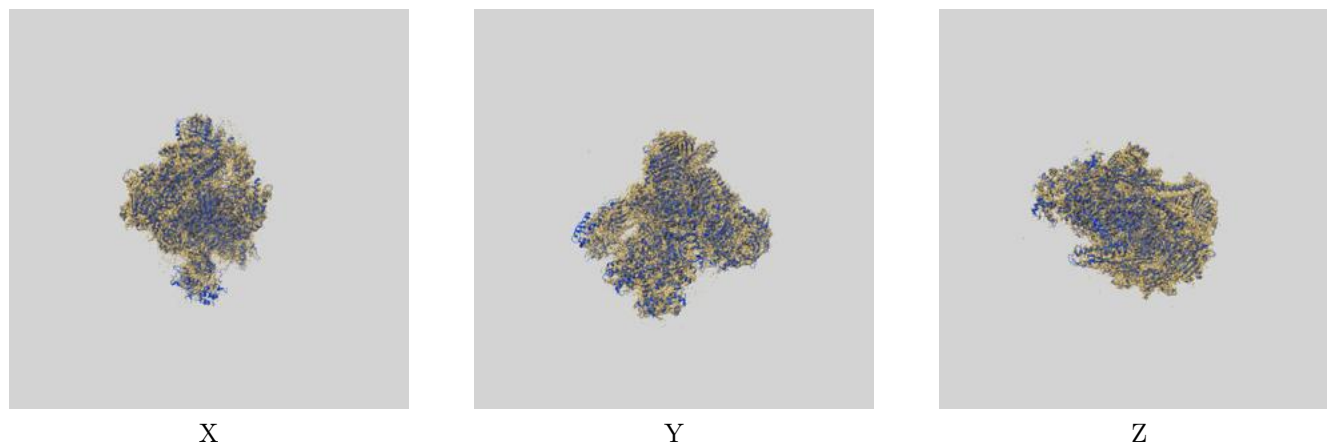
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.5 CUT-OFF 3.49 differs from the reported value 3.07 by more than 10 %

The value from deposited half-maps intersecting FSC 0.5 CUT-OFF 4.08 differs from the reported value 3.07 by more than 10 %

9 Map-model fit [i](#)

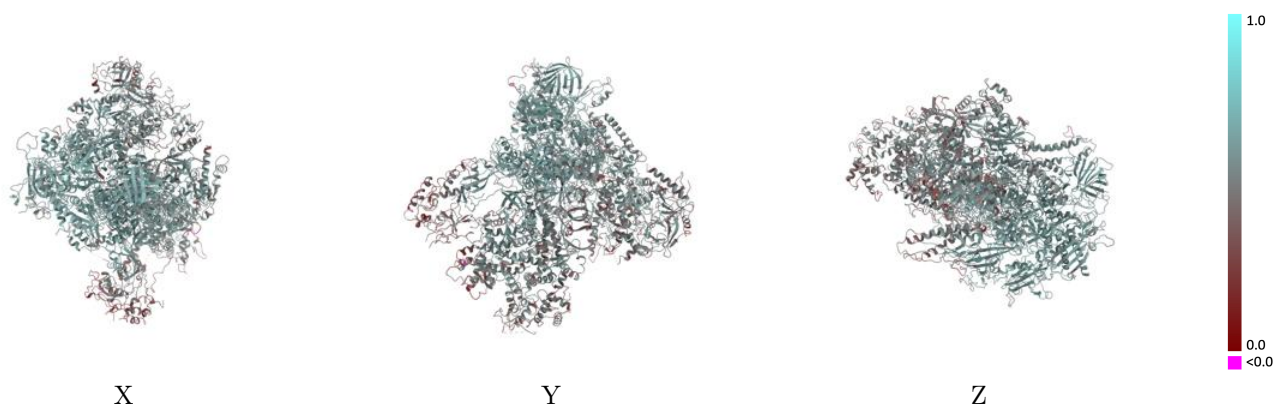
This section contains information regarding the fit between EMDB map EMD-14468 and PDB model 7Z2Z. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



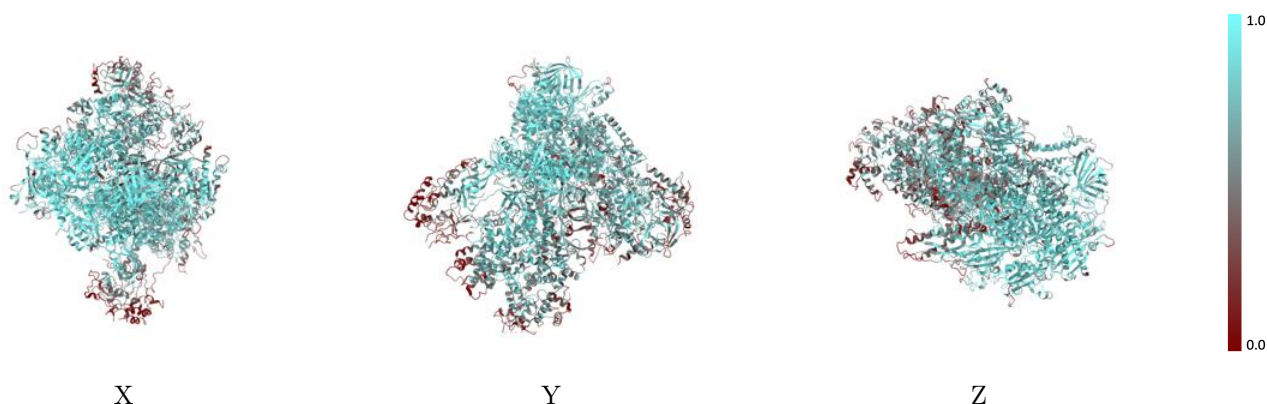
The images above show the 3D surface view of the map at the recommended contour level 0.0235 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



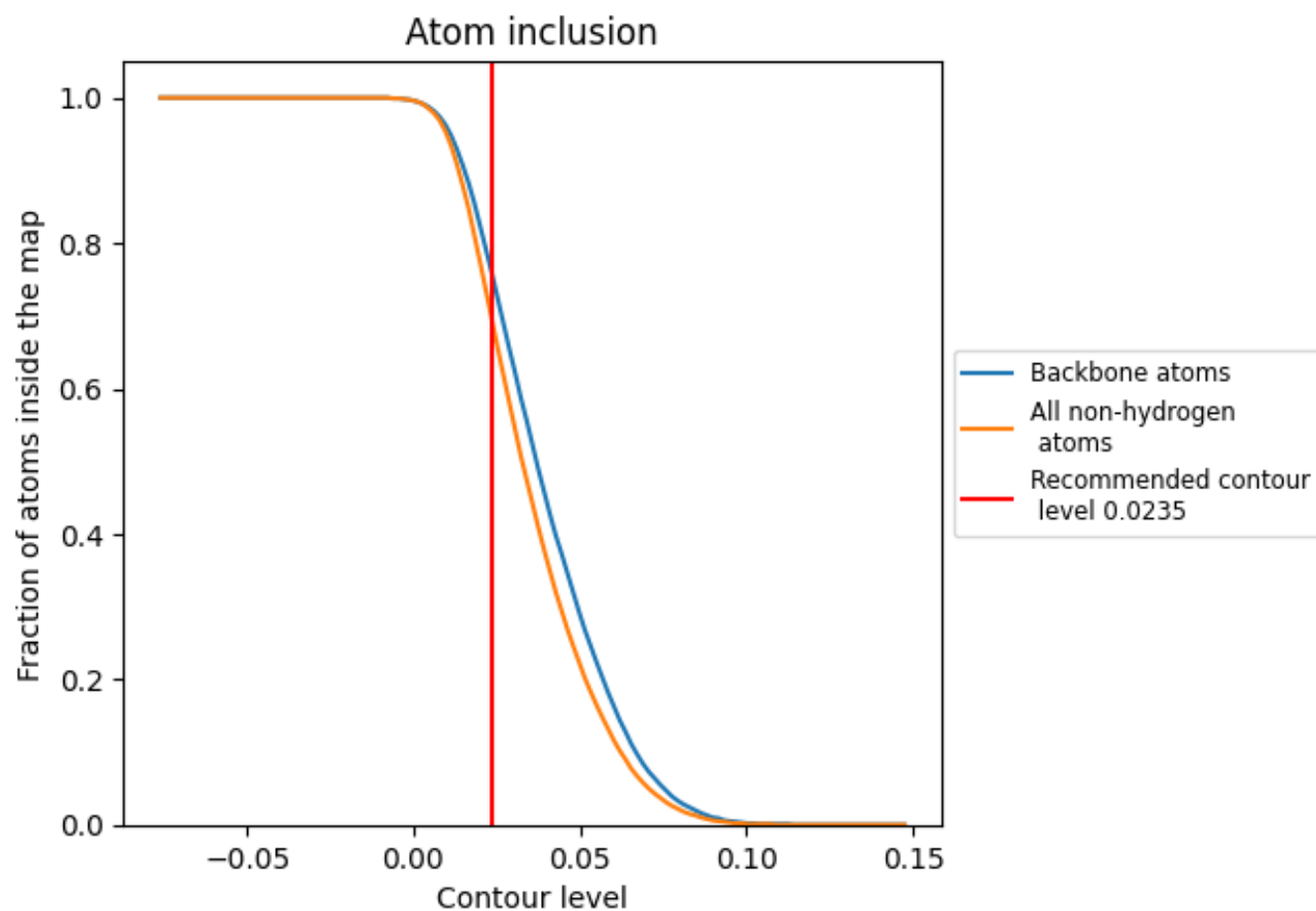
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0235).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0235) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6960	 0.5300
A	 0.7840	 0.5610
B	 0.7790	 0.5590
C	 0.8170	 0.5830
D	 0.2700	 0.3520
E	 0.7550	 0.5500
F	 0.8530	 0.5960
G	 0.5010	 0.4560
H	 0.7910	 0.5760
I	 0.5240	 0.4920
J	 0.8630	 0.6040
K	 0.8540	 0.5980
L	 0.7560	 0.5660
M	 0.4870	 0.4720
N	 0.4660	 0.4770
O	 0.6150	 0.4850
P	 0.4460	 0.4330
Q	 0.5020	 0.4460
R	 0.1470	 0.3500
S	 0.4990	 0.4550
T	 0.4420	 0.4390
W	 0.6120	 0.5650
X	 0.3820	 0.3690

