



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 06:27 AM UTC

PDB ID : 8RAS / pdb_00008ras
EMDB ID : EMD-19023
Title : Plastid-encoded RNA polymerase transcription elongation complex
Authors : Webster, M.W.; Pramanick, I.; Vergara-Cruces, A.
Deposited on : 2023-12-01
Resolution : 2.62 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 ⓘ 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:

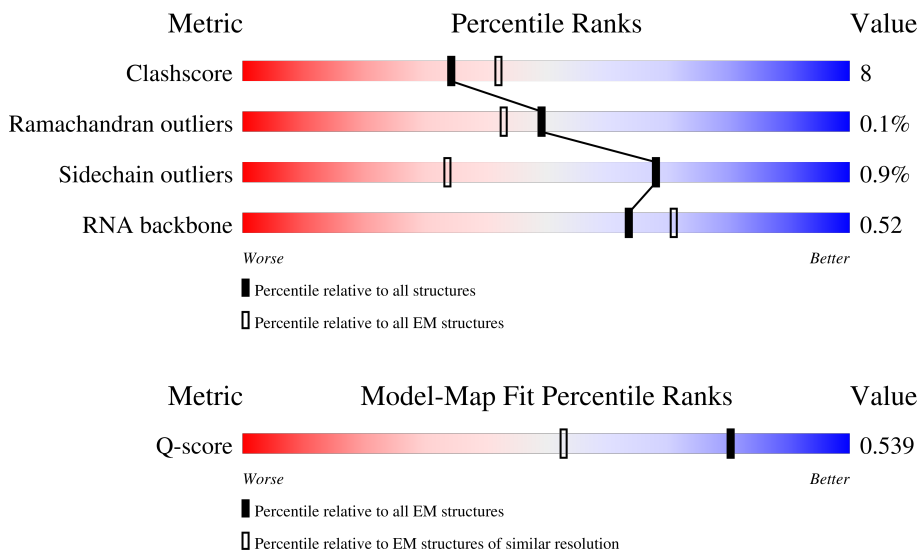
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.62 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.



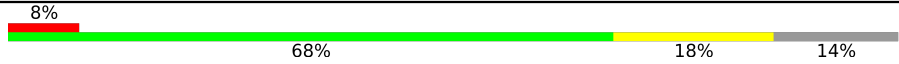
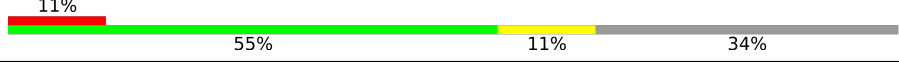
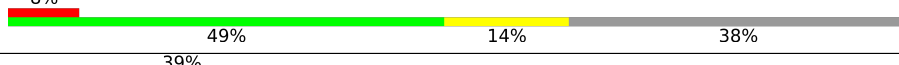



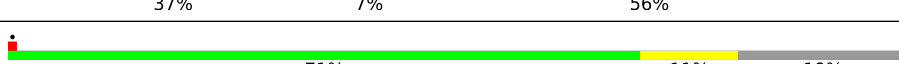
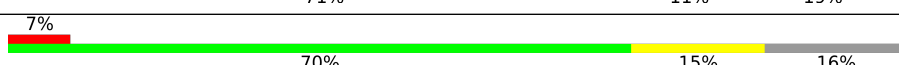


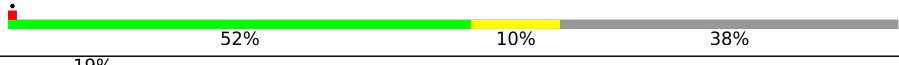
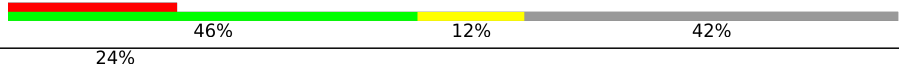



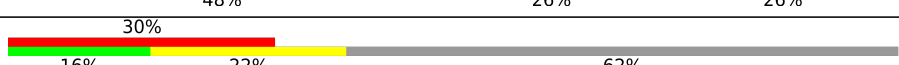
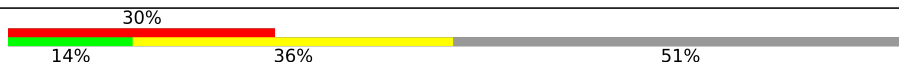



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8810 (2.12 - 3.12)

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	327	
1	B	327	
2	C	1072	

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Mol	Chain	Length	Quality of chain
3	D	680	
4	E	1373	
5	F	911	
6	G	862	
7	H	675	
8	I	263	
9	J	529	
10	K	460	
11	L	483	
12	M	334	
13	N	297	
14	O	185	
14	P	185	
15	Q	768	
16	R	162	
17	S	611	
18	T	140	
19	X	81	
20	Y	81	
21	Z	40	

2 Entry composition [i](#)

There are 26 unique types of molecules in this entry. The entry contains 57315 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 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	301	Total	C	N	O	S	0	0
			2449	1571	422	446	10		
1	B	216	Total	C	N	O	S	0	0
			1722	1091	302	321	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	PHE	SER	conflict	UNP A0A6C0M610
B	67	PHE	SER	conflict	UNP A0A6C0M610

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	726	Total	C	N	O	S	0	0
			5772	3672	1019	1060	21		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	113	PHE	SER	conflict	UNP A0A6C0M5W1
C	657	VAL	ILE	conflict	UNP A0A6C0M5W1

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	585	Total	C	N	O	S	0	0
			4787	3078	847	839	23		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta''.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	912	7308	4683	1294	1305	26	0	0

- Molecule 5 is a protein called PAP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	568	4593	2907	810	849	27	0	0

- Molecule 6 is a protein called PAP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	385	3040	1918	518	583	21	0	0

- Molecule 7 is a protein called PAP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	440	3701	2369	643	676	13	0	0

- Molecule 8 is a protein called PAP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	215	1771	1141	300	324	6	0	0

- Molecule 9 is a protein called PAP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	234	1970	1247	350	363	10	0	0

- Molecule 10 is a protein called PAP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	374	3022	1933	510	564	15	0	0

- Molecule 11 is a protein called PAP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	408	3348	2153	572	603	20	0	0

- Molecule 12 is a protein called PAP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	204	1714	1085	299	323	7	0	0

- Molecule 13 is a protein called PAP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	215	1759	1132	300	323	4	0	0

- Molecule 14 is a protein called PAP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	114	923	588	148	178	9	0	0
14	P	108	865	550	139	167	9	0	0

- Molecule 15 is a protein called PAP11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	Q	220	1740	1082	307	341	10	0	0

- Molecule 16 is a protein called PAP12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	R	114	944	596	167	178	3	0	0

- Molecule 17 is a protein called FLN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	S	386	3056	1941	516	578	21	0	0

- Molecule 18 is a protein called PTAC18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	104	Total	C	N	O	S	0	0
			881	572	148	157	4		

- Molecule 19 is a DNA chain called DNA (81-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	31	Total	C	N	O	P	0	0
			638	304	122	182	30		

- Molecule 20 is a DNA chain called DNA (81-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	40	Total	C	N	O	P	0	0
			813	386	145	242	40		

- Molecule 21 is a RNA chain called RNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	10	Total	C	N	O	P	0	0
			215	95	40	70	10		

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

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

- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
23	E	1	Total	Zn	0
			1	1	

- Molecule 24 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

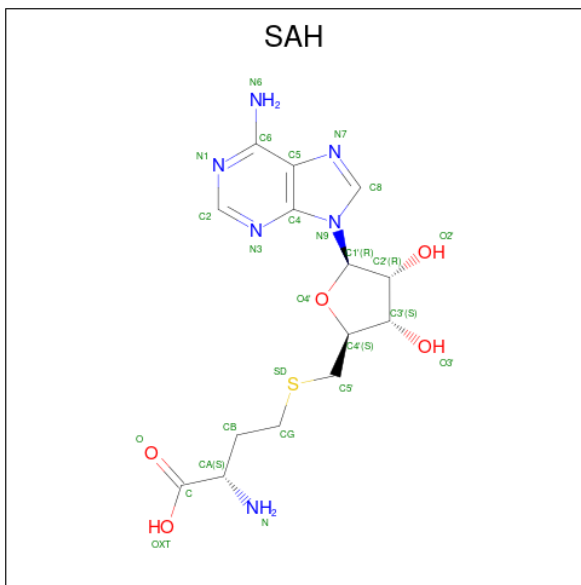
Mol	Chain	Residues	Atoms		AltConf
24	I	1	Total	Fe	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
24	N	1	Total Fe 1 1	0

- Molecule 25 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
25	L	1	Total C N O S 26 14 6 5 1	0

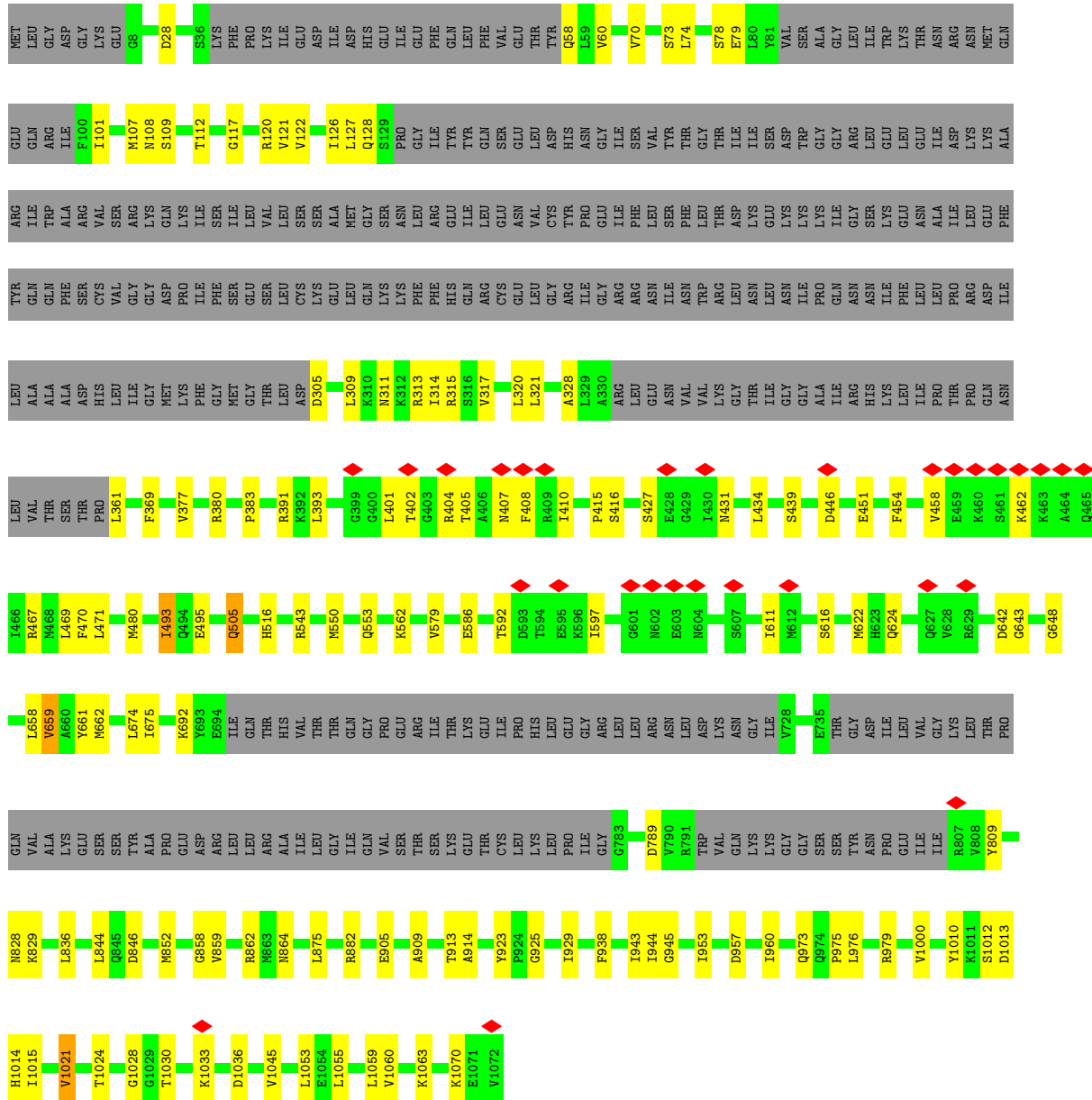
- Molecule 26 is water.

Mol	Chain	Residues	Atoms	AltConf
26	A	18	Total O 18 18	0
26	B	12	Total O 12 12	0
26	C	54	Total O 54 54	0
26	D	18	Total O 18 18	0
26	E	24	Total O 24 24	0
26	F	2	Total O 2 2	0
26	H	6	Total O 6 6	0

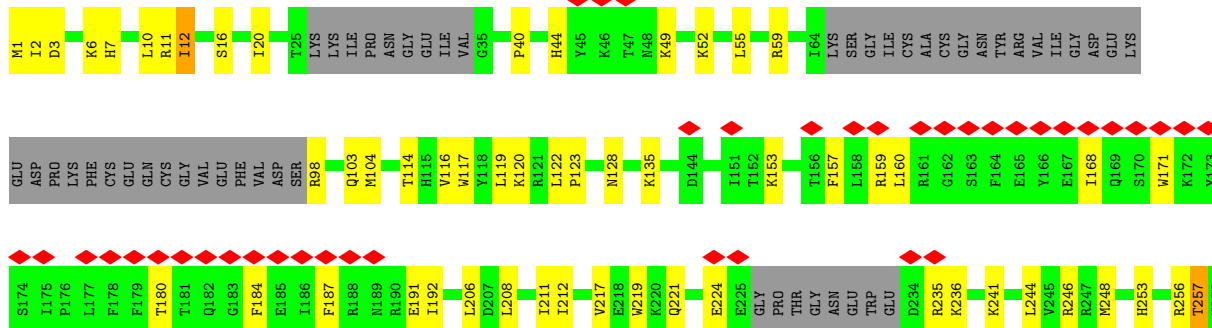
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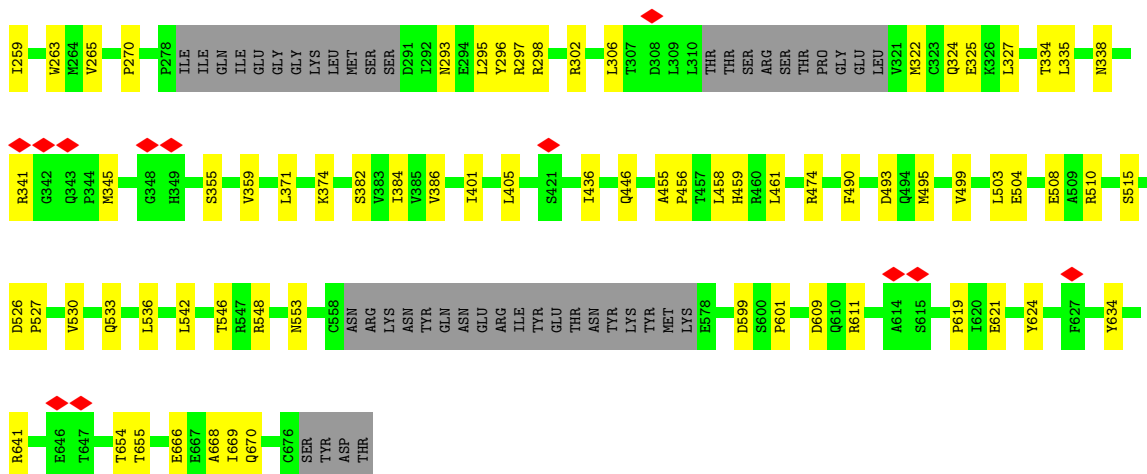
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Mol	Chain	Residues	Atoms		AltConf
26	I	3	Total 3	O 3	0
26	J	32	Total 32	O 32	0
26	K	17	Total 17	O 17	0
26	L	19	Total 19	O 19	0
26	M	15	Total 15	O 15	0
26	N	4	Total 4	O 4	0
26	O	2	Total 2	O 2	0
26	P	2	Total 2	O 2	0
26	R	3	Total 3	O 3	0
26	S	23	Total 23	O 23	0

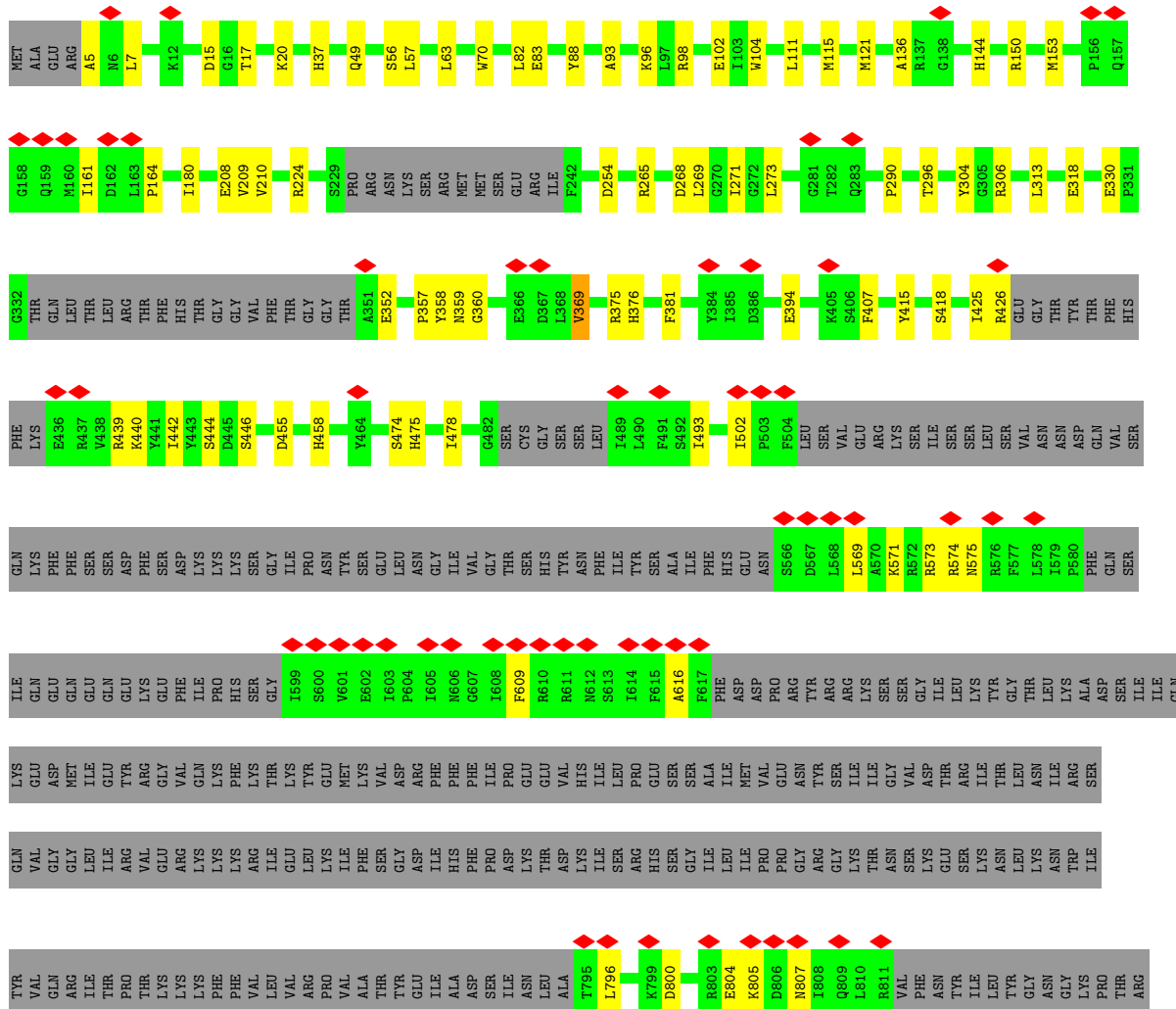


● Molecule 3: DNA-directed RNA polymerase subunit beta'





• Molecule 4: DNA-directed RNA polymerase subunit beta”



• Molecule 21: RNA (40-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	417374	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.48	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.127	Depositor
Minimum map value	-0.951	Depositor
Average map value	0.140	Depositor
Map value standard deviation	0.155	Depositor
Recommended contour level	0.8	Depositor
Map size (\AA)	300.0, 300.0, 300.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.5, 0.5, 0.5	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.11	0/2498	0.26	0/3377
1	B	0.12	0/1755	0.30	0/2378
2	C	0.12	0/5887	0.28	0/7943
3	D	0.12	0/4894	0.28	0/6612
4	E	0.10	0/7449	0.25	0/10057
5	F	0.12	0/4689	0.29	0/6328
6	G	0.11	0/3095	0.33	0/4175
7	H	0.11	0/3809	0.27	0/5147
8	I	0.11	0/1825	0.28	0/2481
9	J	0.11	0/2021	0.27	0/2724
10	K	0.12	0/3100	0.26	0/4204
11	L	0.10	0/3436	0.23	0/4650
12	M	0.09	0/1756	0.23	0/2378
13	N	0.09	0/1812	0.26	0/2464
14	O	0.10	0/939	0.21	0/1268
14	P	0.11	0/879	0.28	0/1187
15	Q	0.11	0/1771	0.31	0/2392
16	R	0.10	0/960	0.23	0/1285
17	S	0.10	0/3123	0.26	0/4226
18	T	0.12	0/906	0.34	0/1225
19	X	0.17	0/716	0.35	0/1102
20	Y	0.17	0/909	0.37	0/1399
21	Z	0.11	0/239	0.30	0/371
All	All	0.11	0/58468	0.28	0/79373

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
4	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	1182	ILE	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	2449	0	2490	36	0
1	B	1722	0	1726	23	0
2	C	5772	0	5790	93	0
3	D	4787	0	4863	100	0
4	E	7308	0	7386	116	0
5	F	4593	0	4529	92	0
6	G	3040	0	2986	61	0
7	H	3701	0	3579	93	0
8	I	1771	0	1696	47	0
9	J	1970	0	1923	31	0
10	K	3022	0	2962	32	0
11	L	3348	0	3304	49	0
12	M	1714	0	1679	24	0
13	N	1759	0	1688	42	0
14	O	923	0	917	15	0
14	P	865	0	867	18	0
15	Q	1740	0	1685	56	0
16	R	944	0	935	21	0
17	S	3056	0	3042	40	0
18	T	881	0	860	34	0
19	X	638	0	351	15	0
20	Y	813	0	450	31	0
21	Z	215	0	110	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	D	1	0	0	0	0
23	E	1	0	0	0	0
24	I	1	0	0	0	0
24	N	1	0	0	0	0
25	L	26	0	19	2	0
26	A	18	0	0	0	0
26	B	12	0	0	0	0
26	C	54	0	0	0	0
26	D	18	0	0	1	0
26	E	24	0	0	1	0
26	F	2	0	0	0	0
26	H	6	0	0	0	0
26	I	3	0	0	0	0
26	J	32	0	0	1	0
26	K	17	0	0	0	0
26	L	19	0	0	0	0
26	M	15	0	0	0	0
26	N	4	0	0	0	0
26	O	2	0	0	0	0
26	P	2	0	0	0	0
26	R	3	0	0	0	0
26	S	23	0	0	0	0
All	All	57315	0	55837	913	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 8.

The worst 5 of 913 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)
3:D:668:ALA:HA	16:R:71:GLN:HE22	1.38	0.87
3:D:384:ILE:HD11	3:D:495:MET:HB2	1.64	0.79
13:N:64:MET:HG2	13:N:69:LEU:HG	1.65	0.79
5:F:74:PHE:HD1	5:F:97:MET:HG2	1.50	0.76
18:T:58:LEU:HD22	18:T:63:VAL:HG11	1.68	0.76

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	295/327 (90%)	287 (97%)	8 (3%)	0	100	100
1	B	212/327 (65%)	206 (97%)	6 (3%)	0	100	100
2	C	710/1072 (66%)	689 (97%)	20 (3%)	1 (0%)	48	69
3	D	571/680 (84%)	554 (97%)	17 (3%)	0	100	100
4	E	874/1373 (64%)	842 (96%)	31 (4%)	1 (0%)	48	69
5	F	558/911 (61%)	535 (96%)	22 (4%)	1 (0%)	43	64
6	G	379/862 (44%)	367 (97%)	12 (3%)	0	100	100
7	H	432/675 (64%)	423 (98%)	9 (2%)	0	100	100
8	I	213/263 (81%)	204 (96%)	9 (4%)	0	100	100
9	J	230/529 (44%)	225 (98%)	5 (2%)	0	100	100
10	K	372/460 (81%)	363 (98%)	9 (2%)	0	100	100
11	L	402/483 (83%)	392 (98%)	9 (2%)	1 (0%)	43	64
12	M	202/334 (60%)	199 (98%)	3 (2%)	0	100	100
13	N	211/297 (71%)	204 (97%)	7 (3%)	0	100	100
14	O	112/185 (60%)	110 (98%)	2 (2%)	0	100	100
14	P	106/185 (57%)	105 (99%)	1 (1%)	0	100	100
15	Q	214/768 (28%)	202 (94%)	12 (6%)	0	100	100
16	R	108/162 (67%)	107 (99%)	1 (1%)	0	100	100
17	S	382/611 (62%)	367 (96%)	15 (4%)	0	100	100
18	T	102/140 (73%)	96 (94%)	6 (6%)	0	100	100
All	All	6685/10644 (63%)	6477 (97%)	204 (3%)	4 (0%)	49	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	553	I LE

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Mol	Chain	Res	Type
2	C	1030	THR
11	L	405	ILE
4	E	1183	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/301 (91%)	273 (99%)	2 (1%)	76	89
1	B	191/301 (64%)	190 (100%)	1 (0%)	81	91
2	C	626/931 (67%)	619 (99%)	7 (1%)	65	83
3	D	524/608 (86%)	518 (99%)	6 (1%)	65	83
4	E	805/1230 (65%)	800 (99%)	5 (1%)	78	90
5	F	484/782 (62%)	480 (99%)	4 (1%)	73	87
6	G	331/740 (45%)	326 (98%)	5 (2%)	57	79
7	H	394/609 (65%)	388 (98%)	6 (2%)	57	79
8	I	187/230 (81%)	186 (100%)	1 (0%)	81	91
9	J	212/469 (45%)	210 (99%)	2 (1%)	70	86
10	K	329/401 (82%)	329 (100%)	0	100	100
11	L	362/431 (84%)	359 (99%)	3 (1%)	73	87
12	M	195/299 (65%)	194 (100%)	1 (0%)	81	91
13	N	185/259 (71%)	182 (98%)	3 (2%)	55	78
14	O	103/169 (61%)	103 (100%)	0	100	100
14	P	97/169 (57%)	97 (100%)	0	100	100
15	Q	190/661 (29%)	185 (97%)	5 (3%)	40	66
16	R	101/144 (70%)	101 (100%)	0	100	100
17	S	336/532 (63%)	332 (99%)	4 (1%)	63	82
18	T	93/126 (74%)	92 (99%)	1 (1%)	65	83
All	All	6020/9392 (64%)	5964 (99%)	56 (1%)	68	86

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	G	711	VAL
18	T	133	CYS
7	H	535	GLN
17	S	389	GLU
15	Q	669	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 110 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	360	ASN
8	I	126	ASN
18	T	55	GLN
15	Q	745	GLN
5	F	788	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	Z	10/40 (25%)	2 (20%)	1 (10%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	Z	32	C
21	Z	34	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	Z	31	C

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 5 ligands modelled in this entry, 4 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	SAH	L	8001	-	27,28,28	1.10	5 (18%)	36,40,40	2.09	10 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	SAH	L	8001	-	-	3/15/31/31	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	L	8001	SAH	C2-N3	2.53	1.38	1.33
25	L	8001	SAH	C2-N1	2.51	1.38	1.33
25	L	8001	SAH	OXT-C	-2.29	1.23	1.30
25	L	8001	SAH	C5-N7	-2.05	1.35	1.39
25	L	8001	SAH	C8-N7	2.04	1.35	1.31

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	L	8001	SAH	N3-C2-N1	-5.49	120.27	128.58
25	L	8001	SAH	C5-C4-N3	-4.68	120.28	126.72
25	L	8001	SAH	C5'-SD-CG	-3.89	90.72	102.26
25	L	8001	SAH	N9-C8-N7	-3.75	108.61	113.94
25	L	8001	SAH	C2-N3-C4	3.45	120.25	111.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

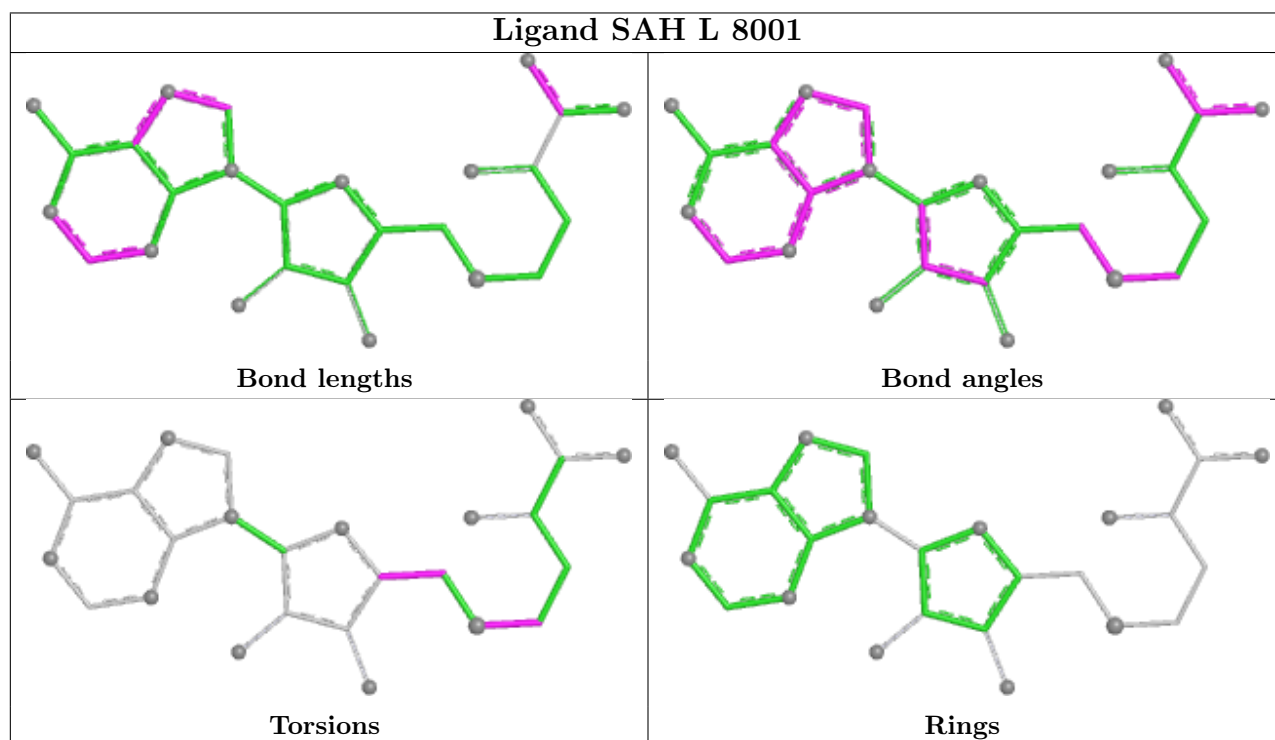
Mol	Chain	Res	Type	Atoms
25	L	8001	SAH	O4'-C4'-C5'-SD
25	L	8001	SAH	C3'-C4'-C5'-SD
25	L	8001	SAH	CB-CG-SD-C5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	L	8001	SAH	2	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.

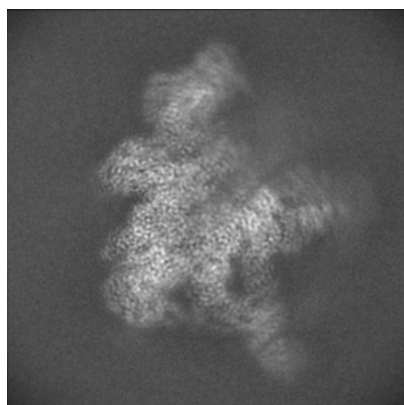
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19023. These allow visual inspection of the internal detail of the map and identification of artifacts.

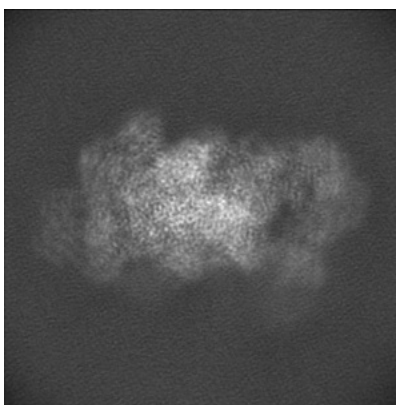
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

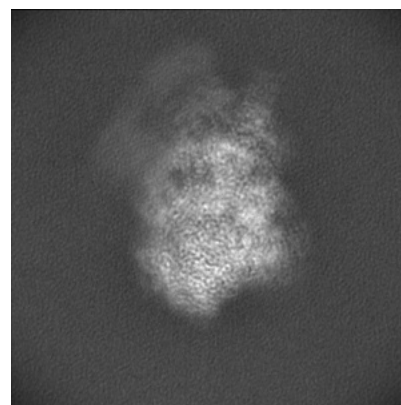
6.1.1 Primary map



X



Y

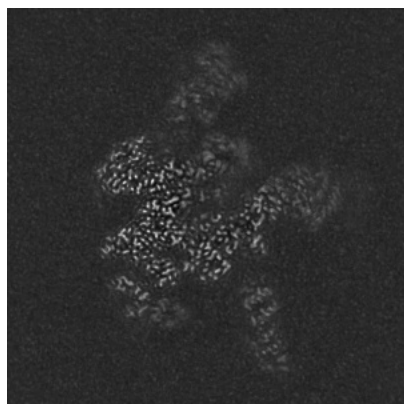


Z

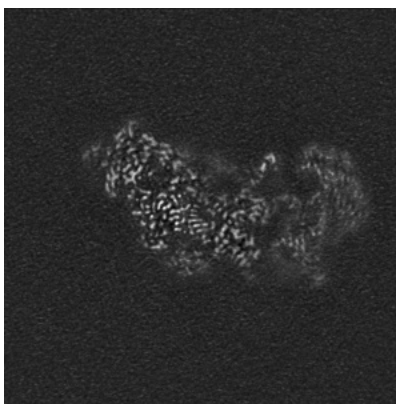
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

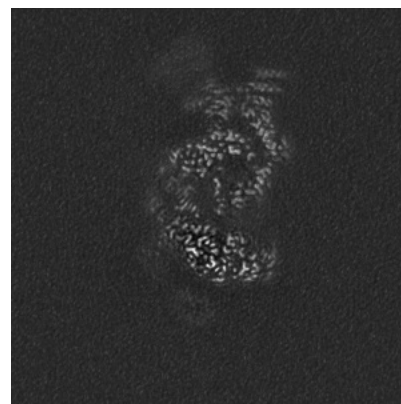
6.2.1 Primary map



X Index: 300



Y Index: 300

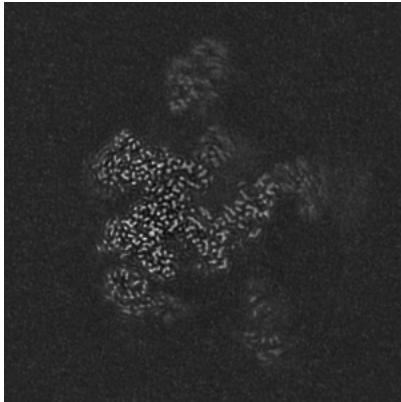


Z Index: 300

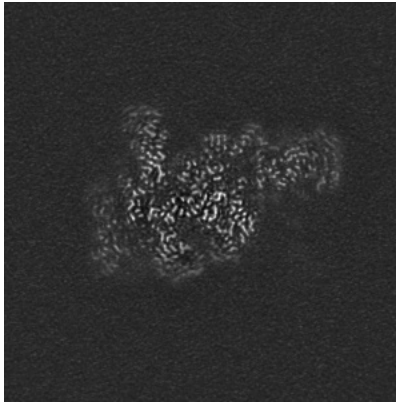
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

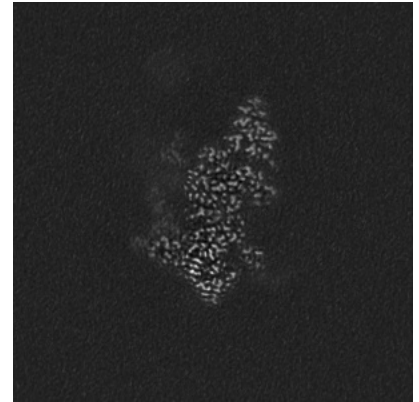
6.3.1 Primary map



X Index: 288



Y Index: 233

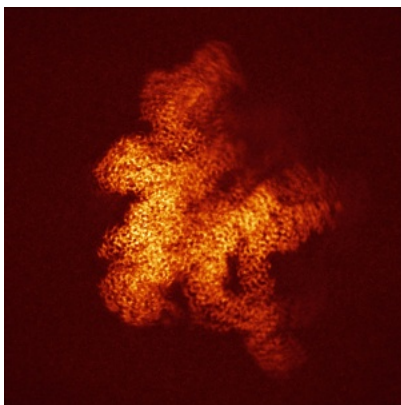


Z Index: 253

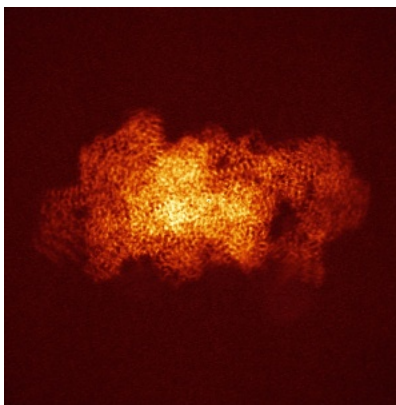
The images above show the largest variance slices of the map in three orthogonal directions.

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

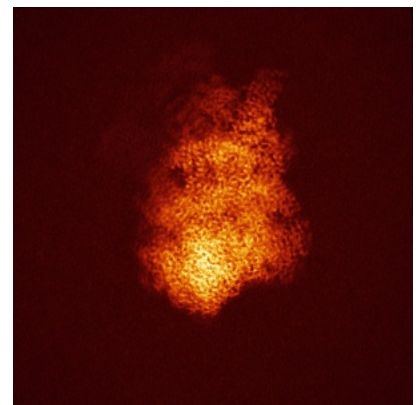
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

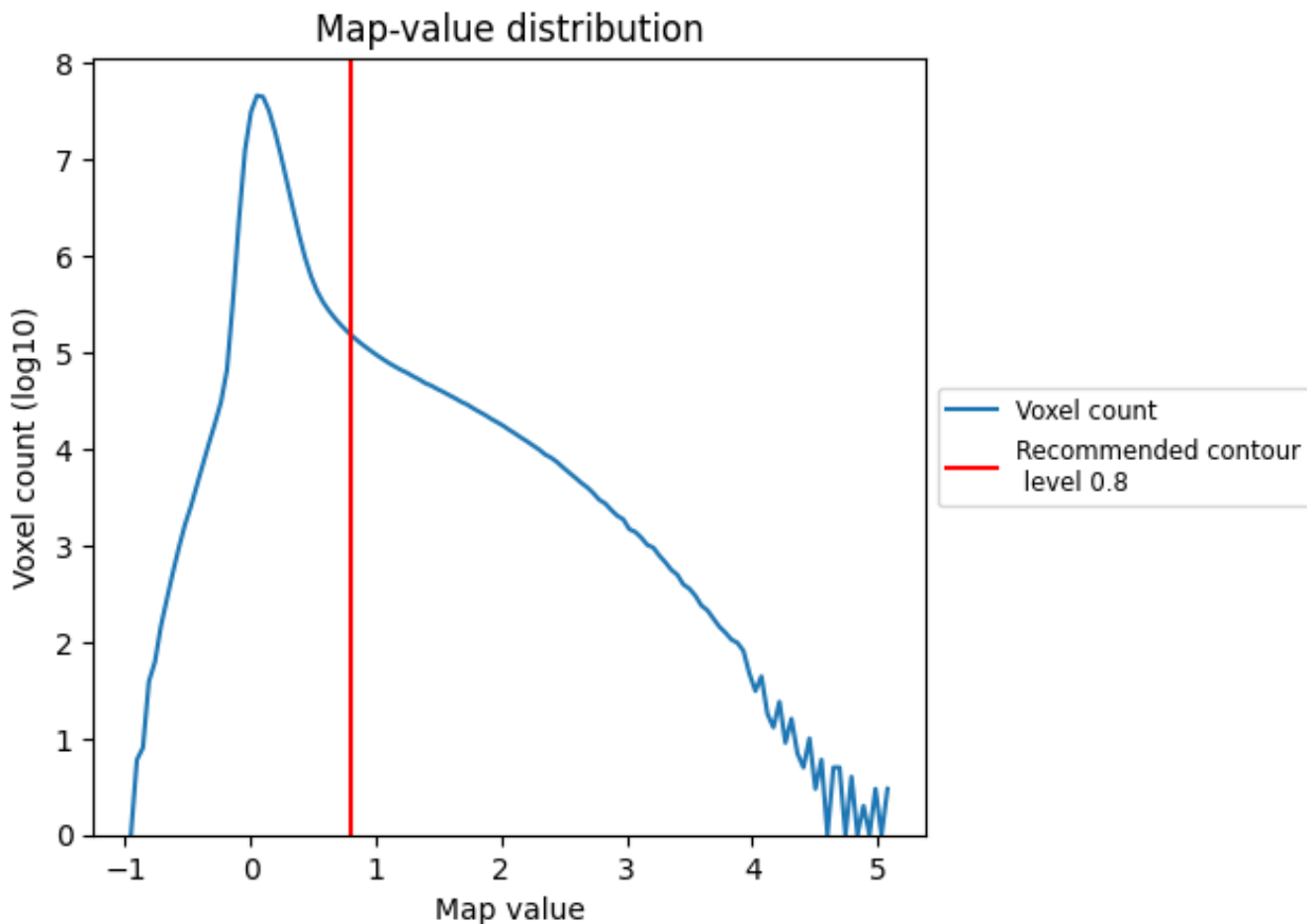
6.6 Mask visualisation

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

7 Map analysis [i](#)

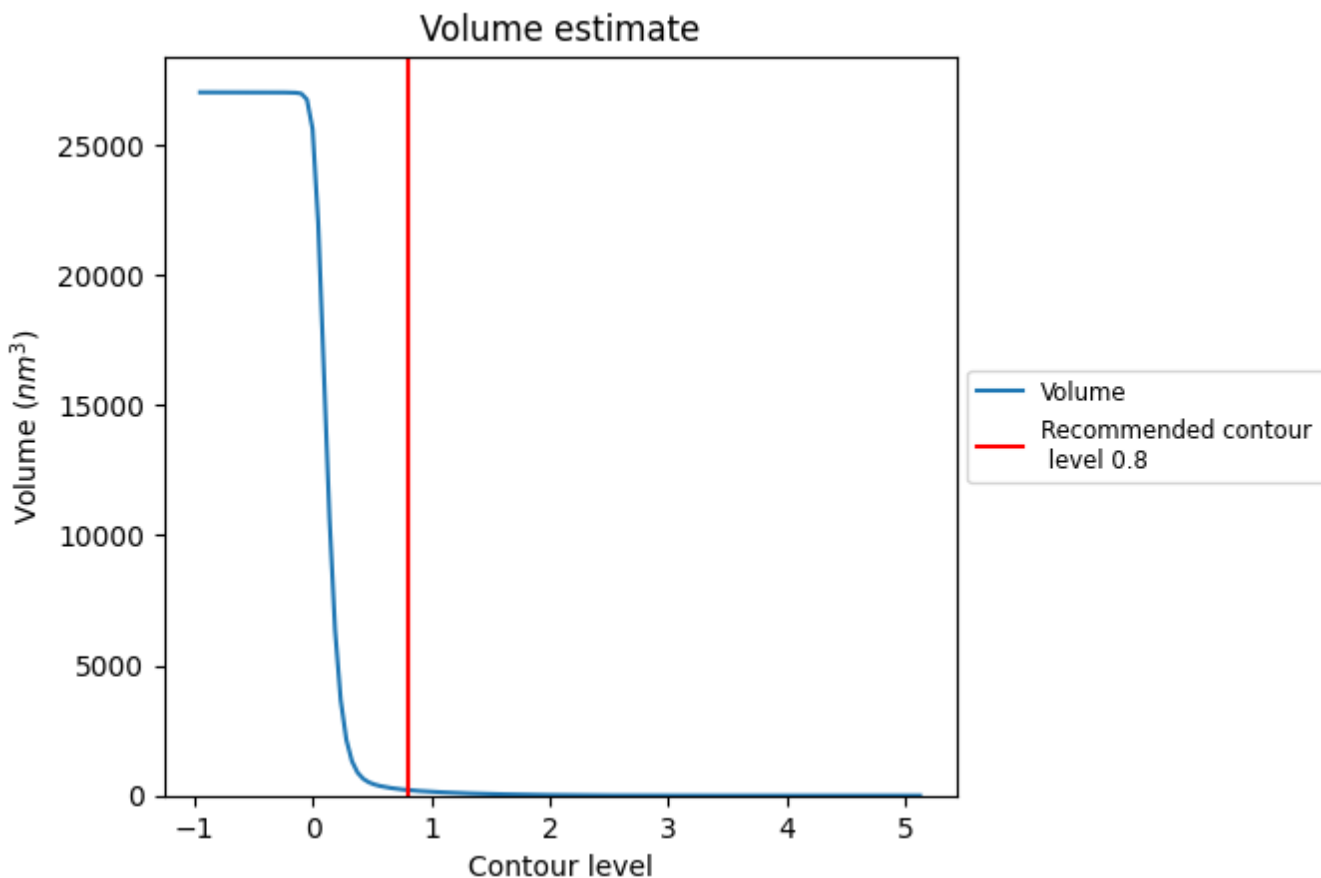
This section contains the results of statistical analysis of the map.

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.

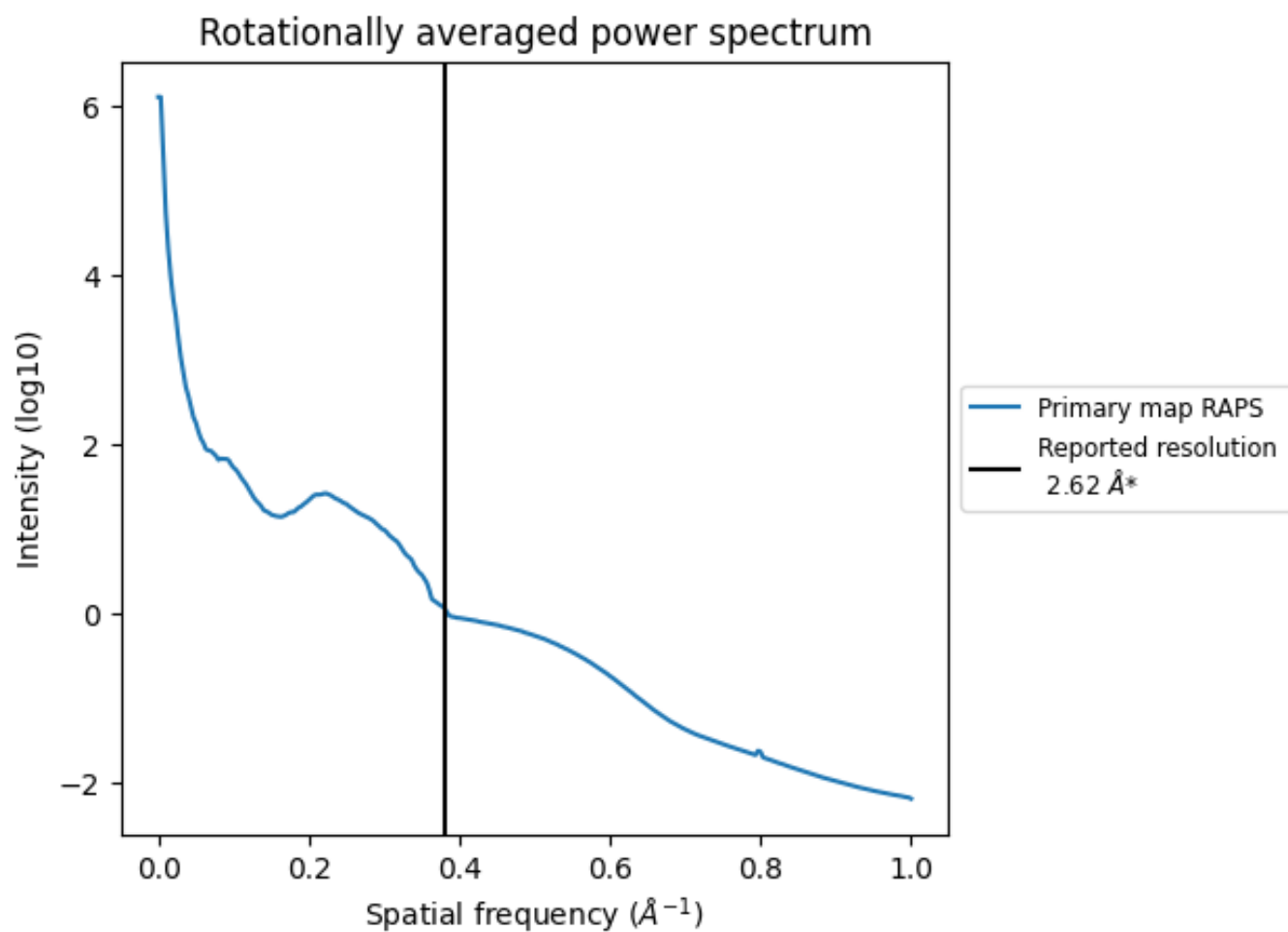
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 214 nm³; this corresponds to an approximate mass of 193 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 0.382 Å⁻¹

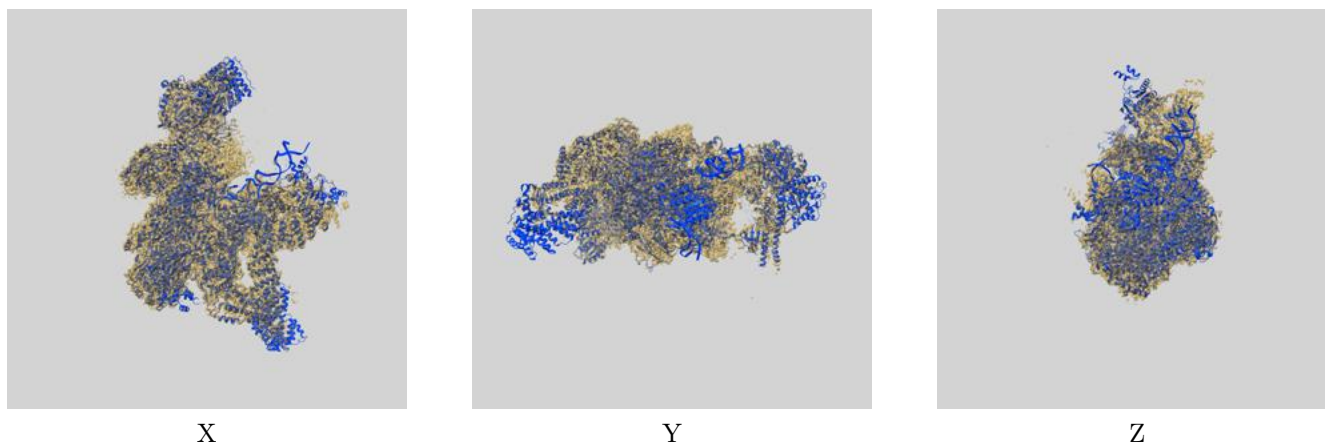
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

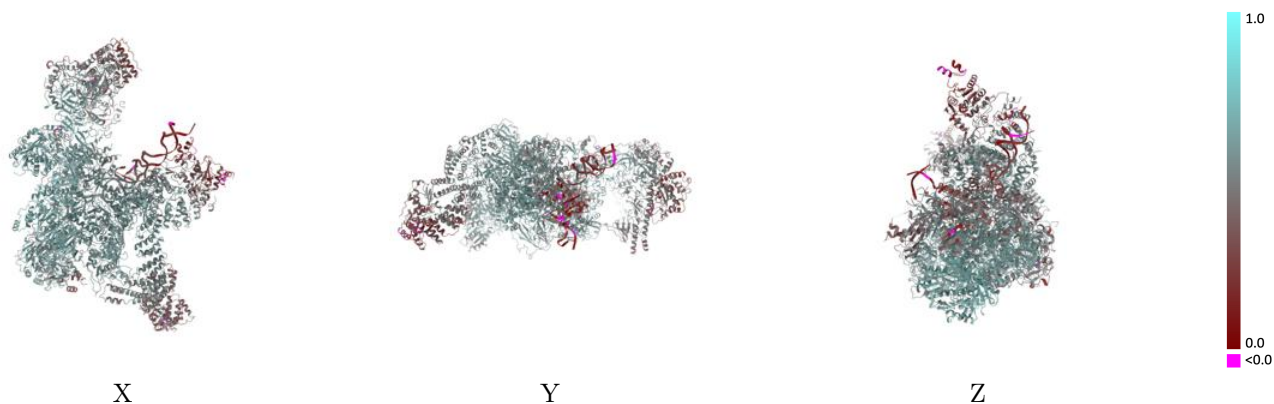
This section contains information regarding the fit between EMDB map EMD-19023 and PDB model 8RAS. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



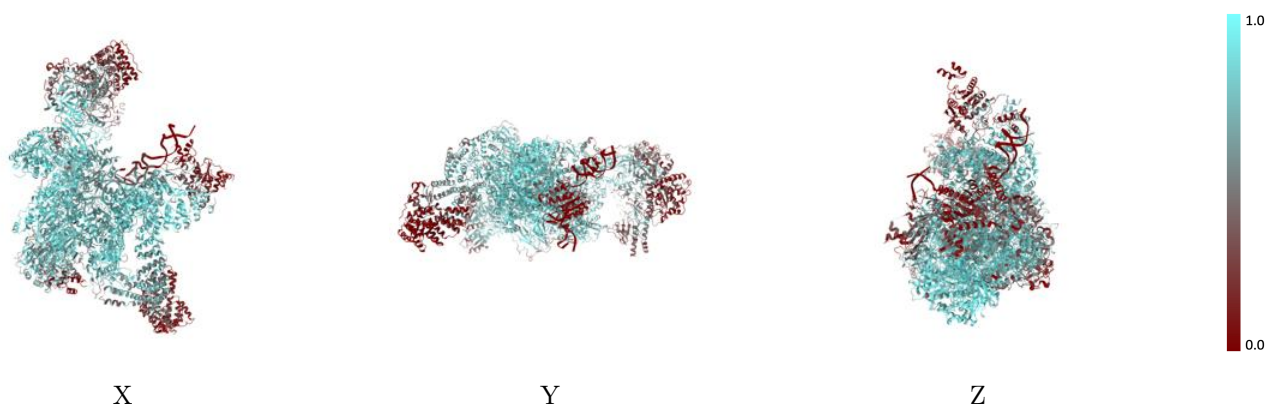
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



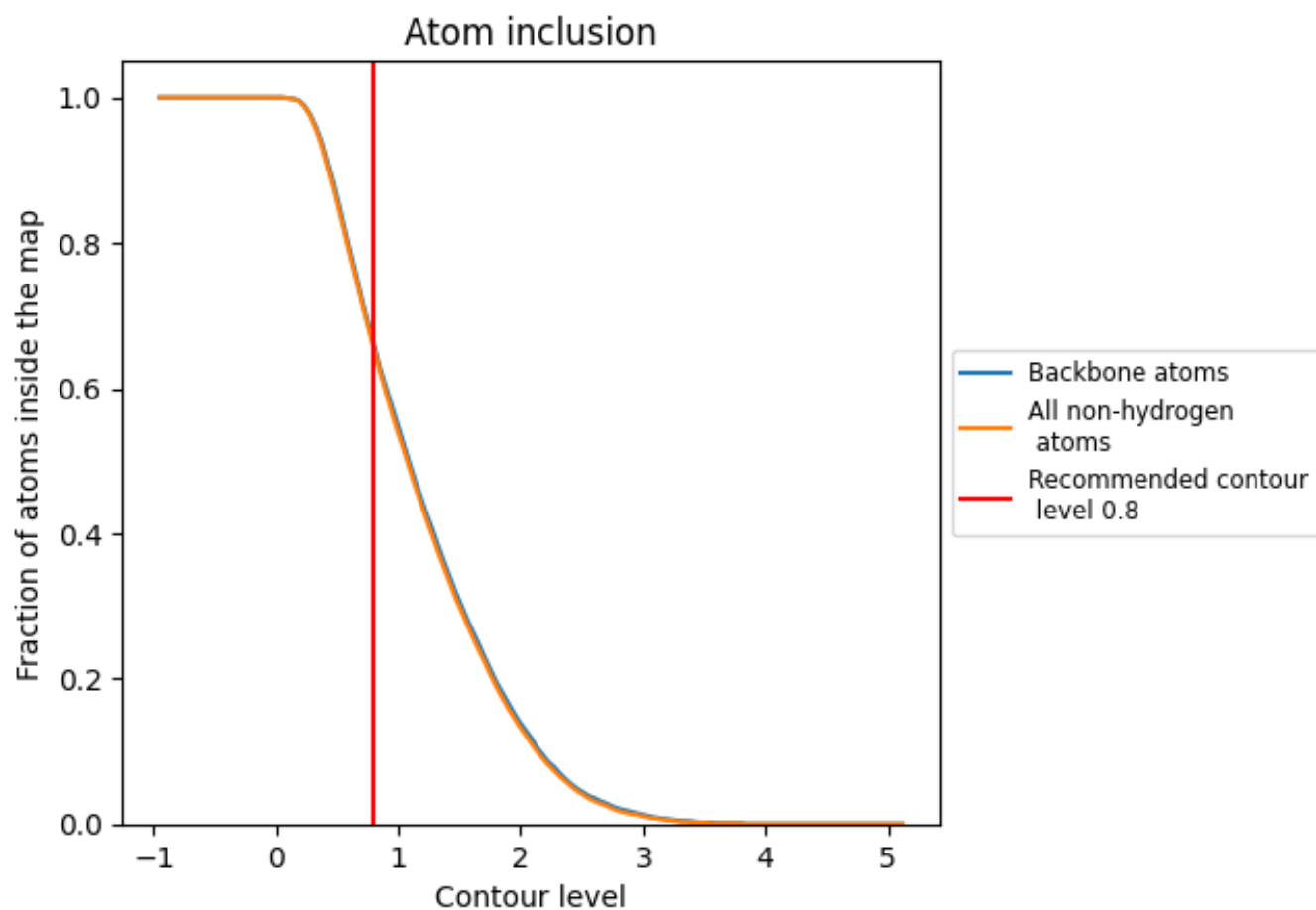
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).

















































9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 66% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6550	 0.5390
A	 0.6730	 0.5750
B	 0.7620	 0.6040
C	 0.8390	 0.6080
D	 0.7920	 0.5650
E	 0.7150	 0.5640
F	 0.7320	 0.5230
G	 0.1440	 0.3750
H	 0.5770	 0.5250
I	 0.4930	 0.5020
J	 0.8690	 0.6380
K	 0.8930	 0.6430
L	 0.7520	 0.5560
M	 0.7220	 0.5800
N	 0.1500	 0.3750
O	 0.8670	 0.6220
P	 0.5610	 0.5510
Q	 0.1670	 0.2750
R	 0.7820	 0.5880
S	 0.7650	 0.6100
T	 0.4640	 0.4750
X	 0.1720	 0.2430
Y	 0.3460	 0.3310
Z	 0.6330	 0.4900

