



wwPDB EM Validation Summary Report ⓘ

Nov 15, 2022 – 11:52 AM EST

PDB ID : 6XH8
EMDB ID : EMD-22185
Title : CueR-transcription activation complex with RNA transcript
Authors : Liu, B.; Shi, W.; Yang, Y.
Deposited on : 2020-06-18
Resolution : 4.10 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.dev43
Mogul : 1.8.5 (274361), 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

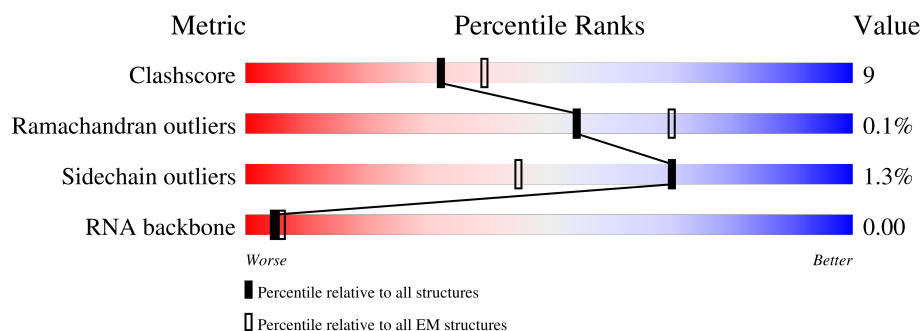
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

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







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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 $\leq 5\%$. 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	329	
1	B	329	
2	C	1342	
3	D	1407	
4	E	91	
5	F	628	
6	G	143	

Continued on next page...

Mol	Chain	Length	Quality of chain
6	H	143	 1% 71% 19% 9%
7	1	54	 1% 80% 20%
8	2	54	 17% 76% 22% 5%
9	3	3	 33% 67% 33% 5%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 65979 atoms, of which 32630 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
1	A	230	Total	C	H	N	O	S	0	0
			3599	1112	1813	317	351	6		
1	B	228	Total	C	H	N	O	S	0	0
			3556	1100	1789	312	349	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	1340	Total	C	H	N	O	S	0	0
			21153	6631	10583	1841	2055	43		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	1337	Total	C	H	N	O	S	0	0
			21011	6531	10615	1853	1962	50		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	59	Total	C	H	N	O	S	0	0
			934	283	476	86	88	1		

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	497	Total	C	H	N	O	S	0	0
			8105	2512	4083	719	768	23		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-14	MET	-	expression tag	UNP P00579

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-13	ARG	-	expression tag	UNP P00579
F	-12	GLY	-	expression tag	UNP P00579
F	-11	SER	-	expression tag	UNP P00579
F	-10	HIS	-	expression tag	UNP P00579
F	-9	HIS	-	expression tag	UNP P00579
F	-8	HIS	-	expression tag	UNP P00579
F	-7	HIS	-	expression tag	UNP P00579
F	-6	HIS	-	expression tag	UNP P00579
F	-5	HIS	-	expression tag	UNP P00579
F	-4	THR	-	expression tag	UNP P00579
F	-3	ASP	-	expression tag	UNP P00579
F	-2	GLN	-	expression tag	UNP P00579
F	-1	PHE	-	expression tag	UNP P00579
F	0	THR	-	expression tag	UNP P00579

- Molecule 6 is a protein called HTH-type transcriptional regulator CueR.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	130	Total	C	H	N	O	S	0	0
			2038	629	1013	186	203	7		
6	H	130	Total	C	H	N	O	S	0	0
			2038	629	1013	186	203	7		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	136	LEU	-	expression tag	UNP P0A9G4
G	137	GLU	-	expression tag	UNP P0A9G4
G	138	HIS	-	expression tag	UNP P0A9G4
G	139	HIS	-	expression tag	UNP P0A9G4
G	140	HIS	-	expression tag	UNP P0A9G4
G	141	HIS	-	expression tag	UNP P0A9G4
G	142	HIS	-	expression tag	UNP P0A9G4
G	143	HIS	-	expression tag	UNP P0A9G4
H	136	LEU	-	expression tag	UNP P0A9G4
H	137	GLU	-	expression tag	UNP P0A9G4
H	138	HIS	-	expression tag	UNP P0A9G4
H	139	HIS	-	expression tag	UNP P0A9G4
H	140	HIS	-	expression tag	UNP P0A9G4
H	141	HIS	-	expression tag	UNP P0A9G4
H	142	HIS	-	expression tag	UNP P0A9G4
H	143	HIS	-	expression tag	UNP P0A9G4

- Molecule 7 is a DNA chain called NONTEMPLATE STRAND DNA (54-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
7	1	54	Total	C	H	N	O	P	0	0
			1713	524	610	193	332	54		

- Molecule 8 is a DNA chain called TEMPLATE STRAND DNA (54-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
8	2	54	Total	C	H	N	O	P	0	0
			1719	526	603	218	318	54		

- Molecule 9 is a RNA chain called NASCENT RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	3	3	Total	C	H	N	O	P	0	0
			109	30	32	15	27	5		

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total	Zn	0
			2	2	

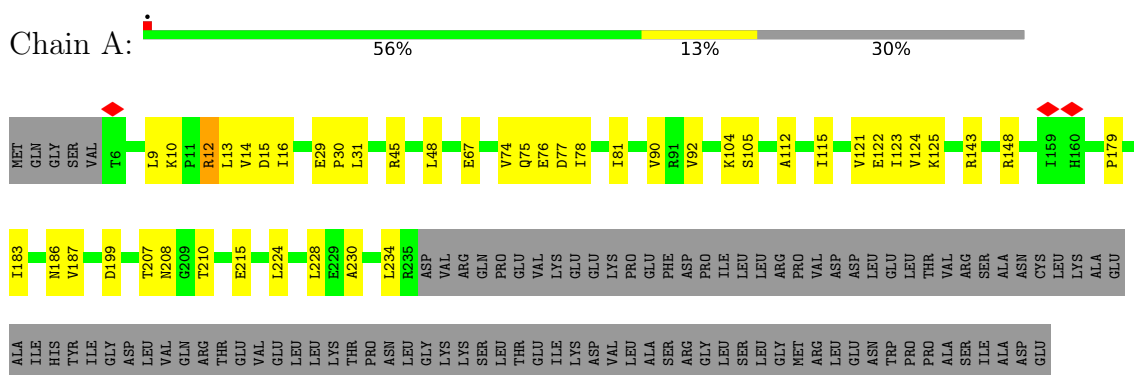
- Molecule 11 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	G	1	Total	Cu	0
			1	1	
11	H	1	Total	Cu	0
			1	1	

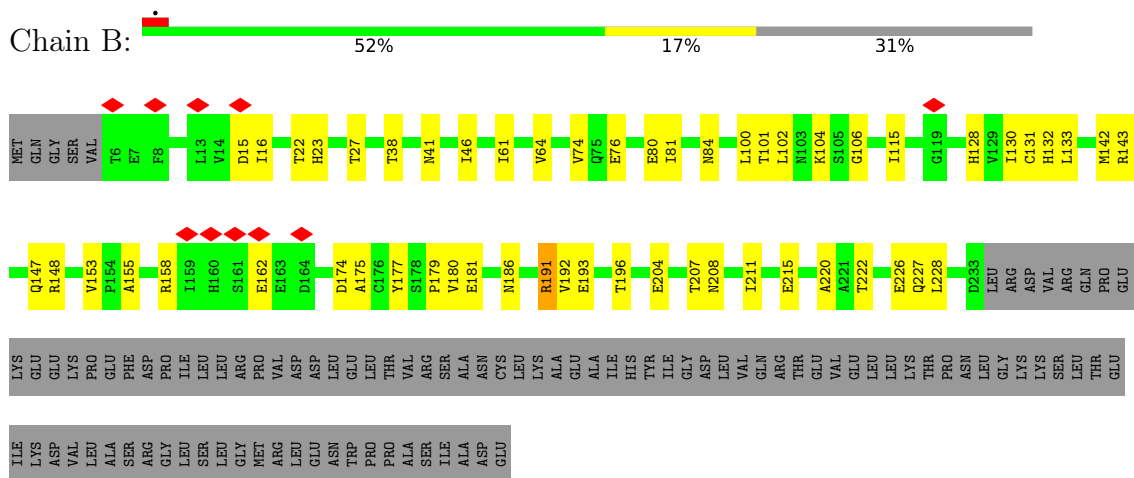
3 Residue-property plots

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

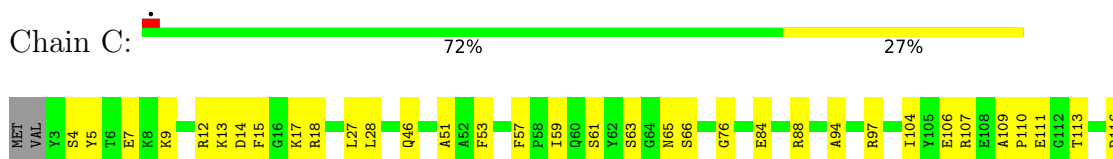
- Molecule 1: DNA-directed RNA polymerase subunit alpha

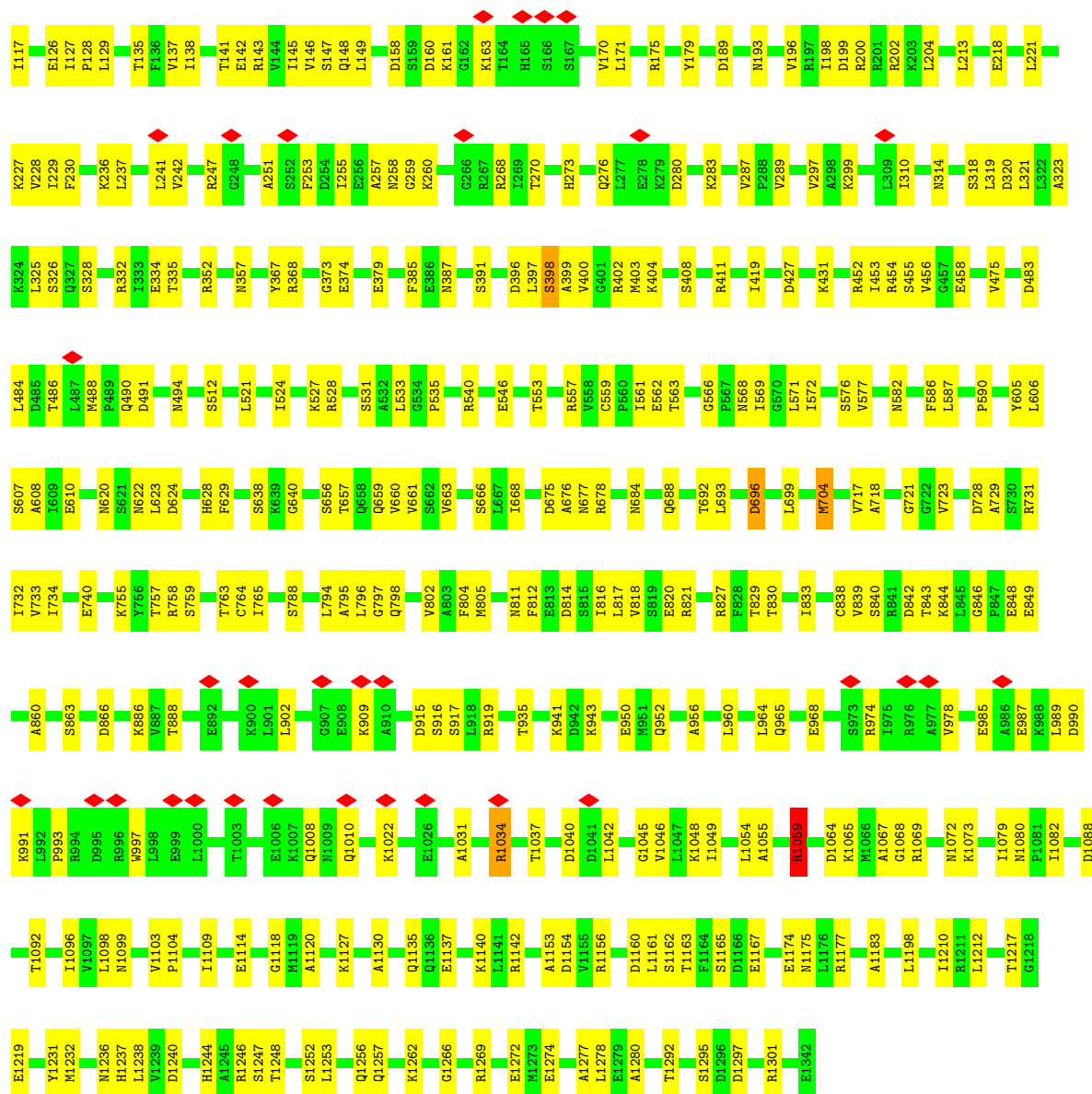


- Molecule 1: DNA-directed RNA polymerase subunit alpha

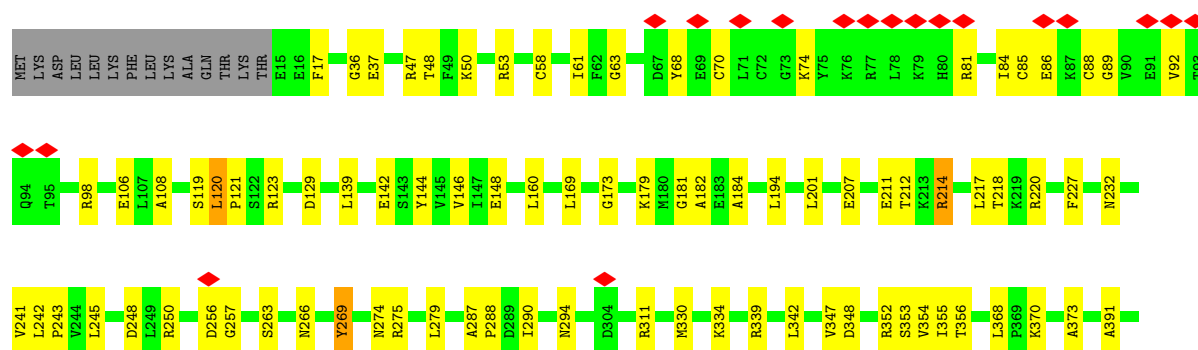


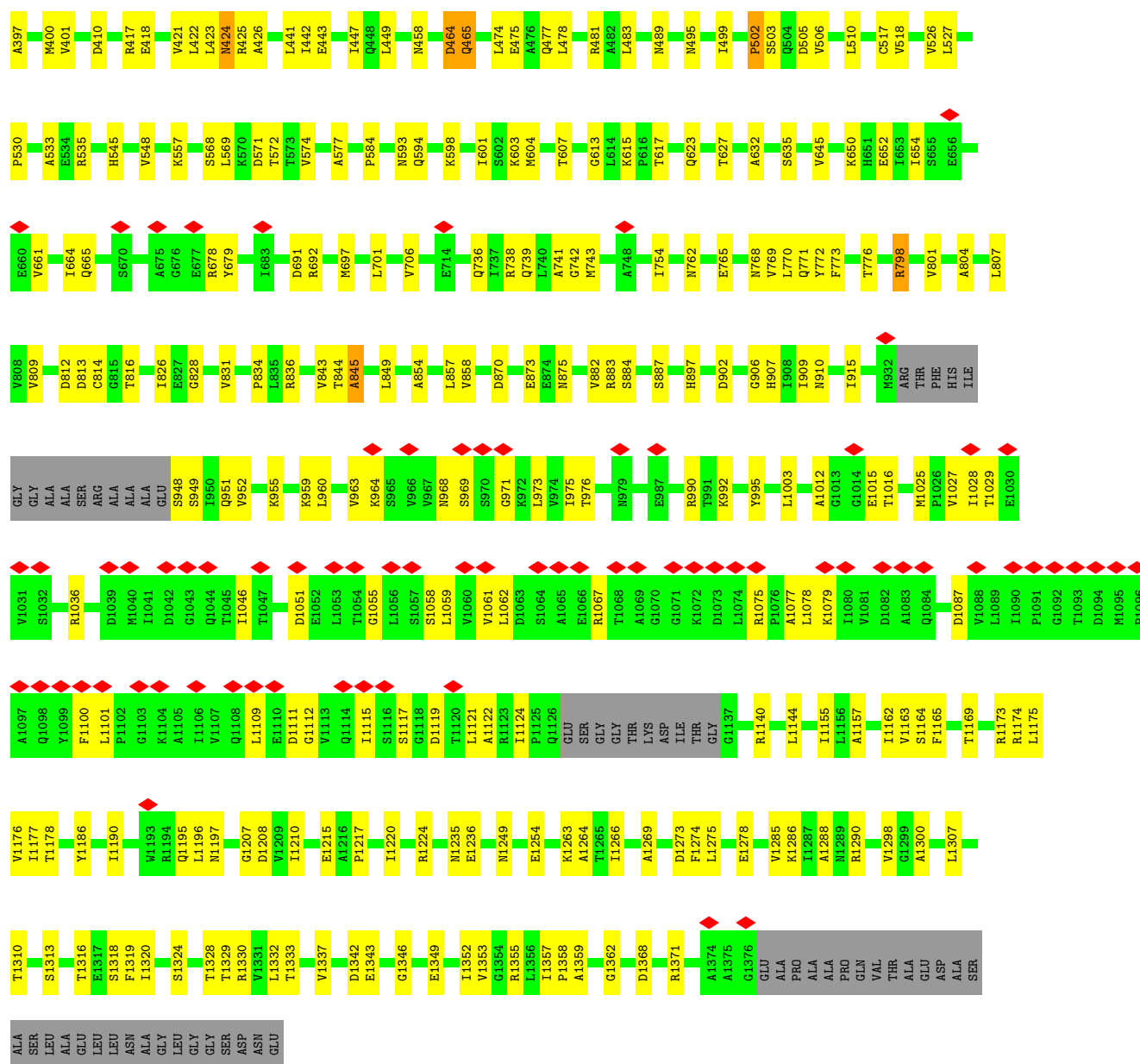
- Molecule 2: DNA-directed RNA polymerase subunit beta





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





• Molecule 4: DNA-directed RNA polymerase subunit omega

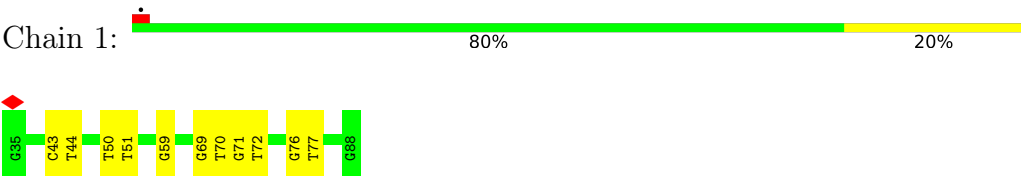


• Molecule 5: RNA polymerase sigma factor RpoD

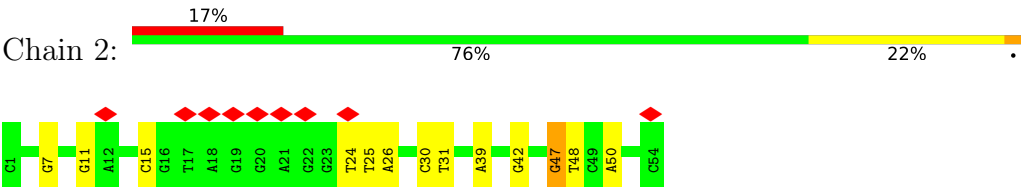


HIS
ARG
ALA
GLY
LEU
GLU
HIS
HIS
HIS
HIS
HIS

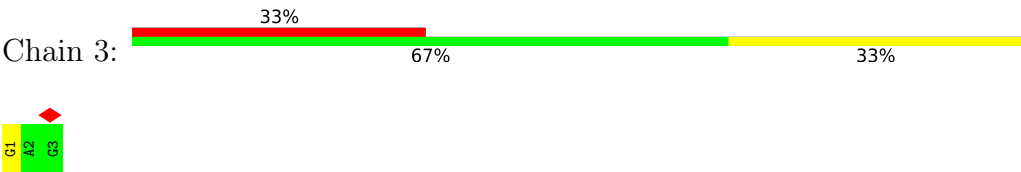
• Molecule 7: NONTEMPLATE STRAND DNA (54-MER)



• Molecule 8: TEMPLATE STRAND DNA (54-MER)



• Molecule 9: NASCENT RNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25244	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00481	Depositor
Map size (Å)	341.76, 341.76, 341.76	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.89000005, 0.89000005, 0.89000005	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, CU, 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	0.57	0/1808	0.69	1/2450 (0.0%)
1	B	0.47	0/1789	0.66	0/2425
2	C	0.62	0/10739	0.70	0/14489
3	D	0.55	0/10553	0.71	1/14248 (0.0%)
4	E	0.37	0/460	0.64	0/620
5	F	0.39	0/4076	0.66	1/5482 (0.0%)
6	G	0.38	0/1038	0.64	0/1400
6	H	0.37	0/1038	0.64	1/1400 (0.1%)
7	1	0.88	1/1233 (0.1%)	1.10	2/1901 (0.1%)
8	2	0.85	0/1255	0.98	2/1936 (0.1%)
9	3	0.56	0/50	1.29	0/76
All	All	0.57	1/34039 (0.0%)	0.73	8/46427 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
2	C	0	5
3	D	0	14
5	F	0	6
All	All	0	28

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1	76	DG	C3'-O3'	5.88	1.51	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	2	47	DG	O4'-C4'-C3'	-7.74	101.36	106.00
5	F	332	ASP	CB-CG-OD1	7.51	125.06	118.30
6	H	51	ARG	NE-CZ-NH2	-6.04	117.28	120.30
7	1	76	DG	P-O3'-C3'	5.98	126.88	119.70
7	1	76	DG	OP1-P-O3'	5.48	117.25	105.20

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	90	VAL	Peptide
1	B	191	ARG	Peptide
1	B	211	ILE	Peptide
2	C	242	VAL	Peptide
2	C	398	SER	Peptide

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	1786	1813	1813	30	0
1	B	1767	1789	1789	40	0
2	C	10570	10583	10582	232	0
3	D	10396	10615	10615	222	0
4	E	458	476	476	11	0
5	F	4022	4083	4083	73	0
6	G	1025	1013	1013	12	0
6	H	1025	1013	1014	19	0
7	1	1103	610	610	7	0
8	2	1116	603	603	13	0
9	3	77	32	34	4	0
10	D	2	0	0	0	0
11	G	1	0	0	0	0
11	H	1	0	0	0	0
All	All	33349	32630	32632	618	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 9.

The worst 5 of 618 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:355:ILE:HD11	3:D:464:ASP:CB	2.04	0.87
3:D:425:ARG:NH1	3:D:426:ALA:O	2.12	0.82
3:D:355:ILE:HD11	3:D:464:ASP:HB2	1.62	0.81
5:F:552:THR:OG1	5:F:597:LYS:NZ	2.15	0.80
2:C:798:GLN:NE2	2:C:827:ARG:O	2.15	0.80

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	228/329 (69%)	192 (84%)	36 (16%)	0	100	100
1	B	226/329 (69%)	202 (89%)	24 (11%)	0	100	100
2	C	1338/1342 (100%)	1156 (86%)	180 (14%)	2 (0%)	51	84
3	D	1331/1407 (95%)	1119 (84%)	211 (16%)	1 (0%)	51	84
4	E	57/91 (63%)	52 (91%)	5 (9%)	0	100	100
5	F	493/628 (78%)	429 (87%)	63 (13%)	1 (0%)	47	80
6	G	128/143 (90%)	116 (91%)	12 (9%)	0	100	100
6	H	128/143 (90%)	120 (94%)	8 (6%)	0	100	100
All	All	3929/4412 (89%)	3386 (86%)	539 (14%)	4 (0%)	54	84

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	399	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	121	PRO
5	F	507	MET
2	C	814	ASP

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	198/286 (69%)	196 (99%)	2 (1%)	76	85
1	B	196/286 (68%)	195 (100%)	1 (0%)	88	93
2	C	1155/1157 (100%)	1134 (98%)	21 (2%)	59	77
3	D	1120/1168 (96%)	1108 (99%)	12 (1%)	73	84
4	E	49/75 (65%)	49 (100%)	0	100	100
5	F	439/554 (79%)	431 (98%)	8 (2%)	59	77
6	G	114/125 (91%)	113 (99%)	1 (1%)	78	87
6	H	114/125 (91%)	114 (100%)	0	100	100
All	All	3385/3776 (90%)	3340 (99%)	45 (1%)	70	81

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

Mol	Chain	Res	Type
3	D	458	ASN
3	D	1249	ASN
3	D	464	ASP
3	D	743	MET
5	F	105	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	186	GLN
6	G	99	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	458	ASN
6	H	104	GLN
5	F	446	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	3	1/3 (33%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

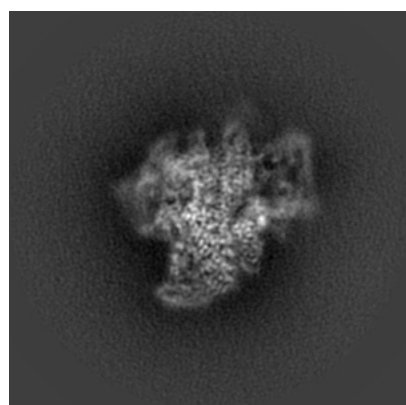
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22185. These allow visual inspection of the internal detail of the map and identification of artifacts.

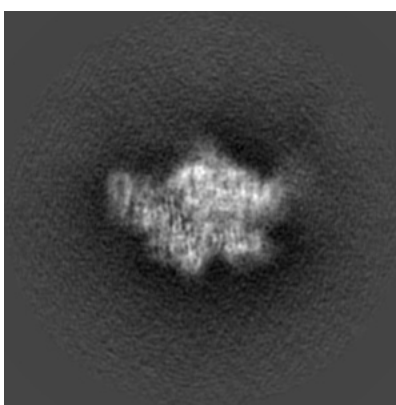
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

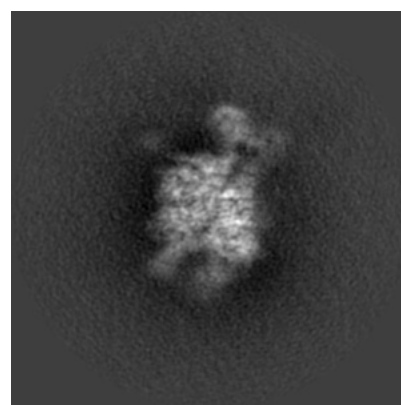
6.1.1 Primary map



X



Y

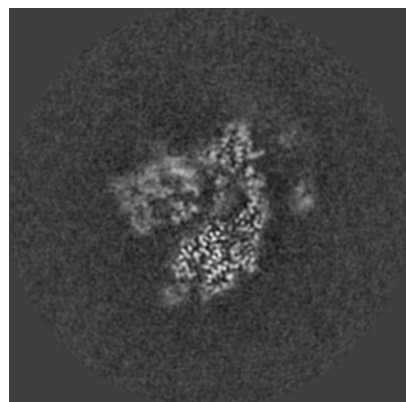


Z

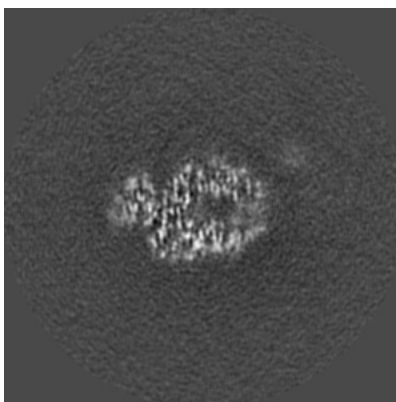
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

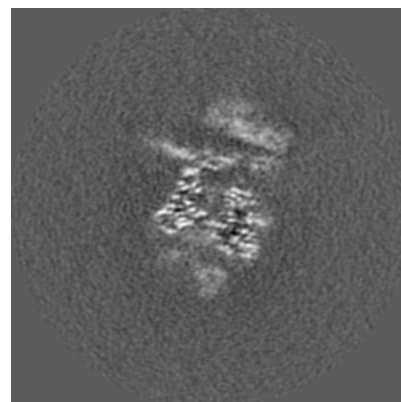
6.2.1 Primary map



X Index: 192



Y Index: 192

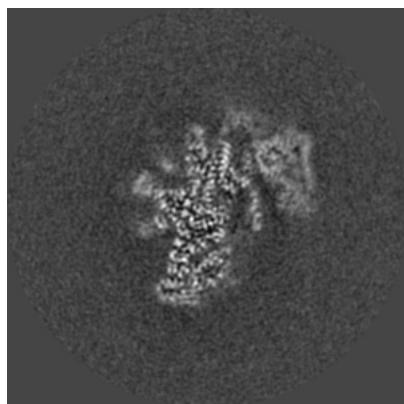


Z Index: 192

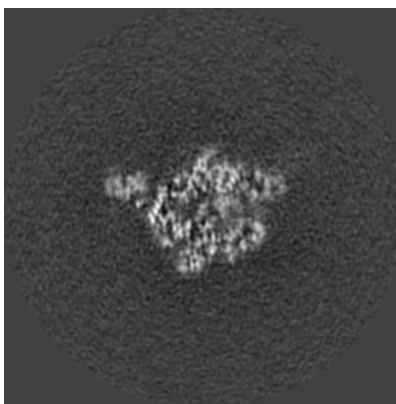
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

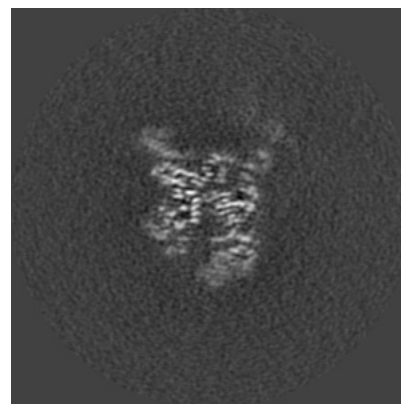
6.3.1 Primary map



X Index: 209



Y Index: 179

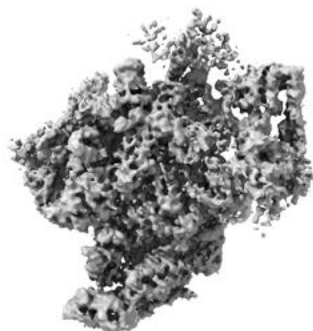


Z Index: 177

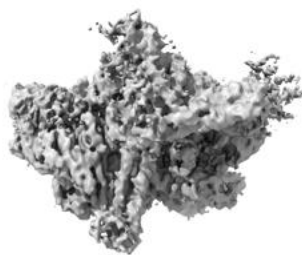
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00481. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

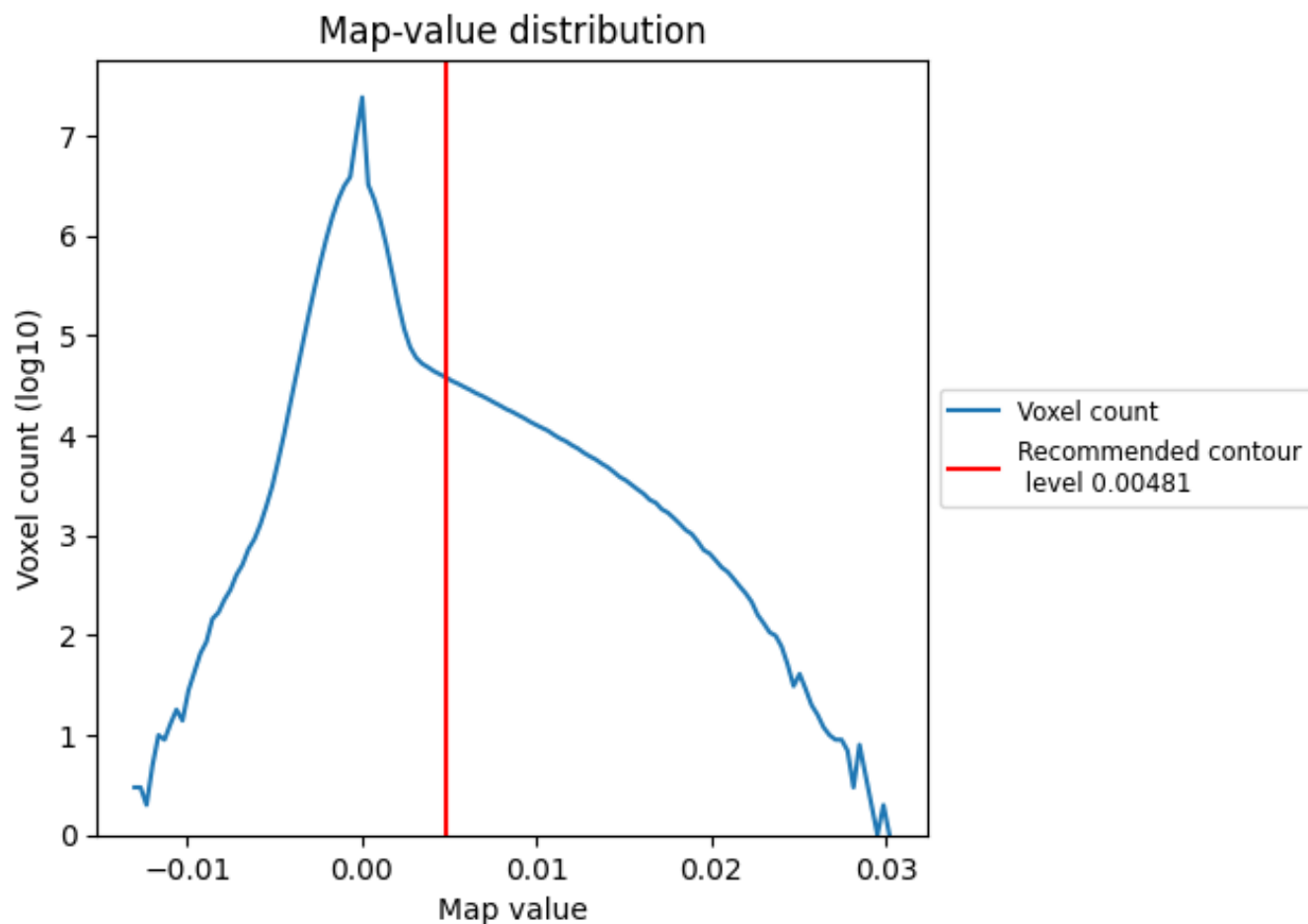
6.5 Mask visualisation

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

7 Map analysis [i](#)

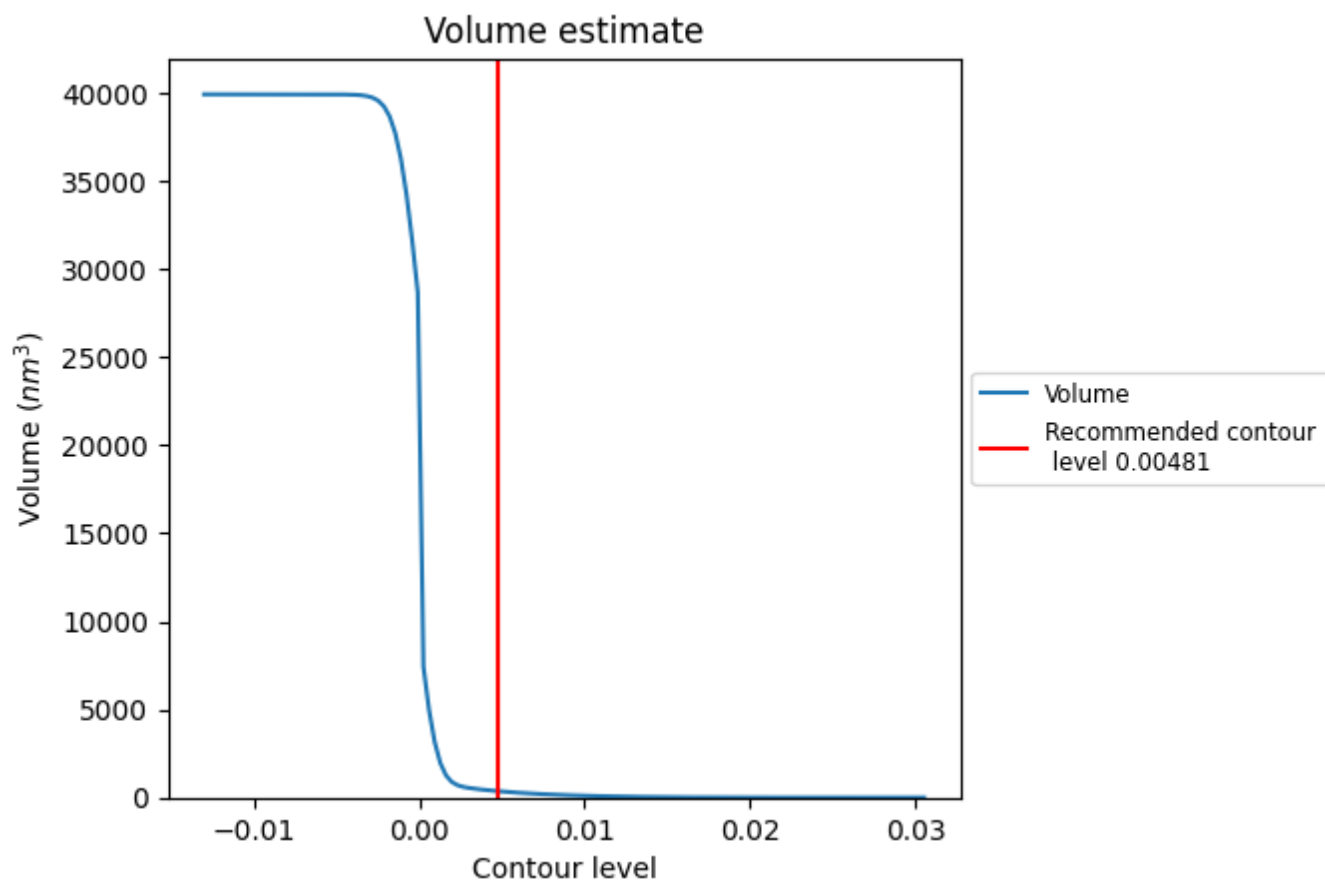
This section contains the results of statistical analysis of the map.

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.

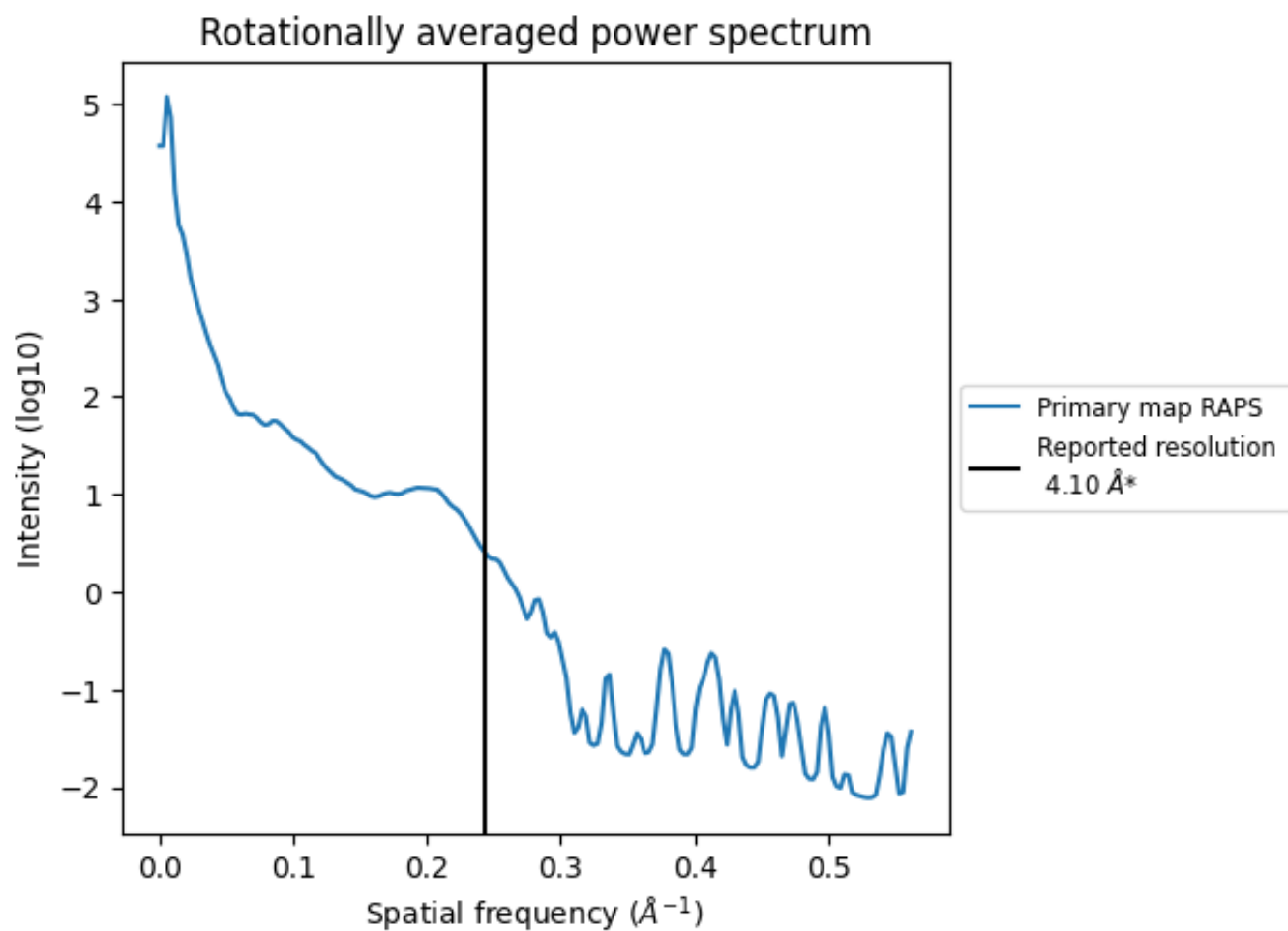
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 360 nm^3 ; this corresponds to an approximate mass of 325 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 0.244 Å⁻¹

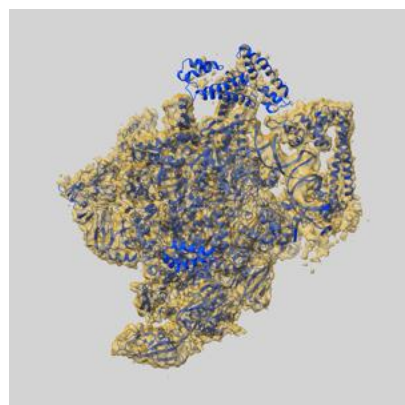
8 Fourier-Shell correlation

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

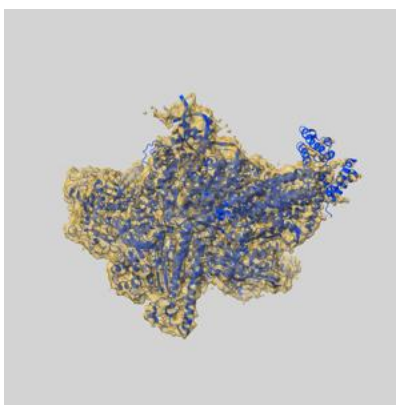
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22185 and PDB model 6XH8. Per-residue inclusion information can be found in section [3](#) on page [7](#).

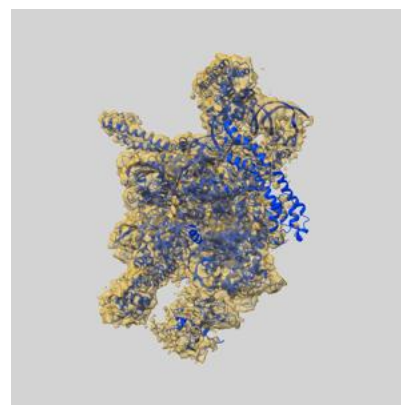
9.1 Map-model overlay [i](#)



X



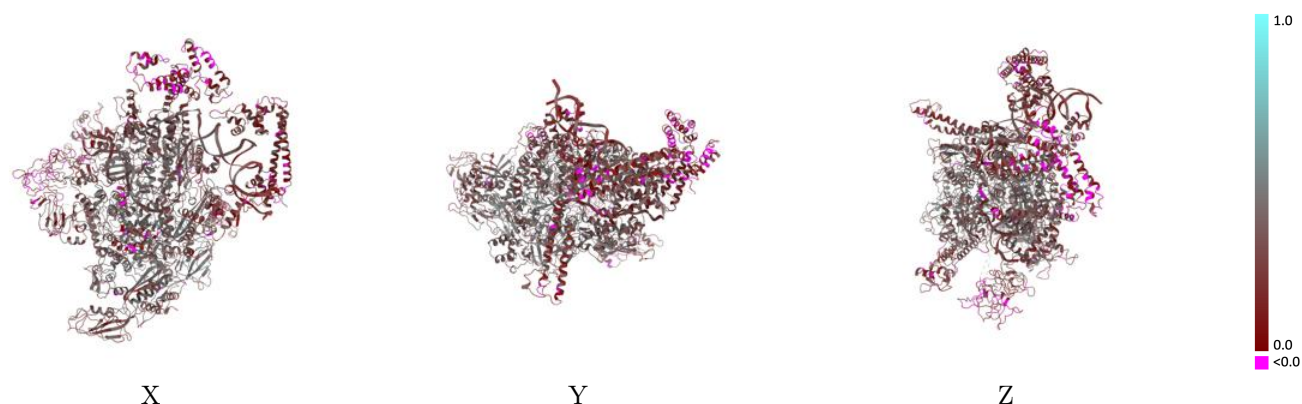
Y



Z

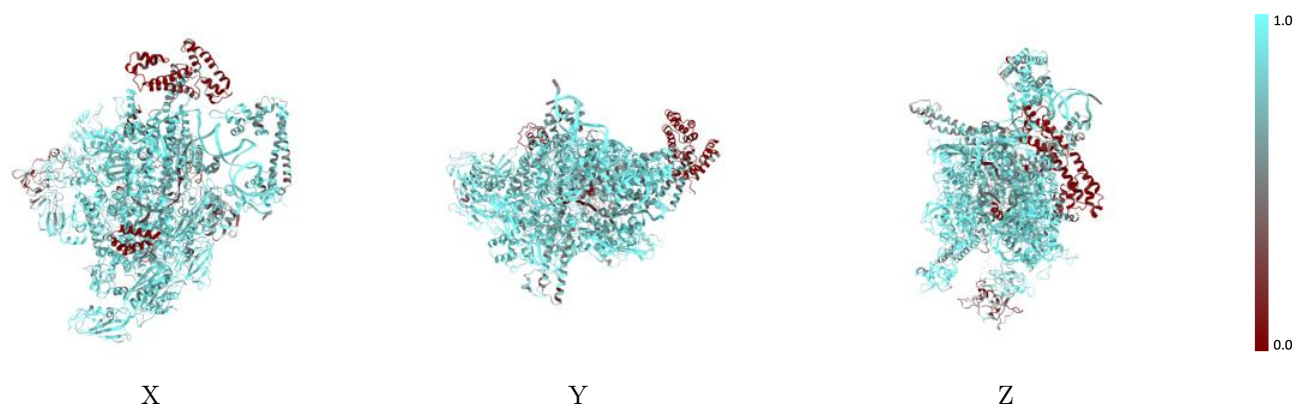
The images above show the 3D surface view of the map at the recommended contour level 0.00481 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



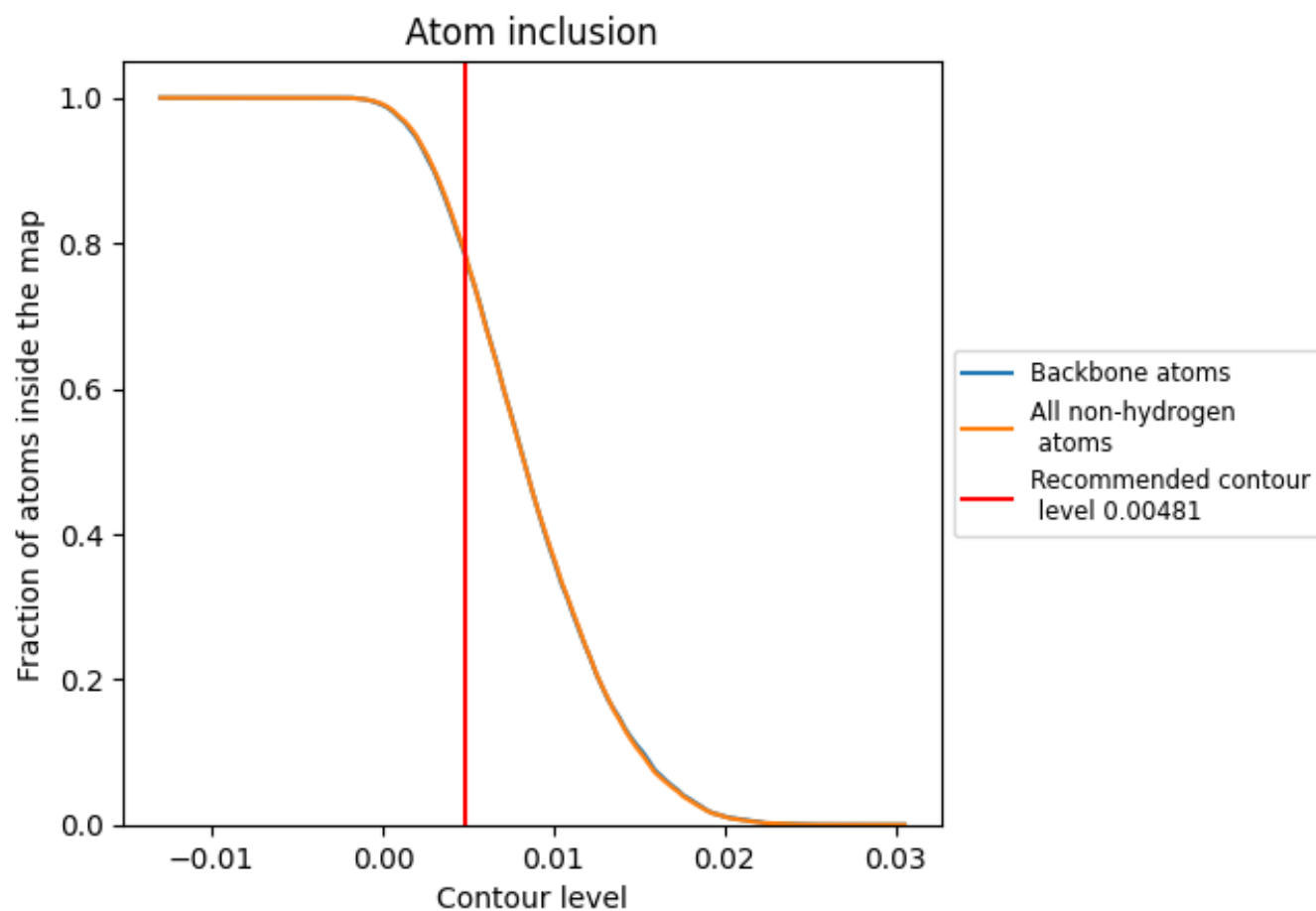
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00481).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 79% 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 (0.00481) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7866	<div></div> 0.3180
1	<div></div> 0.8568	<div></div> 0.2840
2	<div></div> 0.7455	<div></div> 0.2810
3	<div></div> 0.4156	<div></div> 0.3890
A	<div></div> 0.8947	<div></div> 0.3890
B	<div></div> 0.8365	<div></div> 0.3220
C	<div></div> 0.8897	<div></div> 0.3700
D	<div></div> 0.8307	<div></div> 0.3300
E	<div></div> 0.0179	<div></div> 0.1710
F	<div></div> 0.4669	<div></div> 0.2120
G	<div></div> 0.7627	<div></div> 0.2060
H	<div></div> 0.8385	<div></div> 0.1940

1.0

0.0

<0.0