



wwPDB EM Validation Summary Report ⓘ

Dec 10, 2022 – 11:40 pm GMT

PDB ID : 4V1M
EMDB ID : EMD-2784
Title : Architecture of the RNA polymerase II-Mediator core transcription initiation complex
Authors : Plaschka, C.; Lariviere, L.; Wenzek, L.; Hemann, M.; Tegunov, D.; Petrotchenko, E.V.; Borchers, C.H.; Baumeister, W.; Herzog, F.; Villa, E.; Cramer, P.
Deposited on : 2014-09-29
Resolution : 6.60 Å (reported)
Based on initial model : 4A3D

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:

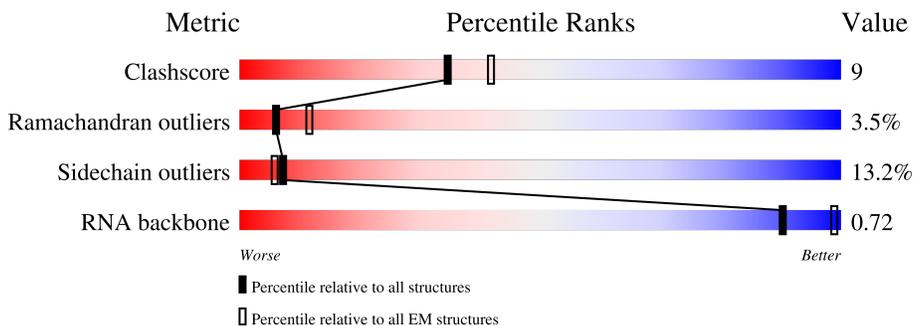
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 6.60 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	1733	
2	B	1224	
3	C	318	
4	E	215	
5	F	155	
6	H	146	
7	I	122	

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Mol	Chain	Length	Quality of chain
8	J	70	
9	K	120	
10	L	70	
11	N	10	
12	P	6	
13	T	20	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 29447 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1422	Total	C	N	O	S	0	0
			11174	7037	1954	2121	62		

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1156	Total	C	N	O	S	0	0
			9143	5784	1606	1697	56		

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	266	Total	C	N	O	S	0	0
			2095	1317	348	417	13		

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	84	Total	C	N	O	S	0	0
			679	434	115	127	3		

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	133	1068	673	180	211	4	0	0

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	119	971	596	179	186	10	0	0

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	J	65	532	339	93	94	6	0	0

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	K	115	920	590	157	171	2	0	1

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L	46	363	224	72	63	4	0	0

- Molecule 11 is a DNA chain called 5'-D(*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	N	10	207	99	39	59	10	0	0

- Molecule 12 is a RNA chain called 5'-D(*CP*CP*AP*GP*GP*AP)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
12	P	6	130	58	26	40	6	0	0

- Molecule 13 is a DNA chain called 5'-D(*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*TP*TP*TP*TP*CP*CP*CP*BRUP*GP*GP*TP*C)-3'.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	Br	C	N	O	P		
13	T	20	404	1	194	63	126	20	0	0

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

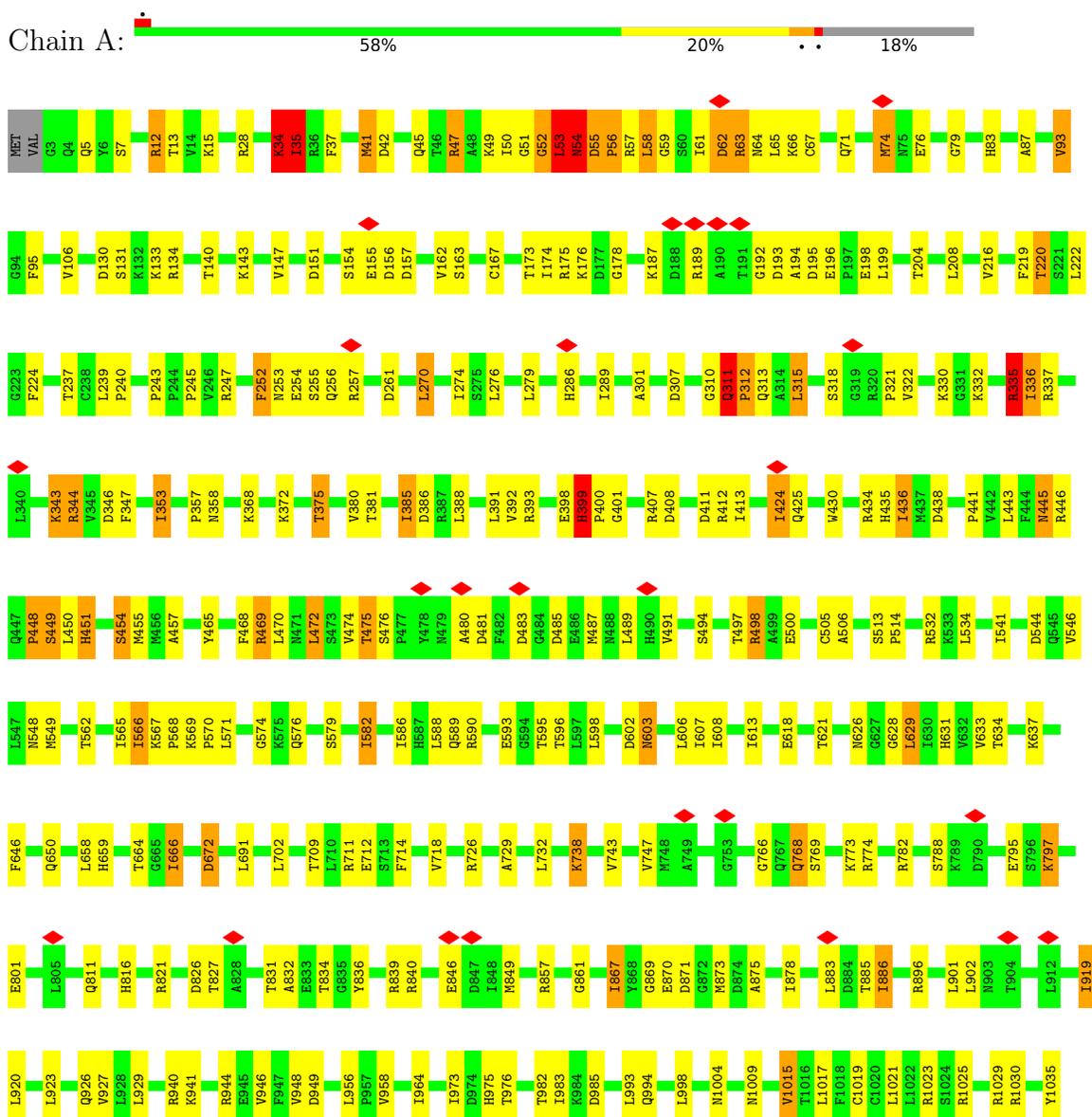
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

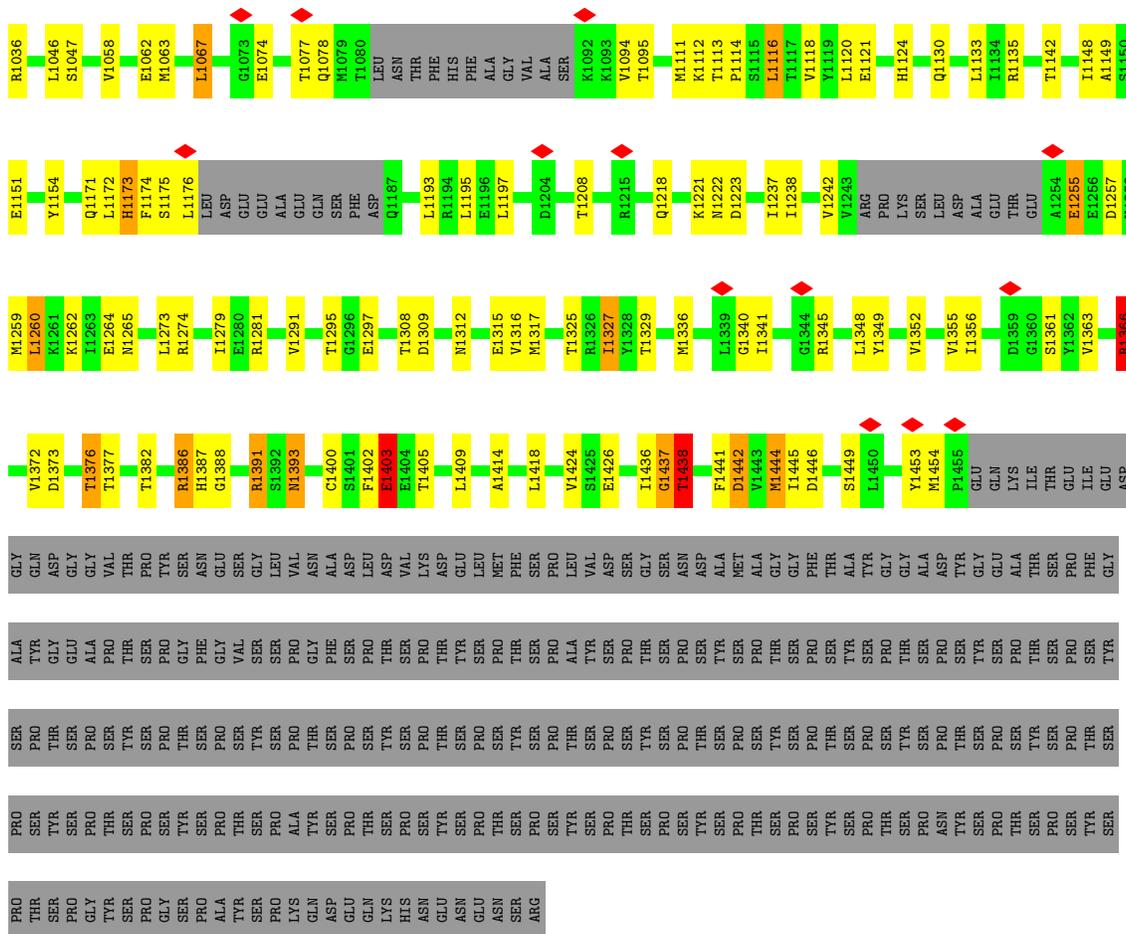
Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total 1	Mg 1	0

3 Residue-property plots

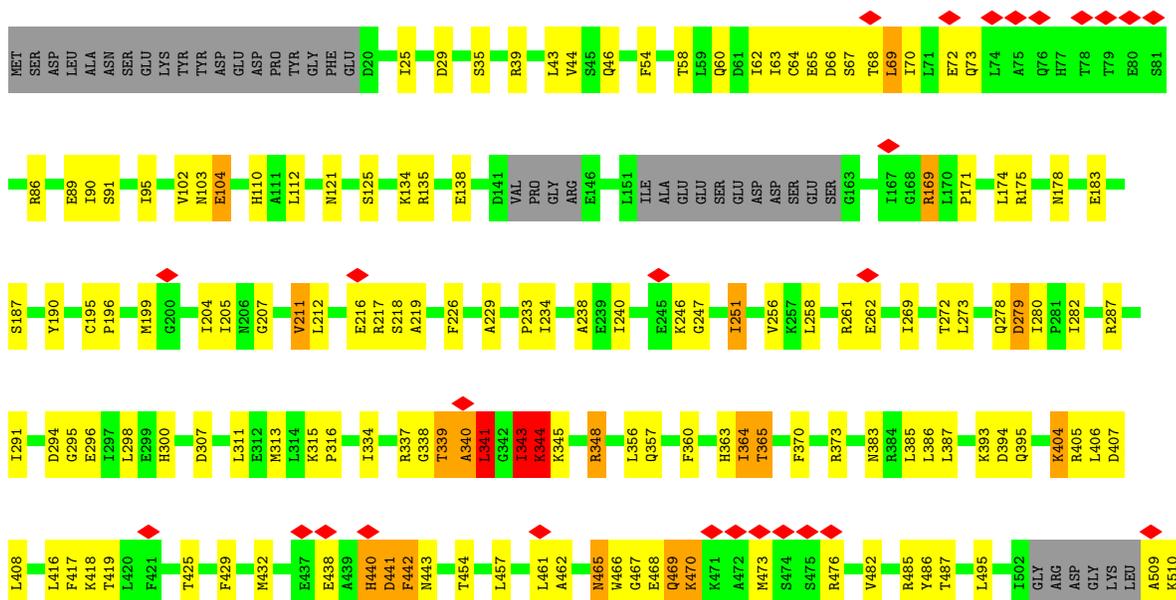
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1



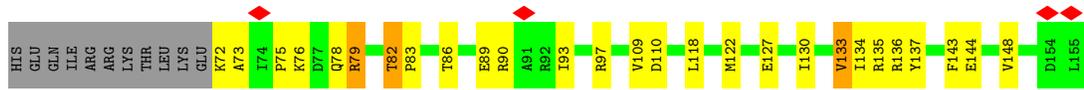
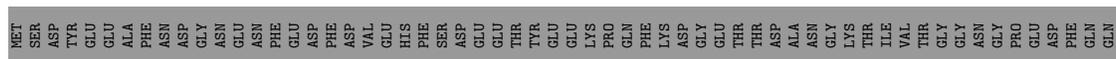
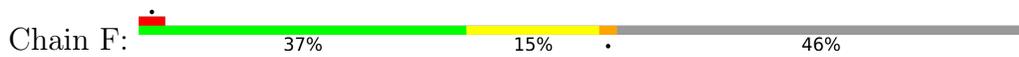


• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2





• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2



• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3



• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14777	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	37169	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.101	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.019	Depositor
Map size (\AA)	378.0, 378.0, 378.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.35, 1.35, 1.35	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.54	0/11374	0.85	10/15383 (0.1%)
2	B	0.49	0/9318	0.79	10/12565 (0.1%)
3	C	0.49	0/2133	0.78	2/2891 (0.1%)
4	E	0.48	0/1788	0.71	0/2406
5	F	0.62	0/691	0.81	0/933
6	H	0.51	0/1086	0.80	0/1470
7	I	0.47	0/989	0.78	0/1331
8	J	0.54	0/541	0.88	1/727 (0.1%)
9	K	0.47	0/938	0.71	0/1267
10	L	0.54	0/365	0.95	0/485
11	N	1.07	0/232	1.06	0/356
12	P	1.21	0/145	0.79	0/224
13	T	1.26	1/426 (0.2%)	1.08	0/652
All	All	0.55	1/30026 (0.0%)	0.82	23/40690 (0.1%)

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	2
2	B	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	26	DC	C1'-N1	5.58	1.56	1.49

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	465	ASN	O-C-N	15.46	147.44	122.70
2	B	465	ASN	CA-C-N	-12.77	89.11	117.20
2	B	465	ASN	C-N-CA	-9.63	97.63	121.70
2	B	218	SER	O-C-N	7.31	134.39	122.70
1	A	399	HIS	N-CA-CB	7.26	123.67	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	LYS	Mainchain,Peptide
2	B	404	LYS	Mainchain
2	B	43	LEU	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11174	0	11233	204	0
2	B	9143	0	9122	204	0
3	C	2095	0	2051	42	0
4	E	1752	0	1776	26	0
5	F	679	0	701	19	0
6	H	1068	0	1040	24	0
7	I	971	0	927	15	0
8	J	532	0	542	15	0
9	K	920	0	929	20	0
10	L	363	0	386	20	0
11	N	207	0	114	0	0
12	P	130	0	66	1	0
13	T	404	0	227	6	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	29447	0	29114	514	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 514 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:ILE:CG1	1:A:867:ILE:CD1	1.83	1.51
2:B:104:GLU:OE2	10:L:54:ARG:HD3	1.50	1.10
1:A:53:LEU:HD23	1:A:54:ASN:H	1.03	1.10
2:B:121:ASN:ND2	2:B:963:PHE:CZ	2.25	1.04
2:B:104:GLU:OE2	10:L:54:ARG:CD	2.10	1.00

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	1414/1733 (82%)	1236 (87%)	126 (9%)	52 (4%)	3	24
2	B	1138/1224 (93%)	1008 (89%)	86 (8%)	44 (4%)	3	23
3	C	264/318 (83%)	242 (92%)	20 (8%)	2 (1%)	19	60
4	E	212/215 (99%)	195 (92%)	13 (6%)	4 (2%)	8	38
5	F	82/155 (53%)	76 (93%)	6 (7%)	0	100	100
6	H	129/146 (88%)	106 (82%)	14 (11%)	9 (7%)	1	14
7	I	117/122 (96%)	98 (84%)	16 (14%)	3 (3%)	5	31
8	J	63/70 (90%)	51 (81%)	9 (14%)	3 (5%)	2	21
9	K	113/120 (94%)	109 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	L	44/70 (63%)	27 (61%)	9 (20%)	8 (18%)	0	2
All	All	3576/4173 (86%)	3148 (88%)	303 (8%)	125 (4%)	6	25

5 of 125 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	58	LEU
1	A	76	GLU
1	A	189	ARG
1	A	195	ASP

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	1240/1520 (82%)	1062 (86%)	178 (14%)	3	16
2	B	986/1061 (93%)	861 (87%)	125 (13%)	4	19
3	C	234/274 (85%)	206 (88%)	28 (12%)	5	20
4	E	196/197 (100%)	175 (89%)	21 (11%)	6	24
5	F	74/137 (54%)	67 (90%)	7 (10%)	8	28
6	H	117/128 (91%)	103 (88%)	14 (12%)	5	20
7	I	113/116 (97%)	106 (94%)	7 (6%)	18	43
8	J	60/65 (92%)	49 (82%)	11 (18%)	1	10
9	K	99/102 (97%)	87 (88%)	12 (12%)	5	20
10	L	40/57 (70%)	27 (68%)	13 (32%)	0	2
All	All	3159/3657 (86%)	2743 (87%)	416 (13%)	7	18

5 of 416 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	615	MET

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Mol	Chain	Res	Type
2	B	1138	MET
9	K	51	LEU
2	B	680	THR
2	B	906	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	325	GLN
2	B	975	GLN
7	I	83	ASN
2	B	842	ASN
2	B	1025	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	P	5/6 (83%)	1 (20%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	P	8	G

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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
13	BRU	T	22	13,12	18,21,22	1.03	1 (5%)	26,30,33	1.63	6 (23%)

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
13	BRU	T	22	13,12	-	0/7/21/22	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	22	BRU	C4-N3	-2.29	1.34	1.38

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	22	BRU	O4'-C1'-N1	4.17	115.31	107.86
13	T	22	BRU	BR-C5-C4	2.84	121.33	118.03
13	T	22	BRU	N3-C2-N1	2.69	118.46	114.89
13	T	22	BRU	BR-C5-C6	-2.61	117.00	120.64
13	T	22	BRU	C2'-C1'-N1	-2.40	108.25	113.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	T	22	BRU	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	934:LYS	C	935:ARG	N	5.39
1	B	351:TYR	C	352:ALA	N	3.28

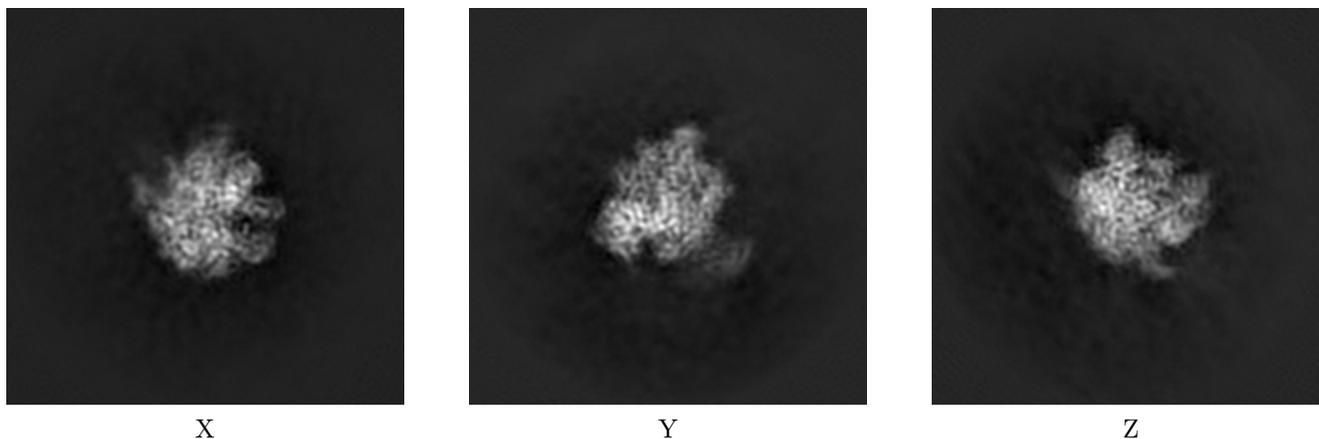
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2784. 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](#)

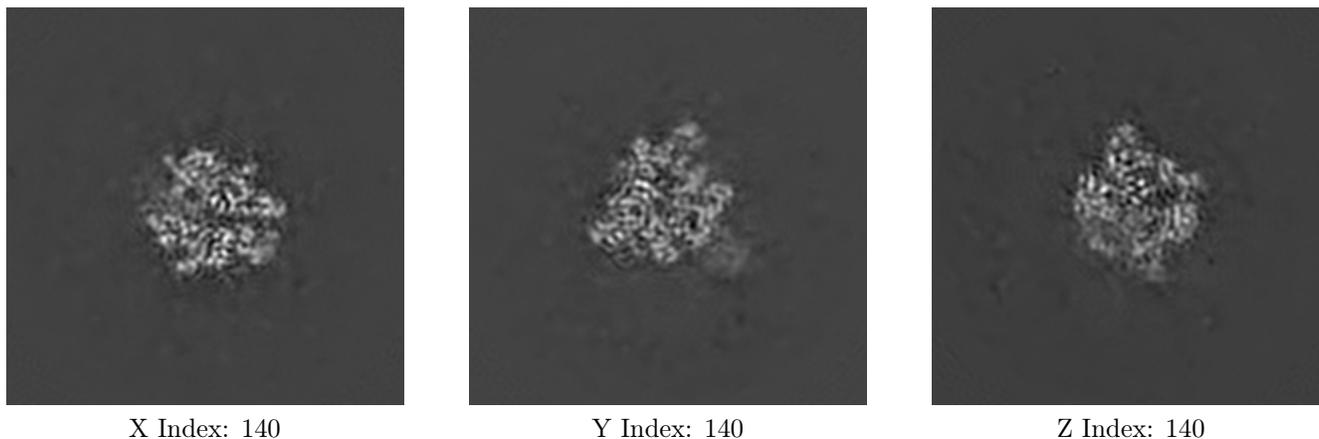
6.1.1 Primary map



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

6.2 Central slices [i](#)

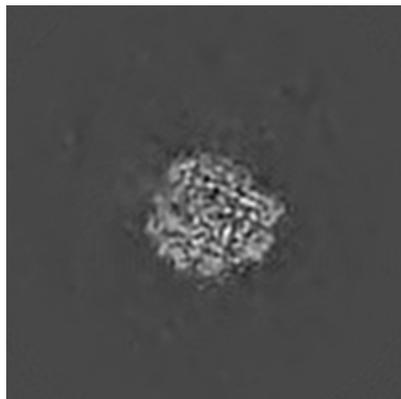
6.2.1 Primary map



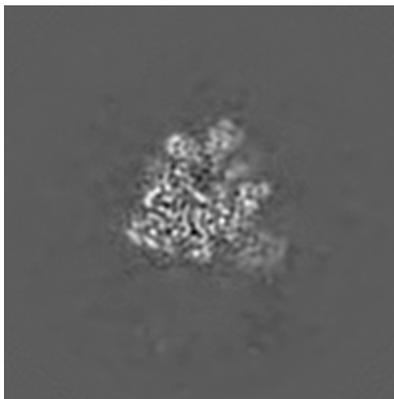
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

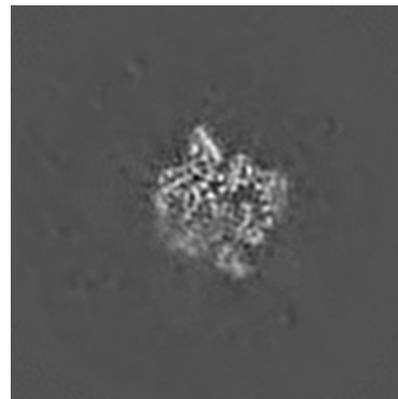
6.3.1 Primary map



X Index: 127



Y Index: 143

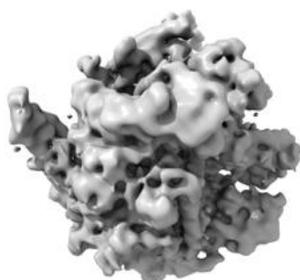


Z Index: 144

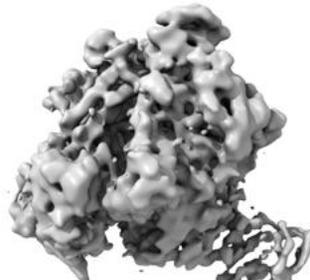
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

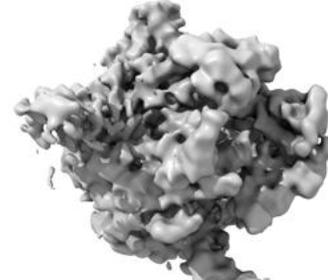
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

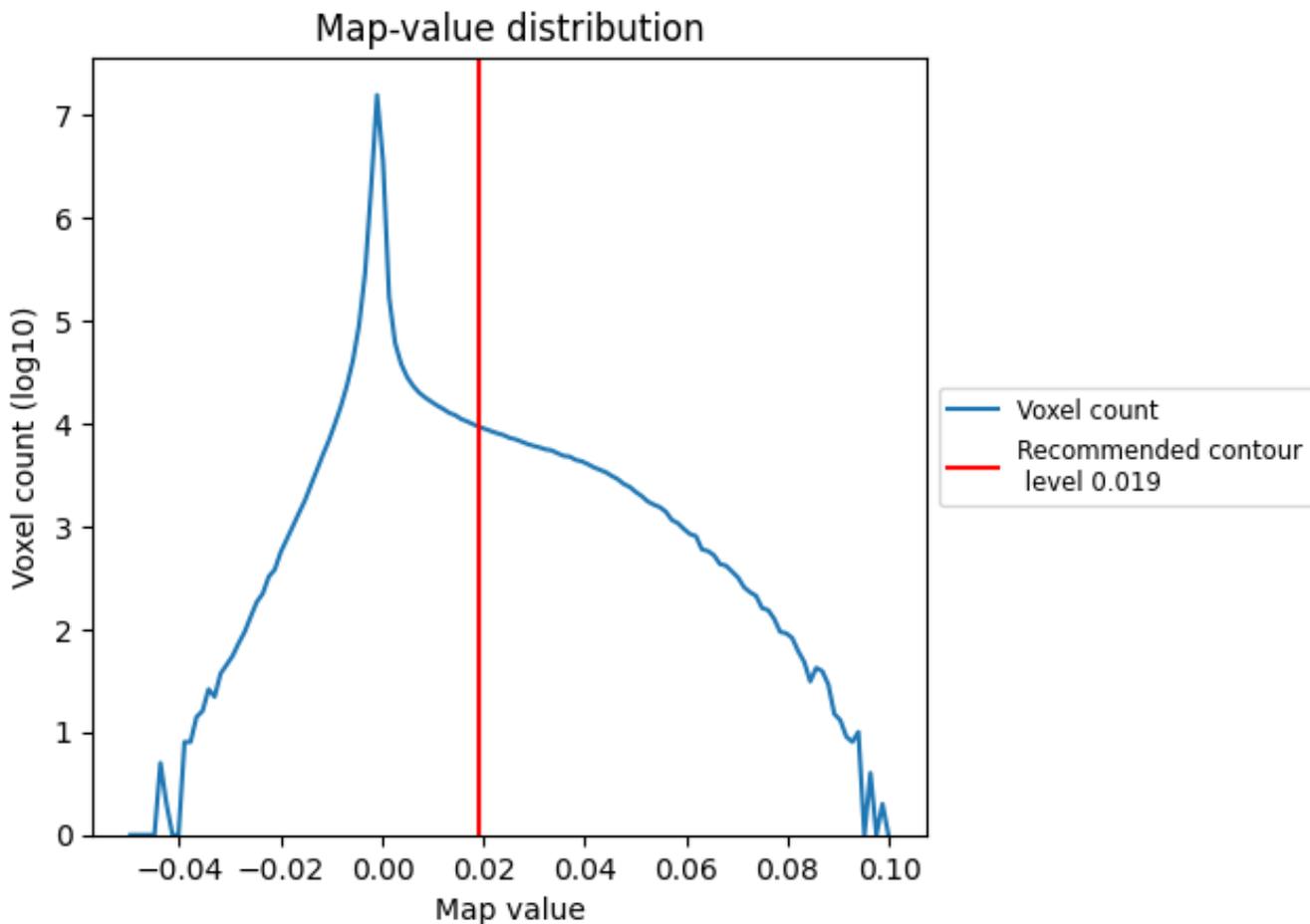
6.5 Mask visualisation

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

7 Map analysis [i](#)

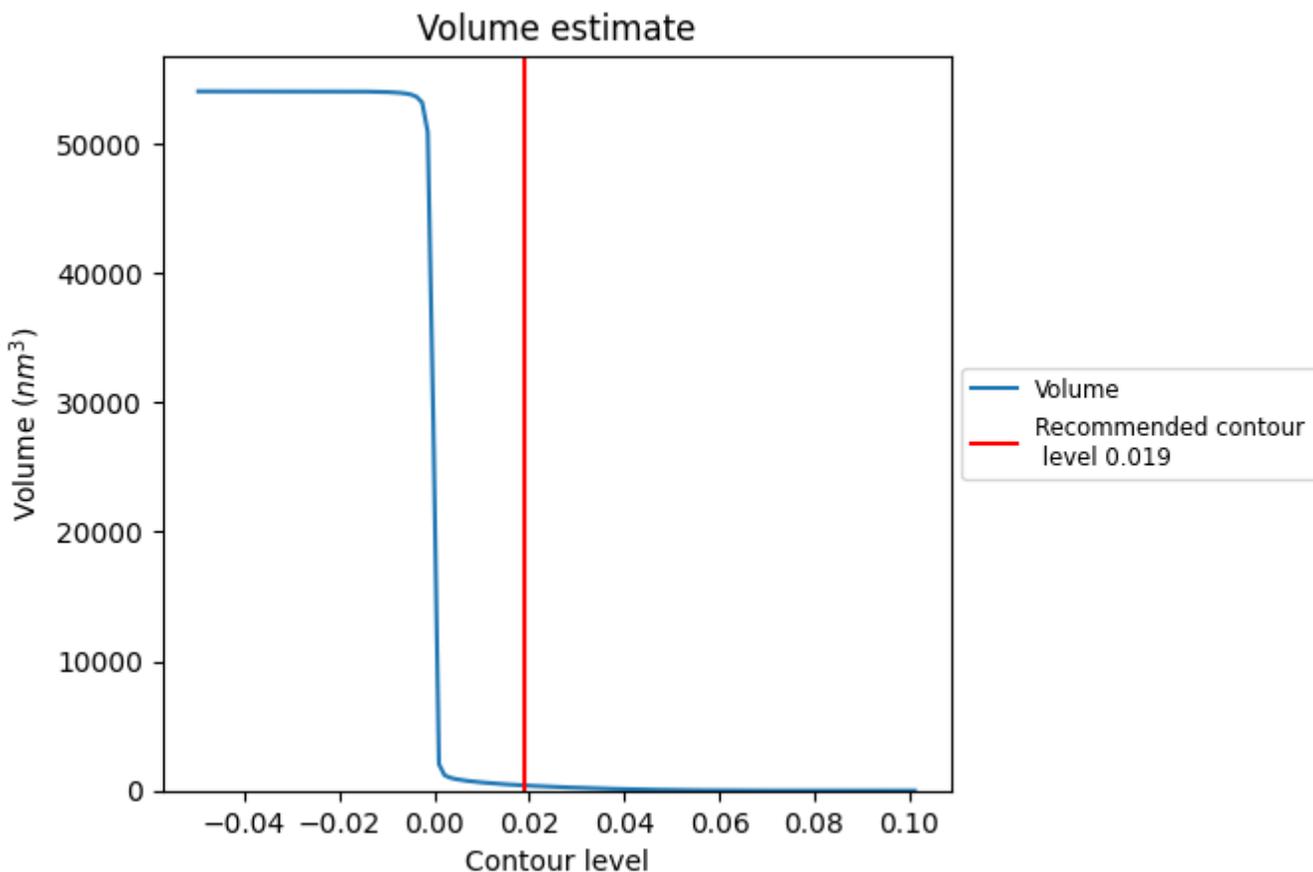
This section contains the results of statistical analysis of the map.

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.

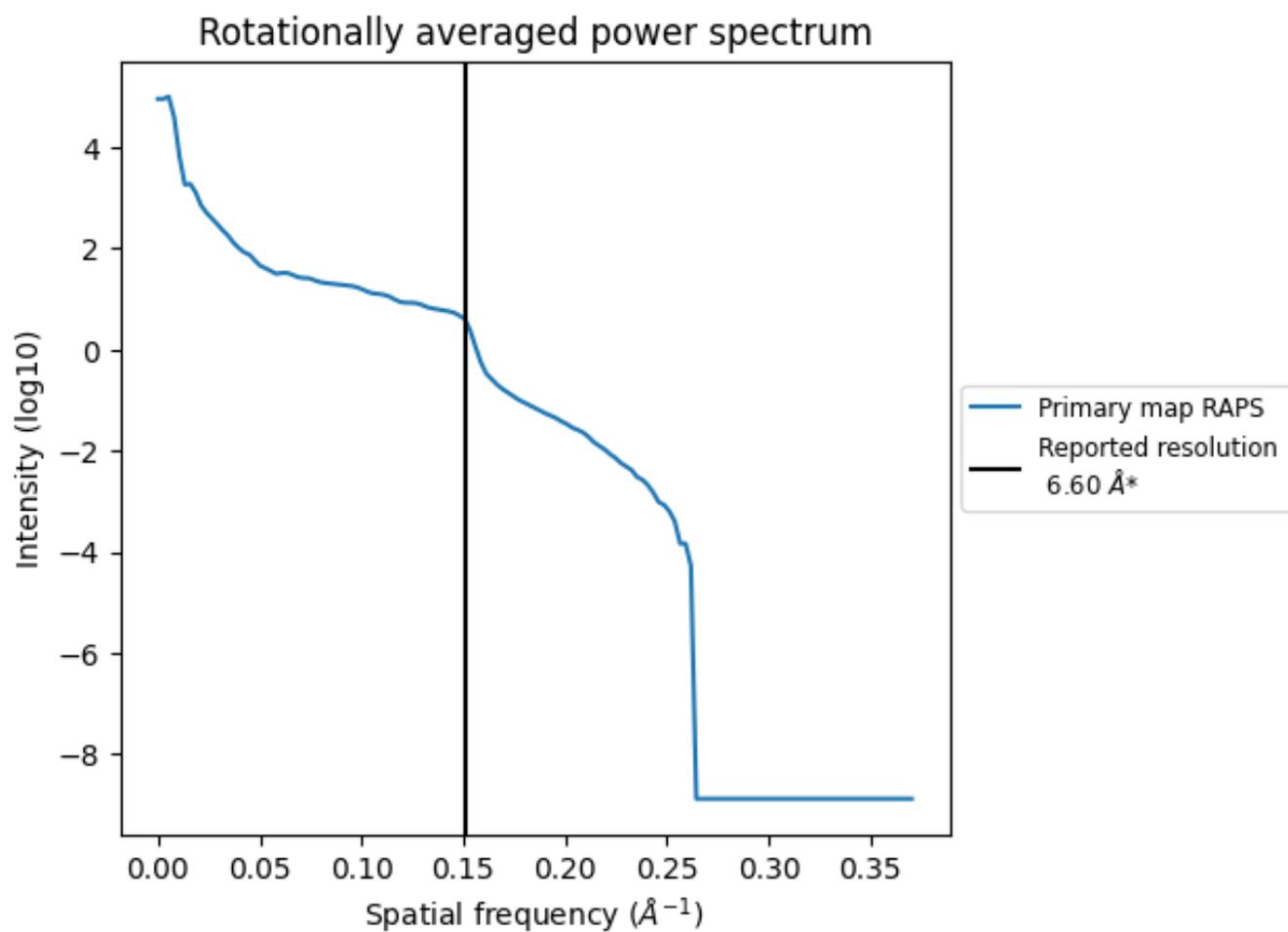
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 400 nm³; this corresponds to an approximate mass of 361 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 0.152 Å⁻¹

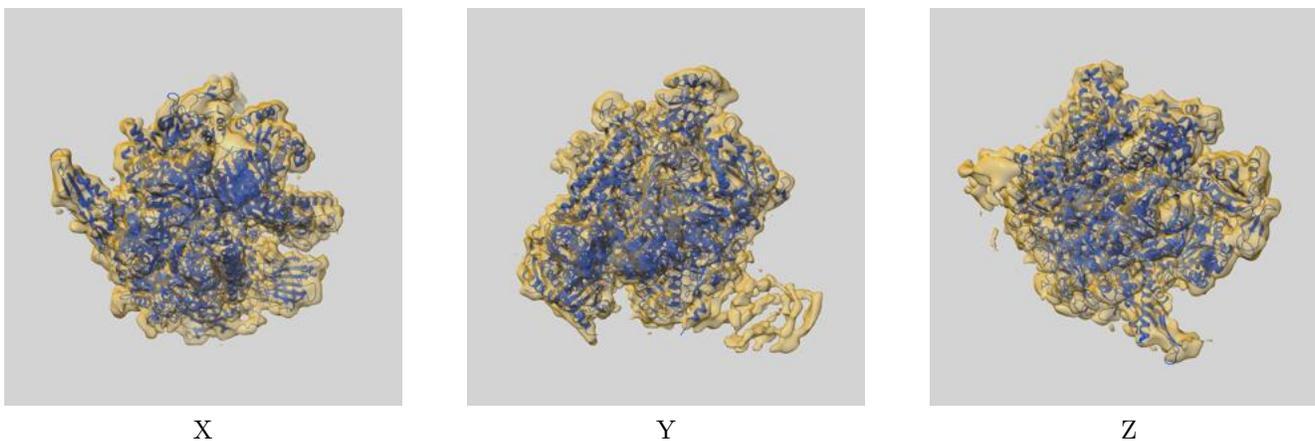
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

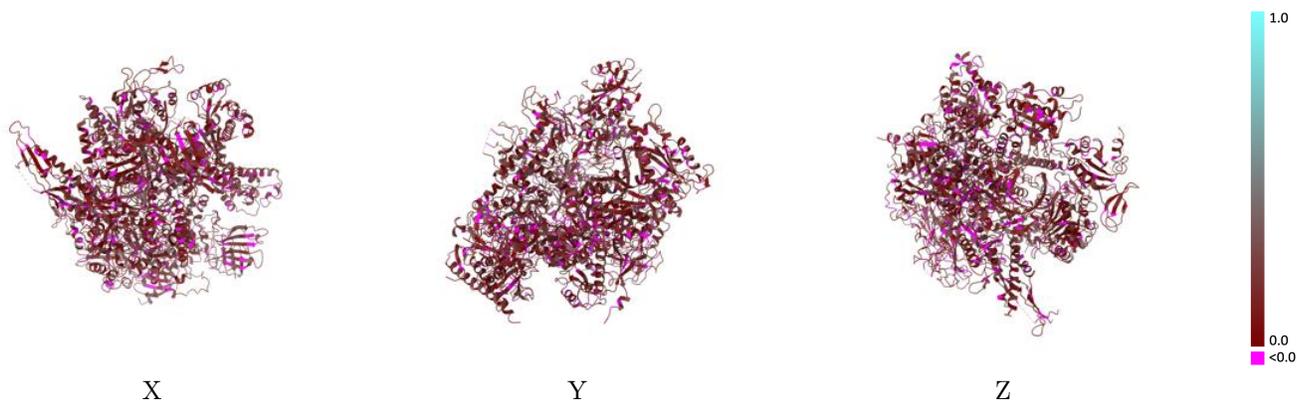
This section contains information regarding the fit between EMDB map EMD-2784 and PDB model 4V1M. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



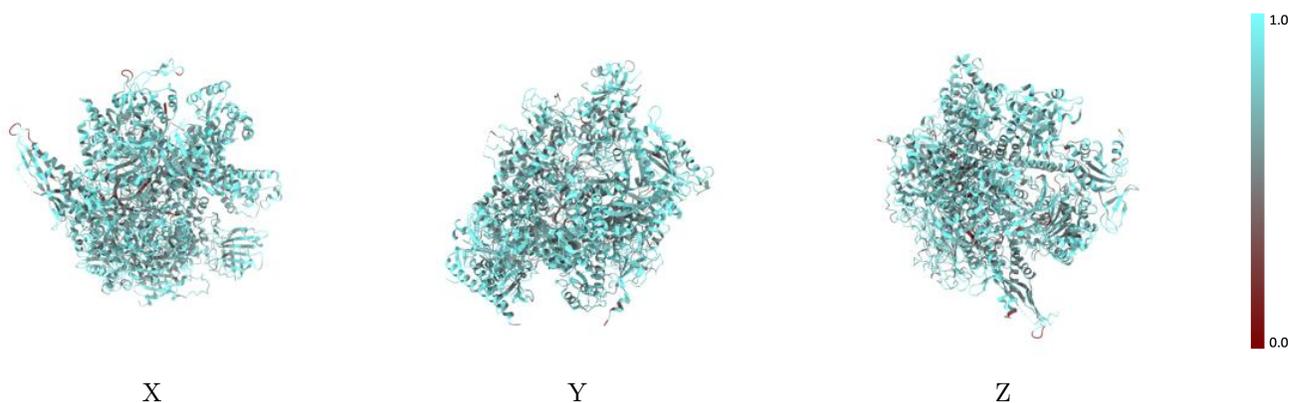
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



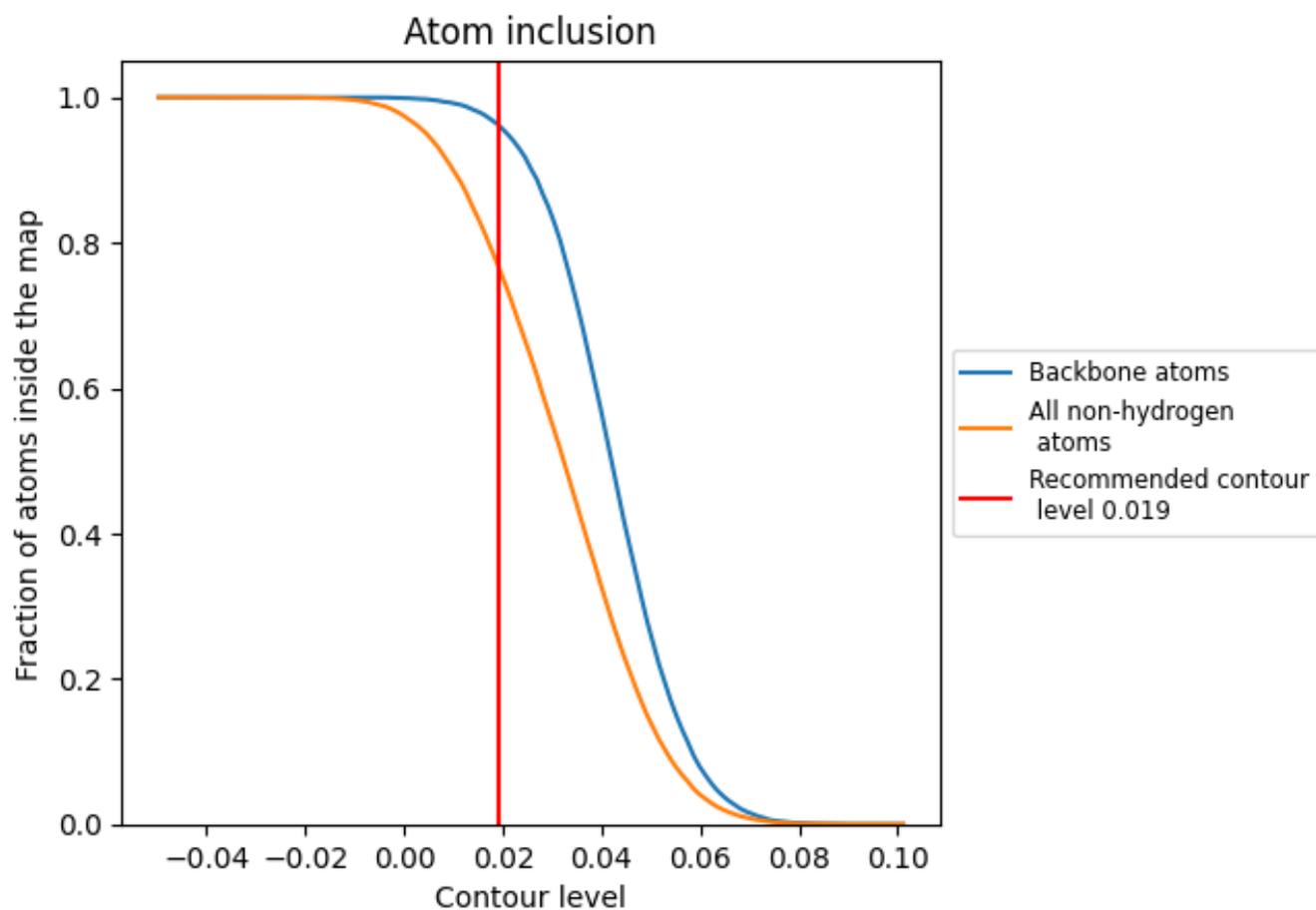
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.019).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 77% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7695	 0.1510
A	 0.7658	 0.1530
B	 0.7615	 0.1480
C	 0.8279	 0.1650
E	 0.7987	 0.1630
F	 0.7685	 0.1520
H	 0.8173	 0.1620
I	 0.7949	 0.1420
J	 0.7563	 0.1280
K	 0.7883	 0.1550
L	 0.7607	 0.1120
N	 0.7778	 0.1840
P	 0.2538	 -0.0070
T	 0.5866	 0.1150

