



## wwPDB EM Validation Summary Report ⓘ

May 7, 2024 – 03:23 pm BST

PDB ID : 8S52  
EMDB ID : EMD-19719  
Title : RNA polymerase II core initially transcribing complex with an ordered RNA of 10 nt  
Authors : Zhan, Y.; Grabbe, F.; Oberbeckmann, E.; Dienemann, C.; Cramer, P.  
Deposited on : 2024-02-22  
Resolution : 2.90 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

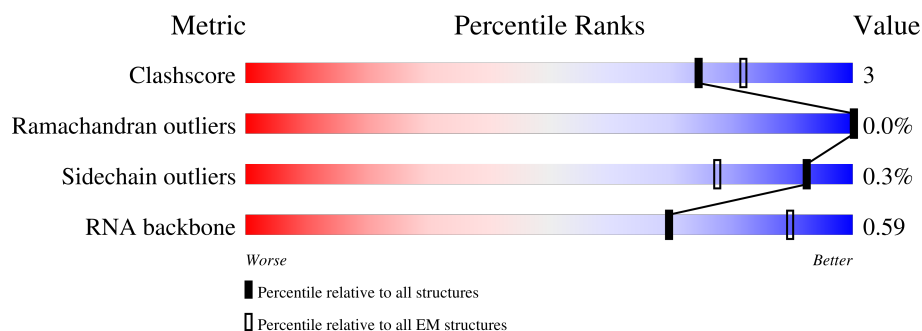
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 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.








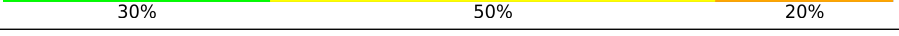

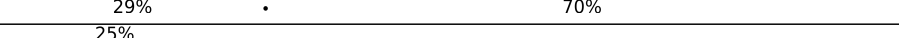

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 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	1984	
2	B	1300	
3	C	275	
4	D	184	
5	E	210	
6	F	127	
7	G	172	

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Mol	Chain	Length	Quality of chain
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	316	
14	N	139	
15	O	339	
16	P	10	
17	Q	517	
18	R	249	
19	T	139	
20	U	376	
21	V	109	
22	W	439	
23	X	291	

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 44875 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1420	Total	C	N	O	S	0	0
			11249	7079	2012	2086	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1130	Total	C	N	O	S	0	0
			9031	5712	1587	1668	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	128	Total	C	N	O	S	0	0
			1050	656	178	212	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	79	Total	C	N	O	S	0	0
			636	406	108	117	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	114	Total	C	N	O	S	0	0
			928	571	166	180	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	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			373	231	72	64	6		

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	289	Total	C	N	O	S	0	0
			2221	1383	395	425	18		

- Molecule 14 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	53	Total	C	N	O	P	0	0
			1117	523	230	311	53		

- Molecule 15 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	179	Total	C	N	O	S	0	0
			1422	923	251	241	7		

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	10	Total	C	N	O	P	0	0
			205	94	38	64	9		

- Molecule 17 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	138	Total	C	N	O	S	0	0
			1138	719	208	208	3		

- Molecule 18 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 19 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	64	Total	C	N	O	P	0	0
			1288	613	218	393	64		

- Molecule 20 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	113	Total	C	N	O	S	0	0
			930	585	152	189	4		

- Molecule 21 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 22 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	187	Total	C	N	O	S	0	0
			1535	964	275	285	11		

- Molecule 23 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	171	Total	C	N	O	S	0	0
			1403	895	243	261	4		

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

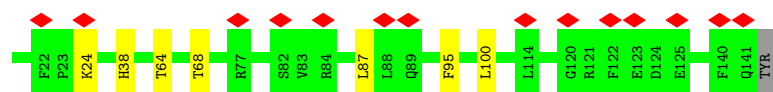
- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
25	P	1	Total	Mg	0
			1	1	









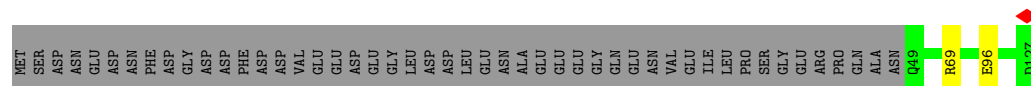
- Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E: 90% 10%



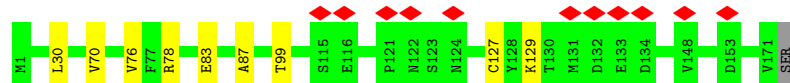
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 61% 38%



- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G: 6% 94% 5%



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

Chain H: 82% 16% 2%



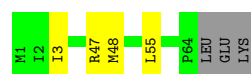
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I: 80% 11% 9%



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

Chain J: 90% 6% 4%

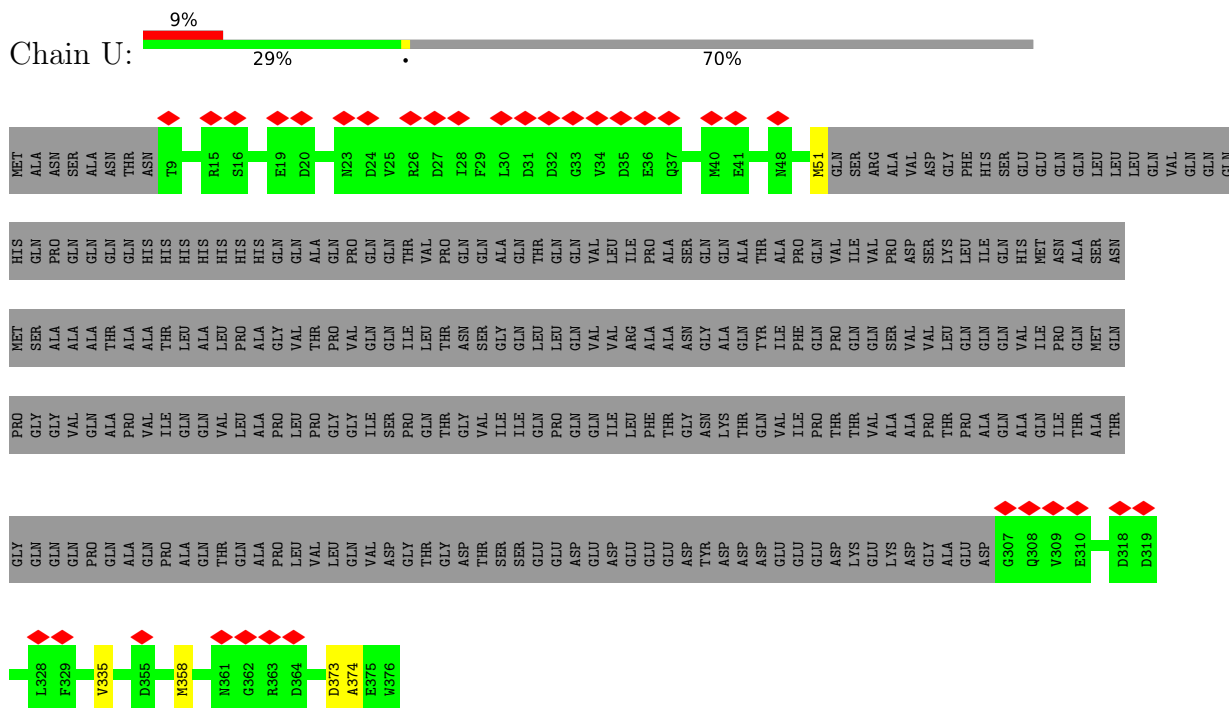


- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

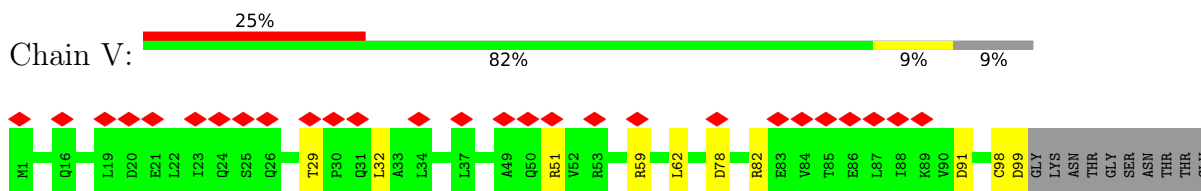
Chain K: 92% 6% 2%



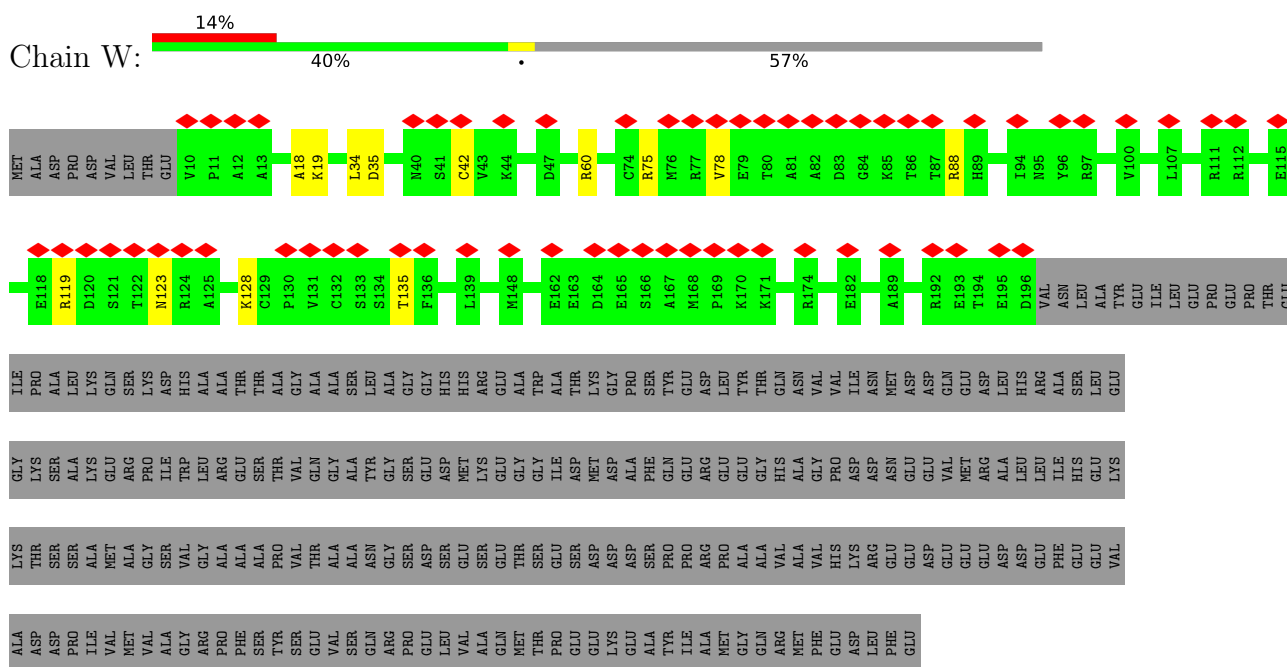




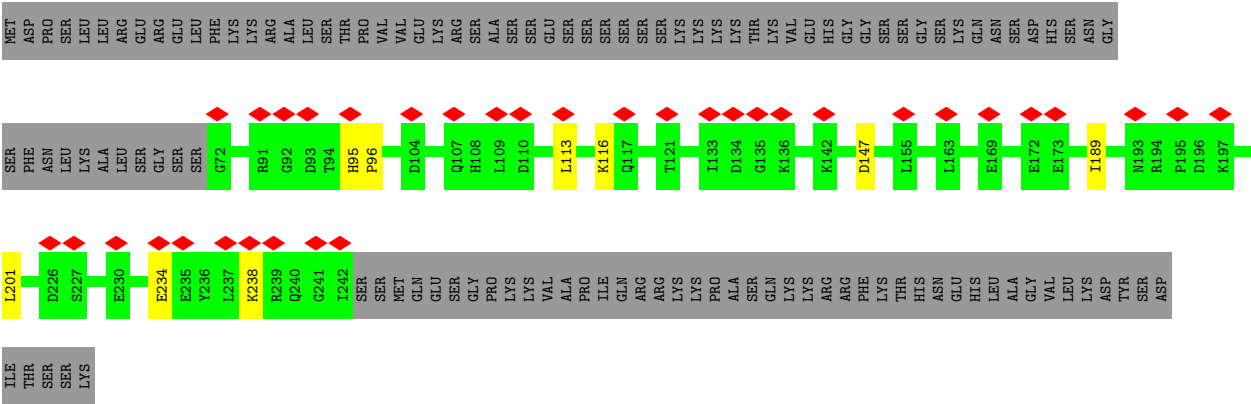
- Molecule 21: Transcription initiation factor IIA subunit 2



- Molecule 22: General transcription factor IIE subunit 1



- Molecule 23: Transcription initiation factor IIE subunit beta



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	151975	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	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	54.796	Depositor
Minimum map value	-28.155	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.55	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.40	0/11454	0.59	0/15462
2	B	0.45	0/9209	0.59	0/12427
3	C	0.44	0/2102	0.54	0/2857
4	D	0.28	0/1064	0.50	0/1428
5	E	0.43	0/1752	0.64	0/2366
6	F	0.44	0/646	0.64	0/871
7	G	0.35	0/1382	0.57	0/1874
8	H	0.48	0/1207	0.63	0/1628
9	I	0.38	0/949	0.62	0/1284
10	J	0.48	0/516	0.59	0/696
11	K	0.42	0/939	0.53	0/1271
12	L	0.51	0/378	0.80	0/500
13	M	0.41	0/2253	0.66	0/3039
14	N	0.85	0/1260	1.14	0/1946
15	O	0.37	0/1448	0.67	0/1948
16	P	0.63	0/228	1.26	0/353
17	Q	0.31	0/1167	0.57	0/1576
18	R	0.30	0/1817	0.54	0/2445
19	T	1.02	0/1435	1.26	0/2205
20	U	0.29	0/945	0.52	0/1274
21	V	0.28	0/816	0.53	0/1105
22	W	0.27	0/1560	0.56	0/2097
23	X	0.28	0/1427	0.52	0/1916
All	All	0.45	0/45954	0.65	0/62568

There are no bond length outliers.

There are no bond angle outliers.

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	11249	0	11390	71	0
2	B	9031	0	9069	64	0
3	C	2059	0	2007	15	0
4	D	1050	0	1033	5	0
5	E	1721	0	1737	12	0
6	F	636	0	665	1	0
7	G	1351	0	1358	5	0
8	H	1186	0	1147	18	0
9	I	928	0	859	8	0
10	J	507	0	523	4	0
11	K	920	0	942	5	0
12	L	373	0	378	6	0
13	M	2221	0	2241	23	0
14	N	1117	0	592	18	0
15	O	1422	0	1514	9	0
16	P	205	0	109	9	0
17	Q	1138	0	1103	10	0
18	R	1788	0	1819	6	0
19	T	1288	0	722	15	0
20	U	930	0	888	4	0
21	V	806	0	818	5	0
22	W	1535	0	1540	7	0
23	X	1403	0	1428	6	0
24	A	2	0	0	0	0
24	B	1	0	0	0	0
24	C	1	0	0	0	0
24	I	2	0	0	0	0
24	J	1	0	0	0	0
24	L	1	0	0	0	0
24	M	1	0	0	0	0
24	W	1	0	0	0	0
25	P	1	0	0	0	0
All	All	44875	0	43882	276	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 3.

The worst 5 of 276 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)
19:T:52:DG:H2''	19:T:53:DT:H5'	1.53	0.88
16:P:1:A:H61	19:T:55:DT:H3	1.21	0.85
19:T:49:DT:H2'	19:T:50:DG:C8	2.17	0.79
3:C:36:ARG:NH1	11:K:41:THR:OG1	2.21	0.73
2:B:1062:ARG:NH2	2:B:1066:PRO:O	2.25	0.70

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	1410/1984 (71%)	1348 (96%)	62 (4%)	0	100	100
2	B	1120/1300 (86%)	1074 (96%)	46 (4%)	0	100	100
3	C	253/275 (92%)	246 (97%)	7 (3%)	0	100	100
4	D	126/184 (68%)	123 (98%)	3 (2%)	0	100	100
5	E	207/210 (99%)	197 (95%)	10 (5%)	0	100	100
6	F	77/127 (61%)	72 (94%)	5 (6%)	0	100	100
7	G	169/172 (98%)	167 (99%)	2 (1%)	0	100	100
8	H	146/150 (97%)	138 (94%)	8 (6%)	0	100	100
9	I	112/125 (90%)	97 (87%)	15 (13%)	0	100	100
10	J	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
12	L	42/58 (72%)	37 (88%)	5 (12%)	0	100	100
13	M	285/316 (90%)	276 (97%)	7 (2%)	2 (1%)	22	54
15	O	177/339 (52%)	174 (98%)	3 (2%)	0	100	100
17	Q	134/517 (26%)	132 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	R	218/249 (88%)	217 (100%)	1 (0%)	0	100	100
20	U	109/376 (29%)	103 (94%)	6 (6%)	0	100	100
21	V	97/109 (89%)	95 (98%)	2 (2%)	0	100	100
22	W	185/439 (42%)	181 (98%)	4 (2%)	0	100	100
23	X	169/291 (58%)	163 (96%)	6 (4%)	0	100	100
All	All	5211/7405 (70%)	5011 (96%)	198 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	M	211	THR
13	M	104	ARG

### 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	1251/1763 (71%)	1249 (100%)	2 (0%)	93	98
2	B	990/1127 (88%)	988 (100%)	2 (0%)	93	98
3	C	234/252 (93%)	234 (100%)	0	100	100
4	D	118/160 (74%)	117 (99%)	1 (1%)	81	94
5	E	191/192 (100%)	190 (100%)	1 (0%)	88	96
6	F	69/111 (62%)	69 (100%)	0	100	100
7	G	152/153 (99%)	152 (100%)	0	100	100
8	H	129/131 (98%)	128 (99%)	1 (1%)	81	94
9	I	103/112 (92%)	102 (99%)	1 (1%)	76	92
10	J	53/56 (95%)	53 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	41/55 (74%)	41 (100%)	0	100	100
13	M	244/268 (91%)	242 (99%)	2 (1%)	81	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	154/293 (53%)	152 (99%)	2 (1%)	69	90
17	Q	121/448 (27%)	120 (99%)	1 (1%)	81	94
18	R	196/218 (90%)	196 (100%)	0	100	100
20	U	105/324 (32%)	105 (100%)	0	100	100
21	V	90/98 (92%)	88 (98%)	2 (2%)	52	81
22	W	169/373 (45%)	169 (100%)	0	100	100
23	X	154/261 (59%)	154 (100%)	0	100	100
All	All	4668/6501 (72%)	4653 (100%)	15 (0%)	92	98

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	15	ARG
21	V	51	ARG
13	M	210	THR
21	V	82	ARG
15	O	258	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	148	HIS
11	K	36	ASN
13	M	229	GLN
9	I	22	ASN
2	B	139	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	10/10 (100%)	1 (10%)	1 (10%)

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	2	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	P	1	A

## 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 11 ligands modelled in this entry, 11 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](#)

There are no chain breaks in this entry.

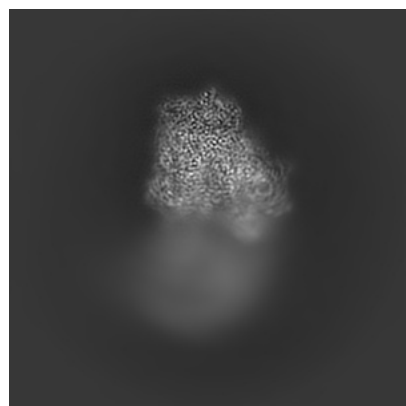
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19719. These allow visual inspection of the internal detail of the map and identification of artifacts.

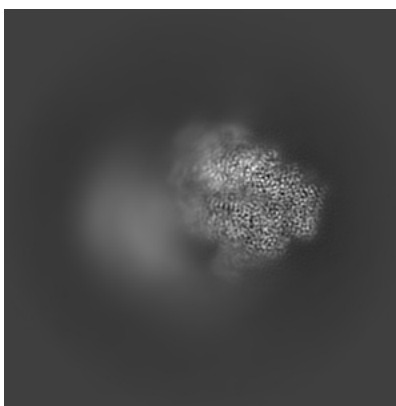
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

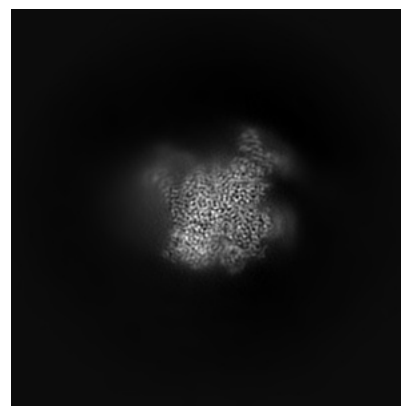
#### 6.1.1 Primary map



X

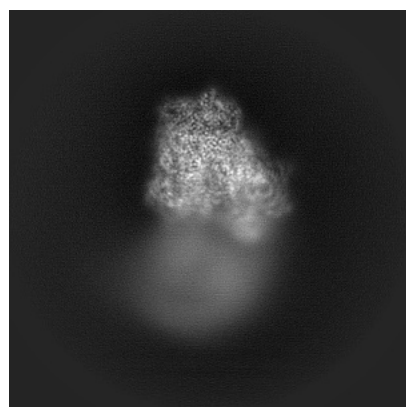


Y

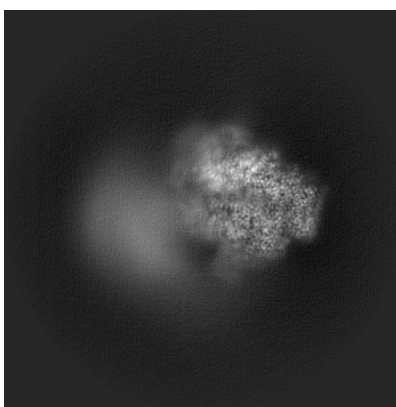


Z

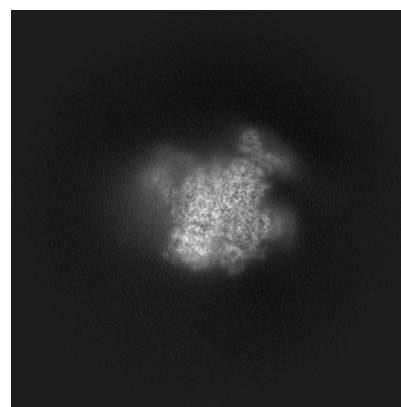
#### 6.1.2 Raw map



X



Y



Z

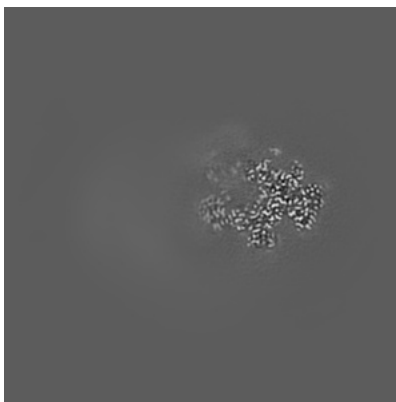
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

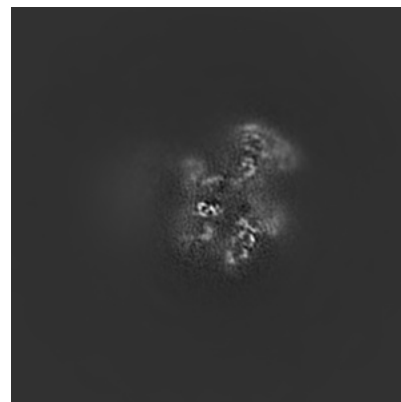
### 6.2.1 Primary map



X Index: 200

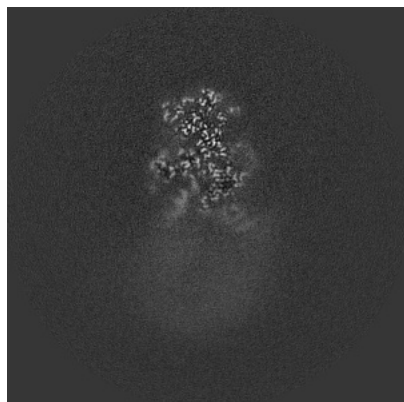


Y Index: 200

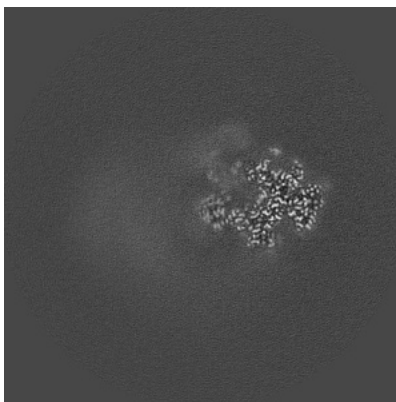


Z Index: 200

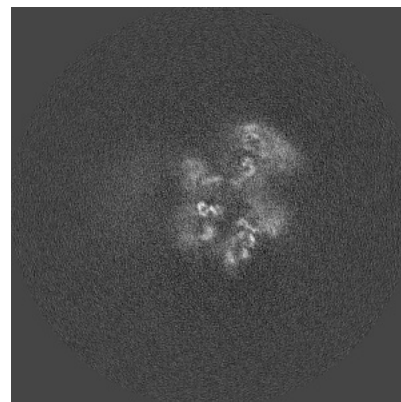
### 6.2.2 Raw map



X Index: 200



Y Index: 200

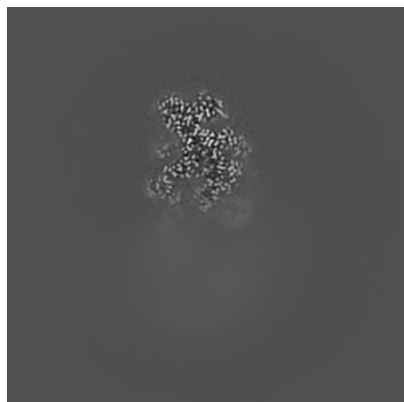


Z Index: 200

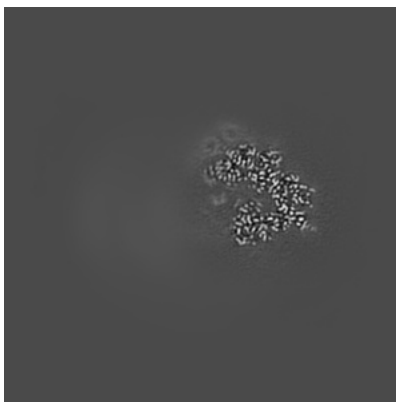
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

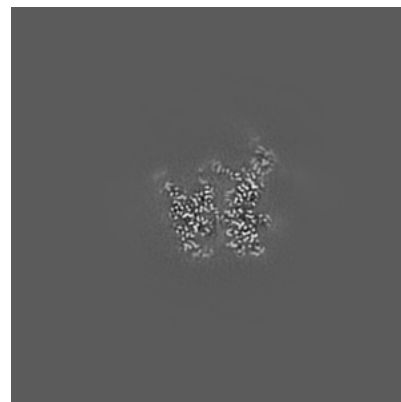
### 6.3.1 Primary map



X Index: 188

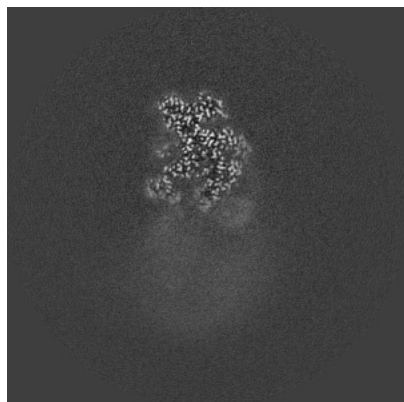


Y Index: 182

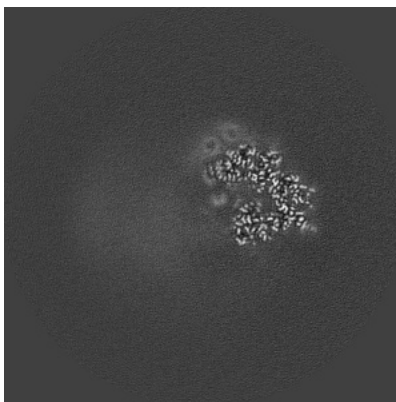


Z Index: 251

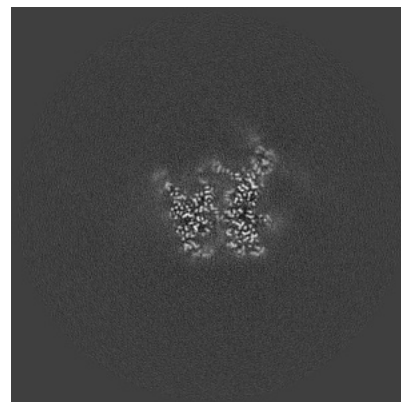
### 6.3.2 Raw map



X Index: 188



Y Index: 182



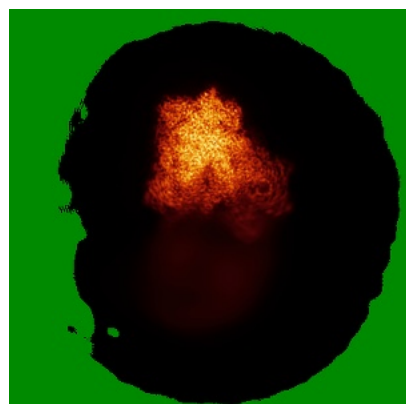
Z Index: 251

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

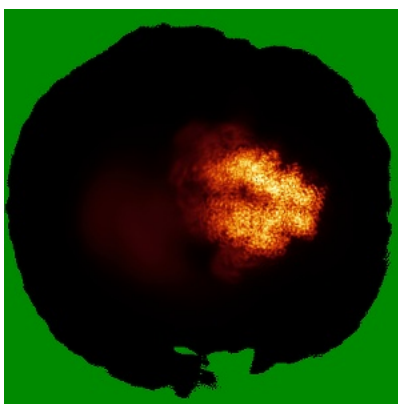


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

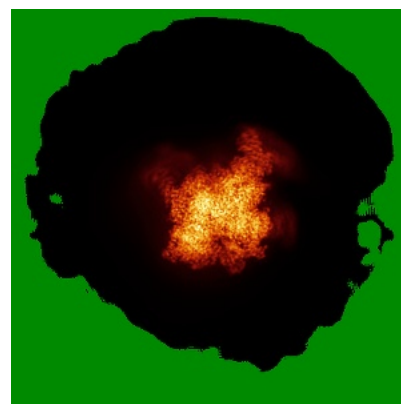
### 6.4.1 Primary map



X

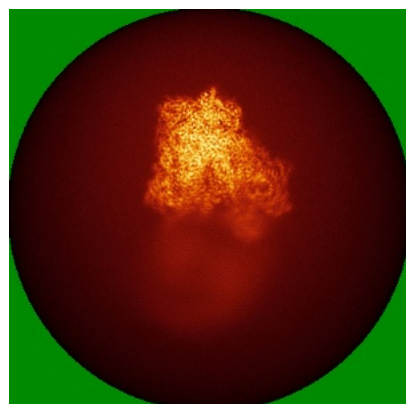


Y

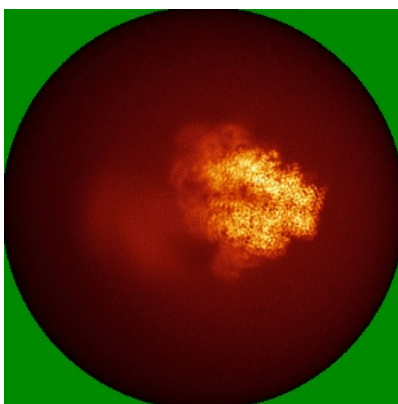


Z

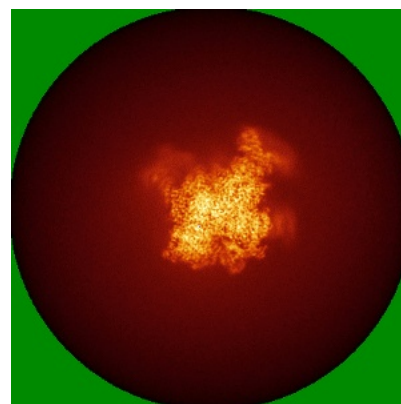
### 6.4.2 Raw map



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.

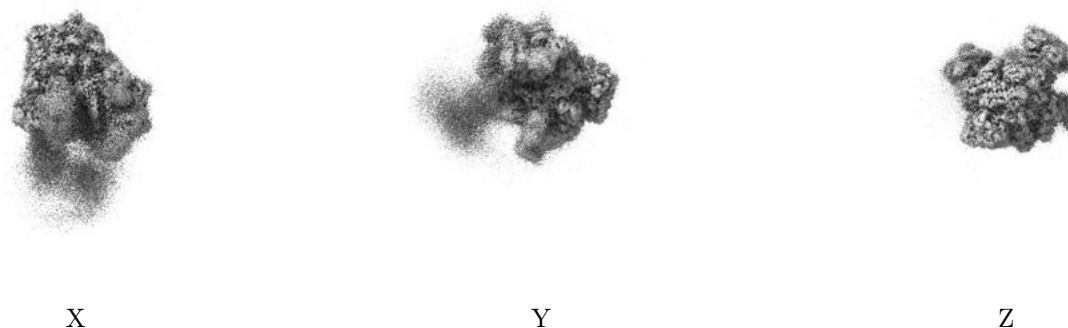
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.55. 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



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.

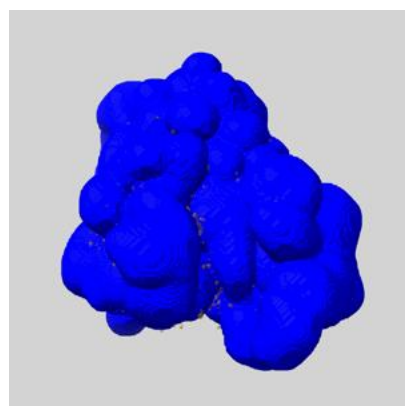
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

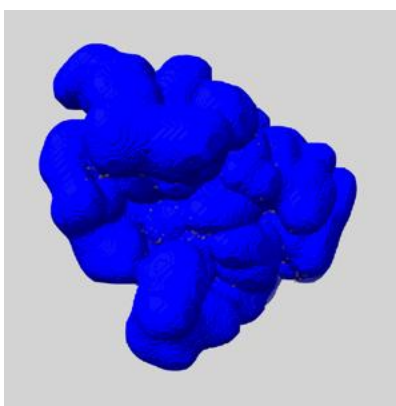
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

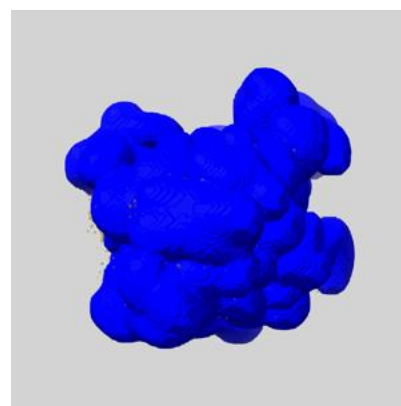
### 6.6.1 emd\_19719\_msk\_1.map [i](#)



X



Y

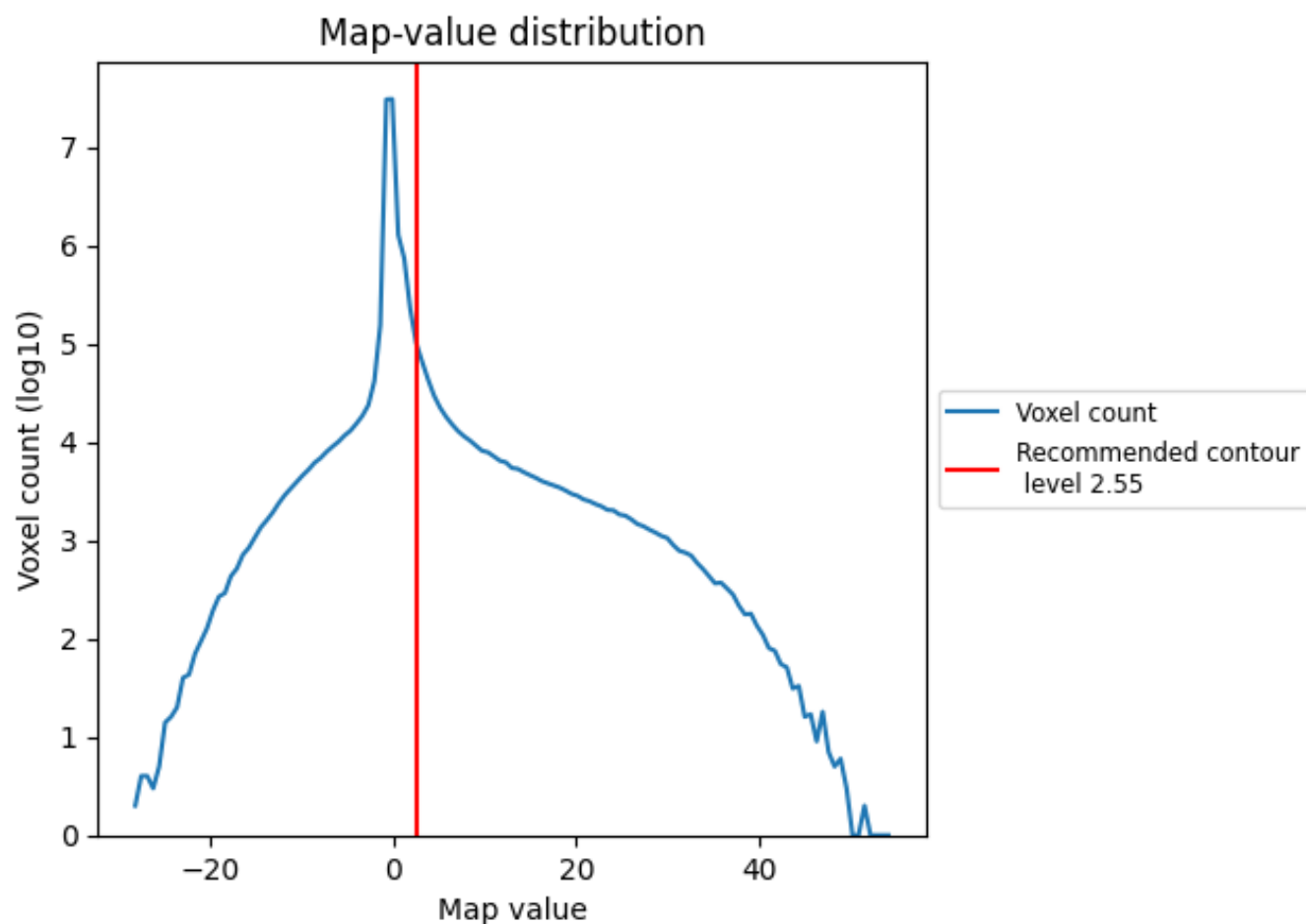


Z

## 7 Map analysis [i](#)

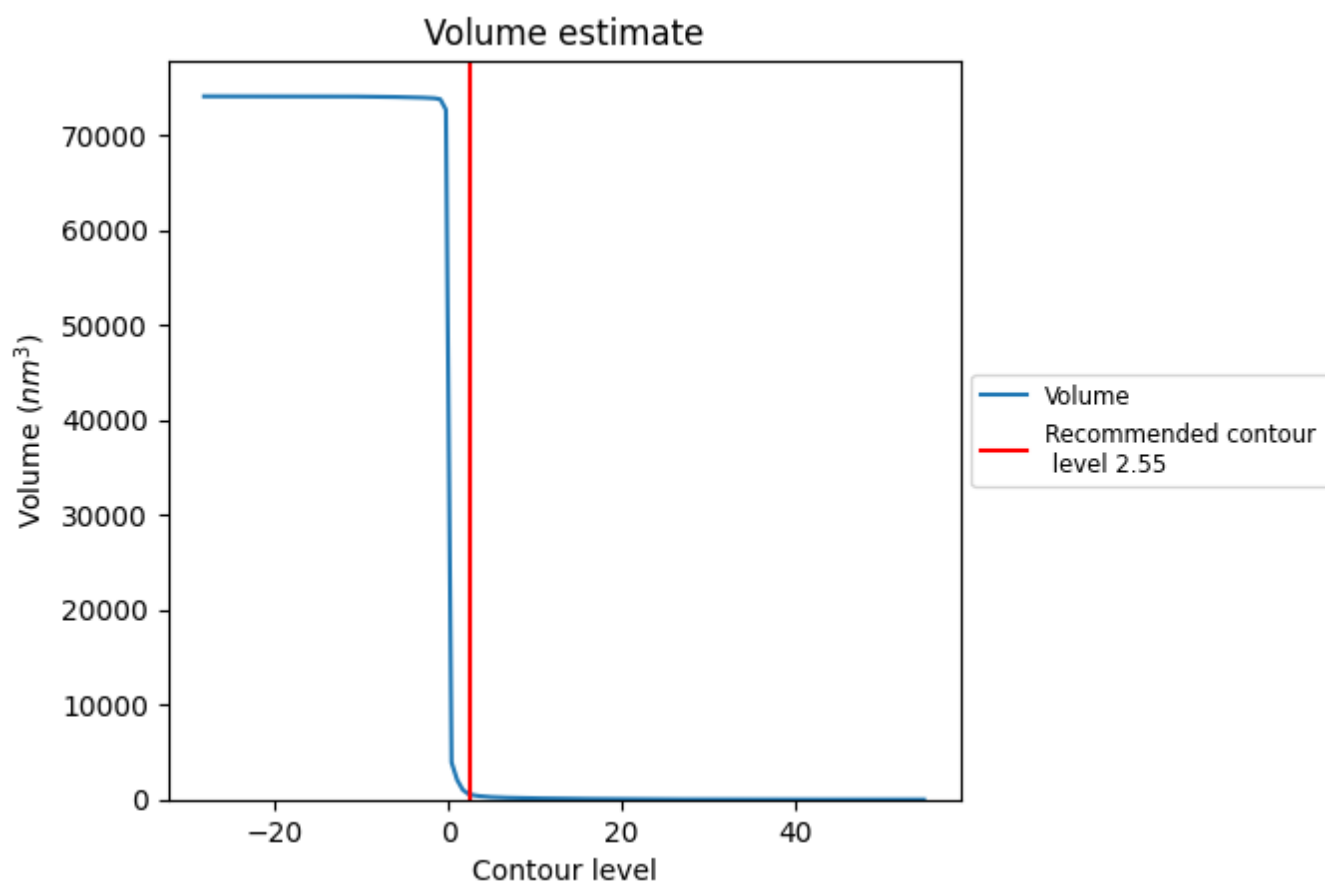
This section contains the results of statistical analysis of the map.

### 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.

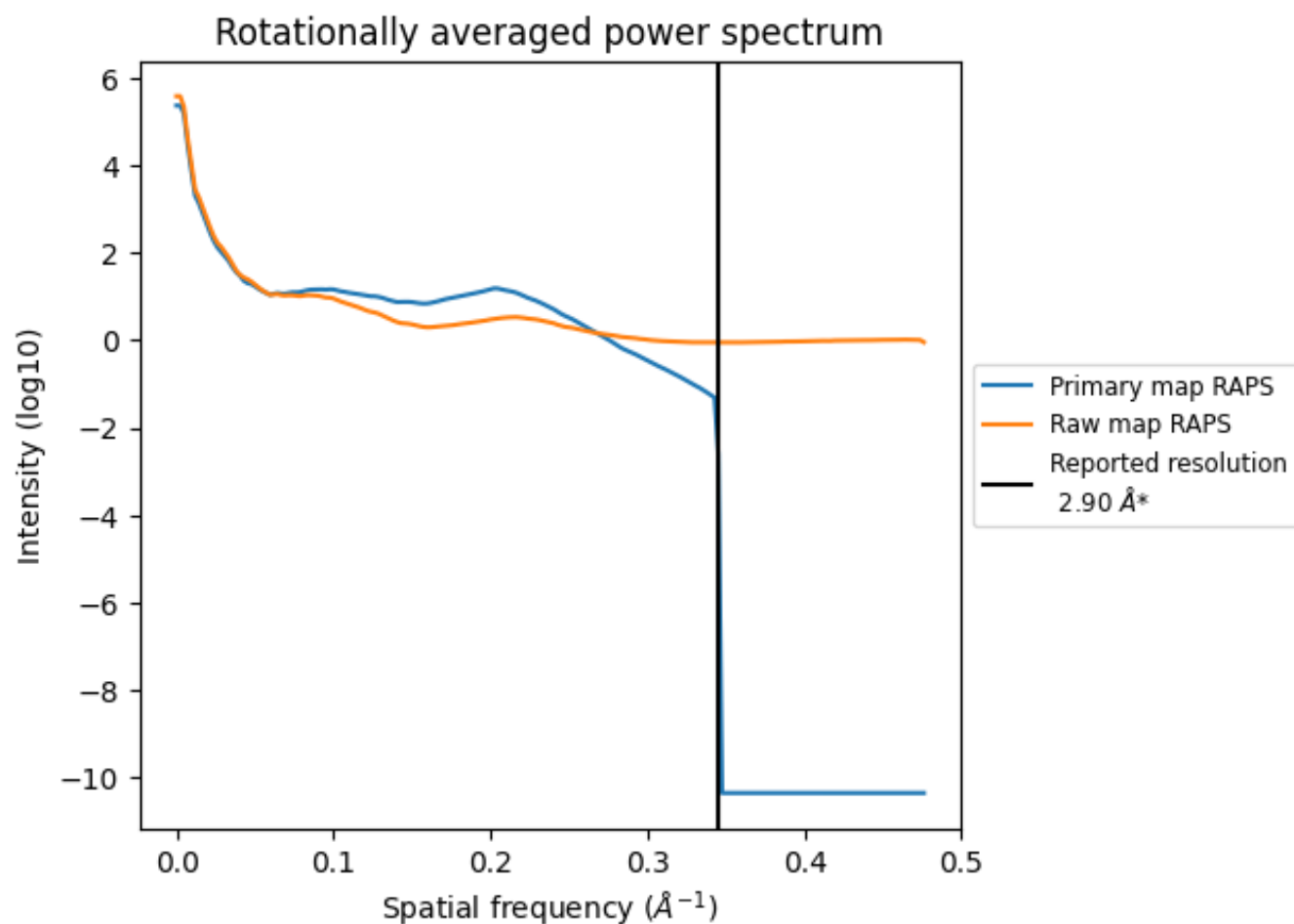
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 533 nm<sup>3</sup>; this corresponds to an approximate mass of 482 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 ⓘ

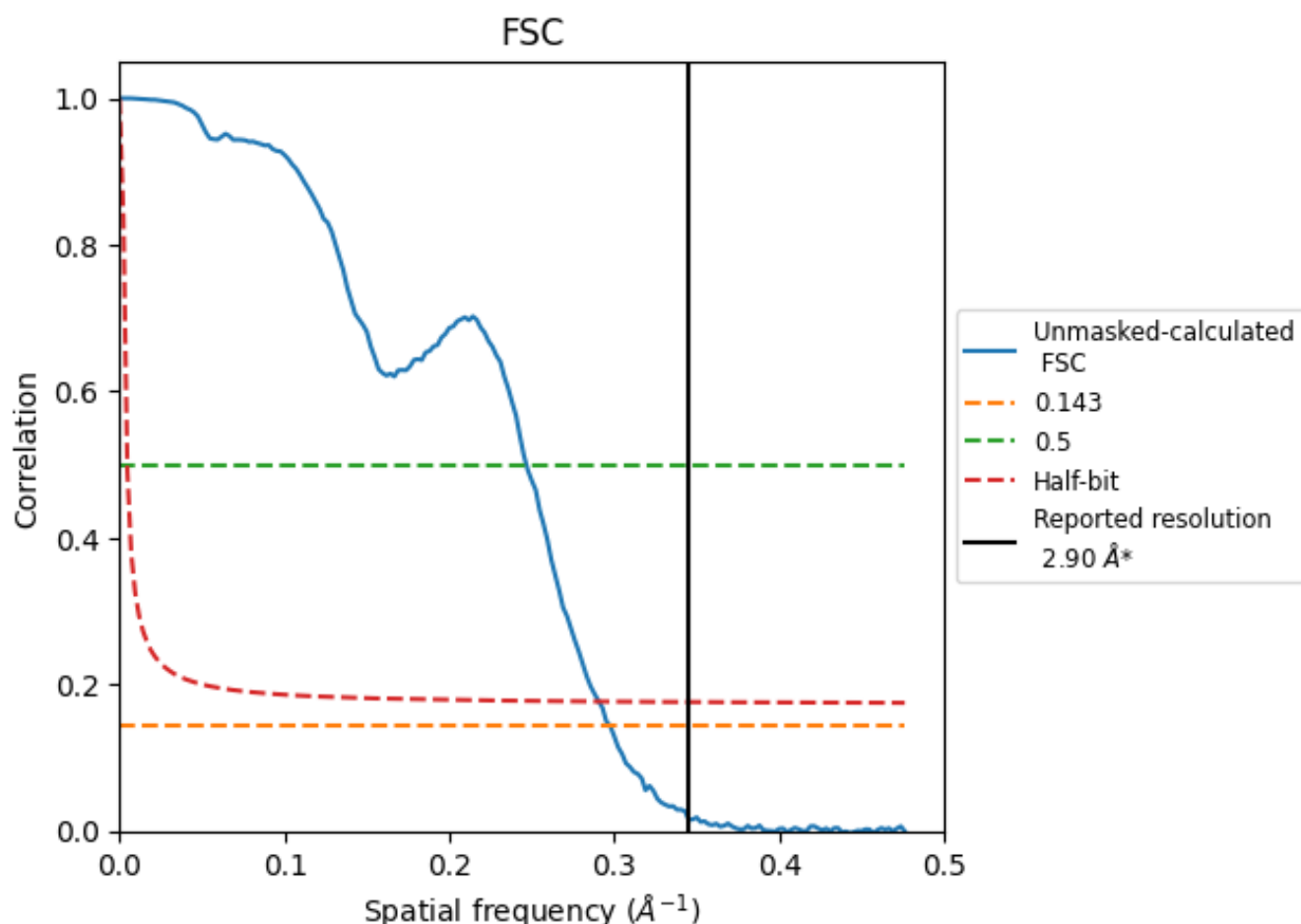


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

## 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 0.345  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.36	4.05	3.44

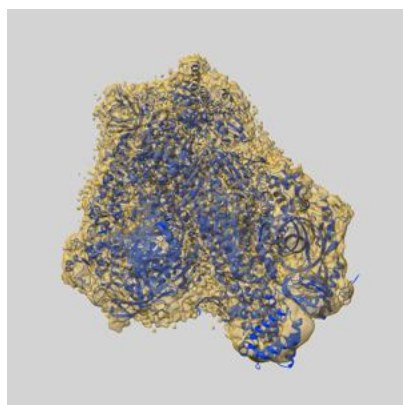
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.36 differs from the reported value 2.9 by more than 10 %



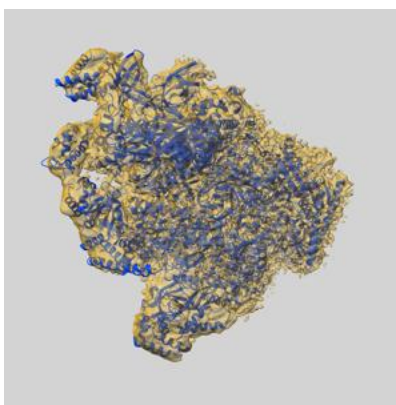
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19719 and PDB model 8S52. Per-residue inclusion information can be found in section [3](#) on page [8](#).

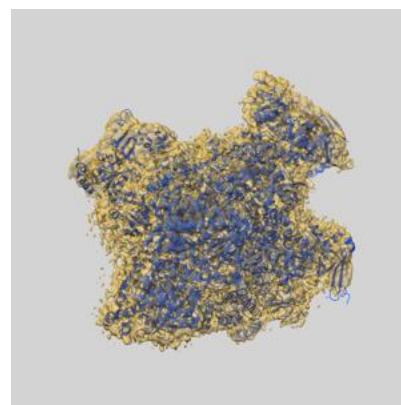
### 9.1 Map-model overlay [i](#)



X



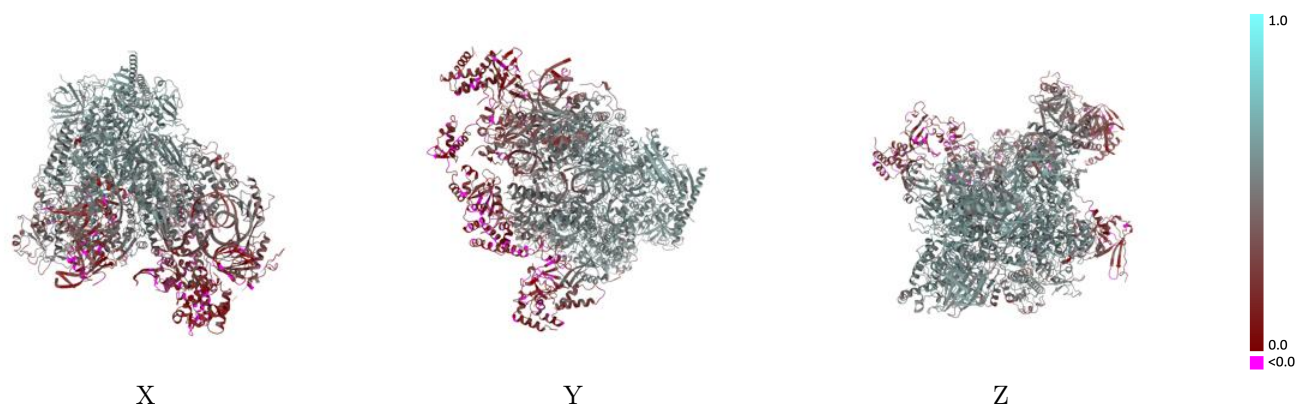
Y



Z

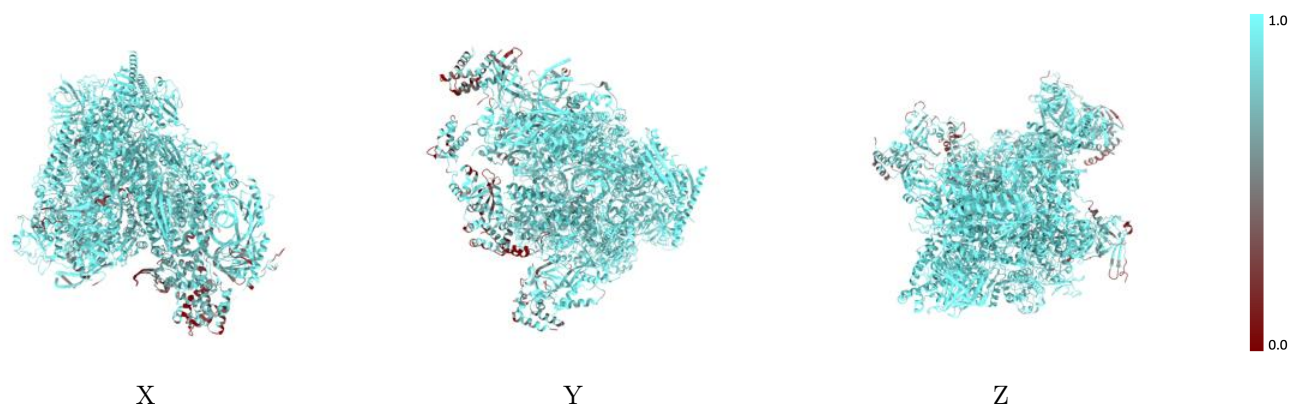
The images above show the 3D surface view of the map at the recommended contour level 2.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



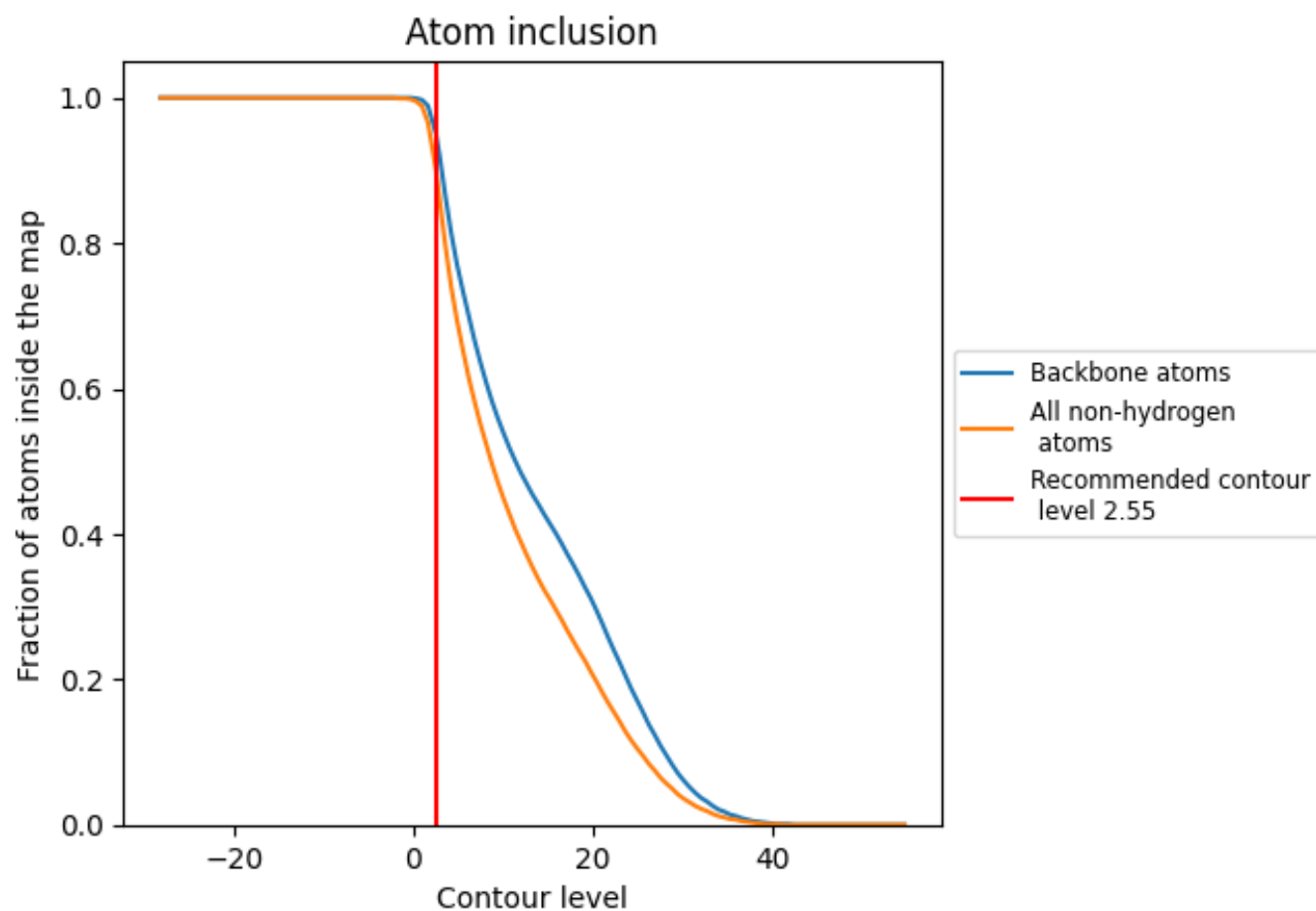
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.55).

















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 90% 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 (2.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9010	 0.4310
A	 0.9550	 0.5170
B	 0.9590	 0.5380
C	 0.9700	 0.5550
D	 0.7480	 0.1790
E	 0.9490	 0.4900
F	 0.9610	 0.5320
G	 0.8460	 0.2800
H	 0.9650	 0.5330
I	 0.9410	 0.4690
J	 0.9860	 0.5650
K	 0.9750	 0.5480
L	 0.9520	 0.5140
M	 0.9200	 0.4680
N	 0.9320	 0.2950
O	 0.9290	 0.3570
P	 0.9760	 0.5270
Q	 0.7810	 0.1930
R	 0.8010	 0.2600
T	 0.9320	 0.3630
U	 0.6110	 0.1600
V	 0.6310	 0.1470
W	 0.5860	 0.1010
X	 0.7030	 0.1220

