



## wwPDB EM Validation Summary Report ⓘ

Sep 28, 2024 – 10:07 PM EDT

PDB ID : 8T9G  
EMDB ID : EMD-41110  
Title : Automethylated PRC2 dimer bound to nucleosome  
Authors : Sauer, P.V.; Pavlenko, E.; Nogales, E.; Poepsel, S.  
Deposited on : 2023-06-23  
Resolution : 6.20 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.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

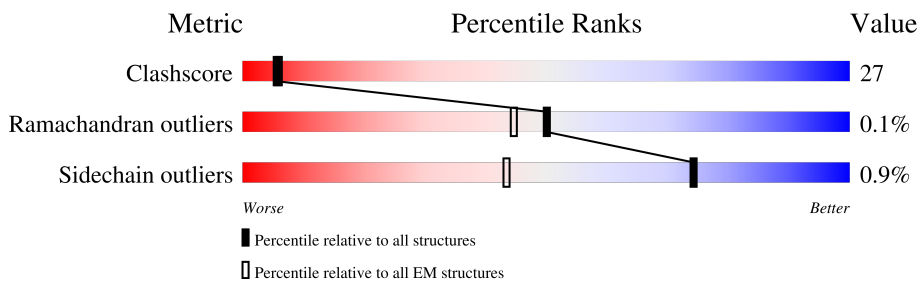
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.20 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.





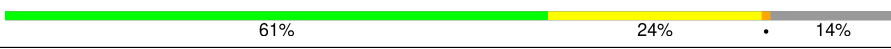
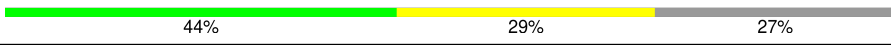
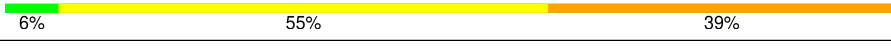
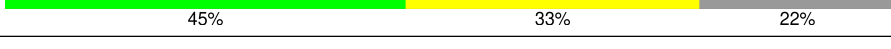

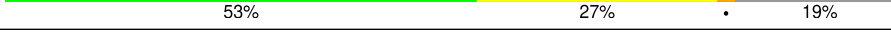
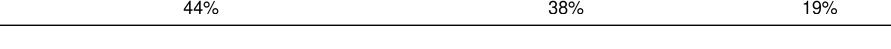
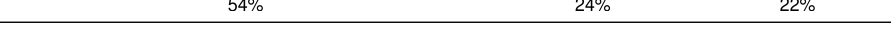
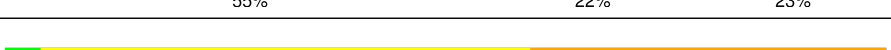
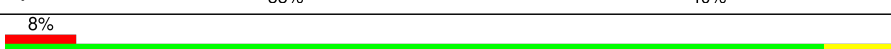
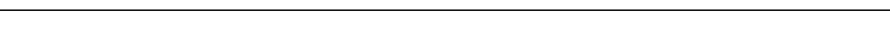
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	B	619	<div> <div>12%</div> <div>35%</div> <div>36%</div> <div>28%</div> </div>
1	G	619	<div> <div>28%</div> <div>43%</div> <div>28%</div> </div>
2	C	753	<div> <div>36%</div> <div>35%</div> <div>29%</div> </div>
2	I	753	<div> <div>38%</div> <div>42%</div> <div>20%</div> </div>
3	F	441	<div> <div>40%</div> <div>42%</div> <div>18%</div> </div>
3	K	441	<div> <div>23%</div> <div>59%</div> <div>18%</div> </div>
4	L	425	<div> <div>40%</div> <div>53%</div> <div>7%</div> </div>
4	O	425	<div> <div>35%</div> <div>58%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
5	M	303	
5	Y	303	
6	A	136	
6	W	136	
7	H	215	
8	J	106	
8	X	106	
9	R	133	
9	U	133	
10	S	123	
10	V	123	
11	T	215	
12	E	12	

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 45911 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 Polycomb protein SUZ12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	443	Total	C	N	O	S	0	0
			3665	2326	656	656	27		
1	G	443	Total	C	N	O	S	0	0
			3665	2326	656	656	27		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	67	MET	-	initiating methionine	UNP Q15022
G	67	MET	-	initiating methionine	UNP Q15022

- Molecule 2 is a protein called Histone-lysine N-methyltransferase EZH2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	536	Total	C	N	O	S	0	0
			4304	2696	765	801	42		
2	I	605	Total	C	N	O	S	0	0
			4863	3049	863	908	43		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP Q15910
C	0	ASN	-	expression tag	UNP Q15910
C	1	ALA	-	expression tag	UNP Q15910
C	14	ALA	CYS	conflict	UNP Q15910
C	15	CYS	TRP	conflict	UNP Q15910
I	-1	SER	-	expression tag	UNP Q15910
I	0	ASN	-	expression tag	UNP Q15910
I	1	ALA	-	expression tag	UNP Q15910
I	14	ALA	CYS	conflict	UNP Q15910
I	15	CYS	TRP	conflict	UNP Q15910

- Molecule 3 is a protein called Polycomb protein EED.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	362	Total	C	N	O	S	0	0
			2930	1855	513	541	21		
3	K	362	Total	C	N	O	S	0	0
			2930	1855	513	541	21		

- Molecule 4 is a protein called Histone-binding protein RBBP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	395	Total	C	N	O	S	0	0
			3139	1981	535	613	10		
4	O	395	Total	C	N	O	S	0	0
			3139	1981	535	613	10		

- Molecule 5 is a protein called Zinc finger protein AEBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	126	Total	C	N	O	S	0	0
			1047	664	206	174	3		
5	Y	126	Total	C	N	O	S	0	0
			1047	664	206	174	3		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	7	SER	-	expression tag	UNP Q6ZN18
M	8	ASN	-	expression tag	UNP Q6ZN18
M	9	ALA	MET	conflict	UNP Q6ZN18
Y	7	SER	-	expression tag	UNP Q6ZN18
Y	8	ASN	-	expression tag	UNP Q6ZN18
Y	9	ALA	MET	conflict	UNP Q6ZN18

- Molecule 6 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	117	Total	C	N	O	S	0	0
			939	590	183	163	3		
6	W	99	Total	C	N	O	S	0	0
			817	515	158	141	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	conflict	UNP P84233
W	102	ALA	GLY	conflict	UNP P84233

- Molecule 7 is a DNA chain called DNA (226-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	215	Total	C	N	O	P	0	0
			4421	2085	846	1275	215		

- Molecule 8 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	83	Total	C	N	O	S	0	0
			661	418	129	113	1		
8	X	87	Total	C	N	O	S	0	0
			702	442	142	117	1		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	103	SER	-	expression tag	UNP P62799
J	104	SER	-	expression tag	UNP P62799
J	105	GLY	-	expression tag	UNP P62799
X	103	SER	-	expression tag	UNP P62799
X	104	SER	-	expression tag	UNP P62799
X	105	GLY	-	expression tag	UNP P62799

- Molecule 9 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	108	Total	C	N	O	S	0	0
			829	522	162	144	1		
9	U	108	Total	C	N	O	S	0	0
			829	522	162	144	1		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-3	SER	-	expression tag	UNP P06897
R	-2	ASN	-	expression tag	UNP P06897
R	-1	ALA	-	expression tag	UNP P06897
R	99	ARG	GLY	conflict	UNP P06897

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Chain	Residue	Modelled	Actual	Comment	Reference
R	119	CYS	LYS	conflict	UNP P06897
R	123	SER	ALA	conflict	UNP P06897
U	-3	SER	-	expression tag	UNP P06897
U	-2	ASN	-	expression tag	UNP P06897
U	-1	ALA	-	expression tag	UNP P06897
U	99	ARG	GLY	conflict	UNP P06897
U	119	CYS	LYS	conflict	UNP P06897
U	123	SER	ALA	conflict	UNP P06897

- Molecule 10 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S	96	Total	C	N	O	S	0	0
			752	472	137	141	2		
10	V	95	Total	C	N	O	S	0	0
			741	466	133	140	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	0	MET	-	initiating methionine	UNP P02281
S	29	THR	SER	conflict	UNP P02281
V	0	MET	-	initiating methionine	UNP P02281
V	29	THR	SER	conflict	UNP P02281

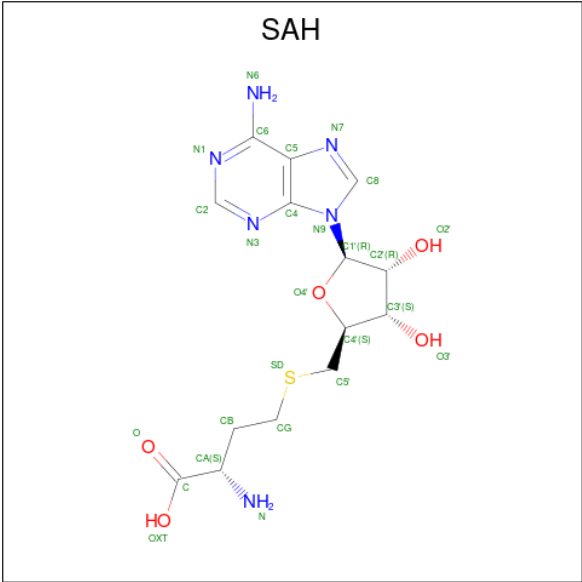
- Molecule 11 is a DNA chain called DNA (226-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	T	215	Total	C	N	O	P	0	0
			4372	2067	807	1283	215		

- Molecule 12 is a protein called activating methylated peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	E	12	Total	C	N	O	0	0
			67	42	13	12		

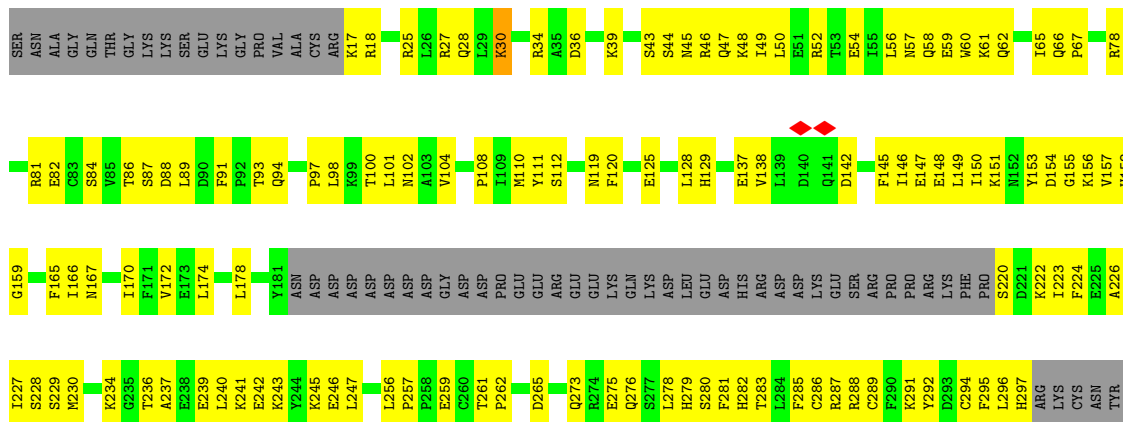
- Molecule 13 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S) (labeled as "Ligand of Interest" by depositor).



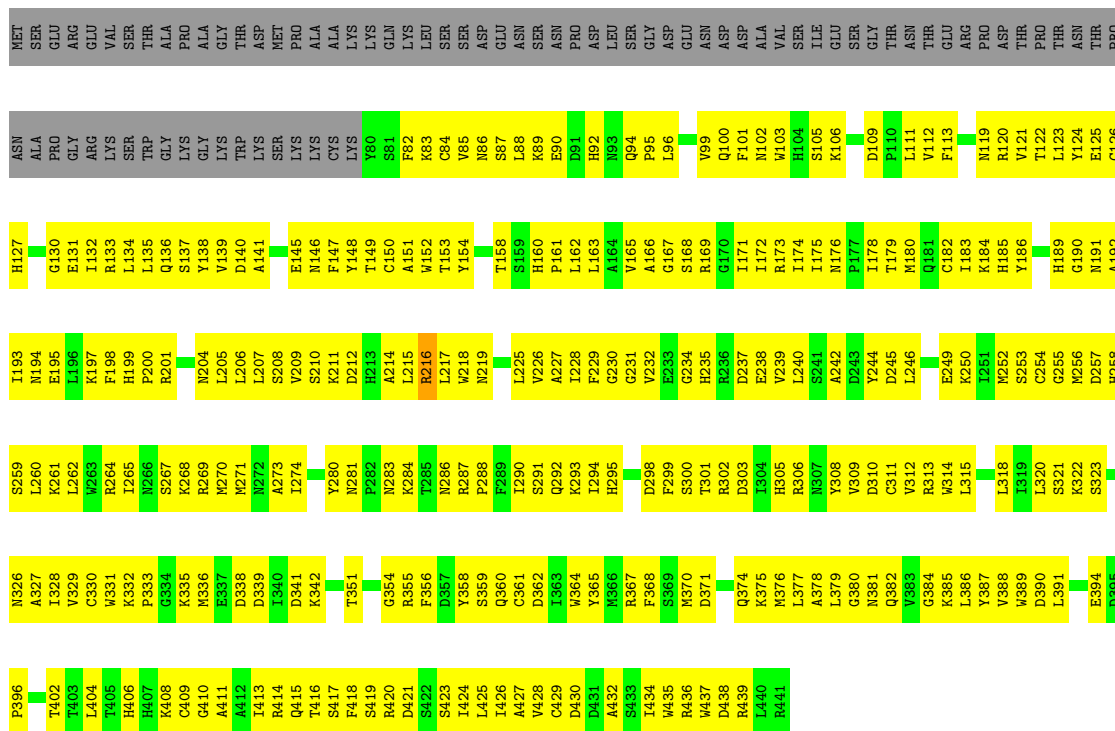
Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	S	0
			26	14	6	5	1	
13	I	1	Total	C	N	O	S	0
			26	14	6	5	1	



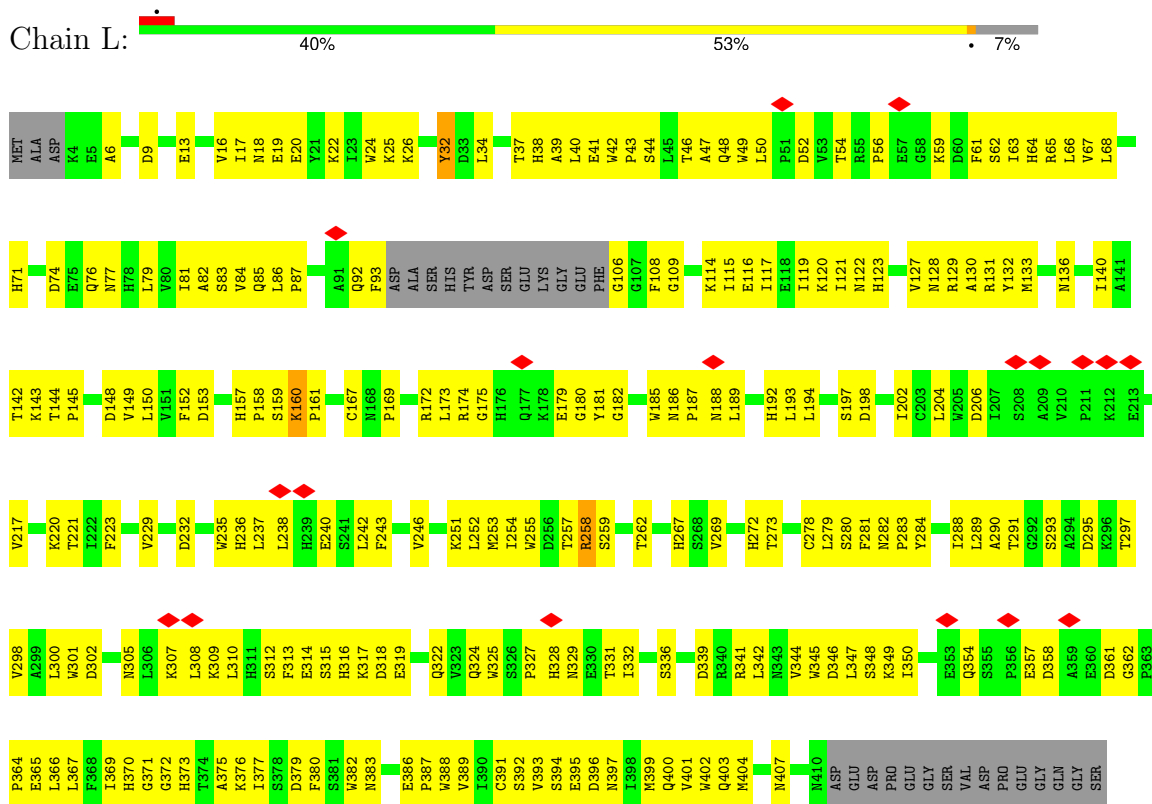






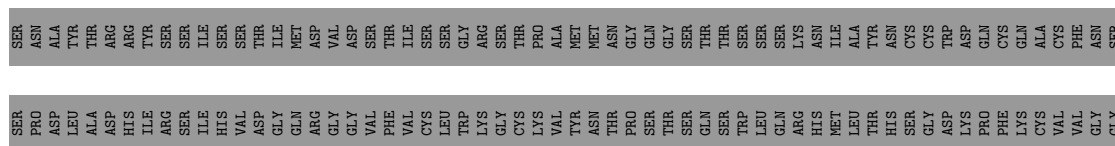


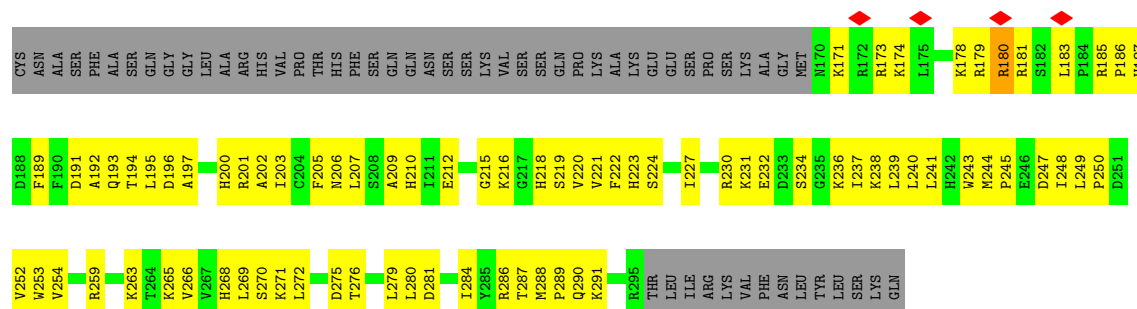
- Molecule 4: Histone-binding protein RBBP4



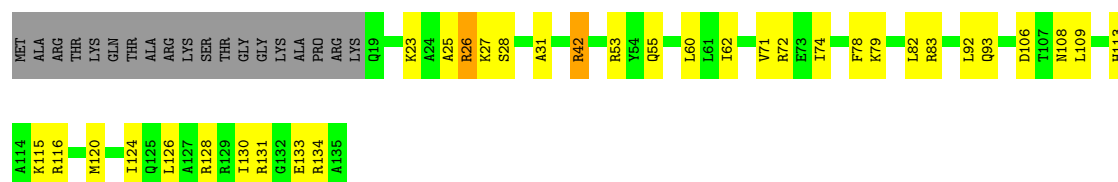
- Molecule 4: Histone-binding protein RBBP4



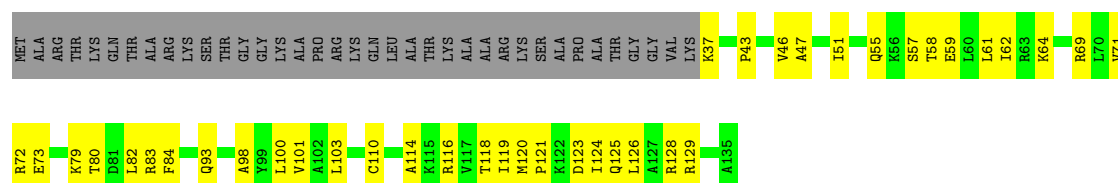




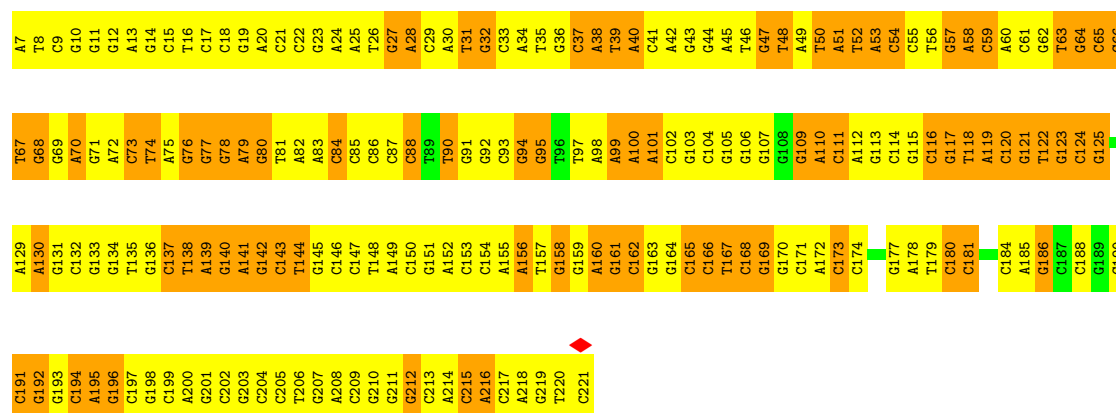
### • Molecule 6: Histone H3.2



### • Molecule 6: Histone H3.2

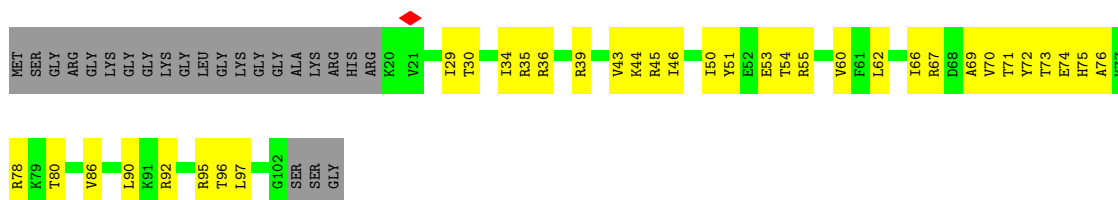


### • Molecule 7: DNA (226-MER)

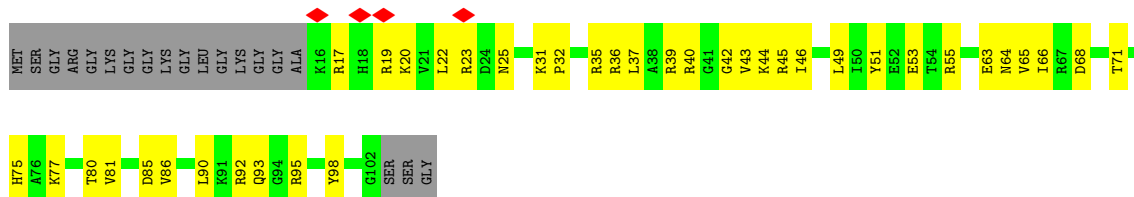


### • Molecule 8: Histone H4

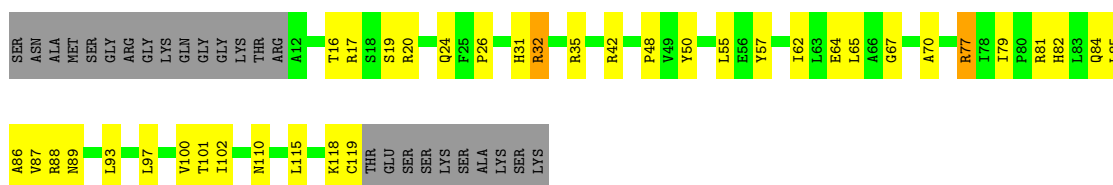




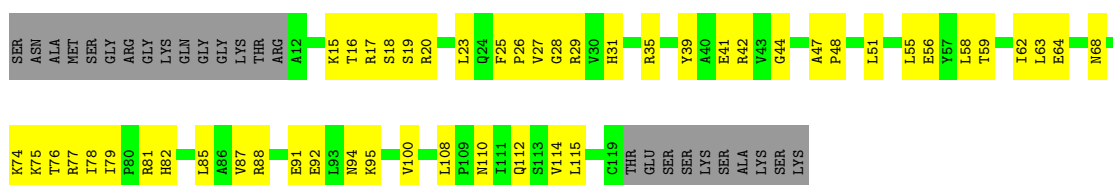
• Molecule 8: Histone H4



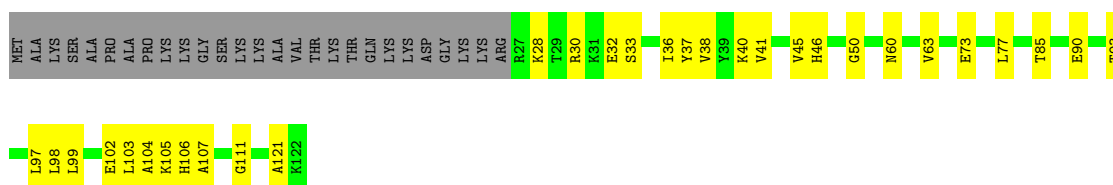
• Molecule 9: Histone H2A type 1



• Molecule 9: Histone H2A type 1



• Molecule 10: Histone H2B 1.1



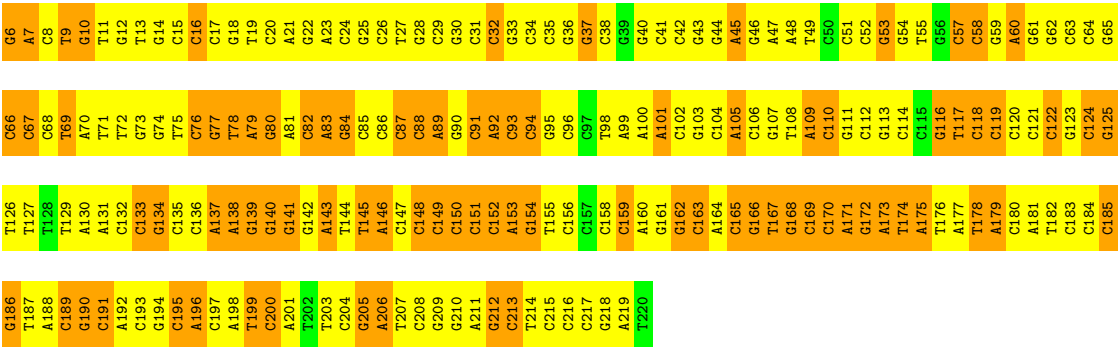
• Molecule 10: Histone H2B 1.1

Chain V:  55% 22% 23%



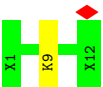
• Molecule 11: DNA (226-MER)

Chain T:  55% 40%



• Molecule 12: activating methylated peptide

Chain E:  8% 92% 8%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34000	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)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.198	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	460.0, 460.0, 460.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.3, 2.3, 2.3	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: M3L, 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	B	0.29	0/3745	0.56	1/5035 (0.0%)
1	G	0.33	0/3745	0.57	2/5035 (0.0%)
2	C	0.26	0/4397	0.53	1/5923 (0.0%)
2	I	0.36	0/4971	0.65	7/6702 (0.1%)
3	F	0.24	0/3005	0.51	0/4070
3	K	0.32	0/3005	0.55	0/4070
4	L	0.27	0/3225	0.51	1/4394 (0.0%)
4	O	0.30	0/3225	0.51	0/4394
5	M	0.27	0/1070	0.59	1/1437 (0.1%)
5	Y	0.28	0/1070	0.56	0/1437
6	A	0.44	0/952	0.76	3/1276 (0.2%)
6	W	0.32	0/829	0.62	0/1111
7	H	0.76	2/4967 (0.0%)	1.74	324/7665 (4.2%)
8	J	0.37	0/668	0.65	1/894 (0.1%)
8	X	0.30	0/710	0.64	0/948
9	R	0.33	0/839	0.61	1/1132 (0.1%)
9	U	0.30	0/839	0.60	0/1132
10	S	0.31	0/763	0.55	0/1025
10	V	0.31	0/752	0.52	0/1011
11	T	0.79	6/4899 (0.1%)	1.73	300/7548 (4.0%)
All	All	0.45	8/47676 (0.0%)	0.97	642/66239 (1.0%)

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	B	0	2
4	L	0	1
6	A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	H	0	3
11	T	0	5
All	All	0	12

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	54	DG	C2-N2	-6.61	1.27	1.34
11	T	124	DC	C4-N4	-6.57	1.28	1.33
11	T	53	DG	C2-N2	-5.49	1.29	1.34
7	H	178	DA	C5-C4	-5.21	1.35	1.38
11	T	48	DA	C5-C4	-5.21	1.35	1.38

The worst 5 of 642 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	93	DC	OP1-P-O3'	-34.70	28.85	105.20
11	T	167	DT	OP1-P-O3'	-34.42	29.47	105.20
11	T	76	DC	OP2-P-O3'	-33.34	31.85	105.20
7	H	85	DC	OP2-P-O3'	-32.65	33.37	105.20
7	H	94	DG	OP1-P-OP2	-14.47	97.90	119.60

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	42	ARG	Sidechain
1	B	461	TYR	Sidechain
1	B	532	ARG	Sidechain
7	H	169	DG	Sidechain
4	L	32	TYR	Sidechain

## 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	B	3665	0	3649	218	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3665	0	3649	275	0
2	C	4304	0	4176	224	0
2	I	4863	0	4751	300	0
3	F	2930	0	2837	172	0
3	K	2930	0	2839	319	0
4	L	3139	0	2986	199	0
4	O	3139	0	2986	250	0
5	M	1047	0	1102	72	0
5	Y	1047	0	1102	87	0
6	A	939	0	995	35	0
6	W	817	0	858	44	0
7	H	4421	0	2399	95	0
8	J	661	0	709	32	0
8	X	702	0	755	43	0
9	R	829	0	887	41	0
9	U	829	0	887	54	0
10	S	752	0	775	33	0
10	V	741	0	762	30	0
11	T	4372	0	2392	87	0
12	E	67	0	32	3	0
13	C	26	0	19	1	0
13	I	26	0	19	4	0
All	All	45911	0	41566	2272	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 27.

The worst 5 of 2272 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)
2:I:101:LEU:HB3	3:K:173:ARG:HH12	1.30	0.94
3:K:145:GLU:HG2	3:K:168:SER:HB2	1.50	0.93
1:G:450:CYS:HB3	1:G:455:LEU:H	1.37	0.89
3:K:147:PHE:HA	3:K:167:GLY:HA3	1.55	0.88
4:O:334:ALA:HB1	4:O:342:LEU:HD21	1.56	0.86

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	B	427/619 (69%)	396 (93%)	31 (7%)	0	100	100
1	G	427/619 (69%)	384 (90%)	42 (10%)	1 (0%)	44	78
2	C	524/753 (70%)	481 (92%)	43 (8%)	0	100	100
2	I	597/753 (79%)	534 (89%)	61 (10%)	2 (0%)	37	73
3	F	360/441 (82%)	334 (93%)	26 (7%)	0	100	100
3	K	360/441 (82%)	313 (87%)	47 (13%)	0	100	100
4	L	391/425 (92%)	370 (95%)	21 (5%)	0	100	100
4	O	391/425 (92%)	362 (93%)	29 (7%)	0	100	100
5	M	124/303 (41%)	110 (89%)	13 (10%)	1 (1%)	16	55
5	Y	124/303 (41%)	106 (86%)	18 (14%)	0	100	100
6	A	115/136 (85%)	107 (93%)	8 (7%)	0	100	100
6	W	97/136 (71%)	96 (99%)	1 (1%)	0	100	100
8	J	81/106 (76%)	80 (99%)	1 (1%)	0	100	100
8	X	85/106 (80%)	81 (95%)	4 (5%)	0	100	100
9	R	106/133 (80%)	103 (97%)	3 (3%)	0	100	100
9	U	106/133 (80%)	102 (96%)	4 (4%)	0	100	100
10	S	94/123 (76%)	89 (95%)	5 (5%)	0	100	100
10	V	93/123 (76%)	90 (97%)	3 (3%)	0	100	100
All	All	4502/6078 (74%)	4138 (92%)	360 (8%)	4 (0%)	50	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	566	ARG
1	G	480	TYR
5	M	176	LYS
2	I	492	THR

### 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	B	415/575 (72%)	409 (99%)	6 (1%)	62	75
1	G	415/575 (72%)	412 (99%)	3 (1%)	81	87
2	C	478/672 (71%)	473 (99%)	5 (1%)	73	82
2	I	539/672 (80%)	533 (99%)	6 (1%)	70	80
3	F	324/392 (83%)	322 (99%)	2 (1%)	84	88
3	K	324/392 (83%)	322 (99%)	2 (1%)	84	88
4	L	351/375 (94%)	347 (99%)	4 (1%)	70	80
4	O	351/375 (94%)	350 (100%)	1 (0%)	91	92
5	M	117/271 (43%)	116 (99%)	1 (1%)	75	83
5	Y	117/271 (43%)	115 (98%)	2 (2%)	56	72
6	A	97/111 (87%)	96 (99%)	1 (1%)	73	82
6	W	86/111 (78%)	85 (99%)	1 (1%)	67	79
8	J	68/81 (84%)	68 (100%)	0	100	100
8	X	72/81 (89%)	71 (99%)	1 (1%)	62	75
9	R	85/104 (82%)	84 (99%)	1 (1%)	67	79
9	U	85/104 (82%)	85 (100%)	0	100	100
10	S	81/103 (79%)	81 (100%)	0	100	100
10	V	80/103 (78%)	80 (100%)	0	100	100
All	All	4085/5368 (76%)	4049 (99%)	36 (1%)	74	83

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	570	GLN
5	Y	291	LYS
2	I	578	CYS
3	K	216	ARG
3	F	313	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	598	HIS
4	O	410	ASN
3	K	94	GLN
4	O	168	ASN
4	L	122	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\# Z  > 2$
12	M3L	E	9	12	10,11,12	0.55	0	9,14,16	0.58	0

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
12	M3L	E	9	12	-	6/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	E	9	M3L	CD-CE-NZ-CM1
12	E	9	M3L	CD-CE-NZ-CM3
12	E	9	M3L	CD-CE-NZ-CM2
12	E	9	M3L	CG-CD-CE-NZ
12	E	9	M3L	CE-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	E	9	M3L	3	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are 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	SAH	I	801	-	23,28,28	1.28	3 (13%)	22,40,40	1.95	3 (13%)
13	SAH	C	801	-	23,28,28	1.28	3 (13%)	22,40,40	1.88	4 (18%)

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	SAH	I	801	-	-	3/11/31/31	0/3/3/3
13	SAH	C	801	-	-	2/11/31/31	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	801	SAH	C2-N3	4.20	1.38	1.32
13	I	801	SAH	C2-N3	4.01	1.38	1.32
13	C	801	SAH	C2-N1	2.55	1.38	1.33
13	I	801	SAH	C2-N1	2.38	1.38	1.33
13	I	801	SAH	OXT-C	-2.34	1.23	1.30

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	I	801	SAH	N3-C2-N1	-6.39	120.00	128.67
13	C	801	SAH	N3-C2-N1	-6.24	120.20	128.67
13	I	801	SAH	C5'-SD-CG	-4.52	88.85	102.26
13	C	801	SAH	C5'-SD-CG	-3.98	90.46	102.26
13	I	801	SAH	OXT-C-O	-2.81	117.71	124.08

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	I	801	SAH	O4'-C4'-C5'-SD
13	I	801	SAH	C3'-C4'-C5'-SD
13	C	801	SAH	CA-CB-CG-SD
13	I	801	SAH	C-CA-CB-CG
13	C	801	SAH	CB-CG-SD-C5'

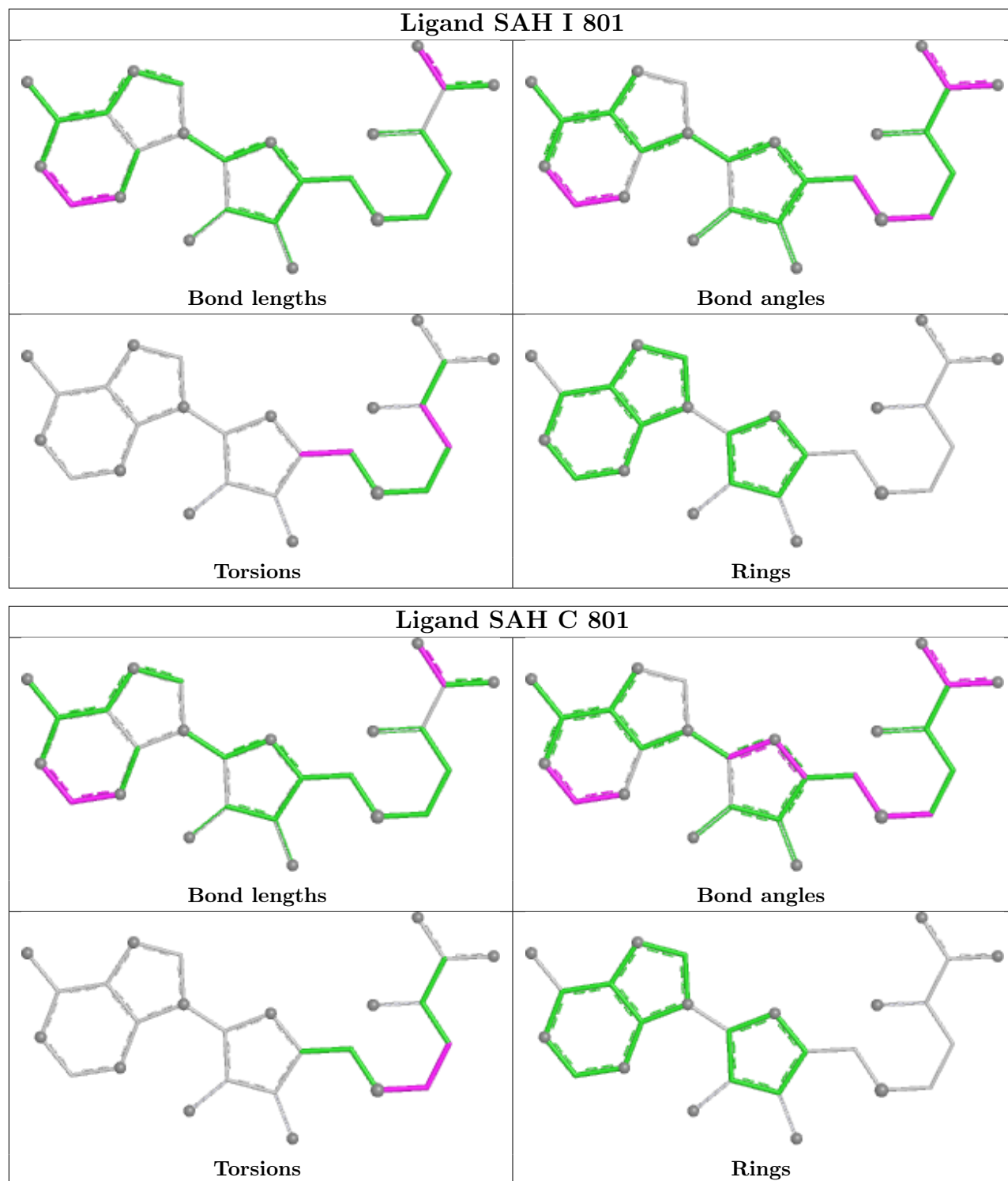
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	I	801	SAH	4	0
13	C	801	SAH	1	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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

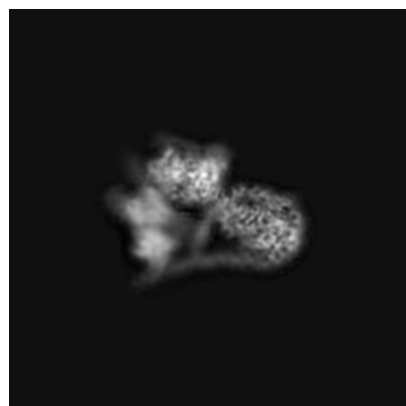
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41110. These allow visual inspection of the internal detail of the map and identification of artifacts.

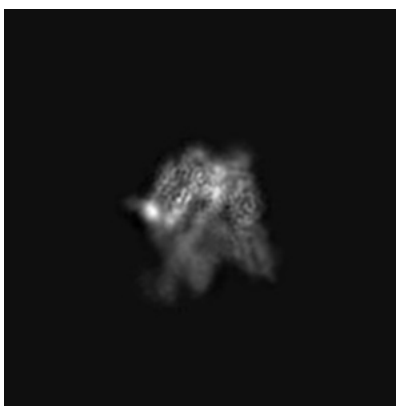
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

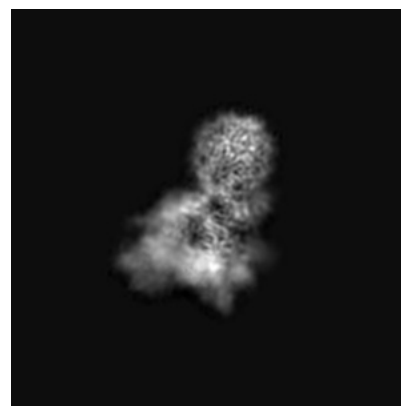
#### 6.1.1 Primary map



X

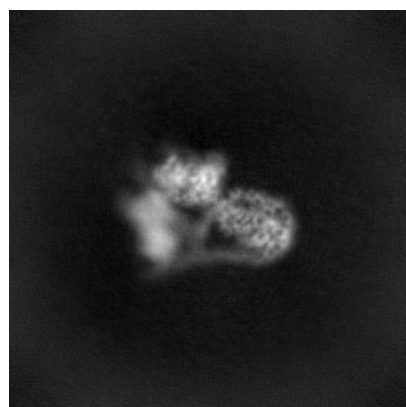


Y

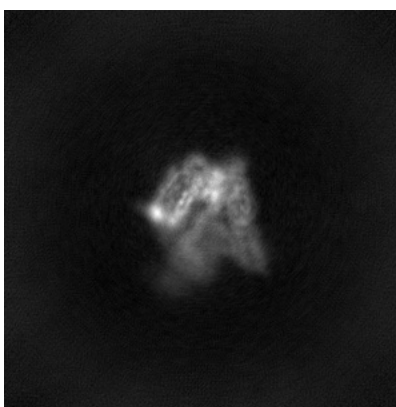


Z

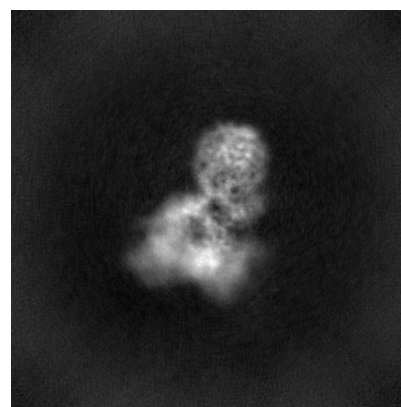
#### 6.1.2 Raw map



X



Y

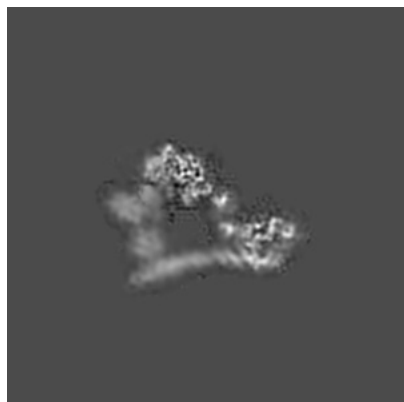


Z

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

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 100

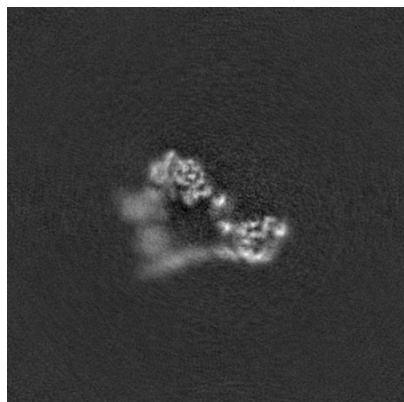


Y Index: 100

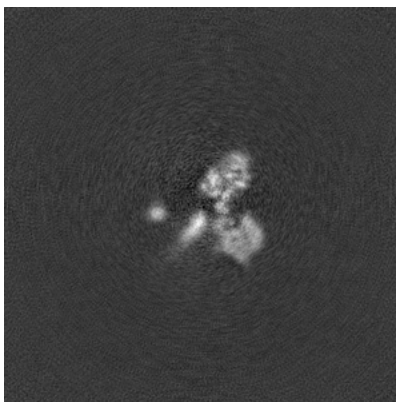


Z Index: 100

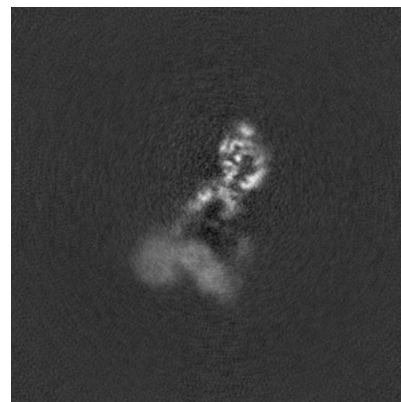
### 6.2.2 Raw map



X Index: 165



Y Index: 165

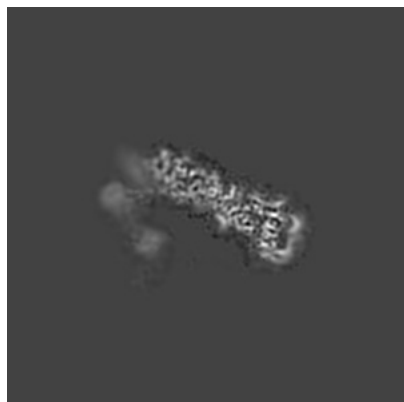


Z Index: 165

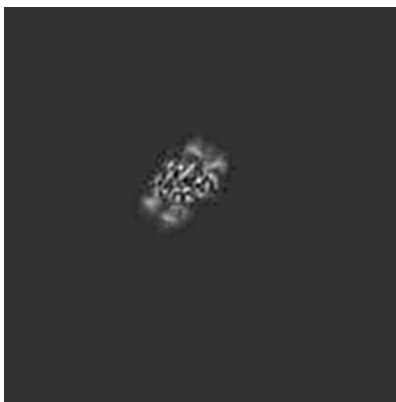
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 108

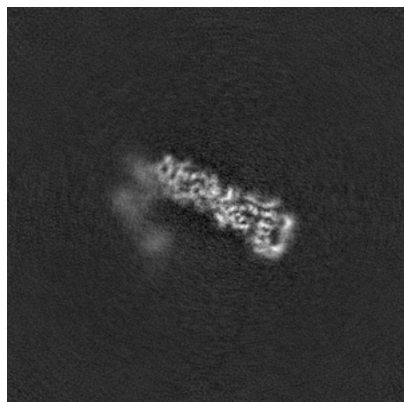


Y Index: 130

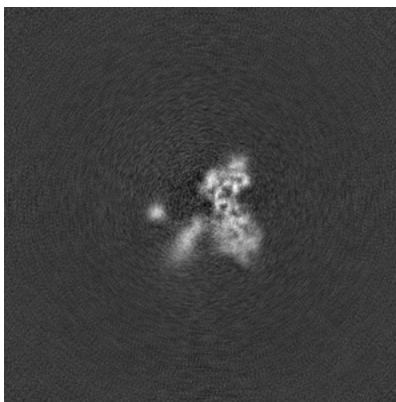


Z Index: 97

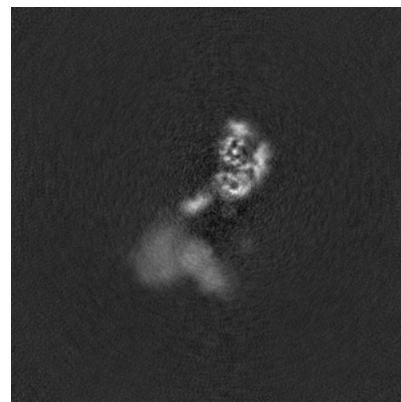
### 6.3.2 Raw map



X Index: 177



Y Index: 161

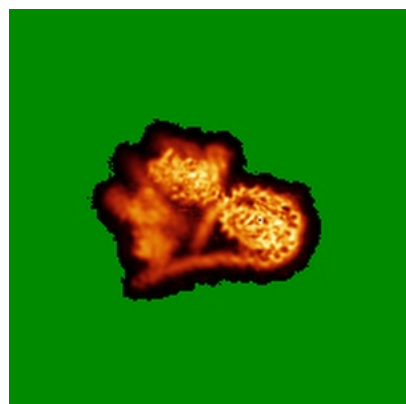


Z Index: 160

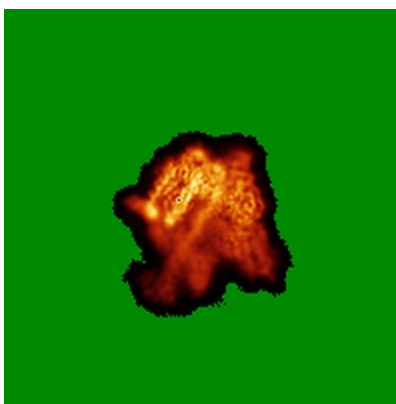
The images above show the largest variance slices of the map in three orthogonal directions.

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

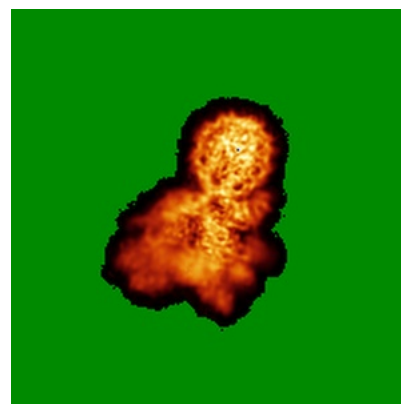
### 6.4.1 Primary map



X

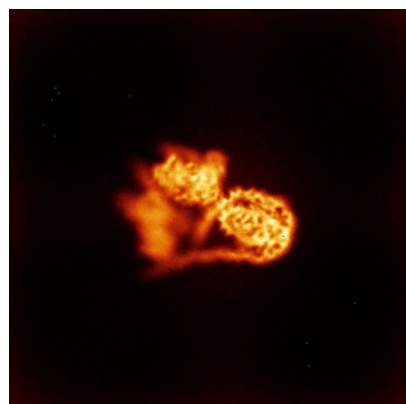


Y

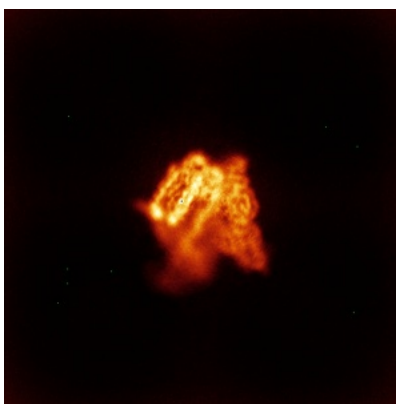


Z

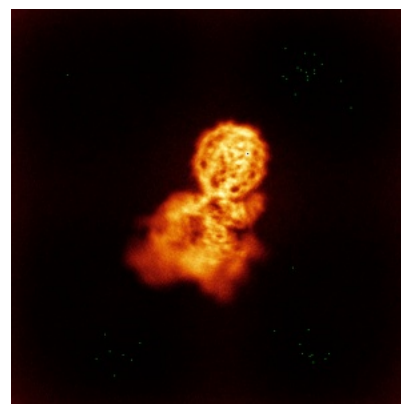
### 6.4.2 Raw map



X



Y

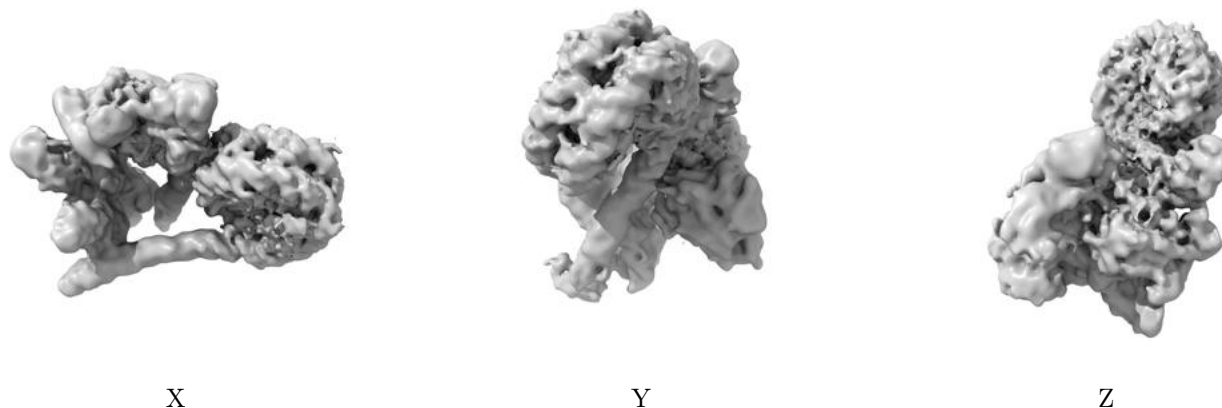


Z

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.

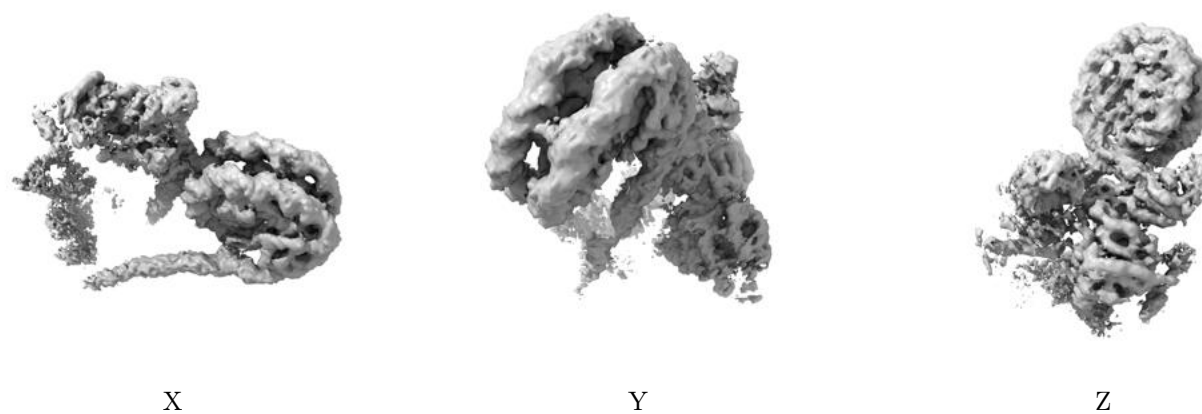
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

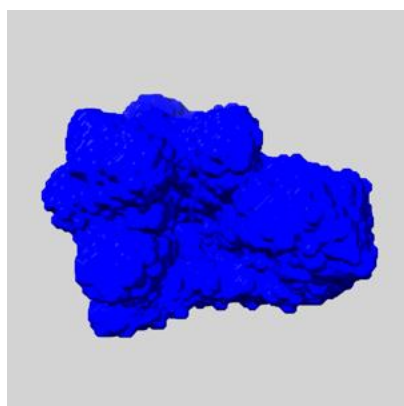
## 6.6 Mask visualisation [i](#)

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

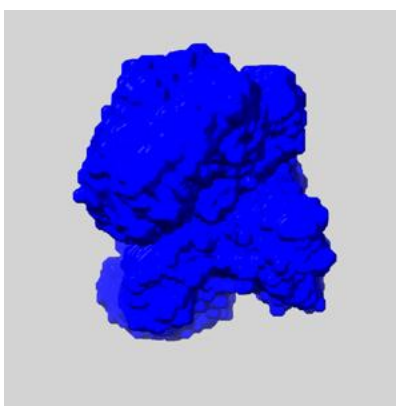
A mask typically either:

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

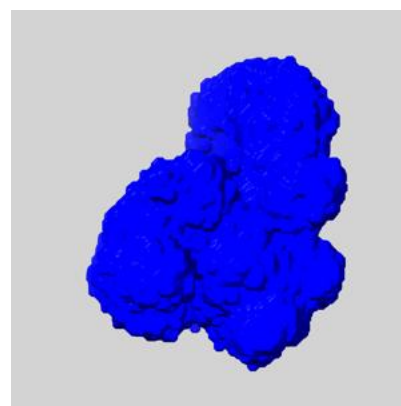
### 6.6.1 emd\_41110\_msk\_1.map [i](#)



X



Y

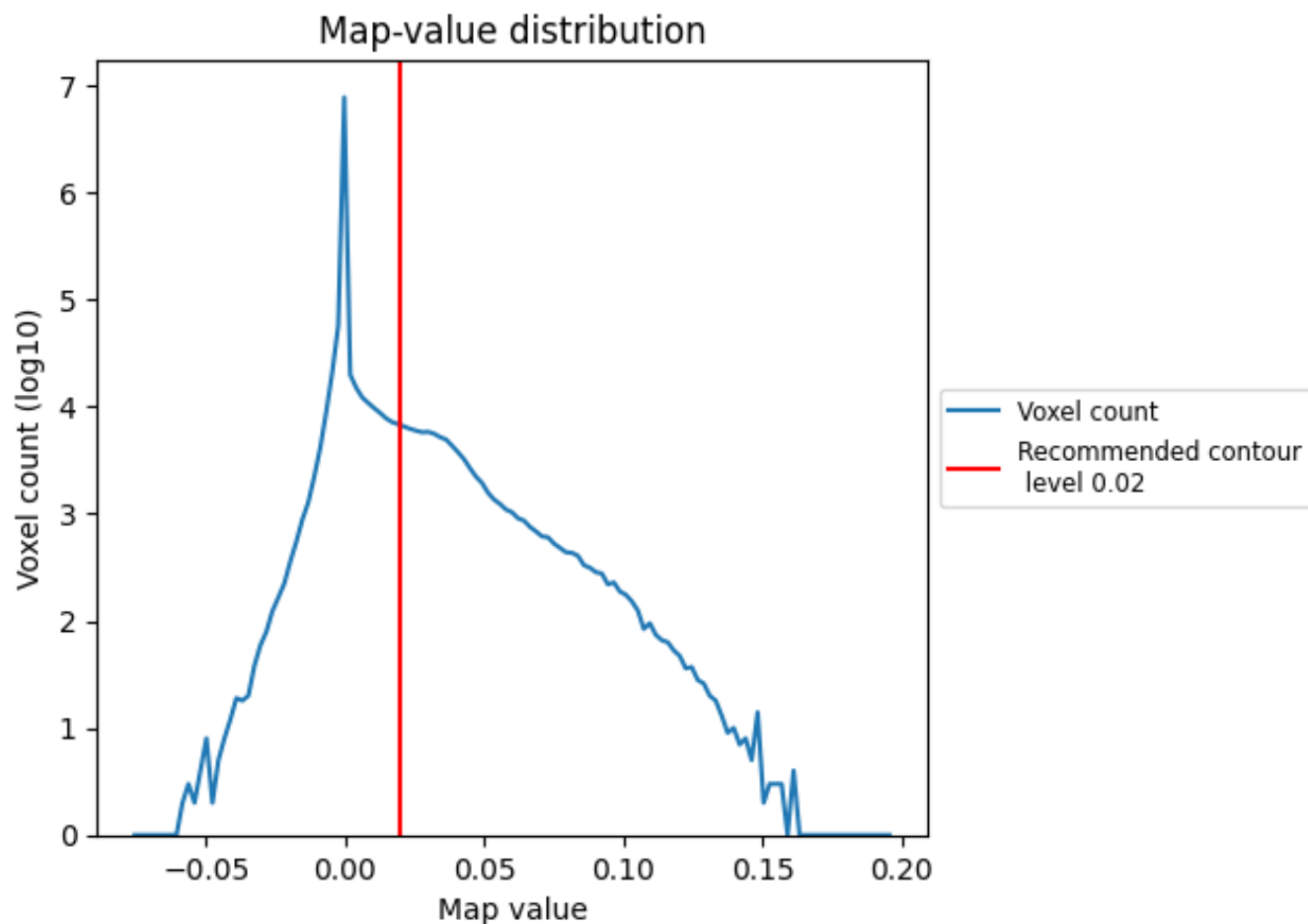


Z

## 7 Map analysis [i](#)

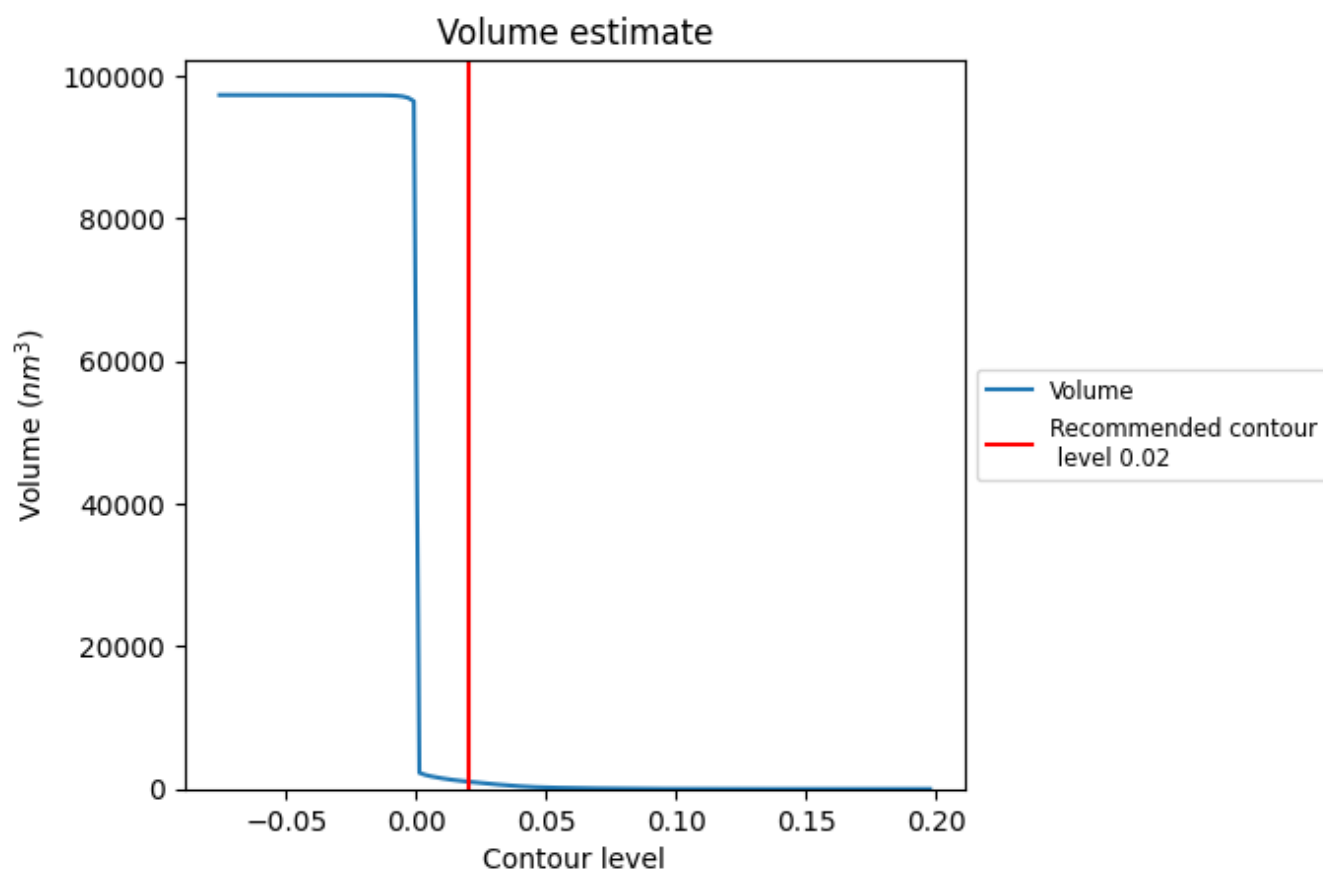
This section contains the results of statistical analysis of the map.

### 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.

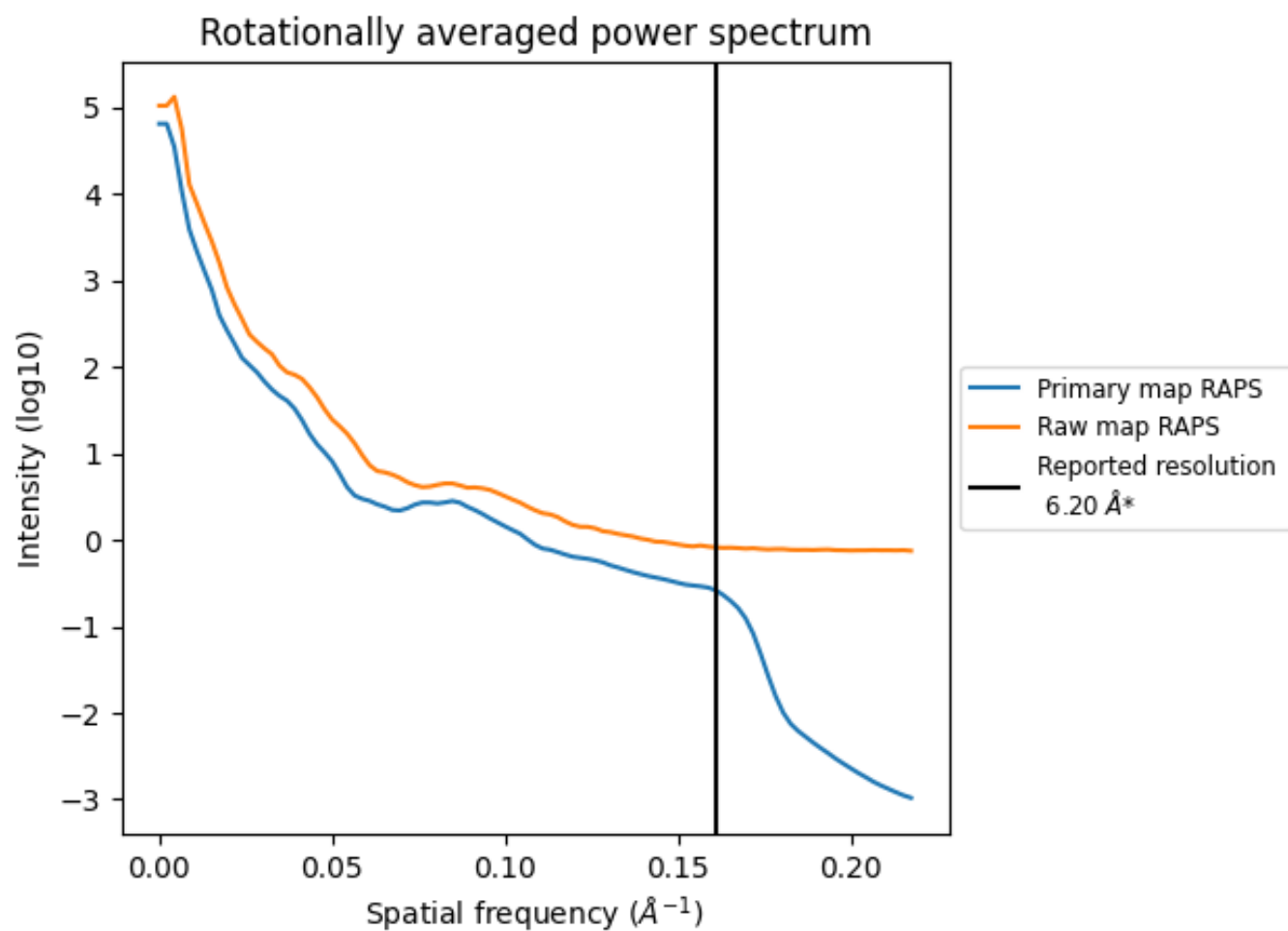
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1023  $\text{nm}^3$ ; this corresponds to an approximate mass of 924 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 ⓘ

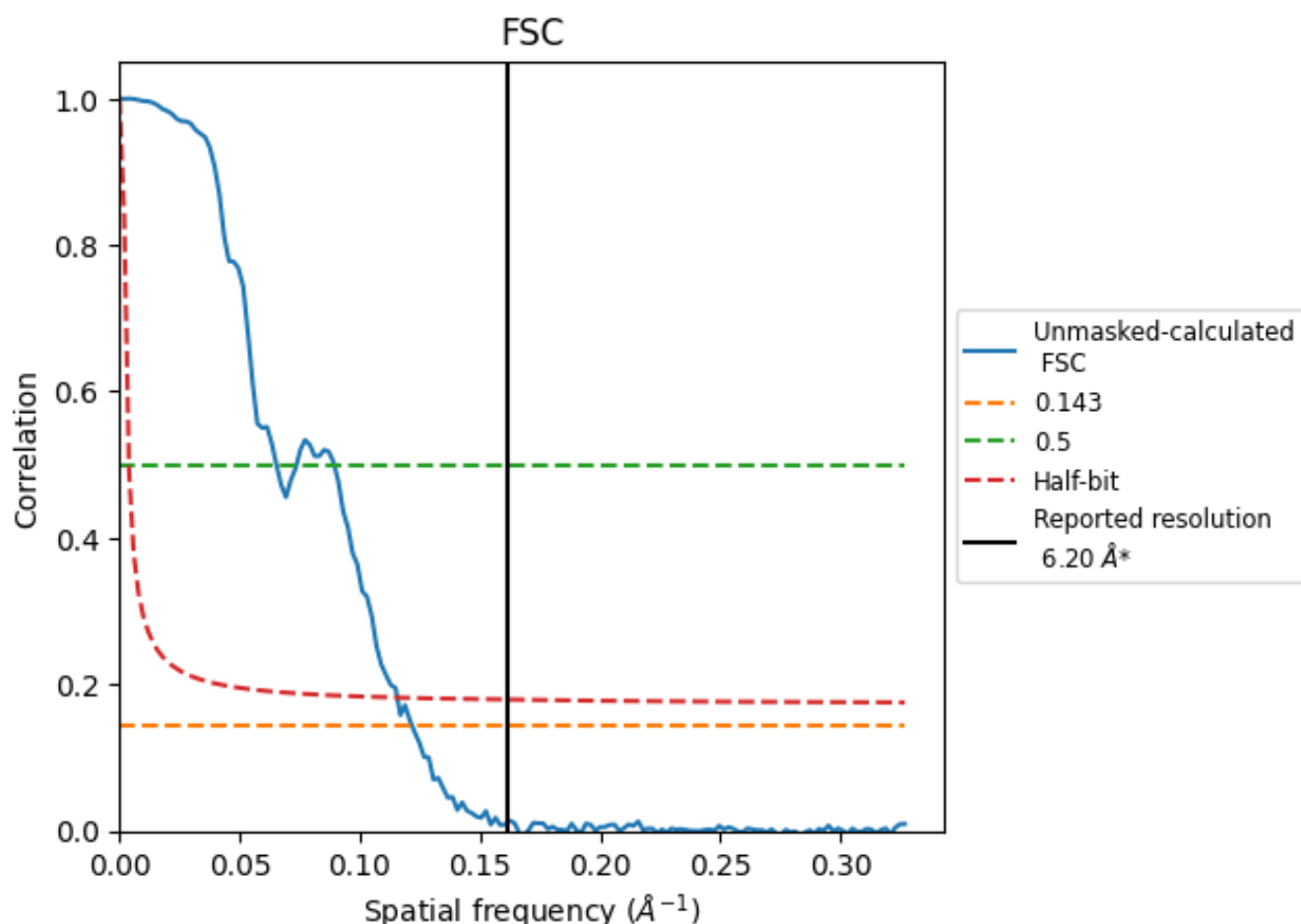


\*Reported resolution corresponds to spatial frequency of 0.161 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

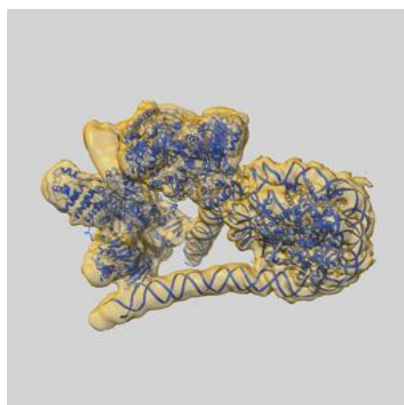
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.21	15.34	8.65

\*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 8.21 differs from the reported value 6.2 by more than 10 %

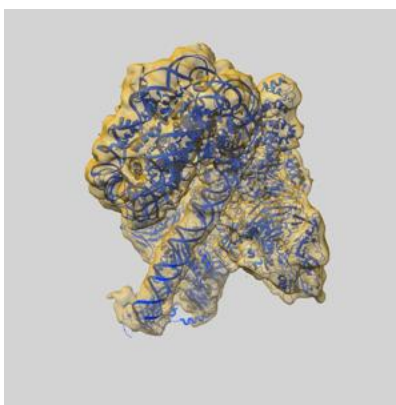
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41110 and PDB model 8T9G. Per-residue inclusion information can be found in section [3](#) on page [9](#).

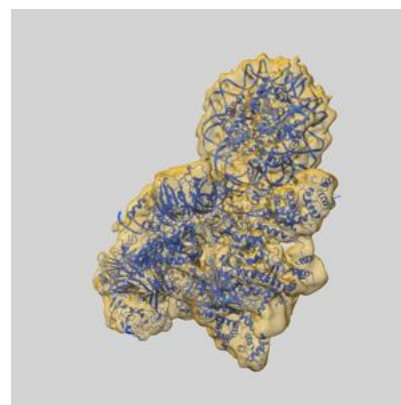
### 9.1 Map-model overlay [i](#)



X



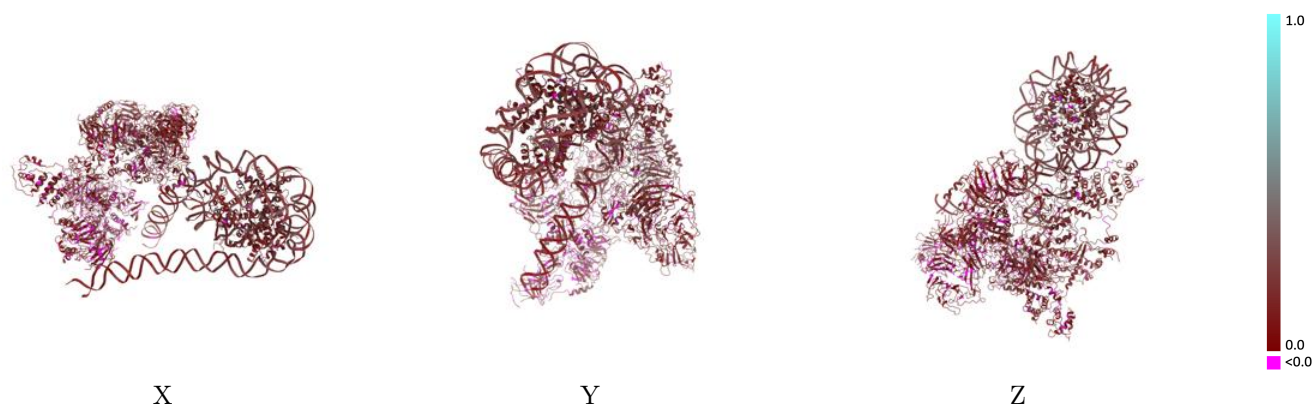
Y



Z

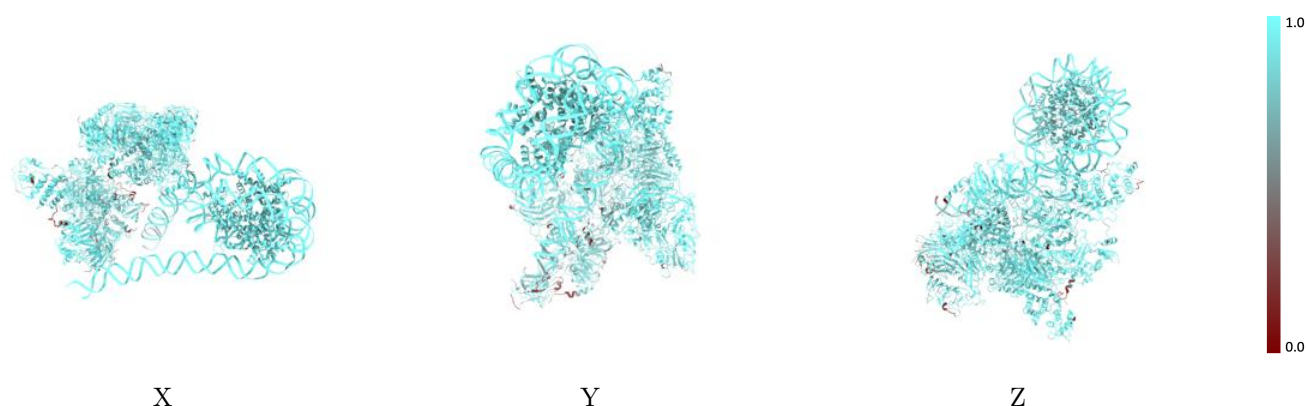
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



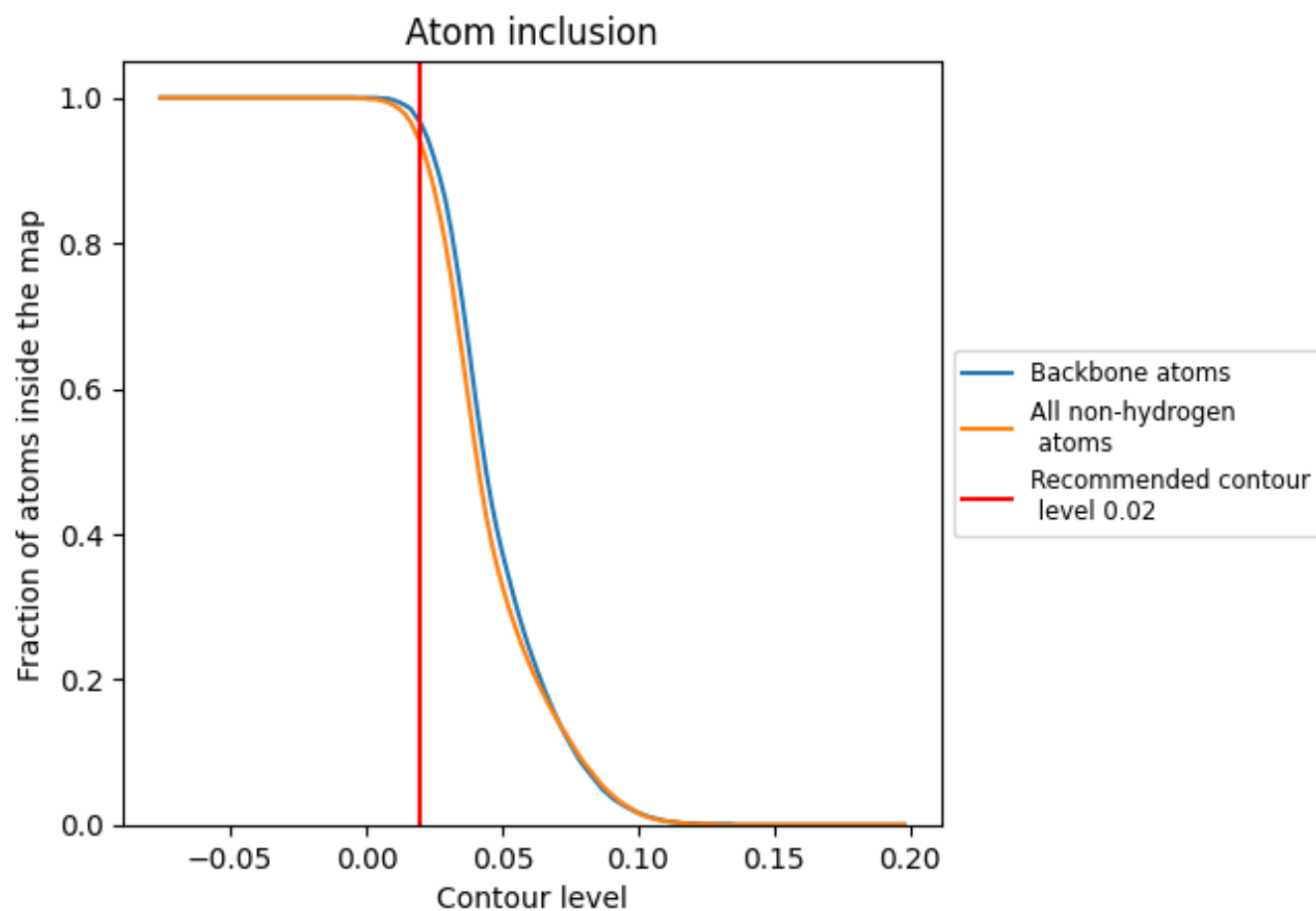
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).













































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 94% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9380	 0.1630
A	 0.9420	 0.1900
B	 0.8110	 0.1060
C	 0.9280	 0.1220
E	 0.8510	 0.1660
F	 0.9740	 0.0960
G	 0.9310	 0.1730
H	 0.9840	 0.2140
I	 0.9480	 0.1860
J	 0.9070	 0.1960
K	 0.9640	 0.1930
L	 0.9200	 0.1010
M	 0.8820	 0.1030
O	 0.9700	 0.1480
R	 0.9400	 0.2140
S	 0.9360	 0.1920
T	 0.9820	 0.2120
U	 0.9420	 0.1980
V	 0.9320	 0.1990
W	 0.9400	 0.1780
X	 0.8780	 0.1710
Y	 0.9050	 0.1640

