



## wwPDB EM Validation Summary Report ⓘ

Nov 9, 2022 – 05:42 PM EST

PDB ID : 6PA7  
EMDB ID : EMD-20281  
Title : The cryo-EM structure of the human DNMT3A2-DNMT3B3 complex bound to nucleosome.  
Authors : Xu, T.H.; Liu, M.; Zhou, X.E.; Liang, G.; Zhao, G.; Xu, H.E.; Melcher, K.; Jones, P.A.  
Deposited on : 2019-06-11  
Resolution : 2.94 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.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

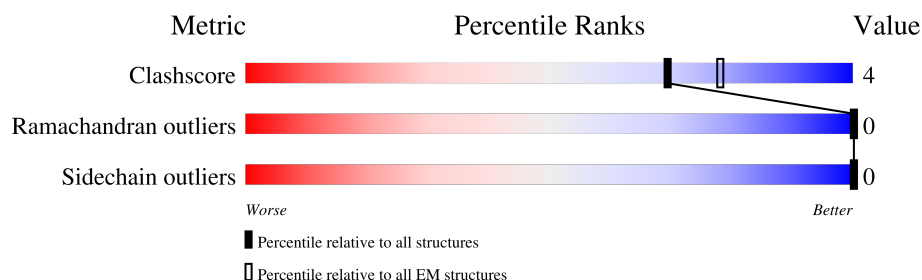
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.94 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

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	135	
1	E	135	
2	B	103	
2	F	103	
3	C	129	
3	G	129	
4	D	123	
4	H	123	

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Mol	Chain	Length	Quality of chain
5	I	167	<div><div><div></div><div></div><div></div></div><div>10%88%11%</div></div>
6	J	167	<div><div><div></div><div></div><div></div></div><div>8%93%7%</div></div>
7	K	689	<div><div><div></div><div></div><div></div></div><div>36%6%58%</div></div>
7	P	689	<div><div><div></div><div></div><div></div></div><div>36%6%58%</div></div>
8	N	770	<div><div><div></div><div></div><div></div></div><div>17%24%73%</div></div>
8	S	770	<div><div><div></div><div></div><div></div></div><div>8%25%73%</div></div>

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 21019 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 Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	99	Total	C	N	O	S	0	0
			817	515	158	141	3		
1	E	98	Total	C	N	O	S	0	0
			805	509	154	139	3		

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	81	Total	C	N	O	S	0	0
			646	407	126	112	1		
2	F	83	Total	C	N	O	S	0	0
			662	418	129	114	1		

- Molecule 3 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	108	Total	C	N	O		0	0
			824	519	161	144			
3	G	111	Total	C	N	O		0	0
			849	533	167	149			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	conflict	UNP P06897
C	123	SER	ALA	conflict	UNP P06897
G	99	ARG	GLY	conflict	UNP P06897

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Chain	Residue	Modelled	Actual	Comment	Reference
G	123	SER	ALA	conflict	UNP P06897

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	94	Total	C	N	O	S	0	0
			731	460	131	138	2		
4	H	96	Total	C	N	O	S	0	0
			752	472	137	141	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP P02281
D	29	THR	SER	engineered mutation	UNP P02281
H	0	MET	-	initiating methionine	UNP P02281
H	29	THR	SER	engineered mutation	UNP P02281

- Molecule 5 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	166	Total	C	N	O	P	0	0
			3385	1605	615	999	166		

- Molecule 6 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	166	Total	C	N	O	P	0	0
			3421	1616	646	993	166		

- Molecule 7 is a protein called DNA (cytosine-5)-methyltransferase 3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	288	Total	C	N	O	S	0	0
			2333	1495	412	413	13		
7	P	288	Total	C	N	O	S	0	0
			2333	1495	412	413	13		

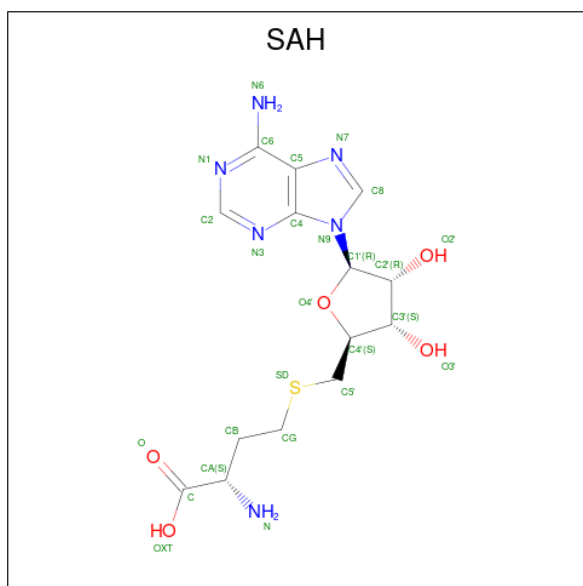
- Molecule 8 is a protein called DNA (cytosine-5)-methyltransferase 3B.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	211	Total	C	N	O	S	0	0
			1703	1105	301	290	7		
8	S	211	Total	C	N	O	S	0	0
			1703	1105	301	290	7		

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total Cl 1 1	0
9	C	1	Total Cl 1 1	0
9	H	1	Total Cl 1 1	0

- Molecule 10 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).

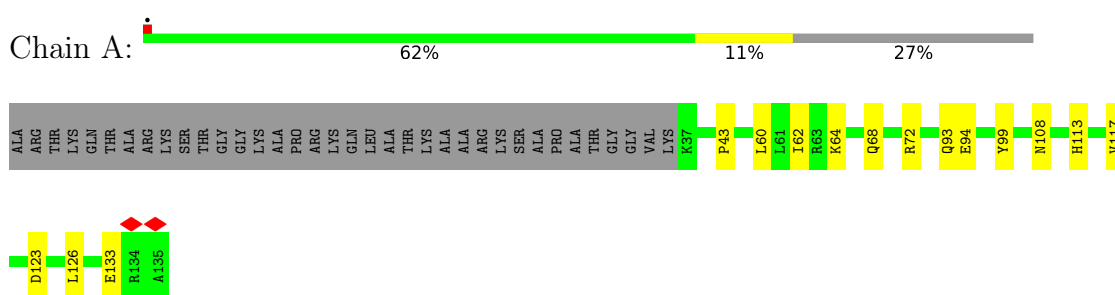


Mol	Chain	Residues	Atoms					AltConf
10	K	1	Total	C	N	O	S	0
			26	14	6	5	1	
10	P	1	Total	C	N	O	S	0
			26	14	6	5	1	

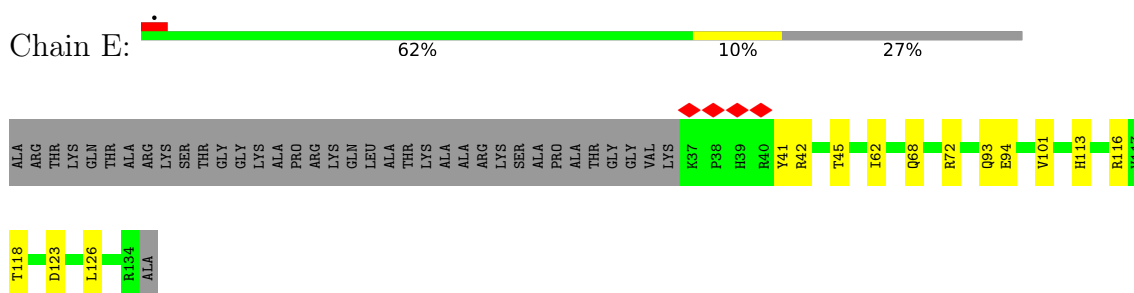
### 3 Residue-property plots [i](#)

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.

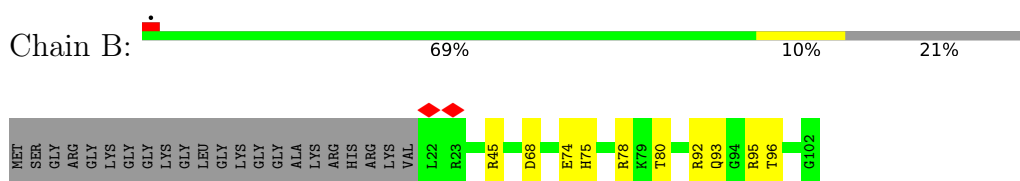
#### • Molecule 1: Histone H3.2



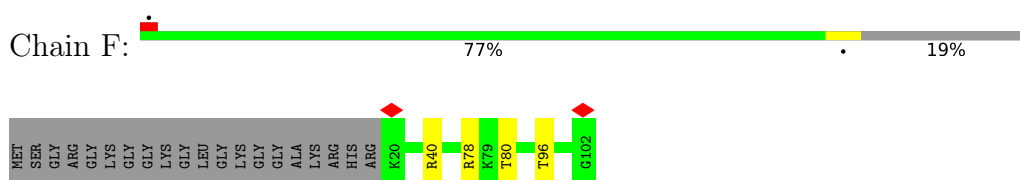
#### • Molecule 1: Histone H3.2



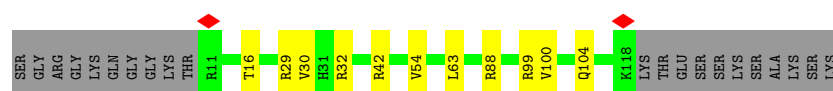
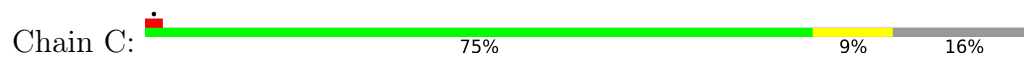
#### • Molecule 2: Histone H4



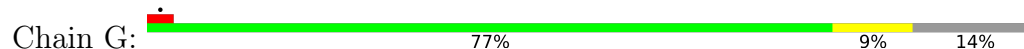
#### • Molecule 2: Histone H4



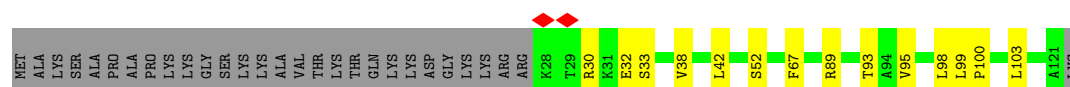
#### • Molecule 3: Histone H2A type 1



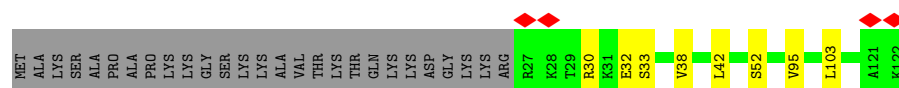
• Molecule 3: Histone H2A type 1



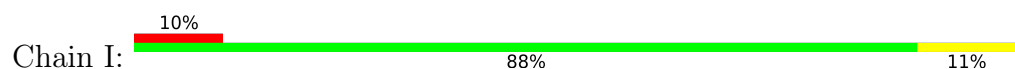
• Molecule 4: Histone H2B 1.1



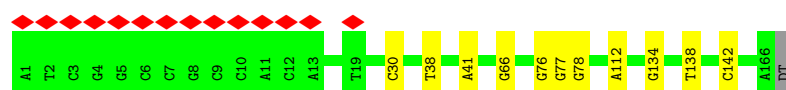
• Molecule 4: Histone H2B 1.1



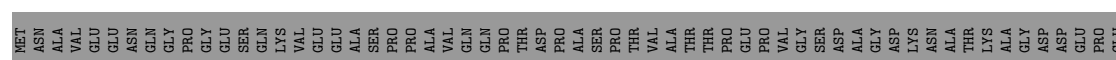
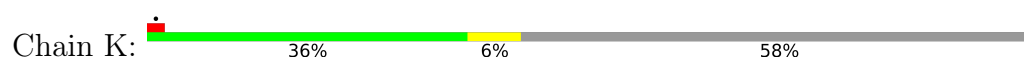
• Molecule 5: DNA (167-MER)



• Molecule 6: DNA (167-MER)

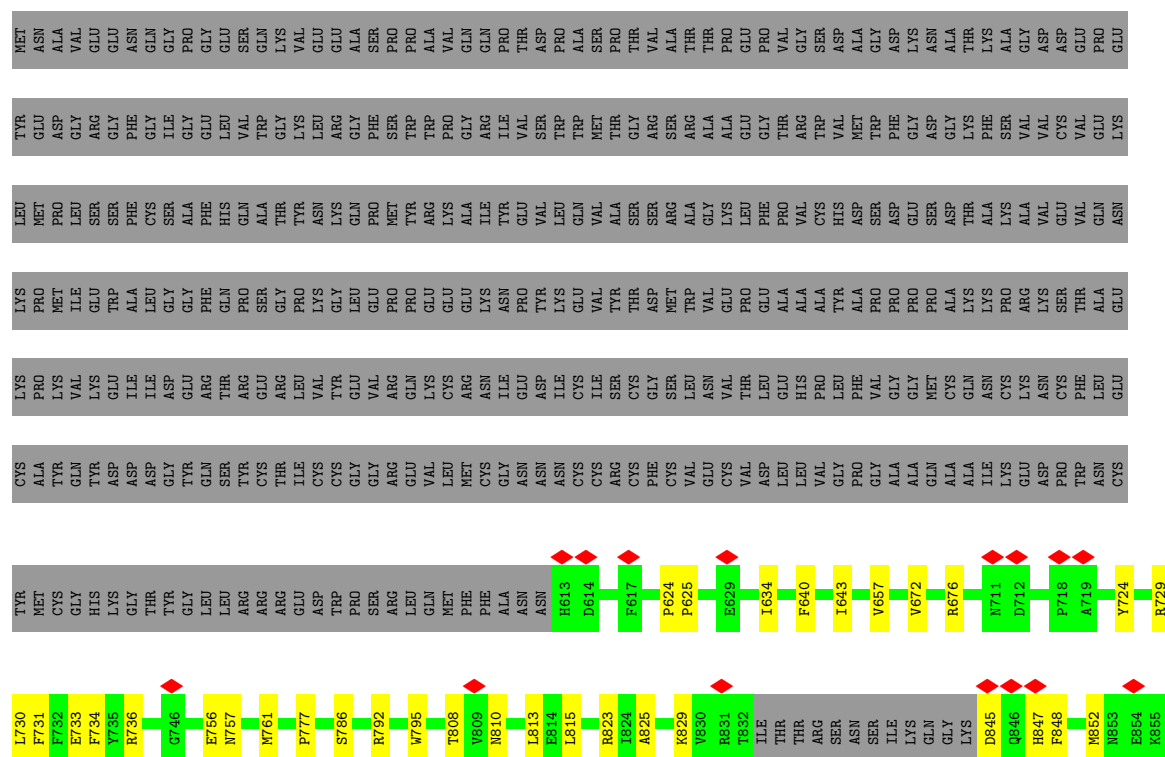
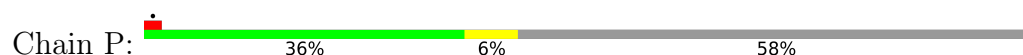


• Molecule 7: DNA (cytosine-5)-methyltransferase 3A



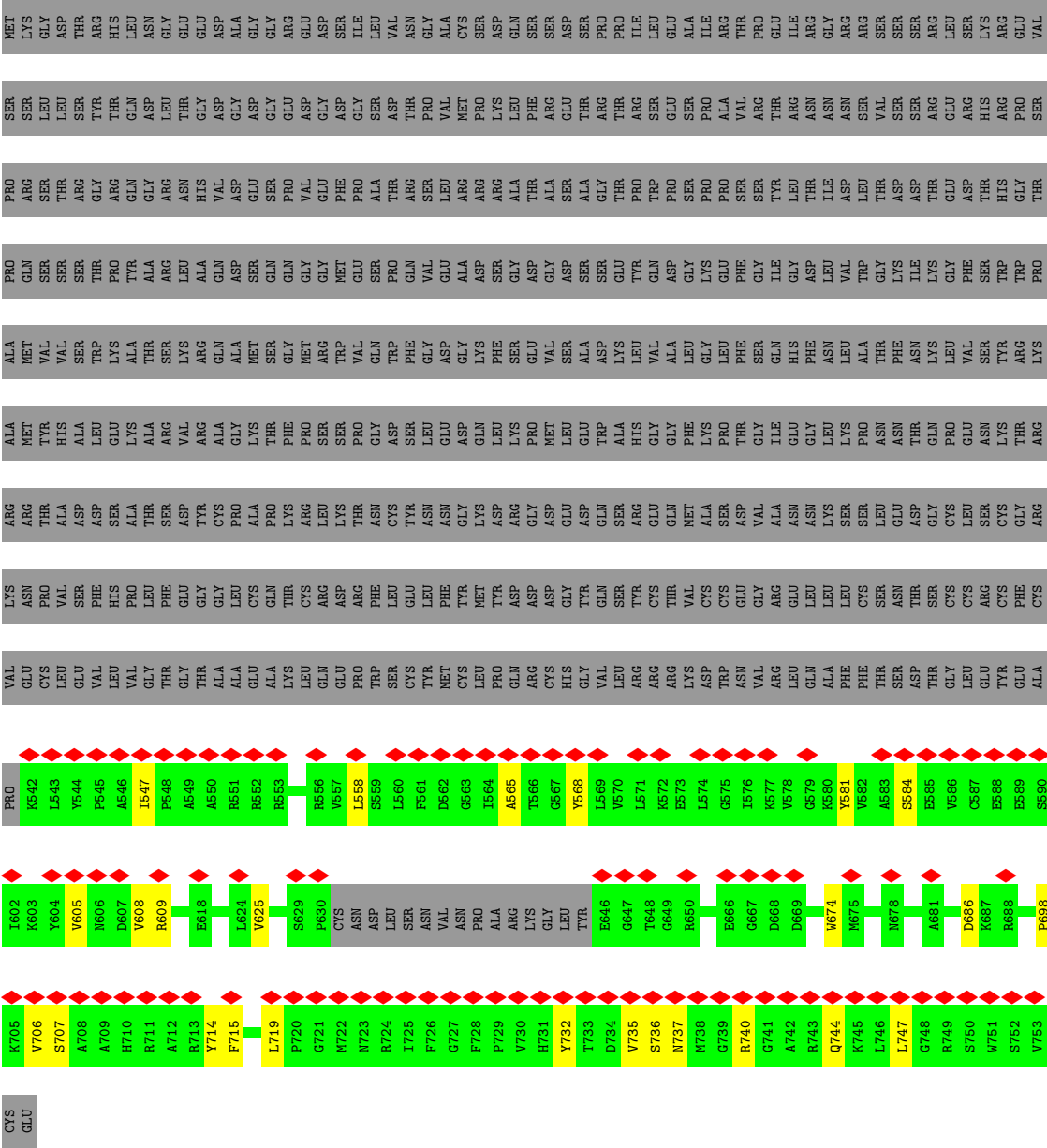


- Molecule 7: DNA (cytosine-5)-methyltransferase 3A

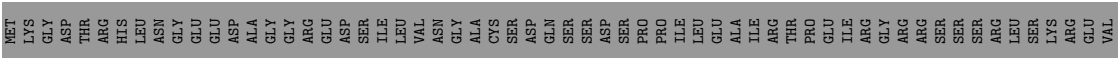




• Molecule 8: DNA (cytosine-5)-methyltransferase 3B



• Molecule 8: DNA (cytosine-5)-methyltransferase 3B



L759	ALA	ARG	PRO	VAL	LYS	ARG	ALA	ALA	LYS	ALA	LYS	ALA	ALA	PRO	GLN	PRO	SER
F760	GLU	GLY	K542	GLU	ASN	ARG	THR	THR	THR	THR	THR	THR	THR	THR	GLN	THR	ARG
F767	GLU	TYR	L543	CYS	VAL	ALA	ALA	ALA	VAL	VAL	VAL	VAL	VAL	VAL	SER	SER	LEU
F787	GLU	TYR	Y544	GLU	PHE	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	THR	GLY	THR
F788	GLU	LEU	P545	VAL	PRO	SER	SER	SER	PHE	PRO	PRO	PRO	PRO	PRO	ARG	ARG	THR
F789	GLU	VAL	A546	VAL	HIS	ASP	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	TYR	GLN	ASP
F790	GLU	THR	A549	GLY	PHE	THR	THR	THR	THR	THR	THR	THR	THR	THR	ARG	ARG	ASP
F791	GLU	THR	A550	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	LEU	GLY	ASP
F792	GLU	THR	R551	ALA	GLY	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	ASN	HIS	THR
F793	GLU	THR	R552	ALA	GLY	CYS	CYS	CYS	CYS	CYS	CYS	CYS	CYS	CYS	GLN	VAL	ASP
F794	GLU	THR	V557	GLU	CYS	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	SER	ALA	SER
F795	GLU	THR	F561	LYS	THR	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	GLN	SER	GLY
F796	GLU	THR	D562	LYS	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	VAL	VAL	ASP
F797	GLU	THR	G563	GLU	ARG	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	MET	PHE	ASP
F798	GLU	THR	I564	GLU	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	VAL	PRO	GLY
F799	GLU	THR	Y568	THR	PHE	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	GLY	ALA	SER
F800	GLU	THR	V578	THR	GLY	CYS	CYS	CYS	CYS	CYS	CYS	CYS	CYS	CYS	PRO	THR	THR
F801	GLU	THR	Y581	THR	GLY	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	GLY	ALA	SER
F802	GLU	THR	E585	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLY	ALA	SER
F803	GLU	THR	V586	THR	GLY	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	GLY	ALA	SER
F804	GLU	THR	C587	THR	GLY	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	MET	VAL	ARG
F805	GLU	THR	E588	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	SER	ALA	THR
F806	GLU	THR	V589	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	SER	GLY	ARG
F807	GLU	THR	S590	THR	THR	SER	SER	SER	SER	SER	SER	SER	SER	SER	GLY	THR	THR
F808	GLU	THR	I591	THR	THR	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	LEU	ALA	PHE
F809	GLU	THR	A592	THR	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	VAL	THR	THR
F810	GLU	THR	V593	THR	THR	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	GLY	ALA	ARG
F811	GLU	THR	R711	THR	CYS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	GLY	ALA	THR
F812	GLU	THR	G594	THR	CYS	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	GLY	ALA	THR
F813	GLU	THR	T595	THR	GLY	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	GLY	ALA	THR
F814	GLU	THR	Y596	THR	GLY	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	GLY	ALA	THR
F815	GLU	THR	K597	THR	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ILE	TYR	THR
F816	GLU	THR	H598	THR	GLU	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLY	LEU	ARG
F817	GLU	THR	E599	THR	LEU	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ILE	ASN	ASN
F818	GLU	THR	G600	THR	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	VAL	ASN	ASN
F819	GLU	THR	N606	THR	CYS	SER	SER	SER	SER	SER	SER	SER	SER	SER	TRP	GLY	VAL
F726	GLU	THR	D607	THR	ASN	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	LYS	ASP	SER
G727	GLU	THR	V608	THR	THR	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ILE	ASN	SER
F728	GLU	THR	R609	THR	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LYS	THR	ARG
F729	GLU	THR	V625	THR	CYS	CYS	CYS	CYS	CYS	CYS	CYS	CYS	CYS	CYS	PRO	GLY	GLU
F730	GLU	THR	H731	THR	ARG	SER	SER	SER	SER	SER	SER	SER	SER	SER	VAL	ASP	THR
F731	GLU	THR	P630	THR	PHE	CYS	CYS	CYS	CYS	CYS	CYS	CYS	CYS	CYS	ASN	THR	HIS
D734	GLU	THR	CYS	THR	THR	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	TRP	GLY	PRO
F735	GLU	THR	ASN	THR	THR	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ARG	GLY	SER
F738	GLU	THR	ASP	THR	THR	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	TRP	GLY	PRO
G739	GLU	THR	SER	THR	THR	SER	SER	SER	SER	SER	SER	SER	SER	SER	VAL	GLY	SER
R743	GLU	THR	VAL	THR	THR	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	ASN	GLY	PRO
L751	GLU	THR	ALA	THR	THR	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	PRO	GLY	SER

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	599344	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 ( $e^-/\text{\AA}^2$ )	65	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.094	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	370.44, 370.44, 370.44	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.029, 1.029, 1.029	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.28	0/829	0.47	0/1111
1	E	0.28	0/817	0.45	0/1097
2	B	0.27	0/653	0.48	0/873
2	F	0.28	0/669	0.49	0/894
3	C	0.26	0/834	0.47	0/1127
3	G	0.28	0/859	0.48	0/1161
4	D	0.26	0/742	0.46	0/1000
4	H	0.28	0/763	0.47	0/1025
5	I	0.57	0/3792	0.96	0/5846
6	J	0.54	0/3842	0.93	0/5932
7	K	0.28	0/2394	0.48	0/3238
7	P	0.28	0/2394	0.48	0/3238
8	N	0.29	0/1749	0.51	0/2361
8	S	0.27	0/1749	0.52	0/2361
All	All	0.39	0/22086	0.70	0/31264

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	817	0	858	14	0
1	E	805	0	842	15	0
2	B	646	0	687	8	0
2	F	662	0	709	3	0
3	C	824	0	873	13	0
3	G	849	0	900	13	0
4	D	731	0	749	14	0
4	H	752	0	775	8	0
5	I	3385	0	1862	19	0
6	J	3421	0	1859	10	0
7	K	2333	0	2310	23	0
7	P	2333	0	2310	22	0
8	N	1703	0	1710	18	0
8	S	1703	0	1710	10	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
9	H	1	0	0	0	0
10	K	26	0	19	1	0
10	P	26	0	19	1	0
All	All	21019	0	18192	141	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 4.

The worst 5 of 141 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)
8:S:698:PRO:HA	8:S:715:PHE:O	1.93	0.68
7:K:729:ARG:NH1	8:N:686:ASP:OD1	2.32	0.62
7:K:676:ARG:NH2	7:K:873:HIS:O	2.34	0.61
7:K:730:LEU:O	7:K:733:GLU:HB2	2.02	0.60
7:P:676:ARG:NH2	7:P:873:HIS:O	2.34	0.60

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	97/135 (72%)	97 (100%)	0	0	100	100
1	E	96/135 (71%)	96 (100%)	0	0	100	100
2	B	79/103 (77%)	78 (99%)	1 (1%)	0	100	100
2	F	81/103 (79%)	80 (99%)	1 (1%)	0	100	100
3	C	106/129 (82%)	104 (98%)	2 (2%)	0	100	100
3	G	109/129 (84%)	108 (99%)	1 (1%)	0	100	100
4	D	92/123 (75%)	91 (99%)	1 (1%)	0	100	100
4	H	94/123 (76%)	92 (98%)	2 (2%)	0	100	100
7	K	284/689 (41%)	275 (97%)	9 (3%)	0	100	100
7	P	284/689 (41%)	275 (97%)	9 (3%)	0	100	100
8	N	207/770 (27%)	194 (94%)	13 (6%)	0	100	100
8	S	207/770 (27%)	193 (93%)	14 (7%)	0	100	100
All	All	1736/3898 (44%)	1683 (97%)	53 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	86/110 (78%)	86 (100%)	0	100	100
1	E	85/110 (77%)	85 (100%)	0	100	100
2	B	66/79 (84%)	66 (100%)	0	100	100
2	F	68/79 (86%)	68 (100%)	0	100	100
3	C	83/101 (82%)	83 (100%)	0	100	100
3	G	86/101 (85%)	86 (100%)	0	100	100
4	D	79/103 (77%)	79 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	81/103 (79%)	81 (100%)	0	100	100
7	K	254/591 (43%)	254 (100%)	0	100	100
7	P	254/591 (43%)	254 (100%)	0	100	100
8	N	179/657 (27%)	179 (100%)	0	100	100
8	S	179/657 (27%)	179 (100%)	0	100	100
All	All	1500/3282 (46%)	1500 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
8	N	731	HIS
7	K	717	ASN
1	E	108	ASN
1	E	68	GLN
3	G	24	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond



length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	SAH	P	1001	-	24,28,28	1.60	8 (33%)	25,40,40	1.75	3 (12%)
10	SAH	K	1001	-	24,28,28	1.60	7 (29%)	25,40,40	1.76	3 (12%)

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
10	SAH	P	1001	-	-	6/11/31/31	0/3/3/3
10	SAH	K	1001	-	-	6/11/31/31	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	P	1001	SAH	C4-N3	-3.30	1.31	1.35
10	K	1001	SAH	C4-N3	-3.22	1.31	1.35
10	P	1001	SAH	C5-C4	-2.83	1.33	1.40
10	K	1001	SAH	C5-C4	-2.81	1.33	1.40
10	K	1001	SAH	C6-N6	2.80	1.44	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	1001	SAH	N3-C2-N1	-6.02	119.27	128.68
10	P	1001	SAH	N3-C2-N1	-5.99	119.32	128.68
10	P	1001	SAH	C5'-SD-CG	2.43	109.55	102.27
10	K	1001	SAH	C5'-SD-CG	2.41	109.49	102.27
10	P	1001	SAH	C3'-C2'-C1'	2.14	104.21	100.98

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	K	1001	SAH	N-CA-CB-CG
10	K	1001	SAH	O-C-CA-N
10	P	1001	SAH	N-CA-CB-CG

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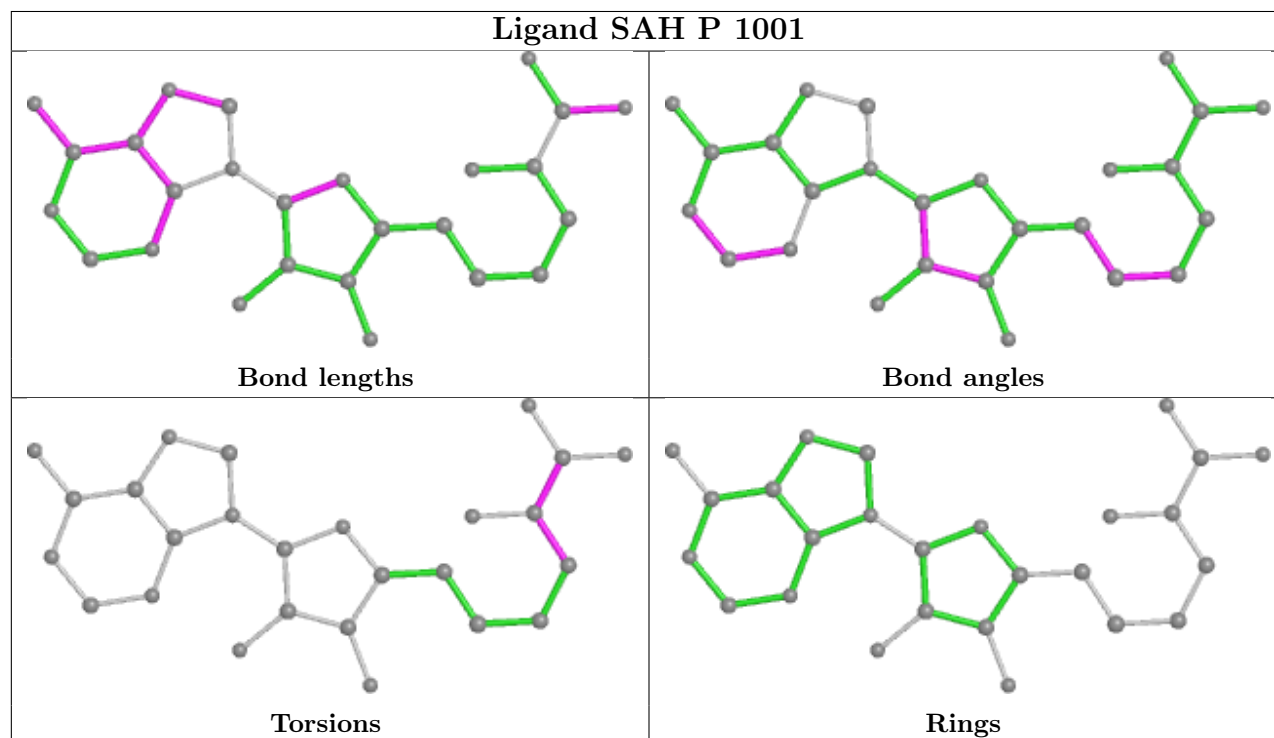
Mol	Chain	Res	Type	Atoms
10	P	1001	SAH	O-C-CA-N
10	K	1001	SAH	OXT-C-CA-N

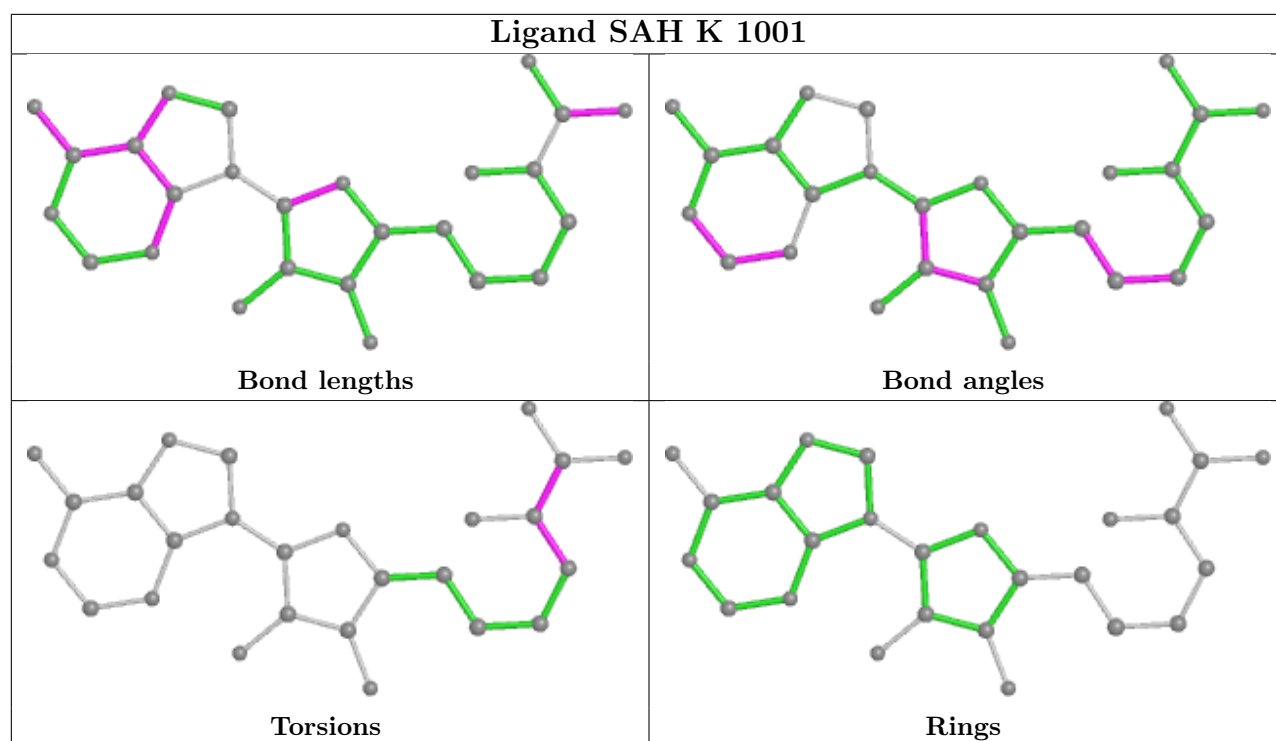
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	P	1001	SAH	1	0
10	K	1001	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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

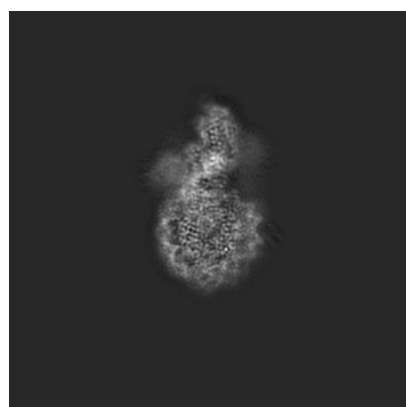
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20281. These allow visual inspection of the internal detail of the map and identification of artifacts.

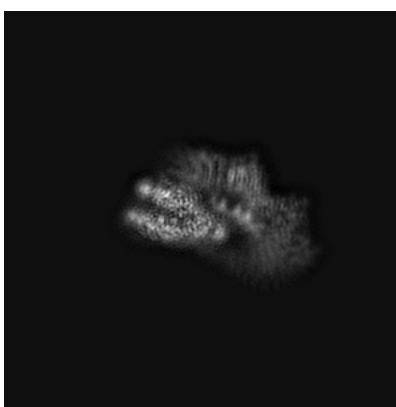
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

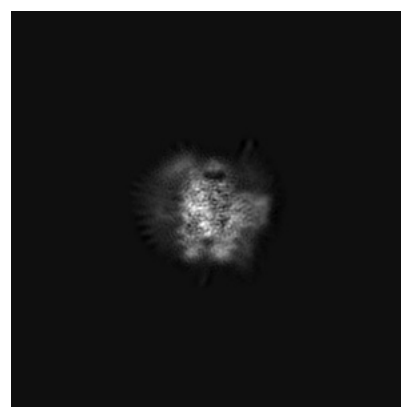
#### 6.1.1 Primary map



X



Y

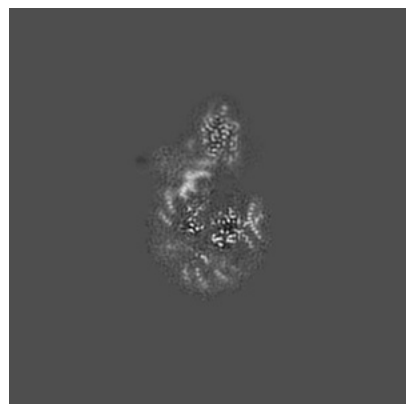


Z

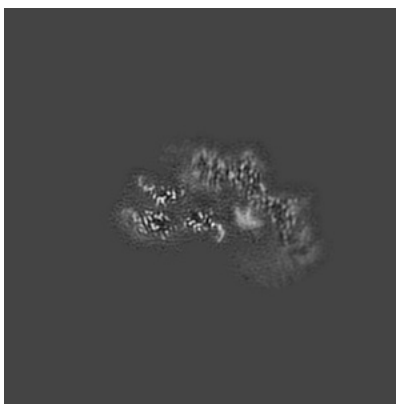
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

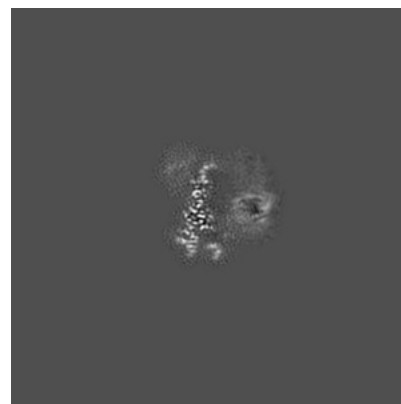
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

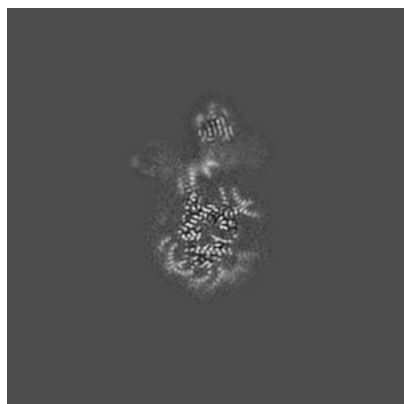


Z Index: 180

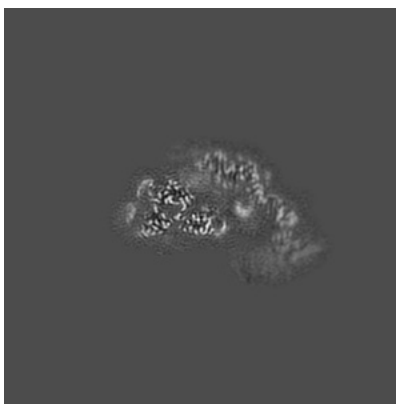
The images above show central slices of the map in three orthogonal directions.

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

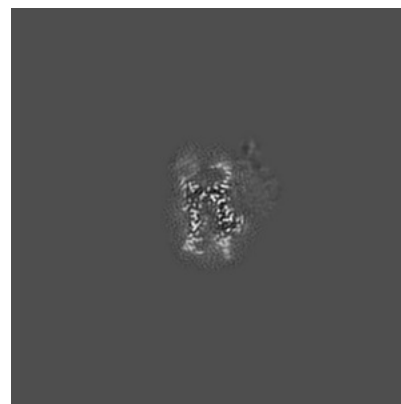
### 6.3.1 Primary map



X Index: 171



Y Index: 173



Z Index: 147

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 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

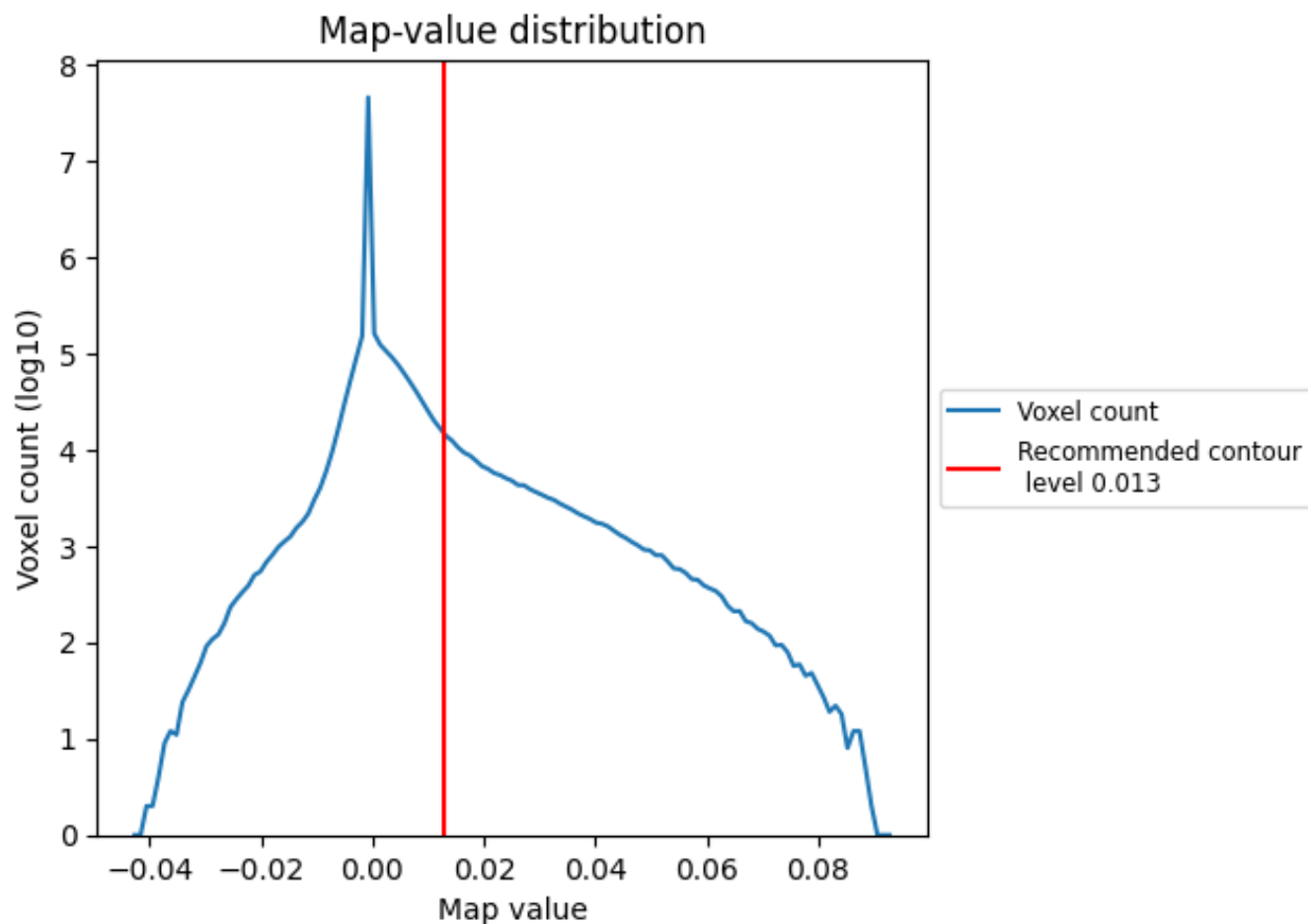
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

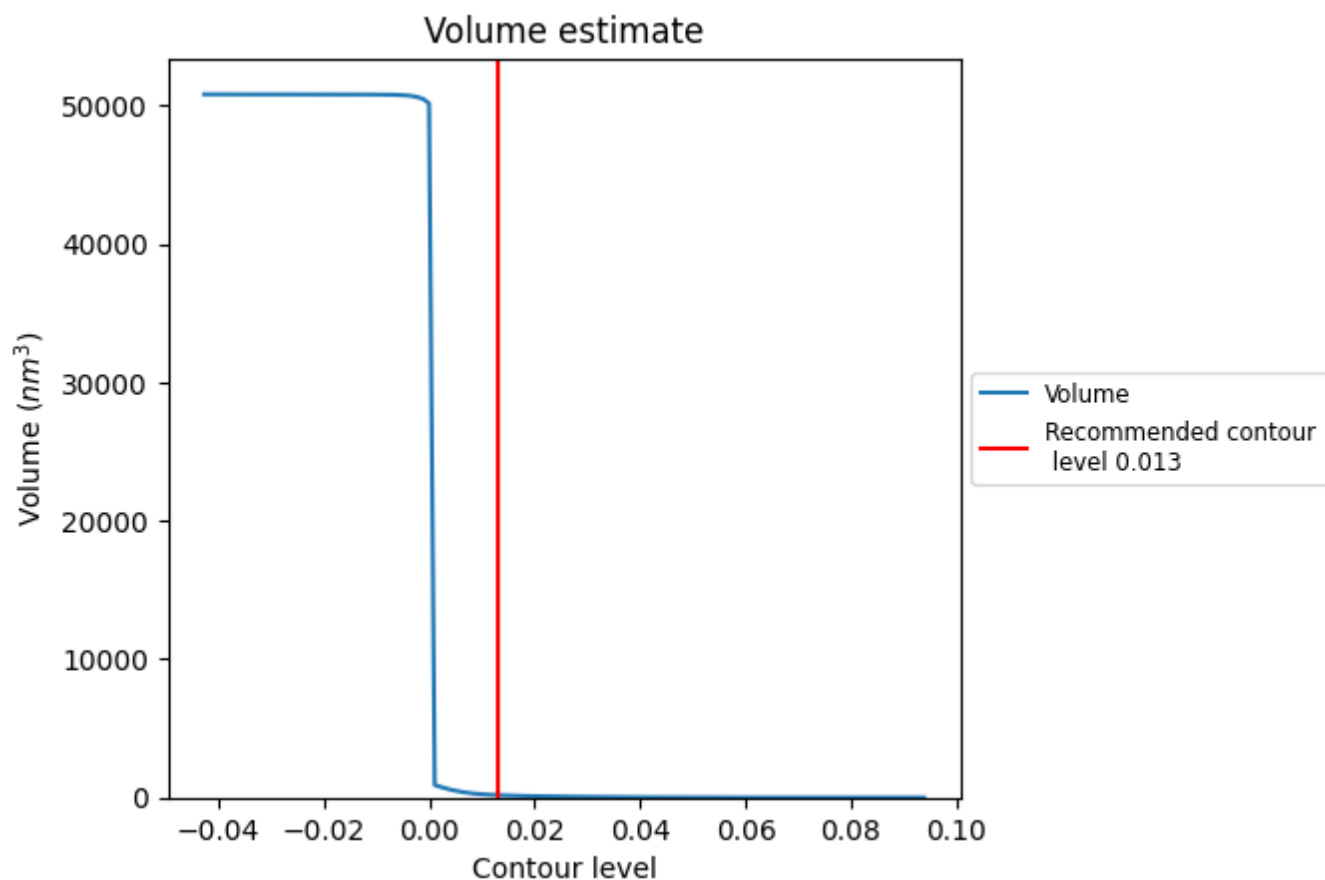
This section contains the results of statistical analysis of the map.

### 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](#)

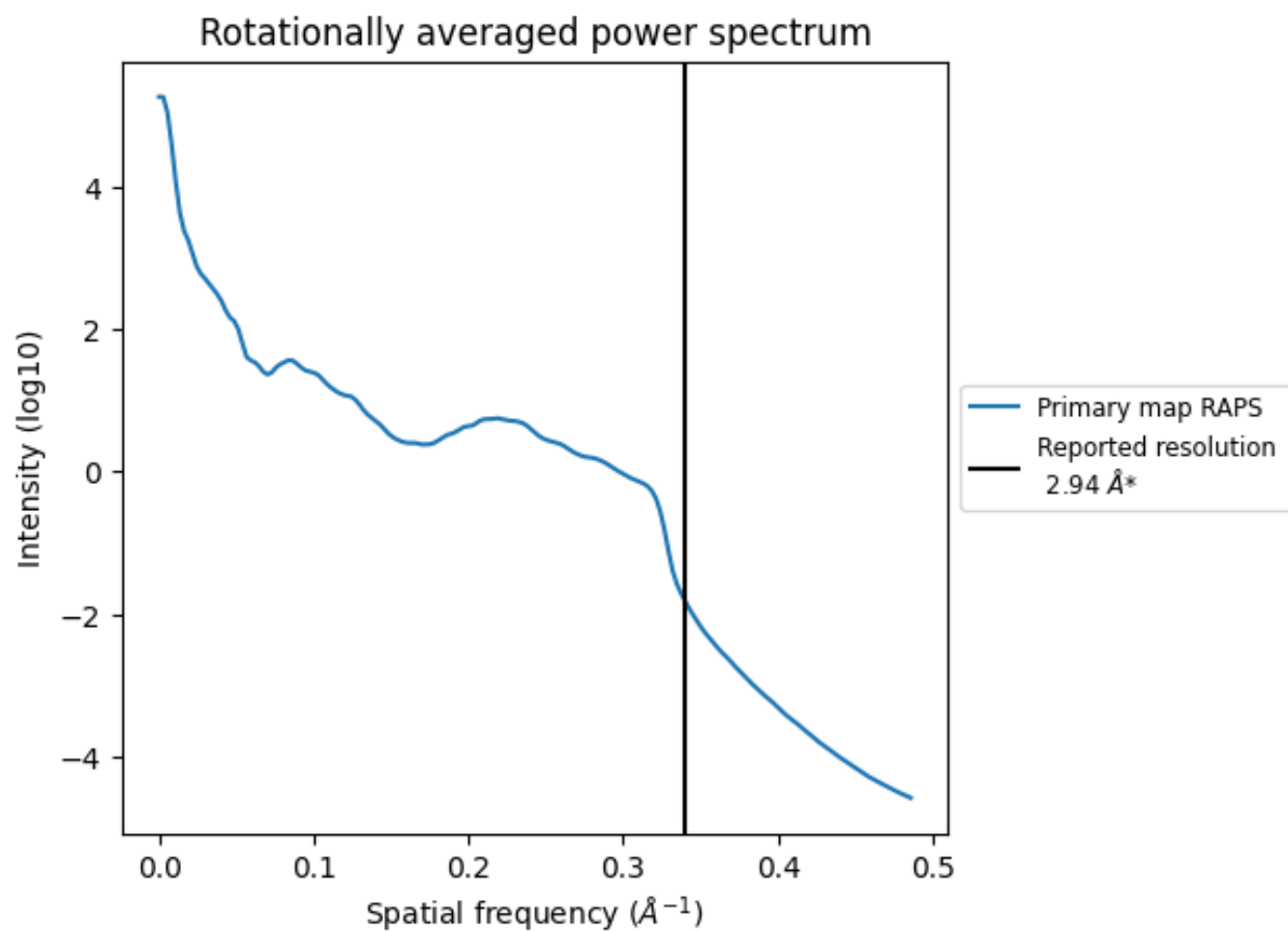


The volume at the recommended contour level is 175 nm<sup>3</sup>; this corresponds to an approximate mass of 158 kDa.

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 0.340 Å<sup>-1</sup>

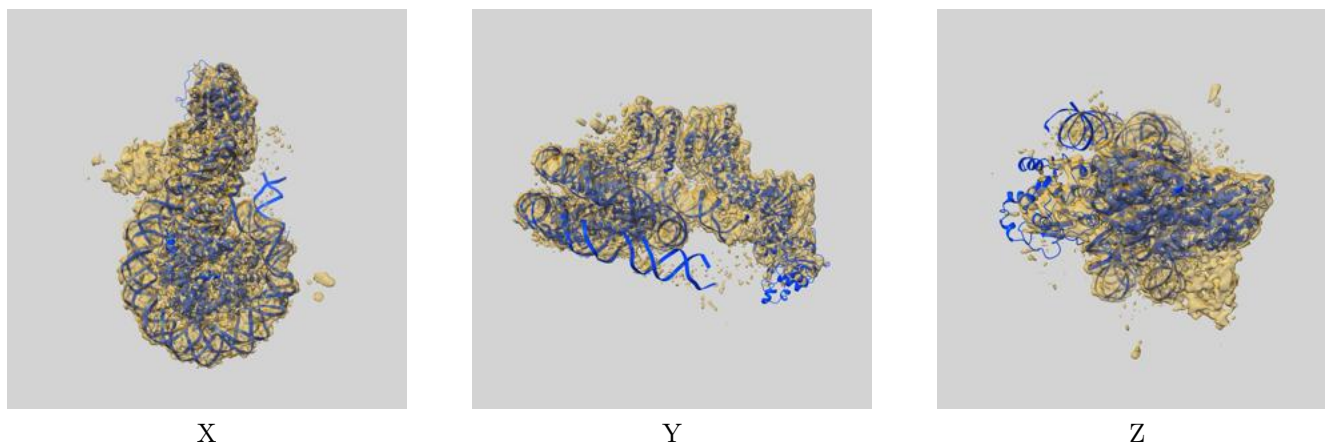
## 8 Fourier-Shell correlation

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

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

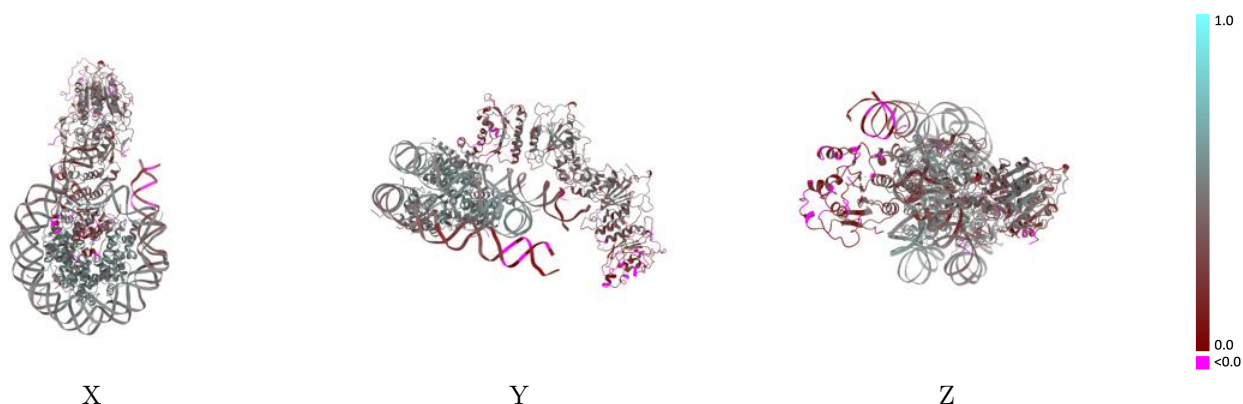
This section contains information regarding the fit between EMDB map EMD-20281 and PDB model 6PA7. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



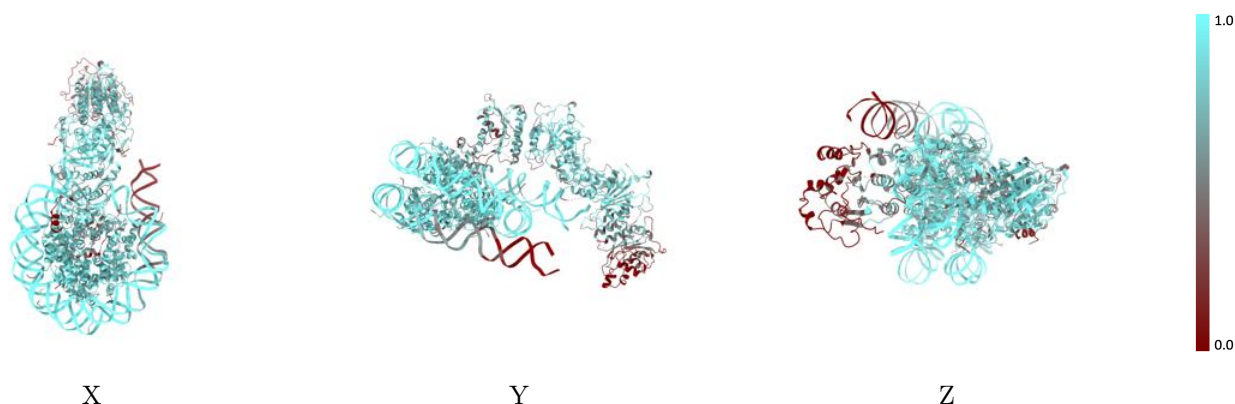
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



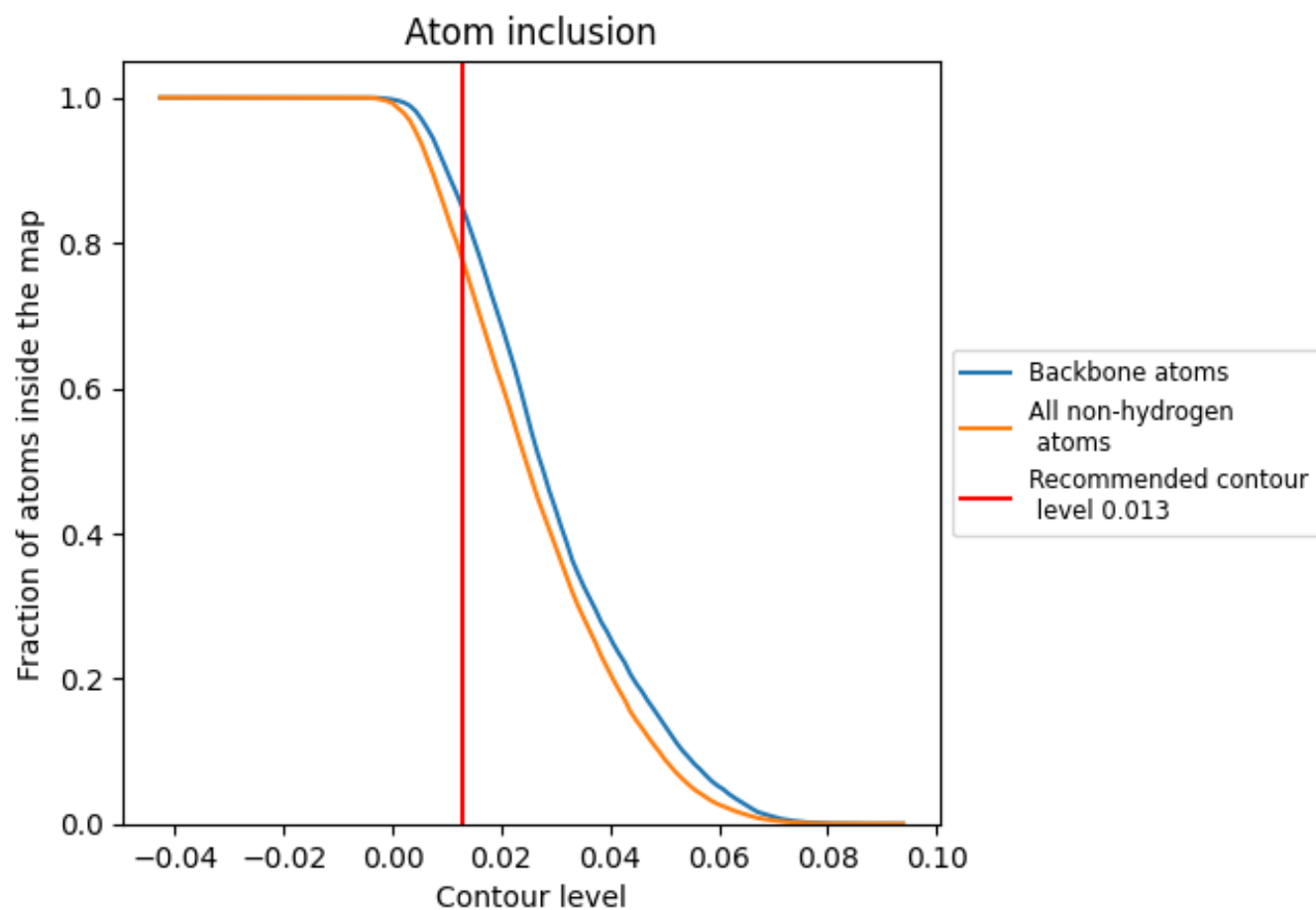
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7727	<div></div> 0.4030
A	<div></div> 0.8844	<div></div> 0.5040
B	<div></div> 0.9161	<div></div> 0.5310
C	<div></div> 0.8325	<div></div> 0.4910
D	<div></div> 0.8683	<div></div> 0.5030
E	<div></div> 0.8260	<div></div> 0.4980
F	<div></div> 0.8789	<div></div> 0.5270
G	<div></div> 0.8467	<div></div> 0.5050
H	<div></div> 0.8597	<div></div> 0.4960
I	<div></div> 0.8576	<div></div> 0.4190
J	<div></div> 0.8576	<div></div> 0.4120
K	<div></div> 0.7487	<div></div> 0.3820
N	<div></div> 0.3092	<div></div> 0.1890
P	<div></div> 0.7809	<div></div> 0.3910
S	<div></div> 0.5918	<div></div> 0.2460

