



## wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 02:25 AM UTC

PDB ID : 9Y4P / pdb\_00009y4p  
EMDB ID : EMD-72487  
Title : Cryo-EM structure of DNMT3A2/3B3 in complex with H3K36me2 di-nucleosome with eight base pair linker  
Authors : Xie, X.; Zhou, X.E.; Worden, E.J.; Jones, P.A.  
Deposited on : 2025-09-03  
Resolution : 3.84 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:

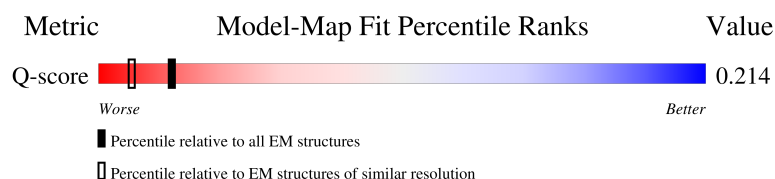
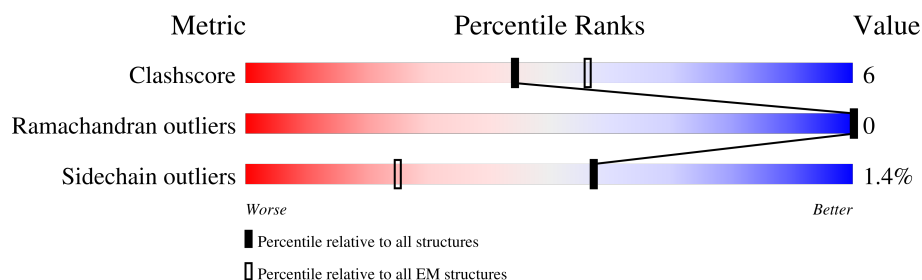
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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 3.84 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.









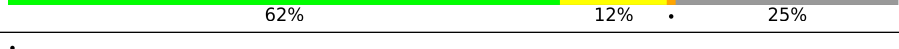
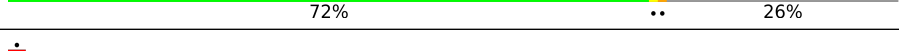
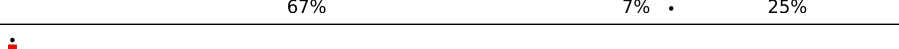
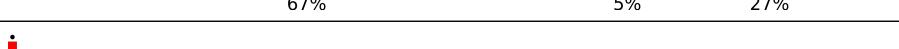
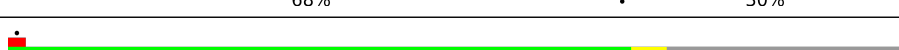

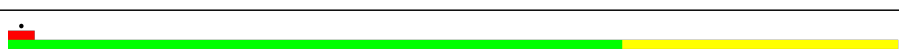


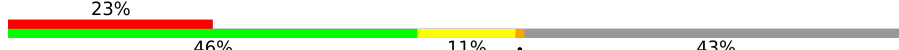




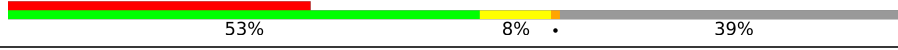

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9033 ( 3.34 - 4.34 )

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	
2	B	103	
2	F	103	
2	R	103	

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Mol	Chain	Length	Quality of chain
2	X	103	
3	C	129	
3	G	129	
3	S	129	
3	Y	129	
4	D	123	
4	H	123	
4	P	123	
4	T	123	
5	E	135	
5	Q	135	
5	W	135	
6	I	321	
7	J	321	
8	Z	580	
8	b	580	
8	e	580	
8	g	580	
9	a	689	
9	c	689	
9	d	689	
9	f	689	

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 91798 atoms, of which 42922 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.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	99	Total	C	H	N	O	S	0	0
			1692	520	870	159	140	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	80	Total	C	H	N	O	S	0	0
			1325	405	684	125	110	1		
2	F	78	Total	C	H	N	O	S	0	0
			1282	393	660	120	108	1		
2	X	78	Total	C	H	N	O	S	0	0
			1282	393	660	120	108	1		
2	R	79	Total	C	H	N	O	S	0	0
			1306	399	673	124	109	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	102	Total	C	H	N	O	0	0
			1618	493	833	154	138		
3	G	98	Total	C	H	N	O	0	0
			1555	474	800	149	132		
3	Y	98	Total	C	H	N	O	0	0
			1555	474	800	149	132		
3	S	98	Total	C	H	N	O	0	0
			1550	473	798	148	131		

There are 8 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
G	123	SER	ALA	engineered mutation	UNP P06897
Y	99	ARG	GLY	engineered mutation	UNP P06897
Y	123	SER	ALA	engineered mutation	UNP P06897
S	99	ARG	GLY	engineered mutation	UNP P06897
S	123	SER	ALA	engineered mutation	UNP P06897

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	93	Total	C	H	N	O	S	0	0
			1473	457	747	130	137	2		
4	H	92	Total	C	H	N	O	S	0	0
			1459	453	740	129	135	2		
4	P	91	Total	C	H	N	O	S	0	0
			1435	447	727	125	134	2		
4	T	92	Total	C	H	N	O	S	0	0
			1459	453	740	129	135	2		

There are 8 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
P	0	MET	-	initiating methionine	UNP P02281
P	29	THR	SER	engineered mutation	UNP P02281
T	0	MET	-	initiating methionine	UNP P02281
T	29	THR	SER	engineered mutation	UNP P02281

- Molecule 5 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	98	Total	C	H	N	O	S	0	0
			1664	512	853	157	139	3		
5	W	99	Total	C	H	N	O	S	0	0
			1686	518	866	159	140	3		
5	Q	95	Total	C	H	N	O	S	0	0
			1611	495	826	151	136	3		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	102	ALA	GLY	variant	UNP P84233
W	102	ALA	GLY	variant	UNP P84233
Q	102	ALA	GLY	variant	UNP P84233

- Molecule 6 is a DNA chain called DNA (321-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
6	I	321	Total	C	H	N	O	P	0	0
			10209	3127	3598	1244	1920	320		

- Molecule 7 is a DNA chain called DNA (321-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
7	J	321	Total	C	H	N	O	P	0	0
			10148	3106	3601	1190	1930	321		

- Molecule 8 is a protein called Isoform 7 of DNA (cytosine-5)-methyltransferase 3B.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	b	344	Total	C	H	N	O	S	0	0
			5426	1751	2673	481	495	26		
8	Z	176	Total	C	H	N	O	S	0	0
			2866	936	1434	244	246	6		
8	e	330	Total	C	H	N	O	S	0	0
			5201	1673	2564	458	481	25		
8	g	176	Total	C	H	N	O	S	0	0
			2870	938	1436	246	245	5		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	391	LYS	-	insertion	UNP Q9UBC3
b	392	ASP	-	insertion	UNP Q9UBC3
b	393	TYR	-	insertion	UNP Q9UBC3
Z	391	LYS	-	insertion	UNP Q9UBC3
Z	392	ASP	-	insertion	UNP Q9UBC3
Z	393	TYR	-	insertion	UNP Q9UBC3
e	391	LYS	-	insertion	UNP Q9UBC3
e	392	ASP	-	insertion	UNP Q9UBC3
e	393	TYR	-	insertion	UNP Q9UBC3
g	391	LYS	-	insertion	UNP Q9UBC3
g	392	ASP	-	insertion	UNP Q9UBC3
g	393	TYR	-	insertion	UNP Q9UBC3

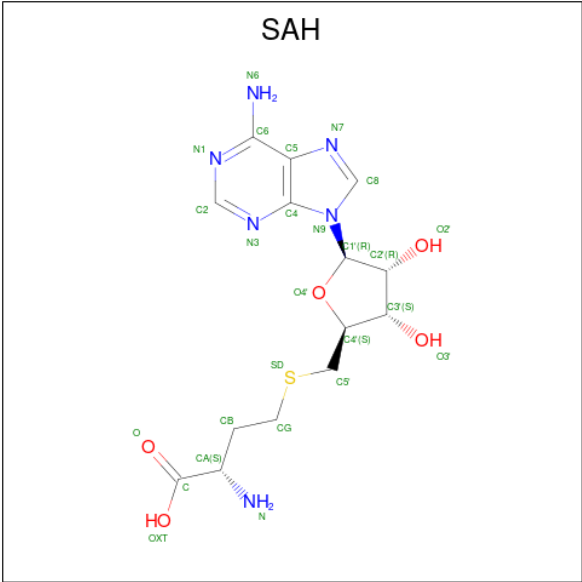
- Molecule 9 is a protein called DNA (cytosine-5)-methyltransferase 3A.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	a	555	Total	C	H	N	O	S	0	0
			8793	2839	4342	784	786	42		
9	c	553	Total	C	H	N	O	S	0	0
			8758	2829	4323	782	782	42		
9	f	423	Total	C	H	N	O	S	0	0
			6714	2154	3314	603	608	35		
9	d	421	Total	C	H	N	O	S	0	0
			6667	2141	3288	598	605	35		

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
10	b	3	Total	Zn	0
			3	3	
10	a	3	Total	Zn	0
			3	3	
10	c	3	Total	Zn	0
			3	3	
10	e	3	Total	Zn	0
			3	3	
10	f	3	Total	Zn	0
			3	3	
10	d	3	Total	Zn	0
			3	3	

- Molecule 11 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: 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).



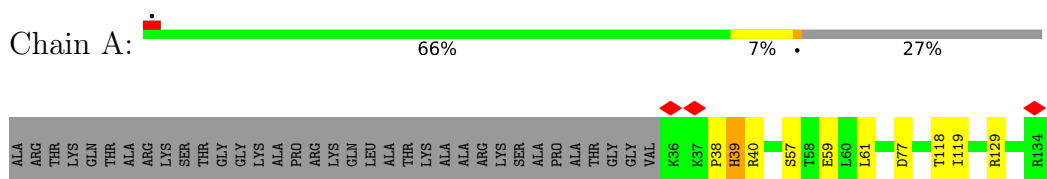
Mol	Chain	Residues	Atoms						AltConf
11	a	1	Total	C	H	N	O	S	0
			44	14	18	6	5	1	
11	c	1	Total	C	H	N	O	S	0
			44	14	18	6	5	1	
11	f	1	Total	C	H	N	O	S	0
			44	14	18	6	5	1	
11	d	1	Total	C	H	N	O	S	0
			44	14	18	6	5	1	



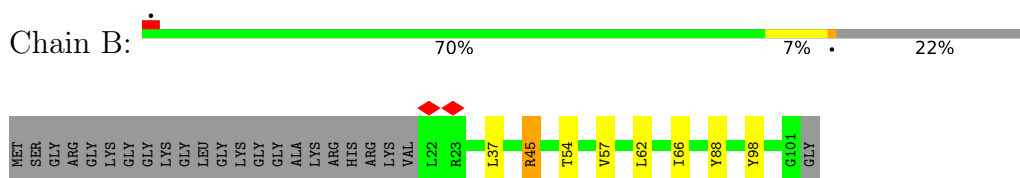
### 3 Residue-property plots [i](#)

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.

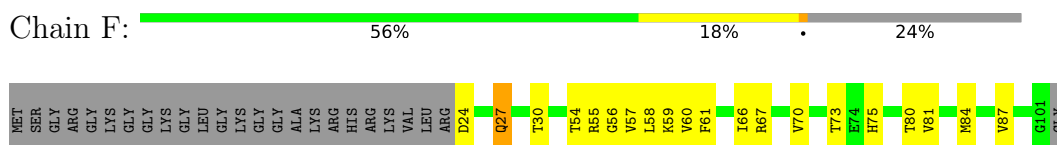
- Molecule 1: Histone H3



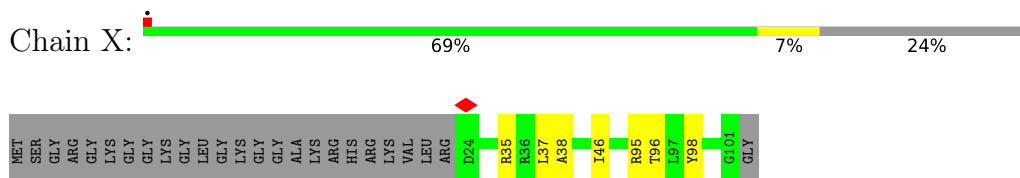
- Molecule 2: Histone H4



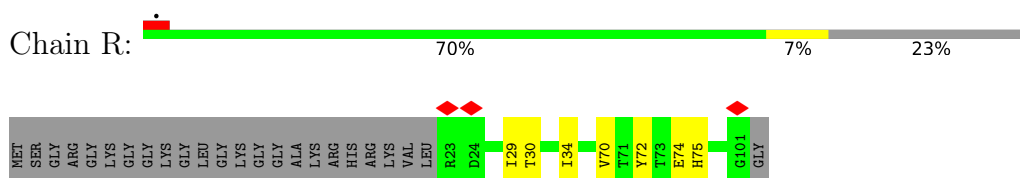
- Molecule 2: Histone H4



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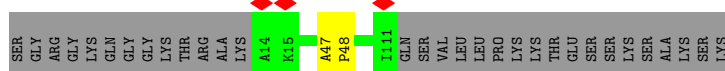
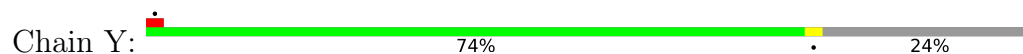
- Molecule 3: Histone H2A type 1



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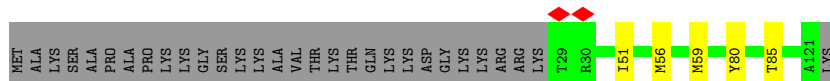
- Molecule 3: Histone H2A type 1



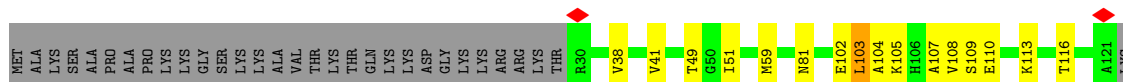
- Molecule 3: Histone H2A type 1



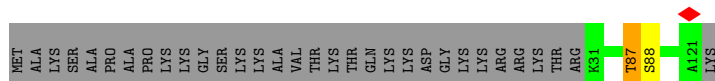
- Molecule 4: Histone H2B 1.1



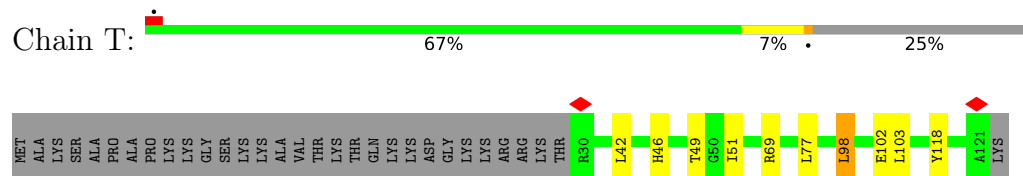
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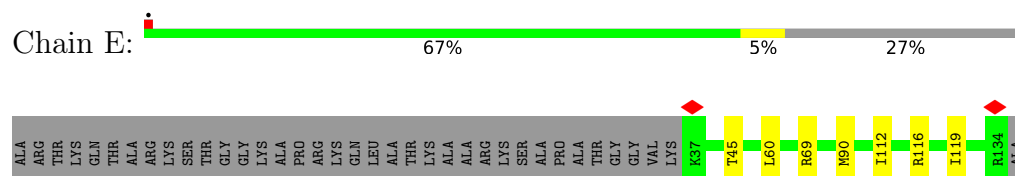
- Molecule 4: Histone H2B 1.1



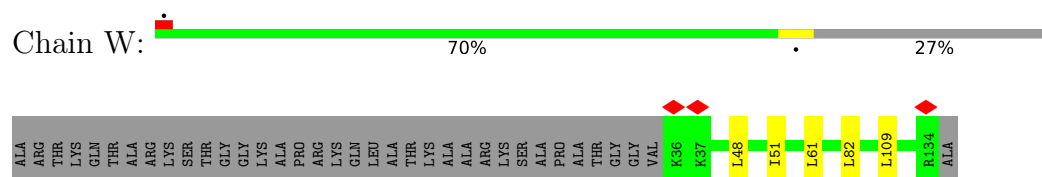
- Molecule 4: Histone H2B 1.1



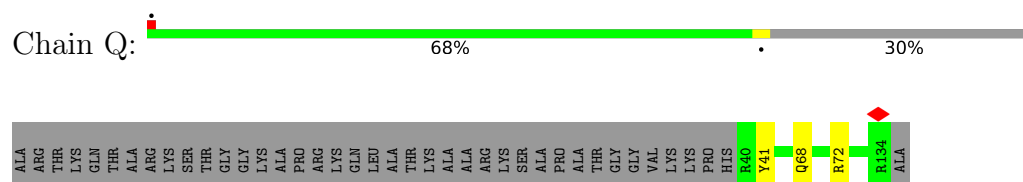
- Molecule 5: Histone H3.2



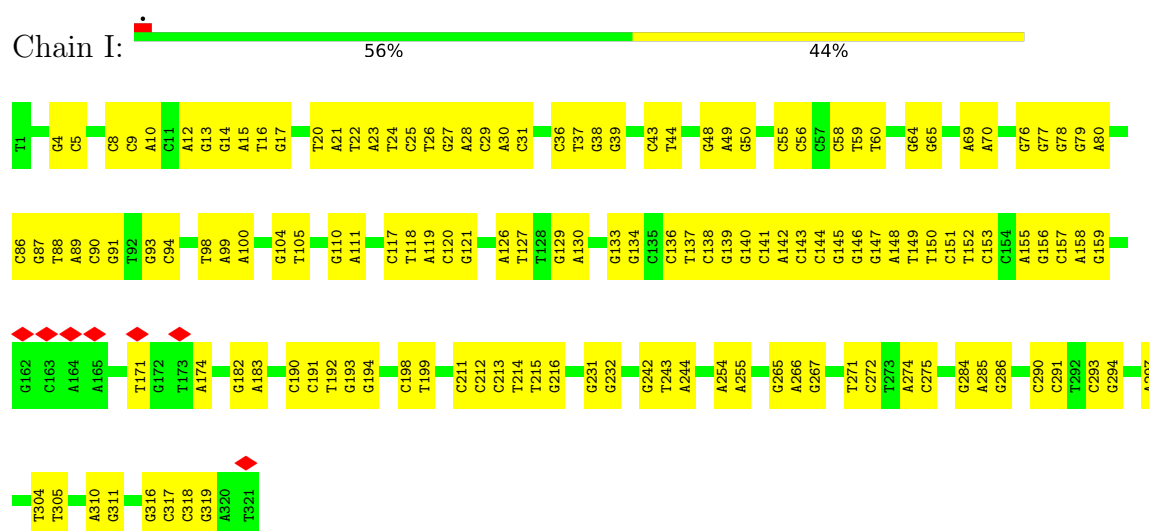
- Molecule 5: Histone H3.2



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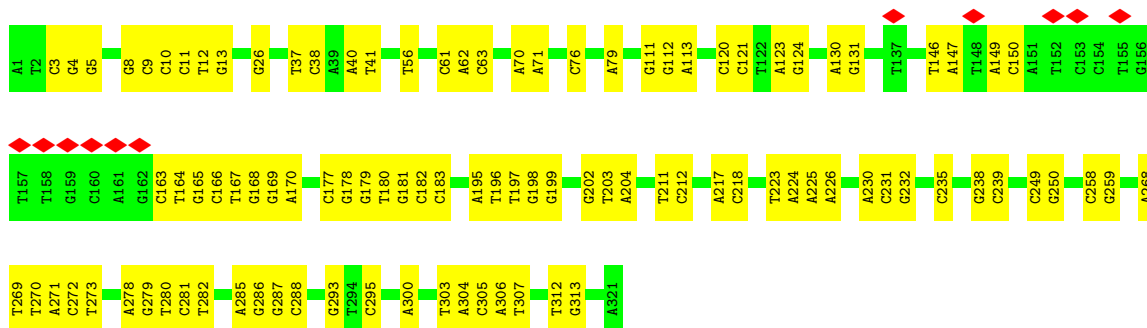


- Molecule 6: DNA (321-MER)

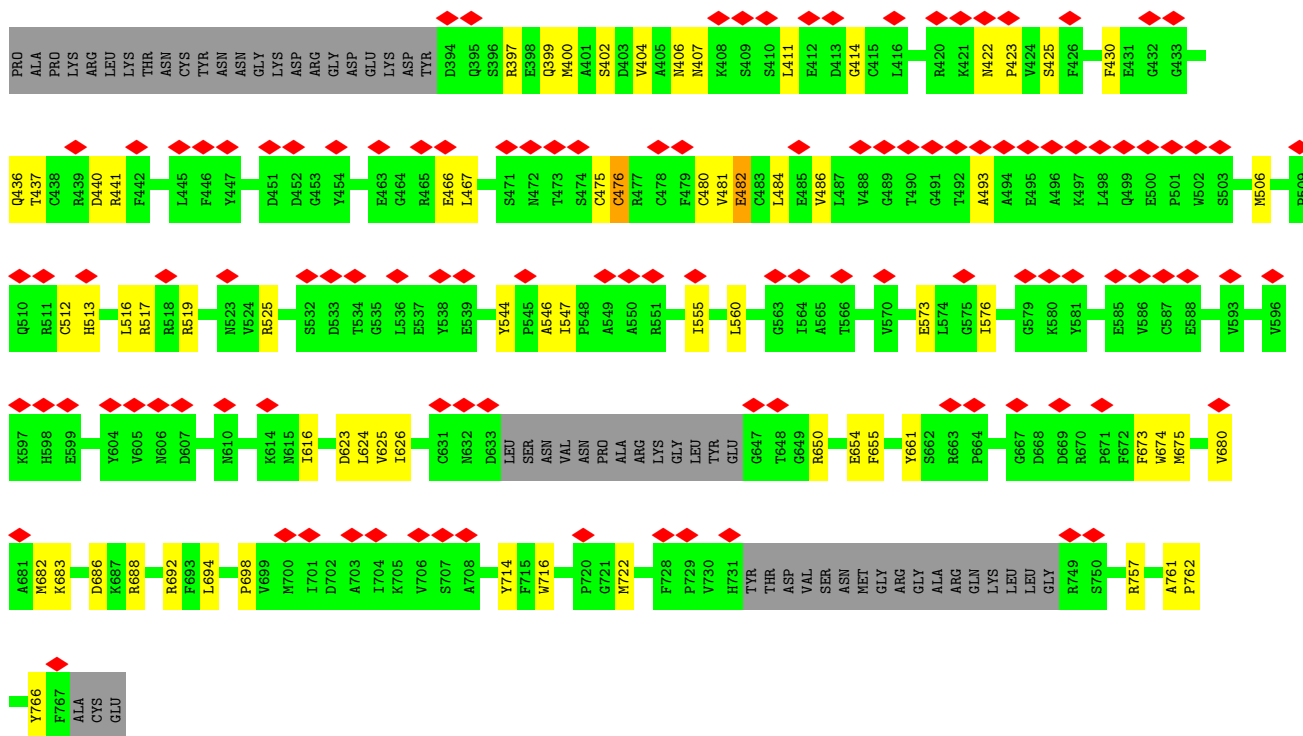
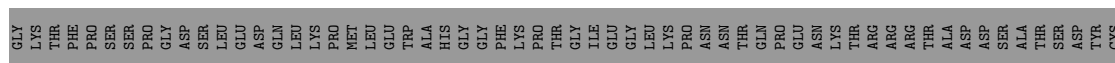
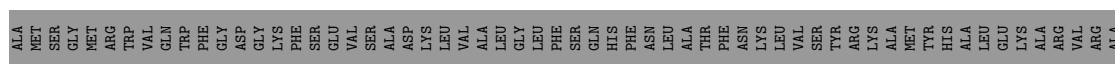
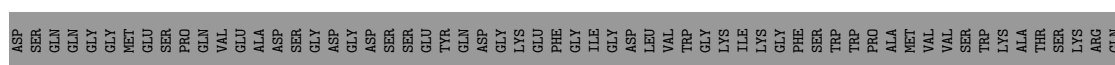


- Molecule 7: DNA (321-MER)

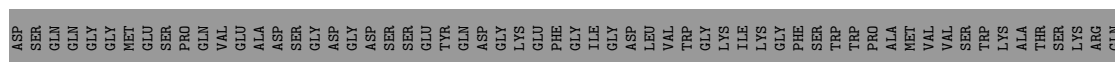


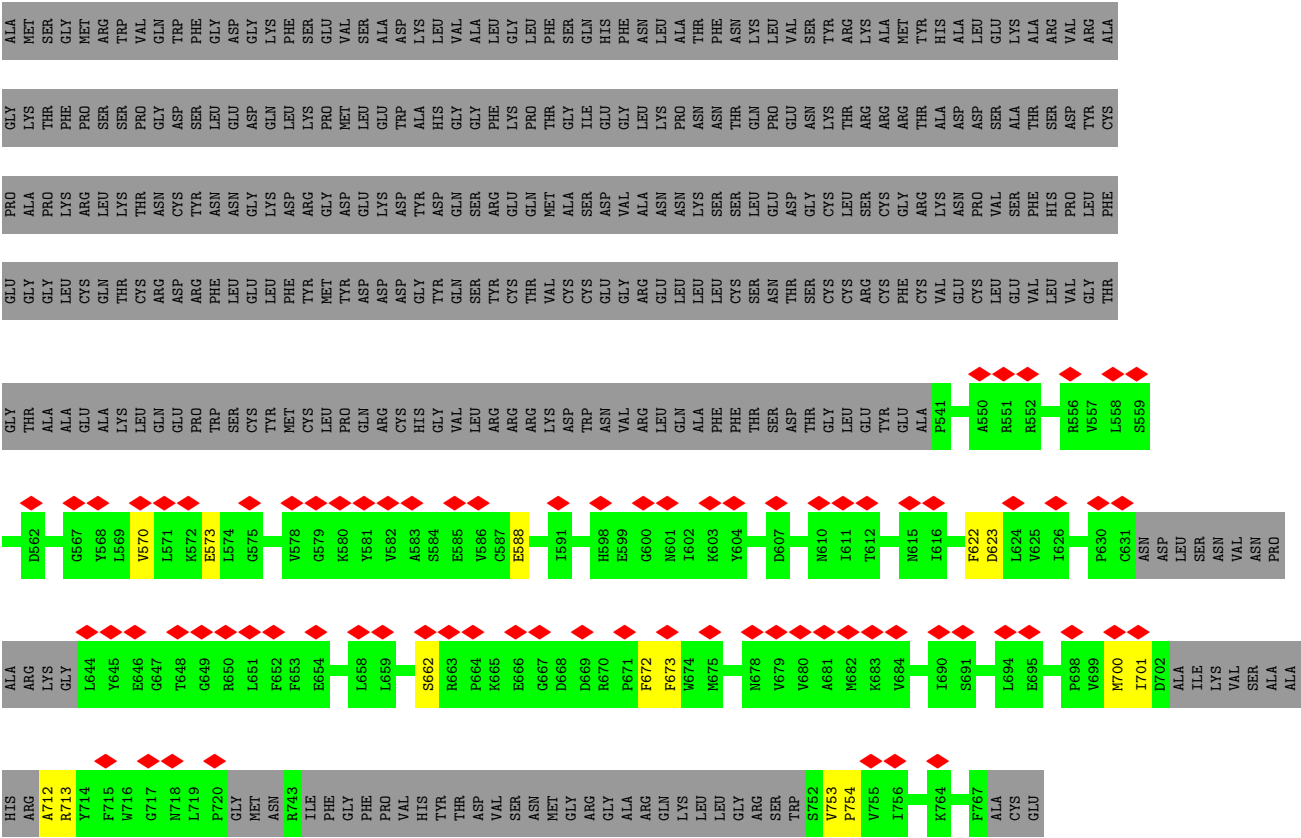


- Molecule 8: Isoform 7 of DNA (cytosine-5)-methyltransferase 3B

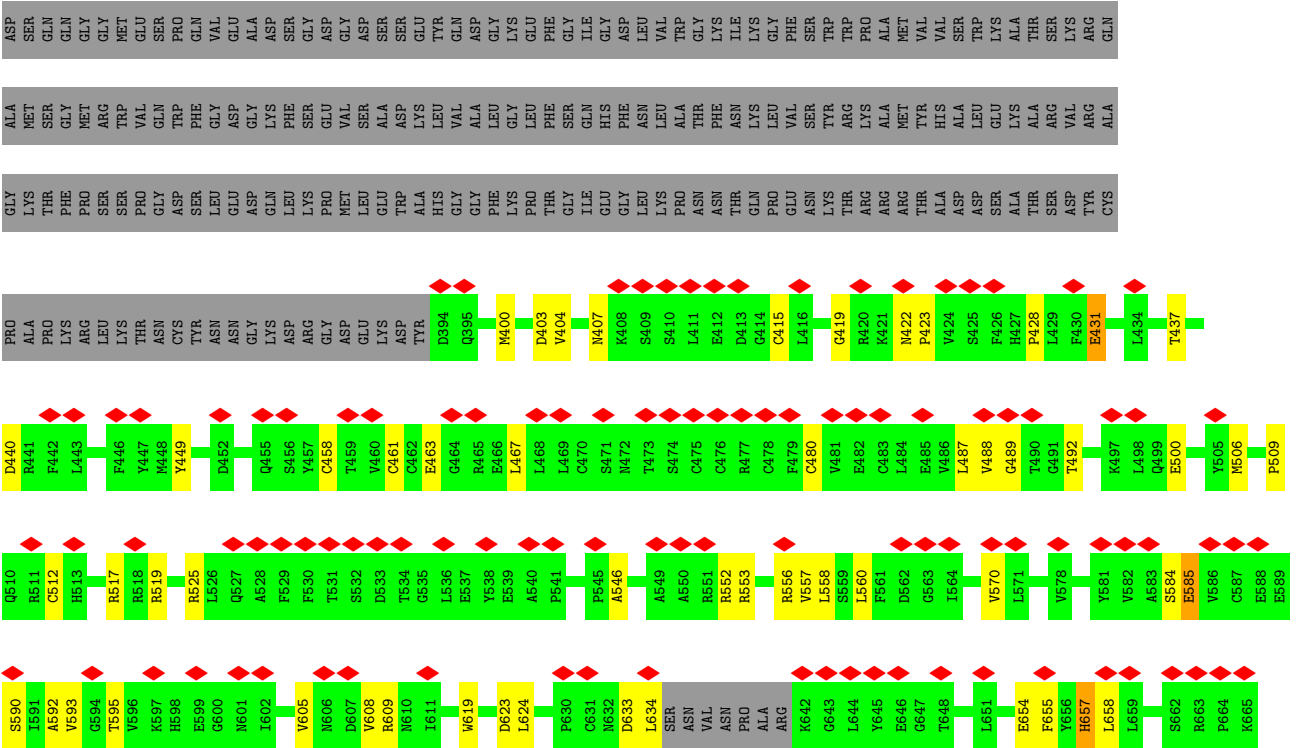


- Molecule 8: Isoform 7 of DNA (cytosine-5)-methyltransferase 3B

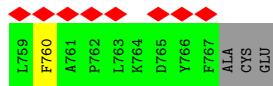
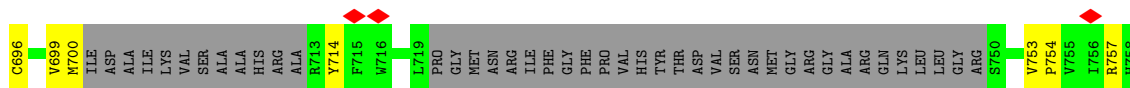
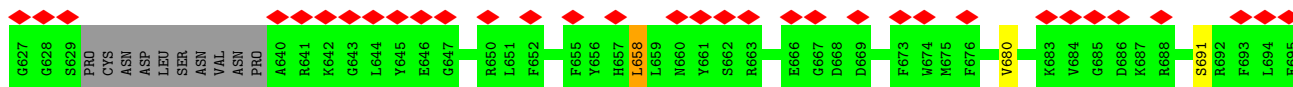
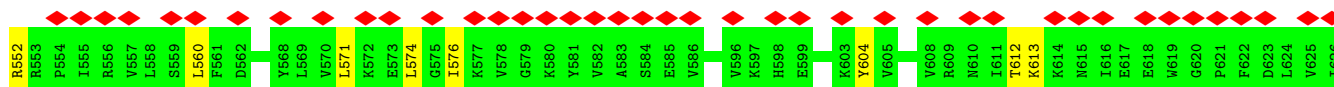
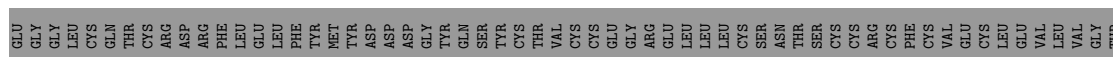
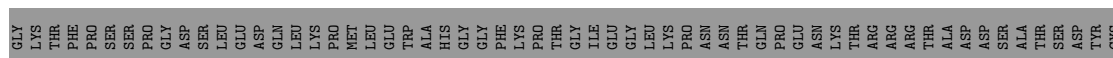
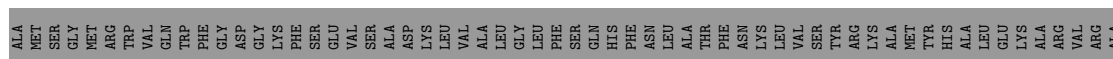
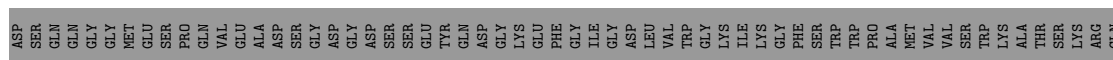




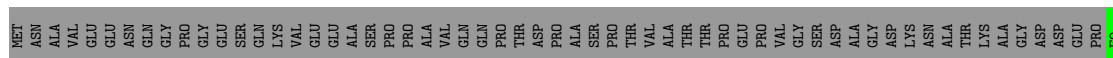
• Molecule 8: Isoform 7 of DNA (cytosine-5)-methyltransferase 3B



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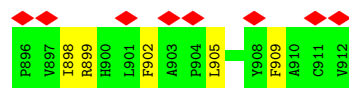
- Molecule 9: DNA (cytosine-5)-methyltransferase 3A



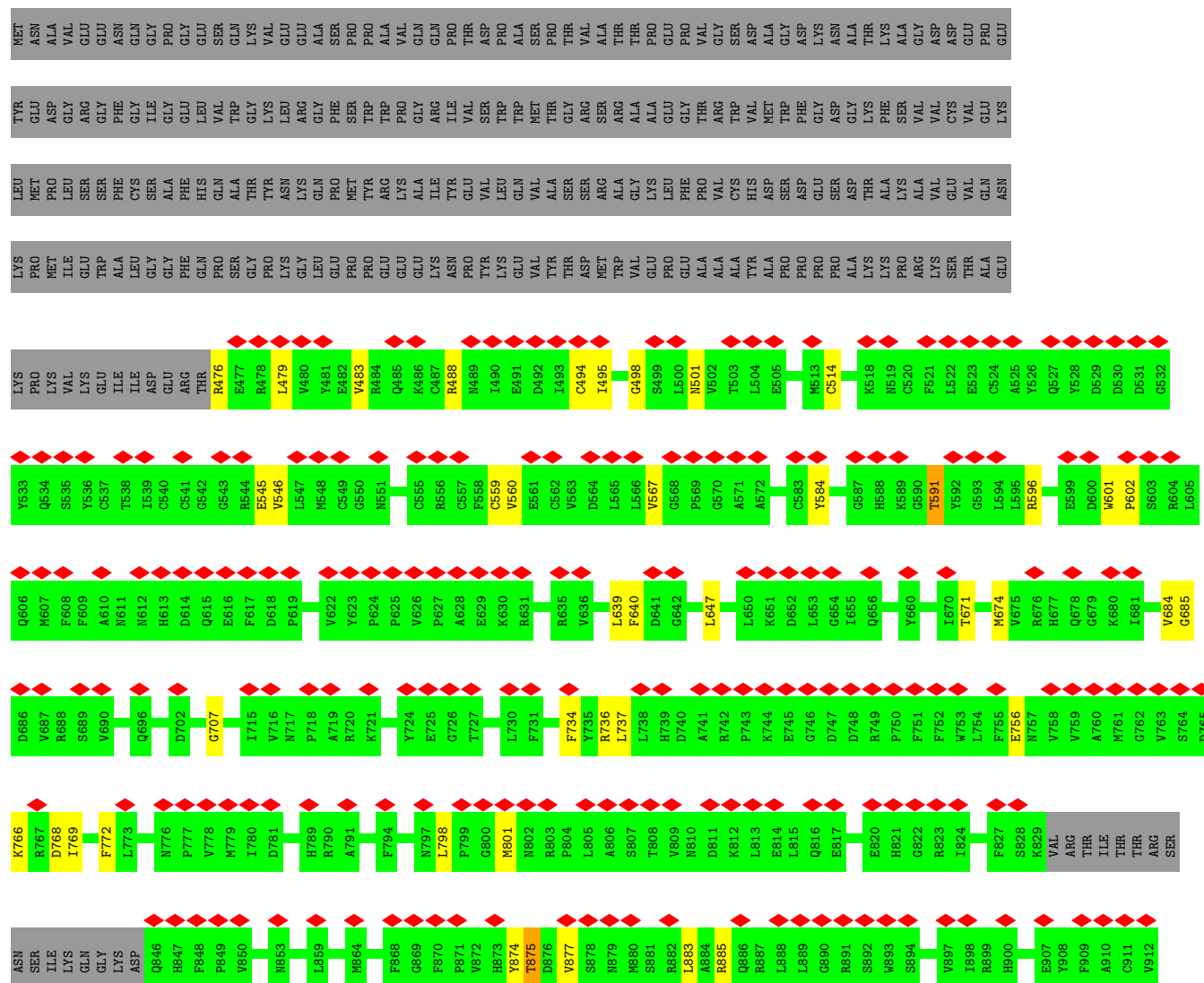








• Molecule 9: DNA (cytosine-5)-methyltransferase 3A



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	176300	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	61	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.796	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.0672	Depositor
Map size ( $\text{\AA}$ )	370.944, 370.944, 370.944	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.828, 0.828, 0.828	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MLY, 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	A	0.62	0/824	0.44	0/1107
2	B	0.65	0/648	0.47	0/868
2	F	0.72	0/629	0.51	0/843
2	R	0.28	0/640	0.30	0/857
2	X	0.27	0/629	0.27	0/843
3	C	0.65	0/794	0.41	0/1072
3	G	0.61	0/764	0.39	0/1031
3	S	0.26	0/761	0.30	0/1027
3	Y	0.25	0/764	0.29	0/1031
4	D	0.67	0/737	0.44	0/993
4	H	0.63	0/730	0.43	0/983
4	P	0.25	0/719	0.26	0/969
4	T	0.27	0/730	0.31	0/983
5	E	0.68	0/823	0.42	0/1104
5	Q	0.25	0/795	0.31	0/1066
5	W	0.25	0/832	0.28	0/1115
6	I	0.45	0/7425	0.50	0/11467
7	J	0.46	0/7336	0.47	0/11312
8	Z	0.14	0/1469	0.26	0/1981
8	b	0.16	0/2821	0.32	0/3810
8	e	0.15	0/2697	0.29	0/3639
8	g	0.12	0/1472	0.26	0/1985
9	a	0.18	0/4570	0.37	1/6176 (0.0%)
9	c	0.15	0/4553	0.29	0/6152
9	d	0.13	0/3462	0.25	0/4678
9	f	0.14	0/3482	0.26	0/4703
All	All	0.36	0/51106	0.38	1/71795 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
9	a	537	CYS	N-CA-C	5.34	117.18	110.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	45	ARG	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	A	822	870	871	10	0
2	B	641	684	684	8	0
2	F	622	660	660	14	0
2	R	633	673	673	6	0
2	X	622	660	660	5	0
3	C	785	833	833	9	0
3	G	755	800	800	5	0
3	S	752	798	796	6	0
3	Y	755	800	800	1	0
4	D	726	747	747	6	0
4	H	719	740	740	11	0
4	P	708	727	727	1	0
4	T	719	740	740	7	0
5	E	811	853	853	6	0
5	Q	785	826	826	2	0
5	W	820	866	866	2	0
6	I	6611	3598	3598	151	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	J	6547	3601	3601	91	0
8	Z	1432	1434	1434	7	0
8	b	2753	2673	2673	49	0
8	e	2637	2564	2564	48	0
8	g	1434	1436	1436	12	0
9	a	4451	4342	4336	54	0
9	c	4435	4323	4323	56	0
9	d	3379	3288	3288	26	0
9	f	3400	3314	3314	37	0
10	a	3	0	0	0	0
10	b	3	0	0	0	0
10	c	3	0	0	0	0
10	d	3	0	0	0	0
10	e	3	0	0	0	0
10	f	3	0	0	0	0
11	a	26	18	19	0	0
11	c	26	18	19	1	0
11	d	26	18	19	0	0
11	f	26	18	19	0	0
All	All	48876	42922	42919	585	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 6.

The worst 5 of 585 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:F:27:GLN:NE2	8:e:512:CYS:SG	2.47	0.88
8:e:585:GLU:N	8:e:585:GLU:OE1	2.14	0.81
8:b:573:GLU:OE2	8:b:757:ARG:NH2	2.16	0.78
8:b:506:MET:N	8:b:506:MET:HE2	1.99	0.77
8:b:482:GLU:N	8:b:482:GLU:OE1	2.18	0.76

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	A	97/135 (72%)	90 (93%)	7 (7%)	0	100	100
2	B	78/103 (76%)	75 (96%)	3 (4%)	0	100	100
2	F	76/103 (74%)	69 (91%)	7 (9%)	0	100	100
2	R	77/103 (75%)	74 (96%)	3 (4%)	0	100	100
2	X	76/103 (74%)	71 (93%)	5 (7%)	0	100	100
3	C	100/129 (78%)	94 (94%)	6 (6%)	0	100	100
3	G	96/129 (74%)	89 (93%)	7 (7%)	0	100	100
3	S	96/129 (74%)	90 (94%)	6 (6%)	0	100	100
3	Y	96/129 (74%)	92 (96%)	4 (4%)	0	100	100
4	D	91/123 (74%)	86 (94%)	5 (6%)	0	100	100
4	H	90/123 (73%)	82 (91%)	8 (9%)	0	100	100
4	P	89/123 (72%)	84 (94%)	5 (6%)	0	100	100
4	T	90/123 (73%)	86 (96%)	4 (4%)	0	100	100
5	E	96/135 (71%)	92 (96%)	4 (4%)	0	100	100
5	Q	93/135 (69%)	90 (97%)	3 (3%)	0	100	100
5	W	97/135 (72%)	95 (98%)	2 (2%)	0	100	100
8	Z	167/580 (29%)	161 (96%)	6 (4%)	0	100	100
8	b	338/580 (58%)	320 (95%)	18 (5%)	0	100	100
8	e	324/580 (56%)	306 (94%)	18 (6%)	0	100	100
8	g	168/580 (29%)	165 (98%)	3 (2%)	0	100	100
9	a	547/689 (79%)	518 (95%)	29 (5%)	0	100	100
9	c	545/689 (79%)	517 (95%)	28 (5%)	0	100	100
9	d	417/689 (60%)	399 (96%)	18 (4%)	0	100	100
9	f	417/689 (60%)	397 (95%)	20 (5%)	0	100	100
All	All	4361/7036 (62%)	4142 (95%)	219 (5%)	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	86/109 (79%)	83 (96%)	3 (4%)	32	55
2	B	66/79 (84%)	66 (100%)	0	100	100
2	F	64/79 (81%)	62 (97%)	2 (3%)	35	57
2	R	65/79 (82%)	65 (100%)	0	100	100
2	X	64/79 (81%)	64 (100%)	0	100	100
3	C	80/101 (79%)	79 (99%)	1 (1%)	61	71
3	G	76/101 (75%)	76 (100%)	0	100	100
3	S	75/101 (74%)	75 (100%)	0	100	100
3	Y	76/101 (75%)	76 (100%)	0	100	100
4	D	79/103 (77%)	79 (100%)	0	100	100
4	H	78/103 (76%)	76 (97%)	2 (3%)	40	61
4	P	77/103 (75%)	76 (99%)	1 (1%)	61	71
4	T	78/103 (76%)	77 (99%)	1 (1%)	61	71
5	E	86/110 (78%)	86 (100%)	0	100	100
5	Q	83/110 (76%)	83 (100%)	0	100	100
5	W	87/110 (79%)	85 (98%)	2 (2%)	44	63
8	Z	153/492 (31%)	151 (99%)	2 (1%)	61	71
8	b	299/492 (61%)	296 (99%)	3 (1%)	68	74
8	e	286/492 (58%)	280 (98%)	6 (2%)	47	64
8	g	151/492 (31%)	149 (99%)	2 (1%)	61	71
9	a	478/591 (81%)	468 (98%)	10 (2%)	47	64
9	c	476/591 (80%)	468 (98%)	8 (2%)	53	68
9	d	369/591 (62%)	366 (99%)	3 (1%)	73	76
9	f	372/591 (63%)	365 (98%)	7 (2%)	50	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3804/5903 (64%)	3751 (99%)	53 (1%)	57 70

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	c	664	GLU
8	e	407	ASN
9	f	786	SER
9	c	671	THR
9	c	740	ASP

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

Mol	Chain	Res	Type
9	a	612	ASN
9	d	515	GLN
9	c	100	GLN
9	d	816	GLN
8	g	610	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	$\# Z  > 2$
1	MLY	A	36	1	9,10,11	0.53	0	6,11,13	0.62	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
1	MLY	A	36	1	-	2/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	36	MLY	N-CA-CB-CG
1	A	36	MLY	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 18 are monoatomic - leaving 4 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	$\# Z  > 2$
11	SAH	f	1004	-	27,28,28	0.69	1 (3%)	36,40,40	0.69	0
11	SAH	d	1004	-	27,28,28	0.65	0	36,40,40	0.61	0
11	SAH	c	1004	-	27,28,28	0.64	0	36,40,40	0.65	0
11	SAH	a	1004	-	27,28,28	0.76	1 (3%)	36,40,40	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
11	SAH	f	1004	-	-	8/15/31/31	0/3/3/3
11	SAH	d	1004	-	-	3/15/31/31	0/3/3/3
11	SAH	c	1004	-	-	6/15/31/31	0/3/3/3
11	SAH	a	1004	-	-	3/15/31/31	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1004	SAH	OXT-C	-2.38	1.23	1.30
11	f	1004	SAH	OXT-C	-2.03	1.24	1.30

There are no bond angle outliers.

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	a	1004	SAH	C2'-C1'-N9-C8
11	a	1004	SAH	C2'-C1'-N9-C4
11	f	1004	SAH	O4'-C4'-C5'-SD
11	f	1004	SAH	C3'-C4'-C5'-SD
11	d	1004	SAH	C2'-C1'-N9-C8

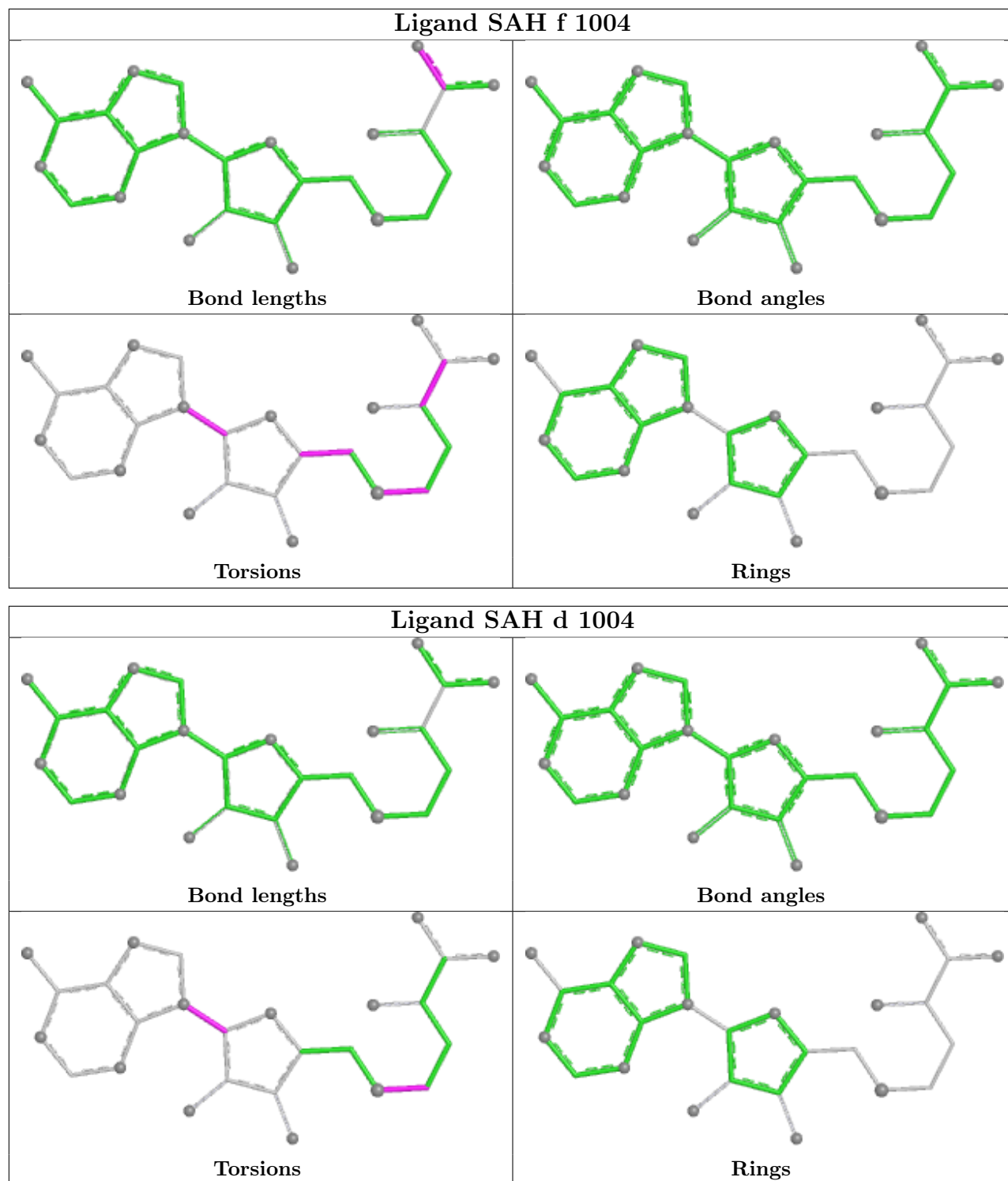
There are no ring outliers.

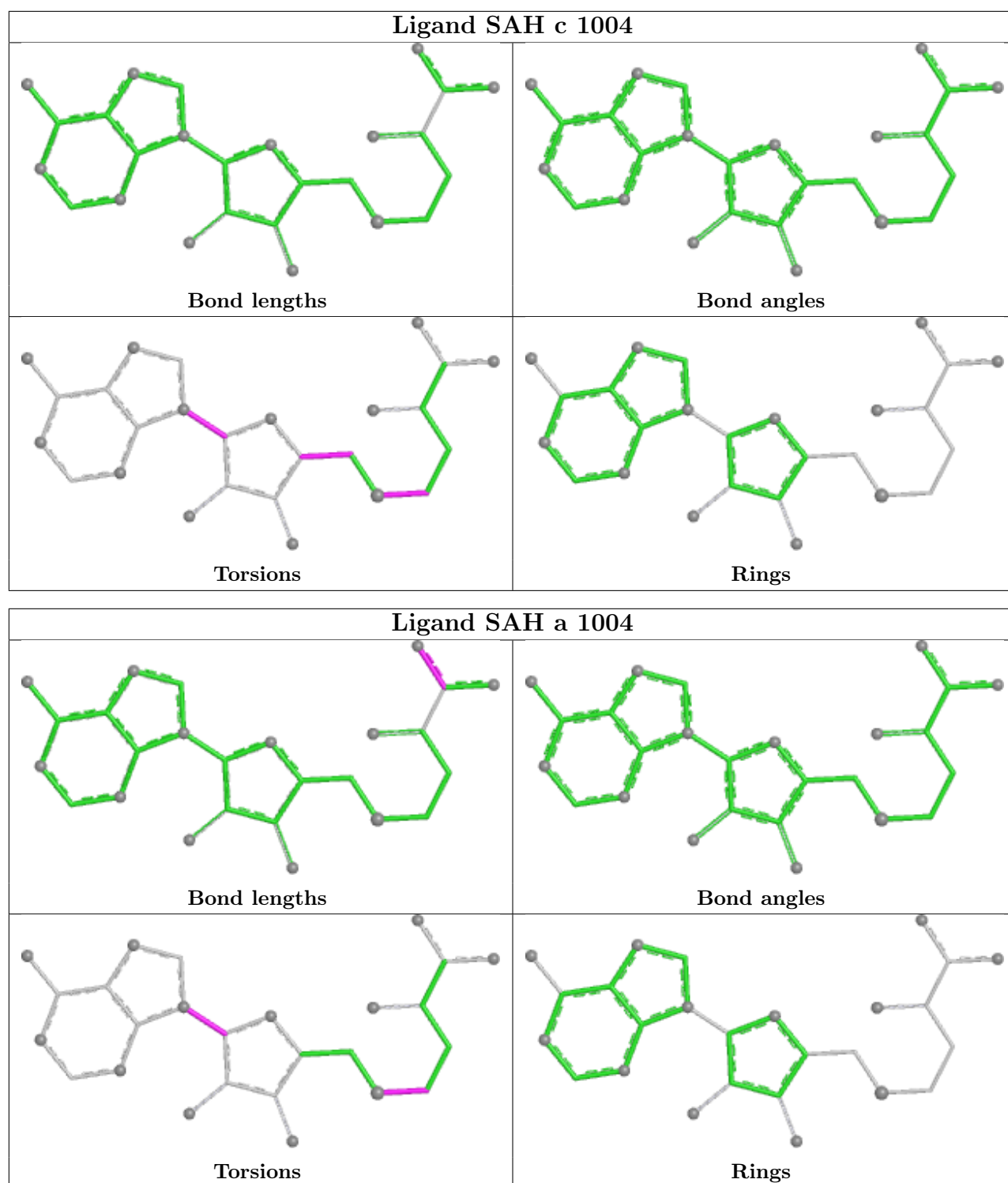
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	c	1004	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 ⓘ

There are no chain breaks in this entry.

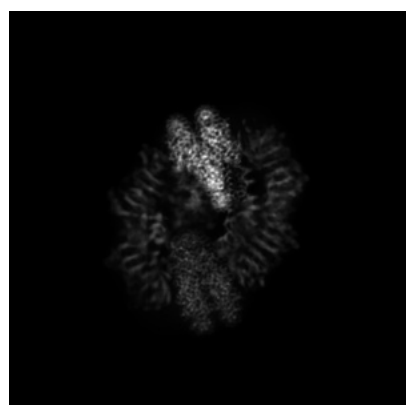
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72487. These allow visual inspection of the internal detail of the map and identification of artifacts.

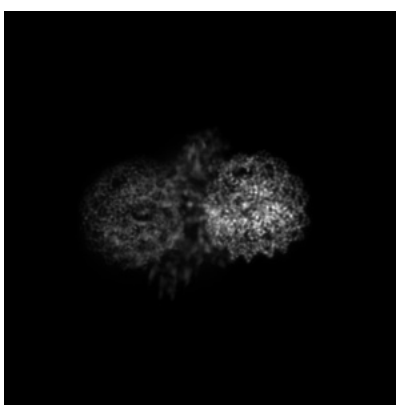
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

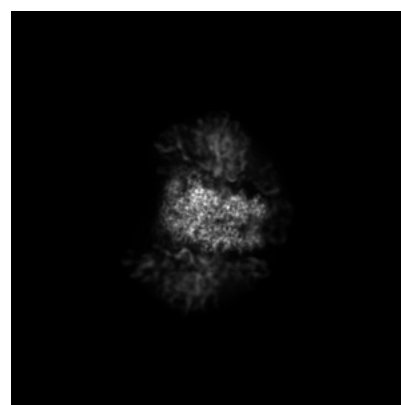
#### 6.1.1 Primary map



X



Y



Z

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

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

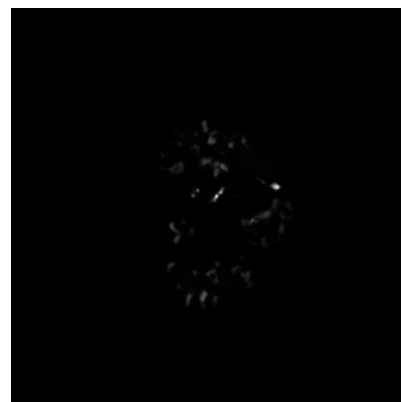
#### 6.2.1 Primary map



X Index: 224



Y Index: 224



Z Index: 224

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: 210



Y Index: 227

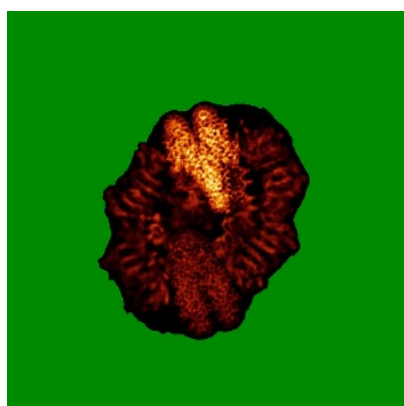


Z Index: 282

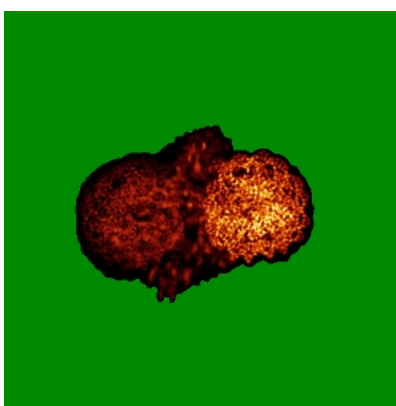
The images above show the largest variance slices of the map in three orthogonal directions.

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

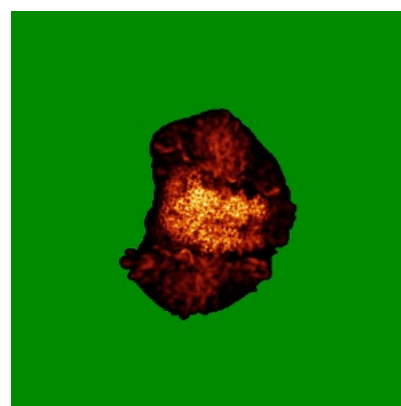
### 6.4.1 Primary map



X



Y

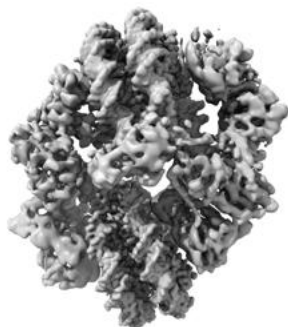


Z

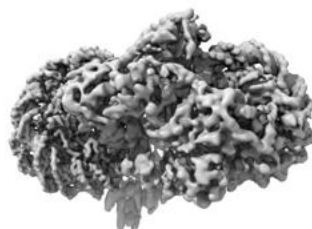
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

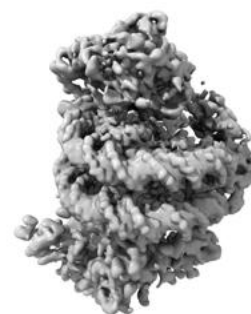
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0672. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

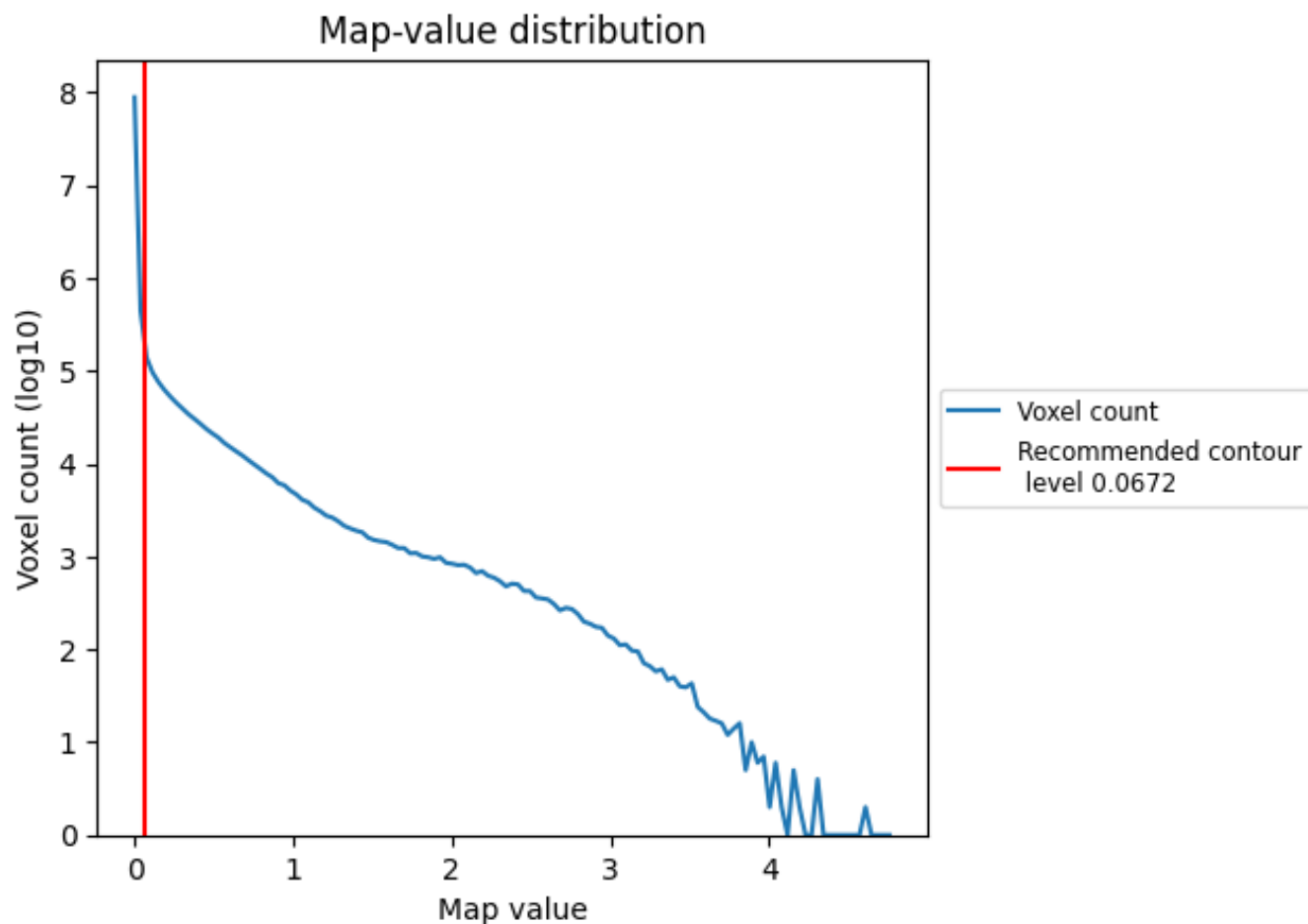
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

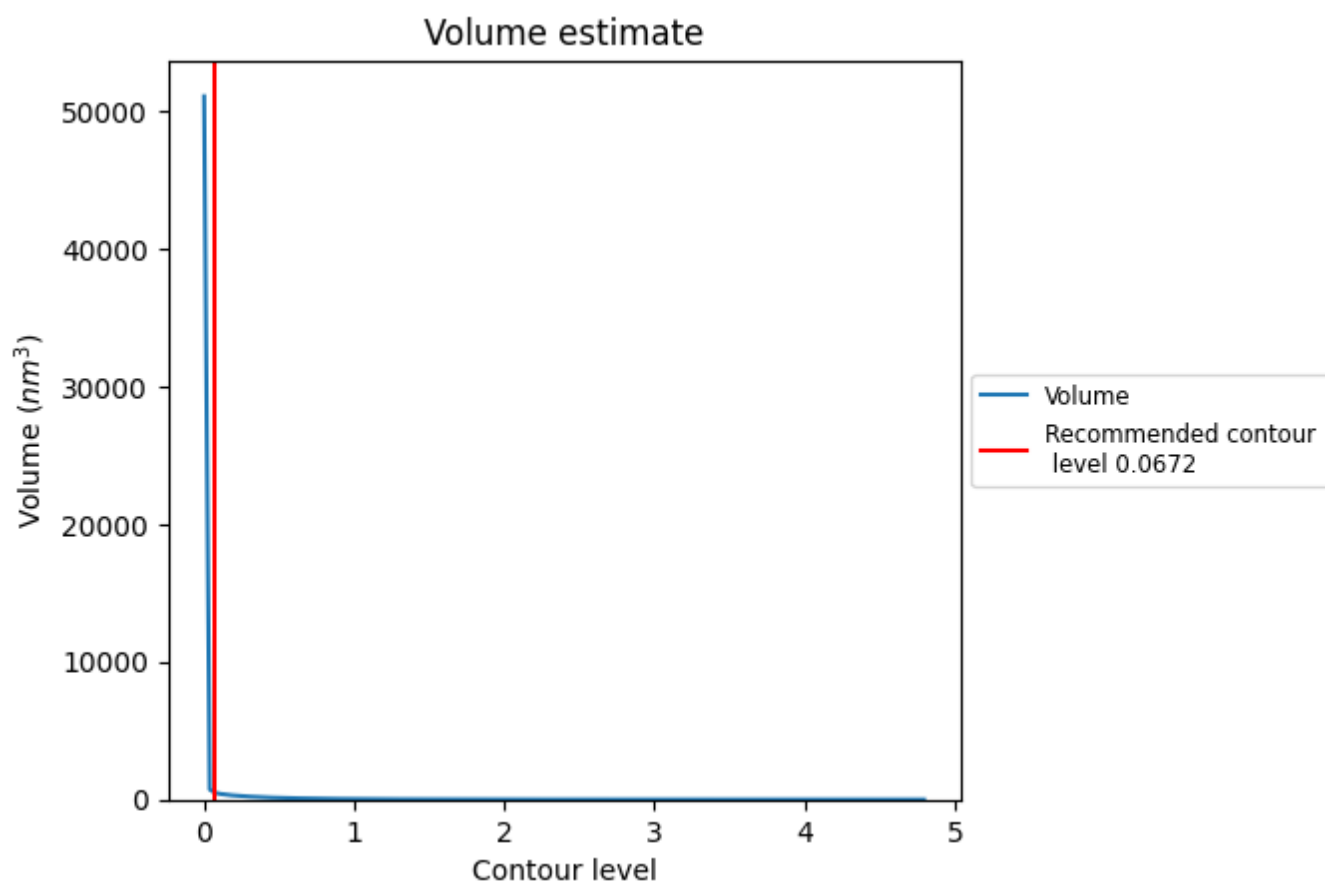
This section contains the results of statistical analysis of the map.

### 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.

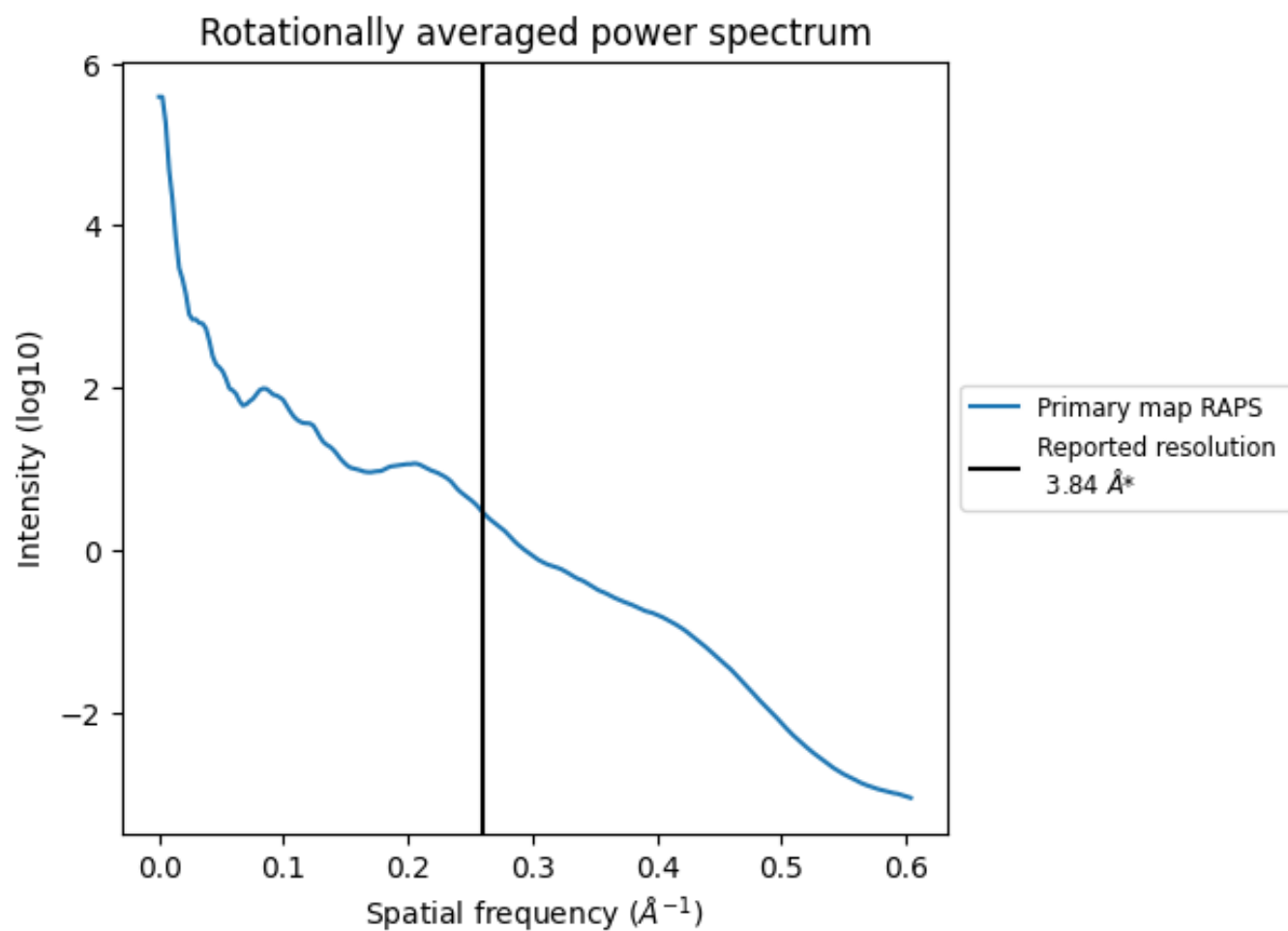
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 534  $\text{nm}^3$ ; 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 0.260  $\text{\AA}^{-1}$

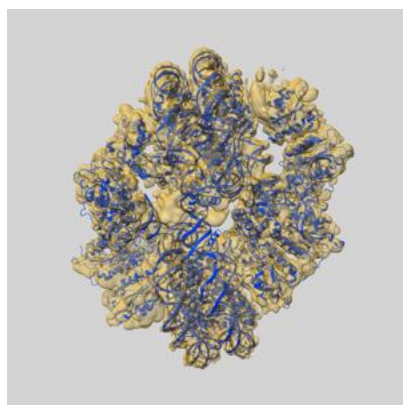
## 8 Fourier-Shell correlation

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

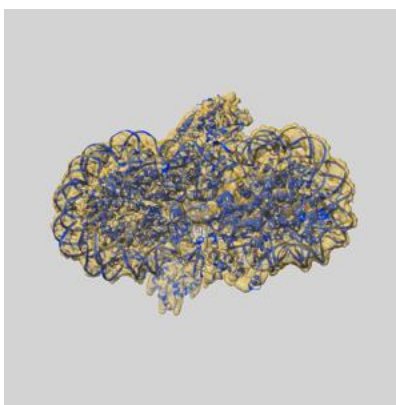
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72487 and PDB model 9Y4P. Per-residue inclusion information can be found in section [3](#) on page [9](#).

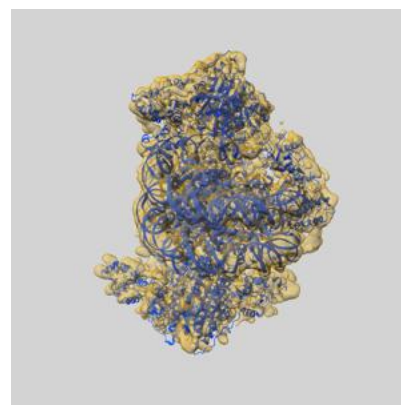
### 9.1 Map-model overlay [i](#)



X



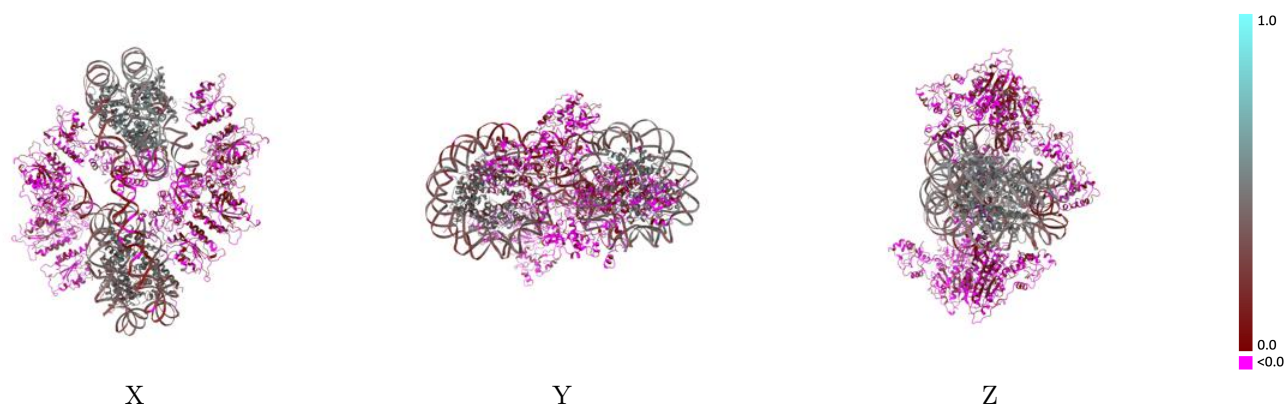
Y



Z

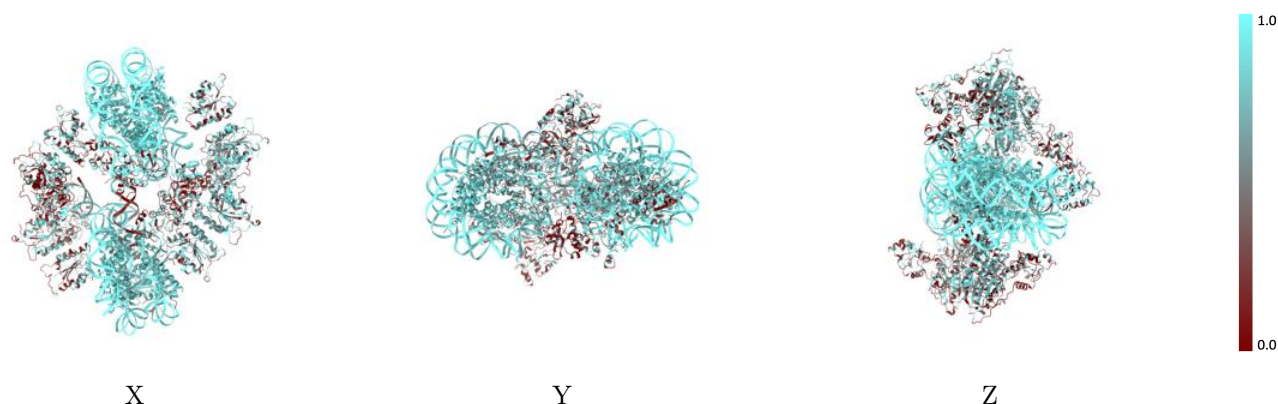
The images above show the 3D surface view of the map at the recommended contour level 0.0672 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



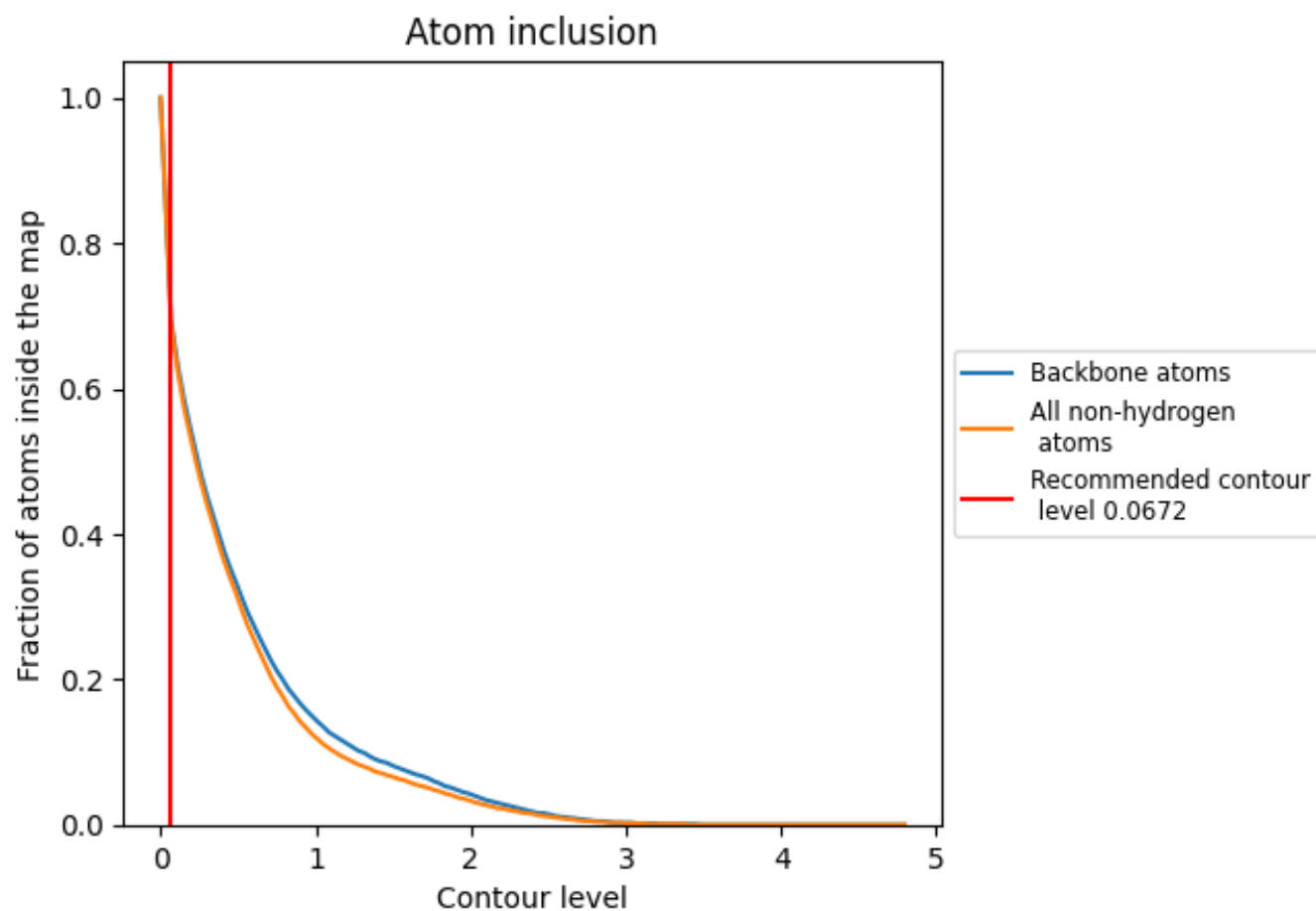
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0672).























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 69% 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 (0.0672) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6900	 0.2140
A	 0.9160	 0.4590
B	 0.9430	 0.4890
C	 0.9070	 0.4830
D	 0.9210	 0.4670
E	 0.9420	 0.4940
F	 0.9630	 0.4970
G	 0.9440	 0.4930
H	 0.9440	 0.4700
I	 0.9090	 0.3260
J	 0.9060	 0.3340
P	 0.8920	 0.4220
Q	 0.8850	 0.4380
R	 0.8880	 0.4350
S	 0.8820	 0.4280
T	 0.8730	 0.4170
W	 0.8760	 0.4350
X	 0.8910	 0.4350
Y	 0.8690	 0.4310
Z	 0.5060	 0.0400
a	 0.5180	 0.0490
b	 0.5600	 0.0620
c	 0.4940	 0.0420
d	 0.4300	 0.0060
e	 0.5140	 0.0380
f	 0.3870	 0.0140
g	 0.4060	 0.0040

