



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:20 AM UTC

PDB ID : 9E3R / pdb\_00009e3r  
EMDB ID : EMD-47495  
Title : Cryo-EM structure of PWWP domain deleted DNMT 3A2/3B3 in complex with a di-nucleosome  
Authors : Xie, X.; Liu, M.; Zhou, X.E.; Worden, E.; Jones, P.  
Deposited on : 2024-10-23  
Resolution : 6.90 Å(reported)

This is a Full wwPDB EM Validation 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 : **NOT EXECUTED**  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

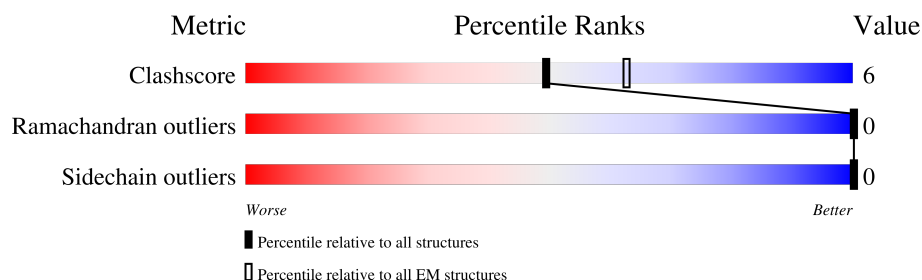
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.















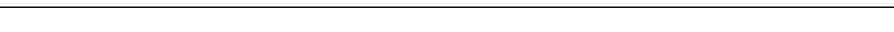



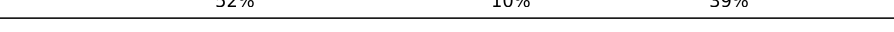
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	135	61% 10% 29%
1	E	135	62% 10% 28%
1	M	135	65% 8% 27%
1	Q	135	61% 10% 30%
2	B	103	66% 11% 23%
2	F	103	67% 9% 24%
2	N	103	64% 12% 24%
2	R	103	70% 6% 24%
3	C	129	65% 12% 23%

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Mol	Chain	Length	Quality of chain
3	G	129	
3	O	129	
3	S	129	
4	D	123	
4	H	123	
4	P	123	
4	T	123	
5	I	321	
6	J	321	
7	L	773	
7	V	773	
7	X	773	
7	Z	773	
8	K	689	
8	U	689	
8	W	689	
8	Y	689	

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 46690 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	96	Total	C	N	O	S	0	0
			795	501	154	137	3		
1	E	97	Total	C	N	O	S	0	0
			802	506	155	138	3		
1	M	99	Total	C	N	O	S	0	0
			820	518	159	140	3		
1	Q	95	Total	C	N	O	S	0	0
			785	495	151	136	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	conflict	UNP Q71DI3
E	102	ALA	GLY	conflict	UNP Q71DI3
M	102	ALA	GLY	conflict	UNP Q71DI3
Q	102	ALA	GLY	conflict	UNP Q71DI3

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	79	Total	C	N	O	S	0	0
			633	399	124	109	1		
2	F	78	Total	C	N	O	S	0	0
			622	393	120	108	1		
2	N	78	Total	C	N	O	S	0	0
			622	393	120	108	1		
2	R	78	Total	C	N	O	S	0	0
			622	393	120	108	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	99	Total	C	N	O	0	0
			764	479	151	134		
3	G	98	Total	C	N	O	0	0
			755	474	149	132		
3	O	98	Total	C	N	O	0	0
			755	474	149	132		
3	S	98	Total	C	N	O	0	0
			752	473	148	131		

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	92	Total	C	N	O	S	0	0
			719	453	129	135	2		
4	H	92	Total	C	N	O	S	0	0
			719	453	129	135	2		
4	P	91	Total	C	N	O	S	0	0
			708	447	125	134	2		
4	T	92	Total	C	N	O	S	0	0
			719	453	129	135	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP A0A1B8Y854
H	0	MET	-	initiating methionine	UNP A0A1B8Y854
P	0	MET	-	initiating methionine	UNP A0A1B8Y854
T	0	MET	-	initiating methionine	UNP A0A1B8Y854

- Molecule 5 is a DNA chain called DNA (320-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	320	Total	C	N	O	P	0	0
			6594	3117	1242	1915	320		

- Molecule 6 is a DNA chain called DNA (319-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	319	Total	C	N	O	P	0	0
			6506	3086	1183	1918	319		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	V	336	Total	C	N	O	S	0	0
			2686	1706	468	486	26		
7	Z	173	Total	C	N	O	S	0	0
			1407	923	238	241	5		
7	L	347	Total	C	N	O	S	0	0
			2769	1753	488	502	26		
7	X	176	Total	C	N	O	S	0	0
			1434	938	246	245	5		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	391	LYS	-	insertion	UNP Q9UBC3
V	392	ASP	-	insertion	UNP Q9UBC3
V	393	TYR	-	insertion	UNP Q9UBC3
Z	391	LYS	-	insertion	UNP Q9UBC3
Z	392	ASP	-	insertion	UNP Q9UBC3
Z	393	TYR	-	insertion	UNP Q9UBC3
L	391	LYS	-	insertion	UNP Q9UBC3
L	392	ASP	-	insertion	UNP Q9UBC3
L	393	TYR	-	insertion	UNP Q9UBC3
X	391	LYS	-	insertion	UNP Q9UBC3
X	392	ASP	-	insertion	UNP Q9UBC3
X	393	TYR	-	insertion	UNP Q9UBC3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	423	Total	C	N	O	S	0	0
			3397	2152	603	607	35		
8	Y	424	Total	C	N	O	S	0	0
			3404	2156	604	609	35		
8	W	423	Total	C	N	O	S	0	0
			3400	2154	603	608	35		
8	K	421	Total	C	N	O	S	0	0
			3379	2141	598	605	35		

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

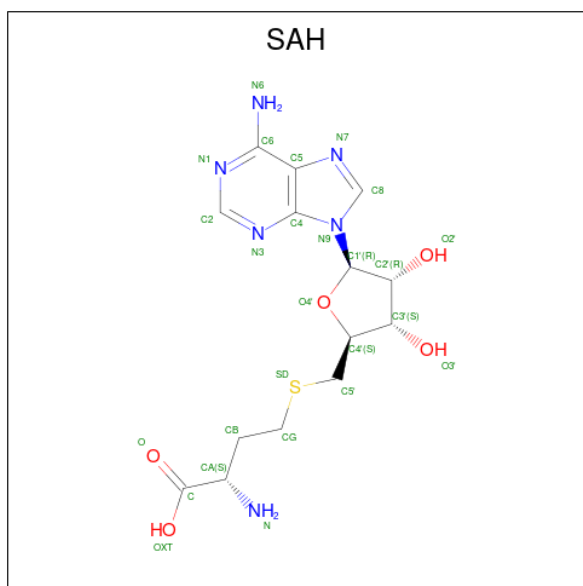
Mol	Chain	Residues	Atoms		AltConf
9	V	3	Total	Zn	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
9	U	3	Total	Zn	0
			3	3	
9	Y	3	Total	Zn	0
			3	3	
9	L	3	Total	Zn	0
			3	3	
9	W	3	Total	Zn	0
			3	3	
9	K	3	Total	Zn	0
			3	3	

- Molecule 10 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).

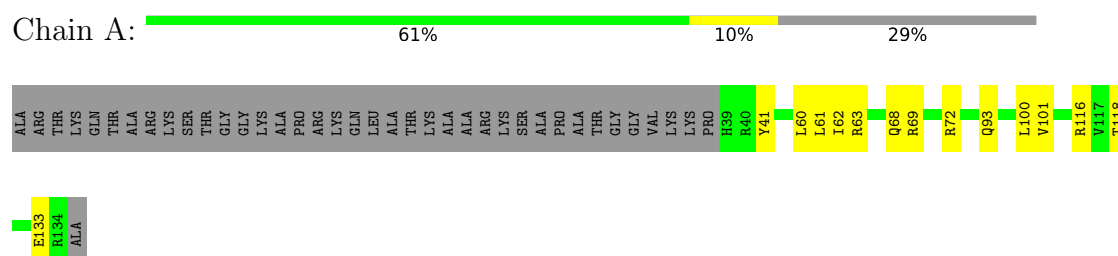


Mol	Chain	Residues	Atoms					AltConf
10	U	1	Total	C	N	O	S	0
			26	14	6	5	1	
10	Y	1	Total	C	N	O	S	0
			26	14	6	5	1	
10	W	1	Total	C	N	O	S	0
			26	14	6	5	1	
10	K	1	Total	C	N	O	S	0
			26	14	6	5	1	

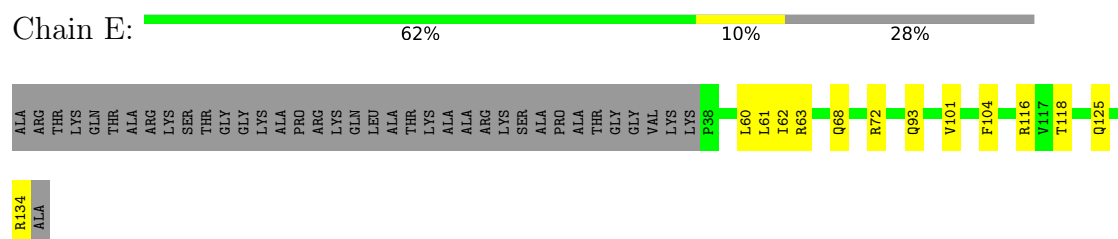
### 3 Residue-property plots [i](#)

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. 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. 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.

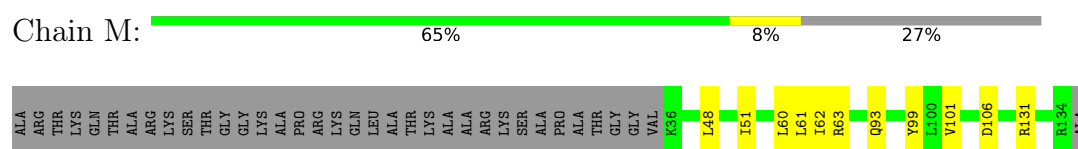
- Molecule 1: Histone H3.2



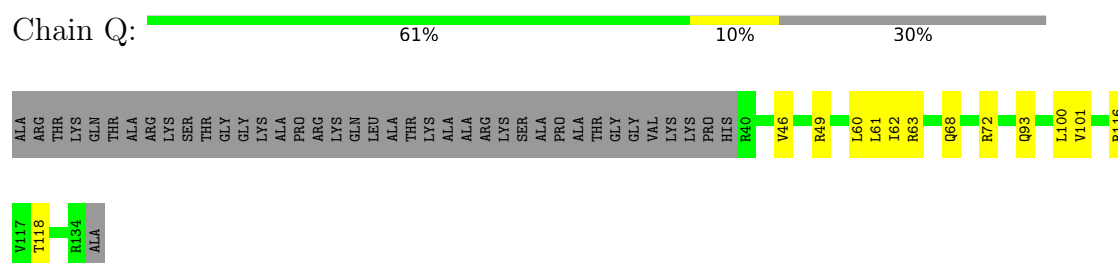
- Molecule 1: Histone H3.2



- Molecule 1: Histone H3.2



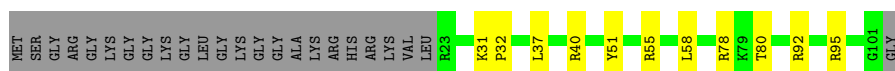
- Molecule 1: Histone H3.2



- Molecule 2: Histone H4

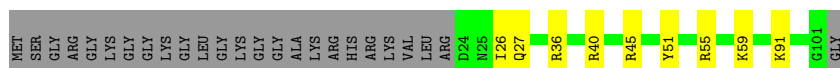






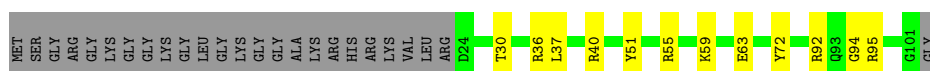
- Molecule 2: Histone H4

Chain F: 67% 9% 24%



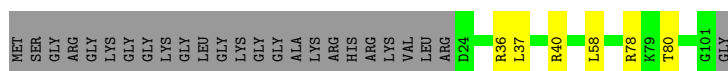
- Molecule 2: Histone H4

Chain N: 64% 12% 24%



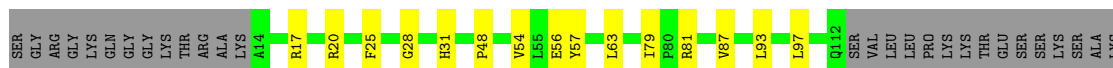
- Molecule 2: Histone H4

Chain R: 70% 6% 24%



- Molecule 3: Histone H2A

Chain C: 65% 12% 23%



- Molecule 3: Histone H2A

Chain G: 67% 9% 24%



- Molecule 3: Histone H2A

Chain O: 70% 6% 24%



- Molecule 3: Histone H2A

Chain S: 66% 10% 24%



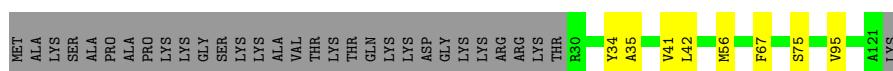
- Molecule 4: Histone H2B

Chain D: 67% 7% 25%



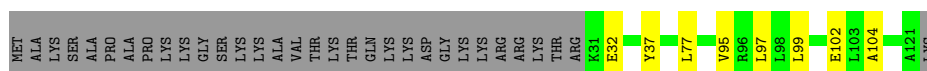
- Molecule 4: Histone H2B

Chain H: 68% 7% 25%



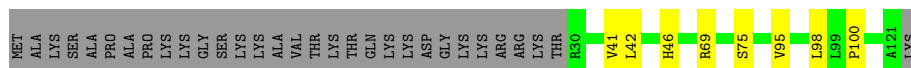
- Molecule 4: Histone H2B

Chain P: 67% 7% 26%



- Molecule 4: Histone H2B

Chain T: 68% 7% 25%



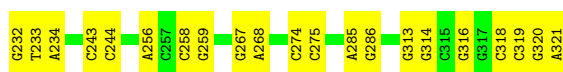
- Molecule 5: DNA (320-MER)

Chain I: 80% 20%

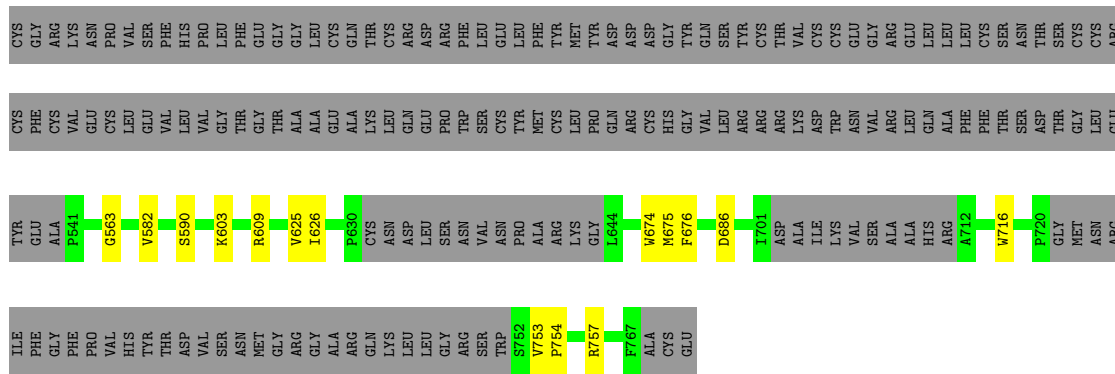


- Molecule 6: DNA (319-MER)

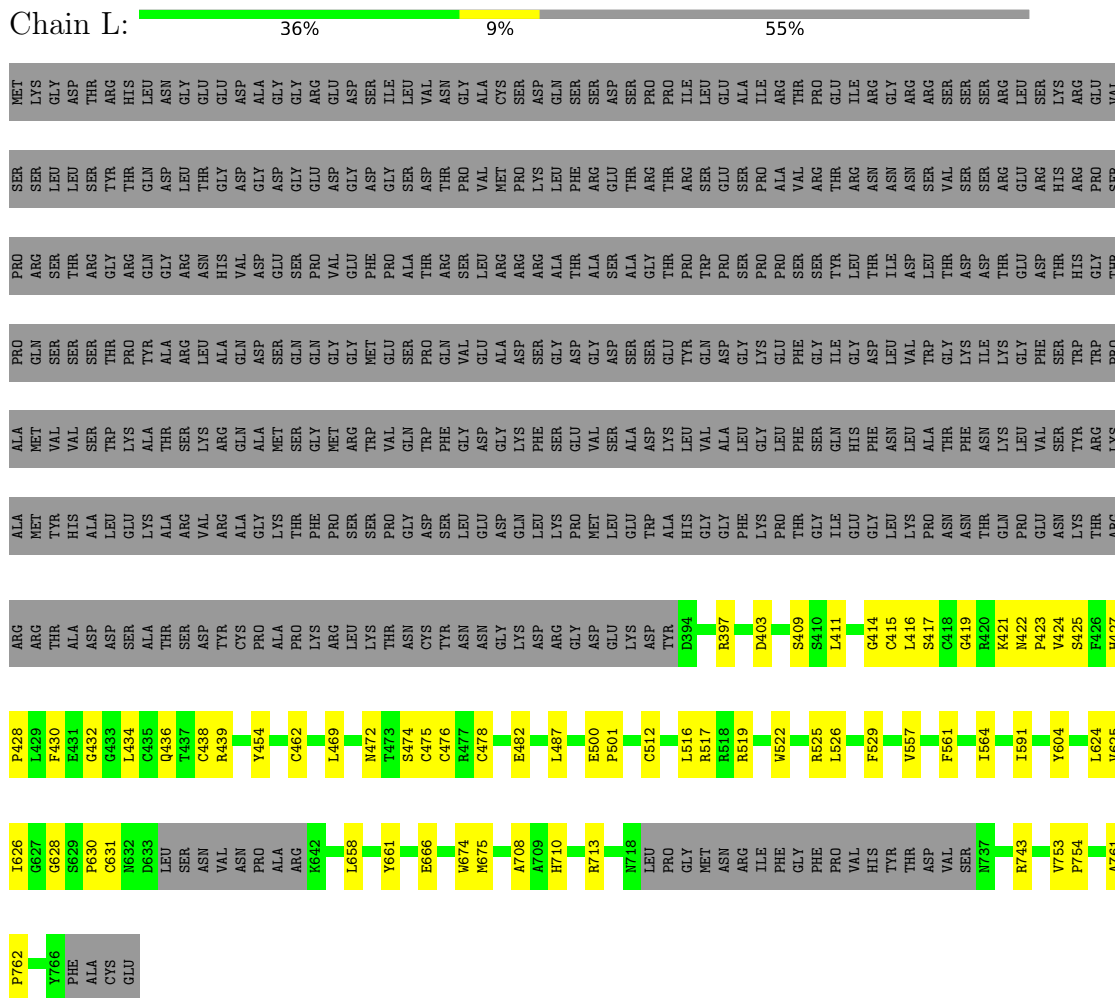
Chain J: 80% 19% .



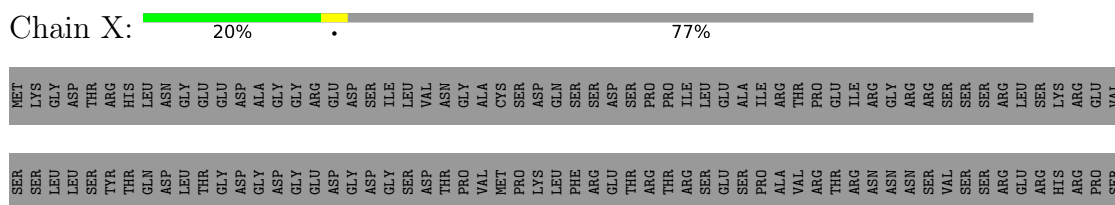


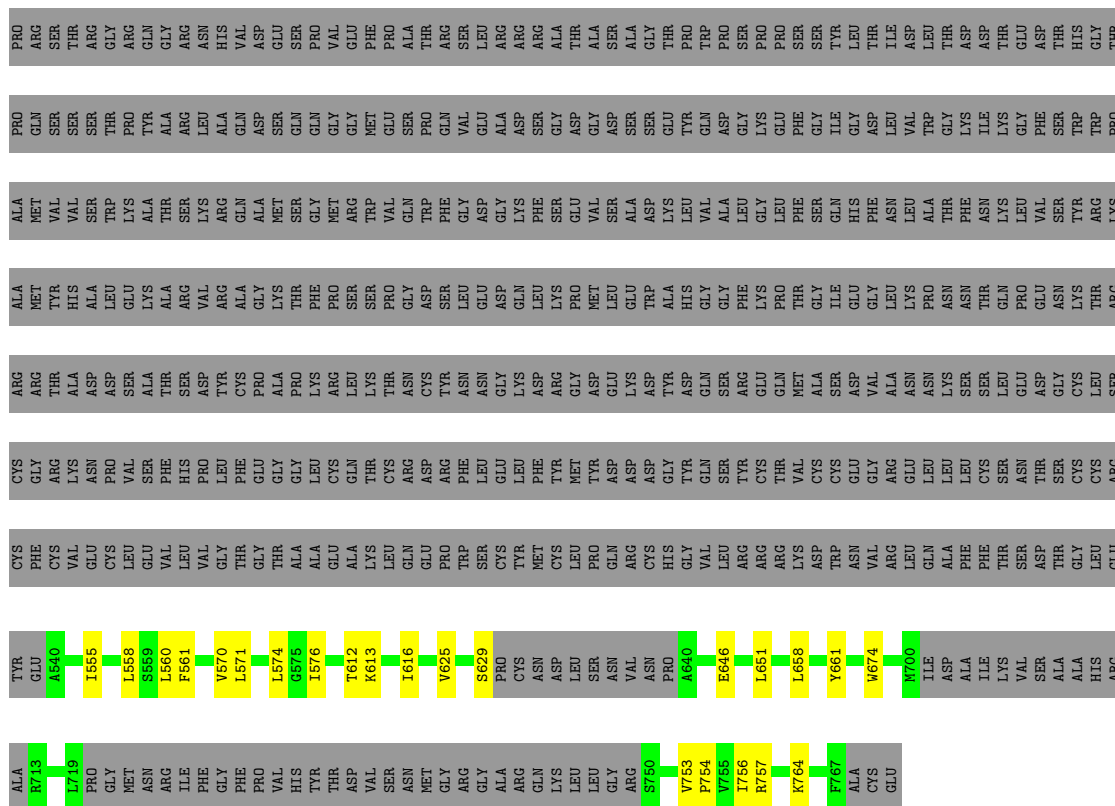


- Molecule 7: Isoform 3 of DNA (cytosine-5)-methyltransferase 3B

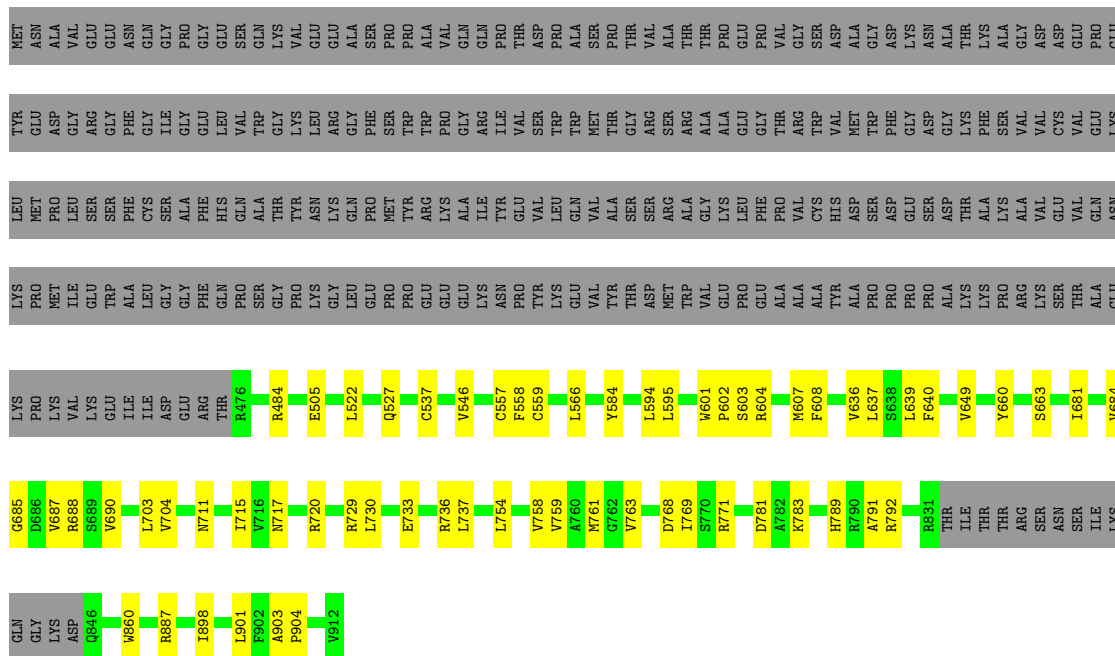


- Molecule 7: Isoform 3 of DNA (cytosine-5)-methyltransferase 3B





- Molecule 8: DNA (cytosine-5)-methyltransferase 3A



- Molecule 8: 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	37292	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.97	0/806	1.41	0/1081
1	E	0.97	0/814	1.39	0/1092
1	M	0.96	0/832	1.39	0/1115
1	Q	0.97	0/795	1.42	0/1066
2	B	0.96	0/640	1.38	0/857
2	F	0.98	0/629	1.40	0/843
2	N	0.96	0/629	1.37	0/843
2	R	0.98	0/629	1.38	0/843
3	C	0.98	0/773	1.38	0/1043
3	G	0.98	0/764	1.45	0/1031
3	O	0.97	0/764	1.39	0/1031
3	S	0.97	0/761	1.42	0/1027
4	D	0.99	0/730	1.48	0/983
4	H	0.99	0/730	1.48	0/983
4	P	1.00	0/719	1.50	0/969
4	T	1.01	0/730	1.49	0/983
5	I	0.28	0/7406	0.58	0/11437
6	J	0.29	0/7290	0.55	1/11241 (0.0%)
7	L	0.99	0/2832	1.35	0/3819
7	V	0.99	0/2750	1.35	2/3714 (0.1%)
7	X	0.97	0/1472	1.29	0/1985
7	Z	0.97	0/1445	1.30	0/1951
8	K	1.00	0/3462	1.33	0/4678
8	U	0.99	0/3480	1.32	0/4702
8	W	0.99	0/3482	1.34	0/4703
8	Y	1.00	0/3487	1.31	0/4712
All	All	0.84	0/48851	1.16	3/68732 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	V	752	SER	CA-C-N	5.99	125.12	120.33
7	V	752	SER	C-N-CA	5.99	125.12	120.33
6	J	313	DG	C2'-C3'-O3'	-5.71	102.94	111.50

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	795	0	833	10	0
1	E	802	0	841	8	0
1	M	820	0	866	8	0
1	Q	785	0	826	12	0
2	B	633	0	673	9	0
2	F	622	0	660	11	0
2	N	622	0	660	11	0
2	R	622	0	660	6	0
3	C	764	0	808	11	0
3	G	755	0	800	16	0
3	O	755	0	800	6	0
3	S	752	0	796	12	0
4	D	719	0	740	9	0
4	H	719	0	740	8	0
4	P	708	0	727	7	0
4	T	719	0	740	8	0
5	I	6594	0	3585	42	0
6	J	6506	0	3578	49	0
7	L	2769	0	2700	65	0
7	V	2686	0	2611	46	0
7	X	1434	0	1436	19	0
7	Z	1407	0	1413	9	0
8	K	3379	0	3288	33	0
8	U	3397	0	3310	57	0
8	W	3400	0	3314	57	0
8	Y	3404	0	3317	54	0
9	K	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	L	3	0	0	0	0
9	U	3	0	0	0	0
9	V	3	0	0	0	0
9	W	3	0	0	0	0
9	Y	3	0	0	0	0
10	K	26	0	19	1	0
10	U	26	0	19	0	0
10	W	26	0	19	0	0
10	Y	26	0	19	2	0
All	All	46690	0	40798	496	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.

All (496) 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)
7:L:626:ILE:HG23	7:L:675:MET:HE3	1.17	1.15
7:L:626:ILE:CG2	7:L:675:MET:HE3	1.80	1.12
7:L:624:LEU:HG	7:L:626:ILE:HD11	1.34	1.06
7:V:464:GLY:O	7:V:467:LEU:HD13	1.57	1.04
8:Y:788:ALA:HB2	8:Y:867:VAL:CG1	1.96	0.95
7:V:463:GLU:O	7:V:467:LEU:HD11	1.65	0.94
7:L:415:CYS:O	7:L:419:GLY:HA2	1.68	0.92
8:Y:788:ALA:HB2	8:Y:867:VAL:HG13	1.53	0.90
8:Y:788:ALA:CB	8:Y:867:VAL:CG1	2.49	0.90
8:W:527:GLN:NE2	8:W:715:ILE:HG13	1.87	0.90
7:L:626:ILE:HG23	7:L:675:MET:CE	2.02	0.88
8:W:527:GLN:HE21	8:W:715:ILE:HG13	1.39	0.88
7:V:467:LEU:HG	7:V:479:PHE:C	1.99	0.88
7:L:624:LEU:CG	7:L:626:ILE:HD11	2.04	0.88
5:I:2:DC:H2"	5:I:3:DG:C8	2.09	0.88
8:U:687:VAL:HG13	8:U:737:LEU:HD12	1.55	0.88
7:L:425:SER:CB	7:L:439:ARG:HD2	2.03	0.87
7:V:457:TYR:HA	7:V:464:GLY:HA2	1.56	0.87
7:L:428:PRO:HB3	7:L:525:ARG:HB3	1.55	0.86
3:G:29:ARG:O	3:G:33:LEU:HG	1.76	0.86
8:Y:788:ALA:CB	8:Y:867:VAL:HG13	2.06	0.85
8:Y:789:HIS:HB2	8:Y:829:LYS:HD2	1.58	0.84
7:V:464:GLY:C	7:V:467:LEU:HD13	2.02	0.84
8:K:640:PHE:CE1	8:K:687:VAL:HG21	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:30:VAL:O	3:G:34:LEU:HG	1.79	0.83
7:L:626:ILE:CG2	7:L:675:MET:CE	2.57	0.82
7:V:692:ARG:HG3	8:U:688:ARG:HG3	1.62	0.81
3:G:39:TYR:HB3	4:H:75:SER:HB2	1.61	0.81
7:L:624:LEU:HG	7:L:626:ILE:CD1	2.11	0.81
8:Y:788:ALA:HA	8:Y:830:VAL:H	1.48	0.79
8:K:640:PHE:CZ	8:K:687:VAL:HG21	2.17	0.78
2:F:59:LYS:HG2	7:V:509:PRO:HB3	1.66	0.76
8:Y:783:LYS:HD3	8:Y:789:HIS:ND1	2.01	0.76
7:L:472:ASN:HB3	7:L:475:CYS:HB3	1.68	0.76
3:G:29:ARG:HG2	3:G:33:LEU:HD11	1.68	0.76
7:X:629:SER:HA	7:X:651:LEU:HD13	1.68	0.76
8:W:522:LEU:HB3	8:W:763:VAL:HG22	1.68	0.76
8:W:555:CYS:SG	8:W:831:ARG:NH1	2.60	0.75
8:W:522:LEU:HB2	8:W:763:VAL:HG21	1.68	0.74
8:U:759:VAL:HB	8:U:791:ALA:O	1.87	0.74
8:U:758:VAL:HA	8:U:792:ARG:CD	2.18	0.74
7:V:467:LEU:HG	7:V:479:PHE:O	1.88	0.73
8:U:687:VAL:CG1	8:U:733:GLU:HB3	2.18	0.73
7:L:425:SER:HB2	7:L:439:ARG:HD2	1.70	0.73
8:W:522:LEU:HB3	8:W:763:VAL:CG2	2.18	0.73
8:W:522:LEU:CB	8:W:763:VAL:CG2	2.67	0.72
8:Y:788:ALA:HB1	8:Y:830:VAL:HB	1.70	0.72
7:L:427:HIS:HB3	7:L:434:LEU:HD22	1.71	0.72
7:V:465:ARG:O	7:V:467:LEU:HD12	1.91	0.71
8:W:640:PHE:CZ	8:W:687:VAL:HG21	2.26	0.71
7:V:454:TYR:CD2	7:V:469:LEU:HD22	2.26	0.71
7:X:612:THR:HG22	7:X:613:LYS:H	1.55	0.71
7:X:560:LEU:HD11	7:X:658:LEU:HD22	1.72	0.70
8:Y:788:ALA:HB2	8:Y:867:VAL:HG11	1.74	0.70
2:F:27:GLN:HE21	7:V:510:GLN:CD	2.00	0.69
7:X:612:THR:HG22	7:X:613:LYS:N	2.07	0.69
6:J:316:DG:P	8:W:882:ARG:HH11	2.15	0.69
8:K:636:VAL:HA	8:K:703:LEU:O	1.93	0.69
6:J:316:DG:OP2	8:W:882:ARG:NE	2.26	0.68
7:L:624:LEU:CD2	7:L:626:ILE:HD11	2.22	0.68
5:I:1:DT:H2"	5:I:2:DC:C5	2.29	0.68
8:Y:785:VAL:O	8:Y:785:VAL:HG22	1.93	0.68
7:V:465:ARG:O	7:V:467:LEU:CD1	2.41	0.67
8:Y:639:LEU:HD22	8:Y:734:PHE:CD1	2.29	0.67
8:U:522:LEU:HD23	8:U:763:VAL:HB	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:484:ARG:HB3	8:W:594:LEU:HD11	1.75	0.67
7:L:417:SER:HB3	7:L:438:CYS:SG	2.34	0.67
8:W:640:PHE:CE1	8:W:687:VAL:HG21	2.30	0.67
8:U:687:VAL:HG13	8:U:737:LEU:CD1	2.23	0.67
8:W:522:LEU:CB	8:W:763:VAL:HG21	2.25	0.67
7:L:474:SER:HB3	7:L:708:ALA:HB1	1.77	0.66
7:V:457:TYR:HA	7:V:464:GLY:CA	2.24	0.66
8:W:527:GLN:HA	8:W:716:VAL:HG12	1.78	0.66
6:J:4:DG:H8	8:U:887:ARG:NH1	1.93	0.65
8:U:484:ARG:HB3	8:U:594:LEU:HD11	1.79	0.65
8:Y:788:ALA:CB	8:Y:830:VAL:HB	2.28	0.64
7:L:428:PRO:CB	7:L:525:ARG:HB3	2.27	0.63
2:F:27:GLN:HG2	7:V:510:GLN:HE22	1.64	0.63
3:S:39:TYR:HB3	4:T:75:SER:HB2	1.79	0.63
7:L:411:LEU:HD11	7:L:432:GLY:H	1.61	0.63
6:J:3:DC:H5''	8:U:711:ASN:ND2	2.13	0.63
7:L:425:SER:HB3	7:L:439:ARG:HD2	1.81	0.63
7:L:626:ILE:HG21	7:L:675:MET:HE3	1.80	0.62
5:I:1:DT:O2	8:W:711:ASN:OD1	2.17	0.62
6:J:316:DG:O5'	8:W:882:ARG:NH1	2.30	0.62
7:L:454:TYR:CD2	7:L:469:LEU:HD23	2.34	0.62
3:G:29:ARG:HG2	3:G:33:LEU:CD1	2.30	0.62
8:U:758:VAL:HA	8:U:792:ARG:HD2	1.79	0.62
8:K:636:VAL:HG22	8:K:703:LEU:HB3	1.82	0.61
8:Y:788:ALA:HB3	8:Y:867:VAL:CG1	2.28	0.61
8:Y:643:ILE:HD11	8:Y:892:SER:HB2	1.82	0.61
8:K:640:PHE:CE1	8:K:687:VAL:CG2	2.82	0.61
2:F:27:GLN:HE21	7:V:510:GLN:NE2	1.98	0.61
2:F:45:ARG:HE	5:I:90:DC:H4'	1.65	0.61
3:S:32:ARG:NH1	6:J:40:DA:OP2	2.34	0.61
7:X:558:LEU:HD21	7:X:658:LEU:HD23	1.82	0.60
3:G:32:ARG:HD2	3:G:32:ARG:C	2.27	0.60
8:U:781:ASP:HA	8:U:791:ALA:HA	1.83	0.60
8:Y:782:ALA:HB3	8:Y:790:ARG:HB3	1.82	0.60
8:U:603:SER:O	8:U:607:MET:HG2	2.01	0.59
7:L:454:TYR:CG	7:L:469:LEU:HD23	2.37	0.59
1:Q:68:GLN:HE21	1:Q:72:ARG:HH21	1.50	0.59
8:Y:643:ILE:HD11	8:Y:892:SER:CB	2.33	0.59
1:Q:46:VAL:HG21	5:I:247:DT:H3'	1.85	0.59
8:U:687:VAL:HG11	8:U:733:GLU:HB3	1.84	0.59
7:X:754:PRO:HA	7:X:757:ARG:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:515:GLN:HA	8:W:518:LYS:HE2	1.85	0.58
4:D:68:GLU:OE1	2:F:91:LYS:NZ	2.36	0.58
3:G:33:LEU:CD1	4:H:34:TYR:OH	2.51	0.58
8:Y:787:ALA:HA	8:Y:813:LEU:O	2.02	0.58
1:E:62:ILE:O	1:E:93:GLN:NE2	2.36	0.58
6:J:314:DG:OP2	8:K:882:ARG:NH1	2.36	0.58
8:W:522:LEU:HB2	8:W:763:VAL:CG2	2.33	0.58
8:K:663:SER:HA	8:K:684:VAL:HB	1.84	0.58
1:E:125:GLN:HG2	1:E:134:ARG:HH12	1.69	0.58
3:S:35:ARG:NH2	5:I:277:DA:OP2	2.37	0.57
1:A:68:GLN:HE21	1:A:72:ARG:HH21	1.53	0.57
5:I:2:DC:H2''	5:I:3:DG:N7	2.19	0.57
7:X:612:THR:CG2	7:X:613:LYS:H	2.17	0.57
8:W:476:ARG:HH11	8:W:565:LEU:HD23	1.70	0.57
8:U:522:LEU:HD23	8:U:763:VAL:CB	2.34	0.57
7:L:487:LEU:HD13	7:L:516:LEU:HB2	1.87	0.57
8:K:637:LEU:HB3	8:K:704:VAL:HG22	1.87	0.57
6:J:321:DA:N7	8:W:719:ALA:CB	2.68	0.57
7:V:692:ARG:HG3	8:U:688:ARG:CG	2.35	0.57
8:W:566:LEU:HD13	8:W:595:LEU:HD22	1.87	0.56
6:J:319:DC:H2''	6:J:320:DG:O4'	2.05	0.56
1:Q:60:LEU:O	1:Q:63:ARG:NH2	2.38	0.56
7:V:609:ARG:NH2	8:U:768:ASP:OD1	2.38	0.56
8:Y:642:GLY:O	8:Y:669:SER:HB2	2.04	0.56
8:W:603:SER:O	8:W:607:MET:HG3	2.06	0.56
7:L:411:LEU:HD11	7:L:432:GLY:N	2.21	0.56
7:V:397:ARG:HH22	7:V:482:GLU:HG2	1.71	0.56
7:L:415:CYS:O	7:L:419:GLY:CA	2.46	0.56
8:Y:589:LYS:NZ	8:Y:591:THR:OG1	2.38	0.56
7:L:430:PHE:O	7:L:519:ARG:NE	2.38	0.56
7:X:612:THR:O	7:X:616:ILE:HG12	2.05	0.56
7:X:625:VAL:O	7:X:674:TRP:HA	2.07	0.55
8:W:515:GLN:HA	8:W:518:LYS:CE	2.36	0.55
3:C:54:VAL:HG21	4:D:95:VAL:HG21	1.89	0.55
1:Q:62:ILE:O	1:Q:93:GLN:NE2	2.40	0.55
5:I:290:DC:H4'	5:I:291:DC:OP1	2.07	0.55
7:L:422:ASN:N	7:L:423:PRO:HD3	2.22	0.55
4:D:100:PRO:HD2	4:D:103:LEU:HD23	1.89	0.54
7:L:428:PRO:HA	7:L:519:ARG:HD2	1.87	0.54
7:V:458:CYS:N	7:V:467:LEU:HD21	2.22	0.54
8:K:754:LEU:HD11	8:K:901:LEU:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:313:DG:H3'	8:Y:882:ARG:HH11	1.72	0.54
7:V:626:ILE:HA	7:V:675:MET:O	2.08	0.54
7:X:646:GLU:HB3	8:K:729:ARG:HH22	1.73	0.54
8:Y:639:LEU:HD12	8:Y:639:LEU:N	2.23	0.54
7:V:609:ARG:HH11	8:U:771:ARG:HD2	1.73	0.54
8:W:636:VAL:HG22	8:W:703:LEU:HB3	1.89	0.54
1:A:62:ILE:O	1:A:93:GLN:NE2	2.41	0.54
3:G:54:VAL:HG21	4:H:95:VAL:HG21	1.89	0.54
8:W:636:VAL:HA	8:W:703:LEU:O	2.08	0.54
7:L:424:VAL:HB	7:L:436:GLN:HB2	1.90	0.53
3:O:57:TYR:OH	7:L:743:ARG:HD2	2.08	0.53
8:Y:761:MET:HE1	8:Y:769:ILE:HD12	1.90	0.53
2:B:92:ARG:HH21	4:D:98:LEU:HD23	1.72	0.53
7:V:467:LEU:CG	7:V:479:PHE:O	2.55	0.53
8:W:562:CYS:O	8:W:566:LEU:HG	2.08	0.53
8:K:641:ASP:OD1	8:K:644:ALA:HA	2.08	0.53
7:V:686:ASP:OD1	8:U:729:ARG:NH1	2.41	0.53
7:V:692:ARG:CG	8:U:688:ARG:HG3	2.36	0.53
8:Y:676:ARG:NH2	8:Y:873:HIS:O	2.42	0.53
8:Y:643:ILE:HD11	8:Y:870:PHE:CZ	2.44	0.53
8:Y:783:LYS:HB3	8:Y:789:HIS:HA	1.91	0.53
8:U:684:VAL:HG11	8:U:690:VAL:HG22	1.91	0.53
5:I:231:DG:H2''	5:I:232:DG:C8	2.44	0.53
8:Y:788:ALA:HB3	8:Y:867:VAL:HG13	1.88	0.53
8:U:687:VAL:HG12	8:U:733:GLU:HB3	1.88	0.52
8:W:715:ILE:HD12	8:W:720:ARG:HD3	1.92	0.52
8:U:754:LEU:HD11	8:U:901:LEU:HD13	1.92	0.52
8:W:578:GLU:HG2	8:W:580:PRO:HD2	1.91	0.52
8:K:482:GLU:HB3	8:K:487:CYS:HB2	1.91	0.52
8:Y:534:GLN:HG3	8:Y:555:CYS:O	2.10	0.52
8:K:483:VAL:HG11	8:K:490:ILE:HD13	1.91	0.52
7:L:591:ILE:HD13	7:L:604:TYR:HB2	1.92	0.52
8:W:754:LEU:HD11	8:W:901:LEU:HD13	1.91	0.52
7:L:625:VAL:O	7:L:674:TRP:HA	2.10	0.52
8:Y:513:MET:HE2	8:Y:518:LYS:HA	1.92	0.52
1:E:116:ARG:NH1	1:E:118:THR:O	2.43	0.52
8:U:783:LYS:HD3	8:U:789:HIS:CD2	2.45	0.52
3:G:32:ARG:HD2	3:G:32:ARG:O	2.11	0.51
7:V:444:GLU:HG2	7:V:683:LYS:HA	1.92	0.51
7:X:612:THR:CG2	7:X:613:LYS:N	2.72	0.51
3:G:33:LEU:HD11	4:H:34:TYR:OH	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:94:GLY:O	3:S:99:ARG:HB3	2.11	0.51
7:V:694:LEU:HD22	7:V:716:TRP:HB3	1.93	0.51
7:L:522:TRP:O	7:L:526:LEU:HB2	2.11	0.51
1:A:60:LEU:O	1:A:63:ARG:NH2	2.43	0.51
1:A:133:GLU:OE2	2:B:95:ARG:NH1	2.37	0.51
7:L:428:PRO:CB	7:L:525:ARG:CB	2.89	0.51
8:K:637:LEU:O	8:K:704:VAL:HA	2.09	0.51
1:Q:116:ARG:NH1	1:Q:118:THR:O	2.43	0.51
6:J:319:DC:C2'	6:J:320:DG:C8	2.94	0.51
1:E:60:LEU:O	1:E:63:ARG:NH2	2.43	0.51
7:V:609:ARG:HD2	8:U:771:ARG:NE	2.25	0.51
6:J:4:DG:H8	8:U:887:ARG:HH12	1.59	0.51
8:K:604:ARG:O	8:K:608:PHE:HB2	2.11	0.51
8:Y:781:ASP:HA	8:Y:791:ALA:HA	1.93	0.51
8:Y:637:LEU:O	8:Y:704:VAL:HA	2.12	0.50
7:L:666:GLU:HB2	8:W:744:LYS:HD3	1.92	0.50
8:K:484:ARG:HB3	8:K:594:LEU:HD11	1.93	0.50
8:K:891:ARG:HD3	10:K:1004:SAH:H3'	1.92	0.50
3:C:20:ARG:NH2	5:I:41:DG:OP1	2.44	0.50
2:F:51:TYR:HB3	2:F:55:ARG:HH12	1.75	0.50
8:U:636:VAL:HG22	8:U:703:LEU:HB3	1.93	0.50
7:V:693:PHE:HD1	8:U:736:ARG:HD3	1.76	0.50
7:L:403:ASP:HB3	7:L:409:SER:HB3	1.93	0.49
8:W:715:ILE:HD12	8:W:720:ARG:CD	2.42	0.49
7:V:467:LEU:CB	7:V:479:PHE:O	2.59	0.49
7:L:417:SER:CB	7:L:438:CYS:SG	3.01	0.49
3:G:63:LEU:HD22	4:H:42:LEU:HD13	1.95	0.49
2:N:51:TYR:HB3	2:N:55:ARG:HH12	1.77	0.49
6:J:130:DA:H2''	6:J:131:DG:C8	2.47	0.49
8:W:637:LEU:HB3	8:W:704:VAL:HG22	1.93	0.49
1:A:101:VAL:HG21	2:B:40:ARG:HD2	1.95	0.49
3:G:30:VAL:HG13	4:H:67:PHE:HE1	1.78	0.49
8:W:567:VAL:HG21	8:W:571:ALA:HB3	1.93	0.49
8:U:636:VAL:HA	8:U:703:LEU:O	2.11	0.49
8:U:684:VAL:HG12	8:U:685:GLY:N	2.27	0.49
6:J:103:DC:H2''	6:J:104:DG:H5''	1.94	0.49
8:Y:787:ALA:O	8:Y:829:LYS:HA	2.13	0.49
2:N:59:LYS:NZ	2:N:63:GLU:OE2	2.45	0.49
6:J:9:DC:H2'	6:J:10:DC:C6	2.48	0.49
6:J:319:DC:H2''	6:J:320:DG:N9	2.27	0.49
7:L:397:ARG:HG3	7:L:416:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:761:MET:HE1	8:K:769:ILE:HD12	1.95	0.49
7:V:458:CYS:CA	7:V:467:LEU:HD21	2.43	0.48
8:W:504:LEU:HG	8:W:505:GLU:O	2.13	0.48
6:J:36:DC:H2"	6:J:37:DT:C5	2.48	0.48
5:I:29:DC:H2"	5:I:30:DA:C8	2.49	0.48
3:O:54:VAL:HG21	4:P:95:VAL:HG21	1.94	0.48
7:Z:676:PHE:HB3	7:Z:716:TRP:HB2	1.94	0.48
1:A:116:ARG:NH1	1:A:118:THR:O	2.47	0.48
2:N:92:ARG:NH1	4:P:97:LEU:HB3	2.29	0.48
7:V:467:LEU:HG	7:V:480:CYS:N	2.28	0.48
7:L:397:ARG:HH22	7:L:482:GLU:HB3	1.77	0.48
6:J:232:DG:H2"	6:J:233:DT:C5	2.48	0.48
1:A:69:ARG:NH2	6:J:256:DA:OP1	2.43	0.48
1:Q:61:LEU:HD13	2:R:36:ARG:HB3	1.95	0.48
1:M:61:LEU:HD13	2:N:36:ARG:HB3	1.96	0.47
3:C:31:HIS:HD2	3:C:48:PRO:HG3	1.79	0.47
6:J:320:DG:H2"	6:J:321:DA:N7	2.29	0.47
8:U:608:PHE:C	8:U:608:PHE:CD2	2.92	0.47
3:C:25:PHE:CE2	4:D:41:VAL:HG21	2.49	0.47
3:O:42:ARG:HG2	6:J:123:DA:H5'	1.96	0.47
5:I:23:DA:H2"	5:I:24:DT:H5"	1.96	0.47
8:W:761:MET:HE1	8:W:769:ILE:HD12	1.96	0.47
7:V:458:CYS:HB3	7:V:463:GLU:H	1.79	0.47
7:V:609:ARG:NH1	8:U:771:ARG:HD2	2.29	0.47
8:U:637:LEU:HB3	8:U:704:VAL:HG22	1.96	0.47
8:Y:783:LYS:HD3	8:Y:789:HIS:CE1	2.48	0.47
3:S:16:THR:HA	6:J:41:DT:H5"	1.97	0.47
5:I:273:DT:H2"	5:I:274:DA:C8	2.50	0.47
6:J:319:DC:H2'	6:J:320:DG:C8	2.49	0.47
8:U:761:MET:HE1	8:U:769:ILE:HD12	1.96	0.47
7:L:474:SER:O	7:L:710:HIS:NE2	2.48	0.47
8:W:618:ASP:OD1	8:W:619:PRO:HD2	2.15	0.47
5:I:319:DG:H2"	5:I:320:DA:H8	1.80	0.47
6:J:46:DC:H2"	6:J:47:DG:C8	2.49	0.47
8:Y:636:VAL:HG22	8:Y:703:LEU:HB3	1.96	0.47
8:Y:550:GLY:N	8:Y:581:TRP:O	2.41	0.47
7:X:574:LEU:HD21	7:X:757:ARG:HB2	1.96	0.47
3:G:25:PHE:CE2	4:H:41:VAL:HG21	2.50	0.47
1:M:106:ASP:OD2	1:M:131:ARG:NH2	2.48	0.47
8:U:758:VAL:HA	8:U:792:ARG:HD3	1.94	0.47
7:L:411:LEU:HD23	7:L:411:LEU:C	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:566:LEU:HD22	8:W:595:LEU:HD13	1.96	0.47
8:K:717:ASN:HB3	8:K:720:ARG:HB3	1.97	0.47
8:Y:484:ARG:HB3	8:Y:594:LEU:HD11	1.98	0.46
3:S:25:PHE:CE2	4:T:41:VAL:HG21	2.49	0.46
6:J:3:DC:H5"	8:U:711:ASN:HD21	1.80	0.46
8:U:860:TRP:CE2	8:Y:878:SER:HA	2.50	0.46
2:F:27:GLN:NE2	7:V:510:GLN:CD	2.71	0.46
1:Q:46:VAL:HG22	1:Q:49:ARG:HH21	1.80	0.46
8:Y:643:ILE:CD1	8:Y:892:SER:CB	2.92	0.46
8:W:522:LEU:HD13	8:W:763:VAL:CG1	2.45	0.46
3:S:54:VAL:HG21	4:T:95:VAL:HG21	1.97	0.46
8:W:604:ARG:HA	8:W:607:MET:CE	2.45	0.46
8:W:710:CYS:HA	8:W:713:LEU:HB2	1.97	0.46
6:J:201:DC:H2"	6:J:202:DG:C8	2.50	0.46
7:L:474:SER:HB2	7:L:708:ALA:O	2.16	0.46
7:X:571:LEU:HD22	7:X:576:ILE:HD11	1.96	0.46
8:K:781:ASP:HA	8:K:791:ALA:HA	1.96	0.46
8:W:504:LEU:HG	8:W:505:GLU:N	2.31	0.46
3:C:79:ILE:HG22	3:C:81:ARG:H	1.80	0.46
2:F:26:ILE:HG21	7:V:510:GLN:HA	1.96	0.46
5:I:184:DC:H2"	5:I:185:DA:C8	2.51	0.46
6:J:191:DC:H2"	6:J:192:DT:C5	2.51	0.46
7:V:522:TRP:O	7:V:526:LEU:HB2	2.15	0.46
8:U:522:LEU:CD2	8:U:763:VAL:HG23	2.45	0.46
8:U:566:LEU:HB3	8:U:595:LEU:HB2	1.96	0.46
8:Y:506:HIS:O	8:Y:598:ARG:NE	2.48	0.46
7:L:557:VAL:HG13	7:L:626:ILE:CD1	2.46	0.46
3:S:64:GLU:HA	4:T:46:HIS:HE1	1.81	0.46
5:I:4:DG:N2	6:J:319:DC:O2	2.48	0.46
7:L:631:CYS:SG	7:L:713:ARG:NH1	2.88	0.46
5:I:138:DC:H2"	5:I:139:DG:C8	2.51	0.46
6:J:274:DC:H2"	6:J:275:DC:C5	2.51	0.46
8:U:687:VAL:CG1	8:U:737:LEU:HD12	2.36	0.46
8:Y:537:CYS:HB2	8:Y:559:CYS:HB3	1.97	0.46
2:B:31:LYS:HB3	2:B:32:PRO:HD3	1.98	0.46
2:B:92:ARG:NH2	4:D:98:LEU:HA	2.31	0.46
1:E:61:LEU:HD13	2:F:36:ARG:HB3	1.98	0.46
5:I:293:DC:H2"	5:I:294:DG:C8	2.51	0.46
6:J:321:DA:N7	8:W:719:ALA:HB3	2.31	0.46
7:L:626:ILE:HG21	7:L:675:MET:CE	2.43	0.46
7:L:626:ILE:HD12	7:L:626:ILE:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:72:TYR:OH	2:N:92:ARG:HD3	2.16	0.45
8:Y:533:TYR:HA	8:Y:555:CYS:HB3	1.98	0.45
8:Y:777:PRO:HB3	8:Y:795:TRP:CE2	2.51	0.45
7:L:474:SER:O	7:L:710:HIS:CE1	2.69	0.45
7:Z:582:VAL:HG22	7:Z:603:LYS:HB2	1.97	0.45
8:U:717:ASN:HB3	8:U:720:ARG:HB3	1.98	0.45
8:U:759:VAL:CB	8:U:791:ALA:O	2.62	0.45
8:Y:788:ALA:CB	8:Y:867:VAL:HG11	2.37	0.45
5:I:26:DT:H2''	5:I:27:DG:C8	2.51	0.45
7:V:466:GLU:O	7:V:481:VAL:HG23	2.16	0.45
7:Z:626:ILE:HB	7:Z:675:MET:HE3	1.97	0.45
8:U:601:TRP:CG	8:U:602:PRO:HD3	2.51	0.45
3:C:57:TYR:HE2	4:D:103:LEU:HD12	1.80	0.45
7:Z:563:GLY:HA3	7:Z:590:SER:HB3	1.98	0.45
1:Q:101:VAL:HG21	2:R:40:ARG:HD2	1.98	0.45
5:I:253:DT:H2''	5:I:254:DA:N7	2.32	0.45
3:S:78:ILE:HD12	4:T:42:LEU:HD11	1.99	0.45
1:A:41:TYR:OH	6:J:172:DA:H5''	2.16	0.45
6:J:319:DC:H2''	6:J:320:DG:C8	2.51	0.45
7:V:467:LEU:HG	7:V:480:CYS:CA	2.47	0.45
7:L:512:CYS:SG	7:L:517:ARG:HG2	2.57	0.45
3:C:87:VAL:HG13	3:C:93:LEU:HB3	1.99	0.45
4:P:37:TYR:OH	6:J:132:DG:OP1	2.33	0.45
8:U:537:CYS:HB2	8:U:559:CYS:HB3	1.97	0.45
7:L:526:LEU:O	7:L:529:PHE:HB3	2.17	0.45
3:C:17:ARG:HH21	3:C:28:GLY:HA2	1.82	0.45
1:M:62:ILE:O	1:M:93:GLN:NE2	2.50	0.45
8:U:546:VAL:HB	8:U:557:CYS:HB3	1.99	0.45
7:V:557:VAL:HA	7:V:624:LEU:O	2.17	0.45
8:Y:783:LYS:HB3	8:Y:789:HIS:ND1	2.31	0.45
8:W:782:ALA:HB3	8:W:790:ARG:HB3	1.99	0.44
4:D:35:ALA:HA	4:D:56:MET:SD	2.57	0.44
1:E:101:VAL:HG21	2:F:40:ARG:HD2	1.98	0.44
5:I:316:DG:H4'	5:I:317:DC:OP1	2.17	0.44
7:Z:609:ARG:HD2	8:Y:771:ARG:HG3	1.98	0.44
3:S:95:LYS:HD2	4:T:100:PRO:HB3	2.00	0.44
8:K:482:GLU:O	8:K:487:CYS:N	2.50	0.44
2:N:30:THR:HG21	5:I:225:DA:H5''	2.00	0.44
4:P:99:LEU:HB2	4:P:104:ALA:HB2	2.00	0.44
7:Z:625:VAL:O	7:Z:674:TRP:HA	2.18	0.44
4:H:35:ALA:HA	4:H:56:MET:SD	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:200:DA:H2"	5:I:201:DG:C8	2.53	0.44
7:Z:754:PRO:HA	7:Z:757:ARG:HG2	1.98	0.44
1:Q:100:LEU:HD11	2:R:58:LEU:HD22	2.00	0.44
8:U:660:TYR:HB3	8:U:681:ILE:HD12	1.99	0.44
5:I:178:DA:H2"	5:I:179:DT:H5"	2.00	0.44
7:V:570:VAL:HG11	7:V:756:ILE:HG22	1.98	0.44
8:W:781:ASP:HA	8:W:791:ALA:HA	2.00	0.44
1:M:99:TYR:CD1	2:N:95:ARG:NH2	2.86	0.44
3:S:63:LEU:HD22	4:T:42:LEU:HD12	2.00	0.44
6:J:119:DC:H2"	6:J:120:DC:C5	2.53	0.44
7:V:467:LEU:HG	7:V:480:CYS:HA	1.99	0.44
7:L:427:HIS:HB3	7:L:434:LEU:CD2	2.46	0.44
7:X:658:LEU:HA	7:X:661:TYR:HD2	1.83	0.44
8:K:601:TRP:CG	8:K:602:PRO:HD3	2.53	0.44
8:K:660:TYR:HB3	8:K:681:ILE:HD12	2.00	0.44
6:J:112:DG:H2"	6:J:113:DA:H5"	2.00	0.43
6:J:285:DA:H2"	6:J:286:DG:C8	2.52	0.43
5:I:232:DG:H2"	5:I:233:DG:C8	2.53	0.43
7:L:462:CYS:O	7:L:462:CYS:SG	2.75	0.43
7:L:564:ILE:HG23	7:L:630:PRO:HB3	2.01	0.43
8:W:601:TRP:CG	8:W:602:PRO:HD3	2.53	0.43
8:K:649:VAL:HG11	8:K:898:ILE:HG22	1.99	0.43
8:K:710:CYS:HA	8:K:713:LEU:HB2	1.99	0.43
6:J:75:DA:H2"	6:J:76:DC:OP2	2.18	0.43
7:X:574:LEU:HD22	7:X:764:LYS:HD2	2.01	0.43
8:W:546:VAL:HB	8:W:557:CYS:HB3	1.99	0.43
8:K:782:ALA:HB3	8:K:790:ARG:HB3	2.00	0.43
1:A:100:LEU:HD11	2:B:58:LEU:HD22	2.00	0.43
6:J:48:DT:H2"	6:J:49:DA:C8	2.52	0.43
7:V:626:ILE:HG22	7:V:675:MET:HB3	2.00	0.43
2:B:51:TYR:HB3	2:B:55:ARG:HH12	1.82	0.43
5:I:36:DC:H2"	5:I:37:DT:C5	2.54	0.43
8:Y:579:ASP:HB3	8:Y:580:PRO:HD3	2.00	0.43
8:W:579:ASP:HB3	8:W:580:PRO:HD3	2.00	0.43
7:L:414:GLY:HA2	7:L:421:LYS:HA	2.01	0.43
8:W:584:TYR:O	8:W:597:ARG:NH1	2.52	0.43
8:K:709:PRO:HG2	8:K:727:THR:HB	2.01	0.43
2:B:78:ARG:NH1	2:B:80:THR:O	2.52	0.43
3:O:31:HIS:HD2	3:O:48:PRO:HG3	1.84	0.43
7:V:473:THR:HA	7:V:476:CYS:SG	2.59	0.43
7:V:678:ASN:HD21	7:V:682:MET:HE3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:521:PHE:HA	8:W:541:CYS:SG	2.59	0.43
6:J:233:DT:H2"	6:J:234:DA:C8	2.53	0.43
7:L:428:PRO:HB2	7:L:525:ARG:HB2	2.00	0.43
8:W:553:ASN:OD1	8:W:827:PHE:CD1	2.71	0.43
5:I:132:DC:H2"	5:I:133:DG:C8	2.53	0.42
7:L:753:VAL:N	7:L:754:PRO:HD2	2.33	0.42
7:X:555:ILE:HG13	7:X:576:ILE:HD12	2.00	0.42
2:N:72:TYR:OH	2:N:92:ARG:CD	2.68	0.42
3:O:32:ARG:NH2	4:P:32:GLU:OE1	2.52	0.42
6:J:203:DT:H2"	6:J:204:DA:C8	2.54	0.42
3:C:87:VAL:HG11	3:C:97:LEU:HD12	2.01	0.42
2:R:78:ARG:NH1	2:R:80:THR:O	2.51	0.42
5:I:69:DA:H2"	5:I:70:DA:C8	2.55	0.42
8:U:640:PHE:CZ	8:U:730:LEU:HB3	2.54	0.42
1:M:61:LEU:HD12	2:N:37:LEU:HD23	2.01	0.42
7:V:527:GLN:HB3	7:V:724:ARG:HH12	1.85	0.42
8:U:663:SER:OG	8:U:685:GLY:O	2.33	0.42
8:Y:546:VAL:HA	8:Y:559:CYS:HA	2.01	0.42
8:Y:566:LEU:HD13	8:Y:595:LEU:HD13	2.02	0.42
8:W:903:ALA:HB3	8:W:904:PRO:HD3	2.00	0.42
5:I:230:DG:H2"	5:I:231:DG:H5"	2.02	0.42
6:J:267:DG:H2"	6:J:268:DA:H5"	2.01	0.42
8:K:546:VAL:HB	8:K:557:CYS:HB3	2.00	0.42
3:G:32:ARG:C	3:G:32:ARG:CD	2.93	0.42
1:M:48:LEU:HA	1:M:51:ILE:HD12	2.01	0.42
8:Y:785:VAL:O	8:Y:785:VAL:CG2	2.63	0.42
8:Y:787:ALA:HB2	8:Y:813:LEU:C	2.44	0.42
7:L:397:ARG:HG3	7:L:416:LEU:CD2	2.50	0.42
7:L:428:PRO:HA	7:L:519:ARG:CD	2.50	0.42
5:I:98:DT:H2"	5:I:99:DA:C8	2.54	0.42
6:J:68:DT:H2"	6:J:69:DA:N7	2.35	0.42
8:U:566:LEU:HD13	8:U:595:LEU:HD13	2.00	0.42
8:W:660:TYR:HB3	8:W:681:ILE:HD12	2.02	0.42
3:O:17:ARG:HH21	3:O:28:GLY:HA2	1.84	0.42
3:S:31:HIS:HD2	3:S:48:PRO:HG3	1.84	0.42
6:J:258:DC:H2"	6:J:259:DG:H5"	2.01	0.42
8:U:783:LYS:HB3	8:U:789:HIS:HA	2.02	0.42
1:M:60:LEU:O	1:M:63:ARG:NH2	2.52	0.42
5:I:118:DT:H2"	5:I:119:DA:C8	2.55	0.42
6:J:243:DC:H2"	6:J:244:DC:C5	2.54	0.42
7:L:557:VAL:HG22	7:L:624:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:518:LYS:HG3	8:K:608:PHE:HZ	1.85	0.42
4:P:102:GLU:HG2	7:L:743:ARG:HH12	1.85	0.42
5:I:242:DG:H2"	5:I:243:DT:C6	2.55	0.42
4:T:69:ARG:HB3	4:T:98:LEU:HD13	2.02	0.41
5:I:212:DC:H2"	5:I:213:DC:C5	2.55	0.41
6:J:38:DC:H2"	6:J:39:DA:C8	2.55	0.41
8:U:759:VAL:CG1	8:U:791:ALA:O	2.68	0.41
7:X:570:VAL:HG21	7:X:756:ILE:HB	2.01	0.41
8:K:578:GLU:HG2	8:K:580:PRO:HD2	2.03	0.41
8:K:579:ASP:HB3	8:K:580:PRO:HD3	2.02	0.41
5:I:253:DT:H2"	5:I:254:DA:C8	2.55	0.41
7:L:761:ALA:N	7:L:762:PRO:HD2	2.34	0.41
3:C:25:PHE:CE2	3:C:56:GLU:HA	2.54	0.41
1:E:68:GLN:HE21	1:E:72:ARG:HH21	1.69	0.41
4:P:77:LEU:HD11	4:P:97:LEU:HD12	2.02	0.41
8:U:505:GLU:OE1	8:U:604:ARG:NH1	2.54	0.41
8:Y:892:SER:HA	10:Y:1001:SAH:C	2.50	0.41
7:X:753:VAL:N	7:X:754:PRO:HD2	2.36	0.41
5:I:287:DC:H2"	5:I:288:DG:C8	2.55	0.41
8:U:527:GLN:HE21	8:U:715:ILE:HG13	1.85	0.41
8:W:493:ILE:HD12	8:W:493:ILE:HA	1.98	0.41
8:W:649:VAL:HG11	8:W:898:ILE:HG22	2.03	0.41
6:J:109:DG:H2"	6:J:110:DG:N7	2.35	0.41
7:L:472:ASN:O	7:L:476:CYS:N	2.54	0.41
6:J:211:DT:H2"	6:J:212:DC:C6	2.56	0.41
8:W:604:ARG:HA	8:W:607:MET:HE3	2.03	0.41
8:W:788:ALA:HA	8:W:830:VAL:H	1.86	0.41
8:U:639:LEU:HD22	8:U:687:VAL:HG22	2.03	0.41
8:Y:676:ARG:NE	8:Y:874:TYR:O	2.54	0.41
10:Y:1001:SAH:HN1	10:Y:1001:SAH:HG1	1.67	0.41
1:M:101:VAL:HG21	2:N:40:ARG:HD2	2.03	0.41
1:Q:61:LEU:HD22	2:R:36:ARG:HD2	2.03	0.41
7:L:561:PHE:O	7:L:628:GLY:O	2.39	0.41
1:A:61:LEU:HD12	2:B:37:LEU:HD23	2.03	0.40
1:Q:46:VAL:HB	5:I:247:DT:P	2.61	0.40
5:I:6:DC:H2"	5:I:7:DG:C8	2.56	0.40
5:I:241:DC:H2"	5:I:242:DG:C8	2.57	0.40
6:J:39:DA:H2"	6:J:40:DA:C8	2.56	0.40
7:V:511:ARG:HG2	7:V:518:ARG:HD3	2.03	0.40
8:U:649:VAL:HG11	8:U:898:ILE:HG22	2.03	0.40
3:C:63:LEU:HD22	4:D:42:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:223:DT:H2''	6:J:224:DA:N7	2.37	0.40
8:U:903:ALA:HB3	8:U:904:PRO:HD3	2.02	0.40
7:L:500:GLU:HA	7:L:501:PRO:HA	1.93	0.40
1:E:101:VAL:HA	1:E:104:PHE:HD2	1.87	0.40
3:G:25:PHE:CE2	3:G:56:GLU:HA	2.56	0.40
1:Q:61:LEU:HD12	2:R:37:LEU:HD23	2.02	0.40
7:Z:686:ASP:OD1	8:Y:729:ARG:NH1	2.52	0.40
7:Z:753:VAL:N	7:Z:754:PRO:HD2	2.36	0.40
8:U:558:PHE:HE2	8:U:584:TYR:H	1.69	0.40
8:Y:731:PHE:O	8:Y:734:PHE:HB3	2.21	0.40
7:X:561:PHE:O	7:X:561:PHE:CG	2.73	0.40
5:I:43:DC:H2'	5:I:44:DT:C6	2.56	0.40
5:I:86:DC:H2''	5:I:87:DG:C8	2.55	0.40
8:Y:639:LEU:N	8:Y:639:LEU:CD1	2.84	0.40
7:L:469:LEU:HG	7:L:478:CYS:SG	2.62	0.40
8:K:567:VAL:HG11	8:K:584:TYR:OH	2.21	0.40
3:G:44:GLY:HA2	5:I:121:DG:H5''	2.04	0.40
6:J:318:DC:H1'	6:J:319:DC:O4'	2.22	0.40
7:L:658:LEU:HA	7:L:661:TYR:HD2	1.86	0.40
8:W:527:GLN:HE21	8:W:715:ILE:CG1	2.23	0.40
8:K:661:ILE:HG13	8:K:682:MET:HB2	2.03	0.40

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	94/135 (70%)	91 (97%)	3 (3%)	0	100	100
1	E	95/135 (70%)	94 (99%)	1 (1%)	0	100	100
1	M	97/135 (72%)	96 (99%)	1 (1%)	0	100	100
1	Q	93/135 (69%)	91 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	77/103 (75%)	76 (99%)	1 (1%)	0	100	100
2	F	76/103 (74%)	73 (96%)	3 (4%)	0	100	100
2	N	76/103 (74%)	75 (99%)	1 (1%)	0	100	100
2	R	76/103 (74%)	74 (97%)	2 (3%)	0	100	100
3	C	97/129 (75%)	94 (97%)	3 (3%)	0	100	100
3	G	96/129 (74%)	93 (97%)	3 (3%)	0	100	100
3	O	96/129 (74%)	92 (96%)	4 (4%)	0	100	100
3	S	96/129 (74%)	93 (97%)	3 (3%)	0	100	100
4	D	90/123 (73%)	86 (96%)	4 (4%)	0	100	100
4	H	90/123 (73%)	88 (98%)	2 (2%)	0	100	100
4	P	89/123 (72%)	88 (99%)	1 (1%)	0	100	100
4	T	90/123 (73%)	89 (99%)	1 (1%)	0	100	100
7	L	341/773 (44%)	326 (96%)	15 (4%)	0	100	100
7	V	330/773 (43%)	318 (96%)	12 (4%)	0	100	100
7	X	168/773 (22%)	160 (95%)	8 (5%)	0	100	100
7	Z	165/773 (21%)	161 (98%)	4 (2%)	0	100	100
8	K	417/689 (60%)	396 (95%)	21 (5%)	0	100	100
8	U	419/689 (61%)	399 (95%)	20 (5%)	0	100	100
8	W	417/689 (60%)	399 (96%)	18 (4%)	0	100	100
8	Y	420/689 (61%)	406 (97%)	14 (3%)	0	100	100
All	All	4105/7808 (53%)	3958 (96%)	147 (4%)	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	84/110 (76%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	85/110 (77%)	85 (100%)	0	100	100
1	M	87/110 (79%)	87 (100%)	0	100	100
1	Q	83/110 (76%)	83 (100%)	0	100	100
2	B	65/79 (82%)	65 (100%)	0	100	100
2	F	64/79 (81%)	64 (100%)	0	100	100
2	N	64/79 (81%)	64 (100%)	0	100	100
2	R	64/79 (81%)	64 (100%)	0	100	100
3	C	77/101 (76%)	77 (100%)	0	100	100
3	G	76/101 (75%)	76 (100%)	0	100	100
3	O	76/101 (75%)	76 (100%)	0	100	100
3	S	75/101 (74%)	75 (100%)	0	100	100
4	D	78/103 (76%)	78 (100%)	0	100	100
4	H	78/103 (76%)	78 (100%)	0	100	100
4	P	77/103 (75%)	77 (100%)	0	100	100
4	T	78/103 (76%)	78 (100%)	0	100	100
7	L	299/660 (45%)	299 (100%)	0	100	100
7	V	292/660 (44%)	292 (100%)	0	100	100
7	X	151/660 (23%)	151 (100%)	0	100	100
7	Z	150/660 (23%)	150 (100%)	0	100	100
8	K	369/591 (62%)	369 (100%)	0	100	100
8	U	371/591 (63%)	371 (100%)	0	100	100
8	W	372/591 (63%)	372 (100%)	0	100	100
8	Y	372/591 (63%)	372 (100%)	0	100	100
All	All	3587/6576 (54%)	3587 (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. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	68	GLN
1	A	108	ASN
3	C	24	GLN

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Mol	Chain	Res	Type
3	C	31	HIS
3	C	73	ASN
3	C	82	HIS
4	D	64	ASN
1	E	68	GLN
2	F	27	GLN
2	F	93	GLN
3	G	24	GLN
3	G	31	HIS
3	G	73	ASN
3	G	82	HIS
4	H	64	ASN
4	H	106	HIS
3	O	31	HIS
3	O	73	ASN
3	O	82	HIS
4	P	64	ASN
1	Q	68	GLN
1	Q	108	ASN
3	S	31	HIS
4	T	64	ASN
4	T	106	HIS
7	V	510	GLN
7	Z	598	HIS
7	Z	601	ASN
8	U	527	GLN
8	U	711	ASN
8	U	739	HIS
8	U	789	HIS
8	U	802	ASN
8	U	900	HIS
8	Y	802	ASN
8	Y	816	GLN
8	Y	847	HIS
8	Y	900	HIS
7	L	399	GLN
7	L	678	ASN
7	L	710	HIS
7	X	601	ASN
7	X	615	ASN
7	X	758	HIS
8	W	527	GLN

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Mol	Chain	Res	Type
8	W	694	HIS
8	W	739	HIS
8	W	821	HIS
8	W	886	GLN
8	W	900	HIS
8	K	612	ASN
8	K	816	GLN
8	K	900	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no 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	$\# Z  > 2$
10	SAH	W	1004	-	27,28,28	0.44	0	36,40,40	0.29	0
10	SAH	K	1004	-	27,28,28	0.43	0	36,40,40	0.29	0
10	SAH	Y	1001	-	27,28,28	0.43	0	36,40,40	0.30	0
10	SAH	U	1004	-	27,28,28	0.43	0	36,40,40	0.29	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
10	SAH	W	1004	-	-	7/15/31/31	0/3/3/3
10	SAH	K	1004	-	-	6/15/31/31	0/3/3/3
10	SAH	Y	1001	-	-	7/15/31/31	0/3/3/3
10	SAH	U	1004	-	-	7/15/31/31	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

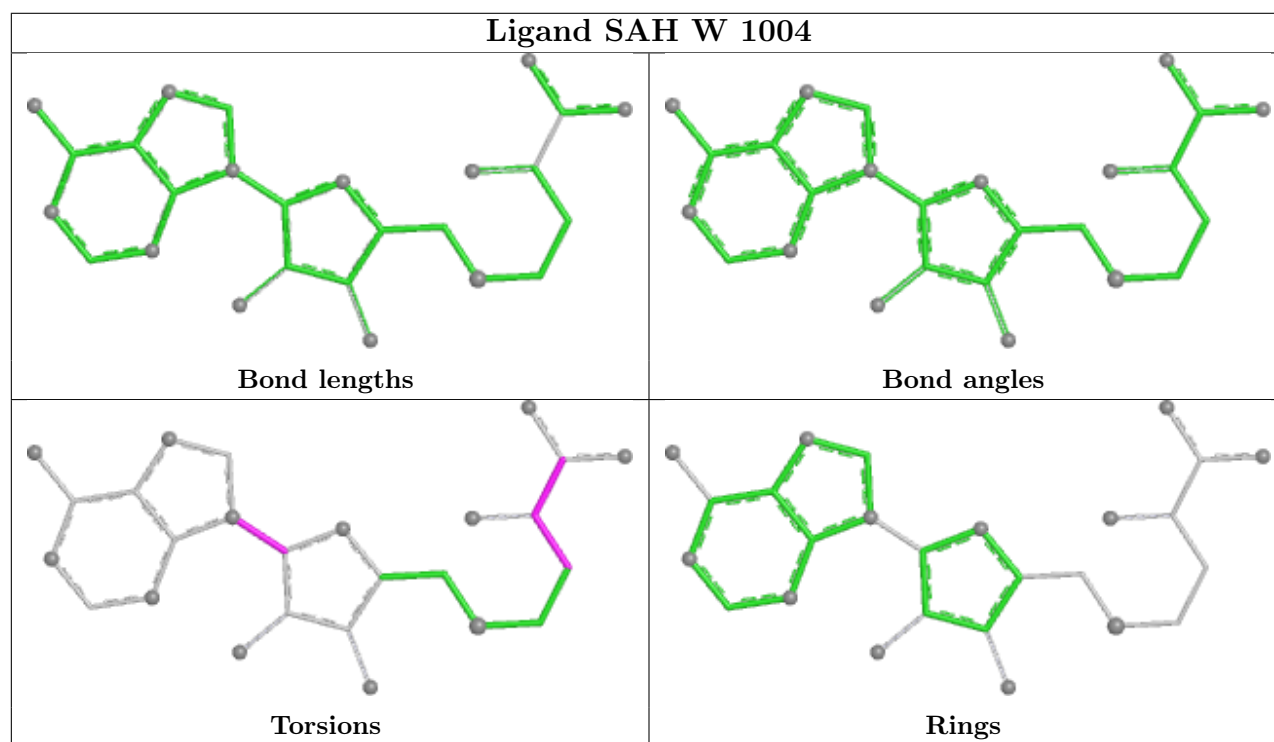
Mol	Chain	Res	Type	Atoms
10	U	1004	SAH	N-CA-CB-CG
10	Y	1001	SAH	N-CA-CB-CG
10	W	1004	SAH	N-CA-CB-CG
10	K	1004	SAH	N-CA-CB-CG
10	U	1004	SAH	C2'-C1'-N9-C8
10	Y	1001	SAH	C2'-C1'-N9-C8
10	W	1004	SAH	C2'-C1'-N9-C8
10	K	1004	SAH	C2'-C1'-N9-C8
10	U	1004	SAH	C-CA-CB-CG
10	Y	1001	SAH	C-CA-CB-CG
10	W	1004	SAH	C-CA-CB-CG
10	K	1004	SAH	C-CA-CB-CG
10	U	1004	SAH	C2'-C1'-N9-C4
10	Y	1001	SAH	C2'-C1'-N9-C4
10	W	1004	SAH	C2'-C1'-N9-C4
10	K	1004	SAH	C2'-C1'-N9-C4
10	U	1004	SAH	OXT-C-CA-CB
10	Y	1001	SAH	OXT-C-CA-CB
10	W	1004	SAH	OXT-C-CA-CB
10	K	1004	SAH	OXT-C-CA-CB
10	U	1004	SAH	O4'-C1'-N9-C8
10	Y	1001	SAH	O4'-C1'-N9-C8
10	W	1004	SAH	O4'-C1'-N9-C8
10	K	1004	SAH	O4'-C1'-N9-C8
10	U	1004	SAH	O-C-CA-CB
10	Y	1001	SAH	O-C-CA-CB
10	W	1004	SAH	O-C-CA-CB

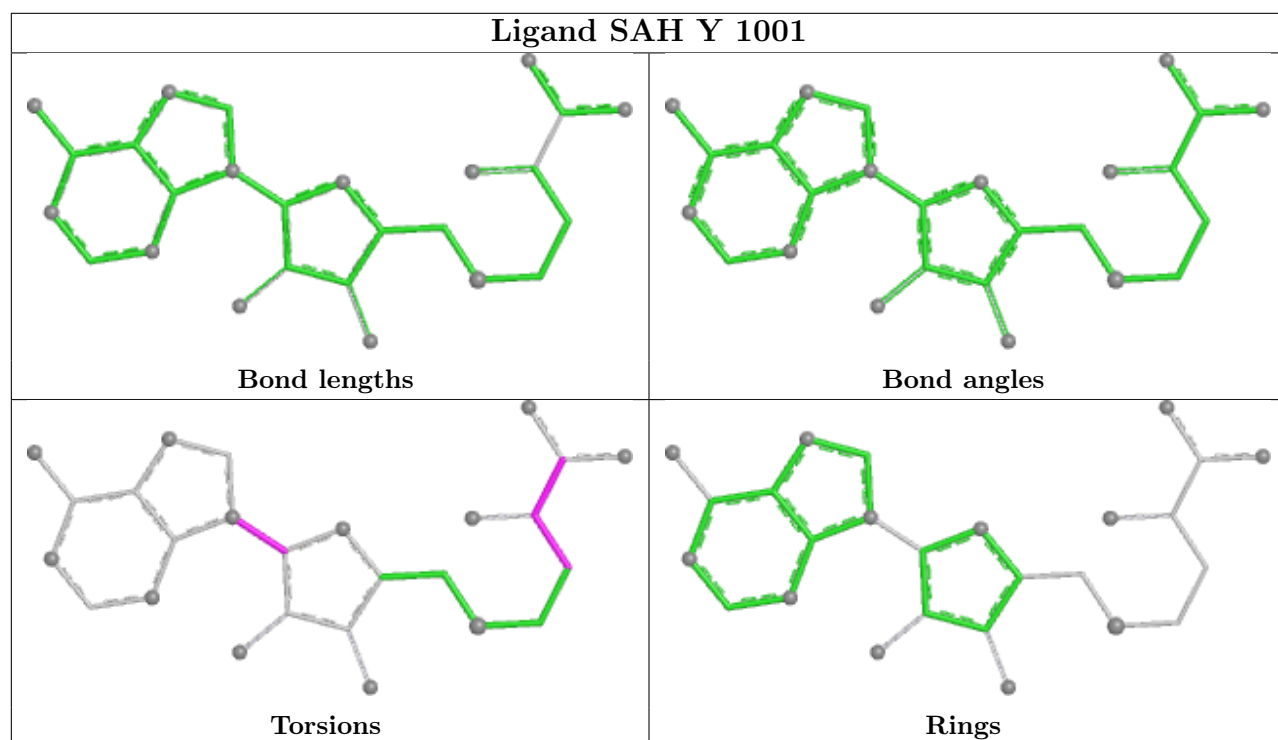
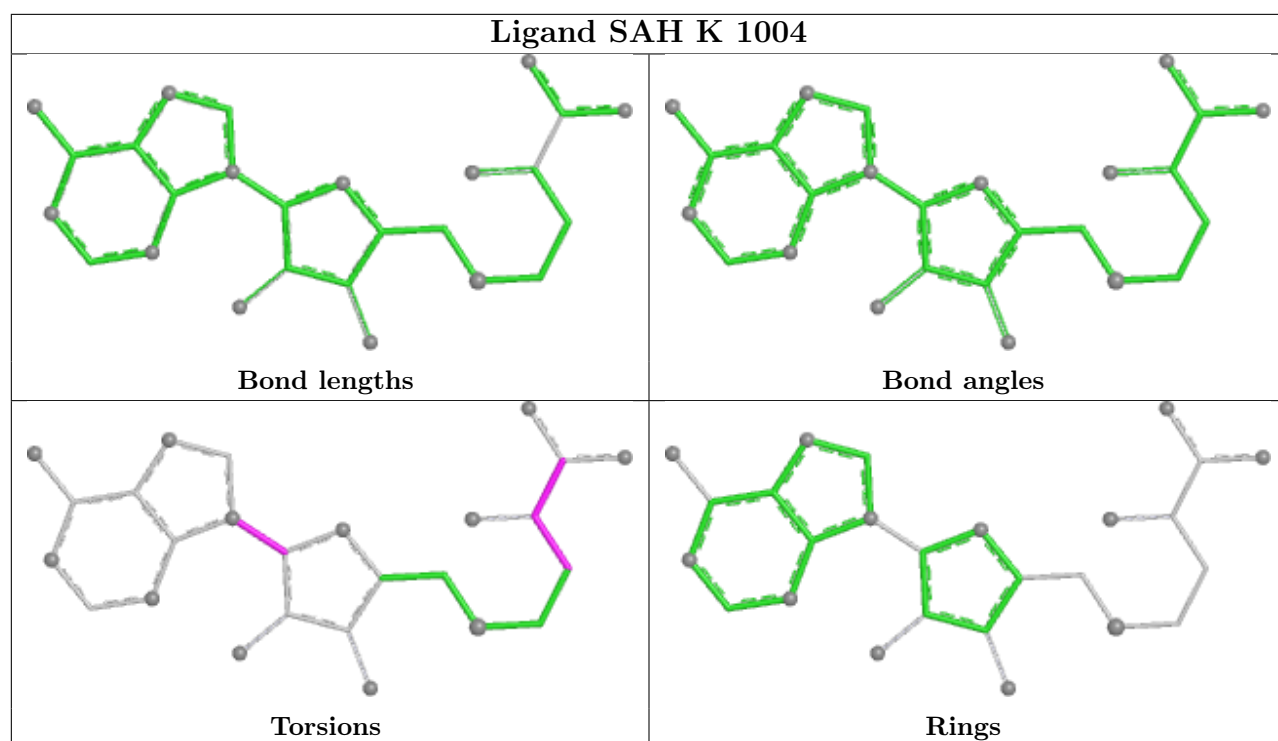
There are no ring outliers.

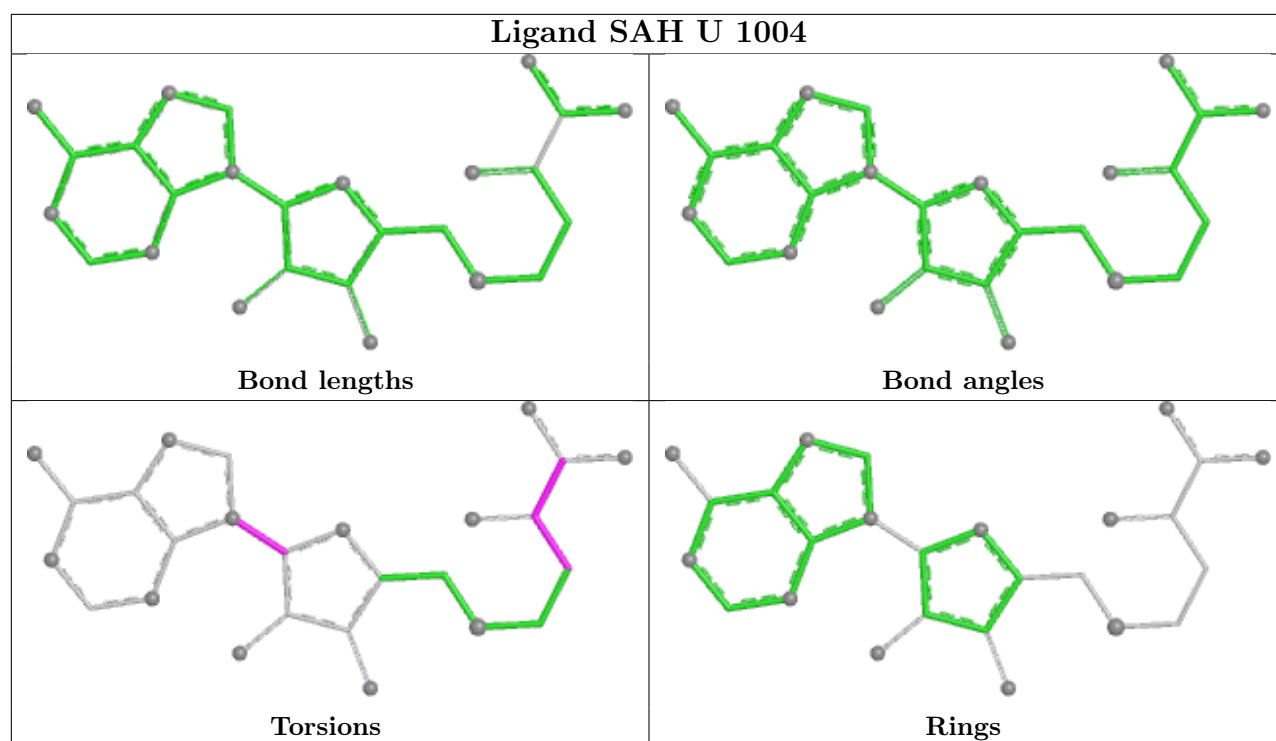
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	K	1004	SAH	1	0
10	Y	1001	SAH	2	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

This section contains visualisations of the EMDB entry EMD-47495. 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

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

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



## 7 Map analysis ⓘ

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

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation

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

## 9 Map-model fit

This section was not generated.