



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:55 pm BST

PDB ID : 4MHT  
Title : TERNARY STRUCTURE OF HHAI METHYLTRANSFERASE WITH NATIVE DNA AND ADOHCY  
Authors : Cheng, X.  
Deposited on : 1996-07-24  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

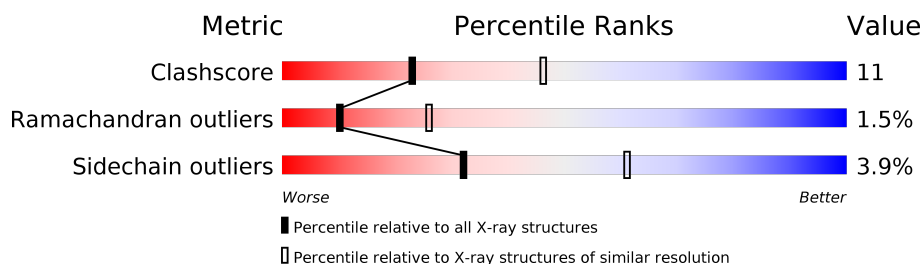
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	12	
2	D	13	
3	A	327	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3254 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 DNA chain called DNA (5'-D(\*GP\*AP\*TP\*AP\*GP\*(5CM)P\*GP\*CP\*TP\*AP\*TP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	12	Total	C	N	O	P	0	0	0
			247	118	45	72	12			

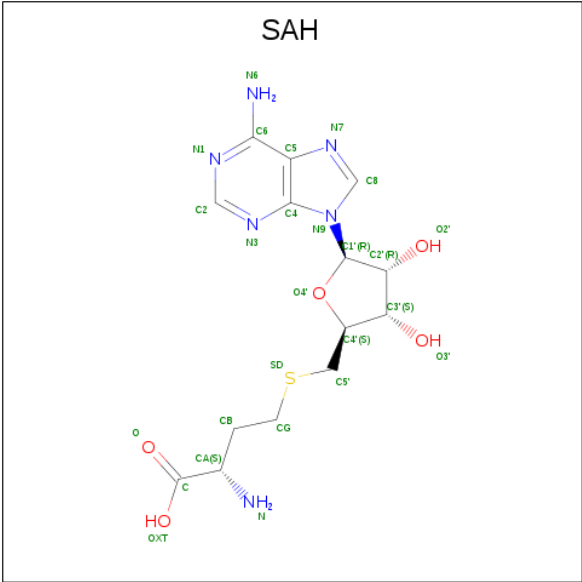
- Molecule 2 is a DNA chain called DNA (5'-D(\*TP\*GP\*AP\*TP\*AP\*GP\*(5CM)P\*GP\*CP\*TP\*AP\*TP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	13	Total	C	N	O	P	0	0	0
			264	128	47	77	12			

- Molecule 3 is a protein called PROTEIN (HHAI METHYLTRANSFERASE (E.C.2.1.1.73)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	327	Total	C	N	O	S	0	0	0
			2606	1662	444	487	13			

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	O	0	0
			1	1		
5	D	7	Total	O	0	0
			7	7		
5	A	103	Total	O	0	0
			103	103		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

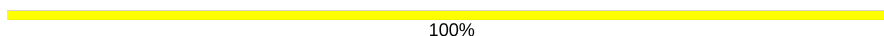
Note EDS was not executed.

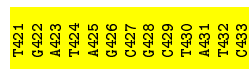
- Molecule 1: DNA (5'-D(\*GP\*AP\*TP\*AP\*GP\*(5CM)P\*GP\*CP\*TP\*AP\*TP\*C)-3')

Chain C: 



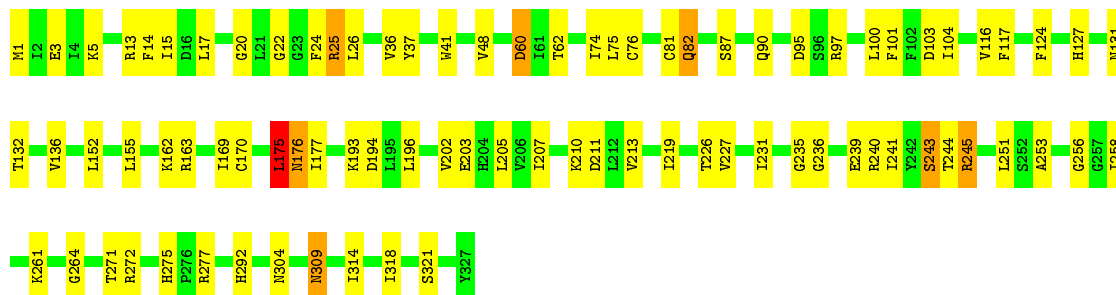
- Molecule 2: DNA (5'-D(\*TP\*GP\*AP\*TP\*AP\*GP\*(5CM)P\*GP\*CP\*TP\*AP\*TP\*C)-3')

Chain D: 



- Molecule 3: PROTEIN (HHA1 METHYLTRANSFERASE (E.C.2.1.1.73))

Chain A: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.86 Å 99.86 Å 325.20 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	90.0 (20.00-2.70)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.178 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3254	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5CM, 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	C	2.56	20/253 (7.9%)	3.73	53/386 (13.7%)
2	D	2.98	26/272 (9.6%)	3.70	61/416 (14.7%)
3	A	0.52	0/2661	0.75	1/3586 (0.0%)
All	All	1.23	46/3186 (1.4%)	1.73	115/4388 (2.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	431	DA	N9-C4	9.40	1.43	1.37
2	D	422	DG	C5'-C4'	9.24	1.61	1.51
2	D	432	DT	N1-C2	8.55	1.44	1.38
2	D	422	DG	N3-C4	8.33	1.41	1.35
2	D	428	DG	C3'-O3'	-8.25	1.33	1.44
2	D	421	DT	C5'-C4'	7.92	1.60	1.51
1	C	408	DG	N9-C4	7.86	1.44	1.38
2	D	428	DG	C2'-C1'	-7.86	1.44	1.52
2	D	424	DT	C5-C7	7.36	1.54	1.50
2	D	421	DT	N1-C2	7.20	1.43	1.38
2	D	425	DA	C5-C6	-7.02	1.34	1.41
2	D	432	DT	C2-O2	7.01	1.28	1.22
2	D	422	DG	C2-N3	7.00	1.38	1.32
1	C	409	DC	C4'-O4'	-6.92	1.38	1.45
2	D	422	DG	C6-N1	6.92	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	413	DC	C4'-C3'	6.80	1.60	1.53
2	D	421	DT	C2'-C1'	-6.79	1.45	1.52
2	D	431	DA	N3-C4	6.78	1.39	1.34
2	D	425	DA	N9-C4	6.77	1.42	1.37
1	C	410	DT	C5-C6	6.61	1.39	1.34
2	D	423	DA	N7-C5	6.46	1.43	1.39
1	C	410	DT	C5-C7	6.38	1.53	1.50
1	C	402	DG	C5'-C4'	6.37	1.58	1.51
1	C	412	DT	N1-C2	6.34	1.43	1.38
2	D	432	DT	C2-N3	6.30	1.42	1.37
2	D	430	DT	C5'-C4'	6.29	1.58	1.51
1	C	404	DT	C5-C7	6.21	1.53	1.50
1	C	403	DA	C4'-C3'	-5.86	1.46	1.52
2	D	430	DT	C5-C7	-5.85	1.46	1.50
2	D	428	DG	N9-C8	-5.79	1.33	1.37
1	C	403	DA	C4'-O4'	-5.78	1.39	1.45
1	C	412	DT	O3'-P	5.74	1.68	1.61
2	D	423	DA	N9-C4	5.59	1.41	1.37
1	C	403	DA	N9-C4	5.58	1.41	1.37
2	D	429	DC	C4'-O4'	-5.49	1.39	1.45
1	C	408	DG	C8-N7	5.41	1.34	1.30
2	D	428	DG	P-O5'	-5.40	1.54	1.59
1	C	412	DT	N1-C6	5.39	1.42	1.38
2	D	431	DA	C3'-O3'	5.37	1.50	1.44
1	C	404	DT	C4'-O4'	-5.37	1.39	1.45
1	C	406	DG	N9-C4	5.30	1.42	1.38
2	D	432	DT	N3-C4	5.29	1.42	1.38
1	C	405	DA	N7-C5	-5.16	1.36	1.39
1	C	410	DT	O3'-P	-5.12	1.55	1.61
1	C	413	DC	C3'-O3'	5.10	1.50	1.44
1	C	402	DG	C6-N1	5.02	1.43	1.39

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	421	DT	O4'-C4'-C3'	-20.41	93.76	106.00
2	D	433	DC	O4'-C1'-C2'	-20.18	89.76	105.90
1	C	409	DC	O4'-C4'-C3'	-17.82	95.31	106.00
1	C	405	DA	O4'-C1'-C2'	-15.60	93.42	105.90
1	C	402	DG	O4'-C4'-C3'	-14.80	97.12	106.00
1	C	410	DT	C4-C5-C7	-13.03	111.18	119.00
1	C	406	DG	O4'-C1'-N9	12.82	116.97	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	429	DC	N1-C2-O2	12.76	126.56	118.90
2	D	425	DA	O4'-C1'-C2'	-12.31	96.05	105.90
2	D	428	DG	O4'-C1'-N9	12.09	116.46	108.00
1	C	402	DG	C5-C6-O6	-11.33	121.80	128.60
2	D	425	DA	N1-C6-N6	10.76	125.06	118.60
1	C	409	DC	O4'-C1'-C2'	-9.87	98.00	105.90
2	D	422	DG	O4'-C4'-C3'	-9.83	100.10	106.00
1	C	402	DG	O4'-C1'-C2'	-9.78	98.08	105.90
1	C	412	DT	O4'-C1'-N1	9.74	114.82	108.00
2	D	426	DG	C2-N3-C4	9.74	116.77	111.90
2	D	429	DC	N3-C2-O2	-9.65	115.14	121.90
1	C	405	DA	N9-C4-C5	9.62	109.65	105.80
2	D	432	DT	C4-C5-C7	-9.25	113.45	119.00
1	C	402	DG	C2-N3-C4	9.04	116.42	111.90
1	C	406	DG	N3-C2-N2	8.98	126.19	119.90
1	C	404	DT	N3-C4-O4	8.80	125.18	119.90
1	C	402	DG	C8-N9-C4	-8.76	102.89	106.40
2	D	430	DT	O4'-C4'-C3'	-8.66	100.80	106.00
1	C	413	DC	C3'-C2'-C1'	-8.25	92.60	102.50
2	D	431	DA	O4'-C1'-N9	8.15	113.70	108.00
1	C	402	DG	N7-C8-N9	8.11	117.16	113.10
2	D	421	DT	C6-C5-C7	-8.00	118.10	122.90
2	D	430	DT	N3-C4-O4	7.99	124.70	119.90
1	C	402	DG	C1'-O4'-C4'	7.94	118.04	110.10
2	D	421	DT	C4'-C3'-C2'	7.88	110.19	103.10
1	C	408	DG	C8-N9-C4	-7.79	103.28	106.40
1	C	404	DT	O4'-C1'-C2'	-7.78	99.67	105.90
2	D	424	DT	O4'-C1'-C2'	-7.78	99.67	105.90
1	C	406	DG	C4'-C3'-C2'	-7.71	96.16	103.10
2	D	423	DA	O4'-C1'-C2'	-7.67	99.76	105.90
2	D	433	DC	N1-C2-O2	7.65	123.49	118.90
2	D	421	DT	N3-C2-O2	-7.49	117.81	122.30
2	D	425	DA	C5-C6-N6	-7.48	117.72	123.70
1	C	406	DG	C2-N3-C4	7.41	115.60	111.90
1	C	405	DA	C8-N9-C4	-7.34	102.86	105.80
2	D	432	DT	C4-C5-C6	7.34	122.41	118.00
2	D	432	DT	N3-C4-O4	7.34	124.30	119.90
2	D	430	DT	C4-C5-C6	7.30	122.38	118.00
1	C	403	DA	O4'-C1'-C2'	-7.29	100.06	105.90
2	D	430	DT	O4'-C1'-N1	7.18	113.03	108.00
2	D	425	DA	O4'-C4'-C3'	7.13	110.28	106.00
1	C	410	DT	C6-C5-C7	6.99	127.09	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	413	DC	C1'-O4'-C4'	-6.90	103.20	110.10
2	D	430	DT	O3'-P-O5'	-6.57	91.52	104.00
1	C	410	DT	C6-N1-C2	-6.57	118.02	121.30
1	C	412	DT	C4-C5-C6	6.52	121.91	118.00
2	D	423	DA	O3'-P-O5'	-6.49	91.67	104.00
2	D	432	DT	O4'-C4'-C3'	6.49	109.89	106.00
2	D	425	DA	C4'-C3'-C2'	-6.45	97.30	103.10
1	C	413	DC	O4'-C1'-N1	6.43	112.50	108.00
2	D	422	DG	C5-C6-O6	-6.41	124.75	128.60
2	D	421	DT	N1-C2-O2	6.41	128.22	123.10
2	D	428	DG	N1-C6-O6	-6.35	116.09	119.90
2	D	428	DG	C4'-C3'-O3'	-6.31	93.93	109.70
2	D	424	DT	C4-C5-C6	6.28	121.77	118.00
1	C	402	DG	C5-N7-C8	-6.28	101.16	104.30
1	C	409	DC	OP1-P-OP2	6.27	129.00	119.60
1	C	402	DG	N1-C6-O6	6.24	123.64	119.90
1	C	406	DG	N1-C2-N3	-6.24	120.16	123.90
2	D	426	DG	N1-C2-N3	-6.23	120.16	123.90
2	D	421	DT	C6-N1-C1'	-6.22	111.07	120.40
1	C	409	DC	C2-N3-C4	6.20	123.00	119.90
1	C	410	DT	C4-C5-C6	6.16	121.70	118.00
1	C	402	DG	N1-C2-N2	6.16	121.74	116.20
1	C	412	DT	O4'-C1'-C2'	-6.15	100.98	105.90
1	C	402	DG	N3-C4-C5	-6.12	125.54	128.60
1	C	406	DG	N1-C6-O6	-6.12	116.23	119.90
1	C	405	DA	C1'-O4'-C4'	6.02	116.12	110.10
1	C	404	DT	C4-C5-C6	6.02	121.61	118.00
1	C	404	DT	O3'-P-O5'	-5.99	92.63	104.00
2	D	431	DA	O4'-C1'-C2'	-5.87	101.21	105.90
2	D	421	DT	C2-N1-C1'	5.85	127.57	118.20
1	C	413	DC	C6-N1-C2	5.81	122.62	120.30
2	D	429	DC	C5-C4-N4	5.78	124.25	120.20
2	D	428	DG	N3-C4-C5	-5.74	125.73	128.60
1	C	409	DC	N1-C2-O2	5.73	122.34	118.90
2	D	432	DT	O4'-C1'-C2'	-5.69	101.35	105.90
2	D	426	DG	O4'-C1'-C2'	-5.67	101.36	105.90
1	C	402	DG	C5-C6-N1	5.67	114.33	111.50
2	D	426	DG	O4'-C1'-N9	5.66	111.96	108.00
1	C	406	DG	C5-C6-N1	5.65	114.33	111.50
1	C	404	DT	P-O3'-C3'	5.58	126.39	119.70
2	D	426	DG	C4'-C3'-C2'	-5.52	98.13	103.10
2	D	430	DT	C3'-C2'-C1'	-5.52	95.88	102.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	425	DA	O5'-P-OP2	-5.46	100.79	105.70
1	C	412	DT	N3-C2-O2	-5.45	119.03	122.30
2	D	424	DT	C6-N1-C2	-5.40	118.60	121.30
1	C	410	DT	O4'-C4'-C3'	5.38	109.23	106.00
2	D	422	DG	N7-C8-N9	5.37	115.78	113.10
2	D	428	DG	O4'-C1'-C2'	5.36	110.19	105.90
1	C	404	DT	C3'-C2'-C1'	5.34	108.91	102.50
2	D	424	DT	N3-C2-O2	-5.33	119.10	122.30
2	D	424	DT	N3-C4-O4	5.32	123.09	119.90
2	D	424	DT	O4'-C1'-N1	-5.26	104.31	108.00
2	D	428	DG	C8-N9-C4	-5.26	104.30	106.40
2	D	432	DT	C5-C4-O4	-5.22	121.25	124.90
3	A	152	LEU	CA-CB-CG	5.21	127.29	115.30
2	D	429	DC	OP2-P-O3'	5.21	116.66	105.20
2	D	425	DA	N1-C2-N3	-5.20	126.70	129.30
2	D	433	DC	C4'-C3'-C2'	-5.19	98.43	103.10
1	C	408	DG	N7-C8-N9	5.18	115.69	113.10
1	C	402	DG	N1-C2-N3	-5.10	120.84	123.90
2	D	432	DT	O4'-C1'-N1	5.10	111.57	108.00
2	D	422	DG	C8-N9-C4	-5.10	104.36	106.40
2	D	421	DT	O4'-C1'-C2'	5.07	109.95	105.90
1	C	409	DC	P-O3'-C3'	5.06	125.77	119.70
1	C	405	DA	P-O3'-C3'	5.05	125.76	119.70
2	D	428	DG	N9-C4-C5	5.00	107.40	105.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	409	DC	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	C	247	0	135	2	0
2	D	264	0	151	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2606	0	2587	65	0
4	A	26	0	19	3	0
5	A	103	0	0	3	0
5	C	1	0	0	0	0
5	D	7	0	0	0	0
All	All	3254	0	2892	68	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 11.

All (68) 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)
3:A:227:VAL:CG2	3:A:243:SER:HB3	2.07	0.83
3:A:227:VAL:HG23	3:A:243:SER:HB3	1.63	0.81
3:A:309:ASN:HD22	3:A:309:ASN:H	1.34	0.74
2:D:427:5CM:C6	3:A:81:CYS:SG	2.77	0.72
3:A:275:HIS:CD2	3:A:277:ARG:H	2.10	0.70
3:A:60:ASP:OD1	3:A:62:THR:HB	1.92	0.69
3:A:202:VAL:HG11	3:A:272:ARG:CZ	2.28	0.64
3:A:202:VAL:HG13	3:A:205:LEU:HD12	1.80	0.63
3:A:275:HIS:HD2	3:A:277:ARG:H	1.45	0.63
2:D:427:5CM:H5A3	4:A:328:SAH:SD	2.39	0.63
2:D:427:5CM:C5A	4:A:328:SAH:SD	2.87	0.62
3:A:309:ASN:HD22	3:A:309:ASN:N	1.97	0.61
3:A:82:GLN:NE2	3:A:82:GLN:H	1.99	0.60
3:A:219:ILE:HD11	3:A:245:ARG:HB3	1.84	0.59
3:A:196:LEU:HD11	3:A:244:THR:HG21	1.84	0.59
3:A:177:ILE:HG23	3:A:321:SER:HB3	1.83	0.59
3:A:241:ILE:HA	3:A:264:GLY:O	2.04	0.57
1:C:406:DG:O6	3:A:256:GLY:HA3	2.06	0.55
3:A:231:ILE:HG13	3:A:235:GLY:CA	2.38	0.54
3:A:231:ILE:HG13	3:A:235:GLY:HA3	1.89	0.54
3:A:207:ILE:HD13	3:A:258:ILE:HG13	1.88	0.54
3:A:15:ILE:HG22	3:A:37:TYR:HB3	1.90	0.54
3:A:193:LYS:HE3	3:A:194:ASP:OD1	2.09	0.53
3:A:127:HIS:HD2	3:A:132:THR:CG2	2.21	0.53
3:A:15:ILE:HD11	3:A:75:LEU:HD12	1.91	0.52
3:A:3:GLU:OE2	3:A:5:LYS:HE3	2.11	0.50
3:A:48:VAL:CG2	3:A:292:HIS:HB2	2.41	0.50
3:A:175:LEU:O	3:A:176:ASN:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:13:ARG:HE	3:A:36:VAL:HG11	1.75	0.50
3:A:162:LYS:O	3:A:162:LYS:HG2	2.12	0.50
2:D:427:5CM:H1'	3:A:304:ASN:HA	1.94	0.50
3:A:236:GLY:N	3:A:239:GLU:HG3	2.27	0.49
3:A:163:ARG:NH2	3:A:251:LEU:O	2.46	0.49
3:A:202:VAL:HG11	3:A:272:ARG:CD	2.43	0.48
3:A:116:VAL:HB	3:A:170:CYS:HB2	1.95	0.48
3:A:95:ASP:OD1	3:A:97:ARG:HD3	2.14	0.48
3:A:100:LEU:O	3:A:103:ASP:HB2	2.14	0.48
3:A:226:THR:HA	5:A:351:HOH:O	2.14	0.48
3:A:127:HIS:CD2	3:A:132:THR:HG21	2.49	0.47
3:A:20:GLY:HA3	4:A:328:SAH:HB1	1.95	0.47
3:A:202:VAL:HG11	3:A:272:ARG:NE	2.29	0.47
1:C:402:DG:O5'	1:C:402:DG:H2'	2.15	0.47
3:A:48:VAL:HG22	3:A:292:HIS:HB2	1.97	0.47
3:A:155:LEU:HD12	3:A:155:LEU:C	2.36	0.46
3:A:207:ILE:O	3:A:271:THR:HG23	2.16	0.46
3:A:202:VAL:HG11	3:A:272:ARG:HD2	1.98	0.45
3:A:22:GLY:O	3:A:25:ARG:HB2	2.16	0.45
3:A:169:ILE:HD12	3:A:318:ILE:HD11	1.97	0.45
3:A:24:PHE:CD2	3:A:76:CYS:HB3	2.51	0.45
3:A:169:ILE:HD11	3:A:314:ILE:HG21	1.98	0.45
3:A:309:ASN:H	3:A:309:ASN:ND2	2.10	0.45
3:A:1:MET:HA	3:A:309:ASN:ND2	2.32	0.44
3:A:202:VAL:HG11	3:A:272:ARG:NH1	2.32	0.44
3:A:253:ALA:O	3:A:261:LYS:HE3	2.18	0.43
2:D:427:5CM:N1	3:A:81:CYS:SG	2.91	0.43
3:A:196:LEU:HD11	3:A:244:THR:CG2	2.49	0.43
3:A:210:LYS:NZ	5:A:440:HOH:O	2.51	0.43
3:A:211:ASP:O	3:A:213:VAL:HG23	2.19	0.43
3:A:177:ILE:CG2	3:A:321:SER:HB3	2.48	0.42
3:A:163:ARG:HD3	5:A:381:HOH:O	2.18	0.42
3:A:15:ILE:HD12	3:A:17:LEU:HD21	2.01	0.42
3:A:101:PHE:O	3:A:104:ILE:HB	2.19	0.42
3:A:14:PHE:HB3	3:A:74:ILE:HB	2.02	0.42
3:A:124:PHE:HZ	3:A:136:VAL:HG21	1.84	0.42
3:A:127:HIS:CD2	3:A:132:THR:CG2	3.02	0.41
3:A:227:VAL:O	3:A:227:VAL:HG23	2.20	0.41
3:A:25:ARG:O	3:A:26:LEU:C	2.59	0.40
3:A:26:LEU:HD23	3:A:26:LEU:HA	1.90	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 X-ray entries followed by that with respect to entries of similar resolution.

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	
3	A	325/327 (99%)	296 (91%)	24 (7%)	5 (2%)	10	26

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	60	ASP
3	A	90	GLN
3	A	175	LEU
3	A	176	ASN
3	A	203	GLU

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	
3	A	283/283 (100%)	272 (96%)	11 (4%)	32	61

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	25	ARG
3	A	41	TRP
3	A	82	GLN
3	A	87	SER
3	A	117	PHE
3	A	131	ASN

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Mol	Chain	Res	Type
3	A	175	LEU
3	A	240	ARG
3	A	243	SER
3	A	245	ARG
3	A	309	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	72	HIS
3	A	82	GLN
3	A	127	HIS
3	A	268	ASN
3	A	275	HIS
3	A	309	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	5CM	D	427	2	15,21,22	2.90	4 (26%)	19,30,33	6.17	10 (52%)
1	5CM	C	407	1,2	15,21,22	3.61	2 (13%)	19,30,33	2.82	5 (26%)

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
2	5CM	D	427	2	-	1/4/21/22	0/2/2/2
1	5CM	C	407	1,2	-	0/4/21/22	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	407	5CM	C5A-C5	-13.22	1.24	1.51
2	D	427	5CM	C5A-C5	9.12	1.69	1.51
2	D	427	5CM	O3'-C3'	3.48	1.50	1.43
2	D	427	5CM	C5'-C4'	2.85	1.60	1.51
1	C	407	5CM	O4'-C4'	-2.32	1.39	1.45
2	D	427	5CM	C1'-N1	2.18	1.55	1.49

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	427	5CM	C5A-C5-C4	-23.21	98.22	121.72
2	D	427	5CM	O4'-C4'-C3'	-7.45	88.29	105.67
1	C	407	5CM	C5A-C5-C4	-6.51	115.13	121.72
2	D	427	5CM	O4'-C1'-C2'	-6.50	93.97	106.25
1	C	407	5CM	C2-N3-C4	6.07	123.35	116.02
1	C	407	5CM	C5A-C5-C6	5.58	130.45	118.68
2	D	427	5CM	C2-N3-C4	4.18	121.06	116.02
1	C	407	5CM	N4-C4-N3	3.94	122.60	117.03
2	D	427	5CM	C2'-C1'-N1	3.88	123.22	114.27
2	D	427	5CM	C4'-O4'-C1'	3.58	118.10	109.45
2	D	427	5CM	C6-N1-C1'	3.40	126.88	119.24
1	C	407	5CM	O4'-C1'-C2'	-3.13	100.33	106.25
2	D	427	5CM	C5A-C5-C6	-2.83	112.71	118.68
2	D	427	5CM	C2'-C3'-C4'	-2.74	97.06	102.76
2	D	427	5CM	O5'-C5'-C4'	2.51	117.52	108.99

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	427	5CM	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 5 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	427	5CM	5	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z  > 2$
4	SAH	A	328	-	21,28,28	1.30	2 (9%)	20,40,40	2.33	3 (15%)

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
4	SAH	A	328	-	-	0/7/31/31	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	328	SAH	C2'-C1'	-4.14	1.47	1.53
4	A	328	SAH	C8-N7	-2.81	1.29	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	328	SAH	O4'-C1'-C2'	-8.14	95.04	106.93
4	A	328	SAH	C5-C6-N6	4.52	127.22	120.35
4	A	328	SAH	CB-CG-SD	-2.00	108.81	113.31

There are no chirality outliers.

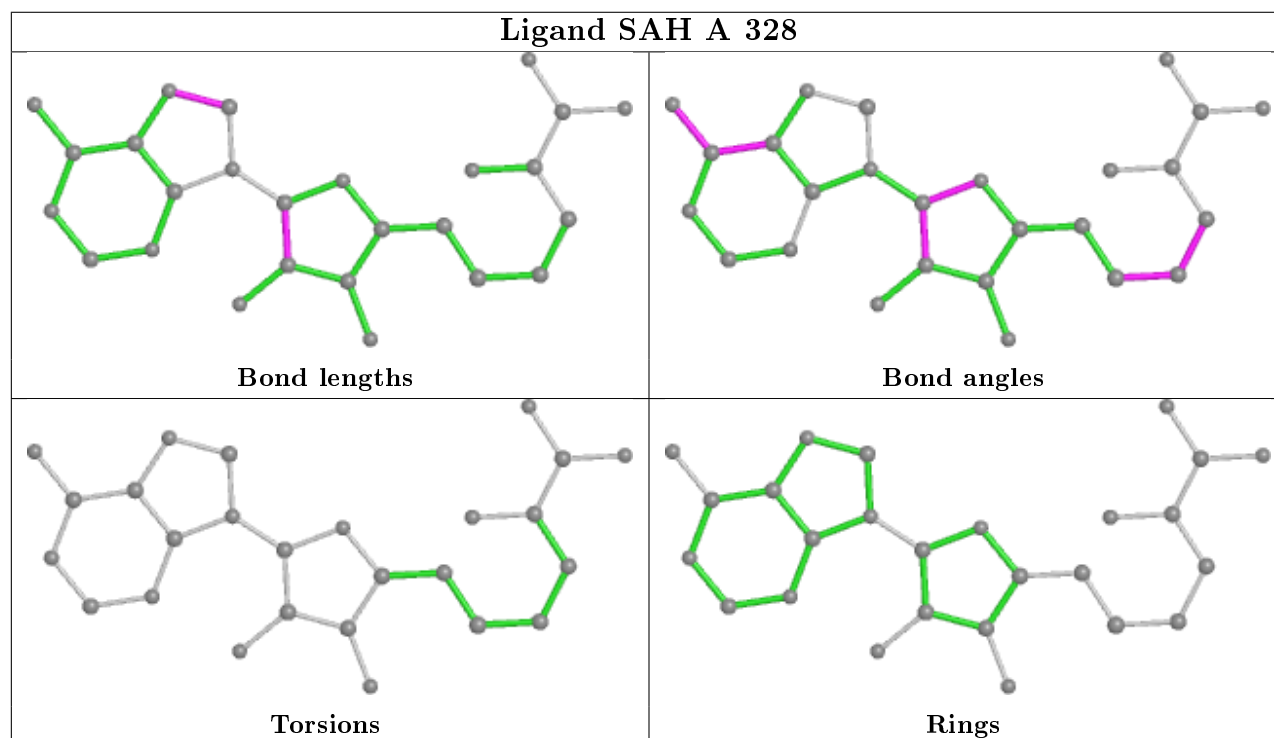
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	328	SAH	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.