



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 11:07 pm BST

PDB ID : 1MHT
Title : COVALENT TERNARY STRUCTURE OF HHAI METHYLTRANSFERASE, DNA AND S-ADENOSYL-L-HOMOCYSTEINE
Authors : Cheng, X.
Deposited on : 1994-12-08
Resolution : 2.60 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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)
Xtrriage (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

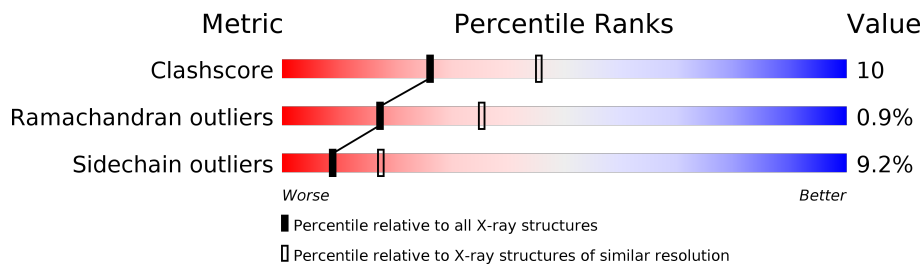
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 ≥ 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	B	12	
2	C	13	
3	A	327	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	C36	B	407	X	-	-	-
2	C36	C	427	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3144 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(P*GP*AP*TP*AP*GP*(C36)P*GP*CP*TP*AP*TP*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	F	N	O	P			
1	B	12	247	117	1	45	72	12	0	0	0

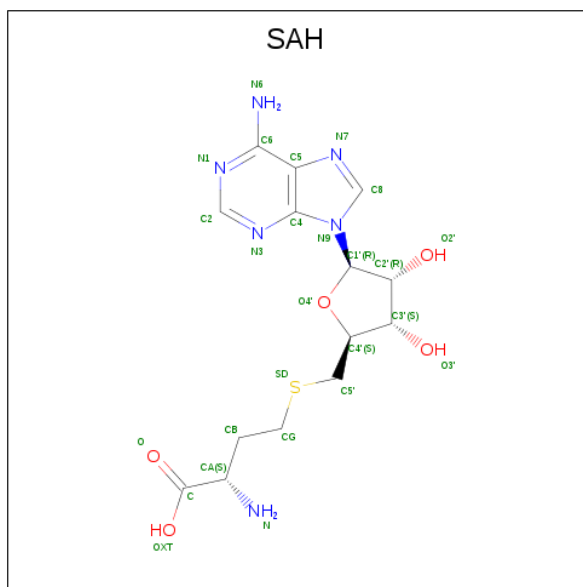
- Molecule 2 is a DNA chain called DNA (5'-D(*TP*GP*AP*TP*AP*GP*(C36)P*GP*CP*TP*AP*TP*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	F	N	O	P			
2	C	13	265	128	1	47	77	12	0	0	0

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

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

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S).



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

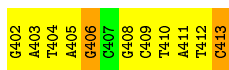
3 Residue-property plots [i](#)

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.

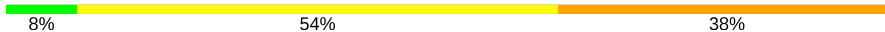
Note EDS was not executed.

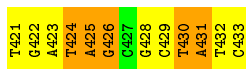
- Molecule 1: DNA (5'-D(P*GP*AP*TP*AP*GP*(C36)P*GP*CP*TP*AP*TP*C)-3')

Chain B: 



- Molecule 2: DNA (5'-D(*TP*GP*AP*TP*AP*GP*(C36)P*GP*CP*TP*AP*TP*C)-3')

Chain C: 




- Molecule 3: PROTEIN (HHA1 METHYLTRANSFERASE)

Chain A: 







4 Data and refinement statistics

Xtrriage (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, α , β , γ	99.86Å 99.86Å 325.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.60)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.174 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3144	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

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, C36

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	B	2.38	13/253 (5.1%)	3.29	51/386 (13.2%)
2	C	2.79	15/272 (5.5%)	3.55	52/416 (12.5%)
3	A	0.52	0/2661	0.72	1/3586 (0.0%)
All	All	1.16	28/3186 (0.9%)	1.61	104/4388 (2.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	1
2	C	1	1
All	All	2	2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	428	DG	C6-N1	-10.65	1.32	1.39
2	C	424	DT	C5-C7	10.17	1.56	1.50
2	C	423	DA	N3-C4	9.11	1.40	1.34
1	B	412	DT	C5-C7	8.90	1.55	1.50
1	B	409	DC	C4'-O4'	-8.56	1.36	1.45
1	B	408	DG	N9-C4	8.36	1.44	1.38
2	C	422	DG	C5'-C4'	7.68	1.59	1.51
2	C	428	DG	C5'-C4'	7.53	1.59	1.51
2	C	433	DC	C2-N3	6.79	1.41	1.35
1	B	402	DG	N1-C2	6.55	1.43	1.37
2	C	423	DA	N9-C4	6.43	1.41	1.37
2	C	425	DA	O3'-P	-6.41	1.53	1.61
2	C	422	DG	C2-N3	6.21	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	421	DT	C5-C7	6.03	1.53	1.50
1	B	413	DC	C4'-C3'	5.99	1.59	1.53
2	C	432	DT	N1-C2	5.93	1.42	1.38
2	C	428	DG	C2'-C1'	-5.92	1.46	1.52
1	B	408	DG	C4'-C3'	-5.73	1.46	1.52
1	B	408	DG	C2'-C1'	-5.69	1.46	1.52
2	C	428	DG	O3'-P	-5.66	1.54	1.61
1	B	405	DA	N7-C5	-5.49	1.35	1.39
1	B	410	DT	P-O5'	-5.34	1.54	1.59
1	B	411	DA	O3'-P	-5.34	1.54	1.61
1	B	405	DA	C4'-C3'	-5.23	1.47	1.52
1	B	412	DT	C1'-N1	5.21	1.56	1.49
1	B	404	DT	P-O5'	-5.19	1.54	1.59
2	C	425	DA	O4'-C1'	-5.07	1.36	1.42
2	C	425	DA	C4'-C3'	-5.00	1.47	1.52

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	421	DT	O4'-C4'-C3'	-19.15	94.51	106.00
2	C	433	DC	O4'-C1'-C2'	-16.51	92.69	105.90
2	C	433	DC	O4'-C4'-C3'	-13.97	97.62	106.00
2	C	429	DC	N1-C2-O2	12.86	126.62	118.90
1	B	405	DA	O4'-C1'-C2'	-12.59	95.83	105.90
1	B	404	DT	O4'-C1'-C2'	-12.10	96.22	105.90
1	B	412	DT	O4'-C1'-C2'	-11.30	96.86	105.90
1	B	412	DT	O4'-C1'-N1	11.11	115.77	108.00
1	B	409	DC	O4'-C4'-C3'	-10.36	99.78	106.00
2	C	433	DC	C1'-O4'-C4'	-10.31	99.79	110.10
1	B	409	DC	C1'-O4'-C4'	-9.82	100.28	110.10
2	C	425	DA	O4'-C1'-N9	-9.71	101.20	108.00
2	C	430	DT	O4'-C1'-C2'	-9.56	98.25	105.90
2	C	422	DG	O4'-C4'-C3'	-9.09	100.55	106.00
2	C	421	DT	N3-C2-O2	-8.99	116.91	122.30
2	C	423	DA	O4'-C1'-C2'	-8.91	98.77	105.90
1	B	410	DT	C4-C5-C6	8.85	123.31	118.00
2	C	430	DT	C4-C5-C6	8.75	123.25	118.00
2	C	426	DG	O4'-C1'-C2'	-8.66	98.97	105.90
2	C	430	DT	N3-C4-O4	8.42	124.95	119.90
2	C	421	DT	N1-C2-O2	8.36	129.79	123.10
2	C	429	DC	N3-C2-O2	-8.26	116.12	121.90
2	C	424	DT	O4'-C1'-C2'	-8.26	99.30	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	424	DT	N3-C4-O4	8.07	124.74	119.90
2	C	423	DA	O3'-P-O5'	-7.90	88.99	104.00
2	C	423	DA	O4'-C1'-N9	7.87	113.51	108.00
1	B	406	DG	N3-C2-N2	7.73	125.31	119.90
1	B	404	DT	O3'-P-O5'	-7.70	89.37	104.00
1	B	405	DA	C4'-C3'-C2'	-7.69	96.18	103.10
1	B	403	DA	O4'-C1'-C2'	-7.64	99.79	105.90
2	C	430	DT	O4'-C4'-C3'	-7.59	101.44	106.00
2	C	429	DC	O4'-C4'-C3'	7.54	110.53	106.00
1	B	404	DT	O4'-C1'-N1	-7.50	102.75	108.00
2	C	426	DG	N1-C6-O6	-7.49	115.41	119.90
1	B	402	DG	C5-C6-O6	-7.44	124.14	128.60
2	C	426	DG	C4'-C3'-C2'	-7.42	96.42	103.10
1	B	412	DT	C4-C5-C6	7.38	122.43	118.00
1	B	410	DT	O5'-P-OP2	-7.34	99.09	105.70
2	C	430	DT	C6-C5-C7	-7.32	118.51	122.90
1	B	406	DG	C4'-C3'-C2'	-7.26	96.57	103.10
2	C	424	DT	O4'-C1'-N1	-7.24	102.93	108.00
2	C	430	DT	O3'-P-O5'	-7.22	90.28	104.00
1	B	402	DG	N3-C2-N2	-7.21	114.86	119.90
1	B	411	DA	O4'-C1'-N9	-7.19	102.97	108.00
2	C	426	DG	C2-N3-C4	7.07	115.44	111.90
2	C	422	DG	O4'-C1'-N9	7.02	112.92	108.00
2	C	432	DT	O4'-C1'-C2'	-7.00	100.30	105.90
2	C	432	DT	C4-C5-C6	6.99	122.20	118.00
1	B	410	DT	C6-N1-C2	-6.99	117.81	121.30
2	C	429	DC	C6-N1-C2	6.98	123.09	120.30
1	B	404	DT	C6-C5-C7	-6.94	118.73	122.90
1	B	412	DT	N3-C2-O2	-6.86	118.18	122.30
1	B	409	DC	P-O3'-C3'	6.78	127.84	119.70
2	C	428	DG	O3'-P-O5'	-6.74	91.20	104.00
2	C	421	DT	C1'-O4'-C4'	-6.71	103.39	110.10
1	B	410	DT	C4-C5-C7	-6.69	114.98	119.00
2	C	432	DT	C4-C5-C7	-6.63	115.02	119.00
2	C	431	DA	O4'-C1'-N9	6.62	112.64	108.00
2	C	424	DT	C4-C5-C7	-6.55	115.07	119.00
1	B	410	DT	N1-C2-N3	6.42	118.45	114.60
2	C	425	DA	O4'-C1'-C2'	-6.33	100.84	105.90
2	C	421	DT	C6-N1-C1'	-6.26	111.01	120.40
1	B	413	DC	N1-C2-O2	6.26	122.66	118.90
2	C	426	DG	N3-C4-C5	-6.25	125.48	128.60
2	C	426	DG	N9-C4-C5	6.24	107.89	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	DG	N1-C2-N2	6.22	121.80	116.20
1	B	412	DT	N1-C2-N3	6.21	118.32	114.60
1	B	412	DT	N3-C4-O4	6.20	123.62	119.90
1	B	409	DC	C6-N1-C2	6.18	122.77	120.30
1	B	410	DT	N3-C4-C5	-6.14	111.52	115.20
1	B	408	DG	N3-C4-C5	-6.14	125.53	128.60
2	C	429	DC	C1'-O4'-C4'	-6.04	104.06	110.10
2	C	421	DT	C2-N1-C1'	6.02	127.83	118.20
1	B	413	DC	C6-N1-C2	5.97	122.69	120.30
2	C	433	DC	C5-C4-N4	-5.96	116.03	120.20
1	B	409	DC	C2-N3-C4	5.92	122.86	119.90
2	C	430	DT	C3'-C2'-C1'	-5.89	95.44	102.50
1	B	402	DG	N1-C6-O6	5.88	123.43	119.90
1	B	406	DG	N1-C2-N3	-5.86	120.38	123.90
1	B	411	DA	P-O3'-C3'	5.84	126.71	119.70
2	C	421	DT	C6-C5-C7	-5.74	119.46	122.90
1	B	408	DG	C2-N3-C4	5.73	114.76	111.90
1	B	406	DG	C2-N3-C4	5.70	114.75	111.90
1	B	402	DG	C8-N9-C4	-5.64	104.14	106.40
1	B	406	DG	O4'-C1'-C2'	-5.62	101.41	105.90
1	B	408	DG	P-O5'-C5'	5.59	129.84	120.90
2	C	421	DT	C4'-C3'-C2'	5.58	108.13	103.10
1	B	404	DT	C4-C5-C6	5.57	121.34	118.00
1	B	408	DG	P-O3'-C3'	-5.54	113.05	119.70
1	B	409	DC	P-O5'-C5'	-5.50	112.10	120.90
1	B	410	DT	N1-C2-O2	-5.43	118.76	123.10
2	C	433	DC	N3-C4-N4	5.42	121.80	118.00
1	B	410	DT	N3-C4-O4	5.25	123.05	119.90
2	C	431	DA	C4'-C3'-C2'	-5.25	98.38	103.10
2	C	425	DA	N1-C6-N6	5.25	121.75	118.60
1	B	403	DA	O3'-P-O5'	-5.22	94.08	104.00
2	C	428	DG	O4'-C1'-N9	5.18	111.63	108.00
3	A	260	ALA	CB-CA-C	-5.17	102.34	110.10
2	C	423	DA	C8-N9-C4	-5.17	103.73	105.80
1	B	412	DT	C5'-C4'-C3'	-5.13	104.86	114.10
2	C	421	DT	O3'-P-O5'	5.11	113.72	104.00
1	B	410	DT	P-O5'-C5'	-5.11	112.72	120.90
1	B	413	DC	C3'-C2'-C1'	-5.07	96.42	102.50
1	B	410	DT	C5'-C4'-C3'	-5.01	105.08	114.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	407	C36	C5
2	C	427	C36	C5

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	413	DC	Sidechain
2	C	430	DT	Sidechain

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	B	247	0	136	1	0
2	C	265	0	147	3	0
3	A	2606	0	2586	61	0
4	A	26	0	19	0	0
All	All	3144	0	2888	63	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 10.

All (63) 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:202:VAL:HG13	3:A:205:LEU:HD12	1.56	0.86
3:A:275:HIS:HD2	3:A:277:ARG:H	1.31	0.79
3:A:309:ASN:HD22	3:A:309:ASN:H	1.31	0.76
3:A:275:HIS:CD2	3:A:277:ARG:H	2.06	0.74
3:A:309:ASN:HD22	3:A:309:ASN:N	1.87	0.70
3:A:69:ILE:O	3:A:111:LYS:HE3	1.94	0.68
1:B:406:DG:O6	3:A:256:GLY:HA3	1.94	0.66
3:A:1:MET:HA	3:A:309:ASN:ND2	2.12	0.65
3:A:275:HIS:HD2	3:A:277:ARG:N	1.95	0.65
3:A:207:ILE:O	3:A:271:THR:HG23	1.98	0.63
3:A:60:ASP:OD1	3:A:62:THR:HB	1.96	0.63
3:A:202:VAL:HG11	3:A:272:ARG:CZ	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:93:PHE:CE2	3:A:132:THR:HG22	2.34	0.62
3:A:223:THR:HG22	3:A:225:LYS:HG2	1.82	0.62
3:A:231:ILE:HG13	3:A:235:GLY:CA	2.32	0.60
3:A:309:ASN:H	3:A:309:ASN:ND2	2.02	0.58
3:A:202:VAL:HG11	3:A:272:ARG:NH1	2.19	0.58
3:A:140:MET:HG2	3:A:170:CYS:SG	2.44	0.57
3:A:223:THR:CG2	3:A:225:LYS:HG2	2.36	0.56
3:A:283:MET:HE2	3:A:305:SER:HB3	1.88	0.55
3:A:25:ARG:O	3:A:29:GLU:HB2	2.08	0.54
3:A:202:VAL:HG11	3:A:272:ARG:HD2	1.91	0.53
3:A:297:GLN:O	3:A:301:GLN:HG3	2.09	0.52
3:A:231:ILE:HG12	3:A:232:VAL:N	2.25	0.51
3:A:232:VAL:HG12	3:A:239:GLU:HB2	1.93	0.51
3:A:202:VAL:HG12	3:A:202:VAL:O	2.11	0.50
3:A:15:ILE:CD1	3:A:37:TYR:HB3	2.42	0.49
2:C:426:DG:N7	3:A:240:ARG:NH2	2.61	0.49
3:A:207:ILE:HD13	3:A:258:ILE:HG13	1.95	0.49
3:A:28:LEU:HD23	3:A:28:LEU:N	2.28	0.49
3:A:236:GLY:N	3:A:239:GLU:HG3	2.28	0.48
3:A:238:GLY:HA3	3:A:257:GLY:HA3	1.94	0.48
3:A:163:ARG:NH2	3:A:251:LEU:O	2.46	0.48
3:A:82:GLN:NE2	3:A:82:GLN:H	2.12	0.48
3:A:127:HIS:HD2	3:A:132:THR:CG2	2.26	0.48
3:A:219:ILE:HD13	3:A:227:VAL:HG11	1.96	0.47
3:A:193:LYS:HG3	3:A:194:ASP:OD1	2.14	0.47
3:A:202:VAL:CG1	3:A:272:ARG:HD2	2.44	0.47
3:A:175:LEU:H	3:A:175:LEU:HG	1.37	0.46
3:A:309:ASN:N	3:A:309:ASN:ND2	2.59	0.46
2:C:424:DT:H2'	2:C:425:DA:C8	2.49	0.46
3:A:231:ILE:HG13	3:A:235:GLY:HA3	1.98	0.46
3:A:95:ASP:OD1	3:A:97:ARG:HD3	2.15	0.46
3:A:25:ARG:HD2	3:A:53:PHE:CE1	2.51	0.46
3:A:127:HIS:CD2	3:A:132:THR:HG21	2.52	0.46
3:A:14:PHE:CZ	3:A:35:CYS:HB2	2.51	0.45
3:A:202:VAL:HG11	3:A:272:ARG:CD	2.46	0.45
3:A:260:ALA:O	3:A:261:LYS:HB2	2.16	0.45
3:A:267:VAL:HG21	3:A:272:ARG:NE	2.31	0.45
3:A:155:LEU:HD12	3:A:155:LEU:C	2.37	0.45
3:A:227:VAL:HG22	3:A:243:SER:HB3	1.99	0.45
2:C:431:DA:O5'	2:C:431:DA:H2'	2.17	0.44
3:A:101:PHE:O	3:A:104:ILE:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:137:LYS:HG2	3:A:141:ASN:HD21	1.84	0.43
3:A:204:HIS:CD2	3:A:204:HIS:H	2.38	0.42
3:A:228:ARG:NH2	3:A:240:ARG:HD2	2.35	0.42
3:A:231:ILE:HG13	3:A:235:GLY:HA2	2.02	0.41
3:A:26:LEU:HD23	3:A:26:LEU:HA	1.86	0.41
3:A:149:ALA:HA	3:A:167:TYR:O	2.21	0.41
3:A:68:THR:HG22	3:A:68:THR:O	2.21	0.41
3:A:127:HIS:CD2	3:A:132:THR:CG2	3.03	0.41
3:A:279:CYS:O	3:A:282:VAL:HG12	2.21	0.41
3:A:15:ILE:HD13	3:A:72:HIS:HB3	2.04	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%)	298 (92%)	24 (7%)	3 (1%)	17 35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	60	ASP
3	A	174	ASP
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%)	257 (91%)	26 (9%)	9 17

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	15	ILE
3	A	25	ARG
3	A	28	LEU
3	A	41	TRP
3	A	48	VAL
3	A	62	THR
3	A	80	PRO
3	A	82	GLN
3	A	96	SER
3	A	106	ARG
3	A	117	PHE
3	A	131	ASN
3	A	132	THR
3	A	169	ILE
3	A	175	LEU
3	A	190	THR
3	A	212	LEU
3	A	227	VAL
3	A	231	ILE
3	A	232	VAL
3	A	240	ARG
3	A	245	ARG
3	A	250	THR
3	A	271	THR
3	A	282	VAL
3	A	309	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	72	HIS
3	A	82	GLN
3	A	90	GLN
3	A	127	HIS
3	A	141	ASN

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Mol	Chain	Res	Type
3	A	204	HIS
3	A	268	ASN
3	A	275	HIS
3	A	309	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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
1	C36	B	407	1,2	15,21,24	3.19	5 (33%)	18,30,37	2.68	8 (44%)
2	C36	C	427	3,2	18,22,24	6.68	8 (44%)	17,33,37	1.15	2 (11%)

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	C36	B	407	1,2	1/1/8/8	2/7/37/44	0/1/2/2
2	C36	C	427	3,2	1/1/8/8	4/7/40/44	0/1/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	427	C36	C-C5	-18.90	1.09	1.51
2	C	427	C36	F-C5	-12.57	1.19	1.42
2	C	427	C36	C6-N1	-12.52	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	427	C36	C6-C5	-9.17	1.31	1.54
1	B	407	C36	C6-N1	-8.35	1.36	1.46
1	B	407	C36	C2-N1	-5.94	1.35	1.41
2	C	427	C36	C1'-N1	4.67	1.51	1.45
1	B	407	C36	C5-C4	-3.80	1.37	1.50
1	B	407	C36	O4'-C4'	-3.53	1.37	1.45
1	B	407	C36	C2'-C1'	-2.45	1.45	1.52
2	C	427	C36	C4-N3	2.30	1.35	1.31
2	C	427	C36	C5'-C4'	2.21	1.58	1.51
2	C	427	C36	C2-N1	2.12	1.43	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	407	C36	O4'-C4'-C3'	-6.42	90.70	105.67
1	B	407	C36	C2-N3-C4	4.94	125.10	119.32
1	B	407	C36	F-C5-C6	4.89	115.88	108.53
1	B	407	C36	O4'-C1'-C2'	-3.52	99.60	106.25
1	B	407	C36	N1-C2-N3	-2.72	115.70	118.45
2	C	427	C36	O4'-C4'-C3'	-2.50	99.84	105.67
1	B	407	C36	O4'-C1'-N1	-2.46	105.28	108.41
1	B	407	C36	C4'-O4'-C1'	-2.29	103.92	109.45
2	C	427	C36	O2-C2-N1	2.14	121.48	119.24
1	B	407	C36	O2-C2-N3	2.08	125.73	122.33

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	407	C36	C5
2	C	427	C36	C5

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	427	C36	O4'-C1'-N1-C6
2	C	427	C36	C2'-C1'-N1-C6
2	C	427	C36	C2'-C1'-N1-C2
1	B	407	C36	O4'-C4'-C5'-O5'
2	C	427	C36	O4'-C1'-N1-C2
1	B	407	C36	O4'-C1'-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

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	1.40	4 (19%)	20,40,40	1.92	6 (30%)

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	-	-	1/7/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	328	SAH	C2'-C1'	-4.17	1.47	1.53
4	A	328	SAH	C4-N3	2.69	1.39	1.35
4	A	328	SAH	C8-N7	-2.61	1.30	1.34
4	A	328	SAH	O4'-C4'	-2.37	1.39	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	328	SAH	O4'-C1'-C2'	-5.93	98.26	106.93
4	A	328	SAH	CB-CG-SD	-2.82	106.99	113.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	328	SAH	C4-C5-N7	2.75	112.27	109.40
4	A	328	SAH	C2-N1-C6	2.31	122.70	118.75
4	A	328	SAH	C5'-SD-CG	2.13	108.65	102.27
4	A	328	SAH	C5-C6-N1	-2.06	115.68	120.35

There are no chirality outliers.

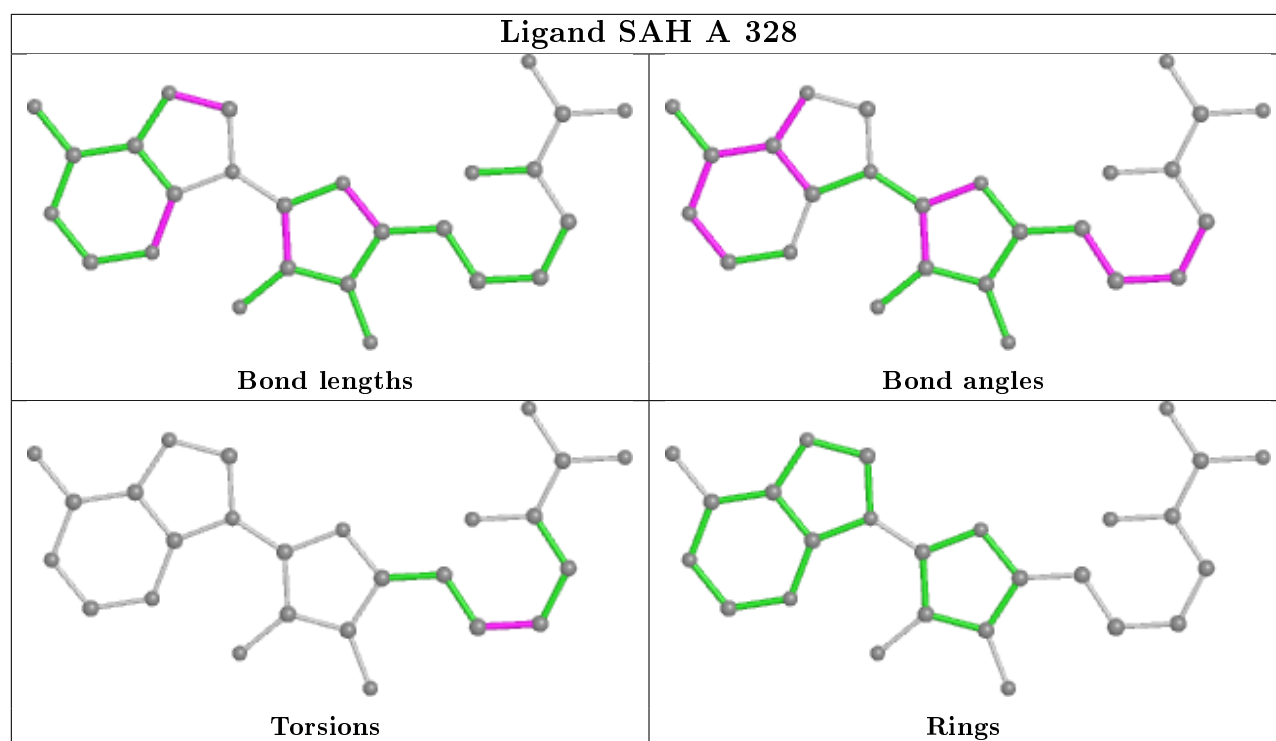
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	328	SAH	CB-CG-SD-C5'

There are no ring outliers.

No monomer is involved in short contacts.

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 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.