



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:54 AM UTC

PDB ID : 3MHT / pdb_00003mht
Title : TERNARY STRUCTURE OF HHAI METHYLTRANSFERASE WITH UN-MODIFIED DNA AND ADOHCY
Authors : O’Gara, M.; Klimasauskas, S.; Roberts, R.J.; 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

A user guide is available at

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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

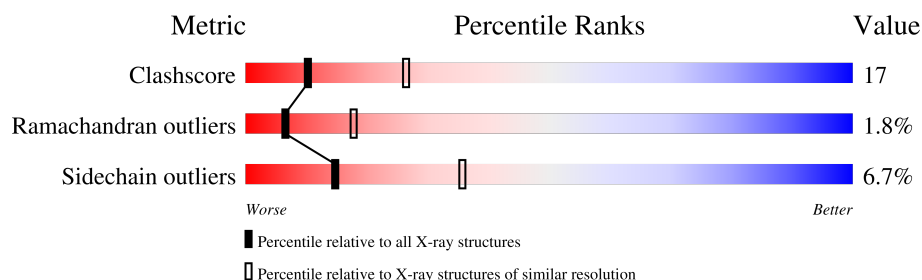
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (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 of 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	C	12	
2	D	13	
3	A	327	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3211 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*CP*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
			246	117	45	72	12			

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*GP*AP*TP*AP*GP*CP*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
			263	127	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 (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).



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	2	Total	O	0	0
			2	2		
5	D	10	Total	O	0	0
			10	10		
5	A	58	Total	O	0	0
			58	58		

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.

Note EDS was not executed.

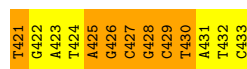
- Molecule 1: DNA (5'-D(*GP*AP*TP*AP*GP*CP*GP*CP*TP*AP*TP*C)-3')

Chain C: 



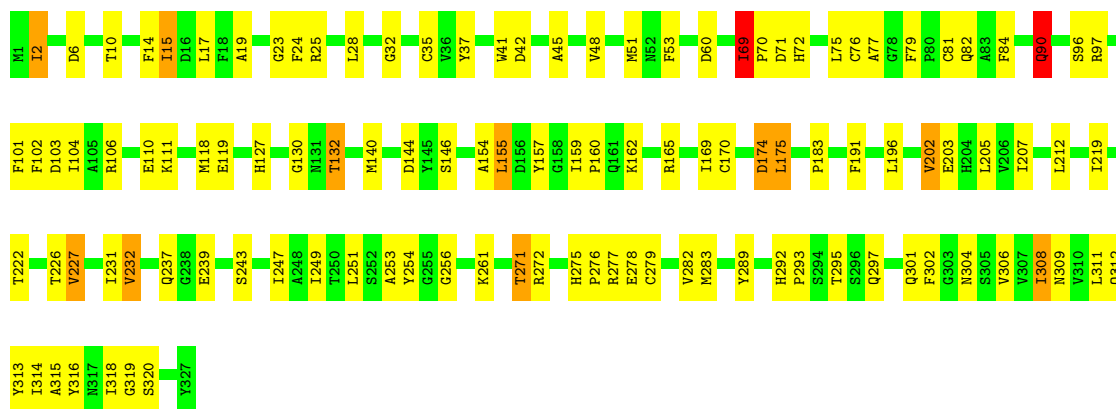
- Molecule 2: DNA (5'-D(*TP*GP*AP*TP*AP*GP*CP*GP*CP*TP*AP*TP*C)-3')

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, α , β , γ	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)	88.7 (20.00-2.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.189 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3211	wwPDB-VP
Average B, all atoms (Å ²)	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: 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	1.42	1/275 (0.4%)	2.93	40/422 (9.5%)
2	D	1.75	7/294 (2.4%)	2.56	30/452 (6.6%)
3	A	0.70	1/2661 (0.0%)	1.09	14/3586 (0.4%)
All	All	0.92	9/3230 (0.3%)	1.56	84/4460 (1.9%)

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	3
2	D	0	3
All	All	0	6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	427	DC	C5'-C4'	6.18	1.64	1.52
2	D	421	DT	C5'-C4'	5.63	1.63	1.52
2	D	428	DG	P-O5'	-5.62	1.49	1.60
2	D	432	DT	O3'-P	-5.51	1.52	1.61
2	D	421	DT	C2'-C1'	-5.38	1.42	1.52
2	D	429	DC	P-O5'	5.27	1.71	1.60
3	A	315	ALA	CA-CB	-5.22	1.45	1.53
1	C	408	DG	N9-C4	5.02	1.48	1.38
2	D	424	DT	O3'-P	-5.02	1.53	1.61

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	407	DC	C1'-O4'-C4'	-15.46	86.50	109.70
1	C	404	DT	O3'-P-O5'	-12.70	84.95	104.00
1	C	407	DC	O4'-C4'-C3'	-11.92	87.52	105.40
1	C	405	DA	O3'-P-O5'	-10.75	87.88	104.00
2	D	430	DT	O3'-P-O5'	-10.59	88.12	104.00
2	D	427	DC	P-O3'-C3'	10.13	135.39	120.20
2	D	421	DT	O4'-C4'-C3'	-9.87	90.60	105.40
1	C	405	DA	O4'-C1'-C2'	-9.41	92.29	106.40
1	C	409	DC	P-O3'-C3'	9.26	134.09	120.20
2	D	427	DC	C4'-C3'-C2'	-9.13	88.70	102.40
1	C	409	DC	C1'-O4'-C4'	-8.53	96.90	109.70
1	C	410	DT	C5'-C4'-C3'	-8.53	102.11	114.90
2	D	423	DA	O3'-P-O5'	-8.52	91.23	104.00
1	C	403	DA	C5'-C4'-C3'	-8.11	102.73	114.90
2	D	421	DT	O5'-C5'-C4'	8.05	122.88	110.80
1	C	410	DT	C6-N1-C1'	7.97	131.31	119.35
2	D	421	DT	O3'-P-O5'	7.69	115.53	104.00
1	C	412	DT	C5'-C4'-C3'	-7.55	103.58	114.90
2	D	428	DG	C4'-C3'-O3'	-7.53	98.71	110.00
1	C	407	DC	O4'-C1'-C2'	-7.50	95.15	106.40
1	C	403	DA	O3'-P-O5'	-7.35	92.98	104.00
1	C	406	DG	C4'-C3'-C2'	-7.26	91.51	102.40
2	D	433	DC	O4'-C4'-C3'	-7.24	94.54	105.40
1	C	410	DT	C4-C5-C7	-7.17	111.64	122.40
1	C	413	DC	C4'-C3'-O3'	7.11	120.67	110.00
1	C	406	DG	P-O5'-C5'	7.09	130.64	120.00
1	C	411	DA	C4'-C3'-O3'	-7.06	99.40	110.00
1	C	404	DT	C5'-C4'-C3'	-7.06	104.31	114.90
2	D	421	DT	C4'-C3'-C2'	6.86	112.69	102.40
2	D	426	DG	C4'-C3'-C2'	-6.71	92.34	102.40
2	D	430	DT	C3'-C2'-C1'	-6.69	91.56	101.60
1	C	408	DG	C4'-C3'-O3'	-6.64	100.04	110.00
2	D	425	DA	P-O5'-C5'	-6.56	110.16	120.00
2	D	433	DC	C1'-O4'-C4'	-6.42	100.08	109.70
2	D	421	DT	C6-N1-C1'	-6.34	109.83	119.35
1	C	408	DG	O3'-P-O5'	6.27	113.41	104.00
3	A	202	VAL	N-CA-C	6.20	117.76	111.00
1	C	410	DT	O3'-P-O5'	-6.18	94.72	104.00
1	C	407	DC	C2'-C3'-O3'	-6.18	102.23	111.50
1	C	406	DG	O4'-C1'-C2'	-6.12	97.22	106.40
1	C	407	DC	N3-C4-N4	6.11	127.06	117.90
1	C	405	DA	C2'-C3'-O3'	-6.00	102.50	111.50
3	A	79	PHE	CA-C-N	5.98	127.32	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	79	PHE	C-N-CA	5.98	127.32	119.84
3	A	318	ILE	N-CA-C	-5.98	104.52	110.62
2	D	432	DT	P-O5'-C5'	-5.94	111.09	120.00
2	D	427	DC	N1-C1'-C2'	5.93	122.39	113.50
1	C	413	DC	C2'-C3'-O3'	-5.91	102.64	111.50
1	C	407	DC	P-O3'-C3'	-5.90	111.36	120.20
2	D	425	DA	C5-C6-N6	-5.85	114.62	123.40
2	D	431	DA	P-O5'-C5'	-5.82	111.27	120.00
2	D	423	DA	C2'-C3'-O3'	5.81	120.22	111.50
2	D	432	DT	O4'-C1'-C2'	-5.77	97.75	106.40
2	D	431	DA	O5'-C5'-C4'	5.76	119.44	110.80
1	C	410	DT	C5'-C4'-O4'	5.67	117.91	109.40
2	D	421	DT	N1-C2-O2	5.66	131.69	123.20
2	D	428	DG	O3'-P-O5'	-5.63	95.55	104.00
3	A	71	ASP	N-CA-C	-5.58	102.75	110.35
1	C	402	DG	O4'-C4'-C3'	-5.55	97.08	105.40
1	C	402	DG	C1'-O4'-C4'	5.54	118.01	109.70
3	A	103	ASP	N-CA-C	-5.50	104.92	111.69
3	A	90	GLN	N-CA-C	5.44	122.39	110.80
1	C	410	DT	C2-N1-C1'	-5.39	111.26	119.35
3	A	69	ILE	CA-C-N	5.37	125.34	120.03
3	A	69	ILE	C-N-CA	5.37	125.34	120.03
1	C	413	DC	O4'-C1'-N1	5.35	116.42	108.40
2	D	429	DC	N1-C2-O2	5.31	127.16	119.20
3	A	45	ALA	N-CA-C	-5.31	105.58	111.36
1	C	407	DC	C3'-C2'-C1'	-5.29	93.66	101.60
3	A	279	CYS	N-CA-C	-5.28	105.42	111.07
2	D	424	DT	C4'-C3'-O3'	-5.27	102.10	110.00
2	D	429	DC	N3-C2-O2	-5.27	114.00	121.90
2	D	424	DT	C4-C5-C7	-5.23	114.56	122.40
1	C	402	DG	O3'-P-O5'	-5.22	96.17	104.00
2	D	427	DC	O4'-C1'-N1	-5.22	100.58	108.40
1	C	404	DT	C6-C5-C7	-5.19	116.21	124.00
1	C	412	DT	O4'-C1'-C2'	-5.14	98.69	106.40
3	A	253	ALA	N-CA-C	5.14	117.67	111.40
2	D	433	DC	O4'-C1'-C2'	-5.11	98.73	106.40
3	A	261	LYS	N-CA-C	5.11	121.69	110.80
1	C	404	DT	O4'-C1'-C2'	-5.05	98.82	106.40
1	C	409	DC	P-O5'-C5'	-5.04	112.44	120.00
1	C	413	DC	C1'-O4'-C4'	-5.02	102.17	109.70
3	A	249	ILE	CB-CA-C	-5.00	104.78	111.13

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	403	DA	Sidechain
1	C	409	DC	Sidechain
1	C	413	DC	Sidechain
2	D	421	DT	Sidechain
2	D	428	DG	Sidechain
2	D	430	DT	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	246	0	135	6	0
2	D	263	0	149	11	0
3	A	2606	0	2587	94	0
4	A	26	0	19	2	0
5	A	58	0	0	8	0
5	C	2	0	0	0	0
5	D	10	0	0	0	0
All	All	3211	0	2890	102	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 17.

All (102) 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:82:GLN:NE2	5:A:376:HOH:O	1.82	1.04
3:A:15:ILE:HD12	3:A:37:TYR:HB3	1.42	0.99
3:A:202:VAL:HG13	3:A:205:LEU:HD12	1.46	0.96
2:D:427:DC:C6	3:A:81:CYS:SG	2.60	0.94
2:D:427:DC:H2'	3:A:304:ASN:HB3	1.58	0.85
3:A:254:TYR:HA	5:A:331:HOH:O	1.87	0.74
1:C:405:DA:H2''	1:C:406:DG:C8	2.23	0.74
3:A:15:ILE:CD1	3:A:37:TYR:HB3	2.18	0.73
3:A:202:VAL:HG11	3:A:272:ARG:CZ	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:DG:O6	3:A:256:GLY:HA3	1.94	0.67
3:A:207:ILE:O	3:A:271:THR:HG23	1.96	0.65
2:D:427:DC:C5	3:A:81:CYS:SG	2.90	0.62
3:A:306:VAL:CG2	3:A:311:LEU:HD11	2.29	0.61
3:A:226:THR:HA	5:A:351:HOH:O	1.99	0.61
3:A:162:LYS:O	3:A:162:LYS:HG2	2.00	0.61
3:A:202:VAL:HG11	3:A:272:ARG:NE	2.15	0.61
3:A:297:GLN:O	3:A:301:GLN:HG3	2.02	0.60
3:A:289:TYR:HA	5:A:361:HOH:O	2.02	0.59
3:A:6:ASP:HB2	3:A:316:TYR:HE1	1.68	0.58
3:A:219:ILE:HD13	3:A:227:VAL:HG11	1.86	0.58
3:A:75:LEU:C	3:A:75:LEU:HD23	2.28	0.58
3:A:155:LEU:HD12	3:A:155:LEU:C	2.29	0.57
3:A:202:VAL:HG11	3:A:272:ARG:HD2	1.85	0.57
3:A:202:VAL:HG11	3:A:272:ARG:CD	2.35	0.56
3:A:275:HIS:CD2	3:A:277:ARG:H	2.23	0.56
3:A:15:ILE:HG22	3:A:17:LEU:HG	1.89	0.55
3:A:41:TRP:HD1	3:A:42:ASP:N	2.03	0.55
3:A:25:ARG:HD2	3:A:53:PHE:CE1	2.43	0.54
3:A:23:GLY:HA2	3:A:308:ILE:HD11	1.89	0.54
3:A:155:LEU:HD12	3:A:155:LEU:O	2.08	0.54
3:A:311:LEU:HD12	3:A:311:LEU:N	2.23	0.53
3:A:24:PHE:CD2	3:A:76:CYS:HB3	2.43	0.53
3:A:41:TRP:CD1	3:A:42:ASP:N	2.75	0.53
2:D:427:DC:H1'	3:A:304:ASN:HA	1.90	0.53
3:A:202:VAL:CG1	3:A:272:ARG:HD2	2.39	0.53
4:A:328:SAH:HG1	5:A:374:HOH:O	2.10	0.52
3:A:275:HIS:HD2	3:A:277:ARG:HB3	1.75	0.51
3:A:232:VAL:HG12	3:A:239:GLU:HB3	1.92	0.51
3:A:306:VAL:HG21	3:A:311:LEU:HD11	1.91	0.51
1:C:406:DG:O5'	1:C:406:DG:H2'	2.11	0.51
3:A:146:SER:O	3:A:170:CYS:HA	2.10	0.51
3:A:140:MET:HG2	3:A:170:CYS:SG	2.51	0.51
3:A:306:VAL:HG22	3:A:311:LEU:HD11	1.93	0.51
3:A:41:TRP:HD1	3:A:42:ASP:H	1.59	0.50
3:A:10:THR:HA	3:A:32:GLY:O	2.11	0.50
2:D:427:DC:C6	3:A:304:ASN:HB2	2.47	0.50
3:A:227:VAL:HG22	3:A:243:SER:HB3	1.92	0.50
3:A:309:ASN:O	3:A:312:GLN:HB2	2.10	0.50
3:A:84:PHE:HE2	3:A:132:THR:HG21	1.76	0.50
3:A:283:MET:HE2	3:A:302:PHE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:101:PHE:O	3:A:104:ILE:HB	2.12	0.49
3:A:311:LEU:HD12	3:A:311:LEU:H	1.78	0.49
2:D:427:DC:C2'	3:A:304:ASN:HB3	2.37	0.48
3:A:15:ILE:HG12	3:A:72:HIS:CG	2.48	0.48
3:A:90:GLN:O	3:A:127:HIS:HE1	1.95	0.48
1:C:402:DG:O5'	1:C:402:DG:H2'	2.13	0.48
3:A:276:PRO:HG2	3:A:295:THR:HG22	1.94	0.47
3:A:119:GLU:OE2	3:A:165:ARG:HD2	2.14	0.47
3:A:202:VAL:CG1	3:A:205:LEU:HD12	2.31	0.47
3:A:155:LEU:HA	3:A:159:ILE:O	2.15	0.47
3:A:127:HIS:HD2	3:A:132:THR:OG1	1.98	0.47
3:A:162:LYS:HB2	3:A:247:ILE:CD1	2.45	0.47
3:A:102:PHE:O	3:A:106:ARG:HG2	2.14	0.46
3:A:275:HIS:CD2	3:A:277:ARG:HB3	2.50	0.46
3:A:306:VAL:HG23	5:A:352:HOH:O	2.16	0.46
3:A:70:PRO:O	3:A:111:LYS:HE2	2.15	0.46
3:A:219:ILE:CD1	3:A:227:VAL:HG11	2.46	0.46
3:A:130:GLY:HA2	5:A:356:HOH:O	2.16	0.46
3:A:19:ALA:O	4:A:328:SAH:HA	2.17	0.45
1:C:413:DC:H42	2:D:422:DG:H1	1.64	0.45
3:A:48:VAL:HG13	3:A:292:HIS:HD2	1.82	0.45
3:A:275:HIS:HB3	3:A:278:GLU:HG3	1.98	0.44
3:A:237:GLN:NE2	5:A:337:HOH:O	2.50	0.44
3:A:313:TYR:O	3:A:314:ILE:C	2.60	0.44
3:A:157:TYR:CE2	3:A:183:PRO:HB2	2.53	0.44
3:A:14:PHE:CZ	3:A:35:CYS:HB2	2.53	0.44
3:A:308:ILE:O	3:A:309:ASN:C	2.61	0.44
3:A:77:ALA:O	3:A:118:MET:HA	2.18	0.43
3:A:319:GLY:O	3:A:320:SER:C	2.61	0.43
3:A:191:PHE:CZ	3:A:222:THR:HB	2.53	0.43
3:A:157:TYR:HE2	3:A:183:PRO:HB2	1.82	0.43
3:A:196:LEU:HA	3:A:278:GLU:OE2	2.18	0.43
3:A:226:THR:HG22	3:A:247:ILE:O	2.19	0.42
1:C:407:DC:N4	3:A:237:GLN:HB2	2.35	0.42
3:A:275:HIS:O	3:A:276:PRO:C	2.60	0.42
3:A:175:LEU:H	3:A:175:LEU:HG	1.59	0.42
3:A:51:MET:HE3	3:A:51:MET:HB2	1.82	0.42
2:D:426:DG:P	3:A:162:LYS:HZ1	2.43	0.41
3:A:227:VAL:HG22	3:A:227:VAL:O	2.20	0.41
3:A:292:HIS:CG	3:A:293:PRO:HD2	2.56	0.41
2:D:422:DG:H2'	2:D:422:DG:O5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:429:DC:O5'	2:D:429:DC:H2'	2.20	0.41
3:A:2:ILE:N	3:A:312:GLN:OE1	2.45	0.41
3:A:23:GLY:HA2	3:A:308:ILE:CD1	2.51	0.41
3:A:69:ILE:HA	3:A:70:PRO:HD3	1.82	0.41
3:A:183:PRO:CG	3:A:313:TYR:HB3	2.50	0.41
3:A:311:LEU:H	3:A:311:LEU:CD1	2.32	0.41
3:A:70:PRO:O	3:A:72:HIS:HD2	2.04	0.41
3:A:174:ASP:O	3:A:175:LEU:C	2.63	0.40
3:A:118:MET:HE3	3:A:118:MET:HB2	1.75	0.40
2:D:425:DA:H2''	2:D:426:DG:O5'	2.20	0.40
3:A:160:PRO:HB3	3:A:191:PHE:HA	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%)	299 (92%)	20 (6%)	6 (2%)	6	18

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	90	GLN
3	A	154	ALA
3	A	174	ASP
3	A	203	GLU
3	A	60	ASP
3	A	144	ASP

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 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%)	264 (93%)	19 (7%)	15	36

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	2	ILE
3	A	15	ILE
3	A	28	LEU
3	A	69	ILE
3	A	96	SER
3	A	97	ARG
3	A	110	GLU
3	A	132	THR
3	A	155	LEU
3	A	169	ILE
3	A	175	LEU
3	A	212	LEU
3	A	227	VAL
3	A	231	ILE
3	A	232	VAL
3	A	251	LEU
3	A	271	THR
3	A	282	VAL
3	A	308	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	8	GLN
3	A	63	GLN
3	A	65	ASN
3	A	72	HIS
3	A	123	ASN
3	A	127	HIS

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Mol	Chain	Res	Type
3	A	141	ASN
3	A	268	ASN
3	A	275	HIS
3	A	297	GLN
3	A	323	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](#)

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](#)

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	-	27,28,28	0.94	1 (3%)	36,40,40	1.61	3 (8%)

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	-	-	3/15/31/31	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	328	SAH	O-C	2.16	1.28	1.22

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	328	SAH	OXT-C-O	-7.10	107.96	124.08
4	A	328	SAH	O4'-C1'-C2'	-3.99	98.08	106.62
4	A	328	SAH	CB-CA-N	2.77	117.35	110.12

There are no chirality outliers.

All (3) torsion outliers are listed below:

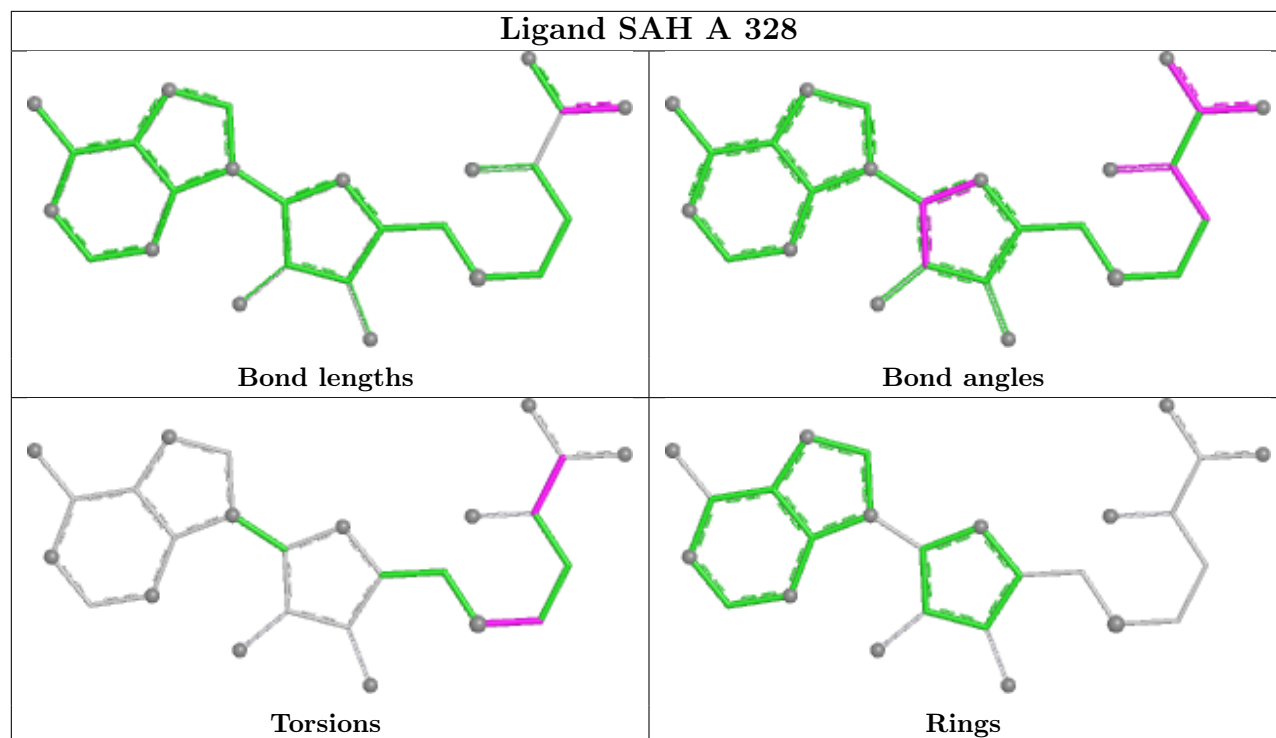
Mol	Chain	Res	Type	Atoms
4	A	328	SAH	OXT-C-CA-CB
4	A	328	SAH	OXT-C-CA-N
4	A	328	SAH	CB-CG-SD-C5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	328	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 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.