



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:56 PM GMT

PDB ID : 5MHT
Title : TERNARY STRUCTURE OF HHAI METHYLTRANSFERASE WITH
HEMIMETHYLATED DNA AND ADOHCY
Authors : Cheng, X.
Deposited on : 1996-10-22
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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

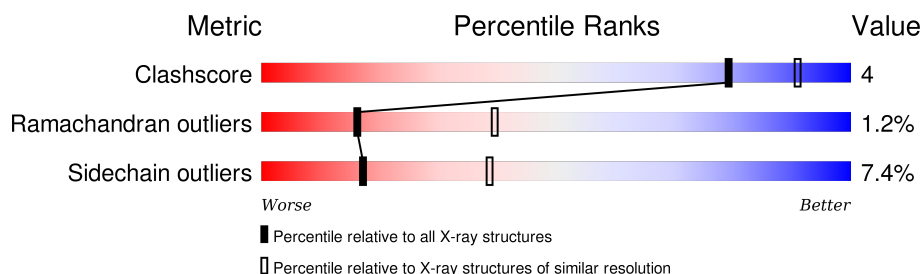
1 Overall quality at a glance

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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	12	<div> <div style="width: 17%; background-color: green;"></div> <div style="width: 83%; background-color: yellow;"></div> </div> <div>17% 83%</div>
2	D	12	<div> <div style="width: 67%; background-color: yellow;"></div> <div style="width: 33%; background-color: orange;"></div> </div> <div>67% 33%</div>
3	A	327	<div> <div style="width: 85%; background-color: green;"></div> <div style="width: 13%; background-color: yellow;"></div> <div style="width: 2%; background-color: red;"></div> </div> <div>85% 13% .</div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3365 atoms, of which 128 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(*CP*CP*AP*TP*GP*(5CM)P*GP*CP*TP*GP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	12	Total	C	N	O	P	0	0	0
			244	116	44	72	12			

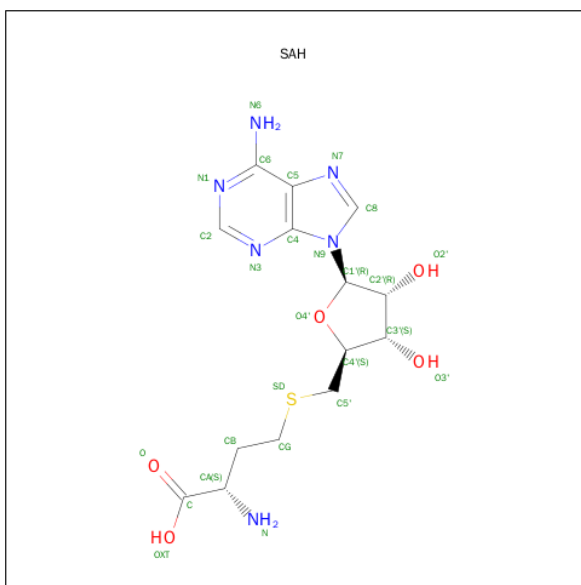
- Molecule 2 is a DNA chain called DNA (5'-D(*GP*TP*CP*AP*GP*CP*GP*CP*AP*TP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	12	Total	C	N	O	P	0	0	0
			249	117	48	72	12			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	327	Total	C	H	N	O	S	0	0	0
			2734	1662	128	444	487	13			

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: 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	A	97	Total O 97 97	0	0
5	C	7	Total O 7 7	0	0
5	D	8	Total O 8 8	0	0

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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(*CP*CP*AP*TP*GP*(5CM)P*GP*CP*TP*GP*AP*C)-3')

Chain C: 




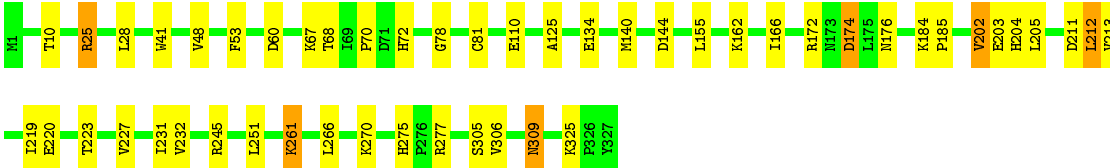
- Molecule 2: DNA (5'-D(*GP*TP*CP*AP*GP*CP*GP*CP*AP*TP*GP*G)-3')

Chain D: 



- Molecule 3: PROTEIN (HHA1 METHYLTRANSFERASE)

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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)	95.1 (20.00-2.70)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3365	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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	2.98	26/249 (10.4%)	3.45	60/379 (15.8%)
2	D	3.07	34/279 (12.2%)	3.79	68/429 (15.9%)
3	A	0.52	0/2661	0.79	2/3586 (0.1%)
All	All	1.32	60/3189 (1.9%)	1.71	130/4394 (3.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	3

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	423	DT	C5-C7	11.00	1.56	1.50
1	C	406	DG	N9-C4	9.66	1.45	1.38
2	D	422	DG	C5'-C4'	9.56	1.61	1.51
1	C	408	DG	N7-C5	9.48	1.45	1.39
2	D	426	DG	N9-C4	8.78	1.45	1.38
2	D	425	DA	N9-C4	8.64	1.43	1.37
1	C	402	DC	C3'-O3'	8.60	1.55	1.44
1	C	402	DC	N3-C4	8.45	1.39	1.33
2	D	427	DC	C2-N3	8.28	1.42	1.35
2	D	422	DG	P-O5'	8.05	1.67	1.59
2	D	430	DA	C5'-C4'	7.98	1.60	1.51
2	D	422	DG	N9-C4	7.90	1.44	1.38
1	C	404	DA	N9-C4	7.80	1.42	1.37
1	C	411	DG	C2-N3	7.51	1.38	1.32
2	D	432	DG	N3-C4	7.50	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	423	DT	C5'-C4'	7.39	1.59	1.51
2	D	425	DA	P-O5'	7.29	1.67	1.59
1	C	402	DC	C5'-C4'	7.25	1.59	1.51
1	C	412	DA	N3-C4	7.18	1.39	1.34
1	C	405	DT	C5-C6	7.00	1.39	1.34
2	D	427	DC	C4'-O4'	-6.96	1.38	1.45
2	D	433	DG	C2-N3	6.84	1.38	1.32
2	D	422	DG	O3'-P	6.83	1.69	1.61
1	C	406	DG	C5'-C4'	6.68	1.58	1.51
2	D	432	DG	C2-N3	6.51	1.38	1.32
2	D	428	DG	C6-N1	-6.48	1.35	1.39
2	D	427	DC	C1'-N1	6.47	1.57	1.49
2	D	432	DG	C6-N1	6.42	1.44	1.39
1	C	408	DG	C4'-C3'	6.39	1.59	1.53
1	C	402	DC	N1-C2	6.27	1.46	1.40
1	C	412	DA	N9-C4	6.20	1.41	1.37
2	D	425	DA	O3'-P	-6.12	1.53	1.61
2	D	432	DG	N9-C4	6.05	1.42	1.38
1	C	402	DC	C4'-C3'	5.90	1.59	1.53
2	D	429	DC	O3'-P	5.88	1.68	1.61
1	C	409	DC	O4'-C1'	-5.83	1.35	1.42
2	D	423	DT	C5-C6	5.83	1.38	1.34
1	C	404	DA	C8-N7	5.78	1.35	1.31
2	D	423	DT	N1-C6	5.75	1.42	1.38
1	C	408	DG	C6-O6	5.69	1.29	1.24
1	C	410	DT	C5'-C4'	5.66	1.57	1.51
2	D	426	DG	C2'-C1'	5.66	1.58	1.52
1	C	412	DA	C5'-C4'	-5.64	1.45	1.51
2	D	433	DG	N3-C4	5.61	1.39	1.35
2	D	426	DG	C2-N3	5.50	1.37	1.32
1	C	406	DG	C8-N7	5.49	1.34	1.30
1	C	402	DC	O3'-P	5.41	1.67	1.61
1	C	411	DG	C3'-C2'	5.39	1.58	1.52
2	D	423	DT	O4'-C1'	5.38	1.48	1.42
2	D	422	DG	C1'-N9	5.30	1.56	1.49
2	D	425	DA	O4'-C1'	-5.29	1.35	1.42
1	C	404	DA	N3-C4	5.28	1.38	1.34
2	D	430	DA	N9-C4	5.20	1.41	1.37
2	D	423	DT	P-O5'	5.17	1.65	1.59
1	C	402	DC	C3'-C2'	5.17	1.58	1.52
1	C	408	DG	O4'-C1'	5.15	1.48	1.42
2	D	429	DC	C5'-C4'	5.12	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	408	DG	C5-C6	5.05	1.47	1.42
2	D	426	DG	O3'-P	-5.02	1.55	1.61
2	D	431	DT	P-O5'	5.01	1.64	1.59

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	427	DC	O4'-C4'-C3'	-24.38	91.37	106.00
2	D	430	DA	O4'-C1'-N9	14.71	118.30	108.00
2	D	422	DG	O4'-C1'-N9	14.68	118.28	108.00
2	D	423	DT	O4'-C1'-N1	14.60	118.22	108.00
1	C	406	DG	O4'-C1'-C2'	-13.57	95.05	105.90
2	D	429	DC	N3-C2-O2	-11.70	113.71	121.90
1	C	402	DC	N1-C2-O2	11.16	125.60	118.90
2	D	431	DT	O4'-C1'-C2'	-11.08	97.03	105.90
2	D	433	DG	O4'-C1'-C2'	-10.40	97.58	105.90
1	C	411	DG	P-O3'-C3'	10.16	131.89	119.70
2	D	422	DG	C8-N9-C4	-10.07	102.37	106.40
2	D	427	DC	N3-C4-C5	-9.87	117.95	121.90
1	C	402	DC	N3-C2-O2	-9.81	115.03	121.90
2	D	422	DG	O4'-C1'-C2'	-9.63	98.19	105.90
1	C	409	DC	O4'-C1'-C2'	-9.58	98.24	105.90
2	D	425	DA	O4'-C1'-C2'	-9.52	98.29	105.90
1	C	404	DA	O4'-C1'-C2'	-9.46	98.33	105.90
1	C	405	DT	N1-C2-N3	9.38	120.23	114.60
2	D	429	DC	N1-C2-O2	9.18	124.41	118.90
2	D	427	DC	N3-C4-N4	9.17	124.42	118.00
1	C	405	DT	O4'-C1'-C2'	-9.02	98.68	105.90
2	D	422	DG	C3'-C2'-C1'	8.98	113.28	102.50
1	C	410	DT	C6-N1-C2	-8.91	116.84	121.30
2	D	432	DG	O4'-C1'-N9	8.91	114.24	108.00
1	C	406	DG	N3-C4-C5	-8.89	124.15	128.60
1	C	406	DG	N3-C2-N2	8.46	125.83	119.90
1	C	410	DT	C4-C5-C6	8.45	123.07	118.00
2	D	427	DC	O4'-C1'-C2'	-8.38	99.20	105.90
2	D	428	DG	C8-N9-C4	-8.34	103.07	106.40
2	D	427	DC	C6-N1-C2	-8.31	116.98	120.30
1	C	411	DG	O4'-C1'-C2'	-8.29	99.27	105.90
2	D	425	DA	C4'-C3'-C2'	-8.27	95.66	103.10
1	C	405	DT	C4-C5-C6	8.19	122.92	118.00
2	D	428	DG	P-O3'-C3'	8.14	129.47	119.70
2	D	428	DG	O4'-C1'-N9	8.10	113.67	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	431	DT	O4'-C1'-N1	8.02	113.61	108.00
1	C	406	DG	N1-C6-O6	-7.75	115.25	119.90
1	C	402	DC	C4'-C3'-C2'	-7.65	96.21	103.10
2	D	422	DG	C1'-O4'-C4'	7.63	117.73	110.10
1	C	406	DG	C8-N9-C4	-7.61	103.36	106.40
2	D	431	DT	C4-C5-C6	7.59	122.55	118.00
1	C	408	DG	O4'-C1'-N9	7.39	113.18	108.00
1	C	409	DC	N3-C4-C5	-7.35	118.96	121.90
2	D	423	DT	N3-C2-O2	-7.22	117.97	122.30
1	C	402	DC	P-O3'-C3'	7.20	128.34	119.70
1	C	412	DA	C1'-O4'-C4'	-7.11	102.99	110.10
1	C	409	DC	C2-N3-C4	7.04	123.42	119.90
2	D	424	DC	P-O3'-C3'	7.02	128.12	119.70
2	D	425	DA	O4'-C4'-C3'	6.96	110.18	106.00
2	D	426	DG	N3-C4-C5	-6.93	125.14	128.60
1	C	412	DA	O4'-C1'-N9	6.91	112.84	108.00
1	C	408	DG	P-O5'-C5'	6.84	131.85	120.90
1	C	412	DA	O4'-C4'-C3'	6.83	110.10	106.00
1	C	405	DT	N3-C2-O2	-6.79	118.22	122.30
1	C	406	DG	C4'-C3'-C2'	-6.74	97.03	103.10
2	D	427	DC	P-O3'-C3'	6.72	127.77	119.70
1	C	410	DT	O4'-C1'-N1	6.72	112.70	108.00
2	D	430	DA	C8-N9-C4	-6.70	103.12	105.80
1	C	403	DC	C5-C6-N1	6.52	124.26	121.00
1	C	405	DT	C5-C4-O4	6.50	129.45	124.90
1	C	411	DG	N1-C6-O6	-6.50	116.00	119.90
1	C	403	DC	O4'-C1'-C2'	-6.48	100.71	105.90
2	D	424	DC	O4'-C1'-C2'	-6.48	100.72	105.90
1	C	404	DA	C8-N9-C4	-6.45	103.22	105.80
2	D	429	DC	O4'-C1'-C2'	-6.42	100.76	105.90
1	C	404	DA	N9-C4-C5	6.27	108.31	105.80
2	D	428	DG	N7-C8-N9	6.26	116.23	113.10
2	D	431	DT	P-O3'-C3'	6.26	127.21	119.70
1	C	403	DC	N3-C4-C5	-6.25	119.40	121.90
2	D	433	DG	O4'-C1'-N9	-6.20	103.66	108.00
2	D	427	DC	N1-C2-O2	-6.15	115.21	118.90
2	D	426	DG	C8-N9-C4	-6.14	103.94	106.40
2	D	427	DC	C5-C6-N1	6.10	124.05	121.00
1	C	410	DT	N1-C2-N3	6.08	118.25	114.60
2	D	424	DC	O4'-C1'-N1	6.06	112.24	108.00
2	D	422	DG	C4-C5-C6	6.02	122.41	118.80
1	C	405	DT	C6-N1-C2	-6.01	118.29	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	405	DT	C4-C5-C7	-6.00	115.40	119.00
1	C	408	DG	P-O3'-C3'	5.97	126.86	119.70
1	C	410	DT	C4-C5-C7	-5.95	115.43	119.00
2	D	426	DG	C4'-C3'-C2'	-5.95	97.75	103.10
1	C	406	DG	C2-N3-C4	5.93	114.86	111.90
2	D	422	DG	N9-C1'-C2'	-5.92	101.36	112.60
1	C	411	DG	N3-C4-C5	-5.89	125.65	128.60
1	C	405	DT	N3-C4-C5	-5.83	111.70	115.20
2	D	432	DG	C2-N3-C4	5.82	114.81	111.90
1	C	410	DT	N3-C4-C5	-5.78	111.73	115.20
2	D	430	DA	O4'-C4'-C3'	-5.77	102.19	104.50
2	D	432	DG	O4'-C1'-C2'	-5.75	101.30	105.90
1	C	409	DC	C4'-C3'-C2'	-5.75	97.93	103.10
2	D	432	DG	N3-C4-N9	5.74	129.44	126.00
1	C	410	DT	C5'-C4'-C3'	-5.71	103.82	114.10
2	D	432	DG	N3-C4-C5	-5.70	125.75	128.60
2	D	422	DG	N3-C4-C5	-5.67	125.76	128.60
1	C	405	DT	P-O3'-C3'	5.65	126.48	119.70
2	D	429	DC	C5-C4-N4	5.65	124.16	120.20
2	D	430	DA	N9-C4-C5	5.65	108.06	105.80
1	C	411	DG	C5-C6-O6	5.63	131.98	128.60
2	D	427	DC	O5'-P-OP1	-5.62	100.64	105.70
1	C	405	DT	C6-N1-C1'	5.60	128.81	120.40
1	C	408	DG	C5-C6-N1	-5.58	108.71	111.50
2	D	423	DT	P-O5'-C5'	5.52	129.73	120.90
1	C	403	DC	C6-N1-C2	-5.51	118.10	120.30
2	D	428	DG	P-O5'-C5'	5.47	129.65	120.90
1	C	405	DT	C5-C6-N1	-5.45	120.43	123.70
1	C	406	DG	C5-C6-O6	5.44	131.87	128.60
2	D	426	DG	P-O3'-C3'	5.41	126.19	119.70
2	D	429	DC	N3-C4-N4	-5.39	114.22	118.00
2	D	425	DA	O3'-P-O5'	-5.35	93.84	104.00
2	D	428	DG	O3'-P-O5'	-5.33	93.86	104.00
3	A	10	THR	N-CA-C	5.33	125.38	111.00
2	D	431	DT	N3-C2-O2	-5.32	119.11	122.30
2	D	429	DC	P-O3'-C3'	5.28	126.04	119.70
1	C	410	DT	N3-C2-O2	-5.26	119.14	122.30
1	C	406	DG	N3-C4-N9	5.25	129.15	126.00
2	D	430	DA	O3'-P-O5'	-5.24	94.04	104.00
2	D	432	DG	C5-C6-O6	-5.21	125.47	128.60
1	C	404	DA	C1'-O4'-C4'	5.19	115.29	110.10
2	D	431	DT	N3-C4-O4	5.18	123.01	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	406	DG	N1-C2-N2	-5.17	111.55	116.20
2	D	425	DA	C8-N9-C4	-5.16	103.74	105.80
1	C	410	DT	C5'-C4'-O4'	5.13	119.05	109.30
2	D	430	DA	C5'-C4'-O4'	5.13	119.04	109.30
2	D	426	DG	C2-N3-C4	5.12	114.46	111.90
2	D	428	DG	N9-C4-C5	5.12	107.45	105.40
2	D	426	DG	O4'-C4'-C3'	5.11	109.07	106.00
3	A	78	GLY	N-CA-C	-5.07	100.42	113.10
1	C	404	DA	O3'-P-O5'	-5.07	94.37	104.00
2	D	423	DT	N1-C1'-C2'	-5.04	103.02	112.60
1	C	405	DT	C4'-C3'-C2'	-5.03	98.58	103.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	422	DG	Sidechain
2	D	424	DC	Sidechain
2	D	428	DG	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	244	0	137	0	0
2	D	249	0	135	3	0
3	A	2606	128	2587	21	0
4	A	26	0	19	0	0
5	A	97	0	0	0	0
5	C	7	0	0	0	0
5	D	8	0	0	0	0
All	All	3237	128	2878	21	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 4.

All (21) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:427:DC:C6	3:A:81:CYS:SG	2.61	0.94
3:A:202:VAL:HG12	3:A:203:GLU:N	2.17	0.60
3:A:309:ASN:N	3:A:309:ASN:HD22	1.97	0.60
2:D:427:DC:H6	3:A:81:CYS:HG	1.32	0.58
3:A:162:LYS:HG2	3:A:162:LYS:O	2.05	0.57
3:A:309:ASN:HD22	3:A:309:ASN:H	1.51	0.57
3:A:125:ALA:HB2	3:A:166:ILE:HD12	1.87	0.57
3:A:211:ASP:O	3:A:213:VAL:HG23	2.06	0.56
3:A:67:LYS:HE2	3:A:110:GLU:OE2	2.11	0.51
3:A:275:HIS:HD2	3:A:277:ARG:H	1.59	0.51
2:D:427:DC:H6	3:A:81:CYS:SG	2.26	0.50
3:A:202:VAL:O	3:A:204:HIS:ND1	2.46	0.48
3:A:212:LEU:HD23	3:A:212:LEU:HA	1.83	0.44
3:A:25:ARG:HD2	3:A:53:PHE:CE1	2.53	0.44
3:A:202:VAL:CG1	3:A:205:LEU:HB2	2.49	0.42
3:A:155:LEU:HD12	3:A:155:LEU:C	2.39	0.42
3:A:172:ARG:NH1	3:A:174:ASP:OD2	2.52	0.42
3:A:184:LYS:HA	3:A:185:PRO:HD3	1.82	0.41
3:A:219:ILE:HD13	3:A:227:VAL:HG21	2.02	0.41
3:A:70:PRO:O	3:A:72:HIS:HD2	2.04	0.40
3:A:305:SER:OG	3:A:306:VAL:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	307 (94%)	14 (4%)	4 (1%)	16	39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	261	LYS

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Mol	Chain	Res	Type
3	A	60	ASP
3	A	144	ASP
3	A	202	VAL

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%)	262 (93%)	21 (7%)	17	39

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	25	ARG
3	A	28	LEU
3	A	41	TRP
3	A	48	VAL
3	A	68	THR
3	A	134	GLU
3	A	140	MET
3	A	174	ASP
3	A	176	ASN
3	A	212	LEU
3	A	220	GLU
3	A	223	THR
3	A	231	ILE
3	A	232	VAL
3	A	245	ARG
3	A	251	LEU
3	A	261	LYS
3	A	266	LEU
3	A	270	LYS
3	A	309	ASN
3	A	325	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
3	A	63	GLN
3	A	72	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 ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	5CM	C	407	1,2	13,21,22	1.35	2 (15%)	17,30,33	1.99	3 (17%)

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	5CM	C	407	1,2	-	0/3/21/22	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	407	5CM	C5A-C5	2.25	1.55	1.51
1	C	407	5CM	C6-N1	2.36	1.38	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	407	5CM	O4'-C1'-C2'	-6.49	93.34	106.27
1	C	407	5CM	C3'-C2'-C1'	2.41	108.20	102.40
1	C	407	5CM	N4-C4-N3	2.54	120.63	116.95

There are no chirality outliers.

There are no torsion outliers.

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	-	20,28,28	1.15	1 (5%)	19,40,40	1.17	2 (10%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	328	SAH	C8-N7	-3.09	1.28	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	328	SAH	C4'-C5'-SD	2.01	119.73	113.53
4	A	328	SAH	C1'-N9-C4	2.69	131.00	126.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.