wwPDB X-ray Structure Validation Summary Report (i)

Apr 7, 2022 – 07:51 PM EDT

PDB ID	:	6MHT
Title	:	TERNARY STRUCTURE OF HHAI METHYLTRANSFERASE WITH ADOHCY AND DNA CONTAINING 4'-THIO-2'DEOXYCYTIDINE AT THE TARGET
Authors	:	Cheng, X.
Deposited on	:	1998-08-05
Resolution	:	2.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

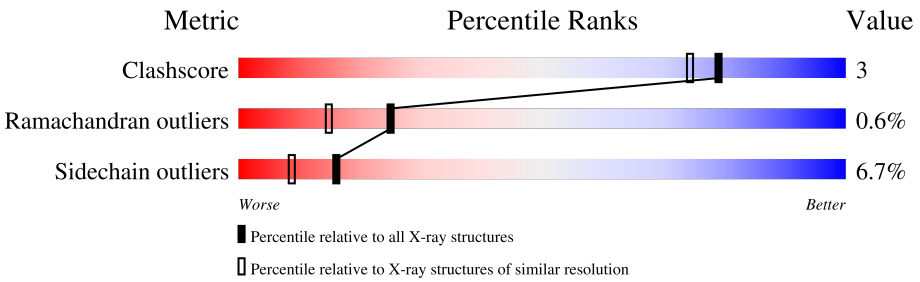
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	12	67% 33%
2	D	12	83% 17%
3	A	327	87% 11% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3276 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*CP*CP*AP*TP*GP*(5CM)P*GP*CP*TP*GP*AP*C)-3').

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

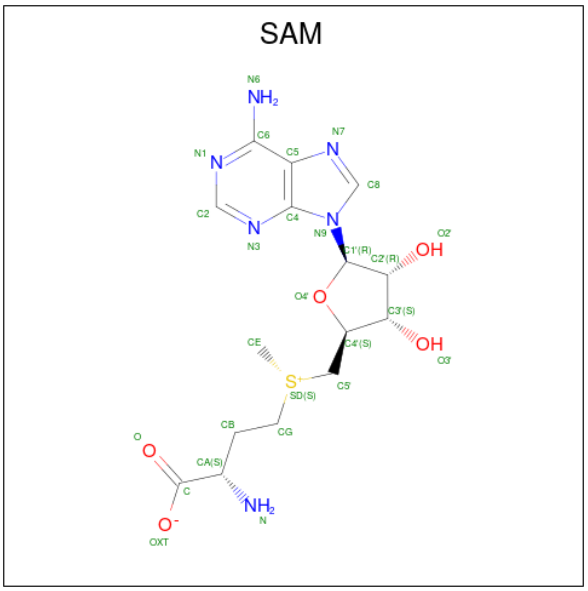
- Molecule 2 is a DNA chain called DNA (5'-D(P*GP*TP*CP*AP*GP*(4SC)P*GP*CP*AP*TP*GP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
2	D	12	250	118	48	71	12	1	0	0	0

- Molecule 3 is a protein called CYTOSINE-SPECIFIC METHYLTRANSFERASE HHAI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	327	2607	1662	444	487	14	0	1	0

- Molecule 4 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	D	1	27	15	6	5	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	C	13	13	13	0	0
			Total	O		
5	D	16	16	16	0	0
			Total	O		
5	A	119	119	119	0	0

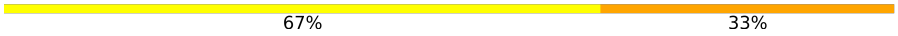
3 Residue-property plots (i)

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.

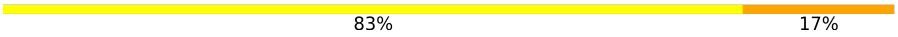
• Molecule 1: DNA (5'-D(P*CP*CP*AP*TP*GP*(5CM)P*GP*CP*TP*GP*AP*C)-3')

Chain C:



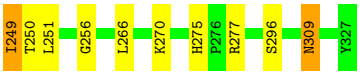
• Molecule 2: DNA (5'-D(P*GP*TP*CP*AP*GP*(4SC)P*GP*CP*AP*TP*GP*G)-3')

Chain D:



• Molecule 3: CYTOSINE-SPECIFIC METHYLTRANSFERASE HHAI

Chain A:



4 Data and refinement statistics (i)

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	99.86Å 99.86Å 325.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	5.00 – 2.05	Depositor
% Data completeness (in resolution range)	81.6 (5.00-2.05)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.186 , 0.231	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3276	wwPDB-VP
Average B, all atoms (Å^2)	19.0	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: 5CM, SAM, 4SC

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	2.76	18/249 (7.2%)	3.46	51/379 (13.5%)
2	D	2.79	23/257 (8.9%)	3.33	53/393 (13.5%)
3	A	0.63	1/2667 (0.0%)	0.86	6/3594 (0.2%)
All	All	1.25	42/3173 (1.3%)	1.63	110/4366 (2.5%)

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
2	D	0	1
3	A	0	2
All	All	0	4

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	405	DT	C5-C7	13.90	1.58	1.50
2	D	431	DT	C5-C7	10.03	1.56	1.50
2	D	429	DC	C5'-C4'	9.49	1.61	1.51
1	C	410	DT	C5-C7	8.82	1.55	1.50
2	D	426	DG	N9-C4	7.97	1.44	1.38

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	193	LYS	CD-CE-NZ	18.03	153.18	111.70
2	D	431	DT	N3-C2-O2	-15.29	113.12	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	406	DG	O4'-C1'-C2'	-14.81	94.05	105.90
1	C	405	DT	O4'-C1'-C2'	-13.52	95.09	105.90
2	D	424	DC	P-O3'-C3'	13.30	135.66	119.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	157	TYR	Sidechain
3	A	249	ILE	Mainchain
1	C	411	DG	Sidechain
2	D	428	DG	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	C	244	0	137	2	0
2	D	250	0	135	3	0
3	A	2607	0	2587	16	0
4	D	27	0	20	0	0
5	A	119	0	0	0	0
5	C	13	0	0	0	0
5	D	16	0	0	0	0
All	All	3276	0	2879	17	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 3.

The worst 5 of 17 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:427:4SC:H62	3:A:81[B]:CYS:SG	1.83	1.18
2:D:427:4SC:C6	3:A:81[B]:CYS:SG	2.70	0.77
3:A:309:ASN:HD22	3:A:309:ASN:N	1.93	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:DG:O6	3:A:256:GLY:HA3	2.00	0.62
3:A:309:ASN:HD22	3:A:309:ASN:H	1.48	0.60

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	326/327 (100%)	316 (97%)	8 (2%)	2 (1%)	25 15

All (2) Ramachandran outliers are listed below:

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

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	284/283 (100%)	264 (93%)	20 (7%)	15 7

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	245	ARG
3	A	270	LYS
3	A	309	ASN
3	A	296	SER
3	A	81[A]	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	141	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	$\#\|Z\| > 2$
2	4SC	D	427	2,4	14,21,22	2.58	6 (42%)	16,30,33	7.55	10 (62%)
1	5CM	C	407	1,2	15,21,22	1.52	4 (26%)	19,30,33	1.69	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
2	4SC	D	427	2,4	-	0/3/21/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5CM	C	407	1,2	-	0/4/21/22	0/2/2/2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	427	4SC	O3'-C3'	4.96	1.53	1.43
2	D	427	4SC	C5-C4	4.85	1.48	1.41
2	D	427	4SC	C5M-C5	4.70	1.60	1.51
1	C	407	5CM	C4-N3	-3.01	1.30	1.35
1	C	407	5CM	C5-C4	2.78	1.45	1.41

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	427	4SC	C5M-C5-C4	-27.63	93.74	121.72
2	D	427	4SC	C5'-C4'-S4'	-5.77	101.68	111.58
1	C	407	5CM	C4-N3-C2	5.57	122.75	116.02
2	D	427	4SC	C4-N3-C2	5.22	122.32	116.02
2	D	427	4SC	C2'-C1'-S4'	4.52	110.75	106.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	427	4SC	3	0
1	C	407	5CM	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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	SAM	D	328	2	21,29,29	1.48	5 (23%)	18,42,42	1.08	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
4	SAM	D	328	2	-	2/8/33/33	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	328	SAM	CE-SD	-3.14	1.59	1.78
4	D	328	SAM	C2-N3	2.51	1.36	1.32
4	D	328	SAM	C4-N3	2.48	1.39	1.35
4	D	328	SAM	C2-N1	2.28	1.38	1.33
4	D	328	SAM	C8-N7	-2.25	1.30	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	328	SAM	O4'-C1'-C2'	-2.46	103.33	106.93
4	D	328	SAM	O3'-C3'-C4'	-2.17	104.78	111.05

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	328	SAM	CB-CG-SD-CE
4	D	328	SAM	CB-CG-SD-C5'

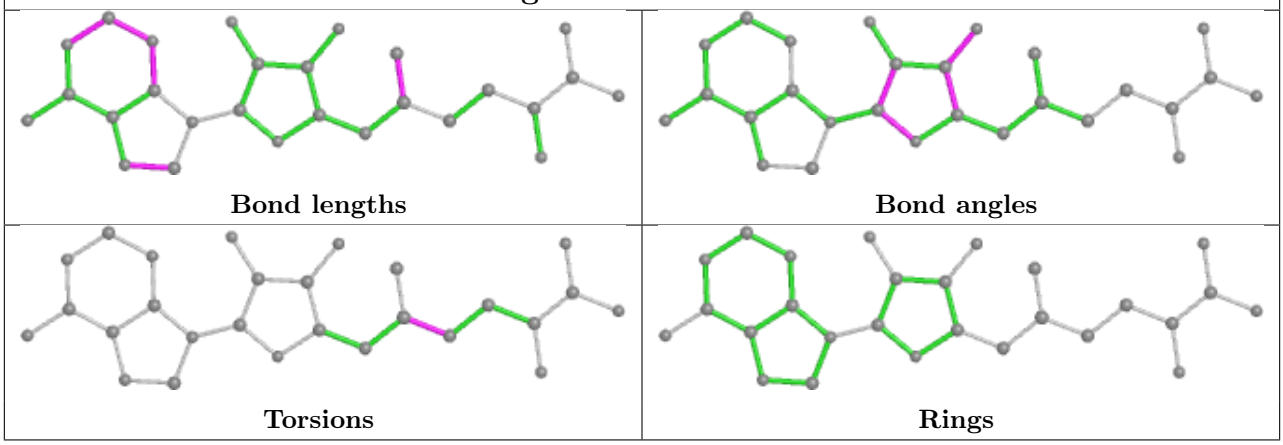
There are no ring outliers.

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 then 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.

Ligand SAM D 328



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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.