

# Full wwPDB X-ray Structure Validation Report (i)

Jan 16, 2023 - 03:21 am GMT

PDB ID	:	7QW5
Title	:	Adenine-specific DNA methyltransferase M.BseCI complexed with AdoHcy
		and cognate unmethylated DNA duplex
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		Glykos, N.M.; Kokkinidis, M.
Deposited on		
Resolution	:	2.30  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 (i) 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 (i)) were used in the production of this report:

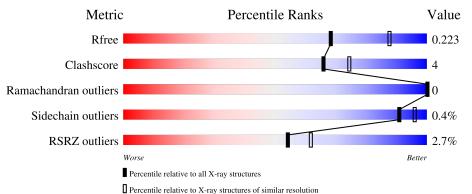
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as $541$ be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.31.3
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.30 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	5042(2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575(2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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% 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.

Mol	Chain	Length	Quality of chain	
1	А	585	3% 83%	10% 7%
2	Z	10	60%	40%
3	Y	10	70%	30%



#### $7 \mathrm{QW5}$

# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5049 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 protein called Modification methylase BseCI.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	544	Total 4380	C 2816	N 736	0 818	S 10	0	1	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	195	GLU	GLY	conflict	UNP P43423
А	580	HIS	-	expression tag	UNP P43423
А	581	HIS	-	expression tag	UNP P43423
А	582	HIS	-	expression tag	UNP P43423
А	583	HIS	-	expression tag	UNP P43423
А	584	HIS	-	expression tag	UNP P43423
А	585	HIS	-	expression tag	UNP P43423

• Molecule 2 is a DNA chain called Unmethylated DNA duplex.

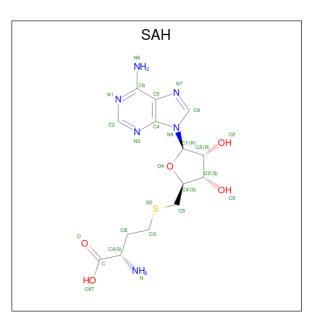
Mol	Chain	Residues		At	$\mathbf{oms}$			ZeroOcc	AltConf	Trace
2	Z	10	Total 200	C 96	N 38	O 57	Р 9	0	0	0

• Molecule 3 is a DNA chain called Unmethylated DNA duplex.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	Y	10	Total 200	C 96	N 38	O 57	Р 9	0	0	0

• Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Atc	$\mathbf{ms}$			ZeroOcc	AltConf
4	А	1	Total	С	Ν	0	$\mathbf{S}$	0	0
	11	Ĩ	26	14	6	5	1		

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	210	Total O 210 210	0	0
5	Ζ	22	Total O 22 22	0	0
5	Y	11	Total O 11 11	0	0



<mark>1 2 8</mark>

# 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 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.

Chain A:	83%	10% 7%	-
MET MET SER SER VIA CIAN CIAN AIA VIO VIO	F37 L48 L48 A51 A51 A51 A51 A51 A51 A52 A52 A52 A52 A52 A52 A52 A52 A52 A52	L124 E125 P126 P127 V127 V127 V126 V150 D140 L161 L161 L162 L179	K199 A221
E236 TYR CTN CTN CTN CTN CTN CTN CTN CTN CTN CTN	V262 N263 S264 E265 E265 E265 K286 K286 K286 K286 K286 K286 K286 K286	1340 A341 K375 W376 S379 LEU VAL VAL 7389 R394 A400 A400	Y412 L413 L420
Y434 E435 1436 1436 1445 1445 7463 7463	1477 472 1477 1477 1478 1478 1478 1486 1486 1486 1486 1486 1486 1486 1521 1535 1535	1541 1541 1750 1753 1553 1554 1559 1559 1550 1560 1560 1560 1560 1567	LEU LEU TYR
HIS HIS HIS HIS HIS HIS			
• Molecule 2: Un	methylated DNA duplex		
Chain Z:	60%	40%	•
C1 88 68 13 13 13 13 13 13 13 14 14 14 14 14 14 14 14 14 14 14 14 14			
• Molecule 3: Un	methylated DNA duplex		
Chain Y:	70%	30%	•

• Molecule 1: Modification methylase BseCI



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants	87.04Å 87.04Å 156.35Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$\frac{90.00^{\circ}  90.00^{\circ}  120.00^{\circ}}{28.49  -  2.30}$	Deperitor
Resolution (Å)		Depositor EDS
% Data completeness	98.7 (28.49-2.30)	Depositor
(in resolution range)	98.7 (42.87-2.20)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	0.06	Depositor
$< I/\sigma(I) > 1$	$1.95 (at 2.20 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
D D	0.197 , $0.224$	Depositor
$R, R_{free}$	0.197 , $0.223$	DCC
$R_{free}$ test set	1685 reflections $(5.02\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	49.9	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.32 , $56.7$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.059 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5049	wwPDB-VP
Average B, all atoms $(Å^2)$	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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

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	А	0.25	0/4473	0.44	0/6040	
2	Ζ	0.58	0/224	0.99	0/344	
3	Y	0.58	0/224	0.98	0/344	
All	All	0.30	0/4921	0.52	0/6728	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	А	4380	0	4360	34	0
2	Ζ	200	0	110	6	0
3	Y	200	0	110	4	0
4	А	26	0	19	3	0
5	А	210	0	0	1	0
5	Y	11	0	0	0	0
5	Ζ	22	0	0	0	0
All	All	5049	0	4599	37	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.



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:339:THR:HG22	1:A:341:ALA:H	1.57	0.69
2:Z:1:DC:H42	3:Y:20:DG:H1	1.44	0.65
1:A:389:TYR:HE2	1:A:442:PRO:HB3	1.67	0.59
1:A:339:THR:HA	1:A:436:ILE:HG23	1.85	0.59
1:A:199:LYS:NZ	5:A:706:HOH:O	2.35	0.57
1:A:190:THR:HA	1:A:304:PRO:HB3	1.86	0.56
1:A:558:ASN:O	1:A:562:ASN:ND2	2.30	0.56
1:A:413:LEU:HD13	1:A:434:TYR:HB2	1.87	0.55
1:A:37:PHE:HA	1:A:179:ILE:HG13	1.89	0.54
1:A:126:PRO:HB2	1:A:175:LYS:HG3	1.89	0.54
1:A:394:ARG:NH2	1:A:400:ALA:O	2.41	0.53
2:Z:2:DG:H1	3:Y:19:DC:H42	1.57	0.53
1:A:140:GLN:HG3	3:Y:18:DT:H5'	1.94	0.50
1:A:51:ALA:O	4:A:601:SAH:N	2.44	0.49
1:A:375:LYS:HB3	1:A:376:TRP:CE3	2.47	0.49
1:A:322:ASN:HD22	1:A:573:ASP:HB3	1.77	0.49
1:A:161:ASP:OD1	1:A:162:LEU:N	2.45	0.49
1:A:221:ALA:HB1	2:Z:8:DT:OP2	2.13	0.49
1:A:199:LYS:HB2	1:A:301:TYR:CD2	2.49	0.48
2:Z:1:DC:N4	3:Y:20:DG:H1	2.11	0.48
1:A:486:ASP:HB3	1:A:541:ILE:HD13	1.96	0.47
1:A:471:ASP:OD1	1:A:472:GLY:N	2.46	0.47
1:A:244:VAL:O	1:A:244:VAL:HG13	2.15	0.47
1:A:339:THR:HG22	1:A:341:ALA:N	2.26	0.46
1:A:479:PRO:HG3	1:A:484:SER:HA	1.98	0.45
1:A:256:ILE:HD12	1:A:280:LEU:HD13	1.98	0.45
1:A:263:ASN:OD1	1:A:265:GLU:HG2	2.17	0.45
1:A:450:ILE:HB	1:A:477:ILE:HB	1.99	0.45
1:A:445:TRP:O	1:A:467:GLY:HA2	2.18	0.44
1:A:48:LEU:HB2	1:A:127:VAL:HG11	1.99	0.43
1:A:521:THR:HG21	2:Z:3:DA:H5"	2.00	0.43
1:A:51:ALA:HB1	4:A:601:SAH:O4'	2.19	0.43
1:A:463:TYR:HB2	1:A:492:MET:HE1	2.00	0.43
1:A:285:ASP:O	1:A:286:LYS:HD3	2.20	0.42
1:A:246:LYS:HA	1:A:294:LYS:HA	2.03	0.41
1:A:18:ALA:HA	4:A:601:SAH:H3'	2.03	0.40
1:A:159:ARG:HH21	2:Z:3:DA:H2	1.70	0.40

All (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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		
1	А	535/585~(92%)	517 (97%)	18 (3%)	0	100 100		

There are no Ramachandran outliers to report.

#### 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	
1	А	475/527~(90%)	473 (100%)	2~(0%)	91 96	

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	79	PHE
1	А	136	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 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	Tuno	Chain	Dog	Link	Bond lengths			Bond angles		
	Type		nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SAH	А	601	-	24,28,28	0.78	1 (4%)	$25,\!40,\!40$	0.81	1 (4%)

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	А	601	-	-	0/11/31/31	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	А	601	SAH	OXT-C	-2.51	1.22	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	601	SAH	C5-C6-N6	2.01	123.40	120.35

There are no chirality outliers.



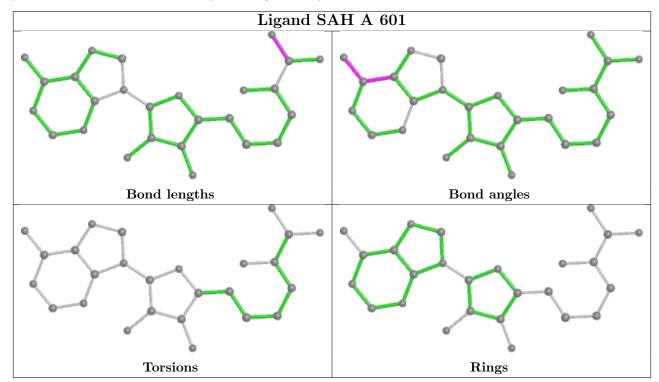
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	601	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 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.



### 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)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	544/585~(92%)	0.06	15 (2%) 53 60	41, 67, 108, 130	0
2	Z	10/10~(100%)	0.42	0 100 100	51, 58, 90, 101	0
3	Y	10/10 (100%)	-0.20	0 100 100	60, 63, 93, 102	0
All	All	564/605~(93%)	0.06	15 (2%) 54 62	41, 67, 108, 130	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	А	535	ILE	3.5	
1	А	412	TYR	3.3	
1	А	555	GLN	3.2	
1	А	489	PHE	3.2	
1	А	409	ALA	3.2	
1	А	568	ILE	2.6	
1	А	262	VAL	2.6	
1	А	420	LEU	2.5	
1	А	483	ASN	2.5	
1	А	567	LEU	2.4	
1	А	538	LYS	2.3	
1	А	560	ILE	2.3	
1	А	554	THR	2.3	
1	А	284	GLU	2.2	
1	А	318	LYS	2.1	

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

There are no non-standard protein/DNA/RNA residues in this entry.



## 6.3 Carbohydrates (i)

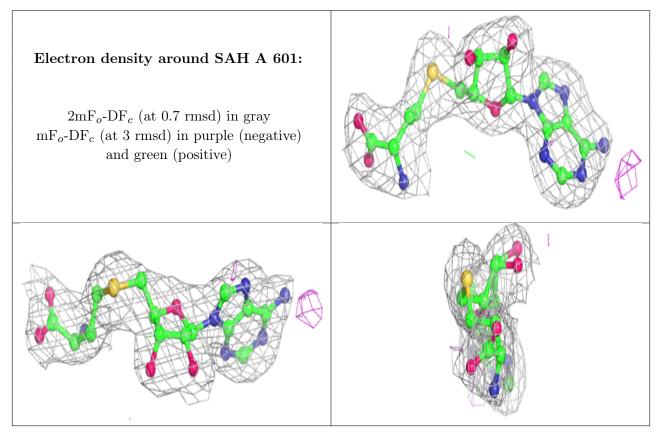
There are no monosaccharides in this entry.

### 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
4	SAH	А	601	26/26	0.95	0.10	$47,\!56,\!59,\!63$	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers (i)

There are no such residues in this entry.

