



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2017 – 10:54 AM EST

PDB ID : 6B3A
Title : AprA Methyltransferase 1 - GNAT didomain in complex with Mn²⁺ and SAM
Authors : Skiba, M.A.; Smith, J.L.
Deposited on : unknown
Resolution : 1.78 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

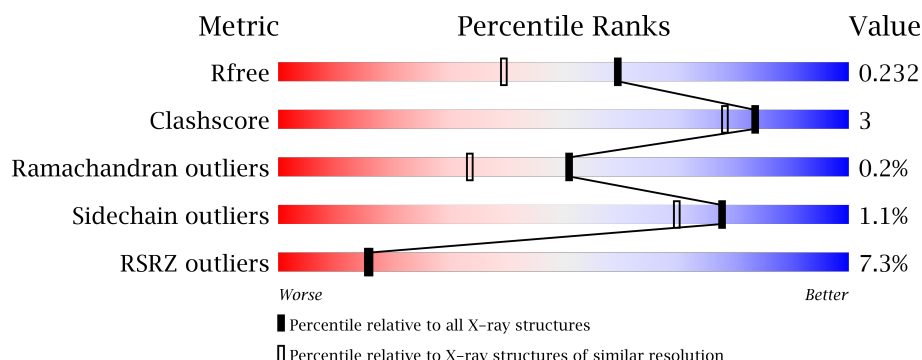
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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))
R_{free}	100719	7172 (1.80-1.76)
Clashscore	112137	8247 (1.80-1.76)
Ramachandran outliers	110173	8154 (1.80-1.76)
Sidechain outliers	110143	8153 (1.80-1.76)
RSRZ outliers	101464	7262 (1.80-1.76)

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.

Mol	Chain	Length	Quality of chain
1	A	652	

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
2	SAM	A	701	-	-	-	X
4	GOL	A	703	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5560 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 AprA Methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	631	5125	3303	865	942	15	0	2	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP A0A1U7N2Z8
A	-21	HIS	-	expression tag	UNP A0A1U7N2Z8
A	-20	HIS	-	expression tag	UNP A0A1U7N2Z8
A	-19	HIS	-	expression tag	UNP A0A1U7N2Z8
A	-18	HIS	-	expression tag	UNP A0A1U7N2Z8
A	-17	HIS	-	expression tag	UNP A0A1U7N2Z8
A	-16	HIS	-	expression tag	UNP A0A1U7N2Z8
A	-15	SER	-	expression tag	UNP A0A1U7N2Z8
A	-14	SER	-	expression tag	UNP A0A1U7N2Z8
A	-13	GLY	-	expression tag	UNP A0A1U7N2Z8
A	-12	VAL	-	expression tag	UNP A0A1U7N2Z8
A	-11	ASP	-	expression tag	UNP A0A1U7N2Z8
A	-10	LEU	-	expression tag	UNP A0A1U7N2Z8
A	-9	GLY	-	expression tag	UNP A0A1U7N2Z8
A	-8	THR	-	expression tag	UNP A0A1U7N2Z8
A	-7	GLU	-	expression tag	UNP A0A1U7N2Z8
A	-6	ASN	-	expression tag	UNP A0A1U7N2Z8
A	-5	LEU	-	expression tag	UNP A0A1U7N2Z8
A	-4	TYR	-	expression tag	UNP A0A1U7N2Z8
A	-3	PHE	-	expression tag	UNP A0A1U7N2Z8
A	-2	GLN	-	expression tag	UNP A0A1U7N2Z8
A	-1	SER	-	expression tag	UNP A0A1U7N2Z8
A	0	ASN	-	expression tag	UNP A0A1U7N2Z8
A	1	ALA	-	expression tag	UNP A0A1U7N2Z8
A	274	ILE	SER	engineered mutation	UNP A0A1U7N2Z8
A	528	PRO	GLN	engineered mutation	UNP A0A1U7N2Z8

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- The chemical structure of S-adenosylmethionine (SAM) is shown with the following atom labels: N6 (amino group), N1, N3, N7, N9 (pyrimidine ring nitrogens), C6, C5, C8, C4, C2 (pyrimidine ring carbons), C1' (ribose C1'), C2' (ribose C2'), C3' (ribose C3'), C4' (ribose C4'), C5' (ribose C5'), O4' (ribose O4'), O2' (ribose O2'), O3' (ribose O3'), CE (methyl group), SD (sulfonium sulfur), CB (methylene group), CG (methylene group), CA (methylene group), C (carboxyl carbon), O (carboxyl oxygen), OXT (carboxylate oxygen), and N (amino group). The structure features a pyrimidine ring connected to a ribose sugar, which is linked via a sulfonium group to a methionine side chain ending in a carboxylate group.

GOL

The diagram shows a skeletal structure of 1,2,3-propanetriol (glycerol). The carbon backbone is represented by three vertices labeled C1, C2, and C3 in green. C1 is on the left, C2 is in the middle, and C3 is on the right. Each carbon is bonded to a hydroxyl group (OH) shown in red. The OH group on C1 is labeled O1 in green below it. The OH group on C2 is labeled O2 in green below it. The OH group on C3 is labeled O3 in green to its right. The bonds between the carbons and between the carbons and the hydroxyl groups are shown as black lines.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

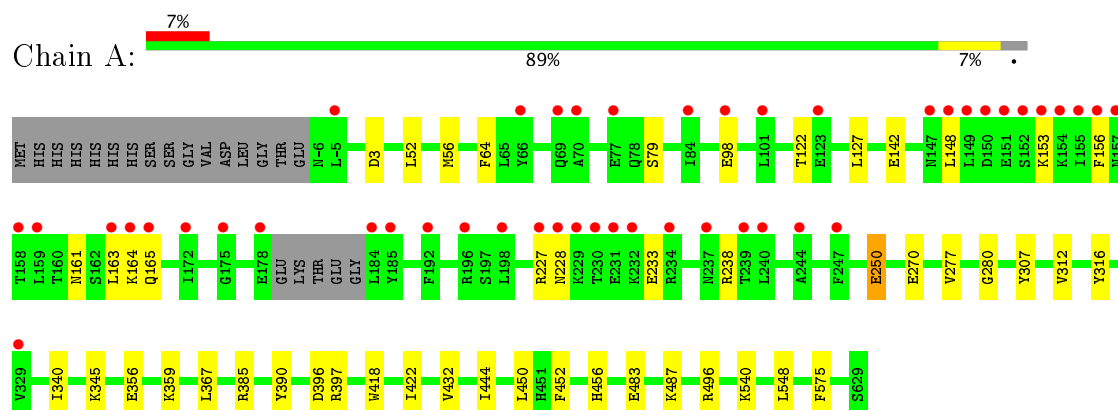
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	401	Total	O	0	0
			401	401		

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 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.

- Molecule 1: AprA Methyltransferase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.52Å 87.05Å 135.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.67 – 1.78 46.67 – 1.78	Depositor EDS
% Data completeness (in resolution range)	90.3 (46.67-1.78) 80.0 (46.67-1.78)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.78Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.180 , 0.226 0.182 , 0.232	Depositor DCC
R_{free} test set	1867 reflections (3.00%)	DCC
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5560	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

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: GOL, MN, SAM

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	A	0.37	0/5234	0.53	2/7086 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	548	LEU	CA-CB-CG	6.20	129.57	115.30
1	A	396	ASP	CB-CG-OD1	5.57	123.31	118.30

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	A	5125	0	5194	27	0
2	A	27	0	22	3	0
3	A	1	0	0	0	0
4	A	6	0	8	1	0
5	A	401	0	0	6	0
All	All	5560	0	5224	29	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.

All (29) 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)
1:A:496:ARG:HH12	4:A:703:GOL:H11	1.53	0.72
1:A:233:GLU:OE2	1:A:238:ARG:HD2	2.01	0.60
1:A:397:ARG:NH2	5:A:804:HOH:O	2.35	0.59
1:A:3:ASP:OD1	5:A:801:HOH:O	2.17	0.56
1:A:270:GLU:HG2	1:A:307:TYR:CE2	2.47	0.50
1:A:270:GLU:HG3	5:A:1047:HOH:O	2.12	0.50
1:A:385:ARG:HG2	1:A:390:TYR:HE2	1.77	0.49
1:A:345:LYS:HE3	5:A:1032:HOH:O	2.11	0.49
2:A:701:SAM:N	2:A:701:SAM:HE2	2.28	0.48
1:A:163:LEU:HA	1:A:163:LEU:HD23	1.78	0.46
2:A:701:SAM:HE2	2:A:701:SAM:HN2	1.81	0.45
1:A:98:GLU:HG2	1:A:142:GLU:CD	2.38	0.44
1:A:452:PHE:CZ	1:A:456:HIS:CE1	3.06	0.44
1:A:280:GLY:HA3	1:A:367:LEU:HD22	2.00	0.43
1:A:250:GLU:HG3	5:A:884:HOH:O	2.18	0.43
1:A:444:ILE:HD11	1:A:450:LEU:HD13	1.99	0.43
1:A:540:LYS:NZ	5:A:816:HOH:O	2.47	0.43
1:A:122:THR:HG21	1:A:127:LEU:HD23	2.00	0.42
1:A:340:ILE:HG22	2:A:701:SAM:N6	2.34	0.42
1:A:277:VAL:HG22	1:A:312:VAL:HB	2.01	0.42
1:A:418:TRP:O	1:A:422:ILE:HG12	2.20	0.42
1:A:52:LEU:O	1:A:56:MET:HG2	2.20	0.42
1:A:161:ASN:O	1:A:165:GLN:HG2	2.20	0.41
1:A:156:PHE:O	1:A:164:LYS:HG2	2.21	0.41
1:A:64:PHE:O	1:A:79:SER:HB3	2.20	0.41
1:A:227:ARG:HA	1:A:227:ARG:HD2	1.97	0.41
1:A:356:GLU:HB2	1:A:359:LYS:HG3	2.03	0.40
1:A:432:VAL:HG21	1:A:452:PHE:CZ	2.57	0.40
1:A:483:GLU:H	1:A:483:GLU:CD	2.25	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	
1	A	629/652 (96%)	613 (98%)	15 (2%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	LYS

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	
1	A	568/584 (97%)	562 (99%)	6 (1%)	78	70

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	LEU
1	A	228	ASN
1	A	250	GLU
1	A	316	TYR
1	A	487	LYS
1	A	575	PHE

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	SAM	A	701	-	21,29,29	1.07	2 (9%)	17,42,42	2.63	2 (11%)
4	GOL	A	703	-	5,5,5	0.32	0	5,5,5	0.20	0

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	SAM	A	701	-	-	0/8/33/33	0/3/3/3
4	GOL	A	703	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	SAM	C2-N1	2.37	1.38	1.33
2	A	701	SAM	C2-N3	3.40	1.37	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	SAM	N3-C2-N1	-10.13	120.04	128.86
2	A	701	SAM	O4'-C4'-C5'	-2.08	103.48	108.87

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	A	701	SAM	3	0
4	A	703	GOL	1	0

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 ⓘ

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, 95th 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	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	631/652 (96%)	0.41	46 (7%) 16 16	20, 31, 72, 133	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	PHE	7.1
1	A	185	TYR	6.6
1	A	230	THR	6.4
1	A	151	GLU	6.3
1	A	158	THR	5.7
1	A	157	ASN	5.5
1	A	152	SER	5.2
1	A	155	ILE	5.1
1	A	227	ARG	4.9
1	A	150	ASP	4.7
1	A	154	LYS	4.5
1	A	123	GLU	4.5
1	A	184	LEU	4.3
1	A	192	PHE	4.1
1	A	229	LYS	3.9
1	A	240	LEU	3.8
1	A	159	LEU	3.8
1	A	232	LYS	3.7
1	A	175	GLY	3.6
1	A	196	ARG	3.6
1	A	153	LYS	3.4
1	A	231	GLU	3.4
1	A	66	TYR	3.2
1	A	147	ASN	3.2
1	A	198	LEU	3.2
1	A	178	GLU	3.1
1	A	149	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	69	GLN	2.8
1	A	172	ILE	2.7
1	A	164	LYS	2.6
1	A	228	ASN	2.5
1	A	234	ARG	2.4
1	A	101	LEU	2.4
1	A	77	GLU	2.3
1	A	70	ALA	2.3
1	A	244	ALA	2.3
1	A	329	VAL	2.2
1	A	148	LEU	2.2
1	A	239	THR	2.2
1	A	237	ASN	2.2
1	A	163	LEU	2.1
1	A	-5	LEU	2.1
1	A	84	ILE	2.1
1	A	165	GLN	2.1
1	A	247	PHE	2.0
1	A	98	GLU	2.0

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
4	GOL	A	703	6/6	0.79	0.19	3.83	63,65,69,69	0
2	SAM	A	701	27/27	0.88	0.13	2.55	30,38,67,81	0
3	MN	A	702	1/1	0.99	0.04	-	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.