



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 2, 2017 – 09:08 AM EDT

PDB ID : 1NBI
Title : Structure of R175K mutated glycine N-methyltransferase complexed with S-adenosylmethionine, R175K:SAM.
Authors : Takata, Y.; Takusagawa, F.
Deposited on : unknown
Resolution : 3.00 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

<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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

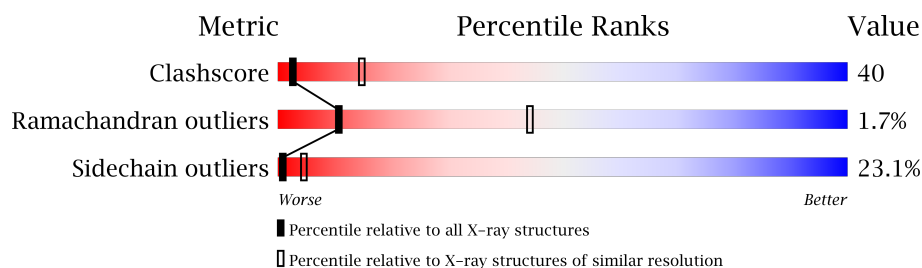
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)

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	A	292	
1	B	292	
1	C	292	
1	D	292	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8984 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 Glycine N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2158	1373	374	400	11			
1	B	275	Total	C	N	O	S	0	0	0
			2158	1373	374	400	11			
1	C	275	Total	C	N	O	S	0	0	0
			2158	1373	374	400	11			
1	D	275	Total	C	N	O	S	0	0	0
			2158	1373	374	400	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	175	LYS	ARG	ENGINEERED	UNP P13255
B	175	LYS	ARG	ENGINEERED	UNP P13255
C	175	LYS	ARG	ENGINEERED	UNP P13255
D	175	LYS	ARG	ENGINEERED	UNP P13255

- Molecule 2 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S).



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

- Molecule 3 is water.

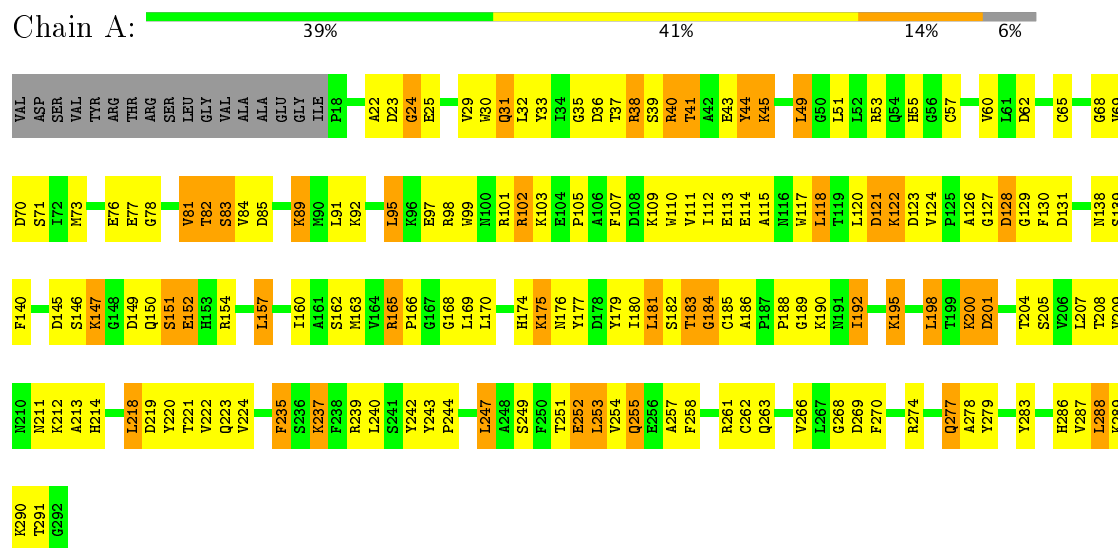
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	70	Total	O	0	0
			70	70		
3	B	55	Total	O	0	0
			55	55		
3	C	63	Total	O	0	0
			63	63		
3	D	56	Total	O	0	0
			56	56		

3 Residue-property plots

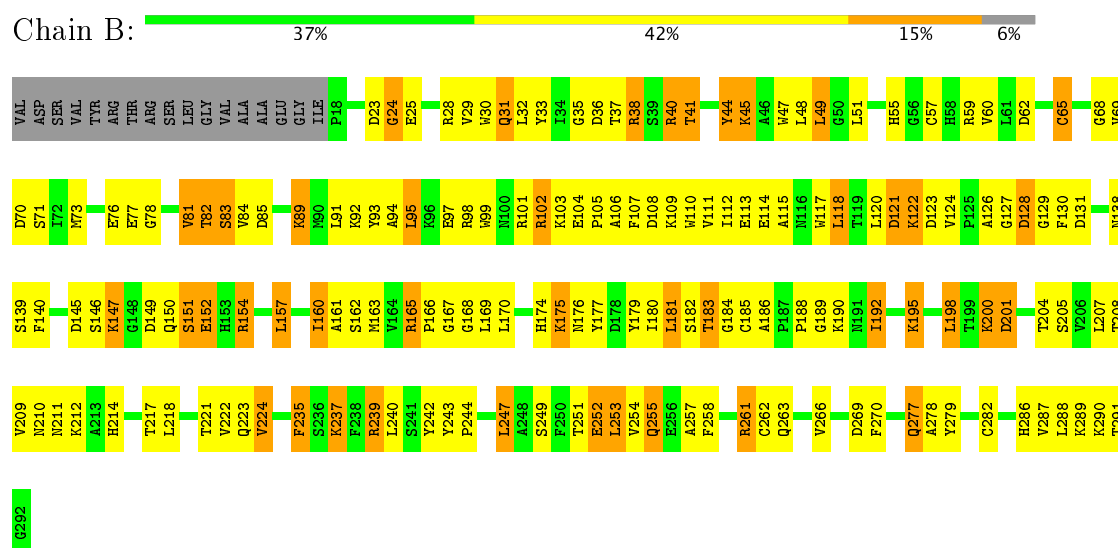
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

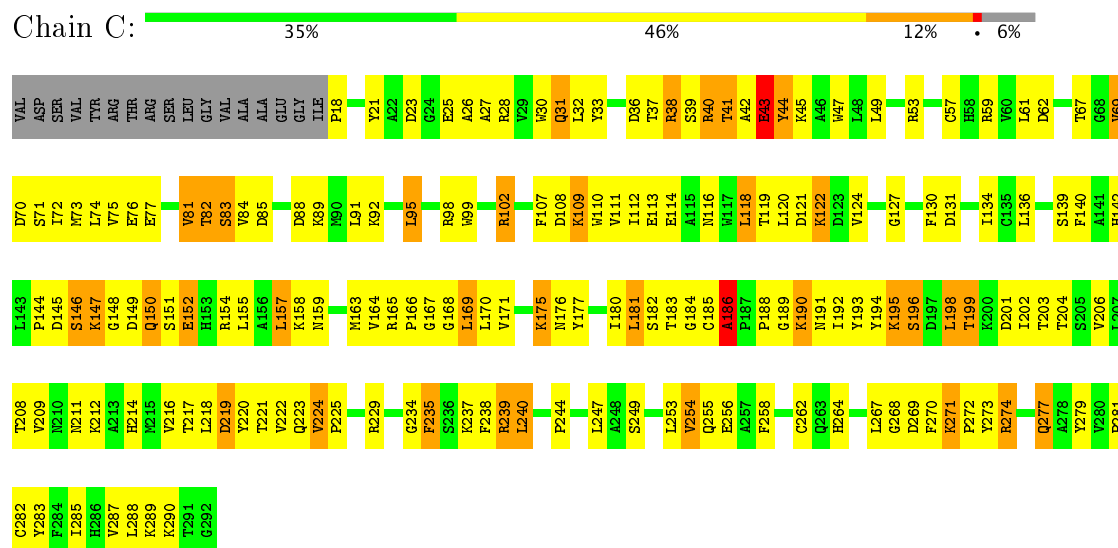
• Molecule 1: Glycine N-methyltransferase



• Molecule 1: Glycine N-methyltransferase



● Molecule 1: Glycine N-methyltransferase



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	77.87Å 77.87Å 227.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-3.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.165 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8984	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: 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	0.39	0/2213	0.63	0/2999
1	B	0.40	0/2213	0.65	0/2999
1	C	0.70	2/2213 (0.1%)	0.83	4/2999 (0.1%)
1	D	0.74	2/2213 (0.1%)	0.85	4/2999 (0.1%)
All	All	0.58	4/8852 (0.0%)	0.75	8/11996 (0.1%)

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	2
1	D	0	2
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	43	GLU	C-N	-28.75	0.68	1.34
1	C	43	GLU	C-N	-26.58	0.72	1.34
1	C	186	ALA	C-N	-8.05	1.19	1.34
1	D	186	ALA	C-N	-7.99	1.19	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	43	GLU	O-C-N	-22.57	86.59	122.70
1	C	43	GLU	C-N-CA	22.29	177.43	121.70
1	D	43	GLU	C-N-CA	20.11	171.98	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	43	GLU	O-C-N	-19.29	91.84	122.70
1	D	43	GLU	CA-C-N	15.44	151.18	117.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	186	ALA	Mainchain
1	C	43	GLU	Peptide
1	D	186	ALA	Mainchain
1	D	43	GLU	Peptide

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	2158	0	2114	145	0
1	B	2158	0	2114	152	0
1	C	2158	0	2113	200	0
1	D	2158	0	2113	199	0
2	A	27	0	22	1	0
2	B	27	0	22	2	0
2	C	27	0	22	3	0
2	D	27	0	22	2	0
3	A	70	0	0	5	0
3	B	55	0	0	2	0
3	C	63	0	0	13	0
3	D	56	0	0	8	0
All	All	8984	0	8542	687	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 40.

The worst 5 of 687 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:C:219:ASP:HA	1:C:239:ARG:HB2	1.42	1.02
1:D:219:ASP:HA	1:D:239:ARG:HB2	1.43	1.00
1:A:186:ALA:O	1:A:188:PRO:HD3	1.59	1.00
1:D:38:ARG:HE	1:D:38:ARG:H	1.00	0.99
1:C:38:ARG:H	1:C:38:ARG:HE	0.97	0.95

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	A	273/292 (94%)	237 (87%)	32 (12%)	4 (2%)	12	48
1	B	273/292 (94%)	239 (88%)	30 (11%)	4 (2%)	12	48
1	C	273/292 (94%)	236 (86%)	31 (11%)	6 (2%)	8	36
1	D	273/292 (94%)	236 (86%)	32 (12%)	5 (2%)	10	43
All	All	1092/1168 (94%)	948 (87%)	125 (11%)	19 (2%)	11	44

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLY
1	C	44	TYR
1	A	44	TYR
1	A	127	GLY
1	B	24	GLY

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	A	229/242 (95%)	170 (74%)	59 (26%)	0	3
1	B	229/242 (95%)	171 (75%)	58 (25%)	0	3
1	C	229/242 (95%)	181 (79%)	48 (21%)	1	6
1	D	229/242 (95%)	182 (80%)	47 (20%)	1	7
All	All	916/968 (95%)	704 (77%)	212 (23%)	1	4

5 of 212 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	183	THR
1	C	31	GLN
1	D	199	THR
1	B	198	LEU
1	B	237	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	214	HIS
1	C	31	GLN
1	D	264	HIS
1	B	277	GLN
1	C	142	HIS

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

4 ligands 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	SAM	A	293	-	21,29,29	1.05	0	17,42,42	1.57	4 (23%)
2	SAM	B	1293	-	21,29,29	1.24	2 (9%)	17,42,42	1.51	3 (17%)
2	SAM	C	2293	-	21,29,29	0.92	0	17,42,42	1.48	3 (17%)
2	SAM	D	3293	-	21,29,29	1.04	1 (4%)	17,42,42	1.50	4 (23%)

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	293	-	-	0/8/33/33	0/3/3/3
2	SAM	B	1293	-	-	0/8/33/33	0/3/3/3
2	SAM	C	2293	-	-	0/8/33/33	0/3/3/3
2	SAM	D	3293	-	-	0/8/33/33	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1293	SAM	O4'-C1'	-2.43	1.37	1.41
2	D	3293	SAM	C2-N3	2.06	1.35	1.32
2	B	1293	SAM	C2-N3	2.42	1.36	1.32

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	293	SAM	O3'-C3'-C4'	-3.04	102.22	111.09
2	D	3293	SAM	C4'-O4'-C1'	-2.96	106.62	109.77
2	B	1293	SAM	O3'-C3'-C4'	-2.75	103.05	111.09
2	C	2293	SAM	C4'-O4'-C1'	-2.67	106.93	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1293	SAM	C4'-O4'-C1'	-2.40	107.22	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	293	SAM	1	0
2	B	1293	SAM	2	0
2	C	2293	SAM	3	0
2	D	3293	SAM	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	2
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	186:ALA	C	187:PRO	N	1.19
1	D	186:ALA	C	187:PRO	N	1.19
1	C	43:GLU	C	44:TYR	N	0.72
1	D	43:GLU	C	44:TYR	N	0.67

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.