



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 11:14 AM UTC

PDB ID : 2AZT / pdb_00002azt
Title : Crystal structure of H176N mutant of human Glycine N-Methyltransferase
Authors : Luka, Z.; Pakhomova, S.; Luka, Y.; Newcomer, M.E.; Wagner, C.
Deposited on : 2005-09-12
Resolution : 2.70 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

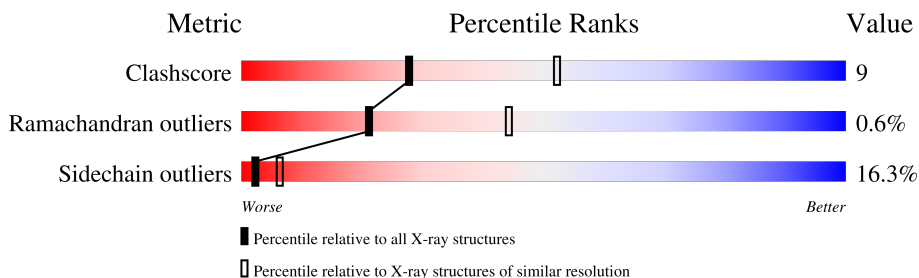
1 Overall quality at a glance

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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (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 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	295	
1	B	295	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4355 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.

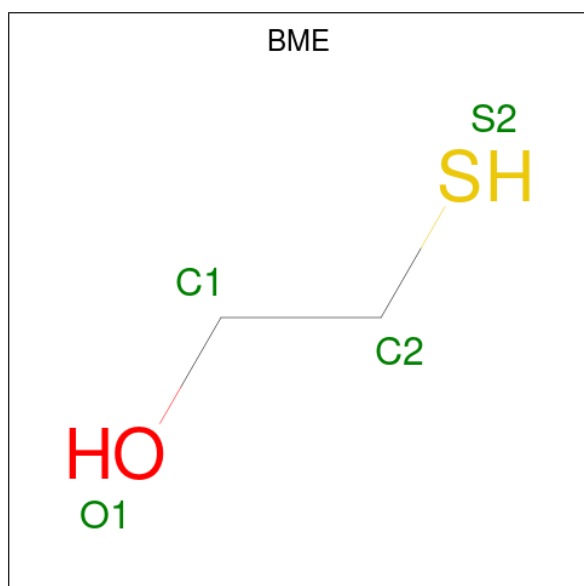
- Molecule 1 is a protein called Glycine N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2109	1343	364	389	13			
1	B	277	Total	C	N	O	S	0	0	0
			2159	1372	375	399	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	ASN	HIS	engineered mutation	UNP Q14749
B	176	ASN	HIS	engineered mutation	UNP Q14749

- Molecule 2 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



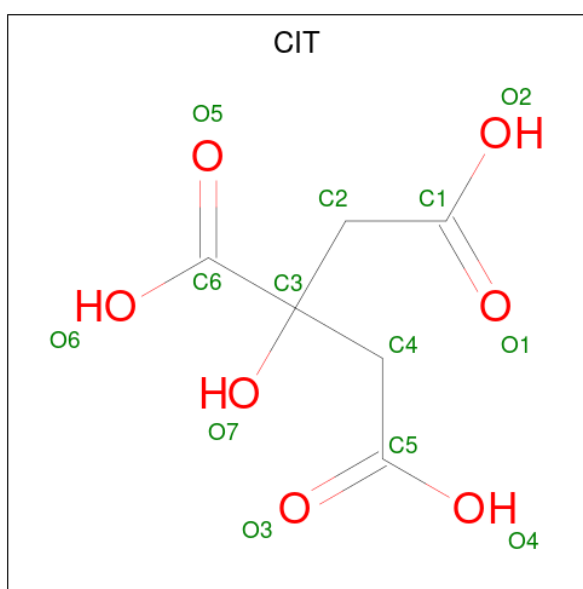
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total 5	O 5	0	0
5	B	35	Total 35	O 35	0	0

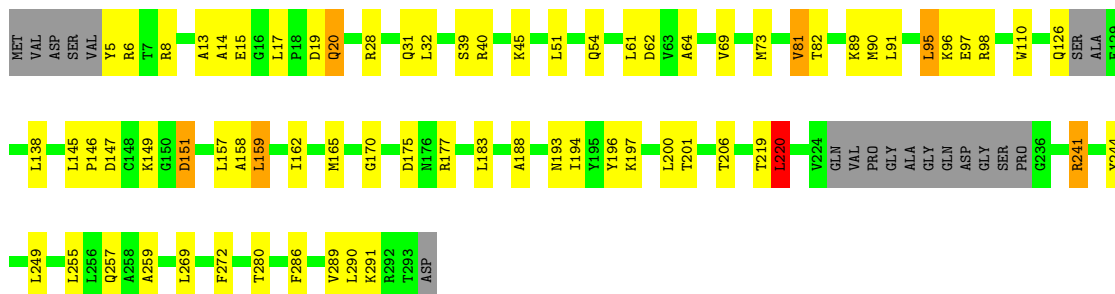
3 Residue-property plots [i](#)

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.

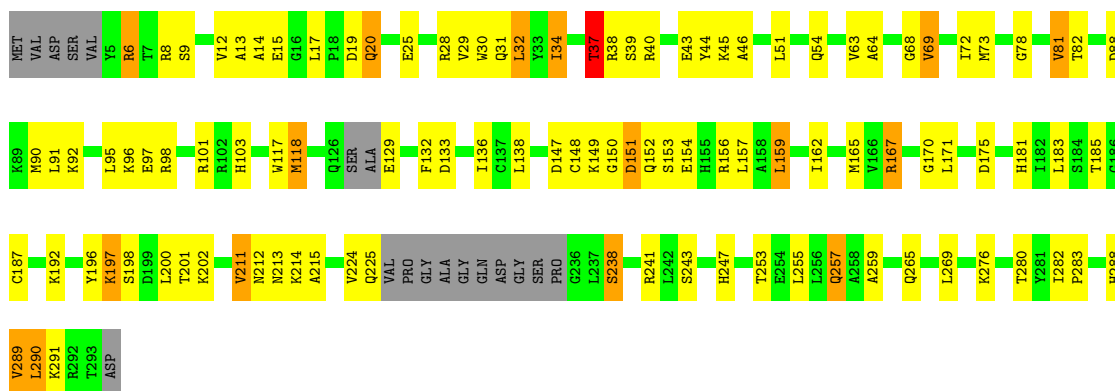
- Molecule 1: Glycine N-methyltransferase

Chain A: 



- Molecule 1: Glycine N-methyltransferase

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	76.12Å 83.28Å 115.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	13.00 – 2.70	Depositor
% Data completeness (in resolution range)	98.9 (13.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.236 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4355	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: BME, CIT, CL

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	0.85	0/2158	1.17	3/2933 (0.1%)
1	B	1.36	7/2208 (0.3%)	1.39	18/2994 (0.6%)
All	All	1.14	7/4366 (0.2%)	1.28	21/5927 (0.4%)

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	A	0	1
1	B	0	1
All	All	0	2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	181	HIS	C-O	8.28	1.33	1.24
1	B	289	VAL	CA-CB	7.79	1.63	1.54
1	B	37	THR	CA-CB	6.58	1.64	1.53
1	B	118	MET	SD-CE	6.29	1.95	1.79
1	B	165	MET	SD-CE	-5.41	1.66	1.79

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	ASP	CA-C-N	-6.85	111.63	122.79
1	B	151	ASP	C-N-CA	-6.85	111.63	122.79
1	B	187	CYS	CA-CB-SG	-6.66	99.09	114.40
1	B	238	SER	N-CA-C	6.33	119.33	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	ALA	N-CA-C	-6.05	101.45	110.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	5	TYR	Peptide
1	B	129	GLU	Peptide

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	A	2109	0	2006	35	0
1	B	2159	0	2098	51	0
2	A	8	0	10	1	0
2	B	12	0	15	1	0
3	A	13	0	5	0	0
3	B	13	0	5	0	0
4	B	1	0	0	0	0
5	A	5	0	0	0	0
5	B	35	0	0	4	0
All	All	4355	0	4139	76	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 9.

The worst 5 of 76 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:B:29:VAL:HG21	1:B:238:SER:HB3	1.53	0.90
1:B:29:VAL:HG21	1:B:238:SER:CB	2.07	0.84
1:A:15:GLU:HB3	1:B:64:ALA:HB1	1.67	0.76
1:B:133:ASP:HA	1:B:167:ARG:HE	1.49	0.74
1:B:37:THR:OG1	1:B:69:VAL:HG21	1.92	0.69

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	270/295 (92%)	251 (93%)	18 (7%)	1 (0%)	30	54
1	B	271/295 (92%)	248 (92%)	21 (8%)	2 (1%)	18	41
All	All	541/590 (92%)	499 (92%)	39 (7%)	3 (1%)	21	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	37	THR
1	A	151	ASP
1	B	38	ARG

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	214/246 (87%)	183 (86%)	31 (14%)	3	8
1	B	227/246 (92%)	186 (82%)	41 (18%)	2	5
All	All	441/492 (90%)	369 (84%)	72 (16%)	2	6

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	197	LYS
1	B	290	LEU
1	B	201	THR
1	B	255	LEU
1	A	241	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	HIS
1	B	58	GLN
1	B	225	GLN
1	B	161	ASN
1	A	161	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	BME	A	1188	1	3,3,3	0.39	0	2,2,2	0.38	0
2	BME	A	1285	1	3,3,3	0.59	0	2,2,2	0.34	0
3	CIT	A	1000	-	12,12,12	1.80	4 (33%)	17,17,17	1.98	6 (35%)
3	CIT	B	2000	-	12,12,12	2.20	3 (25%)	17,17,17	2.54	9 (52%)
2	BME	B	2285	1	3,3,3	0.44	0	2,2,2	0.97	0
2	BME	B	2188	1	3,3,3	0.33	0	2,2,2	0.20	0
2	BME	B	2249	1	3,3,3	0.46	0	2,2,2	0.14	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	BME	A	1188	1	-	1/1/1/1	-
2	BME	A	1285	1	-	1/1/1/1	-
3	CIT	A	1000	-	-	5/16/16/16	-
3	CIT	B	2000	-	-	5/16/16/16	-
2	BME	B	2285	1	-	1/1/1/1	-
2	BME	B	2188	1	-	1/1/1/1	-
2	BME	B	2249	1	-	1/1/1/1	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2000	CIT	C3-C6	4.97	1.58	1.53
3	A	1000	CIT	C3-C6	4.14	1.57	1.53
3	B	2000	CIT	O3-C5	3.99	1.35	1.22
3	B	2000	CIT	O7-C3	2.91	1.48	1.43
3	A	1000	CIT	O7-C3	2.68	1.48	1.43

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2000	CIT	C4-C3-C6	4.31	119.57	110.03
3	B	2000	CIT	O6-C6-C3	4.24	121.27	113.14
3	B	2000	CIT	O7-C3-C4	-3.91	100.46	109.38
3	B	2000	CIT	O3-C5-C4	-3.67	112.55	122.95
3	A	1000	CIT	O7-C3-C4	-3.47	101.45	109.38

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1285	BME	O1-C1-C2-S2
2	B	2285	BME	O1-C1-C2-S2
3	A	1000	CIT	O7-C3-C4-C5
3	A	1000	CIT	C6-C3-C4-C5
3	B	2000	CIT	O7-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1188	BME	1	0
2	B	2285	BME	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 [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.