



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 04:06 pm GMT

PDB ID : 3KPY
Title : Crystal Structure of hPNMT in Complex AdoHcy and 6-Chlorooxindole
Authors : Drinkwater, N.; Martin, J.L.
Deposited on : 2009-11-17
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

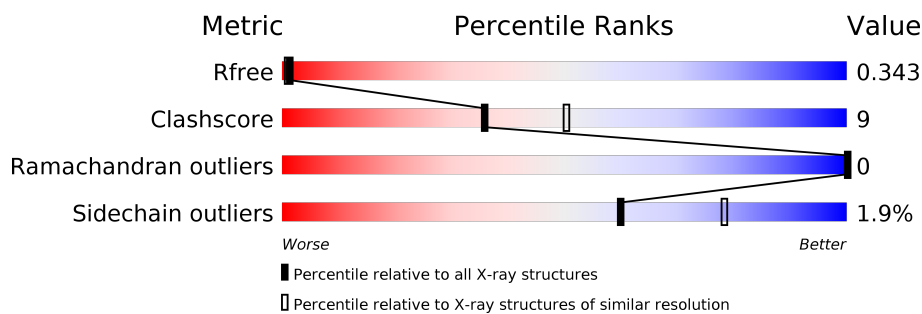
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	289	 70% 18% 11%
1	B	289	 78% 14% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4441 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 Phenylethanolamine N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2016	1280	358	369	9			
1	B	268	Total	C	N	O	S	0	0	0
			2083	1320	370	384	9			

There are 14 discrepancies between the modelled and reference sequences:

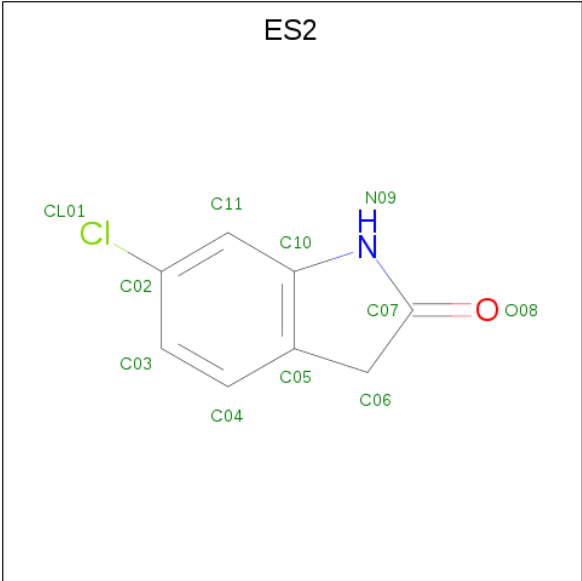
Chain	Residue	Modelled	Actual	Comment	Reference
A	283	GLU	-	EXPRESSION TAG	UNP P11086
A	284	HIS	-	EXPRESSION TAG	UNP P11086
A	285	HIS	-	EXPRESSION TAG	UNP P11086
A	286	HIS	-	EXPRESSION TAG	UNP P11086
A	287	HIS	-	EXPRESSION TAG	UNP P11086
A	288	HIS	-	EXPRESSION TAG	UNP P11086
A	289	HIS	-	EXPRESSION TAG	UNP P11086
B	283	GLU	-	EXPRESSION TAG	UNP P11086
B	284	HIS	-	EXPRESSION TAG	UNP P11086
B	285	HIS	-	EXPRESSION TAG	UNP P11086
B	286	HIS	-	EXPRESSION TAG	UNP P11086
B	287	HIS	-	EXPRESSION TAG	UNP P11086
B	288	HIS	-	EXPRESSION TAG	UNP P11086
B	289	HIS	-	EXPRESSION TAG	UNP P11086

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is 6-chloro-1,3-dihydro-2H-indol-2-one (three-letter code: ES2) (formula: C₈H₆ClNO).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			11	8	1	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	Cl	N	O	0	0
			11	8	1	1	1		

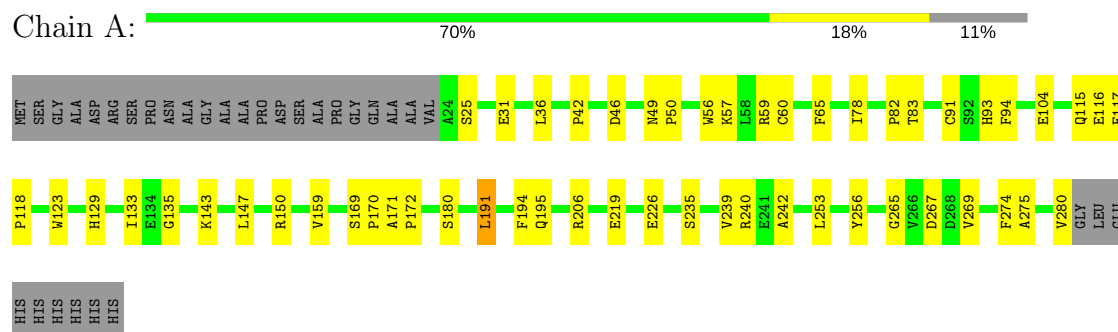
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	115	Total	O	0	0
			115	115		
4	B	153	Total	O	0	0
			153	153		

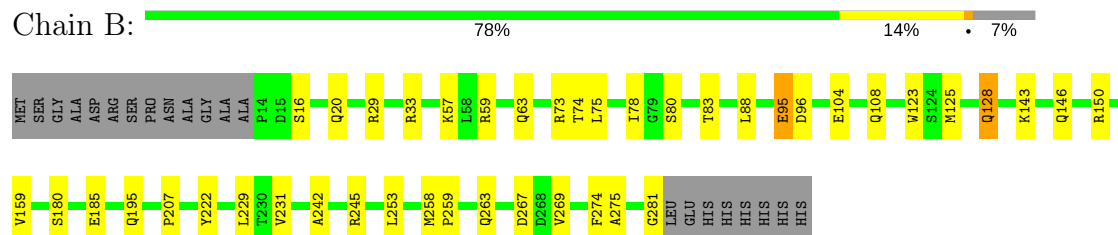
3 Residue-property plots [i](#)

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. 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.

• Molecule 1: Phenylethanolamine N-methyltransferase



• Molecule 1: Phenylethanolamine N-methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	93.91Å 93.91Å 188.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.56 – 2.40 45.56 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.2 (45.56-2.40) 90.2 (45.56-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.39Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.206 , 0.271 0.309 , 0.343	Depositor DCC
R_{free} test set	1583 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4441	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAH, ES2

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	0.29	0/2067	0.46	0/2813
1	B	0.31	0/2136	0.47	0/2908
All	All	0.30	0/4203	0.46	0/5721

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

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	2016	0	1983	38	0
1	B	2083	0	2045	32	0
2	A	26	0	20	2	0
2	B	26	0	20	3	0
3	A	11	0	6	3	0
3	B	11	0	6	3	0
4	A	115	0	0	9	0
4	B	153	0	0	8	0
All	All	4441	0	4080	72	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 72 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:195:GLN:HE22	1:B:242:ALA:HA	1.46	0.79
1:B:263:GLN:HB2	4:B:2039:HOH:O	1.86	0.75
1:A:46:ASP:HB2	4:A:2217:HOH:O	1.91	0.69
1:A:195:GLN:HE22	1:A:242:ALA:HA	1.59	0.67
1:B:263:GLN:HG3	4:B:2159:HOH:O	1.98	0.63

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	255/289 (88%)	250 (98%)	5 (2%)	0	100	100
1	B	266/289 (92%)	261 (98%)	5 (2%)	0	100	100
All	All	521/578 (90%)	511 (98%)	10 (2%)	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	A	212/233 (91%)	208 (98%)	4 (2%)	60	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	218/233 (94%)	214 (98%)	4 (2%)	62	79
All	All	430/466 (92%)	422 (98%)	8 (2%)	60	78

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	ARG
1	B	245	ARG
1	B	95	GLU
1	A	191	LEU
1	B	29	ARG

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

Mol	Chain	Res	Type
1	B	20	GLN
1	B	195	GLN
1	B	106	ASN
1	A	106	ASN
1	B	128	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	SAH	A	2001	-	20,28,28	4.86	10 (50%)	19,40,40	2.85	4 (21%)
3	ES2	A	290	-	12,12,12	4.10	9 (75%)	17,17,17	4.35	3 (17%)
2	SAH	B	2002	-	20,28,28	4.73	9 (45%)	19,40,40	2.82	3 (15%)
3	ES2	B	290	-	12,12,12	4.24	9 (75%)	17,17,17	4.16	3 (17%)

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	SAH	A	2001	-	-	0/7/31/31	0/3/3/3
3	ES2	A	290	-	-	0/0/8/8	0/2/2/2
2	SAH	B	2002	-	-	0/7/31/31	0/3/3/3
3	ES2	B	290	-	-	0/0/8/8	0/2/2/2

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	290	ES2	O08-C07	-2.42	1.18	1.23
3	B	290	ES2	O08-C07	-2.31	1.18	1.23
2	A	2001	SAH	C6-N1	2.12	1.46	1.37
2	B	2002	SAH	C5-N7	2.26	1.47	1.39
2	A	2001	SAH	C5-N7	2.37	1.47	1.39

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	290	ES2	O08-C07-C06	-16.34	119.29	126.95
3	B	290	ES2	O08-C07-C06	-14.91	119.96	126.95
2	A	2001	SAH	N3-C2-N1	-10.60	119.79	128.86
2	B	2002	SAH	N3-C2-N1	-10.33	120.02	128.86
3	B	290	ES2	C10-N09-C07	-6.91	108.35	111.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	SAH	2	0
3	A	290	ES2	3	0
2	B	2002	SAH	3	0
3	B	290	ES2	3	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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.