



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 07:15 PM BST

PDB ID : 5NRR
Title : Human DNMT3B PWWP domain in complex with 5-[(2-Hydroxyethyl)(propyl)amino]-1-pentanol
Authors : Rondelet, G.; Wouters, J.
Deposited on : 2017-04-25
Resolution : 1.70 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

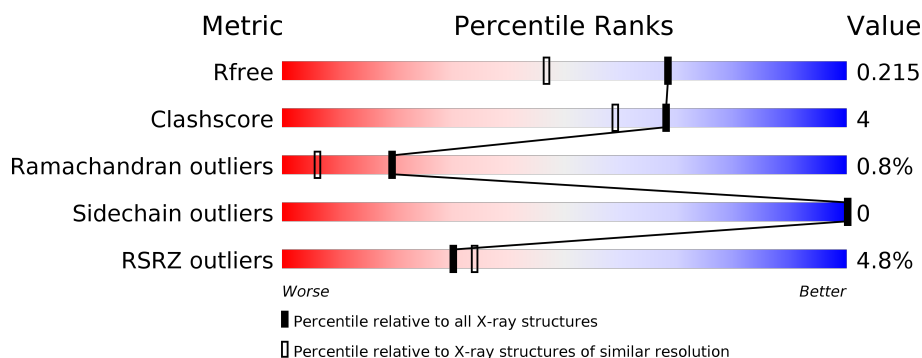
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 on 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 $\leq 5\%$. 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	150	
1	B	150	

2 Entry composition [i](#)

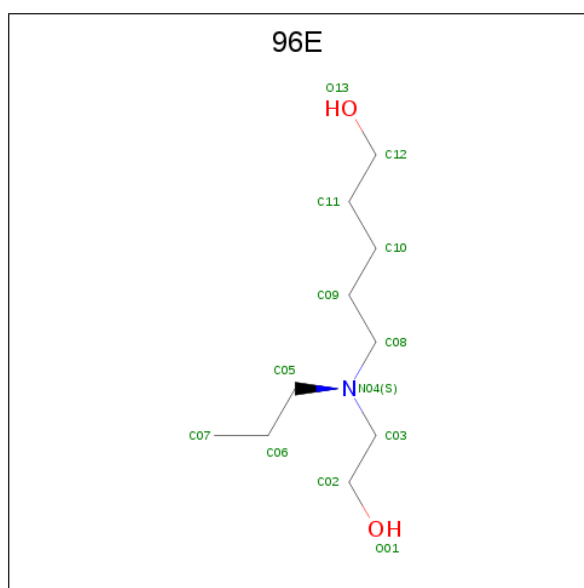
There are 4 unique types of molecules in this entry. The entry contains 2614 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA (cytosine-5)-methyltransferase 3B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	135	Total	C	N	O	S	0	3	0
			1097	715	187	190	5			
1	B	137	Total	C	N	O	S	0	4	0
			1126	733	194	194	5			

- Molecule 2 is 5-[2-hydroxyethyl(propyl)amino]pentan-1-ol (three-letter code: 96E) (formula: C₁₀H₂₃NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	10	1	2		
2	B	1	Total	C	N	O	0	0
			13	10	1	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	177	Total	O	0	0
			177	177		
4	B	163	Total	O	0	0
			163	163		

i

- Molecule 1: DNA (cytosine-5)-methyltransferase 3B



- Molecule 1: DNA (cytosine-5)-methyltransferase 3B



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	73.50 Å 73.50 Å 159.96 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.87 – 1.70 40.87 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.87-1.70) 100.0 (40.87-1.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 1.70 Å)	Xtriage
Refinement program	PHENIX 1.8.1 _1168	Depositor
R, R_{free}	0.194 , 0.213 0.195 , 0.215	Depositor DCC
R_{free} test set	2795 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2614	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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: 96E, SO4

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	0.38	0/1135	0.54	0/1526
1	B	0.35	0/1162	0.49	0/1565
All	All	0.36	0/2297	0.51	0/3091

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	1097	0	1088	8	0
1	B	1126	0	1105	9	0
2	A	13	0	0	0	0
2	B	13	0	0	0	0
3	A	15	0	0	1	0
3	B	10	0	0	0	0
4	A	177	0	0	4	0
4	B	163	0	0	3	0
All	All	2614	0	2193	17	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.

All (17) 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:235:GLY:N	3:A:403:SO4:O3	2.21	0.69
1:B:276:LYS:O	4:B:502:HOH:O	2.15	0.63
1:B:328:GLN:NE2	4:B:503:HOH:O	2.27	0.62
1:B:326:GLU:OE2	4:B:501:HOH:O	2.15	0.60
1:A:275:ASP:OD1	4:A:501:HOH:O	2.16	0.59
1:B:237:SER:O	1:B:239[B]:TRP:HD1	1.90	0.54
1:B:246:TRP:CE2	1:B:253:GLN:HG2	2.48	0.49
1:A:350:PRO:O	1:A:351:ASN:HB2	2.15	0.46
1:A:268:LYS:NZ	4:A:507:HOH:O	2.49	0.45
1:A:239:TRP:CD1	1:A:240:PRO:HD2	2.52	0.44
1:B:321:PRO:HA	1:B:322:GLY:HA2	1.69	0.44
1:B:222:GLU:HB3	1:B:223:PHE:CD2	2.54	0.42
1:A:221:LYS:HD3	4:A:501:HOH:O	2.19	0.42
1:B:230:TRP:HB2	1:B:278:VAL:CG2	2.50	0.41
1:A:351:ASN:ND2	4:A:509:HOH:O	2.53	0.41
1:B:309:ALA:HB1	1:B:348:LEU:HD22	2.02	0.41
1:A:306:LEU:HD23	1:A:306:LEU:HA	1.87	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	134/150 (89%)	132 (98%)	1 (1%)	1 (1%)	22	8
1	B	139/150 (93%)	133 (96%)	5 (4%)	1 (1%)	22	8
All	All	273/300 (91%)	265 (97%)	6 (2%)	2 (1%)	19	8

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	PHE
1	B	223	PHE

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	113/121 (93%)	113 (100%)	0	100	100
1	B	114/121 (94%)	114 (100%)	0	100	100
All	All	227/242 (94%)	227 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some 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](#)

7 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
3	SO4	A	402	-	4,4,4	0.14	0	6,6,6	0.10	0
3	SO4	B	403	-	4,4,4	0.13	0	6,6,6	0.20	0
2	96E	A	401	-	12,12,12	0.86	1 (8%)	12,12,12	1.22	2 (16%)
2	96E	B	401	-	12,12,12	0.83	1 (8%)	12,12,12	1.10	0
3	SO4	A	404	-	4,4,4	0.13	0	6,6,6	0.22	0
3	SO4	B	402	-	4,4,4	0.19	0	6,6,6	0.13	0
3	SO4	A	403	-	4,4,4	0.17	0	6,6,6	0.07	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	96E	A	401	-	-	6/12/12/12	-
2	96E	B	401	-	-	5/12/12/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	96E	C03-N04	-2.43	1.41	1.47
2	B	401	96E	C03-N04	-2.23	1.42	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	96E	C09-C08-N04	2.23	119.46	113.84
2	A	401	96E	C05-N04-C03	-2.13	106.37	111.44

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	96E	O01-C02-C03-N04
2	B	401	96E	O01-C02-C03-N04

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Mol	Chain	Res	Type	Atoms
2	A	401	96E	C06-C05-N04-C08
2	B	401	96E	N04-C05-C06-C07
2	A	401	96E	N04-C08-C09-C10
2	A	401	96E	N04-C05-C06-C07
2	B	401	96E	C06-C05-N04-C03
2	A	401	96E	C08-C09-C10-C11
2	B	401	96E	C06-C05-N04-C08
2	B	401	96E	C10-C11-C12-O13
2	A	401	96E	C09-C10-C11-C12

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	SO4	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](#)

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	135/150 (90%)	0.02	4 (2%) 50 54	26, 34, 62, 87	0
1	B	137/150 (91%)	0.40	9 (6%) 18 20	28, 37, 76, 112	0
All	All	272/300 (90%)	0.21	13 (4%) 30 34	26, 35, 68, 112	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	322	GLY	7.5
1	B	321	PRO	7.5
1	B	320	SER	7.0
1	B	319	SER	5.2
1	A	214	SER	5.0
1	B	323	ASP	4.7
1	B	351	ASN	4.6
1	A	325	LEU	4.6
1	B	317	PHE	4.4
1	A	213	ASP	4.0
1	B	318	PRO	3.5
1	A	318	PRO	2.4
1	B	236	PHE	2.2

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, 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	B-factors(\AA^2)	Q<0.9
2	96E	A	401	13/13	0.72	0.18	45,49,53,55	0
2	96E	B	401	13/13	0.76	0.19	44,48,53,55	13
3	SO4	A	404	5/5	0.93	0.10	45,50,57,61	5
3	SO4	A	402	5/5	0.96	0.10	52,52,63,63	5
3	SO4	A	403	5/5	0.96	0.16	59,62,72,73	5
3	SO4	B	402	5/5	0.97	0.10	42,45,51,54	5
3	SO4	B	403	5/5	0.97	0.09	62,64,71,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.