

Full wwPDB X-ray Structure Validation Report (i)

May 18, 2020 – 11:17 am BST

PDB ID : 1U8B

Title : Crystal structure of the methylated N-ADA/DNA complex

Authors: He, C.; Hus, J.-C.; Sun, L.J.; Zhou, P.; Norman, D.P.G.; Dotsch, V.; Gross,

J.D.; Lane, W.S.; Wagner, G.; Verdine, G.L.

Deposited on : 2004-08-05

Resolution : 2.10 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 (i) symbol.

The following versions of software and data (see references (1)) 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 : 2.11

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

 $\begin{array}{cccc} & CCP4 & : & 7.0.044 \; (Gargrove) \\ Ideal \; geometry \; (proteins) & : & Engh \; \& \; Huber \; (2001) \end{array}$

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

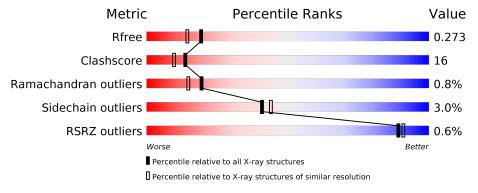
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	В	6	50%	33%	17%
2	С	5	60%	20%	20%
3	D	12	67%		33%
4	Е	13	46%	46%	8%
5	A	133	67%		29% • •



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 1811 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 DNA chain called 5'-D(*TP*AP*AP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	В	5	Total	С	N	0	P	0	0	0
			103	50	19	29	5			

• Molecule 2 is a DNA chain called 5'-D(P*AP*AP*TP*TP*T)-3'.

\mathbf{Mol}	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	С	5	Total 103	C 50	N 16	O 32	P 5	0	0	0

• Molecule 3 is a DNA chain called 5'-D(P*AP*AP*AP*GP*CP*GP*CP*AP*AP*AP*T)-3'.

\mathbf{Mol}	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	12	Total 251	C 118	N 53	O 68	P 12	0	0	0

• Molecule 4 is a DNA chain called 5'-D(*AP*AP*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*TP*TP.3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	19	Total	С	N	О	Р	0	0	0
4	E	12	242	117	36	77	12	0	0	U

• Molecule 5 is a protein called Ada polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
5	A	132	Total 1020	C 638	N 195	O 179	S 5	Se 3	0	0	0

There are 5 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	CLONING ARTIFACT	UNP P06134
A	2	LYS	=	CLONING ARTIFACT	UNP P06134
A	75	ASP	GLU	CONFLICT	UNP P06134
A	79	PRO	ALA	CONFLICT	UNP P06134
A	80	ARG	GLN	CONFLICT	UNP P06134

 \bullet Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Zn 1 1	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	В	6	Total O 6 6	0	0
7	С	12	Total O 12 12	0	0
7	D	13	Total O 13 13	0	0
7	E	11	Total O 11 11	0	0
7	A	49	Total O 49 49	0	0



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 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: 5'-D(*TP*AP*AP*AP*TP*T)-3'

Chain B: 50% 33% 17% • Molecule 2: 5'-D(P*AP*AP*TP*T)-3' Chain C: 60% 20% 20% • Molecule 3: 5'-D(P*AP*AP*AP*GP*CP*GP*CP*AP*AP*AP*T)-3' Chain D: 67% 33% • Molecule 4: 5'-D(*AP*AP*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*T)-3' Chain E: • Molecule 5: Ada polyprotein Chain A: 29%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	28.84Å 84.59Å 108.36Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.40 - 2.10	Depositor
resolution (A)	45.62 - 2.09	EDS
% Data completeness	71.0 (39.40-2.10)	Depositor
(in resolution range)	87.2 (45.62-2.09)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) > 1$	3.51 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
D D.	0.235 , 0.274	Depositor
R, R_{free}	0.235 , 0.273	DCC
R_{free} test set	999 reflections (3.33%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 33.5	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	1811	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.06% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: ZN, SMC

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	Boı	nd lengths	Bond angles		
MIOI	Chain	RMSZ $ \# Z > 5$		RMSZ	# Z > 5	
1	В	0.71	0/115	0.88	0/175	
2	С	0.92	1/114 (0.9%)	0.83	0/172	
3	D	0.66	$1/283 \ (0.4\%)$	0.73	$1/433 \ (0.2\%)$	
4	Е	0.54	0/268	0.75	0/411	
5	A	0.39	0/1036	0.55	0/1401	
All	All	0.53	$2/1816 \ (0.1\%)$	0.67	$1/2592 \ (0.0\%)$	

All (2) bond length outliers are listed below:

N	/Iol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(ext{\AA})$
	2	С	301	DA	OP3-P	-7.13	1.52	1.61
	3	D	401	DA	OP3-P	-6.78	1.53	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
3	D	401	DA	OP1-P-OP2	-5.71	111.04	119.60

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	В	103	0	58	2	0
2	С	103	0	59	2	1
3	D	251	0	134	4	0
4	Е	242	0	139	10	1
5	A	1020	0	968	35	0
6	A	1	0	0	0	0
7	A	49	0	0	1	0
7	В	6	0	0	0	0
7	С	12	0	0	0	0
7	D	13	0	0	0	0
7	E	11	0	0	0	0
All	All	1811	0	1358	49	1

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 16.

All (49) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} ({\rm \AA}) \end{array}$	Clash overlap (Å)
3:D:403:DA:H2"	3:D:404:DG:H5'	1.62	0.81
5:A:82:HIS:CE1	5:A:86:LYS:HE3	2.26	0.69
4:E:512:DT:H5'	4:E:512:DT:H6	1.61	0.65
3:D:403:DA:H2"	3:D:404:DG:C5'	2.27	0.65
5:A:104:ALA:O	5:A:108:GLN:HG3	1.99	0.62
2:C:305:DT:H2'	4:E:501:DA:O4'	2.01	0.60
5:A:111:MSE:CE	5:A:116:LEU:HD13	2.32	0.59
5:A:58:ALA:O	5:A:61:ALA:N	2.35	0.59
5:A:62:LEU:HD22	5:A:62:LEU:H	1.67	0.58
5:A:81:GLN:NE2	5:A:85:ASP:OD1	2.35	0.57
5:A:38:SMC:SG	5:A:69:CYS:HB2	2.45	0.56
4:E:511:DT:C2'	4:E:512:DT:H5"	2.36	0.56
4:E:511:DT:H2"	4:E:512:DT:C5'	2.36	0.55
4:E:511:DT:H2"	4:E:512:DT:H5"	1.88	0.55
5:A:106:ALA:HB1	5:A:111:MSE:O	2.08	0.54
4:E:506:DG:H2"	4:E:507:DC:H5'	1.91	0.53
5:A:96:GLN:NE2	5:A:98:THR:OG1	2.42	0.52
5:A:13:TRP:CD1	5:A:49:ARG:HD3	2.44	0.52
5:A:102:LEU:HD11	5:A:117:HIS:HB2	1.90	0.52
5:A:111:MSE:HE3	5:A:116:LEU:HD13	1.91	0.51
5:A:28:VAL:HG21	5:A:37:PHE:HD2	1.77	0.49
5:A:92:ARG:HA	5:A:95:GLU:HG3	1.93	0.49
4:E:512:DT:H5'	4:E:512:DT:C6	2.45	0.48

Continued on next page...



Continued from previous page...

Continued from pred	-	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}({\rm \AA})$	overlap (Å)
5:A:87:ILE:HD11	5:A:119:LEU:HG	1.95	0.48
4:E:511:DT:H1'	4:E:512:DT:H5"	1.97	0.46
5:A:39:ARG:HG3	5:A:74:PRO:HB3	1.97	0.46
3:D:403:DA:H1'	3:D:404:DG:H5"	1.98	0.46
5:A:109:VAL:HG21	5:A:111:MSE:HE3	1.96	0.46
5:A:91:CYS:O	5:A:95:GLU:HG2	2.15	0.46
5:A:58:ALA:O	5:A:59:SER:C	2.55	0.45
5:A:79:PRO:O	5:A:80:ARG:C	2.54	0.45
1:B:205:DT:OP1	5:A:47:ALA:HB1	2.17	0.45
5:A:111:MSE:HE1	5:A:116:LEU:HD13	1.96	0.45
5:A:21:PRO:HA	5:A:24:ASP:OD2	2.17	0.45
5:A:116:LEU:HD12	5:A:116:LEU:O	2.17	0.44
4:E:507:DC:H2"	4:E:508:DG:C8	2.52	0.44
5:A:62:LEU:CD2	5:A:62:LEU:H	2.31	0.43
5:A:19:ARG:NH2	5:A:44:ALA:O	2.46	0.42
5:A:20:ASP:HA	5:A:21:PRO:HD3	1.89	0.42
5:A:28:VAL:HG22	5:A:38:SMC:O	2.19	0.42
5:A:62:LEU:N	5:A:62:LEU:HD22	2.32	0.42
5:A:19:ARG:HA	5:A:40:PRO:O	2.19	0.42
1:B:201:DA:O4'	3:D:412:DT:H2'	2.20	0.42
5:A:87:ILE:HD11	5:A:119:LEU:CG	2.50	0.42
5:A:9:ASP:OD2	5:A:12:ARG:NH1	2.53	0.41
5:A:102:LEU:HD22	5:A:102:LEU:O	2.20	0.41
5:A:102:LEU:HD23	5:A:102:LEU:HA	1.90	0.41
5:A:14:GLN:NE2	7:A:152:HOH:O	2.53	0.41
2:C:305:DT:H2'	4:E:501:DA:C1'	2.50	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$egin{array}{ll} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{array}$	Clash overlap (Å)
2:C:301:DA:OP2	4:E:512:DT:O3'[2_664]	2.13	0.07

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
5	A	129/133 (97%)	121 (94%)	7 (5%)	1 (1%)	19 15

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	80	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	Analysed Rotameric C		Percentiles
5	A	99/106 (93%)	96 (97%)	3 (3%)	41 44

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	${f Res}$	\mathbf{Type}
5	A	92	ARG
5	A	95	GLU
5	A	102	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	11	GLN
5	A	14	GLN
5	A	82	HIS
5	A	96	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)

1 non-standard protein/DNA/RNA residue is 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	В	ond leng	$_{ m gths}$	Е	ond ang	gles
MIOI	туре	Chain	res	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SMC	A	38	5,6	5,6,7	1.26	1 (20%)	2,6,8	1.71	1 (50%)

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
5	SMC	A	38	5,6	-	0/3/5/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	${ m Observed}({ m \AA})$	$\operatorname{Ideal}(ext{\AA})$
5	A	38	SMC	CB-SG	-2.46	1.77	1.80

All (1) bond angle outliers are listed below:

Mol	Mol Chain Res Type		Atoms Z		$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$	
5	A	38	SMC	CA-CB-SG	2.32	117.80	114.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

\mathbf{Mol}	Chain	Res	Type	Clashes	Symm-Clashes
5	A	38	SMC	2	0



5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	$\langle { m RSRZ} \rangle$	$\# \mathrm{RSRZ} {>} 2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	В	5/6 (83%)	0.19	0 100 100	27, 27, 34, 41	0
2	С	5/5 (100%)	-0.07	0 100 100	29, 30, 32, 35	0
3	D	$12/12 \ (100\%)$	0.10	0 100 100	29, 37, 43, 46	0
4	E	$12/13 \ (92\%)$	0.02	0 100 100	33, 37, 44, 45	0
5	A	128/133~(96%)	0.62	1 (0%) 86 88	24, 36, 45, 47	0
All	All	162/169~(95%)	0.50	1 (0%) 89 91	24, 35, 45, 47	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	A	84	LEU	2.2

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
5	SMC	A	38	7/8	0.90	0.16	30,31,33,34	0

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. The B-factors column lists the minimum, median, 95^{th} 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	${f B-factors}({f A}^2)$	Q < 0.9
	6	ZN	A	150	1/1	0.99	0.13	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.

