Full wwPDB X-ray Structure Validation Report (i)

Dec 4, 2023 – 03:01 am GMT

PDB ID	:	1UWZ
Title	:	Bacillus subtilis cytidine deaminase with an Arg56 - Ala substitution
Authors	:	Johansson, E.; Neuhard, J.; Willemoes, M.; Larsen, S.
Deposited on	:	2004-02-18
Resolution	:	1.99 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

PERCENTILES INFOmissingINFO

1 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2126 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.

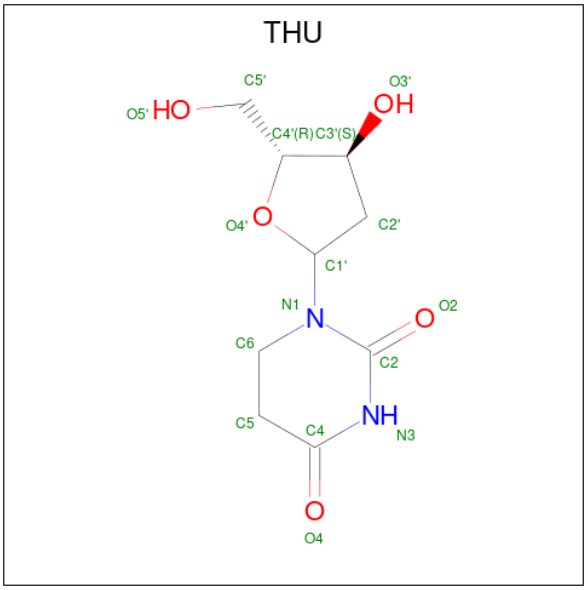
- Molecule 1 is a protein called CYTIDINE DEAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	0	0
			972	607	160	194	11			
1	B	130	Total	C	N	O	S	0	0	0
			972	607	160	194	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	ALA	ARG	engineered mutation	UNP P19079
B	56	ALA	ARG	engineered mutation	UNP P19079

- Molecule 2 is TETRAHYDRODEOXYURIDINE (three-letter code: THU) (formula: $C_9H_{14}N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	9	2	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O 16 9 2 5	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	78	Total O 78 78	0	0
4	B	70	Total O 70 70	0	0

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	73.74Å 66.42Å 55.39Å 90.00° 115.60° 90.00°	Depositor
Resolution (Å)	19.96 – 1.99 19.96 – 1.99	Depositor EDS
% Data completeness (in resolution range)	94.2 (19.96-1.99) 94.3 (19.96-1.99)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 1.99Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.188 , 0.211 0.178 , 0.205	Depositor DCC
R_{free} test set	747 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å^2)	22.5	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2126	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

3 Model quality

3.1 Standard geometry

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

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	0.32	0/984	0.57	0/1331
1	B	0.32	0/984	0.57	0/1331
All	All	0.32	0/1968	0.57	0/2662

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

3.2 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	972	0	969	6	0
1	B	972	0	969	4	0
2	A	16	0	13	0	0
2	B	16	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	78	0	0	0	0
4	B	70	0	0	1	0
All	All	2126	0	1964	10	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 3.

All (10) 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:53:CYS:HB2	1:A:89:CYS:SG	2.44	0.58
1:B:53:CYS:HB2	1:B:89:CYS:SG	2.45	0.56
1:A:1:MET:HG2	1:A:31:LEU:HD13	1.95	0.49
1:B:2:ASN:OD1	1:B:5:GLU:HG3	2.13	0.48
1:B:1:MET:HG2	1:B:31:LEU:HD13	1.95	0.47
1:A:116:THR:OG1	1:A:119:GLU:HG3	2.15	0.47
1:B:3:ARG:HG3	4:B:2002:HOH:O	2.15	0.45
1:A:33:LYS:CG	1:A:69:GLU:HB3	2.50	0.41
1:A:33:LYS:HG3	1:A:69:GLU:HB3	2.02	0.41
1:A:107:ASN:HD21	1:A:111:GLN:HG2	1.86	0.41

There are no symmetry-related clashes.

3.3 Torsion angles (i)

3.3.1 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	128/136 (94%)	127 (99%)	1 (1%)	0	100	100
1	B	128/136 (94%)	127 (99%)	1 (1%)	0	100	100
All	All	256/272 (94%)	254 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

3.3.2 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	105/111 (95%)	104 (99%)	1 (1%)	76	81
1	B	105/111 (95%)	104 (99%)	1 (1%)	76	81
All	All	210/222 (95%)	208 (99%)	2 (1%)	76	81

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	B	4	GLN

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

Mol	Chain	Res	Type
1	A	4	GLN
1	A	71	GLN
1	B	4	GLN
1	B	71	GLN

3.3.3 RNA (i)

There are no RNA molecules in this entry.

3.4 Non-standard residues in protein, DNA, RNA chains (i)

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

3.5 Carbohydrates (i)

There are no monosaccharides in this entry.

3.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	THU	A	138	3	17,17,17	4.47	5 (29%)	21,24,24	6.08	9 (42%)
2	THU	B	138	3	17,17,17	4.48	5 (29%)	21,24,24	6.11	9 (42%)

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	THU	A	138	3	1/1/6/7	2/6/31/31	0/2/2/2
2	THU	B	138	3	1/1/6/7	2/6/31/31	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	138	THU	C1'-N1	13.80	1.64	1.45
2	B	138	THU	C1'-N1	13.77	1.64	1.45
2	B	138	THU	O4-C4	9.54	1.42	1.23
2	A	138	THU	O4-C4	9.46	1.42	1.23
2	B	138	THU	C4-N3	5.76	1.47	1.37
2	A	138	THU	C4-N3	5.41	1.46	1.37
2	A	138	THU	C6-N1	-3.85	1.40	1.47
2	B	138	THU	C6-N1	-3.51	1.40	1.47
2	A	138	THU	C5-C4	2.61	1.56	1.50
2	B	138	THU	C5-C4	2.40	1.55	1.50

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	138	THU	C2'-C1'-N1	23.54	144.38	115.61
2	A	138	THU	C2'-C1'-N1	23.40	144.21	115.61
2	B	138	THU	O4'-C1'-N1	-8.13	98.05	108.41
2	A	138	THU	O4'-C1'-N1	-7.94	98.29	108.41
2	B	138	THU	O4-C4-C5	-7.59	105.96	122.17
2	A	138	THU	O4-C4-C5	-7.43	106.31	122.17
2	B	138	THU	O4'-C1'-C2'	5.98	117.56	106.25
2	A	138	THU	O4'-C1'-C2'	5.95	117.50	106.25
2	A	138	THU	O4-C4-N3	-4.55	113.07	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	138	THU	C4-N3-C2	-4.43	122.11	125.79
2	B	138	THU	C4-N3-C2	-4.31	122.22	125.79
2	B	138	THU	O4-C4-N3	-4.05	113.86	120.28
2	B	138	THU	C2'-C3'-C4'	2.83	108.66	102.76
2	A	138	THU	C2'-C3'-C4'	2.73	108.45	102.76
2	B	138	THU	C1'-N1-C2	-2.70	114.91	118.50
2	A	138	THU	C1'-N1-C2	-2.56	115.09	118.50
2	A	138	THU	C4'-O4'-C1'	-2.54	103.32	109.45
2	B	138	THU	C4'-O4'-C1'	-2.50	103.41	109.45

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	138	THU	C1'
2	B	138	THU	C1'

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	138	THU	O4'-C1'-N1-C6
2	B	138	THU	O4'-C1'-N1-C6
2	B	138	THU	C2'-C1'-N1-C2
2	A	138	THU	C2'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

3.7 Other polymers (i)

There are no such residues in this entry.

3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

4 Fit of model and data

4.1 Protein, DNA and RNA chains

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	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	130/136 (95%)	-0.20	1 (0%) 86 85	15, 21, 35, 41	0
1	B	130/136 (95%)	-0.21	0 100 100	15, 22, 34, 43	0
All	All	260/272 (95%)	-0.21	1 (0%) 92 92	15, 21, 35, 43	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	128	GLU	2.3

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

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

4.3 Carbohydrates

There are no monosaccharides in this entry.

4.4 Ligands

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	B-factors(Å^2)	Q<0.9
2	THU	A	138	16/16	0.90	0.13	19,22,24,24	0
2	THU	B	138	16/16	0.94	0.10	20,23,24,25	0
3	ZN	A	1131	1/1	0.99	0.04	29,29,29,29	0
3	ZN	B	1131	1/1	0.99	0.06	32,32,32,32	0

4.5 Other polymers (i)

There are no such residues in this entry.