

wwPDB X-ray Structure Validation Summary Report (i)

Jun 11, 2024 – 09:48 PM EDT

PDB ID	:	1F8X
Title	:	CRYSTAL STRUCTURE OF NUCLEOSIDE 2-DEOXYRIBOSYLTRANSF
		ERASE
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Deposited on		
Resolution	:	2.50 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 (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:

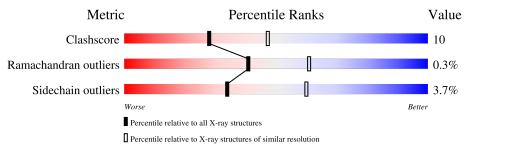
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	А	157	81%	18%	••
1	В	157	78%	18%	• ••



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2616 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.

- AltConf Mol Residues ZeroOcc Trace Chain Atoms Total С Ν 0 S 1 0 0 0 А 1561268816 2012465С Ν \mathbf{S} Total Ο 1 В 0 0 0 15612688162012465
- Molecule 1 is a protein called NUCLEOSIDE 2-DEOXYRIBOSYLTRANSFERASE.

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	49	Total O 49 49	0	0
2	В	31	Total O 31 31	0	0

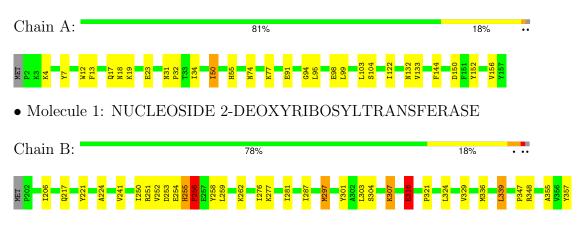


3 Residue-property plots (i)

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: NUCLEOSIDE 2-DEOXYRIBOSYLTRANSFERASE





4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	I 21 3	Depositor	
Cell constants	151.00Å 151.00Å 151.00Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Dopositor	
Resolution (Å)	5.00 - 2.50	Depositor	
% Data completeness	(Not available) (5.00-2.50)	Depositor	
(in resolution range)	(100 available) (0.00 2.00)	Depositor	
R_{merge}	0.12	Depositor	
R _{sym}	(Not available)	Depositor	
Refinement program	X-PLOR	Depositor	
R, R_{free}	0.166 , 0.240	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	2616	wwPDB-VP	
Average B, all atoms $(Å^2)$	22.0	wwPDB-VP	



5 Model quality (i)

5.1 Standard geometry (i)

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	Bo	nd angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.41	0/1301	0.64	1/1762~(0.1%)
1	В	0.37	0/1301	0.70	2/1762~(0.1%)
All	All	0.39	0/2602	0.67	3/3524~(0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	316	GLU	CA-CB-CG	-8.69	94.29	113.40
1	В	256	PRO	N-CA-C	5.79	127.16	112.10
1	А	7	TYR	N-CA-C	-5.01	97.47	111.00

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	А	1268	0	1216	19	0
1	В	1268	0	1216	33	0
2	А	49	0	0	3	0
2	В	31	0	0	0	0
All	All	2616	0	2432	49	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 10.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ILE:HG22	1:B:281:ILE:HB	1.34	1.10
1:B:250:ILE:HA	1:B:255:HIS:HE1	1.33	0.93
1:B:250:ILE:HA	1:B:255:HIS:CE1	2.09	0.87
1:B:250:ILE:CA	1:B:255:HIS:HE1	1.98	0.75
1:A:4:LYS:HE2	2:A:833:HOH:O	1.90	0.71

The worst 5 of 49 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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	Perce	ntiles
1	А	154/157~(98%)	$149 \ (97\%)$	5(3%)	0	100	100
1	В	154/157~(98%)	139 (90%)	14 (9%)	1 (1%)	25	43
All	All	308/314~(98%)	288~(94%)	19~(6%)	1 (0%)	41	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	256	PRO

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	А	136/137~(99%)	135~(99%)	1 (1%)	84 94
1	В	136/137~(99%)	127~(93%)	9~(7%)	16 32
All	All	272/274~(99%)	262~(96%)	10 (4%)	34 60

5 of 10 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	В	316	GLU
1	В	324	LEU
1	В	339	LEU
1	В	255	HIS
1	В	262	LYS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such side chains are listed below:

Mol	Chain	Res	Type
1	В	238	ASN
1	В	255	HIS
1	В	345	ASN
1	В	274	ASN
1	В	279	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.



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.

