Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 01:13 PM EDT

PDB ID	:	6NUA
Title	:	DNA-protein crosslink between E. coli YedK and ssDNA containing an abasic site
Authors	:	Eichman, B.F.; Amidon, K.M.
Deposited on	:	2019-01-31
Resolution	:	1.64 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
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)	:	2.35.1

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 1.64 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7810 atoms, of which 3635 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 SOS response-associated peptidase YedK.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	227	Total	C	H	N	O	S	0	4	0
			3554	1164	1736	316	332	6			
1	B	227	Total	C	H	N	O	S	0	3	0
			3554	1158	1745	315	330	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	LEU	-	expression tag	UNP P76318
A	224	GLU	-	expression tag	UNP P76318
A	225	VAL	-	expression tag	UNP P76318
A	226	LEU	-	expression tag	UNP P76318
A	227	PHE	-	expression tag	UNP P76318
A	228	GLN	-	expression tag	UNP P76318
B	223	LEU	-	expression tag	UNP P76318
B	224	GLU	-	expression tag	UNP P76318
B	225	VAL	-	expression tag	UNP P76318
B	226	LEU	-	expression tag	UNP P76318
B	227	PHE	-	expression tag	UNP P76318
B	228	GLN	-	expression tag	UNP P76318

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*TP*CP*(PED)P*GP*GP*A)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	7	Total	C	H	N	O	P	0	0	0
			211	64	77	25	39	6			
2	D	7	Total	C	H	N	O	P	0	0	0
			211	64	77	25	39	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	113	Total O 113 113	0	0
3	B	133	Total O 133 133	0	0
3	C	18	Total O 18 18	0	0
3	D	16	Total O 16 16	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.26Å 41.89Å 81.42Å 90.00° 95.78° 90.00°	Depositor
Resolution (Å)	40.50 – 1.64	Depositor
% Data completeness (in resolution range)	96.9 (40.50-1.64)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 1.63Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.171 , 0.222	Depositor
Wilson B-factor (Å^2)	18.0	Xtriage
Anisotropy	0.471	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7810	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.67% 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.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

There are no ligands in this entry.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.