



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2023 – 11:15 PM EDT

PDB ID : 6N00
Title : Crystal structure of Tdp1 catalytic domain in complex with compound XZ523
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Deposited on : 2018-11-07
Resolution : 1.94 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)
Xtrriage (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

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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 4 unique types of molecules in this entry. The entry contains 7894 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 Tyrosyl-DNA phosphodiesterase 1.

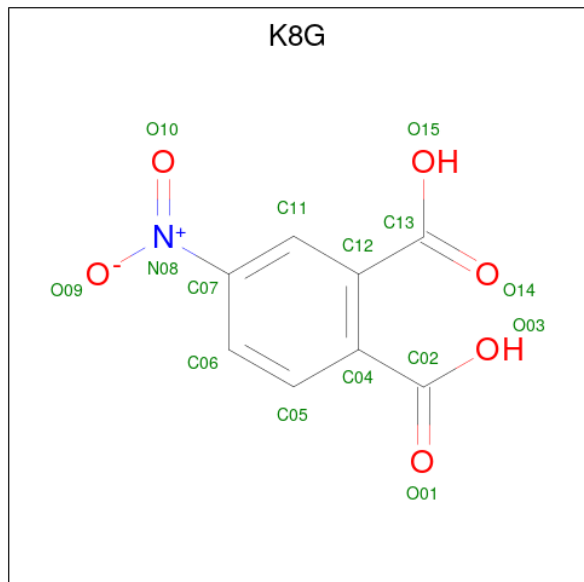
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	438	3597	2330	606	648	13	0	13	0
1	B	438	3578	2320	603	641	14	0	10	0

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0
2	A	1	4	2	2	0	0
2	B	1	4	2	2	0	0
2	B	1	4	2	2	0	0

- Molecule 3 is 4-nitrobenzene-1,2-dicarboxylic acid (three-letter code: K8G) (formula: $C_8H_5NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	15	8	1	6	0	0
3	B	1	15	8	1	6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	377	377	377	0	0
4	B	296	296	296	0	0

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

3 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.77Å 105.15Å 194.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.67 – 1.94	Depositor
% Data completeness (in resolution range)	95.6 (35.67-1.94)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 1.94Å)	Xtrriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.179 , 0.223	Depositor
Wilson B-factor (Å ²)	19.2	Xtrriage
Anisotropy	0.375	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7894	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

6 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	K8G	A	703	-	14,15,15	1.21	1 (7%)	19,21,21	0.86	0
2	EDO	B	701	-	3,3,3	0.50	0	2,2,2	0.23	0
2	EDO	B	702	-	3,3,3	0.42	0	2,2,2	0.45	0
2	EDO	A	701	-	3,3,3	0.55	0	2,2,2	0.17	0
2	EDO	A	702	-	3,3,3	0.32	0	2,2,2	0.62	0
3	K8G	B	703	-	14,15,15	1.25	1 (7%)	19,21,21	1.11	2 (10%)

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
3	K8G	A	703	-	-	8/10/12/12	0/1/1/1
2	EDO	B	701	-	-	0/1/1/1	-
2	EDO	B	702	-	-	0/1/1/1	-
2	EDO	A	701	-	-	0/1/1/1	-
2	EDO	A	702	-	-	1/1/1/1	-
3	K8G	B	703	-	-	8/10/12/12	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	703	K8G	O10-N08	-2.78	1.18	1.22
3	A	703	K8G	O10-N08	-2.34	1.18	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	703	K8G	O15-C13-C12	2.15	121.51	115.31
3	B	703	K8G	C11-C07-N08	2.09	120.59	118.75

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	703	K8G	C06-C07-N08-O10

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Mol	Chain	Res	Type	Atoms
3	A	703	K8G	C11-C07-N08-O10
3	B	703	K8G	C06-C07-N08-O10
3	B	703	K8G	C11-C07-N08-O10
2	A	702	EDO	O1-C1-C2-O2
3	A	703	K8G	O03-C02-C04-C05
3	A	703	K8G	O01-C02-C04-C05
3	B	703	K8G	C11-C12-C13-O15
3	B	703	K8G	O03-C02-C04-C05
3	A	703	K8G	O03-C02-C04-C12
3	A	703	K8G	O01-C02-C04-C12
3	B	703	K8G	O01-C02-C04-C05
3	A	703	K8G	C11-C12-C13-O14
3	A	703	K8G	C11-C12-C13-O15
3	B	703	K8G	C11-C12-C13-O14
3	B	703	K8G	C04-C12-C13-O15
3	B	703	K8G	C04-C12-C13-O14

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

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.