

Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 11:31 PM EDT

PDB ID Title		6VXS Crystal Structure of ADP ribose phosphatase of NSP3 from SARS CoV-2
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Deposited on	:	2020-02-24
1		
Resolution	:	2.03 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	:	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)		
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.03 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.



6VXS

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2715 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.

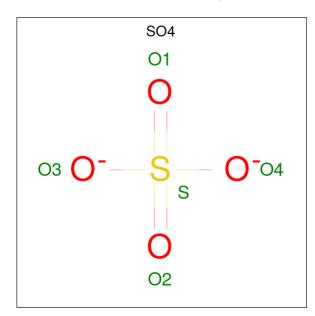
• Molecule 1 is a protein called Non-structural protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	167	Total 1263	C 803	N 217	0 230	${\operatorname{S}}_{{\operatorname{\varDelta}}}$	0	0	0
			Total			$\frac{235}{0}$	S			
	В	167	1263		217	239	4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	GLY	-	expression tag	UNP P0DTD1
В	1	GLY	-	expression tag	UNP P0DTD1

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	А	1	Total 5	0 4	S 1	0	0

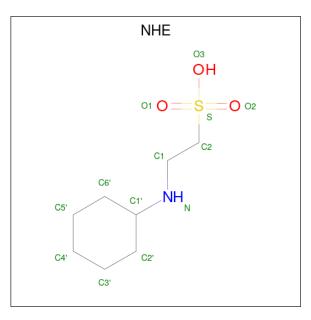
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

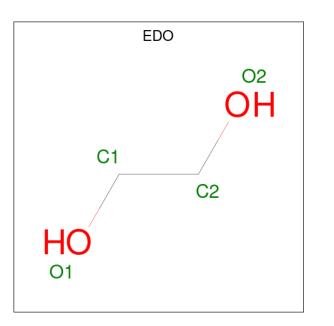
• Molecule 3 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: C₈H₁₇NO₃S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total C N O S 13 8 1 3 1	0	0
3	В	1	Total C N O S 13 8 1 3 1	0	0

• Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	В	1	Total 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	O 2	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	69	Total O 69 69	0	0
5	В	70	Total O 70 70	0	0

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



3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	30.39Å 37.90Å 65.40Å	Depositor
a, b, c, α , β , γ	84.37° 82.11° 90.11°	Depositor
Resolution (Å)	37.71 - 2.03	Depositor
% Data completeness	84.8 (37.71-2.03)	Depositor
(in resolution range)		-
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.89 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.186 , 0.234	Depositor
Wilson B-factor $(Å^2)$	23.1	Xtriage
Anisotropy	0.105	Xtriage
L-test for twinning ²	$ < L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2715	wwPDB-VP
Average B, all atoms $(Å^2)$	24.0	wwPDB-VP

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

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.62% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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)

7 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



Mol	Turne	pe Chain Res		Res Link Bond lengths				Bond angles		
MIOI	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	NHE	В	203	-	$13,\!13,\!13$	0.66	1 (7%)	$16,\!17,\!17$	0.58	0
3	NHE	А	202	-	13,13,13	0.66	1 (7%)	$16,\!17,\!17$	0.67	0
2	SO4	А	201	-	4,4,4	0.13	0	6,6,6	0.06	0
4	EDO	В	202	-	3,3,3	0.44	0	2,2,2	0.44	0
2	SO4	В	201	-	4,4,4	0.14	0	$6,\!6,\!6$	0.07	0
2	SO4	В	204	-	4,4,4	0.14	0	$6,\!6,\!6$	0.08	0
2	SO4	А	203	-	4,4,4	0.15	0	$6,\!6,\!6$	0.08	0

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).

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	NHE	В	203	-	-	0/7/15/15	0/1/1/1
3	NHE	А	202	-	-	0/7/15/15	0/1/1/1
4	EDO	В	202	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
3	В	203	NHE	O3-S	2.18	1.55	1.47
3	А	202	NHE	O3-S	2.17	1.55	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

	Mol	Chain	Res	Type	Atoms
ſ	4	В	202	EDO	O1-C1-C2-O2

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 (i)

5.1 Protein, DNA and RNA chains (i)

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

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

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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

