Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 06:54 AM EDT

PDB ID : 6VKX
Title : Crystal structure of the carbohydrate-binding domain VP8* of human P[8] rotavirus strain BM13851
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Deposited on : 2020-01-22
Resolution : 1.71 Å(reported)

The following versions of software and data (see references (i)) 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 ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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 3956 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 Outer capsid protein VP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total 1277	C 802	N 222	O 251	S 2	0	0	0
1	B	155	Total 1258	C 793	N 216	O 247	S 2	0	0	0
1	C	157	Total 1277	C 802	N 222	O 251	S 2	0	0	0

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).
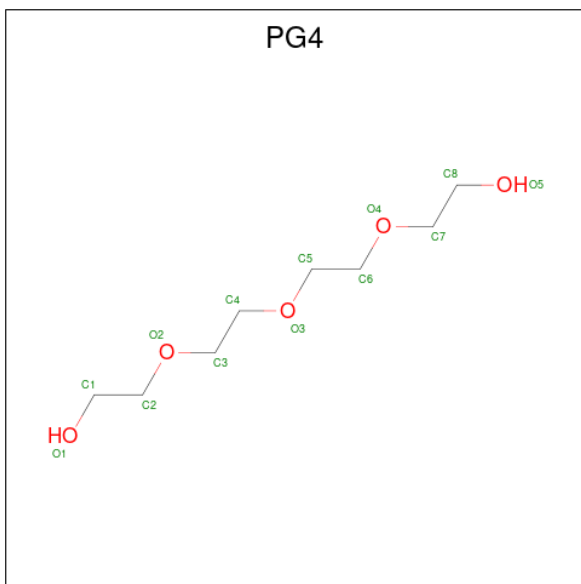
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 13	C 8	O 5	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

PEG

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 7	C 4	O 3	0	0
3	B	1	Total 7	C 4	O 3	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total 53	O 53	0	0
4	B	40	Total 40	O 40	0	0
4	C	24	Total 24	O 24	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	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	112.00Å 63.25Å 71.94Å 90.00° 90.70° 90.00°	Depositor
Resolution (Å)	32.17 – 1.71	Depositor
% Data completeness (in resolution range)	89.8 (32.17-1.71)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.18 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.198 , 0.228	Depositor
Wilson B-factor (Å^2)	19.8	Xtriage
Anisotropy	0.307	Xtriage
L-test for twinning[2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.020 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.017 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.028 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.018 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.028 for -h,-k,l	Xtriage
Total number of atoms	3956	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

3 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	PEG	A	202	-	6,6,6	0.65	0	5,5,5	0.43	0
2	PG4	A	201	-	12,12,12	0.23	0	11,11,11	0.18	0
3	PEG	B	201	-	6,6,6	0.49	0	5,5,5	0.38	0

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	PEG	A	202	-	-	1/4/4/4	-
2	PG4	A	201	-	-	6/10/10/10	-
3	PEG	B	201	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	202	PEG	C4-C3-O2-C2
3	B	201	PEG	O2-C3-C4-O4
2	A	201	PG4	O2-C3-C4-O3
3	B	201	PEG	O1-C1-C2-O2
2	A	201	PG4	O1-C1-C2-O2
2	A	201	PG4	C4-C3-O2-C2
2	A	201	PG4	C6-C5-O3-C4
2	A	201	PG4	C3-C4-O3-C5
2	A	201	PG4	O3-C5-C6-O4

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers ⓘ

There are no such residues in this entry.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

4.8 Polymer linkage issues ⓘ

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.