



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 05:52 AM EDT

PDB ID : 6MSW
Title : Crystal structure of BH1352 2-deoxyribose-5-phosphate from *Bacillus halodurans*, K184L mutant
Authors : Stogios, P.J.; Skarina, T.; Kim, T.; Yim, V.; Yakunin, A.; Savchenko, A.
Deposited on : 2018-10-18
Resolution : 2.17 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 2.17 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

There are 3 unique types of molecules in this entry. The entry contains 10459 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 Deoxyribose-phosphate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	222	Total 1619	C 1013	N 272	O 326	S 8	0	0	0
1	B	221	Total 1622	C 1017	N 269	O 328	S 8	0	3	0
1	C	216	Total 1570	C 985	N 263	O 314	S 8	0	0	0
1	D	216	Total 1576	C 989	N 263	O 316	S 8	0	1	0
1	E	217	Total 1581	C 991	N 267	O 315	S 8	0	0	0
1	F	213	Total 1546	C 972	N 257	O 309	S 8	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	LEU	LYS	engineered mutation	UNP Q9KD67
B	184	LEU	LYS	engineered mutation	UNP Q9KD67
C	184	LEU	LYS	engineered mutation	UNP Q9KD67
D	184	LEU	LYS	engineered mutation	UNP Q9KD67
E	184	LEU	LYS	engineered mutation	UNP Q9KD67
F	184	LEU	LYS	engineered mutation	UNP Q9KD67

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	183	Total O 184 184	0	1
3	B	172	Total O 173 173	0	1
3	C	132	Total O 132 132	0	0
3	D	121	Total O 121 121	0	0
3	E	105	Total O 108 108	0	3
3	F	124	Total O 125 125	0	1

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	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	240.78Å 55.12Å 176.30Å 90.00° 127.71° 90.00°	Depositor
Resolution (Å)	29.98 – 2.17	Depositor
% Data completeness (in resolution range)	99.6 (29.98-2.17)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.18Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.193 , 0.211	Depositor
Wilson B-factor (Å ²)	35.1	Xtrriage
Anisotropy	0.637	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	10459	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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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](#)

17 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
2	GOL	C	302	-	5,5,5	0.93	0	5,5,5	0.97	0
2	GOL	B	301	-	5,5,5	0.91	0	5,5,5	0.98	0
2	GOL	C	303	-	5,5,5	0.90	0	5,5,5	1.02	0
2	GOL	D	303	-	5,5,5	0.90	0	5,5,5	1.00	0
2	GOL	D	302	-	5,5,5	0.84	0	5,5,5	1.03	0
2	GOL	B	303	-	5,5,5	0.92	0	5,5,5	1.00	0
2	GOL	D	301	-	5,5,5	0.26	0	5,5,5	0.28	0
2	GOL	A	302	-	5,5,5	0.92	0	5,5,5	1.02	0
2	GOL	A	303	-	5,5,5	0.90	0	5,5,5	1.02	0
2	GOL	D	304	-	5,5,5	0.92	0	5,5,5	0.98	0
2	GOL	E	302	-	5,5,5	0.89	0	5,5,5	0.99	0
2	GOL	C	301	-	5,5,5	0.92	0	5,5,5	0.99	0
2	GOL	F	302	-	5,5,5	0.90	0	5,5,5	1.00	0
2	GOL	A	301	-	5,5,5	0.83	0	5,5,5	1.03	0
2	GOL	B	302	-	5,5,5	0.90	0	5,5,5	1.02	0
2	GOL	E	301	-	5,5,5	0.26	0	5,5,5	0.28	0
2	GOL	F	301	-	5,5,5	0.26	0	5,5,5	0.29	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
2	GOL	C	302	-	-	0/4/4/4	-
2	GOL	B	301	-	-	0/4/4/4	-
2	GOL	C	303	-	-	2/4/4/4	-
2	GOL	D	303	-	-	0/4/4/4	-
2	GOL	D	302	-	-	0/4/4/4	-
2	GOL	B	303	-	-	2/4/4/4	-
2	GOL	D	301	-	-	2/4/4/4	-
2	GOL	A	302	-	-	4/4/4/4	-
2	GOL	A	303	-	-	0/4/4/4	-
2	GOL	D	304	-	-	0/4/4/4	-
2	GOL	E	302	-	-	0/4/4/4	-
2	GOL	C	301	-	-	0/4/4/4	-
2	GOL	F	302	-	-	0/4/4/4	-
2	GOL	A	301	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	302	-	-	1/4/4/4	-
2	GOL	E	301	-	-	0/4/4/4	-
2	GOL	F	301	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302	GOL	O1-C1-C2-C3
2	B	303	GOL	O2-C2-C3-O3
2	A	302	GOL	C1-C2-C3-O3
2	B	303	GOL	C1-C2-C3-O3
2	D	301	GOL	O1-C1-C2-C3
2	A	302	GOL	O2-C2-C3-O3
2	C	303	GOL	O1-C1-C2-O2
2	A	302	GOL	O1-C1-C2-O2
2	B	302	GOL	O2-C2-C3-O3
2	D	301	GOL	O1-C1-C2-O2
2	C	303	GOL	O1-C1-C2-C3

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.