



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2023 – 06:09 AM EDT

PDB ID : 6VDF
Title : Structure of the periplasmic domain of YejM from *Salmonella typhimurium* (twinned)
Authors : Gabale, U.; Ressler, S.
Deposited on : 2019-12-25
Resolution : 1.92 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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 8 unique types of molecules in this entry. The entry contains 22294 atoms, of which 10549 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 Periplasmic domain of the cardiolipin transporter protein YejM/PbgA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	343	5341	1712	2623	476	522	8	0	0	0
1	B	343	5342	1712	2624	476	522	8	0	0	0
1	C	343	5341	1712	2623	476	522	8	0	0	0
1	D	343	5341	1712	2623	476	522	8	0	0	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	MET	-	expression tag	UNP A0A5K1U4E1
A	220	SER	-	expression tag	UNP A0A5K1U4E1
A	221	GLY	-	expression tag	UNP A0A5K1U4E1
A	222	HIS	-	expression tag	UNP A0A5K1U4E1
A	223	HIS	-	expression tag	UNP A0A5K1U4E1
A	224	HIS	-	expression tag	UNP A0A5K1U4E1
A	225	HIS	-	expression tag	UNP A0A5K1U4E1
A	226	HIS	-	expression tag	UNP A0A5K1U4E1
A	227	HIS	-	expression tag	UNP A0A5K1U4E1
A	228	SER	-	expression tag	UNP A0A5K1U4E1
A	229	SER	-	expression tag	UNP A0A5K1U4E1
A	230	GLY	-	expression tag	UNP A0A5K1U4E1
A	231	LEU	-	expression tag	UNP A0A5K1U4E1
A	232	VAL	-	expression tag	UNP A0A5K1U4E1
A	233	PRO	-	expression tag	UNP A0A5K1U4E1
A	234	ARG	-	expression tag	UNP A0A5K1U4E1
A	235	GLY	-	expression tag	UNP A0A5K1U4E1
A	236	SER	-	expression tag	UNP A0A5K1U4E1
A	237	HIS	-	expression tag	UNP A0A5K1U4E1
A	238	MET	-	expression tag	UNP A0A5K1U4E1

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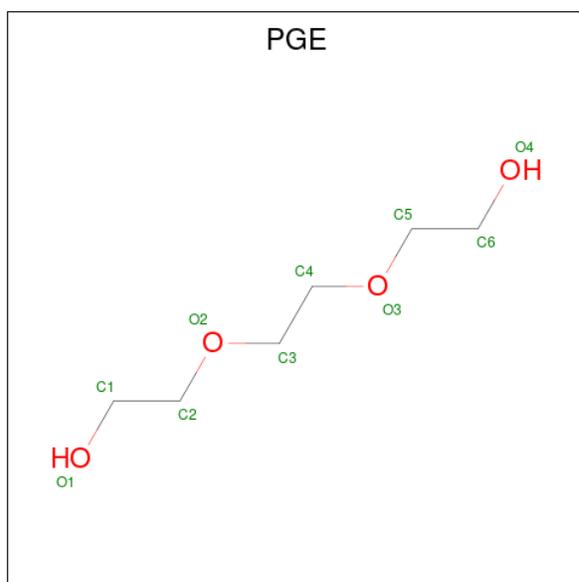
Chain	Residue	Modelled	Actual	Comment	Reference
A	239	ALA	-	expression tag	UNP A0A5K1U4E1
A	240	SER	-	expression tag	UNP A0A5K1U4E1
B	219	MET	-	expression tag	UNP A0A5K1U4E1
B	220	SER	-	expression tag	UNP A0A5K1U4E1
B	221	GLY	-	expression tag	UNP A0A5K1U4E1
B	222	HIS	-	expression tag	UNP A0A5K1U4E1
B	223	HIS	-	expression tag	UNP A0A5K1U4E1
B	224	HIS	-	expression tag	UNP A0A5K1U4E1
B	225	HIS	-	expression tag	UNP A0A5K1U4E1
B	226	HIS	-	expression tag	UNP A0A5K1U4E1
B	227	HIS	-	expression tag	UNP A0A5K1U4E1
B	228	SER	-	expression tag	UNP A0A5K1U4E1
B	229	SER	-	expression tag	UNP A0A5K1U4E1
B	230	GLY	-	expression tag	UNP A0A5K1U4E1
B	231	LEU	-	expression tag	UNP A0A5K1U4E1
B	232	VAL	-	expression tag	UNP A0A5K1U4E1
B	233	PRO	-	expression tag	UNP A0A5K1U4E1
B	234	ARG	-	expression tag	UNP A0A5K1U4E1
B	235	GLY	-	expression tag	UNP A0A5K1U4E1
B	236	SER	-	expression tag	UNP A0A5K1U4E1
B	237	HIS	-	expression tag	UNP A0A5K1U4E1
B	238	MET	-	expression tag	UNP A0A5K1U4E1
B	239	ALA	-	expression tag	UNP A0A5K1U4E1
B	240	SER	-	expression tag	UNP A0A5K1U4E1
C	219	MET	-	expression tag	UNP A0A5K1U4E1
C	220	SER	-	expression tag	UNP A0A5K1U4E1
C	221	GLY	-	expression tag	UNP A0A5K1U4E1
C	222	HIS	-	expression tag	UNP A0A5K1U4E1
C	223	HIS	-	expression tag	UNP A0A5K1U4E1
C	224	HIS	-	expression tag	UNP A0A5K1U4E1
C	225	HIS	-	expression tag	UNP A0A5K1U4E1
C	226	HIS	-	expression tag	UNP A0A5K1U4E1
C	227	HIS	-	expression tag	UNP A0A5K1U4E1
C	228	SER	-	expression tag	UNP A0A5K1U4E1
C	229	SER	-	expression tag	UNP A0A5K1U4E1
C	230	GLY	-	expression tag	UNP A0A5K1U4E1
C	231	LEU	-	expression tag	UNP A0A5K1U4E1
C	232	VAL	-	expression tag	UNP A0A5K1U4E1
C	233	PRO	-	expression tag	UNP A0A5K1U4E1
C	234	ARG	-	expression tag	UNP A0A5K1U4E1
C	235	GLY	-	expression tag	UNP A0A5K1U4E1
C	236	SER	-	expression tag	UNP A0A5K1U4E1

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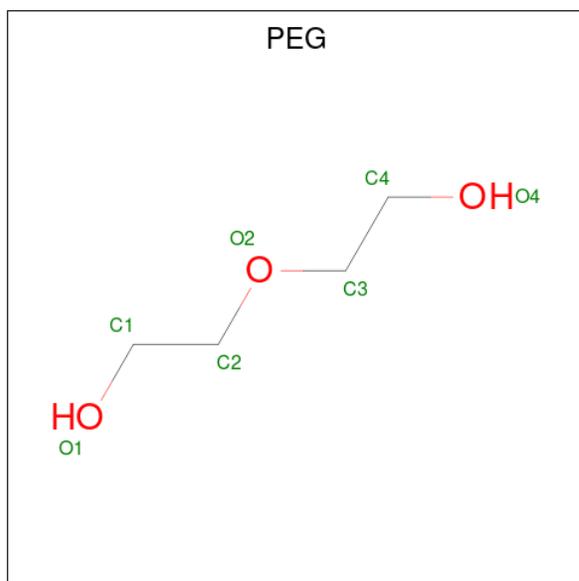
Chain	Residue	Modelled	Actual	Comment	Reference
C	237	HIS	-	expression tag	UNP A0A5K1U4E1
C	238	MET	-	expression tag	UNP A0A5K1U4E1
C	239	ALA	-	expression tag	UNP A0A5K1U4E1
C	240	SER	-	expression tag	UNP A0A5K1U4E1
D	219	MET	-	expression tag	UNP A0A5K1U4E1
D	220	SER	-	expression tag	UNP A0A5K1U4E1
D	221	GLY	-	expression tag	UNP A0A5K1U4E1
D	222	HIS	-	expression tag	UNP A0A5K1U4E1
D	223	HIS	-	expression tag	UNP A0A5K1U4E1
D	224	HIS	-	expression tag	UNP A0A5K1U4E1
D	225	HIS	-	expression tag	UNP A0A5K1U4E1
D	226	HIS	-	expression tag	UNP A0A5K1U4E1
D	227	HIS	-	expression tag	UNP A0A5K1U4E1
D	228	SER	-	expression tag	UNP A0A5K1U4E1
D	229	SER	-	expression tag	UNP A0A5K1U4E1
D	230	GLY	-	expression tag	UNP A0A5K1U4E1
D	231	LEU	-	expression tag	UNP A0A5K1U4E1
D	232	VAL	-	expression tag	UNP A0A5K1U4E1
D	233	PRO	-	expression tag	UNP A0A5K1U4E1
D	234	ARG	-	expression tag	UNP A0A5K1U4E1
D	235	GLY	-	expression tag	UNP A0A5K1U4E1
D	236	SER	-	expression tag	UNP A0A5K1U4E1
D	237	HIS	-	expression tag	UNP A0A5K1U4E1
D	238	MET	-	expression tag	UNP A0A5K1U4E1
D	239	ALA	-	expression tag	UNP A0A5K1U4E1
D	240	SER	-	expression tag	UNP A0A5K1U4E1

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



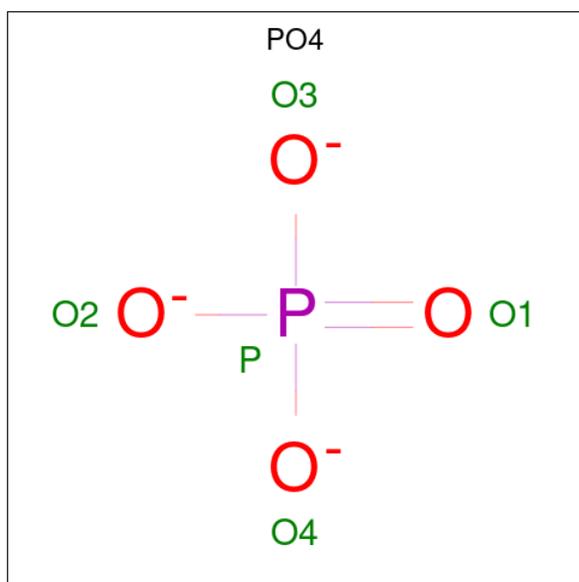
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	24	6	14	4	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	17	4	10	3	0	0
3	D	1	17	4	10	3	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

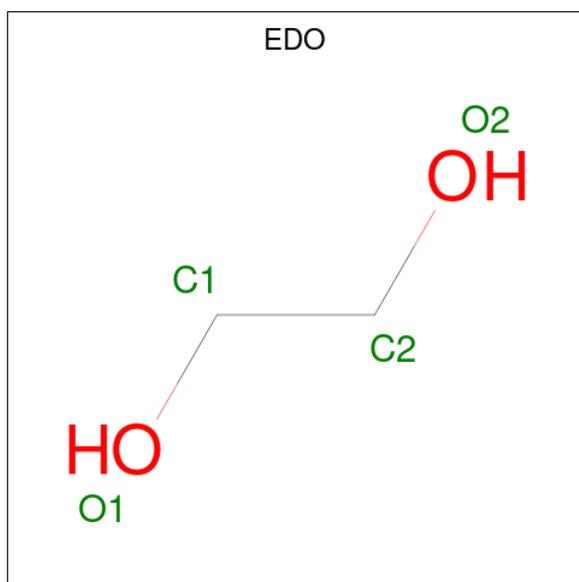


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

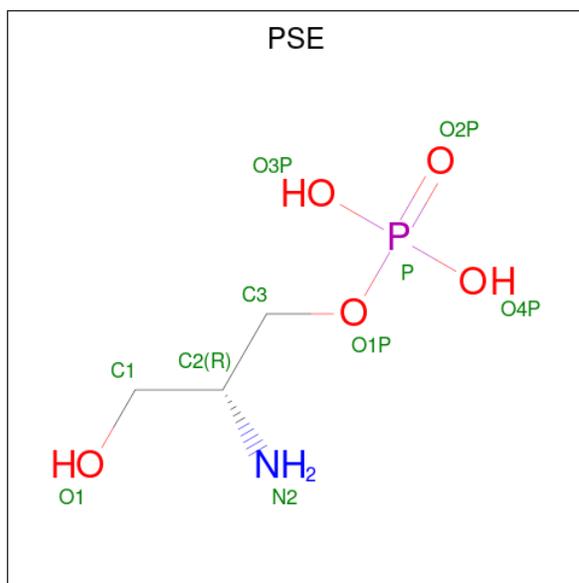
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mn 1 1	0	0
5	B	1	Total Mn 1 1	0	0
5	D	1	Total Mn 1 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	B	1	10	2	6	2	0	0

- Molecule 7 is O-PHOSPHOETHANOLAMINE (three-letter code: PSE) (formula: $C_3H_{10}NO_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
7	C	1	18	3	8	1	5	1	0	0
7	D	1	18	3	8	1	5	1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	183	Total 183	O 183	0	0
8	B	199	Total 199	O 199	0	0
8	C	194	Total 194	O 194	0	0
8	D	236	Total 236	O 236	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	Depositor
Cell constants a, b, c, α , β , γ	42.95Å 42.96Å 181.21Å 94.28° 94.02° 111.78°	Depositor
Resolution (Å)	59.90 – 1.92	Depositor
% Data completeness (in resolution range)	77.2 (59.90-1.92)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	15.55 (at 1.92Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.211 , 0.261	Depositor
Wilson B-factor (Å ²)	19.6	Xtrriage
Anisotropy	0.431	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.428 for k,h,-h-k-l 0.388 for -k,-h,-l 0.387 for -h,-k,h+k+l	Xtrriage
Reported twinning fraction	0.450 for -h,-k,h+k+l	Depositor
Outliers	0 of 70265 reflections	Xtrriage
Total number of atoms	22294	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 for Mogul analysis.

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
4	PO4	D	703	-	4,4,4	0.93	0	6,6,6	0.44	0
7	PSE	D	701	-	9,9,9	0.84	0	9,12,12	0.68	0
2	PGE	A	601	-	9,9,9	0.31	0	8,8,8	0.35	0
6	EDO	B	601	-	3,3,3	0.76	0	2,2,2	0.55	0
3	PEG	D	702	-	6,6,6	0.49	0	5,5,5	0.47	0
3	PEG	A	602	-	6,6,6	0.48	0	5,5,5	0.43	0
7	PSE	C	601	-	9,9,9	0.85	0	9,12,12	0.68	0
4	PO4	A	603	-	4,4,4	0.91	0	6,6,6	0.43	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
7	PSE	D	701	-	-	4/8/8/8	-
2	PGE	A	601	-	-	3/7/7/7	-
6	EDO	B	601	-	-	1/1/1/1	-
3	PEG	D	702	-	-	1/4/4/4	-
3	PEG	A	602	-	-	2/4/4/4	-
7	PSE	C	601	-	-	5/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	601	EDO	O1-C1-C2-O2
7	C	601	PSE	O1-C1-C2-N2
7	C	601	PSE	O1-C1-C2-C3
7	C	601	PSE	C3-O1P-P-O3P
7	C	601	PSE	C3-O1P-P-O4P

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.