Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 10:25 PM EDT

PDB ID	:	6VPU
Title	:	1.90 Angstrom Resolution Crystal Structure Phosphoadenosine Phosphosulfate Reductase (CysH) from Vibrio vulnificus
Authors	:	Minasov, G.; Shuvalova, L.; Dubrovska, I.; Wiersum, G.; Endres, M.; Satchell, K.J.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2020-02-04
Resolution	:	1.90 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
buster-report	:	1.1.7 (2018)
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 (i)

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

The reported resolution of this entry is 1.90 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 5 unique types of molecules in this entry. The entry contains 16978 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 Phosphoadenosine phosphosulfate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	224	1851	1181	316	350	4	0	5	0
1	B	231	1879	1200	320	355	4	0	1	0
1	C	212	1768	1128	300	336	4	0	7	0
1	D	230	1903	1210	325	364	4	0	5	0
1	E	222	1832	1170	314	343	5	0	4	0
1	F	230	1871	1196	319	352	4	0	0	0
1	G	226	1865	1192	318	351	4	0	3	0
1	H	226	1866	1197	318	348	3	0	2	0

There are 24 discrepancies between the modelled and reference sequences:

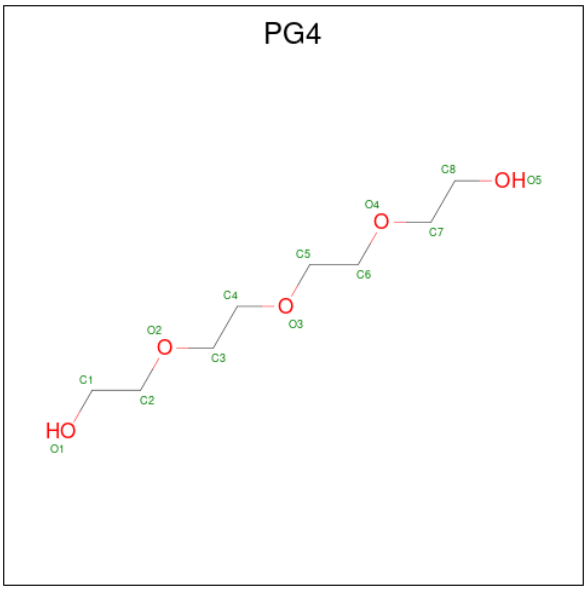
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8CWK6
A	-1	ASN	-	expression tag	UNP Q8CWK6
A	0	ALA	-	expression tag	UNP Q8CWK6
B	-2	SER	-	expression tag	UNP Q8CWK6
B	-1	ASN	-	expression tag	UNP Q8CWK6
B	0	ALA	-	expression tag	UNP Q8CWK6
C	-2	SER	-	expression tag	UNP Q8CWK6
C	-1	ASN	-	expression tag	UNP Q8CWK6
C	0	ALA	-	expression tag	UNP Q8CWK6
D	-2	SER	-	expression tag	UNP Q8CWK6
D	-1	ASN	-	expression tag	UNP Q8CWK6
D	0	ALA	-	expression tag	UNP Q8CWK6
E	-2	SER	-	expression tag	UNP Q8CWK6

Continued on next page...

Continued from previous page...

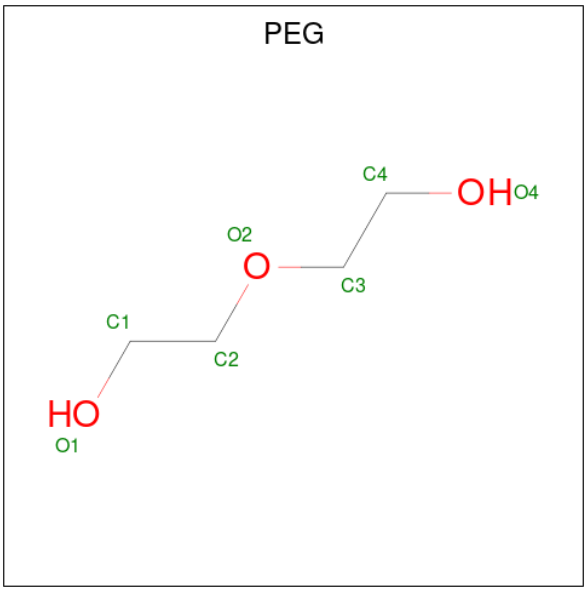
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	expression tag	UNP Q8CWK6
E	0	ALA	-	expression tag	UNP Q8CWK6
F	-2	SER	-	expression tag	UNP Q8CWK6
F	-1	ASN	-	expression tag	UNP Q8CWK6
F	0	ALA	-	expression tag	UNP Q8CWK6
G	-2	SER	-	expression tag	UNP Q8CWK6
G	-1	ASN	-	expression tag	UNP Q8CWK6
G	0	ALA	-	expression tag	UNP Q8CWK6
H	-2	SER	-	expression tag	UNP Q8CWK6
H	-1	ASN	-	expression tag	UNP Q8CWK6
H	0	ALA	-	expression tag	UNP Q8CWK6

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



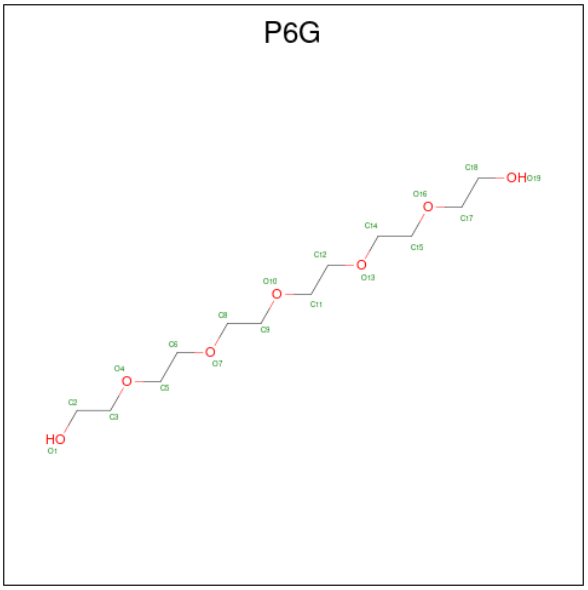
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	13	8	5	0	0

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



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

- Molecule 4 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	D	1	19	12	7	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	284	294	294	0	10
			Total	O		
5	B	266	282	282	0	16
			Total	O		
5	C	262	273	273	0	14
			Total	O		
5	D	292	309	309	0	19
			Total	O		
5	E	268	276	276	0	11
			Total	O		
5	F	208	217	217	0	9
			Total	O		
5	G	216	225	225	0	9
			Total	O		
5	H	213	228	228	0	15

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 21 1	Depositor
Cell constants a, b, c, α, β, γ	107.76Å 76.64Å 143.88Å 90.00° 102.89° 90.00°	Depositor
Resolution (Å)	29.80 – 1.90	Depositor
% Data completeness (in resolution range)	99.9 (29.80-1.90)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.172 , 0.206	Depositor
Wilson B-factor (Å^2)	23.2	Xtriage
Anisotropy	0.196	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16978	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.82 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7231e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (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)

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	B	301	-	6,6,6	0.15	0	5,5,5	0.09	0
2	PG4	A	301	-	12,12,12	0.20	0	11,11,11	0.10	0
4	P6G	D	301	-	18,18,18	0.51	0	17,17,17	0.22	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	B	301	-	-	2/4/4/4	-
2	PG4	A	301	-	-	4/10/10/10	-
4	P6G	D	301	-	-	9/16/16/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

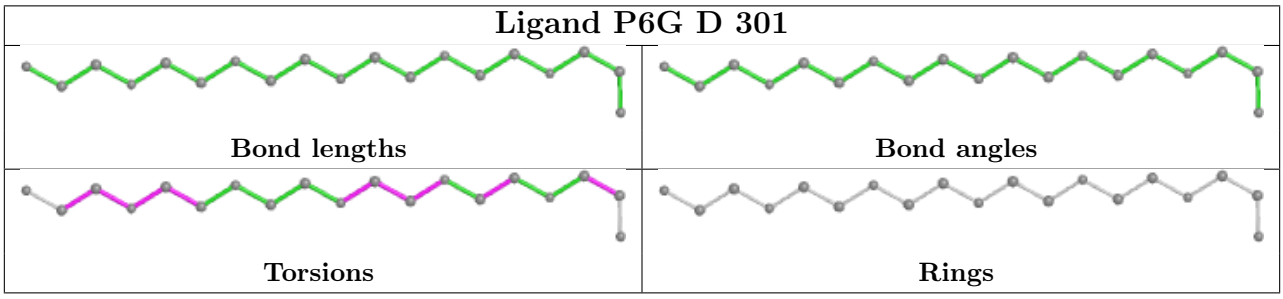
All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	301	P6G	O4-C5-C6-O7
4	D	301	P6G	O7-C8-C9-O10
4	D	301	P6G	O13-C14-C15-O16
4	D	301	P6G	O16-C17-C18-O19
2	A	301	PG4	O2-C3-C4-O3
4	D	301	P6G	O1-C2-C3-O4
3	B	301	PEG	O2-C3-C4-O4
2	A	301	PG4	C1-C2-O2-C3
4	D	301	P6G	C14-C15-O16-C17
4	D	301	P6G	C9-C8-O7-C6
4	D	301	P6G	C8-C9-O10-C11
4	D	301	P6G	C18-C17-O16-C15
3	B	301	PEG	O1-C1-C2-O2
2	A	301	PG4	C6-C5-O3-C4
2	A	301	PG4	O3-C5-C6-O4

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.