

Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 05:38 AM EDT

PDB ID	:	6VVI
Title	:	Arabidopsis thaliana dihydrodipicolinate synthase isoform 1 (DHDPS1)
Authors	:	Lee, M.; Hall, C.J.
Deposited on		
Resolution	:	2.15 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)	:	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: $X\hbox{-}RAY\,DIFFRACTION$

The reported resolution of this entry is 2.15 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 10206 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	308	Total	С	Ν	Ο	\mathbf{S}	0	1	0
	AAA	300	2401	1514	425	448	14	0	1	0
1	BBB	312	Total	С	Ν	0	S	0	4	0
	DDD	312	2455	1545	436	460	14	0	4	0
1	CCC	309	Total	С	Ν	0	S	0	2	0
		309	2413	1522	425	452	14	0	2	0
1	DDD	311	Total	С	Ν	0	S	0	1	0
	עעע	511	2419	1524	426	455	14	0		0

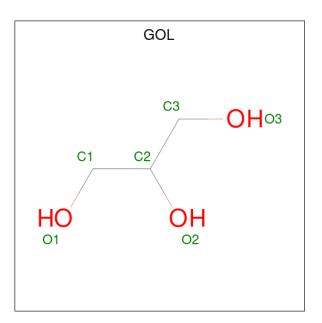
• Molecule 1 is a protein called 4-hydroxy-tetrahydrodipicolinate synthase 1, chloroplastic.

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	45	GLY	-	expression tag	UNP Q9LZX6
AAA	46	PRO	-	expression tag	UNP Q9LZX6
AAA	47	GLY	-	expression tag	UNP Q9LZX6
AAA	48	SER	-	expression tag	UNP Q9LZX6
BBB	45	GLY	-	expression tag	UNP Q9LZX6
BBB	46	PRO	-	expression tag	UNP Q9LZX6
BBB	47	GLY	-	expression tag	UNP Q9LZX6
BBB	48	SER	-	expression tag	UNP Q9LZX6
CCC	45	GLY	-	expression tag	UNP Q9LZX6
CCC	46	PRO	-	expression tag	UNP Q9LZX6
CCC	47	GLY	-	expression tag	UNP Q9LZX6
CCC	48	SER	-	expression tag	UNP Q9LZX6
DDD	45	GLY	-	expression tag	UNP Q9LZX6
DDD	46	PRO	-	expression tag	UNP Q9LZX6
DDD	47	GLY	-	expression tag	UNP Q9LZX6
DDD	48	SER	-	expression tag	UNP Q9LZX6

• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



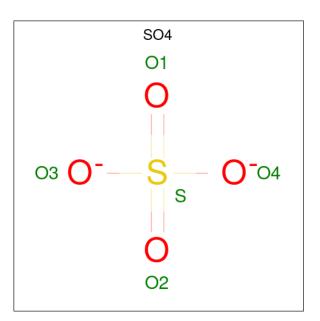


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
2	CCC	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
2	DDD	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
2	DDD	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0

• Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total Na 1 1	0	0
3	BBB	1	Total Na 1 1	0	0
3	CCC	1	Total Na 1 1	0	0
3	DDD	1	Total Na 1 1	0	0





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	BBB	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	CCC	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	CCC	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	DDD	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	DDD	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	85	Total O 85 85	0	0
5	BBB	130	Total O 130 130	0	0
5	CCC	107	Total O 107 107	0	0
5	DDD	143	Total O 143 143	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 21 21 21	Depositor
Cell constants	95.47Å 98.10 Å 176.87 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.10 - 2.15	Depositor
% Data completeness	99.2 (49.10-2.15)	Depositor
(in resolution range)		-
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.29 (at 2.14 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.172 , 0.209	Depositor
Wilson B-factor ($Å^2$)	38.7	Xtriage
Anisotropy	0.505	Xtriage
L-test for twinning ²	$< L > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.032 for k,h,-l	Xtriage
Total number of atoms	10206	wwPDB-VP
Average B, all atoms $(Å^2)$	43.0	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 3.83% 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)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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



Mal	Trune	Chain	Dec	Link	B	ond leng	gths	Bond angles		
Mol	Type	Chain	Res		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	GOL	AAA	401	-	5,5,5	0.13	0	$5,\!5,\!5$	0.38	0
4	SO4	DDD	405	-	4,4,4	0.48	0	$6,\!6,\!6$	0.14	0
2	GOL	CCC	401	-	$5,\!5,\!5$	0.16	0	$5,\!5,\!5$	0.36	0
4	SO4	BBB	402	-	4,4,4	0.37	0	$6,\!6,\!6$	0.08	0
2	GOL	DDD	401	-	$5,\!5,\!5$	0.26	0	$5,\!5,\!5$	0.60	0
4	SO4	CCC	403	-	4,4,4	0.39	0	$6,\!6,\!6$	0.07	0
2	GOL	DDD	402	-	$5,\!5,\!5$	0.13	0	$5,\!5,\!5$	0.40	0
4	SO4	DDD	404	-	4,4,4	0.41	0	$6,\!6,\!6$	0.13	0
4	SO4	CCC	404	-	4,4,4	0.46	0	$6,\!6,\!6$	0.11	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
2	GOL	AAA	401	-	-	2/4/4/4	-
2	GOL	DDD	402	-	-	4/4/4/4	-
2	GOL	DDD	401	-	-	3/4/4/4	-
2	GOL	CCC	401	-	-	2/4/4/4	-

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	CCC	401	GOL	O1-C1-C2-C3
2	DDD	401	GOL	C1-C2-C3-O3
2	DDD	402	GOL	O1-C1-C2-C3
2	DDD	402	GOL	C1-C2-C3-O3
2	DDD	401	GOL	O2-C2-C3-O3
2	AAA	401	GOL	O1-C1-C2-C3
2	AAA	401	GOL	O1-C1-C2-O2
2	CCC	401	GOL	O1-C1-C2-O2
2	DDD	402	GOL	O1-C1-C2-O2

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	DDD	402	GOL	O2-C2-C3-O3
2	DDD	401	GOL	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.

