



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 09:47 PM BST

PDB ID : 6MH4
Title : Crystal Structure of 1-deoxy-D-xylulose-5-phosphate reductoisomerase from *Staphylococcus schleiferi*, Apoenzyme
Authors : Lee, S.G.; Jez, J.M.
Deposited on : 2018-09-17
Resolution : 2.15 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

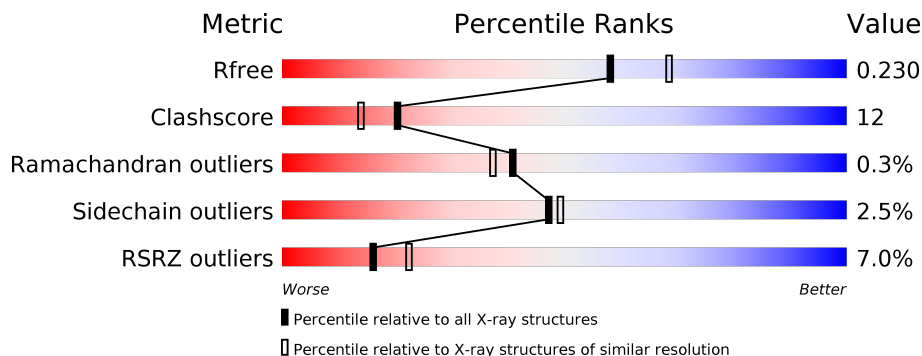
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	376	
1	B	376	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5946 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 1-deoxy-D-xylulose 5-phosphate reductoisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	374	2942	1874	494	558	16	0	0	0
1	B	368	2888	1840	484	549	15	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	GLY	GLU	conflict	UNP A0A0K1A7V6
A	284	VAL	ALA	conflict	UNP A0A0K1A7V6
A	349	SER	ALA	conflict	UNP A0A0K1A7V6
A	367	HIS	TYR	conflict	UNP A0A0K1A7V6
B	188	GLY	GLU	conflict	UNP A0A0K1A7V6
B	284	VAL	ALA	conflict	UNP A0A0K1A7V6
B	349	SER	ALA	conflict	UNP A0A0K1A7V6
B	367	HIS	TYR	conflict	UNP A0A0K1A7V6

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

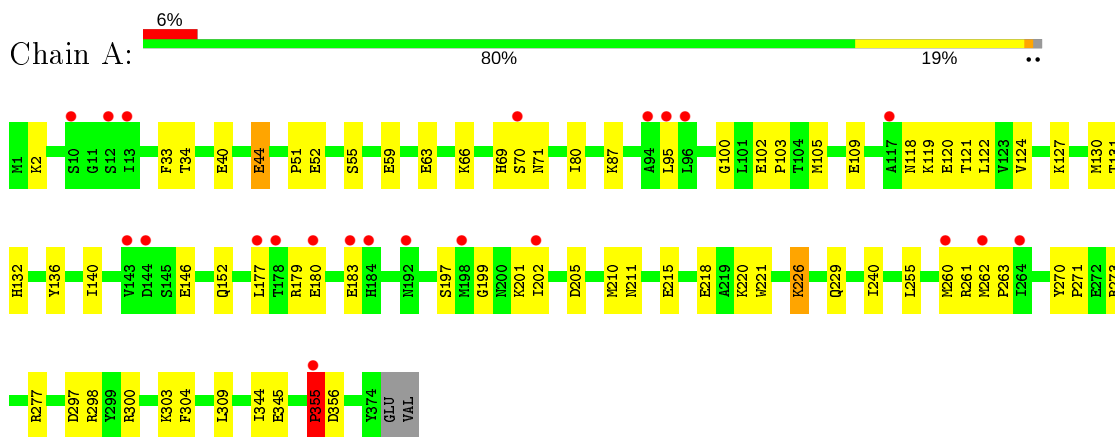
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total	O	0	0
			51	51		
3	B	30	Total	O	0	0
			30	30		

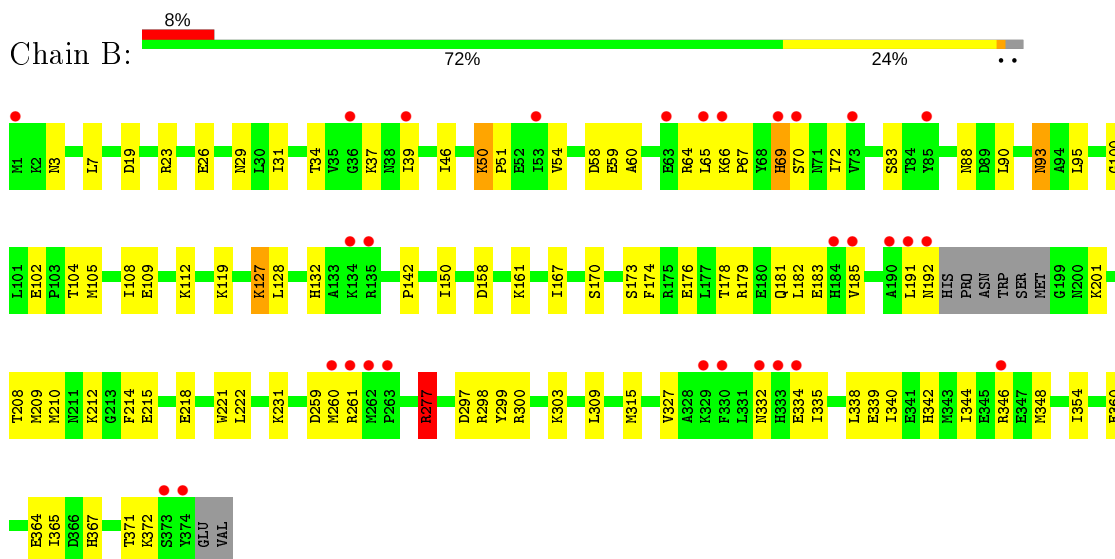
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase



- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	71.37Å 71.37Å 318.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.38 – 2.15 44.38 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.2 (44.38-2.15) 99.2 (44.38-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.16Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.197 , 0.230 0.197 , 0.230	Depositor DCC
R_{free} test set	2581 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtrriage
Anisotropy	0.090	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.057 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5946	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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 $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/2997	0.60	2/4056 (0.0%)
1	B	1.08	1/2938 (0.0%)	1.61	2/3972 (0.1%)
All	All	0.82	1/5935 (0.0%)	1.21	4/8028 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	277	ARG	CZ-NH2	54.27	2.03	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	ARG	NE-CZ-NH2	-85.47	77.56	120.30
1	B	277	ARG	NH1-CZ-NH2	38.37	161.61	119.40
1	A	355	PRO	C-N-CA	6.16	137.09	121.70
1	A	355	PRO	CA-C-N	5.56	129.43	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	69	HIS	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2942	0	2953	62	0
1	B	2888	0	2908	83	2
2	A	20	0	0	0	0
2	B	15	0	0	2	0
3	A	51	0	0	4	1
3	B	30	0	0	3	1
All	All	5946	0	5861	145	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 145 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:ARG:NH2	1:B:277:ARG:CZ	2.03	1.20
1:B:39:ILE:HG21	1:B:64:ARG:NH1	1.79	0.97
1:A:69:HIS:HD2	1:A:71:ASN:H	1.06	0.93
1:A:127:LYS:HG2	1:A:221:TRP:CH2	2.03	0.93
1:B:277:ARG:NH2	1:B:277:ARG:NE	2.18	0.91

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:549:HOH:O	3:B:529:HOH:O[1_455]	1.86	0.34
1:B:277:ARG:CZ	1:B:277:ARG:NH2[6_545]	2.03	0.17
1:B:277:ARG:NE	1:B:277:ARG:NH2[6_545]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	372/376 (99%)	367 (99%)	4 (1%)	1 (0%)	41	37
1	B	364/376 (97%)	351 (96%)	12 (3%)	1 (0%)	41	37
All	All	736/752 (98%)	718 (98%)	16 (2%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	355	PRO
1	B	37	LYS

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	324/327 (99%)	317 (98%)	7 (2%)	52	55
1	B	318/327 (97%)	309 (97%)	9 (3%)	43	44
All	All	642/654 (98%)	626 (98%)	16 (2%)	47	49

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	50	LYS
1	B	83	SER
1	B	173	SER
1	A	303	LYS

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Mol	Chain	Res	Type
1	B	277	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	GLN
1	A	276	HIS
1	B	132	HIS
1	A	152	GLN
1	B	93	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	SO4	A	401	-	4,4,4	0.20	0	6,6,6	0.51	0
2	SO4	A	402	-	4,4,4	0.14	0	6,6,6	0.23	0
2	SO4	B	402	-	4,4,4	0.18	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	401	-	4,4,4	0.40	0	6,6,6	0.93	0
2	SO4	A	404	-	4,4,4	0.15	0	6,6,6	0.18	0
2	SO4	A	403	-	4,4,4	0.42	0	6,6,6	0.32	0
2	SO4	B	403	-	4,4,4	0.13	0	6,6,6	0.33	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	SO4	1	0
2	B	403	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9	
1	A	374/376 (99%)	0.49	22 (5%)	22 30	36, 57, 80, 96	0
1	B	368/376 (97%)	0.57	30 (8%)	11 16	39, 67, 101, 127	0
All	All	742/752 (98%)	0.53	52 (7%)	16 22	36, 61, 94, 127	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	262	MET	6.6
1	B	192	ASN	5.3
1	B	190	ALA	4.7
1	B	260	MET	4.4
1	B	65	LEU	4.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	B	401	5/5	0.81	0.14	89,89,97,99	0
2	SO4	A	403	5/5	0.81	0.23	75,90,93,96	0
2	SO4	B	402	5/5	0.90	0.12	90,99,100,102	0
2	SO4	A	401	5/5	0.92	0.14	66,79,85,90	0
2	SO4	A	404	5/5	0.97	0.10	95,96,98,99	0
2	SO4	A	402	5/5	0.97	0.18	54,63,70,70	0
2	SO4	B	403	5/5	0.98	0.13	70,73,80,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.