



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:10 AM UTC

PDB ID : 2C82 / pdb_00002c82
Title : X-Ray Structure Of 1-Deoxy-D-xylulose 5-phosphate Reductoisomerase, DXR, Rv2870c, From Mycobacterium tuberculosis
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Deposited on : 2005-11-30
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 ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

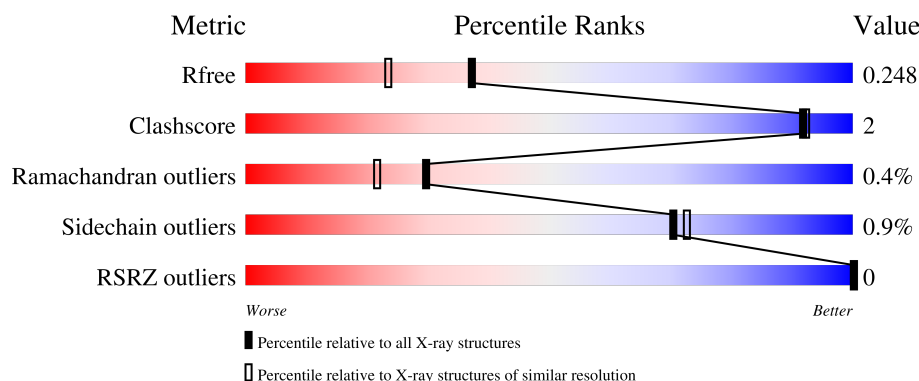
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 of 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	413	 86% 5% 8%
1	B	413	 87% 5% 8%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5906 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
1	A	379	Total	C	N	O	S	0	0	0
			2781	1742	502	528	9			
1	B	379	Total	C	N	O	S	0	0	0
			2781	1742	502	528	9			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	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	168	Total 168	O 168	0	0
3	B	166	Total 166	O 166	0	0

• Molecule 1: 1-DEOXY-D-XYLULOSE 5-PHOSPHATE REDUCTOISOMERASE

- Molecule 1: 1-DEOXY-D-XYLULOSE 5-PHOSPHATE REDUCTOISOMERASE

SER	THR	ALA	LYS	PRO	GLY	ALA	ALA	GLY	ARG	HIS	ALA	SER	THR	LEU	GLU	ARG	SER	MET	THR	ASN	SER	THR	ASP	GLY	ARG	ALA	ASP	G11	R56	Q60	A73	V77	S85	A107	E129	P149	H154	E190	W203	M208	L216	S249	C321	A334	F344	P345	W361	D373	R376	R389	ALA	SER	VAL	ALA	ILE	ALA
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4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	56.93Å 56.93Å 239.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90 40.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-1.90) 99.7 (40.00-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.215 , 0.247 0.214 , 0.248	Depositor DCC
R_{free} test set	2962 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.468 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5906	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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

5.1 Standard geometry

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	0.62	0/2835	0.80	0/3873
1	B	0.63	0/2835	0.79	0/3873
All	All	0.62	0/5670	0.80	0/7746

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2781	0	2768	9	0
1	B	2781	0	2768	9	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	168	0	0	0	0
3	B	166	0	0	1	0
All	All	5906	0	5536	18	0

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 2.

All (18) 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:A:373:ASP:OD1	1:A:376:ARG:NH1	2.32	0.60
1:B:373:ASP:OD1	1:B:376:ARG:NH1	2.34	0.58
1:A:107:ALA:HA	1:A:129:GLU:HG2	1.88	0.56
1:B:107:ALA:HA	1:B:129:GLU:HG2	1.91	0.53
1:A:56:ARG:O	1:A:60:GLN:HG3	2.09	0.52
1:B:56:ARG:O	1:B:60:GLN:HG3	2.12	0.50
1:B:321:CYS:HB2	1:B:361:TRP:HB3	1.92	0.50
1:B:344:PHE:HB3	1:B:345:PRO:HD3	1.93	0.49
1:A:344:PHE:HB3	1:A:345:PRO:HD3	1.93	0.48
1:A:321:CYS:HB2	1:A:361:TRP:HB3	1.95	0.47
1:B:203:TRP:HD1	3:B:2096:HOH:O	1.98	0.47
1:A:208:MET:HE1	1:A:334:ALA:HB3	1.97	0.45
1:B:208:MET:HE1	1:B:334:ALA:HB3	1.98	0.45
1:B:73:ALA:O	1:B:77:VAL:HG22	2.18	0.44
1:A:73:ALA:O	1:A:77:VAL:HG22	2.19	0.43
1:A:247:ILE:HD11	1:A:296:TRP:CE3	2.54	0.42
1:A:170:ALA:O	1:A:236:ARG:HD2	2.20	0.42
1:B:149:PRO:HB2	1:B:154:HIS:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	377/413 (91%)	368 (98%)	8 (2%)	1 (0%)	36	29
1	B	377/413 (91%)	369 (98%)	6 (2%)	2 (0%)	24	16
All	All	754/826 (91%)	737 (98%)	14 (2%)	3 (0%)	30	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	85	SER
1	A	85	SER
1	B	249	SER

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	282/305 (92%)	279 (99%)	3 (1%)	65	67
1	B	282/305 (92%)	280 (99%)	2 (1%)	76	78
All	All	564/610 (92%)	559 (99%)	5 (1%)	70	73

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	SER
1	A	190	GLU
1	A	216	LEU
1	B	190	GLU
1	B	216	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	209	ASN
1	B	94	GLN
1	B	360	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	1390	-	4,4,4	0.31	0	6,6,6	0.20	0
2	SO4	B	1390	-	4,4,4	0.31	0	6,6,6	0.27	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.

No monomer is involved in short contacts.

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	379/413 (91%)	-0.98	0 100 100	18, 32, 56, 70	0
1	B	379/413 (91%)	-1.01	0 100 100	18, 32, 56, 70	0
All	All	758/826 (91%)	-1.00	0 100 100	18, 32, 56, 70	0

There are no RSRZ outliers to report.

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 oligosaccharides 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(Å ²)	Q<0.9
2	SO4	A	1390	5/5	0.99	0.04	48,49,51,51	0
2	SO4	B	1390	5/5	0.99	0.04	49,50,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.