



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 11:06 am BST

PDB ID : 5DZS
Title : 1.5 Angstrom Crystal Structure of Shikimate Dehydrogenase 1 from *Peptoclostridium difficile*.
Authors : Minasov, G.; Wawrzak, Z.; Shuvalova, L.; Dubrovskaya, I.; Flores, K.; Grimshaw, S.; Kwon, K.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2015-09-26
Resolution : 1.50 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 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	:	2.11
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)	:	2.11

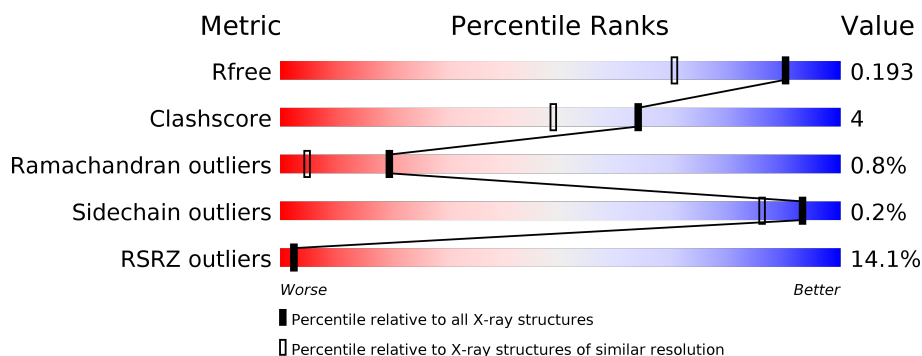
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	276	<div> <div>14%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>5%</div> </div> </div>
1	B	276	<div> <div>13%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>••</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5100 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 Shikimate dehydrogenase (NADP(+)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	31	0
			2330	1498	384	437	11			
1	B	270	Total	C	N	O	S	0	21	0
			2304	1480	383	430	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	270	GLY	-	expression tag	UNP Q187E7
A	271	GLU	-	expression tag	UNP Q187E7
A	272	ASN	-	expression tag	UNP Q187E7
A	273	LEU	-	expression tag	UNP Q187E7
A	274	TYR	-	expression tag	UNP Q187E7
A	275	PHE	-	expression tag	UNP Q187E7
A	276	GLN	-	expression tag	UNP Q187E7
B	270	GLY	-	expression tag	UNP Q187E7
B	271	GLU	-	expression tag	UNP Q187E7
B	272	ASN	-	expression tag	UNP Q187E7
B	273	LEU	-	expression tag	UNP Q187E7
B	274	TYR	-	expression tag	UNP Q187E7
B	275	PHE	-	expression tag	UNP Q187E7
B	276	GLN	-	expression tag	UNP Q187E7

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



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

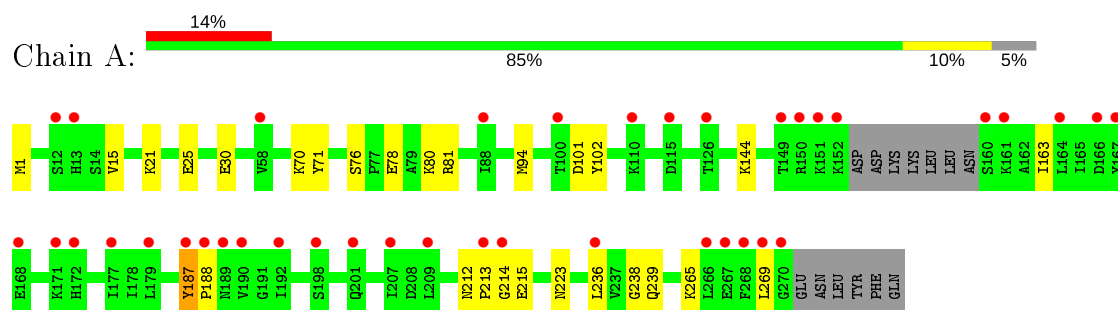
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	216	Total	O	0	26
			232	232		
3	B	207	Total	O	0	13
			219	219		

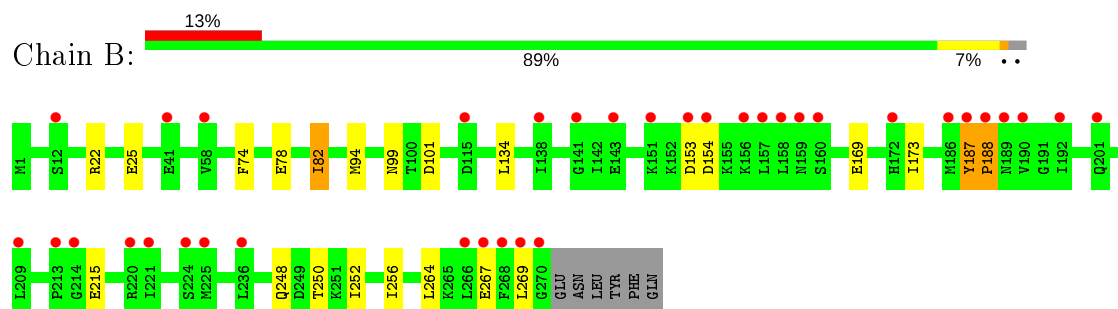
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Shikimate dehydrogenase (NADP(+))



- Molecule 1: Shikimate dehydrogenase (NADP(+))



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.22Å 47.05Å 74.74Å 77.98° 76.44° 89.09°	Depositor
Resolution (Å)	29.70 – 1.50 27.80 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.9 (29.70-1.50) 95.9 (27.80-1.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.163 , 0.185 0.173 , 0.193	Depositor DCC
R_{free} test set	4078 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-k,h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5100	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% 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	0.51	0/2367	0.69	0/3181
1	B	0.48	0/2340	0.68	0/3144
All	All	0.49	0/4707	0.68	0/6325

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	2330	0	2379	27	0
1	B	2304	0	2369	13	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
3	A	232	0	0	7	0
3	B	219	0	0	1	0
All	All	5100	0	4748	40	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 4.

All (40) 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:101:ASP:HA	1:A:239[A]:GLN:OE1	1.78	0.81
1:A:212[A]:ASN:O	1:A:213[A]:PRO:C	2.35	0.65
1:A:78[B]:GLU:H	1:A:78[B]:GLU:CD	2.01	0.64
1:A:212[A]:ASN:O	1:A:214[A]:GLY:N	2.30	0.63
1:A:144:LYS:HE2	1:A:163:ILE:HD11	1.81	0.62
1:A:15[B]:VAL:O	1:A:15[B]:VAL:HG22	1.99	0.61
1:B:187:TYR:CG	1:B:188:PRO:HD3	2.39	0.57
1:A:212[A]:ASN:OD1	1:A:214[A]:GLY:O	2.26	0.54
1:B:82:ILE:HD13	3:B:408:HOH:O	2.08	0.54
1:A:21[A]:LYS:O	1:A:25[A]:GLU:HG3	2.08	0.54
1:B:248[A]:GLN:HB2	1:B:250:THR:HG22	1.95	0.48
1:A:236[A]:LEU:HD12	3:A:430:HOH:O	2.13	0.48
1:B:169:GLU:O	1:B:173:ILE:HD13	2.13	0.47
1:B:269:LEU:O	1:B:269:LEU:HD12	2.15	0.47
1:A:76[B]:SER:OG	1:A:78[B]:GLU:OE1	2.30	0.47
1:A:81[B]:ARG:HD3	3:A:420:HOH:O	2.15	0.47
1:A:15[B]:VAL:CG2	1:A:15[B]:VAL:O	2.63	0.46
1:A:187:TYR:O	1:A:188:PRO:C	2.52	0.46
1:B:252:ILE:HG23	1:B:256:ILE:HD12	1.96	0.46
1:B:22[B]:ARG:HD2	1:B:25:GLU:OE1	2.17	0.45
1:B:78:GLU:O	1:B:82:ILE:HD12	2.18	0.44
1:A:1:MET:HA	1:A:30[B]:GLU:O	2.18	0.43
1:A:187:TYR:HB3	1:A:188:PRO:CD	2.49	0.43
1:A:70[A]:LYS:HE3	1:A:71:TYR:CE2	2.54	0.42
1:A:94[B]:MET:HE2	3:A:480:HOH:O	2.19	0.42
1:B:153:ASP:OD1	1:B:154:ASP:N	2.52	0.42
1:B:74:PHE:CE2	1:B:94[A]:MET:HE3	2.54	0.42
1:A:76[B]:SER:CB	1:A:78[B]:GLU:OE1	2.68	0.42
1:B:264:LEU:HD23	1:B:267:GLU:OE1	2.19	0.42
1:A:238:GLY:HA3	3:A:504:HOH:O	2.19	0.41
1:A:80:LYS:NZ	3:A:407:HOH:O	2.49	0.41
1:A:212[A]:ASN:OD1	1:A:212[A]:ASN:O	2.38	0.41
1:A:15[B]:VAL:HG12	3:A:560:HOH:O	2.20	0.41
1:A:265:LYS:HG2	1:A:269:LEU:HD12	2.03	0.41
1:A:76[B]:SER:HB3	1:A:78[B]:GLU:OE1	2.21	0.41
1:B:99:ASN:OD1	1:B:101:ASP:N	2.44	0.41
1:B:134:LEU:C	1:B:134:LEU:HD23	2.42	0.41
1:A:102:TYR:HB3	3:A:433[A]:HOH:O	2.21	0.41
1:A:187:TYR:HB3	1:A:188:PRO:HD3	2.03	0.40
1:A:215:GLU:OE2	1:A:223:ASN:ND2	2.55	0.40

There are no symmetry-related clashes.

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	290/276 (105%)	283 (98%)	6 (2%)	1 (0%)	41	18
1	B	289/276 (105%)	281 (97%)	5 (2%)	3 (1%)	15	3
All	All	579/552 (105%)	564 (97%)	11 (2%)	4 (1%)	19	6

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	TYR
1	B	188	PRO
1	B	187	TYR
1	B	215	GLU

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	259/242 (107%)	259 (100%)	0	100	100
1	B	255/242 (105%)	254 (100%)	1 (0%)	91	82
All	All	514/484 (106%)	513 (100%)	1 (0%)	93	86

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	82	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 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	$\# Z > 2$
2	SO4	A	301[A]	-	4,4,4	0.43	0	6,6,6	0.47	0
2	SO4	B	302[A]	-	4,4,4	0.33	0	6,6,6	0.12	0
2	SO4	B	301	-	4,4,4	0.48	0	6,6,6	0.28	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	263/276 (95%)	0.81	39 (14%)	2 2	15, 35, 74, 119	0
1	B	270/276 (97%)	0.82	36 (13%)	3 3	16, 36, 79, 127	0
All	All	533/552 (96%)	0.82	75 (14%)	2 2	15, 35, 76, 127	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	187	TYR	16.3
1	B	190	VAL	12.3
1	B	187	TYR	11.3
1	B	269	LEU	10.8
1	B	268	PHE	7.5
1	A	269	LEU	7.4
1	B	270	GLY	7.0
1	B	160	SER	6.7
1	B	153	ASP	6.7
1	A	213[A]	PRO	6.4
1	B	158	LEU	5.8
1	A	268	PHE	5.7
1	A	151	LYS	5.6
1	B	189	ASN	5.5
1	A	214[A]	GLY	5.5
1	B	156	LYS	5.4
1	A	188	PRO	5.3
1	B	201	GLN	5.0
1	A	160	SER	5.0
1	A	172	HIS	4.9
1	A	270	GLY	4.7
1	B	154	ASP	4.6
1	A	266	LEU	4.4
1	A	167	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	188	PRO	4.1
1	B	12[A]	SER	3.9
1	B	220	ARG	3.9
1	B	267	GLU	3.8
1	A	164	LEU	3.8
1	B	214	GLY	3.7
1	B	266	LEU	3.6
1	A	190	VAL	3.6
1	A	152	LYS	3.4
1	B	138	ILE	3.4
1	A	198	SER	3.4
1	A	209	LEU	3.4
1	B	159	ASN	3.3
1	A	236[A]	LEU	3.3
1	B	172	HIS	3.3
1	A	189	ASN	3.2
1	B	192	ILE	3.1
1	A	150	ARG	3.0
1	B	224	SER	2.9
1	B	141	GLY	2.9
1	B	225	MET	2.8
1	A	100	THR	2.8
1	A	161	LYS	2.8
1	A	207	ILE	2.8
1	A	13[A]	HIS	2.8
1	A	192	ILE	2.7
1	B	151	LYS	2.6
1	B	221	ILE	2.6
1	A	12[A]	SER	2.6
1	A	201	GLN	2.6
1	A	168	GLU	2.6
1	A	88	ILE	2.5
1	B	41[A]	GLU	2.4
1	B	58	VAL	2.3
1	A	58	VAL	2.3
1	B	115	ASP	2.3
1	A	115	ASP	2.3
1	A	126	THR	2.2
1	A	149	THR	2.2
1	B	143	GLU	2.2
1	B	209	LEU	2.2
1	A	267	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	166	ASP	2.2
1	B	213	PRO	2.2
1	B	157	LEU	2.1
1	A	177	ILE	2.1
1	B	236	LEU	2.1
1	A	110	LYS	2.1
1	A	171	LYS	2.1
1	A	179	LEU	2.1
1	B	186	MET	2.0

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 carbohydrates 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	B	302[A]	5/5	0.70	0.26	55,57,61,64	5
2	SO4	A	301[A]	5/5	0.90	0.19	21,25,31,34	5
2	SO4	B	301	5/5	0.96	0.09	32,38,50,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.