



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:24 pm GMT

PDB ID : 2GN1
Title : Crystal structure of dimeric biodegradative threonine deaminase (TdcB) from *Salmonella typhimurium* at 2.2Å resolution (Triclinic form with one dimer of TdcB in the asymmetric unit)
Authors : Simanshu, D.K.; Savithri, H.S.; Murthy, M.R.N.
Deposited on : 2006-04-09
Resolution : 2.20 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

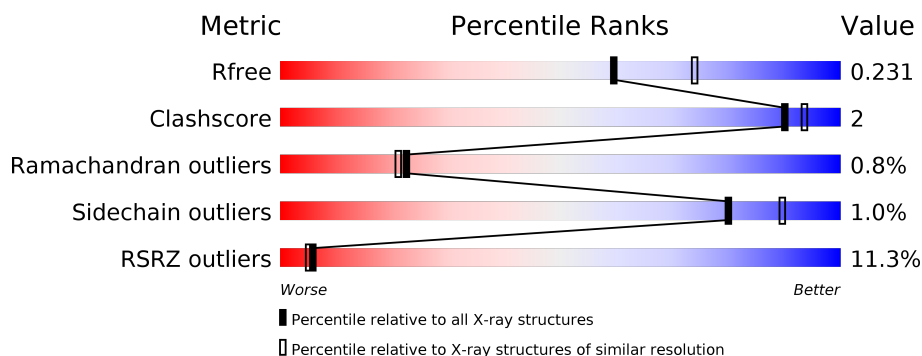
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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. 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	342	
1	B	342	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5070 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 Threonine dehydratase catabolic.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	P	S	0	0	0
			2425	1518	418	474	1	14			
1	B	321	Total	C	N	O	P	S	0	1	0
			2370	1485	409	462	1	13			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	CLONING ARTIFACT	UNP P11954
A	-11	ARG	-	CLONING ARTIFACT	UNP P11954
A	-10	GLY	-	CLONING ARTIFACT	UNP P11954
A	-9	SER	-	CLONING ARTIFACT	UNP P11954
A	-8	HIS	-	EXPRESSION TAG	UNP P11954
A	-7	HIS	-	EXPRESSION TAG	UNP P11954
A	-6	HIS	-	EXPRESSION TAG	UNP P11954
A	-5	HIS	-	EXPRESSION TAG	UNP P11954
A	-4	HIS	-	EXPRESSION TAG	UNP P11954
A	-3	HIS	-	EXPRESSION TAG	UNP P11954
A	-2	GLY	-	CLONING ARTIFACT	UNP P11954
A	-1	MET	-	CLONING ARTIFACT	UNP P11954
A	0	ALA	-	CLONING ARTIFACT	UNP P11954
A	1	SER	-	CLONING ARTIFACT	UNP P11954
A	58	LLP	LYS	MODIFIED RESIDUE	UNP P11954
B	-12	MET	-	CLONING ARTIFACT	UNP P11954
B	-11	ARG	-	CLONING ARTIFACT	UNP P11954
B	-10	GLY	-	CLONING ARTIFACT	UNP P11954
B	-9	SER	-	CLONING ARTIFACT	UNP P11954
B	-8	HIS	-	EXPRESSION TAG	UNP P11954
B	-7	HIS	-	EXPRESSION TAG	UNP P11954
B	-6	HIS	-	EXPRESSION TAG	UNP P11954
B	-5	HIS	-	EXPRESSION TAG	UNP P11954
B	-4	HIS	-	EXPRESSION TAG	UNP P11954
B	-3	HIS	-	EXPRESSION TAG	UNP P11954

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	CLONING ARTIFACT	UNP P11954
B	-1	MET	-	CLONING ARTIFACT	UNP P11954
B	0	ALA	-	CLONING ARTIFACT	UNP P11954
B	1	SER	-	CLONING ARTIFACT	UNP P11954
B	58	LLP	LYS	MODIFIED RESIDUE	UNP P11954

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	153	Total O 153 153	0	0
3	B	121	Total O 121 121	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.32Å 55.30Å 67.23Å 103.09° 94.70° 112.94°	Depositor
Resolution (Å)	25.00 – 2.20 28.22 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.3 (25.00-2.20) 84.9 (28.22-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0009	Depositor
R, R_{free}	0.210 , 0.253 0.217 , 0.231	Depositor DCC
R_{free} test set	1420 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5070	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 8.07% 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: NA, LLP

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	0.37	0/2430	0.54	0/3287
1	B	0.38	0/2377	0.53	0/3213
All	All	0.38	0/4807	0.53	0/6500

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	2425	0	2433	8	0
1	B	2370	0	2364	12	0
2	A	1	0	0	0	0
3	A	153	0	0	0	0
3	B	121	0	0	0	0
All	All	5070	0	4797	20	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 (20) 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:274:ILE:HD13	1:A:320:VAL:HG13	1.76	0.68
1:B:174:TYR:OH	1:B:199:ILE:HG22	1.98	0.62
1:B:131:PHE:CE2	1:B:135:ILE:HD11	2.35	0.62
1:A:178:ASN:HB2	1:A:306:THR:HG23	1.93	0.50
1:A:58:LLP:NZ	1:A:58:LLP:O3	2.45	0.49
1:B:271:ILE:O	1:B:275:GLN:HB2	2.15	0.47
1:B:87:ALA:HB1	1:B:103:VAL:HG11	1.97	0.47
1:A:66:LEU:CD2	1:A:78:VAL:HG11	2.45	0.46
1:B:248:TYR:O	1:B:252:ARG:HG2	2.16	0.46
1:B:58:LLP:H2'3	1:B:284:ALA:HB3	1.98	0.45
1:B:183:ILE:HG23	1:B:186:GLY:HA2	1.99	0.45
1:B:170:MET:HB3	1:B:174:TYR:CE2	2.52	0.43
1:B:48:PHE:CE1	1:B:279:VAL:HG11	2.53	0.43
1:B:62:ALA:O	1:B:66:LEU:HD12	2.18	0.43
1:A:87:ALA:HB1	1:A:103:VAL:HG11	2.00	0.43
1:A:86:HIS:CE1	1:A:152:PRO:HA	2.53	0.42
1:B:120:TYR:O	1:B:121:SER:CB	2.68	0.42
1:A:91:SER:OG	1:A:120:TYR:HB2	2.21	0.41
1:A:300:HIS:O	1:A:304:ARG:HG3	2.21	0.41
1:B:9:VAL:HG22	1:B:250:ILE:HD11	2.03	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	324/342 (95%)	311 (96%)	9 (3%)	4 (1%)	15	12
1	B	319/342 (93%)	306 (96%)	12 (4%)	1 (0%)	44	49
All	All	643/684 (94%)	617 (96%)	21 (3%)	5 (1%)	22	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	121	SER
1	A	120	TYR
1	A	121	SER
1	A	107	LYS
1	A	84	GLY

5.3.2 Protein sidechains ⓘ

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	254/276 (92%)	252 (99%)	2 (1%)	85	92
1	B	244/276 (88%)	241 (99%)	3 (1%)	75	86
All	All	498/552 (90%)	493 (99%)	5 (1%)	80	89

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

Mol	Chain	Res	Type
1	A	162	GLN
1	A	277	ASN
1	B	134	THR
1	B	174	TYR
1	B	277	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	322	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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
1	LLP	A	58	1	24,24,25	1.80	4 (16%)	28,32,34	1.40	3 (10%)
1	LLP	B	58	1	24,24,25	1.79	4 (16%)	28,32,34	1.61	3 (10%)

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
1	LLP	A	58	1	-	0/15/17/19	0/1/1/1
1	LLP	B	58	1	-	0/15/17/19	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	LLP	O3-C3	-6.16	1.22	1.37
1	B	58	LLP	O3-C3	-5.91	1.23	1.37
1	B	58	LLP	C3-C2	-2.29	1.39	1.40
1	A	58	LLP	CA-C	2.03	1.52	1.50
1	A	58	LLP	C4'-NZ	2.22	1.33	1.27
1	B	58	LLP	C4'-NZ	2.39	1.34	1.27
1	A	58	LLP	C4-C4'	3.02	1.52	1.46
1	B	58	LLP	C4-C4'	3.12	1.52	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	LLP	C4-C4'-NZ	-3.15	109.36	124.66
1	B	58	LLP	C4-C4'-NZ	-2.43	112.86	124.66
1	A	58	LLP	C5-C6-N1	-2.24	120.08	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	LLP	OP3-P-OP2	2.15	116.28	107.61
1	A	58	LLP	OP4-C5'-C5	3.85	117.05	109.32
1	B	58	LLP	OP4-C5'-C5	5.85	121.08	109.32

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
1	A	58	LLP	1	0
1	B	58	LLP	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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	326/342 (95%)	0.33	23 (7%) 17 16	29, 34, 46, 50	0
1	B	320/342 (93%)	0.90	50 (15%) 2 2	25, 35, 49, 50	0
All	All	646/684 (94%)	0.61	73 (11%) 6 5	25, 35, 47, 50	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	77	GLY	5.1
1	A	0	ALA	4.8
1	B	110	PRO	4.7
1	B	127	HIS	4.4
1	B	299	SER	4.4
1	A	70	THR	4.3
1	B	120	TYR	4.2
1	B	310	ILE	3.8
1	B	97	LEU	3.8
1	B	129	ASP	3.7
1	B	146	GLY	3.6
1	B	174	TYR	3.6
1	B	139	SER	3.5
1	B	70	THR	3.4
1	B	205	VAL	3.3
1	B	307	VAL	3.3
1	A	188	LEU	3.3
1	B	311	SER	3.3
1	B	6	ASP	3.2
1	B	122	ALA	3.2
1	B	23	GLY	3.1
1	A	187	GLY	3.0
1	B	22	ALA	3.0
1	B	309	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	144	THR	3.0
1	B	112	SER	2.9
1	A	3	ILE	2.9
1	B	5	TYR	2.9
1	B	312	GLY	2.9
1	A	129	ASP	2.8
1	B	188	LEU	2.8
1	B	128	GLY	2.8
1	B	302	GLN	2.8
1	A	4	THR	2.8
1	B	109	ALA	2.7
1	A	75	ARG	2.7
1	B	48	PHE	2.7
1	A	120	TYR	2.7
1	B	99	ILE	2.7
1	B	107	LYS	2.7
1	B	142	VAL	2.7
1	B	141	ILE	2.6
1	B	118	CYS	2.6
1	A	48	PHE	2.6
1	B	63	PHE	2.5
1	B	108	GLY	2.5
1	B	19	LYS	2.5
1	A	189	ILE	2.5
1	A	1	SER	2.4
1	B	7	LEU	2.4
1	B	115	ALA	2.4
1	B	67	SER	2.4
1	B	303	ASN	2.4
1	B	252	ARG	2.4
1	A	310	ILE	2.3
1	B	71	GLU	2.3
1	B	189	ILE	2.3
1	B	193	ALA	2.3
1	A	191	GLY	2.3
1	A	325	GLY	2.3
1	A	309	ILE	2.2
1	A	208	VAL	2.2
1	B	124	VAL	2.2
1	B	280	ILE	2.2
1	A	182	PRO	2.2
1	A	107	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	190	ALA	2.1
1	B	119	ASP	2.1
1	A	57	PHE	2.1
1	B	285	GLY	2.1
1	A	181	VAL	2.1
1	B	143	GLU	2.0
1	A	180	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	LLP	A	58	24/25	0.97	0.19	-	30,33,35,36	0
1	LLP	B	58	24/25	0.95	0.19	-	27,30,34,35	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	NA	A	400	1/1	0.97	0.05	-2.36	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.