



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2014 – 12:12 PM EDT

PDB ID : 4PQ1
Title : Crystal structure and functional implications of a DsbF homologue from *Corynebacterium diphtheriae*
Authors : Um, S.H.; Kim, J.S.; Yoon, B.Y.; Ha, N.C.
Deposited on : 2014-02-28
Resolution : 2.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

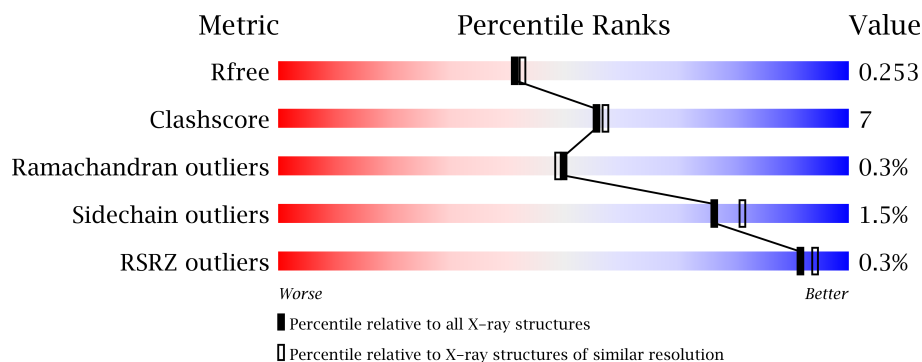
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

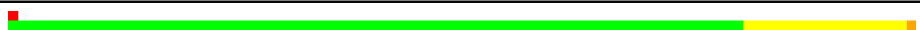

The reported resolution of this entry is 2.10 Å.

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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	158	
1	B	158	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2606 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Putative electron transport related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	2	0
			1228	778	205	243	2			
1	B	158	Total	C	N	O	S	0	1	0
			1229	777	205	245	2			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	91	Total	O	0	0
			91	91		
2	B	58	Total	O	0	0
			58	58		

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- Molecule 1: Putative electron transport related protein

Journal	Publications
G29	185
S35	178
P36	178
E46	178
I55	178
R56	178
G57	178
E58	178
S66	178
L67	178
G81	178
C84	178
A85	178
P86	178
E90	178
S91	178
D92	178
V97	178
L101	178
R113	178
K117	178
F139	178
K140	178
T141	178
Q144	178
V148	178
F149	178
A150	178
I157	178
V158	178
L159	178
H163	178
E172	178
L178	178
I182	178
L185	178

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.10Å 36.16Å 62.52Å 90.00° 67.89° 90.00°	Depositor
Resolution (Å)	36.18 – 2.10 36.18 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.2 (36.18-2.10) 93.4 (36.18-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.09 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.184 , 0.250 0.184 , 0.253	Depositor DCC
R_{free} test set	914 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.4	EDS
Estimated twinning fraction	0.041 for -h+l,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 18104 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2606	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.40	0/1255	0.56	0/1708
1	B	0.39	0/1256	0.53	0/1709
All	All	0.40	0/2511	0.54	0/3417

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1228	0	1194	18	0
1	B	1229	0	1192	14	0
2	A	91	0	0	4	0
2	B	58	0	0	2	0
All	All	2606	0	2386	32	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (32) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:55:ILE:HB	1:A:67:LEU:HG	1.72	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:140:LYS:NZ	2:B:248:HOH:O	2.32	0.62
1:B:65:VAL:HG22	1:B:134:ILE:HG12	1.81	0.61
1:A:56:ARG:HG3	1:A:66:SER:HB3	1.81	0.61
1:B:82:GLN:HG2	1:B:119:ILE:HG22	1.83	0.60
1:A:92:ASP:OD1	2:A:268:HOH:O	2.17	0.59
1:A:90:GLU:HB3	1:A:172:GLU:HG3	1.84	0.59
1:A:101:LEU:HD21	1:A:182:ILE:HD12	1.86	0.56
1:B:30:THR:HB	1:B:50:ALA:HB1	1.91	0.53
1:A:148:VAL:HG21	1:A:157:ILE:HD11	1.92	0.52
1:B:55:ILE:HB	1:B:67:LEU:HG	1.92	0.51
1:B:138:PRO:HG2	1:B:140:LYS:HD3	1.92	0.51
1:A:144:GLN:HG2	2:A:285:HOH:O	2.11	0.51
1:B:60:LEU:O	1:B:121:GLN:NE2	2.45	0.49
1:A:178:LEU:O	1:A:182:ILE:HG12	2.14	0.48
1:B:123:PHE:O	1:B:127:ASN:ND2	2.41	0.47
1:A:148:VAL:HG13	2:A:283:HOH:O	2.16	0.46
1:A:97:VAL:HG21	1:A:178:LEU:HD12	1.97	0.46
1:A:58:GLU:OE2	1:A:117:LYS:NZ	2.28	0.45
1:B:85:ALA:HB3	1:B:86:PRO:HD3	1.98	0.45
1:A:55:ILE:HD12	1:A:141:THR:HG23	1.99	0.44
1:A:46:GLU:HG3	2:A:264:HOH:O	2.18	0.43
1:B:36:PRO:HB2	1:B:39:LYS:HB2	1.99	0.43
1:A:113:ARG:NH2	1:A:150:ALA:O	2.41	0.42
1:A:81:GLY:O	1:A:84:CYS:HB3	2.18	0.42
1:B:97:VAL:HG21	1:B:178:LEU:HD12	2.01	0.42
1:A:159:LEU:HB3	1:A:163:HIS:HA	2.01	0.42
1:B:42:ILE:HD12	2:B:217:HOH:O	2.19	0.41
1:B:87:CYS:SG	1:B:154:PRO:HB3	2.61	0.41
1:A:85:ALA:HB3	1:A:86:PRO:HD3	2.03	0.41
1:A:35:SER:HA	1:A:36:PRO:HD2	1.92	0.40
1:B:159:LEU:HB3	1:B:163:HIS:HA	2.03	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	157/158 (99%)	151 (96%)	6 (4%)	0	100	100
1	B	157/158 (99%)	153 (98%)	3 (2%)	1 (1%)	33	28
All	All	314/316 (99%)	304 (97%)	9 (3%)	1 (0%)	50	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	37	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	135/134 (101%)	133 (98%)	2 (2%)	76	81
1	B	135/134 (101%)	133 (98%)	2 (2%)	76	81
All	All	270/268 (101%)	266 (98%)	4 (2%)	76	81

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	CYS
1	A	139	PHE
1	B	113	ARG
1	B	114	ASP

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

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	157/158 (99%)	-0.30	1 (0%) 86 90	20, 29, 44, 59	0
1	B	158/158 (100%)	-0.18	0 100 100	23, 36, 52, 61	0
All	All	315/316 (99%)	-0.24	1 (0%) 91 94	20, 33, 50, 61	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56	ARG	2.6

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.