



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:00 am BST

PDB ID : 6EEZ
Title : Crystal Structure of the thiol-disulfide exchange protein alpha-DsbA2 from *Wolbachia pipientis*
Authors : Walden, P.M.; Lakshmanane, P.; King, G.J.; Martin, J.L.
Deposited on : 2018-08-15
Resolution : 2.25 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
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

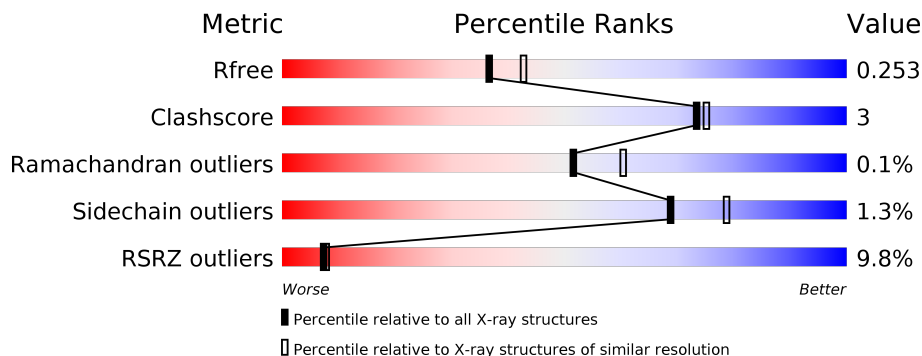
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	190	 4% 91% 7% ••
1	B	190	 5% 88% 11% •
1	C	190	 14% 86% 9% • 5%
1	D	190	 15% 87% 7% • 5%

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 11767 atoms, of which 5750 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 DsbA-like disulfide oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	186	2911	926	1450	244	286	5	0	2	0
1	B	190	2974	945	1480	252	292	5	0	2	0
1	C	181	2830	903	1410	235	279	3	0	0	0
1	D	181	2830	903	1410	235	279	3	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	SER	-	expression tag	UNP Q73FL6
A	64	ASN	-	expression tag	UNP Q73FL6
A	65	ALA	-	expression tag	UNP Q73FL6
B	63	SER	-	expression tag	UNP Q73FL6
B	64	ASN	-	expression tag	UNP Q73FL6
B	65	ALA	-	expression tag	UNP Q73FL6
C	63	SER	-	expression tag	UNP Q73FL6
C	64	ASN	-	expression tag	UNP Q73FL6
C	65	ALA	-	expression tag	UNP Q73FL6
D	63	SER	-	expression tag	UNP Q73FL6
D	64	ASN	-	expression tag	UNP Q73FL6
D	65	ALA	-	expression tag	UNP Q73FL6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	73	Total	O	0	0
			73	73		
2	B	90	Total	O	0	0
			90	90		

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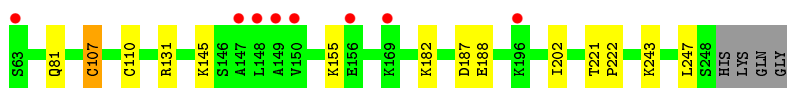
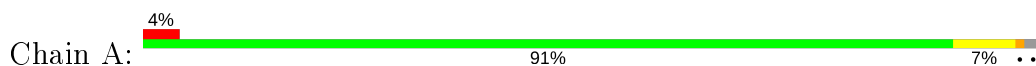
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	43	Total	O	0	0
			43	43		
2	D	16	Total	O	0	0
			16	16		

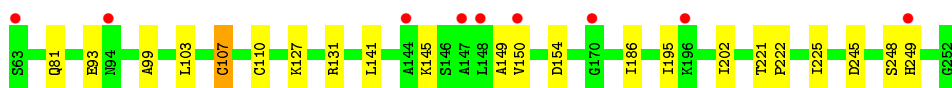
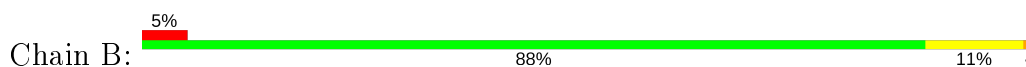
3 Residue-property plots [i](#)

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.

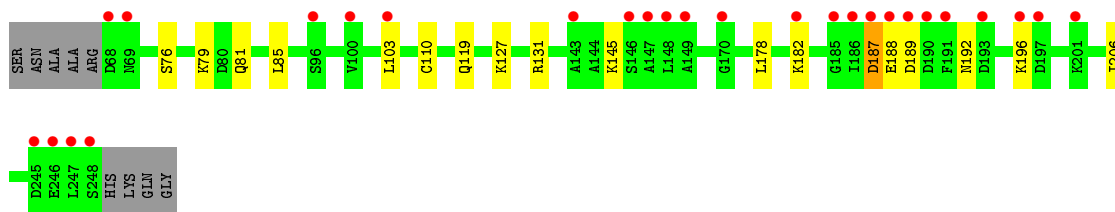
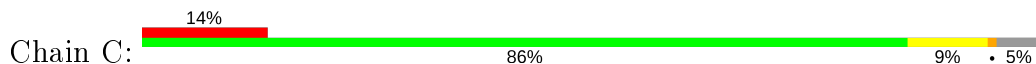
- Molecule 1: DsbA-like disulfide oxidoreductase



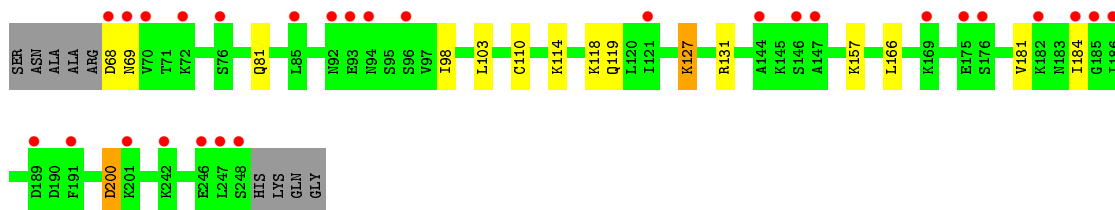
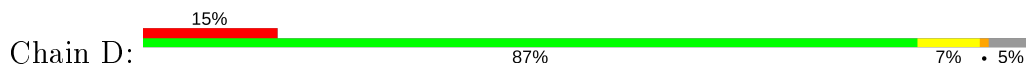
- Molecule 1: DsbA-like disulfide oxidoreductase



- Molecule 1: DsbA-like disulfide oxidoreductase



- Molecule 1: DsbA-like disulfide oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.41Å 104.80Å 67.69Å 90.00° 96.48° 90.00°	Depositor
Resolution (Å)	19.77 – 2.25 19.77 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.77-2.25) 99.0 (19.77-2.25)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.72 (at 2.26Å)	Xtrriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.214 , 0.253 0.214 , 0.253	Depositor DCC
R_{free} test set	1784 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtrriage
Anisotropy	0.577	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11767	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.19% 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](#)

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	0.48	0/1490	0.55	0/2006
1	B	0.54	0/1524	0.62	0/2049
1	C	0.39	0/1443	0.53	0/1943
1	D	0.38	0/1443	0.51	0/1943
All	All	0.45	0/5900	0.56	0/7941

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 [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	1461	1450	1452	8	0
1	B	1494	1480	1483	14	0
1	C	1420	1410	1410	9	0
1	D	1420	1410	1410	9	0
2	A	73	0	0	1	0
2	B	90	0	0	1	0
2	C	43	0	0	0	0
2	D	16	0	0	0	0
All	All	6017	5750	5755	38	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 3.

All (38) 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:107[B]:CYS:SG	2:B:359:HOH:O	2.39	0.61
1:A:155:LYS:NZ	1:C:119:GLN:OE1	2.32	0.57
1:D:81:GLN:O	1:D:131:ARG:NH2	2.39	0.55
1:C:81:GLN:O	1:C:131:ARG:NH2	2.42	0.53
1:D:200:ASP:OD1	1:D:200:ASP:N	2.40	0.52
1:B:145:LYS:HD3	1:B:202:ILE:CG2	2.41	0.51
1:A:221:THR:HB	1:A:222:PRO:HA	1.93	0.50
1:A:107[B]:CYS:SG	2:A:359:HOH:O	2.56	0.50
1:C:76:SER:HA	1:C:79:LYS:HG3	1.93	0.49
1:D:68:ASP:OD1	1:D:69:ASN:N	2.45	0.49
1:B:145:LYS:HD3	1:B:202:ILE:HG22	1.94	0.49
1:B:154:ASP:OD2	1:D:118:LYS:NZ	2.45	0.48
1:C:85:LEU:HD11	1:C:127:LYS:HD2	1.95	0.48
1:B:150:VAL:HG13	1:B:186:ILE:CD1	2.44	0.47
1:B:221:THR:HB	1:B:222:PRO:HA	1.96	0.46
1:D:103:LEU:HB2	1:D:110:CYS:SG	2.56	0.46
1:B:141:LEU:HD11	1:B:145:LYS:HE3	1.98	0.45
1:A:243:LYS:HE3	1:A:247:LEU:HD11	1.98	0.45
1:B:81:GLN:O	1:B:131:ARG:NH2	2.50	0.45
1:B:149:ALA:HB2	1:B:195:ILE:HD13	1.98	0.44
1:B:110[B]:CYS:SG	1:B:222:PRO:HB3	2.57	0.44
1:D:181:VAL:HA	1:D:184:ILE:HD12	1.98	0.44
1:C:192:ASN:O	1:C:196:LYS:HG2	2.19	0.43
1:C:103:LEU:HG	1:C:110:CYS:SG	2.59	0.43
1:B:245:ASP:O	1:B:249:HIS:CD2	2.71	0.43
1:B:93:GLU:HA	1:B:127:LYS:NZ	2.34	0.43
1:C:187:ASP:O	1:C:189:ASP:N	2.52	0.43
1:A:110[B]:CYS:SG	1:A:222:PRO:HB3	2.59	0.42
1:B:103:LEU:HG	1:B:110[B]:CYS:SG	2.59	0.42
1:A:145:LYS:HD3	1:A:202:ILE:HG22	2.02	0.41
1:D:114:LYS:HB3	1:D:166:LEU:HD13	2.02	0.41
1:C:178:LEU:O	1:C:182:LYS:HG2	2.20	0.41
1:A:81:GLN:O	1:A:131:ARG:NH2	2.53	0.41
1:C:145:LYS:HG2	1:C:206:ILE:HD12	2.03	0.41
1:D:157:LYS:CD	1:D:184:ILE:CG2	2.99	0.40
1:D:98:ILE:HG23	1:D:127:LYS:HD2	2.03	0.40
1:A:182:LYS:HE2	1:A:188:GLU:HB2	2.04	0.40
1:B:99:ALA:HA	1:B:225:ILE:O	2.21	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	186/190 (98%)	181 (97%)	5 (3%)	0	100	100
1	B	190/190 (100%)	186 (98%)	4 (2%)	0	100	100
1	C	179/190 (94%)	173 (97%)	5 (3%)	1 (1%)	25	25
1	D	179/190 (94%)	173 (97%)	6 (3%)	0	100	100
All	All	734/760 (97%)	713 (97%)	20 (3%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	188	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	162/163 (99%)	159 (98%)	3 (2%)	57	66
1	B	165/163 (101%)	162 (98%)	3 (2%)	59	68
1	C	157/163 (96%)	156 (99%)	1 (1%)	86	91
1	D	157/163 (96%)	154 (98%)	3 (2%)	57	66
All	All	641/652 (98%)	631 (98%)	10 (2%)	69	73

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107[A]	CYS
1	A	107[B]	CYS
1	A	187	ASP
1	B	107[A]	CYS
1	B	107[B]	CYS
1	B	248	SER
1	C	187	ASP
1	D	119	GLN
1	D	127	LYS
1	D	200	ASP

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](#)

There are no ligands in this entry.

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	186/190 (97%)	0.34	8 (4%) 35 37	26, 42, 69, 82	0
1	B	190/190 (100%)	0.31	9 (4%) 31 34	23, 37, 57, 78	0
1	C	181/190 (95%)	0.87	27 (14%) 2 2	32, 57, 92, 123	0
1	D	181/190 (95%)	0.95	28 (15%) 2 1	36, 64, 102, 117	0
All	All	738/760 (97%)	0.61	72 (9%) 7 8	23, 49, 90, 123	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	190	ASP	8.2
1	C	193	ASP	6.2
1	C	185	GLY	5.9
1	D	184	ILE	5.5
1	D	94	ASN	4.6
1	D	185	GLY	4.4
1	D	96	SER	4.1
1	B	249	HIS	3.6
1	A	147	ALA	3.6
1	D	146	SER	3.6
1	D	85	LEU	3.6
1	A	196	LYS	3.4
1	C	248	SER	3.4
1	D	69	ASN	3.4
1	C	146	SER	3.3
1	D	169	LYS	3.3
1	B	147	ALA	3.3
1	D	176	SER	3.2
1	D	147	ALA	3.1
1	C	245	ASP	3.1
1	D	175	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	247	LEU	3.1
1	A	169	LYS	3.0
1	C	68	ASP	3.0
1	D	182	LYS	3.0
1	D	92	ASN	3.0
1	B	63	SER	2.9
1	C	197	ASP	2.8
1	C	182	LYS	2.8
1	C	191	PHE	2.8
1	C	149	ALA	2.8
1	A	63	SER	2.8
1	C	196	LYS	2.8
1	C	188	GLU	2.7
1	D	248	SER	2.6
1	D	68	ASP	2.6
1	C	103	LEU	2.5
1	A	150	VAL	2.5
1	D	201	LYS	2.5
1	D	93	GLU	2.5
1	B	196	LYS	2.5
1	C	147	ALA	2.5
1	D	242	LYS	2.5
1	C	246	GLU	2.4
1	B	170	GLY	2.4
1	C	186	ILE	2.3
1	D	191	PHE	2.3
1	D	186	ILE	2.3
1	A	156	GLU	2.3
1	A	148	LEU	2.3
1	A	149	ALA	2.3
1	B	94	ASN	2.2
1	B	148	LEU	2.2
1	C	170	GLY	2.2
1	C	189	ASP	2.2
1	C	187	ASP	2.2
1	C	247	LEU	2.1
1	C	96	SER	2.1
1	D	76	SER	2.1
1	D	72	LYS	2.1
1	C	148	LEU	2.1
1	D	70	VAL	2.1
1	D	189	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	201	LYS	2.1
1	C	69	ASN	2.1
1	D	144	ALA	2.1
1	B	150	VAL	2.1
1	D	246	GLU	2.0
1	C	143	ALA	2.0
1	C	100	VAL	2.0
1	D	121	ILE	2.0
1	B	144	ALA	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.