



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2024 – 03:01 PM EDT

PDB ID : 4EXW  
Title : The structure of DdrB from Deinococcus: a new fold for single-stranded DNA binding proteins.  
Authors : Sugiman-Marangos, S.; Junop, M.S.  
Deposited on : 2012-05-01  
Resolution : 2.80 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

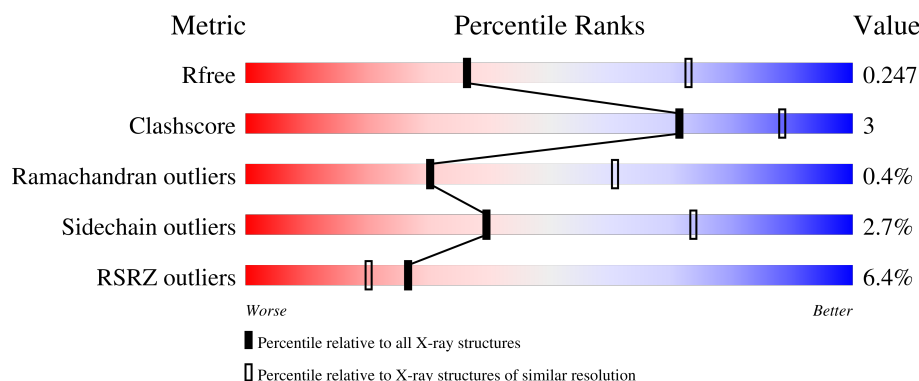
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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  $\geq 3$ , 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	184	<div> <div>64%</div> <div>7%</div> <div>29%</div> </div>
1	B	184	<div> <div>6%</div> <div>59%</div> <div>36%</div> </div>
1	C	184	<div> <div>5%</div> <div>61%</div> <div>33%</div> </div>
1	D	184	<div> <div>3%</div> <div>53%</div> <div>38%</div> </div>
1	E	184	<div> <div>5%</div> <div>60%</div> <div>36%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4603 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 Single-stranded DNA-binding protein DdrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	Se	0	0	0
			996	635	176	183	2			
1	B	117	Total	C	N	O	Se	0	0	0
			856	552	147	156	1			
1	C	124	Total	C	N	O	Se	0	0	0
			912	580	163	167	2			
1	D	115	Total	C	N	O	Se	0	0	0
			872	559	157	154	2			
1	E	117	Total	C	N	O	Se	0	0	0
			899	580	155	162	2			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q1J1N6
A	-4	ILE	-	expression tag	UNP Q1J1N6
A	-3	ASP	-	expression tag	UNP Q1J1N6
A	-2	PRO	-	expression tag	UNP Q1J1N6
A	-1	PHE	-	expression tag	UNP Q1J1N6
A	0	THR	-	expression tag	UNP Q1J1N6
B	-5	GLY	-	expression tag	UNP Q1J1N6
B	-4	ILE	-	expression tag	UNP Q1J1N6
B	-3	ASP	-	expression tag	UNP Q1J1N6
B	-2	PRO	-	expression tag	UNP Q1J1N6
B	-1	PHE	-	expression tag	UNP Q1J1N6
B	0	THR	-	expression tag	UNP Q1J1N6
C	-5	GLY	-	expression tag	UNP Q1J1N6
C	-4	ILE	-	expression tag	UNP Q1J1N6
C	-3	ASP	-	expression tag	UNP Q1J1N6
C	-2	PRO	-	expression tag	UNP Q1J1N6
C	-1	PHE	-	expression tag	UNP Q1J1N6
C	0	THR	-	expression tag	UNP Q1J1N6
D	-5	GLY	-	expression tag	UNP Q1J1N6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	ILE	-	expression tag	UNP Q1J1N6
D	-3	ASP	-	expression tag	UNP Q1J1N6
D	-2	PRO	-	expression tag	UNP Q1J1N6
D	-1	PHE	-	expression tag	UNP Q1J1N6
D	0	THR	-	expression tag	UNP Q1J1N6
E	-5	GLY	-	expression tag	UNP Q1J1N6
E	-4	ILE	-	expression tag	UNP Q1J1N6
E	-3	ASP	-	expression tag	UNP Q1J1N6
E	-2	PRO	-	expression tag	UNP Q1J1N6
E	-1	PHE	-	expression tag	UNP Q1J1N6
E	0	THR	-	expression tag	UNP Q1J1N6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	12	Total O 12 12	0	0
2	B	8	Total O 8 8	0	0
2	C	16	Total O 16 16	0	0
2	D	19	Total O 19 19	0	0
2	E	13	Total O 13 13	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.87Å 102.87Å 96.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.23 – 2.80 35.23 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (35.23-2.80) 98.4 (35.23-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.37 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.231 , 0.254 0.227 , 0.247	Depositor DCC
$R_{free}$ test set	1868 reflections (6.73%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.5	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 96.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,l 0.024 for h,-h-k,-l 0.013 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4603	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.22	0/1017	0.41	0/1376
1	B	0.24	0/876	0.42	0/1189
1	C	0.24	0/931	0.43	0/1261
1	D	0.23	0/890	0.42	0/1203
1	E	0.21	0/920	0.40	0/1244
All	All	0.23	0/4634	0.42	0/6273

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	996	0	937	7	0
1	B	856	0	754	3	0
1	C	912	0	801	7	0
1	D	872	0	803	10	0
1	E	899	0	836	5	0
2	A	12	0	0	0	0
2	B	8	0	0	0	0
2	C	16	0	0	2	0
2	D	19	0	0	0	0
2	E	13	0	0	0	0
All	All	4603	0	4131	28	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 (28) 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:C:39:GLY:O	2:C:213:HOH:O	2.00	0.78
1:C:37:THR:OG1	1:C:78:ARG:NH2	2.26	0.69
1:A:68:ASN:HB2	1:A:69:PRO:HD2	1.79	0.64
1:C:72:GLU:N	2:C:210:HOH:O	2.35	0.58
1:A:39:GLY:HA2	1:B:13:LYS:HE3	1.88	0.55
1:C:74:MSE:HE3	1:C:81:ALA:HB1	1.90	0.53
1:D:1:MSE:HE1	1:D:17:ASP:HB3	1.91	0.53
1:D:0:THR:HA	1:E:1:MSE:HE1	1.90	0.52
1:D:24:LEU:HD21	1:E:14:VAL:HG21	1.92	0.52
1:A:74:MSE:HE3	1:A:81:ALA:HB1	1.94	0.50
1:D:74:MSE:HE3	1:D:81:ALA:HB1	1.93	0.49
1:D:136:ARG:NH1	1:D:138:GLU:OE2	2.43	0.48
1:C:108:LYS:N	1:C:111:ASP:OD1	2.46	0.48
1:E:74:MSE:HE3	1:E:81:ALA:HB1	1.95	0.48
1:D:9:ASP:OD1	1:D:9:ASP:N	2.50	0.44
1:A:1:MSE:HE2	1:A:17:ASP:HB3	2.00	0.44
1:A:9:ASP:OD1	1:A:9:ASP:N	2.51	0.44
1:C:9:ASP:OD1	1:C:9:ASP:N	2.50	0.43
1:D:55:ASP:OD1	1:D:136:ARG:NH2	2.52	0.43
1:B:104:SER:HB3	1:B:127:THR:HA	1.99	0.43
1:C:107:ALA:HB1	1:C:111:ASP:OD1	2.19	0.43
1:D:137:GLN:OE1	1:D:139:ARG:NH1	2.52	0.43
1:D:77:HIS:O	1:D:78:ARG:HB2	2.19	0.42
1:D:139:ARG:NH2	1:E:9:ASP:OD2	2.51	0.42
1:B:111:ASP:HA	1:B:112:PRO:HD2	1.76	0.42
1:E:9:ASP:OD1	1:E:9:ASP:N	2.52	0.42
1:A:82:TYR:OH	1:A:105:ARG:NH1	2.53	0.41
1:A:102:LYS:HD2	1:A:130:ILE:HG12	2.02	0.41

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	124/184 (67%)	121 (98%)	3 (2%)	0	100	100
1	B	109/184 (59%)	102 (94%)	7 (6%)	0	100	100
1	C	114/184 (62%)	110 (96%)	3 (3%)	1 (1%)	14	42
1	D	107/184 (58%)	100 (94%)	6 (6%)	1 (1%)	14	42
1	E	109/184 (59%)	104 (95%)	5 (5%)	0	100	100
All	All	563/920 (61%)	537 (95%)	24 (4%)	2 (0%)	30	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	-1	PHE
1	D	78	ARG

### 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	95/143 (66%)	93 (98%)	2 (2%)	48	80
1	B	73/143 (51%)	69 (94%)	4 (6%)	18	47
1	C	79/143 (55%)	79 (100%)	0	100	100
1	D	79/143 (55%)	75 (95%)	4 (5%)	20	51
1	E	85/143 (59%)	84 (99%)	1 (1%)	67	89
All	All	411/715 (58%)	400 (97%)	11 (3%)	40	74

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	LYS
1	A	127	THR

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Mol	Chain	Res	Type
1	B	-1	PHE
1	B	33	ARG
1	B	104	SER
1	B	136	ARG
1	D	-1	PHE
1	D	64	ARG
1	D	84	ARG
1	D	105	ARG
1	E	78	ARG

Sometimes 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 oligosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	128/184 (69%)	0.01	2 (1%) 70 63	44, 81, 135, 176	0
1	B	116/184 (63%)	0.46	11 (9%) 15 12	48, 108, 165, 183	0
1	C	122/184 (66%)	0.31	10 (8%) 19 14	50, 85, 134, 206	0
1	D	113/184 (61%)	0.26	6 (5%) 33 26	44, 87, 137, 161	0
1	E	115/184 (62%)	0.28	9 (7%) 20 16	46, 98, 173, 192	0
All	All	594/920 (64%)	0.26	38 (6%) 27 20	44, 90, 156, 206	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	110	THR	5.1
1	C	124	GLU	4.0
1	D	67	THR	3.7
1	C	67	THR	3.3
1	C	-1	PHE	3.3
1	C	68	ASN	3.3
1	C	79	GLY	3.2
1	C	69	PRO	3.0
1	B	67	THR	2.9
1	C	125	TYR	2.9
1	D	0	THR	2.9
1	B	0	THR	2.8
1	B	48	PHE	2.8
1	E	-2	PRO	2.7
1	D	51	GLU	2.7
1	B	47	GLN	2.7
1	E	65	LYS	2.6
1	B	58	TRP	2.6
1	A	107	ALA	2.5
1	E	67	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	56	PHE	2.5
1	E	69	PRO	2.4
1	B	109	ASN	2.4
1	C	-2	PRO	2.4
1	E	98	PRO	2.4
1	B	129	ALA	2.4
1	E	144	GLY	2.3
1	E	73	GLU	2.3
1	D	68	ASN	2.3
1	E	88	GLU	2.3
1	B	51	GLU	2.2
1	A	89	ALA	2.2
1	C	104	SER	2.2
1	E	130	ILE	2.1
1	D	107	ALA	2.1
1	B	52	ASN	2.0
1	D	49	PRO	2.0
1	B	131	PHE	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 monosaccharides 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.