

# Full wwPDB X-ray Structure Validation Report (i)

#### Sep 11, 2023 – 11:56 PM EDT

:	4LJR
:	Structural insights into the unique single-stranded DNA binding mode of DNA
	processing protein A from Helicobacter pylori
:	Wang, W.
	2013-07-05
:	1.80  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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

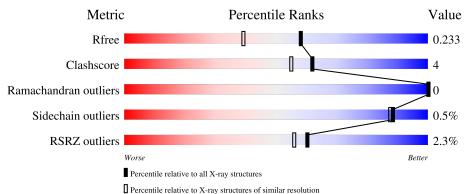
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.80 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	5950(1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 >=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 <=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	А	221	88%	8%	·
1	В	221	4% 86%	10%	·
2	С	35	9% 6% · 83%		
2	D	35	3% • 97%		_



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3845 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	213	Total	С	Ν	Ο	S	0	0	0
		213	1659	1063	282	308	6	0	0	0
1	р	012	Total	С	Ν	0	S	0	0	0
	I B	213	1659	1063	282	308	6	0		0

• Molecule 1 is a protein called DNA processing chain A.

Chain	Residue	Modelled	Actual	Comment	Reference
А	218	LEU	-	expression tag	UNP O25100
А	219	GLU	-	expression tag	UNP O25100
A	220	HIS	-	expression tag	UNP O25100
А	221	HIS	-	expression tag	UNP O25100
А	222	HIS	-	expression tag	UNP O25100
A	223	HIS	-	expression tag	UNP O25100
А	224	HIS	-	expression tag	UNP O25100
А	225	HIS	-	expression tag	UNP O25100
В	218	LEU	-	expression tag	UNP O25100
В	219	GLU	-	expression tag	UNP O25100
В	220	HIS	-	expression tag	UNP O25100
В	221	HIS	-	expression tag	UNP O25100
В	222	HIS	-	expression tag	UNP O25100
В	223	HIS	-	expression tag	UNP O25100
В	224	HIS	-	expression tag	UNP O25100
В	225	HIS	-	expression tag	UNP O25100

There are 16 discrepancies between the modelled and reference sequences:

• Molecule 2 is a DNA chain called single-stranded DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	С	C 6	Total	С	Ν	0	Р	0	0	0
2			121	60	12	43	6	0		
0	а	1	Total	С	Ν	Ο	Р	0	0	0
	2 D	1	21	10	2	8	1	0	0	0





• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	193	Total O 193 193	0	0
3	В	177	Total O 177 177	0	0
3	С	15	Total O 15 15	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

Chain A:	88%	8% •
45 24 16 124 124 187 187 187 187 187 187 186 186 186 186 186 186 186 165 161 161 161 161 161 161 161 161 16	ALTO Q173 P178 P178 P178 A185 N206 N206 CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	214
• Molecule 1: DNA processing chain	n A	
Chain B:	86%	10% •
M5 K30 K45 V46 K45 K57 K59 K59 K59 K59 K59 K59 L69 L69 L99 L99 H113	Li26 Li26 S151 K162 S167 S167 N187 N187 N187 N187 N209 F208 F213 T211 C213 F214 C208 F213 F214 C208 F214 F214 F214 F214 F214 F214 F214 F214	M216 D217 LEU GLU HIS HIS HIS HIS HIS
• Molecule 2: single-stranded DNA		
Chain C: 9% 6% ·	83%	
2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2		
• Molecule 2: single-stranded DNA		
Chain D: •	97%	
• •		

• Molecule 1: DNA processing chain A



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	37.40Å 40.51Å 154.68Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $92.18^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	33.16 - 1.80	Depositor
Resolution (A)	36.01 - 1.80	EDS
% Data completeness	80.5 (33.16-1.80)	Depositor
(in resolution range)	83.2 (36.01-1.80)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.56 (at 1.81 \text{\AA})$	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
D D	0.194 , $0.237$	Depositor
$R, R_{free}$	0.193 , $0.233$	DCC
$R_{free}$ test set	1816 reflections $(5.02\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	22.6	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.35 , $49.1$	EDS
L-test for $twinning^2$	$<  L  > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3845	wwPDB-VP
Average B, all atoms $(Å^2)$	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.07% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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	Boi	nd lengths	Bond angles		
MOI	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.27	0/1688	0.46	0/2284	
1	В	0.26	0/1688	0.45	0/2284	
2	С	1.07	1/132~(0.8%)	1.49	1/200~(0.5%)	
2	D	2.36	1/22~(4.5%)	1.35	0/30	
All	All	0.38	2/3530~(0.1%)	0.55	1/4798~(0.0%)	

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
2	D	5	DT	OP3-P	-10.82	1.48	1.61
2	С	1	DT	OP3-P	-10.65	1.48	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	2	DT	O4'-C4'-C3'	-8.21	101.08	106.00

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	А	1659	0	1728	13	0
1	В	1659	0	1728	16	0
2	С	121	0	73	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	21	0	13	0	0
3	А	193	0	0	6	0
3	В	177	0	0	2	0
3	С	15	0	0	0	0
All	All	3845	0	3542	31	0

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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 (31) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
1 D 010 ACN ()		distance (Å)	overlap (Å)
1:B:212:ASN:O	1:B:216:LYS:HD3	1.89	0.72
2:C:2:DT:H5'	2:C:2:DT:H6	1.56	0.70
1:A:55:THR:H	1:A:158:GLN:HE22	1.43	0.64
2:C:2:DT:H6	2:C:2:DT:C5'	2.14	0.61
1:A:85:ASP:OD2	3:A:423:HOH:O	2.16	0.58
1:B:167:SER:HB2	2:C:6:DT:H4'	1.86	0.58
2:C:2:DT:H5'	2:C:2:DT:C6	2.39	0.58
1:A:30:LYS:NZ	3:A:400:HOH:O	2.39	0.56
1:A:173:GLN:NE2	3:A:405:HOH:O	2.28	0.56
1:A:170:ARG:HG3	3:A:480:HOH:O	2.06	0.56
1:A:24:LEU:HD21	1:A:149:ALA:HB2	1.89	0.55
1:A:59:LYS:HG3	1:A:87:ILE:HD13	1.89	0.54
1:B:113:HIS:NE2	3:B:451:HOH:O	2.33	0.54
1:B:65:LEU:HD23	1:B:207:ILE:HG23	1.90	0.53
1:B:72:ASN:OD1	1:B:215:LEU:HD11	2.08	0.52
1:A:185:ARG:HD3	1:B:57:TYR:CD1	2.45	0.52
1:A:161:LEU:O	3:A:478:HOH:O	2.19	0.49
1:B:186:LEU:O	1:B:187:ASN:HB2	2.13	0.47
2:C:2:DT:C5'	2:C:2:DT:C6	2.96	0.46
1:A:185:ARG:HB3	1:B:57:TYR:CE1	2.52	0.45
1:B:47:ALA:HB2	1:B:151:SER:OG	2.17	0.45
1:B:99:LEU:HD13	1:B:126:LEU:HB2	2.00	0.43
1:B:45:LYS:HG2	1:B:75:VAL:CG1	2.48	0.43
1:A:18:PRO:HB3	3:A:343:HOH:O	2.19	0.42
1:B:30:LYS:NZ	3:B:396:HOH:O	2.51	0.42
1:A:206:ASN:HB3	1:A:209:ASN:HB2	2.02	0.42
1:B:69:LEU:HD23	1:B:69:LEU:HA	1.90	0.41
1:A:152:ASP:O	1:A:178:PRO:HD2	2.21	0.41
1:B:47:ALA:HA	1:B:77:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:LYS:O	1:B:162:LYS:HG3	2.20	0.41
1:B:59:LYS:HG3	1:B:87:ILE:HD13	2.03	0.40

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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	Perce	ntiles
1	А	211/221 (96%)	207~(98%)	4(2%)	0	100	100
1	В	211/221~(96%)	204 (97%)	7 (3%)	0	100	100
All	All	422/442~(96%)	411 (97%)	11 (3%)	0	100	100

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	186/194~(96%)	185 (100%)	1 (0%)	88 87
1	В	186/194~(96%)	185 (100%)	1 (0%)	88 87
All	All	372/388~(96%)	370~(100%)	2~(0%)	88 87

All (2) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	143	ARG
1	В	216	LYS

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

Mol	Chain	Res	Type
1	А	158	GLN
1	В	208	GLN

#### 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 monosaccharides 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 (i)

### 6.1 Protein, DNA and RNA chains (i)

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,  $95^{th}$  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	$OWAB(A^2)$	$\mathbf{Q}{<}0.9$
1	А	213/221~(96%)	-0.31	1 (0%) 91 89	12, 25, 48, 76	0
1	В	213/221~(96%)	-0.02	8 (3%) 40 35	15, 30, 54, 83	0
2	С	6/35~(17%)	-0.25	0 100 100	29, 33, 49, 88	0
2	D	1/35~(2%)	2.55	1 (100%) 0 0	98, 98, 98, 98	0
All	All	433/512~(84%)	-0.16	10 (2%) 60 56	12, 28, 52, 98	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	214	LEU	4.1
1	В	216	LYS	3.7
1	В	217	ASP	3.1
1	В	212	ASN	3.1
1	В	213	THR	3.0
1	А	215	LEU	2.8
2	D	5	DT	2.6
1	В	215	LEU	2.3
1	В	208	GLN	2.3
1	В	210	PHE	2.3

### 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.

