



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 08:21 PM JST

PDB ID : 8IKR  
Title : Crystal structure of DpaA  
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Deposited on : 2023-03-01  
Resolution : 2.90 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  
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

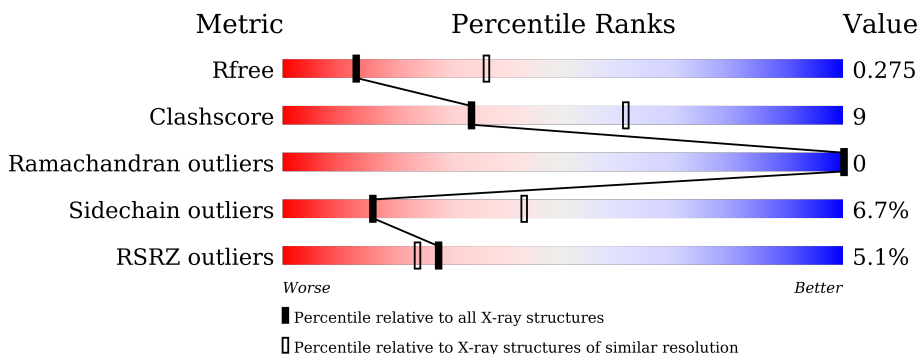
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	236	 58% 21% 18%
1	B	236	 8% 61% 13% 25%

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3033 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 YkuD domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	194	1585	1020	268	288	9	0	0	0
1	B	177	1448	931	243	265	9	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	initiating methionine	UNP V0UTF7
A	247	LEU	-	expression tag	UNP V0UTF7
A	248	GLU	-	expression tag	UNP V0UTF7
A	249	HIS	-	expression tag	UNP V0UTF7
A	250	HIS	-	expression tag	UNP V0UTF7
A	251	HIS	-	expression tag	UNP V0UTF7
A	252	HIS	-	expression tag	UNP V0UTF7
A	253	HIS	-	expression tag	UNP V0UTF7
A	254	HIS	-	expression tag	UNP V0UTF7
B	19	MET	-	initiating methionine	UNP V0UTF7
B	247	LEU	-	expression tag	UNP V0UTF7
B	248	GLU	-	expression tag	UNP V0UTF7
B	249	HIS	-	expression tag	UNP V0UTF7
B	250	HIS	-	expression tag	UNP V0UTF7
B	251	HIS	-	expression tag	UNP V0UTF7
B	252	HIS	-	expression tag	UNP V0UTF7
B	253	HIS	-	expression tag	UNP V0UTF7
B	254	HIS	-	expression tag	UNP V0UTF7



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.88Å 86.88Å 150.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.47 – 2.90 28.47 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (28.47-2.90) 99.7 (28.47-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.90Å)	Xtrriage
Refinement program	REFMAC 5.8.0405	Depositor
R, $R_{free}$	0.215 , 0.274 0.220 , 0.275	Depositor DCC
$R_{free}$ test set	661 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	84.6	Xtrriage
Anisotropy	0.446	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 67.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3033	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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	0.58	1/1629 (0.1%)	1.05	1/2195 (0.0%)
1	B	0.52	0/1477	0.97	2/1974 (0.1%)
All	All	0.55	1/3106 (0.0%)	1.01	3/4169 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	GLU	CD-OE2	5.38	1.31	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	GLN	CB-CA-C	6.42	123.25	110.40
1	A	102	GLN	N-CA-CB	5.40	120.31	110.60
1	B	85	ARG	NE-CZ-NH2	-5.09	117.76	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ARG	Sidechain
1	A	209	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	79	GLY	Peptide
1	B	100	ARG	Sidechain
1	B	133	MET	Peptide

## 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	1585	0	1546	35	0
1	B	1448	0	1408	19	0
All	All	3033	0	2954	51	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 9.

All (51) 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:105:PRO:C	1:B:107:SER:N	2.15	1.00
1:B:105:PRO:O	1:B:107:SER:N	1.94	1.00
1:A:37:GLN:N	1:A:37:GLN:OE1	2.06	0.88
1:A:38:GLN:HA	1:B:104:LYS:HD3	1.59	0.85
1:A:37:GLN:O	1:B:104:LYS:NZ	2.11	0.84
1:B:45:TYR:OH	1:B:172:SER:OG	1.99	0.79
1:B:175:PRO:HG3	1:B:191:PHE:CZ	2.18	0.79
1:B:105:PRO:C	1:B:107:SER:OG	2.38	0.62
1:B:175:PRO:HG3	1:B:191:PHE:HZ	1.63	0.62
1:A:106:ASP:HA	1:A:109:TYR:O	1.99	0.61
1:A:117:PHE:HB3	1:A:132:LEU:HD12	1.81	0.60
1:A:111:LYS:NZ	1:A:152:ASP:OD1	2.30	0.60
1:B:108:ARG:HH11	1:B:108:ARG:HG3	1.66	0.58
1:A:180:ASP:OD1	1:A:180:ASP:N	2.33	0.58
1:A:105:PRO:HB2	1:A:108:ARG:HH21	1.69	0.57
1:A:40:MET:SD	1:A:156:GLN:HG3	2.44	0.57
1:B:100:ARG:HA	1:B:102:GLN:NE2	2.20	0.57
1:A:105:PRO:C	1:A:107:SER:N	2.60	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:LYS:N	1:B:200:PRO:HD2	2.23	0.54
1:A:102:GLN:O	1:A:103:LEU:C	2.46	0.54
1:B:180:ASP:N	1:B:180:ASP:OD1	2.43	0.52
1:A:184:LYS:HG2	1:A:187:LYS:HE2	1.92	0.51
1:B:101:ASN:HB2	1:B:114:ASN:HB3	1.93	0.50
1:B:180:ASP:HA	1:B:183:MET:HB2	1.94	0.49
1:A:191:PHE:O	1:A:192:LYS:C	2.51	0.49
1:A:47:GLN:HG2	1:A:172:SER:HB2	1.95	0.49
1:A:117:PHE:CG	1:A:132:LEU:HD12	2.47	0.49
1:A:199:LYS:N	1:A:200:PRO:CD	2.77	0.48
1:A:217:VAL:HG12	1:A:218:ASN:N	2.30	0.47
1:A:36:LYS:C	1:A:37:GLN:OE1	2.52	0.47
1:A:117:PHE:CD1	1:A:132:LEU:HD12	2.49	0.47
1:B:41:GLY:HA2	1:B:160:GLY:C	2.35	0.47
1:A:117:PHE:CB	1:A:132:LEU:HD12	2.46	0.46
1:A:184:LYS:HG2	1:A:187:LYS:CE	2.45	0.46
1:A:102:GLN:HE21	1:A:102:GLN:HB3	1.48	0.46
1:A:101:ASN:HB3	1:A:114:ASN:HB3	1.98	0.46
1:B:98:VAL:HG22	1:B:169:VAL:O	2.16	0.45
1:A:40:MET:HE2	1:A:40:MET:HB2	1.91	0.45
1:B:84:GLN:O	1:B:127:TYR:HA	2.17	0.44
1:A:104:LYS:HD2	1:A:106:ASP:CG	2.38	0.44
1:A:41:GLY:HA2	1:A:160:GLY:C	2.38	0.44
1:A:121:TYR:HB2	1:A:221:TYR:CE1	2.53	0.43
1:A:58:TYR:HB3	1:A:65:TYR:HB3	2.00	0.43
1:B:75:LYS:HB2	1:B:145:ALA:HB3	2.01	0.42
1:A:136:GLY:O	1:A:138:CYS:N	2.53	0.41
1:A:180:ASP:HA	1:A:183:MET:HB2	2.03	0.41
1:A:187:LYS:O	1:A:188:TYR:HB2	2.20	0.41
1:A:119:ASN:O	1:A:123:ARG:HG3	2.20	0.41
1:A:105:PRO:C	1:A:107:SER:H	2.22	0.41
1:A:163:VAL:HG23	1:B:163:VAL:HG23	2.03	0.40
1:A:194:PHE:O	1:A:197:GLN:HB2	2.20	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	192/236 (81%)	169 (88%)	23 (12%)	0	100	100
1	B	159/236 (67%)	143 (90%)	16 (10%)	0	100	100
All	All	351/472 (74%)	312 (89%)	39 (11%)	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 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	171/209 (82%)	158 (92%)	13 (8%)	13	36
1	B	157/209 (75%)	148 (94%)	9 (6%)	20	51
All	All	328/418 (78%)	306 (93%)	22 (7%)	16	43

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ASP
1	A	101	ASN
1	A	102	GLN
1	A	103	LEU
1	A	107	SER
1	A	128	GLU
1	A	130	LYS
1	A	139	VAL

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Mol	Chain	Res	Type
1	A	141	ILE
1	A	166	GLN
1	A	180	ASP
1	A	192	LYS
1	A	215	SER
1	B	36	LYS
1	B	40	MET
1	B	65	TYR
1	B	102	GLN
1	B	103	LEU
1	B	135	HIS
1	B	162	LEU
1	B	180	ASP
1	B	191	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	101	ASN
1	A	102	GLN
1	A	156	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<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	194/236 (82%)	-0.32	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	63, 81, 114, 146	0
1	B	177/236 (75%)	0.37	19 (10%) <span style="border: 1px solid red; padding: 2px;">6</span> <span style="border: 1px solid red; padding: 2px;">4</span>	90, 140, 193, 202	0
All	All	371/472 (78%)	0.01	19 (5%) <span style="border: 1px solid red; padding: 2px;">28</span> <span style="border: 1px solid red; padding: 2px;">24</span>	63, 100, 186, 202	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	188	TYR	4.3
1	B	218	ASN	3.1
1	B	184	LYS	3.0
1	B	116	GLY	3.0
1	B	117	PHE	2.9
1	B	196	GLU	2.9
1	B	221	TYR	2.9
1	B	194	PHE	2.8
1	B	187	LYS	2.7
1	B	205	PHE	2.7
1	B	165	GLY	2.6
1	B	123	ARG	2.5
1	B	63	GLU	2.4
1	B	182	ASN	2.3
1	B	215	SER	2.2
1	B	203	ASP	2.2
1	B	118	PRO	2.1
1	B	87	GLY	2.1
1	B	207	GLN	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.