



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 14, 2016 – 12:38 AM EST

PDB ID : 4H6Y  
Title : Crystal structure of the DH-PH-PH domain of FARP1  
Authors : He, X.; Zhang, X.  
Deposited on : 2012-09-19  
Resolution : 4.09 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

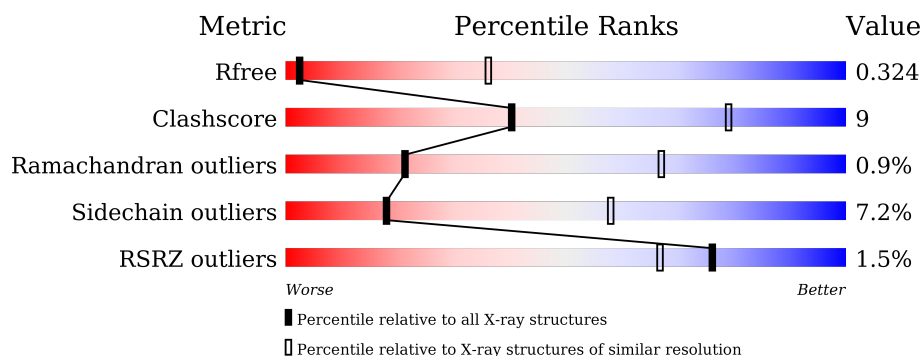
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.09 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))
$R_{free}$	91344	1018 (4.60-3.60)
Clashscore	102246	1117 (4.60-3.60)
Ramachandran outliers	100387	1063 (4.60-3.60)
Sidechain outliers	100360	1049 (4.60-3.60)
RSRZ outliers	91569	1022 (4.60-3.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	501	<div> <div>2%</div> <div>61%</div> <div>17%</div> <div>•</div> <div>20%</div> </div>
1	B	501	<div> <div>%</div> <div>62%</div> <div>18%</div> <div>•</div> <div>19%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5955 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 FERM, RhoGEF and pleckstrin domain-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3005	1949	499	537	20			
1	B	408	Total	C	N	O	S	0	0	0
			2950	1903	496	532	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	535	GLY	-	EXPRESSION TAG	UNP Q9Y4F1
A	536	PRO	-	EXPRESSION TAG	UNP Q9Y4F1
A	537	HIS	-	EXPRESSION TAG	UNP Q9Y4F1
A	538	MET	-	EXPRESSION TAG	UNP Q9Y4F1
B	535	GLY	-	EXPRESSION TAG	UNP Q9Y4F1
B	536	PRO	-	EXPRESSION TAG	UNP Q9Y4F1
B	537	HIS	-	EXPRESSION TAG	UNP Q9Y4F1
B	538	MET	-	EXPRESSION TAG	UNP Q9Y4F1



D969	N970	L976	L979	I985	P986	SER	GLU	SER	GLU	ASN	ILE	GLN	K994	F998	F1009	Y1015	T1016	F1017	E1018	R1019	W1020	M1021	T1028	S1029	SER	ALA	SER	ARG	PRO	HIS
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.24Å 142.24Å 105.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.57 – 4.09 42.57 – 4.09	Depositor EDS
% Data completeness (in resolution range)	96.0 (42.57-4.09) 95.8 (42.57-4.09)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.60 (at 4.13Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.289 , 0.317 0.285 , 0.324	Depositor DCC
$R_{free}$ test set	942 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	145.9	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 155.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l 0.448 for h,-h-k,-l 0.033 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5955	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	176.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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	0.26	0/3070	0.44	1/4178 (0.0%)
1	B	0.26	0/3013	0.43	2/4112 (0.0%)
All	All	0.26	0/6083	0.44	3/8290 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	822	PRO	N-CA-CB	6.13	110.66	103.30
1	B	986	PRO	N-CA-CB	5.83	110.29	103.30
1	A	704	PRO	N-CA-CB	5.62	110.04	103.30

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	3005	0	2704	51	0
1	B	2950	0	2564	47	0
All	All	5955	0	5268	98	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.

The worst 5 of 98 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:961:LEU:HB2	1:B:976:LEU:HB3	1.70	0.74
1:A:760:PHE:HZ	1:A:763:LEU:HD12	1.53	0.73
1:B:810:MET:HB2	1:B:829:GLY:HA2	1.73	0.70
1:A:631:ILE:HD12	1:A:720:ILE:HD11	1.72	0.70
1:A:765:SER:HB3	1:A:919:ASN:HA	1.74	0.69

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	384/501 (77%)	349 (91%)	32 (8%)	3 (1%)	24	69
1	B	390/501 (78%)	357 (92%)	29 (7%)	4 (1%)	19	65
All	All	774/1002 (77%)	706 (91%)	61 (8%)	7 (1%)	21	67

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	767	SER
1	B	807	LEU
1	A	807	LEU
1	A	1003	LYS
1	B	1028	THR

### 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	282/449 (63%)	258 (92%)	24 (8%)	13	51
1	B	263/449 (59%)	248 (94%)	15 (6%)	25	65
All	All	545/898 (61%)	506 (93%)	39 (7%)	18	58

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	911	MET
1	A	952	LEU
1	B	969	ASP
1	A	923	SER
1	A	943	PHE

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 ⓘ

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	402/501 (80%)	-0.02	8 (1%) 68 58	114, 173, 226, 264	0
1	B	408/501 (81%)	-0.07	4 (0%) 84 77	108, 172, 231, 277	0
All	All	810/1002 (80%)	-0.05	12 (1%) 76 67	108, 172, 229, 277	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	588	PHE	2.3
1	A	685	PRO	2.3
1	A	626	VAL	2.2
1	A	827	LEU	2.2
1	A	648	LEU	2.2

### 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.