



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 2QFI  
Title : Structure of the zinc transporter YiiP  
Authors : Lu, M.  
Deposited on : 2007-06-27  
Resolution : 3.80 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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

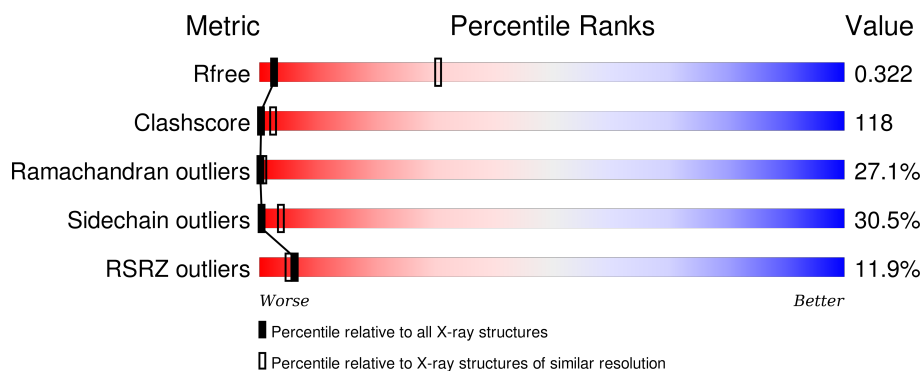
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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))
$R_{free}$	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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	300	
1	B	300	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4417 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 Ferrous-iron efflux pump fieF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2205	1419	378	397	11			
1	B	286	Total	C	N	O	S	0	0	0
			2205	1419	378	397	11			

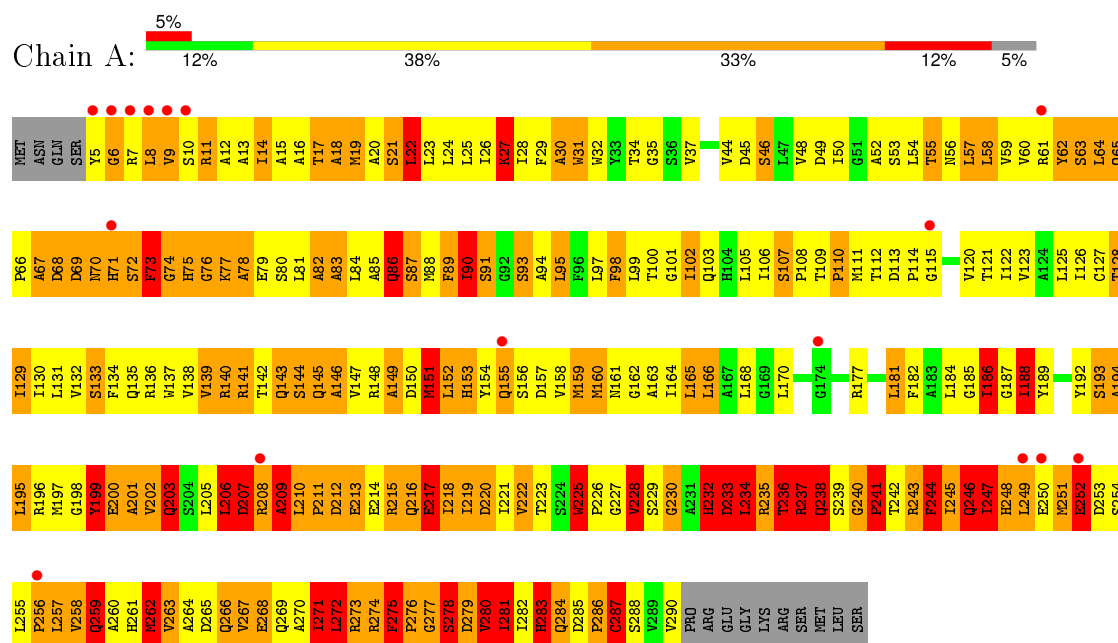
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Zn	0	0
			3	3		
2	A	4	Total	Zn	0	0
			4	4		

### 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 errors 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: Ferrous-iron efflux pump fieF



I245	Q246	I247	H248	L249	E250	H251	E252	D253	S254	L255	P256	L257	V258	Q259	A260	H261	M262	V263	A264	D265	Q266	V267	E268	Q269	A270	I271	L272	R273	R274	F275	P276	G277	S278	D279	V280	I281	L282	H283	Q284	D285	P286	C287	S288	V289	V290	PRO	ARG	GLU	GLY	LYS	ARG	SER	MET	LEU	SER
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.66Å 110.84Å 130.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.80 39.29 – 3.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (12.00-3.80) 97.4 (39.29-3.79)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 3.76Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.322 , 0.329 0.328 , 0.322	Depositor DCC
$R_{free}$ test set	742 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	118.0	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.16 , 155.7	EDS
Estimated twinning fraction	0.086 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	1 of 15522 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	4417	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	200.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	1.41	25/2252 (1.1%)	1.39	37/3069 (1.2%)
1	B	1.07	9/2252 (0.4%)	1.22	18/3069 (0.6%)
All	All	1.25	34/4504 (0.8%)	1.31	55/6138 (0.9%)

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	24
1	B	0	23
All	All	0	47

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	245	ILE	CA-CB	8.52	1.74	1.54
1	A	279	ASP	CB-CG	7.99	1.68	1.51
1	A	247	ILE	CA-CB	7.64	1.72	1.54
1	B	247	ILE	CA-CB	7.59	1.72	1.54
1	A	268	GLU	CG-CD	7.35	1.62	1.51

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	ASP	N-CA-C	8.50	133.95	111.00
1	B	279	ASP	CB-CG-OD1	7.66	125.19	118.30
1	A	247	ILE	N-CA-CB	7.59	128.26	110.80
1	A	249	LEU	CA-CB-CG	7.50	132.56	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	ASP	N-CA-C	7.44	131.09	111.00

There are no chirality outliers.

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	27	LYS	Peptide
1	A	6	GLY	Peptide
1	A	63	SER	Peptide
1	A	76	GLY	Peptide
1	A	97	LEU	Peptide

## 5.2 Too-close contacts

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	2205	0	2239	542	4
1	B	2205	0	2239	514	0
2	A	4	0	0	0	2
2	B	3	0	0	0	0
All	All	4417	0	4478	1052	4

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 118.

The worst 5 of 1052 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:232:HIS:CE1	1:B:245:ILE:HG21	1.36	1.61
1:B:245:ILE:CB	1:B:245:ILE:CA	1.74	1.56
1:B:232:HIS:CE1	1:B:245:ILE:CG2	1.96	1.49
1:B:232:HIS:NE2	1:B:245:ILE:CG2	1.79	1.41
1:B:232:HIS:NE2	1:B:245:ILE:HD12	1.47	1.30

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:HIS:NE2	2:A:306:ZN:ZN[4_556]	1.49	0.71
1:A:68:ASP:N	2:A:303:ZN:ZN[4_556]	1.54	0.66
1:A:261:HIS:CE1	1:A:285:ASP:OD1[4_556]	1.56	0.64
1:A:261:HIS:ND1	1:A:285:ASP:OD1[4_556]	2.09	0.11

## 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	284/300 (95%)	133 (47%)	76 (27%)	75 (26%)	0	1
1	B	284/300 (95%)	129 (45%)	76 (27%)	79 (28%)	0	0
All	All	568/600 (95%)	262 (46%)	152 (27%)	154 (27%)	0	1

5 of 154 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ALA
1	A	21	SER
1	A	55	THR
1	A	67	ALA
1	A	69	ASP

### 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	236/249 (95%)	163 (69%)	73 (31%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	236/249 (95%)	165 (70%)	71 (30%)	0 4
All	All	472/498 (95%)	328 (70%)	144 (30%)	0 4

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	278	SER
1	B	27	LYS
1	B	263	VAL
1	A	281	ILE
1	B	7	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	GLN
1	B	65	GLN
1	B	266	GLN
1	A	284	GLN
1	B	70	ASN

### 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](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	286/300 (95%)	0.10	16 (5%) 28 18	34, 112, 307, 364	0
1	B	286/300 (95%)	0.79	52 (18%) 2 1	48, 212, 575, 683	0
All	All	572/600 (95%)	0.45	68 (11%) 6 5	34, 151, 522, 683	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	42	ALA	15.8
1	B	43	LEU	12.7
1	B	169	GLY	10.2
1	B	167	ALA	9.8
1	B	168	LEU	9.7

### 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	B	304	1/1	0.97	0.14	-0.84	8,8,8,8	0
2	ZN	B	305	1/1	0.96	0.09	-0.96	77,77,77,77	0
2	ZN	A	302	1/1	0.95	0.14	-1.62	28,28,28,28	0
2	ZN	A	303	1/1	0.98	0.02	-2.46	26,26,26,26	0
2	ZN	A	306	1/1	0.97	0.20	-	28,28,28,28	0
2	ZN	A	307	1/1	0.96	0.07	-	109,109,109,109	0
2	ZN	B	301	1/1	0.96	0.23	-	25,25,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.