



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 11:19 am GMT

PDB ID : 3FIP  
Title : Crystal structure of Usher PapC translocation pore  
Authors : Huang, Y.; Deisenhofer, J.  
Deposited on : 2008-12-12  
Resolution : 3.15 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

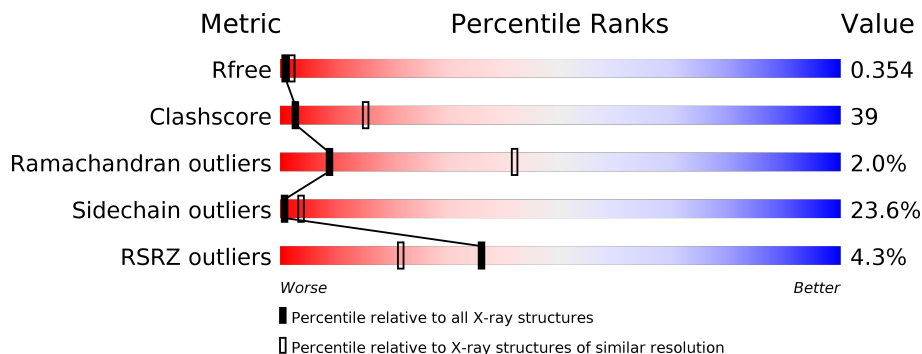
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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))
$R_{free}$	100719	1259 (3.20-3.12)
Clashscore	112137	1397 (3.20-3.12)
Ramachandran outliers	110173	1368 (3.20-3.12)
Sidechain outliers	110143	1367 (3.20-3.12)
RSRZ outliers	101464	1264 (3.20-3.12)

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	493	
1	B	493	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6295 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 Outer membrane usher protein papC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	14	0	0
			3387	2115	605	661	6			
1	B	384	Total	C	N	O	S	4	0	0
			2908	1817	516	569	6			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	624	SER	-	EXPRESSION TAG	UNP P07110
A	625	PHE	-	EXPRESSION TAG	UNP P07110
A	626	GLY	-	EXPRESSION TAG	UNP P07110
A	627	VAL	-	EXPRESSION TAG	UNP P07110
A	628	SER	-	EXPRESSION TAG	UNP P07110
A	629	ALA	-	EXPRESSION TAG	UNP P07110
A	630	SER	-	EXPRESSION TAG	UNP P07110
A	631	GLY	-	EXPRESSION TAG	UNP P07110
A	632	GLY	-	EXPRESSION TAG	UNP P07110
A	633	ALA	-	EXPRESSION TAG	UNP P07110
A	634	THR	-	EXPRESSION TAG	UNP P07110
A	635	ILE	-	EXPRESSION TAG	UNP P07110
A	636	THR	-	EXPRESSION TAG	UNP P07110
B	624	SER	-	EXPRESSION TAG	UNP P07110
B	625	PHE	-	EXPRESSION TAG	UNP P07110
B	626	GLY	-	EXPRESSION TAG	UNP P07110
B	627	VAL	-	EXPRESSION TAG	UNP P07110
B	628	SER	-	EXPRESSION TAG	UNP P07110
B	629	ALA	-	EXPRESSION TAG	UNP P07110
B	630	SER	-	EXPRESSION TAG	UNP P07110
B	631	GLY	-	EXPRESSION TAG	UNP P07110
B	632	GLY	-	EXPRESSION TAG	UNP P07110
B	633	ALA	-	EXPRESSION TAG	UNP P07110
B	634	THR	-	EXPRESSION TAG	UNP P07110
B	635	ILE	-	EXPRESSION TAG	UNP P07110

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Chain	Residue	Modelled	Actual	Comment	Reference
B	636	THR	-	EXPRESSION TAG	UNP P07110



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## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.04Å 120.04Å 354.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.68 – 3.15 49.68 – 3.15	Depositor EDS
% Data completeness (in resolution range)	96.2 (49.68-3.15) 98.0 (49.68-3.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.82 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.285 , 0.359 0.284 , 0.354	Depositor DCC
$R_{free}$ test set	1150 reflections (5.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	115.3	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 106.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	6295	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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

### 5.1 Standard geometry

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	0.59	1/3450 (0.0%)	0.83	14/4668 (0.3%)
1	B	0.44	0/2946	0.83	13/3971 (0.3%)
All	All	0.52	1/6396 (0.0%)	0.83	27/8639 (0.3%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	485	SER	CB-OG	15.64	1.62	1.42

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	317	LYS	N-CA-C	-14.12	72.88	111.00
1	B	317	LYS	CB-CA-C	13.85	138.10	110.40
1	A	190	SER	CB-CA-C	-11.41	88.42	110.10
1	B	579	SER	CB-CA-C	-11.02	89.16	110.10
1	B	318	LYS	N-CA-C	-10.61	82.35	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	367	SER	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	3387	0	3176	239	0
1	B	2908	0	2695	238	0
All	All	6295	0	5871	476	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 39.

The worst 5 of 476 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:267:ILE:HG22	1:B:268:ALA:H	1.10	1.08
1:A:332:ARG:HG2	1:A:332:ARG:HH11	1.14	1.07
1:B:614:ASN:HB3	1:B:626:GLY:HA3	1.32	1.04
1:A:570:THR:HB	1:A:581:SER:HB3	1.35	1.03
1:A:161:GLN:H	1:A:161:GLN:HE21	1.08	1.00

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	408/493 (83%)	349 (86%)	53 (13%)	6 (2%)	12	49
1	B	338/493 (69%)	262 (78%)	67 (20%)	9 (3%)	6	33
All	All	746/986 (76%)	611 (82%)	120 (16%)	15 (2%)	9	42

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	329	TYR
1	B	457	ALA
1	A	333	PRO
1	A	451	MET
1	B	221	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	351/405 (87%)	273 (78%)	78 (22%)	1	5
1	B	292/405 (72%)	218 (75%)	74 (25%)	0	2
All	All	643/810 (79%)	491 (76%)	152 (24%)	1	4

5 of 152 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	581	SER
1	B	201	THR
1	B	542	ARG
1	A	595	GLN
1	A	636	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	565	ASN
1	A	597	GLN
1	B	583	ASN
1	A	587	ASN
1	A	595	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

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	436/493 (88%)	0.17	11 (2%)	58 42	86, 114, 136, 158	11 (2%)
1	B	384/493 (77%)	0.26	24 (6%)	21 11	97, 126, 155, 171	4 (1%)
All	All	820/986 (83%)	0.21	35 (4%)	36 21	86, 120, 150, 171	15 (1%)

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	146	LEU	6.1
1	B	324	THR	5.1
1	A	503	TYR	5.1
1	B	325	ALA	4.8
1	B	361	GLU	3.5

### 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.