



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 12:55 am BST

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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	:	2.11
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)	:	2.11

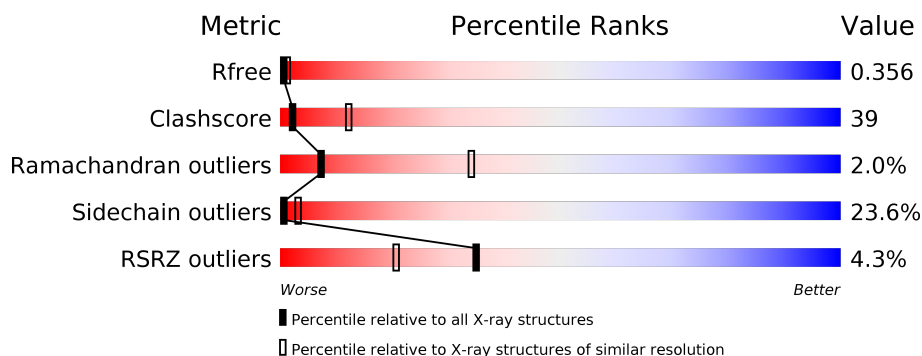
1 Overall quality at a glance ⓘ

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}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (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 ≥ 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	493	<div> <div>2%</div> <div>37%</div> <div>40%</div> <div>12%</div> <div>12%</div> </div>
1	B	493	<div> <div>5%</div> <div>29%</div> <div>37%</div> <div>11%</div> <div>22%</div> </div>

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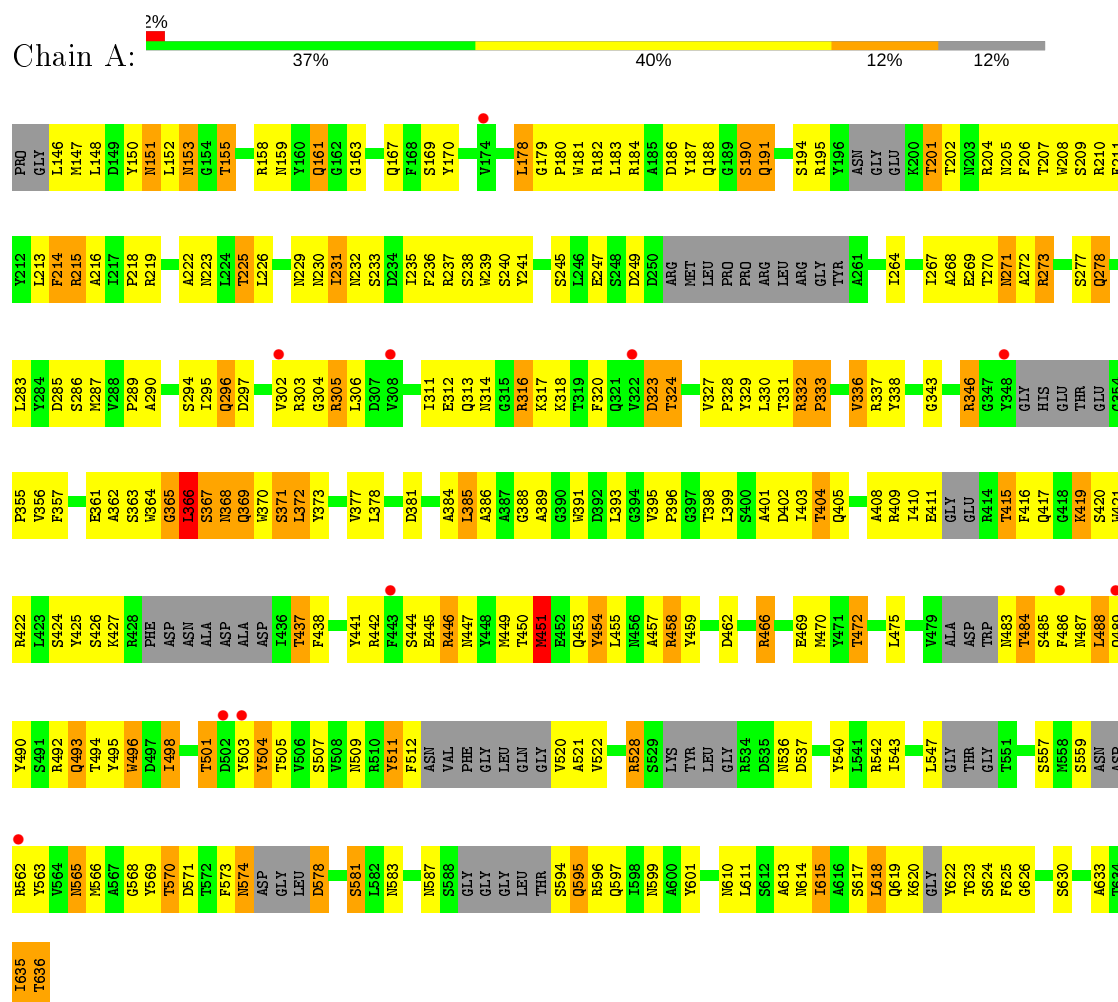
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Chain	Residue	Modelled	Actual	Comment	Reference
B	636	THR	-	EXPRESSION TAG	UNP P07110

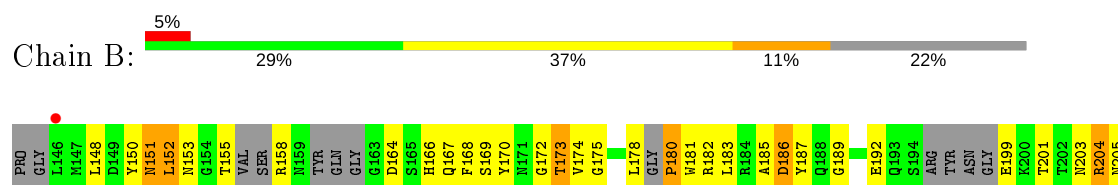
3 Residue-property plots

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

• Molecule 1: Outer membrane usher protein papC



• Molecule 1: Outer membrane usher protein papC



F206	E269	S345	R409	LYS	S538	Y602
T270	ASN	R346	I410	ASN	A539	S603
W208	T270	GLY	E411	VAL	Y540	R604
S209	N271	TYR	G412	ALA	L541	R605
R210	A272	ALA	GLU	ASP	R542	S606
F211	R273	GLY	R414	TRP	I543	P607
Y212	V274	HIS	R414	ASP	SER	L608
L213	GLU	GLU	T415	ASN	VAL	
F214	THR	THR	F416	THR	VAL	
R215	GLU	GLU		PRO	LEU	L611
R216	D285	G354	K419	PHE	S612	S612
A217	S286	P355	S420	ASN	GLY	A613
I217	M287	V356	W421	L488	THR	I614
P218	V288	F357	R422	Q489	GLY	I615
R219		A358	L423	Y490	THR	A616
W220	F293		SER		ALA	S617
R221		E361	TYR	Q493	SER	L618
A222	Q296	A362	SER	T494	Y554	G619
N223	D297	S363	LYS	Y495		LYS
L224	L298		ARG	W496	S559	GLY
T225	ASP		PHE	D497	ASN	Y622
L226	SER		ASP	I498	ASP	T623
G227	ASN	ASN	ASN	R499	R562	S624
E228	V302	Q369	ALA	T501	Y563	F625
N229	R303	N370	ASP	Y504	V564	G626
N230	G304	S371	ALA	D502	M565	Y627
I231	R305	L372	ASP	Y503	S628	S628
N232	L306	V373	ILE	A567	A629	A629
D233	D307	GLY	THR	T505	G568	S630
D234	V308	G375	F438	V506	TYR	G631
I235		A376		S507	THR	G632
F236	E312	V377	Y441	V508	ASP	A633
R237	Q313	L378	R442	ASN	THR	T634
S238	N314	A379	F443	ARG	PHE	I635
W239	G380	D381	R446	TYR	ASN	
S240	K317	X382	N447	PHE	ASP	
Y241	X318	X383	Y448	ASN	GLY	
T242	T319	F320	Y448	VAL	L577	
	Q321	L385	M449	PHE	D578	
L246	Q321	A386	T450	GLY	S579	
E247	V322		N451	LEU	Y580	
S248	D323		E452	GLN	S581	
D249	T324		Q453	GLY	L582	
ASP	A325		Y454	VAL	M583	
ARG	S326		L455	ALA	A584	
M252	X329		N456	V522	N587	
L253	L330		A457	G523	SER	
P254	R332		R458	L524	GLY	
	THR			S525	GLY	
L257	R332		D462	A526	GLY	
ARG			Y463	S527	GLY	
GLY	Q335		R466	R528	LEU	
TYR	R337		E467	S529	THR	
A261	X338			K530	SER	
P262	X339		D402	TYR	GLN	
Q263	L340		I403	LEU	ARG	
I264	X340		Y471	GLY	GLN	
T265	V341		T472	ARG	I598	
G266	S342		Q405	ASN	N599	
I267	G343		S406	D535	A600	
A268	R344		Y407	N536	Y601	

4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.285 , 0.359 0.289 , 0.356	Depositor DCC
R_{free} test set	1151 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	115.3	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 106.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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%)	10	41
1	B	338/493 (69%)	262 (78%)	67 (20%)	9 (3%)	5	27
All	All	746/986 (76%)	611 (82%)	120 (16%)	15 (2%)	7	34

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	4
1	B	292/405 (72%)	218 (75%)	74 (25%)	0	2
All	All	643/810 (79%)	491 (76%)	152 (24%)	1	3

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 [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 [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, 95th 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 ²)	Q<0.9
1	A	436/493 (88%)	0.17	11 (2%)	57 42	86, 114, 136, 158	11 (2%)
1	B	384/493 (77%)	0.26	24 (6%)	20 10	97, 126, 155, 171	4 (1%)
All	All	820/986 (83%)	0.21	35 (4%)	35 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	A	503	TYR	5.1
1	B	324	THR	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.