



# Full wwPDB X-ray Structure Validation Report i

Dec 16, 2023 – 07:48 PM EST

PDB ID : 3NRP  
Title : Crystal structure of 'as isolated' uropathogenic E. coli strain F11 FetP recombinantly expressed in the periplasm of E. coli BL21(DE3)  
Authors : Chan, A.C.K.; Murphy, M.E.P.  
Deposited on : 2010-06-30  
Resolution : 1.60 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 i 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 ①) were used in the production of this report:

MolProbity : **FAILED**  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

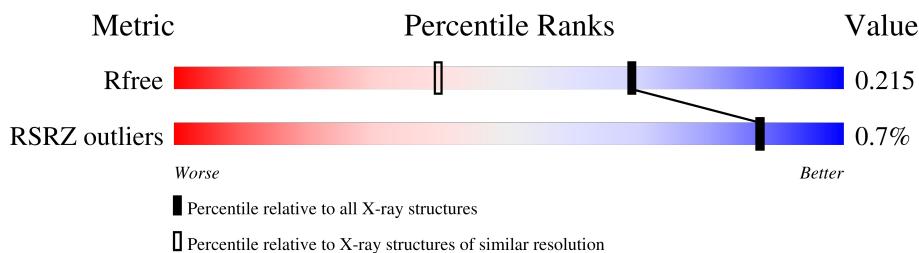
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 5191 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 Periplasmic protein-probably involved in high-affinity Fe2+ transport.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	2	0
			1202	766	201	226	9			
1	B	151	Total	C	N	O	S	0	8	0
			1241	789	207	235	10			
1	C	151	Total	C	N	O	S	0	1	0
			1183	755	194	225	9			
1	D	151	Total	C	N	O	S	0	4	0
			1209	772	200	226	11			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP B3HWD5
A	2	GLY	-	expression tag	UNP B3HWD5
A	154	SER	-	expression tag	UNP B3HWD5
A	155	SER	-	expression tag	UNP B3HWD5
A	156	GLY	-	expression tag	UNP B3HWD5
A	157	LEU	-	expression tag	UNP B3HWD5
A	158	VAL	-	expression tag	UNP B3HWD5
A	159	PRO	-	expression tag	UNP B3HWD5
A	160	ARG	-	expression tag	UNP B3HWD5
B	1	MET	-	expression tag	UNP B3HWD5
B	2	GLY	-	expression tag	UNP B3HWD5
B	154	SER	-	expression tag	UNP B3HWD5
B	155	SER	-	expression tag	UNP B3HWD5
B	156	GLY	-	expression tag	UNP B3HWD5
B	157	LEU	-	expression tag	UNP B3HWD5
B	158	VAL	-	expression tag	UNP B3HWD5
B	159	PRO	-	expression tag	UNP B3HWD5
B	160	ARG	-	expression tag	UNP B3HWD5
C	1	MET	-	expression tag	UNP B3HWD5
C	2	GLY	-	expression tag	UNP B3HWD5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	154	SER	-	expression tag	UNP B3HWD5
C	155	SER	-	expression tag	UNP B3HWD5
C	156	GLY	-	expression tag	UNP B3HWD5
C	157	LEU	-	expression tag	UNP B3HWD5
C	158	VAL	-	expression tag	UNP B3HWD5
C	159	PRO	-	expression tag	UNP B3HWD5
C	160	ARG	-	expression tag	UNP B3HWD5
D	1	MET	-	expression tag	UNP B3HWD5
D	2	GLY	-	expression tag	UNP B3HWD5
D	154	SER	-	expression tag	UNP B3HWD5
D	155	SER	-	expression tag	UNP B3HWD5
D	156	GLY	-	expression tag	UNP B3HWD5
D	157	LEU	-	expression tag	UNP B3HWD5
D	158	VAL	-	expression tag	UNP B3HWD5
D	159	PRO	-	expression tag	UNP B3HWD5
D	160	ARG	-	expression tag	UNP B3HWD5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	86	Total O 87 87	0	1
2	B	92	Total O 92 92	0	0
2	C	91	Total O 91 91	0	0
2	D	86	Total O 86 86	0	0

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### 3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.85Å 134.85Å 45.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.01 – 1.60 42.33 – 1.60	Depositor EDS
% Data completeness (in resolution range)	93.4 (50.01-1.60) 98.9 (42.33-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	2.14 (at 1.60Å)	Xtriage
Refinement program	REFMAC refmac_5.5.0102	Depositor
$R$ , $R_{free}$	0.171 , 0.207 0.180 , 0.215	Depositor DCC
$R_{free}$ test set	6129 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.0	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 33.2	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.51$ , $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.185 for -h,-k,l 0.005 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
Reported twinning fraction	0.408 for H, K, L 0.088 for h+k,-k,-l 0.089 for K, H, -L 0.415 for -h,-k,l	Depositor
Outliers	0 of 120509 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5191	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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  $< |L| >$ ,  $< L^2 >$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 4 Model quality [\(i\)](#)

### 4.1 Standard geometry [\(i\)](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts [\(i\)](#)

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### 4.3 Torsion angles [\(i\)](#)

#### 4.3.1 Protein backbone [\(i\)](#)

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#### 4.3.2 Protein sidechains [\(i\)](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [\(i\)](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

## 4.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

### 4.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 4.8 Polymer linkage issues

There are no chain breaks in this entry.

## 5 Fit of model and data i

### 5.1 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	152/160 (95%)	-0.28	0	100	100	0
1	B	151/160 (94%)	-0.35	1 (0%)	87	87	0
1	C	151/160 (94%)	-0.31	1 (0%)	87	87	0
1	D	151/160 (94%)	-0.26	2 (1%)	77	77	0
All	All	605/640 (94%)	-0.30	4 (0%)	87	87	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	PHE	3.4
1	D	2	GLY	3.3
1	C	3	PHE	2.8
1	B	2	GLY	2.3

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

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

### 5.3 Carbohydrates i

There are no monosaccharides in this entry.

### 5.4 Ligands i

There are no ligands in this entry.

## 5.5 Other polymers [\(i\)](#)

There are no such residues in this entry.