

# wwPDB X-ray Structure Validation Summary Report (i)

#### Aug 7, 2023 – 01:07 PM EDT

PDB ID : 1PO0

Title : Crystal structure of ferric citrate transporter FecA in complex with iron-free

citrate

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Deposited on : 2003-06-13

Resolution : 2.15 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

Mol Probity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.35

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

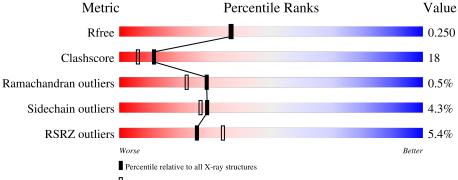
Validation Pipeline (wwPDB-VP) : 2.35

### 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.15 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.



Percentile relative to X-ray structures of similar resolution

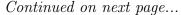
Metric	Whole archive	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 of 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 <=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 cha	in		
			5%			
1	A	751	62%	24%	•	12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FLC	A	742	-	X	-	-





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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FLC	A	743	-	X	=	-



### 2 Entry composition (i)

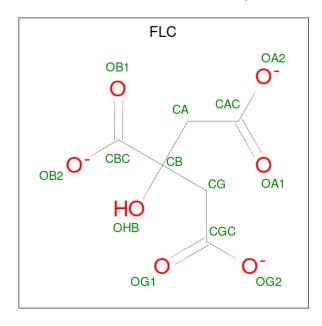
There are 3 unique types of molecules in this entry. The entry contains 5448 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Iron(III) dicitrate transport protein fecA precursor.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	661	Total 5166	C 3235	N 910	O 1008	S 13	0	0	0

• Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: C<sub>6</sub>H<sub>5</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 6 7	0	0
2	A	1	Total C O 13 6 7	0	0

• Molecule 3 is water.

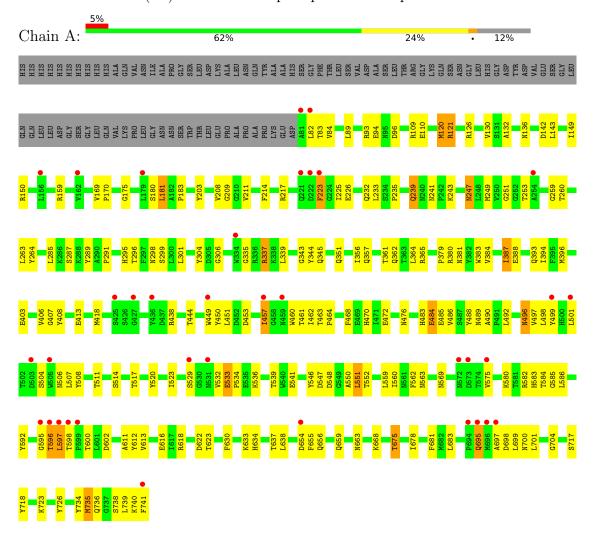
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	256	Total O 256 256	0	0



## 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Iron(III) dicitrate transport protein fecA precursor





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	113.07Å 89.31Å 95.79Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 - 2.15	Depositor
rtesolution (A)	29.06 - 2.08	EDS
% Data completeness	98.1 (19.93-2.15)	Depositor
(in resolution range)	91.6 (29.06-2.08)	EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.31 (at 2.08Å)	Xtriage
Refinement program	CNS 1.1	Depositor
D D.	0.233 , 0.257	Depositor
$R, R_{free}$	0.222 , $0.250$	DCC
$R_{free}$ test set	2608 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.0	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.34, 48.4	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5448	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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: FLC

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).

Mal	Chain	Bond	lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.37	0/5297	0.66	1/7198 (0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	717	SER	N-CA-C	-5.27	96.77	111.00

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	5166	0	4873	178	0
2	A	26	0	10	3	0
3	A	256	0	0	4	0
All	All	5448	0	4883	178	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 18.

The worst 5 of 178 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	$egin{aligned} &  ext{Interatomic} \ &  ext{distance} \ &  ext{(Å)} \end{aligned}$	Clash overlap (Å)
1:A:463:THR:HB	1:A:496:ASN:HD21	1.23	1.03
1:A:463:THR:HB	1:A:496:ASN:ND2	1.88	0.89
1:A:121:ARG:NH1	1:A:132:ALA:O	2.06	0.88
1:A:533:GLU:HG3	1:A:534:PRO:HD2	1.63	0.80
1:A:296:THR:OG1	1:A:345:GLN:HB3	1.83	0.79

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	659/751 (88%)	633 (96%)	23 (4%)	3 (0%)	29 22	

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	596	THR
1	A	695	GLN
1	A	223	PHE

#### 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	539/617 (87%)	516 (96%)	23 (4%)	29 27		



5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	533	GLU
1	A	602	ASP
1	A	597	LEU
1	A	675	THR
1	A	247	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	362	GLN
1	A	489	ASN
1	A	721	ASN
1	A	496	ASN
1	A	275	HIS

#### 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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Type	Chain	Res	Link	Bo	Bond lengths			Bond angles		
IVIOI	туре		nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2	
2	FLC	A	743	-	12,12,12	4.54	7 (58%)	17,17,17	6.05	8 (47%)	
2	FLC	A	742	-	12,12,12	4.56	7 (58%)	17,17,17	5.98	8 (47%)	

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FLC	A	743	-	-	8/16/16/16	-
2	FLC	A	742	-	-	9/16/16/16	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\mathring{\mathbf{A}})$	Ideal(Å)
2	A	742	FLC	CG-CB	9.10	1.65	1.53
2	A	743	FLC	CG-CB	9.08	1.65	1.53
2	A	743	FLC	CB-CBC	8.62	1.62	1.53
2	A	742	FLC	CB-CBC	8.54	1.62	1.53
2	A	743	FLC	CA-CB	7.94	1.63	1.53

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	743	FLC	OHB-CB-CBC	-16.86	85.19	108.86
2	A	742	FLC	OHB-CB-CBC	-16.59	85.57	108.86
2	A	742	FLC	OHB-CB-CG	-13.26	78.38	109.40
2	A	743	FLC	OHB-CB-CG	-13.19	78.54	109.40
2	A	743	FLC	OHB-CB-CA	-9.56	87.03	109.40

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	742	FLC	CAC-CA-CB-CBC
2	A	743	FLC	CAC-CA-CB-CBC
2	A	742	FLC	CBC-CB-CG-CGC
2	A	742	FLC	OHB-CB-CG-CGC
2	A	743	FLC	CBC-CB-CG-CGC

There are no ring outliers.



2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	743	FLC	1	0
2	A	742	FLC	2	0

### 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,  $95^{th}$  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	$\langle { m RSRZ} \rangle$	# RSRZ > 2		$OWAB(A^2)$	Q<0.9
1	A	661/751 (88%)	0.31	36 (5%) 2	25 34	17, 32, 55, 81	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	696	MET	7.9
1	A	81	ALA	7.8
1	A	697	ALA	6.0
1	A	695	GLN	6.0
1	A	741	PHE	5.4

### 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 monosaccharides 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. The B-factors column lists the minimum, median,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	FLC	A	742	13/13	0.88	0.13	33,35,42,44	0
2	FLC	A	743	13/13	0.94	0.14	34,36,43,46	0



## 6.5 Other polymers (i)

There are no such residues in this entry.

