



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 6B05 / pdb\_00006b05  
Title : The Crystal Structure of the Ferredoxin Protease FusC E83A mutant in complex with Arabidopsis Ferredoxin  
Authors : Grinter, R.  
Deposited on : 2017-09-13  
Resolution : 1.90 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

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

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

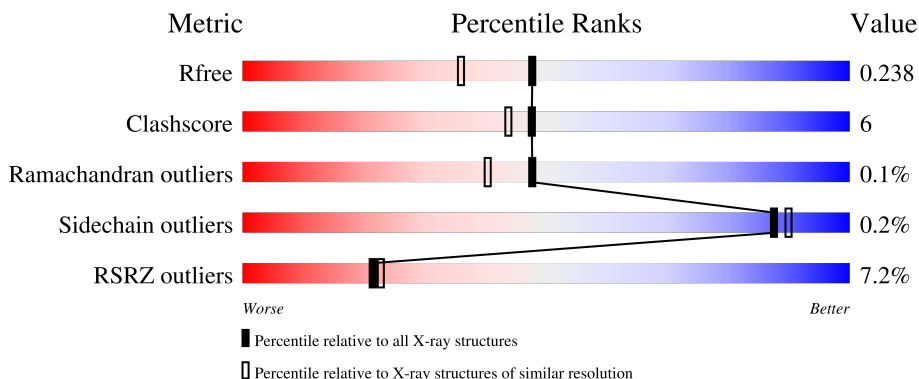
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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  $\geq 3$ , 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	924	
2	B	104	
2	C	104	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8533 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 Putative zinc protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	896	7203	4522	1291	1367	23	0	12	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	ALA	GLU	conflict	UNP Q6D8U3

- Molecule 2 is a protein called Ferredoxin-2, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	41	324	205	44	74	1	0	1	0
2	C	7	48	30	7	11		0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	95	ALA	-	expression tag	UNP P16972
B	96	ILE	-	expression tag	UNP P16972
B	97	MET	-	expression tag	UNP P16972
B	98	LEU	-	expression tag	UNP P16972
B	99	GLU	-	expression tag	UNP P16972
B	100	HIS	-	expression tag	UNP P16972
B	101	HIS	-	expression tag	UNP P16972
B	102	HIS	-	expression tag	UNP P16972
B	103	HIS	-	expression tag	UNP P16972
B	104	HIS	-	expression tag	UNP P16972
B	105	HIS	-	expression tag	UNP P16972
C	95	ALA	-	expression tag	UNP P16972
C	96	ILE	-	expression tag	UNP P16972

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Chain	Residue	Modelled	Actual	Comment	Reference
C	97	MET	-	expression tag	UNP P16972
C	98	LEU	-	expression tag	UNP P16972
C	99	GLU	-	expression tag	UNP P16972
C	100	HIS	-	expression tag	UNP P16972
C	101	HIS	-	expression tag	UNP P16972
C	102	HIS	-	expression tag	UNP P16972
C	103	HIS	-	expression tag	UNP P16972
C	104	HIS	-	expression tag	UNP P16972
C	105	HIS	-	expression tag	UNP P16972

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	938	Total	O	0	0
			938	938		
4	B	16	Total	O	0	0
			16	16		
4	C	3	Total	O	0	0
			3	3		



GLN	GLN	
SER	SER	
PHE	PHE	
LEU	LEU	
ASP	ASP	
GLU	GLU	
GLN	GLN	
ILE	ILE	
GLY	GLY	
GLU	GLU	
GLY	GLY	
PHE	PHE	
VAL	VAL	
LEU	LEU	
THR	THR	
CYS	CYS	
ALA	ALA	
ALA	ALA	
TYR	TYR	
PRO	PRO	
THR	THR	
SER	SER	
SER	D85	●
	V86	●
	T87	●
	I88	●
	E89	●
	T90	●
	H91	●
	LYS	
	GLU	
	GLU	
	ALA	
	ILE	
	MET	
	LEU	
	GLU	
	HIS	
	HIS	
	HIS	
	HIS	
	HIS	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.34Å 126.50Å 133.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.99 – 1.90 39.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.99-1.90) 99.6 (39.99-1.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 1.89Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.195 , 0.239 0.196 , 0.238	Depositor DCC
$R_{free}$ test set	5478 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtrriage
Anisotropy	0.222	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8533	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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

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	0.33	0/7351	0.53	0/9967
2	B	0.21	0/327	0.36	0/445
2	C	0.25	0/47	0.30	0/64
All	All	0.33	0/7725	0.52	0/10476

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	7203	0	7192	78	0
2	B	324	0	302	11	0
2	C	48	0	43	0	0
3	A	1	0	0	0	0
4	A	938	0	0	9	1
4	B	16	0	0	0	0
4	C	3	0	0	0	0
All	All	8533	0	7537	85	1

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 6.

The worst 5 of 85 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:A:512:LYS:NZ	4:A:1101:HOH:O	2.02	0.93
1:A:275:GLN:HE22	1:A:652:VAL:H	1.18	0.89
1:A:318:GLN:HE22	1:A:489:ARG:H	1.19	0.89
1:A:314:GLN:HE21	1:A:318:GLN:HE21	1.28	0.79
1:A:409:THR:HG22	1:A:413:GLN:HE21	1.47	0.78

All (1) 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)
4:A:1126:HOH:O	4:A:1771:HOH:O[2_565]	2.04	0.16

## 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	906/924 (98%)	896 (99%)	10 (1%)	0	100	100
2	B	38/104 (36%)	35 (92%)	2 (5%)	1 (3%)	4	1
2	C	5/104 (5%)	5 (100%)	0	0	100	100
All	All	949/1132 (84%)	936 (99%)	12 (1%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	36	LEU

### 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	776/788 (98%)	773 (100%)	3 (0%)	84	87
2	B	36/88 (41%)	36 (100%)	0	100	100
2	C	5/88 (6%)	5 (100%)	0	100	100
All	All	817/964 (85%)	814 (100%)	3 (0%)	87	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120[A]	ARG
1	A	120[B]	ARG
1	A	364	GLU

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	523	GLN
1	A	571	GLN
1	A	868	GLN
1	A	672	GLN
1	A	275	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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	896/924 (96%)	0.23	33 (3%) 45 48	11, 32, 59, 89	13 (1%)
2	B	41/104 (39%)	3.22	29 (70%) 0 0	20, 92, 136, 140	1 (2%)
2	C	7/104 (6%)	3.25	6 (85%) 0 0	51, 74, 93, 95	0
All	All	944/1132 (83%)	0.38	68 (7%) 21 23	11, 33, 68, 140	14 (1%)

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	208	SER	10.3
2	B	8	PHE	7.9
2	B	88	ILE	6.4
2	B	37	PRO	6.2
2	C	85	ASP	6.1

### 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 oligosaccharides 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<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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	A	1001	1/1	0.99	0.05	37,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.