



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:17 am BST

PDB ID : 3OER  
Title : Crystal structure of trimeric frataxin from the yeast *saccharomyces cerevisiae*, complexed with cobalt  
Authors : Soderberg, C.A.G.; Rajan, S.; Gakh, O.; Ta, C.; Isaya, G.; Al-Karadaghi, S.  
Deposited on : 2010-08-13  
Resolution : 3.20 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 ⓘ 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)	:	1.13
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

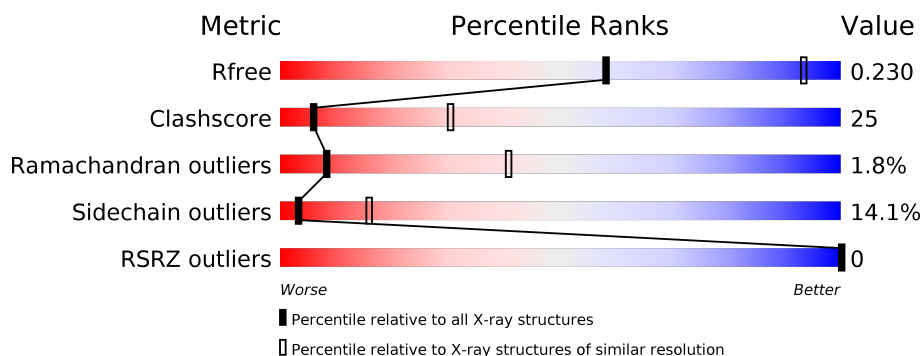
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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	123	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 893 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 Frataxin homolog, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	112	Total	C	N	O	S	0	0	0
			876	557	142	175	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	ALA	TYR	ENGINEERED MUTATION	UNP Q07540

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Co	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		



- Molecule 1: Frataxin homolog, mitochondrial

	VAL	GLU	SER	THR	ASP	GLY	GLN	VAL	P61	P62	P63	P64	P65	P66	P67	P68	P69	L70	L94	L85	D86	S87	L88	E89	E90	S92	E93	A94	H95	P96	D97	C98	I99	S105	H106	L111	P114	T118	Y119	M122	P125	P126	M127	K128	Q129	F130	W131	L132	L136	S137
	N140	R141	F142	D143	L144	E148	V149	S151	L152	R153	N154	G155	T156	K157	L158	T163	E164	E165	V166	E167	K168	K172	SER	GLN																										

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.20Å 121.20Å 121.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.57 – 3.20 28.57 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.57-3.20) 100.0 (28.57-3.20)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 3.17Å)	Xtriage
Refinement program	REFMAC 5.5.0044	Depositor
R, $R_{free}$	0.204 , 0.256 0.210 , 0.230	Depositor DCC
$R_{free}$ test set	491 reflections (9.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 69.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.041 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	893	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:  
CO

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	0.66	1/896 (0.1%)	0.85	2/1225 (0.2%)

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	148	GLU	CB-CG	5.30	1.62	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	LEU	CA-CB-CG	6.31	129.81	115.30
1	A	129	GLN	N-CA-C	5.74	126.51	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	PRO	Peptide

## 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	876	0	852	43	1
2	A	1	0	0	0	0
3	A	16	0	0	2	0
All	All	893	0	852	43	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 25.

All (43) 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:95:HIS:ND1	1:A:95:HIS:O	2.19	0.76
1:A:106:HIS:HD2	3:A:7:HOH:O	1.75	0.70
1:A:95:HIS:HD2	1:A:99:ILE:HG13	1.57	0.69
1:A:95:HIS:CG	1:A:97:ASP:HA	2.31	0.66
1:A:63:GLN:O	1:A:65:VAL:N	2.28	0.63
1:A:95:HIS:CE1	1:A:97:ASP:HA	2.35	0.60
1:A:63:GLN:C	1:A:65:VAL:H	2.04	0.60
1:A:154:ASN:OD1	1:A:156:THR:HG23	2.02	0.59
1:A:95:HIS:HD1	1:A:97:ASP:H	1.50	0.59
1:A:111:LEU:HB3	1:A:119:TYR:HB2	1.84	0.59
1:A:126:PRO:HA	1:A:128:LYS:O	2.05	0.57
1:A:137:SER:HB3	1:A:165:GLU:OE2	2.04	0.56
1:A:122:ASN:HB2	1:A:131:TRP:HB3	1.88	0.56
1:A:95:HIS:HD1	1:A:95:HIS:C	2.09	0.56
1:A:95:HIS:ND1	1:A:97:ASP:HA	2.20	0.56
1:A:61:VAL:N	1:A:62:PRO:CD	2.69	0.55
1:A:106:HIS:CD2	3:A:7:HOH:O	2.57	0.55
1:A:95:HIS:CD2	1:A:99:ILE:HG13	2.40	0.55
1:A:98:CYS:O	1:A:114:PRO:HD2	2.09	0.53
1:A:66:LEU:HA	1:A:70:LEU:HD22	1.91	0.51
1:A:95:HIS:ND1	1:A:97:ASP:N	2.57	0.51
1:A:84:LEU:O	1:A:88:LEU:HB2	2.11	0.50
1:A:128:LYS:HA	1:A:143:ASP:OD1	2.12	0.50
1:A:128:LYS:CB	1:A:152:LEU:HD11	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:HIS:CD2	1:A:97:ASP:HA	2.49	0.46
1:A:125:PRO:HA	1:A:126:PRO:HD3	1.57	0.46
1:A:142:PHE:HA	1:A:150:VAL:O	2.16	0.45
1:A:105:SER:OG	1:A:106:HIS:N	2.50	0.45
1:A:85:LEU:O	1:A:89:GLU:HG2	2.17	0.44
1:A:95:HIS:ND1	1:A:95:HIS:C	2.68	0.44
1:A:70:LEU:HA	1:A:70:LEU:HD12	1.71	0.43
1:A:127:ASN:OD1	1:A:127:ASN:N	2.52	0.43
1:A:63:GLN:HG3	1:A:66:LEU:HD12	2.01	0.43
1:A:132:LEU:HB3	1:A:142:PHE:HE2	1.83	0.43
1:A:144:LEU:HD13	1:A:149:TRP:CE2	2.54	0.42
1:A:99:ILE:O	1:A:99:ILE:CG1	2.67	0.42
1:A:91:LEU:HD13	1:A:166:VAL:HG11	2.02	0.42
1:A:126:PRO:HA	1:A:128:LYS:H	1.85	0.41
1:A:91:LEU:C	1:A:93:GLU:H	2.23	0.41
1:A:95:HIS:ND1	1:A:97:ASP:CA	2.84	0.41
1:A:63:GLN:O	1:A:66:LEU:N	2.51	0.41
1:A:68:LEU:HB2	1:A:70:LEU:HD13	2.02	0.41
1:A:99:ILE:O	1:A:99:ILE:HG13	2.20	0.41

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)
1:A:127:ASN:OD1	1:A:129:GLN:NE2[9_555]	1.89	0.31

## 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	110/123 (89%)	93 (84%)	15 (14%)	2 (2%)	<b>8</b> 41



All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	GLU
1	A	128	LYS

### 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	99/111 (89%)	85 (86%)	14 (14%)	3 16

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	GLU
1	A	66	LEU
1	A	86	ASP
1	A	87	SER
1	A	95	HIS
1	A	99	ILE
1	A	118	THR
1	A	127	ASN
1	A	136	LEU
1	A	140	ASN
1	A	144	LEU
1	A	158	LEU
1	A	163	THR
1	A	168	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	124	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](#)

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	112/123 (91%)	-0.39	0 100 100	65, 90, 154, 171	0

There are no RSRZ outliers to report.

### 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](#)

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(Å <sup>2</sup> )	Q<0.9
2	CO	A	1	1/1	0.92	1.55	79,79,79,79	1

### 6.5 Other polymers [i](#)

There are no such residues in this entry.