

Full wwPDB X-ray Structure Validation Report (i)

Apr 4, 2022 – 08:15 PM EDT

PDB ID	:	5IQS
Title	:	WelO5 bound to Fe(II), Cl, and 2-oxoglutarate
Authors	:	Mitchell, A.J.; Ananth, N.; Boal, A.K.
Deposited on	:	2016-03-11
Resolution	:	2.00 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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

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

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)		
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 Å.

There are no overall percentile quality scores available for this entry.

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



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7153 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	1 A	280	Total	С	Ν	0	\mathbf{S}	0	1	0
			2218	1413	372	423	10	0		
1	В	281	Total	С	Ν	0	S	0	0	0
	I D	201	2219	1414	372	423	10	0		
1	C	C 290	Total	С	Ν	0	S	0	2	0
	280	2224	1417	373	424	10	0	Δ	0	

• Molecule 1 is a protein called WelO5.

Th m = 75	1:	1		l	
There are 75	discrepancies	between	the modelled	ana	reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-24	MET	-	initiating methionine	UNP A0A067YX61
А	-23	LYS	-	expression tag	UNP A0A067YX61
А	-22	HIS	-	expression tag	UNP A0A067YX61
А	-21	HIS	-	expression tag	UNP A0A067YX61
А	-20	HIS	-	expression tag	UNP A0A067YX61
А	-19	HIS	-	expression tag	UNP A0A067YX61
А	-18	HIS	-	expression tag	UNP A0A067YX61
А	-17	HIS	-	expression tag	UNP A0A067YX61
А	-16	HIS	-	expression tag	UNP A0A067YX61
А	-15	SER	-	expression tag	UNP A0A067YX61
А	-14	ASP	-	expression tag	UNP A0A067YX61
А	-13	TYR	-	expression tag	UNP A0A067YX61
А	-12	ASP	-	expression tag	UNP A0A067YX61
А	-11	ILE	-	expression tag	UNP A0A067YX61
А	-10	PRO	-	expression tag	UNP A0A067YX61
А	-9	THR	-	expression tag	UNP A0A067YX61
А	-8	THR	-	expression tag	UNP A0A067YX61
А	-7	GLU	-	expression tag	UNP A0A067YX61
А	-6	ASN	-	expression tag	UNP A0A067YX61
А	-5	LEU	-	expression tag	UNP A0A067YX61
А	-4	TYR	-	expression tag	UNP A0A067YX61
А	-3	PHE	-	expression tag	UNP A0A067YX61
А	-2	GLN	-	expression tag	UNP A0A067YX61

Continued on next page...



Chain	Residue	vious page Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A067YX61
A	0	SER		expression tag	UNP A0A067YX61
B	-24	MET		initiating methionine	UNP A0A067YX61
B	-24	LYS		expression tag	UNP A0A067YX61
B	-23	HIS		expression tag	UNP A0A067YX61
B	-22	HIS	-	expression tag	UNP A0A067YX61
B	-21	HIS		expression tag	UNP A0A067YX61
B	-20	HIS	-		UNP A0A067YX61
B	-19	HIS	-	expression tag	UNP A0A067YX61
B	-18	HIS	-	expression tag	
			-	expression tag	UNP A0A067YX61
B	-16	HIS	-	expression tag	UNP A0A067YX61
B	-15	SER	-	expression tag	UNP A0A067YX61
B	-14	ASP	-	expression tag	UNP A0A067YX61
B	-13	TYR	-	expression tag	UNP A0A067YX61
В	-12	ASP	-	expression tag	UNP A0A067YX61
В	-11	ILE	-	expression tag	UNP A0A067YX61
В	-10	PRO	-	expression tag	UNP A0A067YX61
В	-9	THR	-	expression tag	UNP A0A067YX61
В	-8	THR	-	expression tag	UNP A0A067YX61
В	-7	GLU	-	expression tag	UNP A0A067YX61
В	-6	ASN	-	expression tag	UNP A0A067YX61
В	-5	LEU	-	expression tag	UNP A0A067YX61
В	-4	TYR	-	expression tag	UNP A0A067YX61
В	-3	PHE	-	expression tag	UNP A0A067YX61
В	-2	GLN	-	expression tag	UNP A0A067YX61
В	-1	GLY	_	expression tag	UNP A0A067YX61
В	0	SER	_	expression tag	UNP A0A067YX61
С	-24	MET	-	initiating methionine	UNP A0A067YX61
С	-23	LYS	-	expression tag	UNP A0A067YX61
С	-22	HIS	-	expression tag	UNP A0A067YX61
С	-21	HIS	-	expression tag	UNP A0A067YX61
С	-20	HIS	-	expression tag	UNP A0A067YX61
С	-19	HIS	_	expression tag	UNP A0A067YX61
С	-18	HIS	_	expression tag	UNP A0A067YX61
С	-17	HIS	-	expression tag	UNP A0A067YX61
C	-16	HIS	_	expression tag	UNP A0A067YX61
C	-15	SER	-	expression tag	UNP A0A067YX61
C	-14	ASP	_	expression tag	UNP A0A067YX61
<u> </u>	-13	TYR		expression tag	UNP A0A067YX61
<u> </u>	-12	ASP	_	expression tag	UNP A0A067YX61
<u> </u>	-11	ILE	-	expression tag	UNP A0A067YX61
<u>C</u>	-10	PRO	_	expression tag	UNP A0A067YX61
U	-10	110	_	expression tag	UNI AUAUU/IAU

Continued from previous page...

Continued on next page...



Chain

С

С

С

C C

C C

С

С

С

Comment

expression tag

expression tag

expression tag

expression tag

-9	THR	-	expression tag
-8	THR	-	expression tag
-7	GLU	-	expression tag
-6	ASN	-	expression tag
-5	LEU	-	expression tag
-4	TYR	-	expression tag

_

_

-

_

Actual

Continued from previous page...

Modelled

PHE

GLN

 GLY

SER

Residue

-3

-2

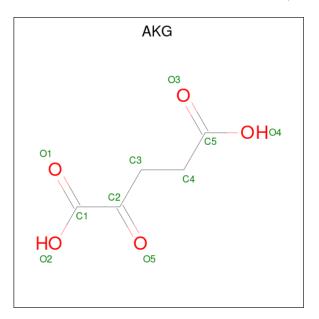
-1

0

• Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Fe 1 1	0	0
2	В	1	Total Fe 1 1	0	0
2	С	1	Total Fe 1 1	0	0

• Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	А	1	Total 10	С 5	O 5	0	0

Continued on next page...

Reference

UNP A0A067YX61

UNP A0A067YX61

UNP A0A067YX61 UNP A0A067YX61

UNP A0A067YX61 UNP A0A067YX61

UNP A0A067YX61

UNP A0A067YX61

UNP A0A067YX61

UNP A0A067YX61



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total C O 10 5 5	0	0
3	С	1	Total C O 10 5 5	0	0

• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Cl 1 1	0	0
4	В	1	Total Cl 1 1	0	0
4	С	1	Total Cl 1 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	141	Total O 141 141	0	0
5	В	152	Total O 152 152	0	0
5	С	163	Total O 163 163	0	0

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



3 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	70.76Å 86.34Å 141.31Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	50.00 - 2.00	Depositor	
% Data completeness	99.3 (50.00-2.00)	Depositor	
(in resolution range)			
R _{merge}	0.12	Depositor	
R _{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$3.47 (at 2.00 \text{\AA})$	Xtriage	
Refinement program	REFMAC 5.8.0073	Depositor	
R, R_{free}	0.189 , 0.219	Depositor	
Wilson B-factor $(Å^2)$	20.1	Xtriage	
Anisotropy	0.223	Xtriage	
L-test for twinning ²	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.34$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	7153	wwPDB-VP	
Average B, all atoms $(Å^2)$	24.0	wwPDB-VP	

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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)

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

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

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)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

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



	Mol	Туре	Chain	Res	Link	Bond lengths			Bond angles		
						Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
	3	AKG	В	302	2	$3,\!9,\!9$	0.29	0	4,11,11	1.08	1 (25%)
Ī	3	AKG	С	302	2	3,9,9	0.32	0	4,11,11	1.04	0
	3	AKG	А	302	2	3,9,9	0.30	0	4,11,11	0.70	0

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).

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
3	AKG	В	302	2	-	0/3/9/9	-
3	AKG	С	302	2	-	0/3/9/9	-
3	AKG	А	302	2	-	0/3/9/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	В	302	AKG	C4-C3-C2	-2.00	108.82	113.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

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

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

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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

