



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 16, 2017 – 02:50 PM EST

PDB ID : 5W1L  
Title : Echinococcus granulosus thioredoxin glutathione reductas (egTGR) with Gold  
Authors : Gao, W.; Wang, Y.; Dai, S.  
Deposited on : unknown  
Resolution : 2.88 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

<http://wwpdb.org/validation/2016/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  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

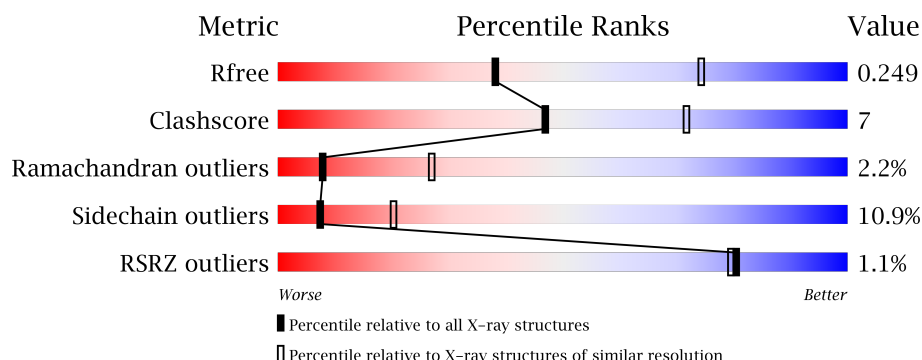
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.88 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))
$R_{free}$	100719	2135 (2.90-2.86)
Clashscore	112137	2400 (2.90-2.86)
Ramachandran outliers	110173	2346 (2.90-2.86)
Sidechain outliers	110143	2349 (2.90-2.86)
RSRZ outliers	101464	2149 (2.90-2.86)

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. 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	586	 77% 20% 2% 1%
2	B	584	 74% 21% 2% 1%



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 Thioredoxin glutathione reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	584	Total	C	N	O	S	0	1	0
			4518	2858	766	865	29			

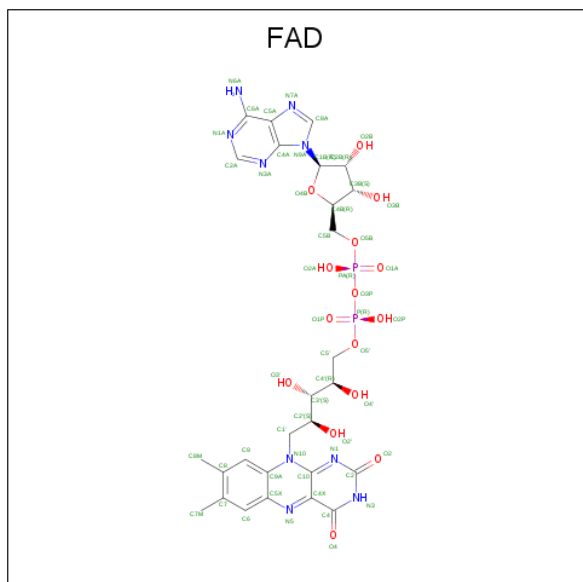
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	-	expression tag	UNP Q869D7
A	3	SEC	-	expression tag	UNP Q869D7

- Molecule 2 is a protein called Thioredoxin glutathione reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	584	Total	C	N	O	S	0	0	0
			4497	2844	762	862	29			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is GOLD ION (three-letter code: AU) (formula: Au).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Au	0	0
			1	1		
4	A	1	Total	Au	0	0
			1	1		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.35Å 109.35Å 258.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.72 – 2.88 49.61 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.0 (100.72-2.88) 99.0 (49.61-2.88)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.185 , 0.249 0.188 , 0.249	Depositor DCC
$R_{free}$ test set	1802 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.9	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 33.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9123	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: AU, FAD

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	0.98	6/4613 (0.1%)	1.05	8/6255 (0.1%)
2	B	0.93	2/4592 (0.0%)	1.05	10/6231 (0.2%)
All	All	0.96	8/9205 (0.1%)	1.05	18/12486 (0.1%)

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
2	B	0	5
All	All	0	6

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	259	GLU	CD-OE2	7.20	1.33	1.25
1	A	438	TYR	CG-CD2	5.92	1.46	1.39
2	B	573	CYS	CB-SG	5.73	1.92	1.82
1	A	300	GLU	CD-OE1	5.69	1.31	1.25
1	A	573	CYS	CB-SG	5.50	1.91	1.82

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	ARG	NE-CZ-NH1	6.90	123.75	120.30
2	B	382	ASP	N-CA-C	6.85	129.50	111.00
2	B	277	ASP	CB-CG-OD1	6.36	124.02	118.30
2	B	260	ARG	CB-CG-CD	6.21	127.74	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	311	ASP	CB-CG-OD1	6.17	123.85	118.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	57	LYS	Peptide
2	B	104	ASN	Peptide
2	B	284	HIS	Peptide
2	B	360	PRO	Peptide
2	B	363	GLY	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	4518	0	4444	64	0
2	B	4497	0	4406	70	0
3	A	53	0	31	0	0
3	B	53	0	31	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	9123	0	8912	128	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 7.

The worst 5 of 128 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:46:GLY:C	1:A:50:TYR:N	2.14	1.01
1:A:46:GLY:O	1:A:50:TYR:N	2.09	0.86
2:B:46:GLY:O	2:B:50:TYR:N	2.10	0.85
2:B:46:GLY:C	2:B:50:TYR:N	2.33	0.82
1:A:471:THR:HG21	1:A:544:GLY:HA2	1.62	0.81



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	581/586 (99%)	534 (92%)	39 (7%)	8 (1%)	13	40
2	B	580/584 (99%)	510 (88%)	52 (9%)	18 (3%)	5	18
All	All	1161/1170 (99%)	1044 (90%)	91 (8%)	26 (2%)	8	27

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ALA
1	A	375	GLU
2	B	5	ALA
2	B	34	VAL
2	B	106	MET

### 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	493/493 (100%)	446 (90%)	47 (10%)	10	27
2	B	489/493 (99%)	428 (88%)	61 (12%)	5	14
All	All	982/986 (100%)	874 (89%)	108 (11%)	7	20

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	33	LYS
2	B	135	VAL
2	B	498	GLU
2	B	43	ILE
2	B	95	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	505	GLN
1	A	517	ASN
2	B	446	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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 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	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	FAD	A	601	-	51,58,58	1.36	10 (19%)	54,89,89	2.37	11 (20%)
3	FAD	B	601	-	51,58,58	1.45	6 (11%)	54,89,89	2.25	13 (24%)

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	FAD	A	601	-	-	0/28/50/50	0/6/6/6
3	FAD	B	601	-	-	0/28/50/50	0/6/6/6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	FAD	C4X-N5	-3.06	1.28	1.33
3	B	601	FAD	C1'-N10	-2.92	1.45	1.48
3	A	601	FAD	C2-N3	-2.66	1.32	1.38
3	A	601	FAD	C2B-C1B	-2.31	1.50	1.53
3	A	601	FAD	C2-N1	-2.22	1.33	1.38

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	FAD	N3A-C2A-N1A	-7.39	122.42	128.86
3	A	601	FAD	N3A-C2A-N1A	-4.13	125.26	128.86
3	A	601	FAD	C4-C4X-C10	-4.09	116.66	119.96
3	B	601	FAD	C4A-C5A-N7A	-3.75	105.79	109.41
3	B	601	FAD	C4-C4X-C10	-3.59	117.06	119.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	FAD	3	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	46:GLY	C	50:TYR	N	2.33
1	A	46:GLY	C	50:TYR	N	2.14

## 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	584/586 (99%)	-0.04	2 (0%) 93 93	46, 69, 109, 142	0
2	B	584/584 (100%)	0.09	11 (1%) 67 65	47, 78, 123, 150	0
All	All	1168/1170 (99%)	0.02	13 (1%) 80 79	46, 72, 118, 150	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	362	SER	3.4
2	B	378	THR	3.0
2	B	99	ILE	2.8
2	B	190	GLY	2.6
1	A	58	ASN	2.6

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FAD	B	601	53/53	0.97	0.18	0.26	54,60,69,71	0
3	FAD	A	601	53/53	0.97	0.19	0.05	49,54,59,60	0
4	AU	B	602	1/1	0.96	0.15	-0.85	126,126,126,126	0
4	AU	A	602	1/1	0.97	0.06	-4.47	116,116,116,116	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.