



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 07:51 PM GMT

PDB ID : 1GXF  
Title : CRYSTAL STRUCTURE OF TRYPANOSOMA CRUZI TRYPANOTHIONE  
REDUCTASE IN COMPLEX WITH THE INHIBITOR QUINACRINE MUS-  
TARD  
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Deposited on : 2002-04-04  
Resolution : 2.70 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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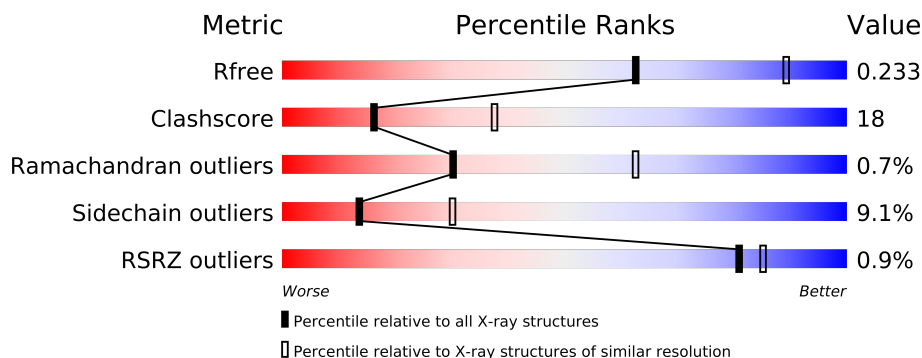
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 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))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	492	
1	B	492	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	QUM	A	1501	-	X
4	QUM	A	1502	-	X
4	QUM	B	1501	-	X
4	QUM	B	1502	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7726 atoms, of which 0 are hydrogen and 0 are deuterium.

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 TRYPTOPHAN REDUCTASE (OXIDIZED FORM).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	1
			3727	2370	635	701	21			
1	B	484	Total	C	N	O	S	0	0	1
			3718	2364	633	700	21			

There are 14 discrepancies between the modelled and reference sequences:

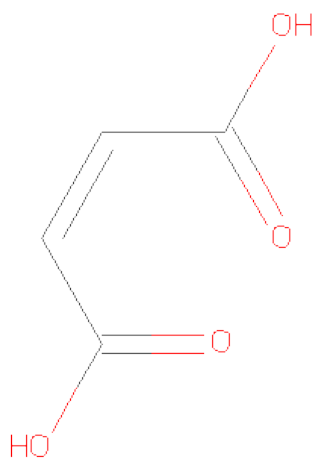
Chain	Residue	Modelled	Actual	Comment	Reference
A	95	ASN	LYS	VARIANT	UNP P28593
A	112	ASP	GLU	VARIANT	UNP P28593
A	156	HIS	ASN	VARIANT	UNP P28593
A	353	THR	ASN	VARIANT	UNP P28593
A	402	LYS	ASN	VARIANT	UNP P28593
A	403	VAL	ILE	VARIANT	UNP P28593
A	441	ILE	VAL	VARIANT	UNP P28593
B	95	ASN	LYS	VARIANT	UNP P28593
B	112	ASP	GLU	VARIANT	UNP P28593
B	156	HIS	ASN	VARIANT	UNP P28593
B	353	THR	ASN	VARIANT	UNP P28593
B	402	LYS	ASN	VARIANT	UNP P28593
B	403	VAL	ILE	VARIANT	UNP P28593
B	441	ILE	VAL	VARIANT	UNP P28593

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



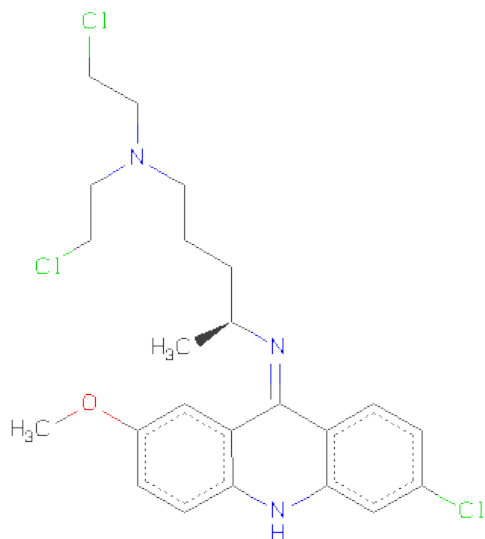
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is MALEIC ACID (three-letter code: MAE) (formula:  $C_4H_4O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	4	4		

- Molecule 4 is QUINACRINE MUSTARD (three-letter code: QUM) (formula:  $C_{23}H_{28}Cl_3N_3O$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			28	23	1	3	1		
4	A	1	Total	C	Cl	N	O	0	0
			29	23	2	3	1		
4	B	1	Total	C	Cl	N	O	0	0
			28	23	1	3	1		
4	B	1	Total	C	Cl	N	O	0	0
			29	23	2	3	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	28	Total	O	0	0
			28	28		
5	B	25	Total	O	0	0
			25	25		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.10Å 93.10Å 156.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.00 – 2.70 29.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	79.0 (21.00-2.70) 79.5 (29.96-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.50 (at 2.68Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.190 , 0.250 0.188 , 0.233	Depositor DCC
$R_{free}$ test set	1466 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 31.4	EDS
Estimated twinning fraction	0.056 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 29072 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7726	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QUM, MAE, 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	0.41	0/3804	1.15	23/5154 (0.4%)
1	B	0.41	0/3795	1.20	23/5143 (0.4%)
All	All	0.41	0/7599	1.18	46/10297 (0.4%)

There are no bond length outliers.

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	472	ARG	CD-NE-CZ	26.14	160.19	123.60
1	A	472	ARG	CD-NE-CZ	23.57	156.60	123.60
1	B	361	ARG	NE-CZ-NH2	11.73	126.17	120.30
1	A	139	ARG	CD-NE-CZ	11.66	139.92	123.60
1	B	139	ARG	CD-NE-CZ	10.80	138.72	123.60

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3727	0	3739	130	1
1	B	3718	0	3726	142	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	53	0	31	1	0
2	B	53	0	31	3	0
3	A	8	0	2	3	0
4	A	57	0	48	33	0
4	B	57	0	48	14	0
5	A	28	0	0	4	0
5	B	25	0	0	5	0
All	All	7726	0	7625	278	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

The worst 5 of 278 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:1502:QUM:H1	4:A:1502:QUM:C20	1.28	1.61
4:A:1502:QUM:C1	4:A:1502:QUM:C20	2.22	1.18
1:B:232:ASP:HB3	1:B:235:LEU:HD12	1.21	1.12
1:A:232:ASP:HB3	1:A:235:LEU:HD12	1.26	1.10
4:A:1502:QUM:H1	4:A:1502:QUM:H203	1.15	1.08

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	Distance(Å)	Clash(Å)
1:A:299:ASN:ND2	1:B:407:LYS:NZ[3_554]	2.18	0.02

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	483/492 (98%)	450 (93%)	30 (6%)	3 (1%)	33	66
1	B	482/492 (98%)	442 (92%)	36 (8%)	4 (1%)	27	58
All	All	965/984 (98%)	892 (92%)	66 (7%)	7 (1%)	30	62

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	LYS
1	B	299	ASN
1	A	41	HIS
1	B	320	SER
1	B	21	ALA

### 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	405/412 (98%)	369 (91%)	36 (9%)	14	31
1	B	404/412 (98%)	366 (91%)	38 (9%)	13	28
All	All	809/824 (98%)	735 (91%)	74 (9%)	14	30

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	450	LYS
1	B	90	ARG
1	B	395	SER
1	A	480	LYS
1	B	47	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	69	GLN
1	B	106	ASN
1	B	255	ASN
1	B	55	ASN
1	B	299	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

7 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	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	FAD	A	1492	-	58,58,58	1.44	4 (6%)	85,89,89	1.76	15 (17%)
3	MAE	A	1500	-	7,7,7	0.83	0	8,8,8	0.53	0
4	QUM	A	1501	1	30,30,32	5.30	6 (20%)	37,41,43	1.69	4 (10%)
4	QUM	A	1502	1	31,31,32	2.28	4 (12%)	39,42,43	2.16	6 (15%)
2	FAD	B	1492	-	58,58,58	1.42	4 (6%)	85,89,89	1.81	13 (15%)
4	QUM	B	1501	1	30,30,32	5.14	6 (20%)	37,41,43	1.72	4 (10%)
4	QUM	B	1502	1	31,31,32	2.20	4 (12%)	39,42,43	1.75	4 (10%)

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	FAD	A	1492	-	-	0/34/50/50	0/1/6/6
3	MAE	A	1500	-	-	0/5/5/5	0/0/0/0
4	QUM	A	1501	1	-	1/14/16/18	0/0/3/3
4	QUM	A	1502	1	-	1/15/17/18	0/0/3/3
2	FAD	B	1492	-	-	0/34/50/50	0/1/6/6
4	QUM	B	1501	1	-	1/14/16/18	0/0/3/3
4	QUM	B	1502	1	-	1/15/17/18	0/0/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1501	QUM	C28-C27	-26.26	1.44	1.55
4	B	1501	QUM	C28-C27	-25.25	1.45	1.55
4	A	1502	QUM	C26-C25	-10.78	1.50	1.55
4	B	1502	QUM	C26-C25	-10.28	1.51	1.55
4	B	1501	QUM	C26-C25	-10.18	1.51	1.55

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1502	QUM	C9-N18-C19	11.56	142.17	122.21
2	B	1492	FAD	C2-N1-C10	8.90	123.94	114.98
4	B	1502	QUM	C9-N18-C19	8.69	137.22	122.21
4	B	1501	QUM	C9-N18-C19	7.71	135.52	122.21
2	A	1492	FAD	C2-N1-C10	7.56	122.59	114.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1502	QUM	C20-C19-N18-C9
4	B	1502	QUM	C20-C19-N18-C9
4	A	1501	QUM	C20-C19-N18-C9
4	B	1501	QUM	C20-C19-N18-C9

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	485/492 (98%)	-0.47	2 (0%) 90 93	19, 42, 73, 90	0
1	B	484/492 (98%)	-0.48	7 (1%) 72 77	19, 42, 73, 90	0
All	All	969/984 (98%)	-0.48	9 (0%) 81 85	19, 42, 73, 90	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	354	PRO	3.2
1	B	353	THR	3.1
1	B	263	ALA	3.1
1	B	352	THR	3.0
1	B	488	SER	2.7

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	QUM	A	1502	29/30	0.38	8.83	47,55,57,58	29
4	QUM	B	1501	28/30	0.53	6.01	53,55,68,71	28
4	QUM	A	1501	28/30	0.39	5.10	53,56,68,71	28
4	QUM	B	1502	29/30	0.38	4.75	47,55,57,58	29
3	MAE	A	1500	8/8	0.18	1.68	29,31,33,35	0
2	FAD	B	1492	53/53	0.11	0.01	17,33,49,50	0
2	FAD	A	1492	53/53	0.14	-0.08	16,33,49,50	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.