



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:41 PM GMT

PDB ID : 1GTA  
Title : CRYSTAL STRUCTURES OF A SCHISTOSOMAL DRUG AND VACCINE TARGET: GLUTATHIONE S-TRANSFERASE FROM SCHISTOSOMA JAPONICA AND ITS COMPLEX WITH THE LEADING ANTISCHISTOSOMAL DRUG PRAZIQUANTEL  
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Deposited on : 1994-12-01  
Resolution : 2.40 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  
<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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

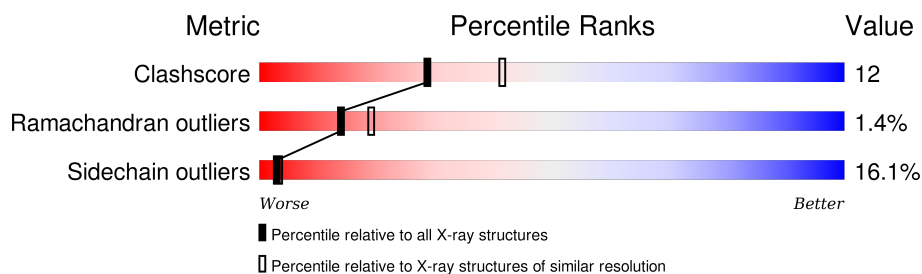
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	218	 57% 28% 12% •

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1900 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 GLUTATHIONE S-TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1786	1163	288	322	13			

- Molecule 2 is water.

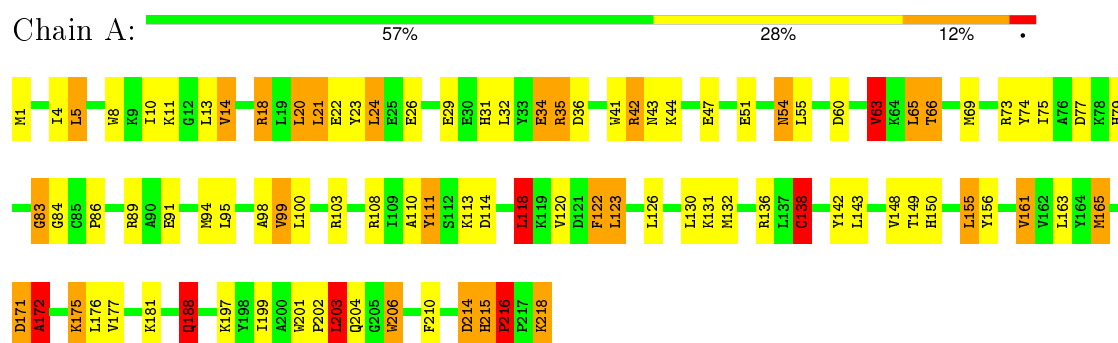
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	114	Total	O	0	0
			114	114		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

#### • Molecule 1: GLUTATHIONE S-TRANSFERASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.20 Å   125.20 Å   70.20 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	7.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.40)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.197 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1900	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

## 5 Model quality [i](#)

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

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	1.16	2/1834 (0.1%)	2.20	73/2475 (2.9%)

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	VAL	CA-CB	5.24	1.65	1.54
1	A	51	GLU	CA-CB	-5.13	1.42	1.53

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	ARG	NE-CZ-NH1	23.62	132.11	120.30
1	A	94	MET	CG-SD-CE	-16.41	73.95	100.20
1	A	69	MET	CG-SD-CE	-16.08	74.48	100.20
1	A	18	ARG	NE-CZ-NH2	-12.06	114.27	120.30
1	A	165	MET	CG-SD-CE	-11.39	81.98	100.20
1	A	8	TRP	CD1-CG-CD2	11.20	115.26	106.30
1	A	156	TYR	CB-CG-CD2	-11.08	114.35	121.00
1	A	216	PRO	N-CA-C	11.02	140.75	112.10
1	A	41	TRP	CD1-CG-CD2	10.22	114.47	106.30
1	A	148	VAL	CG1-CB-CG2	-9.89	95.07	110.90
1	A	35	ARG	NE-CZ-NH2	-9.87	115.37	120.30
1	A	83	GLY	CA-C-N	9.48	135.15	116.20
1	A	73	ARG	NE-CZ-NH1	8.91	124.75	120.30
1	A	41	TRP	CE2-CD2-CG	-8.50	100.50	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	A	42	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	A	23	TYR	CB-CG-CD1	-8.02	116.19	121.00
1	A	201	TRP	CD1-CG-CD2	7.96	112.67	106.30
1	A	111	TYR	CB-CG-CD2	-7.93	116.24	121.00
1	A	138	CYS	CA-CB-SG	-7.75	100.04	114.00
1	A	214	ASP	CB-CG-OD1	7.67	125.21	118.30
1	A	8	TRP	CE2-CD2-CG	-7.61	101.22	107.30
1	A	66	THR	N-CA-C	7.49	131.21	111.00
1	A	41	TRP	CG-CD2-CE3	7.29	140.46	133.90
1	A	201	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	A	172	ALA	N-CA-CB	6.83	119.66	110.10
1	A	8	TRP	CG-CD1-NE1	-6.70	103.40	110.10
1	A	74	TYR	CB-CG-CD1	-6.69	116.99	121.00
1	A	42	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	41	TRP	CB-CG-CD1	-6.66	118.34	127.00
1	A	172	ALA	CB-CA-C	-6.66	100.12	110.10
1	A	63	VAL	N-CA-CB	-6.62	96.93	111.50
1	A	41	TRP	CG-CD1-NE1	-6.59	103.51	110.10
1	A	14	VAL	CG1-CB-CG2	-6.49	100.52	110.90
1	A	34	GLU	CA-CB-CG	-6.47	99.16	113.40
1	A	206	TRP	CD1-CG-CD2	6.43	111.44	106.30
1	A	136	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	A	215	HIS	N-CA-C	6.31	128.04	111.00
1	A	103	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	23	TYR	CD1-CG-CD2	6.18	124.70	117.90
1	A	35	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	122	PHE	CB-CG-CD2	-6.04	116.57	120.80
1	A	216	PRO	CA-N-CD	-6.04	103.05	111.50
1	A	65	LEU	CA-CB-CG	6.01	129.13	115.30
1	A	155	LEU	CB-CG-CD1	-5.94	100.90	111.00
1	A	83	GLY	CA-C-O	-5.90	109.98	120.60
1	A	171	ASP	CA-C-N	5.89	130.17	117.20
1	A	149	THR	O-C-N	-5.87	113.31	122.70
1	A	118	LEU	CB-CG-CD2	-5.83	101.09	111.00
1	A	65	LEU	CB-CG-CD2	-5.79	101.16	111.00
1	A	142	TYR	CB-CG-CD1	-5.78	117.53	121.00
1	A	203	LEU	CA-CB-CG	5.65	128.29	115.30
1	A	91	GLU	CA-CB-CG	5.65	125.83	113.40
1	A	161	VAL	CA-C-N	5.64	129.62	117.20
1	A	29	GLU	CA-C-N	5.63	129.59	117.20
1	A	206	TRP	CE2-CD2-CG	-5.63	102.80	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	GLN	CA-CB-CG	5.59	125.70	113.40
1	A	29	GLU	O-C-N	-5.57	113.79	122.70
1	A	63	VAL	CG1-CB-CG2	5.50	119.70	110.90
1	A	132	MET	CG-SD-CE	5.46	108.94	100.20
1	A	150	HIS	CA-CB-CG	5.44	122.84	113.60
1	A	77	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	26	GLU	CA-CB-CG	-5.34	101.64	113.40
1	A	111	TYR	O-C-N	-5.29	114.23	122.70
1	A	18	ARG	NH1-CZ-NH2	-5.27	113.60	119.40
1	A	122	PHE	CB-CG-CD1	5.21	124.45	120.80
1	A	98	ALA	CA-C-N	5.19	128.62	117.20
1	A	111	TYR	CB-CG-CD1	5.12	124.07	121.00
1	A	155	LEU	CA-CB-CG	5.08	126.97	115.30
1	A	83	GLY	O-C-N	-5.06	114.59	123.20
1	A	218	LYS	N-CA-C	5.05	124.63	111.00
1	A	21	LEU	CA-CB-CG	5.03	126.86	115.30
1	A	5	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	HIS	Mainchain,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	1786	0	1780	41	0
2	A	114	0	0	13	0
All	All	1900	0	1780	41	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 12.

All (41) 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:83:GLY:HA3	1:A:89:ARG:HG3	1.54	0.89
1:A:123:LEU:HD13	1:A:165:MET:HE2	1.57	0.86
1:A:66:THR:N	2:A:379:HOH:O	2.27	0.66
1:A:75:ILE:O	1:A:79:HIS:HD2	1.80	0.64
1:A:210:PHE:HD1	1:A:218:LYS:HA	1.62	0.64
1:A:210:PHE:CD1	1:A:218:LYS:HA	2.32	0.64
1:A:138:CYS:HB3	2:A:339:HOH:O	1.99	0.62
1:A:203:LEU:HB3	2:A:414:HOH:O	2.04	0.57
1:A:204:GLN:HG2	2:A:414:HOH:O	2.05	0.55
1:A:10:ILE:HG22	1:A:202:PRO:HG2	1.89	0.55
1:A:95:LEU:O	1:A:99:VAL:HG13	2.08	0.54
1:A:210:PHE:HD2	2:A:395:HOH:O	1.92	0.53
1:A:122:PHE:HA	2:A:324:HOH:O	2.09	0.52
1:A:123:LEU:CD1	1:A:165:MET:HE2	2.35	0.52
1:A:60:ASP:HB2	1:A:63:VAL:HG12	1.90	0.52
1:A:44:LYS:HA	1:A:47:GLU:HG2	1.93	0.51
1:A:138:CYS:SG	1:A:175:LYS:HE3	2.51	0.50
1:A:114:ASP:O	1:A:118:LEU:HD22	2.13	0.49
1:A:188:GLN:NE2	1:A:188:GLN:H	2.11	0.48
1:A:188:GLN:NE2	1:A:188:GLN:N	2.61	0.48
1:A:114:ASP:C	1:A:118:LEU:HD22	2.35	0.47
1:A:54:ASN:HD22	1:A:55:LEU:H	1.62	0.47
1:A:118:LEU:HD21	2:A:418:HOH:O	2.15	0.47
1:A:34:GLU:HB3	2:A:365:HOH:O	2.13	0.47
1:A:161:VAL:HG22	1:A:203:LEU:HG	1.97	0.47
1:A:35:ARG:HB3	1:A:206:TRP:CE2	2.51	0.46
1:A:10:ILE:O	1:A:18:ARG:NH2	2.49	0.45
1:A:13:LEU:HD23	2:A:303:HOH:O	2.17	0.45
1:A:18:ARG:O	1:A:22:GLU:HG2	2.16	0.45
1:A:197:LYS:HD3	2:A:330:HOH:O	2.16	0.45
1:A:4:ILE:HD12	2:A:389:HOH:O	2.16	0.45
1:A:84:GLY:N	2:A:380:HOH:O	2.49	0.45
1:A:165:MET:HB2	1:A:210:PHE:CZ	2.52	0.44
1:A:20:LEU:O	1:A:24:LEU:HB2	2.18	0.43
1:A:4:ILE:HG21	1:A:31:HIS:CE1	2.54	0.42
1:A:63:VAL:HG13	1:A:65:LEU:HD22	2.01	0.42
1:A:171:ASP:O	1:A:172:ALA:CB	2.66	0.42
1:A:35:ARG:HB3	1:A:206:TRP:CD2	2.55	0.42
1:A:110:ALA:HB2	2:A:395:HOH:O	2.20	0.41
1:A:177:VAL:O	1:A:181:LYS:HG3	2.21	0.41
1:A:11:LYS:HE3	1:A:199:ILE:O	2.22	0.40

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	216/218 (99%)	202 (94%)	11 (5%)	3 (1%)	14 19

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	PRO
1	A	111	TYR
1	A	172	ALA

### 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	192/194 (99%)	161 (84%)	31 (16%)	3 3

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	LEU
1	A	14	VAL
1	A	20	LEU
1	A	21	LEU
1	A	24	LEU
1	A	32	LEU
1	A	36	ASP

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Mol	Chain	Res	Type
1	A	42	ARG
1	A	43	ASN
1	A	54	ASN
1	A	63	VAL
1	A	86	PRO
1	A	100	LEU
1	A	113	LYS
1	A	118	LEU
1	A	120	VAL
1	A	123	LEU
1	A	126	LEU
1	A	130	LEU
1	A	131	LYS
1	A	138	CYS
1	A	143	LEU
1	A	155	LEU
1	A	163	LEU
1	A	175	LYS
1	A	176	LEU
1	A	188	GLN
1	A	203	LEU
1	A	214	ASP
1	A	216	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	54	ASN
1	A	67	GLN
1	A	79	HIS
1	A	188	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.