



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:01 PM GMT

PDB ID : 4WO8  
Title : The substrate-free duplicated taurocyamine kinase from *Schistosoma mansoni*  
Authors : Merceron, R.; Awama, A.; Montserret, R.; Marcillat, O.; Gouet, P.  
Deposited on : 2014-10-15  
Resolution : 2.20 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  
<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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

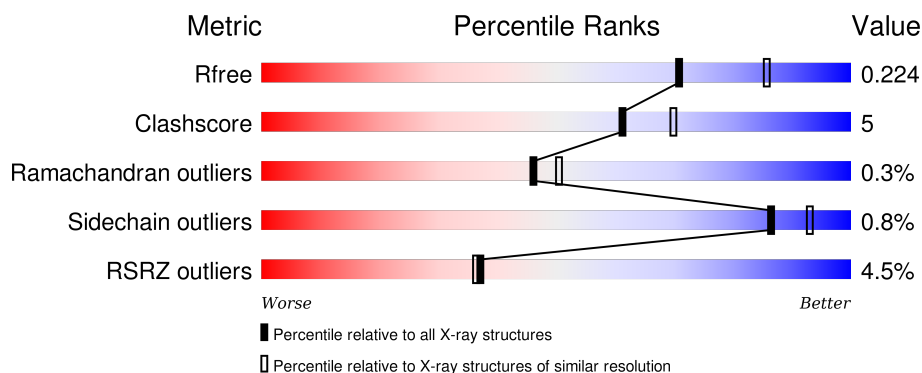
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 2.20 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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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. 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	716	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5930 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 Taurocyamine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	706	Total	C	N	O	S	0	0	0
			5568	3521	973	1045	29			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	VAL	ALA	engineered mutation	UNP P16641
A	235	GLY	ASP	engineered mutation	UNP P16641
A	237	THR	ILE	engineered mutation	UNP P16641
A	493	GLY	ASP	engineered mutation	UNP P16641

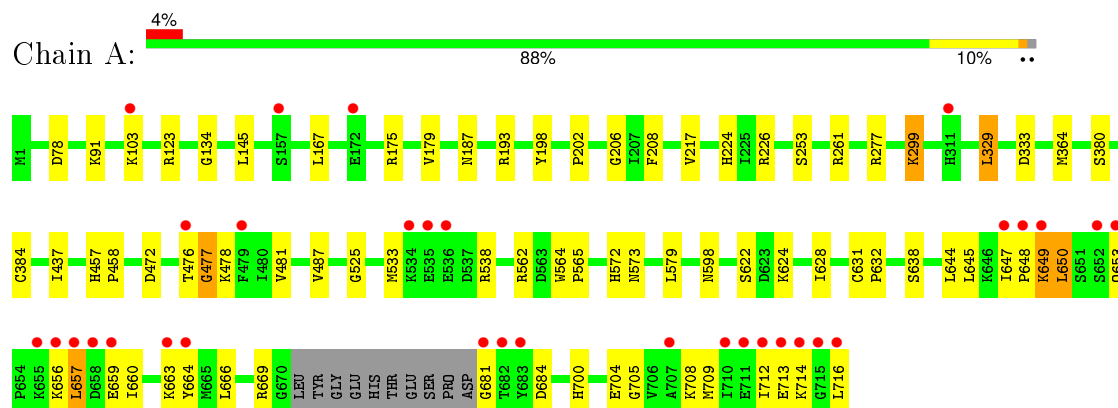
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	362	Total	O	0	0
			362	362		

### 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 ( $\text{RSRZ} > 2$ ). 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.

- Molecule 1: Taurocyamine kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.84Å 122.02Å 62.97Å 90.00° 108.10° 90.00°	Depositor
Resolution (Å)	46.18 – 2.20 46.18 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.18-2.20) 98.9 (46.18-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.176 , 0.224 0.176 , 0.224	Depositor DCC
$R_{free}$ test set	1900 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.1	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 38030 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5930	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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	0.43	0/5680	0.59	2/7660 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	716	LEU	CA-CB-CG	6.18	129.52	115.30
1	A	650	LEU	CB-CG-CD2	-5.74	101.24	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	5568	0	5572	61	0
2	A	362	0	0	6	0
All	All	5930	0	5572	61	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 5.

All (61) 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:572:HIS:HB3	1:A:579:LEU:HD12	1.63	0.78
1:A:663:LYS:HE2	1:A:708:LYS:NZ	2.10	0.67
1:A:709:MET:O	1:A:713:GLU:HG2	1.97	0.65
1:A:663:LYS:HG2	1:A:664:TYR:CD1	2.32	0.65
1:A:123:ARG:HD2	1:A:226:ARG:HD3	1.79	0.64
1:A:123:ARG:NH1	2:A:1103:HOH:O	2.32	0.63
1:A:167:LEU:HD13	1:A:206:GLY:HA2	1.79	0.63
1:A:666:LEU:HD11	1:A:705:GLY:HA3	1.87	0.57
1:A:650:LEU:HD23	1:A:657:LEU:HG	1.86	0.57
1:A:656:LYS:O	1:A:660:ILE:HG12	2.05	0.57
1:A:649:LYS:HE3	1:A:713:GLU:HB3	1.85	0.57
1:A:123:ARG:NH2	2:A:1119:HOH:O	2.38	0.56
1:A:650:LEU:CD2	1:A:657:LEU:HG	2.36	0.55
1:A:663:LYS:HE2	1:A:708:LYS:HZ1	1.70	0.55
1:A:663:LYS:HG2	1:A:664:TYR:HD1	1.72	0.55
1:A:78:ASP:OD1	1:A:261:ARG:NH1	2.40	0.54
1:A:653:GLN:OE1	1:A:656:LYS:N	2.29	0.53
1:A:659:GLU:O	1:A:663:LYS:HB3	2.08	0.53
1:A:647:ILE:HG22	1:A:713:GLU:HG3	1.91	0.52
1:A:175:ARG:O	1:A:179:VAL:HG12	2.08	0.52
1:A:650:LEU:HD22	1:A:713:GLU:OE2	2.09	0.52
1:A:123:ARG:HH21	1:A:277:ARG:HD3	1.74	0.52
1:A:648:PRO:HA	1:A:681:GLY:HA3	1.93	0.51
1:A:472:ASP:HA	1:A:598:ASN:HA	1.93	0.51
1:A:656:LYS:HG3	1:A:659:GLU:OE1	2.12	0.49
1:A:457:HIS:NE2	2:A:1158:HOH:O	2.32	0.49
1:A:299:LYS:HE3	2:A:1027:HOH:O	2.13	0.48
1:A:478:LYS:HE3	1:A:481:VAL:HA	1.96	0.48
1:A:187:ASN:O	1:A:193:ARG:NH1	2.45	0.48
1:A:533:MET:HB3	1:A:538:ARG:CZ	2.45	0.47
1:A:167:LEU:HB3	1:A:202:PRO:HB2	1.97	0.47
1:A:653:GLN:CD	1:A:656:LYS:HB2	2.35	0.47
1:A:708:LYS:O	1:A:712:ILE:HG12	2.14	0.47
1:A:645:LEU:HG	1:A:647:ILE:HG23	1.97	0.46
1:A:669:ARG:HG2	1:A:684:ASP:HB3	1.98	0.46
1:A:487:VAL:HA	1:A:638:SER:O	2.15	0.46
1:A:329:LEU:HB2	1:A:333:ASP:HB2	1.97	0.46
1:A:476:THR:OG1	1:A:477:GLY:N	2.49	0.46
1:A:657:LEU:HA	1:A:657:LEU:HD23	1.69	0.46
1:A:187:ASN:HA	1:A:198:TYR:CZ	2.52	0.45
1:A:714:LYS:HA	1:A:714:LYS:HD2	1.43	0.44
1:A:145:LEU:HD21	1:A:224:HIS:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:PRO:HG2	2:A:1038:HOH:O	2.18	0.44
1:A:622:SER:HB2	1:A:628:ILE:HD11	1.99	0.44
1:A:525:GLY:HA3	1:A:573:ASN:HA	1.99	0.43
1:A:364:MET:HG3	1:A:562:ARG:HD3	2.00	0.43
1:A:380:SER:O	1:A:384:CYS:HB3	2.18	0.43
1:A:644:LEU:HA	1:A:644:LEU:HD12	1.70	0.43
1:A:437:ILE:HD12	1:A:624:LYS:HE3	2.01	0.43
1:A:533:MET:O	1:A:538:ARG:NH1	2.50	0.42
1:A:664:TYR:CE2	1:A:708:LYS:HD3	2.54	0.42
1:A:663:LYS:HE2	1:A:708:LYS:HZ3	1.81	0.42
1:A:700:HIS:NE2	1:A:704:GLU:OE2	2.53	0.41
1:A:299:LYS:HB2	1:A:299:LYS:HE2	1.83	0.41
1:A:664:TYR:CD2	1:A:705:GLY:HA2	2.55	0.41
1:A:208:PHE:HB3	1:A:217:VAL:HB	2.02	0.41
1:A:103:LYS:HE2	2:A:1011:HOH:O	2.20	0.41
1:A:656:LYS:HA	1:A:659:GLU:HB3	2.03	0.40
1:A:91:LYS:HD3	1:A:91:LYS:HA	1.86	0.40
1:A:631:CYS:HA	1:A:632:PRO:HD3	1.98	0.40
1:A:564:TRP:HA	1:A:565:PRO:HA	1.94	0.40

There are no symmetry-related clashes.

## 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	702/716 (98%)	677 (96%)	23 (3%)	2 (0%)	46 50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	477	GLY
1	A	134	GLY

### 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	604/613 (98%)	599 (99%)	5 (1%)	86	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	SER
1	A	299	LYS
1	A	329	LEU
1	A	649	LYS
1	A	657	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	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](#)

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 ⓘ

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	706/716 (98%)	-0.11	32 (4%) 37 36	20, 28, 65, 108	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	716	LEU	9.6
1	A	715	GLY	6.4
1	A	664	TYR	5.2
1	A	648	PRO	4.6
1	A	656	LYS	4.6
1	A	713	GLU	4.2
1	A	653	GLN	4.1
1	A	714	LYS	3.8
1	A	649	LYS	3.7
1	A	657	LEU	3.5
1	A	479	PHE	3.3
1	A	476	THR	3.1
1	A	681	GLY	3.0
1	A	711	GLU	2.9
1	A	682	THR	2.8
1	A	683	TYR	2.8
1	A	535	GLU	2.6
1	A	172	GLU	2.6
1	A	659	GLU	2.6
1	A	655	LYS	2.5
1	A	157	SER	2.5
1	A	311	HIS	2.5
1	A	647	ILE	2.5
1	A	707	ALA	2.4
1	A	536	GLU	2.3
1	A	710	ILE	2.3
1	A	103	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	652	SER	2.3
1	A	663	LYS	2.2
1	A	534	LYS	2.2
1	A	712	ILE	2.1
1	A	658	ASP	2.0

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.