

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	3WXI
Title	:	Crystal structure of trypanosoma brucei gambiense glycerol kinase (ligand-free
		form)
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Deposited on	:	2014-08-01
Resolution	:	2.90 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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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.



Matria	Whole archive	Similar resolution		
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R_{free}	130704	1957 (2.90-2.90)		
Clashscore	141614	2172(2.90-2.90)		
Ramachandran outliers	138981	2115 (2.90-2.90)		
Sidechain outliers	138945	2117 (2.90-2.90)		

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5%

Mol	Chain	Length	Quality of chain						
1	А	518	63%	29%	7%	•			
1	В	518	53%	37%	9%	•			



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7906 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 Glycerol kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	513	Total 3957	C 2499	N 694	0 731	S 33	0	0	0
1	В	512	Total 3940	C 2486	N 692	0 729	S 33	0	0	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	-5	GLY	-	expression tag	UNP D3KVM3
А	-4	ILE	-	expression tag	UNP D3KVM3
A	-3	ASP	-	expression tag	UNP D3KVM3
A	-2	PRO	-	expression tag	UNP D3KVM3
A	-1	PHE	-	expression tag	UNP D3KVM3
А	0	THR	-	expression tag	UNP D3KVM3
В	-5	GLY	-	expression tag	UNP D3KVM3
В	-4	ILE	-	expression tag	UNP D3KVM3
В	-3	ASP	-	expression tag	UNP D3KVM3
В	-2	PRO	-	expression tag	UNP D3KVM3
В	-1	PHE	-	expression tag	UNP D3KVM3
В	0	THR	-	expression tag	UNP D3KVM3

There are 12 discrepancies between the modelled and reference sequences:

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total O 2 2	0	0
2	В	7	Total O 7 7	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Glycerol kinase



P440 Q351 1441 1441 1441 1442 1441 A58 1444 A58 1444 A58 1444 A58 1444 A58 1444 A58 1445 A58 1445 A58 1445 A58 1450 A58 1451 A58 A453 A54 A545 A54 A454 A54 A47 A54 <



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	68.76Å 131.98Å 148.61Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	30.00 - 2.90	Depositor
Resolution (A)	29.75 - 2.90	EDS
% Data completeness	99.5 (30.00-2.90)	Depositor
(in resolution range)	99.5 (29.75-2.90)	EDS
R_{merge}	0.05	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.24 (at 2.90\AA)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
D D.	0.202 , 0.282	Depositor
II, II, <i>free</i>	0.255 , 0.312	DCC
R_{free} test set	1539 reflections (5.04%)	wwPDB-VP
Wilson B-factor $(Å^2)$	101.7	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 35.2	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7906	wwPDB-VP
Average B, all atoms $(Å^2)$	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.70% 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.

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).

Mal	Chain	Bo	nd lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.77	0/4039	0.85	2/5465~(0.0%)	
1	В	0.67	1/4021~(0.0%)	0.76	0/5442	
All	All	0.72	1/8060~(0.0%)	0.81	2/10907~(0.0%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	В	307	GLY	N-CA	5.10	1.53	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	А	369	PRO	CA-N-CD	-8.29	99.90	111.50
1	А	70	ALA	N-CA-C	-5.51	96.12	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	А	3957	0	3968	265	0
1	В	3940	0	3943	304	0
2	А	2	0	0	0	0
2	В	7	0	0	0	0
All	All	7906	0	7911	563	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 36.

The worst 5 of 563 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:B:238:VAL:CG1	1:B:240:ALA:HB3	1.44	1.43
1:B:481:TRP:HZ3	1:B:483:THR:CG2	1.33	1.40
1:A:364:ALA:HB3	1:A:366:TYR:CE2	1.56	1.40
1:B:238:VAL:CG2	1:B:240:ALA:H	1.46	1.28
1:B:238:VAL:HG11	1:B:240:ALA:CB	1.65	1.27

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	Pe	erce	entile	es
1	А	511/518~(99%)	465 (91%)	39~(8%)	7 (1%)	1	11	36	
1	В	510/518~(98%)	456 (89%)	44 (9%)	10 (2%)		7	27	
All	All	1021/1036 (99%)	921 (90%)	83 (8%)	17 (2%)		9	31	

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	335	SER
1	А	337	ILE
1	А	226	GLU
1	А	244	GLU
1	В	340	CYS



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	Pe	rce	\mathbf{nti}	les
1	А	421/425~(99%)	360~(86%)	61 (14%)		3	9	
1	В	418/425~(98%)	350 (84%)	68 (16%)		2	7	
All	All	839/850~(99%)	710~(85%)	129~(15%)		2	8	

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	440	ASP
1	В	468	LEU
1	А	420	ASP
1	А	412	LEU
1	В	476	ARG

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such side chains are listed below:

Mol	Chain	Res	Type
1	В	105	ASN
1	В	243	ASN
1	В	479	ASN
1	В	293	HIS
1	В	224	ASN

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

