



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:20 AM GMT

PDB ID : 4A5B  
Title : Crystal structure of the C258S/C268S variant of Toxoplasma gondii nucleoside triphosphate diphosphohydrolase 1 (NTPDase1)  
Authors : Krug, U.; Zebisch, M.; Strater, N.  
Deposited on : 2011-10-24  
Resolution : 2.48 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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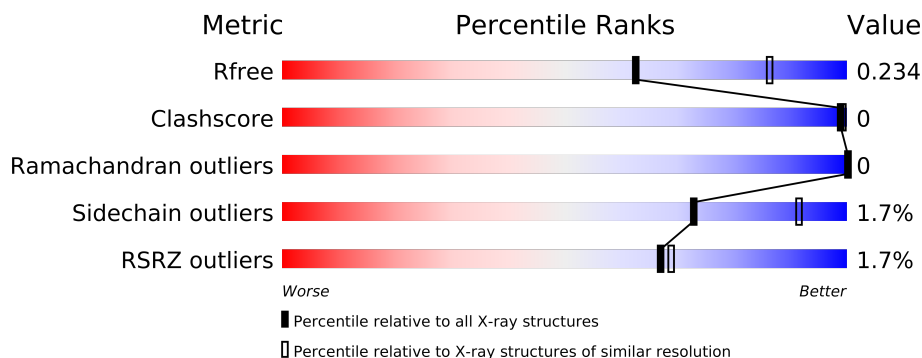
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.48 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	3277 (2.50-2.46)
Clashscore	79885	4136 (2.50-2.46)
Ramachandran outliers	78287	4052 (2.50-2.46)
Sidechain outliers	78261	4054 (2.50-2.46)
RSRZ outliers	66119	3279 (2.50-2.46)

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	611	
1	B	611	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9496 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 NUCLEOSIDE-TRIPHOSPHATASE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	592	Total	C	N	O	S	0	0	0
			4619	2902	810	882	25			
1	B	593	Total	C	N	O	S	0	0	0
			4630	2908	815	882	25			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	EXPRESSION TAG	UNP Q27895
A	629	GLU	-	EXPRESSION TAG	UNP Q27895
A	630	HIS	-	EXPRESSION TAG	UNP Q27895
A	631	HIS	-	EXPRESSION TAG	UNP Q27895
A	632	HIS	-	EXPRESSION TAG	UNP Q27895
A	633	HIS	-	EXPRESSION TAG	UNP Q27895
A	634	HIS	-	EXPRESSION TAG	UNP Q27895
A	635	HIS	-	EXPRESSION TAG	UNP Q27895
A	258	SER	CYS	ENGINEERED MUTATION	UNP Q27895
A	268	SER	CYS	ENGINEERED MUTATION	UNP Q27895
B	25	MET	-	EXPRESSION TAG	UNP Q27895
B	629	GLU	-	EXPRESSION TAG	UNP Q27895
B	630	HIS	-	EXPRESSION TAG	UNP Q27895
B	631	HIS	-	EXPRESSION TAG	UNP Q27895
B	632	HIS	-	EXPRESSION TAG	UNP Q27895
B	633	HIS	-	EXPRESSION TAG	UNP Q27895
B	634	HIS	-	EXPRESSION TAG	UNP Q27895
B	635	HIS	-	EXPRESSION TAG	UNP Q27895
B	258	SER	CYS	ENGINEERED MUTATION	UNP Q27895
B	268	SER	CYS	ENGINEERED MUTATION	UNP Q27895

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	140	Total 140	O 140	0	0
2	B	107	Total 107	O 107	0	0

### 3 Residue-property plots

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.

#### • Molecule 1: NUCLEOSIDE-TRIPHOSPHATASE2

Chain A: 



#### • Molecule 1: NUCLEOSIDE-TRIPHOSPHATASE2

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.73Å 150.40Å 242.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.22 – 2.48 39.11 – 2.48	Depositor EDS
% Data completeness (in resolution range)	(Not available) (39.22-2.48) 99.1 (39.11-2.48)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 2.48Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.176 , 0.226 0.183 , 0.234	Depositor DCC
$R_{free}$ test set	972 reflections (2.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.2	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 26.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 47551 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9496	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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

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	0.51	0/4710	0.72	0/6376
1	B	0.50	0/4722	0.71	0/6393
All	All	0.51	0/9432	0.71	0/12769

There are no bond length outliers.

There are no bond angle outliers.

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	4619	0	0	1	0
1	B	4630	0	0	2	0
2	A	140	0	0	0	0
2	B	107	0	0	1	0
All	All	9496	0	0	3	0

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 0.

All (3) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:124:ALA:O	1:B:131:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:412:GLN:NE2	2:B:2082:HOH:O	2.50	0.44
1:A:473:SER:OG	1:A:475:ASP:OD1	2.36	0.43

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	588/611 (96%)	580 (99%)	8 (1%)	0	100	100
1	B	591/611 (97%)	575 (97%)	16 (3%)	0	100	100
All	All	1179/1222 (96%)	1155 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	510/527 (97%)	501 (98%)	9 (2%)	71	90
1	B	511/527 (97%)	503 (98%)	8 (2%)	75	92
All	All	1021/1054 (97%)	1004 (98%)	17 (2%)	73	91

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	302	VAL

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Mol	Chain	Res	Type
1	A	388	ARG
1	A	447	SER
1	A	469	SER
1	A	475	ASP
1	A	524	GLU
1	A	548	GLN
1	A	591	ASP
1	B	42	ILE
1	B	307	GLU
1	B	309	LEU
1	B	312	GLU
1	B	351	ILE
1	B	366	SER
1	B	451	SER
1	B	549	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

There are no ligands in this entry.

### 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	592/611 (96%)	-0.40	7 (1%) 75 77	16, 31, 56, 109	0
1	B	593/611 (97%)	-0.23	13 (2%) 59 61	17, 35, 70, 93	0
All	All	1185/1222 (96%)	-0.31	20 (1%) 67 69	16, 33, 63, 109	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	ASP	5.3
1	A	291	GLU	4.6
1	B	590	PRO	4.2
1	A	629	GLU	4.0
1	B	591	ASP	4.0
1	A	35	ASP	3.8
1	B	532	ILE	3.8
1	B	535	ASP	3.8
1	B	292	GLY	3.6
1	B	531	ILE	3.5
1	B	293	THR	2.9
1	A	590	PRO	2.7
1	B	294	VAL	2.7
1	A	541	LEU	2.6
1	B	43	ASN	2.4
1	A	40	LYS	2.4
1	B	536	GLY	2.3
1	B	628	LEU	2.3
1	B	533	ARG	2.1
1	B	42	ILE	2.1

## 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 ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.