



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:15 AM GMT

PDB ID : 3DZO
Title : Crystal structure of a rhopty kinase from toxoplasma gondii
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Deposited on : 2008-07-30
Resolution : 1.80 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

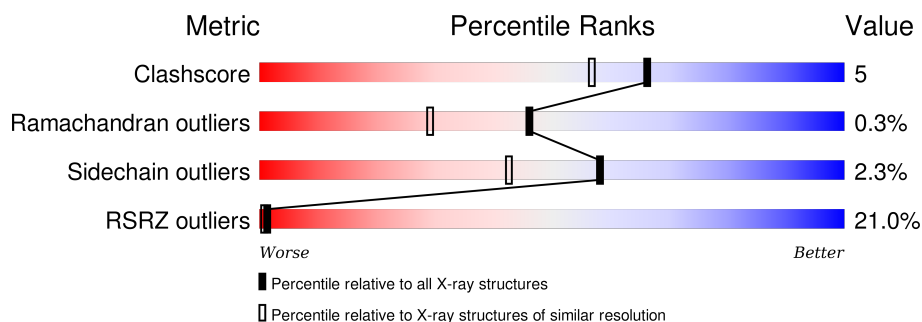
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 ≥ 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	413	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2828 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 Rhoptyr kinase domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	7	0
			2709	1755	460	487	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	178	MET	-	EXPRESSION TAG	PDB 3DZO
A	179	HIS	-	EXPRESSION TAG	PDB 3DZO
A	180	HIS	-	EXPRESSION TAG	PDB 3DZO
A	181	HIS	-	EXPRESSION TAG	PDB 3DZO
A	182	HIS	-	EXPRESSION TAG	PDB 3DZO
A	183	HIS	-	EXPRESSION TAG	PDB 3DZO
A	184	HIS	-	EXPRESSION TAG	PDB 3DZO
A	185	SER	-	EXPRESSION TAG	PDB 3DZO
A	186	SER	-	EXPRESSION TAG	PDB 3DZO
A	187	GLY	-	EXPRESSION TAG	PDB 3DZO
A	188	ARG	-	EXPRESSION TAG	PDB 3DZO
A	189	GLU	-	EXPRESSION TAG	PDB 3DZO
A	190	ASN	-	EXPRESSION TAG	PDB 3DZO
A	191	LEU	-	EXPRESSION TAG	PDB 3DZO
A	192	TYR	-	EXPRESSION TAG	PDB 3DZO
A	193	PHE	-	EXPRESSION TAG	PDB 3DZO
A	194	GLN	-	EXPRESSION TAG	PDB 3DZO
A	195	GLY	-	EXPRESSION TAG	PDB 3DZO

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

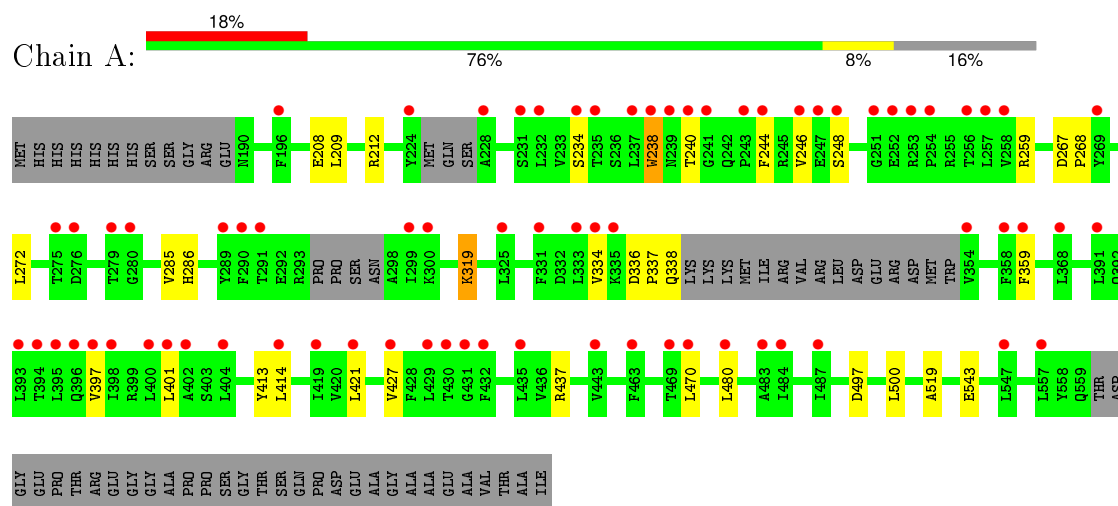
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	118	Total 118	O 118	0	0

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: Rhoptry kinase domain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.26 Å 44.29 Å 105.30 Å 90.00° 98.90° 90.00°	Depositor
Resolution (Å)	35.00 – 1.80 29.99 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (35.00-1.80) 93.6 (29.99-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.04 (at 1.79 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.244 , 0.270 0.237 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.1	EDS
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 34402 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2828	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.39	0/2800	0.53	0/3820

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2709	0	2584	26	0
2	A	1	0	0	0	0
3	A	118	0	0	0	0
All	All	2828	0	2584	26	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 (26) 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:246:VAL:HB	1:A:334:VAL:HG11	1.31	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:LEU:HD11	1:A:414:LEU:HD22	1.57	0.82
1:A:246:VAL:HB	1:A:334:VAL:CG1	2.11	0.78
1:A:208:GLU:OE1	1:A:212:ARG:HD2	1.84	0.77
1:A:319[A]:LYS:H	1:A:319[A]:LYS:HD2	1.50	0.76
1:A:401:LEU:HD12	1:A:480:LEU:HD13	1.67	0.76
1:A:401:LEU:HD11	1:A:414:LEU:CD2	2.25	0.66
1:A:259:ARG:HG2	1:A:259:ARG:HH11	1.67	0.60
1:A:497:ASP:HA	1:A:500:LEU:HD13	1.84	0.60
1:A:259:ARG:NH1	1:A:259:ARG:HG2	2.18	0.59
1:A:519:ALA:HB3	1:A:543:GLU:HG2	1.85	0.59
1:A:259:ARG:HG3	1:A:272:LEU:HD13	1.89	0.55
1:A:401:LEU:CD1	1:A:480:LEU:HB2	2.39	0.52
1:A:259:ARG:CG	1:A:259:ARG:HH11	2.23	0.51
1:A:240:THR:HA	1:A:259:ARG:HH12	1.76	0.49
1:A:248:SER:HA	1:A:334:VAL:HG22	1.95	0.48
1:A:272:LEU:HG	1:A:285:VAL:HB	1.96	0.47
1:A:234:SER:HA	1:A:238:TRP:O	2.15	0.46
1:A:240:THR:HA	1:A:259:ARG:NH1	2.30	0.45
1:A:267:ASP:HA	1:A:268:PRO:HA	1.80	0.45
1:A:421[B]:LEU:HD22	1:A:427:VAL:HG22	2.00	0.43
1:A:397[B]:VAL:HG12	1:A:480:LEU:CD1	2.49	0.42
1:A:336:ASP:O	1:A:338:GLN:N	2.53	0.42
1:A:319[A]:LYS:CD	1:A:319[A]:LYS:H	2.27	0.41
1:A:286:HIS:HB2	1:A:359:PHE:HB2	2.03	0.41
1:A:244:PHE:HE2	1:A:259:ARG:HB2	1.85	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	347/413 (84%)	333 (96%)	13 (4%)	1 (0%)	46	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	PRO

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	273/357 (76%)	266 (97%)	7 (3%)	54 37

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	209	LEU
1	A	238	TRP
1	A	319[A]	LYS
1	A	319[B]	LYS
1	A	413	TYR
1	A	437	ARG
1	A	470	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	A	546	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th 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 ²)	Q<0.9
1	A	348/413 (84%)	1.12	73 (20%) 1 1	20, 31, 35, 37	8 (2%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	THR	8.8
1	A	291	THR	7.4
1	A	397[A]	VAL	6.9
1	A	258	VAL	6.2
1	A	400	LEU	5.3
1	A	429	LEU	5.3
1	A	276	ASP	5.2
1	A	254	PRO	5.1
1	A	244	PHE	5.0
1	A	257	LEU	4.7
1	A	228	ALA	4.6
1	A	393	LEU	4.6
1	A	401	LEU	4.5
1	A	358	PHE	4.3
1	A	290	PHE	4.2
1	A	333	LEU	4.0
1	A	414	LEU	3.9
1	A	421[A]	LEU	3.8
1	A	246	VAL	3.8
1	A	232	LEU	3.7
1	A	231	SER	3.7
1	A	241	GLY	3.6
1	A	354	VAL	3.5
1	A	469	THR	3.5
1	A	275	THR	3.2
1	A	395	LEU	3.2
1	A	234	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	239	ASN	3.1
1	A	398	ILE	3.1
1	A	419	ILE	3.1
1	A	443	VAL	3.0
1	A	480	LEU	3.0
1	A	430	THR	3.0
1	A	404	LEU	3.0
1	A	427	VAL	3.0
1	A	256	THR	3.0
1	A	280	GLY	3.0
1	A	463	PHE	2.9
1	A	331	PHE	2.9
1	A	251	GLY	2.9
1	A	483	ALA	2.8
1	A	243	PRO	2.8
1	A	435	LEU	2.7
1	A	394	THR	2.7
1	A	402	ALA	2.7
1	A	300	LYS	2.7
1	A	432	PHE	2.7
1	A	431	GLY	2.7
1	A	557	LEU	2.5
1	A	224	TYR	2.5
1	A	237	LEU	2.5
1	A	334	VAL	2.4
1	A	253	ARG	2.4
1	A	238	TRP	2.4
1	A	289	TYR	2.4
1	A	359	PHE	2.3
1	A	484	ILE	2.3
1	A	487	ILE	2.3
1	A	396	GLN	2.3
1	A	470	LEU	2.2
1	A	196	PHE	2.2
1	A	335	LYS	2.2
1	A	391	LEU	2.2
1	A	299	ILE	2.2
1	A	240	THR	2.2
1	A	247	GLU	2.2
1	A	252	GLU	2.2
1	A	368	LEU	2.2
1	A	269	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	248	SER	2.1
1	A	279	THR	2.1
1	A	325	LEU	2.1
1	A	547	LEU	2.1

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](#)

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, 95th 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	A	601	1/1	0.92	0.15	-	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.