



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:02 am GMT

PDB ID : 4S1J
Title : Crystal structure of cyclophilin mutant V33A from Leishmania donovani at 2.3 angstrom.
Authors : Roy, S.; Datta, A.K.; Banerjee, R.
Deposited on : 2015-01-14
Resolution : 2.30 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

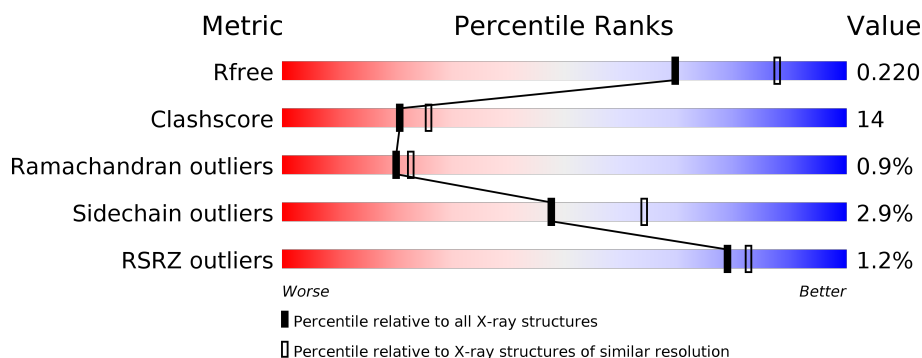
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	172	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>• •</div> </div> </div>
1	B	172	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2677 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 Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1284	820	218	241	5			
1	B	166	Total	C	N	O	S	0	0	0
			1284	820	218	241	5			

There are 14 discrepancies between the modelled and reference sequences:

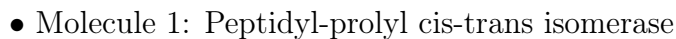
Chain	Residue	Modelled	Actual	Comment	Reference
A	16	HIS	-	EXPRESSION TAG	UNP E9B8M3
A	17	HIS	-	EXPRESSION TAG	UNP E9B8M3
A	18	HIS	-	EXPRESSION TAG	UNP E9B8M3
A	19	HIS	-	EXPRESSION TAG	UNP E9B8M3
A	20	HIS	-	EXPRESSION TAG	UNP E9B8M3
A	21	HIS	-	EXPRESSION TAG	UNP E9B8M3
A	33	ALA	VAL	ENGINEERED MUTATION	UNP E9B8M3
B	16	HIS	-	EXPRESSION TAG	UNP E9B8M3
B	17	HIS	-	EXPRESSION TAG	UNP E9B8M3
B	18	HIS	-	EXPRESSION TAG	UNP E9B8M3
B	19	HIS	-	EXPRESSION TAG	UNP E9B8M3
B	20	HIS	-	EXPRESSION TAG	UNP E9B8M3
B	21	HIS	-	EXPRESSION TAG	UNP E9B8M3
B	33	ALA	VAL	ENGINEERED MUTATION	UNP E9B8M3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	56	Total	O	0	0
			56	56		
2	B	53	Total	O	0	0
			53	53		

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- Molecule 1: Peptidyl-prolyl cis-trans isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	48.53Å 48.53Å 141.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.50 – 2.30 48.53 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.4 (48.50-2.30) 95.1 (48.53-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.191 , 0.222 0.191 , 0.220	Depositor DCC
R_{free} test set	693 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.487 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2677	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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	0.37	0/1315	0.63	0/1776
1	B	0.36	0/1315	0.65	0/1776
All	All	0.37	0/2630	0.64	0/3552

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	1284	0	1261	37	0
1	B	1284	0	1261	33	0
2	A	56	0	0	1	0
2	B	53	0	0	0	0
All	All	2677	0	2522	70	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 14.

All (70) 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:45:ILE:HD12	1:A:120:LEU:HD11	1.10	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ILE:HD12	1:A:120:LEU:CD1	1.86	1.05
1:A:45:ILE:CD1	1:A:120:LEU:HD11	1.95	0.96
1:A:78:ARG:NH1	1:A:80:ILE:HD11	1.97	0.79
1:B:104:GLU:HG2	1:B:105:LYS:HG2	1.63	0.78
1:A:104:GLU:HG2	1:A:105:LYS:HG2	1.72	0.71
1:A:104:GLU:O	1:A:105:LYS:HD3	1.94	0.67
1:A:58:ASN:HA	1:A:101:ILE:HD12	1.75	0.67
1:A:78:ARG:HH12	1:A:80:ILE:HD11	1.62	0.65
1:B:45:ILE:HG23	1:B:120:LEU:HD13	1.80	0.63
1:A:170:ASN:HD22	1:A:171:SER:N	1.98	0.61
1:B:104:GLU:O	1:B:105:LYS:HD3	2.01	0.60
1:A:75:ILE:HD13	2:A:205:HOH:O	2.03	0.59
1:A:45:ILE:HG23	1:A:120:LEU:HD13	1.87	0.57
1:B:92:ASN:HD22	1:B:97:GLY:HA3	1.69	0.57
1:A:101:ILE:H	1:A:101:ILE:HD13	1.70	0.56
1:B:45:ILE:HD13	1:B:120:LEU:HD21	1.88	0.55
1:A:64:THR:OG1	1:A:66:GLU:HG3	2.07	0.55
1:A:75:ILE:HD13	1:A:75:ILE:H	1.72	0.55
1:A:72:LYS:O	1:A:73:ASP:HB2	2.07	0.55
1:A:35:ILE:HD11	1:A:40:LEU:HD21	1.89	0.54
1:B:110:ASN:ND2	1:B:113:VAL:HG23	2.22	0.54
1:B:80:ILE:HG22	1:B:83:PHE:HB3	1.89	0.54
1:B:22:GLU:OE2	1:B:153:LYS:HD3	2.08	0.53
1:B:80:ILE:HD13	1:B:84:MET:CE	2.38	0.53
1:B:72:LYS:O	1:B:73:ASP:HB2	2.08	0.53
1:B:80:ILE:HD13	1:B:84:MET:HE1	1.91	0.52
1:A:45:ILE:HD13	1:A:154:VAL:HA	1.91	0.52
1:B:171:SER:O	1:B:174:ARG:HG2	2.10	0.52
1:B:142:PRO:HA	1:B:145:ASP:OD2	2.11	0.51
1:B:64:THR:OG1	1:B:66:GLU:HG3	2.10	0.51
1:B:60:ARG:NH1	1:B:61:GLN:HG3	2.26	0.51
1:A:170:ASN:ND2	1:A:171:SER:N	2.59	0.51
1:A:34:MET:HG2	1:A:39:PRO:HA	1.92	0.50
1:A:35:ILE:CD1	1:A:40:LEU:HD21	2.43	0.49
1:A:174:ARG:HH11	1:A:174:ARG:HG3	1.78	0.49
1:A:24:GLU:HB3	1:A:50:LYS:HE2	1.94	0.49
1:B:60:ARG:HH12	1:B:61:GLN:HG3	1.77	0.48
1:B:73:ASP:HA	1:B:180:LYS:HE3	1.94	0.48
1:B:34:MET:HG2	1:B:39:PRO:HA	1.96	0.48
1:B:30:TYR:CD1	1:B:187:LEU:HD13	2.49	0.47
1:B:45:ILE:CG2	1:B:120:LEU:HD13	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:VAL:C	1:B:80:ILE:HD12	2.34	0.47
1:B:35:ILE:CD1	1:B:40:LEU:HD21	2.45	0.47
1:B:174:ARG:HG3	1:B:174:ARG:HH11	1.80	0.46
1:B:110:ASN:HD21	1:B:113:VAL:HG23	1.81	0.46
1:A:158:MET:O	1:A:162:LEU:HG	2.16	0.46
1:B:168:LYS:O	1:B:176:VAL:HG23	2.17	0.45
1:A:171:SER:O	1:A:174:ARG:HG2	2.17	0.45
1:B:164:ILE:O	1:B:167:THR:HG22	2.16	0.45
1:B:153:LYS:HE3	1:B:155:LEU:HD23	1.99	0.44
1:A:101:ILE:N	1:A:101:ILE:HD13	2.34	0.43
1:A:164:ILE:O	1:A:167:THR:HG22	2.19	0.43
1:A:101:ILE:CD1	1:A:101:ILE:H	2.31	0.43
1:B:23:PRO:HG2	1:B:48:PHE:CZ	2.54	0.43
1:A:101:ILE:HD11	1:A:102:TYR:CZ	2.54	0.42
1:B:158:MET:O	1:B:162:LEU:HG	2.18	0.42
1:B:105:LYS:HA	1:B:130:ASN:O	2.20	0.42
1:B:144:LEU:HD22	1:B:148:HIS:CD2	2.55	0.42
1:B:88:GLY:HA3	1:B:133:GLN:HA	2.02	0.42
1:A:23:PRO:HG2	1:A:48:PHE:CZ	2.55	0.41
1:A:60:ARG:NH1	1:A:61:GLN:HG3	2.36	0.41
1:A:104:GLU:HG2	1:A:105:LYS:HE2	2.03	0.41
1:A:45:ILE:CD1	1:A:154:VAL:HG22	2.51	0.41
1:B:170:ASN:CG	1:B:171:SER:H	2.24	0.41
1:A:73:ASP:HA	1:A:180:LYS:HE3	2.02	0.41
1:A:58:ASN:O	1:A:62:LEU:HG	2.21	0.40
1:A:170:ASN:HD22	1:A:170:ASN:C	2.22	0.40
1:A:35:ILE:O	1:A:38:GLU:HB3	2.21	0.40
1:A:142:PRO:HA	1:A:145:ASP:OD2	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	164/172 (95%)	154 (94%)	9 (6%)	1 (1%)	28	34
1	B	164/172 (95%)	156 (95%)	6 (4%)	2 (1%)	15	16
All	All	328/344 (95%)	310 (94%)	15 (5%)	3 (1%)	20	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	170	ASN
1	A	36	ASP
1	B	36	ASP

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	138/144 (96%)	134 (97%)	4 (3%)	48	64
1	B	138/144 (96%)	134 (97%)	4 (3%)	48	64
All	All	276/288 (96%)	268 (97%)	8 (3%)	48	64

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ILE
1	A	84	MET
1	A	101	ILE
1	A	170	ASN
1	B	84	MET
1	B	120	LEU
1	B	163	ARG
1	B	170	ASN

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	92	ASN
1	A	170	ASN
1	A	172	HIS
1	B	92	ASN
1	B	170	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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	166/172 (96%)	-0.26	3 (1%) 69 74	17, 30, 59, 81	0
1	B	166/172 (96%)	-0.31	1 (0%) 89 92	19, 30, 58, 86	0
All	All	332/344 (96%)	-0.28	4 (1%) 79 82	17, 30, 59, 86	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	172	HIS	3.0
1	A	171	SER	2.2
1	A	170	ASN	2.2
1	A	172	HIS	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.