



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2018 – 01:01 AM EST

PDB ID : 5OL0
Title : Structure of Leishmania infantum Silent Information Regulator 2 related protein 1 (LiSIR2rp1) in complex with acetylated p53 peptide
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Deposited on : 2017-07-26
Resolution : 1.99 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
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) : rb-20030736

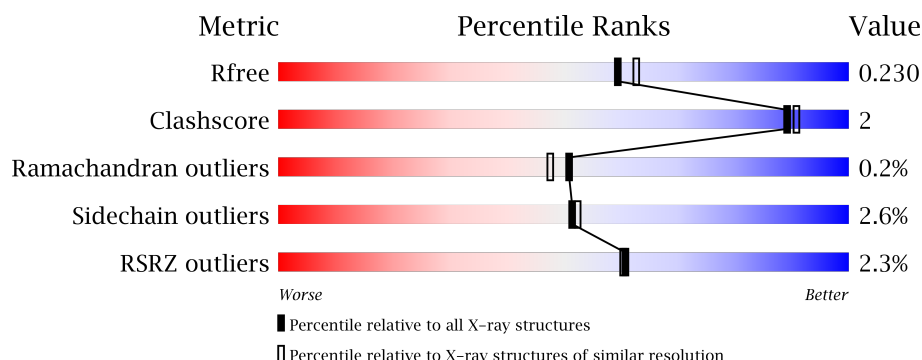
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	324	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>7%</div> <div>13%</div> </div> </div>
1	B	324	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>5%</div> <div>19%</div> </div> </div>
2	C	18	<div> <div></div> <div> <div>44%</div> <div>56%</div> </div> </div>
2	D	18	<div> <div>6%</div> <div> <div></div> <div>39%</div> <div>11%</div> <div>50%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4626 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 Putative silent information regulator 2, Putative silent information regulator 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2190	1394	384	399	13			
1	B	263	Total	C	N	O	S	0	0	0
			2033	1297	358	365	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q8I6E4
A	0	HIS	-	expression tag	UNP Q8I6E4
B	-1	GLY	-	expression tag	UNP Q8I6E4
B	0	HIS	-	expression tag	UNP Q8I6E4

- Molecule 2 is a protein called Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	S	0	0	0
			78	52	16	9	1			
2	D	9	Total	C	N	O	S	0	0	0
			84	55	17	11	1			

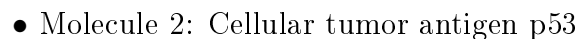
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	109	Total 109	O 109	0	0
4	B	115	Total 115	O 115	0	0
4	C	7	Total 7	O 7	0	0
4	D	8	Total 8	O 8	0	0

- Molecule 1: Putative silent information regulator 2, Putative silent information regulator 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.02Å 65.67Å 66.62Å 90.00° 97.75° 90.00°	Depositor
Resolution (Å)	46.56 – 1.99 46.56 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.56-1.99) 98.8 (46.56-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.167 , 0.226 0.177 , 0.230	Depositor DCC
R_{free} test set	1917 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4626	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.69% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.83	0/2239	0.94	8/3041 (0.3%)
1	B	0.83	0/2077	0.90	6/2818 (0.2%)
2	C	0.74	0/66	1.08	0/82
2	D	0.73	0/72	1.06	0/90
All	All	0.83	0/4454	0.93	14/6031 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	327	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	A	327	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	117	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	B	334	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	110	ARG	NE-CZ-NH2	5.83	123.22	120.30
1	B	332	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	327	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	B	249	LEU	CB-CG-CD2	-5.59	101.50	111.00
1	A	244	ARG	CG-CD-NE	5.47	123.28	111.80
1	A	244	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	334	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	114	ASP	CB-CG-OD1	5.35	123.12	118.30
1	B	110	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	A	249	LEU	CA-CB-CG	-5.15	103.45	115.30

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	2190	0	2173	14	0
1	B	2033	0	2028	4	0
2	C	78	0	88	0	0
2	D	84	0	93	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	109	0	0	1	0
4	B	115	0	0	1	0
4	C	7	0	0	0	0
4	D	8	0	0	1	0
All	All	4626	0	4382	19	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 2.

All (19) 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:68:GLU:O	1:A:69:ASP:HB2	1.63	0.96
1:A:124:GLN:NE2	1:A:217:THR:OG1	2.10	0.84
1:A:106:HIS:HE1	4:A:1131:HOH:O	1.78	0.66
1:B:106:HIS:HE1	4:B:1128:HOH:O	1.79	0.65
1:A:63:GLY:O	1:A:66:ASN:ND2	2.30	0.65
1:A:58:ILE:HD11	1:A:89:ILE:HG23	1.89	0.54
1:A:43:SER:HB3	1:A:48:ILE:HD12	1.91	0.52
1:A:214:ILE:HG22	1:A:217:THR:HG22	1.92	0.51
1:A:68:GLU:O	1:A:69:ASP:CB	2.47	0.51
1:A:218:SER:O	1:A:219:MET:HB2	2.12	0.49
1:B:336:GLN:O	1:B:340:VAL:HG23	2.15	0.47
1:B:103:THR:H	1:B:106:HIS:HD2	1.63	0.46
1:A:85:ILE:O	1:A:89:ILE:HD12	2.20	0.41
1:A:103:THR:H	1:A:106:HIS:HD2	1.68	0.41
1:A:214:ILE:CG2	1:A:217:THR:HG22	2.50	0.41
1:A:52:ARG:O	1:A:54:PRO:HD3	2.21	0.41
2:D:378:SER:HB3	4:D:408:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:VAL:CG1	1:A:237:ARG:HG2	2.51	0.40
1:B:241:ASN:O	1:B:332:ARG:HA	2.21	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	279/324 (86%)	266 (95%)	12 (4%)	1 (0%)	38	33
1	B	257/324 (79%)	253 (98%)	4 (2%)	0	100	100
2	C	5/18 (28%)	5 (100%)	0	0	100	100
2	D	6/18 (33%)	6 (100%)	0	0	100	100
All	All	547/684 (80%)	530 (97%)	16 (3%)	1 (0%)	51	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	ASP

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	236/265 (89%)	232 (98%)	4 (2%)	66	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	219/265 (83%)	212 (97%)	7 (3%)	44	42
2	C	7/15 (47%)	7 (100%)	0	100	100
2	D	8/15 (53%)	7 (88%)	1 (12%)	5	3
All	All	470/560 (84%)	458 (97%)	12 (3%)	51	52

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LEU
1	A	69	ASP
1	A	249	LEU
1	A	327	ARG
1	B	71	THR
1	B	72	ASP
1	B	75	SER
1	B	242	ARG
1	B	243	GLU
1	B	327	ARG
1	B	339	VAL
2	D	379	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	106	HIS
1	A	124	GLN
1	A	164	ASN
1	B	106	HIS
1	B	164	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ALY	C	382	2	11,11,12	1.18	2 (18%)	9,12,14	1.43	1 (11%)
2	ALY	D	382	2	11,11,12	0.90	0	9,12,14	1.04	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ALY	C	382	2	-	0/8/10/12	0/0/0/0
2	ALY	D	382	2	-	0/8/10/12	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	382	ALY	CB-CA	-2.10	1.50	1.53
2	C	382	ALY	CA-C	2.22	1.53	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	382	ALY	CE-NZ-CH	2.69	126.82	122.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are 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

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 [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	283/324 (87%)	-0.14	8 (2%) 53 53	27, 37, 73, 95	0
1	B	263/324 (81%)	-0.25	4 (1%) 74 73	26, 36, 65, 95	0
2	C	7/18 (38%)	0.01	0 100 100	35, 42, 67, 75	0
2	D	8/18 (44%)	0.57	1 (12%) 4 4	32, 47, 74, 83	0
All	All	561/684 (82%)	-0.18	13 (2%) 61 60	26, 37, 72, 95	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	325	VAL	4.7
1	B	51	PHE	4.5
1	A	62	LEU	3.4
2	D	378	SER	3.0
1	A	61	ASN	2.5
1	A	51	PHE	2.4
1	A	358	LEU	2.4
1	A	324	ASP	2.3
1	A	66	ASN	2.2
1	B	8	PRO	2.2
1	B	9	HIS	2.1
1	B	360	ASP	2.1
1	A	357	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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	ALY	C	382	12/13	0.97	0.11	-	27,31,33,42	0
2	ALY	D	382	12/13	0.97	0.08	-	26,28,33,34	0

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
3	ZN	B	1001	1/1	0.93	0.07	-1.01	58,58,58,58	0
3	ZN	A	1001	1/1	0.98	0.05	-2.21	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.