



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 08:08 pm BST

PDB ID : 5OL0  
Title : Structure of Leishmania infantum Silent Information Regulator 2 related protein 1 (LiSIR2rp1) in complex with acetylated p53 peptide  
Authors : Ronin, C.; Ciesielski, F.; Ciapetti, P.  
Deposited on : 2017-07-26  
Resolution : 1.99 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](mailto: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 ⓘ symbol.

---

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

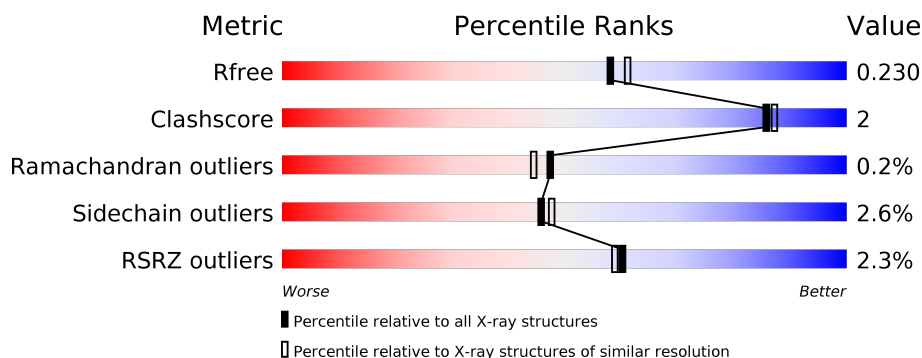
# 1 Overall quality at a glance

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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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  $\geq 3$ , 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  $\leq 5\%$ . 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.6	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

The worst 5 of 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

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	A	2190	0	2173	14	0
1	B	2033	0	2028	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

The worst 5 of 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

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%)	34	30
1	B	257/324 (79%)	253 (98%)	4 (2%)	0	100	100
2	C	5/18 (28%)	5 (100%)	0	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	6/18 (33%)	6 (100%)	0	0	100	100
All	All	547/684 (80%)	530 (97%)	16 (3%)	1 (0%)	47	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	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	236/265 (89%)	232 (98%)	4 (2%)	60	65
1	B	219/265 (83%)	212 (97%)	7 (3%)	39	38
2	C	7/15 (47%)	7 (100%)	0	100	100
2	D	8/15 (53%)	7 (88%)	1 (12%)	4	2
All	All	470/560 (84%)	458 (97%)	12 (3%)	46	48

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	72	ASP
1	B	75	SER
1	B	327	ARG
1	B	71	THR
1	B	243	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	B	164	ASN
1	A	164	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	106	HIS
1	B	106	HIS

### 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	10,11,12	1.06	1 (10%)	7,12,14	1.33	1 (14%)
2	ALY	D	382	2	10,11,12	0.98	0	7,12,14	0.82	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	-	0/9/10/12	-
2	ALY	D	382	2	-	0/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	382	ALY	CB-CA	-2.12	1.50	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	C	382	ALY	CE-NZ-CH	2.77	126.82	122.56

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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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 [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, 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	283/324 (87%)	-0.14	8 (2%) 53 51	27, 37, 73, 95	0
1	B	263/324 (81%)	-0.25	4 (1%) 73 72	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%)	0.58	1 (12%) 3 3	32, 47, 74, 83	0
All	All	561/684 (82%)	-0.18	13 (2%) 60 59	26, 37, 72, 95	0

The worst 5 of 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	3.1
1	A	51	PHE	2.5

### 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	ALY	C	382	12/13	0.97	0.10	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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	B	1001	1/1	0.93	0.07	58,58,58,58	0
3	ZN	A	1001	1/1	0.98	0.05	53,53,53,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.