

Full wwPDB X-ray Structure Validation Report (i)

Apr 8, 2024 – 12:51 PM EDT

PDB ID	:	8G91
Title	:	LaM domain of human LARP1 in complex with Rp phosphorothioate isomer
		of AAAAA(SRA) RNA
Authors	:	Kozlov, G.; Jiang, J.; Gehring, K.
Deposited on		
Resolution	:	1.20 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

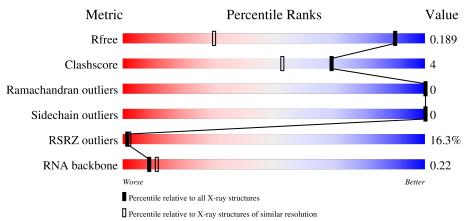
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.20 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)
RSRZ outliers	127900	1200 (1.22-1.18)
RNA backbone	3102	1000 (2.34-0.62)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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				
			13%				
1	A	99		83%		6% • 10%	
			33%				
2	В	6	17%	33%	17%	33%	



8G91

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 936 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 Isoform 2 of La-related protein 1.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	89	Total 749	C 485	N 125	0 138	S 1	0	1	0

There are 11 discrepancies between the modelled and reference sequences:

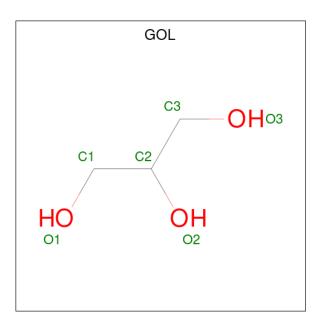
Chain	Residue	Modelled	Actual	Comment	Reference
А	312	MET	-	initiating methionine	UNP Q6PKG0-3
А	313	GLY	-	expression tag	UNP Q6PKG0-3
А	314	SER	-	expression tag	UNP Q6PKG0-3
А	315	SER	-	expression tag	UNP Q6PKG0-3
А	316	HIS	-	expression tag	UNP Q6PKG0-3
A	317	HIS	-	expression tag	UNP Q6PKG0-3
А	318	HIS	-	expression tag	UNP Q6PKG0-3
A	319	HIS	-	expression tag	UNP Q6PKG0-3
А	320	HIS	-	expression tag	UNP Q6PKG0-3
А	321	HIS	-	expression tag	UNP Q6PKG0-3
А	322	SER	-	expression tag	UNP Q6PKG0-3

• Molecule 2 is a RNA chain called RNA (5'-R(*AP*AP*AP*AP*AP*(SRA))-3').

Mol	Chain	Residues		A	tom	ıs			ZeroOcc	AltConf	Trace
2	В	4	Total 75	C 35	N 15	O 21	Р 3	S 1	0	0	0

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





I	Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
	3	А	1	Total 6	${ m C} { m 3}$	O 3	0	0

• Molecule 4 is water.

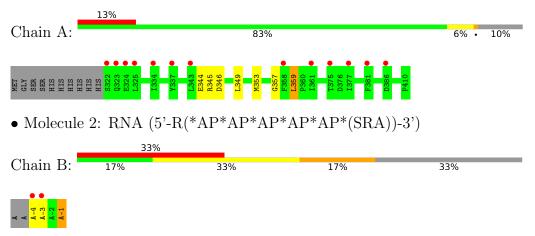
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	97	Total O 97 97	0	0
4	В	9	Total O 9 9	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Isoform 2 of La-related protein 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants	53.78Å 53.78Å 90.45Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.06 - 1.20	Depositor
Resolution (A)	35.06 - 1.20	EDS
% Data completeness	99.1 (35.06-1.20)	Depositor
(in resolution range)	99.1 (35.06-1.20)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.30 (at 1.20 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
D D	0.178 , 0.189	Depositor
R, R_{free}	0.177 , 0.189	DCC
R_{free} test set	2085 reflections $(4.99%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	13.2	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.39, 51.6	EDS
L-test for twinning ²	$ \langle L \rangle = 0.46, \langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	936	wwPDB-VP
Average B, all atoms $(Å^2)$	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.30% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: GOL, SRA

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		
	CHAIN RMSZ # Z > 5		RMSZ = # Z > 5			
1	А	0.31	0/768	0.71	1/1037~(0.1%)	
2	В	0.34	0/59	0.71	0/90	
All	All	0.32	0/827	0.71	1/1127~(0.1%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	A	359	LEU	CA-CB-CG	-5.35	102.99	115.30

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	А	749	0	746	5	0
2	В	75	0	39	2	0
3	А	6	0	8	0	0
4	А	97	0	0	2	0
4	В	9	0	0	1	0
All	All	936	0	793	6	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 4.

All (6) 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:345:ARG:NH2	4:A:601:HOH:O	2.02	0.91
1:A:344[B]:GLU:OE1	4:A:601:HOH:O	2.01	0.79
1:A:349:LEU:HD11	1:A:359:LEU:HD13	1.97	0.47
1:A:346:ASP:OD1	2:B:-1:SRA:O2'	2.33	0.46
1:A:353:MET:HG2	1:A:357:GLY:O	2.17	0.44
2:B:-4:A:O2'	4:B:101:HOH:O	2.22	0.41

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	avoured Allowed		Percentiles		
1	А	88/99~(89%)	86~(98%)	2(2%)	0	100 100		

There are no Ramachandran outliers to report.

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			
1	А	81/92~(88%)	81 (100%)	0	100 100)	



There are no protein residues with a non-rotameric sidechain to report.

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

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	В	2/6~(33%)	1 (50%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	В	-3	А

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is 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		
IVIOI					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	SRA	В	-1	2	18,24,25	<mark>3.90</mark>	10 (55%)	18,35,38	3.00	7 (38%)

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	SRA	В	-1	2	-	0/3/25/26	0/3/3/3

All (10) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
2	В	-1	SRA	C2'-C3'	-9.75	1.26	1.53
2	В	-1	SRA	O4'-C1'	6.42	1.50	1.41
2	В	-1	SRA	O4'-C4'	-6.07	1.31	1.45
2	В	-1	SRA	C2'-C1'	5.30	1.61	1.53
2	В	-1	SRA	C3'-C4'	4.90	1.65	1.53
2	В	-1	SRA	C6-N6	3.39	1.46	1.34
2	В	-1	SRA	O2'-C2'	3.28	1.50	1.43
2	В	-1	SRA	C2-N3	2.77	1.36	1.32
2	В	-1	SRA	O3'-C3'	2.30	1.48	1.43
2	В	-1	SRA	C5-C4	-2.25	1.35	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	-1	SRA	C5-C6-N6	6.58	130.35	120.35
2	В	-1	SRA	C3'-C2'-C1'	5.70	109.56	100.98
2	В	-1	SRA	N3-C2-N1	-5.28	120.42	128.68
2	В	-1	SRA	O4'-C1'-C2'	-4.65	100.13	106.93
2	В	-1	SRA	N6-C6-N1	-4.29	109.66	118.57
2	В	-1	SRA	C1'-N9-C4	-2.35	122.50	126.64
2	В	-1	SRA	O3'-C3'-C4'	-2.22	104.64	111.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

\mathbf{N}	ſol	Chain	Res	Type	Clashes	Symm-Clashes
	2	В	-1	SRA	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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		
					LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
	3	GOL	А	501	-	$5,\!5,\!5$	0.89	0	$5,\!5,\!5$	0.98	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
3	GOL	А	501	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	501	GOL	O1-C1-C2-C3
3	А	501	GOL	O1-C1-C2-O2
3	А	501	GOL	C1-C2-C3-O3

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^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2		$OWAB(Å^2)$	Q<0.9	
1	А	89/99~(89%)	1.26	13 (14%)	2	3	9, 15, 29, 68	0
2	В	3/6~(50%)	3.99	2~(66%)	0	0	21, 21, 30, 88	0
All	All	92/105~(87%)	1.35	15~(16%)	1	2	9, 16, 36, 88	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	322	SER	9.9
2	В	-3	А	6.8
1	А	325	LEU	5.2
1	А	323	GLN	4.4
2	В	-4	А	4.1
1	А	324	GLU	3.7
1	А	386	ASP	3.1
1	А	361	ILE	2.5
1	А	375	THR	2.4
1	А	358	PHE	2.4
1	А	377	ILE	2.2
1	А	334	ILE	2.0
1	А	337	TYR	2.0
1	А	381	PHE	2.0
1	А	343	LEU	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. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q < 0.9
2	SRA	В	-1	22/23	0.95	0.13	$11,\!16,\!25,\!35$	0

6.3 Carbohydrates (i)

There are no monosaccharides 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^{th} 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 ²)	Q<0.9
3	GOL	А	501	6/6	0.92	0.21	22,34,37,44	0

6.5 Other polymers (i)

There are no such residues in this entry.

