



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 09:35 AM EDT

PDB ID : 6D12
Title : Crystal structure of C-terminal xRRM domain of human Larp7 bound to 7SK stem-loop 4 RNA
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Deposited on : 2018-04-11
Resolution : 2.21 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 ⓘ 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 ⓘ](#)) 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 : 2.37.1
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) : 2.37.1

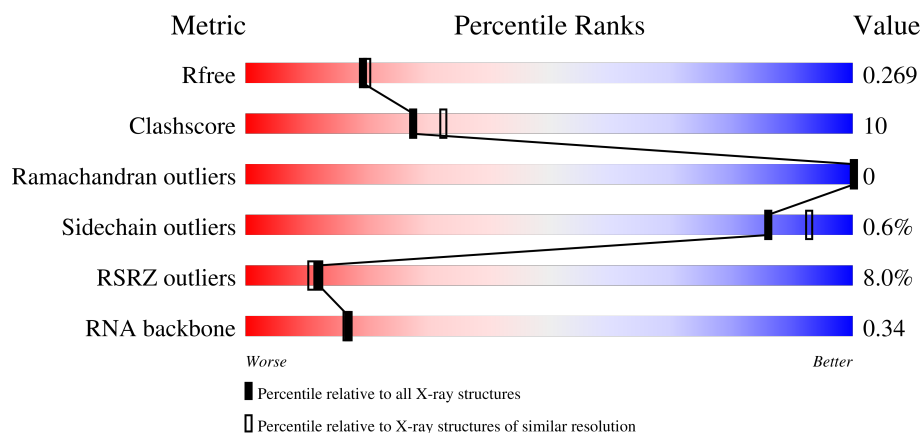
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)
RNA backbone	3102	1032 (2.60-1.80)

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 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 $\leq 5\%$. 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	113	<div> <div>4%</div> <div>74%</div> <div>14%</div> <div>12%</div> </div>
1	B	113	<div> <div>7%</div> <div>73%</div> <div>18%</div> <div>9%</div> </div>
2	C	38	<div> <div>18%</div> <div>24%</div> <div>53%</div> <div>24%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2421 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 La-related protein 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	100	Total	C	N	O	S	Se	0	0	0
			761	485	134	138	2	2			
1	B	103	Total	C	N	O	S	Se	0	0	0
			798	507	143	144	2	2			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	444	SER	-	expression tag	UNP Q4G0J3
A	475	MSE	LEU	engineered mutation	UNP Q4G0J3
A	501	LEU	GLU	engineered mutation	UNP Q4G0J3
A	504	LEU	GLN	engineered mutation	UNP Q4G0J3
A	521	MSE	LEU	engineered mutation	UNP Q4G0J3
B	444	SER	-	expression tag	UNP Q4G0J3
B	475	MSE	LEU	engineered mutation	UNP Q4G0J3
B	501	LEU	GLU	engineered mutation	UNP Q4G0J3
B	504	LEU	GLN	engineered mutation	UNP Q4G0J3
B	521	MSE	LEU	engineered mutation	UNP Q4G0J3

- Molecule 2 is a RNA chain called human 7SK RNA stem-loop 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	38	Total	C	N	O	P	0	0	0
			816	362	146	270	38			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	30	Total	O	0	0
			30	30		

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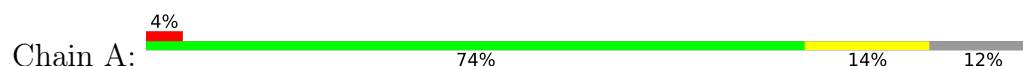
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	O	0	0
			1	1		

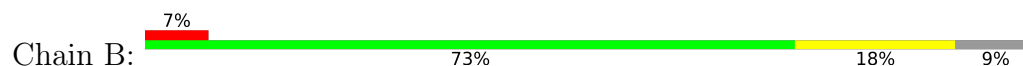
3 Residue-property plots [i](#)

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.

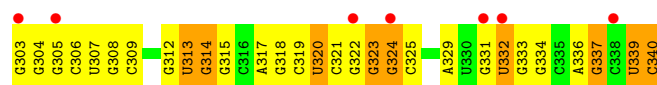
- Molecule 1: La-related protein 7



- Molecule 1: La-related protein 7



- Molecule 2: human 7SK RNA stem-loop 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.91Å 34.03Å 95.01Å 90.00° 95.18° 90.00°	Depositor
Resolution (Å)	94.62 – 2.21 94.62 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.5 (94.62-2.21) 90.5 (94.62-2.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.69 (at 2.20Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.228 , 0.267 0.228 , 0.269	Depositor DCC
R_{free} test set	719 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2421	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.07% 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	0.41	0/774	0.62	0/1049
1	B	0.57	0/812	0.64	0/1099
2	C	0.46	0/911	1.07	0/1420
All	All	0.48	0/2497	0.84	0/3568

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	761	0	744	11	0
1	B	798	0	788	14	0
2	C	816	0	411	22	0
3	A	15	0	0	0	0
3	B	30	0	0	0	0
3	C	1	0	0	0	0
All	All	2421	0	1943	43	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 10.

All (43) 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)
2:C:303:G:H2'	2:C:304:G:H8	1.55	0.71
1:B:468:ARG:HD2	2:C:314:G:C2	2.26	0.70
2:C:321:C:H2'	2:C:322:G:C8	2.28	0.69
1:B:543:LYS:NZ	2:C:313:U:OP2	2.21	0.67
1:B:468:ARG:HH11	1:B:468:ARG:HG2	1.63	0.63
2:C:317:A:H2'	2:C:318:G:C8	2.35	0.61
2:C:320:U:H2'	2:C:321:C:C6	2.34	0.61
1:B:548:ARG:NH1	2:C:308:G:O6	2.28	0.61
2:C:323:G:H1	2:C:339:U:H3	1.47	0.60
1:B:464:PRO:HA	1:B:491:THR:HG22	1.85	0.58
2:C:303:G:H2'	2:C:304:G:C8	2.38	0.57
1:A:527:ASP:HB3	1:A:531:ARG:NH1	2.20	0.57
1:B:459:ILE:HG12	1:B:521:MSE:HG2	1.87	0.56
1:B:509:ALA:HB3	1:B:513:ILE:HD12	1.88	0.56
2:C:324:G:H2'	2:C:325:C:C6	2.42	0.55
1:B:465:LEU:HD13	1:B:486:LEU:HD13	1.90	0.54
1:A:479:SER:HB3	1:A:502:ASP:HB3	1.89	0.54
1:A:527:ASP:HB3	1:A:531:ARG:HH12	1.75	0.50
1:B:543:LYS:O	1:B:546:GLN:HG2	2.11	0.49
2:C:303:G:C2	2:C:322:G:C2	3.00	0.49
1:A:456:ILE:HD12	1:A:532:TYR:CD2	2.47	0.48
2:C:306:C:H2'	2:C:307:U:C6	2.49	0.47
2:C:317:A:H2'	2:C:318:G:H8	1.79	0.47
1:A:527:ASP:O	1:A:531:ARG:HG3	2.14	0.47
1:A:504:LEU:O	1:A:507:ILE:HG13	2.13	0.47
1:B:468:ARG:HG2	1:B:468:ARG:NH1	2.30	0.47
1:B:472:ARG:HB2	1:B:484:VAL:HG21	1.97	0.47
1:A:475:MSE:HE2	1:A:513:ILE:CD1	2.45	0.46
1:B:476:ALA:HA	1:B:479:SER:O	2.15	0.46
1:A:531:ARG:HA	1:A:534:GLN:HG3	1.98	0.46
2:C:304:G:H2'	2:C:305:G:H8	1.82	0.45
1:A:483:TYR:HE2	2:C:332:U:H5''	1.82	0.45
2:C:339:U:H2'	2:C:340:C:O4'	2.17	0.45
2:C:336:A:H2'	2:C:337:G:O4'	2.17	0.45
1:B:467:GLY:O	1:B:470:GLN:N	2.49	0.45
2:C:324:G:H2'	2:C:325:C:H6	1.81	0.44
1:A:475:MSE:HB2	1:A:481:VAL:HG21	2.00	0.42
2:C:323:G:H2'	2:C:324:G:H8	1.83	0.42
1:B:466:PRO:HG2	1:B:471:VAL:HG23	2.02	0.42
2:C:319:C:C4	2:C:320:U:C4	3.08	0.42
2:C:308:G:H2'	2:C:309:C:O4'	2.21	0.41
2:C:306:C:H2'	2:C:307:U:H6	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:LYS:HD3	1:A:517:HIS:NE2	2.36	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	Allowed	Outliers	Percentiles	
1	A	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	B	101/113 (89%)	96 (95%)	5 (5%)	0	100	100
All	All	199/226 (88%)	193 (97%)	6 (3%)	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	Percentiles	
1	A	77/97 (79%)	76 (99%)	1 (1%)	69	81
1	B	82/97 (84%)	82 (100%)	0	100	100
All	All	159/194 (82%)	158 (99%)	1 (1%)	86	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	472	ARG

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	37/38 (97%)	15 (40%)	0

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	312	G
2	C	313	U
2	C	314	G
2	C	315	G
2	C	320	U
2	C	323	G
2	C	324	G
2	C	329	A
2	C	331	G
2	C	332	U
2	C	333	G
2	C	334	G
2	C	337	G
2	C	339	U
2	C	340	C

There are no RNA pucker outliers to report.

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

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	98/113 (86%)	0.49	4 (4%)	37 35	26, 41, 63, 74	0
1	B	101/113 (89%)	0.43	8 (7%)	12 11	20, 33, 58, 101	2 (1%)
2	C	38/38 (100%)	1.19	7 (18%)	1 1	48, 107, 133, 136	0
All	All	237/264 (89%)	0.58	19 (8%)	12 11	20, 40, 120, 136	2 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	466	PRO	3.9
1	A	447	THR	3.3
1	A	518	CYS	3.1
2	C	324	G	3.1
1	B	545	ASN	3.0
1	B	546	GLN	3.0
2	C	332	U	2.9
1	A	510	TYR	2.9
1	B	548	ARG	2.8
1	B	547	PRO	2.7
2	C	303	G	2.7
2	C	338	C	2.6
2	C	305	G	2.6
1	B	543	LYS	2.5
2	C	322	G	2.4
2	C	331	G	2.2
1	B	478	ILE	2.2
1	B	544	LEU	2.2
1	A	465	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 monosaccharides 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.