



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:01 PM GMT

PDB ID : 4WKR
Title : LaRP7 wrapping up the 3' hairpin of 7SK non-coding RNA (302-332)
Authors : Uchikawa, E.; Natchiar, K.S.; Han, X.; Proux, F.; Roblin, P.; Zhang, E.;
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Deposited on : 2014-10-03
Resolution : 3.20 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
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

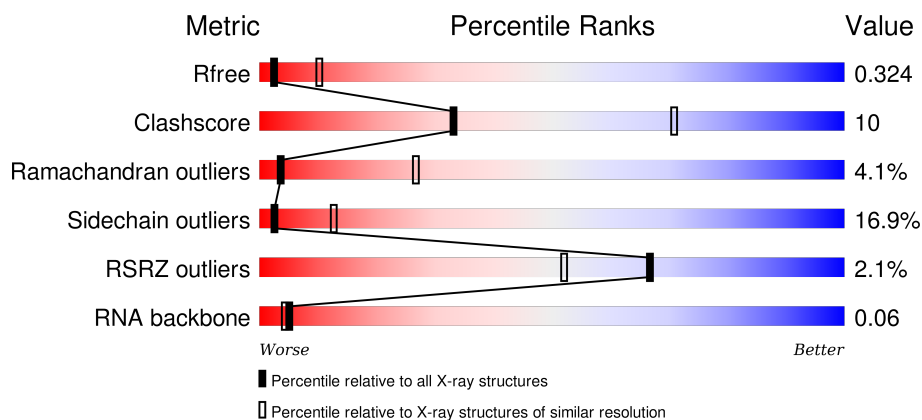
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)
RNA backbone	2183	1079 (3.70-2.70)

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	208	<div> <div> <div></div> <div>52%</div> <div>19%</div> <div>5%</div> <div>23%</div> </div> </div>
1	B	208	<div> <div> <div></div> <div>51%</div> <div>19%</div> <div>7%</div> <div>23%</div> </div> </div>
2	C	31	<div> <div> <div>3%</div> <div>10%</div> <div>6%</div> <div>84%</div> </div> </div>
2	D	31	<div> <div> <div>3%</div> <div>6%</div> <div>6%</div> <div>84%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2701 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	161	Total	C	N	O	S	0	0	0
			1261	803	224	232	2			
1	B	161	Total	C	N	O	S	0	0	0
			1267	808	227	230	2			

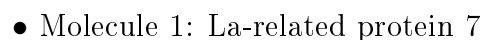
- Molecule 2 is a RNA chain called 7SK GGHP4 (300-332).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	P	0	0	0
			68	27	6	30	5			
2	D	5	Total	C	N	O	P	0	0	0
			100	45	11	39	5			

- Molecule 3 is water.

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

- Molecule 1: La-related protein 7



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.45Å 33.50Å 119.08Å 90.00° 128.99° 90.00°	Depositor
Resolution (Å)	59.06 – 3.20 59.06 – 3.20	Depositor EDS
% Data completeness (in resolution range)	94.0 (59.06-3.20) 94.0 (59.06-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.221 , 0.274 0.273 , 0.324	Depositor DCC
R_{free} test set	382 reflections (4.91%)	DCC
Wilson B-factor (Å ²)	90.5	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 67.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 8156 reflections (0.012%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2701	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.31% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.59	1/1286 (0.1%)	1.19	12/1741 (0.7%)
1	B	0.86	3/1291 (0.2%)	1.08	13/1743 (0.7%)
2	C	1.08	0/71	1.69	0/104
2	D	1.52	1/109 (0.9%)	2.25	6/166 (3.6%)
All	All	0.79	5/2757 (0.2%)	1.23	31/3754 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	188	ASN	C-N	20.89	1.74	1.34
1	B	104	LEU	C-N	-10.96	1.08	1.34
2	D	-5	C	C1'-N1	9.03	1.62	1.48
1	A	68	TYR	C-N	-8.94	1.13	1.34
1	B	105	GLU	C-N	7.80	1.47	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	LEU	C-N-CA	18.82	168.74	121.70
1	A	105	GLU	N-CA-CB	-15.45	82.79	110.60
1	B	105	GLU	N-CA-C	11.90	143.13	111.00
1	B	104	LEU	O-C-N	-11.57	104.18	122.70
1	A	188	ASN	O-C-N	-11.48	99.28	121.10
2	D	-4	U	P-O3'-C3'	11.35	133.32	119.70
1	B	105	GLU	CB-CA-C	-10.89	88.62	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	TYR	N-CA-C	10.08	138.20	111.00
1	A	161	SER	CB-CA-C	9.40	127.97	110.10
1	B	161	SER	CB-CA-C	9.13	127.45	110.10
1	A	68	TYR	O-C-N	-8.89	108.47	122.70
1	B	105	GLU	CA-C-N	-8.61	98.99	116.20
1	B	161	SER	N-CA-C	-8.28	88.64	111.00
1	A	161	SER	N-CA-C	-8.17	88.94	111.00
2	D	-5	C	C3'-C2'-C1'	-7.95	95.14	101.50
1	B	104	LEU	CA-C-N	7.81	134.38	117.20
1	A	105	GLU	N-CA-C	6.99	129.87	111.00
1	B	102	LEU	N-CA-C	-6.85	92.49	111.00
1	B	188	ASN	CA-C-N	-6.82	98.00	117.10
2	D	-4	U	C3'-C2'-C1'	6.48	106.68	101.50
1	A	104	LEU	CB-CA-C	-6.19	98.44	110.20
1	A	68	TYR	CB-CA-C	-5.69	99.01	110.40
1	A	162	THR	N-CA-CB	-5.63	99.61	110.30
1	B	162	THR	N-CA-CB	-5.59	99.68	110.30
1	B	101	GLU	N-CA-CB	5.56	120.61	110.60
2	D	-4	U	O4'-C1'-N1	5.49	112.59	108.20
2	D	-4	U	N1-C2-O2	5.36	126.55	122.80
1	A	68	TYR	CA-C-N	5.32	128.90	117.20
1	B	112	LYS	CB-CA-C	-5.27	99.86	110.40
1	B	105	GLU	O-C-N	5.19	132.02	123.20
2	D	-5	C	C2'-C3'-O3'	5.06	121.79	113.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	ASN	Mainchain

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	1261	0	1225	19	0
1	B	1267	0	1249	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	68	0	31	0	0
2	D	100	0	52	0	0
3	A	3	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	2701	0	2557	54	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 (54) 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:B:188:ASN:C	1:B:189:PRO:N	1.74	1.40
1:B:105:GLU:HB2	1:B:107:THR:HG22	1.18	1.16
1:B:105:GLU:HB2	1:B:107:THR:CG2	2.05	0.84
1:B:188:ASN:ND2	1:B:189:PRO:CD	2.46	0.79
1:B:105:GLU:CB	1:B:107:THR:HG22	2.07	0.79
1:B:97:SER:OG	1:B:100:VAL:HG12	1.84	0.76
1:B:188:ASN:CA	1:B:189:PRO:N	2.48	0.75
1:B:188:ASN:ND2	1:B:189:PRO:HD2	2.05	0.71
1:B:188:ASN:ND2	1:B:189:PRO:HD3	2.05	0.71
1:A:52:HIS:HB3	1:A:118:ARG:HD2	1.71	0.71
1:B:99:VAL:O	1:B:100:VAL:HB	1.92	0.68
1:A:100:VAL:HA	1:A:110:ARG:O	1.96	0.64
1:A:188:ASN:HB3	1:A:189:PRO:CD	2.26	0.64
1:B:188:ASN:CG	1:B:189:PRO:HD2	2.20	0.62
1:B:100:VAL:O	1:B:112:LYS:HD2	2.00	0.62
1:A:99:VAL:O	1:A:100:VAL:HG12	2.01	0.61
1:B:99:VAL:HG21	1:B:111:ARG:HH21	1.66	0.60
1:B:99:VAL:O	1:B:99:VAL:HG13	2.03	0.59
1:B:188:ASN:C	1:B:189:PRO:CA	2.68	0.59
1:A:178:GLN:HA	1:A:181:LYS:HE3	1.86	0.58
1:B:188:ASN:CG	1:B:189:PRO:CD	2.74	0.55
1:A:188:ASN:HB3	1:A:189:PRO:HD3	1.88	0.55
1:B:102:LEU:HG	1:B:109:ILE:HG22	1.88	0.54
1:A:102:LEU:HG	1:A:109:ILE:HG22	1.88	0.54
1:A:140:TRP:HD1	1:A:143:ARG:HH21	1.54	0.54
1:A:105:GLU:HB3	1:A:107:THR:HG22	1.89	0.53
1:B:52:HIS:HB3	1:B:118:ARG:HD3	1.91	0.53
1:B:175:THR:C	1:B:177:GLU:H	2.13	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:HIS:HB3	1:B:118:ARG:CD	2.42	0.48
1:B:183:ILE:O	1:B:186:LEU:HB3	2.13	0.48
1:A:183:ILE:O	1:A:186:LEU:HB3	2.13	0.48
1:B:103:ASP:N	1:B:103:ASP:OD1	2.24	0.48
1:B:126:THR:HA	1:B:172:GLU:HA	1.95	0.48
1:A:84:THR:HG22	1:A:86:ASP:H	1.79	0.47
1:A:52:HIS:HB3	1:A:118:ARG:CD	2.44	0.47
1:B:134:LYS:C	1:B:136:VAL:H	2.18	0.47
1:B:84:THR:HG22	1:B:86:ASP:H	1.79	0.47
1:A:134:LYS:C	1:A:136:VAL:H	2.18	0.47
1:B:140:TRP:O	1:B:144:VAL:HG22	2.15	0.46
1:B:188:ASN:HA	1:B:189:PRO:N	2.31	0.46
1:B:126:THR:HG22	1:B:172:GLU:HB2	1.97	0.46
1:A:188:ASN:O	1:A:189:PRO:C	2.55	0.45
1:B:105:GLU:CB	1:B:107:THR:CG2	2.81	0.45
1:B:155:SER:HB3	1:B:170:PHE:HB2	1.98	0.45
1:A:157:PRO:HB2	1:A:166:LYS:HD2	1.99	0.44
1:A:155:SER:HB3	1:A:170:PHE:HB2	1.99	0.44
1:A:152:VAL:HG21	1:A:174:GLU:HG2	2.00	0.43
1:B:68:TYR:HB3	1:B:108:ARG:HB3	2.01	0.43
1:B:154:ILE:HG12	1:B:171:VAL:HG13	2.01	0.42
1:B:105:GLU:OE1	1:B:105:GLU:N	2.53	0.42
1:A:154:ILE:HG12	1:A:171:VAL:HG13	2.01	0.42
1:A:87:GLY:HA2	1:A:90:ILE:HD12	2.01	0.42
1:B:91:ALA:HB1	1:B:95:ARG:HH12	1.85	0.41
1:B:87:GLY:HA2	1:B:90:ILE:HD12	2.02	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	159/208 (76%)	139 (87%)	13 (8%)	7 (4%)	3	24
1	B	159/208 (76%)	132 (83%)	21 (13%)	6 (4%)	4	28
All	All	318/416 (76%)	271 (85%)	34 (11%)	13 (4%)	3	27

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	VAL
1	B	136	VAL
1	A	48	ASP
1	A	64	SER
1	B	48	ASP
1	B	100	VAL
1	A	137	ASN
1	B	137	ASN
1	A	100	VAL
1	B	68	TYR
1	A	65	ARG
1	A	135	ASN
1	B	135	ASN

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	130/186 (70%)	107 (82%)	23 (18%)	2	11
1	B	131/186 (70%)	110 (84%)	21 (16%)	3	14
All	All	261/372 (70%)	217 (83%)	44 (17%)	2	13

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	SER
1	A	54	ASP
1	A	61	ILE

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Mol	Chain	Res	Type
1	A	65	ARG
1	A	69	VAL
1	A	73	LEU
1	A	84	THR
1	A	89	LEU
1	A	100	VAL
1	A	103	ASP
1	A	104	LEU
1	A	105	GLU
1	A	109	ILE
1	A	110	ARG
1	A	111	ARG
1	A	113	LYS
1	A	118	ARG
1	A	132	LEU
1	A	137	ASN
1	A	164	ASP
1	A	175	THR
1	A	183	ILE
1	A	186	LEU
1	B	41	GLN
1	B	43	ASP
1	B	54	ASP
1	B	61	ILE
1	B	64	SER
1	B	73	LEU
1	B	84	THR
1	B	89	LEU
1	B	100	VAL
1	B	103	ASP
1	B	109	ILE
1	B	110	ARG
1	B	111	ARG
1	B	118	ARG
1	B	132	LEU
1	B	137	ASN
1	B	164	ASP
1	B	174	GLU
1	B	183	ILE
1	B	184	GLU
1	B	186	LEU

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	52	HIS
1	A	137	ASN
1	A	178	GLN
1	B	52	HIS
1	B	137	ASN
1	B	188	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	3/31 (9%)	1 (33%)	1 (33%)
2	D	5/31 (16%)	3 (60%)	3 (60%)
All	All	8/62 (12%)	4 (50%)	4 (50%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	-2	U
2	D	-4	U
2	D	-3	U
2	D	-2	U

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	-3	U
2	D	-5	C
2	D	-4	U
2	D	-3	U

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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	188:ASN	C	189:PRO	N	1.74
1	A	68:TYR	C	69:VAL	N	1.13
1	B	104:LEU	C	105:GLU	N	1.08

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	161/208 (77%)	-0.13	2 (1%) 81 69	45, 86, 123, 139	0
1	B	161/208 (77%)	-0.06	3 (1%) 70 55	43, 92, 128, 160	0
2	C	5/31 (16%)	1.10	1 (20%) 1 1	93, 99, 139, 165	0
2	D	5/31 (16%)	0.74	1 (20%) 1 1	100, 106, 138, 155	0
All	All	332/478 (69%)	-0.06	7 (2%) 67 52	43, 91, 129, 165	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	135	ASN	4.9
1	A	189	PRO	4.4
2	C	-5	C	3.8
1	B	106	GLY	3.3
1	B	145	PHE	3.1
1	B	189	PRO	3.1
2	D	-5	C	2.3

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.