Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 12:12 AM BST

PDB ID	:	6PPQ
Title	:	Structure of S. pombe Lsm1-7 with RNA, polyuridine with 3' adenosine
Authors	:	Montemayor, E.J.; Butcher, S.E.
Deposited on	:	2019-07-08
Resolution	:	1.81 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 following versions of software and data (see references ①) were used in the production of this report:

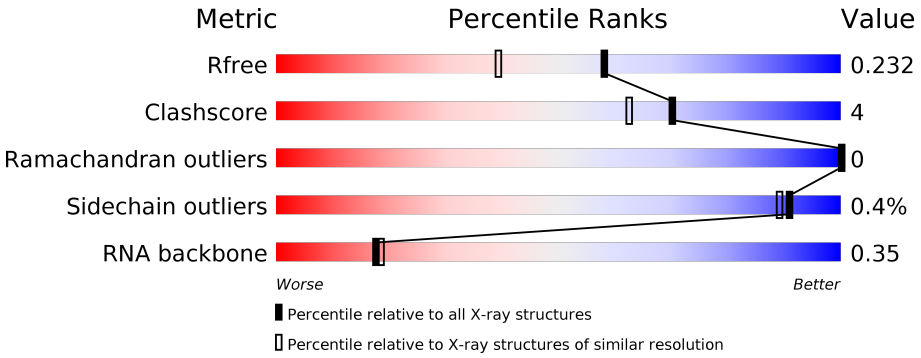
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RNA backbone	3102	1047 (2.40-1.24)

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 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%

Mol	Chain	Length	Quality of chain
1	A	86	78% · 20%
2	B	96	85% 10% · ·
3	C	95	72% 7% 21%
4	D	129	51% 12% 36%
5	E	80	93% · 6%
6	F	77	86% 6% 8%

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Mol	Chain	Length	Quality of chain
7	G	119	
8	H	6	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4677 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 U6 snRNA-associated Sm-like protein LSm1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	69	Total	C	N	O	S	0	0	0
			556	360	91	103	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P87173
A	0	SER	-	expression tag	UNP P87173

- Molecule 2 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	93	Total	C	N	O	S	0	0	0
			727	469	121	132	5			

- Molecule 3 is a protein called Probable U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	75	Total	C	N	O	S	0	0	0
			599	383	104	110	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP Q9Y7M4
C	0	SER	-	expression tag	UNP Q9Y7M4

- Molecule 4 is a protein called Probable U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	82	Total	C	N	O	S	0	0	0
			630	397	111	117	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	122	TRP	-	expression tag	UNP O14352
D	123	SER	-	expression tag	UNP O14352
D	124	HIS	-	expression tag	UNP O14352
D	125	PRO	-	expression tag	UNP O14352
D	126	GLN	-	expression tag	UNP O14352
D	127	PHE	-	expression tag	UNP O14352
D	128	GLU	-	expression tag	UNP O14352
D	129	LYS	-	expression tag	UNP O14352

- Molecule 5 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	75	Total	C	N	O	S	0	0	0
			572	366	89	111	6			

- Molecule 6 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	71	Total	C	N	O	S	0	0	0
			544	346	91	105	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	GLY	-	expression tag	UNP Q9UUI1
F	0	SER	-	expression tag	UNP Q9UUI1

- Molecule 7 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	85	Total	C	N	O	S	0	1	0
			645	406	115	122	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	114	HIS	-	expression tag	UNP O74499
G	115	HIS	-	expression tag	UNP O74499
G	116	HIS	-	expression tag	UNP O74499
G	117	HIS	-	expression tag	UNP O74499
G	118	HIS	-	expression tag	UNP O74499

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Chain	Residue	Modelled	Actual	Comment	Reference
G	119	HIS	-	expression tag	UNP O74499

- Molecule 8 is a RNA chain called RNA (5'-R(*UP*UP*UP*UP*UP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	5	Total	C	N	O	P	0	0	0
			102	46	13	38	5			

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	41	Total	O	0	0
			41	41		
9	B	34	Total	O	0	0
			34	34		
9	C	51	Total	O	0	0
			51	51		
9	D	36	Total	O	0	0
			36	36		
9	E	51	Total	O	0	0
			51	51		
9	F	31	Total	O	0	0
			31	31		
9	G	46	Total	O	0	0
			46	46		
9	H	12	Total	O	0	0
			12	12		

3 Residue-property plots (i)

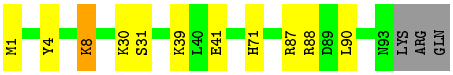
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: U6 snRNA-associated Sm-like protein LSm1

Chain A:

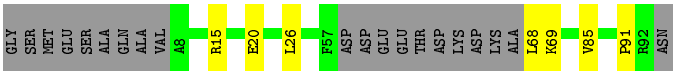
- Molecule 2: U6 snRNA-associated Sm-like protein LSm2

Chain B:



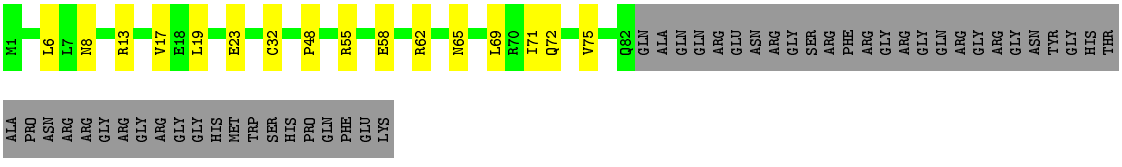
- Molecule 3: Probable U6 snRNA-associated Sm-like protein LSm3

Chain C:



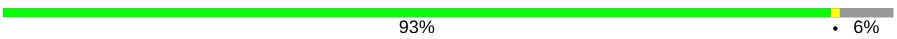
- Molecule 4: Probable U6 snRNA-associated Sm-like protein LSm4

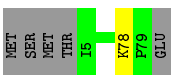
Chain D:



- Molecule 5: U6 snRNA-associated Sm-like protein LSm5

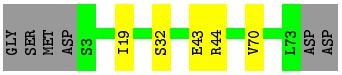
Chain E:





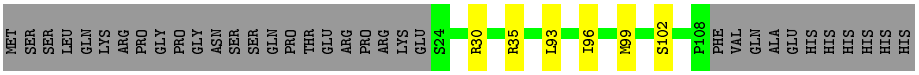
- Molecule 6: U6 snRNA-associated Sm-like protein LSm6

Chain F:



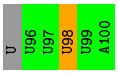
• Molecule 7: U6 snRNA-associated Sm-like protein LSm7

Chain G:



• Molecule 8: RNA (5'-R(*UP*UP*UP*UP*UP*A)-3')

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	68.86Å 68.86Å 296.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.50 – 1.81 98.77 – 1.81	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.50-1.81) 99.9 (98.77-1.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.93 (at 1.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	(Not available) , (Not available) 0.207 , 0.232	Depositor DCC
R_{free} test set	1995 reflections (2.63%)	wwPDB-VP
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 58.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4677	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.35	0/562	0.62	0/758
2	B	0.33	0/738	0.56	0/998
3	C	0.32	0/607	0.59	0/820
4	D	0.38	0/639	0.56	0/867
5	E	0.36	0/581	0.62	0/787
6	F	0.37	0/551	0.60	0/744
7	G	0.33	0/654	0.55	0/885
8	H	0.58	0/112	1.19	1/171 (0.6%)
All	All	0.36	0/4444	0.61	1/6030 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	98	U	C5-C6-N1	-5.77	119.82	122.70

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	556	0	570	2	0
2	B	727	0	736	10	0
3	C	599	0	610	5	0
4	D	630	0	615	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	572	0	573	1	0
6	F	544	0	542	2	0
7	G	645	0	661	5	0
8	H	102	0	52	0	0
9	A	41	0	0	0	0
9	B	34	0	0	3	0
9	C	51	0	0	0	0
9	D	36	0	0	1	0
9	E	51	0	0	1	0
9	F	31	0	0	0	0
9	G	46	0	0	0	0
9	H	12	0	0	0	0
All	All	4677	0	4359	31	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 (31) 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:B:30:LYS:NZ	2:B:41:GLU:OE1	2.21	0.74
5:E:78:LYS:NZ	9:E:101:HOH:O	2.21	0.73
7:G:93:LEU:HD13	7:G:96:ILE:HD11	1.81	0.61
2:B:88:ARG:NH2	9:B:102:HOH:O	2.29	0.61
3:C:68:LEU:HG	3:C:69:LYS:HD3	1.88	0.55
1:A:60:ASP:OD1	1:A:60:ASP:N	2.40	0.54
4:D:8:ASN:ND2	4:D:32:CYS:SG	2.81	0.54
2:B:87:ARG:NH2	9:B:101:HOH:O	2.26	0.53
3:C:68:LEU:HG	3:C:69:LYS:CD	2.40	0.52
4:D:17:VAL:HG22	4:D:69:LEU:HD22	1.91	0.51
2:B:4:TYR:CZ	2:B:8:LYS:HD2	2.46	0.51
4:D:13:ARG:HD3	4:D:75:VAL:HG22	1.92	0.50
3:C:20:GLU:HB3	3:C:91:PRO:HG3	1.95	0.48
4:D:19:LEU:HD13	4:D:65:ASN:ND2	2.29	0.48
2:B:1:MET:HB3	2:B:4:TYR:HB3	1.96	0.47
4:D:6:LEU:HD21	4:D:71:ILE:HD11	1.95	0.47
2:B:71:HIS:HD2	9:B:131:HOH:O	1.98	0.46
6:F:32:SER:OG	6:F:43:GLU:HG3	2.16	0.46
4:D:58:GLU:OE1	7:G:30:ARG:NH2	2.35	0.45
2:B:90:LEU:HD22	3:C:15:ARG:HD3	1.98	0.45
7:G:35:ARG:HG2	7:G:99:MET:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:26:LEU:HD23	3:C:85:VAL:HA	1.98	0.44
4:D:62:ARG:HD2	7:G:93:LEU:O	2.18	0.44
1:A:18:ASP:OD2	2:B:39:LYS:NZ	2.52	0.42
4:D:55:ARG:O	7:G:102:SER:HA	2.19	0.42
4:D:23:GLU:HG3	4:D:48:PRO:HD3	2.02	0.42
2:B:31:SER:HB3	2:B:39:LYS:HB2	2.01	0.41
4:D:72:GLN:HB2	4:D:75:VAL:HG23	2.02	0.41
6:F:19:ILE:HD12	6:F:70:VAL:HG22	2.03	0.41
2:B:30:LYS:HG3	2:B:41:GLU:CD	2.41	0.40
4:D:75:VAL:HG21	9:D:207:HOH:O	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	67/86 (78%)	65 (97%)	2 (3%)	0	100	100
2	B	91/96 (95%)	91 (100%)	0	0	100	100
3	C	71/95 (75%)	71 (100%)	0	0	100	100
4	D	80/129 (62%)	78 (98%)	2 (2%)	0	100	100
5	E	73/80 (91%)	71 (97%)	2 (3%)	0	100	100
6	F	69/77 (90%)	68 (99%)	1 (1%)	0	100	100
7	G	84/119 (71%)	82 (98%)	2 (2%)	0	100	100
All	All	535/682 (78%)	526 (98%)	9 (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	Percentiles	
1	A	61/76 (80%)	61 (100%)	0	100	100
2	B	79/87 (91%)	78 (99%)	1 (1%)	69	61
3	C	65/83 (78%)	65 (100%)	0	100	100
4	D	66/110 (60%)	66 (100%)	0	100	100
5	E	65/71 (92%)	65 (100%)	0	100	100
6	F	59/66 (89%)	58 (98%)	1 (2%)	60	50
7	G	69/104 (66%)	69 (100%)	0	100	100
All	All	464/597 (78%)	462 (100%)	2 (0%)	91	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
6	F	44	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	42	ASN
4	D	8	ASN
4	D	34	ASN
4	D	65	ASN
7	G	32	GLN
7	G	34	GLN
7	G	45	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	H	4/6 (66%)	1 (25%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	H	98	U

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides 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)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.