



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 05:39 am BST

PDB ID : 4M75  
Title : Crystal structure of Lsm1-7 complex  
Authors : Zhou, L.; Hang, J.; Zhou, Y.; Wan, R.; Lu, G.; Yan, C.; Shi, Y.  
Deposited on : 2013-08-12  
Resolution : 2.95 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.

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

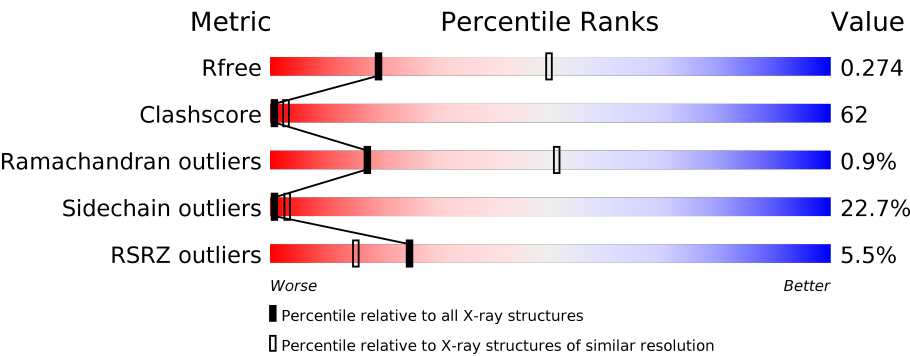
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	144	<div><div>6%</div><div><div></div><div>36%</div><div>44%</div><div>16%</div><div></div></div><div></div></div>
1	H	144	<div><div>3%</div><div><div></div><div>35%</div><div>47%</div><div>11%</div><div>7%</div></div><div></div></div>
2	B	95	<div><div>3%</div><div><div></div><div>38%</div><div>41%</div><div>17%</div><div></div></div><div></div></div>
2	I	95	<div><div>8%</div><div><div></div><div>28%</div><div>51%</div><div>12%</div><div>9%</div></div><div></div></div>
3	C	89	<div><div>3%</div><div><div></div><div>25%</div><div>40%</div><div>13%</div><div>21%</div></div><div></div></div>
3	J	89	<div><div>8%</div><div><div></div><div>13%</div><div>52%</div><div>19%</div><div>16%</div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
4	D	86	
4	K	86	
5	E	93	
5	L	93	
6	F	115	
6	M	115	
7	G	122	
7	N	122	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	CL	B	101	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9319 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	139	Total	C	N	O	S	Se	0	0	0
			1145	730	192	216	1	6			
1	H	134	Total	C	N	O	S	Se	0	0	0
			1036	659	178	192	1	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MSE	-	EXPRESSION TAG	UNP P47017
H	29	MSE	-	EXPRESSION TAG	UNP P47017

- Molecule 2 is a protein called U6 snRNA-associated Sm-like protein Lsm2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	91	Total	C	N	O	Se	0	0	0
			744	475	125	141	3			
2	I	86	Total	C	N	O	Se	0	0	0
			693	444	117	130	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	45	SER	CYS	ENGINEERED MUTATION	UNP P38203
I	45	SER	CYS	ENGINEERED MUTATION	UNP P38203

- Molecule 3 is a protein called U6 snRNA-associated Sm-like protein Lsm3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	70	Total	C	N	O	Se	0	0	0
			553	348	96	108	1			
3	J	75	Total	C	N	O	Se	0	0	0
			587	370	101	115	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	37	SER	CYS	ENGINEERED MUTATION	UNP P57743
C	63	SER	CYS	ENGINEERED MUTATION	UNP P57743
J	37	SER	CYS	ENGINEERED MUTATION	UNP P57743
J	63	SER	CYS	ENGINEERED MUTATION	UNP P57743

- Molecule 4 is a protein called U6 snRNA-associated Sm-like protein Lsm6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	72	Total	C	N	O	Se	0	0	0
			561	355	94	110	2			
4	K	71	Total	C	N	O	Se	0	0	0
			525	333	86	104	2			

- 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	Se	0	0	0
			588	378	98	110	2			
5	L	75	Total	C	N	O	Se	0	0	0
			587	374	101	110	2			

- Molecule 6 is a protein called U6 snRNA-associated Sm-like protein Lsm7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	75	Total	C	N	O	Se	0	0	0
			523	331	92	97	3			
6	M	62	Total	C	N	O	Se	0	0	0
			460	295	77	85	3			

- Molecule 7 is a protein called U6 snRNA-associated Sm-like protein Lsm4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	82	Total	C	N	O	Se	0	0	0
			659	428	107	121	3			
7	N	82	Total	C	N	O	Se	0	0	0
			656	424	108	121	3			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-28	MSE	-	EXPRESSION TAG	UNP P40070

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-27	LYS	-	EXPRESSION TAG	UNP P40070
G	-26	HIS	-	EXPRESSION TAG	UNP P40070
G	-25	HIS	-	EXPRESSION TAG	UNP P40070
G	-24	HIS	-	EXPRESSION TAG	UNP P40070
G	-23	HIS	-	EXPRESSION TAG	UNP P40070
G	-22	HIS	-	EXPRESSION TAG	UNP P40070
G	-21	HIS	-	EXPRESSION TAG	UNP P40070
G	-20	HIS	-	EXPRESSION TAG	UNP P40070
G	-19	GLY	-	EXPRESSION TAG	UNP P40070
G	-18	ALA	-	EXPRESSION TAG	UNP P40070
G	-17	ALA	-	EXPRESSION TAG	UNP P40070
G	-16	GLY	-	EXPRESSION TAG	UNP P40070
G	-15	THR	-	EXPRESSION TAG	UNP P40070
G	-14	SER	-	EXPRESSION TAG	UNP P40070
G	-13	LEU	-	EXPRESSION TAG	UNP P40070
G	-12	TYR	-	EXPRESSION TAG	UNP P40070
G	-11	LYS	-	EXPRESSION TAG	UNP P40070
G	-10	LYS	-	EXPRESSION TAG	UNP P40070
G	-9	ALA	-	EXPRESSION TAG	UNP P40070
G	-8	GLY	-	EXPRESSION TAG	UNP P40070
G	-7	GLU	-	EXPRESSION TAG	UNP P40070
G	-6	ASN	-	EXPRESSION TAG	UNP P40070
G	-5	LEU	-	EXPRESSION TAG	UNP P40070
G	-4	TYR	-	EXPRESSION TAG	UNP P40070
G	-3	PHE	-	EXPRESSION TAG	UNP P40070
G	-2	GLN	-	EXPRESSION TAG	UNP P40070
G	-1	GLY	-	EXPRESSION TAG	UNP P40070
G	0	SER	-	EXPRESSION TAG	UNP P40070
N	-28	MSE	-	EXPRESSION TAG	UNP P40070
N	-27	LYS	-	EXPRESSION TAG	UNP P40070
N	-26	HIS	-	EXPRESSION TAG	UNP P40070
N	-25	HIS	-	EXPRESSION TAG	UNP P40070
N	-24	HIS	-	EXPRESSION TAG	UNP P40070
N	-23	HIS	-	EXPRESSION TAG	UNP P40070
N	-22	HIS	-	EXPRESSION TAG	UNP P40070
N	-21	HIS	-	EXPRESSION TAG	UNP P40070
N	-20	HIS	-	EXPRESSION TAG	UNP P40070
N	-19	GLY	-	EXPRESSION TAG	UNP P40070
N	-18	ALA	-	EXPRESSION TAG	UNP P40070
N	-17	ALA	-	EXPRESSION TAG	UNP P40070
N	-16	GLY	-	EXPRESSION TAG	UNP P40070
N	-15	THR	-	EXPRESSION TAG	UNP P40070

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-14	SER	-	EXPRESSION TAG	UNP P40070
N	-13	LEU	-	EXPRESSION TAG	UNP P40070
N	-12	TYR	-	EXPRESSION TAG	UNP P40070
N	-11	LYS	-	EXPRESSION TAG	UNP P40070
N	-10	LYS	-	EXPRESSION TAG	UNP P40070
N	-9	ALA	-	EXPRESSION TAG	UNP P40070
N	-8	GLY	-	EXPRESSION TAG	UNP P40070
N	-7	GLU	-	EXPRESSION TAG	UNP P40070
N	-6	ASN	-	EXPRESSION TAG	UNP P40070
N	-5	LEU	-	EXPRESSION TAG	UNP P40070
N	-4	TYR	-	EXPRESSION TAG	UNP P40070
N	-3	PHE	-	EXPRESSION TAG	UNP P40070
N	-2	GLN	-	EXPRESSION TAG	UNP P40070
N	-1	GLY	-	EXPRESSION TAG	UNP P40070
N	0	SER	-	EXPRESSION TAG	UNP P40070

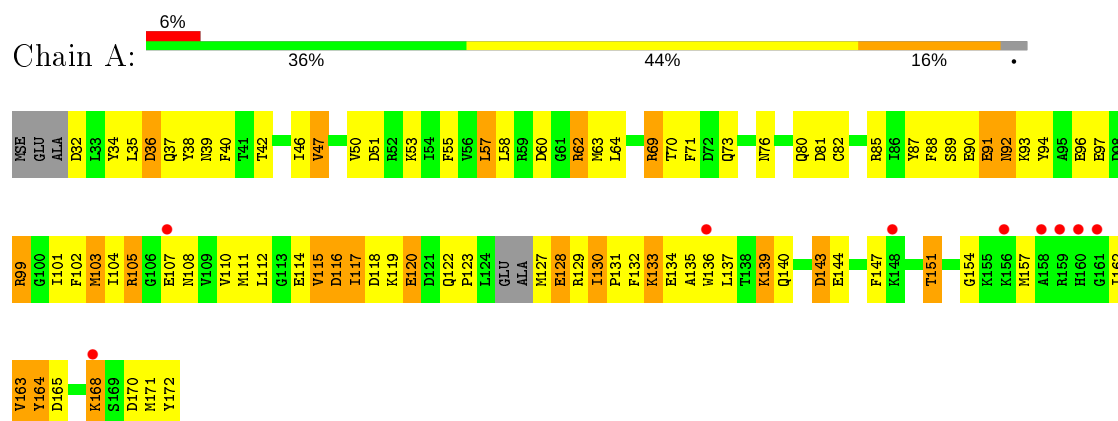
- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Cl 1 1	0	0
8	C	1	Total Cl 1 1	0	0

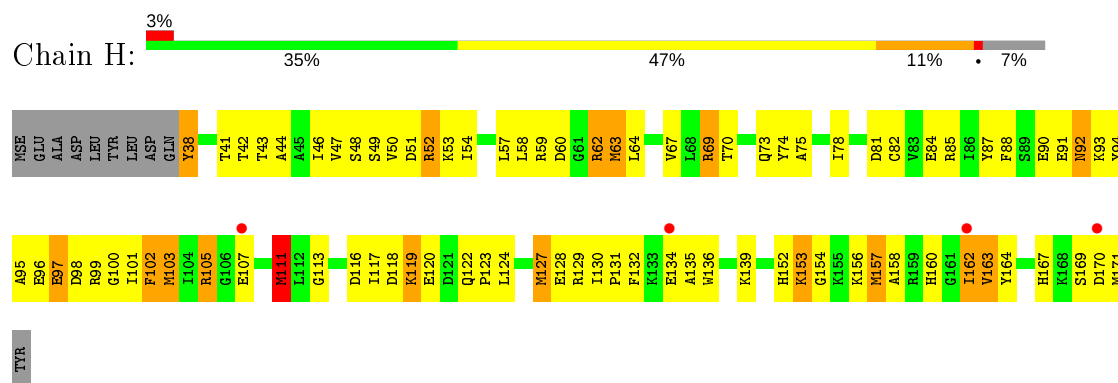
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

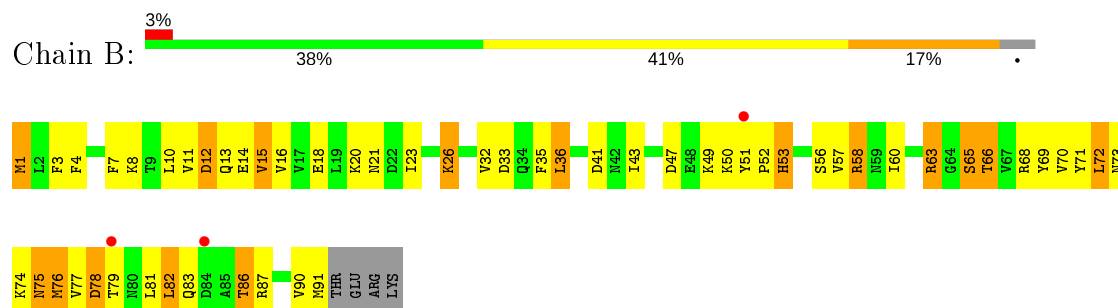
#### • Molecule 1: U6 snRNA-associated Sm-like protein Lsm1



#### • Molecule 1: U6 snRNA-associated Sm-like protein Lsm1

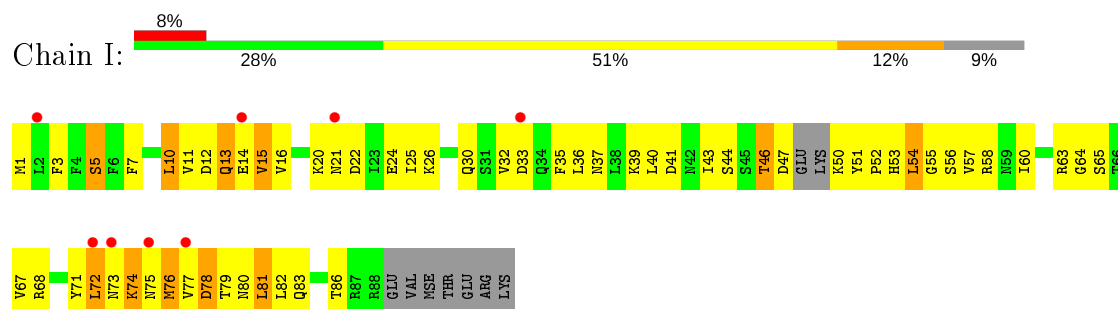


#### • Molecule 2: U6 snRNA-associated Sm-like protein Lsm2

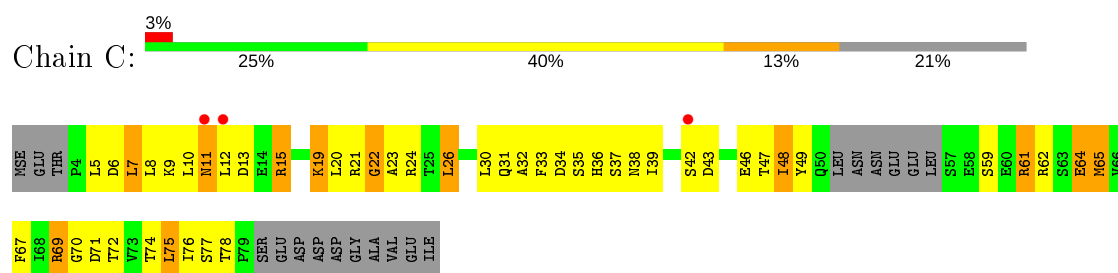




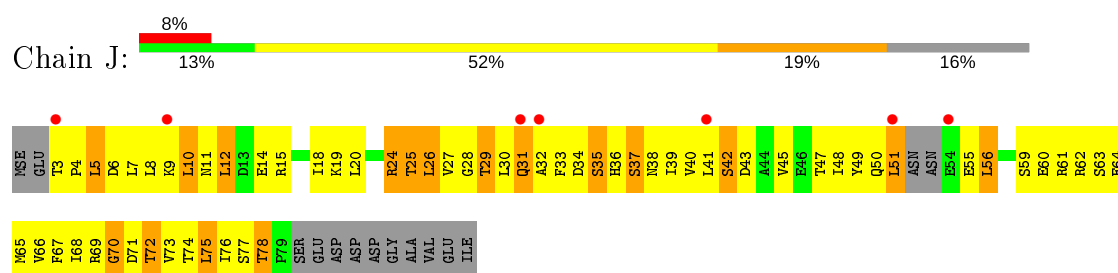
- Molecule 2: U6 snRNA-associated Sm-like protein Lsm2



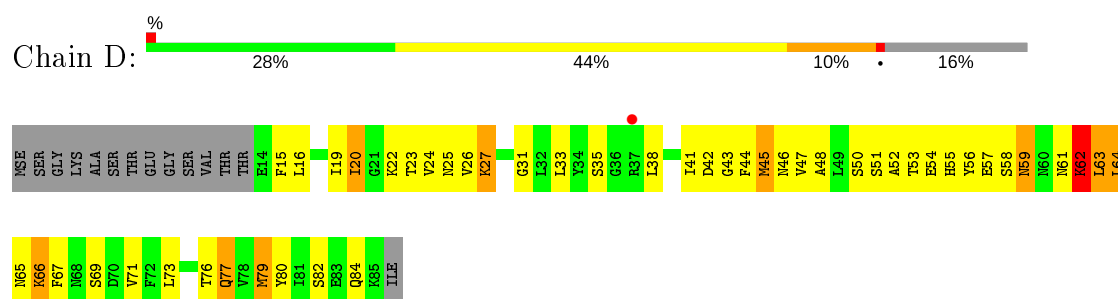
- Molecule 3: U6 snRNA-associated Sm-like protein Lsm3



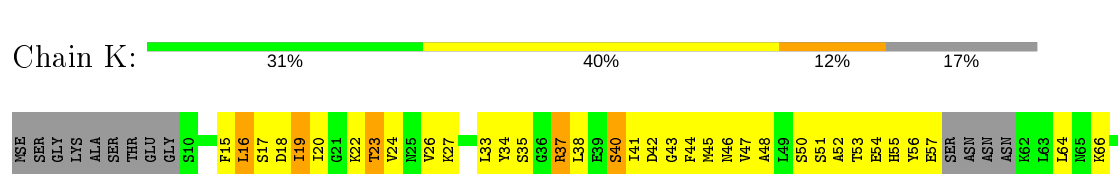
- Molecule 3: U6 snRNA-associated Sm-like protein Lsm3



- Molecule 4: U6 snRNA-associated Sm-like protein Lsm6

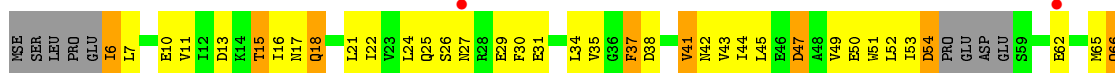


- Molecule 4: U6 snRNA-associated Sm-like protein Lsm6

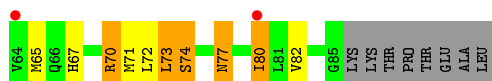
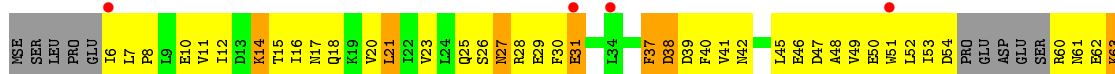




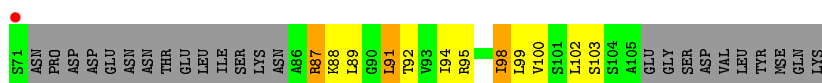
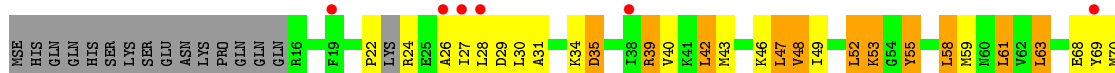
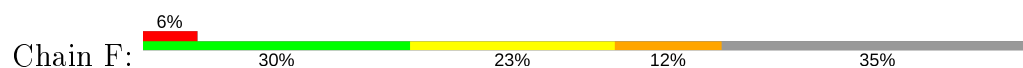
- Molecule 5: U6 snRNA-associated Sm-like protein Lsm5



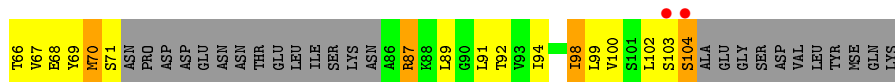
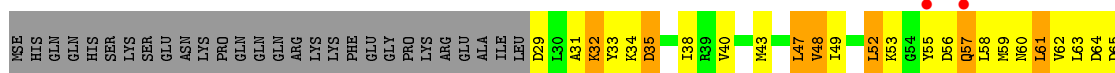
- Molecule 5: U6 snRNA-associated Sm-like protein Lsm5



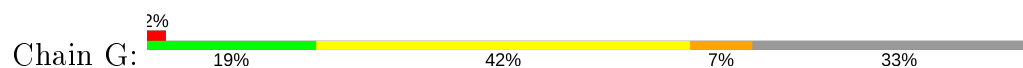
- Molecule 6: U6 snRNA-associated Sm-like protein Lsm7

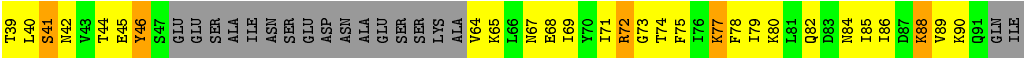


- Molecule 6: U6 snRNA-associated Sm-like protein Lsm7

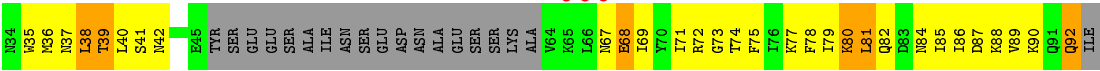
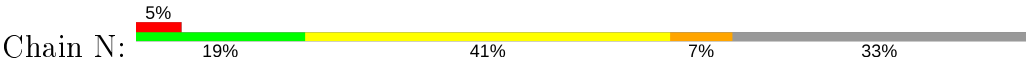


- Molecule 7: U6 snRNA-associated Sm-like protein Lsm4





● Molecule 7: U6 snRNA-associated Sm-like protein Lsm4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.67Å 67.83Å 98.23Å 93.14° 108.21° 116.30°	Depositor
Resolution (Å)	38.66 – 2.95 38.66 – 2.95	Depositor EDS
% Data completeness (in resolution range)	96.7 (38.66-2.95) 98.4 (38.66-2.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 2.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.266 , 0.291 0.253 , 0.274	Depositor DCC
$R_{free}$ test set	1504 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.3	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 61.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for k,h,-h-k-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9319	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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:  
CL

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	0.61	0/1160	0.61	0/1547
1	H	0.61	0/1049	0.66	1/1408 (0.1%)
2	B	0.60	0/752	0.64	0/1010
2	I	0.56	0/700	0.62	0/942
3	C	0.62	0/557	0.65	0/750
3	J	0.52	0/591	0.66	0/798
4	D	0.61	0/566	0.65	0/757
4	K	0.53	0/529	0.66	0/710
5	E	0.52	0/593	0.66	0/800
5	L	0.53	0/592	0.68	0/797
6	F	0.50	0/519	0.70	1/690 (0.1%)
6	M	0.58	0/458	0.73	0/609
7	G	0.62	0/664	0.61	0/889
7	N	0.62	0/660	0.65	0/883
All	All	0.58	0/9390	0.65	2/12590 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	22	PRO	N-CA-CB	6.12	110.64	103.30
1	H	111	MSE	N-CA-CB	-5.11	101.39	110.60

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	1145	0	1108	122	0
1	H	1036	0	956	159	0
2	B	744	0	755	110	0
2	I	693	0	702	92	0
3	C	553	0	564	84	0
3	J	587	0	599	121	0
4	D	561	0	558	89	0
4	K	525	0	485	75	0
5	E	588	0	594	75	1
5	L	587	0	588	95	1
6	F	523	0	526	90	0
6	M	460	0	488	71	0
7	G	659	0	675	72	0
7	N	656	0	674	109	0
8	B	1	0	0	1	0
8	C	1	0	0	0	0
All	All	9319	0	9272	1152	1

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 62.

The worst 5 of 1152 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)
7:N:15:MSE:CE	7:N:79:ILE:HG21	1.34	1.57
4:K:53:THR:HG22	4:K:66:LYS:CB	1.39	1.51
2:B:91:MSE:HE1	3:C:33:PHE:CE2	1.45	1.48
3:J:26:LEU:HD11	3:J:41:LEU:CD1	1.56	1.36
1:A:35:LEU:CD1	7:N:36:MSE:HE3	1.57	1.33

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:62:GLU:OE1	5:L:60:ARG:NH1[1_554]	2.05	0.15

## 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	135/144 (94%)	124 (92%)	8 (6%)	3 (2%)	6	28
1	H	132/144 (92%)	123 (93%)	9 (7%)	0	100	100
2	B	89/95 (94%)	76 (85%)	13 (15%)	0	100	100
2	I	82/95 (86%)	72 (88%)	8 (10%)	2 (2%)	6	26
3	C	66/89 (74%)	61 (92%)	4 (6%)	1 (2%)	10	38
3	J	71/89 (80%)	64 (90%)	6 (8%)	1 (1%)	11	39
4	D	70/86 (81%)	64 (91%)	5 (7%)	1 (1%)	11	39
4	K	67/86 (78%)	63 (94%)	4 (6%)	0	100	100
5	E	71/93 (76%)	67 (94%)	3 (4%)	1 (1%)	11	39
5	L	71/93 (76%)	61 (86%)	10 (14%)	0	100	100
6	F	69/115 (60%)	65 (94%)	4 (6%)	0	100	100
6	M	58/115 (50%)	52 (90%)	5 (9%)	1 (2%)	9	34
7	G	78/122 (64%)	72 (92%)	6 (8%)	0	100	100
7	N	78/122 (64%)	74 (95%)	4 (5%)	0	100	100
All	All	1137/1488 (76%)	1038 (91%)	89 (8%)	10 (1%)	17	51

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	M	34	LYS
1	A	89	SER
5	E	41	VAL
4	D	62	LYS

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Mol	Chain	Res	Type
2	I	74	LYS

### 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	121/122 (99%)	91 (75%)	30 (25%)	0	2
1	H	100/122 (82%)	73 (73%)	27 (27%)	0	2
2	B	86/88 (98%)	67 (78%)	19 (22%)	1	3
2	I	79/88 (90%)	63 (80%)	16 (20%)	1	5
3	C	63/79 (80%)	48 (76%)	15 (24%)	0	2
3	J	67/79 (85%)	47 (70%)	20 (30%)	0	1
4	D	63/72 (88%)	50 (79%)	13 (21%)	1	4
4	K	53/72 (74%)	43 (81%)	10 (19%)	1	7
5	E	66/81 (82%)	56 (85%)	10 (15%)	3	12
5	L	65/81 (80%)	50 (77%)	15 (23%)	1	3
6	F	50/98 (51%)	34 (68%)	16 (32%)	0	1
6	M	50/98 (51%)	37 (74%)	13 (26%)	0	2
7	G	72/103 (70%)	59 (82%)	13 (18%)	1	7
7	N	72/103 (70%)	60 (83%)	12 (17%)	2	9
All	All	1007/1286 (78%)	778 (77%)	229 (23%)	1	3

5 of 229 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	0	SER
1	H	96	GLU
6	M	61	LEU
7	G	26	GLN
1	H	38	TYR



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	68	HIS
7	G	82	GLN
7	N	82	GLN
7	G	16	GLN
7	G	21	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 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 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 ⓘ

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, 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	133/144 (92%)	0.40	9 (6%) 17 10	25, 58, 153, 180	0
1	H	128/144 (88%)	0.33	4 (3%) 49 32	24, 77, 151, 249	0
2	B	88/95 (92%)	0.28	3 (3%) 45 29	24, 62, 123, 195	0
2	I	84/95 (88%)	0.48	8 (9%) 8 5	37, 80, 145, 182	0
3	C	69/89 (77%)	0.22	3 (4%) 35 22	31, 59, 100, 118	0
3	J	74/89 (83%)	0.53	7 (9%) 8 5	51, 83, 151, 250	0
4	D	70/86 (81%)	0.03	1 (1%) 75 59	31, 71, 119, 135	0
4	K	69/86 (80%)	0.25	0 100 100	44, 79, 132, 160	0
5	E	73/93 (78%)	0.26	3 (4%) 37 24	40, 73, 129, 164	0
5	L	73/93 (78%)	0.44	6 (8%) 11 6	43, 72, 128, 154	0
6	F	72/115 (62%)	0.39	7 (9%) 7 4	35, 75, 102, 325	0
6	M	59/115 (51%)	0.29	4 (6%) 17 10	27, 73, 105, 128	0
7	G	79/122 (64%)	0.07	2 (2%) 57 40	27, 60, 124, 242	0
7	N	79/122 (64%)	0.18	6 (7%) 13 7	34, 58, 90, 146	0
All	All	1150/1488 (77%)	0.30	63 (5%) 25 15	24, 71, 136, 325	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	L	6	ILE	6.9
6	F	27	ILE	6.7
2	I	72	LEU	6.1
5	E	62	GLU	4.5
7	G	0	SER	4.3

## 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](#)

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
8	CL	B	101	1/1	0.60	0.70	179,179,179,179	0
8	CL	C	101	1/1	0.90	1.08	150,150,150,150	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.