Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:38 PM GMT

PDB ID	:	4M77
Title	:	Crystal structure of Lsm2-8 complex, space group I212121
Authors	:	Zhou, L.; Hang, J.; Zhou, Y.; Wan, R.; Lu, G.; Yan, C.; Shi, Y.
Deposited on	:	2013-08-12
Resolution	:	3.11 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:

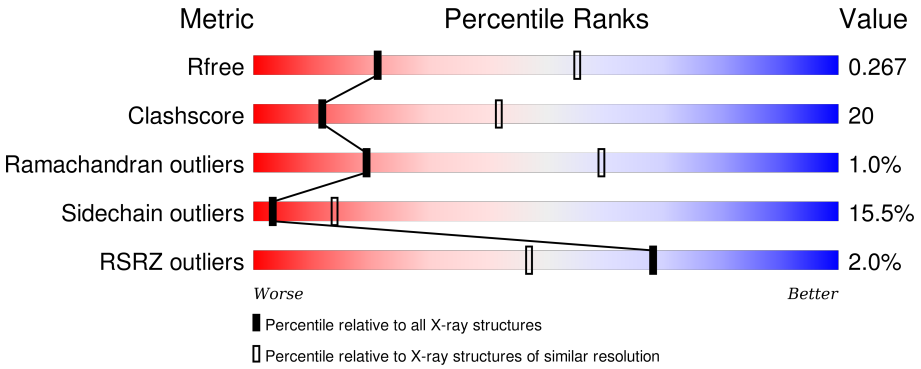
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.11 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	1112 (3.16-3.08)
Clashscore	102246	1218 (3.16-3.08)
Ramachandran outliers	100387	1175 (3.16-3.08)
Sidechain outliers	100360	1175 (3.16-3.08)
RSRZ outliers	91569	1114 (3.16-3.08)

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 <=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	109	4% 31% 34% 11% 24%
1	H	109	3% 42% 30% 6% 22%
2	B	95	47% 46%
2	I	95	52% 36% 8%
3	C	89	% 43% 26% 9% 22%

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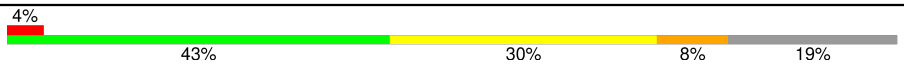
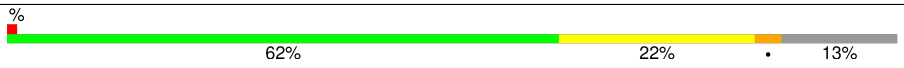
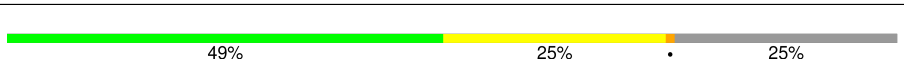
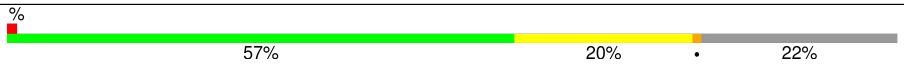
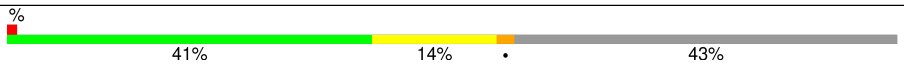
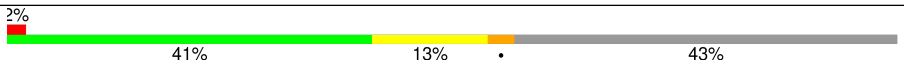
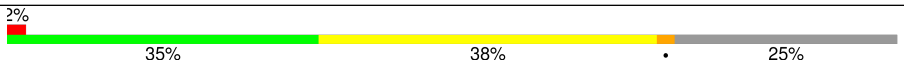
Mol	Chain	Length	Quality of chain
3	J	89	
4	D	86	
4	K	86	
5	E	93	
5	L	93	
6	F	115	
6	M	115	
7	G	93	
7	N	93	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8312 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 LSm8.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	83	Total	C	N	O	0	0	0
			637	408	108	121			
1	H	85	Total	C	N	O	0	0	0
			663	425	111	127			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	LEU	LYS	ENGINEERED MUTATION	UNP P47093
A	22	SER	CYS	ENGINEERED MUTATION	UNP P47093
A	38	LEU	ILE	ENGINEERED MUTATION	UNP P47093
A	51	SER	CYS	ENGINEERED MUTATION	UNP P47093
H	17	LEU	LYS	ENGINEERED MUTATION	UNP P47093
H	22	SER	CYS	ENGINEERED MUTATION	UNP P47093
H	38	LEU	ILE	ENGINEERED MUTATION	UNP P47093
H	51	SER	CYS	ENGINEERED MUTATION	UNP P47093

- 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	S	0	0	0
			739	471	124	141	3			
2	I	91	Total	C	N	O	S	0	0	0
			739	471	124	141	3			

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	69	Total	C	N	O	S	0	0	0
			546	344	94	107	1			
3	J	72	Total	C	N	O	S	0	0	0
			571	359	99	112	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	75	Total	C	N	O	S	0	0	0
			582	367	96	117	2			
4	K	75	Total	C	N	O	S	0	0	0
			578	364	95	117	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	70	Total	C	N	O	S	0	0	0
			545	352	91	100	2			
5	L	73	Total	C	N	O	S	0	0	0
			578	372	96	108	2			

- Molecule 6 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	65	Total	C	N	O	S	0	0	0
			499	322	84	90	3			
6	M	65	Total	C	N	O	S	0	0	0
			499	322	84	90	3			

- Molecule 7 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	70	Total	C	N	O	S	0	0	0
			568	369	92	104	3			

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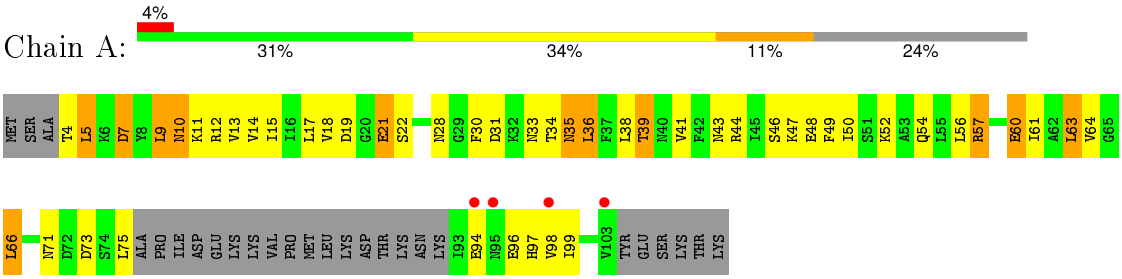
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	N	70	Total	C	N	O	S	0	0	0
			568	369	92	104	3			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

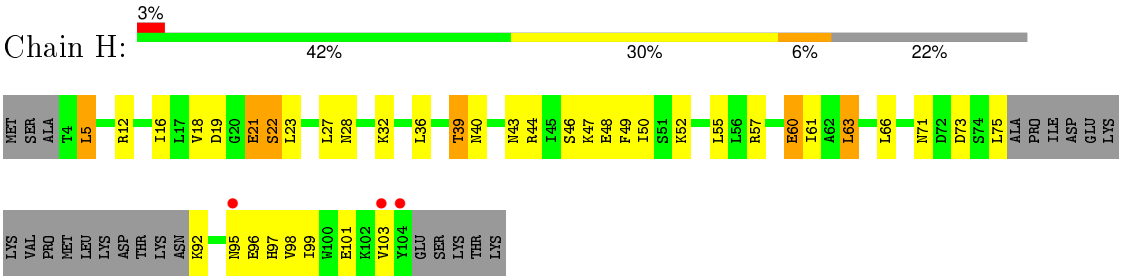
- Molecule 1: U6 snRNA-associated Sm-like protein LSm8

Chain A:



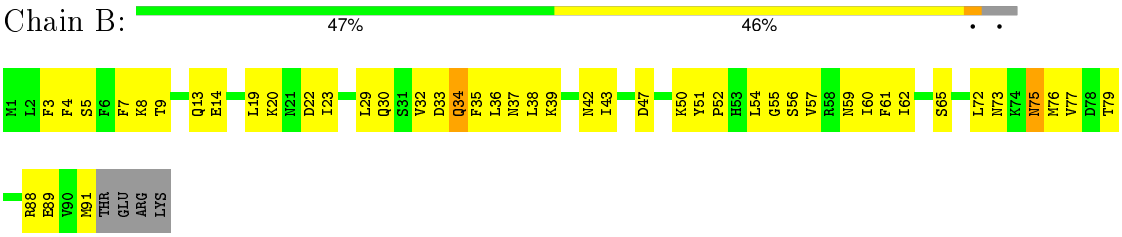
- Molecule 1: U6 snRNA-associated Sm-like protein LSm8

Chain H:



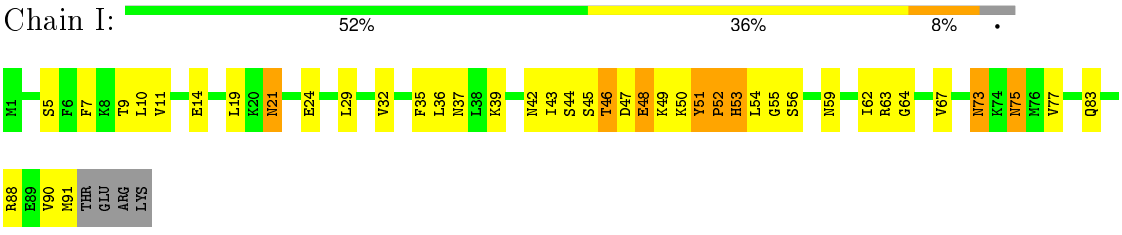
- Molecule 2: U6 snRNA-associated Sm-like protein LSm2

Chain B:



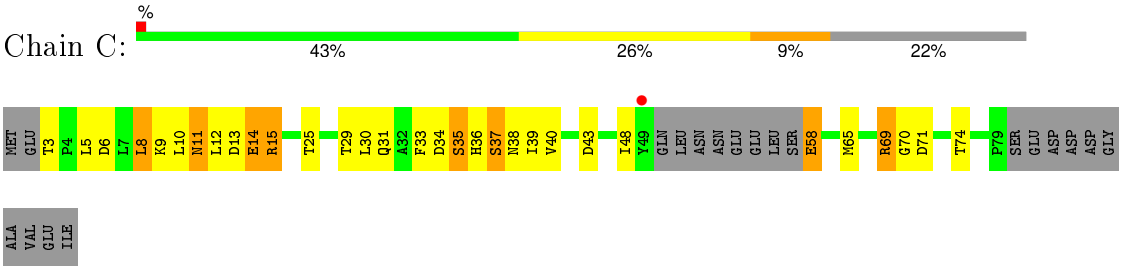
- Molecule 2: U6 snRNA-associated Sm-like protein LSm2

Chain I:



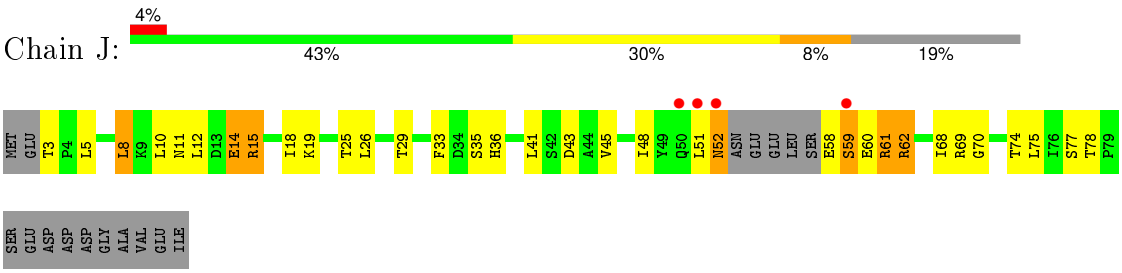
• Molecule 3: U6 snRNA-associated Sm-like protein LSm3

Chain C:



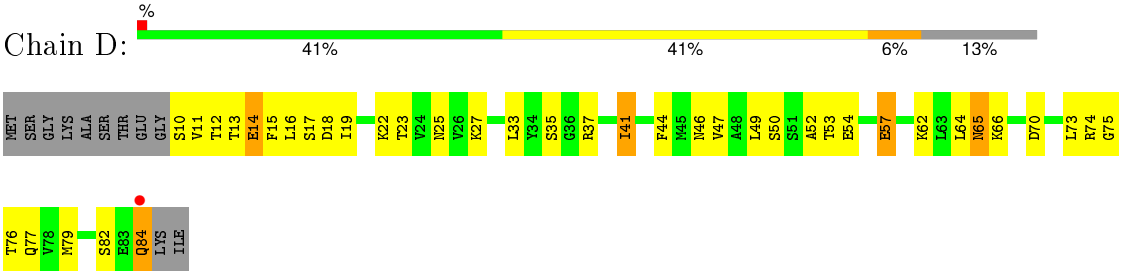
• Molecule 3: U6 snRNA-associated Sm-like protein LSm3

Chain J:



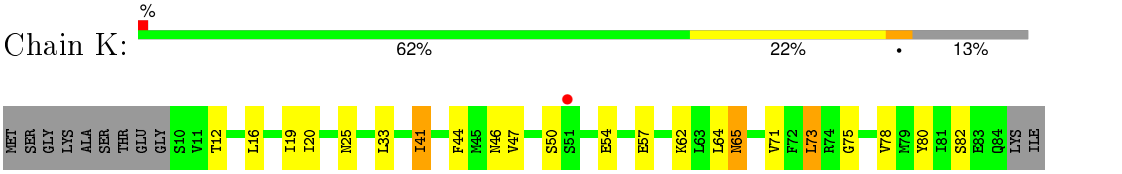
• Molecule 4: U6 snRNA-associated Sm-like protein LSm6

Chain D:



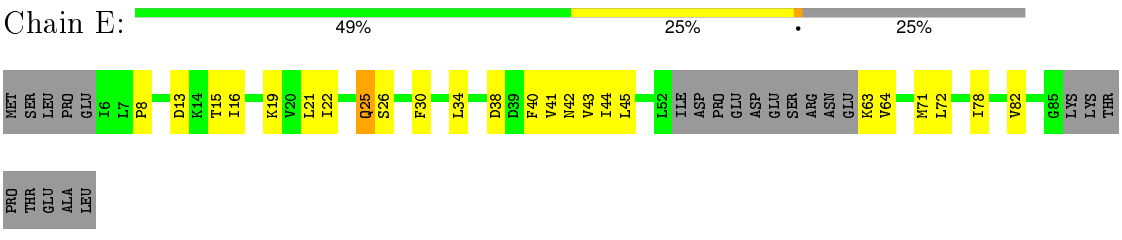
• Molecule 4: U6 snRNA-associated Sm-like protein LSm6

Chain K:



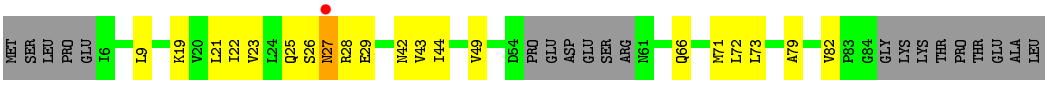
• Molecule 5: U6 snRNA-associated Sm-like protein LSm5

Chain E:



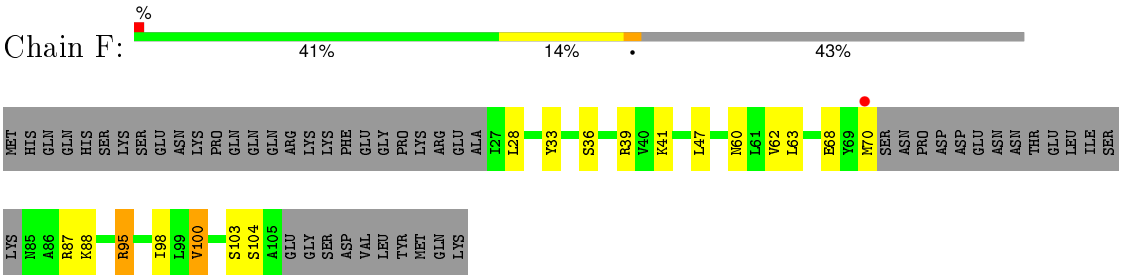
• Molecule 5: U6 snRNA-associated Sm-like protein LSm5

Chain L:



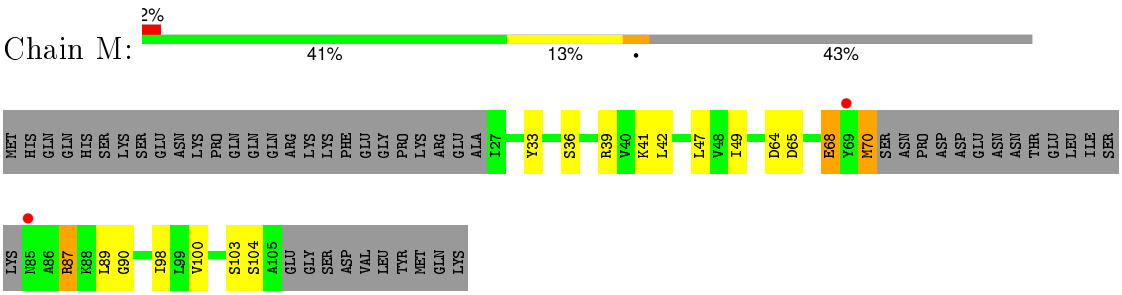
- Molecule 6: U6 snRNA-associated Sm-like protein LSm7

Chain F:



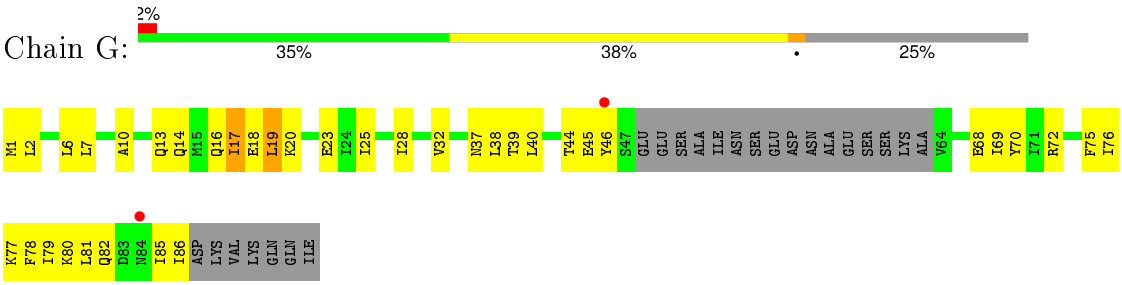
- Molecule 6: U6 snRNA-associated Sm-like protein LSm7

Chain M:



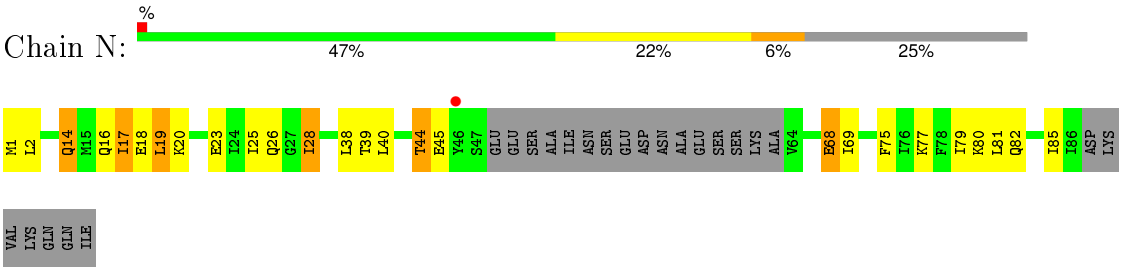
- Molecule 7: U6 snRNA-associated Sm-like protein LSm4

Chain G:



- Molecule 7: U6 snRNA-associated Sm-like protein LSm4

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	139.10Å 145.88Å 149.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 3.11 29.98 – 3.11	Depositor EDS
% Data completeness (in resolution range)	96.0 (29.98-3.11) 96.0 (29.98-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 3.11Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.247 , 0.267 0.242 , 0.267	Depositor DCC
R_{free} test set	1328 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	79.2	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 59.9	EDS
Estimated twinning fraction	0.017 for -h,-l,-k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 26475 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8312	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.45	0/643	0.62	0/869
1	H	0.52	0/670	0.68	0/906
2	B	0.47	0/749	0.67	0/1011
2	I	0.51	1/749 (0.1%)	0.71	2/1011 (0.2%)
3	C	0.42	0/551	0.72	0/745
3	J	0.41	0/576	0.73	0/779
4	D	0.39	0/589	0.63	0/794
4	K	0.41	0/585	0.58	0/790
5	E	0.44	0/552	0.64	0/748
5	L	0.49	0/585	0.67	0/792
6	F	0.40	0/500	0.64	0/668
6	M	0.43	0/500	0.65	0/668
7	G	0.43	0/574	0.67	1/774 (0.1%)
7	N	0.49	0/574	0.69	0/774
All	All	0.45	1/8397 (0.0%)	0.67	3/11329 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	52	PRO	N-CD	5.01	1.54	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	6	LEU	CA-CB-CG	6.12	129.38	115.30
2	I	51	TYR	C-N-CD	6.04	141.08	128.40
2	I	10	LEU	CA-CB-CG	5.63	128.24	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	A	637	0	633	64	0
1	H	663	0	659	24	0
2	B	739	0	742	66	0
2	I	739	0	742	44	1
3	C	546	0	560	31	0
3	J	571	0	585	24	1
4	D	582	0	574	34	0
4	K	578	0	563	15	0
5	E	545	0	555	15	0
5	L	578	0	590	14	0
6	F	499	0	552	14	0
6	M	499	0	552	12	0
7	G	568	0	594	23	0
7	N	568	0	594	18	0
All	All	8312	0	8495	339	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 20.

All (339) 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)
4:D:23:THR:CG2	4:D:84:GLN:HE21	1.13	1.54
4:D:23:THR:CG2	4:D:84:GLN:NE2	1.90	1.34
1:A:7:ASP:O	1:A:11:LYS:HE2	1.27	1.30
2:I:43:ILE:HD12	2:I:51:TYR:OH	1.37	1.23
4:D:23:THR:HG21	4:D:84:GLN:NE2	1.45	1.22
1:A:63:LEU:CD1	2:B:62:ILE:HG12	1.73	1.17
2:I:51:TYR:CE2	2:I:54:LEU:HD11	1.81	1.14
1:A:63:LEU:HD12	2:B:62:ILE:HG12	1.33	1.11
4:D:23:THR:HG22	4:D:84:GLN:HE21	0.91	1.05
1:H:44:ARG:NH2	2:I:53:HIS:O	1.92	1.01
2:I:43:ILE:CD1	2:I:51:TYR:OH	2.09	1.00
4:D:23:THR:HG21	4:D:84:GLN:HE21	1.04	0.99
2:B:52:PRO:HG2	2:B:54:LEU:HD12	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:74:ARG:NH1	4:D:76:THR:OG1	1.98	0.97
2:B:52:PRO:HG2	2:B:54:LEU:CD1	1.97	0.95
2:B:73:ASN:OD1	2:B:76:MET:HB2	1.66	0.94
1:A:7:ASP:O	1:A:11:LYS:CE	2.16	0.93
2:B:73:ASN:OD1	2:B:76:MET:CE	2.18	0.91
3:C:37:SER:O	3:C:39:ILE:HG13	1.72	0.90
4:D:23:THR:HG22	4:D:84:GLN:NE2	1.68	0.89
1:A:63:LEU:HD11	2:B:62:ILE:HG12	1.54	0.88
2:I:51:TYR:HE2	2:I:54:LEU:HD11	1.29	0.88
1:A:18:VAL:HG23	1:A:60:GLU:O	1.74	0.88
1:H:95:ASN:ND2	3:J:51:LEU:HD23	1.89	0.87
2:I:51:TYR:HE2	2:I:54:LEU:CD1	1.87	0.87
1:A:28:ASN:OD1	1:A:39:THR:OG1	1.92	0.86
2:I:51:TYR:CE2	2:I:54:LEU:CD1	2.60	0.84
2:B:73:ASN:OD1	2:B:76:MET:HE3	1.79	0.82
5:E:21:LEU:HB3	5:E:82:VAL:HB	1.62	0.81
4:K:57:GLU:OE2	5:L:28:ARG:NH1	2.13	0.80
1:H:43:ASN:HB2	1:H:50:ILE:HD11	1.63	0.80
2:I:44:SER:O	2:I:51:TYR:CE1	2.35	0.79
1:A:43:ASN:HB2	1:A:50:ILE:HD11	1.65	0.78
6:F:95:ARG:HG2	6:F:95:ARG:HH21	1.49	0.77
1:H:32:LYS:O	2:I:35:PHE:HE2	1.68	0.77
2:I:43:ILE:HD12	2:I:51:TYR:HH	1.50	0.76
6:F:95:ARG:NH2	6:F:95:ARG:HG2	2.02	0.75
2:B:3:PHE:HE1	3:C:40:VAL:HG23	1.50	0.75
2:I:44:SER:O	2:I:51:TYR:HE1	1.70	0.75
2:I:47:ASP:HB3	2:I:50:LYS:HG2	1.68	0.75
1:A:63:LEU:HD11	2:B:62:ILE:CG1	2.15	0.75
4:D:10:SER:O	4:D:14:GLU:HG2	1.87	0.74
3:C:38:ASN:OD1	3:C:70:GLY:N	2.18	0.74
2:I:45:SER:HB2	2:I:51:TYR:HB2	1.69	0.74
4:D:23:THR:HG21	4:D:84:GLN:HE22	1.49	0.73
1:H:22:SER:HB2	1:H:44:ARG:HE	1.54	0.72
5:L:21:LEU:HB3	5:L:82:VAL:HB	1.71	0.72
7:G:18:GLU:HG2	7:G:77:LYS:HD3	1.72	0.72
1:A:63:LEU:HD21	2:B:60:ILE:HB	1.72	0.71
1:H:28:ASN:OD1	1:H:39:THR:OG1	2.08	0.71
2:B:13:GLN:HB3	2:B:76:MET:SD	2.31	0.71
4:D:15:PHE:O	4:D:19:ILE:HG23	1.90	0.71
1:A:57:ARG:NH1	1:A:57:ARG:HG2	2.06	0.70
1:A:31:ASP:OD1	1:A:33:ASN:HB2	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:ASP:OD1	2:B:37:ASN:HB2	1.92	0.70
3:J:15:ARG:NH2	3:J:43:ASP:O	2.25	0.70
3:J:26:LEU:HD22	3:J:68:ILE:HD11	1.73	0.70
1:A:63:LEU:HG	2:B:61:PHE:O	1.92	0.70
2:I:51:TYR:CZ	2:I:54:LEU:HD11	2.25	0.69
4:K:25:ASN:HB3	4:K:33:LEU:HD11	1.73	0.69
3:C:15:ARG:NH2	3:C:43:ASP:O	2.25	0.69
2:B:33:ASP:OD1	2:B:37:ASN:N	2.24	0.69
1:A:33:ASN:HB2	1:A:35:ASN:ND2	2.08	0.68
1:A:63:LEU:CD1	2:B:62:ILE:CG1	2.62	0.68
1:A:96:GLU:HA	1:A:99:ILE:HD12	1.76	0.68
2:B:47:ASP:HB3	2:B:50:LYS:HB2	1.76	0.67
1:A:57:ARG:HG2	1:A:57:ARG:HH11	1.58	0.67
2:B:35:PHE:O	2:B:36:LEU:HB2	1.95	0.67
2:B:13:GLN:CD	2:B:76:MET:SD	2.74	0.67
1:A:63:LEU:HD21	2:B:60:ILE:CG2	2.25	0.66
4:D:82:SER:HB2	5:E:71:MET:HG3	1.76	0.66
1:H:99:ILE:O	1:H:103:VAL:HG23	1.95	0.66
2:B:73:ASN:OD1	2:B:76:MET:CB	2.43	0.66
3:C:36:HIS:O	3:C:37:SER:CB	2.43	0.66
2:I:35:PHE:O	2:I:36:LEU:HB2	1.95	0.66
1:A:36:LEU:HD11	1:A:61:ILE:HD13	1.77	0.66
2:I:52:PRO:HG2	2:I:54:LEU:HD23	1.79	0.65
2:B:75:ASN:N	2:B:75:ASN:OD1	2.25	0.65
2:B:3:PHE:CE1	3:C:40:VAL:HG23	2.32	0.64
6:F:100:VAL:HG22	7:G:75:PHE:HB2	1.80	0.64
3:C:34:ASP:OD2	3:C:36:HIS:HB2	1.98	0.64
2:I:37:ASN:OD1	2:I:64:GLY:N	2.25	0.64
5:L:49:VAL:HG22	5:L:66:GLN:NE2	2.13	0.64
2:B:52:PRO:HG2	2:B:54:LEU:HD11	1.79	0.63
2:I:83:GLN:HB3	3:J:12:LEU:HD23	1.80	0.63
2:B:73:ASN:OD1	2:B:76:MET:HE2	1.97	0.63
7:G:19:LEU:HD21	7:G:25:ILE:HD13	1.81	0.62
3:C:48:ILE:O	3:C:58:GLU:HA	1.99	0.62
3:J:8:LEU:HB3	3:J:33:PHE:CZ	2.34	0.62
2:B:43:ILE:HD12	2:B:51:TYR:OH	1.99	0.62
2:I:44:SER:OG	2:I:45:SER:N	2.31	0.62
1:A:5:LEU:HD13	2:B:61:PHE:CD2	2.33	0.62
1:H:92:LYS:O	1:H:96:GLU:HB2	2.00	0.61
6:M:41:LYS:NZ	7:N:23:GLU:OE1	2.32	0.61
1:A:63:LEU:HD21	2:B:60:ILE:CB	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:PHE:HE1	3:C:40:VAL:CG2	2.13	0.61
1:A:57:ARG:CG	1:A:57:ARG:HH11	2.14	0.61
2:I:47:ASP:HB3	2:I:50:LYS:CG	2.31	0.61
1:A:34:THR:O	1:A:34:THR:HG22	2.01	0.61
2:I:75:ASN:OD1	2:I:75:ASN:N	2.33	0.61
4:K:16:LEU:HD22	4:K:41:ILE:HG12	1.81	0.60
3:C:30:LEU:CD1	3:C:39:ILE:CG2	2.79	0.60
2:B:7:PHE:HB3	2:B:32:VAL:HG21	1.82	0.60
2:I:21:ASN:OD1	2:I:21:ASN:N	2.35	0.60
6:F:95:ARG:CG	6:F:95:ARG:HH21	2.14	0.60
1:H:95:ASN:OD1	1:H:98:VAL:HG21	2.01	0.60
4:K:54:GLU:HG3	4:K:64:LEU:HB2	1.83	0.60
4:D:10:SER:CB	4:D:13:THR:HG23	2.32	0.59
7:G:17:ILE:HD13	7:G:79:ILE:HG23	1.84	0.59
5:L:49:VAL:HG22	5:L:66:GLN:HE21	1.65	0.59
1:A:33:ASN:CB	1:A:35:ASN:HD21	2.16	0.59
1:A:97:HIS:CE1	1:A:98:VAL:HG22	2.38	0.59
4:D:74:ARG:HB2	4:D:77:GLN:HG3	1.85	0.58
1:A:39:THR:HG22	1:A:52:LYS:O	2.03	0.58
6:M:39:ARG:HG2	6:M:47:LEU:HD11	1.84	0.58
1:A:63:LEU:HD21	2:B:60:ILE:HG21	1.84	0.58
1:A:22:SER:HB3	1:A:44:ARG:HE	1.68	0.58
2:I:35:PHE:HB2	2:I:37:ASN:ND2	2.18	0.58
1:H:61:ILE:O	2:I:63:ARG:HD3	2.04	0.58
1:A:33:ASN:HB2	1:A:35:ASN:HD21	1.68	0.58
1:H:101:GLU:HA	4:K:64:LEU:HD22	1.86	0.58
6:F:41:LYS:HG2	6:F:47:LEU:HD13	1.84	0.57
1:A:22:SER:CB	1:A:44:ARG:HE	2.17	0.57
3:C:30:LEU:HD11	3:C:39:ILE:HG23	1.87	0.56
1:H:16:ILE:HB	1:H:63:LEU:HB3	1.88	0.56
2:B:65:SER:HA	3:C:69:ARG:NH1	2.22	0.55
7:N:25:ILE:HD11	7:N:45:GLU:HG3	1.88	0.55
1:H:95:ASN:HD22	3:J:51:LEU:HD23	1.69	0.55
7:N:18:GLU:HG2	7:N:77:LYS:HD3	1.88	0.55
1:H:23:LEU:HD23	1:H:43:ASN:HA	1.88	0.55
2:B:13:GLN:OE1	2:B:76:MET:SD	2.65	0.55
3:J:51:LEU:HG	3:J:52:ASN:H	1.71	0.55
2:B:33:ASP:CG	2:B:37:ASN:HB2	2.27	0.54
4:K:12:THR:HA	5:L:44:ILE:HD11	1.89	0.54
4:K:82:SER:HB2	5:L:71:MET:HG3	1.90	0.54
2:B:39:LYS:HA	2:B:60:ILE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LEU:O	1:A:10:ASN:HB2	2.08	0.53
1:A:57:ARG:CD	7:G:76:ILE:O	2.57	0.53
4:D:53:THR:HG22	4:D:66:LYS:HG3	1.90	0.53
2:I:37:ASN:HB3	2:I:62:ILE:O	2.08	0.53
3:J:19:LYS:HB2	3:J:75:LEU:HB3	1.91	0.53
2:B:35:PHE:CD1	2:B:35:PHE:N	2.74	0.53
3:J:18:ILE:HD13	3:J:41:LEU:HD11	1.90	0.52
7:N:19:LEU:HD21	7:N:25:ILE:HD13	1.91	0.52
3:J:26:LEU:HD22	3:J:68:ILE:CD1	2.40	0.52
6:F:39:ARG:HG2	6:F:47:LEU:HD11	1.92	0.52
1:A:9:LEU:HD11	1:A:30:PHE:HD1	1.75	0.52
4:D:25:ASN:HB3	4:D:33:LEU:HD11	1.91	0.52
4:D:54:GLU:HG2	4:D:65:ASN:HB2	1.91	0.52
3:J:15:ARG:HE	3:J:29:THR:HG22	1.75	0.52
1:A:9:LEU:CD1	1:A:30:PHE:CD1	2.93	0.52
6:M:103:SER:HB3	7:N:69:ILE:HG13	1.91	0.52
5:E:13:ASP:O	5:E:16:ILE:HG13	2.10	0.52
4:D:41:ILE:HD12	4:D:47:VAL:HG22	1.91	0.52
7:N:81:LEU:HB3	7:N:85:ILE:HD12	1.90	0.52
3:C:36:HIS:O	3:C:37:SER:HB2	2.09	0.52
7:G:19:LEU:HD23	7:G:23:GLU:HB3	1.92	0.52
1:A:9:LEU:CD1	1:A:30:PHE:HD1	2.23	0.52
4:K:80:TYR:HB3	5:L:73:LEU:HD12	1.92	0.52
2:I:64:GLY:O	2:I:67:VAL:HG13	2.09	0.51
3:C:8:LEU:HB3	3:C:33:PHE:CZ	2.46	0.51
3:C:6:ASP:HA	3:C:9:LYS:HD2	1.92	0.51
2:I:52:PRO:HG2	2:I:54:LEU:CD2	2.40	0.51
4:D:53:THR:HG22	4:D:66:LYS:CG	2.41	0.51
4:D:11:VAL:HG12	5:E:44:ILE:HD12	1.92	0.51
1:H:95:ASN:ND2	3:J:51:LEU:CD2	2.69	0.51
7:N:17:ILE:HD13	7:N:79:ILE:HG23	1.93	0.51
2:B:79:THR:HB	3:C:31:GLN:HE21	1.75	0.51
1:A:43:ASN:HB2	1:A:50:ILE:CD1	2.39	0.50
3:J:61:ARG:HG3	3:J:62:ARG:N	2.26	0.50
2:B:52:PRO:CG	2:B:54:LEU:HD11	2.42	0.50
6:M:39:ARG:NH2	7:N:45:GLU:OE1	2.34	0.50
4:D:54:GLU:HG3	4:D:64:LEU:HB2	1.92	0.50
7:G:16:GLN:HB3	7:G:80:LYS:HB2	1.93	0.50
4:D:13:THR:O	4:D:16:LEU:HB2	2.11	0.50
2:I:39:LYS:HE3	2:I:59:ASN:OD1	2.12	0.50
5:L:79:ALA:HA	6:M:98:ILE:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:64:LEU:O	4:K:65:ASN:ND2	2.40	0.50
1:A:33:ASN:CB	1:A:35:ASN:ND2	2.73	0.50
2:I:35:PHE:N	2:I:35:PHE:CD1	2.78	0.49
3:J:48:ILE:O	3:J:58:GLU:HA	2.12	0.49
6:M:68:GLU:HG2	6:M:89:LEU:HD13	1.95	0.49
5:E:22:ILE:HD11	5:E:43:VAL:HG11	1.93	0.49
4:K:41:ILE:HD12	4:K:47:VAL:HG22	1.93	0.49
3:C:12:LEU:C	3:C:14:GLU:H	2.16	0.49
1:A:60:GLU:OE1	7:G:77:LYS:HG2	2.12	0.49
1:A:17:LEU:HD12	1:A:21:GLU:HB3	1.95	0.48
5:L:22:ILE:HD11	5:L:43:VAL:HG11	1.94	0.48
2:B:72:LEU:HB2	3:C:65:MET:HB3	1.96	0.48
6:F:62:VAL:O	6:F:63:LEU:HD23	2.14	0.48
2:I:47:ASP:HB3	2:I:50:LYS:HB2	1.94	0.48
4:K:80:TYR:HB3	5:L:73:LEU:CD1	2.43	0.48
2:B:79:THR:HB	3:C:31:GLN:CG	2.44	0.48
7:G:39:THR:O	7:G:40:LEU:HD23	2.13	0.48
1:A:19:ASP:OD1	1:A:21:GLU:HB2	2.13	0.48
4:D:79:MET:HE2	5:E:30:PHE:HZ	1.76	0.48
4:K:54:GLU:HG2	4:K:65:ASN:HB2	1.96	0.47
1:A:9:LEU:HD13	1:A:30:PHE:CE1	2.49	0.47
3:J:36:HIS:O	3:J:70:GLY:HA3	2.14	0.47
3:J:15:ARG:HG2	3:J:29:THR:HG22	1.96	0.47
2:I:24:GLU:HB3	2:I:46:THR:CG2	2.44	0.47
4:D:12:THR:HG21	5:E:38:ASP:OD2	2.14	0.47
2:B:89:GLU:HB2	3:C:9:LYS:HE3	1.97	0.47
1:A:11:LYS:O	1:A:13:VAL:HG13	2.14	0.47
1:A:18:VAL:N	1:A:60:GLU:O	2.42	0.47
2:B:47:ASP:HB3	2:B:50:LYS:HG2	1.97	0.47
1:H:12:ARG:HH12	1:H:40:ASN:HB2	1.79	0.47
2:B:4:PHE:CZ	2:B:8:LYS:HE2	2.50	0.47
1:H:32:LYS:O	2:I:35:PHE:CE2	2.58	0.47
2:B:34:GLN:H	2:B:34:GLN:HG3	1.48	0.46
3:C:5:LEU:HG	3:C:33:PHE:HE1	1.81	0.46
3:J:51:LEU:O	3:J:52:ASN:HB2	2.14	0.46
1:A:94:GLU:O	1:A:97:HIS:HD2	1.98	0.46
5:E:63:LYS:O	5:E:64:VAL:HG22	2.14	0.46
2:I:11:VAL:HG13	2:I:29:LEU:O	2.15	0.46
1:A:49:PHE:HE2	1:A:52:LYS:HD2	1.80	0.46
7:N:39:THR:HA	7:N:69:ILE:O	2.16	0.46
3:C:5:LEU:HD13	3:C:35:SER:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:25:GLN:OE1	6:F:98:ILE:HG21	2.15	0.46
6:F:28:LEU:HD22	7:G:70:TYR:HB2	1.98	0.46
1:A:63:LEU:CD2	2:B:60:ILE:CG2	2.94	0.46
4:D:16:LEU:C	4:D:18:ASP:N	2.69	0.46
4:D:16:LEU:C	4:D:18:ASP:H	2.19	0.46
3:J:48:ILE:HB	3:J:59:SER:HB3	1.98	0.46
2:B:13:GLN:NE2	2:B:76:MET:HG2	2.31	0.46
1:A:56:LEU:HD12	7:G:78:PHE:HB3	1.96	0.46
5:L:29:GLU:OE1	6:M:87:ARG:NH2	2.49	0.46
3:C:37:SER:O	3:C:39:ILE:CG1	2.53	0.45
2:I:35:PHE:HB2	2:I:37:ASN:HD21	1.81	0.45
5:L:73:LEU:HD12	5:L:73:LEU:HA	1.75	0.45
7:N:16:GLN:HB3	7:N:80:LYS:HB2	1.98	0.45
2:B:47:ASP:HB3	2:B:50:LYS:CB	2.43	0.45
5:L:42:ASN:HB3	5:L:72:LEU:HD11	1.99	0.45
3:J:60:GLU:HG3	3:J:61:ARG:H	1.80	0.45
1:A:14:VAL:O	1:A:14:VAL:HG13	2.16	0.45
7:N:19:LEU:HD23	7:N:23:GLU:HB3	1.99	0.45
4:D:35:SER:O	4:D:52:ALA:HA	2.17	0.45
2:I:43:ILE:HD12	2:I:51:TYR:CZ	2.41	0.45
1:A:5:LEU:HD12	1:A:5:LEU:HA	1.83	0.45
6:M:70:MET:HE2	6:M:70:MET:HB2	1.78	0.45
1:A:66:LEU:O	2:B:57:VAL:HG13	2.17	0.45
7:G:39:THR:HA	7:G:69:ILE:O	2.17	0.45
1:A:57:ARG:HD3	7:G:76:ILE:O	2.17	0.45
2:B:51:TYR:CD1	2:B:52:PRO:HD2	2.52	0.44
2:I:24:GLU:CG	2:I:46:THR:HG21	2.47	0.44
2:B:13:GLN:CG	2:B:76:MET:SD	3.05	0.44
7:G:23:GLU:HG2	7:G:46:TYR:O	2.17	0.44
1:A:33:ASN:O	1:A:34:THR:HB	2.17	0.44
4:D:16:LEU:O	4:D:18:ASP:N	2.50	0.44
1:A:15:ILE:CG2	1:A:61:ILE:HG23	2.47	0.44
7:N:19:LEU:HB3	7:N:75:PHE:CD2	2.52	0.44
3:J:60:GLU:CG	3:J:61:ARG:N	2.81	0.44
2:B:13:GLN:CB	2:B:76:MET:SD	3.05	0.44
7:G:10:ALA:HA	7:G:13:GLN:NE2	2.33	0.44
5:E:63:LYS:C	5:E:64:VAL:CG2	2.86	0.43
5:E:41:VAL:O	5:E:78:ILE:HD12	2.18	0.43
6:M:39:ARG:HG3	6:M:49:ILE:HG12	2.00	0.43
4:D:44:PHE:O	4:D:75:GLY:HA3	2.18	0.43
6:F:33:TYR:O	6:F:36:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:47:ASP:HB3	2:I:50:LYS:CB	2.48	0.43
4:D:13:THR:HA	4:D:16:LEU:HD12	2.00	0.43
1:A:9:LEU:HD13	1:A:30:PHE:HE1	1.82	0.43
2:B:73:ASN:OD1	2:B:76:MET:CG	2.67	0.43
2:B:34:GLN:C	2:B:36:LEU:H	2.21	0.43
1:A:94:GLU:O	1:A:97:HIS:CD2	2.70	0.43
7:G:81:LEU:HB3	7:G:85:ILE:HD12	2.01	0.43
2:B:33:ASP:OD1	2:B:37:ASN:CB	2.65	0.43
5:E:25:GLN:OE1	6:F:98:ILE:CG2	2.66	0.43
2:I:47:ASP:O	2:I:49:LYS:N	2.52	0.43
6:F:103:SER:HB3	7:G:69:ILE:HG13	2.01	0.43
2:B:23:ILE:HG23	2:B:52:PRO:HD3	2.01	0.43
3:C:15:ARG:HE	3:C:29:THR:HG22	1.85	0.42
2:B:79:THR:CB	3:C:31:GLN:HE21	2.32	0.42
5:L:27:ASN:OD1	5:L:27:ASN:N	2.51	0.42
3:J:77:SER:OG	3:J:78:THR:N	2.52	0.42
2:I:51:TYR:HE2	2:I:54:LEU:HD12	1.79	0.42
2:I:43:ILE:HD11	2:I:51:TYR:OH	2.12	0.42
3:C:12:LEU:O	3:C:14:GLU:N	2.52	0.42
6:M:33:TYR:O	6:M:36:SER:HB3	2.20	0.42
6:F:39:ARG:NH2	7:G:45:GLU:OE1	2.43	0.42
4:D:41:ILE:HA	4:D:46:ASN:O	2.19	0.42
5:E:42:ASN:HB3	5:E:72:LEU:HD11	2.00	0.42
7:G:82:GLN:O	7:G:85:ILE:HB	2.20	0.42
1:H:19:ASP:OD1	1:H:21:GLU:HB2	2.19	0.42
2:B:39:LYS:HE3	2:B:59:ASN:OD1	2.19	0.42
7:N:14:GLN:O	7:N:82:GLN:HG3	2.20	0.42
7:N:26:GLN:HB3	7:N:44:THR:HG23	2.02	0.42
3:C:69:ARG:NH1	3:C:71:ASP:OD2	2.52	0.42
2:I:47:ASP:C	2:I:49:LYS:N	2.73	0.42
4:K:41:ILE:HA	4:K:46:ASN:O	2.20	0.42
7:N:28:ILE:HG13	7:N:28:ILE:O	2.20	0.42
7:G:7:LEU:HG	7:G:32:VAL:HG21	2.01	0.42
2:B:30:GLN:HB3	2:B:39:LYS:O	2.20	0.42
3:C:30:LEU:HD11	3:C:39:ILE:CG2	2.47	0.42
4:D:22:LYS:O	4:D:37:ARG:HA	2.19	0.42
1:H:18:VAL:HG23	1:H:60:GLU:O	2.19	0.42
1:A:13:VAL:HG12	1:A:66:LEU:HD23	2.02	0.41
3:C:34:ASP:OD1	3:C:37:SER:N	2.52	0.41
2:B:36:LEU:HA	2:B:36:LEU:HD23	1.84	0.41
3:J:12:LEU:C	3:J:14:GLU:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:37:ASN:OD1	7:G:72:ARG:HD3	2.18	0.41
3:C:11:ASN:HB2	3:C:14:GLU:HG2	2.01	0.41
1:A:41:VAL:HG21	1:A:54:GLN:HG2	2.03	0.41
1:A:15:ILE:HG23	1:A:64:VAL:HG22	2.02	0.41
1:A:56:LEU:CD1	7:G:78:PHE:HB3	2.50	0.41
6:M:64:ASP:OD1	6:M:65:ASP:N	2.52	0.41
2:B:29:LEU:HA	2:B:29:LEU:HD12	1.80	0.41
1:A:66:LEU:HA	1:A:66:LEU:HD23	1.86	0.41
4:D:14:GLU:HG2	4:D:14:GLU:H	1.49	0.41
3:J:5:LEU:HG	3:J:33:PHE:HE1	1.86	0.41
4:K:44:PHE:O	4:K:75:GLY:HA3	2.21	0.41
1:H:27:LEU:HD11	1:H:36:LEU:HD22	2.03	0.41
1:A:18:VAL:CG2	1:A:60:GLU:O	2.58	0.41
2:I:54:LEU:O	2:I:54:LEU:HD12	2.21	0.41
2:B:4:PHE:CE2	2:B:8:LYS:HE3	2.56	0.41
1:H:49:PHE:HE2	1:H:52:LYS:HD2	1.86	0.41
1:H:5:LEU:HA	1:H:5:LEU:HD12	1.74	0.41
5:E:8:PRO:HG2	6:F:60:ASN:O	2.20	0.41
1:H:97:HIS:CE1	1:H:98:VAL:HG22	2.56	0.41
4:D:49:LEU:O	4:D:70:ASP:HA	2.21	0.41
2:I:24:GLU:HG2	2:I:46:THR:HG21	2.02	0.41
1:A:9:LEU:O	1:A:10:ASN:CB	2.69	0.40
2:I:7:PHE:HB3	2:I:32:VAL:HG21	2.02	0.40
2:B:20:LYS:C	2:B:22:ASP:H	2.24	0.40
1:A:4:THR:HG21	2:B:61:PHE:HE2	1.86	0.40
7:N:18:GLU:HA	7:N:23:GLU:O	2.22	0.40
3:J:19:LYS:HE2	3:J:19:LYS:HB3	1.82	0.40
7:N:40:LEU:HB2	7:N:69:ILE:HG22	2.03	0.40
7:N:40:LEU:O	7:N:68:GLU:HA	2.21	0.40
7:G:85:ILE:O	7:G:86:ILE:HD13	2.21	0.40
1:A:4:THR:HG21	2:B:61:PHE:CE2	2.55	0.40
1:H:22:SER:CB	1:H:44:ARG:HE	2.27	0.40
2:B:34:GLN:OE1	2:B:35:PHE:CE1	2.74	0.40
5:E:15:THR:HB	5:E:34:LEU:HD23	2.04	0.40
4:D:27:LYS:HZ3	4:D:57:GLU:HA	1.87	0.40
3:C:30:LEU:CD1	3:C:39:ILE:HG23	2.47	0.40
4:K:71:VAL:HG12	4:K:73:LEU:HD13	2.02	0.40
2:B:47:ASP:HB3	2:B:50:LYS:CG	2.51	0.40
6:M:42:LEU:HD22	6:M:98:ILE:HD12	2.03	0.40

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)
2:I:73:ASN:OD1	3:J:62:ARG:NH1[8_555]	2.04	0.16

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	79/109 (72%)	69 (87%)	10 (13%)	0	100 100
1	H	81/109 (74%)	76 (94%)	5 (6%)	0	100 100
2	B	89/95 (94%)	76 (85%)	12 (14%)	1 (1%)	17 56
2	I	89/95 (94%)	74 (83%)	11 (12%)	4 (4%)	3 18
3	C	65/89 (73%)	62 (95%)	1 (2%)	2 (3%)	5 28
3	J	68/89 (76%)	63 (93%)	5 (7%)	0	100 100
4	D	73/86 (85%)	68 (93%)	4 (6%)	1 (1%)	14 49
4	K	73/86 (85%)	69 (94%)	4 (6%)	0	100 100
5	E	66/93 (71%)	62 (94%)	4 (6%)	0	100 100
5	L	69/93 (74%)	65 (94%)	3 (4%)	1 (1%)	14 49
6	F	61/115 (53%)	56 (92%)	5 (8%)	0	100 100
6	M	61/115 (53%)	58 (95%)	2 (3%)	1 (2%)	12 45
7	G	66/93 (71%)	63 (96%)	3 (4%)	0	100 100
7	N	66/93 (71%)	59 (89%)	7 (11%)	0	100 100
All	All	1006/1360 (74%)	920 (92%)	76 (8%)	10 (1%)	19 59

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	55	GLY
3	C	13	ASP
6	M	90	GLY
2	I	55	GLY

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Mol	Chain	Res	Type
3	C	37	SER
2	I	48	GLU
4	D	17	SER
2	I	53	HIS
5	L	9	LEU
2	I	90	VAL

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	68/99 (69%)	48 (71%)	20 (29%)	0 1
1	H	72/99 (73%)	57 (79%)	15 (21%)	1 6
2	B	85/91 (93%)	73 (86%)	12 (14%)	4 18
2	I	85/91 (93%)	71 (84%)	14 (16%)	3 12
3	C	63/81 (78%)	52 (82%)	11 (18%)	2 10
3	J	66/81 (82%)	51 (77%)	15 (23%)	1 4
4	D	66/75 (88%)	58 (88%)	8 (12%)	6 24
4	K	65/75 (87%)	57 (88%)	8 (12%)	6 24
5	E	61/84 (73%)	56 (92%)	5 (8%)	14 47
5	L	66/84 (79%)	61 (92%)	5 (8%)	16 51
6	F	56/103 (54%)	49 (88%)	7 (12%)	6 23
6	M	56/103 (54%)	51 (91%)	5 (9%)	12 42
7	G	64/85 (75%)	54 (84%)	10 (16%)	3 14
7	N	64/85 (75%)	54 (84%)	10 (16%)	3 14
All	All	937/1236 (76%)	792 (84%)	145 (16%)	3 14

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU

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Mol	Chain	Res	Type
1	A	7	ASP
1	A	9	LEU
1	A	10	ASN
1	A	12	ARG
1	A	21	GLU
1	A	35	ASN
1	A	36	LEU
1	A	38	LEU
1	A	39	THR
1	A	46	SER
1	A	47	LYS
1	A	48	GLU
1	A	57	ARG
1	A	60	GLU
1	A	63	LEU
1	A	66	LEU
1	A	71	ASN
1	A	73	ASP
1	A	75	LEU
2	B	5	SER
2	B	9	THR
2	B	14	GLU
2	B	19	LEU
2	B	34	GLN
2	B	38	LEU
2	B	42	ASN
2	B	56	SER
2	B	75	ASN
2	B	77	VAL
2	B	88	ARG
2	B	91	MET
3	C	3	THR
3	C	8	LEU
3	C	10	LEU
3	C	11	ASN
3	C	14	GLU
3	C	15	ARG
3	C	25	THR
3	C	35	SER
3	C	58	GLU
3	C	69	ARG
3	C	74	THR

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Mol	Chain	Res	Type
4	D	14	GLU
4	D	41	ILE
4	D	50	SER
4	D	57	GLU
4	D	62	LYS
4	D	65	ASN
4	D	73	LEU
4	D	84	GLN
5	E	19	LYS
5	E	25	GLN
5	E	26	SER
5	E	40	PHE
5	E	45	LEU
6	F	68	GLU
6	F	70	MET
6	F	87	ARG
6	F	88	LYS
6	F	95	ARG
6	F	100	VAL
6	F	104	SER
7	G	1	MET
7	G	2	LEU
7	G	14	GLN
7	G	17	ILE
7	G	19	LEU
7	G	20	LYS
7	G	28	ILE
7	G	38	LEU
7	G	44	THR
7	G	68	GLU
1	H	5	LEU
1	H	21	GLU
1	H	22	SER
1	H	39	THR
1	H	46	SER
1	H	47	LYS
1	H	48	GLU
1	H	55	LEU
1	H	57	ARG
1	H	60	GLU
1	H	63	LEU
1	H	66	LEU

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Mol	Chain	Res	Type
1	H	71	ASN
1	H	73	ASP
1	H	75	LEU
2	I	5	SER
2	I	9	THR
2	I	14	GLU
2	I	19	LEU
2	I	21	ASN
2	I	42	ASN
2	I	46	THR
2	I	48	GLU
2	I	56	SER
2	I	73	ASN
2	I	75	ASN
2	I	77	VAL
2	I	88	ARG
2	I	91	MET
3	J	3	THR
3	J	8	LEU
3	J	10	LEU
3	J	11	ASN
3	J	14	GLU
3	J	15	ARG
3	J	25	THR
3	J	35	SER
3	J	45	VAL
3	J	52	ASN
3	J	59	SER
3	J	61	ARG
3	J	62	ARG
3	J	69	ARG
3	J	74	THR
4	K	19	ILE
4	K	20	ILE
4	K	41	ILE
4	K	50	SER
4	K	62	LYS
4	K	65	ASN
4	K	73	LEU
4	K	78	VAL
5	L	19	LYS
5	L	23	VAL

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Mol	Chain	Res	Type
5	L	25	GLN
5	L	26	SER
5	L	27	ASN
6	M	68	GLU
6	M	70	MET
6	M	87	ARG
6	M	100	VAL
6	M	104	SER
7	N	1	MET
7	N	2	LEU
7	N	14	GLN
7	N	17	ILE
7	N	19	LEU
7	N	20	LYS
7	N	28	ILE
7	N	38	LEU
7	N	44	THR
7	N	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
4	D	84	GLN
5	E	67	HIS
2	I	42	ASN
3	J	31	GLN
4	K	25	ASN
5	L	17	ASN
5	L	66	GLN

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

There are no carbohydrates 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, 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	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	83/109 (76%)	0.05	4 (4%) 34 15	50, 76, 155, 198	0
1	H	85/109 (77%)	0.05	3 (3%) 48 24	43, 77, 130, 155	0
2	B	91/95 (95%)	-0.40	0 100 100	46, 72, 121, 137	0
2	I	91/95 (95%)	-0.37	0 100 100	52, 76, 122, 177	0
3	C	69/89 (77%)	-0.24	1 (1%) 78 61	53, 78, 115, 135	0
3	J	72/89 (80%)	-0.12	4 (5%) 28 11	47, 80, 120, 173	0
4	D	75/86 (87%)	0.03	1 (1%) 79 63	55, 82, 133, 169	0
4	K	75/86 (87%)	-0.11	1 (1%) 79 63	54, 87, 135, 178	0
5	E	70/93 (75%)	-0.34	0 100 100	46, 72, 101, 123	0
5	L	73/93 (78%)	-0.23	1 (1%) 78 61	46, 77, 123, 129	0
6	F	65/115 (56%)	-0.27	1 (1%) 76 58	56, 84, 119, 188	0
6	M	65/115 (56%)	-0.27	2 (3%) 52 28	58, 90, 120, 188	0
7	G	70/93 (75%)	-0.08	2 (2%) 55 32	59, 84, 123, 151	0
7	N	70/93 (75%)	-0.17	1 (1%) 78 61	62, 98, 146, 188	0
All	All	1054/1360 (77%)	-0.18	21 (1%) 68 47	43, 81, 133, 198	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	51	LEU	4.9
3	J	59	SER	3.9
1	H	95	ASN	3.4
3	J	52	ASN	3.4
1	H	104	TYR	3.1
7	N	46	TYR	3.1
3	J	50	GLN	2.9
7	G	46	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
7	G	84	ASN	2.8
1	A	103	VAL	2.7
1	H	103	VAL	2.6
3	C	49	TYR	2.5
4	D	84	GLN	2.5
6	M	85	ASN	2.5
1	A	94	GLU	2.5
1	A	95	ASN	2.3
5	L	27	ASN	2.3
1	A	98	VAL	2.2
4	K	51	SER	2.2
6	M	69	TYR	2.1
6	F	70	MET	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 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.