



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:17 am BST

PDB ID : 3CW1
Title : Crystal Structure of Human Spliceosomal U1 snRNP
Authors : Pomeranz Krummel, D.A.; Oubridge, C.; Leung, A.K.; Li, J.; Nagai, K.
Deposited on : 2008-04-21
Resolution : 5.49 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
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

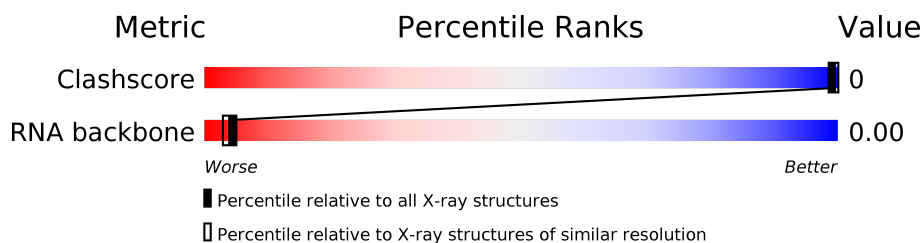
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


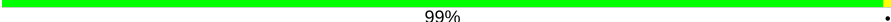
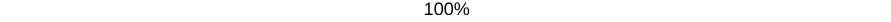



The reported resolution of this entry is 5.49 Å.

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.



















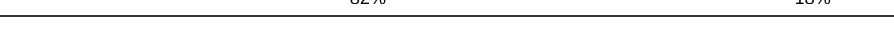

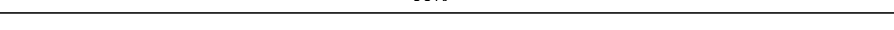
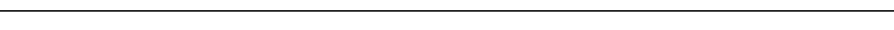
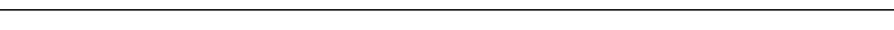
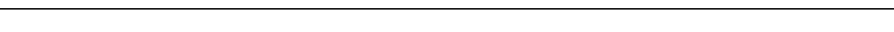
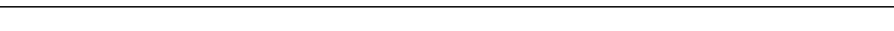
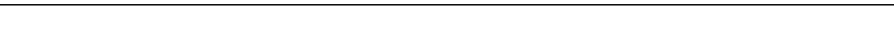

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1010 (7.10-3.90)
RNA backbone	3102	1074 (7.80-3.00)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	V	138	 100%
1	v	138	 99% .
1	w	138	 100%
1	x	138	 100%
2	D	126	 60% 40%
2	S	126	 60% 40%
2	T	126	 60% 40%
2	U	126	 60% 40%
3	A	174	 37% 63%
3	H	174	 37% 63%

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Mol	Chain	Length	Quality of chain
3	I	174	
3	J	174	
4	B	119	
4	M	119	
4	N	119	
4	O	119	
5	C	118	
5	P	118	
5	Q	118	
5	R	118	
6	1	86	
6	2	86	
6	F	86	
6	Z	86	
7	E	92	
7	W	92	
7	X	92	
7	Y	92	
8	3	76	
8	4	76	
8	5	76	
8	G	76	
9	6	216	
9	7	216	
9	8	216	

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Mol	Chain	Length	Quality of chain
9	K	216	<div><div></div><div>55%</div><div>44%</div></div>
10	0	77	<div><div></div><div>70%</div><div>30%</div></div>
10	9	77	<div><div></div><div>75%</div><div>25%</div></div>
10	L	77	<div><div></div><div>74%</div><div>26%</div></div>
10	l	77	<div><div></div><div>75%</div><div>25%</div></div>

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 3365 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 RNA chain called U1 snRNA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	V	138	Total P 138 138	0	0	138
1	v	138	Total P 138 138	0	0	138
1	w	138	Total P 138 138	0	0	138
1	x	138	Total P 138 138	0	0	138

- Molecule 2 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	D	76	Total C 76 76	0	0	76
2	S	76	Total C 76 76	0	0	76
2	T	76	Total C 76 76	0	0	76
2	U	76	Total C 76 76	0	0	76

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	66	CYS	SER	CONFLICT	UNP P62318
S	266	CYS	SER	CONFLICT	UNP P62318
T	466	CYS	SER	CONFLICT	UNP P62318
U	666	CYS	SER	CONFLICT	UNP P62318

- Molecule 3 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	A	64	Total C 64 64	0	0	64
3	H	64	Total C 64 64	0	0	64
3	I	63	Total C 63 63	0	0	63
3	J	63	Total C 63 63	0	0	63

- Molecule 4 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	B	77	Total C 77 77	0	0	77
4	M	77	Total C 77 77	0	0	77
4	N	76	Total C 76 76	0	0	76
4	O	77	Total C 77 77	0	0	77

- Molecule 5 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	C	88	Total C 88 88	0	0	88
5	P	86	Total C 86 86	0	0	86
5	Q	89	Total C 89 89	0	0	89
5	R	85	Total C 85 85	0	0	85

- Molecule 6 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	F	76	Total C 76 76	0	0	76
6	Z	70	Total C 70 70	0	0	70
6	1	75	Total C 75 75	0	0	75

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	2	76	Total C 76 76	0	0	76

- Molecule 7 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	E	75	Total C 75 75	0	0	75
7	W	75	Total C 75 75	0	0	75
7	X	75	Total C 75 75	0	0	75
7	Y	75	Total C 75 75	0	0	75

- Molecule 8 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	G	73	Total C 73 73	0	0	73
8	3	73	Total C 73 73	0	0	73
8	4	73	Total C 73 73	0	0	73
8	5	73	Total C 73 73	0	0	73

- Molecule 9 is a protein called U1 small nuclear ribonucleoprotein 70 kDa.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	K	120	Total C 120 120	0	0	120
9	6	120	Total C 120 120	0	0	120
9	7	120	Total C 120 120	0	0	120
9	8	120	Total C 120 120	0	0	120

- Molecule 10 is a protein called U1 small nuclear ribonucleoprotein C.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	L	57	Total C 57 57	0	0	57
10	9	58	Total C 58 58	0	0	58
10	0	54	Total C 54 54	0	0	54
10	1	58	Total C 58 58	0	0	58

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	39	CYS	GLN	CONFLICT	UNP P09234
9	239	CYS	GLN	CONFLICT	UNP P09234
0	439	CYS	GLN	CONFLICT	UNP P09234
1	639	CYS	GLN	CONFLICT	UNP P09234

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	0	1	Total Zn 1 1	0	0
11	1	1	Total Zn 1 1	0	0
11	9	1	Total Zn 1 1	0	0
11	L	1	Total Zn 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. 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: U1 snRNA

Chain V:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: U1 snRNA

Chain v:  99%



- Molecule 1: U1 snRNA

Chain w:  100%

There are no outlier residues recorded for this chain.

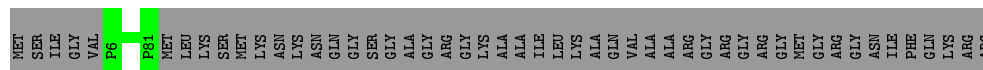
- Molecule 1: U1 snRNA

Chain x:  100%

There are no outlier residues recorded for this chain.

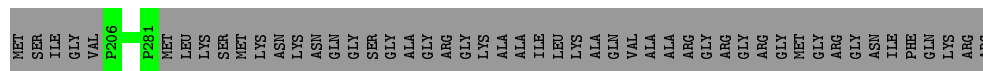
- Molecule 2: Small nuclear ribonucleoprotein Sm D3

Chain D:  60% 40%



- Molecule 2: Small nuclear ribonucleoprotein Sm D3

Chain S:  60% 40%



- Molecule 2: Small nuclear ribonucleoprotein Sm D3

Chain T:  60% 40%

MET	SER	ILE	GLY	VAL	P406	P481	MET	LEU	LYS	SER	MET	LYS	ASN	ASN	GLN	GLY	SER	GLY	ALA	GLY	ARG	GLY	LYS	ALA	ALA	TLE	LEU	LYS	ALA	GLN	VAL	ALA	ALA	ARG	GLY	ARG	GLY	ARG	GLY	MET	GLY	ARG	GLY	ASN	TLE	PHE	GLN	LYS	ARG
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- Molecule 2: Small nuclear ribonucleoprotein Sm D3

Chain U:  60% 40%

MET	SER	ILE	GLY	VAL	P606	P681	MET	LEU	LYS	SER	MET	LYS	ASN	ASN	GLN	GLY	SER	GLY	ALA	GLY	ARG	GLY	LYS	ALA	ALA	ILE	LEU	LYS	ALA	GLN	VAL	ALA	ALA	ARG	GLY	ARG	GLY	ARG	GLY	MET	GLY	ARG	GLY	ASN	ILE	PHE	GLN	LYS	ARG
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- Molecule 3: Small nuclear ribonucleoprotein-associated proteins B and B

Chain A:  37% 63%

MET	THR	VAL	GLY	LYS	SER	S7	P47	E4E	PHE	ARG	LYS	ILE	LYS	PRO	LYS	ASN	SER	LYS	GLN	ALA	GLU	ARG	GLU	GLU	R65	R65	P67	LYS	ASP	THR	THR	GLY	ILE	ALA	ARG	VAL	PRO	PRO	LEU	ALA	ALA	GLY	ALA	ALA	GLY	GLY	PRO	PRO	GLY	ILE	GLY	ARG	ALA	ALA	GLY	ALA	GLY	ARG	GLY	ILE	PRO	PRO	ALA	ALA	GLY	VAL
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[illegible]

- Molecule 3: Small nuclear ribonucleoprotein-associated proteins B and B

Chain H: 37% 63%

MET	THR	VAL	GLY	LYS	SER	S207	P247	PHE	ARG	LYS	ILE	LYS	PRO	ASN	SER	LYS	GLN	ALA	GLU	ARG	GLU	GLU	LYS	R265	P287	LYS	ASP	THR	GLY	ILE	ALA	ARG	VAL	PRO	LEU	ALA	GLY	GLY	GLY	GLY	ILE	ARG	ALA	ALA	GLY	ARG	GLY	ILE	PRO	ALA	GLY
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	PRO	MET	PRO	GLN	ALA	PRO	ALA	GLY	LEU	GLY	VAL	ARG	GLY	VAL	GLY	GLY	PRO	SER	GLN	GLN	VAL	VAL	MET	THR	PRO	GLN	GLY	ARG	GLY	THR	VAL	VAL	ALA	ALA	ALA	ALA	ALA	SER	ILE	ALA	GLY	ALA	PRO	THR	GLN	Tyr	PRO	GLY	ARG	GLY
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- Molecule 3: Small nuclear ribonucleoprotein-associated proteins B and B

Chain I: 

MET	THR	VAL	GLY	LYS	SER	SER	R407	F446	PRE	ARG	LYS	LYS	LYS	PRO	LYS	ASN	SER	LYS	GLN	ALA	GLU	ARG	GLU	GLY	LYS	R465	F487	LYS	ASP	THR	THR	GLY	ILE	ALA	ALA	ARG	VAL	PRO	PRO	LEU	ALA	GLY	GLY	PRO	GLY	ILE	GLY	ARG	ALA	ALA	GLY	GLY	GLY	ILE	PRO	ALA
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VAL	PRO	MET	PRO	GLN	ALA	ALA	PRO	GLY	ALA	ALA	GLY	PRO	ARG	GLY	VAL	VAL	GLY	GLY	PRO	SER	GLN	GLN	VAL	MET	THR	PRO	PRO	GLN	GLY	GLY	ARG	GLY	THR	VAL	VAL	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	THR	THR	PRO	PRO	GLY	ARG	GLY	GLY
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- Molecule 3: Small nuclear ribonucleoprotein-associated proteins B and B

Chain J: 36% 64%

MET	THR	VAL	GLY	LYS	SER	S607	E647	PHE	ARG	LYS	ILE	LYS	PRO	LYS	ASN	SER	LYS	GLN	ALA	GLU	ARG	GLU	GLU	LYS	R665	P686	PRO	LYS	ASP	THR	THR	GLY	ILE	ALA	ALA	ARG	VAL	PRO	LEU	ALA	GLY	ALA	ALA	GLY	PRO	GLY	ILE	GLY	ARG	ALA	ALA	GLY	ARG	GLY	ILE	PRO	ALA
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VAL	PRO	PRO	GLN	ALA	PRO	ALA	ALA	LEU	GLY	ALA	GLY	PRO	VAL	ARG	GLY	VAL	GLY	GLY	PRO	PRO	SER	GLN	GLN	VAL	VAL	MET	THR	THR	GLN	GLY	ARG	GLY	THR	VAL	ALA	ALA	ALA	ALA	ALA	ALA	ALA	THR	THR	THR	PRO	PRO	PRO	GLY	ARG	GLY	GLY
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- Molecule 4: Small nuclear ribonucleoprotein Sm D1

Chain B: 65% 35%



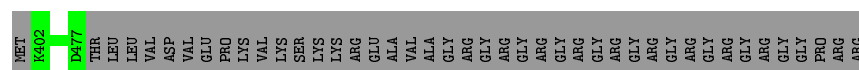
- Molecule 4: Small nuclear ribonucleoprotein Sm D1

Chain M: 65% 35%



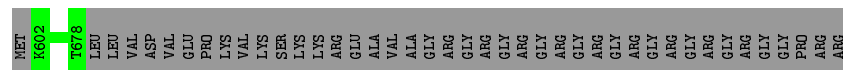
- Molecule 4: Small nuclear ribonucleoprotein Sm D1

Chain N: 64% 36%




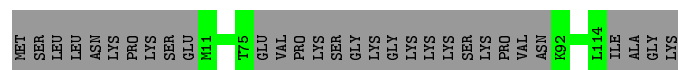
- Molecule 4: Small nuclear ribonucleoprotein Sm D1

Chain O:  65% 35%



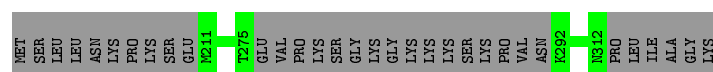
- Molecule 5: Small nuclear ribonucleoprotein Sm D2

Chain C:  75% 25%

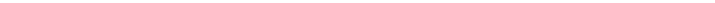


- Molecule 5: Small nuclear ribonucleoprotein Sm D2

Chain P:  73% 27%



- Molecule 5: Small nuclear ribonucleoprotein Sm D2

Chain Q: 



- Molecule 5: Small nuclear ribonucleoprotein Sm D2

Chain R:  72% 28%


MET SER LEU LEU ASN LYS PRO LYS SER SER P611 P673 TRP THR GLU VAL PRO LYS SER SER LYS GLY GLY LYS LYS LYS SER LYS LYS PRO VAL ASN P692 P713 LEU ILE ALA GLY LYS

- Molecule 6: Small nuclear ribonucleoprotein F

Chain F:  88% 12%

MET SER LEU PRO LEU D6 D61 GLY GLU MET ARG GLU

- Molecule 6: Small nuclear ribonucleoprotein F

Chain Z:  81% 19%


MET SER LEU PRO LEU N206 V278 GLU GLU GLU GLU ASP GLY GLU MET ARG GLU

- Molecule 6: Small nuclear ribonucleoprotein F

Chain 1:  87% 13%


MET SER LEU PRO LEU ASN P407 D481 GLY GLU MET ARG GLU

- Molecule 6: Small nuclear ribonucleoprotein F

Chain 2:  88% 12%


MET SER LEU PRO LEU N606 D681 GLY GLU MET ARG GLU

- Molecule 7: Small nuclear ribonucleoprotein E

Chain E:  82% 18%


MET ALA TYR ARG GLY GLN GLN LYS VAL VAL LYS LYS VAL MET VAL VAL PRO I18 H92

- Molecule 7: Small nuclear ribonucleoprotein E

Chain W:  82% 18%


MET ALA TYR ARG GLY GLN GLN LYS VAL VAL LYS LYS VAL MET VAL VAL PRO I218 H292

- Molecule 7: Small nuclear ribonucleoprotein E

Chain X:  82% 18%

MET	ALA	TYR	ARG	GLY	GLN	GLY	GLN	LYS	VAL	GLN	LYS	VAL	VAL	MET	VAL	GLN	PRO	I418	I492
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- Molecule 7: Small nuclear ribonucleoprotein E

Chain Y:  82% 18%

MET	ALA	TYR	ARG	GLY	GLN	GLY	GLN	LYS	VAL	GLN	LYS	VAL	VAL	MET	VAL	GLN	PRO	I618	I692
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- Molecule 8: Small nuclear ribonucleoprotein G

Chain G:  96% .

MET	SER	LYS	A4	V76
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- Molecule 8: Small nuclear ribonucleoprotein G

Chain 3:  96% .

MET	SER	LYS	A204	V276
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- Molecule 8: Small nuclear ribonucleoprotein G

Chain 4:  96% .

MET	SER	LYS	A404	V476
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- Molecule 8: Small nuclear ribonucleoprotein G

Chain 5:  96% .

MET	SER	LYS	A604	V676
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- Molecule 9: U1 small nuclear ribonucleoprotein 70 kDa

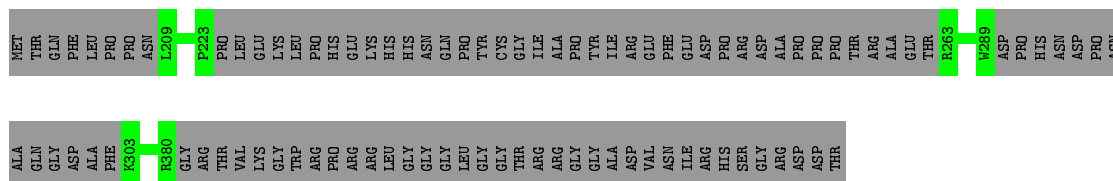
Chain K:  55% 44%

MET	THR	GLN	PHE	LEU	PRO	ASN	L9	P23	PRO	LEU	GLU	LYS	LEU	PRO	HIS	GLU	LYS	HIS	HIS	ASN	GLN	PRO	TYR	CYS	GLY	ILE	ALA	PRO	TYR	ILE	ARG	GLU	ALA	PHE	GLU	ASP	PRO	ARG	ASP	ALA	PRO	PRO	THR	ARG	ALA	GLU	THR	R63	R89	ASP	PRO	HIS	ASN	ASP	PRO	ASN
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ALA	GLN	GLY	ASP	ALA	PHE	K103	H153	R190	GLY	ARG	THR	VAL	LYS	GLY	TRP	ARG	PRO	ARG	ARG	LEU	GLY	GLY	GLY	LEU	GLY	THR	ARG	ARG	GLY	GLY	ALA	ASP	VAL	ASN	THR	ARG	HIS	SER	GLY	ARG	ASP	ASP	THR
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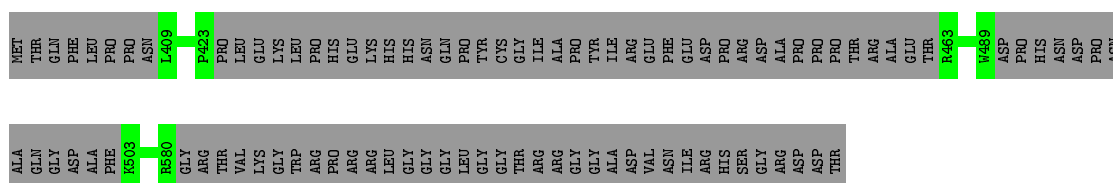
- Molecule 9: U1 small nuclear ribonucleoprotein 70 kDa

Chain 6:  56% 44%



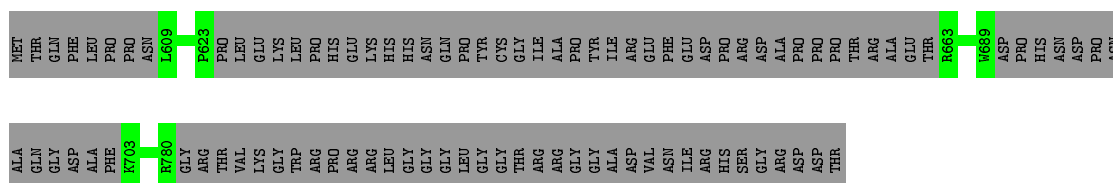
- Molecule 9: U1 small nuclear ribonucleoprotein 70 kDa

Chain 7:  56% 44%



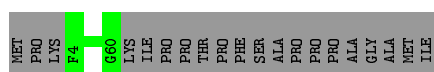
- Molecule 9: U1 small nuclear ribonucleoprotein 70 kDa

Chain 8:  56% 44%




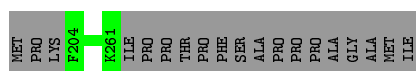
- Molecule 10: U1 small nuclear ribonucleoprotein C

Chain L:  74% 26%



- Molecule 10: U1 small nuclear ribonucleoprotein C

Chain 9:  75% 25%



- Molecule 10: U1 small nuclear ribonucleoprotein C

Chain 0:  70% 30%

MET	PRO	LYS	F404	F457	GLN	GLN	GLY	LYS	ILE	PRO	THR	PRO	PHE	SER	ALA	PRO	PRO	ALA	GLY	ALA	MET	ILE
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- Molecule 10: U1 small nuclear ribonucleoprotein C

Chain 1:

75%

25%

MET	PRO	LYS	F604	K661	ILE	PRO	THR	PRO	PHE	SER	ALA	PRO	PRO	ALA	GLY	ALA	MET	ILE
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	126.47 Å 127.08 Å 152.02 Å 95.42° 105.92° 101.80°	Depositor
Resolution (Å)	123.09 – 5.49 122.79 – 5.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) (123.09-5.49) 99.0 (122.79-5.49)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 5.42 Å)	Xtriage
Refinement program		Depositor
R, R_{free}	(Not available) , (Not available) 0.469 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	251.7	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.59 , -6.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	3365	wwPDB-VP
Average B, all atoms (Å ²)	231.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	V	138	0	0	0	0
1	v	138	0	0	0	1
1	w	138	0	0	0	0
1	x	138	0	0	0	0
2	D	76	0	0	0	0
2	S	76	0	0	0	0
2	T	76	0	0	0	0
2	U	76	0	0	0	0
3	A	64	0	0	0	0
3	H	64	0	0	0	0
3	I	63	0	0	0	0
3	J	63	0	0	0	0
4	B	77	0	0	0	0
4	M	77	0	0	0	0
4	N	76	0	0	0	0
4	O	77	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	88	0	0	0	0
5	P	86	0	0	0	0
5	Q	89	0	0	0	0
5	R	85	0	0	0	0
6	1	75	0	0	0	0
6	2	76	0	0	0	0
6	F	76	0	0	0	0
6	Z	70	0	0	0	0
7	E	75	0	0	0	0
7	W	75	0	0	0	0
7	X	75	0	0	0	0
7	Y	75	0	0	0	0
8	3	73	0	0	0	0
8	4	73	0	0	0	0
8	5	73	0	0	0	0
8	G	73	0	0	0	0
9	6	120	0	0	0	0
9	7	120	0	0	0	0
9	8	120	0	0	0	0
9	K	120	0	0	0	1
10	0	54	0	0	0	0
10	9	58	0	0	0	0
10	L	57	0	0	0	0
10	l	58	0	0	0	0
11	0	1	0	0	0	0
11	9	1	0	0	0	0
11	L	1	0	0	0	0
11	l	1	0	0	0	0
All	All	3365	0	0	0	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 0.

There are no clashes within the asymmetric unit.

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)
1:v:214:A:P	9:k:153:HIS:CA[1_545]	2.05	0.15

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	V	0/138	-	-
1	v	0/138	-	-
1	w	0/138	-	-
1	x	0/138	-	-
All	All	0/552	-	-

There are no RNA backbone outliers to report.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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

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 ⓘ

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.