



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:12 PM UTC

PDB ID : 4WZJ / pdb_00004wzj
Title : Spliceosomal U4 snRNP core domain
Authors : Leung, A.K.W.; Nagai, K.; Li, J.
Deposited on : 2014-11-19
Resolution : 3.60 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

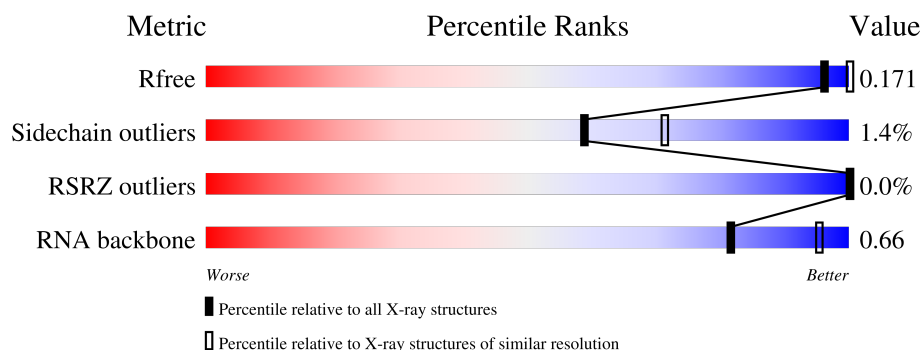
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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.



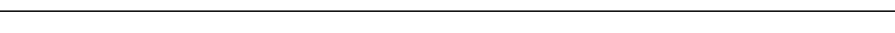
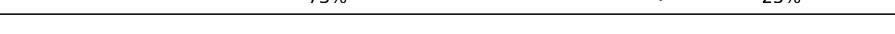
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

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 of 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 $\leq 5\%$. 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	125	66% 34%
1	AA	125	66% 34%
1	AAA	125	66% 34%
1	AAAA	125	65% 34%
1	H	125	66% 33%
1	HH	125	67% 33%

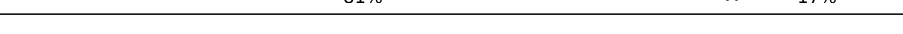
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Mol	Chain	Length	Quality of chain
1	HHH	125	
1	HHHH	125	
1	O	125	
1	OO	125	
1	OOO	125	
1	OOOO	125	
2	B	95	
2	BB	95	
2	BBB	95	
2	BBBB	95	
2	I	95	
2	II	95	
2	III	95	
2	III	95	
2	P	95	
2	PP	95	
2	PPP	95	
2	PPPP	95	
3	C	118	
3	CC	118	
3	CCC	118	
3	CCCC	118	
3	J	118	
3	JJ	118	
3	JJJ	118	

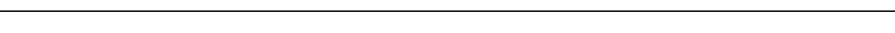
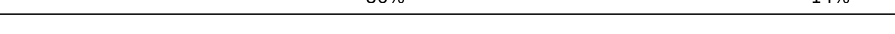
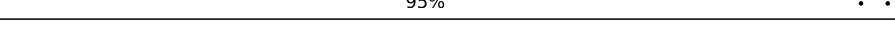
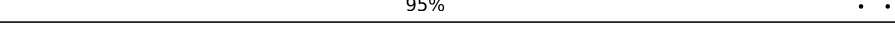
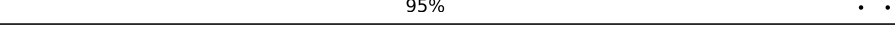
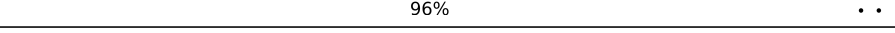
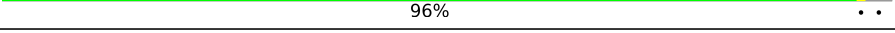
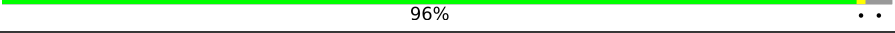
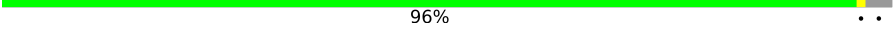
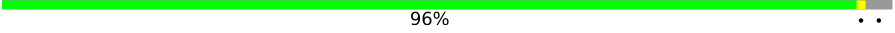
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Mol	Chain	Length	Quality of chain
3	JJJJ	118	
3	Q	118	
3	QQ	118	
3	QQQ	118	
3	QQQQ	118	
4	D	118	
4	DD	118	
4	DDD	118	
4	DDDD	118	
4	K	118	
4	KK	118	
4	KKK	118	
4	KKKK	118	
4	R	118	
4	RR	118	
4	RRR	118	
4	RRRR	118	
5	F	86	
5	FF	86	
5	FFF	86	
5	FFFF	86	
5	M	86	
5	MM	86	
5	MMM	86	
5	MMMM	86	

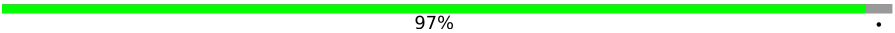
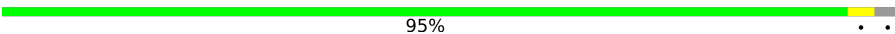
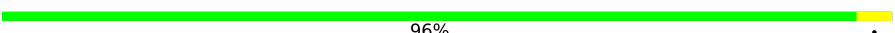
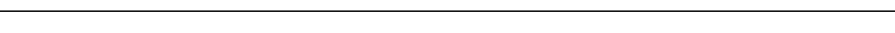
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Mol	Chain	Length	Quality of chain
5	T	86	 85% 12%
5	TT	86	 84% 7% 9%
5	TTT	86	 86% 12%
5	TTTT	86	 87% 10%
6	E	92	 85% 14%
6	EE	92	 86% 14%
6	EEE	92	 86% 14%
6	EEEE	92	 85% 14%
6	L	92	 86% 14%
6	LL	92	 86% 14%
6	LLL	92	 86% 14%
6	LLLL	92	 83% 16%
6	S	92	 86% 14%
6	SS	92	 86% 14%
6	SSS	92	 86% 14%
6	SSSS	92	 86% 14%
7	G	76	 95% 2%
7	GG	76	 95% 2%
7	GGG	76	 95% 2%
7	GGGG	76	 96% 2%
7	N	76	 96% 2%
7	NN	76	 96% 2%
7	NNN	76	 96% 2%
7	NNNN	76	 96% 2%
7	U	76	 96% 2%

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Mol	Chain	Length	Quality of chain
7	UU	76	 97% .
7	UUU	76	 95% . .
7	UUUU	76	 96% . .
8	V	68	 96% .
8	VV	68	 91% 7% .
8	VVV	68	 93% 7%
8	VVVV	68	 94% 6%
8	X	68	 91% 9%
8	XX	68	 90% 9% .
8	XXX	68	 94% . .
8	XXXX	68	 91% 9%
8	Y	68	 93% 7%
8	YY	68	 94% 6%
8	YYY	68	 93% 7%
8	YYYY	68	 94% 6%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 71485 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 Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	83	Total	C	N	O	S	0	0	0
			652	409	115	122	6			
1	H	84	Total	C	N	O	S	0	0	0
			658	412	116	124	6			
1	O	83	Total	C	N	O	S	0	0	0
			652	409	115	122	6			
1	AA	83	Total	C	N	O	S	0	0	0
			652	409	115	122	6			
1	HH	84	Total	C	N	O	S	0	0	0
			653	409	115	123	6			
1	OO	81	Total	C	N	O	S	0	0	0
			637	400	112	119	6			
1	AAA	83	Total	C	N	O	S	0	0	0
			648	406	114	122	6			
1	HHH	84	Total	C	N	O	S	0	0	0
			658	412	116	124	6			
1	OOO	82	Total	C	N	O	S	0	0	0
			646	406	114	120	6			
1	AAAA	82	Total	C	N	O	S	0	0	0
			646	406	114	120	6			
1	HHHH	82	Total	C	N	O	S	0	0	0
			643	403	113	121	6			
1	OOOO	82	Total	C	N	O	S	0	0	0
			646	406	114	120	6			

- Molecule 2 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	86	Total	C	N	O	S	0	0	0
			690	434	126	123	7			
2	I	72	Total	C	N	O	S	0	0	0
			574	364	103	100	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	71	Total	C	N	O	S	0	0	0
			569	361	102	99	7			
2	BB	71	Total	C	N	O	S	0	0	0
			565	358	101	99	7			
2	II	75	Total	C	N	O	S	0	0	0
			585	370	105	103	7			
2	PP	71	Total	C	N	O	S	0	0	0
			569	361	102	99	7			
2	BBB	71	Total	C	N	O	S	0	0	0
			565	358	101	99	7			
2	III	71	Total	C	N	O	S	0	0	0
			565	358	101	99	7			
2	PPP	71	Total	C	N	O	S	0	0	0
			559	355	98	99	7			
2	BBBB	74	Total	C	N	O	S	0	0	0
			592	375	106	104	7			
2	IIII	75	Total	C	N	O	S	0	0	0
			602	381	109	105	7			
2	PPPP	75	Total	C	N	O	S	0	0	0
			598	381	107	103	7			

- Molecule 3 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	82	Total	C	N	O	S	0	0	0
			649	413	113	119	4			
3	J	82	Total	C	N	O	S	0	0	0
			649	413	113	119	4			
3	Q	82	Total	C	N	O	S	0	0	0
			649	413	113	119	4			
3	CC	82	Total	C	N	O	S	0	0	0
			649	413	113	119	4			
3	JJ	82	Total	C	N	O	S	0	0	0
			649	413	113	119	4			
3	QQ	82	Total	C	N	O	S	0	0	0
			649	413	113	119	4			
3	CCC	82	Total	C	N	O	S	0	0	0
			649	413	113	119	4			
3	JJJ	82	Total	C	N	O	S	0	0	0
			649	413	113	119	4			
3	QQQ	82	Total	C	N	O	S	0	0	0
			649	413	113	119	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CCCC	82	Total	C	N	O	S	0	0	0
			649	413	113	119	4			
3	JJJJ	82	Total	C	N	O	S	0	0	0
			649	413	113	119	4			
3	QQQQ	82	Total	C	N	O	S	0	0	0
			649	413	113	119	4			

- Molecule 4 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	97	Total	C	N	O	S	0	0	0
			776	488	143	140	5			
4	K	100	Total	C	N	O	S	0	0	0
			796	499	149	143	5			
4	R	98	Total	C	N	O	S	0	0	0
			787	494	147	141	5			
4	DD	98	Total	C	N	O	S	0	0	0
			783	491	146	141	5			
4	KK	104	Total	C	N	O	S	0	0	0
			838	526	155	152	5			
4	RR	98	Total	C	N	O	S	0	0	0
			787	494	147	141	5			
4	DDD	98	Total	C	N	O	S	0	0	0
			787	494	147	141	5			
4	KKK	99	Total	C	N	O	S	0	0	0
			786	494	146	141	5			
4	RRR	98	Total	C	N	O	S	0	0	0
			787	494	147	141	5			
4	DDDD	104	Total	C	N	O	S	0	0	0
			838	526	155	152	5			
4	KKKK	104	Total	C	N	O	S	0	0	0
			838	526	155	152	5			
4	RRRR	98	Total	C	N	O	S	0	0	0
			787	494	147	141	5			

- Molecule 5 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	74	Total	C	N	O	S	0	0	0
			576	373	95	103	5			
5	M	79	Total	C	N	O	S	0	0	0
			609	392	100	112	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	T	76	Total	C	N	O	S	0	0	0
			594	383	97	109	5			
5	FF	75	Total	C	N	O	S	0	0	0
			585	378	96	106	5			
5	MM	80	Total	C	N	O	S	0	0	0
			621	399	101	115	6			
5	TT	78	Total	C	N	O	S	0	0	0
			596	385	99	107	5			
5	FFF	74	Total	C	N	O	S	0	0	0
			576	373	95	103	5			
5	MMM	76	Total	C	N	O	S	0	0	0
			590	381	97	107	5			
5	TTT	76	Total	C	N	O	S	0	0	0
			590	381	97	107	5			
5	FFFF	74	Total	C	N	O	S	0	0	0
			576	373	95	103	5			
5	MMMM	78	Total	C	N	O	S	0	0	0
			604	389	99	111	5			
5	TTTT	77	Total	C	N	O	S	0	0	0
			599	386	98	110	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	79	Total	C	N	O	S	0	0	0
			652	412	116	119	5			
6	L	79	Total	C	N	O	S	0	0	0
			652	412	116	119	5			
6	S	79	Total	C	N	O	S	0	0	0
			652	412	116	119	5			
6	EE	79	Total	C	N	O	S	0	0	0
			652	412	116	119	5			
6	LL	79	Total	C	N	O	S	0	0	0
			652	412	116	119	5			
6	SS	79	Total	C	N	O	S	0	0	0
			652	412	116	119	5			
6	EEE	79	Total	C	N	O	S	0	0	0
			652	412	116	119	5			
6	LLL	79	Total	C	N	O	S	0	0	0
			652	412	116	119	5			
6	SSS	79	Total	C	N	O	S	0	0	0
			652	412	116	119	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	EEEE	79	Total	C	N	O	S	0	0	0
			652	412	116	119	5			
6	LLLL	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
6	SSSS	79	Total	C	N	O	S	0	0	0
			652	412	116	119	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	74	Total	C	N	O	S	0	0	0
			577	364	104	103	6			
7	N	74	Total	C	N	O	S	0	0	0
			577	364	104	103	6			
7	U	74	Total	C	N	O	S	0	0	0
			577	364	104	103	6			
7	GG	74	Total	C	N	O	S	0	0	0
			577	364	104	103	6			
7	NN	74	Total	C	N	O	S	0	0	0
			577	364	104	103	6			
7	UU	74	Total	C	N	O	S	0	0	0
			571	361	101	103	6			
7	GGG	74	Total	C	N	O	S	0	0	0
			577	364	104	103	6			
7	NNN	74	Total	C	N	O	S	0	0	0
			577	364	104	103	6			
7	UUU	74	Total	C	N	O	S	0	0	0
			577	364	104	103	6			
7	GGGG	74	Total	C	N	O	S	0	0	0
			577	364	104	103	6			
7	NNNN	74	Total	C	N	O	S	0	0	0
			577	364	104	103	6			
7	UUUU	74	Total	C	N	O	S	0	0	0
			577	364	104	103	6			

- Molecule 8 is a RNA chain called U4 small nuclear RNA variant: Native sequence 85-145, of which nucleotides 97-104 are replaced with GAAA tetraloop and nucleotides 134-137 are replaced with GAAA tetraloop receptor..

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	V	68	Total	C	N	O	P	0	0	0
			1453	650	263	473	67			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	X	68	Total 1453	C 650	N 263	O 473	P 67	0	0	0
8	Y	68	Total 1453	C 650	N 263	O 473	P 67	0	0	0
8	VV	68	Total 1453	C 650	N 263	O 473	P 67	0	0	0
8	XX	68	Total 1453	C 650	N 263	O 473	P 67	0	0	0
8	YY	68	Total 1453	C 650	N 263	O 473	P 67	0	0	0
8	VVV	68	Total 1453	C 650	N 263	O 473	P 67	0	0	0
8	XXX	68	Total 1453	C 650	N 263	O 473	P 67	0	0	0
8	YYY	68	Total 1453	C 650	N 263	O 473	P 67	0	0	0
8	VVVV	68	Total 1453	C 650	N 263	O 473	P 67	0	0	0
8	XXXX	68	Total 1453	C 650	N 263	O 473	P 67	0	0	0
8	YYYY	68	Total 1453	C 650	N 263	O 473	P 67	0	0	0

- Molecule 9 is water.

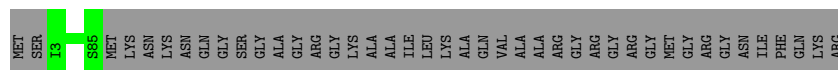
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	R	1	Total 1	O 1	0	0
9	DD	1	Total 1	O 1	0	0
9	RR	1	Total 1	O 1	0	0

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 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.

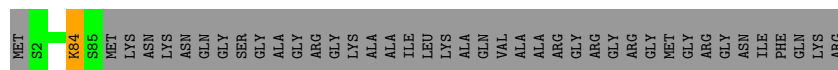
- Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain A:  66% 34%



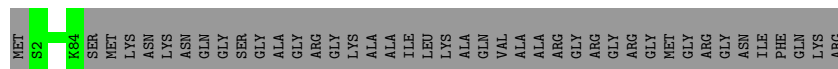
- Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain H:  66% 33%



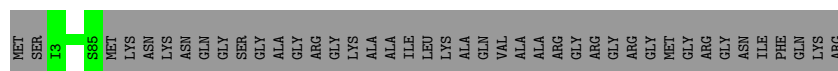
- Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain O:  66% 34%



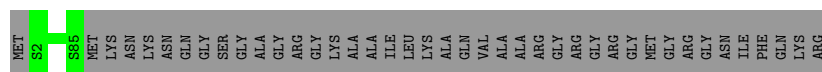
- Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain AA:  66% 34%



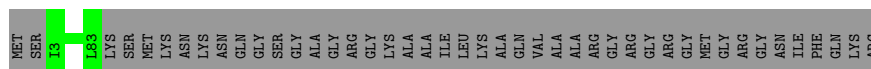
- Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain HH:  67% 33%



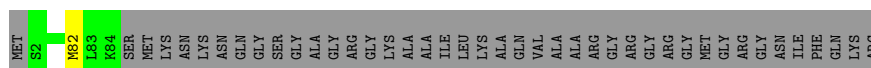
- Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain OO:  65% 35%



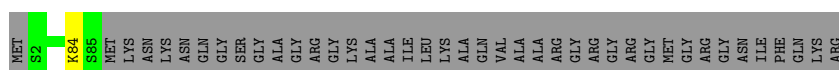
- Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain AAA: 66% 34%



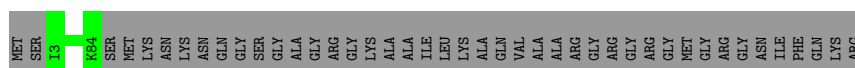
- Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain HHH: 66% 33%



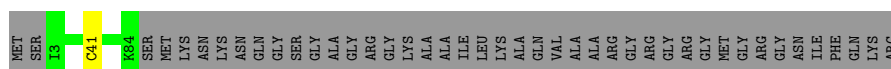
- Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain OOO: 66% 34%



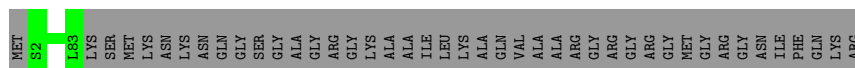
- Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain AAAA: 65% 34%



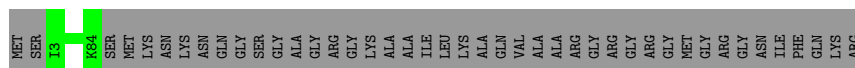
- Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain HHHH: 66% 34%



- Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain OOOO: 66% 34%



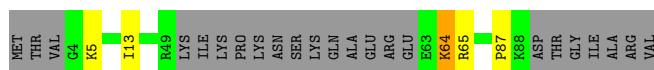
- Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain B: 84% 6% 9%



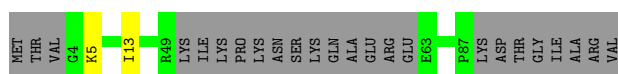
- Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain I: 71% 24%



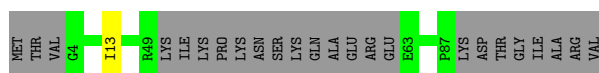
- Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain P: 73% 25%



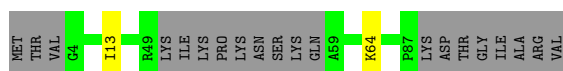
- Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain BB: 74% 25%



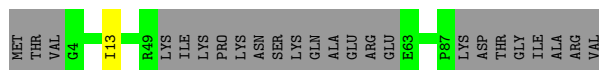
- Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain II: 77% 21%



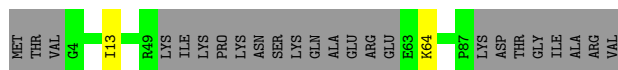
- Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain PP: 74% 25%



- Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

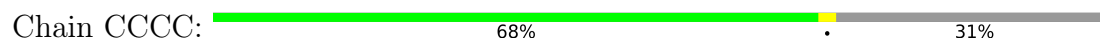
Chain BBB: 73% 25%



- Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain III: 74% 25%



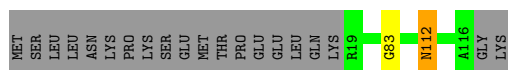






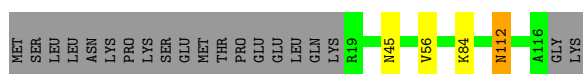
- Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain RR: 81% 17%



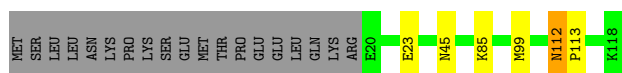
- Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain DDD: 80% 17%



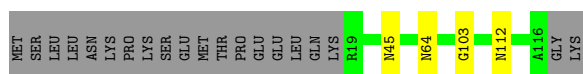
- Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain KKK: 79% 16%



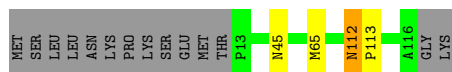
- Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain RRR: 80% 17%



- Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain DDDD: 85% 12%



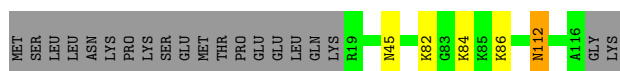
- Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain KKKK: 85% 12%

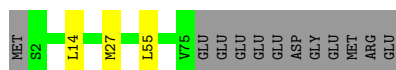
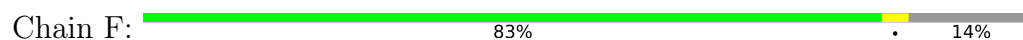


- Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain RRRR: 79% 17%



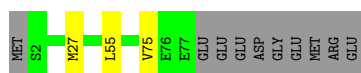
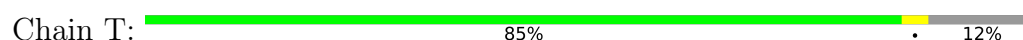
- Molecule 5: Small nuclear ribonucleoprotein F



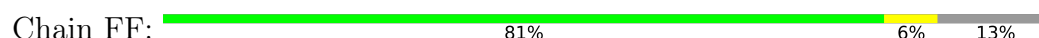
- Molecule 5: Small nuclear ribonucleoprotein F



- Molecule 5: Small nuclear ribonucleoprotein F



- Molecule 5: Small nuclear ribonucleoprotein F



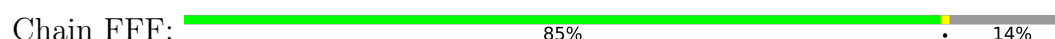
- Molecule 5: Small nuclear ribonucleoprotein F

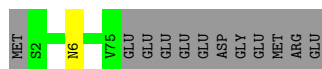


- Molecule 5: Small nuclear ribonucleoprotein F



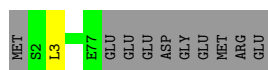
- Molecule 5: Small nuclear ribonucleoprotein F





- Molecule 5: Small nuclear ribonucleoprotein F

Chain MMM: 87% 12%



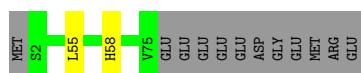
- Molecule 5: Small nuclear ribonucleoprotein F

Chain TTT: 86% 12%



- Molecule 5: Small nuclear ribonucleoprotein F

Chain FFFF: 84% 14%



- Molecule 5: Small nuclear ribonucleoprotein F

Chain MMMM: 85% 6% 9%



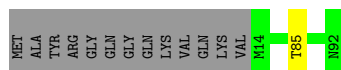
- Molecule 5: Small nuclear ribonucleoprotein F

Chain TTTT: 87% 10%



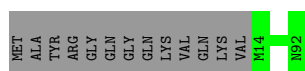
- Molecule 6: Small nuclear ribonucleoprotein E

Chain E: 85% 14%



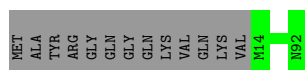
- Molecule 6: Small nuclear ribonucleoprotein E

Chain L: 86% 14%



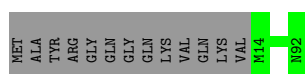
- Molecule 6: Small nuclear ribonucleoprotein E

Chain S: 86% 14%



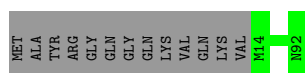
- Molecule 6: Small nuclear ribonucleoprotein E

Chain EE: 86% 14%



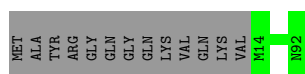
- Molecule 6: Small nuclear ribonucleoprotein E

Chain LL: 86% 14%



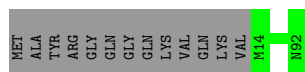
- Molecule 6: Small nuclear ribonucleoprotein E

Chain SS: 86% 14%



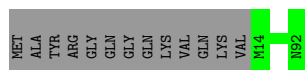
- Molecule 6: Small nuclear ribonucleoprotein E

Chain EEE: 86% 14%



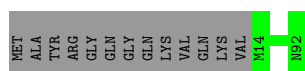
- Molecule 6: Small nuclear ribonucleoprotein E

Chain LLL: 86% 14%



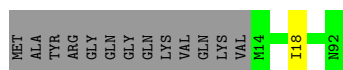
- Molecule 6: Small nuclear ribonucleoprotein E

Chain SSS: 86% 14%



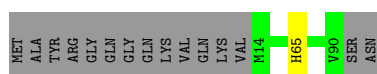
- Molecule 6: Small nuclear ribonucleoprotein E

Chain EEEE: 85% 14%



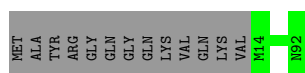
- Molecule 6: Small nuclear ribonucleoprotein E

Chain LLLL: 83% 16%



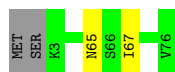
- Molecule 6: Small nuclear ribonucleoprotein E

Chain SSSS: 86% 14%



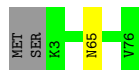
- Molecule 7: Small nuclear ribonucleoprotein G

Chain G: 95%



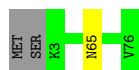
- Molecule 7: Small nuclear ribonucleoprotein G

Chain N: 96%



- Molecule 7: Small nuclear ribonucleoprotein G

Chain U: 96%



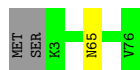
- Molecule 7: Small nuclear ribonucleoprotein G

Chain GG: 95%



- Molecule 7: Small nuclear ribonucleoprotein G

Chain NN: 96%



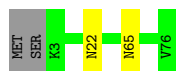
- Molecule 7: Small nuclear ribonucleoprotein G

Chain UU: 97%



- Molecule 7: Small nuclear ribonucleoprotein G

Chain GGG: 95%



- Molecule 7: Small nuclear ribonucleoprotein G

Chain NNN: 96%



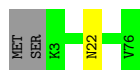
- Molecule 7: Small nuclear ribonucleoprotein G

Chain UUU: 95%



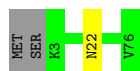
- Molecule 7: Small nuclear ribonucleoprotein G

Chain GGGG: 96%



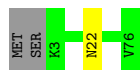
- Molecule 7: Small nuclear ribonucleoprotein G

Chain NNNN: 96%



- Molecule 7: Small nuclear ribonucleoprotein G

Chain UUUU: 96%



- Molecule 8: U4 small nuclear RNA variant: Native sequence 85-145, of which nucleotides 97-104 are replaced with GAAA tetraloop and nucleotides 134-137 are replaced with GAAA tetraloop receptor.

Chain V: 96%



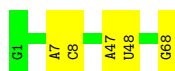
- Molecule 8: U4 small nuclear RNA variant: Native sequence 85-145, of which nucleotides 97-104 are replaced with GAAA tetraloop and nucleotides 134-137 are replaced with GAAA tetraloop receptor.

Chain X: 91%



- Molecule 8: U4 small nuclear RNA variant: Native sequence 85-145, of which nucleotides 97-104 are replaced with GAAA tetraloop and nucleotides 134-137 are replaced with GAAA tetraloop receptor.

Chain Y: 93%



- Molecule 8: U4 small nuclear RNA variant: Native sequence 85-145, of which nucleotides 97-104 are replaced with GAAA tetraloop and nucleotides 134-137 are replaced with GAAA tetraloop receptor.

Chain VV: 91%



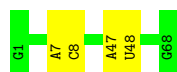
- Molecule 8: U4 small nuclear RNA variant: Native sequence 85-145, of which nucleotides 97-104 are replaced with GAAA tetraloop and nucleotides 134-137 are replaced with GAAA tetraloop receptor.

Chain XX:  90% 9%

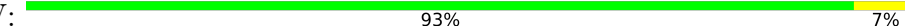


- Molecule 8: U4 small nuclear RNA variant: Native sequence 85-145, of which nucleotides 97-104 are replaced with GAAA tetraloop and nucleotides 134-137 are replaced with GAAA tetraloop receptor.

Chain YY:  94% 6%

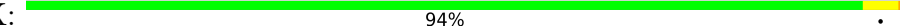


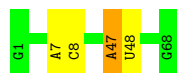
- Molecule 8: U4 small nuclear RNA variant: Native sequence 85-145, of which nucleotides 97-104 are replaced with GAAA tetraloop and nucleotides 134-137 are replaced with GAAA tetraloop receptor.

Chain VVV:  93% 7%

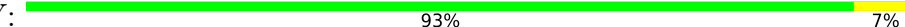


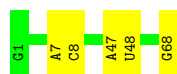
- Molecule 8: U4 small nuclear RNA variant: Native sequence 85-145, of which nucleotides 97-104 are replaced with GAAA tetraloop and nucleotides 134-137 are replaced with GAAA tetraloop receptor.

Chain XXX:  94% 0%

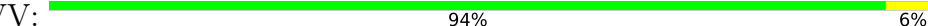


- Molecule 8: U4 small nuclear RNA variant: Native sequence 85-145, of which nucleotides 97-104 are replaced with GAAA tetraloop and nucleotides 134-137 are replaced with GAAA tetraloop receptor.

Chain YYY:  93% 7%



- Molecule 8: U4 small nuclear RNA variant: Native sequence 85-145, of which nucleotides 97-104 are replaced with GAAA tetraloop and nucleotides 134-137 are replaced with GAAA tetraloop receptor.

Chain VVVV:  94% 6%



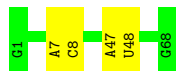
- Molecule 8: U4 small nuclear RNA variant: Native sequence 85-145, of which nucleotides 97-104 are replaced with GAAA tetraloop and nucleotides 134-137 are replaced with GAAA tetraloop receptor.

Chain XXXX:  91% 9%



- Molecule 8: U4 small nuclear RNA variant: Native sequence 85-145, of which nucleotides 97-104 are replaced with GAAA tetraloop and nucleotides 134-137 are replaced with GAAA tetraloop receptor.

Chain YYYY:  94% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	248.01Å 248.01Å 251.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	66.15 – 3.60 66.15 – 3.60	Depositor EDS
% Data completeness (in resolution range)	83.1 (66.15-3.60) 83.1 (66.15-3.60)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.177 , 0.224 (Not available) , 0.171	Depositor DCC
R_{free} test set	8492 reflections (3.73%)	wwPDB-VP
Wilson B-factor (Å ²)	84.3	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	0.309 for -h,-k,l 0.306 for h,-h-k,-l 0.306 for -k,-h,-l	Xtriage
Reported twinning fraction	0.218 for H, K, L 0.282 for -K, -H, -L 0.283 for K, H, -L 0.216 for -h,-k,l	Depositor
Outliers	0 of 169321 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	71485	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.59% 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 ⓘ

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	0.64	0/660	0.85	0/889
1	AA	0.63	0/660	0.89	0/889
1	AAA	0.63	0/656	0.89	1/885 (0.1%)
1	AAAA	0.66	0/654	0.88	1/881 (0.1%)
1	H	0.68	1/666 (0.2%)	0.90	1/897 (0.1%)
1	HH	0.70	0/661	0.87	0/892
1	HHH	0.69	0/666	0.90	1/897 (0.1%)
1	HHHH	0.63	0/651	0.88	0/878
1	O	0.62	0/660	0.86	0/889
1	OO	0.62	0/645	0.85	0/870
1	OOO	0.64	0/654	0.86	0/881
1	OOOO	0.60	0/654	0.85	0/881
2	B	0.72	0/700	1.03	4/933 (0.4%)
2	BB	0.66	0/573	0.89	0/765
2	BBB	0.62	0/573	0.85	0/765
2	BBBB	0.67	0/600	0.98	2/799 (0.3%)
2	I	0.72	1/582 (0.2%)	0.99	3/776 (0.4%)
2	II	0.70	0/593	0.92	0/793
2	III	0.66	0/573	0.88	0/765
2	IIII	0.72	0/610	0.93	0/813
2	P	0.60	0/577	0.91	2/769 (0.3%)
2	PP	0.66	0/577	0.84	0/769
2	PPP	0.62	0/567	0.89	2/758 (0.3%)
2	PPPP	0.61	0/607	0.89	1/810 (0.1%)
3	C	0.74	0/657	0.98	0/888
3	CC	0.75	0/657	0.95	0/888
3	CCC	0.73	0/657	0.94	0/888
3	CCCC	0.72	0/657	0.95	0/888
3	J	0.72	0/657	0.95	0/888
3	JJ	0.70	0/657	0.97	1/888 (0.1%)
3	JJJ	0.72	0/657	0.94	0/888
3	JJJJ	0.70	0/657	0.96	0/888
3	Q	0.70	0/657	0.93	1/888 (0.1%)
3	QQ	0.70	0/657	0.94	0/888

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	QQQ	0.71	0/657	0.97	0/888
3	QQQQ	0.67	0/657	0.91	1/888 (0.1%)
4	D	0.94	0/786	1.10	2/1053 (0.2%)
4	DD	0.89	1/793 (0.1%)	1.09	1/1063 (0.1%)
4	DDD	0.89	0/797	1.07	3/1067 (0.3%)
4	DDDD	0.88	0/849	1.07	1/1136 (0.1%)
4	K	0.96	0/806	1.05	1/1079 (0.1%)
4	KK	0.93	1/849 (0.1%)	1.09	3/1136 (0.3%)
4	KKK	0.92	1/796 (0.1%)	1.12	4/1064 (0.4%)
4	KKKK	1.05	3/849 (0.4%)	1.13	0/1136
4	R	0.86	0/797	1.06	2/1067 (0.2%)
4	RR	0.88	0/797	1.07	1/1067 (0.1%)
4	RRR	0.87	0/797	1.04	2/1067 (0.2%)
4	RRRR	0.88	0/797	1.10	3/1067 (0.3%)
5	F	1.03	1/588 (0.2%)	1.08	0/795
5	FF	0.97	1/597 (0.2%)	1.07	1/807 (0.1%)
5	FFF	0.90	0/588	1.06	1/795 (0.1%)
5	FFFF	0.90	1/588 (0.2%)	1.02	0/795
5	M	0.98	0/621	1.06	0/840
5	MM	1.00	2/633 (0.3%)	1.08	0/855
5	MMM	0.87	0/602	1.02	0/814
5	MMMM	1.06	3/616 (0.5%)	1.07	1/833 (0.1%)
5	T	0.92	0/606	1.10	3/819 (0.4%)
5	TT	0.94	1/608 (0.2%)	1.11	1/823 (0.1%)
5	TTT	0.96	0/602	1.02	0/814
5	TTTT	0.93	0/611	1.04	1/826 (0.1%)
6	E	0.84	0/660	1.06	1/886 (0.1%)
6	EE	0.82	0/660	1.05	0/886
6	EEE	0.86	0/660	1.06	0/886
6	EEEE	0.87	0/660	1.06	1/886 (0.1%)
6	L	0.80	0/660	1.04	0/886
6	LL	0.76	0/660	1.02	0/886
6	LLL	0.78	0/660	1.03	0/886
6	LLLL	0.90	0/646	1.09	1/867 (0.1%)
6	S	0.80	0/660	1.03	0/886
6	SS	0.87	0/660	1.06	0/886
6	SSS	0.79	0/660	1.04	0/886
6	SSSS	0.83	0/660	1.02	0/886
7	G	0.71	0/584	0.95	1/779 (0.1%)
7	GG	0.74	0/584	0.96	2/779 (0.3%)
7	GGG	0.67	0/584	0.91	0/779
7	GGGG	0.72	0/584	0.95	0/779
7	N	0.68	0/584	0.94	0/779

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	NN	0.71	0/584	0.94	0/779
7	NNN	0.68	0/584	0.94	1/779 (0.1%)
7	NNNN	0.77	0/584	0.91	0/779
7	U	0.68	0/584	0.90	0/779
7	UU	0.68	0/578	0.92	0/772
7	UUU	0.68	0/584	0.93	0/779
7	UUUU	0.68	0/584	0.92	0/779
8	V	0.58	0/1626	0.75	3/2534 (0.1%)
8	VV	0.54	0/1626	0.78	5/2534 (0.2%)
8	VVV	0.49	0/1626	0.79	7/2534 (0.3%)
8	VVVV	0.53	0/1626	0.74	4/2534 (0.2%)
8	X	0.55	1/1626 (0.1%)	0.84	11/2534 (0.4%)
8	XX	0.49	0/1626	0.78	4/2534 (0.2%)
8	XXX	0.46	0/1626	0.74	5/2534 (0.2%)
8	XXXX	0.52	0/1626	0.82	7/2534 (0.3%)
8	Y	0.49	0/1626	0.75	5/2534 (0.2%)
8	YY	0.47	0/1626	0.74	5/2534 (0.2%)
8	YYY	0.46	0/1626	0.73	5/2534 (0.2%)
8	YYYY	0.49	0/1626	0.75	5/2534 (0.2%)
All	All	0.73	18/74296 (0.0%)	0.93	125/103980 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	PPPP	0	1
4	D	0	1
4	DD	0	1
4	DDD	0	1
4	DDDD	0	1
4	K	0	1
4	KK	0	1
4	KKK	0	1
4	KKKK	0	1
4	R	0	1
4	RR	0	1
4	RRR	0	1
4	RRRR	0	1
5	M	0	1
5	MM	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	MMM	0	1
5	MMMM	0	1
5	TT	0	2
5	TTT	0	1
8	V	0	1
8	VVVV	0	1
All	All	0	23

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	84	LYS	N-CA	6.50	1.54	1.46
4	KKKK	22	GLU	CA-CB	6.46	1.63	1.53
5	FFFF	58	HIS	C-O	-5.96	1.17	1.24
2	I	87	PRO	CA-C	5.93	1.60	1.52
4	DD	84	LYS	C-O	-5.88	1.17	1.24

The worst 5 of 125 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	XXX	47	A	C2'-C3'-O3'	-14.04	88.44	109.50
8	X	47	A	C2'-C3'-O3'	-13.85	88.72	109.50
8	YYYY	47	A	C2'-C3'-O3'	-13.80	88.79	109.50
8	XX	47	A	C2'-C3'-O3'	-13.76	88.87	109.50
8	YY	47	A	C2'-C3'-O3'	-13.14	89.78	109.50

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	112	ASN	Peptide
4	DD	112	ASN	Peptide
4	K	112	ASN	Peptide
5	M	3	LEU	Peptide
4	R	112	ASN	Peptide

5.2 Too-close contacts [\(i\)](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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

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	73/100 (73%)	73 (100%)	0	100	100
1	AA	73/100 (73%)	73 (100%)	0	100	100
1	AAA	72/100 (72%)	72 (100%)	0	100	100
1	AAAA	72/100 (72%)	72 (100%)	0	100	100
1	H	74/100 (74%)	73 (99%)	1 (1%)	59	71
1	HH	72/100 (72%)	72 (100%)	0	100	100
1	HHH	74/100 (74%)	74 (100%)	0	100	100
1	HHHH	72/100 (72%)	72 (100%)	0	100	100
1	O	73/100 (73%)	73 (100%)	0	100	100
1	OO	71/100 (71%)	71 (100%)	0	100	100
1	OOO	72/100 (72%)	72 (100%)	0	100	100
1	OOOO	72/100 (72%)	72 (100%)	0	100	100
2	B	77/85 (91%)	74 (96%)	3 (4%)	28	54
2	BB	63/85 (74%)	62 (98%)	1 (2%)	55	69
2	BBB	63/85 (74%)	61 (97%)	2 (3%)	34	58
2	BBBB	66/85 (78%)	65 (98%)	1 (2%)	57	70
2	I	64/85 (75%)	62 (97%)	2 (3%)	35	59
2	II	63/85 (74%)	61 (97%)	2 (3%)	34	58
2	III	63/85 (74%)	62 (98%)	1 (2%)	55	69
2	IIII	67/85 (79%)	66 (98%)	1 (2%)	57	70
2	P	64/85 (75%)	63 (98%)	1 (2%)	55	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	PP	64/85 (75%)	63 (98%)	1 (2%)	55	69
2	PPP	62/85 (73%)	62 (100%)	0	100	100
2	PPPP	67/85 (79%)	65 (97%)	2 (3%)	36	59
3	C	77/100 (77%)	75 (97%)	2 (3%)	40	62
3	CC	77/100 (77%)	75 (97%)	2 (3%)	40	62
3	CCC	77/100 (77%)	75 (97%)	2 (3%)	40	62
3	CCCC	77/100 (77%)	75 (97%)	2 (3%)	40	62
3	J	77/100 (77%)	75 (97%)	2 (3%)	40	62
3	JJ	77/100 (77%)	75 (97%)	2 (3%)	40	62
3	JJJ	77/100 (77%)	75 (97%)	2 (3%)	40	62
3	JJJJ	77/100 (77%)	75 (97%)	2 (3%)	40	62
3	Q	77/100 (77%)	75 (97%)	2 (3%)	40	62
3	QQ	77/100 (77%)	75 (97%)	2 (3%)	40	62
3	QQQ	77/100 (77%)	75 (97%)	2 (3%)	40	62
3	QQQQ	77/100 (77%)	75 (97%)	2 (3%)	40	62
4	D	90/110 (82%)	89 (99%)	1 (1%)	65	74
4	DD	90/110 (82%)	88 (98%)	2 (2%)	45	65
4	DDD	91/110 (83%)	90 (99%)	1 (1%)	65	74
4	DDDD	97/110 (88%)	95 (98%)	2 (2%)	47	65
4	K	91/110 (83%)	90 (99%)	1 (1%)	65	74
4	KK	97/110 (88%)	96 (99%)	1 (1%)	68	75
4	KKK	90/110 (82%)	89 (99%)	1 (1%)	65	74
4	KKKK	97/110 (88%)	95 (98%)	2 (2%)	47	65
4	R	91/110 (83%)	90 (99%)	1 (1%)	65	74
4	RR	91/110 (83%)	90 (99%)	1 (1%)	65	74
4	RRR	91/110 (83%)	90 (99%)	1 (1%)	65	74
4	RRRR	91/110 (83%)	89 (98%)	2 (2%)	45	65
5	F	63/74 (85%)	61 (97%)	2 (3%)	34	58
5	FF	64/74 (86%)	61 (95%)	3 (5%)	23	50
5	FFF	63/74 (85%)	63 (100%)	0	100	100
5	FFFF	63/74 (85%)	62 (98%)	1 (2%)	55	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	M	65/74 (88%)	62 (95%)	3 (5%)	24	51
5	MM	67/74 (90%)	65 (97%)	2 (3%)	36	59
5	MMM	64/74 (86%)	64 (100%)	0	100	100
5	MMMM	65/74 (88%)	64 (98%)	1 (2%)	57	70
5	T	65/74 (88%)	63 (97%)	2 (3%)	35	59
5	TT	63/74 (85%)	61 (97%)	2 (3%)	34	58
5	TTT	64/74 (86%)	63 (98%)	1 (2%)	55	69
5	TTTT	65/74 (88%)	65 (100%)	0	100	100
6	E	74/84 (88%)	74 (100%)	0	100	100
6	EE	74/84 (88%)	74 (100%)	0	100	100
6	EEE	74/84 (88%)	74 (100%)	0	100	100
6	EEEE	74/84 (88%)	74 (100%)	0	100	100
6	L	74/84 (88%)	74 (100%)	0	100	100
6	LL	74/84 (88%)	74 (100%)	0	100	100
6	LLL	74/84 (88%)	74 (100%)	0	100	100
6	LLLL	72/84 (86%)	72 (100%)	0	100	100
6	S	74/84 (88%)	74 (100%)	0	100	100
6	SS	74/84 (88%)	74 (100%)	0	100	100
6	SSS	74/84 (88%)	74 (100%)	0	100	100
6	SSSS	74/84 (88%)	74 (100%)	0	100	100
7	G	64/66 (97%)	63 (98%)	1 (2%)	55	69
7	GG	64/66 (97%)	64 (100%)	0	100	100
7	GGG	64/66 (97%)	62 (97%)	2 (3%)	35	59
7	GGGG	64/66 (97%)	63 (98%)	1 (2%)	55	69
7	N	64/66 (97%)	63 (98%)	1 (2%)	55	69
7	NN	64/66 (97%)	63 (98%)	1 (2%)	55	69
7	NNN	64/66 (97%)	64 (100%)	0	100	100
7	NNNN	64/66 (97%)	63 (98%)	1 (2%)	55	69
7	U	64/66 (97%)	63 (98%)	1 (2%)	55	69
7	UU	63/66 (96%)	63 (100%)	0	100	100
7	UUU	64/66 (97%)	62 (97%)	2 (3%)	35	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	UUUU	64/66 (97%)	63 (98%)	1 (2%)	55 69
All	All	6108/7428 (82%)	6022 (99%)	86 (1%)	59 71

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	JJJ	54	GLN
7	GGGG	22	ASN
3	QQQ	40	LEU
2	BBBB	13	ILE
4	KKKK	45	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
2	BB	76	ASN
2	II	76	ASN
4	RR	34	GLN
3	CC	64	ASN
1	HH	23	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	V	67/68 (98%)	0	0
8	VV	67/68 (98%)	2 (2%)	1 (1%)
8	VVV	67/68 (98%)	1 (1%)	0
8	VVVV	67/68 (98%)	0	0
8	X	67/68 (98%)	0	0
8	XX	67/68 (98%)	3 (4%)	2 (2%)
8	XXX	67/68 (98%)	1 (1%)	1 (1%)
8	XXXX	67/68 (98%)	2 (2%)	0
8	Y	67/68 (98%)	2 (2%)	0
8	YY	67/68 (98%)	1 (1%)	0
8	YYY	67/68 (98%)	2 (2%)	0
8	YYYY	67/68 (98%)	1 (1%)	0
All	All	804/816 (98%)	15 (1%)	4 (0%)

5 of 15 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	Y	8	C
8	Y	68	G
8	VV	8	C
8	VV	68	G
8	XX	8	C

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	VV	67	G
8	XX	47	A
8	XX	67	G
8	XXX	47	A

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 oligosaccharides 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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	83/125 (66%)	-1.22	0 100 100	58, 143, 193, 230	0
1	AA	83/125 (66%)	-1.25	0 100 100	82, 130, 175, 210	0
1	AAA	83/125 (66%)	-1.25	0 100 100	63, 130, 180, 217	0
1	AAAA	82/125 (65%)	-1.28	0 100 100	56, 136, 187, 201	0
1	H	84/125 (67%)	-1.13	0 100 100	58, 144, 210, 248	0
1	HH	84/125 (67%)	-1.24	0 100 100	84, 139, 195, 231	0
1	HHH	84/125 (67%)	-1.20	0 100 100	70, 143, 195, 230	0
1	HHHH	82/125 (65%)	-1.29	0 100 100	71, 142, 192, 240	0
1	O	83/125 (66%)	-1.21	0 100 100	92, 164, 222, 306	0
1	OO	81/125 (64%)	-1.20	0 100 100	64, 143, 192, 213	0
1	OOO	82/125 (65%)	-1.25	0 100 100	74, 146, 192, 214	0
1	OOOO	82/125 (65%)	-1.11	0 100 100	50, 152, 202, 231	0
2	B	86/95 (90%)	-1.19	0 100 100	72, 139, 198, 223	0
2	BB	71/95 (74%)	-1.27	0 100 100	63, 125, 171, 191	0
2	BBB	71/95 (74%)	-1.15	0 100 100	2, 136, 190, 273	1 (1%)
2	BBBB	74/95 (77%)	-1.27	0 100 100	57, 128, 164, 201	0
2	I	72/95 (75%)	-1.15	0 100 100	79, 131, 178, 240	0
2	II	75/95 (78%)	-1.20	0 100 100	68, 126, 202, 302	0
2	III	71/95 (74%)	-1.13	0 100 100	59, 129, 183, 202	0
2	IIII	75/95 (78%)	-1.11	0 100 100	89, 154, 220, 250	0
2	P	71/95 (74%)	-1.15	0 100 100	82, 146, 184, 219	0
2	PP	71/95 (74%)	-1.20	0 100 100	84, 138, 195, 207	0
2	PPP	71/95 (74%)	-1.18	0 100 100	79, 137, 191, 204	0
2	PPPP	75/95 (78%)	-1.16	0 100 100	63, 135, 191, 222	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
3	C	82/118 (69%)	-1.34	0	100	100	70, 104, 135, 172	0
3	CC	82/118 (69%)	-1.34	0	100	100	57, 91, 139, 162	0
3	CCC	82/118 (69%)	-1.40	0	100	100	43, 96, 151, 213	0
3	CCCC	82/118 (69%)	-1.22	0	100	100	56, 99, 159, 214	0
3	J	82/118 (69%)	-1.33	0	100	100	51, 102, 146, 168	0
3	JJ	82/118 (69%)	-1.24	0	100	100	56, 104, 168, 212	0
3	JJJ	82/118 (69%)	-1.33	0	100	100	57, 101, 144, 178	0
3	JJJJ	82/118 (69%)	-1.36	0	100	100	49, 90, 150, 191	0
3	Q	82/118 (69%)	-1.33	0	100	100	57, 108, 151, 275	0
3	QQ	82/118 (69%)	-1.32	0	100	100	46, 98, 152, 208	0
3	QQQ	82/118 (69%)	-1.32	0	100	100	46, 103, 157, 174	0
3	QQQQ	82/118 (69%)	-1.29	0	100	100	64, 103, 178, 220	0
4	D	97/118 (82%)	-1.31	0	100	100	48, 93, 168, 229	0
4	DD	98/118 (83%)	-1.25	0	100	100	57, 106, 187, 244	0
4	DDD	98/118 (83%)	-1.31	0	100	100	34, 92, 211, 237	0
4	DDDD	104/118 (88%)	-1.27	0	100	100	36, 96, 184, 219	0
4	K	100/118 (84%)	-1.32	0	100	100	29, 99, 180, 200	0
4	KK	104/118 (88%)	-1.23	0	100	100	45, 106, 191, 249	0
4	KKK	99/118 (83%)	-1.27	0	100	100	59, 110, 173, 200	0
4	KKKK	104/118 (88%)	-1.19	2 (1%)	66	39	47, 100, 198, 262	0
4	R	98/118 (83%)	-1.19	1 (1%)	79	54	48, 103, 175, 212	0
4	RR	98/118 (83%)	-1.30	0	100	100	49, 100, 207, 227	0
4	RRR	98/118 (83%)	-1.21	0	100	100	26, 95, 263, 292	0
4	RRRR	98/118 (83%)	-1.36	0	100	100	36, 96, 189, 246	0
5	F	74/86 (86%)	-1.49	0	100	100	25, 74, 117, 136	0
5	FF	75/86 (87%)	-1.46	0	100	100	25, 88, 149, 188	0
5	FFF	74/86 (86%)	-1.36	0	100	100	47, 89, 139, 166	0
5	FFFF	74/86 (86%)	-1.44	0	100	100	42, 88, 131, 165	0
5	M	79/86 (91%)	-1.42	0	100	100	45, 90, 153, 171	0
5	MM	80/86 (93%)	-1.43	0	100	100	39, 89, 139, 167	0
5	MMM	76/86 (88%)	-1.41	0	100	100	45, 97, 143, 167	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	MMMM	78/86 (90%)	-1.46	0 100 100	37, 85, 136, 165	0
5	T	76/86 (88%)	-1.37	0 100 100	49, 94, 153, 219	0
5	TT	78/86 (90%)	-1.40	0 100 100	45, 89, 138, 174	0
5	TTT	76/86 (88%)	-1.41	0 100 100	46, 91, 142, 213	0
5	TTTT	77/86 (89%)	-1.38	0 100 100	44, 92, 156, 203	0
6	E	79/92 (85%)	-1.36	0 100 100	46, 100, 142, 181	0
6	EE	79/92 (85%)	-1.28	0 100 100	53, 102, 159, 210	0
6	EEE	79/92 (85%)	-1.27	0 100 100	51, 100, 158, 195	0
6	EEEE	79/92 (85%)	-1.31	0 100 100	54, 96, 149, 168	0
6	L	79/92 (85%)	-1.27	0 100 100	57, 100, 157, 221	0
6	LL	79/92 (85%)	-1.32	0 100 100	62, 103, 154, 173	0
6	LLL	79/92 (85%)	-1.14	0 100 100	57, 114, 193, 234	0
6	LLLL	77/92 (83%)	-1.30	0 100 100	42, 91, 157, 190	0
6	S	79/92 (85%)	-1.31	0 100 100	47, 112, 180, 205	0
6	SS	79/92 (85%)	-1.23	0 100 100	52, 98, 157, 202	0
6	SSS	79/92 (85%)	-1.28	0 100 100	58, 109, 179, 203	0
6	SSSS	79/92 (85%)	-1.21	0 100 100	51, 107, 180, 227	0
7	G	74/76 (97%)	-1.32	0 100 100	58, 130, 187, 200	0
7	GG	74/76 (97%)	-1.33	0 100 100	45, 120, 173, 204	0
7	GGG	74/76 (97%)	-1.30	0 100 100	64, 133, 182, 222	0
7	GGGG	74/76 (97%)	-1.29	0 100 100	57, 129, 183, 233	0
7	N	74/76 (97%)	-1.26	0 100 100	76, 128, 186, 212	0
7	NN	74/76 (97%)	-1.31	0 100 100	70, 120, 172, 243	0
7	NNN	74/76 (97%)	-1.23	0 100 100	75, 142, 187, 214	0
7	NNNN	74/76 (97%)	-1.31	0 100 100	63, 111, 186, 233	0
7	U	74/76 (97%)	-1.29	0 100 100	86, 132, 212, 239	0
7	UU	74/76 (97%)	-1.26	0 100 100	61, 133, 181, 226	0
7	UUU	74/76 (97%)	-1.24	0 100 100	50, 141, 213, 254	0
7	UUUU	74/76 (97%)	-1.19	0 100 100	74, 144, 188, 206	0
8	V	68/68 (100%)	-1.75	0 100 100	67, 171, 209, 272	0
8	VV	68/68 (100%)	-1.64	0 100 100	63, 148, 219, 272	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
8	VVV	68/68 (100%)	-1.72	0	100	100	75, 163, 213, 248	0
8	VVVV	68/68 (100%)	-1.62	0	100	100	67, 168, 222, 263	0
8	X	68/68 (100%)	-1.49	0	100	100	81, 164, 218, 272	0
8	XX	68/68 (100%)	-1.70	0	100	100	74, 161, 218, 267	0
8	XXX	68/68 (100%)	-1.61	0	100	100	85, 158, 210, 221	0
8	XXXX	68/68 (100%)	-1.69	0	100	100	69, 158, 220, 249	0
8	Y	68/68 (100%)	-1.63	0	100	100	79, 173, 228, 245	0
8	YY	68/68 (100%)	-1.69	0	100	100	81, 155, 229, 291	0
8	YYY	68/68 (100%)	-1.61	0	100	100	78, 164, 247, 310	0
8	YYYY	68/68 (100%)	-1.67	0	100	100	83, 164, 226, 341	0
All	All	7623/9336 (81%)	-1.32	3 (0%)	100	100	2, 118, 195, 341	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	KKKK	81	GLY	3.6
4	R	83	GLY	2.2
4	KKKK	82	LYS	2.2

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 oligosaccharides 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.