Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 04:40 PM EDT

PDB ID	:	4WZJ
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 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 (i) 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 (1)) were used in the production of this report:

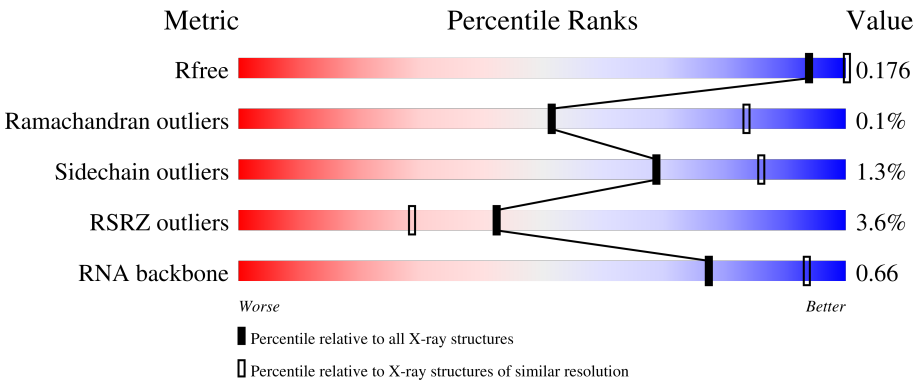
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	1257 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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 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 <=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	3% 66% 34%
1	AA	125	% 66% 34%
1	AAA	125	4% 66% · 34%
1	AAAA	125	3% 66% 34%
1	H	125	4% 66% · 33%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	HH	125	3% 67% 33%
1	HHH	125	2% 67% 33%
1	HHHH	125	2% 65% 34%
1	O	125	11% 66% 34%
1	OO	125	5% 65% 35%
1	OOO	125	3% 66% 34%
1	OOOO	125	5% 66% 34%
2	B	95	7% 88% 9%
2	BB	95	% 73% 25%
2	BBB	95	11% 73% 25%
2	BBBB	95	3% 77% 22%
2	I	95	7% 73% 24%
2	II	95	6% 78% 21%
2	III	95	5% 73% 25%
2	IIII	95	8% 77% 21%
2	P	95	4% 74% 25%
2	PP	95	5% 74% 25%
2	PPP	95	4% 73% 25%
2	PPPP	95	9% 76% 21%
3	C	118	68% 31%
3	CC	118	% 68% 31%
3	CCC	118	% 68% 31%
3	CCCC	118	2% 68% 31%
3	J	118	68% 31%
3	JJ	118	2% 68% 31%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	JJJ	118	%, 68%, 31%
3	JJJJ	118	68%, 31%
3	Q	118	%, 68%, 31%
3	QQ	118	68%, 31%
3	QQQ	118	68%, 31%
3	QQQQ	118	%, 68%, 31%
4	D	118	3%, 81%, 18%
4	DD	118	3%, 78%, 17%
4	DDD	118	4%, 81%, 17%
4	DDDD	118	6%, 85%, 12%
4	K	118	3%, 80%, 15%
4	KK	118	5%, 86%, 12%
4	KKK	118	80%, 16%
4	KKKK	118	3%, 85%, 12%
4	R	118	3%, 81%, 17%
4	RR	118	4%, 80%, 17%
4	RRR	118	6%, 81%, 17%
4	RRRR	118	3%, 79%, 17%
5	F	86	85%, 14%
5	FF	86	87%, 13%
5	FFF	86	86%, 14%
5	FFFF	86	%, 84%, 14%
5	M	86	2%, 90%, 8%
5	MM	86	90%, 7%
5	MMM	86	87%, 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	MMMM	86	87% 9%
5	T	86	2% 88% 12%
5	TT	86	87% 9%
5	TTT	86	2% 85% 12%
5	TTTT	86	2% 88% 10%
6	E	92	86% 14%
6	EE	92	% 86% 14%
6	EEE	92	2% 86% 14%
6	EEEE	92	% 86% 14%
6	L	92	3% 85% 14%
6	LL	92	% 86% 14%
6	LLL	92	4% 86% 14%
6	LLLL	92	2% 84% 16%
6	S	92	2% 86% 14%
6	SS	92	86% 14%
6	SSS	92	4% 86% 14%
6	SSSS	92	3% 86% 14%
7	G	76	96%
7	GG	76	5% 96%
7	GGG	76	4% 95%
7	GGGG	76	5% 95%
7	N	76	7% 96%
7	NN	76	7% 97%
7	NNN	76	4% 96%
7	NNNN	76	7% 95%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	U	76	11% 93%
7	UU	76	7% 96%
7	UUU	76	12% 93%
7	UUUU	76	7% 96%
8	V	68	% 93% 7%
8	VV	68	88% 12%
8	VVV	68	% 91% 9%
8	VVVV	68	94% 6%
8	X	68	93% 7%
8	XX	68	87% 10%
8	XXX	68	94%
8	XXXX	68	90% 9%
8	Y	68	% 91% 9%
8	YY	68	94% 6%
8	YYY	68	% 93% 6%
8	YYYY	68	93% 7%

2 Entry composition (i)

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

- 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
			Total	C	N	O	P			
8	V	68	1453	650	263	473	67	0	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 9 is water.

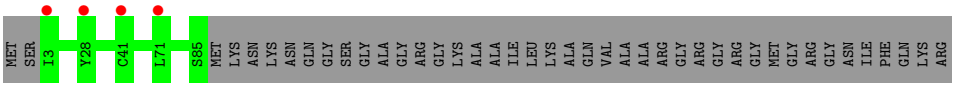
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	R	1	1	1	0	0
9	DD	1	1	1	0	0
9	RR	1	1	1	0	0

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.

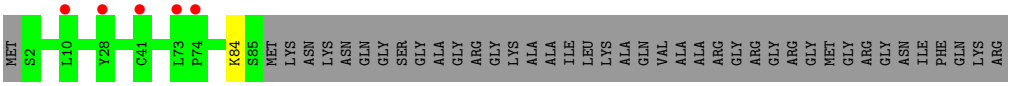
• Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain A:



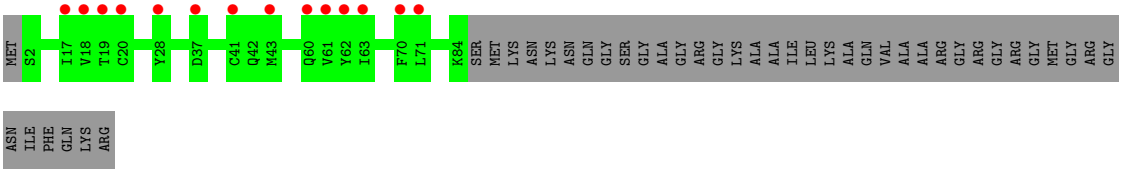
• Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain H:



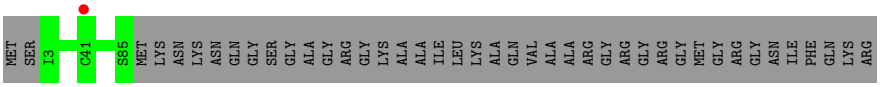
• Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain O:



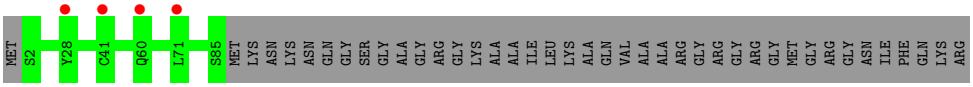
• Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain AA:



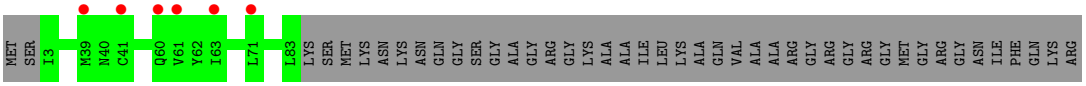
• Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain HH:



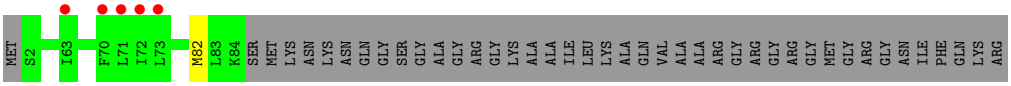
• Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain OO:



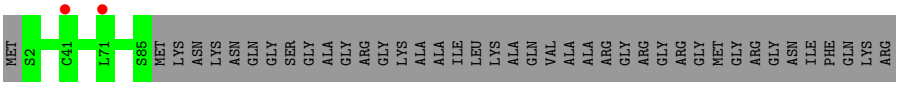
• Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain AAA:



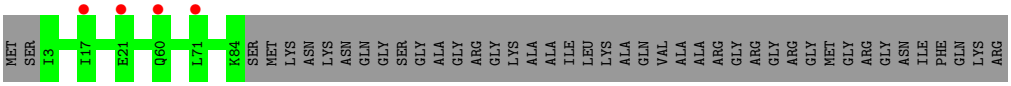
• Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain HHH:



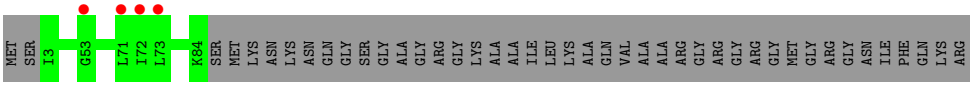
• Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain OOO:



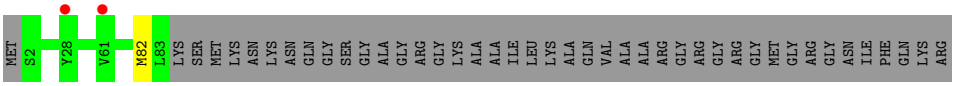
• Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain AAAA:



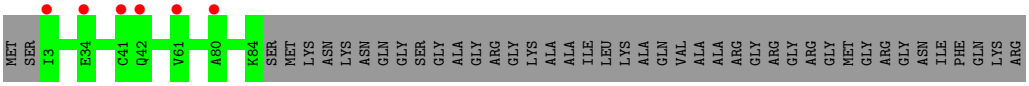
• Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain HHHH:



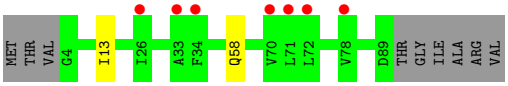
• Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain OOOO:



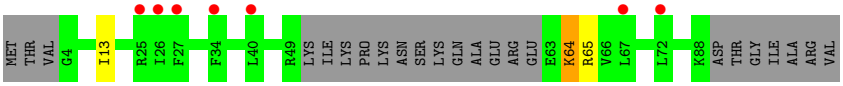
• Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain B:



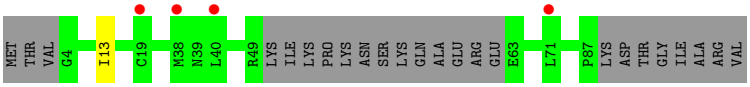
• Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain I:



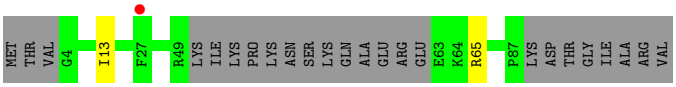
• Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain P:



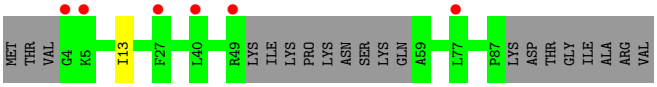
• Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain BB:



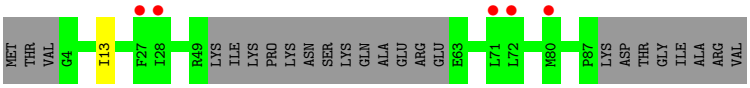
• Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain II:



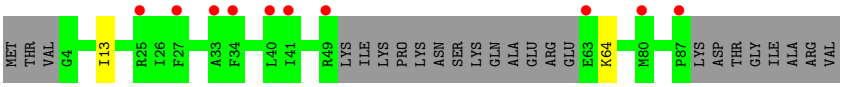
• Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain PP:



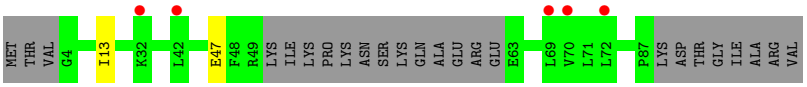
• Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain BBB:



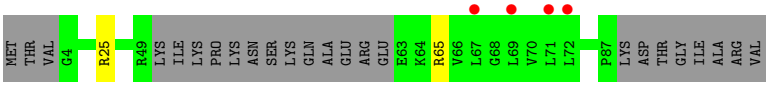
• Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain III:



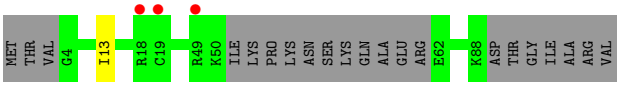
• Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain PPP:



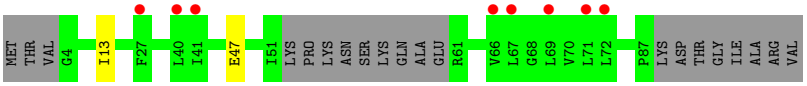
• Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain BBBB:



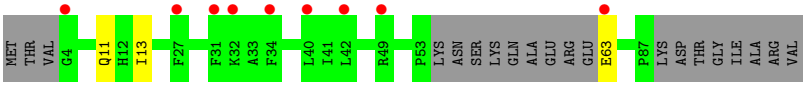
• Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain IIII:



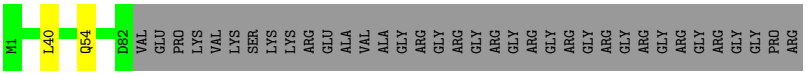
• Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain PPPP:



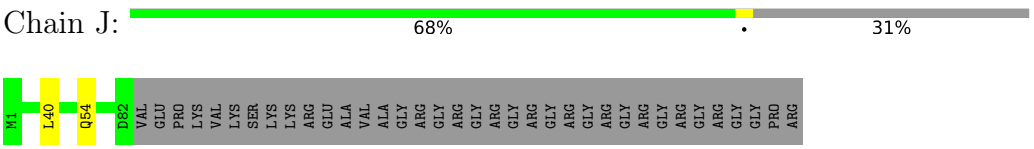
• Molecule 3: Small nuclear ribonucleoprotein Sm D1

Chain C:



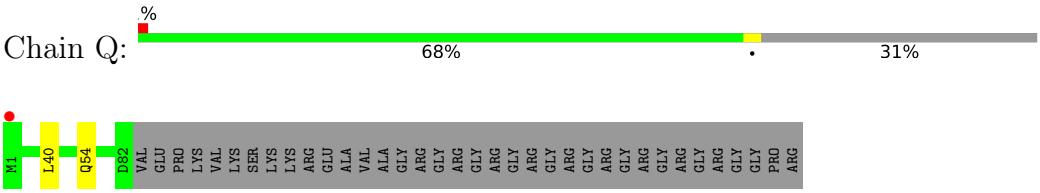
• Molecule 3: Small nuclear ribonucleoprotein Sm D1

Chain J:



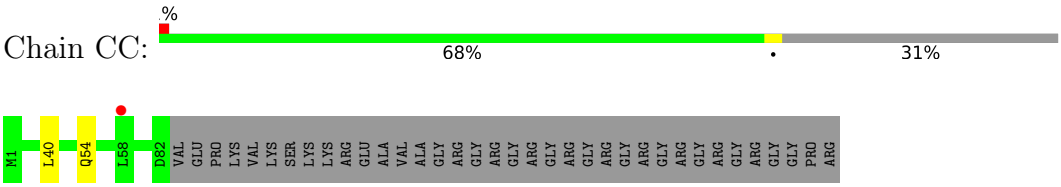
• Molecule 3: Small nuclear ribonucleoprotein Sm D1

Chain Q:



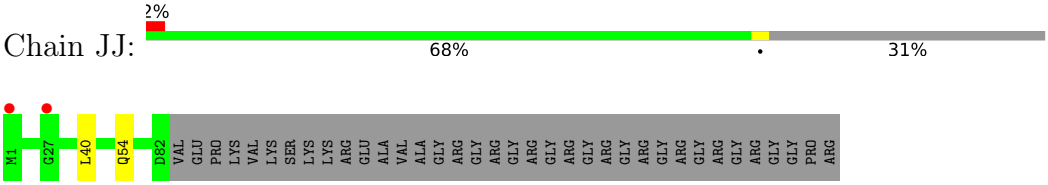
• Molecule 3: Small nuclear ribonucleoprotein Sm D1

Chain CC:



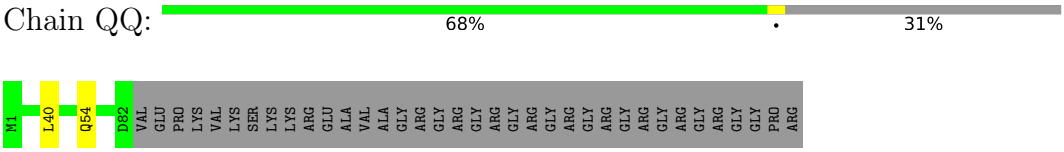
• Molecule 3: Small nuclear ribonucleoprotein Sm D1

Chain JJ:



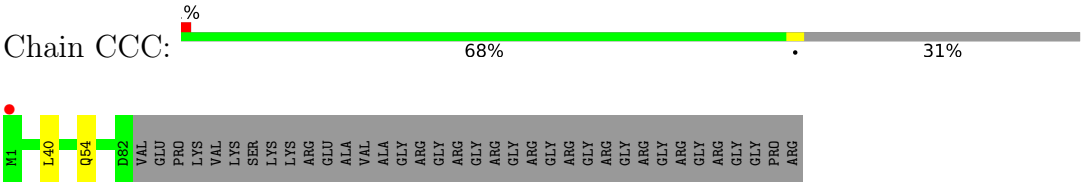
• Molecule 3: Small nuclear ribonucleoprotein Sm D1

Chain QQ:



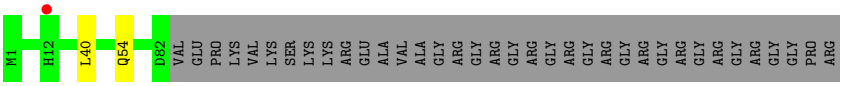
• Molecule 3: Small nuclear ribonucleoprotein Sm D1

Chain CCC:



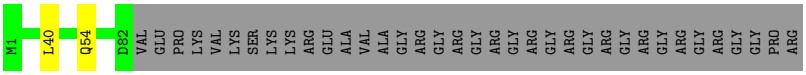
• Molecule 3: Small nuclear ribonucleoprotein Sm D1

Chain JJJ:



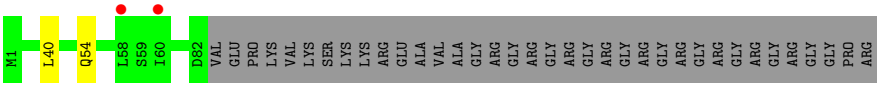
• Molecule 3: Small nuclear ribonucleoprotein Sm D1

Chain QQQ:



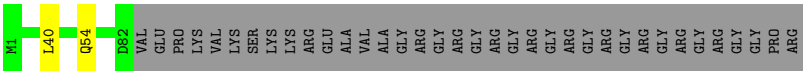
• Molecule 3: Small nuclear ribonucleoprotein Sm D1

Chain CCCC:



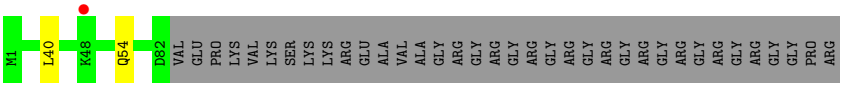
• Molecule 3: Small nuclear ribonucleoprotein Sm D1

Chain JJJJ:



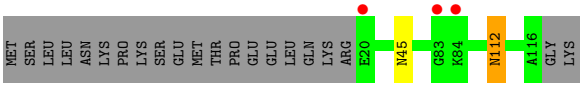
• Molecule 3: Small nuclear ribonucleoprotein Sm D1

Chain QQQQ:



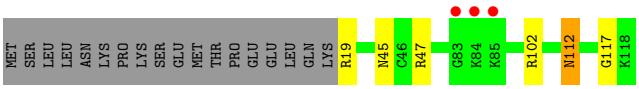
• Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain D:



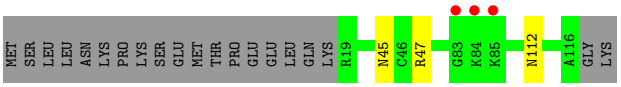
• Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain K:



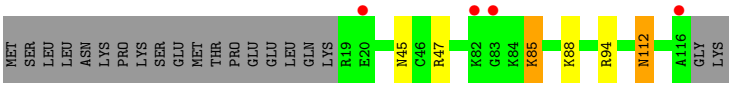
• Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain R:



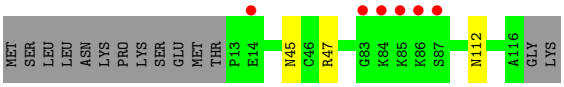
• Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain DD:



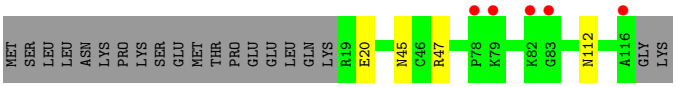
• Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain KK:



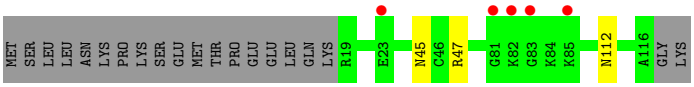
• Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain RR:



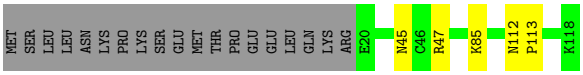
• Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain DDD:



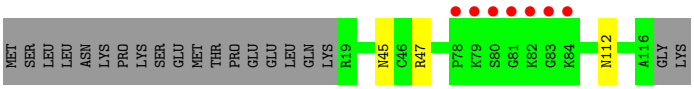
• Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain KKK:



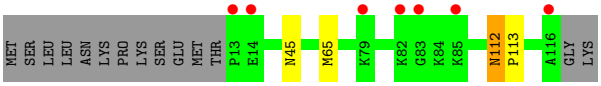
• Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain RRR:



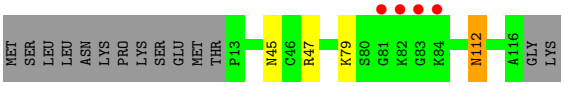
• Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain DDDD:



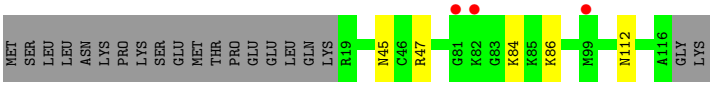
• Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain KKKK:



• Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain RRRR:



• Molecule 5: Small nuclear ribonucleoprotein F

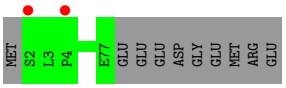
Chain F:

• Molecule 5: Small nuclear ribonucleoprotein F

Chain M:

• Molecule 5: Small nuclear ribonucleoprotein F

Chain T:

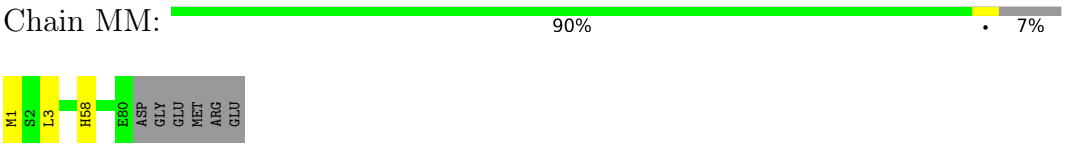


• Molecule 5: Small nuclear ribonucleoprotein F

Chain FF:

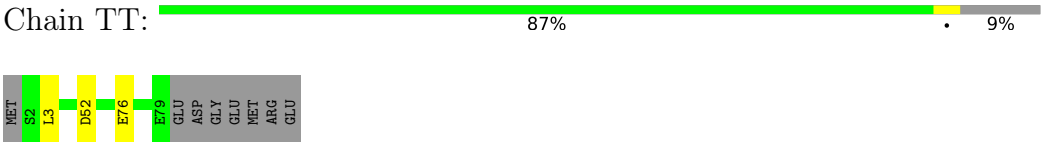
• Molecule 5: Small nuclear ribonucleoprotein F

Chain MM:



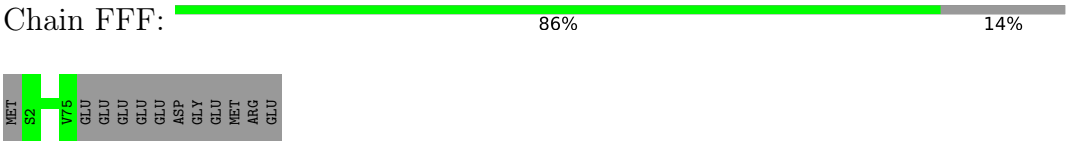
• Molecule 5: Small nuclear ribonucleoprotein F

Chain TT:



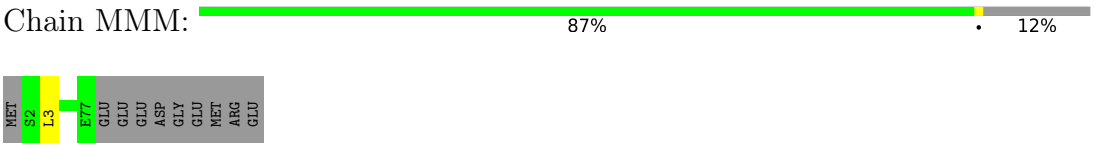
• Molecule 5: Small nuclear ribonucleoprotein F

Chain FFF:



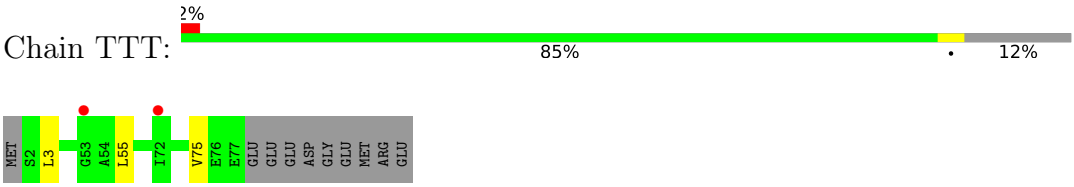
• Molecule 5: Small nuclear ribonucleoprotein F

Chain MMM:



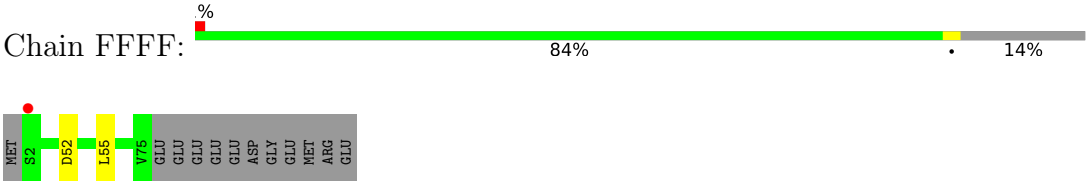
• Molecule 5: Small nuclear ribonucleoprotein F

Chain TTT:



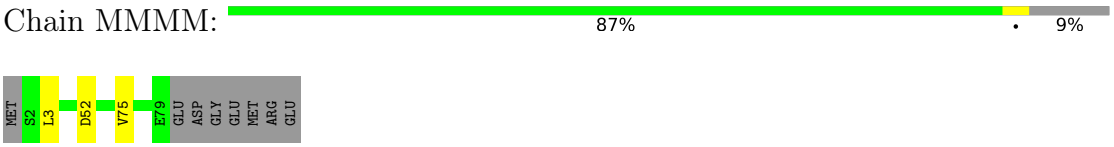
• Molecule 5: Small nuclear ribonucleoprotein F

Chain FFFF:



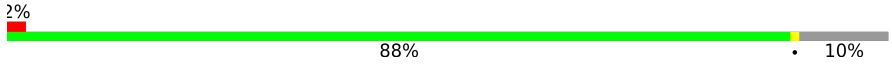
• Molecule 5: Small nuclear ribonucleoprotein F

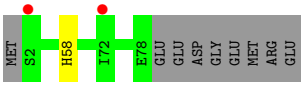
Chain MMMM:



• Molecule 5: Small nuclear ribonucleoprotein F

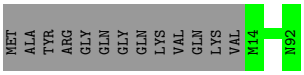
Chain TTTT:





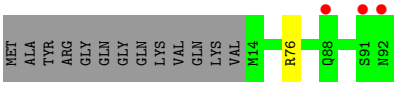
• Molecule 6: Small nuclear ribonucleoprotein E

Chain E:



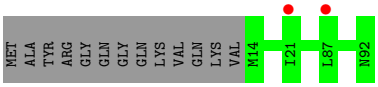
• Molecule 6: Small nuclear ribonucleoprotein E

Chain L:



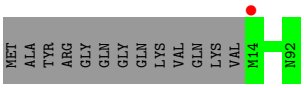
• Molecule 6: Small nuclear ribonucleoprotein E

Chain S:



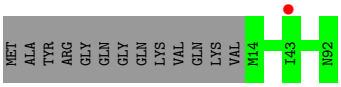
• Molecule 6: Small nuclear ribonucleoprotein E

Chain EE:



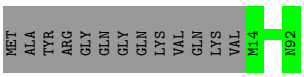
• Molecule 6: Small nuclear ribonucleoprotein E

Chain LL:



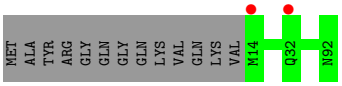
• Molecule 6: Small nuclear ribonucleoprotein E

Chain SS:



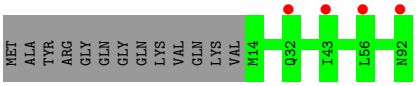
• Molecule 6: Small nuclear ribonucleoprotein E

Chain EEE:



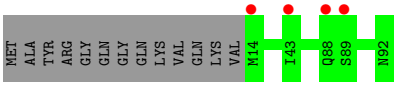
• Molecule 6: Small nuclear ribonucleoprotein E

Chain LLL:



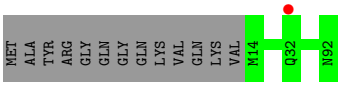
• Molecule 6: Small nuclear ribonucleoprotein E

Chain SSS:



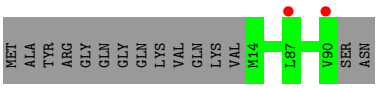
• Molecule 6: Small nuclear ribonucleoprotein E

Chain EEEE:



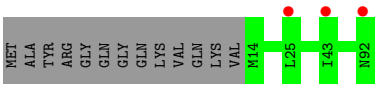
• Molecule 6: Small nuclear ribonucleoprotein E

Chain LLLL:



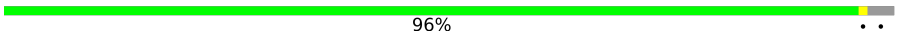
• Molecule 6: Small nuclear ribonucleoprotein E

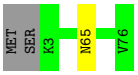
Chain SSSS:



• Molecule 7: Small nuclear ribonucleoprotein G

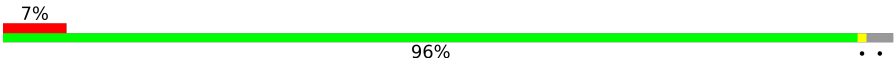
Chain G:

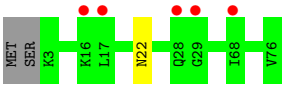




• Molecule 7: Small nuclear ribonucleoprotein G

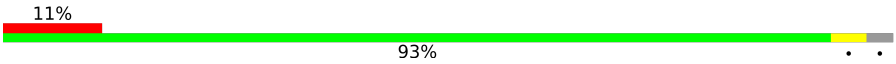
Chain N:

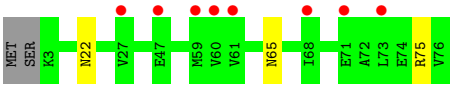




• Molecule 7: Small nuclear ribonucleoprotein G

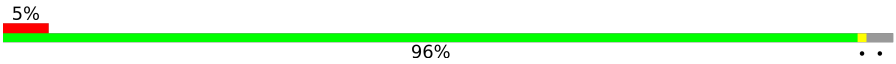
Chain U:

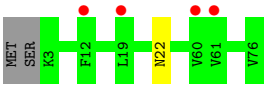




• Molecule 7: Small nuclear ribonucleoprotein G

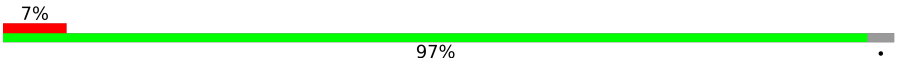
Chain GG:

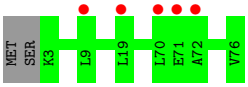




• Molecule 7: Small nuclear ribonucleoprotein G

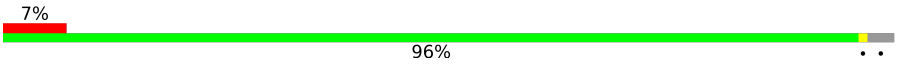
Chain NN:

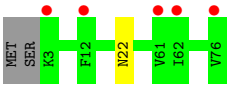




• Molecule 7: Small nuclear ribonucleoprotein G

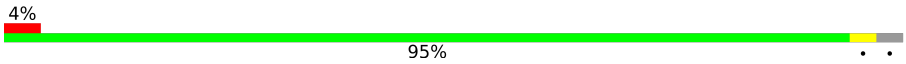
Chain UU:

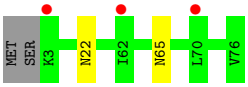




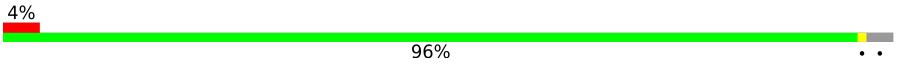
• Molecule 7: Small nuclear ribonucleoprotein G

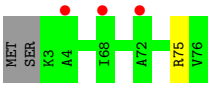
Chain GGG:



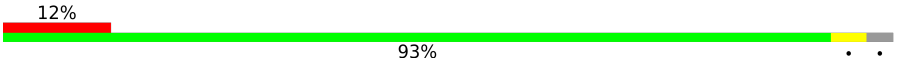


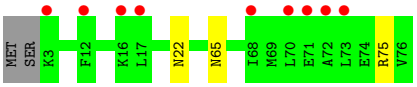
• Molecule 7: Small nuclear ribonucleoprotein G

Chain NNN: 

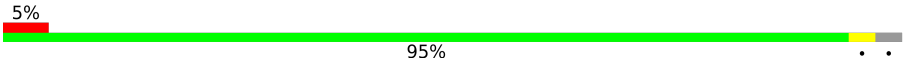


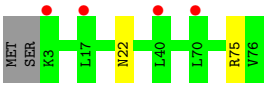
• Molecule 7: Small nuclear ribonucleoprotein G

Chain UUU: 

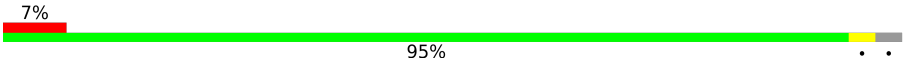


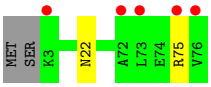
• Molecule 7: Small nuclear ribonucleoprotein G

Chain GGGG: 

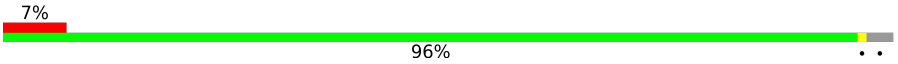


• Molecule 7: Small nuclear ribonucleoprotein G

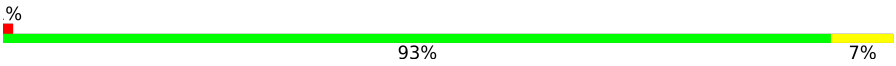
Chain NNNN: 

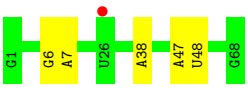


• Molecule 7: Small nuclear ribonucleoprotein G

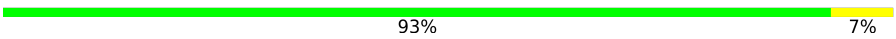
Chain UUUU: 

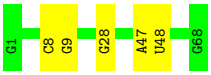
• Molecule 8: U4 small nuclear RNA variant: Native sequence 85-145, of which nucleotides 97-104 are replaced with GAAA tetraloop and nucleotides 134-137 are replaced with GAAA tetraloop receptor.

Chain V: 



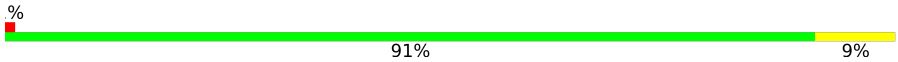
• Molecule 8: U4 small nuclear RNA variant: Native sequence 85-145, of which nucleotides 97-104 are replaced with GAAA tetraloop and nucleotides 134-137 are replaced with GAAA tetraloop receptor.

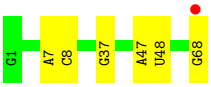
Chain X: 



• 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.

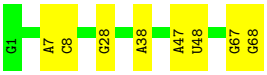
Chain Y:





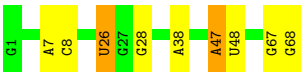
• Molecule 8: U4 small nuclear RNA variant: Native sequence 85-145, of which nucleotides 97-104 are replaced with GAAA tetraloop and nucleotides 134-137 are replaced with GAAA tetraloop receptor.

Chain VV:



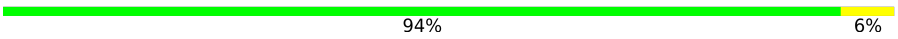
• Molecule 8: U4 small nuclear RNA variant: Native sequence 85-145, of which nucleotides 97-104 are replaced with GAAA tetraloop and nucleotides 134-137 are replaced with GAAA tetraloop receptor.

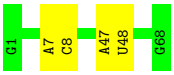
Chain XX:



• 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.

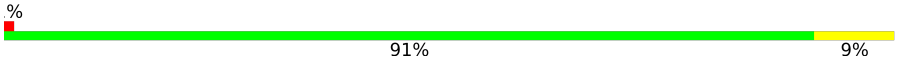
Chain YY:



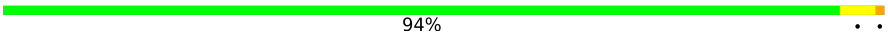


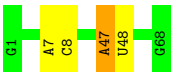
• Molecule 8: U4 small nuclear RNA variant: Native sequence 85-145, of which nucleotides 97-104 are replaced with GAAA tetraloop and nucleotides 134-137 are replaced with GAAA tetraloop receptor.

Chain VVV:

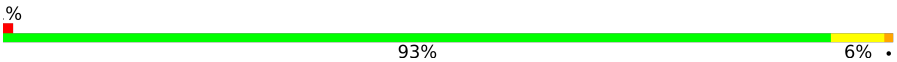


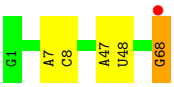
• Molecule 8: U4 small nuclear RNA variant: Native sequence 85-145, of which nucleotides 97-104 are replaced with GAAA tetraloop and nucleotides 134-137 are replaced with GAAA tetraloop receptor.

Chain XXX: 

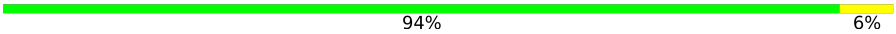


• Molecule 8: U4 small nuclear RNA variant: Native sequence 85-145, of which nucleotides 97-104 are replaced with GAAA tetraloop and nucleotides 134-137 are replaced with GAAA tetraloop receptor.

Chain YYY: 



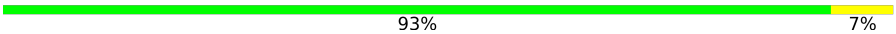
• Molecule 8: U4 small nuclear RNA variant: Native sequence 85-145, of which nucleotides 97-104 are replaced with GAAA tetraloop and nucleotides 134-137 are replaced with GAAA tetraloop receptor.

Chain VVVV: 

• 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:

• 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: 

4 Data and refinement statistics (i)

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 – 3.48	Depositor EDS
% Data completeness (in resolution range)	83.1 (66.15-3.60) 75.9 (66.15-3.48)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.177 , 0.224 0.179 , 0.176	Depositor DCC
R_{free} test set	8492 reflections (5.02%)	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 , 35.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.32$, $< L^2 > = 0.15$	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	0.92	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.46	0/660	0.67	0/889
1	AA	0.45	0/660	0.69	0/889
1	AAA	0.46	0/656	0.71	1/885 (0.1%)
1	AAAA	0.49	0/654	0.69	0/881
1	H	0.50	0/666	0.71	0/897
1	HH	0.49	0/661	0.68	0/892
1	HHH	0.49	0/666	0.67	0/897
1	HHHH	0.45	0/651	0.71	1/878 (0.1%)
1	O	0.45	0/660	0.68	0/889
1	OO	0.44	0/645	0.66	0/870
1	OOO	0.46	0/654	0.67	0/881
1	OOOO	0.44	0/654	0.69	0/881
2	B	0.53	0/700	0.82	0/933
2	BB	0.56	0/573	0.81	1/765 (0.1%)
2	BBB	0.49	0/573	0.73	0/765
2	BBBB	0.50	0/600	0.84	0/799
2	I	0.56	0/582	0.83	2/776 (0.3%)
2	II	0.49	0/593	0.77	0/793
2	III	0.61	2/573 (0.3%)	0.76	1/765 (0.1%)
2	IIII	0.61	0/610	0.84	1/813 (0.1%)
2	P	0.46	0/577	0.74	0/769
2	PP	0.49	0/577	0.69	0/769
2	PPP	0.49	0/567	0.92	3/758 (0.4%)
2	PPPP	0.46	0/607	0.73	0/810
3	C	0.56	0/657	0.77	0/888
3	CC	0.55	0/657	0.78	0/888
3	CCC	0.56	0/657	0.76	0/888
3	CCCC	0.54	0/657	0.76	0/888
3	J	0.54	0/657	0.76	0/888
3	JJ	0.53	0/657	0.76	0/888
3	JJJ	0.53	0/657	0.75	0/888
3	JJJJ	0.54	0/657	0.78	0/888
3	Q	0.52	0/657	0.74	0/888
3	QQ	0.53	0/657	0.76	0/888

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	QQQ	0.56	0/657	0.77	0/888
3	QQQQ	0.51	0/657	0.75	0/888
4	D	0.69	0/786	0.86	0/1053
4	DD	0.66	0/793	0.88	1/1063 (0.1%)
4	DDD	0.62	0/797	0.86	1/1067 (0.1%)
4	DDDD	0.62	0/849	0.88	1/1136 (0.1%)
4	K	0.69	0/806	0.88	4/1079 (0.4%)
4	KK	0.65	0/849	0.84	1/1136 (0.1%)
4	KKK	0.63	0/796	0.86	2/1064 (0.2%)
4	KKKK	0.76	0/849	0.93	2/1136 (0.2%)
4	R	0.63	0/797	0.85	1/1067 (0.1%)
4	RR	0.68	1/797 (0.1%)	0.89	2/1067 (0.2%)
4	RRR	0.63	0/797	0.84	1/1067 (0.1%)
4	RRRR	0.66	0/797	0.89	2/1067 (0.2%)
5	F	0.81	0/588	0.83	0/795
5	FF	0.72	0/597	0.80	0/807
5	FFF	0.69	0/588	0.82	0/795
5	FFFF	0.70	0/588	0.85	2/795 (0.3%)
5	M	0.73	0/621	0.81	0/840
5	MM	0.74	0/633	0.83	0/855
5	MMM	0.68	0/602	0.80	0/814
5	MMMM	0.76	0/616	0.84	0/833
5	T	0.72	0/606	0.80	0/819
5	TT	0.71	0/608	0.82	0/823
5	TTT	0.74	0/602	0.77	0/814
5	TTTT	0.69	0/611	0.79	0/826
6	E	0.61	0/660	0.83	0/886
6	EE	0.60	0/660	0.86	0/886
6	EEE	0.63	0/660	0.86	0/886
6	EEEE	0.62	0/660	0.86	0/886
6	L	0.59	0/660	0.86	1/886 (0.1%)
6	LL	0.57	0/660	0.82	0/886
6	LLL	0.58	0/660	0.82	0/886
6	LLLL	0.66	0/646	0.85	0/867
6	S	0.60	0/660	0.83	0/886
6	SS	0.62	0/660	0.84	0/886
6	SSS	0.57	0/660	0.83	0/886
6	SSSS	0.59	0/660	0.80	0/886
7	G	0.52	0/584	0.78	0/779
7	GG	0.54	0/584	0.78	0/779
7	GGG	0.49	0/584	0.75	0/779
7	GGGG	0.50	0/584	0.79	1/779 (0.1%)
7	N	0.50	0/584	0.77	0/779

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
7	NN	0.52	0/584	0.79	0/779
7	NNN	0.49	0/584	0.83	2/779 (0.3%)
7	NNNN	0.55	0/584	0.82	2/779 (0.3%)
7	U	0.49	0/584	0.79	2/779 (0.3%)
7	UU	0.48	0/578	0.74	0/772
7	UUU	0.53	0/584	0.81	1/779 (0.1%)
7	UUUU	0.49	0/584	0.76	0/779
8	V	0.59	1/1626 (0.1%)	0.80	3/2534 (0.1%)
8	VV	0.53	0/1626	0.79	7/2534 (0.3%)
8	VVV	0.46	0/1626	0.80	5/2534 (0.2%)
8	VVVV	0.53	0/1626	0.76	4/2534 (0.2%)
8	X	0.58	1/1626 (0.1%)	0.83	6/2534 (0.2%)
8	XX	0.46	0/1626	0.81	8/2534 (0.3%)
8	XXX	0.42	0/1626	0.76	4/2534 (0.2%)
8	XXXX	0.51	0/1626	0.99	12/2534 (0.5%)
8	Y	0.46	0/1626	0.78	6/2534 (0.2%)
8	YY	0.43	0/1626	0.75	4/2534 (0.2%)
8	YYY	0.41	0/1626	0.75	4/2534 (0.2%)
8	YYYY	0.48	0/1626	0.77	4/2534 (0.2%)
All	All	0.56	5/74296 (0.0%)	0.80	106/103980 (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

Continued on next page...

Continued from previous page...

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	RR	20	GLU	CB-CG	6.88	1.65	1.52
8	X	8	C	O3'-P	-6.72	1.53	1.61
2	III	47	GLU	CD-OE1	5.94	1.32	1.25
8	V	7	A	O3'-P	-5.39	1.54	1.61
2	III	47	GLU	CD-OE2	-5.10	1.20	1.25

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	XXXX	48	U	O5'-P-OP2	-23.61	82.36	110.70
2	PPP	25	ARG	NE-CZ-NH2	-11.55	114.52	120.30
8	XXXX	18	G	O5'-P-OP2	-11.18	95.64	105.70
2	PPP	25	ARG	NE-CZ-NH1	10.24	125.42	120.30
8	XXX	47	A	C2'-C3'-O3'	-9.57	88.44	109.50
8	XXXX	18	G	O5'-P-OP1	9.50	122.10	110.70
8	VVV	28	G	C5'-C4'-C3'	9.48	131.17	116.00
8	X	47	A	C2'-C3'-O3'	-9.45	88.72	109.50
8	YYYY	47	A	C2'-C3'-O3'	-9.41	88.79	109.50
4	DDDD	65	MET	CG-SD-CE	9.40	115.24	100.20
8	XX	47	A	C2'-C3'-O3'	-9.38	88.87	109.50
8	YY	47	A	C2'-C3'-O3'	-8.96	89.78	109.50
8	VVV	47	A	C2'-C3'-O3'	-8.94	89.84	109.50
8	YYY	47	A	C2'-C3'-O3'	-8.86	90.01	109.50
8	X	28	G	C5'-C4'-C3'	8.83	130.13	116.00
8	Y	47	A	C2'-C3'-O3'	-8.61	90.56	109.50
8	VVVV	47	A	C2'-C3'-O3'	-8.58	90.62	109.50
8	XX	26	U	O5'-P-OP2	8.56	120.97	110.70
8	XXXX	47	A	C2'-C3'-O3'	-8.14	91.58	109.50
8	VV	47	A	C2'-C3'-O3'	-8.09	91.71	109.50
1	AAA	82	MET	CG-SD-CE	7.77	112.63	100.20
5	FFFF	52	ASP	CB-CG-OD2	7.58	125.12	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	XXXX	68	G	O5'-P-OP2	7.36	119.53	110.70
1	HHHH	82	MET	CG-SD-CE	7.28	111.85	100.20
8	XX	48	U	P-O5'-C5'	6.92	131.97	120.90
8	VVV	38	A	O5'-P-OP1	6.91	118.99	110.70
8	XXXX	48	U	P-O5'-C5'	6.91	131.95	120.90
8	YYYY	48	U	P-O5'-C5'	6.86	131.88	120.90
8	V	47	A	C2'-C3'-O3'	-6.80	94.54	109.50
4	KKKK	79	LYS	CD-CE-NZ	6.67	127.03	111.70
8	XXXX	48	U	OP1-P-OP2	6.59	129.49	119.60
8	VV	47	A	O3'-P-O5'	-6.54	91.57	104.00
7	NNN	75	ARG	NE-CZ-NH1	6.50	123.55	120.30
8	YYY	48	U	P-O5'-C5'	6.44	131.21	120.90
8	V	48	U	P-O5'-C5'	6.42	131.18	120.90
8	VV	38	A	O5'-P-OP1	6.40	118.38	110.70
8	XXXX	7	A	C2'-C3'-O3'	-6.37	95.48	109.50
8	XXXX	47	A	P-O3'-C3'	6.37	127.35	119.70
7	NNN	75	ARG	NE-CZ-NH2	-6.32	117.14	120.30
8	XX	7	A	C2'-C3'-O3'	-6.28	95.68	109.50
8	XXXX	38	A	O5'-P-OP1	6.26	118.22	110.70
8	VV	47	A	P-O3'-C3'	6.14	127.07	119.70
5	FFFF	52	ASP	CB-CG-OD1	-6.13	112.78	118.30
2	BB	65	ARG	NE-CZ-NH1	6.10	123.35	120.30
8	YY	7	A	C2'-C3'-O3'	-6.10	96.09	109.50
8	XXX	48	U	P-O5'-C5'	6.09	130.65	120.90
8	VVV	48	U	P-O5'-C5'	6.06	130.60	120.90
8	YYY	68	G	O5'-P-OP1	-5.97	100.33	105.70
8	VVV	7	A	C2'-C3'-O3'	-5.95	96.41	109.50
8	XXX	7	A	C2'-C3'-O3'	-5.95	96.42	109.50
8	VVVV	38	A	O5'-P-OP1	5.93	117.81	110.70
4	KKK	85	LYS	N-CA-CB	5.91	121.24	110.60
8	YY	48	U	P-O5'-C5'	5.88	130.32	120.90
8	Y	48	U	P-O5'-C5'	5.85	130.26	120.90
8	X	48	U	O5'-P-OP1	5.81	117.68	110.70
8	XX	48	U	O5'-P-OP1	5.80	117.66	110.70
2	I	65	ARG	CB-CG-CD	-5.78	96.57	111.60
2	IIII	47	GLU	CG-CD-OE2	5.78	129.85	118.30
8	X	48	U	P-O5'-C5'	5.75	130.09	120.90
8	YYY	7	A	C2'-C3'-O3'	-5.74	96.88	109.50
8	VVVV	47	A	P-O3'-C3'	5.71	126.56	119.70
4	KKK	47	ARG	NE-CZ-NH2	-5.68	117.46	120.30
8	YYYY	38	A	O5'-P-OP1	5.67	117.50	110.70
8	XX	28	G	O5'-P-OP2	-5.62	100.64	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	KKKK	47	ARG	NE-CZ-NH2	-5.60	117.50	120.30
4	DDD	47	ARG	NE-CZ-NH2	-5.58	117.51	120.30
4	K	19	ARG	NE-CZ-NH2	-5.55	117.52	120.30
2	I	64	LYS	CB-CG-CD	5.55	126.03	111.60
7	NNNN	75	ARG	NE-CZ-NH1	5.51	123.05	120.30
8	XX	47	A	P-O3'-C3'	5.50	126.30	119.70
8	X	8	C	C2'-C3'-O3'	5.49	122.48	113.70
4	K	102	ARG	NE-CZ-NH2	5.49	123.04	120.30
4	KK	47	ARG	NE-CZ-NH2	-5.45	117.58	120.30
4	RR	47	ARG	NE-CZ-NH2	-5.44	117.58	120.30
4	K	47	ARG	NE-CZ-NH2	-5.44	117.58	120.30
4	DD	47	ARG	NE-CZ-NH2	-5.43	117.58	120.30
4	K	19	ARG	NE-CZ-NH1	5.33	122.97	120.30
8	V	38	A	O5'-P-OP1	5.33	117.09	110.70
8	XXXX	47	A	OP2-P-O3'	5.32	116.90	105.20
7	UUU	75	ARG	NE-CZ-NH2	-5.31	117.65	120.30
4	RRRR	47	ARG	NE-CZ-NH2	-5.29	117.65	120.30
8	Y	48	U	O5'-P-OP1	5.29	117.05	110.70
2	III	47	GLU	CG-CD-OE2	-5.28	107.73	118.30
7	NNNN	75	ARG	NE-CZ-NH2	-5.24	117.68	120.30
7	U	75	ARG	NE-CZ-NH2	-5.24	117.68	120.30
7	GGGG	75	ARG	NE-CZ-NH1	5.23	122.92	120.30
8	VV	7	A	C2'-C3'-O3'	-5.23	97.99	109.50
8	XX	38	A	O5'-P-OP1	5.21	116.96	110.70
8	Y	37	G	C5'-C4'-O4'	5.21	115.36	109.10
8	YY	48	U	O5'-P-OP1	5.20	116.94	110.70
8	XXXX	18	G	C5'-C4'-C3'	-5.20	107.68	116.00
2	PPP	65	ARG	NE-CZ-NH1	5.18	122.89	120.30
8	VV	28	G	C5'-C4'-C3'	5.14	124.22	116.00
6	L	76	ARG	NE-CZ-NH2	5.12	122.86	120.30
8	YYYY	7	A	C2'-C3'-O3'	-5.12	98.25	109.50
4	RRRR	84	LYS	CA-CB-CG	5.10	124.63	113.40
4	RR	20	GLU	OE1-CD-OE2	-5.10	117.18	123.30
8	X	9	G	C2'-C3'-O3'	5.09	121.85	113.70
8	Y	7	A	P-O3'-C3'	5.08	125.80	119.70
7	U	75	ARG	NE-CZ-NH1	5.08	122.84	120.30
8	Y	47	A	P-O3'-C3'	5.08	125.80	119.70
8	VVVV	48	U	P-O5'-C5'	5.08	129.03	120.90
8	XXX	48	U	O5'-P-OP1	5.06	116.78	110.70
4	R	47	ARG	NE-CZ-NH2	-5.04	117.78	120.30
8	VV	48	U	O5'-P-OP1	5.04	116.74	110.70
4	RRR	47	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	112	ASN	Peptide
4	DD	112	ASN	Peptide
4	DDD	112	ASN	Peptide
4	DDDD	112	ASN	Peptide
4	K	112	ASN	Peptide
4	KK	112	ASN	Peptide
4	KKK	112	ASN	Peptide
4	KKKK	112	ASN	Peptide
5	M	3	LEU	Peptide
5	MM	1	MET	Peptide
5	MM	3	LEU	Peptide
5	MMM	3	LEU	Peptide
5	MMMM	3	LEU	Peptide
2	PPPP	63	GLU	Peptide
4	R	112	ASN	Peptide
4	RR	112	ASN	Peptide
4	RRR	112	ASN	Peptide
4	RRRR	112	ASN	Peptide
5	TT	3	LEU	Peptide
5	TT	76	GLU	Peptide
5	TTT	3	LEU	Peptide
8	V	6	G	Sidechain
8	VVVV	67	G	Sidechain

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 (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	81/125 (65%)	80 (99%)	1 (1%)	0	100	100
1	AA	81/125 (65%)	78 (96%)	3 (4%)	0	100	100
1	AAA	81/125 (65%)	80 (99%)	1 (1%)	0	100	100
1	AAAA	80/125 (64%)	78 (98%)	2 (2%)	0	100	100
1	H	82/125 (66%)	81 (99%)	1 (1%)	0	100	100
1	HH	82/125 (66%)	78 (95%)	4 (5%)	0	100	100
1	HHH	82/125 (66%)	81 (99%)	1 (1%)	0	100	100
1	HHHH	80/125 (64%)	78 (98%)	2 (2%)	0	100	100
1	O	81/125 (65%)	80 (99%)	1 (1%)	0	100	100
1	OO	79/125 (63%)	78 (99%)	1 (1%)	0	100	100
1	OOO	80/125 (64%)	78 (98%)	2 (2%)	0	100	100
1	OOOO	80/125 (64%)	79 (99%)	1 (1%)	0	100	100
2	B	84/95 (88%)	82 (98%)	2 (2%)	0	100	100
2	BB	67/95 (70%)	66 (98%)	1 (2%)	0	100	100
2	BBB	67/95 (70%)	66 (98%)	1 (2%)	0	100	100
2	BBBB	70/95 (74%)	69 (99%)	1 (1%)	0	100	100
2	I	68/95 (72%)	66 (97%)	2 (3%)	0	100	100
2	II	71/95 (75%)	70 (99%)	1 (1%)	0	100	100
2	III	67/95 (70%)	65 (97%)	2 (3%)	0	100	100
2	IIII	71/95 (75%)	70 (99%)	1 (1%)	0	100	100
2	P	67/95 (70%)	65 (97%)	2 (3%)	0	100	100
2	PP	67/95 (70%)	65 (97%)	2 (3%)	0	100	100
2	PPP	67/95 (70%)	66 (98%)	1 (2%)	0	100	100
2	PPPP	71/95 (75%)	69 (97%)	2 (3%)	0	100	100
3	C	80/118 (68%)	77 (96%)	3 (4%)	0	100	100
3	CC	80/118 (68%)	77 (96%)	3 (4%)	0	100	100
3	CCC	80/118 (68%)	77 (96%)	3 (4%)	0	100	100
3	CCCC	80/118 (68%)	78 (98%)	2 (2%)	0	100	100
3	J	80/118 (68%)	77 (96%)	3 (4%)	0	100	100
3	JJ	80/118 (68%)	77 (96%)	3 (4%)	0	100	100
3	JJJ	80/118 (68%)	77 (96%)	3 (4%)	0	100	100
3	JJJJ	80/118 (68%)	77 (96%)	3 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Q	80/118 (68%)	77 (96%)	3 (4%)	0	100	100
3	QQ	80/118 (68%)	78 (98%)	2 (2%)	0	100	100
3	QQQ	80/118 (68%)	78 (98%)	2 (2%)	0	100	100
3	QQQQ	80/118 (68%)	78 (98%)	2 (2%)	0	100	100
4	D	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
4	DD	96/118 (81%)	92 (96%)	3 (3%)	1 (1%)	15	55
4	DDD	96/118 (81%)	92 (96%)	4 (4%)	0	100	100
4	DDDD	102/118 (86%)	98 (96%)	4 (4%)	0	100	100
4	K	98/118 (83%)	93 (95%)	4 (4%)	1 (1%)	15	55
4	KK	102/118 (86%)	98 (96%)	4 (4%)	0	100	100
4	KKK	97/118 (82%)	93 (96%)	4 (4%)	0	100	100
4	KKKK	102/118 (86%)	98 (96%)	4 (4%)	0	100	100
4	R	96/118 (81%)	92 (96%)	4 (4%)	0	100	100
4	RR	96/118 (81%)	90 (94%)	6 (6%)	0	100	100
4	RRR	96/118 (81%)	92 (96%)	4 (4%)	0	100	100
4	RRRR	96/118 (81%)	92 (96%)	4 (4%)	0	100	100
5	F	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
5	FF	73/86 (85%)	69 (94%)	4 (6%)	0	100	100
5	FFF	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
5	FFFF	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
5	M	77/86 (90%)	73 (95%)	4 (5%)	0	100	100
5	MM	78/86 (91%)	74 (95%)	4 (5%)	0	100	100
5	MMM	74/86 (86%)	69 (93%)	5 (7%)	0	100	100
5	MMMM	76/86 (88%)	69 (91%)	6 (8%)	1 (1%)	12	50
5	T	74/86 (86%)	70 (95%)	4 (5%)	0	100	100
5	TT	76/86 (88%)	73 (96%)	3 (4%)	0	100	100
5	TTT	74/86 (86%)	70 (95%)	3 (4%)	1 (1%)	11	48
5	TTTT	75/86 (87%)	71 (95%)	4 (5%)	0	100	100
6	E	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
6	EE	77/92 (84%)	75 (97%)	2 (3%)	0	100	100
6	EEE	77/92 (84%)	75 (97%)	2 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	EEEE	77/92 (84%)	75 (97%)	2 (3%)	0	100	100
6	L	77/92 (84%)	74 (96%)	3 (4%)	0	100	100
6	LL	77/92 (84%)	75 (97%)	2 (3%)	0	100	100
6	LLL	77/92 (84%)	75 (97%)	2 (3%)	0	100	100
6	LLLL	75/92 (82%)	74 (99%)	1 (1%)	0	100	100
6	S	77/92 (84%)	75 (97%)	2 (3%)	0	100	100
6	SS	77/92 (84%)	75 (97%)	2 (3%)	0	100	100
6	SSS	77/92 (84%)	75 (97%)	2 (3%)	0	100	100
6	SSSS	77/92 (84%)	75 (97%)	2 (3%)	0	100	100
7	G	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
7	GG	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
7	GGG	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
7	GGGG	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
7	N	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
7	NN	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
7	NNN	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
7	NNNN	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
7	U	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
7	UU	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
7	UUU	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
7	UUUU	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
All	All	6617/8520 (78%)	6400 (97%)	213 (3%)	4 (0%)	51	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	DD	85	LYS
5	TTT	75	VAL
4	K	117	GLY
5	MMMM	75	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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%)	67	85
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%)	75 (97%)	2 (3%)	46	74
2	BB	63/85 (74%)	62 (98%)	1 (2%)	62	83
2	BBB	63/85 (74%)	61 (97%)	2 (3%)	39	70
2	BBBB	66/85 (78%)	65 (98%)	1 (2%)	65	84
2	I	64/85 (75%)	62 (97%)	2 (3%)	40	71
2	II	63/85 (74%)	62 (98%)	1 (2%)	62	83
2	III	63/85 (74%)	62 (98%)	1 (2%)	62	83
2	IIII	67/85 (79%)	66 (98%)	1 (2%)	65	84
2	P	64/85 (75%)	63 (98%)	1 (2%)	62	83
2	PP	64/85 (75%)	63 (98%)	1 (2%)	62	83
2	PPP	62/85 (73%)	62 (100%)	0	100	100
2	PPPP	67/85 (79%)	65 (97%)	2 (3%)	41	71
3	C	77/100 (77%)	75 (97%)	2 (3%)	46	74
3	CC	77/100 (77%)	75 (97%)	2 (3%)	46	74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	CCC	77/100 (77%)	75 (97%)	2 (3%)	46	74
3	CCCC	77/100 (77%)	75 (97%)	2 (3%)	46	74
3	J	77/100 (77%)	75 (97%)	2 (3%)	46	74
3	JJ	77/100 (77%)	75 (97%)	2 (3%)	46	74
3	JJJ	77/100 (77%)	75 (97%)	2 (3%)	46	74
3	JJJJ	77/100 (77%)	75 (97%)	2 (3%)	46	74
3	Q	77/100 (77%)	75 (97%)	2 (3%)	46	74
3	QQ	77/100 (77%)	75 (97%)	2 (3%)	46	74
3	QQQ	77/100 (77%)	75 (97%)	2 (3%)	46	74
3	QQQQ	77/100 (77%)	75 (97%)	2 (3%)	46	74
4	D	90/110 (82%)	88 (98%)	2 (2%)	52	77
4	DD	90/110 (82%)	85 (94%)	5 (6%)	21	56
4	DDD	91/110 (83%)	90 (99%)	1 (1%)	73	88
4	DDDD	97/110 (88%)	95 (98%)	2 (2%)	53	78
4	K	91/110 (83%)	89 (98%)	2 (2%)	52	77
4	KK	97/110 (88%)	96 (99%)	1 (1%)	76	88
4	KKK	90/110 (82%)	89 (99%)	1 (1%)	73	88
4	KKKK	97/110 (88%)	95 (98%)	2 (2%)	53	78
4	R	91/110 (83%)	90 (99%)	1 (1%)	73	88
4	RR	91/110 (83%)	90 (99%)	1 (1%)	73	88
4	RRR	91/110 (83%)	90 (99%)	1 (1%)	73	88
4	RRRR	91/110 (83%)	89 (98%)	2 (2%)	52	77
5	F	63/74 (85%)	62 (98%)	1 (2%)	62	83
5	FF	64/74 (86%)	64 (100%)	0	100	100
5	FFF	63/74 (85%)	63 (100%)	0	100	100
5	FFFF	63/74 (85%)	62 (98%)	1 (2%)	62	83
5	M	65/74 (88%)	64 (98%)	1 (2%)	65	84
5	MM	67/74 (90%)	67 (100%)	0	100	100
5	MMM	64/74 (86%)	64 (100%)	0	100	100
5	MMMM	65/74 (88%)	64 (98%)	1 (2%)	65	84
5	T	65/74 (88%)	65 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	TT	63/74 (85%)	62 (98%)	1 (2%)	62	83
5	TTT	64/74 (86%)	63 (98%)	1 (2%)	62	83
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%)	62	83
7	GG	64/66 (97%)	63 (98%)	1 (2%)	62	83
7	GGG	64/66 (97%)	62 (97%)	2 (3%)	40	71
7	GGGG	64/66 (97%)	63 (98%)	1 (2%)	62	83
7	N	64/66 (97%)	63 (98%)	1 (2%)	62	83
7	NN	64/66 (97%)	64 (100%)	0	100	100
7	NNN	64/66 (97%)	64 (100%)	0	100	100
7	NNNN	64/66 (97%)	63 (98%)	1 (2%)	62	83
7	U	64/66 (97%)	62 (97%)	2 (3%)	40	71
7	UU	63/66 (96%)	62 (98%)	1 (2%)	62	83
7	UUU	64/66 (97%)	62 (97%)	2 (3%)	40	71
7	UUUU	64/66 (97%)	63 (98%)	1 (2%)	62	83
All	All	6108/7428 (82%)	6028 (99%)	80 (1%)	69	86

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	13	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	58	GLN
3	C	40	LEU
3	C	54	GLN
4	D	45	ASN
4	D	112	ASN
5	F	55	LEU
7	G	65	ASN
1	H	84	LYS
2	I	13	ILE
2	I	64	LYS
3	J	40	LEU
3	J	54	GLN
4	K	45	ASN
4	K	112	ASN
5	M	55	LEU
7	N	22	ASN
2	P	13	ILE
3	Q	40	LEU
3	Q	54	GLN
4	R	45	ASN
7	U	22	ASN
7	U	65	ASN
2	BB	13	ILE
3	CC	40	LEU
3	CC	54	GLN
4	DD	45	ASN
4	DD	85	LYS
4	DD	88	LYS
4	DD	94	ARG
4	DD	112	ASN
7	GG	22	ASN
2	II	13	ILE
3	JJ	40	LEU
3	JJ	54	GLN
4	KK	45	ASN
2	PP	13	ILE
3	QQ	40	LEU
3	QQ	54	GLN
4	RR	45	ASN
5	TT	52	ASP
7	UU	22	ASN
2	BBB	13	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	BBB	64	LYS
3	CCC	40	LEU
3	CCC	54	GLN
4	DDD	45	ASN
7	GGG	22	ASN
7	GGG	65	ASN
2	III	13	ILE
3	JJJ	40	LEU
3	JJJ	54	GLN
4	KKK	45	ASN
3	QQQ	40	LEU
3	QQQ	54	GLN
4	RRR	45	ASN
5	TTT	55	LEU
7	UUU	22	ASN
7	UUU	65	ASN
2	BBBB	13	ILE
3	CCCC	40	LEU
3	CCCC	54	GLN
4	DDDD	45	ASN
4	DDDD	112	ASN
5	FFFF	55	LEU
7	GGGG	22	ASN
2	IIII	13	ILE
3	JJJJ	40	LEU
3	JJJJ	54	GLN
4	KKKK	45	ASN
4	KKKK	112	ASN
5	MMMM	52	ASP
7	NNNN	22	ASN
2	PPPP	11	GLN
2	PPPP	13	ILE
3	QQQQ	40	LEU
3	QQQQ	54	GLN
4	RRRR	45	ASN
4	RRRR	86	LYS
7	UUUU	22	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	22	GLN
2	B	76	ASN
3	C	12	HIS
3	C	64	ASN
4	D	69	ASN
4	D	91	ASN
7	G	65	ASN
1	H	60	GLN
2	I	22	GLN
2	I	76	ASN
3	J	64	ASN
4	K	69	ASN
7	N	53	GLN
7	N	55	ASN
7	N	65	ASN
1	O	60	GLN
2	P	22	GLN
2	P	76	ASN
3	Q	64	ASN
4	R	69	ASN
4	R	91	ASN
7	U	65	ASN
1	AA	60	GLN
2	BB	22	GLN
2	BB	76	ASN
3	CC	64	ASN
4	DD	69	ASN
7	GG	65	ASN
1	HH	23	ASN
1	HH	60	GLN
2	II	22	GLN
2	II	76	ASN
3	JJ	64	ASN
4	KK	69	ASN
6	LL	27	ASN
6	LL	65	HIS
7	NN	65	ASN
1	OO	60	GLN
2	PP	22	GLN
2	PP	76	ASN
3	QQ	64	ASN
4	RR	69	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	SS	27	ASN
7	UU	53	GLN
7	UU	55	ASN
7	UU	65	ASN

5.3.3 RNA (i)

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%)

All (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
8	XX	26	U
8	XX	68	G
8	YY	8	C
8	VVV	8	C
8	XXX	8	C
8	YYY	8	C
8	YYY	68	G
8	XXXX	8	C
8	XXXX	68	G
8	YYYY	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.26	4 (4%)	30	19	58, 143, 193, 230	0
1	AA	83/125 (66%)	0.09	1 (1%)	79	66	82, 130, 175, 210	0
1	AAA	83/125 (66%)	0.06	5 (6%)	21	12	63, 130, 180, 217	0
1	AAAA	82/125 (65%)	0.18	4 (4%)	29	18	56, 136, 187, 201	0
1	H	84/125 (67%)	0.31	5 (5%)	21	12	58, 144, 210, 248	0
1	HH	84/125 (67%)	0.17	4 (4%)	30	19	84, 139, 195, 231	0
1	HHH	84/125 (67%)	0.21	2 (2%)	59	42	70, 143, 195, 230	0
1	HHHH	82/125 (65%)	0.10	2 (2%)	59	42	71, 142, 192, 240	0
1	O	83/125 (66%)	0.69	14 (16%)	1	1	92, 164, 222, 306	0
1	OO	81/125 (64%)	0.25	6 (7%)	14	9	64, 143, 192, 213	0
1	OOO	82/125 (65%)	0.28	4 (4%)	29	18	74, 146, 192, 214	0
1	OOOO	82/125 (65%)	0.36	6 (7%)	15	9	50, 152, 202, 231	0
2	B	86/95 (90%)	0.31	7 (8%)	12	7	72, 139, 198, 223	0
2	BB	71/95 (74%)	0.25	1 (1%)	75	61	63, 125, 171, 191	0
2	BBB	71/95 (74%)	0.63	10 (14%)	2	2	78, 136, 190, 273	1 (1%)
2	BBBB	74/95 (77%)	0.21	3 (4%)	37	24	57, 128, 164, 201	0
2	I	72/95 (75%)	0.34	7 (9%)	7	4	79, 131, 178, 240	0
2	II	75/95 (78%)	0.32	6 (8%)	12	7	68, 126, 202, 302	0
2	III	71/95 (74%)	0.28	5 (7%)	16	9	60, 129, 183, 202	0
2	IIII	75/95 (78%)	0.46	8 (10%)	6	3	89, 154, 220, 250	0
2	P	71/95 (74%)	0.29	4 (5%)	24	14	82, 146, 184, 219	0
2	PP	71/95 (74%)	0.39	5 (7%)	16	9	84, 138, 195, 207	0
2	PPP	71/95 (74%)	0.16	4 (5%)	24	14	79, 137, 191, 204	0
2	PPPP	75/95 (78%)	0.54	9 (12%)	4	3	63, 135, 191, 222	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
3	C	82/118 (69%)	-0.02	0	100	100	70, 104, 135, 172	0
3	CC	82/118 (69%)	-0.05	1 (1%)	79	66	57, 91, 139, 162	0
3	CCC	82/118 (69%)	0.05	1 (1%)	79	66	43, 96, 151, 213	0
3	CCCC	82/118 (69%)	0.09	2 (2%)	59	42	56, 99, 159, 214	0
3	J	82/118 (69%)	-0.00	0	100	100	51, 102, 146, 168	0
3	JJ	82/118 (69%)	0.03	2 (2%)	59	42	56, 104, 168, 212	0
3	JJJ	82/118 (69%)	-0.07	1 (1%)	79	66	57, 101, 144, 178	0
3	JJJJ	82/118 (69%)	0.05	0	100	100	49, 90, 150, 191	0
3	Q	82/118 (69%)	0.13	1 (1%)	79	66	57, 108, 151, 275	0
3	QQ	82/118 (69%)	-0.02	0	100	100	46, 98, 152, 208	0
3	QQQ	82/118 (69%)	0.03	0	100	100	46, 103, 157, 174	0
3	QQQQ	82/118 (69%)	0.03	1 (1%)	79	66	64, 103, 178, 220	0
4	D	97/118 (82%)	0.00	3 (3%)	49	33	48, 93, 168, 229	0
4	DD	98/118 (83%)	0.14	4 (4%)	37	24	57, 106, 187, 244	0
4	DDD	98/118 (83%)	0.13	5 (5%)	28	17	34, 92, 211, 237	0
4	DDDD	104/118 (88%)	0.18	7 (6%)	17	10	36, 96, 184, 219	0
4	K	100/118 (84%)	0.02	3 (3%)	50	34	29, 99, 180, 200	0
4	KK	104/118 (88%)	0.09	6 (5%)	23	13	45, 106, 191, 249	0
4	KKK	99/118 (83%)	-0.04	0	100	100	59, 110, 173, 200	0
4	KKKK	104/118 (88%)	0.06	4 (3%)	40	26	47, 100, 198, 262	0
4	R	98/118 (83%)	0.04	3 (3%)	49	33	48, 103, 175, 212	0
4	RR	98/118 (83%)	0.06	5 (5%)	28	17	49, 100, 207, 227	0
4	RRR	98/118 (83%)	0.41	7 (7%)	16	9	26, 95, 263, 292	0
4	RRRR	98/118 (83%)	0.02	3 (3%)	49	33	36, 96, 189, 246	0
5	F	74/86 (86%)	-0.01	0	100	100	25, 74, 117, 136	0
5	FF	75/86 (87%)	-0.04	0	100	100	25, 88, 149, 188	0
5	FFF	74/86 (86%)	0.11	0	100	100	47, 89, 139, 166	0
5	FFFF	74/86 (86%)	0.10	1 (1%)	75	61	42, 88, 131, 165	0
5	M	79/86 (91%)	0.05	2 (2%)	57	41	45, 90, 153, 171	0
5	MM	80/86 (93%)	-0.10	0	100	100	39, 89, 139, 167	0
5	MMM	76/86 (88%)	0.13	0	100	100	45, 97, 143, 167	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
5	MMMM	78/86 (90%)	-0.07	0	100	100	37, 85, 136, 165	0
5	T	76/86 (88%)	0.10	2 (2%)	56	40	49, 94, 153, 219	0
5	TT	78/86 (90%)	-0.08	0	100	100	45, 89, 138, 174	0
5	TTT	76/86 (88%)	0.13	2 (2%)	56	40	46, 91, 142, 213	0
5	TTTT	77/86 (89%)	0.05	2 (2%)	56	40	44, 92, 156, 203	0
6	E	79/92 (85%)	-0.06	0	100	100	46, 100, 142, 181	0
6	EE	79/92 (85%)	0.06	1 (1%)	77	63	53, 102, 159, 210	0
6	EEE	79/92 (85%)	0.10	2 (2%)	57	41	51, 100, 158, 195	0
6	EEEE	79/92 (85%)	0.04	1 (1%)	77	63	54, 96, 149, 168	0
6	L	79/92 (85%)	0.14	3 (3%)	40	26	57, 100, 157, 221	0
6	LL	79/92 (85%)	0.04	1 (1%)	77	63	62, 103, 154, 173	0
6	LLL	79/92 (85%)	0.27	4 (5%)	28	17	57, 114, 193, 234	0
6	LLLL	77/92 (83%)	-0.03	2 (2%)	56	40	42, 91, 157, 190	0
6	S	79/92 (85%)	0.09	2 (2%)	57	41	47, 112, 180, 205	0
6	SS	79/92 (85%)	-0.01	0	100	100	52, 98, 157, 202	0
6	SSS	79/92 (85%)	0.09	4 (5%)	28	17	58, 109, 179, 203	0
6	SSSS	79/92 (85%)	0.17	3 (3%)	40	26	51, 107, 180, 227	0
7	G	74/76 (97%)	0.24	0	100	100	58, 130, 187, 200	0
7	GG	74/76 (97%)	0.12	4 (5%)	25	16	45, 120, 173, 204	0
7	GGG	74/76 (97%)	0.17	3 (4%)	37	24	64, 133, 182, 222	0
7	GGGG	74/76 (97%)	0.16	4 (5%)	25	16	57, 129, 183, 233	0
7	N	74/76 (97%)	0.31	5 (6%)	17	10	76, 128, 186, 212	0
7	NN	74/76 (97%)	0.24	5 (6%)	17	10	70, 120, 172, 243	0
7	NNN	74/76 (97%)	0.31	3 (4%)	37	24	75, 142, 187, 214	0
7	NNNN	74/76 (97%)	0.31	5 (6%)	17	10	63, 111, 186, 233	0
7	U	74/76 (97%)	0.38	8 (10%)	5	3	86, 132, 212, 239	0
7	UU	74/76 (97%)	0.31	5 (6%)	17	10	61, 133, 181, 226	0
7	UUU	74/76 (97%)	0.49	9 (12%)	4	3	50, 141, 213, 254	0
7	UUUU	74/76 (97%)	0.33	5 (6%)	17	10	74, 144, 188, 206	0
8	V	68/68 (100%)	-0.63	1 (1%)	73	60	67, 171, 209, 272	0
8	VV	68/68 (100%)	-0.60	0	100	100	63, 148, 219, 272	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
8	VVV	68/68 (100%)	-0.63	1 (1%) 73 60	75, 163, 213, 248	0
8	VVVV	68/68 (100%)	-0.60	0 100 100	67, 168, 222, 263	0
8	X	68/68 (100%)	-0.60	0 100 100	81, 164, 218, 272	0
8	XX	68/68 (100%)	-0.60	0 100 100	74, 161, 218, 267	0
8	XXX	68/68 (100%)	-0.66	0 100 100	85, 158, 210, 221	0
8	XXXX	68/68 (100%)	-0.55	0 100 100	69, 158, 220, 249	0
8	Y	68/68 (100%)	-0.62	1 (1%) 73 60	79, 173, 228, 245	0
8	YY	68/68 (100%)	-0.61	0 100 100	81, 155, 229, 291	0
8	YYY	68/68 (100%)	-0.57	1 (1%) 73 60	78, 164, 247, 310	0
8	YYYY	68/68 (100%)	-0.62	0 100 100	83, 164, 226, 341	0
All	All	7623/9336 (81%)	0.07	277 (3%) 42 28	25, 118, 195, 341	1 (0%)

All (277) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	1	MET	8.9
4	RRR	83	GLY	7.8
4	RRR	82	LYS	7.8
2	II	4	GLY	7.4
4	KKKK	83	GLY	7.4
4	DDDD	14	GLU	7.2
7	UUU	72	ALA	6.6
1	O	18	VAL	6.6
2	BBB	40	LEU	6.1
4	RRR	79	LYS	5.8
7	UU	76	VAL	5.7
4	RRR	80	SER	5.3
2	B	71	LEU	5.2
7	N	17	LEU	5.1
3	CCC	1	MET	4.9
1	AAA	71	LEU	4.8
4	RRR	78	PRO	4.8
1	O	63	ILE	4.8
2	BBB	49	ARG	4.7
4	KKKK	82	LYS	4.7
7	UUU	17	LEU	4.7
1	A	41	CYS	4.7
5	T	2	SER	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	UUU	3	LYS	4.4
7	U	68	ILE	4.4
7	GGG	3	LYS	4.3
1	A	3	ILE	4.3
1	O	60	GLN	4.3
6	L	92	ASN	4.2
7	UUU	73	LEU	4.2
2	BB	27	PHE	4.2
4	DDDD	13	PRO	4.1
4	RR	83	GLY	4.1
2	PPPP	63	GLU	4.0
1	HH	41	CYS	4.0
2	B	72	LEU	3.9
6	S	87	LEU	3.9
6	EEE	32	GLN	3.9
4	DD	83	GLY	3.8
1	O	19	THR	3.8
4	KK	85	LYS	3.8
4	D	83	GLY	3.7
2	I	26	ILE	3.7
1	O	71	LEU	3.6
4	RRR	81	GLY	3.6
4	KK	83	GLY	3.6
7	U	61	VAL	3.6
2	PPPP	34	PHE	3.5
1	H	28	TYR	3.5
1	A	28	TYR	3.5
1	O	37	ASP	3.5
2	IIII	72	LEU	3.5
7	U	47	GLU	3.4
4	RR	79	LYS	3.4
4	DDD	85	LYS	3.4
7	GGGG	3	LYS	3.4
1	OO	71	LEU	3.4
1	AAAA	71	LEU	3.4
4	DDD	83	GLY	3.4
2	B	33	ALA	3.4
2	I	27	PHE	3.3
6	L	91	SER	3.3
1	O	43	MET	3.3
1	AA	41	CYS	3.3
7	UU	61	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	JJ	1	MET	3.2
7	NNNN	73	LEU	3.2
4	KK	14	GLU	3.2
2	II	40	LEU	3.2
4	RRRR	82	LYS	3.2
4	DDD	23	GLU	3.1
8	VVV	68	G	3.1
5	TTT	72	ILE	3.1
4	DDDD	85	LYS	3.1
4	RRR	84	LYS	3.1
7	NN	71	GLU	3.1
2	II	77	LEU	3.1
2	IIII	67	LEU	3.1
4	RR	82	LYS	3.1
4	KK	86	LYS	3.1
6	LLLL	90	VAL	3.1
1	OOOO	34	GLU	3.0
1	HH	28	TYR	3.0
1	OOOO	42	GLN	3.0
7	UUUU	70	LEU	3.0
2	BBBB	18	ARG	3.0
4	KKKK	84	LYS	3.0
2	PPPP	4	GLY	3.0
1	OO	41	CYS	3.0
4	DDDD	79	LYS	3.0
7	NNNN	76	VAL	3.0
4	RR	78	PRO	3.0
8	Y	68	G	3.0
7	UU	62	ILE	3.0
6	LL	43	ILE	3.0
1	H	10	LEU	3.0
4	KKKK	81	GLY	3.0
2	BBB	41	ILE	3.0
7	U	27	VAL	3.0
4	KK	84	LYS	3.0
7	NNNN	75	ARG	3.0
2	PPP	69	LEU	2.9
2	BBB	87	PRO	2.9
7	NN	9	LEU	2.9
1	H	41	CYS	2.9
1	HHHH	28	TYR	2.9
7	N	29	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	BBB	27	PHE	2.9
2	P	19	CYS	2.8
2	B	70	VAL	2.8
2	B	26	ILE	2.8
7	N	16	LYS	2.8
4	DDDD	82	LYS	2.8
1	O	70	PHE	2.8
7	NNN	68	ILE	2.8
4	DD	116	ALA	2.8
1	O	62	TYR	2.8
6	LLL	32	GLN	2.8
1	OO	61	VAL	2.8
2	PPPP	27	PHE	2.8
2	I	25	ARG	2.7
2	PP	28	ILE	2.7
2	BBB	63	GLU	2.7
1	HHH	71	LEU	2.7
4	R	83	GLY	2.7
2	B	78	VAL	2.7
6	LLL	92	ASN	2.7
5	M	42	MET	2.7
7	NNNN	3	LYS	2.7
1	OOOO	3	ILE	2.7
6	L	88	GLN	2.7
7	U	60	VAL	2.7
1	AAA	72	ILE	2.7
1	OOO	60	GLN	2.6
2	PPP	67	LEU	2.6
3	CC	58	LEU	2.6
1	OOO	17	ILE	2.6
2	III	70	VAL	2.6
1	AAA	70	PHE	2.6
7	GGGG	40	LEU	2.6
5	M	30	LYS	2.6
2	PPPP	31	PHE	2.6
2	II	5	LYS	2.6
2	I	40	LEU	2.6
1	O	61	VAL	2.6
6	LLL	43	ILE	2.6
2	I	34	PHE	2.6
2	III	69	LEU	2.5
2	PPP	71	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	PPPP	40	LEU	2.5
5	FFFF	2	SER	2.5
2	IIII	27	PHE	2.5
1	AAAA	73	LEU	2.5
2	BBB	80	MET	2.5
1	OO	60	GLN	2.5
2	BBB	34	PHE	2.5
2	IIII	71	LEU	2.5
4	K	85	LYS	2.5
7	UUU	71	GLU	2.5
6	EE	14	MET	2.5
5	TTT	53	GLY	2.5
2	PP	71	LEU	2.5
2	II	27	PHE	2.5
4	K	84	LYS	2.5
7	GG	60	VAL	2.5
1	AAAA	53	GLY	2.5
2	PPP	72	LEU	2.5
2	PPPP	32	LYS	2.5
7	UUUU	44	GLU	2.5
7	U	73	LEU	2.5
8	V	26	U	2.5
2	I	72	LEU	2.4
2	IIII	69	LEU	2.4
7	NNNN	72	ALA	2.4
7	N	68	ILE	2.4
2	P	71	LEU	2.4
7	UUU	16	LYS	2.4
1	OOOO	41	CYS	2.4
2	B	34	PHE	2.4
3	QQQQ	48	LYS	2.4
7	GG	12	PHE	2.4
3	JJJ	12	HIS	2.4
2	IIII	40	LEU	2.4
7	GG	19	LEU	2.4
6	S	21	ILE	2.4
7	NN	72	ALA	2.4
4	DDD	82	LYS	2.4
4	DDDD	83	GLY	2.4
1	OOOO	61	VAL	2.4
1	A	71	LEU	2.4
7	UUU	12	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	NN	19	LEU	2.4
7	GGGG	17	LEU	2.4
1	OOO	21	GLU	2.3
6	EEEE	32	GLN	2.3
6	LLLL	87	LEU	2.3
1	O	28	TYR	2.3
1	HH	60	GLN	2.3
7	U	59	MET	2.3
4	DDD	81	GLY	2.3
7	GGGG	70	LEU	2.3
2	III	32	LYS	2.3
1	HHH	41	CYS	2.3
1	OO	63	ILE	2.3
1	OOO	71	LEU	2.3
6	SSS	14	MET	2.3
2	I	67	LEU	2.3
5	TTTT	2	SER	2.3
7	N	28	GLN	2.3
4	KK	87	SER	2.3
3	CCCC	58	LEU	2.3
4	DD	82	LYS	2.3
2	II	49	ARG	2.2
7	UU	12	PHE	2.2
1	O	20	CYS	2.2
2	PPPP	42	LEU	2.2
3	CCCC	60	ILE	2.2
8	YYY	68	G	2.2
1	OO	39	MET	2.2
2	P	38	MET	2.2
7	NNN	72	ALA	2.2
1	O	41	CYS	2.2
4	K	83	GLY	2.2
6	SSSS	92	ASN	2.2
5	T	4	PRO	2.2
4	RRRR	81	GLY	2.2
7	UUUU	9	LEU	2.2
2	P	40	LEU	2.2
7	UUU	68	ILE	2.2
2	III	42	LEU	2.2
2	PPPP	49	ARG	2.2
2	BBBB	49	ARG	2.2
7	NN	70	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	GGG	62	ILE	2.2
7	GGG	70	LEU	2.2
1	H	73	LEU	2.1
6	SSS	88	GLN	2.1
7	U	71	GLU	2.1
2	PP	80	MET	2.1
7	UUUU	3	LYS	2.1
1	OOOO	80	ALA	2.1
4	R	84	LYS	2.1
1	O	17	ILE	2.1
1	AAAA	72	ILE	2.1
4	R	85	LYS	2.1
2	BBB	33	ALA	2.1
4	D	20	GLU	2.1
7	UU	3	LYS	2.1
4	RR	116	ALA	2.1
7	UUU	70	LEU	2.1
6	SSSS	43	ILE	2.1
5	TTTT	72	ILE	2.1
4	DD	20	GLU	2.1
6	SSS	43	ILE	2.1
2	BBB	25	ARG	2.1
6	EEE	14	MET	2.1
2	PP	72	LEU	2.1
7	UUUU	19	LEU	2.1
1	H	74	PRO	2.1
1	AAA	73	LEU	2.1
3	JJ	27	GLY	2.1
7	GG	61	VAL	2.0
2	IIII	41	ILE	2.0
6	SSS	89	SER	2.0
1	HH	71	LEU	2.0
4	D	84	LYS	2.0
7	NNN	4	ALA	2.0
2	IIII	66	VAL	2.0
1	AAA	63	ILE	2.0
4	DDDD	116	ALA	2.0
2	PP	27	PHE	2.0
6	SSSS	25	LEU	2.0
2	BBBB	19	CYS	2.0
1	HHHH	61	VAL	2.0
2	III	72	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	RRRR	99	MET	2.0
6	LLL	56	LEU	2.0

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 monosaccharides 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.